



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:38 AM UTC

PDB ID : 2QJK / pdb_00002qjk
Title : Crystal Structure Analysis of mutant rhodobacter sphaeroides bc1 with stigmatellin and antimycin
Authors : Esser, L.
Deposited on : 2007-07-07
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

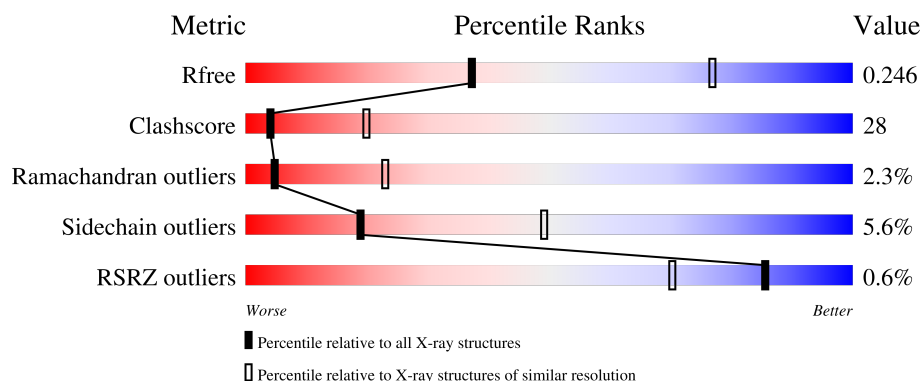
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



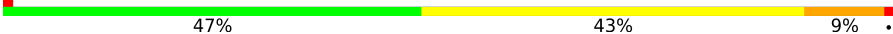
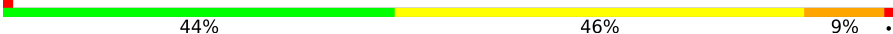
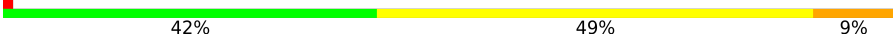
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	428	48% 45% 7%
1	D	428	50% 45% 5%
1	G	428	49% 44% 7%
1	J	428	46% 49% 6%
1	M	428	44% 49% 7%

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Mol	Chain	Length	Quality of chain
1	P	428	
2	B	256	
2	E	256	
2	H	256	
2	K	256	
2	N	256	
2	Q	256	
3	C	179	
3	F	179	
3	I	179	
3	L	179	
3	O	179	
3	R	179	

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	FES	C	200	-	-	X	-
10	FES	F	200	-	-	X	-
10	FES	I	200	-	-	X	-
10	FES	L	200	-	-	X	-
10	FES	O	200	-	-	X	-
10	FES	R	200	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 42048 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	287	ARG	SER	engineered mutation	UNP Q02761
D	287	ARG	SER	engineered mutation	UNP Q02761
G	287	ARG	SER	engineered mutation	UNP Q02761
J	287	ARG	SER	engineered mutation	UNP Q02761
M	287	ARG	SER	engineered mutation	UNP Q02761
P	287	ARG	SER	engineered mutation	UNP Q02761

- Molecule 2 is a protein called Cytochrome c1.

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

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

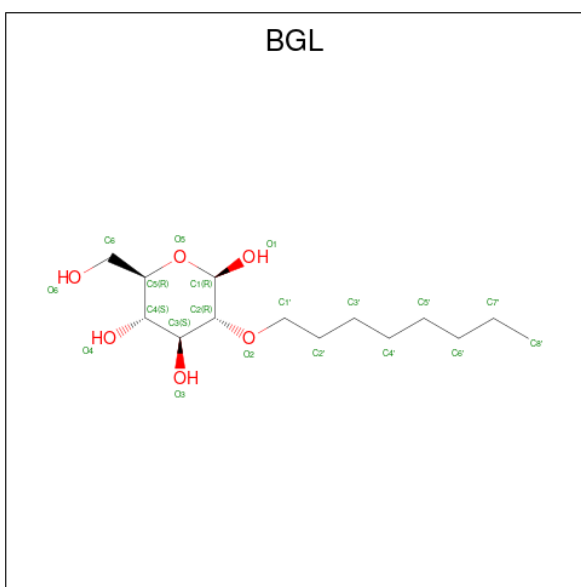
- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

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

There are 6 discrepancies between the modelled and reference sequences:

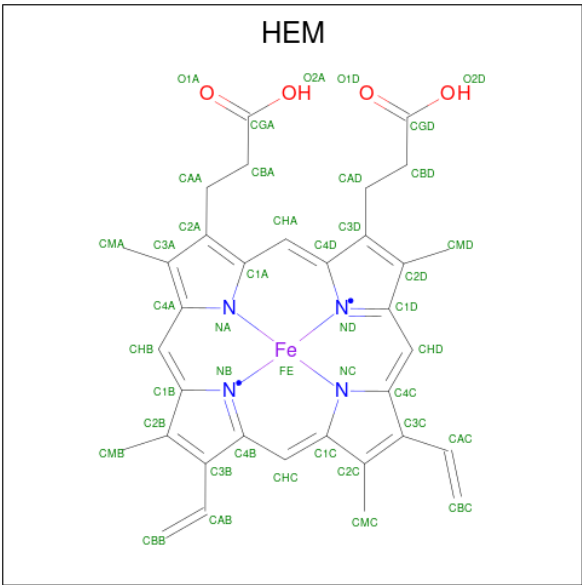
Chain	Residue	Modelled	Actual	Comment	Reference
C	135	SER	VAL	engineered mutation	UNP Q02762
F	135	SER	VAL	engineered mutation	UNP Q02762
I	135	SER	VAL	engineered mutation	UNP Q02762
L	135	SER	VAL	engineered mutation	UNP Q02762
O	135	SER	VAL	engineered mutation	UNP Q02762
R	135	SER	VAL	engineered mutation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

- Molecule 4 is 2-O-octyl-beta-D-glucopyranose (CCD ID: BGL) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	D	1	Total	C	O	0	0
			20	14	6		
4	G	1	Total	C	O	0	0
			20	14	6		
4	J	1	Total	C	O	0	0
			20	14	6		
4	M	1	Total	C	O	0	0
			20	14	6		
4	Q	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



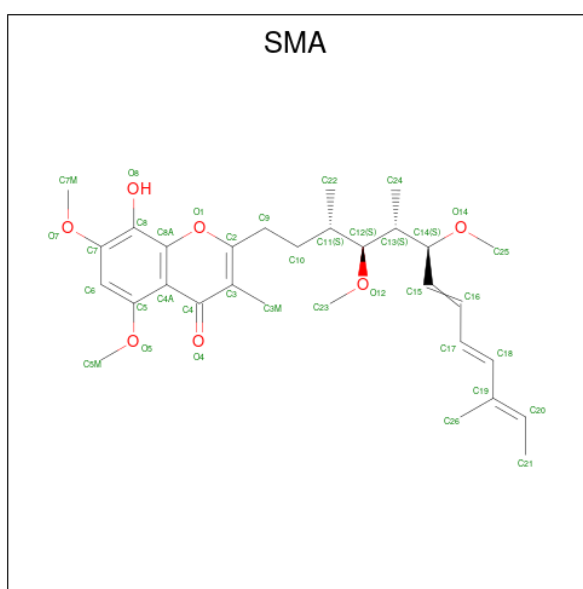
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	G	1	Total 43	C 34	Fe 1	N 4	O 4	0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

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

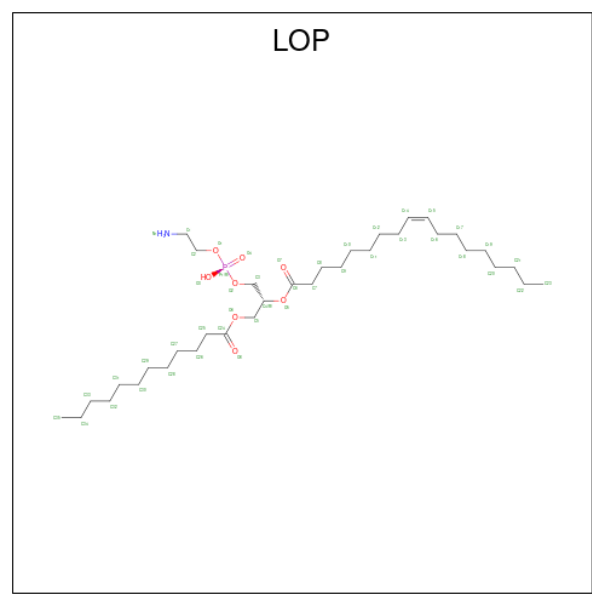
- Molecule 6 is STIGMATELLIN A (CCD ID: SMA) (formula: C₃₀H₄₂O₇).



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

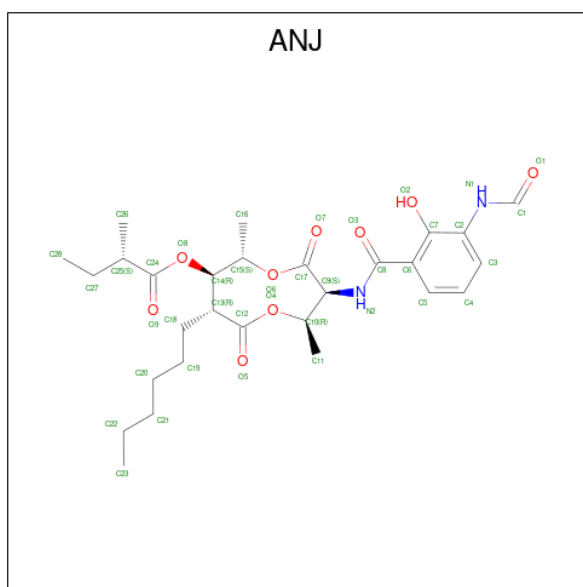
- Molecule 7 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (CCD ID: LOP)

(formula: C₃₅H₆₈NO₈P).



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

- Molecule 8 is (2R,3S,6S,7R,8R)-3-{[3-(FORMYLAMINO)-2-HYDROXYBENZOYL]AMINO O}-8-HEXYL-2,6-DIMETHYL-4,9-DIOXO-1,5-DIOXONAN-7-YL (2S)-2-METHYLBUTANOATE (CCD ID: ANJ) (formula: C₂₈H₄₀N₂O₉).

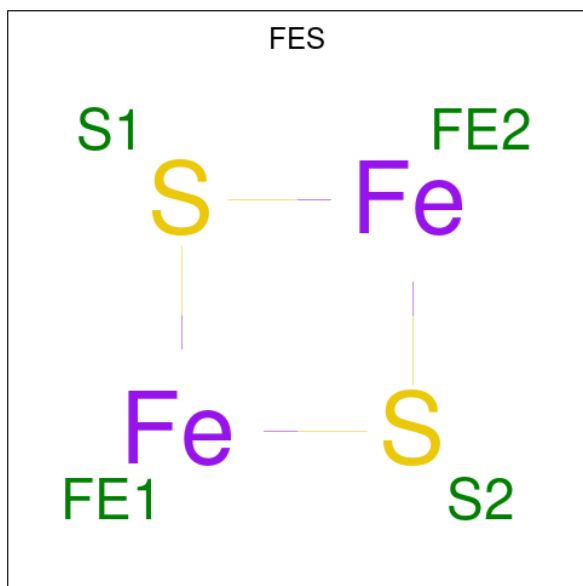


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			39	28	2	9		
8	D	1	Total	C	N	O	0	0
			39	28	2	9		
8	G	1	Total	C	N	O	0	0
			39	28	2	9		
8	J	1	Total	C	N	O	0	0
			39	28	2	9		
8	M	1	Total	C	N	O	0	0
			39	28	2	9		
8	P	1	Total	C	N	O	0	0
			39	28	2	9		

- Molecule 9 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Sr	0	0
			1	1		
9	E	1	Total	Sr	0	0
			1	1		
9	H	1	Total	Sr	0	0
			1	1		
9	K	1	Total	Sr	0	0
			1	1		
9	N	1	Total	Sr	0	0
			1	1		
9	Q	1	Total	Sr	0	0
			1	1		

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

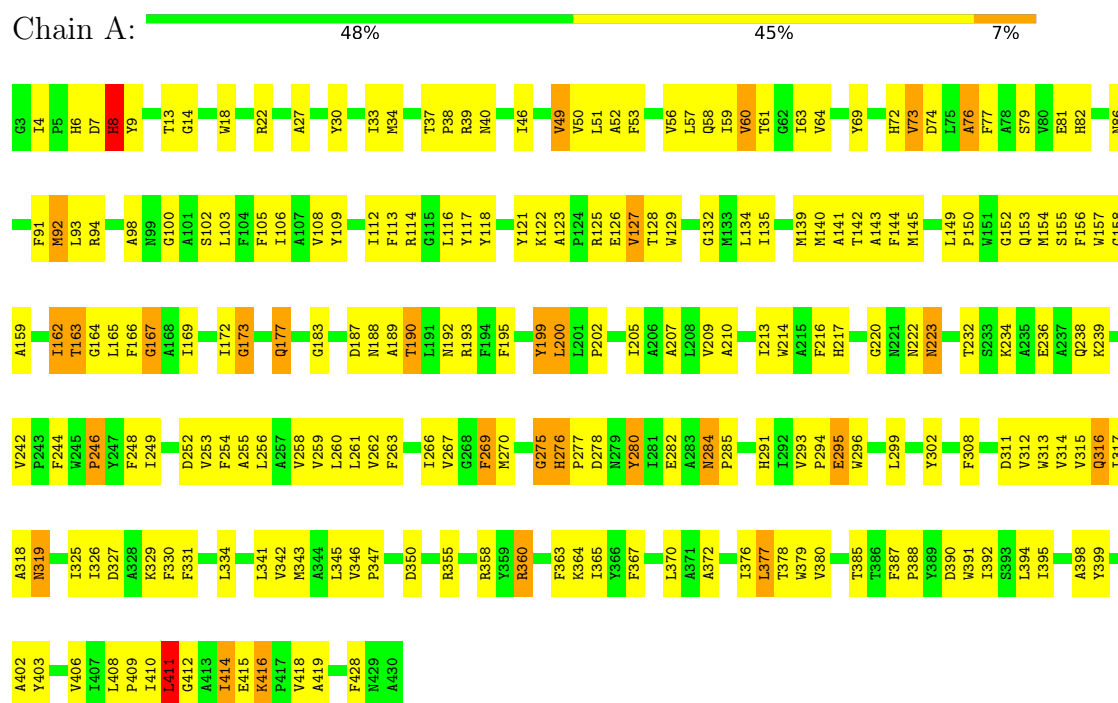


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total 4	Fe 2	S 2	0	0
10	F	1	Total 4	Fe 2	S 2	0	0
10	I	1	Total 4	Fe 2	S 2	0	0
10	L	1	Total 4	Fe 2	S 2	0	0
10	O	1	Total 4	Fe 2	S 2	0	0
10	R	1	Total 4	Fe 2	S 2	0	0

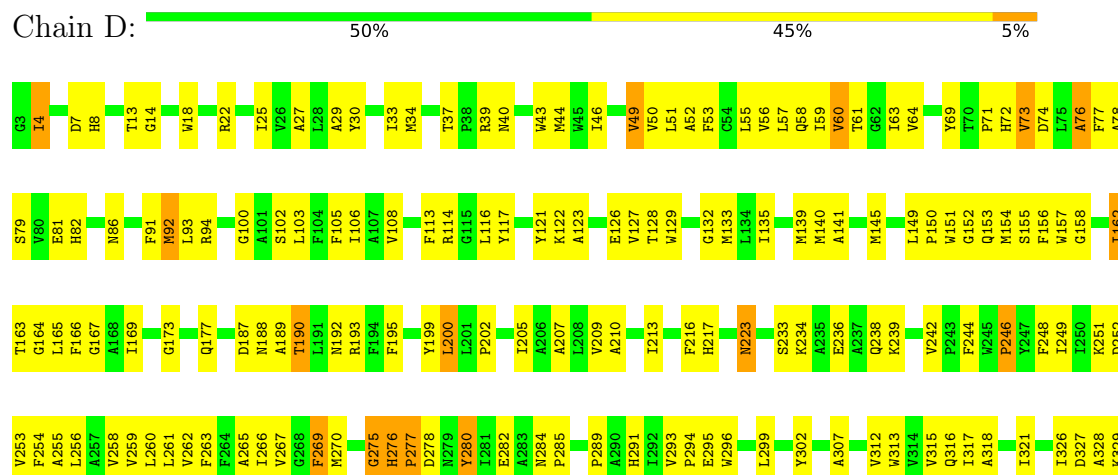
3 Residue-property plots

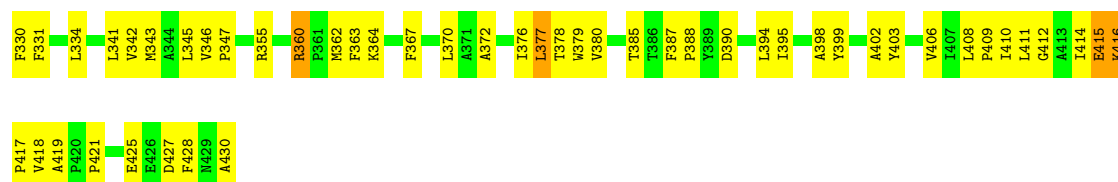
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Cytochrome b



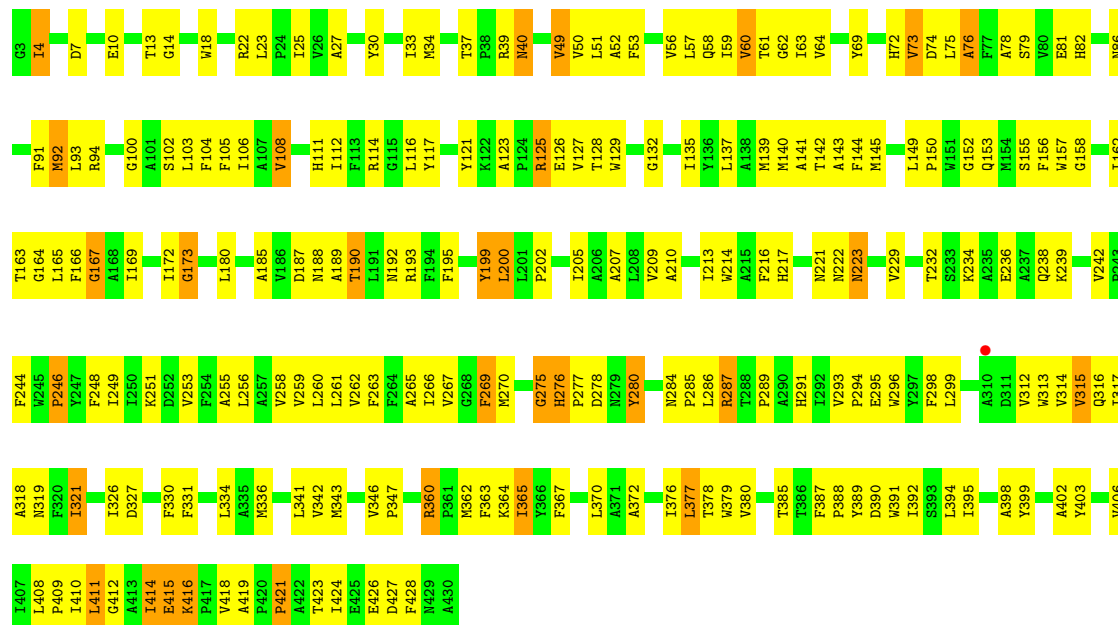
• Molecule 1: Cytochrome b





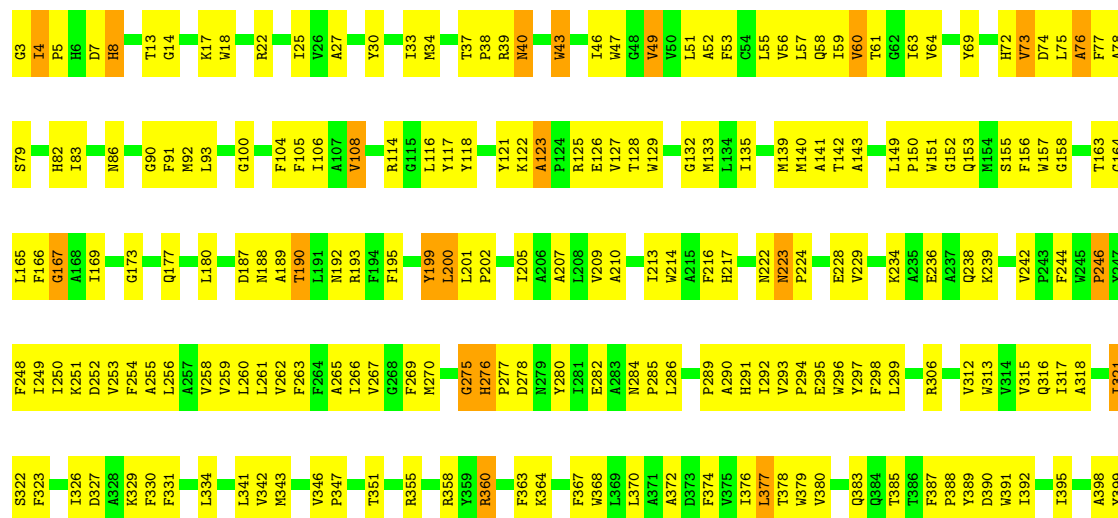
• Molecule 1: Cytochrome b

Chain G: 49% 44% 7%



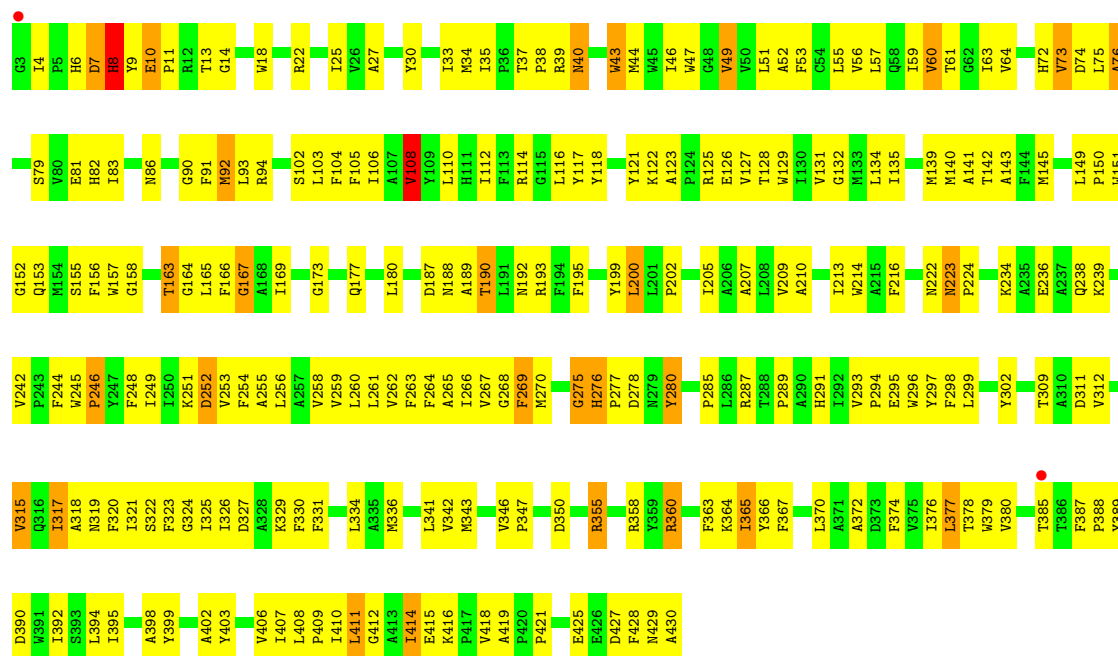
• Molecule 1: Cytochrome b

Chain J: 46% 49% 6%

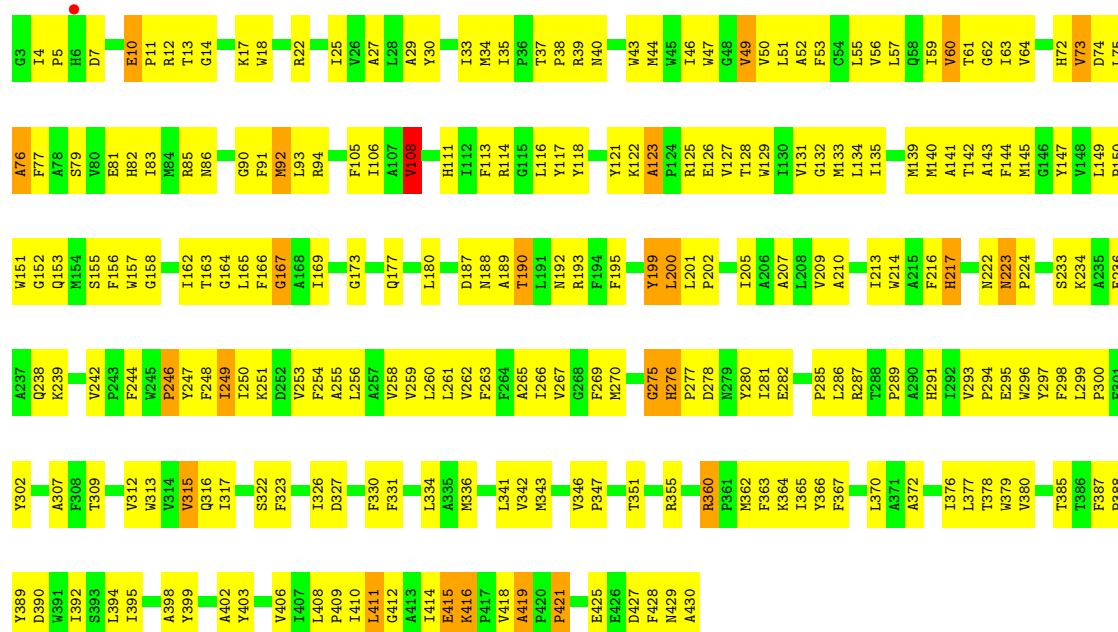




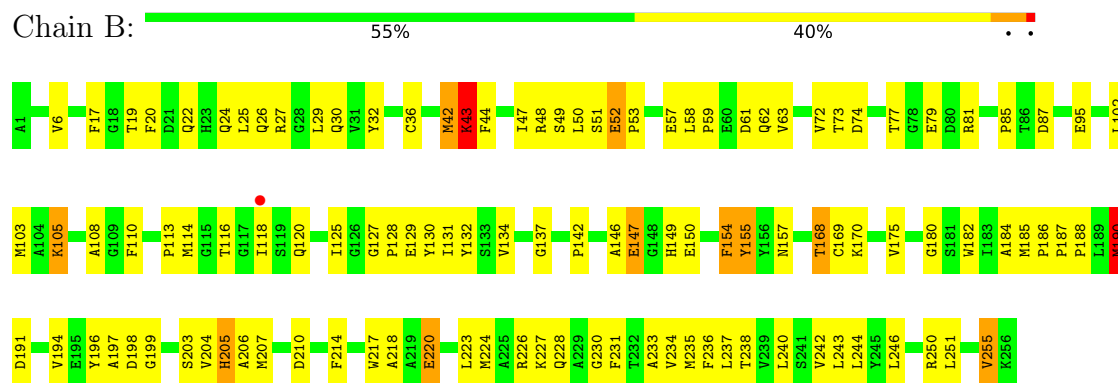
• Molecule 1: Cytochrome b



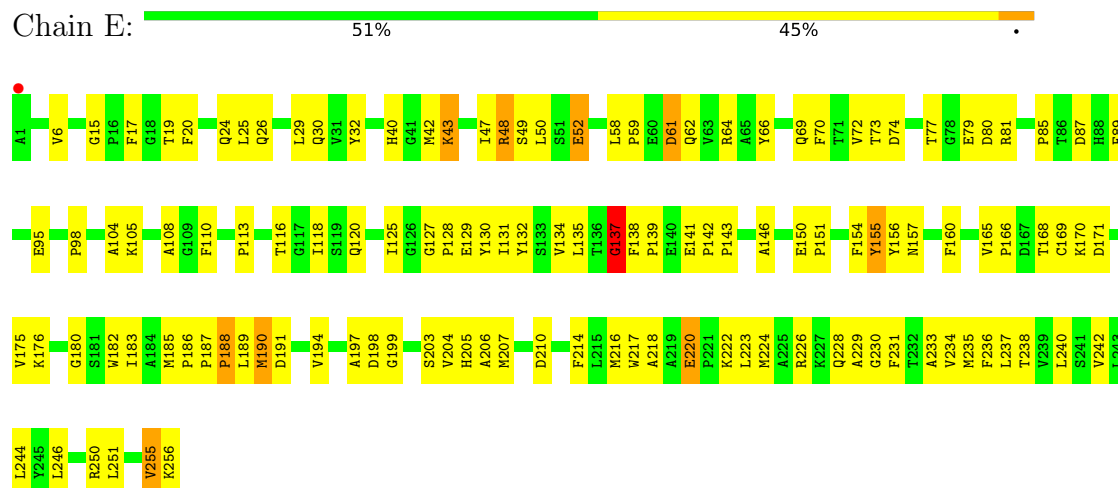
• Molecule 1: Cytochrome b



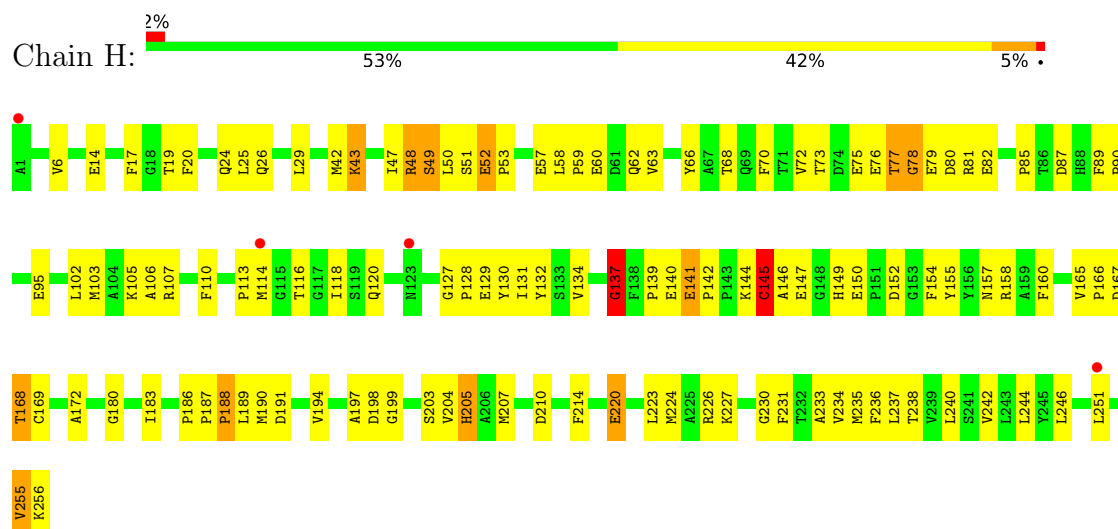
• Molecule 2: Cytochrome c1



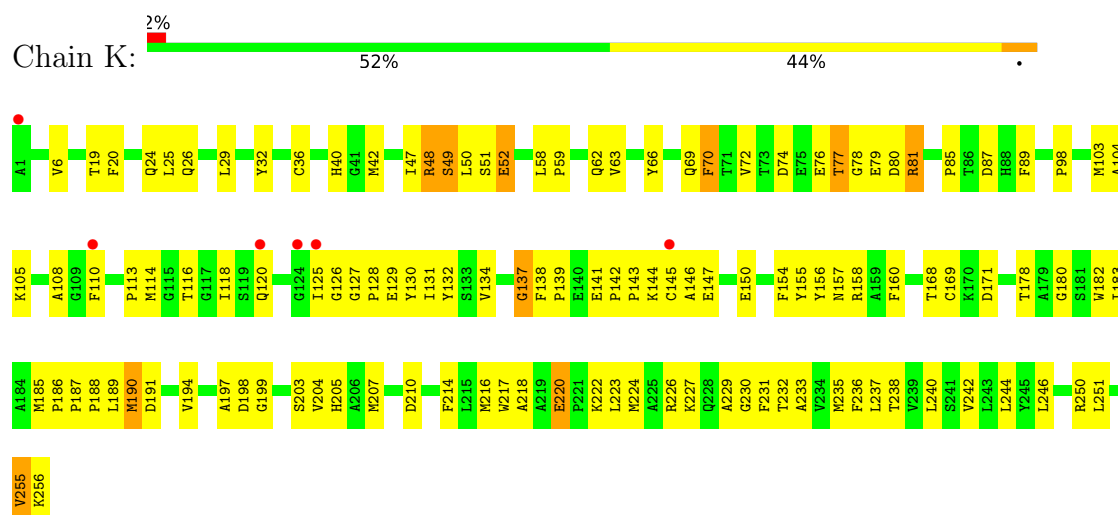
• Molecule 2: Cytochrome c1



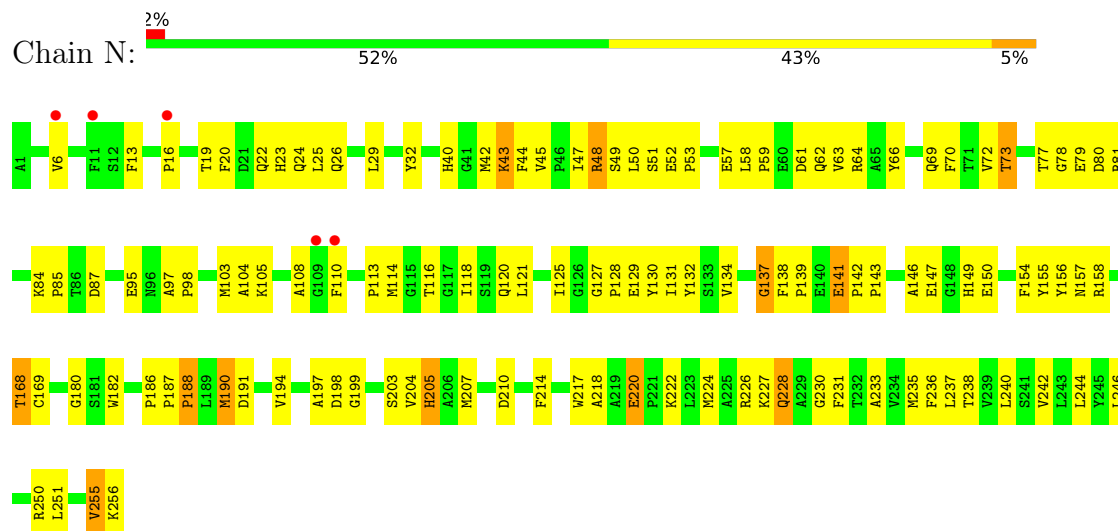
• Molecule 2: Cytochrome c1



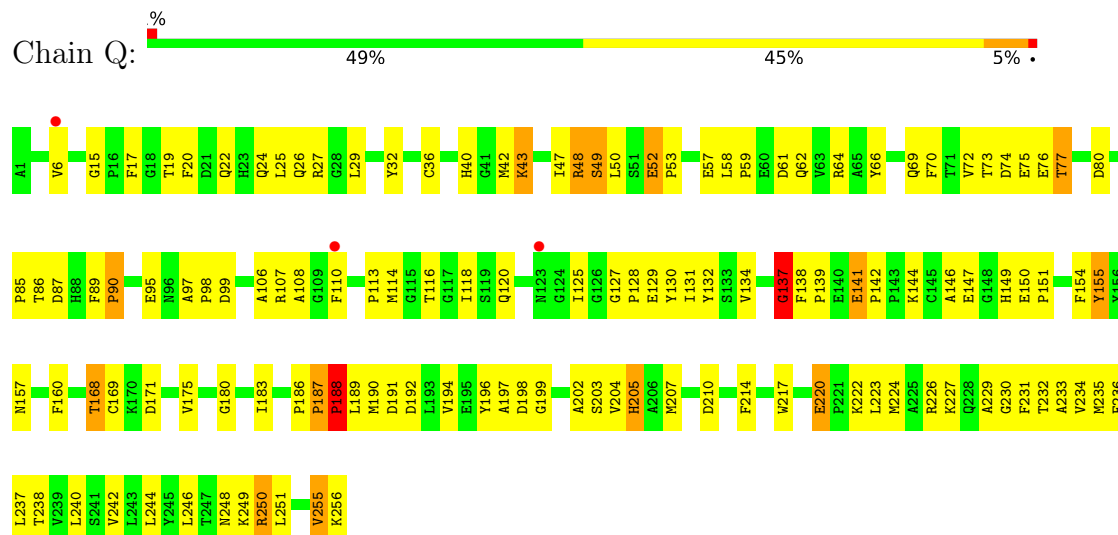
• Molecule 2: Cytochrome c1



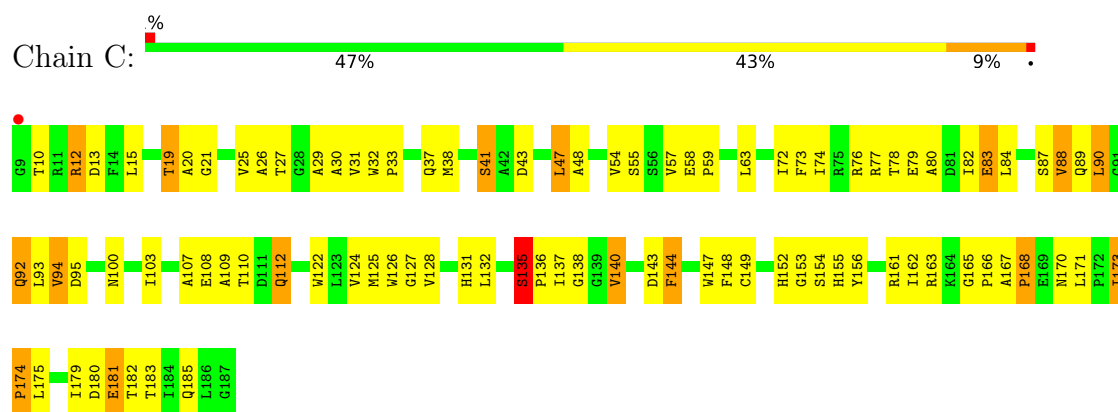
• Molecule 2: Cytochrome c1



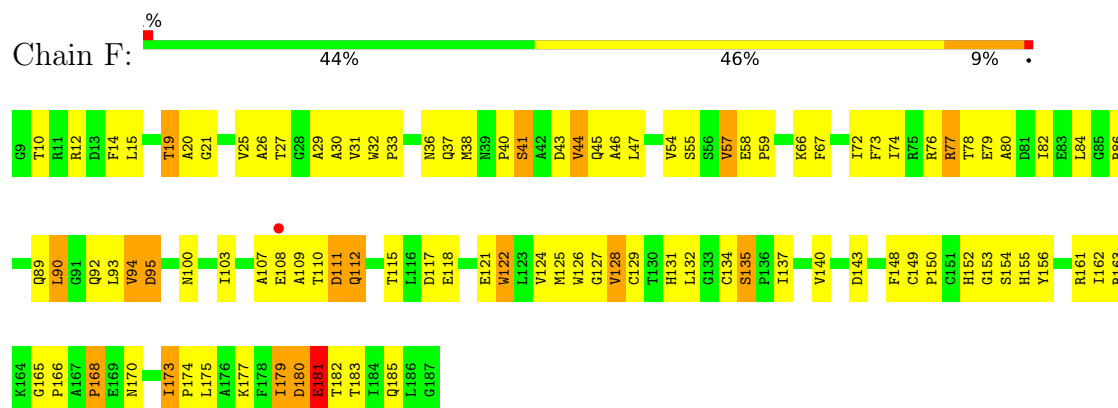
• Molecule 2: Cytochrome c1



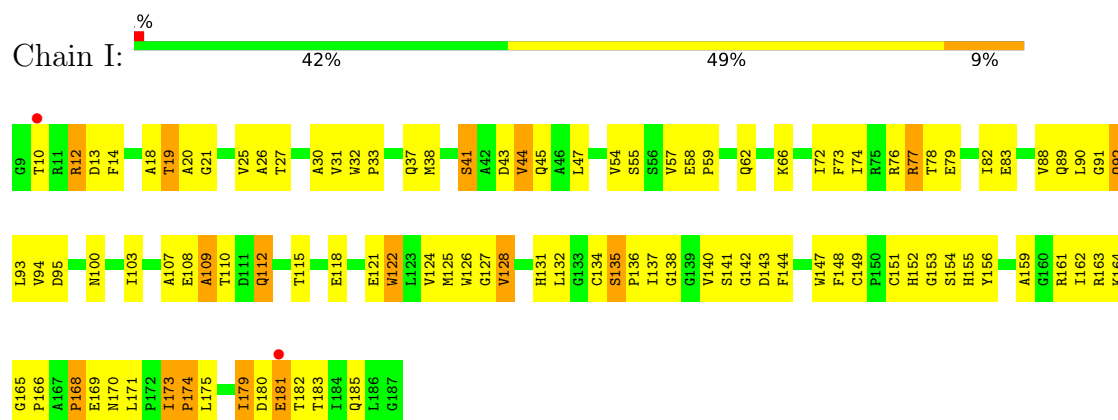
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



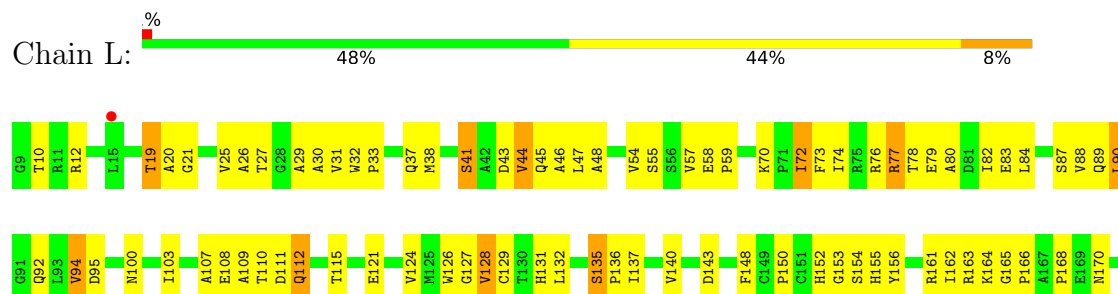
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



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



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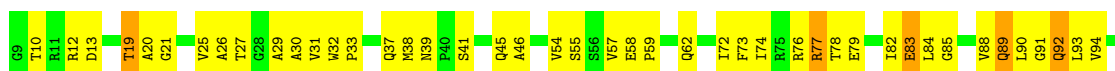




• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	352.29Å 147.40Å 160.76Å 90.00° 104.13° 90.00°	Depositor
Resolution (Å)	18.00 – 3.10 18.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (18.00-3.10) 86.4 (18.00-3.10)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 3.06Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.266 0.226 , 0.246	Depositor DCC
R_{free} test set	5751 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å ²)	78.9	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	42048	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.75	1/3570 (0.0%)	1.11	27/4897 (0.6%)
1	D	0.76	0/3570	1.11	25/4897 (0.5%)
1	G	0.71	0/3570	1.11	27/4897 (0.6%)
1	J	0.68	0/3570	1.13	27/4897 (0.6%)
1	M	0.64	0/3570	1.14	25/4897 (0.5%)
1	P	0.72	1/3570 (0.0%)	1.14	30/4897 (0.6%)
2	B	0.62	0/2010	1.07	6/2733 (0.2%)
2	E	0.59	0/2010	1.07	6/2733 (0.2%)
2	H	0.63	0/2010	1.05	6/2733 (0.2%)
2	K	0.56	0/2010	1.06	9/2733 (0.3%)
2	N	0.55	0/2010	1.06	7/2733 (0.3%)
2	Q	0.56	0/2010	1.07	8/2733 (0.3%)
3	C	0.76	1/1370 (0.1%)	1.27	17/1866 (0.9%)
3	F	0.77	1/1370 (0.1%)	1.24	18/1866 (1.0%)
3	I	0.77	1/1370 (0.1%)	1.30	19/1866 (1.0%)
3	L	0.77	1/1370 (0.1%)	1.25	16/1866 (0.9%)
3	O	0.73	1/1370 (0.1%)	1.24	12/1866 (0.6%)
3	R	0.70	1/1370 (0.1%)	1.23	12/1866 (0.6%)
All	All	0.69	8/41700 (0.0%)	1.13	297/56976 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	G	0	1
1	J	0	1
1	P	0	1
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	181	GLU	CB-CG	-8.51	1.26	1.52
3	F	181	GLU	CB-CG	-7.81	1.29	1.52
3	L	181	GLU	CB-CG	-7.69	1.29	1.52
3	C	181	GLU	CB-CG	-7.05	1.31	1.52
3	I	181	GLU	CB-CG	-6.58	1.32	1.52
1	P	315	VAL	CA-CB	-5.27	1.48	1.54
1	A	127	VAL	CA-CB	-5.10	1.48	1.54
3	R	181	GLU	CA-C	-5.01	1.45	1.52

All (297) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	416	LYS	CA-C-N	12.18	132.30	119.76
1	P	416	LYS	C-N-CA	12.18	132.30	119.76
3	C	181	GLU	N-CA-C	11.86	125.35	111.71
3	O	181	GLU	N-CA-C	11.77	125.25	111.71
3	R	181	GLU	N-CA-C	11.61	125.06	111.71
3	I	181	GLU	N-CA-C	11.20	124.59	111.71
3	I	44	VAL	N-CA-C	11.09	123.09	111.00
3	L	181	GLU	N-CA-C	9.56	122.71	111.71
1	P	414	ILE	N-CA-C	9.24	119.22	110.53
1	A	416	LYS	CA-C-N	9.15	129.19	119.76
1	A	416	LYS	C-N-CA	9.15	129.19	119.76
3	F	181	GLU	N-CA-C	9.04	122.10	111.71
1	M	414	ILE	N-CA-C	8.99	118.98	110.53
3	L	165	GLY	CA-C-N	8.61	128.25	119.56
3	L	165	GLY	C-N-CA	8.61	128.25	119.56
1	G	414	ILE	N-CA-C	8.43	120.19	111.00
1	D	414	ILE	N-CA-C	8.42	119.22	110.72
3	O	165	GLY	CA-C-N	8.31	127.95	119.56
3	O	165	GLY	C-N-CA	8.31	127.95	119.56
3	R	165	GLY	CA-C-N	8.21	127.85	119.56
3	R	165	GLY	C-N-CA	8.21	127.85	119.56
3	R	135	SER	CA-C-N	8.18	128.18	119.76
3	R	135	SER	C-N-CA	8.18	128.18	119.76
3	I	135	SER	CA-C-N	8.16	128.16	119.76
3	I	135	SER	C-N-CA	8.16	128.16	119.76
1	G	416	LYS	CA-C-N	8.11	128.12	119.76
1	G	416	LYS	C-N-CA	8.11	128.12	119.76
1	J	280	TYR	N-CA-C	-8.09	103.50	112.72
3	O	181	GLU	CA-CB-CG	-8.08	97.94	114.10
3	L	44	VAL	N-CA-C	-8.07	102.57	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	165	GLY	CA-C-N	7.93	127.57	119.56
3	C	165	GLY	C-N-CA	7.93	127.57	119.56
3	I	165	GLY	CA-C-N	7.88	127.52	119.56
3	I	165	GLY	C-N-CA	7.88	127.52	119.56
1	M	280	TYR	N-CA-C	-7.85	103.77	112.72
1	D	280	TYR	N-CA-C	-7.84	103.79	112.72
1	J	414	ILE	N-CA-C	7.84	119.54	111.00
3	F	165	GLY	CA-C-N	7.82	127.46	119.56
3	F	165	GLY	C-N-CA	7.82	127.46	119.56
3	C	181	GLU	CG-CD-OE2	-7.72	100.64	118.40
1	A	414	ILE	N-CA-C	7.72	119.42	111.00
1	G	280	TYR	N-CA-C	-7.71	103.93	112.72
2	Q	52	GLU	CA-C-N	7.71	127.47	119.76
2	Q	52	GLU	C-N-CA	7.71	127.47	119.76
1	P	280	TYR	N-CA-C	-7.66	103.98	112.72
1	P	108	VAL	CB-CA-C	-7.58	102.17	111.88
3	C	135	SER	CA-C-N	7.55	127.54	119.76
3	C	135	SER	C-N-CA	7.55	127.54	119.76
1	M	416	LYS	CA-C-N	7.44	127.42	119.76
1	M	416	LYS	C-N-CA	7.44	127.42	119.76
1	J	416	LYS	CA-C-N	7.40	127.16	119.76
1	J	416	LYS	C-N-CA	7.40	127.16	119.76
3	O	135	SER	CA-C-N	7.40	127.38	119.76
3	O	135	SER	C-N-CA	7.40	127.38	119.76
2	H	52	GLU	CA-C-N	7.39	127.15	119.76
2	H	52	GLU	C-N-CA	7.39	127.15	119.76
3	F	128	VAL	N-CA-C	7.32	116.85	106.53
2	B	52	GLU	CA-C-N	7.23	127.15	119.85
2	B	52	GLU	C-N-CA	7.23	127.15	119.85
3	L	88	VAL	N-CA-C	7.23	118.23	108.11
2	E	52	GLU	CA-C-N	7.21	127.13	119.85
2	E	52	GLU	C-N-CA	7.21	127.13	119.85
3	I	79	GLU	N-CA-C	-7.20	103.36	111.14
2	K	52	GLU	CA-C-N	7.19	126.95	119.76
2	K	52	GLU	C-N-CA	7.19	126.95	119.76
3	L	135	SER	CA-C-N	7.16	127.14	119.76
3	L	135	SER	C-N-CA	7.16	127.14	119.76
1	A	280	TYR	N-CA-C	-7.15	104.57	112.72
1	A	200	LEU	N-CA-C	7.13	119.66	111.11
3	F	135	SER	CA-C-N	7.10	127.08	119.76
3	F	135	SER	C-N-CA	7.10	127.08	119.76
1	D	416	LYS	CA-C-N	7.07	126.83	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	416	LYS	C-N-CA	7.07	126.83	119.76
2	N	52	GLU	CA-C-N	7.07	126.99	119.85
2	N	52	GLU	C-N-CA	7.07	126.99	119.85
1	G	200	LEU	N-CA-C	7.00	119.56	111.02
3	R	128	VAL	N-CA-C	6.98	116.37	106.53
1	P	360	ARG	CA-C-N	6.97	127.27	119.32
1	P	360	ARG	C-N-CA	6.97	127.27	119.32
3	I	181	GLU	CA-CB-CG	-6.97	100.17	114.10
3	O	128	VAL	N-CA-C	6.95	116.32	106.53
1	M	200	LEU	N-CA-C	6.91	119.45	111.02
1	M	360	ARG	CA-C-N	6.82	127.09	119.32
1	M	360	ARG	C-N-CA	6.82	127.09	119.32
3	I	128	VAL	N-CA-C	6.81	116.13	106.53
1	J	360	ARG	CA-C-N	6.81	127.08	119.32
1	J	360	ARG	C-N-CA	6.81	127.08	119.32
3	R	79	GLU	N-CA-C	-6.77	103.83	111.14
1	J	200	LEU	N-CA-C	6.76	119.27	111.02
3	L	128	VAL	N-CA-C	6.76	116.07	106.53
3	L	79	GLU	N-CA-C	-6.75	103.85	111.14
1	P	200	LEU	N-CA-C	6.72	119.22	111.02
3	C	79	GLU	N-CA-C	-6.67	103.94	111.14
1	D	360	ARG	CA-C-N	6.61	126.86	119.32
1	D	360	ARG	C-N-CA	6.61	126.86	119.32
1	G	360	ARG	CA-C-N	6.61	126.86	119.32
1	G	360	ARG	C-N-CA	6.61	126.86	119.32
3	O	79	GLU	N-CA-C	-6.58	104.03	111.14
3	L	94	VAL	N-CA-C	-6.57	104.61	111.58
1	M	10	GLU	CA-C-N	6.57	126.93	119.83
1	M	10	GLU	C-N-CA	6.57	126.93	119.83
3	F	79	GLU	N-CA-C	-6.53	104.09	111.14
3	C	181	GLU	CA-CB-CG	-6.52	101.06	114.10
1	P	276	HIS	CA-C-N	6.51	127.03	119.47
1	P	276	HIS	C-N-CA	6.51	127.03	119.47
1	A	163	THR	N-CA-C	-6.51	104.27	111.82
1	A	331	PHE	N-CA-C	-6.51	104.11	111.14
1	J	276	HIS	CA-C-N	6.48	126.99	119.47
1	J	276	HIS	C-N-CA	6.48	126.99	119.47
3	I	94	VAL	CB-CA-C	-6.47	104.17	111.80
1	P	40	ASN	N-CA-C	6.46	120.76	113.01
1	M	415	GLU	N-CA-C	6.45	119.12	110.35
2	N	141	GLU	CA-C-N	6.45	124.36	119.66
2	N	141	GLU	C-N-CA	6.45	124.36	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	78	GLY	N-CA-C	-6.42	106.22	115.27
3	I	94	VAL	N-CA-C	-6.36	105.62	111.67
1	M	269	PHE	N-CA-C	6.30	121.09	113.41
1	M	40	ASN	N-CA-C	6.28	120.54	113.01
1	D	200	LEU	N-CA-C	6.28	118.68	111.02
1	A	360	ARG	CA-C-N	6.24	126.44	119.32
1	A	360	ARG	C-N-CA	6.24	126.44	119.32
1	M	276	HIS	CA-C-N	6.19	127.58	119.84
1	M	276	HIS	C-N-CA	6.19	127.58	119.84
2	H	145	CYS	CA-CB-SG	-6.17	100.22	114.40
1	P	365	ILE	N-CA-C	6.17	116.83	110.36
1	P	163	THR	N-CA-C	-6.15	104.69	111.82
3	C	128	VAL	N-CA-C	6.13	115.17	106.53
1	P	10	GLU	CA-C-N	6.11	126.43	119.83
1	P	10	GLU	C-N-CA	6.11	126.43	119.83
1	D	415	GLU	N-CA-C	6.11	118.66	110.35
1	M	108	VAL	CB-CA-C	-6.10	104.07	111.88
1	G	276	HIS	CA-C-N	6.09	127.45	119.84
1	G	276	HIS	C-N-CA	6.09	127.45	119.84
1	G	163	THR	N-CA-C	-6.08	104.77	111.82
1	A	276	HIS	CA-C-N	6.06	127.41	119.84
1	A	276	HIS	C-N-CA	6.06	127.41	119.84
1	G	415	GLU	N-CA-C	6.05	118.58	110.35
1	J	331	PHE	N-CA-C	-6.03	104.62	111.14
1	D	331	PHE	N-CA-C	-6.02	104.63	111.14
1	M	163	THR	N-CA-C	-5.99	104.87	111.82
1	M	8	HIS	N-CA-C	5.96	118.72	109.60
3	L	173	ILE	N-CA-C	-5.93	101.42	107.89
1	D	8	HIS	N-CA-C	5.93	117.54	110.19
1	J	275	GLY	N-CA-C	5.92	121.87	111.57
1	P	269	PHE	N-CA-C	5.87	120.59	112.90
3	F	180	ASP	CA-C-N	5.83	128.68	120.28
3	F	180	ASP	C-N-CA	5.83	128.68	120.28
1	P	307	ALA	N-CA-C	-5.83	105.01	111.36
1	A	276	HIS	N-CA-C	5.82	118.89	108.47
1	J	163	THR	N-CA-C	-5.82	105.07	111.82
1	D	163	THR	N-CA-C	-5.79	105.10	111.82
1	J	78	ALA	N-CA-C	-5.79	104.16	111.11
1	A	40	ASN	N-CA-C	5.78	119.94	113.01
2	N	78	GLY	N-CA-C	-5.78	107.13	115.27
1	J	40	ASN	N-CA-C	5.77	119.94	113.01
1	D	284	ASN	CA-C-N	5.77	125.87	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	284	ASN	C-N-CA	5.77	125.87	119.87
1	G	365	ILE	N-CA-C	5.76	115.95	110.42
1	J	269	PHE	N-CA-C	5.76	120.44	112.90
1	M	275	GLY	N-CA-C	5.76	121.59	111.57
2	Q	187	PRO	CA-C-N	5.74	127.01	119.84
2	Q	187	PRO	C-N-CA	5.74	127.01	119.84
1	D	269	PHE	N-CA-C	5.72	120.39	112.90
1	G	40	ASN	N-CA-C	5.71	119.87	113.01
1	D	276	HIS	CA-C-N	5.68	126.94	119.84
1	D	276	HIS	C-N-CA	5.68	126.94	119.84
1	A	415	GLU	N-CA-C	5.68	118.07	110.35
1	D	276	HIS	N-CA-C	5.67	118.63	108.47
1	M	331	PHE	N-CA-C	-5.66	105.02	111.07
1	M	317	ILE	N-CA-C	-5.65	104.36	110.23
1	A	269	PHE	N-CA-C	5.64	120.29	112.90
1	D	270	MET	CA-C-N	5.63	125.48	119.28
1	D	270	MET	C-N-CA	5.63	125.48	119.28
3	L	181	GLU	CA-CB-CG	-5.62	102.86	114.10
1	G	275	GLY	N-CA-C	5.61	121.33	111.57
3	C	144	PHE	N-CA-C	5.61	119.30	111.56
1	J	86	ASN	N-CA-C	5.60	119.80	112.13
2	B	105	LYS	N-CA-C	-5.59	106.82	113.97
1	J	415	GLU	N-CA-C	5.58	117.94	110.35
3	F	122	TRP	N-CA-C	5.57	118.12	107.75
1	G	276	HIS	N-CA-C	5.57	118.44	108.47
1	P	270	MET	CA-C-N	5.56	125.22	119.05
1	P	270	MET	C-N-CA	5.56	125.22	119.05
1	D	40	ASN	N-CA-C	5.56	119.68	113.01
1	M	81	GLU	N-CA-C	-5.55	105.31	111.36
3	F	95	ASP	N-CA-C	-5.54	100.67	109.59
1	P	415	GLU	N-CA-C	5.54	118.26	110.23
1	G	81	GLU	N-CA-C	-5.54	105.39	111.82
3	L	87	SER	CA-C-N	-5.54	115.89	123.14
3	L	87	SER	C-N-CA	-5.54	115.89	123.14
3	C	149	CYS	CA-C-N	5.51	125.60	119.87
3	C	149	CYS	C-N-CA	5.51	125.60	119.87
1	G	78	ALA	N-CA-C	-5.51	104.50	111.11
1	P	275	GLY	N-CA-C	5.51	121.16	111.57
1	A	365	ILE	N-CA-C	5.50	115.70	110.42
3	C	77	ARG	N-CA-C	5.50	118.25	110.50
1	G	269	PHE	N-CA-C	5.49	120.11	113.41
3	F	181	GLU	N-CA-CB	-5.46	101.81	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	331	PHE	N-CA-C	-5.46	105.25	111.14
3	O	181	GLU	CG-CD-OE2	-5.46	105.84	118.40
1	G	86	ASN	N-CA-C	5.45	119.42	112.12
1	G	10	GLU	CA-C-N	5.43	126.27	119.98
1	G	10	GLU	C-N-CA	5.43	126.27	119.98
1	A	284	ASN	CA-C-N	5.42	125.51	119.87
1	A	284	ASN	C-N-CA	5.42	125.51	119.87
1	J	270	MET	CA-C-N	5.42	125.24	119.28
1	J	270	MET	C-N-CA	5.42	125.24	119.28
3	O	149	CYS	CA-C-N	5.42	125.50	119.87
3	O	149	CYS	C-N-CA	5.42	125.50	119.87
3	C	88	VAL	N-CA-C	5.41	120.58	109.34
1	M	276	HIS	N-CA-C	5.38	118.11	108.47
3	I	122	TRP	N-CA-C	5.38	118.10	107.98
3	C	92	GLN	N-CA-C	-5.38	106.56	113.23
1	A	81	GLU	N-CA-C	-5.38	105.50	111.36
1	A	275	GLY	N-CA-C	5.38	120.92	111.57
3	O	181	GLU	CB-CG-CD	5.37	121.73	112.60
2	K	137	GLY	N-CA-C	5.36	125.89	113.18
1	J	276	HIS	N-CA-C	5.34	118.03	108.47
1	A	270	MET	CA-C-N	5.34	125.15	119.28
1	A	270	MET	C-N-CA	5.34	125.15	119.28
1	D	78	ALA	N-CA-C	-5.32	104.73	111.11
3	F	173	ILE	N-CA-C	-5.30	102.11	107.89
3	R	173	ILE	N-CA-C	-5.30	102.11	107.89
1	A	8	HIS	N-CA-C	5.29	118.36	110.52
1	G	167	GLY	N-CA-C	-5.29	108.85	114.67
3	L	77	ARG	N-CA-C	5.29	117.95	110.50
1	M	365	ILE	N-CA-C	5.28	115.49	110.53
2	B	72	VAL	N-CA-C	5.27	116.31	108.46
1	P	86	ASN	N-CA-C	5.27	119.35	112.13
2	H	49	SER	N-CA-C	-5.26	106.81	113.18
1	J	424	ILE	N-CA-C	-5.26	105.41	110.72
2	Q	49	SER	N-CA-C	-5.26	106.82	113.18
3	C	173	ILE	CA-C-N	5.25	125.46	120.31
3	C	173	ILE	C-N-CA	5.25	125.46	120.31
1	P	331	PHE	N-CA-C	-5.25	105.47	111.14
3	I	149	CYS	CA-C-N	5.25	125.33	119.87
3	I	149	CYS	C-N-CA	5.25	125.33	119.87
1	D	86	ASN	N-CA-C	5.23	119.13	112.12
1	J	167	GLY	N-CA-C	-5.23	108.92	114.67
1	J	284	ASN	CA-C-N	5.23	125.31	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	284	ASN	C-N-CA	5.23	125.31	119.87
2	K	49	SER	N-CA-C	-5.22	106.86	113.18
1	P	81	GLU	N-CA-C	-5.21	105.68	111.36
1	J	313	TRP	N-CA-C	5.21	116.65	110.97
1	M	86	ASN	N-CA-C	5.21	119.26	112.13
1	G	321	ILE	CB-CA-C	-5.20	105.23	112.04
3	F	77	ARG	N-CA-C	5.20	117.83	110.50
3	I	173	ILE	CA-C-N	5.20	125.40	120.31
3	I	173	ILE	C-N-CA	5.20	125.40	120.31
2	Q	141	GLU	CA-C-N	5.19	125.73	120.38
2	Q	141	GLU	C-N-CA	5.19	125.73	120.38
1	A	232	THR	N-CA-C	5.19	118.76	112.23
1	J	321	ILE	CB-CA-C	-5.18	104.48	112.05
1	D	81	GLU	N-CA-C	-5.18	105.71	111.36
1	D	275	GLY	N-CA-C	5.18	120.58	111.57
3	R	77	ARG	N-CA-C	5.17	117.79	110.50
2	E	89	PHE	CA-C-N	-5.17	115.40	120.52
2	E	89	PHE	C-N-CA	-5.17	115.40	120.52
2	E	137	GLY	N-CA-C	5.16	125.41	113.18
2	B	43	LYS	N-CA-C	5.16	121.79	110.80
2	K	70	PHE	N-CA-C	5.15	117.95	109.76
1	D	307	ALA	N-CA-C	-5.14	105.75	111.36
3	I	173	ILE	N-CA-C	-5.14	102.28	107.89
3	I	77	ARG	N-CA-C	5.14	117.75	110.50
3	F	149	CYS	CA-C-N	5.13	125.21	119.87
3	F	149	CYS	C-N-CA	5.13	125.21	119.87
2	B	73	THR	N-CA-C	-5.13	102.05	109.59
1	M	167	GLY	N-CA-C	-5.13	109.03	114.67
3	L	181	GLU	CG-CD-OE2	-5.13	106.61	118.40
1	P	167	GLY	N-CA-C	-5.12	109.03	114.67
2	H	137	GLY	N-CA-C	5.12	125.31	113.18
3	R	143	ASP	N-CA-C	-5.12	105.51	112.26
2	K	216	MET	N-CA-C	-5.10	105.64	111.14
1	A	308	PHE	N-CA-C	5.08	116.97	108.23
1	G	270	MET	CA-C-N	5.08	124.87	119.28
1	G	270	MET	C-N-CA	5.08	124.87	119.28
1	P	217	HIS	N-CA-C	-5.08	106.93	113.23
2	Q	137	GLY	N-CA-C	5.08	125.21	113.18
3	I	159	ALA	N-CA-C	-5.07	106.00	113.61
1	P	276	HIS	N-CA-C	5.06	117.53	108.47
1	G	232	THR	N-CA-C	5.06	118.61	112.23
1	P	419	ALA	N-CA-C	5.06	116.27	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	43	LYS	N-CA-C	5.06	121.57	110.80
3	F	57	VAL	N-CA-C	5.06	114.03	106.85
3	F	143	ASP	N-CA-C	-5.06	106.53	113.30
2	N	45	VAL	N-CA-C	5.04	112.54	107.55
1	P	108	VAL	N-CA-CB	5.04	116.11	110.51
3	R	173	ILE	CA-C-N	5.04	125.25	120.31
3	R	173	ILE	C-N-CA	5.04	125.25	120.31
1	P	85	ARG	N-CA-C	5.04	118.58	112.23
2	N	228	GLN	N-CA-C	-5.03	105.69	111.07
1	A	167	GLY	N-CA-C	-5.03	109.14	114.67
2	K	89	PHE	CA-C-N	-5.03	115.54	120.52
2	K	89	PHE	C-N-CA	-5.03	115.54	120.52
1	A	86	ASN	N-CA-C	5.03	118.86	112.12
1	J	317	ILE	CB-CA-C	-5.03	105.27	111.70
2	H	43	LYS	N-CA-C	5.02	121.49	110.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	TYR	Sidechain
1	G	199	TYR	Sidechain
1	J	199	TYR	Sidechain
1	P	199	TYR	Sidechain

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	3440	0	3428	209	0
1	D	3440	0	3428	213	0
1	G	3440	0	3428	224	0
1	J	3440	0	3428	225	0
1	M	3440	0	3428	232	0
1	P	3440	0	3428	221	0
2	B	1953	0	1848	99	0
2	E	1953	0	1848	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1953	0	1848	97	0
2	K	1953	0	1848	101	0
2	N	1953	0	1848	107	0
2	Q	1953	0	1848	119	0
3	C	1340	0	1303	88	0
3	F	1340	0	1303	81	0
3	I	1340	0	1303	83	0
3	L	1340	0	1303	74	0
3	O	1340	0	1303	68	0
3	R	1340	0	1303	72	0
4	A	20	0	28	1	0
4	D	20	0	28	2	0
4	G	20	0	28	2	0
4	J	20	0	28	0	0
4	M	20	0	28	2	0
4	Q	20	0	28	0	0
5	A	86	0	60	8	0
5	B	43	0	30	6	0
5	D	86	0	60	14	0
5	E	43	0	30	2	0
5	G	86	0	60	12	0
5	H	43	0	30	1	0
5	J	86	0	60	12	0
5	K	43	0	30	2	0
5	M	86	0	60	6	0
5	N	43	0	30	0	0
5	P	86	0	60	17	0
5	Q	43	0	30	1	0
6	A	37	0	42	7	0
6	D	37	0	42	3	0
6	G	37	0	42	8	0
6	J	37	0	42	4	0
6	M	37	0	42	4	0
6	P	37	0	42	5	0
7	A	45	0	67	5	0
7	D	45	0	67	4	0
7	G	45	0	67	4	0
7	J	45	0	67	3	0
7	M	45	0	67	7	0
7	P	45	0	67	3	0
8	A	39	0	40	7	0
8	D	39	0	39	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	39	0	39	7	0
8	J	39	0	40	7	0
8	M	39	0	39	6	0
8	P	39	0	39	7	0
9	B	1	0	0	0	0
9	E	1	0	0	0	0
9	H	1	0	0	0	0
9	K	1	0	0	0	0
9	N	1	0	0	0	0
9	Q	1	0	0	0	0
10	C	4	0	0	2	0
10	F	4	0	0	2	0
10	I	4	0	0	2	0
10	L	4	0	0	2	0
10	O	4	0	0	2	0
10	R	4	0	0	3	0
All	All	42048	0	41072	2296	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (2296) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:250:ARG:CZ	3:L:12:ARG:HB3	1.85	1.04
1:J:236:GLU:HA	1:J:239:LYS:HD3	1.37	1.03
3:C:143:ASP:HA	3:L:89:GLN:HE21	1.24	1.01
1:M:200:LEU:HD22	1:P:63:ILE:HD13	1.41	1.01
2:E:138:PHE:CD2	2:E:187:PRO:HG3	1.95	1.01
1:A:200:LEU:HD22	1:D:63:ILE:HD13	1.40	0.99
1:G:63:ILE:HD13	1:J:200:LEU:HD22	1.46	0.97
1:P:33:ILE:HD11	1:P:249:ILE:HD11	1.48	0.96
1:G:195:PHE:HE2	1:J:195:PHE:HE2	1.11	0.94
1:M:63:ILE:HD13	1:P:200:LEU:HD22	1.47	0.94
1:A:195:PHE:HE2	1:D:195:PHE:HE2	1.01	0.94
1:J:33:ILE:HD11	1:J:249:ILE:HD11	1.46	0.94
1:M:33:ILE:HD11	1:M:249:ILE:HD11	1.48	0.93
1:G:33:ILE:HD11	1:G:249:ILE:HD11	1.47	0.93
1:A:63:ILE:HD13	1:D:200:LEU:HD22	1.48	0.93
1:M:195:PHE:HE2	1:P:195:PHE:HE2	1.06	0.92
1:G:294:PRO:HA	6:G:503:SMA:H10	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:329:LYS:HE3	3:R:131:HIS:O	1.71	0.91
1:D:294:PRO:HA	6:D:2:SMA:H10	1.53	0.91
2:B:223:LEU:HD21	2:B:227:LYS:HE3	1.54	0.90
1:G:248:PHE:HD1	1:G:251:LYS:HD3	1.36	0.90
2:N:138:PHE:CD2	2:N:187:PRO:HG3	2.06	0.90
1:A:33:ILE:HD11	1:A:249:ILE:HD11	1.52	0.89
1:D:33:ILE:HD11	1:D:249:ILE:HD11	1.52	0.89
1:G:200:LEU:HD22	1:J:63:ILE:HD13	1.56	0.87
3:R:89:GLN:HB2	3:R:92:GLN:HG2	1.58	0.86
1:D:39:ARG:HH12	2:E:255:VAL:HG12	1.41	0.85
2:E:250:ARG:HD3	3:F:12:ARG:CD	2.06	0.85
2:K:250:ARG:NE	3:L:12:ARG:HB3	1.90	0.84
2:K:77:THR:HG22	2:K:79:GLU:H	1.42	0.84
1:A:195:PHE:CE2	1:D:195:PHE:HE2	1.93	0.84
1:J:125:ARG:CZ	1:J:222:ASN:HB2	2.07	0.84
2:B:103:MET:HE3	5:B:301:HEM:HAA2	1.59	0.84
2:Q:138:PHE:CD2	2:Q:187:PRO:HG3	2.12	0.84
1:G:236:GLU:HA	1:G:239:LYS:HD3	1.58	0.83
1:J:294:PRO:HA	6:J:503:SMA:H10	1.58	0.83
1:P:39:ARG:HH12	2:Q:255:VAL:HG12	1.44	0.83
2:Q:142:PRO:HG2	2:Q:150:GLU:OE2	1.77	0.83
1:J:142:THR:HG21	5:J:502:HEM:HBB2	1.59	0.82
2:K:128:PRO:HG2	2:K:129:GLU:OE1	1.80	0.82
1:A:195:PHE:HE2	1:D:195:PHE:CE2	1.94	0.81
1:P:418:VAL:HG12	1:P:419:ALA:H	1.44	0.81
1:G:103:LEU:HD13	7:G:504:LOP:H212	1.61	0.81
2:K:250:ARG:NH2	3:L:12:ARG:HB3	1.95	0.81
3:R:74:ILE:HG12	3:R:124:VAL:HG22	1.63	0.81
2:H:128:PRO:HG2	2:H:129:GLU:OE1	1.80	0.80
1:G:39:ARG:HD3	1:G:428:PHE:CD2	2.16	0.80
2:K:74:ASP:HB3	2:K:77:THR:HB	1.62	0.80
1:D:246:PRO:HG2	2:E:251:LEU:HD21	1.62	0.80
1:G:410:ILE:HG23	1:G:414:ILE:HD12	1.63	0.80
1:G:125:ARG:CZ	1:G:222:ASN:HB2	2.12	0.79
2:N:149:HIS:CE1	2:N:168:THR:HG21	2.17	0.79
2:E:74:ASP:HB3	2:E:77:THR:HB	1.64	0.79
3:F:74:ILE:HG12	3:F:124:VAL:HG22	1.64	0.79
1:M:195:PHE:HE2	1:P:195:PHE:CE2	1.97	0.79
1:M:195:PHE:CE2	1:P:195:PHE:HE2	1.96	0.79
1:D:406:VAL:O	1:D:409:PRO:HD2	1.83	0.79
1:P:294:PRO:HA	6:P:503:SMA:H10	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:76:ALA:O	1:G:79:SER:HB3	1.84	0.78
1:J:105:PHE:O	1:J:108:VAL:HG23	1.82	0.78
2:N:128:PRO:HG2	2:N:129:GLU:OE1	1.82	0.78
1:D:236:GLU:HA	1:D:239:LYS:HD3	1.63	0.78
2:E:250:ARG:HD3	3:F:12:ARG:NE	1.99	0.78
3:I:89:GLN:H	3:I:92:GLN:HE21	1.31	0.78
2:K:42:MET:HE1	2:K:214:PHE:CE2	2.19	0.78
3:L:89:GLN:HB2	3:L:92:GLN:HG3	1.65	0.78
1:P:418:VAL:HG12	1:P:419:ALA:N	1.98	0.77
1:G:213:ILE:HA	1:G:216:PHE:CE2	2.20	0.77
3:I:90:LEU:HD11	3:I:108:GLU:HB3	1.65	0.77
3:O:74:ILE:HG12	3:O:124:VAL:HG22	1.67	0.77
1:G:39:ARG:HH12	2:H:255:VAL:HG12	1.49	0.77
1:G:248:PHE:CD1	1:G:251:LYS:HD3	2.18	0.77
2:B:147:GLU:HG3	2:B:147:GLU:O	1.85	0.77
1:M:44:MET:HE3	7:M:504:LOP:H101	1.65	0.77
1:D:30:TYR:CE1	1:D:34:MET:HG3	2.21	0.76
8:P:505:ANJ:C12	8:P:505:ANJ:O6	2.33	0.76
1:G:410:ILE:CG2	1:G:414:ILE:HD12	2.16	0.76
2:Q:61:ASP:HA	2:Q:64:ARG:NH1	2.00	0.76
1:D:213:ILE:HA	1:D:216:PHE:CE2	2.20	0.76
1:P:199:TYR:CE2	5:P:502:HEM:HBC1	2.21	0.76
1:A:213:ILE:HA	1:A:216:PHE:CE2	2.21	0.76
1:A:91:PHE:CE1	1:A:92:MET:HG2	2.20	0.76
1:D:418:VAL:HG12	1:D:419:ALA:N	2.00	0.76
2:E:142:PRO:HG2	2:E:150:GLU:OE2	1.86	0.75
3:L:74:ILE:HG12	3:L:124:VAL:HG22	1.66	0.75
2:N:194:VAL:HB	2:N:207:MET:HE3	1.68	0.75
1:P:44:MET:HE3	7:P:504:LOP:H92	1.67	0.75
1:J:213:ILE:HA	1:J:216:PHE:CE2	2.21	0.75
3:I:74:ILE:HG12	3:I:124:VAL:HG22	1.68	0.75
2:K:194:VAL:HB	2:K:207:MET:HE3	1.69	0.75
1:M:213:ILE:HA	1:M:216:PHE:CE2	2.22	0.75
1:M:406:VAL:O	1:M:409:PRO:HD2	1.86	0.75
2:Q:194:VAL:HB	2:Q:207:MET:HE3	1.69	0.75
2:E:108:ALA:HA	2:E:125:ILE:HG22	1.69	0.75
1:M:236:GLU:HA	1:M:239:LYS:HD3	1.67	0.75
2:E:77:THR:HG22	2:E:79:GLU:H	1.52	0.74
2:Q:61:ASP:HA	2:Q:64:ARG:HH12	1.49	0.74
2:B:194:VAL:HB	2:B:207:MET:HE3	1.69	0.74
3:C:74:ILE:HG12	3:C:124:VAL:HG22	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:PHE:HE1	1:G:92:MET:HE3	1.52	0.74
1:G:195:PHE:CE2	1:J:195:PHE:HE2	2.02	0.74
2:Q:128:PRO:HG2	2:Q:129:GLU:OE1	1.86	0.74
3:O:95:ASP:HB3	3:O:170:ASN:ND2	2.00	0.74
2:H:194:VAL:HB	2:H:207:MET:HE3	1.68	0.74
1:J:199:TYR:HA	5:J:502:HEM:HBC2	1.69	0.74
1:P:55:LEU:HD23	8:P:505:ANJ:H281	1.67	0.74
6:A:1:SMA:H33	6:A:1:SMA:H39	1.68	0.73
1:J:406:VAL:O	1:J:409:PRO:HD2	1.87	0.73
1:J:59:ILE:O	1:J:63:ILE:HG13	1.88	0.73
8:M:505:ANJ:O6	8:M:505:ANJ:C12	2.37	0.73
2:B:184:ALA:HB3	5:B:301:HEM:HBD2	1.71	0.73
1:D:132:GLY:C	5:D:501:HEM:HBC2	2.14	0.73
2:Q:32:TYR:CE2	2:Q:42:MET:HE2	2.24	0.73
2:B:103:MET:CE	5:B:301:HEM:HAA2	2.18	0.73
2:B:250:ARG:NE	3:C:12:ARG:HB2	2.03	0.73
1:M:76:ALA:O	1:M:79:SER:HB3	1.88	0.73
1:J:76:ALA:O	1:J:79:SER:HB3	1.88	0.73
1:P:213:ILE:HA	1:P:216:PHE:CE2	2.23	0.73
8:D:504:ANJ:O6	8:D:504:ANJ:C12	2.37	0.73
2:N:220:GLU:OE2	2:N:226:ARG:NH1	2.22	0.72
2:B:250:ARG:HE	3:C:12:ARG:HB2	1.54	0.72
2:N:250:ARG:NE	3:O:12:ARG:HB2	2.04	0.72
1:G:195:PHE:HE2	1:J:195:PHE:CE2	2.03	0.72
2:Q:48:ARG:HG3	2:Q:48:ARG:HH11	1.53	0.72
1:G:91:PHE:CE1	1:G:92:MET:HE3	2.24	0.72
1:P:59:ILE:O	1:P:63:ILE:HG13	1.90	0.72
8:A:504:ANJ:O6	8:A:504:ANJ:C12	2.36	0.72
1:G:387:PHE:CD1	1:G:388:PRO:HA	2.25	0.72
1:D:76:ALA:O	1:D:79:SER:HB3	1.89	0.72
2:E:194:VAL:HB	2:E:207:MET:HE3	1.71	0.71
1:G:317:ILE:O	1:G:321:ILE:HG13	1.90	0.71
8:J:505:ANJ:O6	8:J:505:ANJ:C12	2.37	0.71
6:P:503:SMA:H33	6:P:503:SMA:H39	1.71	0.71
2:E:66:TYR:O	2:E:69:GLN:HG2	1.91	0.71
1:A:76:ALA:O	1:A:79:SER:HB3	1.90	0.71
1:A:294:PRO:HA	6:A:1:SMA:H10	1.72	0.71
2:H:48:ARG:HH11	2:H:48:ARG:HG3	1.56	0.71
2:K:66:TYR:O	2:K:69:GLN:HG2	1.90	0.71
1:P:236:GLU:HA	1:P:239:LYS:HD3	1.71	0.71
8:G:505:ANJ:O6	8:G:505:ANJ:C12	2.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4:ILE:N	1:J:4:ILE:HD12	2.06	0.71
5:D:502:HEM:HBB2	5:D:502:HEM:CMB	2.20	0.71
1:J:358:ARG:HH21	7:J:504:LOP:H21	1.56	0.71
1:M:105:PHE:O	1:M:108:VAL:HG23	1.91	0.71
1:J:105:PHE:HA	1:J:108:VAL:CG2	2.20	0.70
1:J:312:VAL:O	1:J:316:GLN:HG3	1.89	0.70
2:N:48:ARG:HG3	2:N:48:ARG:HH11	1.53	0.70
1:M:59:ILE:O	1:M:63:ILE:HG13	1.91	0.70
1:M:317:ILE:HG22	1:M:321:ILE:HD11	1.72	0.70
1:P:326:ILE:HG22	1:P:326:ILE:O	1.91	0.70
1:P:76:ALA:O	1:P:79:SER:HB3	1.91	0.70
1:D:360:ARG:O	1:D:364:LYS:HG3	1.92	0.70
3:R:89:GLN:C	3:R:91:GLY:H	1.97	0.70
1:A:263:PHE:O	1:A:267:VAL:HG23	1.92	0.70
2:B:250:ARG:NH2	3:C:12:ARG:HB3	2.07	0.70
1:G:213:ILE:CD1	8:G:505:ANJ:H14	2.22	0.70
1:A:39:ARG:HH12	2:B:255:VAL:HG12	1.57	0.69
3:O:55:SER:HB3	3:O:182:THR:OG1	1.91	0.69
1:A:408:LEU:HB2	1:A:409:PRO:HD3	1.73	0.69
1:D:263:PHE:O	1:D:267:VAL:HG23	1.92	0.69
2:H:146:ALA:HB2	2:H:169:CYS:SG	2.32	0.69
1:P:406:VAL:C	1:P:409:PRO:HD2	2.17	0.69
1:A:213:ILE:CD1	8:A:504:ANJ:H14	2.22	0.69
3:R:124:VAL:O	3:R:173:ILE:HG23	1.91	0.69
2:H:141:GLU:O	2:H:141:GLU:HG3	1.93	0.69
1:A:372:ALA:O	1:A:376:ILE:HG13	1.93	0.69
1:D:43:TRP:CZ3	1:D:251:LYS:HE3	2.27	0.69
2:E:138:PHE:HD2	2:E:187:PRO:HG3	1.51	0.69
1:J:39:ARG:HG2	1:J:242:VAL:HG13	1.75	0.69
3:O:138:GLY:CA	3:O:147:TRP:CD1	2.75	0.69
3:F:55:SER:HB3	3:F:182:THR:OG1	1.93	0.69
1:J:91:PHE:HE1	1:J:92:MET:HE3	1.58	0.69
3:F:124:VAL:O	3:F:173:ILE:HG23	1.92	0.69
2:K:77:THR:HG22	2:K:79:GLU:N	2.07	0.69
1:M:105:PHE:HA	1:M:108:VAL:CG2	2.23	0.69
1:M:108:VAL:O	1:M:112:ILE:HG13	1.92	0.69
1:A:291:HIS:O	1:A:293:VAL:HG23	1.93	0.69
1:A:319:ASN:HD22	1:A:319:ASN:C	2.00	0.69
1:G:52:ALA:HB2	8:G:505:ANJ:H163	1.74	0.68
1:M:326:ILE:HG22	1:M:326:ILE:O	1.91	0.68
2:N:66:TYR:HE1	2:N:70:PHE:HE2	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:VAL:HG22	1:A:188:ASN:OD1	1.93	0.68
3:F:84:LEU:HD12	3:F:84:LEU:H	1.57	0.68
3:F:93:LEU:HD13	3:F:161:ARG:HD2	1.74	0.68
1:M:156:PHE:CE2	1:M:285:PRO:HA	2.29	0.68
3:R:89:GLN:O	3:R:91:GLY:N	2.25	0.68
2:N:156:TYR:HB2	2:N:182:TRP:CZ2	2.28	0.68
2:Q:223:LEU:HD21	2:Q:227:LYS:HE3	1.76	0.68
3:R:55:SER:HB3	3:R:182:THR:OG1	1.93	0.68
4:D:431:BGL:H5	2:E:15:GLY:H	1.56	0.68
1:G:39:ARG:HG2	1:G:242:VAL:HG13	1.76	0.68
2:Q:42:MET:HE1	2:Q:214:PHE:CZ	2.27	0.68
1:A:280:TYR:CZ	2:B:105:LYS:HD2	2.29	0.68
1:G:59:ILE:O	1:G:63:ILE:HG13	1.93	0.68
1:P:39:ARG:HH12	2:Q:255:VAL:CG1	2.05	0.68
2:Q:32:TYR:CD2	2:Q:42:MET:HE2	2.28	0.68
3:R:84:LEU:O	3:R:88:VAL:HG23	1.93	0.68
2:H:145:CYS:O	2:H:145:CYS:SG	2.49	0.68
2:B:48:ARG:HH11	2:B:48:ARG:HG3	1.59	0.67
1:P:105:PHE:HA	1:P:108:VAL:HG22	1.74	0.67
1:J:105:PHE:HA	1:J:108:VAL:HG23	1.75	0.67
1:P:30:TYR:CE1	1:P:34:MET:HG3	2.29	0.67
2:N:138:PHE:HD2	2:N:187:PRO:HG3	1.58	0.67
1:G:209:VAL:HG22	5:G:501:HEM:HBB2	1.76	0.67
3:L:55:SER:HB3	3:L:182:THR:OG1	1.95	0.67
2:Q:89:PHE:HB3	2:Q:90:PRO:HD2	1.75	0.67
1:M:164:GLY:HA2	1:M:177:GLN:NE2	2.09	0.67
1:G:4:ILE:HD12	1:G:4:ILE:N	2.09	0.67
1:P:291:HIS:O	1:P:293:VAL:HG23	1.94	0.67
1:A:166:PHE:O	1:A:169:ILE:HD12	1.94	0.67
1:A:330:PHE:CE2	1:A:334:LEU:HD11	2.30	0.67
1:A:406:VAL:O	1:A:409:PRO:HD2	1.95	0.67
1:D:39:ARG:HG2	1:D:242:VAL:HG13	1.76	0.67
3:I:55:SER:HB3	3:I:182:THR:OG1	1.93	0.67
2:K:48:ARG:HH11	2:K:48:ARG:HG3	1.58	0.67
2:Q:242:VAL:O	2:Q:246:LEU:HG	1.95	0.67
3:I:124:VAL:O	3:I:173:ILE:HG23	1.95	0.67
2:N:242:VAL:O	2:N:246:LEU:HG	1.94	0.67
1:A:236:GLU:HA	1:A:239:LYS:HG3	1.75	0.67
1:D:91:PHE:HE1	1:D:92:MET:HE3	1.60	0.67
2:E:48:ARG:HH11	2:E:48:ARG:HG3	1.60	0.67
3:L:124:VAL:O	3:L:173:ILE:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:235:MET:HE2	2:N:235:MET:HA	1.76	0.67
1:P:128:THR:HG21	5:P:501:HEM:HBD1	1.77	0.67
1:D:59:ILE:O	1:D:63:ILE:HG13	1.94	0.66
1:A:39:ARG:HG2	1:A:242:VAL:HG13	1.78	0.66
1:A:418:VAL:HG12	1:A:419:ALA:N	2.09	0.66
1:J:30:TYR:CE1	1:J:34:MET:HG3	2.31	0.66
1:J:263:PHE:O	1:J:267:VAL:HG23	1.95	0.66
1:M:418:VAL:HG12	1:M:419:ALA:H	1.59	0.66
3:O:124:VAL:O	3:O:173:ILE:HG23	1.95	0.66
2:K:139:PRO:HB3	2:K:158:ARG:NH1	2.10	0.66
1:G:286:LEU:O	1:G:287:ARG:HG3	1.96	0.66
3:C:55:SER:HB3	3:C:182:THR:OG1	1.95	0.66
2:K:220:GLU:OE2	2:K:226:ARG:NH1	2.29	0.66
1:M:39:ARG:HG2	1:M:242:VAL:HG13	1.77	0.66
1:P:39:ARG:HG2	1:P:242:VAL:HG13	1.78	0.66
1:A:193:ARG:HD3	3:F:38:MET:HE3	1.77	0.66
1:J:418:VAL:HG12	1:J:419:ALA:N	2.10	0.66
2:K:138:PHE:CD1	2:K:187:PRO:HG3	2.31	0.66
1:M:117:TYR:HB2	1:M:367:PHE:CZ	2.31	0.66
1:D:105:PHE:HA	1:D:108:VAL:HG22	1.77	0.66
1:D:128:THR:HG21	5:D:501:HEM:HBD1	1.78	0.65
1:G:105:PHE:HA	1:G:108:VAL:CG2	2.26	0.65
1:M:418:VAL:HG12	1:M:419:ALA:N	2.10	0.65
1:P:117:TYR:HB2	1:P:367:PHE:CZ	2.31	0.65
1:P:406:VAL:O	1:P:409:PRO:HD2	1.95	0.65
1:J:39:ARG:HH12	2:K:255:VAL:HG12	1.60	0.65
1:J:166:PHE:O	1:J:169:ILE:HD12	1.96	0.65
3:R:155:HIS:O	3:R:162:ILE:HD12	1.96	0.65
3:C:19:THR:HG22	3:C:20:ALA:N	2.11	0.65
2:E:72:VAL:HG12	2:E:73:THR:N	2.10	0.65
1:G:263:PHE:O	1:G:267:VAL:HG23	1.96	0.65
1:D:418:VAL:HG12	1:D:419:ALA:H	1.61	0.65
1:G:39:ARG:HH12	2:H:255:VAL:CG1	2.09	0.65
1:G:330:PHE:CE2	1:G:334:LEU:HD11	2.32	0.65
1:J:132:GLY:C	5:J:501:HEM:HBC2	2.21	0.65
3:F:54:VAL:HG22	3:F:54:VAL:O	1.97	0.65
1:M:123:ALA:O	1:M:355:ARG:NH1	2.30	0.65
1:M:425:GLU:HG2	1:M:429:ASN:HD21	1.60	0.65
3:R:138:GLY:HA2	3:R:147:TRP:CD1	2.31	0.65
1:A:312:VAL:O	1:A:315:VAL:HB	1.97	0.65
1:J:418:VAL:CG1	1:J:419:ALA:N	2.58	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:108:ALA:HA	2:K:125:ILE:HG22	1.79	0.65
1:P:91:PHE:HE1	1:P:92:MET:HE3	1.61	0.65
1:P:263:PHE:O	1:P:267:VAL:HG23	1.95	0.65
1:D:73:VAL:HG22	1:D:188:ASN:OD1	1.96	0.65
1:G:4:ILE:HD12	1:G:4:ILE:H	1.60	0.65
3:I:131:HIS:O	1:J:329:LYS:HE3	1.97	0.65
1:M:294:PRO:HA	6:M:503:SMA:H10	1.78	0.65
2:Q:47:ILE:HG13	2:Q:87:ASP:O	1.96	0.65
2:B:74:ASP:HB2	2:B:81:ARG:HE	1.62	0.65
2:E:17:PHE:CE1	2:E:231:PHE:HE1	2.14	0.65
1:M:236:GLU:HA	1:M:239:LYS:CD	2.26	0.65
1:A:59:ILE:O	1:A:63:ILE:HG13	1.97	0.65
1:D:4:ILE:HD12	1:D:4:ILE:N	2.12	0.65
3:F:37:GLN:NE2	3:F:38:MET:HG3	2.12	0.65
2:H:77:THR:C	2:H:79:GLU:H	2.04	0.65
2:N:47:ILE:HG13	2:N:87:ASP:O	1.97	0.65
1:D:164:GLY:HA2	1:D:177:GLN:NE2	2.12	0.64
1:D:326:ILE:O	1:D:326:ILE:HG22	1.97	0.64
1:G:166:PHE:O	1:G:169:ILE:HD12	1.97	0.64
1:J:330:PHE:CE2	1:J:334:LEU:HD11	2.32	0.64
1:D:166:PHE:O	1:D:169:ILE:HD12	1.97	0.64
1:D:372:ALA:O	1:D:376:ILE:HG13	1.97	0.64
2:E:146:ALA:HB2	2:E:169:CYS:SG	2.37	0.64
1:A:105:PHE:HA	1:A:108:VAL:HG12	1.79	0.64
1:D:291:HIS:O	1:D:293:VAL:HG23	1.97	0.64
1:A:30:TYR:CE1	1:A:34:MET:HG3	2.32	0.64
2:H:220:GLU:OE2	2:H:226:ARG:NH1	2.31	0.64
2:K:42:MET:HE1	2:K:214:PHE:CZ	2.31	0.64
2:N:149:HIS:ND1	2:N:168:THR:HG21	2.13	0.64
2:E:250:ARG:HD3	3:F:12:ARG:HD2	1.79	0.64
1:M:234:LYS:O	1:M:238:GLN:HG3	1.97	0.64
1:G:291:HIS:O	1:G:293:VAL:HG23	1.97	0.64
1:J:117:TYR:HB2	1:J:367:PHE:CZ	2.33	0.64
2:K:48:ARG:HB3	2:K:85:PRO:O	1.98	0.64
1:M:263:PHE:O	1:M:267:VAL:HG23	1.97	0.64
1:P:418:VAL:CG1	1:P:419:ALA:H	2.11	0.64
2:Q:220:GLU:OE2	2:Q:226:ARG:NH1	2.30	0.64
1:G:418:VAL:HG12	1:G:419:ALA:N	2.13	0.64
2:N:51:SER:OG	2:N:63:VAL:HG21	1.98	0.64
1:G:117:TYR:HB2	1:G:367:PHE:CZ	2.32	0.64
1:G:326:ILE:O	1:G:326:ILE:HG22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:104:PHE:O	1:J:108:VAL:HG22	1.97	0.64
3:L:155:HIS:O	3:L:162:ILE:HD12	1.98	0.64
3:O:138:GLY:HA2	3:O:147:TRP:CD1	2.33	0.64
1:A:144:PHE:HE2	6:A:1:SMA:H43	1.63	0.63
1:J:291:HIS:O	1:J:293:VAL:HG23	1.98	0.63
1:M:291:HIS:O	1:M:293:VAL:HG23	1.98	0.63
1:A:326:ILE:O	1:A:326:ILE:HG22	1.97	0.63
3:L:54:VAL:O	3:L:54:VAL:HG22	1.97	0.63
1:P:114:ARG:HD2	1:P:114:ARG:C	2.23	0.63
1:J:306:ARG:NH2	1:J:383:GLN:O	2.27	0.63
1:D:51:LEU:HD21	1:D:108:VAL:HG13	1.79	0.63
1:M:408:LEU:HB2	1:M:409:PRO:HD3	1.81	0.63
8:A:504:ANJ:O6	8:A:504:ANJ:O4	2.16	0.63
3:I:155:HIS:O	3:I:162:ILE:HD12	1.99	0.63
3:C:131:HIS:O	1:D:329:LYS:HE3	1.98	0.63
1:M:64:VAL:HG11	1:M:93:LEU:HD13	1.81	0.63
1:A:108:VAL:HG22	1:A:112:ILE:HD11	1.80	0.63
1:P:156:PHE:CE2	1:P:285:PRO:HA	2.33	0.63
1:A:105:PHE:O	1:A:108:VAL:HG12	1.98	0.63
1:D:406:VAL:C	1:D:409:PRO:HD2	2.24	0.63
1:G:39:ARG:HH11	1:G:428:PHE:HE2	1.45	0.63
1:P:376:ILE:O	1:P:380:VAL:HG22	1.99	0.63
2:Q:171:ASP:OD2	2:Q:175:VAL:HB	1.99	0.63
2:E:128:PRO:HG2	2:E:129:GLU:OE1	1.99	0.62
3:O:90:LEU:HD11	3:O:108:GLU:HB3	1.81	0.62
1:P:44:MET:CE	7:P:504:LOP:H92	2.29	0.62
1:P:158:GLY:O	1:P:162:ILE:HG13	1.98	0.62
2:Q:114:MET:HG2	2:Q:114:MET:O	1.98	0.62
3:R:89:GLN:C	3:R:91:GLY:N	2.56	0.62
3:L:148:PHE:CE1	3:L:153:GLY:HA2	2.34	0.62
3:I:162:ILE:HD11	3:I:164:LYS:O	1.99	0.62
1:M:114:ARG:HD2	1:M:114:ARG:C	2.23	0.62
1:M:370:LEU:HD22	1:M:403:TYR:CE2	2.35	0.62
1:M:372:ALA:O	1:M:376:ILE:HG13	1.99	0.62
2:N:77:THR:HG22	2:N:79:GLU:H	1.65	0.62
1:A:108:VAL:O	1:A:112:ILE:HG13	1.99	0.62
1:J:3:GLY:C	1:J:4:ILE:HD12	2.25	0.62
1:M:330:PHE:CE2	1:M:334:LEU:HD11	2.34	0.62
1:A:199:TYR:O	1:A:202:PRO:HD2	2.00	0.62
1:A:246:PRO:HG2	2:B:251:LEU:HD21	1.81	0.62
1:M:103:LEU:HD13	7:M:504:LOP:H222	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:502:HEM:O1A	5:P:502:HEM:O2D	2.17	0.62
3:R:148:PHE:CE1	3:R:153:GLY:HA2	2.35	0.62
1:J:180:LEU:HD13	6:J:503:SMA:H25	1.81	0.62
1:M:410:ILE:CG2	1:M:414:ILE:HD12	2.30	0.62
8:M:505:ANJ:O6	8:M:505:ANJ:O4	2.18	0.62
1:A:117:TYR:HB2	1:A:367:PHE:CZ	2.35	0.62
1:G:313:TRP:O	1:G:317:ILE:HG13	1.98	0.62
1:J:326:ILE:HG22	1:J:326:ILE:O	2.00	0.62
1:J:114:ARG:HD2	1:J:114:ARG:C	2.25	0.62
1:J:213:ILE:CD1	8:J:505:ANJ:H14	2.30	0.62
2:N:66:TYR:O	2:N:69:GLN:HG2	1.99	0.62
3:R:54:VAL:O	3:R:54:VAL:HG22	1.99	0.62
1:M:91:PHE:HE1	1:M:92:MET:HE3	1.65	0.61
2:N:66:TYR:CE1	2:N:70:PHE:HE2	2.17	0.61
3:O:54:VAL:O	3:O:54:VAL:HG22	1.99	0.61
2:E:171:ASP:OD2	2:E:175:VAL:HB	2.00	0.61
3:F:137:ILE:HD13	3:F:150:PRO:HD3	1.81	0.61
2:N:48:ARG:HB3	2:N:85:PRO:O	2.00	0.61
1:G:105:PHE:O	1:G:108:VAL:HG23	1.99	0.61
3:I:19:THR:HG22	3:I:20:ALA:N	2.15	0.61
3:C:54:VAL:HG22	3:C:54:VAL:O	1.99	0.61
3:C:127:GLY:O	3:C:135:SER:HA	2.00	0.61
1:D:39:ARG:HH12	2:E:255:VAL:CG1	2.11	0.61
1:G:64:VAL:HG11	1:G:93:LEU:HD13	1.81	0.61
1:J:428:PHE:CZ	2:K:256:LYS:HB2	2.35	0.61
2:K:160:PHE:CD2	2:K:183:ILE:HB	2.35	0.61
1:D:91:PHE:CE1	1:D:92:MET:HE3	2.35	0.61
1:G:372:ALA:O	1:G:376:ILE:HG13	1.99	0.61
1:J:64:VAL:HG11	1:J:93:LEU:HD13	1.82	0.61
1:J:199:TYR:CE2	5:J:502:HEM:HBC1	2.36	0.61
2:K:242:VAL:O	2:K:246:LEU:HG	2.01	0.61
1:P:213:ILE:CD1	8:P:505:ANJ:H14	2.31	0.61
1:A:8:HIS:H	1:A:8:HIS:CD2	2.18	0.61
1:A:418:VAL:CG1	1:A:419:ALA:N	2.63	0.61
1:D:376:ILE:O	1:D:380:VAL:HG22	2.01	0.61
2:E:61:ASP:HA	2:E:64:ARG:NH1	2.14	0.61
3:C:80:ALA:O	3:C:84:LEU:HD13	2.00	0.61
1:G:193:ARG:HH11	3:L:38:MET:HE2	1.65	0.61
3:I:62:GLN:NE2	3:I:73:PHE:CG	2.68	0.61
1:A:4:ILE:H	1:A:4:ILE:HD12	1.66	0.61
1:A:118:TYR:OH	7:A:503:LOP:H32	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ASN:C	1:A:319:ASN:ND2	2.58	0.61
1:P:199:TYR:CD2	5:P:502:HEM:HBC1	2.36	0.61
3:R:19:THR:HG22	3:R:20:ALA:N	2.15	0.61
1:A:193:ARG:HH11	3:F:38:MET:CE	2.14	0.61
2:B:146:ALA:HB2	2:B:169:CYS:SG	2.41	0.61
8:D:504:ANJ:O6	8:D:504:ANJ:O4	2.19	0.61
2:E:42:MET:HE1	2:E:214:PHE:CZ	2.36	0.61
1:J:234:LYS:O	1:J:238:GLN:HG3	2.01	0.61
1:P:64:VAL:HG11	1:P:93:LEU:HD13	1.82	0.61
3:I:95:ASP:HB3	3:I:170:ASN:ND2	2.16	0.60
1:M:406:VAL:C	1:M:409:PRO:HD2	2.25	0.60
2:E:48:ARG:HB3	2:E:85:PRO:O	2.00	0.60
2:H:42:MET:HE1	2:H:214:PHE:CZ	2.36	0.60
3:L:19:THR:HG22	3:L:20:ALA:N	2.14	0.60
1:A:73:VAL:HG23	1:A:74:ASP:H	1.65	0.60
2:K:139:PRO:HB3	2:K:158:ARG:HH12	1.64	0.60
3:C:124:VAL:O	3:C:173:ILE:HG23	2.01	0.60
3:C:155:HIS:O	3:C:162:ILE:HD12	2.02	0.60
1:D:91:PHE:CD2	2:E:222:LYS:HG2	2.36	0.60
1:J:92:MET:HE2	1:J:92:MET:HA	1.83	0.60
1:M:60:VAL:CG2	1:M:61:THR:N	2.65	0.60
1:M:199:TYR:O	1:M:202:PRO:HD2	2.02	0.60
2:N:66:TYR:HE1	2:N:70:PHE:CE2	2.18	0.60
2:N:66:TYR:CE1	2:N:70:PHE:CE2	2.90	0.60
3:C:148:PHE:CE1	3:C:153:GLY:HA2	2.37	0.60
1:G:411:LEU:HD22	1:G:415:GLU:HB2	1.84	0.60
1:J:91:PHE:CE1	1:J:92:MET:HE3	2.35	0.60
1:P:166:PHE:O	1:P:169:ILE:HD12	2.01	0.60
1:A:193:ARG:HH11	3:F:38:MET:HE2	1.65	0.60
1:D:213:ILE:CD1	8:D:504:ANJ:H14	2.32	0.60
1:D:312:VAL:O	1:D:316:GLN:HG3	2.00	0.60
1:G:418:VAL:CG1	1:G:419:ALA:N	2.64	0.60
2:H:48:ARG:HB3	2:H:85:PRO:O	2.02	0.60
1:A:4:ILE:HD12	1:A:4:ILE:N	2.16	0.60
2:B:17:PHE:CE1	2:B:231:PHE:CE1	2.90	0.60
1:G:114:ARG:HD2	1:G:114:ARG:C	2.25	0.60
1:J:51:LEU:HD13	5:J:501:HEM:C3B	2.37	0.60
1:D:29:ALA:HB2	8:D:504:ANJ:H233	1.84	0.60
1:G:156:PHE:CE2	1:G:285:PRO:HA	2.36	0.60
3:I:12:ARG:HG2	3:I:13:ASP:N	2.16	0.60
1:M:317:ILE:O	1:M:321:ILE:HG13	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:156:TYR:HA	3:R:161:ARG:O	2.02	0.60
2:K:77:THR:CG2	2:K:79:GLU:HB2	2.32	0.60
1:P:51:LEU:HD13	5:P:501:HEM:C3B	2.37	0.60
1:P:62:GLY:C	5:P:502:HEM:HAC	2.27	0.60
2:Q:48:ARG:HB3	2:Q:85:PRO:O	2.02	0.60
2:K:130:TYR:O	2:K:134:VAL:HG23	2.01	0.60
1:M:4:ILE:N	1:M:4:ILE:HD12	2.17	0.60
1:A:60:VAL:CG2	1:A:61:THR:N	2.64	0.59
2:B:184:ALA:HB3	5:B:301:HEM:CBD	2.31	0.59
2:E:17:PHE:CE1	2:E:231:PHE:CE1	2.90	0.59
1:J:213:ILE:HD11	8:J:505:ANJ:H162	1.84	0.59
8:P:505:ANJ:O6	8:P:505:ANJ:O4	2.20	0.59
1:D:117:TYR:HB2	1:D:367:PHE:CZ	2.36	0.59
1:D:199:TYR:O	1:D:202:PRO:HD2	2.01	0.59
1:D:418:VAL:CG1	1:D:419:ALA:N	2.65	0.59
3:I:148:PHE:CE1	3:I:153:GLY:HA2	2.36	0.59
1:M:91:PHE:CD1	1:M:92:MET:N	2.71	0.59
1:A:64:VAL:HG11	1:A:93:LEU:HD13	1.83	0.59
2:H:142:PRO:HG2	2:H:150:GLU:OE2	2.02	0.59
2:H:242:VAL:O	2:H:246:LEU:HG	2.02	0.59
1:J:322:SER:O	1:J:323:PHE:HB2	2.02	0.59
1:P:199:TYR:O	1:P:202:PRO:HD2	2.01	0.59
1:A:125:ARG:NH1	1:A:220:GLY:O	2.35	0.59
1:D:330:PHE:CE2	1:D:334:LEU:HD11	2.37	0.59
2:H:130:TYR:O	2:H:134:VAL:HG23	2.02	0.59
3:R:10:THR:O	3:R:10:THR:HG22	2.02	0.59
1:A:91:PHE:CD1	1:A:92:MET:N	2.70	0.59
1:D:91:PHE:CD1	1:D:92:MET:N	2.71	0.59
3:I:54:VAL:O	3:I:54:VAL:HG22	2.02	0.59
1:J:73:VAL:HG22	1:J:188:ASN:OD1	2.03	0.59
1:M:213:ILE:CD1	8:M:505:ANJ:H14	2.32	0.59
1:P:370:LEU:HD22	1:P:403:TYR:CE2	2.38	0.59
3:F:148:PHE:CE1	3:F:153:GLY:HA2	2.38	0.59
1:G:92:MET:HA	1:G:92:MET:HE2	1.85	0.59
2:K:40:HIS:HE1	2:K:98:PRO:HD2	1.67	0.59
1:M:39:ARG:HH12	2:N:255:VAL:HG12	1.67	0.59
3:O:37:GLN:NE2	3:O:38:MET:HG3	2.17	0.59
1:A:329:LYS:HE3	3:F:131:HIS:O	2.03	0.59
2:B:220:GLU:OE2	2:B:226:ARG:NH1	2.36	0.59
1:D:370:LEU:HD22	1:D:403:TYR:CE2	2.37	0.59
1:J:376:ILE:O	1:J:380:VAL:HG22	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:91:PHE:CD2	2:Q:222:LYS:HG2	2.38	0.59
1:A:52:ALA:HB2	8:A:504:ANJ:H163	1.83	0.59
3:I:89:GLN:O	3:I:92:GLN:N	2.36	0.59
1:J:199:TYR:O	1:J:202:PRO:HD2	2.03	0.59
3:O:89:GLN:O	3:O:91:GLY:N	2.36	0.59
1:D:280:TYR:CE2	2:E:105:LYS:HD2	2.37	0.59
3:I:156:TYR:HA	3:I:161:ARG:O	2.03	0.59
1:J:164:GLY:HA2	1:J:177:GLN:NE2	2.18	0.59
1:M:376:ILE:O	1:M:380:VAL:HG22	2.02	0.59
3:O:148:PHE:CE1	3:O:153:GLY:HA2	2.38	0.59
3:C:152:HIS:HB2	10:C:200:FES:S1	2.43	0.58
2:E:220:GLU:OE2	2:E:226:ARG:NH1	2.36	0.58
3:F:54:VAL:HG23	3:F:57:VAL:HG21	1.84	0.58
1:G:102:SER:O	1:G:106:ILE:HG13	2.03	0.58
2:B:74:ASP:HB2	2:B:81:ARG:NE	2.18	0.58
1:J:91:PHE:HE1	1:J:92:MET:CE	2.16	0.58
1:P:52:ALA:HB2	8:P:505:ANJ:H163	1.85	0.58
1:A:370:LEU:HD22	1:A:403:TYR:CE2	2.38	0.58
1:D:43:TRP:CH2	1:D:251:LYS:HE3	2.37	0.58
1:G:370:LEU:HD22	1:G:403:TYR:CE2	2.38	0.58
1:P:39:ARG:NH1	2:Q:255:VAL:HG12	2.15	0.58
1:P:346:VAL:HG12	1:P:347:PRO:HD3	1.85	0.58
2:Q:53:PRO:HA	2:Q:57:GLU:CD	2.27	0.58
2:B:48:ARG:HB3	2:B:85:PRO:O	2.03	0.58
3:F:19:THR:HG22	3:F:20:ALA:N	2.17	0.58
3:I:89:GLN:C	3:I:91:GLY:N	2.55	0.58
3:L:162:ILE:HD12	3:L:163:ARG:H	1.69	0.58
3:C:54:VAL:HG23	3:C:57:VAL:HG21	1.85	0.58
1:D:164:GLY:HA2	1:D:177:GLN:HE21	1.66	0.58
3:F:78:THR:O	3:F:82:ILE:HG13	2.03	0.58
8:J:505:ANJ:O6	8:J:505:ANJ:O4	2.19	0.58
3:R:162:ILE:HD11	3:R:164:LYS:O	2.04	0.58
1:A:341:LEU:HD12	1:A:341:LEU:O	2.04	0.58
2:E:32:TYR:CE2	2:E:42:MET:HE2	2.39	0.58
8:G:505:ANJ:O6	8:G:505:ANJ:O4	2.20	0.58
3:I:10:THR:HG22	3:I:10:THR:O	2.03	0.58
3:R:21:GLY:O	3:R:25:VAL:HG23	2.02	0.58
1:A:296:TRP:HA	1:A:299:LEU:HG	1.85	0.58
3:F:10:THR:O	3:F:10:THR:HG22	2.04	0.58
2:K:80:ASP:O	2:K:81:ARG:HB3	2.03	0.58
3:O:155:HIS:O	3:O:162:ILE:HD12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:330:PHE:CE2	1:P:334:LEU:HD11	2.38	0.58
1:P:372:ALA:O	1:P:376:ILE:HG13	2.03	0.58
1:A:51:LEU:HD13	5:A:501:HEM:C3B	2.39	0.58
1:A:91:PHE:CE1	1:A:92:MET:CG	2.86	0.58
3:C:10:THR:O	3:C:10:THR:HG22	2.03	0.58
2:E:130:TYR:O	2:E:134:VAL:HG23	2.04	0.58
1:G:30:TYR:CE1	1:G:34:MET:HG3	2.38	0.58
1:J:60:VAL:CG2	1:J:61:THR:N	2.66	0.58
2:N:250:ARG:NH2	3:O:12:ARG:HB3	2.19	0.58
1:P:346:VAL:CG1	1:P:347:PRO:HD3	2.34	0.58
1:D:64:VAL:HG11	1:D:93:LEU:HD13	1.85	0.58
1:D:418:VAL:CG1	1:D:419:ALA:H	2.16	0.58
1:G:60:VAL:CG2	1:G:61:THR:N	2.65	0.58
1:G:144:PHE:CE2	6:G:503:SMA:H42	2.38	0.58
1:G:199:TYR:O	1:G:202:PRO:HD2	2.04	0.58
3:L:10:THR:HG22	3:L:10:THR:O	2.03	0.58
1:M:44:MET:HE3	7:M:504:LOP:C10	2.34	0.58
1:M:166:PHE:O	1:M:169:ILE:HD12	2.04	0.58
2:N:157:ASN:O	2:N:180:GLY:HA3	2.04	0.58
1:P:60:VAL:CG2	1:P:61:THR:N	2.67	0.58
2:B:242:VAL:O	2:B:246:LEU:HG	2.04	0.58
3:C:78:THR:O	3:C:82:ILE:HG13	2.04	0.58
1:D:346:VAL:HG12	1:D:347:PRO:HD3	1.86	0.58
1:A:114:ARG:HD2	1:A:114:ARG:C	2.29	0.57
1:A:125:ARG:HD3	5:A:501:HEM:O2D	2.04	0.57
2:E:142:PRO:CG	2:E:150:GLU:OE2	2.52	0.57
1:J:43:TRP:HZ3	1:J:251:LYS:HE2	1.69	0.57
3:O:78:THR:O	3:O:82:ILE:HG13	2.04	0.57
1:A:280:TYR:CE2	2:B:105:LYS:HD2	2.39	0.57
2:B:17:PHE:CE1	2:B:231:PHE:HE1	2.22	0.57
2:B:250:ARG:NE	3:C:12:ARG:CB	2.66	0.57
3:C:162:ILE:HD12	3:C:163:ARG:H	1.69	0.57
1:D:346:VAL:CG1	1:D:347:PRO:HD3	2.34	0.57
5:G:502:HEM:HBA2	5:G:502:HEM:O1D	2.04	0.57
3:I:78:THR:O	3:I:82:ILE:HG13	2.04	0.57
1:M:7:ASP:HB3	1:M:234:LYS:HZ1	1.69	0.57
1:M:341:LEU:HD12	1:M:341:LEU:O	2.04	0.57
3:O:95:ASP:HB3	3:O:170:ASN:HD21	1.69	0.57
1:G:376:ILE:O	1:G:380:VAL:HG22	2.03	0.57
1:J:133:MET:N	5:J:501:HEM:HBC2	2.20	0.57
2:K:250:ARG:HH21	3:L:12:ARG:HD3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ILE:O	1:A:380:VAL:HG22	2.05	0.57
2:E:42:MET:HE1	2:E:214:PHE:CE2	2.39	0.57
1:G:418:VAL:CG1	1:G:419:ALA:H	2.18	0.57
1:J:418:VAL:CG1	1:J:419:ALA:H	2.17	0.57
3:O:10:THR:HG22	3:O:10:THR:O	2.03	0.57
3:O:19:THR:HG22	3:O:20:ALA:N	2.18	0.57
1:P:125:ARG:NE	1:P:222:ASN:HB2	2.19	0.57
2:Q:106:ALA:O	2:Q:107:ARG:HG2	2.04	0.57
2:B:27:ARG:HB3	2:B:196:TYR:CZ	2.39	0.57
1:P:105:PHE:HA	1:P:108:VAL:CG2	2.34	0.57
1:A:406:VAL:C	1:A:409:PRO:HD2	2.30	0.57
2:E:242:VAL:O	2:E:246:LEU:HG	2.05	0.57
1:G:248:PHE:HA	1:G:251:LYS:HG2	1.85	0.57
3:I:89:GLN:H	3:I:92:GLN:NE2	2.02	0.57
3:O:131:HIS:HB3	10:O:200:FES:S2	2.45	0.57
1:P:418:VAL:CG1	1:P:419:ALA:N	2.66	0.57
3:F:90:LEU:CD1	3:F:108:GLU:HB3	2.34	0.57
3:F:132:LEU:HD12	3:F:152:HIS:CE1	2.39	0.57
1:J:5:PRO:HB3	1:J:234:LYS:HG2	1.87	0.57
1:J:406:VAL:C	1:J:409:PRO:HD2	2.29	0.57
3:L:84:LEU:H	3:L:84:LEU:HD12	1.69	0.57
3:L:90:LEU:CD1	3:L:108:GLU:HB3	2.35	0.57
6:M:503:SMA:H35	6:M:503:SMA:H21	1.86	0.57
1:A:91:PHE:HE1	1:A:92:MET:HG2	1.66	0.57
2:B:113:PRO:HD2	2:B:118:ILE:HB	1.86	0.57
3:I:88:VAL:HG11	3:I:93:LEU:HD21	1.85	0.57
3:R:78:THR:O	3:R:82:ILE:HG13	2.04	0.57
2:B:108:ALA:HA	2:B:125:ILE:HG22	1.85	0.57
2:B:149:HIS:CE1	2:B:168:THR:HG21	2.40	0.57
2:E:47:ILE:HG13	2:E:87:ASP:O	2.05	0.57
3:F:155:HIS:O	3:F:162:ILE:HD12	2.04	0.57
3:F:162:ILE:HD12	3:F:163:ARG:H	1.69	0.57
1:G:406:VAL:O	1:G:409:PRO:HD2	2.04	0.57
1:J:370:LEU:HD22	1:J:403:TYR:CE2	2.40	0.57
1:J:372:ALA:O	1:J:376:ILE:HG13	2.05	0.57
2:E:40:HIS:HE1	2:E:98:PRO:HD2	1.70	0.57
2:H:17:PHE:CE1	2:H:231:PHE:CE1	2.93	0.57
3:I:21:GLY:O	3:I:25:VAL:HG23	2.05	0.57
3:I:38:MET:HE3	1:J:193:ARG:HD3	1.85	0.57
2:K:189:LEU:O	2:K:190:MET:HB2	2.05	0.57
1:M:190:THR:O	1:M:193:ARG:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:GLN:O	1:A:317:ILE:C	2.48	0.56
3:I:162:ILE:HD12	3:I:163:ARG:H	1.70	0.56
1:J:246:PRO:HG2	2:K:251:LEU:HD21	1.87	0.56
2:N:191:ASP:N	2:N:204:VAL:HG23	2.19	0.56
1:J:156:PHE:CE2	1:J:285:PRO:HA	2.40	0.56
1:M:249:ILE:O	1:M:253:VAL:HG23	2.05	0.56
1:P:205:ILE:O	1:P:209:VAL:HG23	2.06	0.56
1:P:296:TRP:HA	1:P:299:LEU:HG	1.87	0.56
1:A:73:VAL:HG23	1:A:74:ASP:N	2.20	0.56
2:B:157:ASN:O	2:B:180:GLY:HA3	2.05	0.56
1:G:269:PHE:HB3	4:G:431:BGL:H1'2	1.86	0.56
1:G:312:VAL:O	1:G:316:GLN:HG3	2.05	0.56
1:M:73:VAL:HG22	1:M:188:ASN:OD1	2.06	0.56
1:D:236:GLU:O	1:D:239:LYS:HB2	2.05	0.56
1:G:91:PHE:CD1	1:G:92:MET:N	2.73	0.56
1:J:27:ALA:O	1:J:30:TYR:HB3	2.05	0.56
3:L:54:VAL:HG23	3:L:57:VAL:HG21	1.86	0.56
1:G:312:VAL:O	1:G:315:VAL:HB	2.05	0.56
3:I:38:MET:CE	1:J:193:ARG:HH11	2.17	0.56
3:I:38:MET:HG2	1:J:193:ARG:NH1	2.21	0.56
2:K:250:ARG:NE	3:L:12:ARG:CB	2.66	0.56
3:O:54:VAL:HG23	3:O:57:VAL:HG21	1.88	0.56
2:Q:19:THR:CG2	2:Q:224:MET:HE3	2.35	0.56
3:R:138:GLY:CA	3:R:147:TRP:CD1	2.88	0.56
1:A:156:PHE:CE2	1:A:285:PRO:HA	2.40	0.56
1:G:229:VAL:HG22	1:G:424:ILE:CD1	2.36	0.56
3:L:37:GLN:NE2	3:L:38:MET:HG3	2.20	0.56
1:M:128:THR:HG21	5:M:501:HEM:HBD1	1.86	0.56
2:Q:157:ASN:O	2:Q:180:GLY:HA3	2.06	0.56
3:R:127:GLY:O	3:R:135:SER:HA	2.06	0.56
1:D:428:PHE:CE1	2:E:256:LYS:HD3	2.41	0.56
3:O:156:TYR:HA	3:O:161:ARG:O	2.05	0.56
1:P:295:GLU:OE1	1:P:295:GLU:N	2.37	0.56
1:P:316:GLN:O	1:P:317:ILE:C	2.49	0.56
1:A:125:ARG:CZ	1:A:222:ASN:HB2	2.36	0.56
3:I:131:HIS:O	1:J:329:LYS:CE	2.54	0.56
3:L:21:GLY:O	3:L:25:VAL:HG23	2.06	0.56
1:M:37:THR:HB	1:M:248:PHE:HE2	1.71	0.56
2:N:48:ARG:HG3	2:N:48:ARG:NH1	2.21	0.56
2:Q:191:ASP:N	2:Q:204:VAL:HG23	2.21	0.56
1:D:116:LEU:HA	1:D:121:TYR:HE2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:362:MET:N	1:G:415:GLU:OE2	2.37	0.56
1:J:91:PHE:CE1	1:J:92:MET:CE	2.89	0.56
1:J:116:LEU:HA	1:J:121:TYR:HE2	1.71	0.56
1:P:312:VAL:O	1:P:315:VAL:HB	2.04	0.56
3:R:54:VAL:HG23	3:R:57:VAL:HG21	1.88	0.56
1:A:39:ARG:HH12	2:B:255:VAL:CG1	2.19	0.56
1:A:410:ILE:CG2	1:A:414:ILE:HD12	2.36	0.56
1:D:341:LEU:HD12	1:D:341:LEU:O	2.06	0.56
1:J:91:PHE:CD1	1:J:92:MET:N	2.75	0.56
2:N:59:PRO:HD2	2:N:62:GLN:NE2	2.21	0.56
1:M:377:LEU:O	1:M:380:VAL:HG23	2.05	0.55
1:G:62:GLY:C	5:G:502:HEM:HAC	2.31	0.55
1:G:346:VAL:HG12	1:G:347:PRO:HD3	1.88	0.55
1:J:190:THR:O	1:J:193:ARG:HG2	2.07	0.55
1:J:205:ILE:O	1:J:209:VAL:HG23	2.06	0.55
1:J:346:VAL:CG1	1:J:347:PRO:HD3	2.36	0.55
3:L:78:THR:O	3:L:82:ILE:HG13	2.06	0.55
1:M:91:PHE:CD2	2:N:222:LYS:HG2	2.41	0.55
1:D:27:ALA:O	1:D:30:TYR:HB3	2.06	0.55
2:E:59:PRO:HD2	2:E:62:GLN:NE2	2.22	0.55
1:G:39:ARG:NH1	1:G:428:PHE:HE2	2.03	0.55
1:G:199:TYR:CE2	5:G:502:HEM:HBC1	2.41	0.55
1:G:261:LEU:HD11	2:H:234:VAL:HG13	1.88	0.55
2:H:59:PRO:HD2	2:H:62:GLN:NE2	2.21	0.55
1:J:199:TYR:CD2	5:J:502:HEM:HBC1	2.41	0.55
1:J:341:LEU:HD12	1:J:341:LEU:O	2.06	0.55
1:M:193:ARG:HH11	3:R:38:MET:CE	2.20	0.55
1:P:27:ALA:O	1:P:30:TYR:HB3	2.07	0.55
2:Q:235:MET:HE2	2:Q:235:MET:N	2.21	0.55
1:D:149:LEU:HB2	1:D:150:PRO:HD3	1.87	0.55
3:F:21:GLY:O	3:F:25:VAL:HG23	2.06	0.55
1:G:193:ARG:HH11	3:L:38:MET:CE	2.19	0.55
1:J:149:LEU:HB2	1:J:150:PRO:HD3	1.88	0.55
2:N:72:VAL:HG12	2:N:73:THR:N	2.22	0.55
3:R:132:LEU:HD12	3:R:152:HIS:CE1	2.42	0.55
2:B:129:GLU:O	2:B:132:TYR:HB3	2.06	0.55
1:D:114:ARG:HD2	1:D:114:ARG:C	2.31	0.55
1:D:295:GLU:O	1:D:296:TRP:C	2.50	0.55
1:D:387:PHE:CD1	1:D:387:PHE:C	2.84	0.55
2:E:32:TYR:CD2	2:E:42:MET:HE2	2.41	0.55
2:E:113:PRO:HD2	2:E:118:ILE:HB	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:THR:HB	1:G:248:PHE:HE2	1.72	0.55
1:G:387:PHE:HA	1:G:390:ASP:OD1	2.06	0.55
1:J:43:TRP:CZ3	1:J:251:LYS:HE2	2.42	0.55
1:J:296:TRP:HA	1:J:299:LEU:HG	1.89	0.55
2:K:47:ILE:HG13	2:K:87:ASP:O	2.07	0.55
1:P:91:PHE:CD1	1:P:92:MET:N	2.75	0.55
2:Q:66:TYR:CE1	2:Q:70:PHE:HE2	2.23	0.55
3:C:38:MET:CE	1:D:193:ARG:HH11	2.19	0.55
1:M:374:PHE:CD2	7:M:504:LOP:H321	2.42	0.55
3:O:95:ASP:HB3	3:O:170:ASN:CG	2.30	0.55
1:P:52:ALA:HB2	8:P:505:ANJ:C16	2.37	0.55
1:P:91:PHE:CE1	1:P:92:MET:HE3	2.41	0.55
2:Q:108:ALA:HA	2:Q:125:ILE:O	2.07	0.55
1:A:276:HIS:CE1	1:A:278:ASP:HB2	2.42	0.55
2:B:47:ILE:HG13	2:B:87:ASP:O	2.06	0.55
3:I:77:ARG:HH21	3:I:115:THR:HG21	1.72	0.55
3:I:89:GLN:O	3:I:90:LEU:C	2.49	0.55
3:O:84:LEU:H	3:O:84:LEU:HD12	1.72	0.55
1:D:60:VAL:CG2	1:D:61:THR:N	2.69	0.55
2:H:113:PRO:HD2	2:H:118:ILE:HB	1.88	0.55
3:I:88:VAL:CG1	3:I:93:LEU:HD21	2.37	0.55
1:J:91:PHE:CD2	2:K:222:LYS:HG2	2.42	0.55
2:N:156:TYR:HB2	2:N:182:TRP:CE2	2.41	0.55
1:A:234:LYS:O	1:A:238:GLN:HG3	2.07	0.55
2:B:59:PRO:HD2	2:B:62:GLN:NE2	2.22	0.55
2:B:128:PRO:HG2	2:B:129:GLU:OE1	2.07	0.55
1:G:116:LEU:HA	1:G:121:TYR:HE2	1.72	0.55
1:G:141:ALA:O	1:G:145:MET:HE2	2.06	0.55
1:G:341:LEU:HD12	1:G:341:LEU:O	2.07	0.55
1:J:346:VAL:HG12	1:J:347:PRO:HD3	1.88	0.55
1:J:425:GLU:CG	1:J:429:ASN:HD21	2.19	0.55
3:C:138:GLY:HA2	3:C:147:TRP:CD1	2.41	0.55
2:H:47:ILE:HG13	2:H:87:ASP:O	2.06	0.55
2:K:59:PRO:HD2	2:K:62:GLN:NE2	2.21	0.55
3:L:137:ILE:HD12	3:L:150:PRO:HD3	1.89	0.55
2:B:130:TYR:O	2:B:134:VAL:HG23	2.06	0.54
5:D:502:HEM:HBB2	5:D:502:HEM:HMB1	1.88	0.54
2:E:238:THR:O	2:E:242:VAL:HG23	2.07	0.54
3:F:156:TYR:HA	3:F:161:ARG:O	2.06	0.54
1:G:27:ALA:O	1:G:30:TYR:HB3	2.07	0.54
1:G:185:ALA:HB2	3:L:70:LYS:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:113:PRO:HD2	2:K:118:ILE:HB	1.88	0.54
2:N:77:THR:CG2	2:N:79:GLU:HB2	2.37	0.54
2:N:77:THR:HG21	2:N:79:GLU:HB2	1.89	0.54
3:C:156:TYR:HA	3:C:161:ARG:O	2.07	0.54
1:G:296:TRP:HA	1:G:299:LEU:HG	1.89	0.54
1:G:319:ASN:C	1:G:319:ASN:ND2	2.66	0.54
3:I:76:ARG:HG2	3:I:121:GLU:HG2	1.88	0.54
3:I:127:GLY:O	3:I:135:SER:HA	2.06	0.54
2:K:129:GLU:O	2:K:132:TYR:HB3	2.07	0.54
1:M:296:TRP:HA	1:M:299:LEU:HG	1.87	0.54
2:Q:48:ARG:HG3	2:Q:48:ARG:NH1	2.22	0.54
3:L:44:VAL:C	3:L:46:ALA:H	2.15	0.54
1:M:49:VAL:CG1	1:M:256:LEU:HD13	2.37	0.54
1:M:346:VAL:HG12	1:M:347:PRO:HD3	1.89	0.54
2:N:103:MET:C	2:N:105:LYS:H	2.14	0.54
3:O:162:ILE:HD12	3:O:163:ARG:H	1.73	0.54
1:P:190:THR:O	1:P:193:ARG:HG2	2.08	0.54
1:A:9:TYR:HB2	1:A:30:TYR:CG	2.43	0.54
3:C:95:ASP:HB3	3:C:170:ASN:ND2	2.21	0.54
2:E:129:GLU:O	2:E:132:TYR:HB3	2.06	0.54
1:G:249:ILE:O	1:G:253:VAL:HG23	2.08	0.54
1:M:37:THR:HB	1:M:248:PHE:CE2	2.42	0.54
1:M:132:GLY:HA3	5:M:501:HEM:HBC2	1.89	0.54
2:N:40:HIS:HE1	2:N:98:PRO:HD2	1.72	0.54
2:N:103:MET:O	2:N:105:LYS:N	2.40	0.54
3:O:162:ILE:HD11	3:O:164:LYS:O	2.07	0.54
2:Q:59:PRO:HD2	2:Q:62:GLN:NE2	2.21	0.54
1:D:123:ALA:O	1:D:355:ARG:NH1	2.40	0.54
1:D:261:LEU:HD11	2:E:234:VAL:HG13	1.89	0.54
1:G:37:THR:HB	1:G:248:PHE:CE2	2.43	0.54
3:L:127:GLY:O	3:L:135:SER:HA	2.07	0.54
3:O:21:GLY:O	3:O:25:VAL:HG23	2.06	0.54
1:A:263:PHE:HA	7:A:503:LOP:H221	1.90	0.54
3:C:140:VAL:O	3:C:140:VAL:HG12	2.07	0.54
1:M:214:TRP:CH2	1:P:25:ILE:HA	2.43	0.54
1:M:360:ARG:O	1:M:364:LYS:HG3	2.08	0.54
2:N:113:PRO:HD2	2:N:118:ILE:HB	1.90	0.54
1:P:132:GLY:C	5:P:501:HEM:HBC2	2.32	0.54
1:A:193:ARG:NH1	3:F:38:MET:HG2	2.23	0.54
1:D:276:HIS:CE1	1:D:278:ASP:HB2	2.42	0.54
1:G:125:ARG:NE	1:G:222:ASN:HB2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:377:LEU:O	1:P:380:VAL:HG23	2.08	0.54
2:Q:74:ASP:HB3	2:Q:77:THR:HB	1.88	0.54
2:Q:189:LEU:HB2	2:Q:204:VAL:HG13	1.89	0.54
1:A:141:ALA:O	1:A:145:MET:HE2	2.08	0.54
3:F:84:LEU:HD12	3:F:84:LEU:N	2.21	0.54
1:J:123:ALA:O	1:J:355:ARG:NH1	2.41	0.54
2:K:114:MET:O	2:K:114:MET:HG2	2.07	0.54
3:R:77:ARG:HH21	3:R:115:THR:HG21	1.72	0.54
5:D:502:HEM:O2D	5:D:502:HEM:O1A	2.26	0.54
1:G:205:ILE:O	1:G:209:VAL:HG23	2.07	0.54
1:J:13:THR:O	1:J:17:LYS:HG3	2.07	0.54
1:M:425:GLU:O	1:M:429:ASN:ND2	2.41	0.54
3:O:127:GLY:O	3:O:135:SER:HA	2.08	0.54
1:P:77:PHE:CD2	1:P:282:GLU:HG2	2.43	0.54
1:P:341:LEU:HD12	1:P:341:LEU:O	2.08	0.54
3:R:93:LEU:HD13	3:R:161:ARG:HD2	1.90	0.54
1:A:193:ARG:HH12	3:F:38:MET:CB	2.21	0.54
1:A:399:TYR:O	1:A:402:ALA:HB3	2.08	0.54
3:C:73:PHE:CE1	3:C:127:GLY:HA3	2.42	0.54
3:I:54:VAL:HG23	3:I:57:VAL:HG21	1.88	0.54
1:J:387:PHE:HA	1:J:390:ASP:OD1	2.08	0.54
1:M:4:ILE:HD12	1:M:4:ILE:H	1.73	0.54
3:O:132:LEU:HD12	3:O:152:HIS:CE1	2.43	0.54
1:P:144:PHE:HE2	6:P:503:SMA:H43	1.72	0.54
1:A:315:VAL:O	1:A:318:ALA:HB3	2.09	0.53
1:D:39:ARG:NH1	2:E:255:VAL:HG12	2.17	0.53
1:G:315:VAL:HG12	1:G:316:GLN:N	2.23	0.53
2:H:66:TYR:CE1	2:H:70:PHE:HE2	2.26	0.53
1:G:190:THR:O	1:G:193:ARG:HG2	2.08	0.53
1:G:377:LEU:O	1:G:380:VAL:HG23	2.08	0.53
1:A:116:LEU:HA	1:A:121:TYR:HE2	1.72	0.53
1:G:213:ILE:HA	1:G:216:PHE:CD2	2.43	0.53
1:G:346:VAL:CG1	1:G:347:PRO:HD3	2.38	0.53
1:J:377:LEU:O	1:J:380:VAL:HG23	2.08	0.53
2:K:231:PHE:O	2:K:235:MET:HG2	2.08	0.53
1:M:125:ARG:NE	1:M:222:ASN:HB2	2.22	0.53
2:Q:129:GLU:O	2:Q:132:TYR:HB3	2.08	0.53
1:D:377:LEU:O	1:D:380:VAL:HG23	2.09	0.53
3:F:44:VAL:C	3:F:46:ALA:H	2.17	0.53
1:G:105:PHE:HA	1:G:108:VAL:HG23	1.91	0.53
1:G:144:PHE:CD1	1:G:162:ILE:HD13	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:131:HIS:HB3	10:I:200:FES:S2	2.49	0.53
1:M:276:HIS:CE1	1:M:278:ASP:HB2	2.43	0.53
1:P:427:ASP:O	1:P:430:ALA:HB3	2.08	0.53
2:B:250:ARG:CZ	3:C:12:ARG:HB3	2.39	0.53
3:C:138:GLY:CA	3:C:147:TRP:CD1	2.92	0.53
3:L:132:LEU:HD12	3:L:152:HIS:CE1	2.43	0.53
1:A:377:LEU:O	1:A:380:VAL:HG23	2.08	0.53
1:D:77:PHE:CD2	1:D:282:GLU:HG2	2.44	0.53
2:H:149:HIS:CD2	2:H:168:THR:HG21	2.43	0.53
2:K:76:GLU:O	2:K:77:THR:C	2.52	0.53
3:L:156:TYR:HA	3:L:161:ARG:O	2.07	0.53
1:M:388:PRO:O	1:M:392:ILE:HG13	2.08	0.53
1:A:387:PHE:HA	1:A:390:ASP:OD1	2.07	0.53
2:B:74:ASP:CB	2:B:81:ARG:HE	2.21	0.53
3:C:12:ARG:CG	3:C:13:ASP:N	2.71	0.53
3:F:80:ALA:O	3:F:84:LEU:HD13	2.09	0.53
3:F:95:ASP:HB3	3:F:170:ASN:ND2	2.23	0.53
2:H:155:TYR:CD1	2:H:155:TYR:N	2.77	0.53
1:J:37:THR:HB	1:J:248:PHE:HE2	1.73	0.53
2:K:66:TYR:CE1	2:K:70:PHE:HE2	2.27	0.53
3:L:154:SER:OG	3:L:166:PRO:HD2	2.09	0.53
2:N:77:THR:HG22	2:N:79:GLU:N	2.24	0.53
1:P:249:ILE:O	1:P:253:VAL:HG23	2.08	0.53
1:A:295:GLU:O	1:A:296:TRP:C	2.50	0.53
2:B:238:THR:O	2:B:242:VAL:HG23	2.08	0.53
2:N:154:PHE:C	2:N:155:TYR:CD1	2.86	0.53
2:Q:188:PRO:HG2	2:Q:189:LEU:H	1.73	0.53
3:C:38:MET:HE2	1:D:193:ARG:HH11	1.74	0.53
1:D:387:PHE:CE1	1:D:388:PRO:HB3	2.44	0.53
1:J:399:TYR:O	1:J:402:ALA:HB3	2.09	0.53
2:K:157:ASN:O	2:K:180:GLY:HA3	2.08	0.53
1:P:123:ALA:O	1:P:355:ARG:NH1	2.42	0.53
1:A:105:PHE:O	1:A:106:ILE:C	2.51	0.53
1:A:190:THR:O	1:A:193:ARG:HG2	2.09	0.53
1:A:410:ILE:HG23	1:A:414:ILE:HD12	1.90	0.53
2:E:191:ASP:N	2:E:204:VAL:HG23	2.24	0.53
3:F:111:ASP:C	3:F:111:ASP:OD1	2.51	0.53
1:G:406:VAL:C	1:G:409:PRO:HD2	2.34	0.53
1:J:123:ALA:HB2	1:J:126:GLU:OE2	2.08	0.53
1:J:249:ILE:O	1:J:253:VAL:HG23	2.09	0.53
2:N:114:MET:HG2	2:N:114:MET:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:127:GLY:O	3:F:135:SER:HA	2.09	0.52
3:I:100:ASN:HB3	3:I:103:ILE:HG12	1.91	0.52
1:M:205:ILE:O	1:M:209:VAL:HG23	2.09	0.52
2:N:129:GLU:O	2:N:132:TYR:HB3	2.08	0.52
2:N:230:GLY:O	2:N:231:PHE:C	2.51	0.52
1:P:363:PHE:O	1:P:364:LYS:C	2.51	0.52
1:A:249:ILE:O	1:A:253:VAL:HG23	2.08	0.52
1:D:213:ILE:HA	1:D:216:PHE:CD2	2.44	0.52
1:G:399:TYR:O	1:G:402:ALA:HB3	2.09	0.52
2:H:49:SER:HA	2:H:52:GLU:HG3	1.89	0.52
1:J:37:THR:HB	1:J:248:PHE:CE2	2.43	0.52
2:H:236:PHE:CZ	3:I:25:VAL:HG12	2.44	0.52
2:K:32:TYR:CD2	2:K:42:MET:HE2	2.45	0.52
3:L:73:PHE:CE1	3:L:127:GLY:HA3	2.44	0.52
1:M:407:ILE:HG22	1:M:411:LEU:HD12	1.92	0.52
1:P:246:PRO:HG2	2:Q:251:LEU:HD21	1.90	0.52
1:P:360:ARG:O	1:P:364:LYS:HG3	2.10	0.52
2:Q:66:TYR:CE1	2:Q:70:PHE:CE2	2.98	0.52
1:M:319:ASN:OD1	1:M:324:GLY:HA2	2.09	0.52
1:M:399:TYR:O	1:M:402:ALA:HB3	2.09	0.52
2:Q:113:PRO:HD2	2:Q:118:ILE:HB	1.92	0.52
1:D:105:PHE:O	1:D:106:ILE:C	2.51	0.52
1:D:256:LEU:O	1:D:260:LEU:HG	2.09	0.52
1:D:296:TRP:HA	1:D:299:LEU:HG	1.91	0.52
1:G:125:ARG:HH21	1:G:221:ASN:C	2.18	0.52
3:R:73:PHE:CE1	3:R:127:GLY:HA3	2.45	0.52
1:G:49:VAL:CG1	1:G:256:LEU:HD13	2.39	0.52
1:G:123:ALA:HB2	1:G:126:GLU:OE2	2.10	0.52
1:G:246:PRO:HG2	2:H:251:LEU:HD21	1.91	0.52
2:H:52:GLU:HB3	2:H:53:PRO:HD2	1.92	0.52
1:J:427:ASP:O	1:J:430:ALA:HB3	2.09	0.52
1:M:116:LEU:HA	1:M:121:TYR:HE2	1.74	0.52
1:G:295:GLU:O	1:G:296:TRP:C	2.53	0.52
1:G:408:LEU:HB2	1:G:409:PRO:HD3	1.91	0.52
1:J:140:MET:O	1:J:141:ALA:C	2.51	0.52
1:J:213:ILE:HA	1:J:216:PHE:CD2	2.45	0.52
3:O:109:ALA:O	3:O:161:ARG:NH1	2.37	0.52
2:Q:250:ARG:CZ	3:R:12:ARG:HB3	2.39	0.52
3:R:162:ILE:HD12	3:R:163:ARG:H	1.75	0.52
1:A:27:ALA:O	1:A:30:TYR:HB3	2.10	0.52
1:A:37:THR:HB	1:A:248:PHE:HE2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:VAL:HG12	1:A:347:PRO:HD3	1.90	0.52
3:C:100:ASN:HB3	3:C:103:ILE:HG12	1.92	0.52
1:D:123:ALA:HB2	1:D:126:GLU:OE2	2.09	0.52
3:F:84:LEU:H	3:F:84:LEU:CD1	2.23	0.52
2:H:53:PRO:HA	2:H:57:GLU:CG	2.39	0.52
3:O:77:ARG:HH21	3:O:115:THR:HG21	1.75	0.52
1:D:49:VAL:HG21	1:D:252:ASP:OD2	2.10	0.52
1:D:190:THR:O	1:D:193:ARG:HG2	2.10	0.52
2:E:157:ASN:O	2:E:180:GLY:HA3	2.10	0.52
2:H:154:PHE:C	2:H:155:TYR:CD1	2.88	0.52
2:K:191:ASP:N	2:K:204:VAL:HG23	2.25	0.52
1:P:37:THR:HB	1:P:248:PHE:CE2	2.45	0.52
1:P:39:ARG:HD3	1:P:428:PHE:CD2	2.45	0.52
2:Q:154:PHE:C	2:Q:155:TYR:CD1	2.88	0.52
3:R:37:GLN:NE2	3:R:38:MET:HG3	2.25	0.52
1:A:123:ALA:HB2	1:A:126:GLU:OE2	2.09	0.52
1:D:156:PHE:CE2	1:D:285:PRO:HA	2.45	0.52
1:D:213:ILE:HD11	8:D:504:ANJ:H162	1.91	0.52
2:E:236:PHE:HE1	3:F:25:VAL:CG1	2.23	0.52
2:H:77:THR:C	2:H:79:GLU:N	2.68	0.52
1:M:44:MET:CE	7:M:504:LOP:H101	2.37	0.52
1:P:116:LEU:HA	1:P:121:TYR:HE2	1.74	0.52
1:D:269:PHE:HB3	4:D:431:BGL:O1	2.10	0.51
1:D:399:TYR:O	1:D:402:ALA:HB3	2.09	0.51
1:J:73:VAL:HG12	1:J:151:TRP:CE2	2.44	0.51
1:J:275:GLY:O	1:J:277:PRO:HD3	2.11	0.51
1:M:193:ARG:HD3	3:R:38:MET:HE3	1.91	0.51
1:M:213:ILE:HA	1:M:216:PHE:CD2	2.44	0.51
1:P:37:THR:HB	1:P:248:PHE:HE2	1.75	0.51
1:P:147:TYR:HA	5:P:502:HEM:HAA2	1.92	0.51
1:P:295:GLU:O	1:P:296:TRP:C	2.53	0.51
1:A:152:GLY:H	1:A:155:SER:HB2	1.75	0.51
2:B:191:ASP:N	2:B:204:VAL:HG23	2.26	0.51
3:C:154:SER:OG	3:C:166:PRO:HD2	2.10	0.51
1:D:187:ASP:CG	1:D:188:ASN:H	2.18	0.51
1:G:39:ARG:NH1	2:H:255:VAL:HG12	2.22	0.51
1:G:104:PHE:O	1:G:108:VAL:HG22	2.11	0.51
2:K:20:PHE:HB3	2:K:25:LEU:HD11	1.92	0.51
1:M:27:ALA:O	1:M:30:TYR:HB3	2.09	0.51
1:M:317:ILE:O	1:M:320:PHE:HB3	2.11	0.51
2:N:40:HIS:CE1	2:N:97:ALA:HB1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:213:ILE:HA	1:P:216:PHE:CD2	2.45	0.51
3:R:152:HIS:N	10:R:200:FES:S1	2.83	0.51
1:G:234:LYS:O	1:G:238:GLN:HG3	2.10	0.51
2:H:154:PHE:N	2:H:154:PHE:CD1	2.78	0.51
1:P:234:LYS:O	1:P:238:GLN:HG3	2.10	0.51
1:A:37:THR:HB	1:A:248:PHE:CE2	2.46	0.51
2:B:27:ARG:HD2	2:B:196:TYR:CE2	2.45	0.51
2:B:154:PHE:CD1	2:B:154:PHE:N	2.76	0.51
3:F:154:SER:OG	3:F:166:PRO:HD2	2.10	0.51
2:H:230:GLY:O	2:H:231:PHE:C	2.53	0.51
3:O:180:ASP:OD2	3:O:183:THR:HB	2.11	0.51
1:P:73:VAL:HG22	1:P:188:ASN:OD1	2.10	0.51
1:P:123:ALA:HB2	1:P:126:GLU:OE2	2.11	0.51
1:A:162:ILE:CG2	6:A:1:SMA:H19	2.41	0.51
2:B:42:MET:HE1	2:B:214:PHE:CZ	2.46	0.51
1:D:362:MET:HB2	1:D:415:GLU:OE2	2.10	0.51
5:D:502:HEM:O2D	5:D:502:HEM:HHA	2.11	0.51
3:I:131:HIS:O	1:J:329:LYS:NZ	2.41	0.51
1:J:295:GLU:O	1:J:296:TRP:C	2.52	0.51
1:M:7:ASP:HB3	1:M:234:LYS:NZ	2.25	0.51
1:M:51:LEU:HD13	5:M:501:HEM:C3B	2.46	0.51
1:A:346:VAL:CG1	1:A:347:PRO:HD3	2.41	0.51
2:B:243:LEU:HD13	3:C:19:THR:HA	1.92	0.51
2:E:61:ASP:HA	2:E:64:ARG:HH12	1.74	0.51
1:M:52:ALA:HB2	8:M:505:ANJ:H163	1.91	0.51
2:N:130:TYR:O	2:N:134:VAL:HG23	2.10	0.51
1:P:199:TYR:HA	5:P:502:HEM:HBC2	1.91	0.51
1:P:366:TYR:CD2	1:P:411:LEU:HD11	2.45	0.51
3:C:21:GLY:O	3:C:25:VAL:HG23	2.09	0.51
3:C:180:ASP:OD2	3:C:183:THR:HB	2.11	0.51
3:I:73:PHE:CE1	3:I:127:GLY:HA3	2.45	0.51
1:J:315:VAL:O	1:J:318:ALA:HB3	2.10	0.51
2:K:29:LEU:HD22	2:K:50:LEU:HD22	1.91	0.51
1:M:346:VAL:CG1	1:M:347:PRO:HD3	2.40	0.51
2:N:154:PHE:N	2:N:154:PHE:CD1	2.79	0.51
1:P:105:PHE:O	1:P:108:VAL:HG23	2.10	0.51
1:A:313:TRP:HA	1:A:316:GLN:HG3	1.93	0.51
1:G:103:LEU:CD1	7:G:504:LOP:H212	2.37	0.51
1:G:214:TRP:CH2	1:J:25:ILE:HA	2.46	0.51
1:J:395:ILE:O	1:J:398:ALA:HB3	2.11	0.51
1:J:425:GLU:HG3	1:J:429:ASN:HD21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:25:ILE:HA	1:P:214:TRP:CH2	2.46	0.51
1:M:49:VAL:HG21	1:M:252:ASP:OD2	2.10	0.51
1:A:213:ILE:HA	1:A:216:PHE:CD2	2.45	0.51
3:C:37:GLN:NE2	3:C:38:MET:HG3	2.25	0.51
1:D:52:ALA:HB2	8:D:504:ANJ:H163	1.92	0.51
3:F:180:ASP:OD2	3:F:183:THR:HB	2.11	0.51
1:G:360:ARG:HB3	1:G:415:GLU:OE1	2.10	0.51
2:H:191:ASP:N	2:H:204:VAL:HG23	2.25	0.51
1:P:256:LEU:O	1:P:260:LEU:HG	2.10	0.51
3:R:100:ASN:HB3	3:R:103:ILE:HG12	1.91	0.51
1:M:49:VAL:HG12	1:M:256:LEU:HD13	1.92	0.51
1:P:39:ARG:NH1	2:Q:255:VAL:CG1	2.71	0.51
2:Q:142:PRO:CG	2:Q:150:GLU:OE2	2.56	0.51
1:A:327:ASP:C	1:A:327:ASP:OD1	2.55	0.50
1:J:43:TRP:CZ3	1:J:251:LYS:CE	2.93	0.50
1:M:73:VAL:HG23	1:M:74:ASP:H	1.77	0.50
1:M:91:PHE:CE1	1:M:92:MET:HE3	2.46	0.50
2:Q:76:GLU:H	2:Q:76:GLU:CD	2.19	0.50
1:A:193:ARG:HH12	3:F:38:MET:HB3	1.75	0.50
1:D:158:GLY:O	1:D:162:ILE:HG13	2.11	0.50
2:E:155:TYR:N	2:E:155:TYR:CD1	2.78	0.50
2:H:107:ARG:HH21	5:H:301:HEM:CGA	2.23	0.50
1:M:123:ALA:HB2	1:M:126:GLU:OE2	2.12	0.50
1:P:49:VAL:CG1	1:P:256:LEU:HD13	2.41	0.50
1:P:92:MET:HE2	1:P:92:MET:HA	1.93	0.50
1:P:140:MET:O	1:P:141:ALA:C	2.54	0.50
2:Q:42:MET:HE1	2:Q:214:PHE:HZ	1.75	0.50
2:Q:113:PRO:O	2:Q:114:MET:HB3	2.11	0.50
3:R:62:GLN:NE2	3:R:73:PHE:CG	2.79	0.50
1:A:256:LEU:O	1:A:260:LEU:HG	2.12	0.50
1:D:239:LYS:HE2	1:D:425:GLU:OE1	2.11	0.50
2:E:154:PHE:C	2:E:155:TYR:CD1	2.89	0.50
2:H:53:PRO:HA	2:H:57:GLU:HG2	1.93	0.50
3:I:76:ARG:HG3	3:I:122:TRP:CH2	2.47	0.50
1:J:209:VAL:HG22	5:J:501:HEM:HBB2	1.94	0.50
1:J:312:VAL:O	1:J:316:GLN:CG	2.59	0.50
1:D:213:ILE:HG22	1:D:217:HIS:CD2	2.47	0.50
1:G:73:VAL:HG23	1:G:74:ASP:N	2.27	0.50
1:G:164:GLY:O	1:G:165:LEU:C	2.55	0.50
2:H:29:LEU:HD22	2:H:50:LEU:HD22	1.92	0.50
2:H:106:ALA:O	2:H:107:ARG:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:129:GLU:O	2:H:132:TYR:HB3	2.10	0.50
2:K:77:THR:HG21	2:K:79:GLU:HB2	1.94	0.50
2:K:144:LYS:O	2:K:147:GLU:N	2.44	0.50
2:K:155:TYR:CD1	2:K:155:TYR:N	2.79	0.50
3:L:180:ASP:OD2	3:L:183:THR:HB	2.12	0.50
1:M:125:ARG:CZ	1:M:222:ASN:HB2	2.41	0.50
3:O:90:LEU:CD1	3:O:108:GLU:HB3	2.41	0.50
1:P:149:LEU:HB2	1:P:150:PRO:HD3	1.93	0.50
1:D:113:PHE:HB3	7:D:503:LOP:H272	1.93	0.50
2:H:165:VAL:CG1	2:H:169:CYS:HB2	2.41	0.50
1:J:364:LYS:O	1:J:368:TRP:HD1	1.94	0.50
3:O:12:ARG:HG2	3:O:13:ASP:N	2.26	0.50
1:P:113:PHE:HB3	7:P:504:LOP:H272	1.94	0.50
2:Q:233:ALA:O	2:Q:237:LEU:HD12	2.12	0.50
1:A:121:TYR:HB3	1:A:129:TRP:CE3	2.47	0.50
2:B:155:TYR:N	2:B:155:TYR:CD1	2.79	0.50
3:C:162:ILE:HD12	3:C:163:ARG:N	2.27	0.50
3:I:180:ASP:OD2	3:I:183:THR:HB	2.12	0.50
1:J:125:ARG:NE	1:J:222:ASN:HB2	2.27	0.50
1:P:188:ASN:O	1:P:189:ALA:C	2.55	0.50
1:A:418:VAL:CG1	1:A:419:ALA:H	2.23	0.50
1:D:103:LEU:HD13	7:D:503:LOP:H202	1.93	0.50
1:D:141:ALA:O	1:D:145:MET:HE2	2.12	0.50
2:H:238:THR:O	2:H:242:VAL:HG23	2.11	0.50
3:I:37:GLN:NE2	3:I:38:MET:HG3	2.27	0.50
3:I:125:MET:CE	3:I:171:LEU:HD12	2.42	0.50
1:J:105:PHE:O	1:J:106:ILE:C	2.54	0.50
2:K:238:THR:O	2:K:242:VAL:HG23	2.11	0.50
3:L:100:ASN:HB3	3:L:103:ILE:HG12	1.93	0.50
1:D:133:MET:N	5:D:501:HEM:HBC2	2.27	0.50
1:D:223:ASN:ND2	1:D:223:ASN:H	2.10	0.50
1:D:249:ILE:O	1:D:253:VAL:HG23	2.12	0.50
2:H:20:PHE:HB3	2:H:25:LEU:HD11	1.94	0.50
2:N:20:PHE:HB3	2:N:25:LEU:HD11	1.93	0.50
2:N:155:TYR:CD1	2:N:155:TYR:N	2.79	0.50
2:Q:20:PHE:HB3	2:Q:25:LEU:HD11	1.94	0.50
2:Q:130:TYR:O	2:Q:134:VAL:HG23	2.12	0.50
3:C:112:GLN:NE2	3:C:112:GLN:H	2.10	0.50
2:H:17:PHE:CE1	2:H:231:PHE:HE1	2.30	0.50
2:K:230:GLY:O	2:K:231:PHE:C	2.55	0.50
2:K:233:ALA:O	2:K:237:LEU:HD12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:8:HIS:H	1:M:8:HIS:CD2	2.29	0.50
1:M:193:ARG:NH1	3:R:38:MET:HG2	2.27	0.50
2:N:53:PRO:HA	2:N:57:GLU:CD	2.37	0.50
2:N:146:ALA:HB2	2:N:169:CYS:SG	2.51	0.50
2:B:154:PHE:C	2:B:155:TYR:CD1	2.90	0.49
1:D:37:THR:HB	1:D:248:PHE:HE2	1.76	0.49
1:D:92:MET:HA	1:D:92:MET:HE2	1.93	0.49
5:D:502:HEM:CMB	5:D:502:HEM:CBB	2.88	0.49
2:E:66:TYR:CE1	2:E:70:PHE:HE2	2.29	0.49
1:G:121:TYR:HB3	1:G:129:TRP:CE3	2.47	0.49
3:I:62:GLN:NE2	3:I:73:PHE:CD1	2.80	0.49
2:K:143:PRO:HG3	2:K:178:THR:HG21	1.94	0.49
1:M:39:ARG:HH12	2:N:255:VAL:CG1	2.24	0.49
1:M:379:TRP:CZ2	2:N:114:MET:HE3	2.47	0.49
2:N:19:THR:CG2	2:N:224:MET:HE3	2.42	0.49
2:N:42:MET:HE1	2:N:214:PHE:CE2	2.47	0.49
2:N:233:ALA:O	2:N:237:LEU:HD12	2.11	0.49
3:O:154:SER:OG	3:O:166:PRO:HD2	2.12	0.49
1:P:342:VAL:HG23	1:P:343:MET:N	2.27	0.49
2:Q:15:GLY:O	2:Q:227:LYS:NZ	2.43	0.49
2:Q:42:MET:HE1	2:Q:214:PHE:CE2	2.46	0.49
2:Q:89:PHE:HB3	2:Q:90:PRO:CD	2.41	0.49
2:E:236:PHE:HE1	3:F:25:VAL:HG12	1.76	0.49
1:G:123:ALA:HA	1:G:126:GLU:OE1	2.12	0.49
2:H:48:ARG:HG3	2:H:48:ARG:NH1	2.24	0.49
3:I:132:LEU:HD12	3:I:152:HIS:CE1	2.47	0.49
2:K:142:PRO:HG2	2:K:150:GLU:OE2	2.12	0.49
1:M:73:VAL:HG23	1:M:74:ASP:N	2.28	0.49
1:M:121:TYR:HB3	1:M:129:TRP:CE3	2.46	0.49
1:A:187:ASP:CG	1:A:188:ASN:H	2.20	0.49
3:C:38:MET:HE3	1:D:193:ARG:HD3	1.95	0.49
1:D:152:GLY:H	1:D:155:SER:HB2	1.77	0.49
3:I:89:GLN:O	3:I:91:GLY:N	2.45	0.49
1:J:52:ALA:HB2	8:J:505:ANJ:H163	1.94	0.49
3:O:89:GLN:C	3:O:91:GLY:H	2.21	0.49
2:B:250:ARG:HE	3:C:12:ARG:CB	2.22	0.49
3:C:90:LEU:HB2	2:H:172:ALA:HB1	1.93	0.49
1:G:152:GLY:H	1:G:155:SER:HB2	1.77	0.49
2:H:157:ASN:O	2:H:180:GLY:HA3	2.11	0.49
1:J:256:LEU:O	1:J:260:LEU:HG	2.12	0.49
2:K:154:PHE:N	2:K:154:PHE:CD1	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:156:TYR:HD1	2:K:182:TRP:CZ3	2.30	0.49
1:M:149:LEU:HB2	1:M:150:PRO:HD3	1.94	0.49
1:M:280:TYR:CE2	2:N:105:LYS:HD2	2.47	0.49
2:N:127:GLY:N	2:N:128:PRO:HD2	2.27	0.49
2:N:137:GLY:O	2:N:139:PRO:HD3	2.11	0.49
1:P:366:TYR:HD2	1:P:411:LEU:HD11	1.78	0.49
2:Q:110:PHE:O	2:Q:120:GLN:HG2	2.12	0.49
2:B:29:LEU:HD22	2:B:50:LEU:HD22	1.93	0.49
3:C:125:MET:CE	3:C:171:LEU:HD12	2.43	0.49
1:D:37:THR:HB	1:D:248:PHE:CE2	2.47	0.49
3:F:162:ILE:HD12	3:F:163:ARG:N	2.26	0.49
1:G:49:VAL:HG12	1:G:256:LEU:HD13	1.94	0.49
1:G:63:ILE:HD13	1:J:200:LEU:CD2	2.33	0.49
1:G:276:HIS:CE1	1:G:278:ASP:HB2	2.47	0.49
1:J:4:ILE:N	1:J:4:ILE:CD1	2.74	0.49
2:K:154:PHE:C	2:K:155:TYR:CD1	2.90	0.49
3:L:162:ILE:HD12	3:L:163:ARG:N	2.27	0.49
1:M:91:PHE:HE1	1:M:92:MET:CE	2.25	0.49
1:M:125:ARG:HH11	1:M:125:ARG:HG3	1.77	0.49
1:M:140:MET:O	1:M:141:ALA:C	2.55	0.49
1:M:428:PHE:CE1	2:N:256:LYS:HD3	2.48	0.49
2:N:238:THR:O	2:N:242:VAL:HG23	2.12	0.49
3:O:100:ASN:HB3	3:O:103:ILE:HG12	1.94	0.49
1:P:152:GLY:H	1:P:155:SER:HB2	1.77	0.49
3:R:143:ASP:C	3:R:144:PHE:CD1	2.91	0.49
3:R:180:ASP:OD2	3:R:183:THR:HB	2.12	0.49
1:D:162:ILE:HD13	6:D:2:SMA:H14	1.95	0.49
2:H:81:ARG:NH1	2:H:82:GLU:O	2.46	0.49
3:O:44:VAL:C	3:O:46:ALA:H	2.19	0.49
1:P:49:VAL:HG12	1:P:256:LEU:HD13	1.94	0.49
1:P:275:GLY:O	1:P:277:PRO:HD3	2.12	0.49
1:D:258:VAL:O	1:D:261:LEU:HB3	2.12	0.49
1:D:294:PRO:HA	6:D:2:SMA:C7M	2.34	0.49
2:E:20:PHE:HB3	2:E:25:LEU:HD11	1.95	0.49
2:E:29:LEU:HD22	2:E:50:LEU:HD22	1.95	0.49
3:I:162:ILE:HD12	3:I:163:ARG:N	2.28	0.49
1:J:123:ALA:HA	1:J:126:GLU:OE1	2.12	0.49
1:M:51:LEU:HB3	5:M:501:HEM:HMB1	1.93	0.49
2:N:110:PHE:O	2:N:120:GLN:HG2	2.13	0.49
2:N:149:HIS:CG	2:N:168:THR:HG21	2.48	0.49
1:A:358:ARG:HH21	7:A:503:LOP:H21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ILE:O	1:A:398:ALA:HB3	2.13	0.49
1:G:60:VAL:HG23	1:G:61:THR:N	2.28	0.49
1:J:122:LYS:O	1:J:123:ALA:C	2.55	0.49
2:K:142:PRO:CG	2:K:150:GLU:OE2	2.61	0.49
1:M:275:GLY:O	1:M:277:PRO:HD3	2.12	0.49
1:M:427:ASP:O	1:M:430:ALA:HB3	2.12	0.49
2:Q:155:TYR:CD1	2:Q:155:TYR:N	2.80	0.49
2:Q:189:LEU:CB	2:Q:204:VAL:HG13	2.42	0.49
1:D:51:LEU:HD13	5:D:501:HEM:C3B	2.48	0.49
2:H:19:THR:CG2	2:H:224:MET:HE3	2.43	0.49
3:I:88:VAL:HA	3:I:92:GLN:NE2	2.28	0.49
1:J:152:GLY:H	1:J:155:SER:HB2	1.77	0.49
1:J:157:TRP:O	1:J:158:GLY:C	2.55	0.49
1:J:276:HIS:CE1	1:J:278:ASP:HB2	2.47	0.49
2:N:42:MET:HE1	2:N:214:PHE:CZ	2.48	0.49
1:P:12:ARG:O	1:P:17:LYS:HE2	2.13	0.49
1:P:387:PHE:CD1	1:P:387:PHE:C	2.91	0.49
1:P:390:ASP:N	1:P:390:ASP:OD1	2.46	0.49
2:Q:230:GLY:O	2:Q:231:PHE:C	2.53	0.49
1:D:313:TRP:O	1:D:317:ILE:HG13	2.13	0.49
2:E:233:ALA:O	2:E:237:LEU:HD12	2.13	0.49
1:M:135:ILE:O	1:M:139:MET:HG3	2.13	0.49
1:M:389:TYR:HA	1:M:392:ILE:HD12	1.95	0.49
2:N:72:VAL:O	2:N:80:ASP:HA	2.12	0.49
2:N:235:MET:HE2	2:N:235:MET:CA	2.42	0.49
1:A:319:ASN:ND2	1:A:319:ASN:O	2.46	0.48
2:H:205:HIS:ND1	2:H:205:HIS:C	2.71	0.48
1:J:51:LEU:HB3	5:J:501:HEM:HMB1	1.95	0.48
1:J:60:VAL:HG23	1:J:61:THR:N	2.28	0.48
1:J:121:TYR:HB3	1:J:129:TRP:CE3	2.48	0.48
1:J:228:GLU:O	1:J:424:ILE:HD11	2.13	0.48
1:J:295:GLU:OE1	1:J:295:GLU:N	2.46	0.48
2:N:205:HIS:ND1	2:N:205:HIS:C	2.71	0.48
2:N:235:MET:O	2:N:236:PHE:C	2.56	0.48
3:O:108:GLU:O	3:O:110:THR:N	2.40	0.48
1:P:121:TYR:HB3	1:P:129:TRP:CE3	2.48	0.48
1:P:261:LEU:HD11	2:Q:234:VAL:HG13	1.95	0.48
1:P:399:TYR:O	1:P:402:ALA:HB3	2.13	0.48
2:Q:250:ARG:HH21	3:R:12:ARG:HD3	1.77	0.48
2:K:32:TYR:CE2	2:K:42:MET:CE	2.96	0.48
1:P:351:THR:OG1	1:P:412:GLY:HA3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:389:TYR:HA	1:P:392:ILE:HD12	1.95	0.48
3:L:128:VAL:O	3:L:129:CYS:C	2.57	0.48
3:L:143:ASP:OD2	3:L:164:LYS:NZ	2.40	0.48
1:M:295:GLU:O	1:M:296:TRP:C	2.56	0.48
2:N:108:ALA:HA	2:N:125:ILE:O	2.13	0.48
1:P:262:VAL:O	1:P:265:ALA:HB3	2.13	0.48
1:A:60:VAL:HG23	1:A:61:THR:N	2.27	0.48
2:B:205:HIS:C	2:B:205:HIS:ND1	2.71	0.48
1:D:316:GLN:O	1:D:317:ILE:C	2.56	0.48
2:E:230:GLY:O	2:E:231:PHE:C	2.56	0.48
1:J:105:PHE:CA	1:J:108:VAL:HG23	2.44	0.48
3:R:62:GLN:NE2	3:R:73:PHE:CD1	2.82	0.48
1:D:327:ASP:C	1:D:327:ASP:OD1	2.56	0.48
1:J:351:THR:OG1	1:J:412:GLY:HA3	2.13	0.48
1:M:156:PHE:HE2	1:M:285:PRO:HA	1.74	0.48
3:O:89:GLN:C	3:O:91:GLY:N	2.70	0.48
1:P:4:ILE:HG22	1:P:5:PRO:N	2.28	0.48
3:C:12:ARG:HG2	3:C:13:ASP:N	2.28	0.48
1:D:255:ALA:O	1:D:259:VAL:HG23	2.14	0.48
1:J:49:VAL:CG1	1:J:256:LEU:HD13	2.43	0.48
1:M:342:VAL:HG23	1:M:343:MET:N	2.29	0.48
1:P:248:PHE:O	1:P:249:ILE:C	2.56	0.48
1:G:149:LEU:HB2	1:G:150:PRO:HD3	1.94	0.48
2:H:160:PHE:CD2	2:H:183:ILE:HB	2.48	0.48
1:J:164:GLY:O	1:J:165:LEU:C	2.56	0.48
3:L:80:ALA:O	3:L:84:LEU:HD13	2.14	0.48
3:O:30:ALA:O	3:O:33:PRO:HG2	2.14	0.48
1:A:379:TRP:CZ2	2:B:114:MET:HE3	2.48	0.48
2:E:116:THR:O	2:E:116:THR:HG22	2.14	0.48
2:E:205:HIS:C	2:E:205:HIS:ND1	2.72	0.48
1:G:116:LEU:HA	1:G:121:TYR:CE2	2.49	0.48
2:H:89:PHE:HB3	2:H:90:PRO:HD2	1.96	0.48
3:I:138:GLY:HA2	3:I:147:TRP:CD1	2.48	0.48
2:K:144:LYS:O	2:K:146:ALA:N	2.47	0.48
1:P:132:GLY:HA3	5:P:501:HEM:HBC2	1.95	0.48
1:P:281:ILE:HD11	2:Q:107:ARG:HH12	1.78	0.48
2:Q:238:THR:O	2:Q:242:VAL:HG23	2.14	0.48
1:A:46:ILE:O	1:A:50:VAL:HG23	2.13	0.48
1:A:72:HIS:C	1:A:72:HIS:ND1	2.72	0.48
1:A:262:VAL:O	1:A:266:ILE:HG12	2.13	0.48
2:B:48:ARG:HG3	2:B:48:ARG:NH1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:236:PHE:HZ	3:I:25:VAL:HG12	1.78	0.48
1:M:255:ALA:O	1:M:259:VAL:HG23	2.13	0.48
2:N:29:LEU:HD22	2:N:50:LEU:HD22	1.96	0.48
1:P:276:HIS:CE1	1:P:278:ASP:HB2	2.49	0.48
2:B:149:HIS:CD2	2:B:168:THR:HG21	2.49	0.48
3:C:143:ASP:HA	3:L:89:GLN:NE2	2.09	0.48
1:D:58:GLN:OE1	1:D:100:GLY:HA3	2.14	0.48
3:F:100:ASN:HB3	3:F:103:ILE:HG12	1.96	0.48
1:G:244:PHE:CD1	1:G:248:PHE:HB2	2.49	0.48
1:M:123:ALA:HA	1:M:126:GLU:OE1	2.14	0.48
1:M:188:ASN:O	1:M:189:ALA:C	2.56	0.48
1:M:223:ASN:H	1:M:223:ASN:ND2	2.12	0.48
3:R:112:GLN:NE2	3:R:112:GLN:H	2.12	0.48
1:A:52:ALA:HB2	8:A:504:ANJ:C16	2.44	0.47
1:A:213:ILE:HD11	8:A:504:ANJ:H14	1.95	0.47
1:A:255:ALA:O	1:A:259:VAL:HG23	2.14	0.47
1:A:342:VAL:HG23	1:A:343:MET:N	2.29	0.47
2:B:20:PHE:HB3	2:B:25:LEU:HD11	1.94	0.47
1:D:248:PHE:O	1:D:249:ILE:C	2.57	0.47
1:D:387:PHE:HA	1:D:390:ASP:OD1	2.14	0.47
1:G:193:ARG:HD3	3:L:38:MET:HE3	1.96	0.47
1:G:315:VAL:O	1:G:318:ALA:HB3	2.14	0.47
3:I:180:ASP:OD1	3:I:181:GLU:N	2.47	0.47
1:M:60:VAL:HG23	1:M:61:THR:N	2.28	0.47
1:P:135:ILE:O	1:P:139:MET:HG3	2.15	0.47
1:P:388:PRO:O	1:P:392:ILE:HG13	2.14	0.47
2:Q:53:PRO:HA	2:Q:57:GLU:CG	2.44	0.47
2:Q:186:PRO:O	2:Q:187:PRO:C	2.57	0.47
3:R:174:PRO:O	3:R:175:LEU:C	2.57	0.47
2:B:230:GLY:O	2:B:231:PHE:C	2.57	0.47
5:D:502:HEM:HMB1	5:D:502:HEM:CBB	2.43	0.47
2:E:72:VAL:HG12	2:E:73:THR:H	1.76	0.47
3:F:89:GLN:HB2	3:F:92:GLN:HG3	1.95	0.47
2:K:110:PHE:O	2:K:120:GLN:HG2	2.14	0.47
2:K:141:GLU:HA	2:K:142:PRO:HD3	1.76	0.47
1:M:244:PHE:CD1	1:M:248:PHE:HB2	2.49	0.47
1:M:251:LYS:HA	1:M:254:PHE:HB3	1.95	0.47
1:P:164:GLY:O	1:P:167:GLY:N	2.47	0.47
1:P:223:ASN:ND2	1:P:223:ASN:H	2.12	0.47
2:Q:29:LEU:HD22	2:Q:50:LEU:HD22	1.96	0.47
2:Q:66:TYR:O	2:Q:69:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:HA	1:A:121:TYR:CE2	2.50	0.47
1:A:149:LEU:HB2	1:A:150:PRO:HD3	1.95	0.47
2:B:125:ILE:HD13	2:B:125:ILE:N	2.29	0.47
3:C:76:ARG:HG3	3:C:122:TRP:CH2	2.49	0.47
1:D:92:MET:HE3	1:D:92:MET:HB2	1.78	0.47
1:G:166:PHE:HA	1:G:169:ILE:HD12	1.96	0.47
1:J:5:PRO:HB2	1:J:234:LYS:HA	1.96	0.47
3:L:112:GLN:NE2	3:L:112:GLN:H	2.13	0.47
1:M:164:GLY:O	1:M:167:GLY:N	2.47	0.47
1:M:269:PHE:HB3	4:M:431:BGL:H1'2	1.96	0.47
1:A:58:GLN:OE1	1:A:100:GLY:HA3	2.15	0.47
1:A:109:TYR:HA	1:A:112:ILE:HD12	1.96	0.47
1:A:244:PHE:CD1	1:A:248:PHE:HB2	2.49	0.47
3:C:90:LEU:HD11	3:C:108:GLU:HB3	1.96	0.47
1:D:275:GLY:O	1:D:277:PRO:HD3	2.14	0.47
3:F:30:ALA:O	3:F:33:PRO:HG2	2.13	0.47
2:H:127:GLY:N	2:H:128:PRO:HD2	2.29	0.47
1:J:244:PHE:CD1	1:J:248:PHE:HB2	2.50	0.47
2:K:32:TYR:CE2	2:K:42:MET:HE2	2.49	0.47
1:M:164:GLY:O	1:M:165:LEU:C	2.58	0.47
1:P:125:ARG:CZ	1:P:222:ASN:HB2	2.44	0.47
2:Q:26:GLN:HG2	2:Q:58:LEU:HD21	1.96	0.47
1:A:13:THR:HG22	1:A:14:GLY:N	2.30	0.47
1:A:199:TYR:CD2	5:A:502:HEM:HBC1	2.49	0.47
1:D:44:MET:HE3	7:D:503:LOP:H92	1.96	0.47
1:D:315:VAL:O	1:D:318:ALA:HB3	2.13	0.47
1:D:342:VAL:HG23	1:D:343:MET:N	2.29	0.47
2:E:26:GLN:HG2	2:E:58:LEU:HD21	1.97	0.47
2:E:48:ARG:HG3	2:E:48:ARG:NH1	2.29	0.47
1:G:144:PHE:CD2	6:G:503:SMA:H42	2.50	0.47
1:G:275:GLY:O	1:G:277:PRO:HD3	2.15	0.47
2:K:32:TYR:CD2	2:K:42:MET:CE	2.98	0.47
1:M:358:ARG:NE	7:M:504:LOP:H21	2.29	0.47
1:P:43:TRP:CZ3	1:P:251:LYS:HE3	2.49	0.47
3:R:77:ARG:NH2	3:R:115:THR:HG21	2.29	0.47
1:A:102:SER:O	1:A:106:ILE:HG13	2.15	0.47
3:C:108:GLU:O	3:C:110:THR:N	2.43	0.47
1:D:244:PHE:CD1	1:D:248:PHE:HB2	2.50	0.47
1:D:261:LEU:CD1	2:E:234:VAL:HG13	2.44	0.47
2:E:80:ASP:O	2:E:81:ARG:HB3	2.14	0.47
2:E:224:MET:O	2:E:228:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:TYR:HB2	1:G:367:PHE:CE1	2.49	0.47
1:G:125:ARG:NH2	1:G:221:ASN:C	2.73	0.47
1:G:236:GLU:HA	1:G:239:LYS:CD	2.36	0.47
1:J:49:VAL:HG12	1:J:256:LEU:HD13	1.95	0.47
1:M:276:HIS:ND1	1:M:278:ASP:HB2	2.30	0.47
1:P:117:TYR:HB2	1:P:367:PHE:CE1	2.49	0.47
1:A:275:GLY:O	1:A:277:PRO:HD3	2.14	0.47
2:B:127:GLY:N	2:B:128:PRO:HD2	2.29	0.47
2:B:235:MET:O	2:B:236:PHE:C	2.57	0.47
3:C:131:HIS:HB3	10:C:200:FES:S2	2.54	0.47
2:E:160:PHE:CG	2:E:183:ILE:HD12	2.50	0.47
3:F:26:ALA:O	3:F:27:THR:C	2.58	0.47
3:F:73:PHE:CE1	3:F:127:GLY:HA3	2.49	0.47
3:F:77:ARG:HH21	3:F:115:THR:HG21	1.79	0.47
1:G:342:VAL:HG23	1:G:343:MET:N	2.30	0.47
1:G:411:LEU:HA	1:G:411:LEU:HD23	1.63	0.47
2:H:102:LEU:O	2:H:103:MET:C	2.57	0.47
2:H:188:PRO:HG2	2:H:189:LEU:H	1.80	0.47
1:J:248:PHE:HD1	1:J:251:LYS:HD3	1.79	0.47
2:K:127:GLY:N	2:K:128:PRO:HD2	2.30	0.47
3:L:90:LEU:HD11	3:L:108:GLU:HB3	1.96	0.47
1:M:13:THR:HG22	1:M:14:GLY:N	2.30	0.47
1:M:105:PHE:O	1:M:106:ILE:C	2.57	0.47
1:M:117:TYR:HB2	1:M:367:PHE:CE1	2.49	0.47
1:M:370:LEU:HD22	1:M:403:TYR:CD2	2.49	0.47
2:N:158:ARG:HH11	2:N:158:ARG:HG3	1.80	0.47
1:P:164:GLY:HA2	1:P:177:GLN:NE2	2.29	0.47
2:Q:48:ARG:HH11	2:Q:48:ARG:CG	2.26	0.47
1:A:117:TYR:HB2	1:A:367:PHE:CE1	2.50	0.47
3:C:144:PHE:N	3:C:144:PHE:CD1	2.82	0.47
1:D:370:LEU:HD22	1:D:403:TYR:CD2	2.50	0.47
2:E:72:VAL:CG1	2:E:73:THR:N	2.78	0.47
2:E:170:LYS:HA	2:E:175:VAL:O	2.15	0.47
1:G:379:TRP:CZ2	2:H:114:MET:HE3	2.50	0.47
3:L:26:ALA:O	3:L:27:THR:C	2.57	0.47
1:M:34:MET:SD	1:M:245:TRP:HB3	2.55	0.47
1:P:18:TRP:CD1	1:P:22:ARG:NH1	2.83	0.47
1:A:49:VAL:CG1	1:A:256:LEU:HD13	2.45	0.47
1:A:223:ASN:ND2	1:A:223:ASN:H	2.13	0.47
2:B:49:SER:HA	2:B:52:GLU:CD	2.40	0.47
1:D:123:ALA:HA	1:D:126:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:280:TYR:CE2	2:H:105:LYS:HD2	2.49	0.47
1:M:214:TRP:HH2	1:P:25:ILE:HA	1.80	0.47
1:M:367:PHE:O	1:M:370:LEU:HB3	2.15	0.47
1:D:51:LEU:CD2	1:D:108:VAL:HG13	2.45	0.47
1:D:395:ILE:O	1:D:398:ALA:HB3	2.15	0.47
2:E:185:MET:HB2	5:E:301:HEM:C1D	2.50	0.47
1:G:263:PHE:HD1	7:G:504:LOP:H232	1.80	0.47
1:G:395:ILE:O	1:G:398:ALA:HB3	2.15	0.47
2:H:66:TYR:HE1	2:H:70:PHE:HE2	1.63	0.47
2:H:110:PHE:O	2:H:120:GLN:HG2	2.15	0.47
3:I:77:ARG:NH2	3:I:115:THR:HG21	2.30	0.47
1:J:53:PHE:CE2	1:J:260:LEU:HD21	2.50	0.47
1:J:213:ILE:HD12	8:J:505:ANJ:O9	2.15	0.47
2:K:19:THR:CG2	2:K:224:MET:HE3	2.45	0.47
3:L:174:PRO:O	3:L:175:LEU:C	2.58	0.47
1:M:72:HIS:HE1	1:M:74:ASP:OD2	1.98	0.47
1:M:116:LEU:HA	1:M:121:TYR:CE2	2.50	0.47
3:O:73:PHE:CE1	3:O:127:GLY:HA3	2.50	0.47
1:P:60:VAL:HG23	1:P:61:THR:N	2.30	0.47
1:A:79:SER:O	1:A:82:HIS:HB3	2.15	0.46
1:A:162:ILE:CD1	6:A:1:SMA:H14	2.45	0.46
1:D:121:TYR:HB3	1:D:129:TRP:CE3	2.50	0.46
2:E:183:ILE:HG23	2:E:185:MET:H	1.80	0.46
2:H:197:ALA:C	2:H:199:GLY:H	2.24	0.46
2:K:116:THR:O	2:K:116:THR:HG22	2.15	0.46
2:K:186:PRO:O	2:K:187:PRO:C	2.56	0.46
1:M:209:VAL:HG22	5:M:501:HEM:HBB2	1.97	0.46
1:M:256:LEU:O	1:M:260:LEU:HG	2.14	0.46
1:M:329:LYS:CE	3:R:131:HIS:O	2.56	0.46
2:N:108:ALA:HA	2:N:125:ILE:HG22	1.97	0.46
1:P:255:ALA:O	1:P:259:VAL:HG23	2.15	0.46
1:D:56:VAL:O	1:D:57:LEU:C	2.58	0.46
1:D:102:SER:O	1:D:103:LEU:C	2.58	0.46
1:D:205:ILE:O	1:D:209:VAL:HG23	2.16	0.46
2:E:66:TYR:CE1	2:E:70:PHE:CE2	3.03	0.46
1:G:105:PHE:O	1:G:106:ILE:C	2.57	0.46
1:G:128:THR:HG21	5:G:501:HEM:HBD1	1.97	0.46
2:H:235:MET:O	2:H:236:PHE:C	2.57	0.46
1:J:8:HIS:CD2	1:J:8:HIS:H	2.33	0.46
1:J:213:ILE:HD13	8:J:505:ANJ:H14	1.98	0.46
3:L:108:GLU:O	3:L:110:THR:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:295:GLU:O	1:M:298:PHE:N	2.39	0.46
1:P:83:ILE:O	1:P:90:GLY:HA3	2.16	0.46
1:P:157:TRP:O	1:P:158:GLY:C	2.58	0.46
1:P:367:PHE:O	1:P:370:LEU:HB3	2.15	0.46
1:A:135:ILE:O	1:A:139:MET:HG3	2.15	0.46
1:G:299:LEU:HB2	1:G:378:THR:HG23	1.98	0.46
2:H:68:THR:HG23	2:H:82:GLU:HG2	1.96	0.46
2:H:77:THR:O	2:H:79:GLU:N	2.48	0.46
1:J:117:TYR:HB2	1:J:367:PHE:CE1	2.51	0.46
1:J:358:ARG:NH2	7:J:504:LOP:H21	2.27	0.46
1:M:39:ARG:HD3	1:M:428:PHE:CD2	2.50	0.46
1:M:79:SER:O	1:M:82:HIS:HB3	2.15	0.46
1:P:295:GLU:O	1:P:298:PHE:N	2.38	0.46
1:A:108:VAL:HG22	1:A:112:ILE:CD1	2.46	0.46
2:B:142:PRO:HG2	2:B:150:GLU:OE2	2.14	0.46
2:B:217:TRP:O	2:B:218:ALA:C	2.59	0.46
1:D:105:PHE:HA	1:D:108:VAL:CG2	2.42	0.46
1:D:223:ASN:ND2	1:D:223:ASN:N	2.63	0.46
2:E:154:PHE:CD1	2:E:154:PHE:N	2.83	0.46
3:F:108:GLU:O	3:F:110:THR:N	2.41	0.46
1:G:209:VAL:O	1:G:213:ILE:HG13	2.16	0.46
1:M:248:PHE:O	1:M:249:ILE:C	2.58	0.46
3:O:138:GLY:HA3	3:O:147:TRP:CD1	2.49	0.46
1:P:123:ALA:HA	1:P:126:GLU:OE1	2.15	0.46
1:D:49:VAL:HG12	1:D:256:LEU:HD13	1.98	0.46
1:D:140:MET:O	1:D:141:ALA:C	2.58	0.46
1:D:223:ASN:N	1:D:223:ASN:HD22	2.13	0.46
1:G:92:MET:HE1	2:H:226:ARG:HG3	1.97	0.46
1:G:132:GLY:HA3	5:G:501:HEM:HBC2	1.97	0.46
1:G:180:LEU:O	1:G:193:ARG:HD2	2.15	0.46
2:H:223:LEU:HD21	2:H:227:LYS:HE3	1.96	0.46
3:I:26:ALA:O	3:I:27:THR:C	2.58	0.46
3:I:38:MET:HE2	1:J:193:ARG:HH11	1.80	0.46
1:J:105:PHE:C	1:J:108:VAL:HG23	2.41	0.46
1:J:116:LEU:HA	1:J:121:TYR:CE2	2.49	0.46
1:J:187:ASP:CG	1:J:188:ASN:H	2.23	0.46
1:J:258:VAL:O	1:J:261:LEU:HB3	2.15	0.46
1:M:418:VAL:CG1	1:M:419:ALA:H	2.28	0.46
2:Q:127:GLY:N	2:Q:128:PRO:HD2	2.30	0.46
1:A:248:PHE:O	1:A:249:ILE:C	2.59	0.46
2:B:43:LYS:HE3	2:B:44:PHE:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:MET:O	2:B:228:GLN:HG3	2.16	0.46
1:D:49:VAL:CG1	1:D:256:LEU:HD13	2.46	0.46
3:I:152:HIS:HB2	10:I:200:FES:S1	2.56	0.46
1:J:295:GLU:O	1:J:298:PHE:N	2.38	0.46
1:M:387:PHE:HA	1:M:390:ASP:OD1	2.15	0.46
2:Q:19:THR:HG22	2:Q:224:MET:HE3	1.96	0.46
2:Q:43:LYS:HG2	2:Q:99:ASP:OD1	2.16	0.46
1:D:73:VAL:HG12	1:D:151:TRP:CE2	2.51	0.46
1:D:116:LEU:HA	1:D:121:TYR:CE2	2.50	0.46
1:G:53:PHE:CE2	1:G:260:LEU:HD21	2.50	0.46
1:J:43:TRP:HA	1:J:43:TRP:HE3	1.81	0.46
1:J:389:TYR:HA	1:J:392:ILE:HD12	1.97	0.46
3:L:148:PHE:HE1	3:L:153:GLY:HA2	1.80	0.46
1:A:53:PHE:CE2	1:A:260:LEU:HD21	2.50	0.46
1:A:132:GLY:HA3	5:A:501:HEM:HBC2	1.98	0.46
2:B:6:VAL:HG23	2:B:6:VAL:O	2.16	0.46
3:F:117:ASP:OD2	3:F:121:GLU:N	2.45	0.46
1:G:72:HIS:ND1	1:G:72:HIS:C	2.74	0.46
1:G:103:LEU:HB2	7:G:504:LOP:H233	1.98	0.46
1:G:157:TRP:O	1:G:158:GLY:C	2.59	0.46
1:G:370:LEU:HD22	1:G:403:TYR:CD2	2.51	0.46
3:I:138:GLY:CA	3:I:147:TRP:CD1	2.98	0.46
2:K:26:GLN:HG2	2:K:58:LEU:HD21	1.98	0.46
1:P:79:SER:O	1:P:82:HIS:HB3	2.16	0.46
3:R:30:ALA:O	3:R:33:PRO:HG2	2.15	0.46
1:A:209:VAL:HG22	5:A:501:HEM:HBB2	1.97	0.46
1:A:341:LEU:HD11	1:A:345:LEU:HD11	1.98	0.46
1:D:4:ILE:HD12	1:D:4:ILE:H	1.81	0.46
1:D:29:ALA:CB	8:D:504:ANJ:H233	2.45	0.46
3:F:77:ARG:NH2	3:F:115:THR:HG21	2.31	0.46
1:G:73:VAL:HG13	1:G:188:ASN:OD1	2.16	0.46
1:G:298:PHE:CZ	6:G:503:SMA:H36	2.51	0.46
2:H:6:VAL:HG23	2:H:6:VAL:O	2.16	0.46
3:I:14:PHE:CE1	3:I:18:ALA:HB2	2.51	0.46
3:I:59:PRO:HD3	3:I:76:ARG:NH1	2.31	0.46
3:I:88:VAL:HG13	3:I:92:GLN:HG3	1.98	0.46
2:K:126:GLY:HA2	2:K:129:GLU:OE2	2.16	0.46
2:N:197:ALA:C	2:N:199:GLY:H	2.24	0.46
1:P:244:PHE:CD1	1:P:248:PHE:HB2	2.50	0.46
2:Q:116:THR:HG22	2:Q:116:THR:O	2.16	0.46
3:C:47:LEU:HD23	3:C:48:ALA:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:PHE:CD1	1:D:388:PRO:N	2.84	0.46
2:E:197:ALA:C	2:E:199:GLY:H	2.24	0.46
1:G:25:ILE:HA	1:J:214:TRP:CH2	2.51	0.46
1:G:312:VAL:HB	1:G:315:VAL:HB	1.96	0.46
1:G:336:MET:HE3	6:G:503:SMA:H32	1.98	0.46
1:M:114:ARG:C	1:M:114:ARG:CD	2.89	0.46
2:N:32:TYR:CE2	2:N:42:MET:HE2	2.51	0.46
1:P:53:PHE:CE2	1:P:260:LEU:HD21	2.51	0.46
1:P:144:PHE:CD1	1:P:162:ILE:HD12	2.50	0.46
2:Q:76:GLU:CD	2:Q:76:GLU:N	2.74	0.46
2:Q:154:PHE:N	2:Q:154:PHE:CD1	2.83	0.46
2:E:235:MET:N	2:E:235:MET:HE2	2.30	0.45
3:F:110:THR:O	3:F:111:ASP:C	2.57	0.45
1:G:256:LEU:O	1:G:260:LEU:HG	2.16	0.45
1:G:394:LEU:HA	1:G:394:LEU:HD23	1.73	0.45
2:H:233:ALA:O	2:H:237:LEU:HD12	2.15	0.45
3:I:93:LEU:HD12	3:I:109:ALA:HB3	1.98	0.45
3:I:154:SER:OG	3:I:166:PRO:HD2	2.15	0.45
1:J:164:GLY:HA2	1:J:177:GLN:HE22	1.80	0.45
1:M:10:GLU:HA	1:M:11:PRO:HD3	1.77	0.45
1:M:262:VAL:O	1:M:265:ALA:HB3	2.16	0.45
2:N:186:PRO:O	2:N:187:PRO:C	2.59	0.45
1:P:394:LEU:HD23	1:P:394:LEU:HA	1.72	0.45
2:Q:72:VAL:HG12	2:Q:73:THR:N	2.30	0.45
1:A:205:ILE:O	1:A:209:VAL:HG23	2.17	0.45
2:B:197:ALA:C	2:B:199:GLY:H	2.23	0.45
2:E:186:PRO:O	2:E:187:PRO:C	2.58	0.45
1:G:388:PRO:O	1:G:392:ILE:HG13	2.15	0.45
3:I:30:ALA:O	3:I:33:PRO:HG2	2.16	0.45
1:J:39:ARG:HG2	1:J:242:VAL:CG1	2.44	0.45
1:J:39:ARG:NH1	2:K:255:VAL:HG12	2.30	0.45
1:J:72:HIS:ND1	1:J:72:HIS:C	2.74	0.45
1:J:164:GLY:O	1:J:167:GLY:N	2.49	0.45
1:J:229:VAL:HG22	1:J:424:ILE:HD12	1.99	0.45
1:M:91:PHE:CD1	1:M:91:PHE:C	2.93	0.45
3:O:26:ALA:O	3:O:27:THR:C	2.58	0.45
1:P:133:MET:N	5:P:501:HEM:HBC2	2.31	0.45
2:Q:127:GLY:O	2:Q:131:ILE:HG13	2.17	0.45
2:Q:203:SER:O	2:Q:204:VAL:C	2.60	0.45
2:Q:235:MET:O	2:Q:236:PHE:C	2.57	0.45
3:R:76:ARG:HG3	3:R:122:TRP:CH2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ALA:O	1:A:210:ALA:HB3	2.16	0.45
1:A:258:VAL:O	1:A:261:LEU:HB3	2.16	0.45
1:A:312:VAL:HB	1:A:315:VAL:CG2	2.46	0.45
2:B:19:THR:CG2	2:B:224:MET:HE3	2.46	0.45
2:B:105:LYS:HE2	2:B:220:GLU:HG2	1.98	0.45
1:G:258:VAL:O	1:G:261:LEU:HB3	2.17	0.45
1:M:246:PRO:HG2	2:N:251:LEU:HD21	1.98	0.45
1:M:327:ASP:C	1:M:327:ASP:OD1	2.60	0.45
2:N:103:MET:C	2:N:105:LYS:N	2.74	0.45
1:P:73:VAL:HG23	1:P:74:ASP:N	2.31	0.45
1:A:123:ALA:HA	1:A:126:GLU:OE1	2.16	0.45
2:B:51:SER:OG	2:B:63:VAL:HG21	2.16	0.45
2:B:206:ALA:O	2:B:207:MET:C	2.59	0.45
1:G:187:ASP:CG	1:G:188:ASN:H	2.24	0.45
3:I:108:GLU:O	3:I:110:THR:N	2.43	0.45
2:K:205:HIS:ND1	2:K:205:HIS:C	2.73	0.45
2:K:235:MET:O	2:K:236:PHE:C	2.59	0.45
1:M:91:PHE:CE1	1:M:92:MET:HB2	2.51	0.45
1:M:125:ARG:HG3	1:M:125:ARG:NH1	2.31	0.45
2:N:141:GLU:HG3	2:N:141:GLU:O	2.16	0.45
1:P:164:GLY:O	1:P:165:LEU:C	2.56	0.45
2:Q:226:ARG:O	2:Q:229:ALA:HB3	2.17	0.45
1:A:113:PHE:CD2	7:A:503:LOP:H301	2.52	0.45
1:A:128:THR:HG21	5:A:501:HEM:HBD1	1.98	0.45
2:B:110:PHE:O	2:B:120:GLN:HG2	2.16	0.45
2:E:127:GLY:O	2:E:131:ILE:HG13	2.16	0.45
1:G:18:TRP:CD1	1:G:22:ARG:NH1	2.85	0.45
1:G:363:PHE:O	1:G:364:LYS:C	2.58	0.45
1:J:13:THR:HG22	1:J:14:GLY:N	2.32	0.45
1:J:43:TRP:HA	1:J:43:TRP:CE3	2.52	0.45
1:J:56:VAL:O	1:J:57:LEU:C	2.59	0.45
1:J:188:ASN:O	1:J:189:ALA:C	2.58	0.45
1:J:248:PHE:O	1:J:249:ILE:C	2.58	0.45
2:K:47:ILE:C	2:K:49:SER:N	2.75	0.45
1:M:25:ILE:HA	1:P:214:TRP:HH2	1.82	0.45
1:M:374:PHE:HD2	7:M:504:LOP:H321	1.80	0.45
3:O:76:ARG:HG3	3:O:122:TRP:CH2	2.52	0.45
1:P:416:LYS:HD3	1:P:416:LYS:HA	1.80	0.45
2:Q:141:GLU:HA	2:Q:142:PRO:HD3	1.83	0.45
2:Q:189:LEU:HD23	2:Q:189:LEU:N	2.30	0.45
2:Q:197:ALA:C	2:Q:199:GLY:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:205:HIS:C	2:Q:205:HIS:ND1	2.73	0.45
1:A:370:LEU:HD22	1:A:403:TYR:CD2	2.52	0.45
1:G:13:THR:HG22	1:G:14:GLY:N	2.32	0.45
1:G:52:ALA:HB2	8:G:505:ANJ:C16	2.46	0.45
1:G:56:VAL:O	1:G:57:LEU:C	2.58	0.45
1:G:140:MET:O	1:G:141:ALA:C	2.59	0.45
2:H:116:THR:O	2:H:116:THR:HG22	2.17	0.45
1:J:296:TRP:CD2	1:J:297:TYR:N	2.85	0.45
1:J:327:ASP:C	1:J:327:ASP:OD1	2.59	0.45
1:J:379:TRP:CE2	2:K:114:MET:HE3	2.51	0.45
2:K:42:MET:HE1	2:K:214:PHE:HE2	1.74	0.45
2:K:103:MET:O	2:K:105:LYS:N	2.49	0.45
3:O:162:ILE:HD12	3:O:163:ARG:N	2.31	0.45
3:O:180:ASP:OD1	3:O:181:GLU:N	2.50	0.45
1:P:13:THR:HG22	1:P:14:GLY:N	2.32	0.45
1:P:122:LYS:NZ	1:P:360:ARG:NH1	2.65	0.45
1:P:209:VAL:O	1:P:213:ILE:HG13	2.16	0.45
2:Q:149:HIS:CG	2:Q:168:THR:HG21	2.52	0.45
3:R:185:GLN:O	3:R:185:GLN:HG2	2.17	0.45
1:D:188:ASN:O	1:D:189:ALA:C	2.60	0.45
2:E:127:GLY:N	2:E:128:PRO:HD2	2.32	0.45
2:E:203:SER:O	2:E:204:VAL:C	2.58	0.45
1:J:58:GLN:OE1	1:J:100:GLY:HA3	2.17	0.45
2:K:197:ALA:C	2:K:199:GLY:H	2.25	0.45
3:L:47:LEU:HD23	3:L:48:ALA:O	2.16	0.45
1:M:53:PHE:CE2	1:M:260:LEU:HD21	2.51	0.45
1:M:180:LEU:O	1:M:193:ARG:HD2	2.16	0.45
2:N:16:PRO:O	2:N:231:PHE:CZ	2.70	0.45
1:P:395:ILE:O	1:P:398:ALA:HB3	2.17	0.45
1:A:56:VAL:O	1:A:57:LEU:C	2.58	0.45
1:A:127:VAL:O	1:A:128:THR:C	2.60	0.45
3:C:87:SER:OG	3:C:88:VAL:N	2.50	0.45
3:C:185:GLN:O	3:C:185:GLN:HG2	2.16	0.45
2:E:30:GLN:NE2	2:E:194:VAL:HG13	2.32	0.45
3:I:66:LYS:HB2	1:J:286:LEU:HD11	1.98	0.45
1:J:209:VAL:O	1:J:213:ILE:HG13	2.16	0.45
1:J:299:LEU:HB2	1:J:378:THR:HG23	1.99	0.45
2:K:48:ARG:HG3	2:K:48:ARG:NH1	2.27	0.45
2:K:203:SER:O	2:K:204:VAL:C	2.60	0.45
2:N:240:LEU:HG	2:N:244:LEU:HD12	1.99	0.45
2:Q:189:LEU:HD21	5:Q:301:HEM:HBB1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:26:ALA:O	3:R:27:THR:C	2.59	0.45
1:A:213:ILE:HD11	8:A:504:ANJ:H162	1.97	0.45
1:G:91:PHE:CD1	1:G:91:PHE:C	2.95	0.45
1:G:135:ILE:O	1:G:139:MET:HG3	2.17	0.45
1:G:223:ASN:ND2	1:G:223:ASN:H	2.15	0.45
1:G:248:PHE:O	1:G:249:ILE:C	2.59	0.45
3:I:58:GLU:HB3	3:I:59:PRO:HD2	1.99	0.45
3:I:112:GLN:NE2	3:I:112:GLN:H	2.15	0.45
3:I:174:PRO:O	3:I:175:LEU:C	2.57	0.45
1:J:18:TRP:CD1	1:J:22:ARG:NH1	2.84	0.45
2:K:156:TYR:CD1	2:K:182:TRP:CZ3	3.05	0.45
1:M:46:ILE:HG13	1:M:47:TRP:N	2.31	0.45
1:M:127:VAL:O	1:M:128:THR:C	2.60	0.45
2:N:250:ARG:NE	3:O:12:ARG:CB	2.75	0.45
1:A:39:ARG:HD3	1:A:428:PHE:CD2	2.51	0.45
3:C:12:ARG:HG2	3:C:13:ASP:H	1.82	0.45
1:D:317:ILE:HG22	1:D:321:ILE:HD12	1.99	0.45
3:L:32:TRP:HB3	3:L:33:PRO:CD	2.47	0.45
1:M:209:VAL:O	1:M:213:ILE:HG13	2.17	0.45
1:M:262:VAL:O	1:M:266:ILE:HG12	2.17	0.45
1:M:329:LYS:HG3	3:R:131:HIS:HD2	1.82	0.45
1:P:379:TRP:NE1	2:Q:114:MET:HE2	2.32	0.45
1:A:188:ASN:O	1:A:189:ALA:C	2.59	0.44
3:C:59:PRO:HD3	3:C:76:ARG:NH1	2.33	0.44
1:D:234:LYS:O	1:D:238:GLN:HG3	2.17	0.44
1:D:262:VAL:O	1:D:265:ALA:HB3	2.17	0.44
2:E:190:MET:O	2:E:191:ASP:C	2.58	0.44
1:G:79:SER:O	1:G:82:HIS:HB3	2.17	0.44
1:G:269:PHE:HB3	4:G:431:BGL:O1	2.17	0.44
3:I:109:ALA:O	3:I:161:ARG:NH1	2.38	0.44
3:I:185:GLN:O	3:I:185:GLN:HG2	2.17	0.44
1:J:342:VAL:HG23	1:J:343:MET:N	2.32	0.44
1:M:73:VAL:HG12	1:M:151:TRP:CE2	2.52	0.44
1:M:299:LEU:HB2	1:M:378:THR:HG23	1.99	0.44
1:M:336:MET:HE3	6:M:503:SMA:H32	1.98	0.44
3:O:58:GLU:HB3	3:O:59:PRO:HD2	1.97	0.44
3:R:32:TRP:HB3	3:R:33:PRO:CD	2.46	0.44
3:R:83:GLU:O	3:R:84:LEU:C	2.58	0.44
3:C:58:GLU:HB3	3:C:59:PRO:HD2	1.99	0.44
3:C:174:PRO:O	3:C:175:LEU:C	2.58	0.44
3:F:174:PRO:O	3:F:175:LEU:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:77:ARG:HH21	3:L:115:THR:HG21	1.82	0.44
1:P:10:GLU:HA	1:P:11:PRO:HD3	1.78	0.44
1:P:116:LEU:HA	1:P:121:TYR:CE2	2.51	0.44
3:R:128:VAL:O	3:R:129:CYS:C	2.59	0.44
1:A:91:PHE:CD1	1:A:91:PHE:C	2.96	0.44
2:B:116:THR:O	2:B:116:THR:HG22	2.17	0.44
3:C:94:VAL:HG23	3:C:162:ILE:O	2.17	0.44
3:C:180:ASP:OD1	3:C:181:GLU:N	2.51	0.44
1:D:79:SER:O	1:D:82:HIS:HB3	2.18	0.44
1:D:209:VAL:O	1:D:213:ILE:HG13	2.17	0.44
1:D:262:VAL:O	1:D:266:ILE:HG12	2.17	0.44
3:F:32:TRP:CE2	3:F:36:ASN:HB2	2.53	0.44
1:G:327:ASP:C	1:G:327:ASP:OD1	2.59	0.44
3:L:58:GLU:HB3	3:L:59:PRO:HD2	1.99	0.44
1:M:30:TYR:CE1	1:M:34:MET:HG3	2.53	0.44
1:M:56:VAL:O	1:M:57:LEU:C	2.61	0.44
1:M:157:TRP:O	1:M:158:GLY:C	2.59	0.44
1:M:418:VAL:CG1	1:M:419:ALA:N	2.78	0.44
2:Q:248:ASN:O	2:Q:249:LYS:C	2.60	0.44
3:R:31:VAL:O	3:R:32:TRP:C	2.58	0.44
1:A:164:GLY:O	1:A:165:LEU:C	2.59	0.44
2:B:190:MET:O	2:B:191:ASP:C	2.59	0.44
1:D:164:GLY:O	1:D:167:GLY:N	2.50	0.44
3:F:31:VAL:O	3:F:32:TRP:C	2.61	0.44
3:F:128:VAL:O	3:F:129:CYS:C	2.61	0.44
1:G:39:ARG:HG2	1:G:242:VAL:CG1	2.46	0.44
1:M:60:VAL:O	1:M:64:VAL:HG23	2.18	0.44
2:N:26:GLN:HG2	2:N:58:LEU:HD21	1.99	0.44
1:P:156:PHE:HE2	1:P:285:PRO:HA	1.82	0.44
1:A:49:VAL:HG12	1:A:256:LEU:HD13	2.00	0.44
1:A:122:LYS:HZ1	1:A:350:ASP:CG	2.26	0.44
1:A:163:THR:O	1:A:177:GLN:HG3	2.18	0.44
1:A:223:ASN:HD22	1:A:223:ASN:N	2.15	0.44
3:C:84:LEU:H	3:C:84:LEU:HD12	1.83	0.44
1:D:117:TYR:HB2	1:D:367:PHE:CE1	2.53	0.44
1:D:157:TRP:O	1:D:158:GLY:C	2.57	0.44
1:D:295:GLU:N	1:D:295:GLU:OE1	2.49	0.44
3:I:89:GLN:N	3:I:92:GLN:HE21	2.07	0.44
1:J:139:MET:O	1:J:142:THR:HB	2.17	0.44
1:J:367:PHE:O	1:J:370:LEU:HB3	2.17	0.44
1:M:139:MET:O	1:M:142:THR:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:41:SER:HB2	3:O:43:ASP:OD1	2.17	0.44
1:P:13:THR:O	1:P:17:LYS:HG3	2.17	0.44
1:P:370:LEU:HD22	1:P:403:TYR:CD2	2.52	0.44
2:Q:27:ARG:HB3	2:Q:196:TYR:CE1	2.53	0.44
2:Q:40:HIS:HE1	2:Q:98:PRO:HD2	1.82	0.44
1:A:103:LEU:HD13	7:A:503:LOP:H222	2.00	0.44
1:A:388:PRO:O	1:A:392:ILE:HG13	2.18	0.44
3:C:83:GLU:O	3:C:84:LEU:C	2.61	0.44
3:C:132:LEU:HD12	3:C:152:HIS:CE1	2.52	0.44
1:D:13:THR:HG22	1:D:14:GLY:N	2.32	0.44
1:D:43:TRP:HA	1:D:43:TRP:CE3	2.52	0.44
3:F:112:GLN:NE2	3:F:112:GLN:H	2.16	0.44
1:G:114:ARG:C	1:G:114:ARG:CD	2.91	0.44
1:G:410:ILE:O	1:G:412:GLY:N	2.50	0.44
1:J:418:VAL:HG13	1:J:419:ALA:H	1.82	0.44
3:L:32:TRP:HB3	3:L:33:PRO:HD3	2.00	0.44
3:L:44:VAL:O	3:L:46:ALA:N	2.51	0.44
1:M:9:TYR:CD2	1:M:27:ALA:HA	2.53	0.44
1:M:18:TRP:CD1	1:M:22:ARG:NH1	2.85	0.44
1:M:193:ARG:HH11	3:R:38:MET:HE2	1.82	0.44
2:N:127:GLY:O	2:N:131:ILE:HG13	2.18	0.44
1:P:254:PHE:CD1	1:P:254:PHE:C	2.95	0.44
2:Q:53:PRO:HA	2:Q:57:GLU:HG2	2.00	0.44
3:R:132:LEU:HB2	10:R:200:FES:S2	2.58	0.44
1:A:157:TRP:O	1:A:158:GLY:C	2.61	0.44
2:B:26:GLN:HG2	2:B:58:LEU:HD21	1.98	0.44
2:B:102:LEU:O	2:B:103:MET:C	2.60	0.44
3:F:110:THR:HB	3:F:112:GLN:NE2	2.33	0.44
1:G:262:VAL:O	1:G:265:ALA:HB3	2.18	0.44
6:G:503:SMA:H11	6:G:503:SMA:H30	1.73	0.44
1:J:43:TRP:HZ3	1:J:251:LYS:CE	2.29	0.44
2:K:24:GLN:HG3	2:K:210:ASP:OD1	2.18	0.44
2:K:47:ILE:C	2:K:49:SER:H	2.25	0.44
1:M:104:PHE:O	1:M:108:VAL:HG22	2.18	0.44
1:M:223:ASN:ND2	1:M:223:ASN:N	2.66	0.44
2:N:81:ARG:HH22	2:N:87:ASP:CG	2.26	0.44
3:O:31:VAL:O	3:O:32:TRP:C	2.61	0.44
3:O:174:PRO:O	3:O:175:LEU:C	2.59	0.44
1:P:56:VAL:O	1:P:57:LEU:C	2.60	0.44
1:P:247:TYR:CE1	2:Q:251:LEU:HD11	2.53	0.44
2:Q:106:ALA:C	2:Q:107:ARG:HG2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:240:LEU:HG	2:Q:244:LEU:HD12	1.99	0.44
1:A:122:LYS:HD2	1:A:355:ARG:HA	1.99	0.44
1:A:223:ASN:ND2	1:A:223:ASN:N	2.66	0.44
2:B:233:ALA:O	2:B:237:LEU:HD12	2.18	0.44
3:C:143:ASP:C	3:C:144:PHE:CD1	2.96	0.44
2:E:235:MET:O	2:E:236:PHE:C	2.61	0.44
1:G:389:TYR:HA	1:G:392:ILE:HD12	2.00	0.44
1:G:423:THR:O	1:G:426:GLU:HB3	2.18	0.44
2:H:42:MET:HE1	2:H:214:PHE:CE2	2.52	0.44
1:J:180:LEU:O	1:J:193:ARG:HD2	2.18	0.44
1:M:122:LYS:HE2	1:M:350:ASP:CG	2.42	0.44
3:O:71:PRO:HB3	1:P:286:LEU:HD22	2.00	0.44
1:P:56:VAL:O	1:P:60:VAL:HG13	2.18	0.44
1:P:105:PHE:O	1:P:108:VAL:CG2	2.66	0.44
2:Q:24:GLN:HG3	2:Q:210:ASP:OD1	2.16	0.44
1:A:140:MET:O	1:A:141:ALA:C	2.60	0.44
1:A:145:MET:HE3	1:A:145:MET:HB2	1.91	0.44
2:B:250:ARG:HH21	3:C:12:ARG:HB3	1.76	0.44
1:D:252:ASP:O	1:D:256:LEU:HB2	2.18	0.44
1:G:140:MET:HB3	6:G:503:SMA:H37	1.99	0.44
2:K:77:THR:HG22	2:K:79:GLU:CB	2.48	0.44
2:K:77:THR:CG2	2:K:79:GLU:H	2.24	0.44
2:K:251:LEU:O	2:K:251:LEU:HD12	2.17	0.44
3:L:110:THR:O	3:L:111:ASP:C	2.60	0.44
1:M:153:GLN:HB3	1:M:289:PRO:HG2	2.00	0.44
2:N:142:PRO:HG2	2:N:150:GLU:OE2	2.18	0.44
3:O:76:ARG:HA	3:O:121:GLU:O	2.18	0.44
3:O:185:GLN:O	3:O:185:GLN:HG2	2.17	0.44
1:P:34:MET:O	1:P:35:ILE:C	2.61	0.44
1:P:111:HIS:HE1	5:P:501:HEM:C1A	2.36	0.44
1:P:180:LEU:O	1:P:193:ARG:HD2	2.18	0.44
1:P:209:VAL:HG22	5:P:501:HEM:HBB2	2.00	0.44
1:A:302:TYR:CE1	6:A:1:SMA:H5	2.52	0.43
1:D:72:HIS:C	1:D:72:HIS:ND1	2.76	0.43
6:J:503:SMA:H11	6:J:503:SMA:H30	1.66	0.43
3:L:44:VAL:C	3:L:46:ALA:N	2.76	0.43
1:M:223:ASN:N	1:M:223:ASN:HD22	2.16	0.43
2:N:224:MET:O	2:N:228:GLN:HG3	2.18	0.43
1:P:114:ARG:C	1:P:114:ARG:CD	2.89	0.43
1:P:223:ASN:ND2	1:P:223:ASN:N	2.66	0.43
2:Q:6:VAL:O	2:Q:6:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLY:O	1:A:167:GLY:N	2.51	0.43
1:D:213:ILE:CG2	1:D:217:HIS:HD2	2.31	0.43
2:E:206:ALA:O	2:E:207:MET:C	2.61	0.43
2:E:236:PHE:CE1	3:F:25:VAL:HG12	2.54	0.43
3:F:126:TRP:C	3:F:128:VAL:H	2.27	0.43
3:F:132:LEU:HA	3:F:132:LEU:HD23	1.84	0.43
3:F:185:GLN:O	3:F:185:GLN:HG2	2.18	0.43
1:G:255:ALA:O	1:G:259:VAL:HG23	2.18	0.43
2:H:26:GLN:HG2	2:H:58:LEU:HD21	1.99	0.43
1:J:73:VAL:HG23	1:J:74:ASP:N	2.33	0.43
1:M:34:MET:O	1:M:35:ILE:C	2.61	0.43
1:M:379:TRP:CE3	1:M:380:VAL:HG13	2.53	0.43
1:P:72:HIS:HE1	1:P:74:ASP:OD2	2.01	0.43
1:A:39:ARG:HG2	1:A:242:VAL:CG1	2.47	0.43
2:B:170:LYS:HA	2:B:175:VAL:O	2.18	0.43
2:B:223:LEU:HD23	2:B:223:LEU:C	2.43	0.43
3:C:38:MET:HG2	1:D:193:ARG:NH1	2.33	0.43
1:D:39:ARG:HD3	1:D:428:PHE:CD2	2.53	0.43
1:D:132:GLY:CA	5:D:501:HEM:HBC2	2.49	0.43
2:E:160:PHE:CE2	2:E:183:ILE:HG13	2.54	0.43
2:H:24:GLN:HG3	2:H:210:ASP:OD1	2.18	0.43
3:I:32:TRP:HB3	3:I:33:PRO:CD	2.48	0.43
1:J:77:PHE:CD2	1:J:282:GLU:HG2	2.53	0.43
1:J:114:ARG:C	1:J:114:ARG:CD	2.90	0.43
1:J:228:GLU:C	1:J:424:ILE:HD11	2.42	0.43
2:Q:22:GLN:HE21	2:Q:22:GLN:HB2	1.70	0.43
2:Q:47:ILE:C	2:Q:49:SER:N	2.76	0.43
2:B:185:MET:HB2	5:B:301:HEM:C1D	2.54	0.43
3:C:31:VAL:O	3:C:32:TRP:C	2.60	0.43
3:C:95:ASP:HB3	3:C:170:ASN:HD21	1.83	0.43
1:D:103:LEU:CD1	7:D:503:LOP:H202	2.48	0.43
1:G:4:ILE:N	1:G:4:ILE:CD1	2.77	0.43
2:H:203:SER:O	2:H:204:VAL:C	2.60	0.43
1:J:39:ARG:HH12	2:K:255:VAL:CG1	2.29	0.43
1:J:127:VAL:O	1:J:128:THR:C	2.60	0.43
1:J:180:LEU:CD1	6:J:503:SMA:H25	2.47	0.43
2:K:6:VAL:HG23	2:K:6:VAL:O	2.18	0.43
3:L:179:ILE:HD13	3:L:179:ILE:HA	1.86	0.43
1:M:39:ARG:HB3	1:M:428:PHE:CE1	2.54	0.43
1:M:43:TRP:CZ3	1:M:251:LYS:HE3	2.53	0.43
1:M:270:MET:HE1	2:N:121:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:365:ILE:HD13	1:M:365:ILE:HA	1.78	0.43
3:O:30:ALA:O	3:O:33:PRO:HD2	2.18	0.43
3:O:112:GLN:NE2	3:O:112:GLN:H	2.17	0.43
1:P:75:LEU:O	1:P:76:ALA:C	2.61	0.43
1:P:408:LEU:HB2	1:P:409:PRO:HD3	1.99	0.43
2:Q:223:LEU:HD23	2:Q:223:LEU:C	2.43	0.43
1:A:102:SER:O	1:A:103:LEU:C	2.60	0.43
1:A:276:HIS:ND1	1:A:278:ASP:HB2	2.33	0.43
1:A:394:LEU:HA	1:A:394:LEU:HD23	1.75	0.43
2:B:127:GLY:O	2:B:131:ILE:HG13	2.18	0.43
3:C:90:LEU:CD1	3:C:108:GLU:HB3	2.49	0.43
1:D:122:LYS:O	1:D:123:ALA:C	2.61	0.43
3:F:82:ILE:O	3:F:86:ARG:HG3	2.19	0.43
2:H:223:LEU:C	2:H:223:LEU:HD23	2.43	0.43
3:I:142:GLY:C	3:I:144:PHE:H	2.26	0.43
1:J:79:SER:O	1:J:82:HIS:HB3	2.17	0.43
2:K:127:GLY:O	2:K:131:ILE:HG13	2.19	0.43
5:K:301:HEM:CBB	5:K:301:HEM:HMB1	2.48	0.43
1:M:83:ILE:O	1:M:90:GLY:HA3	2.19	0.43
1:P:135:ILE:HG21	5:P:501:HEM:CBB	2.48	0.43
1:P:278:ASP:OD2	1:P:289:PRO:HB3	2.19	0.43
1:P:379:TRP:CE3	1:P:380:VAL:HG13	2.53	0.43
2:Q:47:ILE:C	2:Q:49:SER:H	2.26	0.43
1:A:391:TRP:O	1:A:395:ILE:HG13	2.18	0.43
3:C:41:SER:HB2	3:C:43:ASP:OD1	2.19	0.43
3:F:58:GLU:HB3	3:F:59:PRO:HD2	1.99	0.43
1:G:58:GLN:OE1	1:G:100:GLY:HA3	2.18	0.43
1:G:214:TRP:HH2	1:J:25:ILE:HA	1.84	0.43
3:I:137:ILE:HD11	1:J:290:ALA:HA	1.99	0.43
1:J:37:THR:O	1:J:38:PRO:C	2.62	0.43
2:K:240:LEU:HG	2:K:244:LEU:HD12	2.01	0.43
2:N:19:THR:HB	2:N:224:MET:HE3	2.00	0.43
3:R:162:ILE:HD12	3:R:163:ARG:N	2.33	0.43
1:A:9:TYR:CD2	1:A:27:ALA:HA	2.54	0.43
1:A:22:ARG:HH11	1:A:22:ARG:HG3	1.83	0.43
3:C:30:ALA:O	3:C:33:PRO:HG2	2.18	0.43
3:C:32:TRP:HB3	3:C:33:PRO:CD	2.49	0.43
1:D:254:PHE:CD1	1:D:254:PHE:C	2.97	0.43
1:D:379:TRP:CE3	1:D:380:VAL:HG13	2.54	0.43
2:E:223:LEU:HD23	2:E:223:LEU:C	2.44	0.43
1:G:137:LEU:HD23	1:G:137:LEU:HA	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:47:ILE:C	2:H:49:SER:N	2.76	0.43
2:H:152:ASP:C	2:H:152:ASP:OD1	2.61	0.43
1:J:255:ALA:O	1:J:259:VAL:HG23	2.18	0.43
3:L:30:ALA:O	3:L:33:PRO:HG2	2.19	0.43
3:L:76:ARG:HG2	3:L:121:GLU:HG2	2.00	0.43
1:M:390:ASP:OD1	1:M:390:ASP:N	2.51	0.43
2:N:69:GLN:HG3	2:N:70:PHE:N	2.33	0.43
1:P:72:HIS:ND1	1:P:72:HIS:C	2.76	0.43
1:P:105:PHE:O	1:P:106:ILE:C	2.61	0.43
1:P:202:PRO:O	1:P:205:ILE:HB	2.18	0.43
1:P:336:MET:HE3	6:P:503:SMA:H32	2.01	0.43
1:P:362:MET:HB2	1:P:415:GLU:OE2	2.18	0.43
2:Q:144:LYS:O	2:Q:147:GLU:HB2	2.19	0.43
1:A:139:MET:O	1:A:142:THR:HB	2.19	0.43
1:D:22:ARG:HH11	1:D:22:ARG:HG3	1.84	0.43
1:D:39:ARG:NH1	2:E:255:VAL:CG1	2.79	0.43
1:D:135:ILE:O	1:D:139:MET:HG3	2.18	0.43
3:F:41:SER:HB2	3:F:43:ASP:OD1	2.19	0.43
1:G:261:LEU:CD1	2:H:234:VAL:HG13	2.49	0.43
1:J:51:LEU:HD13	5:J:501:HEM:C4B	2.53	0.43
1:J:135:ILE:HG21	5:J:501:HEM:CBB	2.48	0.43
3:L:83:GLU:O	3:L:84:LEU:C	2.61	0.43
1:M:207:ALA:O	1:M:210:ALA:HB3	2.19	0.43
1:M:299:LEU:O	1:M:302:TYR:HB3	2.18	0.43
2:N:81:ARG:NH1	2:N:84:LYS:HG3	2.34	0.43
1:A:122:LYS:NZ	1:A:350:ASP:CG	2.77	0.43
1:D:150:PRO:HG2	5:D:502:HEM:O1A	2.19	0.43
1:D:276:HIS:ND1	1:D:278:ASP:HB2	2.34	0.43
2:E:6:VAL:O	2:E:6:VAL:HG23	2.17	0.43
1:G:63:ILE:N	5:G:502:HEM:HAC	2.34	0.43
1:G:135:ILE:HG21	5:G:501:HEM:CBB	2.48	0.43
1:J:166:PHE:HA	1:J:169:ILE:HD12	2.00	0.43
1:J:425:GLU:O	1:J:429:ASN:ND2	2.52	0.43
3:L:31:VAL:O	3:L:32:TRP:C	2.60	0.43
1:M:51:LEU:O	1:M:52:ALA:C	2.62	0.43
6:M:503:SMA:H30	6:M:503:SMA:H11	1.76	0.43
2:Q:108:ALA:HA	2:Q:125:ILE:HG22	2.01	0.43
3:R:148:PHE:HE1	3:R:153:GLY:HA2	1.81	0.43
2:B:154:PHE:HB3	2:B:182:TRP:HB3	2.01	0.43
1:D:72:HIS:HE1	1:D:74:ASP:OD2	2.01	0.43
1:D:91:PHE:CG	1:D:92:MET:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:VAL:O	1:G:128:THR:C	2.62	0.43
1:G:262:VAL:O	1:G:266:ILE:HG12	2.18	0.43
3:I:135:SER:HA	3:I:136:PRO:HD3	1.76	0.43
1:J:83:ILE:O	1:J:90:GLY:HA3	2.19	0.43
1:M:425:GLU:CG	1:M:429:ASN:HD21	2.29	0.43
1:P:428:PHE:CZ	2:Q:256:LYS:HB2	2.54	0.43
1:A:363:PHE:O	1:A:364:LYS:C	2.61	0.42
2:B:30:GLN:NE2	2:B:194:VAL:HG13	2.34	0.42
2:B:243:LEU:HB3	3:C:19:THR:OG1	2.19	0.42
3:F:152:HIS:HB2	10:F:200:FES:S1	2.59	0.42
1:G:139:MET:O	1:G:142:THR:HB	2.18	0.42
1:G:188:ASN:O	1:G:189:ALA:C	2.60	0.42
2:H:47:ILE:C	2:H:49:SER:H	2.27	0.42
1:J:370:LEU:HD22	1:J:403:TYR:CD2	2.54	0.42
2:N:43:LYS:HE3	2:N:44:PHE:CZ	2.54	0.42
3:O:59:PRO:HD3	3:O:76:ARG:NH1	2.34	0.42
1:P:207:ALA:O	1:P:210:ALA:HB3	2.19	0.42
3:R:154:SER:OG	3:R:166:PRO:HD2	2.18	0.42
1:D:91:PHE:CD1	1:D:91:PHE:C	2.97	0.42
1:D:233:SER:O	1:D:234:LYS:C	2.60	0.42
3:F:66:LYS:HG2	3:F:67:PHE:N	2.33	0.42
1:G:51:LEU:HD13	5:G:501:HEM:C3B	2.54	0.42
1:J:55:LEU:HD12	1:J:55:LEU:HA	1.84	0.42
2:K:185:MET:HB2	5:K:301:HEM:C1D	2.53	0.42
1:M:312:VAL:O	1:M:315:VAL:HB	2.19	0.42
2:N:61:ASP:HA	2:N:64:ARG:CZ	2.50	0.42
3:O:38:MET:HG2	1:P:193:ARG:NH1	2.34	0.42
1:P:46:ILE:HG13	1:P:47:TRP:N	2.33	0.42
3:C:26:ALA:O	3:C:27:THR:C	2.61	0.42
3:C:132:LEU:HA	3:C:132:LEU:HD23	1.81	0.42
1:D:71:PRO:O	1:D:72:HIS:HB2	2.19	0.42
1:D:213:ILE:HG22	1:D:217:HIS:HD2	1.84	0.42
2:E:217:TRP:O	2:E:218:ALA:C	2.62	0.42
2:K:190:MET:O	2:K:191:ASP:C	2.61	0.42
3:L:95:ASP:HB3	3:L:170:ASN:ND2	2.35	0.42
1:M:102:SER:O	1:M:103:LEU:C	2.63	0.42
1:M:315:VAL:O	1:M:318:ALA:HB3	2.19	0.42
2:N:23:HIS:O	2:N:26:GLN:HB2	2.19	0.42
3:R:85:GLY:HA3	3:R:111:ASP:OD2	2.19	0.42
1:A:69:TYR:HA	1:A:79:SER:OG	2.19	0.42
1:A:166:PHE:HA	1:A:169:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LEU:O	1:A:302:TYR:HB3	2.20	0.42
2:B:223:LEU:CD2	2:B:227:LYS:HE3	2.39	0.42
1:D:278:ASP:OD2	1:D:289:PRO:HB3	2.19	0.42
1:D:299:LEU:HB2	1:D:378:THR:HG23	2.02	0.42
1:D:312:VAL:O	1:D:315:VAL:HB	2.19	0.42
3:I:41:SER:HB2	3:I:43:ASP:OD1	2.18	0.42
3:L:135:SER:HA	3:L:136:PRO:HD3	1.84	0.42
1:M:131:VAL:HA	1:M:134:LEU:HD12	2.02	0.42
1:M:394:LEU:HD23	1:M:394:LEU:HA	1.73	0.42
1:P:18:TRP:NE1	1:P:22:ARG:CZ	2.82	0.42
1:P:410:ILE:O	1:P:412:GLY:N	2.52	0.42
2:B:203:SER:O	2:B:204:VAL:C	2.60	0.42
1:D:213:ILE:CG2	1:D:217:HIS:CD2	3.02	0.42
1:D:367:PHE:O	1:D:370:LEU:HB3	2.20	0.42
3:F:32:TRP:CZ2	3:F:36:ASN:HB2	2.54	0.42
3:F:137:ILE:HD12	3:F:137:ILE:N	2.35	0.42
1:G:223:ASN:HD22	1:G:223:ASN:N	2.17	0.42
1:G:317:ILE:HG22	1:G:321:ILE:CD1	2.50	0.42
6:G:503:SMA:H12	6:G:503:SMA:H1	1.79	0.42
2:K:51:SER:OG	2:K:63:VAL:HG21	2.20	0.42
1:M:410:ILE:O	1:M:412:GLY:N	2.53	0.42
2:N:24:GLN:HG3	2:N:210:ASP:OD1	2.19	0.42
3:O:108:GLU:C	3:O:110:THR:H	2.27	0.42
1:P:312:VAL:HB	1:P:315:VAL:CG2	2.49	0.42
2:Q:27:ARG:HD2	2:Q:196:TYR:CE2	2.55	0.42
1:A:39:ARG:NH1	2:B:255:VAL:HG12	2.31	0.42
1:A:367:PHE:O	1:A:370:LEU:HB3	2.19	0.42
2:B:114:MET:O	2:B:114:MET:HG2	2.20	0.42
1:D:60:VAL:HG23	1:D:61:THR:N	2.33	0.42
1:D:73:VAL:HG23	1:D:74:ASP:H	1.83	0.42
2:E:66:TYR:HE1	2:E:70:PHE:HE2	1.67	0.42
3:F:94:VAL:HG23	3:F:162:ILE:O	2.19	0.42
1:G:156:PHE:HE2	1:G:285:PRO:HA	1.82	0.42
1:G:428:PHE:CZ	2:H:256:LYS:HB2	2.55	0.42
1:J:75:LEU:O	1:J:76:ALA:C	2.62	0.42
1:J:250:ILE:HD12	2:K:251:LEU:CD2	2.48	0.42
1:J:379:TRP:CE3	1:J:380:VAL:HG13	2.55	0.42
2:N:105:LYS:HE2	2:N:220:GLU:HG2	2.02	0.42
3:O:126:TRP:NE1	3:O:174:PRO:HB3	2.34	0.42
1:P:312:VAL:O	1:P:313:TRP:C	2.61	0.42
3:R:59:PRO:HD3	3:R:76:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:126:TRP:C	3:R:128:VAL:H	2.26	0.42
1:A:156:PHE:O	1:A:159:ALA:HB3	2.20	0.42
3:C:166:PRO:O	3:C:167:ALA:C	2.60	0.42
1:D:39:ARG:HG2	1:D:242:VAL:CG1	2.46	0.42
1:D:53:PHE:CE2	1:D:260:LEU:HD21	2.55	0.42
1:D:69:TYR:HA	1:D:79:SER:OG	2.19	0.42
1:D:91:PHE:CE1	1:D:92:MET:HB2	2.55	0.42
2:E:137:GLY:O	2:E:139:PRO:HD3	2.20	0.42
1:G:22:ARG:HH11	1:G:22:ARG:HG3	1.84	0.42
2:H:187:PRO:HA	2:H:188:PRO:HD2	1.85	0.42
1:J:254:PHE:CD1	1:J:254:PHE:C	2.98	0.42
1:J:388:PRO:O	1:J:392:ILE:HG13	2.20	0.42
2:K:32:TYR:CD1	2:K:36:CYS:HB2	2.54	0.42
1:M:114:ARG:HD2	1:M:114:ARG:O	2.20	0.42
1:M:258:VAL:O	1:M:261:LEU:HB3	2.20	0.42
1:M:269:PHE:CB	4:M:431:BGL:H1'2	2.49	0.42
1:M:278:ASP:OD2	1:M:289:PRO:HB3	2.20	0.42
2:N:203:SER:O	2:N:204:VAL:C	2.62	0.42
3:O:32:TRP:CE2	3:O:36:ASN:HB2	2.55	0.42
1:P:51:LEU:HB3	5:P:501:HEM:HMB1	2.02	0.42
1:P:327:ASP:C	1:P:327:ASP:OD1	2.62	0.42
1:A:269:PHE:HB3	4:A:431:BGL:H1'2	2.02	0.42
1:A:299:LEU:HB2	1:A:378:THR:HG23	2.00	0.42
3:C:30:ALA:O	3:C:33:PRO:HD2	2.20	0.42
1:D:164:GLY:O	1:D:165:LEU:C	2.63	0.42
1:D:390:ASP:OD1	1:D:390:ASP:N	2.53	0.42
1:D:394:LEU:HA	1:D:394:LEU:HD23	1.73	0.42
3:F:93:LEU:CD1	3:F:161:ARG:HD2	2.45	0.42
1:G:60:VAL:O	1:G:64:VAL:HG23	2.20	0.42
1:G:295:GLU:O	1:G:298:PHE:N	2.37	0.42
2:H:48:ARG:NH1	2:H:48:ARG:CG	2.83	0.42
3:I:151:CYS:SG	1:J:292:ILE:HD13	2.60	0.42
1:J:199:TYR:CZ	5:J:502:HEM:HBC1	2.55	0.42
1:J:321:ILE:O	1:J:321:ILE:HG22	2.19	0.42
2:K:146:ALA:HB2	2:K:169:CYS:SG	2.60	0.42
1:M:22:ARG:HH11	1:M:22:ARG:HG3	1.85	0.42
1:M:152:GLY:H	1:M:155:SER:HB2	1.85	0.42
1:M:296:TRP:CD2	1:M:297:TYR:N	2.88	0.42
2:N:250:ARG:CZ	3:O:12:ARG:HB3	2.50	0.42
3:O:152:HIS:HB2	10:O:200:FES:S1	2.60	0.42
1:P:132:GLY:CA	5:P:501:HEM:HBC2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:20:PHE:CZ	2:Q:217:TRP:HA	2.55	0.42
2:Q:48:ARG:NH1	2:Q:48:ARG:CG	2.81	0.42
1:A:18:TRP:CD1	1:A:22:ARG:NH1	2.88	0.42
1:A:346:VAL:N	1:A:347:PRO:CD	2.83	0.42
2:B:185:MET:HA	2:B:186:PRO:HD2	1.97	0.42
3:C:63:LEU:HB3	3:C:74:ILE:HB	2.01	0.42
1:D:410:ILE:C	1:D:412:GLY:N	2.78	0.42
1:D:410:ILE:O	1:D:412:GLY:N	2.53	0.42
2:E:151:PRO:HD2	2:E:182:TRP:CD1	2.55	0.42
1:G:391:TRP:O	1:G:395:ILE:HG13	2.20	0.42
2:H:72:VAL:O	2:H:80:ASP:HA	2.20	0.42
2:H:110:PHE:HE2	2:H:129:GLU:OE2	2.02	0.42
1:J:391:TRP:O	1:J:395:ILE:HG13	2.20	0.42
2:K:47:ILE:O	2:K:49:SER:N	2.53	0.42
3:L:26:ALA:O	3:L:29:ALA:N	2.53	0.42
3:L:152:HIS:HB2	10:L:200:FES:S1	2.59	0.42
1:M:52:ALA:HB2	8:M:505:ANJ:C16	2.50	0.42
1:M:366:TYR:CD2	1:M:411:LEU:HD11	2.55	0.42
1:P:111:HIS:CE1	5:P:501:HEM:C1A	3.07	0.42
1:P:118:TYR:CD1	1:P:224:PRO:HA	2.55	0.42
1:P:387:PHE:HA	1:P:390:ASP:OD1	2.20	0.42
3:C:87:SER:HB2	3:L:84:LEU:HD21	2.02	0.42
3:C:89:GLN:HG3	3:C:92:GLN:OE1	2.20	0.42
1:D:427:ASP:O	1:D:430:ALA:HB3	2.19	0.42
3:F:32:TRP:HB3	3:F:33:PRO:CD	2.50	0.42
1:G:111:HIS:HE1	5:G:501:HEM:C1A	2.38	0.42
1:G:284:ASN:HA	1:G:285:PRO:HD3	1.88	0.42
2:H:240:LEU:HG	2:H:244:LEU:HD12	2.02	0.42
1:J:360:ARG:HB2	1:J:363:PHE:HB3	2.02	0.42
1:M:105:PHE:HA	1:M:108:VAL:HG23	1.97	0.42
1:M:166:PHE:HA	1:M:169:ILE:HD12	2.01	0.42
1:M:287:ARG:HG2	1:M:287:ARG:HH11	1.84	0.42
5:M:502:HEM:CMB	5:M:502:HEM:CBB	2.97	0.42
2:N:141:GLU:HA	2:N:142:PRO:HD3	1.95	0.42
3:O:32:TRP:CZ2	3:O:36:ASN:HB2	2.55	0.42
1:P:37:THR:O	1:P:38:PRO:C	2.62	0.42
1:P:114:ARG:HD2	1:P:114:ARG:O	2.19	0.42
1:P:296:TRP:CD2	1:P:297:TYR:N	2.88	0.42
1:P:425:GLU:HG2	1:P:429:ASN:ND2	2.35	0.42
1:A:125:ARG:NE	1:A:222:ASN:HB2	2.35	0.41
3:C:126:TRP:NE1	3:C:174:PRO:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:LEU:HD11	1:D:345:LEU:HD11	2.01	0.41
2:H:51:SER:OG	2:H:63:VAL:HG21	2.20	0.41
3:I:179:ILE:HD13	3:I:179:ILE:HA	1.90	0.41
1:J:250:ILE:O	1:J:251:LYS:C	2.62	0.41
2:K:66:TYR:HE1	2:K:70:PHE:HE2	1.67	0.41
3:L:155:HIS:CD2	3:L:164:LYS:HD3	2.56	0.41
1:M:43:TRP:HA	1:M:43:TRP:HE3	1.86	0.41
1:P:49:VAL:O	1:P:50:VAL:C	2.63	0.41
1:P:258:VAL:O	1:P:261:LEU:HB3	2.20	0.41
2:Q:137:GLY:O	2:Q:139:PRO:HD3	2.20	0.41
3:R:131:HIS:CD2	3:R:132:LEU:HG	2.55	0.41
1:A:60:VAL:O	1:A:64:VAL:HG23	2.20	0.41
1:A:183:GLY:HA2	3:F:40:PRO:HG3	2.01	0.41
1:A:214:TRP:CH2	1:D:25:ILE:HA	2.55	0.41
2:E:77:THR:CG2	2:E:79:GLU:HB2	2.50	0.41
3:F:54:VAL:O	3:F:54:VAL:CG2	2.68	0.41
3:F:76:ARG:HG3	3:F:122:TRP:CH2	2.55	0.41
1:G:172:ILE:HG13	1:G:173:GLY:N	2.35	0.41
1:G:207:ALA:O	1:G:210:ALA:HB3	2.20	0.41
1:G:213:ILE:HD13	8:G:505:ANJ:H14	2.01	0.41
1:G:379:TRP:CE3	1:G:380:VAL:HG13	2.54	0.41
2:H:186:PRO:O	2:H:187:PRO:C	2.60	0.41
3:I:95:ASP:OD2	3:I:169:GLU:HA	2.21	0.41
3:I:138:GLY:O	3:I:141:SER:OG	2.35	0.41
1:J:374:PHE:HD2	7:J:504:LOP:H322	1.85	0.41
1:J:407:ILE:O	1:J:411:LEU:HG	2.20	0.41
3:L:180:ASP:OD1	3:L:181:GLU:N	2.53	0.41
1:M:187:ASP:CG	1:M:188:ASN:H	2.28	0.41
3:O:77:ARG:NH2	3:O:115:THR:HG21	2.35	0.41
1:P:153:GLN:HB3	1:P:289:PRO:HG2	2.02	0.41
1:P:223:ASN:N	1:P:223:ASN:HD22	2.17	0.41
2:Q:187:PRO:HA	2:Q:188:PRO:HD3	1.91	0.41
3:R:58:GLU:HB3	3:R:59:PRO:HD2	2.01	0.41
2:B:186:PRO:O	2:B:187:PRO:C	2.61	0.41
1:D:360:ARG:HB2	1:D:363:PHE:HB3	2.02	0.41
1:G:39:ARG:NH1	2:H:255:VAL:CG1	2.78	0.41
1:G:223:ASN:ND2	1:G:223:ASN:N	2.67	0.41
1:G:421:PRO:HB3	1:G:426:GLU:CD	2.45	0.41
2:H:165:VAL:HA	2:H:166:PRO:HD3	1.96	0.41
1:J:114:ARG:HD2	1:J:114:ARG:O	2.20	0.41
1:J:251:LYS:O	1:J:252:ASP:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:41:SER:HB2	3:L:43:ASP:OD1	2.20	0.41
1:M:8:HIS:CD2	1:M:8:HIS:N	2.88	0.41
1:M:360:ARG:HB2	1:M:363:PHE:HB3	2.03	0.41
2:N:13:PHE:O	2:N:227:LYS:NZ	2.53	0.41
2:N:22:GLN:HE21	2:N:22:GLN:HB2	1.68	0.41
3:O:84:LEU:HD12	3:O:84:LEU:N	2.34	0.41
1:P:122:LYS:O	1:P:123:ALA:C	2.62	0.41
2:Q:146:ALA:HB2	2:Q:169:CYS:SG	2.60	0.41
1:A:132:GLY:C	5:A:501:HEM:HBC2	2.44	0.41
1:A:254:PHE:CD1	1:A:254:PHE:C	2.98	0.41
3:C:93:LEU:HD23	3:C:163:ARG:HD3	2.01	0.41
1:D:153:GLN:HB3	1:D:289:PRO:HG2	2.02	0.41
2:E:143:PRO:HD3	2:E:156:TYR:CD2	2.56	0.41
3:F:137:ILE:CD1	3:F:150:PRO:HD3	2.47	0.41
1:G:18:TRP:NE1	1:G:22:ARG:CZ	2.83	0.41
2:H:145:CYS:SG	2:H:168:THR:O	2.78	0.41
2:K:144:LYS:O	2:K:147:GLU:HB2	2.20	0.41
1:M:55:LEU:HA	1:M:55:LEU:HD12	1.81	0.41
2:N:190:MET:O	2:N:191:ASP:C	2.64	0.41
1:P:201:LEU:HA	1:P:201:LEU:HD23	1.83	0.41
2:Q:231:PHE:O	2:Q:232:THR:C	2.63	0.41
2:Q:251:LEU:HD12	2:Q:251:LEU:O	2.21	0.41
2:B:22:GLN:HE21	2:B:22:GLN:HB2	1.72	0.41
1:D:4:ILE:N	1:D:4:ILE:CD1	2.82	0.41
2:E:24:GLN:HG3	2:E:210:ASP:OD1	2.20	0.41
2:E:110:PHE:O	2:E:120:GLN:HG2	2.20	0.41
1:G:111:HIS:CE1	5:G:501:HEM:C1A	3.08	0.41
1:G:114:ARG:HD2	1:G:114:ARG:O	2.21	0.41
2:H:127:GLY:O	2:H:131:ILE:HG13	2.21	0.41
2:H:251:LEU:HD12	2:H:251:LEU:O	2.21	0.41
1:J:40:ASN:HD21	1:J:223:ASN:HB2	1.86	0.41
1:J:358:ARG:HA	1:J:364:LYS:HE2	2.03	0.41
2:K:217:TRP:O	2:K:218:ALA:C	2.64	0.41
1:M:6:HIS:ND1	1:M:6:HIS:C	2.78	0.41
1:M:309:THR:C	1:M:311:ASP:H	2.28	0.41
1:P:39:ARG:HG2	1:P:242:VAL:CG1	2.48	0.41
1:P:91:PHE:CE1	1:P:92:MET:HB2	2.54	0.41
1:P:139:MET:O	1:P:142:THR:HB	2.21	0.41
1:P:187:ASP:CG	1:P:188:ASN:H	2.29	0.41
1:P:322:SER:O	1:P:323:PHE:HB2	2.20	0.41
2:Q:190:MET:O	2:Q:191:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ILE:HG13	1:A:173:GLY:N	2.35	0.41
2:B:77:THR:HG22	2:B:79:GLU:H	1.85	0.41
2:B:149:HIS:NE2	2:B:168:THR:HG21	2.36	0.41
1:D:18:TRP:CD1	1:D:22:ARG:NH1	2.88	0.41
1:D:209:VAL:HG22	5:D:501:HEM:HBB2	2.03	0.41
2:E:19:THR:CG2	2:E:224:MET:HE3	2.51	0.41
2:E:135:LEU:HD21	5:E:301:HEM:C2B	2.56	0.41
1:G:39:ARG:HD3	1:G:428:PHE:CE2	2.55	0.41
1:G:125:ARG:NH2	1:G:222:ASN:CA	2.83	0.41
2:H:144:LYS:HD3	2:H:147:GLU:CD	2.45	0.41
1:J:153:GLN:HB3	1:J:289:PRO:HG2	2.02	0.41
3:L:72:ILE:HG13	3:L:126:TRP:CE3	2.56	0.41
1:M:40:ASN:HD21	1:M:223:ASN:HB2	1.86	0.41
1:M:91:PHE:CG	1:M:92:MET:N	2.88	0.41
1:M:91:PHE:HD2	2:N:222:LYS:HG2	1.84	0.41
3:R:12:ARG:CG	3:R:13:ASP:N	2.83	0.41
1:A:91:PHE:CG	1:A:92:MET:N	2.89	0.41
1:A:261:LEU:HD11	2:B:234:VAL:HG13	2.01	0.41
1:A:410:ILE:O	1:A:412:GLY:N	2.54	0.41
1:D:299:LEU:O	1:D:302:TYR:HB3	2.21	0.41
2:E:47:ILE:C	2:E:49:SER:H	2.29	0.41
2:E:189:LEU:O	2:E:190:MET:HB2	2.21	0.41
1:G:23:LEU:C	1:G:25:ILE:H	2.29	0.41
1:G:49:VAL:O	1:G:50:VAL:C	2.63	0.41
1:G:153:GLN:HB3	1:G:289:PRO:HG2	2.02	0.41
2:H:66:TYR:CE1	2:H:70:PHE:CE2	3.07	0.41
3:I:131:HIS:CD2	3:I:132:LEU:HG	2.56	0.41
1:J:18:TRP:NE1	1:J:22:ARG:CZ	2.83	0.41
1:J:72:HIS:HE1	1:J:74:ASP:OD2	2.03	0.41
1:M:43:TRP:HA	1:M:43:TRP:CE3	2.55	0.41
1:M:118:TYR:CD1	1:M:224:PRO:HA	2.56	0.41
1:M:322:SER:O	1:M:323:PHE:HB2	2.20	0.41
1:M:395:ILE:O	1:M:398:ALA:HB3	2.20	0.41
1:P:299:LEU:HB2	1:P:378:THR:HG23	2.02	0.41
2:Q:40:HIS:CE1	2:Q:97:ALA:HB1	2.55	0.41
3:R:164:LYS:HG2	3:R:165:GLY:N	2.35	0.41
1:A:77:PHE:CD2	1:A:282:GLU:HG2	2.55	0.41
6:A:1:SMA:H1	6:A:1:SMA:H12	1.86	0.41
2:B:24:GLN:HG3	2:B:210:ASP:OD1	2.21	0.41
2:B:53:PRO:HA	2:B:57:GLU:CD	2.45	0.41
2:B:251:LEU:HD12	2:B:251:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:THR:O	3:C:20:ALA:C	2.64	0.41
1:D:127:VAL:O	1:D:128:THR:C	2.63	0.41
1:G:317:ILE:CG2	1:G:321:ILE:HD11	2.51	0.41
1:J:37:THR:HA	1:J:38:PRO:HD2	1.93	0.41
2:K:231:PHE:O	2:K:232:THR:C	2.63	0.41
3:L:59:PRO:HD3	3:L:76:ARG:NH1	2.36	0.41
2:N:116:THR:HG22	2:N:116:THR:O	2.20	0.41
1:P:29:ALA:CB	8:P:505:ANJ:H233	2.51	0.41
2:Q:250:ARG:NE	3:R:12:ARG:HB3	2.35	0.41
1:A:37:THR:O	1:A:38:PRO:C	2.63	0.41
1:A:114:ARG:HD2	1:A:114:ARG:O	2.20	0.41
1:A:252:ASP:O	1:A:256:LEU:HB2	2.21	0.41
1:A:410:ILE:HG22	1:A:411:LEU:N	2.35	0.41
2:B:32:TYR:CD1	2:B:36:CYS:HB2	2.56	0.41
2:B:185:MET:HB2	5:B:301:HEM:C4D	2.56	0.41
2:B:240:LEU:HG	2:B:244:LEU:HD12	2.02	0.41
1:D:55:LEU:O	1:D:59:ILE:HG13	2.21	0.41
1:D:76:ALA:C	1:D:79:SER:HB3	2.45	0.41
1:D:114:ARG:C	1:D:114:ARG:CD	2.94	0.41
1:D:149:LEU:C	1:D:151:TRP:N	2.79	0.41
1:D:199:TYR:CZ	5:D:502:HEM:HBC1	2.55	0.41
1:D:207:ALA:O	1:D:210:ALA:HB3	2.20	0.41
1:D:328:ALA:O	1:D:329:LYS:C	2.64	0.41
1:D:362:MET:N	1:D:415:GLU:OE2	2.52	0.41
1:D:403:TYR:CE2	1:D:408:LEU:HD11	2.56	0.41
2:E:47:ILE:C	2:E:49:SER:N	2.78	0.41
2:E:104:ALA:CB	2:E:216:MET:HA	2.51	0.41
2:E:251:LEU:HD12	2:E:251:LEU:O	2.20	0.41
3:F:179:ILE:HD13	3:F:179:ILE:HA	1.87	0.41
1:G:69:TYR:HA	1:G:79:SER:OG	2.20	0.41
1:G:112:ILE:HG12	5:G:501:HEM:HAC	2.02	0.41
1:G:367:PHE:O	1:G:370:LEU:HB3	2.21	0.41
2:H:142:PRO:CG	2:H:150:GLU:OE2	2.69	0.41
2:H:190:MET:O	2:H:191:ASP:C	2.62	0.41
3:I:126:TRP:C	3:I:128:VAL:H	2.29	0.41
1:J:201:LEU:HD23	1:J:201:LEU:HA	1.80	0.41
1:J:207:ALA:O	1:J:210:ALA:HB3	2.21	0.41
1:J:262:VAL:O	1:J:265:ALA:HB3	2.20	0.41
1:M:408:LEU:N	1:M:409:PRO:CD	2.84	0.41
2:N:6:VAL:O	2:N:6:VAL:HG23	2.20	0.41
2:N:47:ILE:C	2:N:49:SER:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:147:GLU:O	2:N:147:GLU:HG3	2.21	0.41
3:O:12:ARG:CG	3:O:13:ASP:N	2.83	0.41
1:P:122:LYS:NZ	1:P:360:ARG:HH11	2.19	0.41
1:P:248:PHE:C	1:P:250:ILE:N	2.77	0.41
2:Q:150:GLU:HA	2:Q:151:PRO:HD3	1.93	0.41
3:R:12:ARG:HG3	3:R:13:ASP:N	2.36	0.41
1:A:209:VAL:O	1:A:213:ILE:HG13	2.21	0.41
1:A:360:ARG:HB2	1:A:363:PHE:HB3	2.03	0.41
2:B:246:LEU:HB2	3:C:15:LEU:HD21	2.03	0.41
3:F:32:TRP:N	3:F:33:PRO:HD2	2.36	0.41
3:F:180:ASP:OD1	3:F:181:GLU:N	2.54	0.41
1:G:365:ILE:HA	1:G:365:ILE:HD13	1.79	0.41
2:H:76:GLU:O	2:H:78:GLY:N	2.54	0.41
1:J:46:ILE:HG13	1:J:47:TRP:N	2.36	0.41
1:J:118:TYR:CD1	1:J:224:PRO:HA	2.56	0.41
1:J:223:ASN:H	1:J:223:ASN:ND2	2.18	0.41
3:L:126:TRP:C	3:L:128:VAL:H	2.29	0.41
1:M:75:LEU:O	1:M:76:ALA:C	2.64	0.41
1:P:91:PHE:CD1	1:P:91:PHE:C	2.98	0.41
1:P:127:VAL:O	1:P:128:THR:C	2.62	0.41
1:P:180:LEU:HD23	1:P:180:LEU:HA	1.85	0.41
1:P:262:VAL:O	1:P:266:ILE:HG12	2.21	0.41
2:Q:86:THR:CG2	3:R:46:ALA:HB1	2.51	0.41
1:A:134:LEU:HD23	1:A:134:LEU:HA	1.92	0.40
1:A:153:GLN:O	1:A:154:MET:C	2.64	0.40
3:C:84:LEU:H	3:C:84:LEU:CD1	2.34	0.40
1:D:30:TYR:CZ	1:D:34:MET:HG3	2.55	0.40
2:E:165:VAL:HA	2:E:166:PRO:HD3	1.98	0.40
3:F:132:LEU:HB2	10:F:200:FES:S2	2.61	0.40
1:G:40:ASN:HD21	1:G:223:ASN:HB2	1.86	0.40
1:G:213:ILE:HD11	8:G:505:ANJ:H14	2.00	0.40
1:J:276:HIS:HA	1:J:277:PRO:HD3	1.90	0.40
3:L:84:LEU:HD12	3:L:84:LEU:N	2.34	0.40
3:L:131:HIS:HB3	10:L:200:FES:S2	2.61	0.40
1:M:18:TRP:NE1	1:M:22:ARG:CZ	2.84	0.40
1:M:145:MET:HE3	1:M:145:MET:HB2	1.96	0.40
1:M:264:PHE:O	1:M:268:GLY:N	2.51	0.40
2:N:64:ARG:HA	2:N:85:PRO:HG3	2.03	0.40
2:N:143:PRO:HD3	2:N:156:TYR:CD2	2.56	0.40
1:P:131:VAL:HA	1:P:134:LEU:HD12	2.02	0.40
1:P:145:MET:HE3	1:P:145:MET:HB2	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:64:ARG:HA	2:Q:85:PRO:HG3	2.04	0.40
3:R:39:ASN:HD22	3:R:39:ASN:HA	1.72	0.40
2:B:27:ARG:HB3	2:B:196:TYR:CE1	2.56	0.40
3:F:26:ALA:O	3:F:29:ALA:N	2.54	0.40
1:G:164:GLY:O	1:G:167:GLY:N	2.54	0.40
1:G:216:PHE:CD1	1:G:216:PHE:C	2.99	0.40
1:J:69:TYR:HA	1:J:79:SER:OG	2.21	0.40
1:J:278:ASP:OD2	1:J:289:PRO:HB3	2.21	0.40
2:K:226:ARG:O	2:K:229:ALA:HB3	2.21	0.40
1:M:213:ILE:HD13	8:M:505:ANJ:H14	2.01	0.40
3:O:38:MET:CE	1:P:193:ARG:HH11	2.34	0.40
3:R:152:HIS:HB2	10:R:200:FES:S1	2.61	0.40
1:A:51:LEU:HD13	5:A:501:HEM:C4B	2.56	0.40
1:A:98:ALA:C	1:A:100:GLY:N	2.78	0.40
1:A:114:ARG:C	1:A:114:ARG:CD	2.93	0.40
1:A:284:ASN:HA	1:A:285:PRO:HD3	1.85	0.40
3:C:26:ALA:O	3:C:29:ALA:N	2.54	0.40
3:C:108:GLU:C	3:C:110:THR:H	2.27	0.40
1:D:153:GLN:O	1:D:154:MET:C	2.64	0.40
1:D:416:LYS:HA	1:D:417:PRO:HD2	1.93	0.40
2:E:226:ARG:O	2:E:229:ALA:HB3	2.21	0.40
2:E:237:LEU:O	2:E:238:THR:C	2.64	0.40
2:E:240:LEU:HG	2:E:244:LEU:HD12	2.02	0.40
3:F:14:PHE:CD2	3:F:15:LEU:N	2.89	0.40
1:G:316:GLN:O	1:G:317:ILE:C	2.64	0.40
2:H:137:GLY:O	2:H:139:PRO:HD3	2.22	0.40
2:H:189:LEU:HD23	2:H:189:LEU:HA	1.88	0.40
3:I:59:PRO:HD3	3:I:76:ARG:HH11	1.86	0.40
3:I:132:LEU:HA	3:I:132:LEU:HD23	1.89	0.40
1:J:262:VAL:O	1:J:266:ILE:HG12	2.21	0.40
1:J:410:ILE:O	1:J:412:GLY:N	2.54	0.40
3:L:90:LEU:O	3:L:90:LEU:HG	2.22	0.40
1:P:299:LEU:O	1:P:302:TYR:HB3	2.21	0.40
3:R:137:ILE:O	3:R:147:TRP:HA	2.21	0.40
1:A:8:HIS:CD2	1:A:8:HIS:N	2.86	0.40
1:A:72:HIS:HE1	1:A:74:ASP:OD2	2.03	0.40
3:C:73:PHE:CZ	3:C:127:GLY:HA3	2.56	0.40
1:D:114:ARG:HD2	1:D:114:ARG:O	2.22	0.40
2:E:185:MET:HA	2:E:186:PRO:HD2	1.99	0.40
1:G:248:PHE:HD1	1:G:251:LYS:CD	2.20	0.40
1:J:425:GLU:HG2	1:J:429:ASN:HD21	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:110:LEU:HA	1:M:110:LEU:HD23	1.92	0.40
2:N:217:TRP:O	2:N:218:ALA:C	2.63	0.40
6:P:503:SMA:H30	6:P:503:SMA:H11	1.82	0.40
2:Q:160:PHE:CD2	2:Q:183:ILE:HB	2.56	0.40
2:Q:192:ASP:HA	2:Q:202:ALA:HB3	2.03	0.40
3:C:32:TRP:HB3	3:C:33:PRO:HD3	2.04	0.40
3:C:135:SER:HA	3:C:136:PRO:HD3	1.79	0.40
1:D:46:ILE:O	1:D:50:VAL:HG23	2.22	0.40
2:E:150:GLU:HA	2:E:151:PRO:HD3	1.96	0.40
1:G:75:LEU:O	1:G:76:ALA:C	2.65	0.40
3:I:31:VAL:O	3:I:32:TRP:C	2.64	0.40
1:J:223:ASN:ND2	1:J:223:ASN:N	2.69	0.40
2:K:223:LEU:HD21	2:K:227:LYS:HE3	2.04	0.40
3:L:185:GLN:O	3:L:185:GLN:HG2	2.20	0.40
1:M:37:THR:O	1:M:38:PRO:C	2.62	0.40
1:M:163:THR:O	1:M:177:GLN:HG3	2.22	0.40
2:N:32:TYR:CE2	2:N:42:MET:CE	3.05	0.40
1:P:149:LEU:C	1:P:151:TRP:N	2.79	0.40
1:P:233:SER:O	1:P:234:LYS:C	2.63	0.40
1:P:299:LEU:O	1:P:300:PRO:C	2.62	0.40
2:Q:17:PHE:CE1	2:Q:231:PHE:CE1	3.09	0.40
2:Q:32:TYR:CD1	2:Q:36:CYS:HB2	2.56	0.40
2:Q:236:PHE:CZ	3:R:25:VAL:HG12	2.56	0.40
3:R:26:ALA:O	3:R:29:ALA:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	426/428 (100%)	366 (86%)	54 (13%)	6 (1%)	9 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	426/428 (100%)	365 (86%)	57 (13%)	4 (1%)	14	44
1	G	426/428 (100%)	368 (86%)	53 (12%)	5 (1%)	10	37
1	J	426/428 (100%)	361 (85%)	58 (14%)	7 (2%)	7	30
1	M	426/428 (100%)	364 (85%)	54 (13%)	8 (2%)	6	27
1	P	426/428 (100%)	364 (85%)	54 (13%)	8 (2%)	6	27
2	B	254/256 (99%)	210 (83%)	38 (15%)	6 (2%)	4	22
2	E	254/256 (99%)	210 (83%)	37 (15%)	7 (3%)	4	20
2	H	254/256 (99%)	205 (81%)	42 (16%)	7 (3%)	4	20
2	K	254/256 (99%)	205 (81%)	41 (16%)	8 (3%)	3	18
2	N	254/256 (99%)	210 (83%)	36 (14%)	8 (3%)	3	18
2	Q	254/256 (99%)	212 (84%)	34 (13%)	8 (3%)	3	18
3	C	177/179 (99%)	143 (81%)	28 (16%)	6 (3%)	3	16
3	F	177/179 (99%)	148 (84%)	23 (13%)	6 (3%)	3	16
3	I	177/179 (99%)	145 (82%)	24 (14%)	8 (4%)	2	12
3	L	177/179 (99%)	144 (81%)	29 (16%)	4 (2%)	5	23
3	O	177/179 (99%)	148 (84%)	22 (12%)	7 (4%)	2	13
3	R	177/179 (99%)	143 (81%)	28 (16%)	6 (3%)	3	16
All	All	5142/5178 (99%)	4311 (84%)	712 (14%)	119 (2%)	5	23

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	VAL
3	C	109	ALA
1	D	73	VAL
1	D	76	ALA
3	F	45	GLN
3	F	107	ALA
3	F	109	ALA
1	G	73	VAL
1	G	76	ALA
3	I	45	GLN
3	I	109	ALA
1	J	73	VAL
1	J	76	ALA
3	L	107	ALA

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Mol	Chain	Res	Type
3	L	109	ALA
1	M	73	VAL
1	M	76	ALA
3	O	107	ALA
3	O	109	ALA
1	P	73	VAL
1	P	76	ALA
3	R	45	GLN
3	R	107	ALA
3	R	109	ALA
1	A	76	ALA
1	A	173	GLY
2	B	43	LYS
3	C	107	ALA
1	D	173	GLY
2	E	43	LYS
2	E	190	MET
1	G	173	GLY
1	G	411	LEU
3	I	107	ALA
3	I	143	ASP
1	J	173	GLY
2	K	104	ALA
2	K	145	CYS
2	K	190	MET
3	L	45	GLN
1	M	173	GLY
1	M	411	LEU
2	N	43	LYS
2	N	104	ALA
3	O	90	LEU
1	P	173	GLY
2	Q	43	LYS
2	Q	137	GLY
3	R	83	GLU
3	R	90	LEU
3	R	140	VAL
1	A	411	LEU
2	B	198	ASP
2	E	137	GLY
2	E	198	ASP
2	H	43	LYS

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Mol	Chain	Res	Type
2	H	77	THR
2	H	188	PRO
2	H	198	ASP
2	K	77	THR
2	K	137	GLY
2	K	198	ASP
2	N	198	ASP
3	O	45	GLN
3	O	134	CYS
1	P	143	ALA
1	P	411	LEU
2	Q	77	THR
2	Q	188	PRO
2	Q	198	ASP
2	B	137	GLY
3	C	90	LEU
1	D	411	LEU
2	E	95	GLU
3	F	140	VAL
2	H	137	GLY
1	J	143	ALA
1	J	411	LEU
2	K	48	ARG
1	M	143	ALA
1	M	355	ARG
2	N	48	ARG
2	N	137	GLY
2	N	188	PRO
2	Q	48	ARG
2	Q	75	GLU
1	A	6	HIS
1	A	143	ALA
2	B	95	GLU
2	B	188	PRO
2	B	190	MET
2	E	48	ARG
2	H	48	ARG
2	H	78	GLY
3	I	83	GLU
3	I	134	CYS
3	I	140	VAL
2	K	81	ARG

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Mol	Chain	Res	Type
2	Q	95	GLU
3	C	83	GLU
3	F	134	CYS
1	G	143	ALA
2	N	95	GLU
2	N	190	MET
3	C	168	PRO
2	E	188	PRO
3	L	140	VAL
3	O	140	VAL
3	C	140	VAL
1	J	123	ALA
1	M	421	PRO
3	O	168	PRO
1	P	421	PRO
3	F	168	PRO
3	I	168	PRO
1	M	325	ILE
1	J	421	PRO
1	P	123	ALA
1	P	249	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/353 (100%)	330 (94%)	23 (6%)	15	44
1	D	353/353 (100%)	338 (96%)	15 (4%)	26	58
1	G	353/353 (100%)	332 (94%)	21 (6%)	18	48
1	J	353/353 (100%)	337 (96%)	16 (4%)	24	56
1	M	353/353 (100%)	337 (96%)	16 (4%)	24	56
1	P	353/353 (100%)	338 (96%)	15 (4%)	26	58
2	B	203/203 (100%)	193 (95%)	10 (5%)	22	53
2	E	203/203 (100%)	194 (96%)	9 (4%)	25	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	203/203 (100%)	189 (93%)	14 (7%)	14	41
2	K	203/203 (100%)	196 (97%)	7 (3%)	32	63
2	N	203/203 (100%)	197 (97%)	6 (3%)	36	65
2	Q	203/203 (100%)	193 (95%)	10 (5%)	22	53
3	C	138/138 (100%)	126 (91%)	12 (9%)	9	34
3	F	138/138 (100%)	123 (89%)	15 (11%)	6	24
3	I	138/138 (100%)	126 (91%)	12 (9%)	9	34
3	L	138/138 (100%)	128 (93%)	10 (7%)	13	40
3	O	138/138 (100%)	128 (93%)	10 (7%)	13	40
3	R	138/138 (100%)	125 (91%)	13 (9%)	8	31
All	All	4164/4164 (100%)	3930 (94%)	234 (6%)	19	49

All (234) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	8	HIS
1	A	49	VAL
1	A	60	VAL
1	A	92	MET
1	A	94	ARG
1	A	162	ILE
1	A	177	GLN
1	A	190	THR
1	A	192	ASN
1	A	217	HIS
1	A	223	ASN
1	A	246	PRO
1	A	295	GLU
1	A	311	ASP
1	A	314	VAL
1	A	316	GLN
1	A	319	ASN
1	A	325	ILE
1	A	377	LEU
1	A	385	THR
1	A	411	LEU
1	A	416	LYS

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Mol	Chain	Res	Type
2	B	42	MET
2	B	61	ASP
2	B	147	GLU
2	B	154	PHE
2	B	155	TYR
2	B	168	THR
2	B	190	MET
2	B	205	HIS
2	B	220	GLU
2	B	255	VAL
3	C	12	ARG
3	C	19	THR
3	C	41	SER
3	C	47	LEU
3	C	72	ILE
3	C	94	VAL
3	C	112	GLN
3	C	135	SER
3	C	137	ILE
3	C	168	PRO
3	C	174	PRO
3	C	179	ILE
1	D	4	ILE
1	D	7	ASP
1	D	49	VAL
1	D	60	VAL
1	D	92	MET
1	D	94	ARG
1	D	162	ILE
1	D	190	THR
1	D	192	ASN
1	D	223	ASN
1	D	246	PRO
1	D	277	PRO
1	D	377	LEU
1	D	385	THR
1	D	421	PRO
2	E	52	GLU
2	E	61	ASP
2	E	141	GLU
2	E	155	TYR
2	E	168	THR

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Mol	Chain	Res	Type
2	E	176	LYS
2	E	188	PRO
2	E	220	GLU
2	E	255	VAL
3	F	19	THR
3	F	41	SER
3	F	44	VAL
3	F	47	LEU
3	F	72	ILE
3	F	90	LEU
3	F	94	VAL
3	F	111	ASP
3	F	112	GLN
3	F	118	GLU
3	F	125	MET
3	F	168	PRO
3	F	177	LYS
3	F	179	ILE
3	F	181	GLU
1	G	4	ILE
1	G	7	ASP
1	G	49	VAL
1	G	60	VAL
1	G	92	MET
1	G	94	ARG
1	G	108	VAL
1	G	125	ARG
1	G	190	THR
1	G	192	ASN
1	G	217	HIS
1	G	223	ASN
1	G	246	PRO
1	G	287	ARG
1	G	314	VAL
1	G	315	VAL
1	G	377	LEU
1	G	385	THR
1	G	416	LYS
1	G	421	PRO
1	G	427	ASP
2	H	14	GLU
2	H	60	GLU

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Mol	Chain	Res	Type
2	H	73	THR
2	H	75	GLU
2	H	95	GLU
2	H	140	GLU
2	H	141	GLU
2	H	145	CYS
2	H	158	ARG
2	H	167	ASP
2	H	168	THR
2	H	205	HIS
2	H	220	GLU
2	H	255	VAL
3	I	12	ARG
3	I	19	THR
3	I	41	SER
3	I	44	VAL
3	I	47	LEU
3	I	72	ILE
3	I	92	GLN
3	I	112	GLN
3	I	118	GLU
3	I	168	PRO
3	I	174	PRO
3	I	179	ILE
1	J	4	ILE
1	J	7	ASP
1	J	8	HIS
1	J	43	TRP
1	J	49	VAL
1	J	60	VAL
1	J	108	VAL
1	J	190	THR
1	J	192	ASN
1	J	217	HIS
1	J	223	ASN
1	J	246	PRO
1	J	377	LEU
1	J	385	THR
1	J	416	LYS
1	J	421	PRO
2	K	52	GLU
2	K	72	VAL

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Mol	Chain	Res	Type
2	K	168	THR
2	K	171	ASP
2	K	188	PRO
2	K	220	GLU
2	K	255	VAL
3	L	19	THR
3	L	41	SER
3	L	72	ILE
3	L	90	LEU
3	L	94	VAL
3	L	112	GLN
3	L	168	PRO
3	L	174	PRO
3	L	177	LYS
3	L	179	ILE
1	M	7	ASP
1	M	8	HIS
1	M	43	TRP
1	M	49	VAL
1	M	60	VAL
1	M	92	MET
1	M	94	ARG
1	M	108	VAL
1	M	190	THR
1	M	192	ASN
1	M	223	ASN
1	M	246	PRO
1	M	252	ASP
1	M	315	VAL
1	M	377	LEU
1	M	385	THR
2	N	73	THR
2	N	168	THR
2	N	188	PRO
2	N	205	HIS
2	N	220	GLU
2	N	255	VAL
3	O	19	THR
3	O	41	SER
3	O	44	VAL
3	O	72	ILE
3	O	94	VAL

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Mol	Chain	Res	Type
3	O	112	GLN
3	O	125	MET
3	O	168	PRO
3	O	174	PRO
3	O	179	ILE
1	P	7	ASP
1	P	49	VAL
1	P	60	VAL
1	P	92	MET
1	P	94	ARG
1	P	108	VAL
1	P	190	THR
1	P	192	ASN
1	P	217	HIS
1	P	223	ASN
1	P	246	PRO
1	P	287	ARG
1	P	309	THR
1	P	385	THR
1	P	421	PRO
2	Q	52	GLU
2	Q	80	ASP
2	Q	90	PRO
2	Q	155	TYR
2	Q	168	THR
2	Q	188	PRO
2	Q	205	HIS
2	Q	220	GLU
2	Q	250	ARG
2	Q	255	VAL
3	R	19	THR
3	R	41	SER
3	R	72	ILE
3	R	89	GLN
3	R	92	GLN
3	R	94	VAL
3	R	112	GLN
3	R	118	GLU
3	R	140	VAL
3	R	168	PRO
3	R	174	PRO
3	R	177	LYS

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Mol	Chain	Res	Type
3	R	179	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	86	ASN
1	A	177	GLN
1	A	222	ASN
1	A	272	ASN
1	A	319	ASN
2	B	22	GLN
2	B	26	GLN
2	B	62	GLN
2	B	111	HIS
2	B	162	ASN
2	B	228	GLN
3	C	36	ASN
3	C	39	ASN
3	C	89	GLN
3	C	112	GLN
3	C	185	GLN
1	D	217	HIS
1	D	221	ASN
1	D	316	GLN
2	E	22	GLN
2	E	26	GLN
2	E	30	GLN
2	E	62	GLN
2	E	111	HIS
2	E	149	HIS
2	E	162	ASN
2	E	173	ASN
3	F	36	ASN
3	F	39	ASN
3	F	112	GLN
3	F	185	GLN
1	G	8	HIS
1	G	86	ASN
1	G	221	ASN
1	G	319	ASN
2	H	22	GLN

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Mol	Chain	Res	Type
2	H	26	GLN
2	H	62	GLN
2	H	149	HIS
2	H	162	ASN
3	I	36	ASN
3	I	39	ASN
3	I	92	GLN
3	I	112	GLN
3	I	185	GLN
1	J	8	HIS
1	J	177	GLN
1	J	221	ASN
1	J	429	ASN
2	K	22	GLN
2	K	26	GLN
2	K	30	GLN
2	K	62	GLN
2	K	162	ASN
3	L	36	ASN
3	L	39	ASN
3	L	45	GLN
3	L	89	GLN
3	L	92	GLN
3	L	112	GLN
3	L	155	HIS
3	L	185	GLN
1	M	8	HIS
1	M	86	ASN
1	M	177	GLN
1	M	217	HIS
1	M	221	ASN
1	M	316	GLN
1	M	429	ASN
2	N	22	GLN
2	N	26	GLN
2	N	30	GLN
2	N	62	GLN
2	N	96	ASN
2	N	162	ASN
2	N	228	GLN
3	O	36	ASN
3	O	39	ASN

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Mol	Chain	Res	Type
3	O	112	GLN
3	O	185	GLN
1	P	8	HIS
1	P	221	ASN
1	P	316	GLN
1	P	429	ASN
2	Q	22	GLN
2	Q	26	GLN
2	Q	30	GLN
2	Q	62	GLN
2	Q	162	ASN
3	R	36	ASN
3	R	39	ASN
3	R	112	GLN
3	R	185	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 6 are monoatomic - leaving 48 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	FES	O	200	3	0,4,4	-	-	-		
5	HEM	E	301	2	50,50,50	1.49	4 (8%)	67,82,82	1.13	4 (5%)
4	BGL	G	431	-	20,20,20	1.79	1 (5%)	24,25,25	0.85	0
4	BGL	J	431	-	20,20,20	1.58	2 (10%)	24,25,25	1.01	3 (12%)
4	BGL	M	431	-	20,20,20	1.75	2 (10%)	24,25,25	0.65	0
7	LOP	P	504	-	44,44,44	0.64	0	47,49,49	1.28	5 (10%)
8	ANJ	M	505	-	40,40,40	1.81	10 (25%)	34,54,54	1.79	8 (23%)
6	SMA	G	503	-	38,38,38	1.92	8 (21%)	47,52,52	2.24	12 (25%)
6	SMA	J	503	-	38,38,38	1.88	7 (18%)	47,52,52	2.00	11 (23%)
5	HEM	D	501	1	50,50,50	1.53	7 (14%)	67,82,82	1.20	3 (4%)
7	LOP	A	503	-	44,44,44	0.57	0	47,49,49	1.27	6 (12%)
5	HEM	A	502	1	50,50,50	1.74	9 (18%)	67,82,82	1.29	4 (5%)
5	HEM	K	301	2	50,50,50	1.49	4 (8%)	67,82,82	1.11	4 (5%)
7	LOP	D	503	-	44,44,44	0.58	0	47,49,49	1.31	5 (10%)
5	HEM	D	502	1	50,50,50	1.48	6 (12%)	67,82,82	1.15	4 (5%)
6	SMA	D	2	-	38,38,38	2.24	10 (26%)	47,52,52	2.00	13 (27%)
5	HEM	H	301	2	50,50,50	1.58	6 (12%)	67,82,82	1.21	5 (7%)
5	HEM	G	502	1	50,50,50	1.61	8 (16%)	67,82,82	1.21	4 (5%)
10	FES	R	200	3	0,4,4	-	-	-		
8	ANJ	D	504	-	40,40,40	1.80	11 (27%)	34,54,54	1.65	8 (23%)
6	SMA	M	503	-	38,38,38	2.11	8 (21%)	47,52,52	2.10	12 (25%)
5	HEM	G	501	1	50,50,50	1.48	6 (12%)	67,82,82	1.16	3 (4%)
8	ANJ	J	505	-	40,40,40	1.92	12 (30%)	34,54,54	1.64	6 (17%)
10	FES	L	200	3	0,4,4	-	-	-		
5	HEM	A	501	1	50,50,50	1.43	5 (10%)	67,82,82	1.12	3 (4%)
5	HEM	Q	301	2	50,50,50	1.39	4 (8%)	67,82,82	1.13	4 (5%)
4	BGL	Q	257	-	20,20,20	1.46	2 (10%)	24,25,25	1.02	1 (4%)
5	HEM	J	502	1	50,50,50	1.49	6 (12%)	67,82,82	1.17	3 (4%)
7	LOP	M	504	-	44,44,44	0.65	0	47,49,49	1.33	6 (12%)
5	HEM	M	502	1	50,50,50	1.53	6 (12%)	67,82,82	1.14	4 (5%)
5	HEM	P	501	1	50,50,50	1.54	7 (14%)	67,82,82	1.23	3 (4%)
5	HEM	J	501	1	50,50,50	1.43	5 (10%)	67,82,82	1.08	3 (4%)
5	HEM	B	301	2	50,50,50	1.54	5 (10%)	67,82,82	1.12	3 (4%)
5	HEM	P	502	1	50,50,50	1.52	6 (12%)	67,82,82	1.26	3 (4%)
5	HEM	M	501	1	50,50,50	1.43	6 (12%)	67,82,82	1.15	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	FES	F	200	3	0,4,4	-	-	-		
5	HEM	N	301	2	50,50,50	1.36	3 (6%)	67,82,82	1.10	3 (4%)
4	BGL	A	431	-	20,20,20	1.62	2 (10%)	24,25,25	1.07	3 (12%)
8	ANJ	P	505	-	40,40,40	1.75	11 (27%)	34,54,54	1.65	7 (20%)
8	ANJ	G	505	-	40,40,40	1.66	10 (25%)	34,54,54	1.81	8 (23%)
10	FES	I	200	3	0,4,4	-	-	-		
4	BGL	D	431	-	20,20,20	1.41	1 (5%)	24,25,25	1.17	2 (8%)
6	SMA	A	1	-	38,38,38	1.95	7 (18%)	47,52,52	2.26	12 (25%)
7	LOP	G	504	-	44,44,44	0.64	0	47,49,49	1.22	4 (8%)
10	FES	C	200	3	0,4,4	-	-	-		
8	ANJ	A	504	-	40,40,40	1.79	12 (30%)	34,54,54	1.72	8 (23%)
7	LOP	J	504	-	44,44,44	0.69	1 (2%)	47,49,49	1.17	2 (4%)
6	SMA	P	503	-	38,38,38	1.95	9 (23%)	47,52,52	1.69	7 (14%)

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
10	FES	O	200	3	-	-	0/1/1/1
5	HEM	E	301	2	-	6/14/54/54	-
4	BGL	G	431	-	-	0/11/31/31	0/1/1/1
4	BGL	J	431	-	-	0/11/31/31	0/1/1/1
4	BGL	M	431	-	-	0/11/31/31	0/1/1/1
7	LOP	P	504	-	-	4/48/48/48	-
8	ANJ	M	505	-	-	3/40/55/55	0/1/2/2
6	SMA	G	503	-	-	8/34/34/34	0/2/2/2
6	SMA	J	503	-	-	9/34/34/34	0/2/2/2
5	HEM	D	501	1	-	6/14/54/54	-
7	LOP	A	503	-	-	11/48/48/48	-
5	HEM	A	502	1	-	7/14/54/54	-
5	HEM	K	301	2	-	8/14/54/54	-
7	LOP	D	503	-	-	3/48/48/48	-
5	HEM	D	502	1	-	5/14/54/54	-
6	SMA	D	2	-	-	6/34/34/34	0/2/2/2
5	HEM	H	301	2	-	9/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	G	502	1	-	9/14/54/54	-
10	FES	R	200	3	-	-	0/1/1/1
8	ANJ	D	504	-	-	4/40/55/55	0/1/2/2
6	SMA	M	503	-	-	10/34/34/34	0/2/2/2
5	HEM	G	501	1	-	6/14/54/54	-
8	ANJ	J	505	-	-	4/40/55/55	0/1/2/2
10	FES	L	200	3	-	-	0/1/1/1
5	HEM	A	501	1	-	8/14/54/54	-
5	HEM	Q	301	2	-	10/14/54/54	-
4	BGL	Q	257	-	-	0/11/31/31	0/1/1/1
5	HEM	J	502	1	-	6/14/54/54	-
7	LOP	M	504	-	-	6/48/48/48	-
5	HEM	M	502	1	-	8/14/54/54	-
5	HEM	P	501	1	-	9/14/54/54	-
5	HEM	J	501	1	-	6/14/54/54	-
5	HEM	B	301	2	-	7/14/54/54	-
5	HEM	P	502	1	-	8/14/54/54	-
5	HEM	M	501	1	-	9/14/54/54	-
10	FES	F	200	3	-	-	0/1/1/1
5	HEM	N	301	2	-	7/14/54/54	-
4	BGL	A	431	-	-	0/11/31/31	0/1/1/1
8	ANJ	P	505	-	-	6/40/55/55	0/1/2/2
8	ANJ	G	505	-	-	5/40/55/55	0/1/2/2
10	FES	I	200	3	-	-	0/1/1/1
4	BGL	D	431	-	-	0/11/31/31	0/1/1/1
6	SMA	A	1	-	-	8/34/34/34	0/2/2/2
7	LOP	G	504	-	-	11/48/48/48	-
10	FES	C	200	3	-	-	0/1/1/1
8	ANJ	A	504	-	-	4/40/55/55	0/1/2/2
7	LOP	J	504	-	-	10/48/48/48	-
6	SMA	P	503	-	-	7/34/34/34	0/2/2/2

All (229) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	431	BGL	C1-C2	6.84	1.58	1.52
6	M	503	SMA	O7-C7	6.79	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2	SMA	O5-C5	6.62	1.47	1.37
6	P	503	SMA	O5-C5	6.34	1.47	1.37
4	M	431	BGL	C1-C2	6.13	1.57	1.52
6	D	2	SMA	O7-C7	5.93	1.46	1.37
4	A	431	BGL	C1-C2	5.79	1.57	1.52
6	M	503	SMA	O5-C5	5.71	1.46	1.37
6	A	1	SMA	O7-C7	5.68	1.46	1.37
6	J	503	SMA	O5-C5	5.55	1.46	1.37
4	J	431	BGL	C1-C2	5.41	1.57	1.52
6	J	503	SMA	O7-C7	5.34	1.45	1.37
5	G	502	HEM	CBB-CAB	5.11	1.54	1.30
5	D	502	HEM	CBB-CAB	5.04	1.54	1.30
5	M	502	HEM	CBB-CAB	5.00	1.54	1.30
6	G	503	SMA	O5-C5	5.00	1.45	1.37
4	Q	257	BGL	C1-C2	5.00	1.57	1.52
5	H	301	HEM	CBB-CAB	4.99	1.54	1.30
5	B	301	HEM	CBC-CAC	4.99	1.54	1.30
5	N	301	HEM	CBC-CAC	4.98	1.54	1.30
5	P	502	HEM	CBB-CAB	4.97	1.54	1.30
5	B	301	HEM	CBB-CAB	4.95	1.54	1.30
5	K	301	HEM	CBB-CAB	4.92	1.54	1.30
5	K	301	HEM	CBC-CAC	4.91	1.54	1.30
5	Q	301	HEM	CBB-CAB	4.85	1.53	1.30
6	A	1	SMA	O5-C5	4.85	1.45	1.37
5	M	501	HEM	CBC-CAC	4.82	1.53	1.30
5	E	301	HEM	CBB-CAB	4.81	1.53	1.30
6	P	503	SMA	O7-C7	4.80	1.45	1.37
4	D	431	BGL	C1-C2	4.79	1.56	1.52
5	N	301	HEM	CBB-CAB	4.75	1.53	1.30
5	D	502	HEM	CBC-CAC	4.74	1.53	1.30
5	Q	301	HEM	CBC-CAC	4.72	1.53	1.30
6	G	503	SMA	O7-C7	4.72	1.44	1.37
5	A	502	HEM	CBB-CAB	4.68	1.52	1.30
5	A	501	HEM	CBC-CAC	4.66	1.52	1.30
5	E	301	HEM	CBC-CAC	4.65	1.52	1.30
5	H	301	HEM	CBC-CAC	4.64	1.52	1.30
5	M	501	HEM	CBB-CAB	4.62	1.52	1.30
5	D	501	HEM	CBB-CAB	4.61	1.52	1.30
8	J	505	ANJ	C5-C6	4.60	1.46	1.39
5	D	501	HEM	CBC-CAC	4.59	1.52	1.30
8	A	504	ANJ	C5-C6	4.55	1.46	1.39
5	J	502	HEM	CBB-CAB	4.54	1.52	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	502	HEM	CBC-CAC	4.50	1.52	1.30
5	G	501	HEM	CBB-CAB	4.49	1.52	1.30
5	J	501	HEM	CBB-CAB	4.49	1.51	1.30
5	P	501	HEM	CBB-CAB	4.48	1.51	1.30
5	P	501	HEM	CBC-CAC	4.47	1.51	1.30
5	G	501	HEM	CBC-CAC	4.42	1.51	1.30
5	G	502	HEM	CBC-CAC	4.38	1.51	1.30
5	J	501	HEM	CBC-CAC	4.37	1.51	1.30
5	A	502	HEM	CBC-CAC	4.36	1.51	1.30
6	D	2	SMA	O1-C2	4.34	1.41	1.36
5	A	501	HEM	CBB-CAB	4.31	1.51	1.30
6	A	1	SMA	C20-C19	4.20	1.36	1.33
5	J	502	HEM	CBC-CAC	4.18	1.50	1.30
6	G	503	SMA	O1-C2	4.17	1.41	1.36
5	P	502	HEM	CBC-CAC	4.15	1.50	1.30
8	M	505	ANJ	C5-C6	4.04	1.46	1.39
6	D	2	SMA	C3-C4	-3.96	1.38	1.47
8	J	505	ANJ	O8-C14	3.95	1.50	1.44
8	G	505	ANJ	C13-C12	3.94	1.59	1.51
8	P	505	ANJ	C10-C9	3.90	1.62	1.53
6	M	503	SMA	O1-C2	3.86	1.41	1.36
6	A	1	SMA	O8-C8	3.83	1.45	1.36
6	M	503	SMA	C20-C19	3.78	1.36	1.33
6	G	503	SMA	O8-C8	3.78	1.45	1.36
5	J	502	HEM	CAB-C3B	-3.75	1.37	1.47
8	D	504	ANJ	C13-C12	3.66	1.58	1.51
5	A	502	HEM	C4D-ND	-3.66	1.33	1.40
8	G	505	ANJ	C5-C6	3.65	1.45	1.39
8	A	504	ANJ	O4-C10	3.65	1.52	1.46
8	M	505	ANJ	O4-C12	3.59	1.42	1.34
6	P	503	SMA	C7-C8	-3.55	1.35	1.40
6	G	503	SMA	C3-C4	-3.55	1.39	1.47
8	M	505	ANJ	C13-C12	3.53	1.58	1.51
8	A	504	ANJ	O4-C12	3.52	1.42	1.34
8	J	505	ANJ	C4-C3	3.52	1.44	1.38
6	J	503	SMA	O8-C8	3.51	1.44	1.36
8	P	505	ANJ	C5-C6	3.47	1.45	1.39
8	J	505	ANJ	C13-C12	3.42	1.58	1.51
8	P	505	ANJ	C4-C3	3.41	1.44	1.38
6	J	503	SMA	O1-C2	3.41	1.40	1.36
5	J	501	HEM	CAB-C3B	-3.41	1.38	1.47
6	A	1	SMA	C3-C4	-3.40	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2	SMA	O8-C8	3.39	1.44	1.36
6	A	1	SMA	O1-C2	3.38	1.40	1.36
6	M	503	SMA	O8-C8	3.36	1.44	1.36
8	D	504	ANJ	C5-C6	3.34	1.45	1.39
6	P	503	SMA	O8-C8	3.33	1.44	1.36
5	J	502	HEM	CAC-C3C	-3.31	1.38	1.47
6	P	503	SMA	C3-C4	-3.26	1.40	1.47
5	A	502	HEM	CAC-C3C	-3.24	1.38	1.47
8	J	505	ANJ	C2-N1	3.20	1.46	1.41
8	G	505	ANJ	C4-C3	3.19	1.44	1.38
5	J	501	HEM	FE-NB	3.18	2.04	1.94
5	P	502	HEM	CAC-C3C	-3.16	1.39	1.47
8	D	504	ANJ	O8-C14	3.15	1.49	1.44
8	P	505	ANJ	C26-C25	3.12	1.63	1.52
8	M	505	ANJ	C10-C9	3.12	1.60	1.53
5	H	301	HEM	CAC-C3C	-3.09	1.39	1.47
8	P	505	ANJ	C2-N1	3.06	1.45	1.41
6	G	503	SMA	C4A-C4	-3.05	1.38	1.46
5	G	502	HEM	CAB-C3B	-3.05	1.39	1.47
8	M	505	ANJ	C4-C3	3.05	1.44	1.38
6	J	503	SMA	C3-C4	-3.04	1.40	1.47
8	D	504	ANJ	O4-C12	3.04	1.41	1.34
8	D	504	ANJ	C1-N1	3.03	1.38	1.34
5	G	501	HEM	CAB-C3B	-3.02	1.39	1.47
5	K	301	HEM	CAB-C3B	-3.01	1.39	1.47
5	P	501	HEM	CAB-C3B	-2.99	1.39	1.47
8	M	505	ANJ	C2-N1	2.98	1.45	1.41
6	D	2	SMA	C4A-C4	-2.98	1.39	1.46
8	P	505	ANJ	C13-C12	2.97	1.57	1.51
5	A	502	HEM	CHA-C4D	-2.97	1.32	1.38
8	D	504	ANJ	C2-N1	2.95	1.45	1.41
6	P	503	SMA	C4A-C4	-2.95	1.39	1.46
8	P	505	ANJ	C6-C8	-2.94	1.44	1.50
8	M	505	ANJ	O8-C14	2.94	1.49	1.44
8	D	504	ANJ	C10-C9	2.94	1.60	1.53
8	A	504	ANJ	C13-C12	2.92	1.57	1.51
8	J	505	ANJ	C10-C9	2.91	1.60	1.53
5	M	502	HEM	CAB-C3B	-2.91	1.39	1.47
8	D	504	ANJ	C4-C3	2.91	1.43	1.38
8	G	505	ANJ	O4-C12	2.90	1.40	1.34
5	A	502	HEM	FE-ND	-2.88	1.86	1.94
8	J	505	ANJ	O4-C12	2.87	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	503	SMA	C4A-C4	-2.85	1.39	1.46
5	Q	301	HEM	CAC-C3C	-2.82	1.39	1.47
5	G	501	HEM	CAC-C3C	-2.82	1.39	1.47
5	E	301	HEM	CAC-C3C	-2.79	1.39	1.47
5	P	502	HEM	CAB-C3B	-2.79	1.39	1.47
5	A	501	HEM	CAB-C3B	-2.79	1.40	1.47
5	P	501	HEM	CAC-C3C	-2.78	1.40	1.47
8	A	504	ANJ	C26-C25	2.78	1.62	1.52
5	D	501	HEM	CAC-C3C	-2.77	1.40	1.47
8	J	505	ANJ	C6-C8	-2.77	1.44	1.50
8	A	504	ANJ	C4-C3	2.76	1.43	1.38
8	P	505	ANJ	C1-N1	2.75	1.38	1.34
8	M	505	ANJ	O4-C10	2.74	1.50	1.46
5	A	502	HEM	CAB-C3B	-2.73	1.40	1.47
6	D	2	SMA	C7-C8	-2.73	1.36	1.40
6	G	503	SMA	C6-C7	-2.72	1.34	1.38
5	G	502	HEM	CAC-C3C	-2.72	1.40	1.47
6	A	1	SMA	C4A-C4	-2.71	1.39	1.46
6	M	503	SMA	C3-C4	-2.69	1.41	1.47
5	D	501	HEM	C2A-C3A	-2.69	1.31	1.38
8	G	505	ANJ	C10-C9	2.67	1.59	1.53
8	A	504	ANJ	C2-C7	2.66	1.44	1.40
6	D	2	SMA	C3-C2	2.63	1.39	1.34
8	M	505	ANJ	C26-C25	2.62	1.61	1.52
5	D	501	HEM	CHA-C4D	-2.59	1.33	1.38
5	H	301	HEM	CAB-C3B	-2.58	1.40	1.47
5	J	502	HEM	CMA-C3A	2.56	1.56	1.50
5	B	301	HEM	CHA-C1A	-2.54	1.33	1.39
6	G	503	SMA	C20-C19	2.53	1.35	1.33
8	J	505	ANJ	O4-C10	2.52	1.50	1.46
8	D	504	ANJ	O7-C17	-2.51	1.14	1.21
5	Q	301	HEM	CAB-C3B	-2.48	1.40	1.47
5	P	502	HEM	C2A-C3A	-2.47	1.32	1.38
5	J	501	HEM	CAC-C3C	-2.46	1.40	1.47
6	D	2	SMA	O12-C12	2.45	1.48	1.42
8	J	505	ANJ	C26-C25	2.44	1.61	1.52
8	G	505	ANJ	O8-C14	2.43	1.48	1.44
6	P	503	SMA	C20-C19	2.43	1.35	1.33
5	E	301	HEM	CAB-C3B	-2.43	1.40	1.47
5	M	502	HEM	CAC-C3C	-2.42	1.40	1.47
6	P	503	SMA	O1-C2	2.41	1.39	1.36
5	G	502	HEM	CHA-C4D	-2.41	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	502	HEM	C2A-C3A	-2.41	1.32	1.38
8	P	505	ANJ	O8-C14	2.40	1.48	1.44
5	A	502	HEM	FE-NB	2.40	2.02	1.94
5	K	301	HEM	CAC-C3C	-2.38	1.41	1.47
5	P	501	HEM	CHA-C1A	-2.38	1.34	1.39
6	M	503	SMA	C4A-C4	-2.36	1.40	1.46
5	A	501	HEM	CAC-C3C	-2.35	1.41	1.47
8	A	504	ANJ	O7-C17	-2.34	1.15	1.21
5	N	301	HEM	CAC-C3C	-2.34	1.41	1.47
8	G	505	ANJ	C2-N1	2.33	1.44	1.41
8	G	505	ANJ	C26-C25	2.33	1.60	1.52
4	A	431	BGL	O5-C1	2.33	1.48	1.42
8	D	504	ANJ	C26-C25	2.31	1.60	1.52
8	J	505	ANJ	C1-N1	2.31	1.37	1.34
5	D	502	HEM	CMB-C2B	2.29	1.55	1.50
8	A	504	ANJ	C2-N1	2.29	1.44	1.41
5	B	301	HEM	CAC-C3C	-2.28	1.41	1.47
8	A	504	ANJ	C18-C13	2.27	1.58	1.54
5	G	502	HEM	CBD-CGD	2.27	1.55	1.50
5	H	301	HEM	C2A-C3A	-2.24	1.33	1.38
4	M	431	BGL	O2-C2	2.24	1.46	1.43
5	D	502	HEM	CAB-C3B	-2.23	1.41	1.47
5	G	502	HEM	CHA-C1A	-2.23	1.34	1.39
8	G	505	ANJ	C1-N1	2.23	1.37	1.34
8	P	505	ANJ	O4-C12	2.22	1.39	1.34
5	P	501	HEM	C2A-C3A	-2.22	1.33	1.38
5	M	502	HEM	C4D-ND	-2.21	1.36	1.40
4	Q	257	BGL	O5-C1	2.21	1.48	1.42
5	G	502	HEM	CHC-C4B	-2.20	1.34	1.39
6	J	503	SMA	C20-C19	2.20	1.35	1.33
8	D	504	ANJ	O4-C10	2.20	1.49	1.46
5	D	501	HEM	CAB-C3B	-2.18	1.41	1.47
5	B	301	HEM	CAB-C3B	-2.18	1.41	1.47
5	M	501	HEM	CAB-C3B	-2.16	1.41	1.47
5	J	502	HEM	CHC-C4B	-2.16	1.34	1.39
8	A	504	ANJ	C10-C9	2.15	1.58	1.53
8	P	505	ANJ	O3-C8	2.15	1.28	1.23
5	D	502	HEM	CAC-C3C	-2.15	1.41	1.47
5	P	502	HEM	C4D-ND	-2.15	1.36	1.40
5	M	501	HEM	FE-NB	2.14	2.01	1.94
6	D	2	SMA	O1-C8A	2.13	1.41	1.38
6	M	503	SMA	C3-C2	2.12	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	431	BGL	O2-C2	2.11	1.46	1.43
5	G	501	HEM	FE-NC	2.11	2.02	1.95
5	G	501	HEM	C4D-ND	-2.10	1.36	1.40
8	A	504	ANJ	C1-N1	2.10	1.37	1.34
5	M	502	HEM	CHA-C1A	-2.10	1.34	1.39
5	D	502	HEM	C1B-NB	-2.10	1.36	1.40
8	G	505	ANJ	C6-C8	-2.09	1.46	1.50
8	J	505	ANJ	C13-C14	2.09	1.57	1.53
7	J	504	LOP	O5-C6	2.07	1.40	1.34
5	M	501	HEM	C2A-C3A	-2.06	1.33	1.38
5	H	301	HEM	CHC-C4B	-2.05	1.34	1.39
5	P	501	HEM	CHA-C4D	-2.05	1.34	1.38
5	A	501	HEM	C1B-NB	-2.03	1.36	1.40
8	M	505	ANJ	C1-N1	2.02	1.37	1.34
5	D	501	HEM	C4D-ND	-2.01	1.36	1.40
5	M	501	HEM	CAC-C3C	-2.01	1.42	1.47
6	P	503	SMA	O1-C8A	2.01	1.41	1.38

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	503	SMA	O7-C7-C8	7.48	122.36	114.53
6	A	1	SMA	O7-C7-C8	6.65	121.49	114.53
6	M	503	SMA	O7-C7-C8	6.51	121.34	114.53
6	A	1	SMA	C5M-O5-C5	-6.46	108.04	117.51
6	D	2	SMA	O7-C7-C8	5.80	120.59	114.53
6	J	503	SMA	O7-C7-C8	5.69	120.48	114.53
8	G	505	ANJ	O6-C17-C9	-5.47	101.68	110.28
6	G	503	SMA	C5M-O5-C5	-5.46	109.51	117.51
6	M	503	SMA	C5M-O5-C5	-5.31	109.72	117.51
8	J	505	ANJ	O6-C17-C9	-5.23	102.05	110.28
6	J	503	SMA	C5M-O5-C5	-5.11	110.02	117.51
8	P	505	ANJ	O6-C17-C9	-5.10	102.26	110.28
6	G	503	SMA	O1-C2-C9	5.05	120.85	110.12
8	M	505	ANJ	O6-C17-C9	-4.98	102.44	110.28
6	P	503	SMA	O1-C2-C9	4.87	120.46	110.12
6	A	1	SMA	O1-C2-C9	4.82	120.35	110.12
8	D	504	ANJ	O6-C17-C9	-4.69	102.90	110.28
6	D	2	SMA	O1-C2-C9	4.63	119.95	110.12
8	A	504	ANJ	O6-C17-C9	-4.61	103.02	110.28
8	G	505	ANJ	O6-C17-O7	4.60	129.80	124.10
8	J	505	ANJ	O6-C17-O7	4.56	129.75	124.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	503	SMA	O1-C2-C9	4.44	119.55	110.12
8	M	505	ANJ	O6-C17-O7	4.42	129.58	124.10
6	J	503	SMA	C7M-O7-C7	-4.39	111.08	117.51
8	P	505	ANJ	O6-C17-O7	4.36	129.51	124.10
8	A	504	ANJ	O6-C17-O7	4.34	129.48	124.10
7	G	504	LOP	O5-C6-C7	4.32	120.83	111.48
6	M	503	SMA	O5-C5-C4A	4.26	121.88	115.84
8	D	504	ANJ	O6-C17-O7	4.22	129.33	124.10
6	G	503	SMA	C7M-O7-C7	-4.17	111.40	117.51
5	A	502	HEM	C3B-C4B-NB	4.17	112.46	109.47
7	J	504	LOP	O5-C6-C7	4.12	120.40	111.48
6	M	503	SMA	O1-C2-C9	4.12	118.86	110.12
5	D	501	HEM	C3B-C4B-NB	4.11	112.42	109.47
5	G	502	HEM	C3B-C4B-NB	4.04	112.37	109.47
6	A	1	SMA	C7M-O7-C7	-4.03	111.60	117.51
6	G	503	SMA	O7-C7-C6	-4.00	117.19	124.08
6	J	503	SMA	O5-C5-C4A	3.97	121.47	115.84
6	A	1	SMA	O5-C5-C4A	3.84	121.28	115.84
6	D	2	SMA	C7M-O7-C7	-3.83	111.89	117.51
5	H	301	HEM	C3B-C4B-NB	3.82	112.21	109.47
5	P	502	HEM	C3B-C4B-NB	3.79	112.19	109.47
5	J	502	HEM	CBC-CAC-C3C	-3.79	108.58	127.53
5	P	502	HEM	CBC-CAC-C3C	-3.76	108.73	127.53
5	J	502	HEM	C3B-C4B-NB	3.72	112.14	109.47
6	P	503	SMA	O7-C7-C8	3.72	118.42	114.53
8	A	504	ANJ	C5-C6-C7	-3.69	115.18	118.76
5	A	502	HEM	CBC-CAC-C3C	-3.69	109.10	127.53
6	G	503	SMA	O5-C5-C4A	3.68	121.05	115.84
5	J	502	HEM	CBB-CAB-C3B	-3.67	109.18	127.53
6	A	1	SMA	C16-C17-C18	-3.66	115.99	124.65
7	D	503	LOP	C19-C18-C17	-3.66	95.87	114.37
5	J	501	HEM	CBB-CAB-C3B	-3.64	109.33	127.53
5	P	501	HEM	CBB-CAB-C3B	-3.62	109.42	127.53
5	N	301	HEM	C3B-C4B-NB	3.60	112.06	109.47
5	G	501	HEM	CBB-CAB-C3B	-3.60	109.53	127.53
7	M	504	LOP	C12-C11-C10	-3.59	96.22	114.37
5	A	501	HEM	CBB-CAB-C3B	-3.58	109.64	127.53
5	D	502	HEM	C3B-C4B-NB	3.57	112.03	109.47
5	H	301	HEM	CBC-CAC-C3C	-3.55	109.79	127.53
5	K	301	HEM	CBB-CAB-C3B	-3.55	109.81	127.53
5	D	501	HEM	CBC-CAC-C3C	-3.53	109.87	127.53
5	E	301	HEM	CBB-CAB-C3B	-3.52	109.92	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	501	HEM	C3B-C4B-NB	3.52	112.00	109.47
5	G	502	HEM	CBC-CAC-C3C	-3.52	109.96	127.53
5	M	501	HEM	C3B-C4B-NB	3.51	111.99	109.47
5	G	501	HEM	CBC-CAC-C3C	-3.51	110.01	127.53
6	P	503	SMA	C7M-O7-C7	-3.50	112.38	117.51
5	M	502	HEM	CBB-CAB-C3B	-3.49	110.08	127.53
8	M	505	ANJ	C5-C6-C7	-3.48	115.39	118.76
5	H	301	HEM	CBB-CAB-C3B	-3.46	110.22	127.53
5	M	501	HEM	CBB-CAB-C3B	-3.45	110.29	127.53
6	A	1	SMA	O7-C7-C6	-3.45	118.14	124.08
5	Q	301	HEM	CBB-CAB-C3B	-3.44	110.34	127.53
5	P	501	HEM	CBC-CAC-C3C	-3.44	110.35	127.53
5	K	301	HEM	CBC-CAC-C3C	-3.43	110.36	127.53
5	B	301	HEM	C3B-C4B-NB	3.43	111.93	109.47
5	P	502	HEM	CBB-CAB-C3B	-3.42	110.46	127.53
5	G	502	HEM	CBB-CAB-C3B	-3.39	110.61	127.53
8	D	504	ANJ	C5-C6-C7	-3.38	115.48	118.76
5	D	501	HEM	CBB-CAB-C3B	-3.37	110.70	127.53
5	N	301	HEM	CBC-CAC-C3C	-3.36	110.73	127.53
8	M	505	ANJ	C19-C18-C13	-3.35	108.37	114.28
5	J	501	HEM	CBC-CAC-C3C	-3.35	110.81	127.53
5	M	501	HEM	CBC-CAC-C3C	-3.34	110.84	127.53
5	N	301	HEM	CBB-CAB-C3B	-3.34	110.84	127.53
6	D	2	SMA	O1-C2-C3	-3.34	118.88	121.81
5	A	502	HEM	CBB-CAB-C3B	-3.33	110.88	127.53
7	A	503	LOP	C19-C18-C17	-3.33	97.53	114.37
5	E	301	HEM	CBC-CAC-C3C	-3.33	110.89	127.53
5	A	501	HEM	CBC-CAC-C3C	-3.32	110.94	127.53
5	B	301	HEM	CBB-CAB-C3B	-3.32	110.95	127.53
5	G	501	HEM	C3B-C4B-NB	3.30	111.84	109.47
5	Q	301	HEM	CBC-CAC-C3C	-3.29	111.07	127.53
5	D	502	HEM	CBB-CAB-C3B	-3.29	111.09	127.53
5	B	301	HEM	CBC-CAC-C3C	-3.28	111.12	127.53
5	M	502	HEM	CBC-CAC-C3C	-3.28	111.14	127.53
6	D	2	SMA	O5-C5-C4A	3.27	120.47	115.84
8	G	505	ANJ	C5-C6-C7	-3.27	115.59	118.76
5	A	501	HEM	C3B-C4B-NB	3.26	111.81	109.47
4	D	431	BGL	C1'-O2-C2	-3.20	106.91	114.02
7	P	504	LOP	C19-C18-C17	-3.19	98.27	114.37
6	M	503	SMA	C7M-O7-C7	-3.17	112.86	117.51
5	D	502	HEM	CBC-CAC-C3C	-3.13	111.89	127.53
5	M	502	HEM	C3B-C4B-NB	3.11	111.70	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	503	SMA	O5-C5-C4A	3.08	120.20	115.84
6	M	503	SMA	O5-C5-C6	-3.08	118.78	124.08
5	K	301	HEM	C3B-C4B-NB	3.06	111.67	109.47
5	Q	301	HEM	C3B-C4B-NB	3.02	111.64	109.47
6	P	503	SMA	O1-C2-C3	-3.01	119.17	121.81
6	G	503	SMA	O5-C5-C6	-3.00	118.91	124.08
7	A	503	LOP	O5-C6-C7	3.00	117.96	111.48
7	M	504	LOP	O5-C6-C7	2.97	117.91	111.48
6	D	2	SMA	C17-C18-C19	-2.96	118.25	126.36
7	D	503	LOP	O6-C24-C25	2.93	120.77	111.83
4	D	431	BGL	C3'-C2'-C1'	-2.91	100.84	113.47
4	Q	257	BGL	C1'-O2-C2	-2.89	107.60	114.02
8	P	505	ANJ	C5-C6-C7	-2.87	115.98	118.76
6	A	1	SMA	C9-C10-C11	-2.86	109.11	114.46
7	P	504	LOP	C9-C8-C7	-2.85	102.66	113.13
4	A	431	BGL	C1'-O2-C2	-2.85	107.70	114.02
5	J	501	HEM	C3B-C4B-NB	2.84	111.51	109.47
6	M	503	SMA	O7-C7-C6	-2.84	119.19	124.08
7	D	503	LOP	O5-C6-C7	2.83	117.61	111.48
6	A	1	SMA	O5-C5-C6	-2.82	119.21	124.08
6	J	503	SMA	O5-C5-C6	-2.82	119.22	124.08
8	J	505	ANJ	C5-C6-C7	-2.81	116.04	118.76
6	D	2	SMA	C5M-O5-C5	-2.80	113.40	117.51
8	A	504	ANJ	C3-C2-C7	2.80	121.56	119.75
6	J	503	SMA	O7-C7-C6	-2.76	119.32	124.08
8	G	505	ANJ	C3-C2-C7	2.76	121.53	119.75
8	A	504	ANJ	O3-C8-N2	-2.75	117.24	122.47
7	M	504	LOP	C10-C9-C8	-2.75	100.49	114.37
7	P	504	LOP	O5-C6-C7	2.71	117.34	111.48
6	G	503	SMA	O1-C2-C3	-2.69	119.44	121.81
6	D	2	SMA	O7-C7-C6	-2.67	119.47	124.08
8	A	504	ANJ	C6-C8-N2	2.67	122.45	116.67
8	G	505	ANJ	O3-C8-N2	-2.67	117.40	122.47
5	E	301	HEM	C3B-C4B-NB	2.66	111.38	109.47
6	M	503	SMA	C16-C17-C18	-2.65	118.38	124.65
6	D	2	SMA	C9-C10-C11	-2.62	109.56	114.46
7	A	503	LOP	C31-C30-C29	-2.60	101.22	114.37
8	G	505	ANJ	C19-C18-C13	-2.59	109.72	114.28
7	P	504	LOP	O6-C24-C25	2.57	119.69	111.83
7	A	503	LOP	C21-C20-C19	-2.57	101.39	114.37
8	D	504	ANJ	C3-C2-C7	2.56	121.41	119.75
8	M	505	ANJ	C3-C2-C7	2.54	121.40	119.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	505	ANJ	C6-C8-N2	2.50	122.10	116.67
6	G	503	SMA	O1-C8A-C8	2.49	121.20	116.28
8	G	505	ANJ	C6-C8-N2	2.48	122.05	116.67
7	D	503	LOP	C21-C20-C19	-2.48	101.84	114.37
6	M	503	SMA	O1-C2-C3	-2.47	119.64	121.81
7	G	504	LOP	C31-C30-C29	-2.46	101.95	114.37
6	D	2	SMA	C13-C14-C15	2.45	117.42	112.11
7	M	504	LOP	O6-C24-C25	2.44	119.29	111.83
6	P	503	SMA	C3M-C3-C2	-2.44	119.65	123.28
4	A	431	BGL	C3'-C2'-C1'	-2.43	102.89	113.47
6	A	1	SMA	O1-C2-C3	-2.41	119.69	121.81
6	A	1	SMA	O1-C8A-C8	2.41	121.06	116.28
4	J	431	BGL	C3'-C2'-C1'	-2.39	103.08	113.47
6	A	1	SMA	C26-C19-C18	2.38	121.72	118.09
6	P	503	SMA	C5M-O5-C5	-2.33	114.10	117.51
5	G	502	HEM	C3D-C4D-ND	2.32	112.72	110.17
8	D	504	ANJ	O3-C8-N2	-2.32	118.05	122.47
7	G	504	LOP	O6-C24-C25	2.32	118.90	111.83
8	M	505	ANJ	O3-C8-N2	-2.29	118.11	122.47
8	J	505	ANJ	O3-C8-N2	-2.28	118.14	122.47
6	J	503	SMA	O1-C2-C3	-2.23	119.86	121.81
6	G	503	SMA	C11-C12-C13	-2.22	108.37	114.29
7	A	503	LOP	C29-C28-C27	-2.21	103.21	114.37
5	A	502	HEM	C3D-C4D-ND	2.20	112.58	110.17
4	J	431	BGL	C1'-O2-C2	-2.19	109.15	114.02
7	D	503	LOP	P1-O1-C2	-2.19	110.83	121.26
8	P	505	ANJ	C3-C2-C7	2.19	121.17	119.75
8	G	505	ANJ	O1-C1-N1	2.18	128.71	125.72
5	M	502	HEM	C3D-C4D-ND	2.17	112.55	110.17
6	J	503	SMA	C3M-C3-C2	-2.16	120.07	123.28
6	M	503	SMA	C14-C15-C16	-2.16	121.50	125.88
8	D	504	ANJ	C6-C8-N2	2.16	121.35	116.67
7	J	504	LOP	C19-C18-C17	-2.15	103.50	114.37
6	D	2	SMA	C4A-C4-C3	2.15	121.94	118.78
5	H	301	HEM	O1A-CGA-CBA	-2.14	116.31	123.09
7	M	504	LOP	C29-C28-C27	-2.14	103.56	114.37
6	G	503	SMA	C17-C18-C19	-2.13	120.51	126.36
8	D	504	ANJ	C14-O8-C24	2.13	121.30	117.76
6	J	503	SMA	C17-C16-C15	-2.12	110.12	124.25
5	D	502	HEM	C2B-C1B-NB	2.12	112.28	109.84
6	D	2	SMA	O1-C8A-C8	2.11	120.47	116.28
8	M	505	ANJ	O1-C1-N1	2.11	128.61	125.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	505	ANJ	C14-O8-C24	2.10	121.26	117.76
6	M	503	SMA	C26-C19-C18	2.10	121.29	118.09
8	M	505	ANJ	C6-C8-N2	2.09	121.20	116.67
6	J	503	SMA	C17-C18-C19	-2.09	120.64	126.36
8	A	504	ANJ	O1-C1-N1	2.08	128.57	125.72
5	H	301	HEM	CAD-C3D-C4D	2.08	128.32	124.70
5	K	301	HEM	O1A-CGA-CBA	-2.08	116.51	123.09
8	J	505	ANJ	C3-C2-C7	2.07	121.09	119.75
4	A	431	BGL	C5'-C4'-C3'	-2.05	103.98	114.37
7	G	504	LOP	C12-C13-C14	-2.05	101.12	112.60
4	J	431	BGL	C5'-C4'-C3'	-2.04	104.06	114.37
8	P	505	ANJ	O1-C1-N1	2.04	128.51	125.72
8	P	505	ANJ	O3-C8-N2	-2.04	118.59	122.47
7	M	504	LOP	P1-O1-C2	-2.03	111.57	121.26
6	G	503	SMA	C24-C13-C12	-2.03	107.82	111.40
7	P	504	LOP	C21-C20-C19	-2.03	104.13	114.37
7	A	503	LOP	P1-O2-C3	-2.02	109.76	121.35
8	A	504	ANJ	C4-C5-C6	2.02	123.45	119.80
6	D	2	SMA	C22-C11-C12	-2.02	107.85	111.14
5	E	301	HEM	C2B-C1B-NB	2.02	112.16	109.84
8	D	504	ANJ	O1-C1-N1	2.01	128.47	125.72
6	M	503	SMA	C23-O12-C12	-2.01	109.32	114.47
5	Q	301	HEM	C2B-C1B-NB	2.01	112.14	109.84

There are no chirality outliers.

All (253) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	HEM	C2B-C3B-CAB-CBB
5	A	501	HEM	C2C-C3C-CAC-CBC
5	A	501	HEM	C4C-C3C-CAC-CBC
5	A	502	HEM	C2C-C3C-CAC-CBC
5	B	301	HEM	C2B-C3B-CAB-CBB
5	D	501	HEM	C2C-C3C-CAC-CBC
5	D	501	HEM	C4C-C3C-CAC-CBC
5	E	301	HEM	C2B-C3B-CAB-CBB
5	E	301	HEM	C2C-C3C-CAC-CBC
5	G	501	HEM	C2B-C3B-CAB-CBB
5	G	501	HEM	C2C-C3C-CAC-CBC
5	G	501	HEM	C4C-C3C-CAC-CBC
5	G	502	HEM	C2C-C3C-CAC-CBC
5	G	502	HEM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
5	H	301	HEM	C2B-C3B-CAB-CBB
5	J	501	HEM	C2B-C3B-CAB-CBB
5	J	501	HEM	C4B-C3B-CAB-CBB
5	J	501	HEM	C2C-C3C-CAC-CBC
5	J	501	HEM	C4C-C3C-CAC-CBC
5	J	502	HEM	C2B-C3B-CAB-CBB
5	J	502	HEM	C2C-C3C-CAC-CBC
5	M	501	HEM	C2B-C3B-CAB-CBB
5	M	501	HEM	C2C-C3C-CAC-CBC
5	M	501	HEM	C4C-C3C-CAC-CBC
5	N	301	HEM	C2B-C3B-CAB-CBB
5	N	301	HEM	C2C-C3C-CAC-CBC
5	P	501	HEM	C2B-C3B-CAB-CBB
5	P	501	HEM	C2C-C3C-CAC-CBC
5	P	501	HEM	C4C-C3C-CAC-CBC
5	P	502	HEM	C2C-C3C-CAC-CBC
5	P	502	HEM	C4C-C3C-CAC-CBC
6	J	503	SMA	C11-C10-C9-C2
6	M	503	SMA	O14-C14-C15-C16
7	A	503	LOP	C2-O1-P1-O2
7	G	504	LOP	C2-O1-P1-O2
7	G	504	LOP	C2-O1-P1-O3
7	G	504	LOP	C2-O1-P1-O4
7	G	504	LOP	O5-C4-C5-O6
7	J	504	LOP	C2-O1-P1-O2
7	J	504	LOP	C2-O1-P1-O4
7	P	504	LOP	C2-O1-P1-O4
8	A	504	ANJ	C16-C15-O6-C17
8	A	504	ANJ	O8-C24-C25-C27
8	A	504	ANJ	O9-C24-C25-C27
8	D	504	ANJ	C16-C15-O6-C17
8	G	505	ANJ	C16-C15-O6-C17
8	J	505	ANJ	C16-C15-O6-C17
8	M	505	ANJ	C16-C15-O6-C17
8	P	505	ANJ	C16-C15-O6-C17
6	J	503	SMA	C9-C10-C11-C22
6	G	503	SMA	C9-C10-C11-C22
6	P	503	SMA	C9-C10-C11-C22
6	G	503	SMA	C8-C7-O7-C7M
6	A	1	SMA	C8-C7-O7-C7M
6	J	503	SMA	C8-C7-O7-C7M
6	M	503	SMA	C8-C7-O7-C7M

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Mol	Chain	Res	Type	Atoms
6	P	503	SMA	C8-C7-O7-C7M
5	P	502	HEM	C2A-CAA-CBA-CGA
6	M	503	SMA	C9-C10-C11-C22
6	D	2	SMA	C9-C10-C11-C22
6	J	503	SMA	C6-C7-O7-C7M
6	M	503	SMA	C6-C5-O5-C5M
6	M	503	SMA	C6-C7-O7-C7M
6	G	503	SMA	C6-C5-O5-C5M
6	D	2	SMA	C6-C7-O7-C7M
6	J	503	SMA	C6-C5-O5-C5M
6	A	1	SMA	C6-C5-O5-C5M
6	A	1	SMA	C6-C7-O7-C7M
6	G	503	SMA	C6-C7-O7-C7M
6	P	503	SMA	C6-C7-O7-C7M
6	M	503	SMA	C11-C10-C9-C2
5	B	301	HEM	C3D-CAD-CBD-CGD
5	M	501	HEM	C2A-CAA-CBA-CGA
5	N	301	HEM	C3D-CAD-CBD-CGD
6	D	2	SMA	C8-C7-O7-C7M
6	A	1	SMA	C9-C10-C11-C22
6	A	1	SMA	C4A-C5-O5-C5M
6	J	503	SMA	C4A-C5-O5-C5M
6	M	503	SMA	C4A-C5-O5-C5M
6	G	503	SMA	C4A-C5-O5-C5M
5	M	501	HEM	C1A-C2A-CAA-CBA
8	D	504	ANJ	C24-C25-C27-C28
8	G	505	ANJ	C24-C25-C27-C28
8	J	505	ANJ	C24-C25-C27-C28
8	P	505	ANJ	C24-C25-C27-C28
8	G	505	ANJ	C26-C25-C27-C28
8	P	505	ANJ	C26-C25-C27-C28
6	G	503	SMA	C11-C10-C9-C2
6	P	503	SMA	C11-C10-C9-C2
5	P	501	HEM	C2A-CAA-CBA-CGA
8	P	505	ANJ	O8-C24-C25-C26
5	B	301	HEM	C2C-C3C-CAC-CBC
5	D	501	HEM	C2B-C3B-CAB-CBB
5	M	502	HEM	C2C-C3C-CAC-CBC
5	B	301	HEM	C4B-C3B-CAB-CBB
5	G	501	HEM	C4B-C3B-CAB-CBB
5	J	502	HEM	C4B-C3B-CAB-CBB
5	J	502	HEM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
5	M	501	HEM	C4B-C3B-CAB-CBB
5	P	501	HEM	C4B-C3B-CAB-CBB
8	D	504	ANJ	C26-C25-C27-C28
8	J	505	ANJ	C26-C25-C27-C28
6	P	503	SMA	C9-C10-C11-C12
5	Q	301	HEM	C4D-C3D-CAD-CBD
7	G	504	LOP	C3-C4-C5-O6
6	A	1	SMA	C11-C10-C9-C2
5	P	501	HEM	C1A-C2A-CAA-CBA
7	A	503	LOP	O2-C3-C4-C5
7	A	503	LOP	O2-C3-C4-O5
7	J	504	LOP	O5-C4-C5-O6
8	P	505	ANJ	O9-C24-C25-C26
5	A	502	HEM	C2B-C3B-CAB-CBB
5	H	301	HEM	C2C-C3C-CAC-CBC
5	K	301	HEM	C2B-C3B-CAB-CBB
5	K	301	HEM	C2C-C3C-CAC-CBC
5	Q	301	HEM	C2B-C3B-CAB-CBB
5	Q	301	HEM	C2C-C3C-CAC-CBC
6	A	1	SMA	C15-C14-O14-C25
6	M	503	SMA	C15-C14-O14-C25
6	P	503	SMA	C15-C14-O14-C25
5	A	502	HEM	C4C-C3C-CAC-CBC
5	N	301	HEM	C4B-C3B-CAB-CBB
6	J	503	SMA	C24-C13-C14-C15
6	J	503	SMA	C24-C13-C14-O14
6	D	2	SMA	C13-C14-C15-C16
6	M	503	SMA	C13-C14-C15-C16
7	J	504	LOP	O2-C3-C4-C5
6	D	2	SMA	O14-C14-C15-C16
7	A	503	LOP	C2-O1-P1-O4
7	M	504	LOP	C3-O2-P1-O4
5	G	502	HEM	C3D-CAD-CBD-CGD
7	G	504	LOP	O5-C6-C7-C8
7	M	504	LOP	C12-C13-C14-C15
7	M	504	LOP	O2-C3-C4-O5
7	D	503	LOP	O6-C24-C25-C26
6	D	2	SMA	C11-C10-C9-C2
5	G	502	HEM	C2B-C3B-CAB-CBB
7	G	504	LOP	O2-C3-C4-O5
7	A	503	LOP	C14-C15-C16-C17
7	M	504	LOP	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
5	A	501	HEM	C4B-C3B-CAB-CBB
5	E	301	HEM	C4B-C3B-CAB-CBB
5	E	301	HEM	C4C-C3C-CAC-CBC
5	H	301	HEM	C4B-C3B-CAB-CBB
5	K	301	HEM	C4C-C3C-CAC-CBC
5	N	301	HEM	C4C-C3C-CAC-CBC
5	Q	301	HEM	C4B-C3B-CAB-CBB
7	A	503	LOP	O5-C4-C5-O6
5	P	502	HEM	CAA-CBA-CGA-O1A
5	P	502	HEM	CAD-CBD-CGD-O2D
5	G	501	HEM	CAA-CBA-CGA-O1A
5	P	502	HEM	CAD-CBD-CGD-O1D
5	G	501	HEM	CAA-CBA-CGA-O2A
5	D	502	HEM	CAA-CBA-CGA-O1A
6	M	503	SMA	C13-C14-O14-C25
7	J	504	LOP	C3-C4-O5-C6
5	K	301	HEM	CAA-CBA-CGA-O2A
5	A	501	HEM	CAA-CBA-CGA-O2A
5	A	502	HEM	CAA-CBA-CGA-O1A
5	A	502	HEM	CAD-CBD-CGD-O1D
5	P	502	HEM	CAA-CBA-CGA-O2A
7	G	504	LOP	C14-C15-C16-C17
5	A	501	HEM	CAA-CBA-CGA-O1A
7	G	504	LOP	O2-C3-C4-C5
5	A	502	HEM	CAA-CBA-CGA-O2A
5	D	502	HEM	CAA-CBA-CGA-O2A
5	M	502	HEM	CAA-CBA-CGA-O2A
7	D	503	LOP	C14-C15-C16-C17
5	A	502	HEM	CAD-CBD-CGD-O2D
5	G	502	HEM	CAD-CBD-CGD-O2D
5	M	502	HEM	CAA-CBA-CGA-O1A
5	K	301	HEM	CAD-CBD-CGD-O2D
5	Q	301	HEM	C2D-C3D-CAD-CBD
5	K	301	HEM	CAA-CBA-CGA-O1A
5	E	301	HEM	CAA-CBA-CGA-O2A
7	P	504	LOP	O2-C3-C4-O5
5	H	301	HEM	CAA-CBA-CGA-O2A
5	N	301	HEM	CAA-CBA-CGA-O2A
7	D	503	LOP	C12-C13-C14-C15
7	G	504	LOP	C12-C13-C14-C15
7	J	504	LOP	C14-C15-C16-C17
7	P	504	LOP	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
5	G	502	HEM	CAD-CBD-CGD-O1D
5	J	501	HEM	CAA-CBA-CGA-O2A
7	M	504	LOP	O2-C3-C4-C5
7	G	504	LOP	O7-C6-C7-C8
5	H	301	HEM	CAD-CBD-CGD-O2D
5	M	502	HEM	CAD-CBD-CGD-O1D
5	P	501	HEM	CAA-CBA-CGA-O2A
5	Q	301	HEM	CAA-CBA-CGA-O2A
5	Q	301	HEM	CAA-CBA-CGA-O1A
5	E	301	HEM	CAA-CBA-CGA-O1A
5	M	502	HEM	CAD-CBD-CGD-O2D
5	D	502	HEM	C2C-C3C-CAC-CBC
5	M	502	HEM	C2B-C3B-CAB-CBB
5	G	502	HEM	CAA-CBA-CGA-O1A
7	A	503	LOP	C12-C13-C14-C15
5	G	502	HEM	CAA-CBA-CGA-O2A
5	K	301	HEM	CAD-CBD-CGD-O1D
5	J	501	HEM	CAA-CBA-CGA-O1A
5	N	301	HEM	CAA-CBA-CGA-O1A
8	A	504	ANJ	C14-C15-O6-C17
8	D	504	ANJ	C14-C15-O6-C17
8	G	505	ANJ	C14-C15-O6-C17
8	J	505	ANJ	C14-C15-O6-C17
8	M	505	ANJ	C14-C15-O6-C17
8	P	505	ANJ	C14-C15-O6-C17
7	J	504	LOP	C3-C4-C5-O6
5	B	301	HEM	C4C-C3C-CAC-CBC
5	D	501	HEM	C4B-C3B-CAB-CBB
5	G	502	HEM	C4B-C3B-CAB-CBB
5	H	301	HEM	C4C-C3C-CAC-CBC
5	K	301	HEM	C4B-C3B-CAB-CBB
5	M	502	HEM	C4B-C3B-CAB-CBB
5	M	502	HEM	C4C-C3C-CAC-CBC
5	Q	301	HEM	C4C-C3C-CAC-CBC
5	D	502	HEM	CAD-CBD-CGD-O1D
5	H	301	HEM	CAA-CBA-CGA-O1A
7	P	504	LOP	C12-C13-C14-C15
5	H	301	HEM	CAD-CBD-CGD-O1D
5	J	502	HEM	CAA-CBA-CGA-O1A
5	J	502	HEM	CAA-CBA-CGA-O2A
5	D	501	HEM	CAA-CBA-CGA-O1A
5	P	501	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
5	D	501	HEM	CAA-CBA-CGA-O2A
5	A	501	HEM	CAD-CBD-CGD-O2D
7	J	504	LOP	C12-C13-C14-C15
7	A	503	LOP	O5-C6-C7-C8
6	G	503	SMA	C13-C14-C15-C16
5	M	501	HEM	CAD-CBD-CGD-O2D
6	J	503	SMA	C12-C13-C14-O14
5	B	301	HEM	CAA-CBA-CGA-O2A
7	J	504	LOP	O5-C6-C7-C8
6	A	1	SMA	C13-C14-O14-C25
6	P	503	SMA	C13-C14-O14-C25
8	M	505	ANJ	O9-C24-C25-C27
5	M	501	HEM	C3A-C2A-CAA-CBA
7	A	503	LOP	O6-C24-C25-C26
5	H	301	HEM	C4D-C3D-CAD-CBD
8	G	505	ANJ	C12-C13-C18-C19
5	Q	301	HEM	CAD-CBD-CGD-O2D
5	D	502	HEM	CAD-CBD-CGD-O2D
5	M	501	HEM	CAD-CBD-CGD-O1D
5	A	501	HEM	CAD-CBD-CGD-O1D
7	A	503	LOP	O7-C6-C7-C8
5	B	301	HEM	CAA-CBA-CGA-O1A
5	P	501	HEM	CAD-CBD-CGD-O2D
7	M	504	LOP	O6-C24-C25-C26
7	J	504	LOP	O7-C6-C7-C8
7	A	503	LOP	O8-C24-C25-C26
5	P	502	HEM	C2B-C3B-CAB-CBB
6	G	503	SMA	O14-C14-C15-C16
5	Q	301	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

45 monomers are involved in 199 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	O	200	FES	2	0
5	E	301	HEM	2	0
4	G	431	BGL	2	0
4	M	431	BGL	2	0
7	P	504	LOP	3	0
8	M	505	ANJ	6	0
6	G	503	SMA	8	0
6	J	503	SMA	4	0

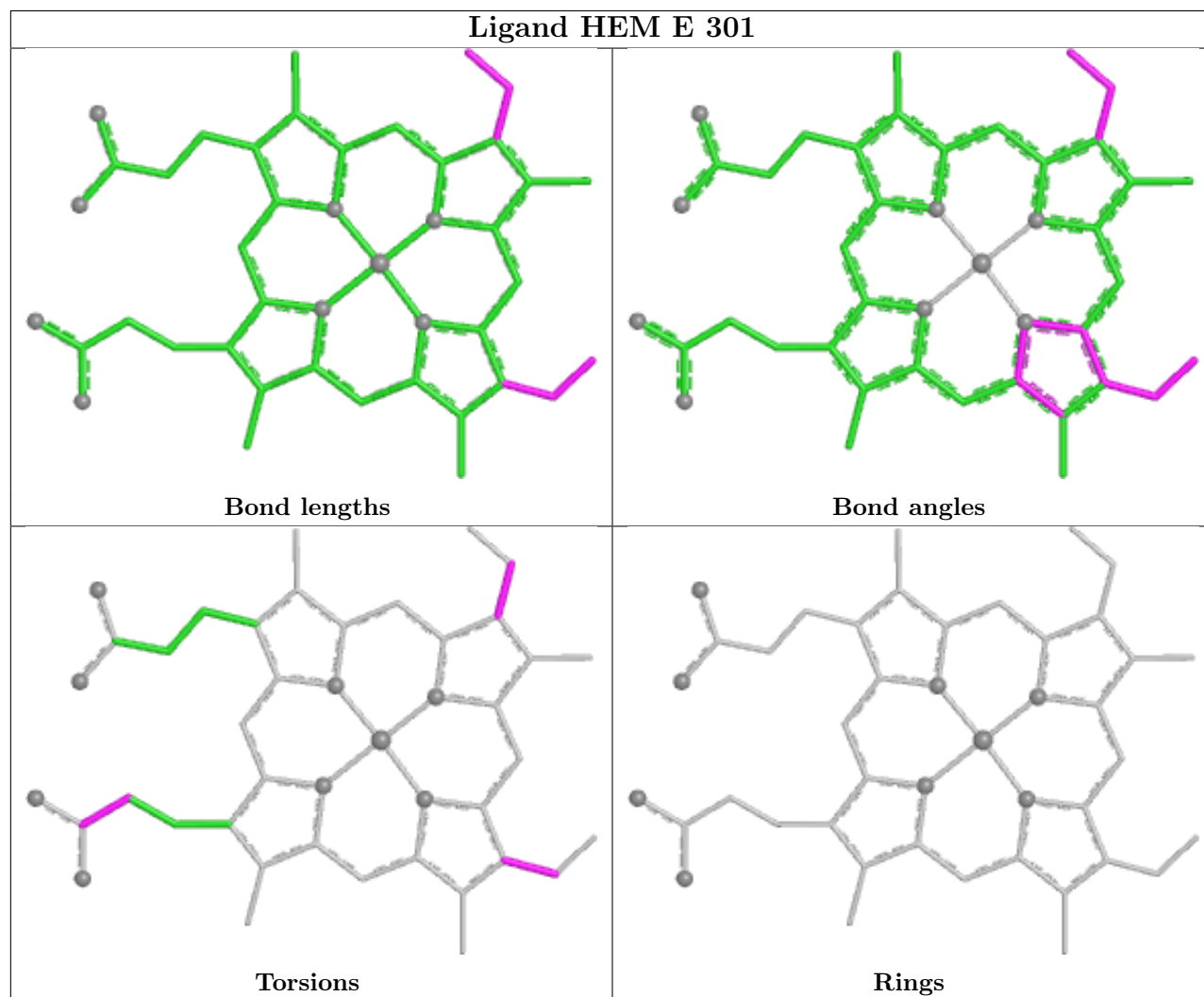
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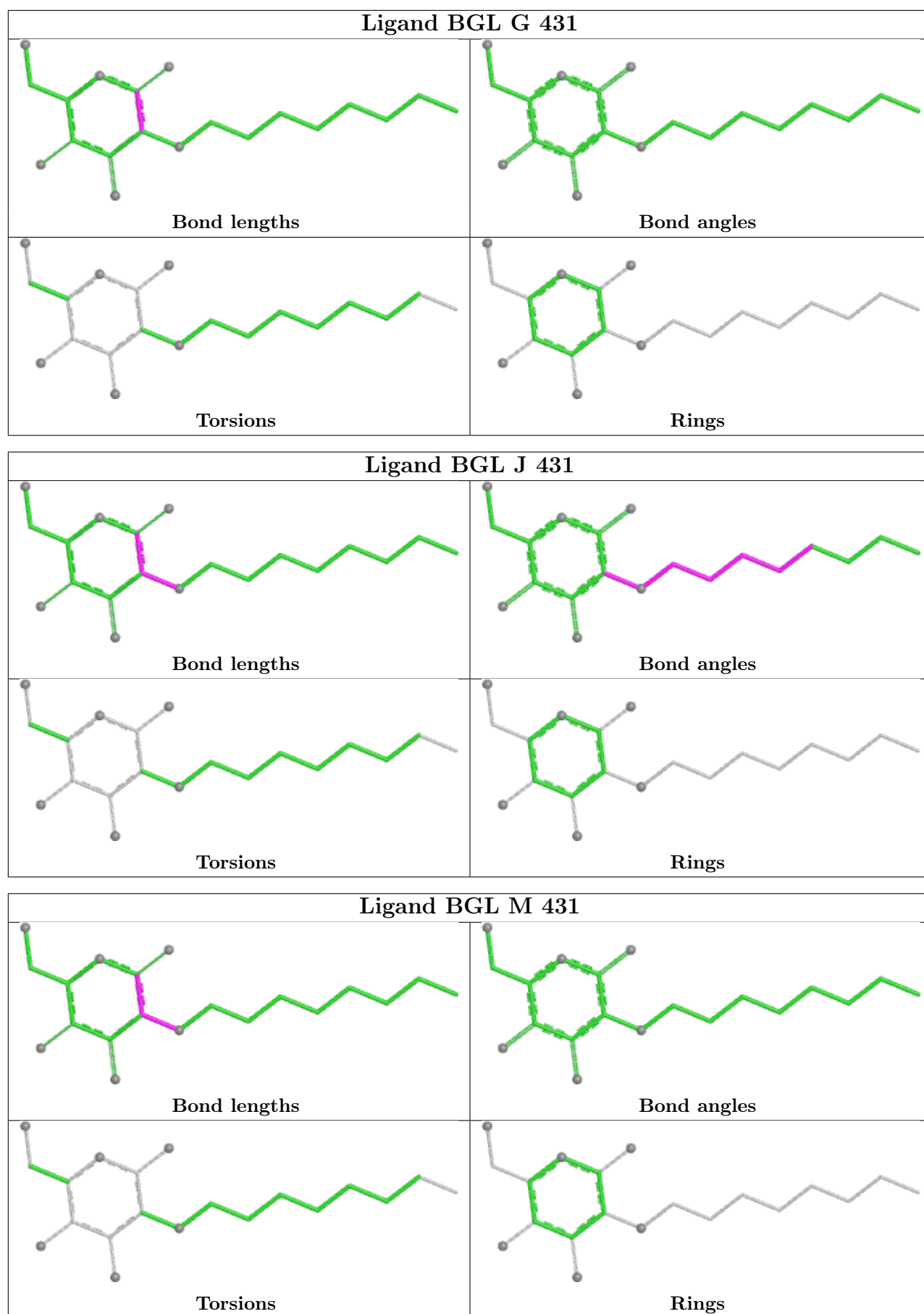
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	501	HEM	6	0
7	A	503	LOP	5	0
5	A	502	HEM	1	0
5	K	301	HEM	2	0
7	D	503	LOP	4	0
5	D	502	HEM	8	0
6	D	2	SMA	3	0
5	H	301	HEM	1	0
5	G	502	HEM	4	0
10	R	200	FES	3	0
8	D	504	ANJ	7	0
6	M	503	SMA	4	0
5	G	501	HEM	8	0
8	J	505	ANJ	7	0
10	L	200	FES	2	0
5	A	501	HEM	7	0
5	Q	301	HEM	1	0
5	J	502	HEM	5	0
7	M	504	LOP	7	0
5	M	502	HEM	1	0
5	P	501	HEM	11	0
5	J	501	HEM	7	0
5	B	301	HEM	6	0
5	P	502	HEM	6	0
5	M	501	HEM	5	0
10	F	200	FES	2	0
4	A	431	BGL	1	0
8	P	505	ANJ	7	0
8	G	505	ANJ	7	0
10	I	200	FES	2	0
4	D	431	BGL	2	0
6	A	1	SMA	7	0
7	G	504	LOP	4	0
10	C	200	FES	2	0
8	A	504	ANJ	7	0
7	J	504	LOP	3	0
6	P	503	SMA	5	0

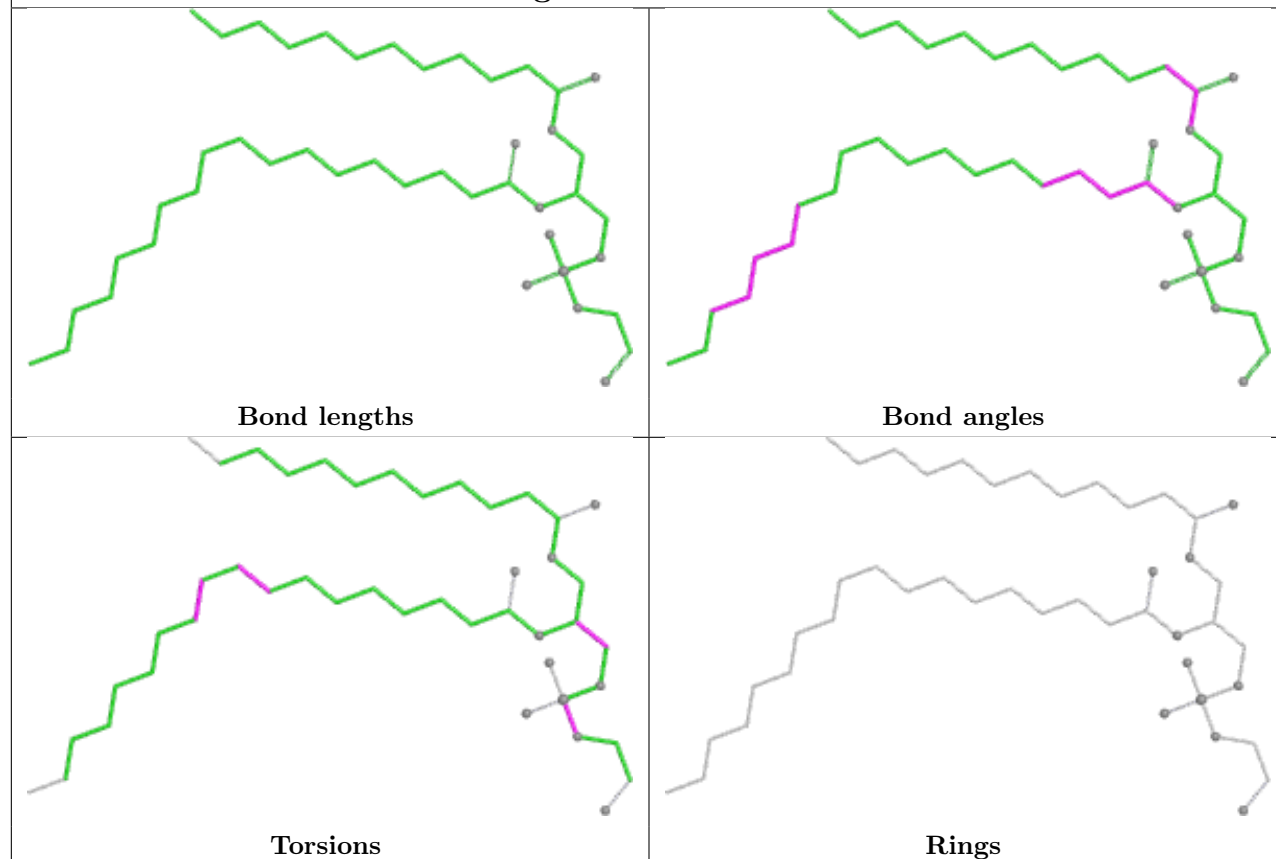
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

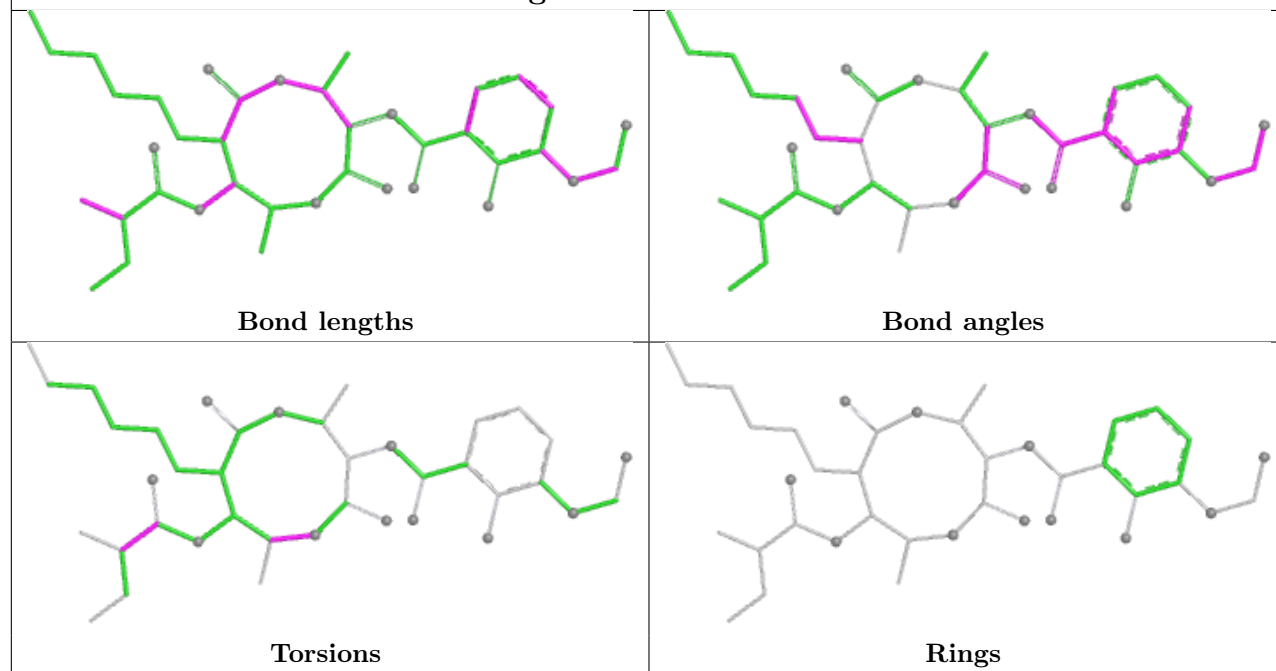


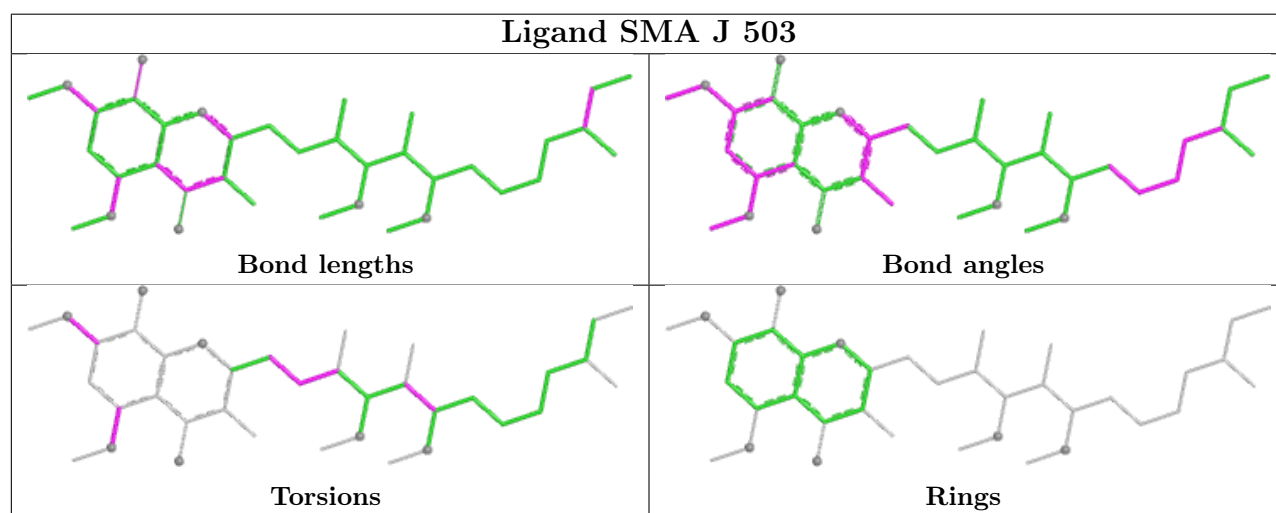
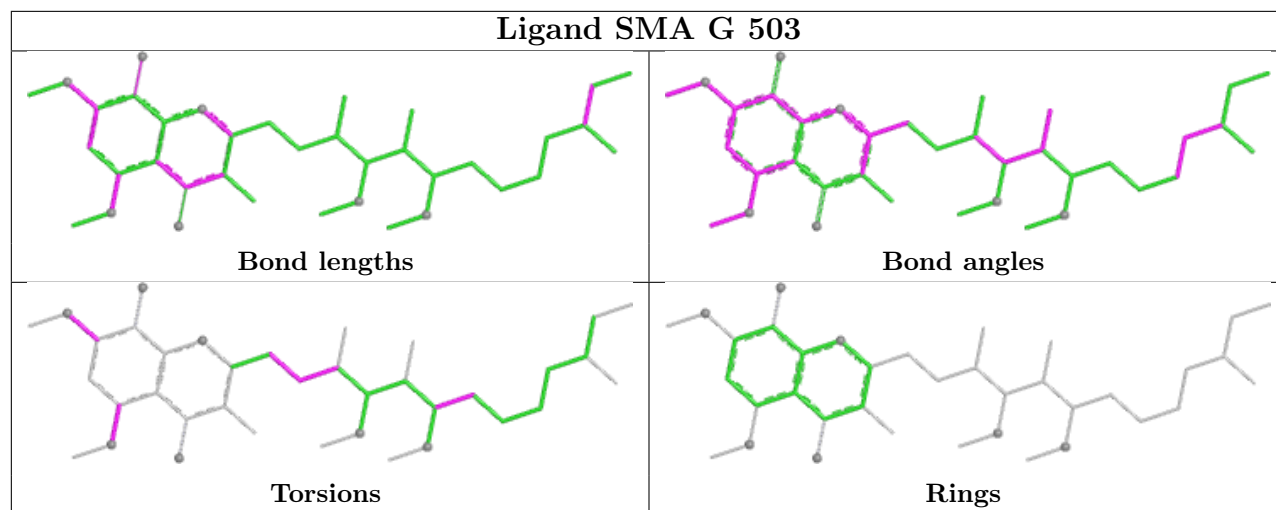


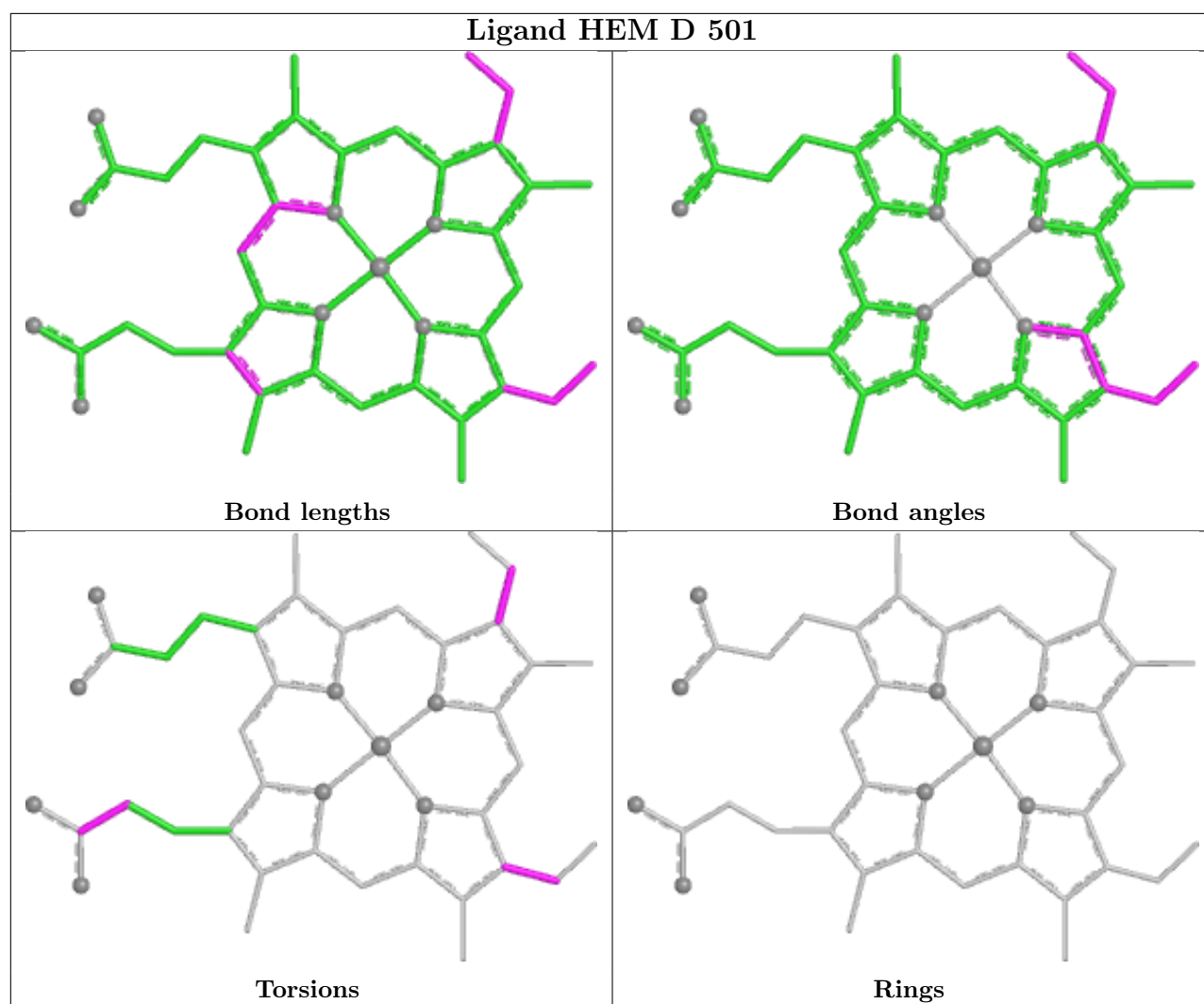
Ligand LOP P 504

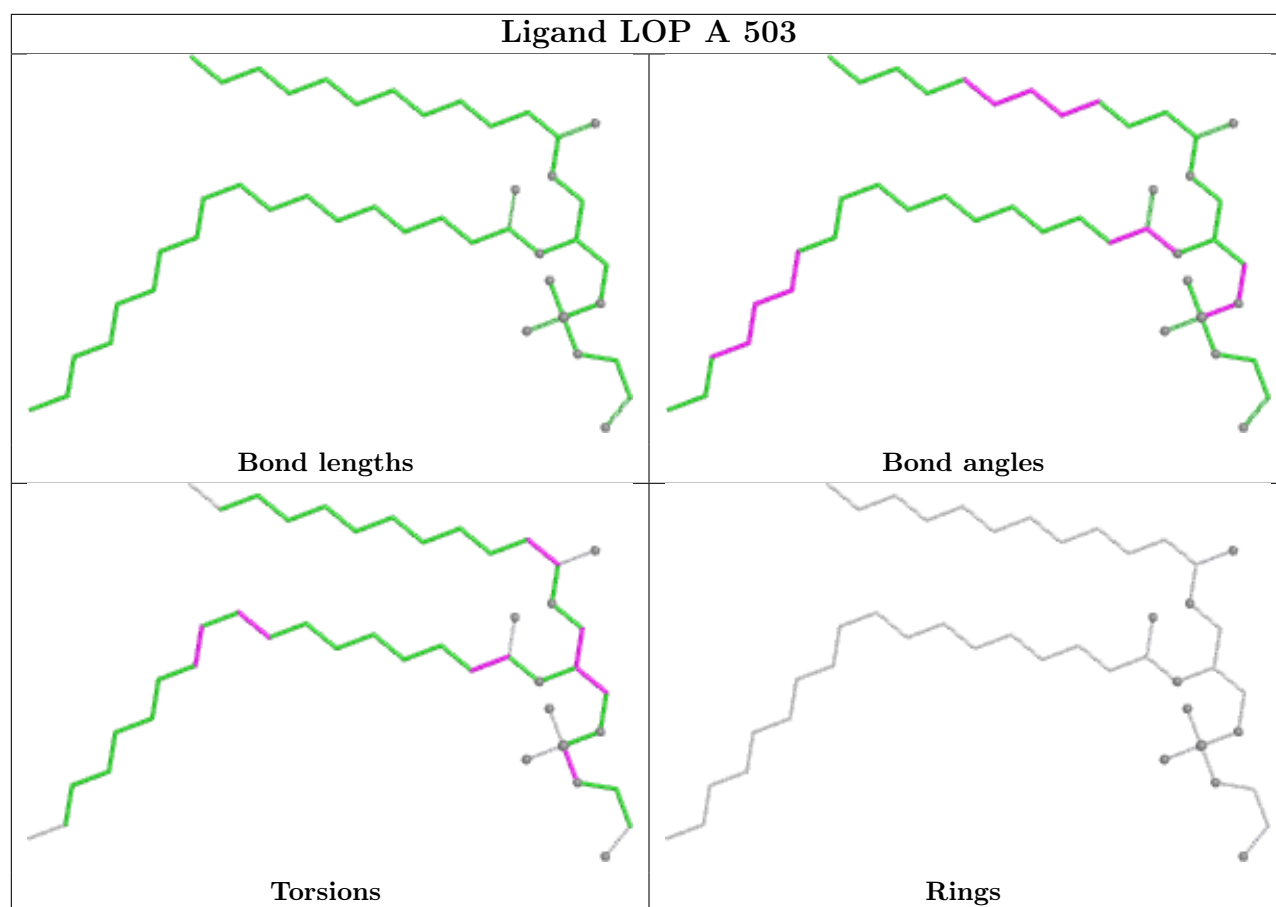


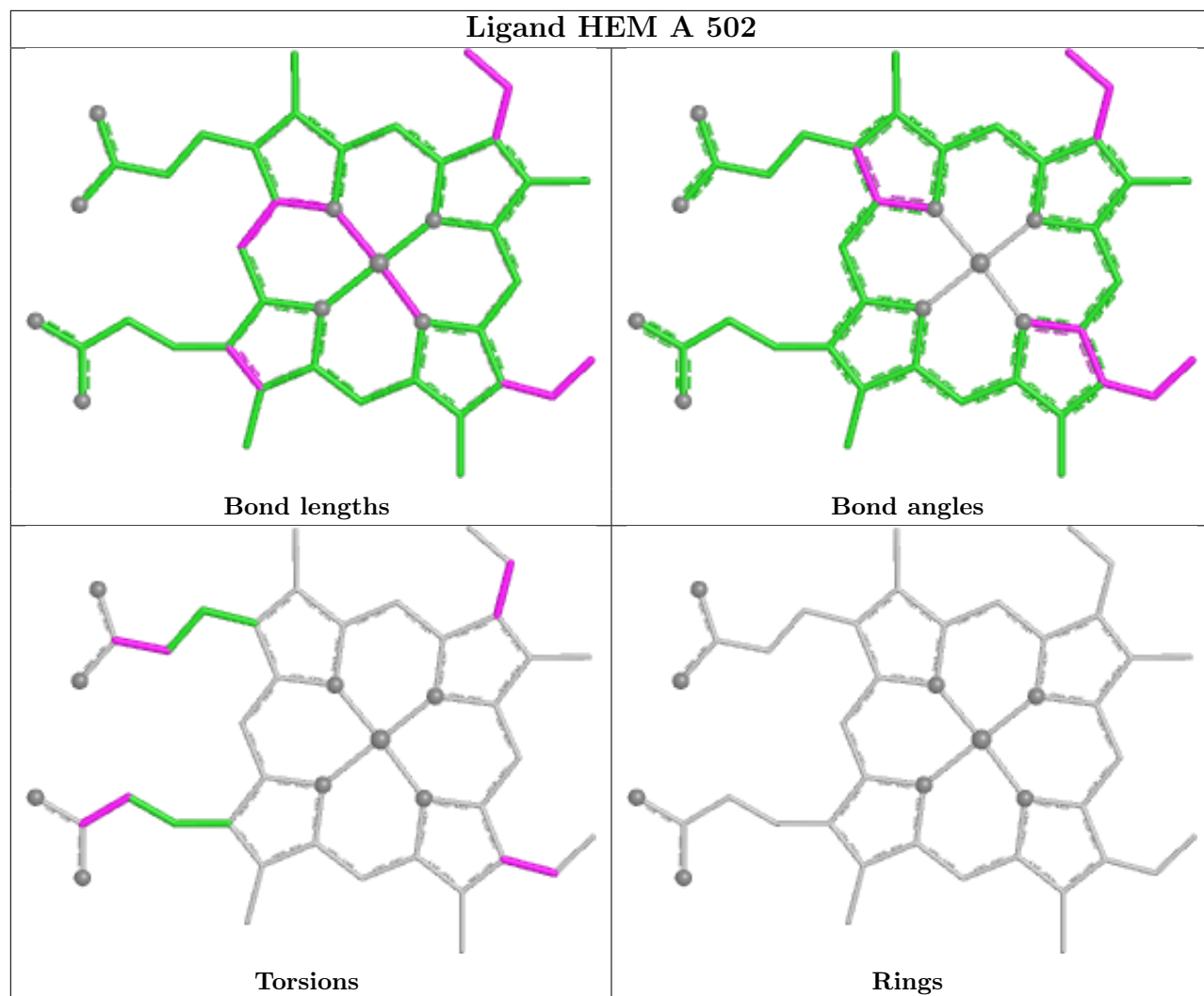
Ligand ANJ M 505

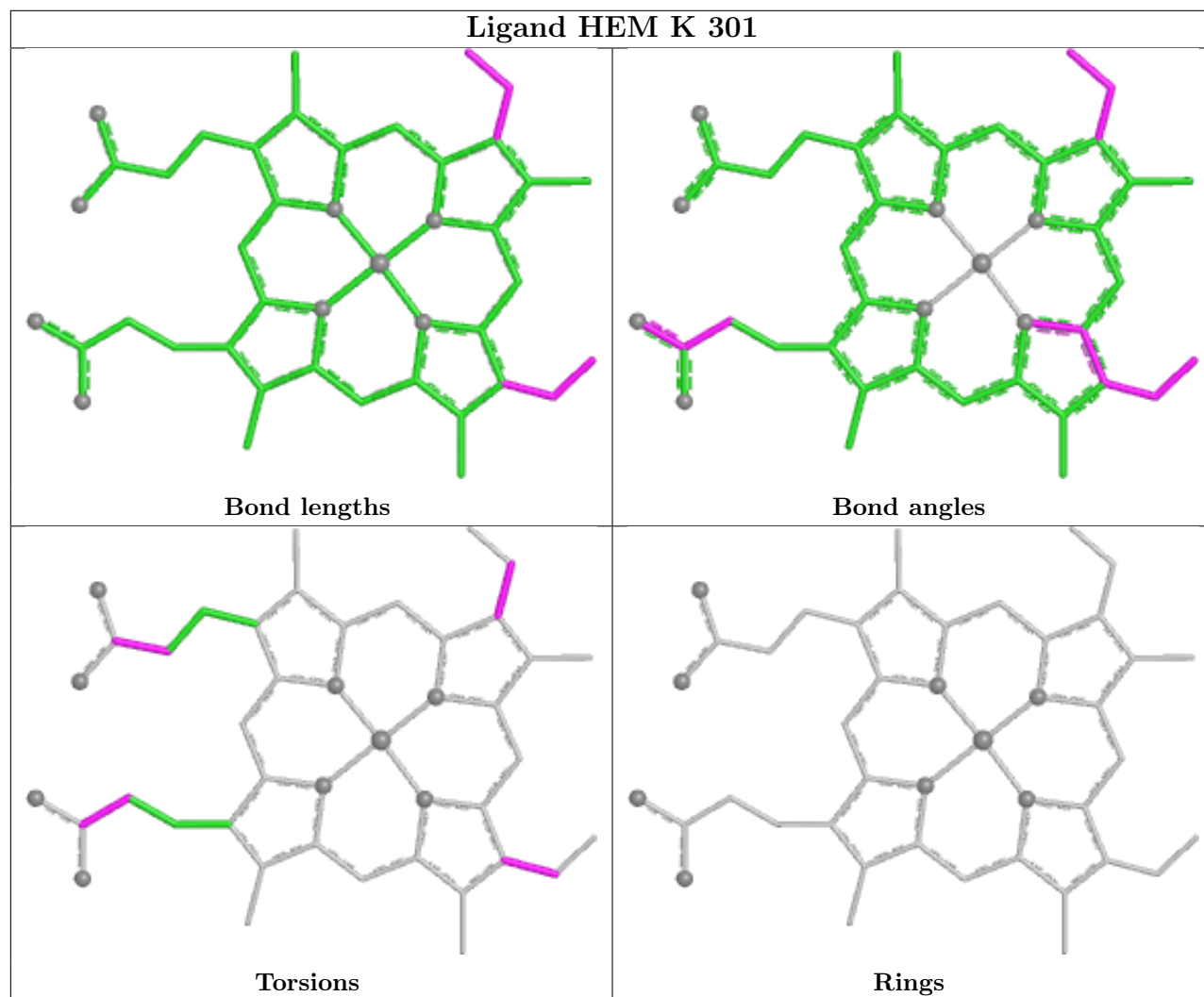


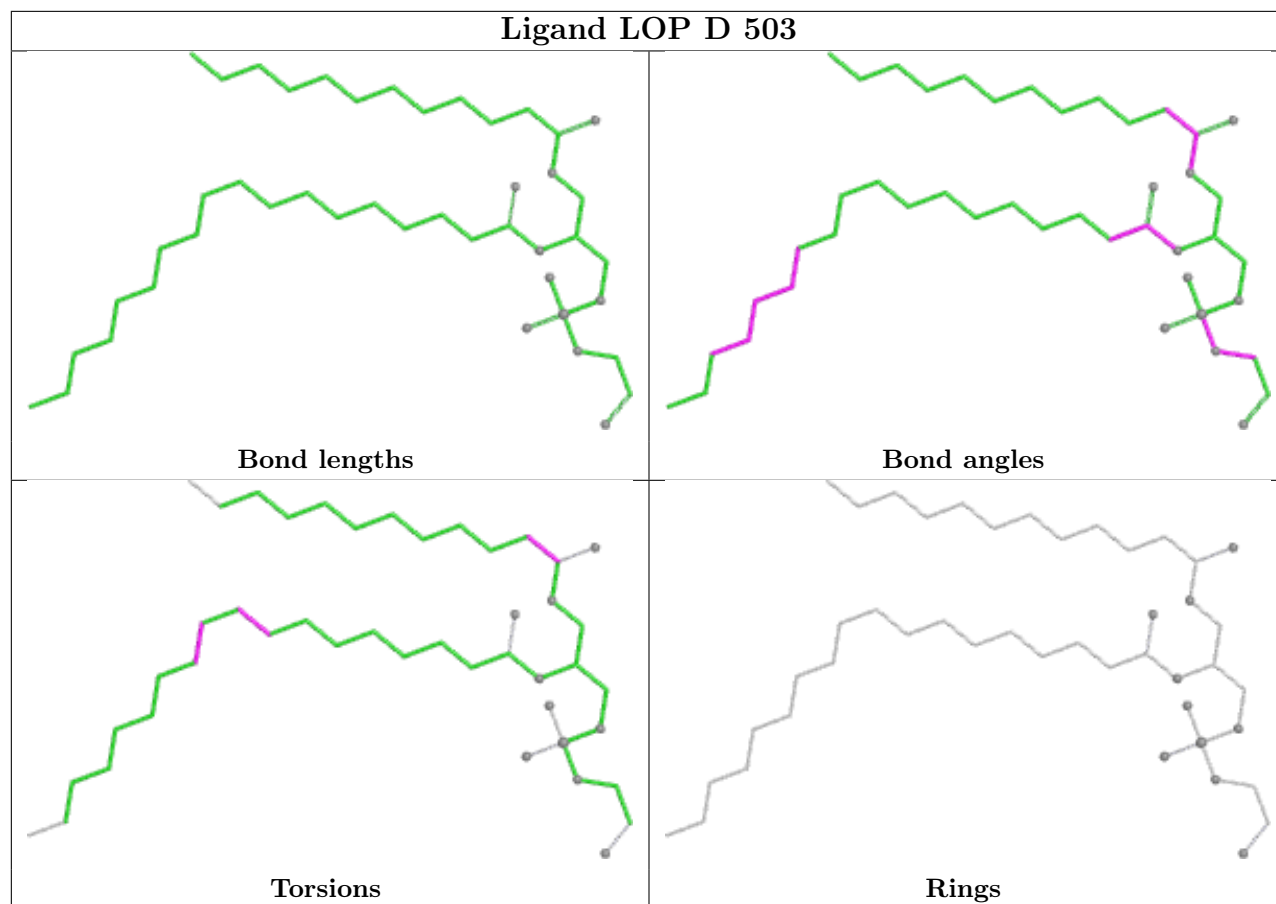


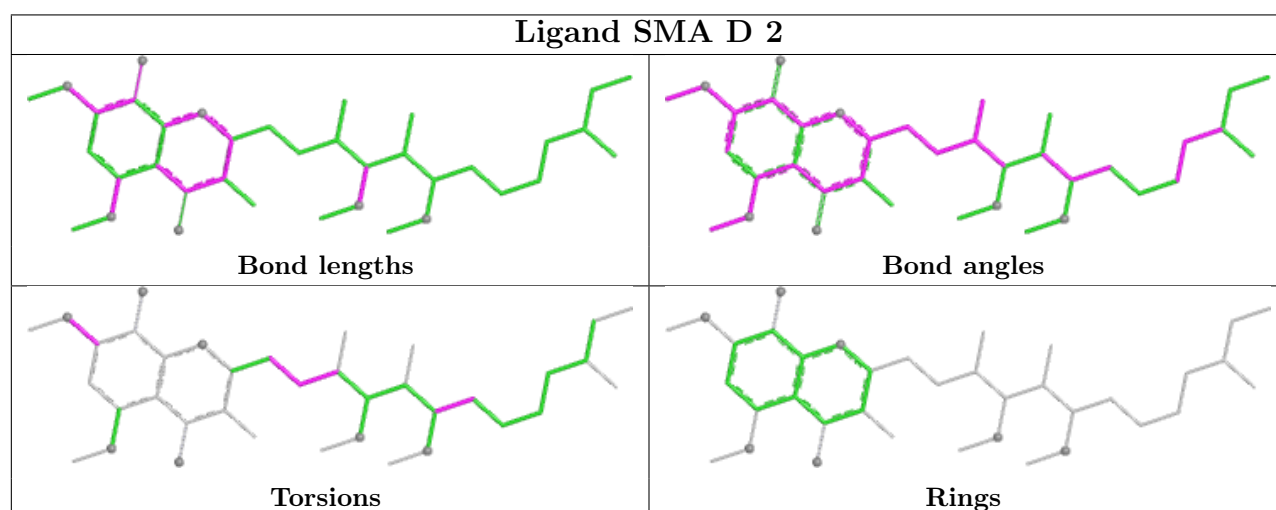
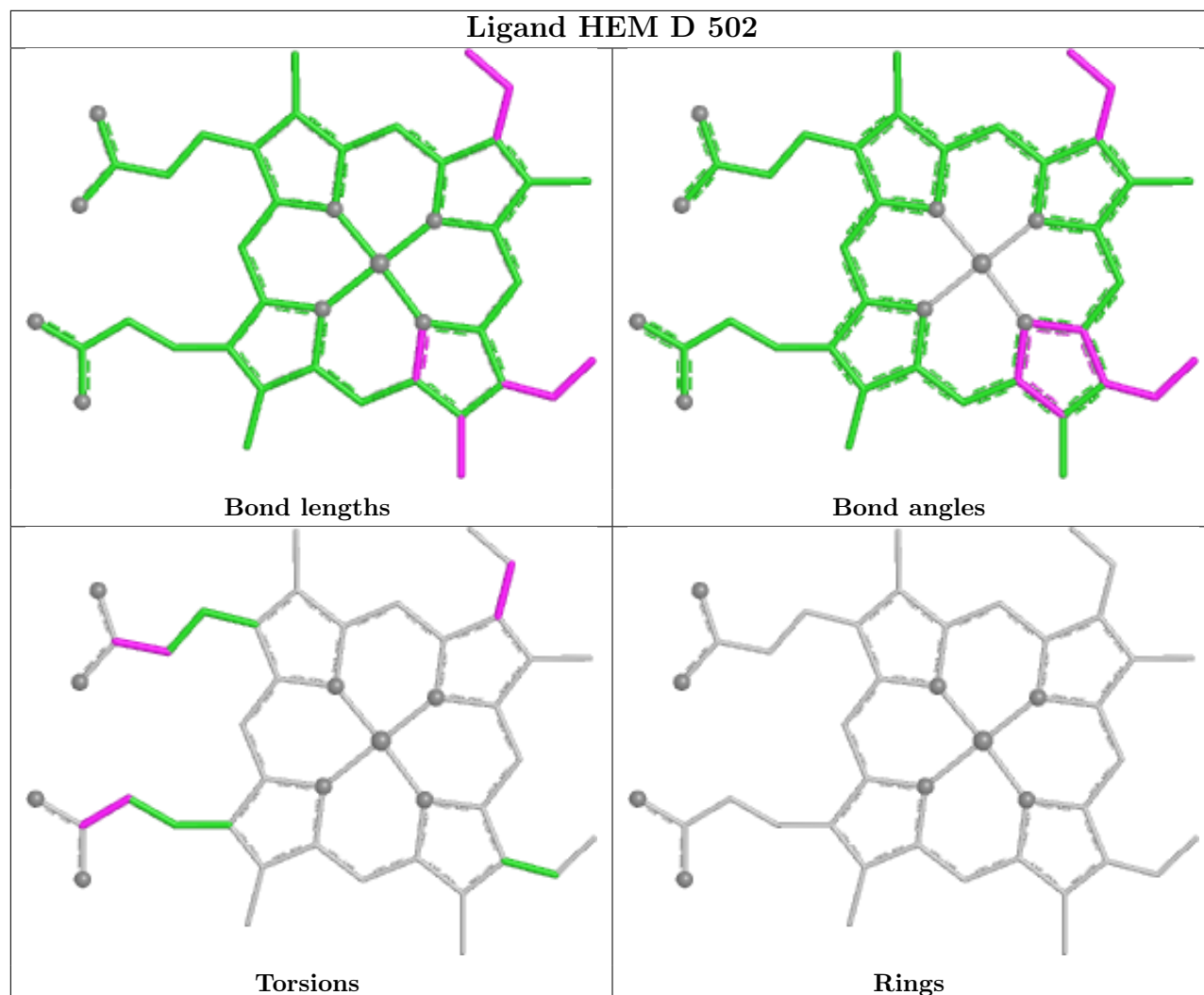


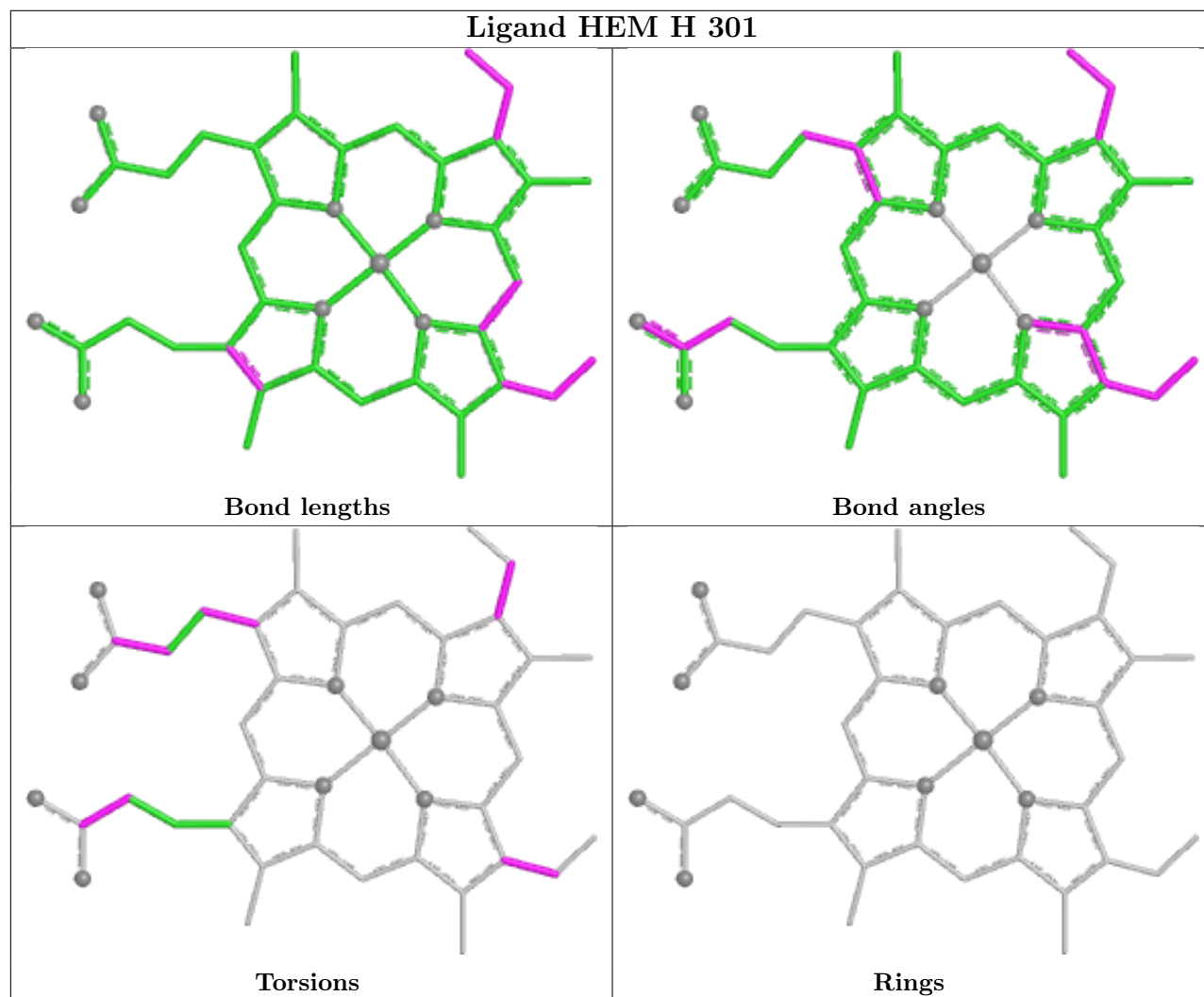




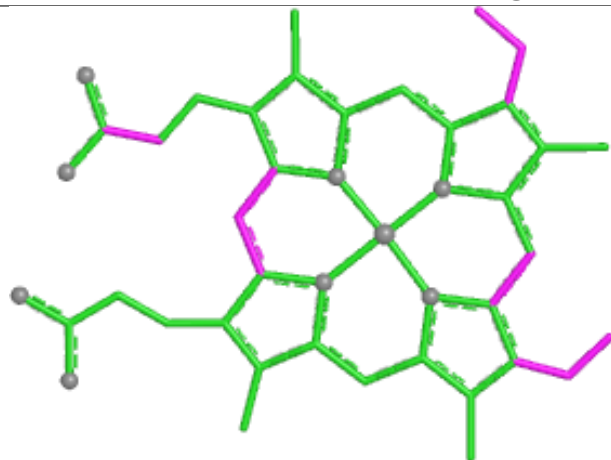




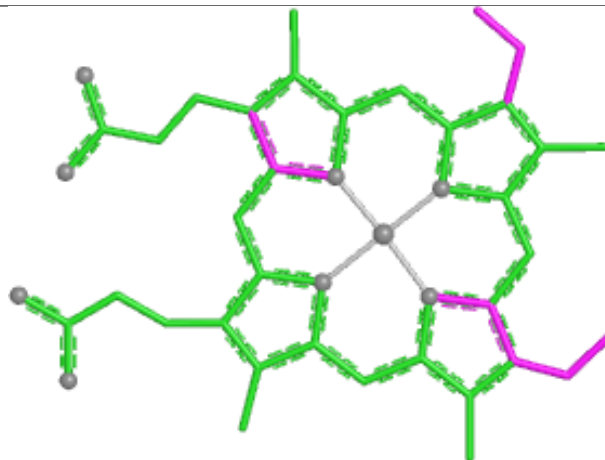




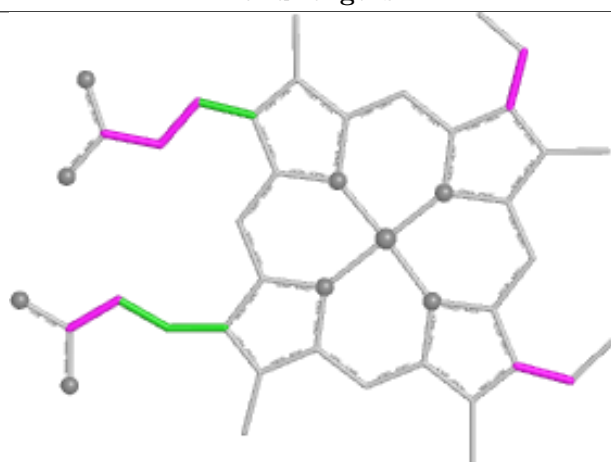
Ligand HEM G 502



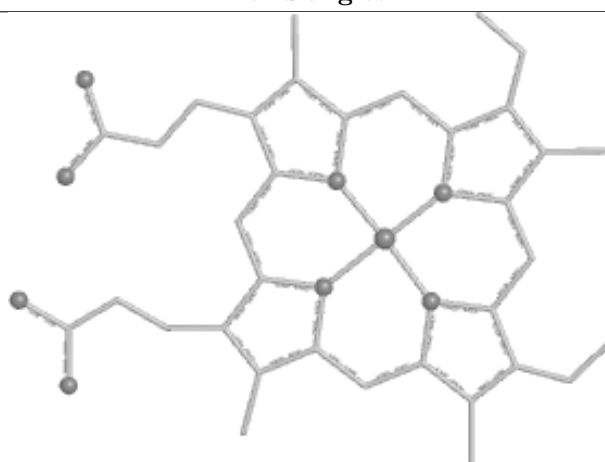
Bond lengths



Bond angles

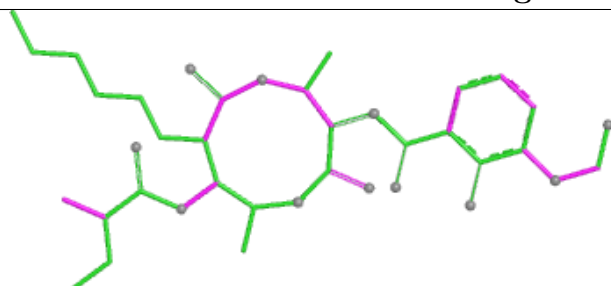


Torsions

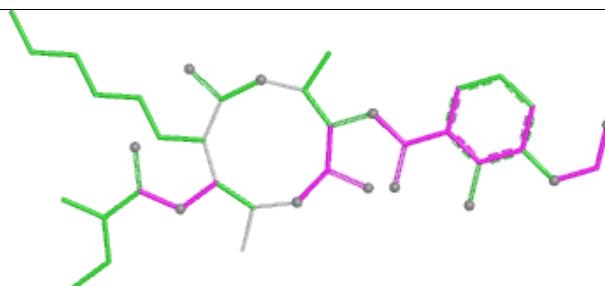


Rings

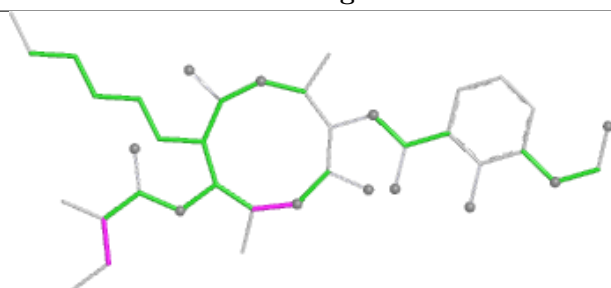
Ligand ANJ D 504



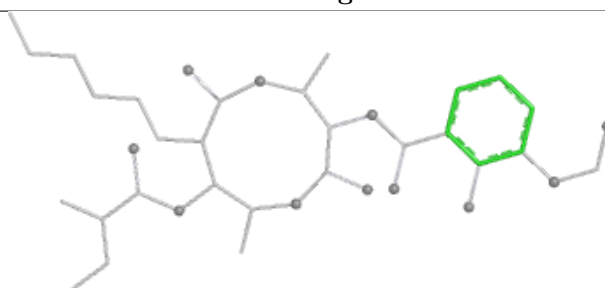
Bond lengths



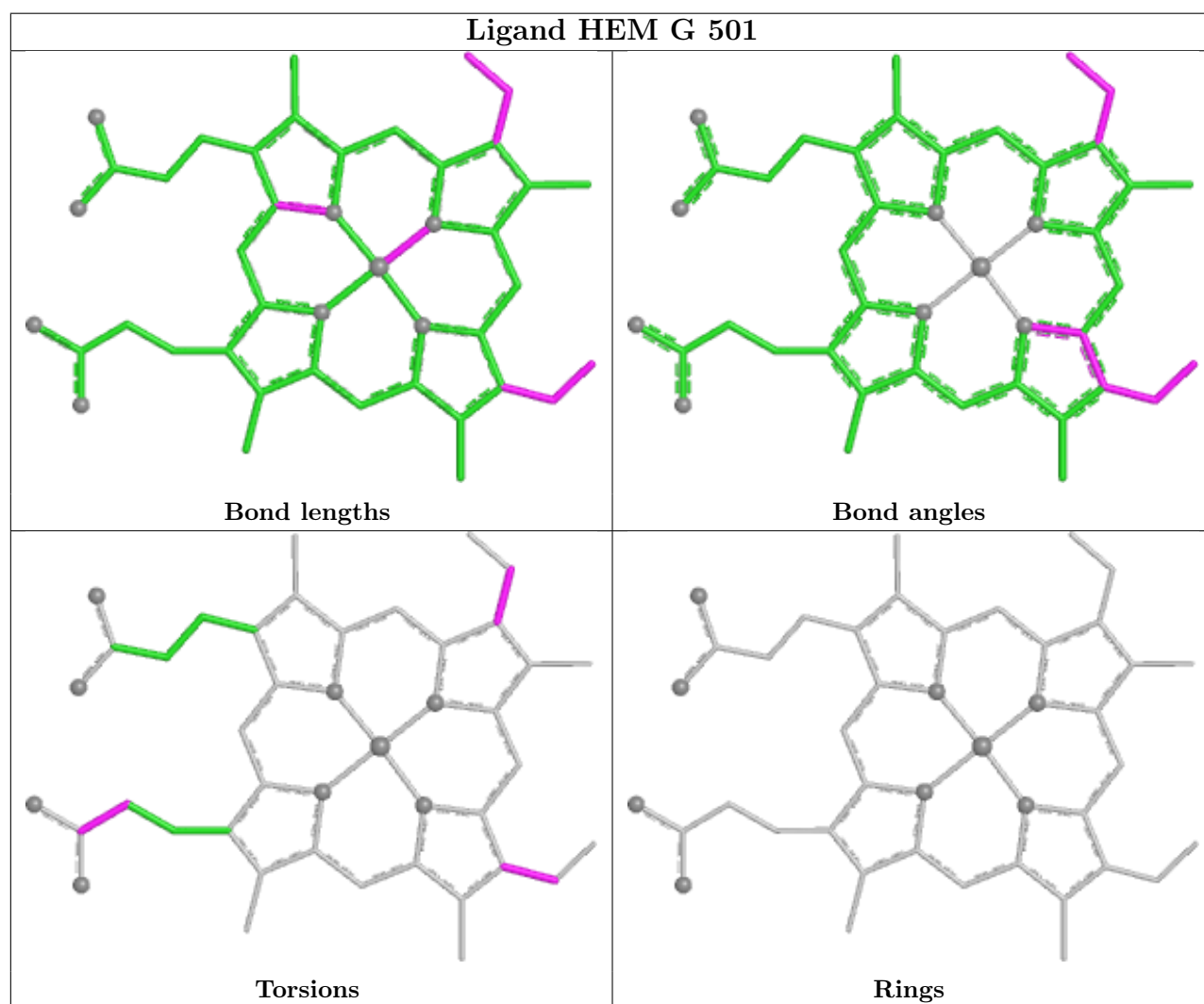
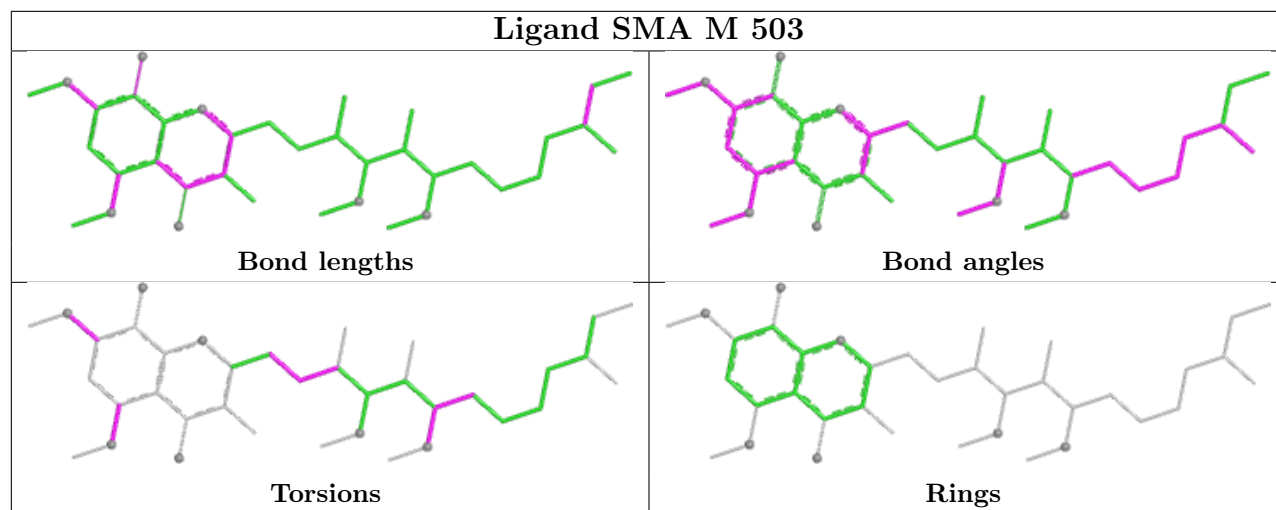
Bond angles



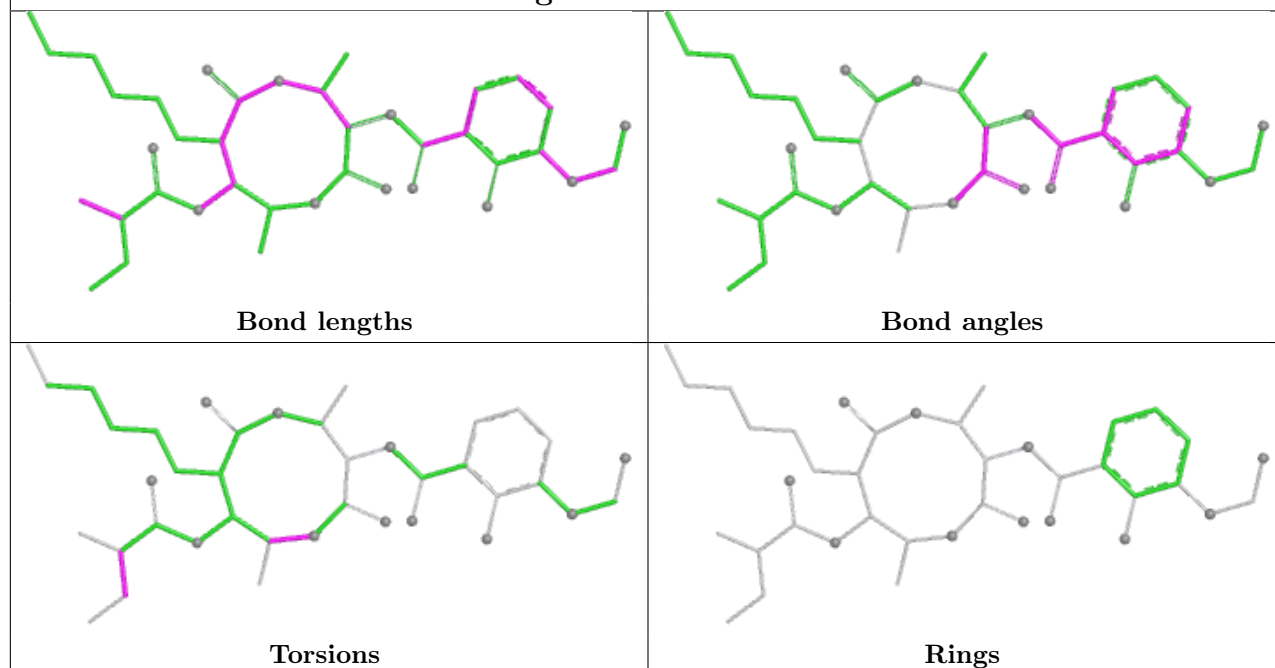
Torsions



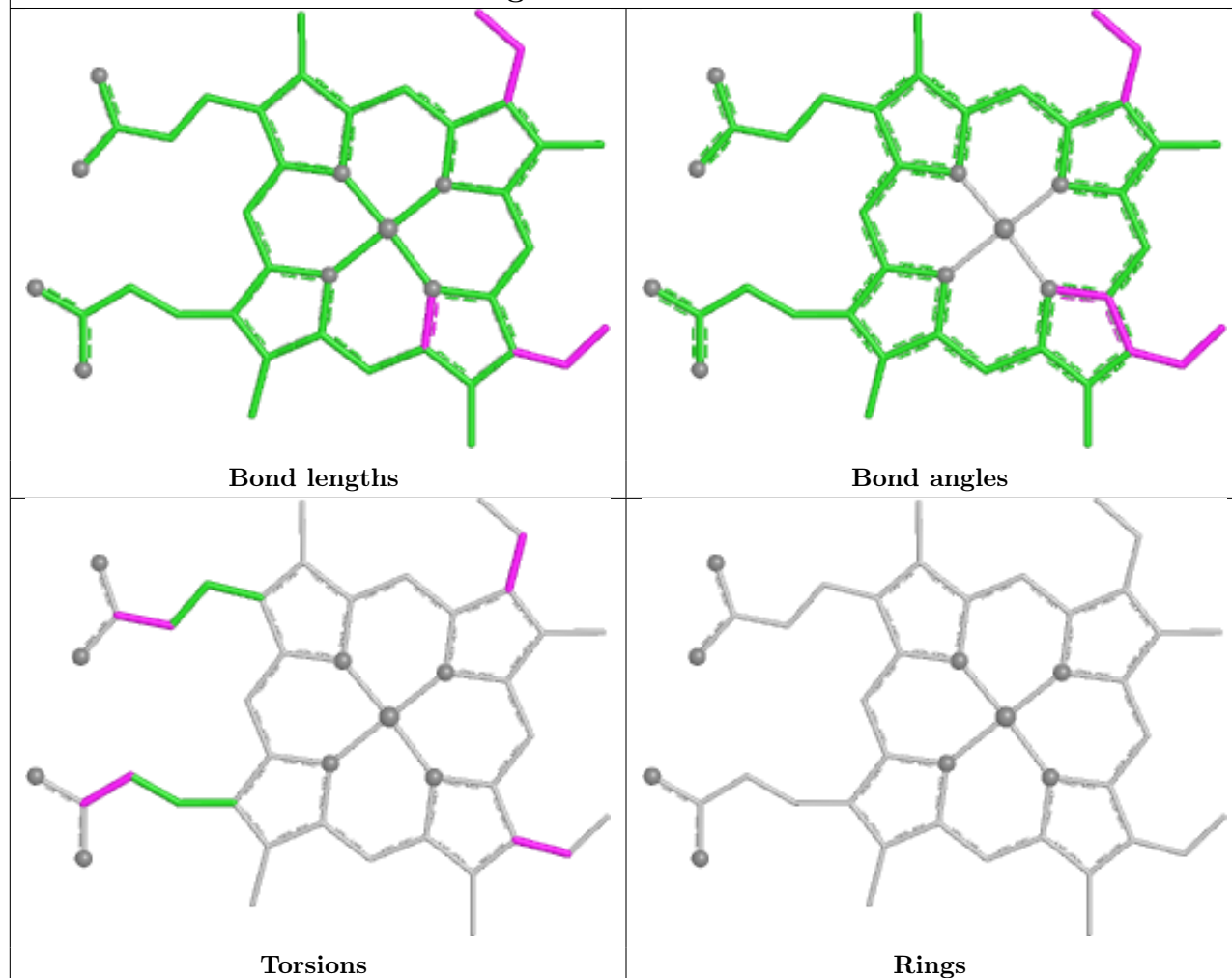
Rings

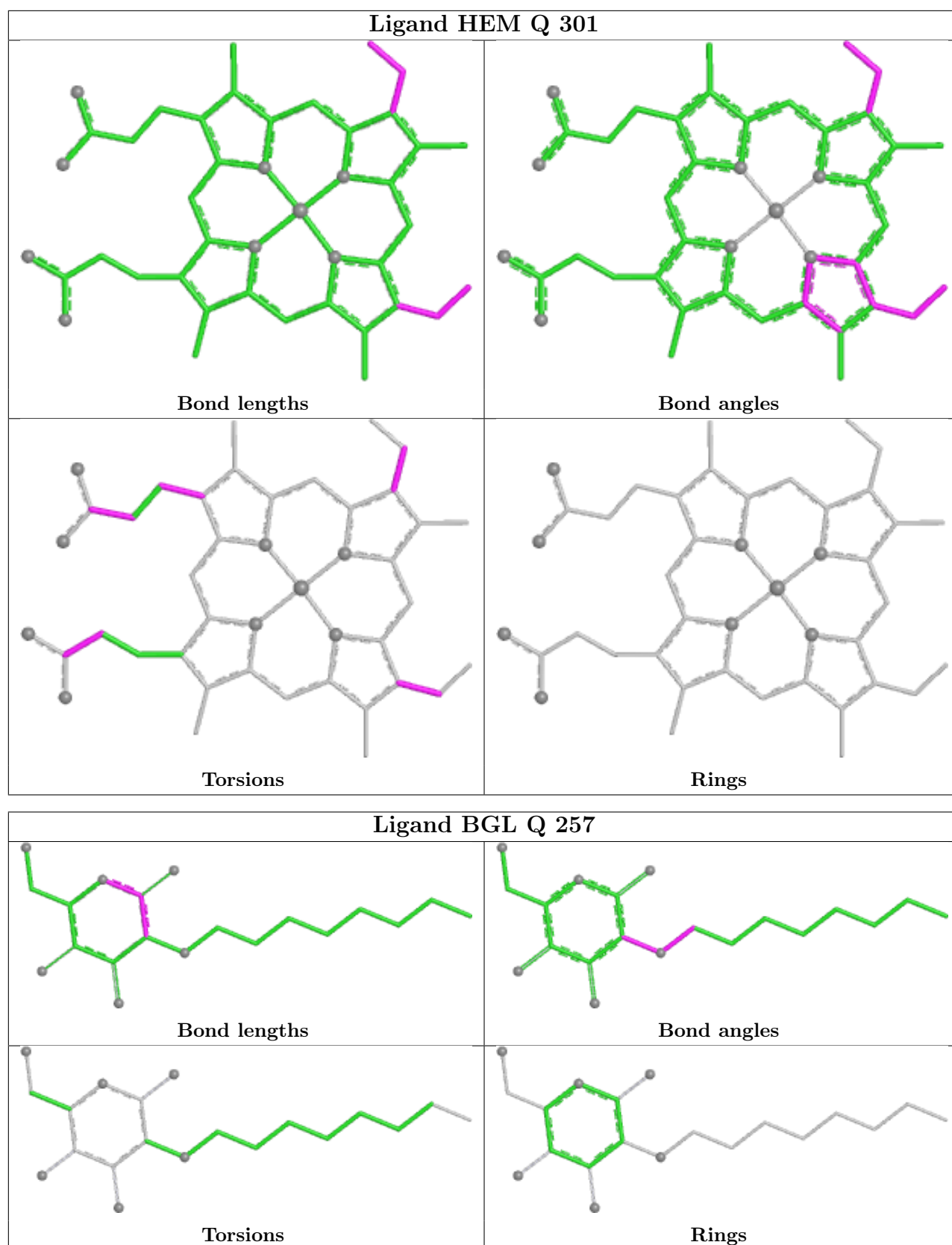


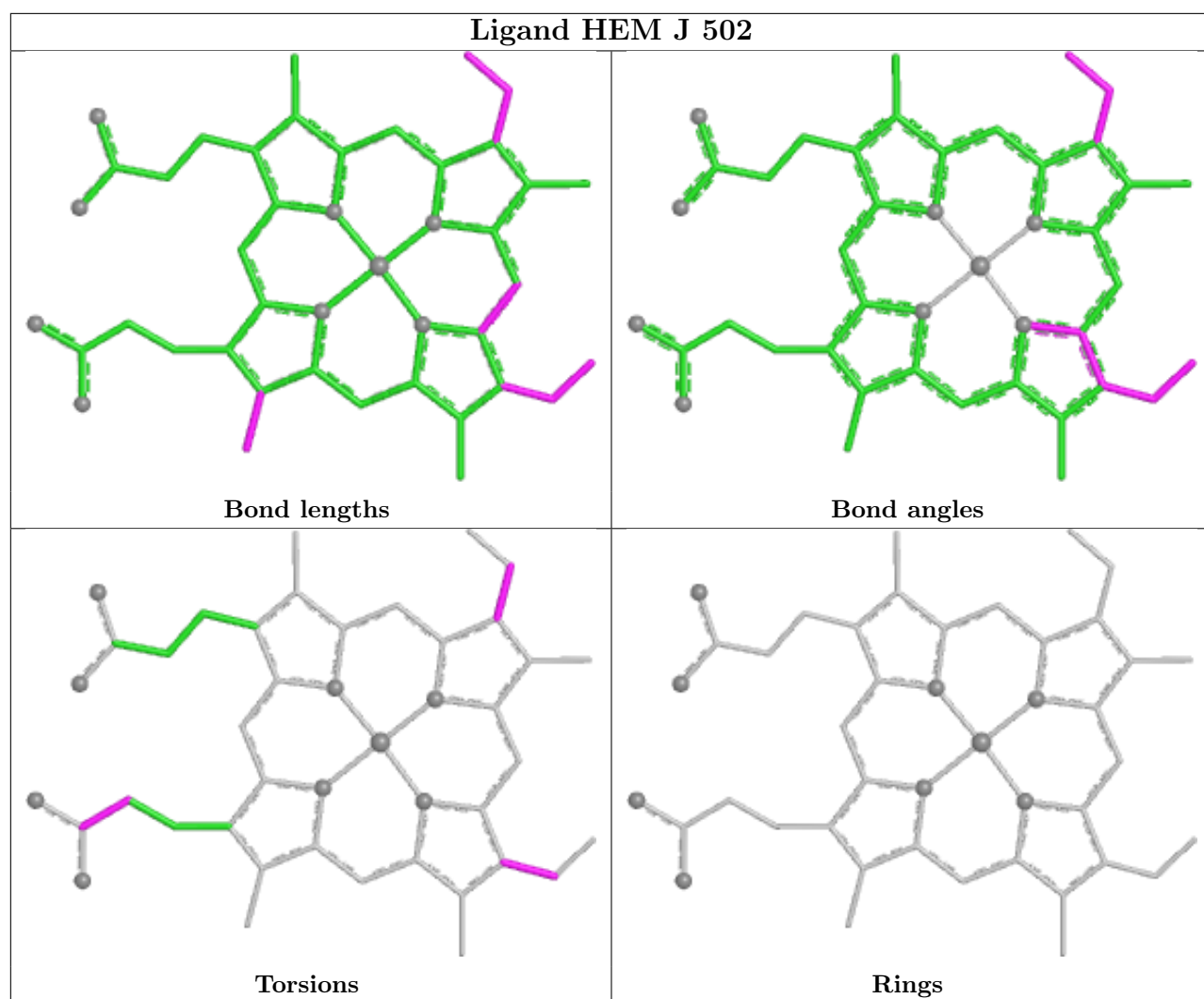
Ligand ANJ J 505

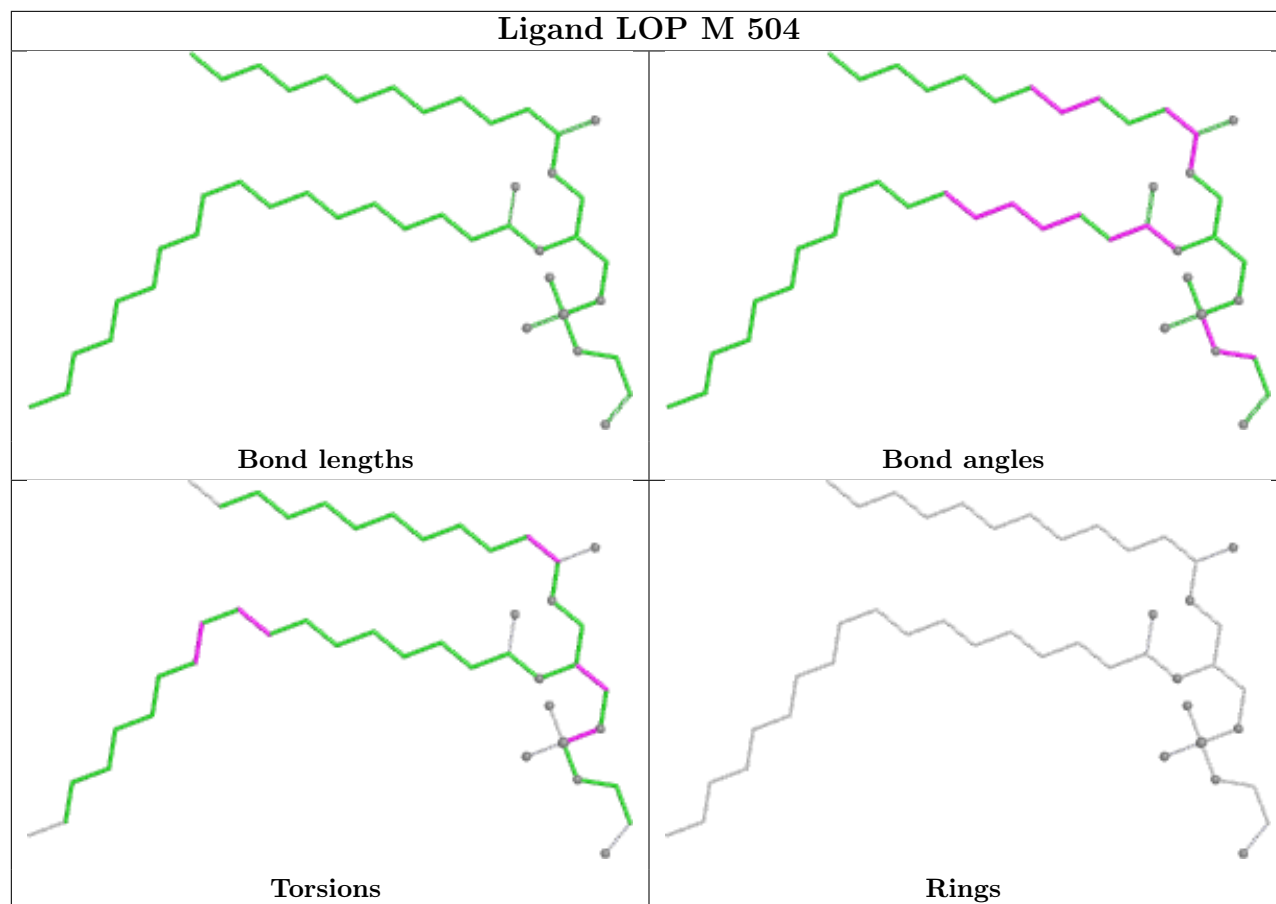


Ligand HEM A 501

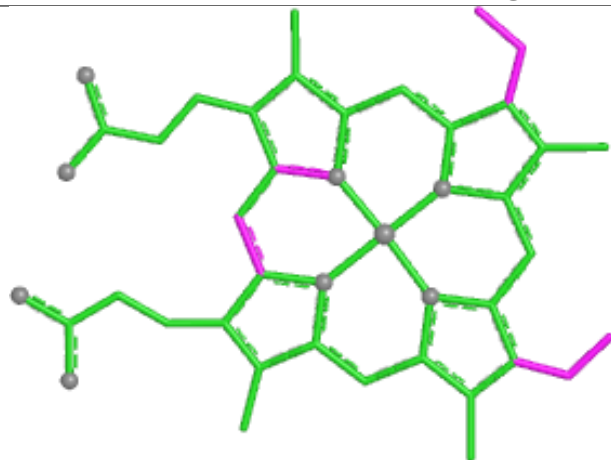




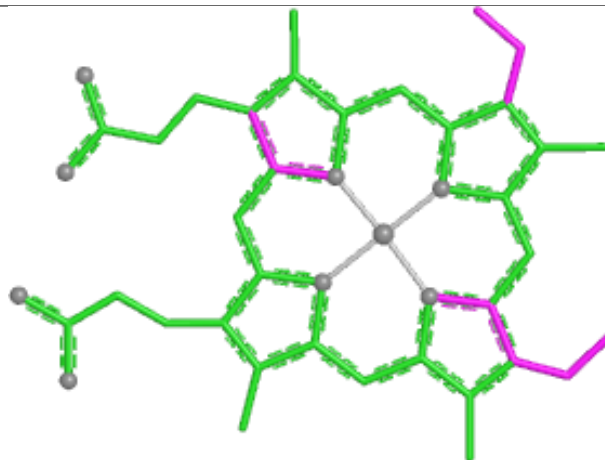




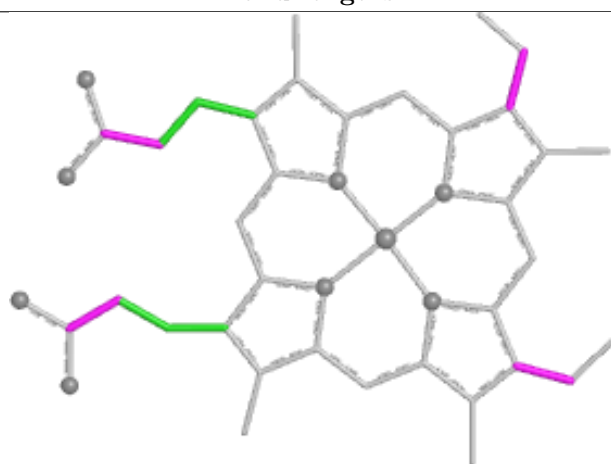
Ligand HEM M 502



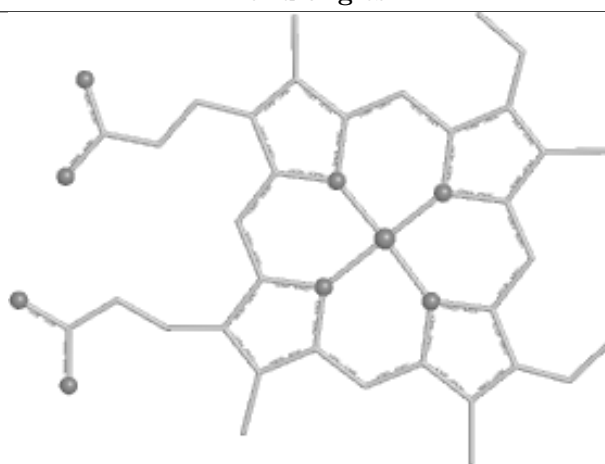
Bond lengths



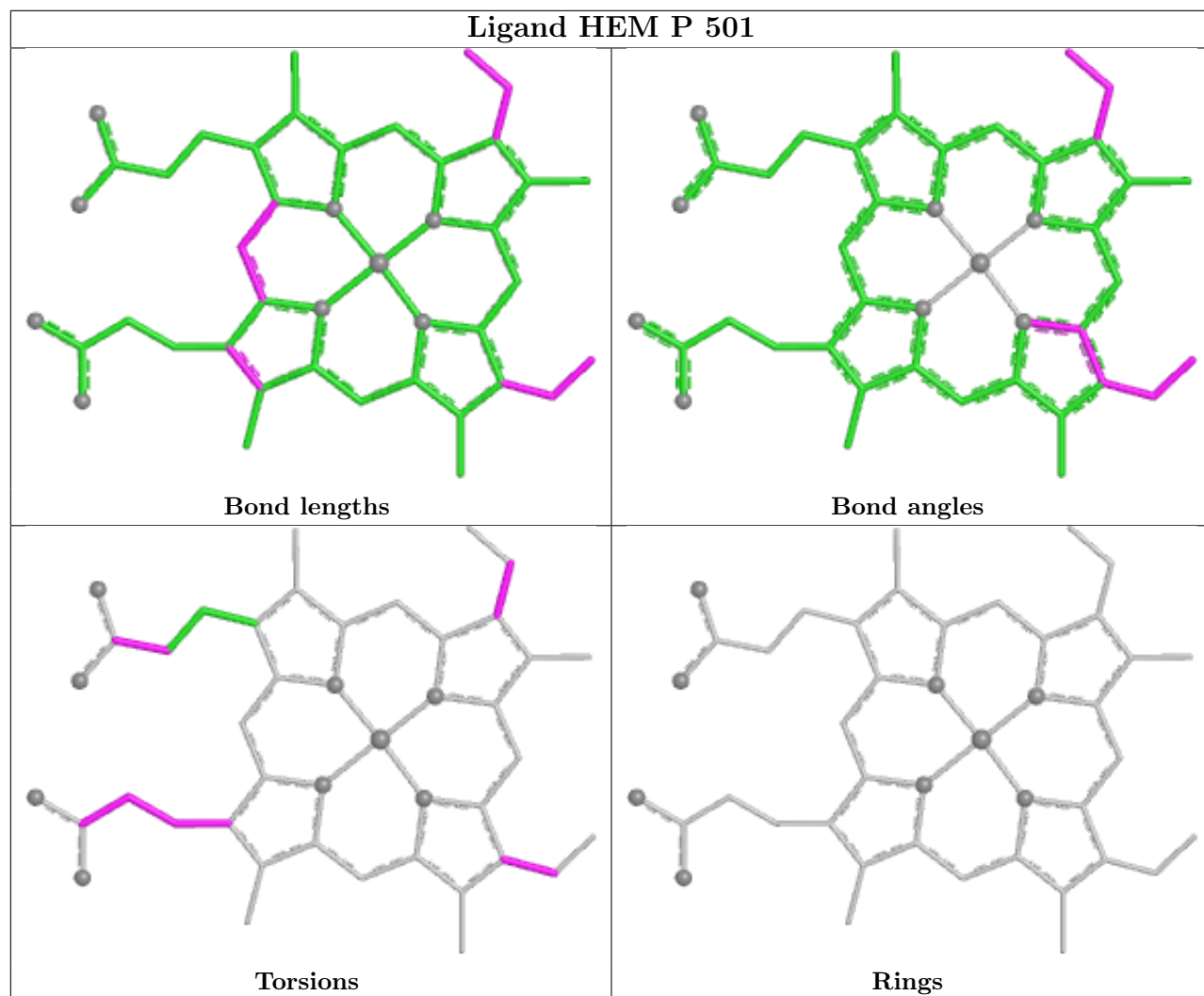
Bond angles

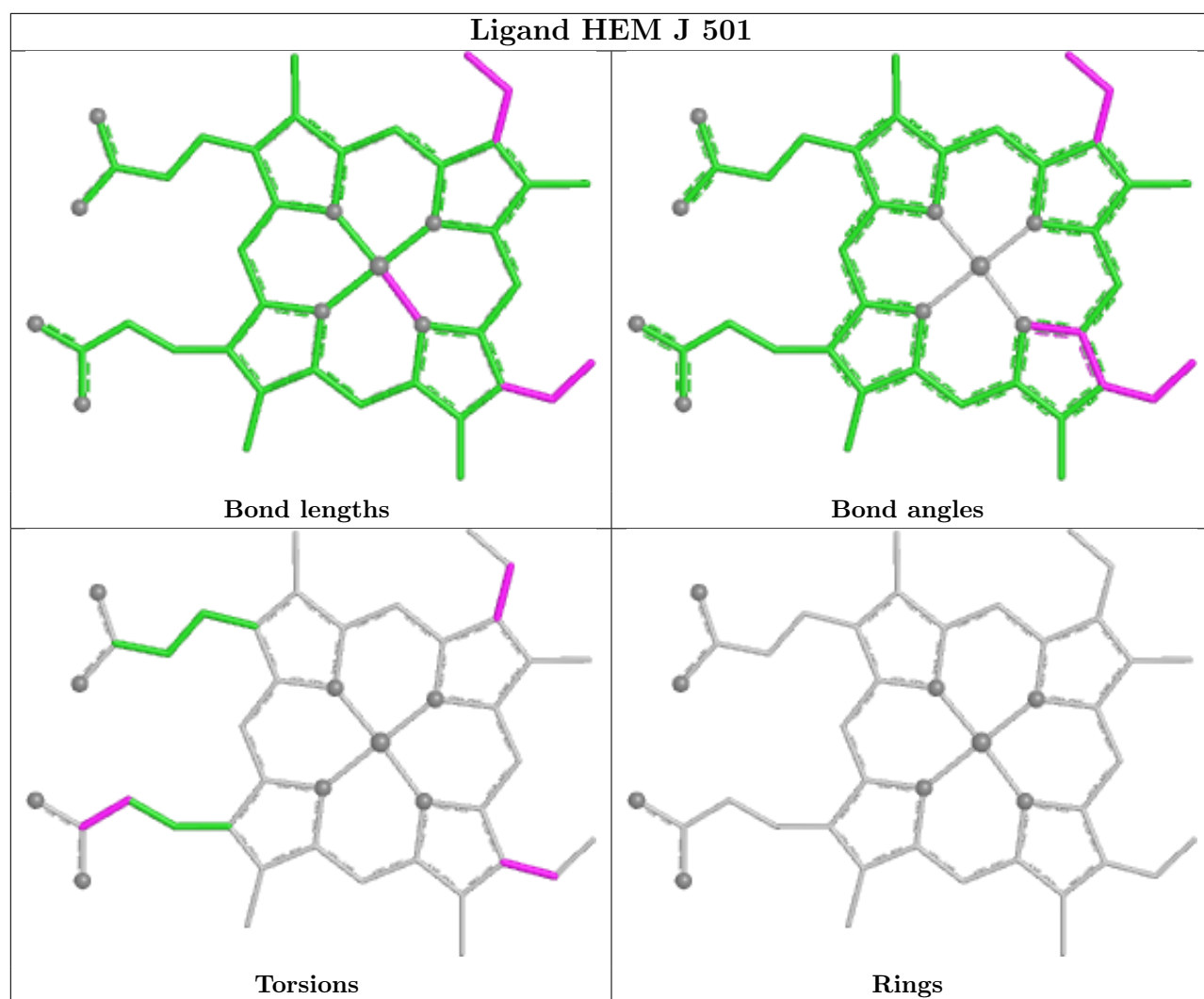


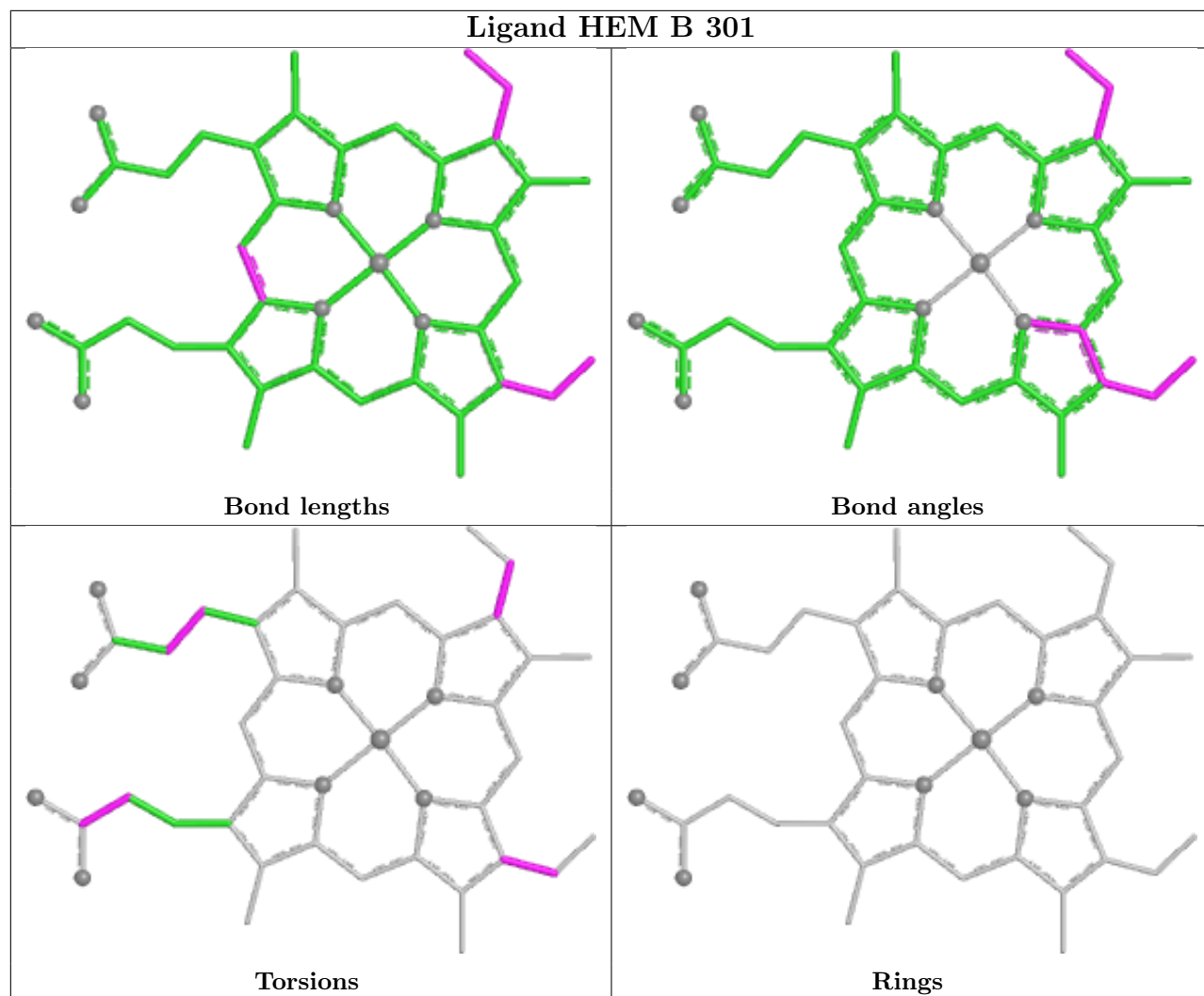
Torsions

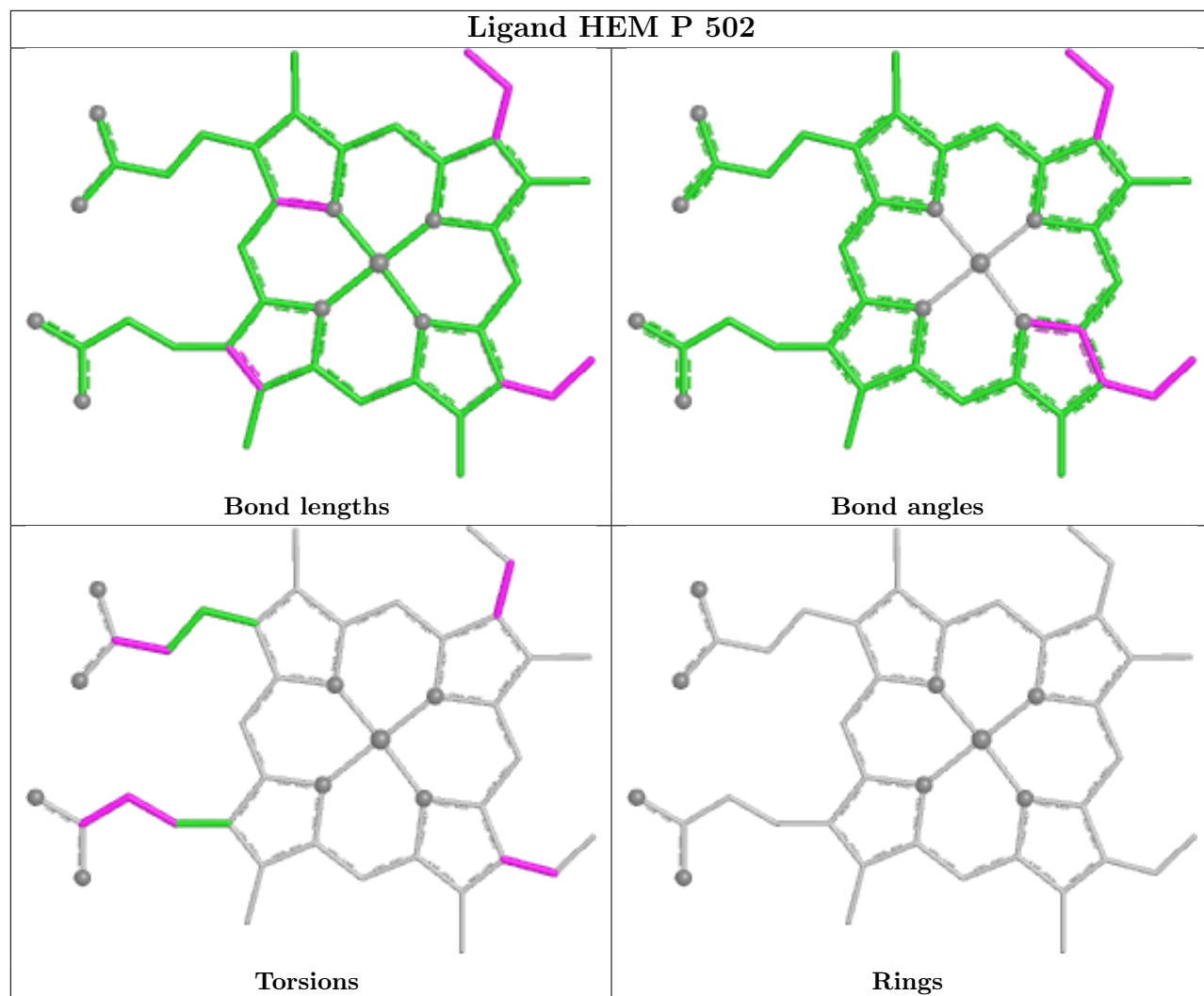


Rings

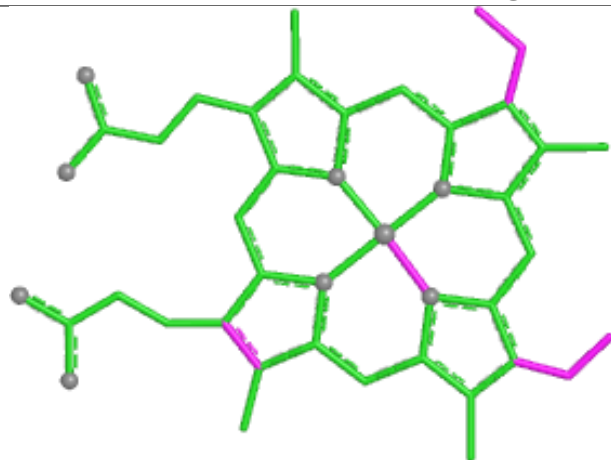




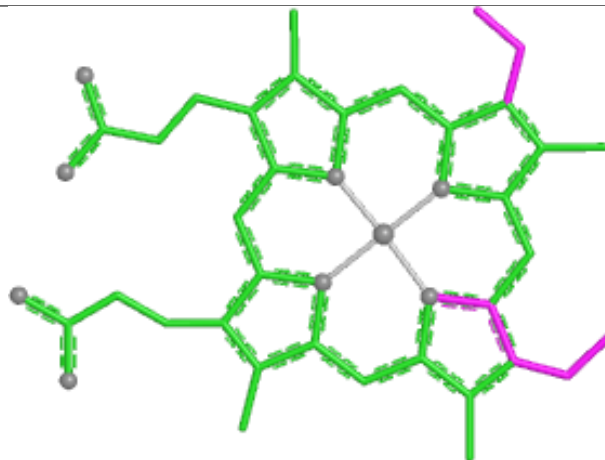




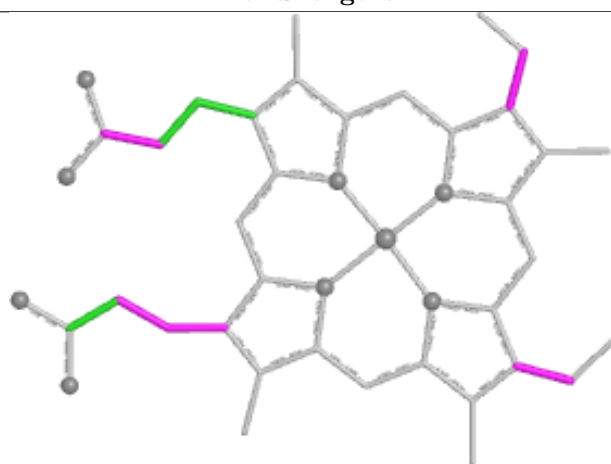
Ligand HEM M 501



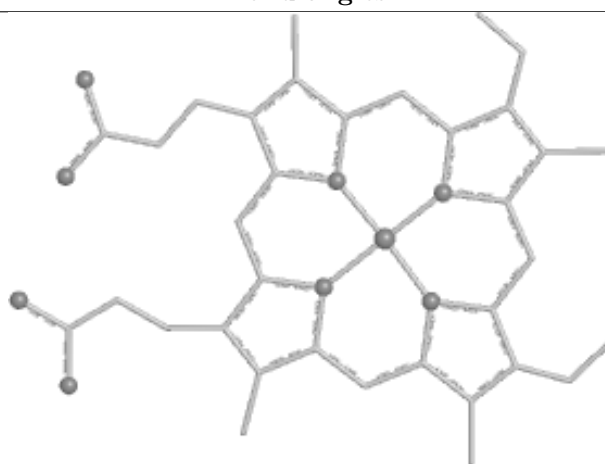
Bond lengths



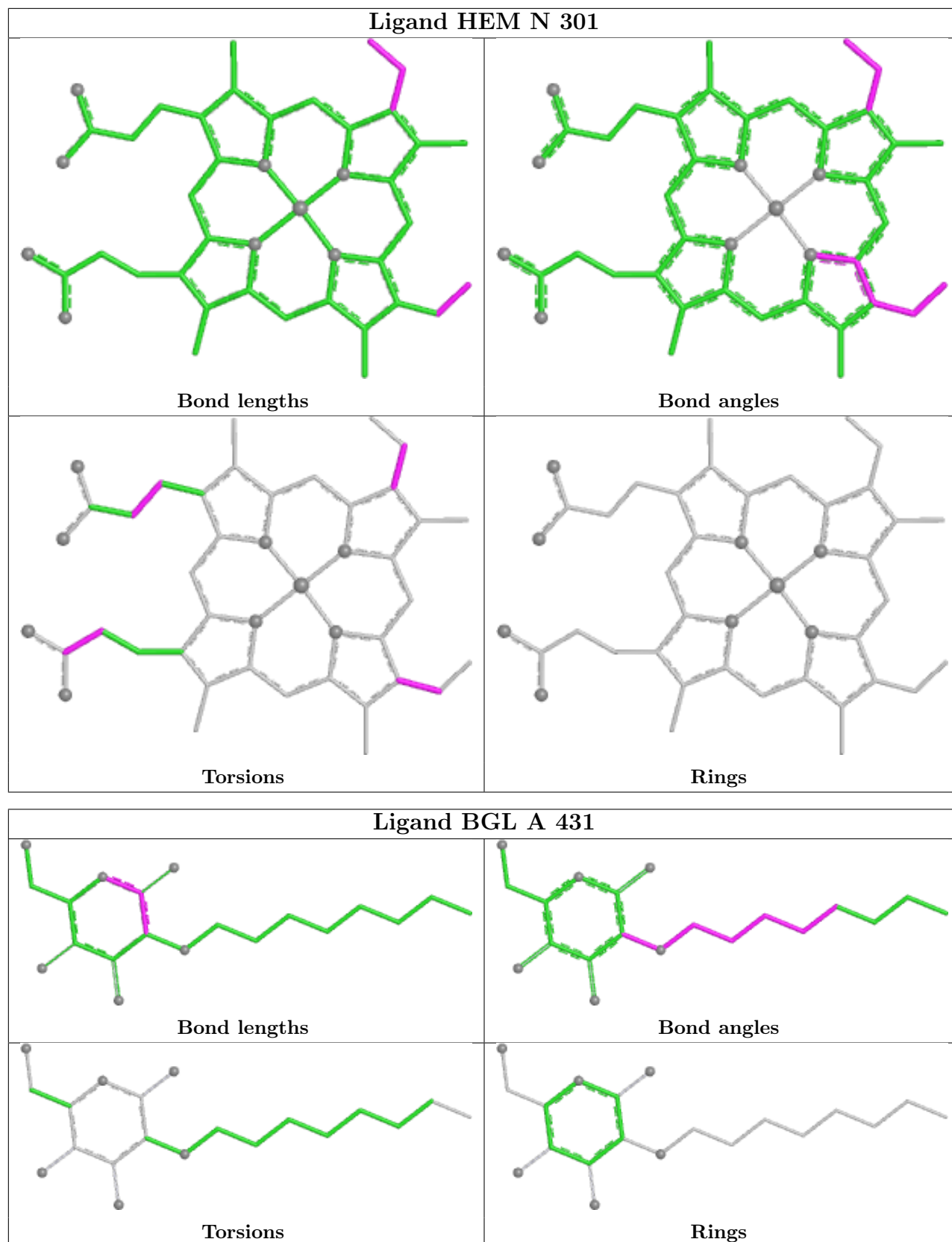
Bond angles



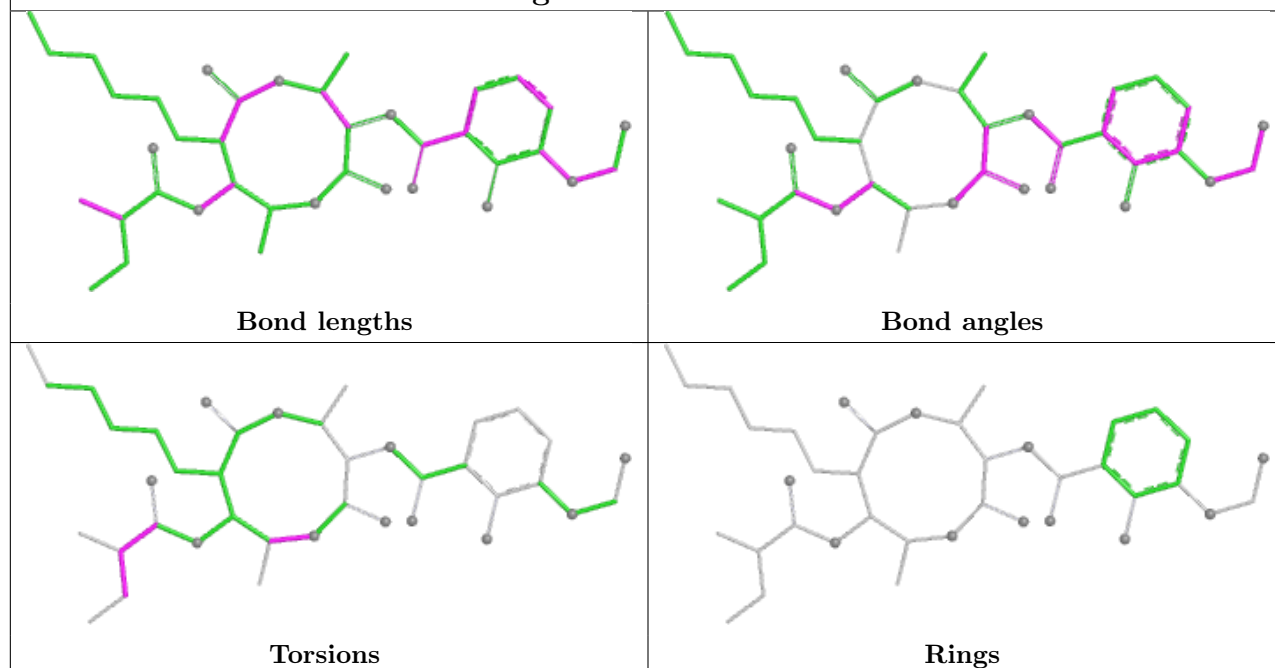
Torsions



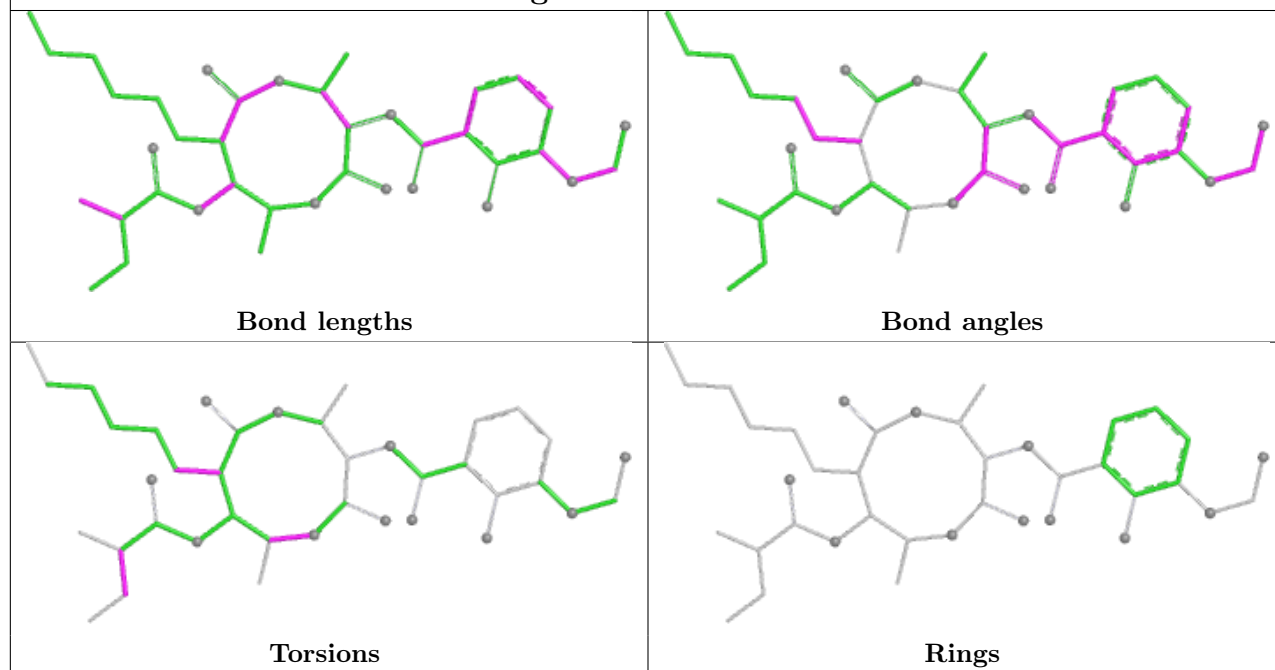
Rings

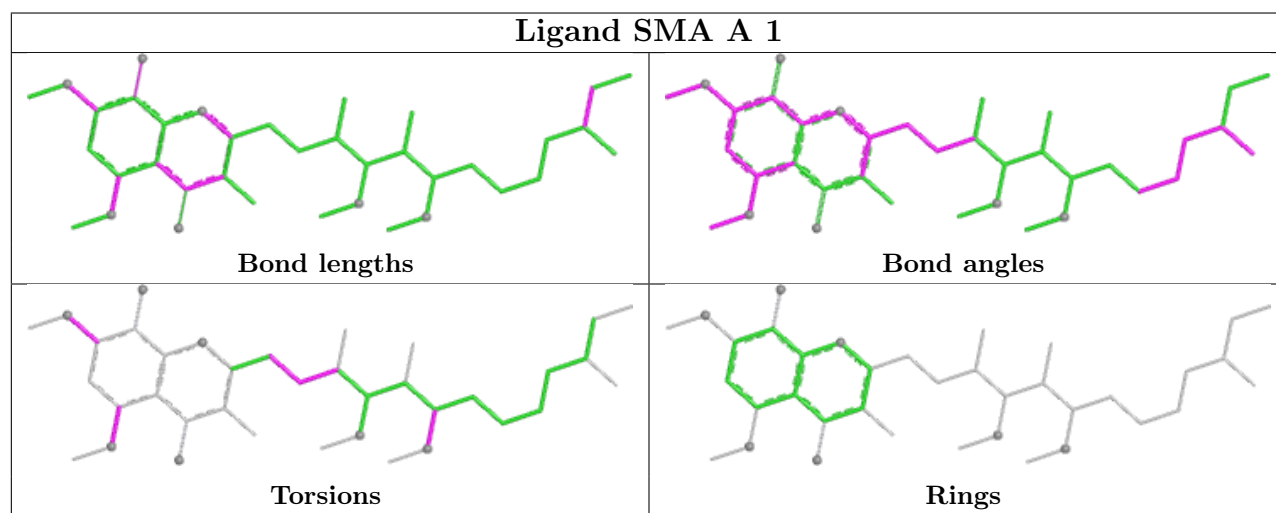
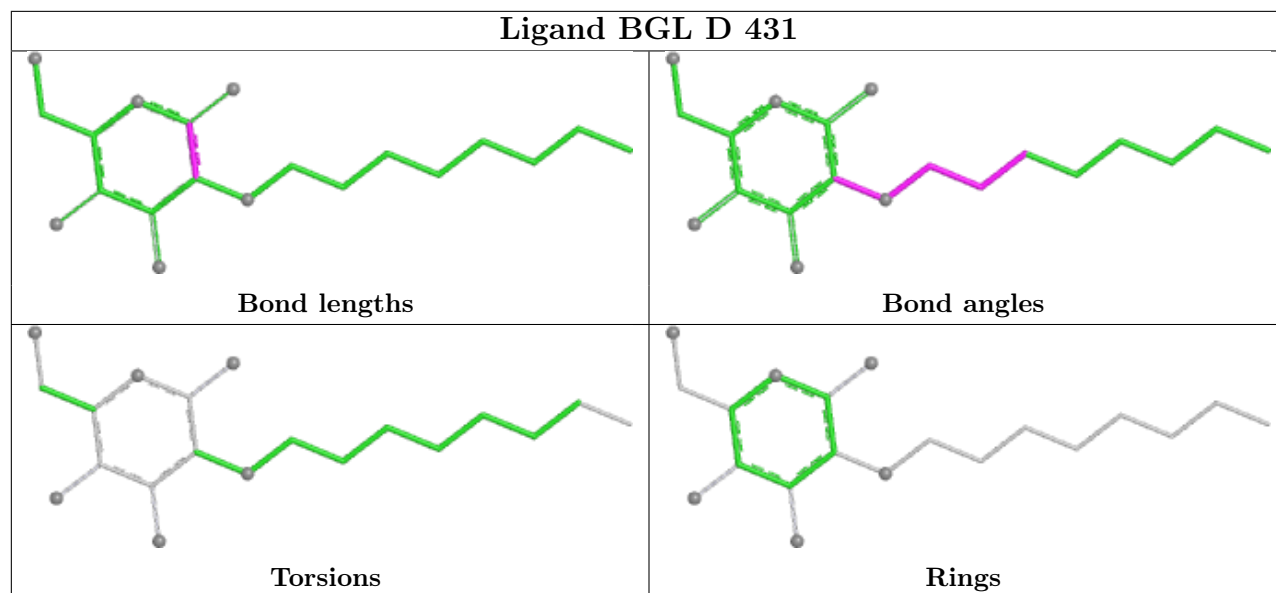


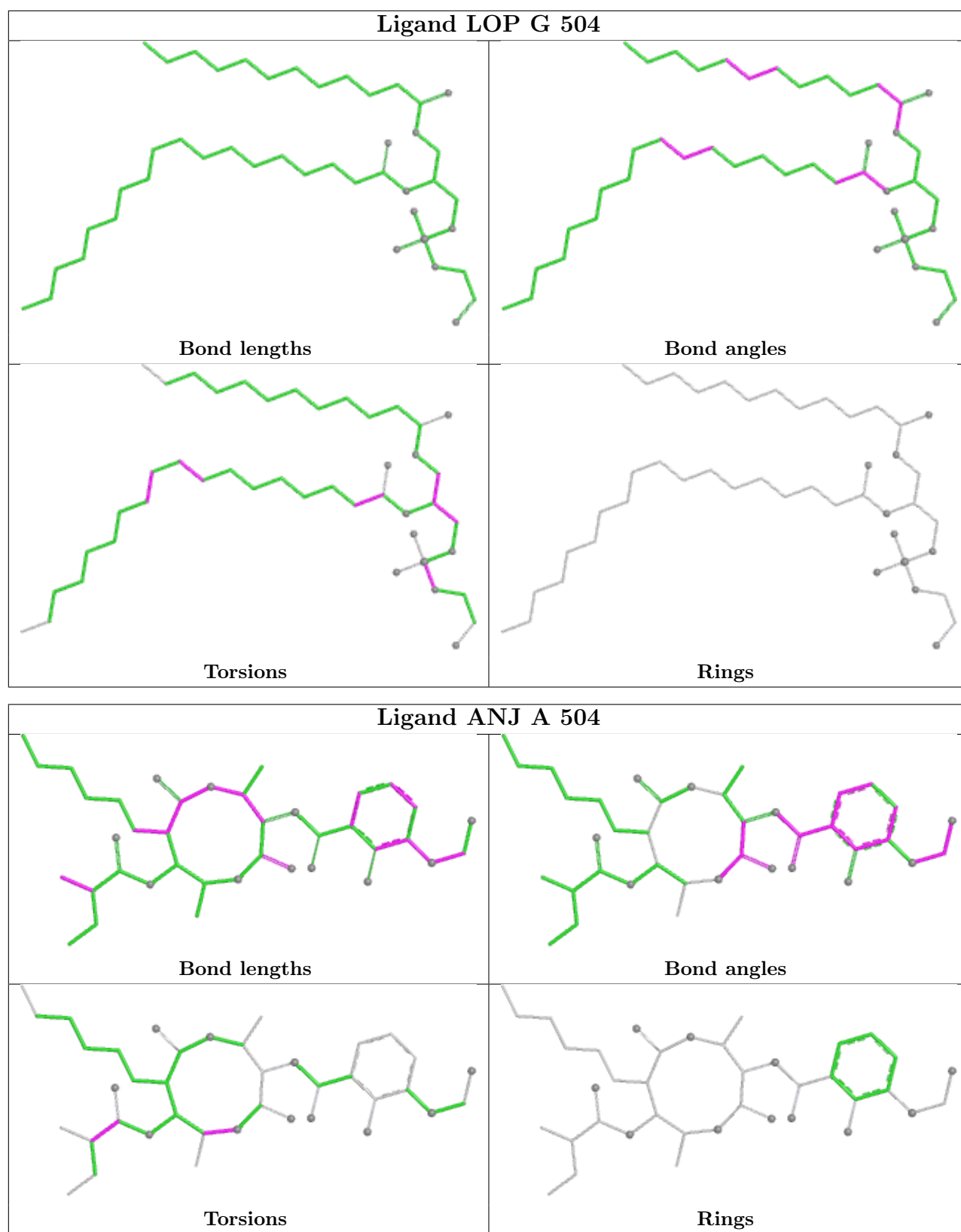
Ligand ANJ P 505

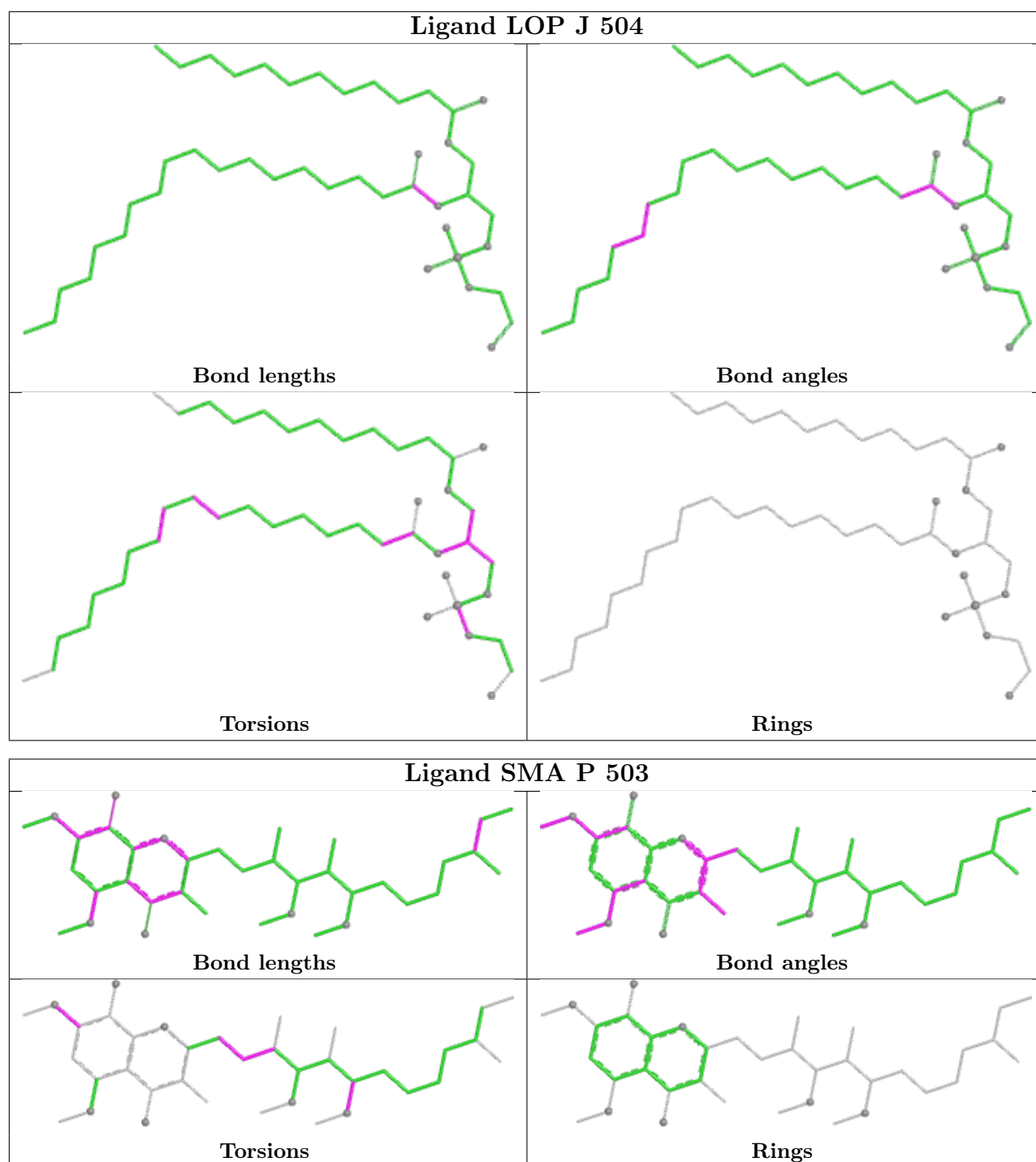


Ligand ANJ G 505









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	428/428 (100%)	-0.50	0 100 100	31, 60, 105, 139	0
1	D	428/428 (100%)	-0.46	0 100 100	33, 59, 109, 147	0
1	G	428/428 (100%)	-0.36	1 (0%) 91 83	34, 63, 113, 153	0
1	J	428/428 (100%)	-0.32	0 100 100	36, 65, 113, 164	0
1	M	428/428 (100%)	-0.29	2 (0%) 87 73	41, 71, 117, 157	0
1	P	428/428 (100%)	-0.40	1 (0%) 91 83	40, 64, 116, 162	0
2	B	256/256 (100%)	-0.10	1 (0%) 88 76	54, 90, 138, 176	0
2	E	256/256 (100%)	-0.02	1 (0%) 88 76	47, 89, 141, 172	0
2	H	256/256 (100%)	0.06	4 (1%) 70 49	41, 88, 139, 179	0
2	K	256/256 (100%)	0.05	6 (2%) 61 39	49, 95, 141, 173	0
2	N	256/256 (100%)	0.21	5 (1%) 65 44	64, 104, 148, 177	0
2	Q	256/256 (100%)	0.17	3 (1%) 76 58	59, 99, 148, 174	0
3	C	179/179 (100%)	-0.41	1 (0%) 85 70	38, 67, 125, 186	0
3	F	179/179 (100%)	-0.27	1 (0%) 85 70	42, 70, 127, 184	0
3	I	179/179 (100%)	-0.24	2 (1%) 78 59	44, 70, 124, 183	0
3	L	179/179 (100%)	-0.29	1 (0%) 85 70	39, 68, 129, 183	0
3	O	179/179 (100%)	-0.28	1 (0%) 85 70	44, 75, 131, 184	0
3	R	179/179 (100%)	0.05	0 100 100	49, 86, 130, 181	0
All	All	5178/5178 (100%)	-0.22	30 (0%) 85 70	31, 75, 132, 186	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	124	GLY	5.6
2	H	1	ALA	3.9
2	Q	123	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
2	K	120	GLN	3.3
2	H	251	LEU	3.2
2	K	1	ALA	3.1
3	I	181	GLU	3.1
3	O	16	TYR	2.5
2	K	110	PHE	2.5
1	M	385	THR	2.5
1	M	3	GLY	2.4
2	N	109	GLY	2.4
2	H	114	MET	2.4
3	C	9	GLY	2.4
3	L	15	LEU	2.4
1	G	310	ALA	2.3
2	K	145	CYS	2.2
3	F	108	GLU	2.2
2	Q	110	PHE	2.2
2	H	123	ASN	2.2
2	N	16	PRO	2.2
1	P	6	HIS	2.2
2	Q	6	VAL	2.1
2	E	1	ALA	2.1
2	N	11	PHE	2.1
2	N	6	VAL	2.1
2	K	125	ILE	2.1
3	I	10	THR	2.1
2	B	118	ILE	2.0
2	N	110	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

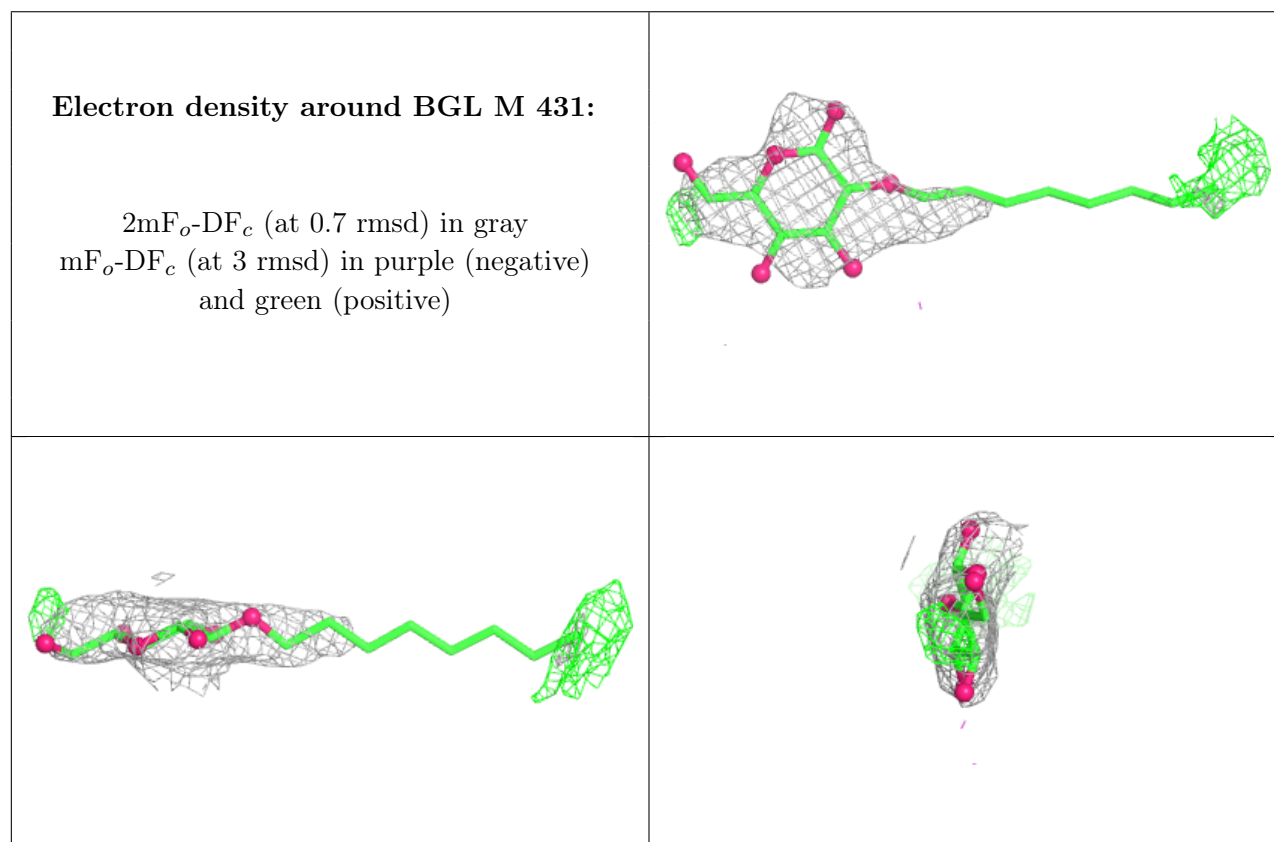
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BGL	M	431	20/20	0.64	0.23	120,124,128,129	0
4	BGL	Q	257	20/20	0.76	0.18	94,99,103,103	0
7	LOP	G	504	45/45	0.79	0.19	91,111,130,131	0
7	LOP	J	504	45/45	0.80	0.20	105,143,157,158	0
7	LOP	M	504	45/45	0.80	0.19	91,121,132,133	0
4	BGL	G	431	20/20	0.81	0.18	93,98,109,109	0
4	BGL	J	431	20/20	0.82	0.15	94,99,103,104	0
4	BGL	A	431	20/20	0.82	0.19	90,98,102,104	0
4	BGL	D	431	20/20	0.85	0.12	79,86,88,89	0
7	LOP	P	504	45/45	0.85	0.16	63,98,114,118	0
7	LOP	A	503	45/45	0.86	0.14	62,89,101,105	0
8	ANJ	J	505	39/39	0.89	0.14	88,96,102,104	0
8	ANJ	A	504	39/39	0.91	0.12	57,73,93,96	0
8	ANJ	G	505	39/39	0.91	0.12	52,75,95,98	0
7	LOP	D	503	45/45	0.91	0.12	49,102,111,113	0
9	SR	Q	258	1/1	0.91	0.05	139,139,139,139	0
8	ANJ	P	505	39/39	0.92	0.12	63,74,89,96	0
8	ANJ	M	505	39/39	0.92	0.12	82,96,101,103	0
9	SR	K	257	1/1	0.93	0.05	134,134,134,134	0
8	ANJ	D	504	39/39	0.93	0.10	57,69,84,85	0
6	SMA	A	1	37/37	0.94	0.09	34,49,61,66	0
6	SMA	M	503	37/37	0.94	0.09	50,68,78,80	0
5	HEM	J	501	43/43	0.95	0.11	74,84,95,99	0
6	SMA	D	2	37/37	0.95	0.08	32,44,52,54	0
6	SMA	G	503	37/37	0.95	0.09	37,47,64,67	0
6	SMA	J	503	37/37	0.96	0.09	42,60,69,72	0
9	SR	N	257	1/1	0.96	0.04	153,153,153,153	0
5	HEM	N	301	43/43	0.96	0.10	71,81,87,89	0
5	HEM	G	501	43/43	0.97	0.11	58,71,84,91	0
5	HEM	A	501	43/43	0.97	0.08	39,56,61,62	0
9	SR	E	257	1/1	0.97	0.03	111,111,111,111	0
5	HEM	D	501	43/43	0.97	0.09	50,56,68,73	0
5	HEM	E	301	43/43	0.97	0.09	55,63,79,80	0
6	SMA	P	503	37/37	0.97	0.09	33,47,68,70	0
5	HEM	M	501	43/43	0.98	0.09	73,78,88,91	0
5	HEM	M	502	43/43	0.98	0.09	49,54,64,66	0
5	HEM	B	301	43/43	0.98	0.08	54,59,74,78	0
5	HEM	P	501	43/43	0.98	0.09	58,67,79,85	0
5	HEM	Q	301	43/43	0.98	0.08	64,75,81,82	0
9	SR	B	257	1/1	0.98	0.02	136,136,136,136	0
5	HEM	A	502	43/43	0.98	0.07	14,29,45,49	0

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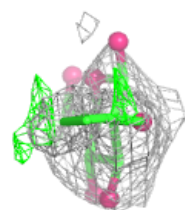
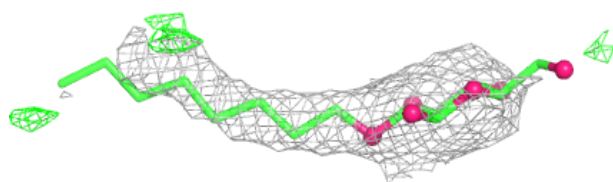
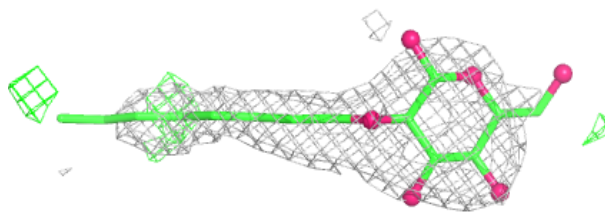
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	SR	H	257	1/1	0.98	0.02	106,106,106,106	0
5	HEM	H	301	43/43	0.98	0.07	39,50,58,60	0
5	HEM	D	502	43/43	0.98	0.07	16,29,46,53	0
5	HEM	K	301	43/43	0.98	0.07	49,60,74,75	0
5	HEM	G	502	43/43	0.99	0.06	22,34,45,51	0
5	HEM	P	502	43/43	0.99	0.07	25,36,48,59	0
5	HEM	J	502	43/43	0.99	0.06	27,37,52,60	0
10	FES	C	200	4/4	0.99	0.03	33,36,40,42	0
10	FES	F	200	4/4	0.99	0.03	42,42,42,45	0
10	FES	O	200	4/4	0.99	0.03	40,43,43,50	0
10	FES	R	200	4/4	0.99	0.03	56,57,58,59	0
10	FES	I	200	4/4	1.00	0.03	45,47,48,50	0
10	FES	L	200	4/4	1.00	0.02	32,34,36,39	0

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

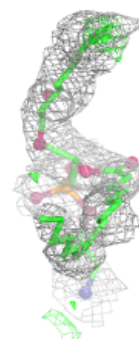
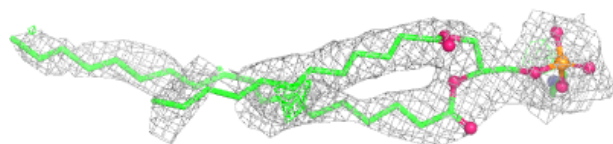
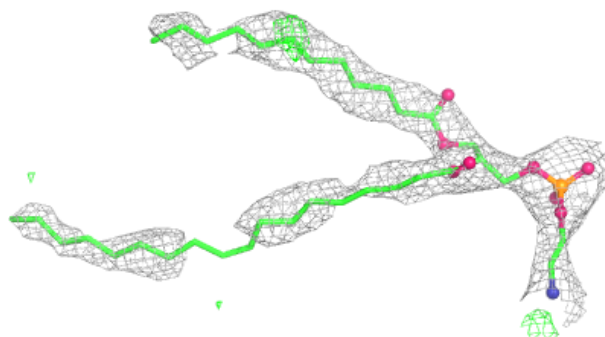


Electron density around BGL Q 257:

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

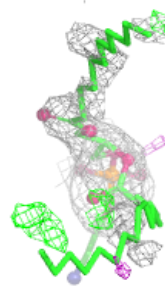
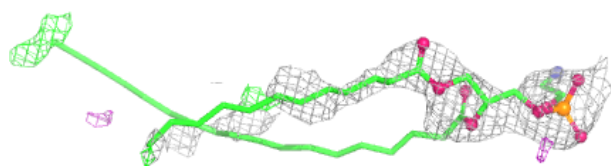
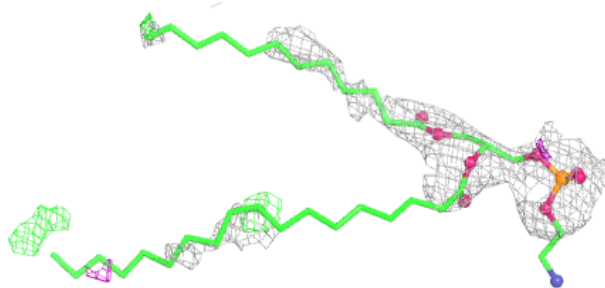
**Electron density around LOP G 504:**

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

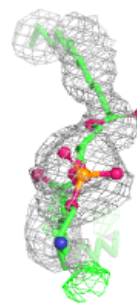
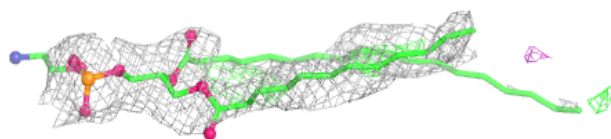
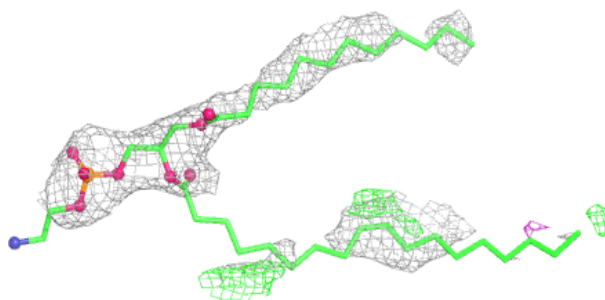


Electron density around LOP J 504:

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

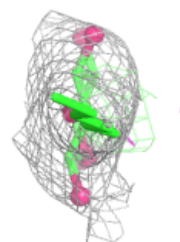
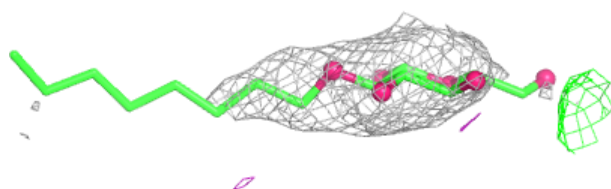
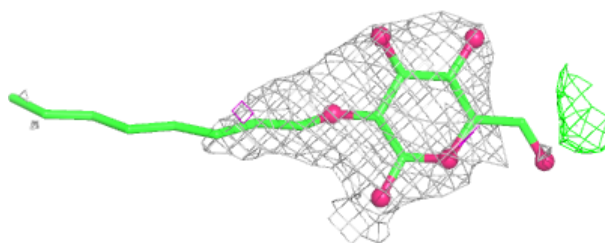
**Electron density around LOP M 504:**

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

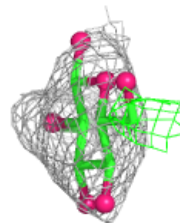
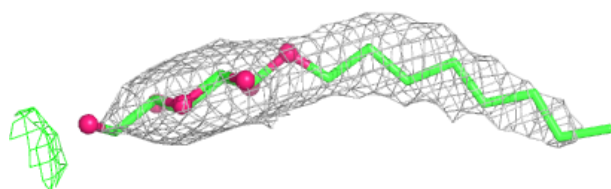
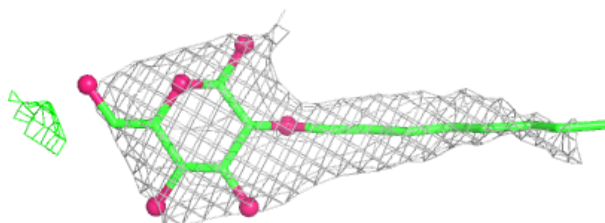


Electron density around BGL G 431:

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

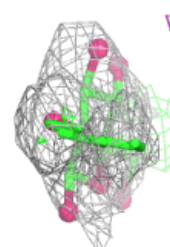
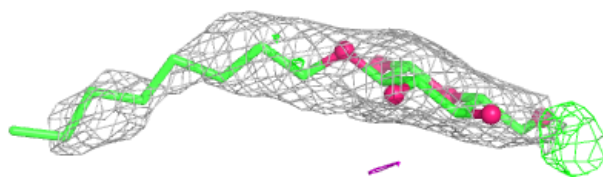
**Electron density around BGL J 431:**

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

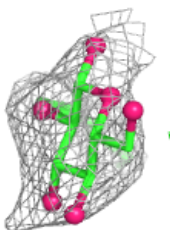
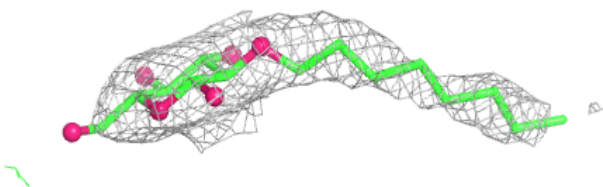


Electron density around BGL A 431:

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

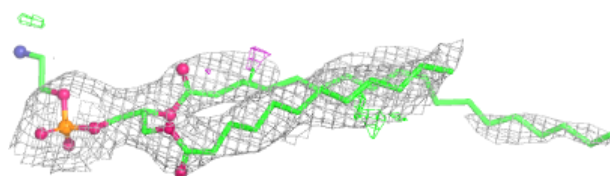
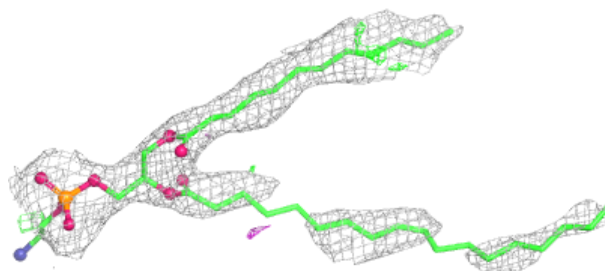
**Electron density around BGL D 431:**

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

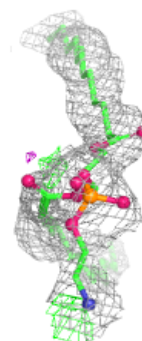
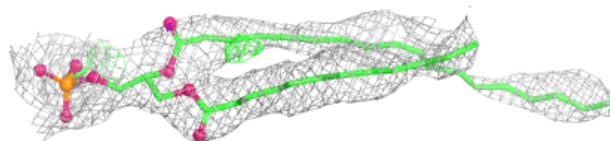
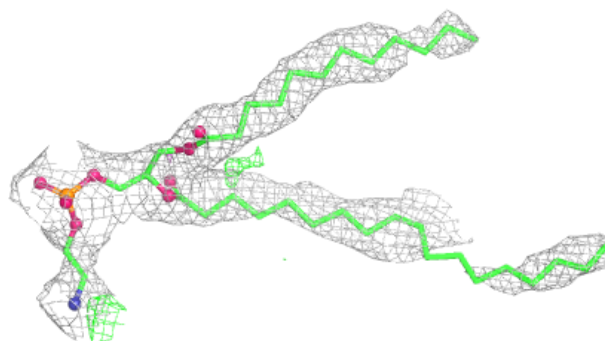


Electron density around LOP P 504:

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

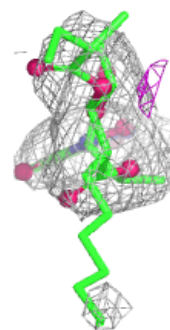
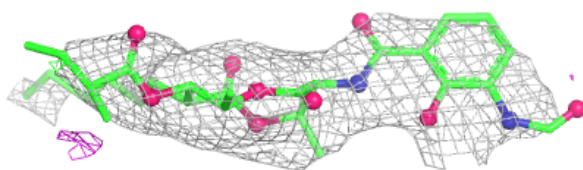
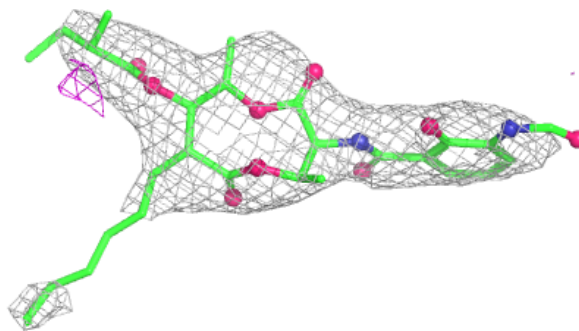
**Electron density around LOP A 503:**

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and green (positive)

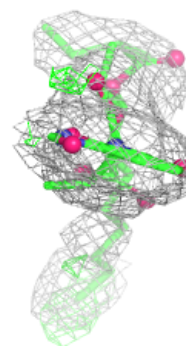
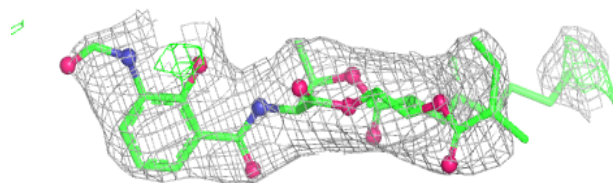
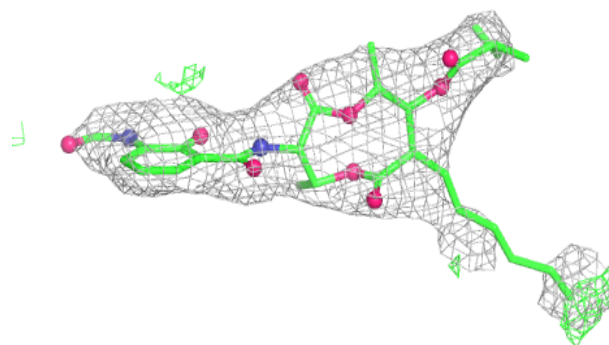


Electron density around ANJ J 505:

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

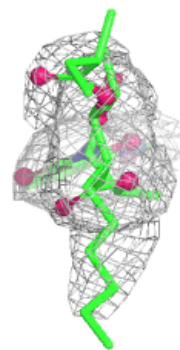
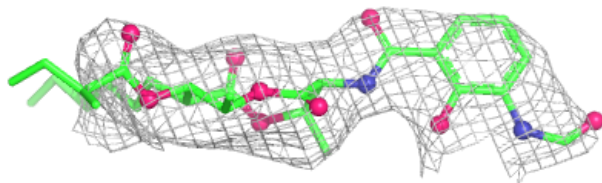
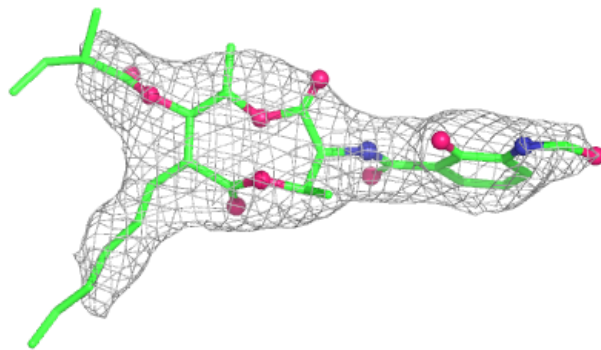
**Electron density around ANJ A 504:**

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

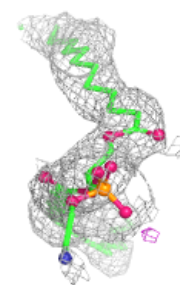
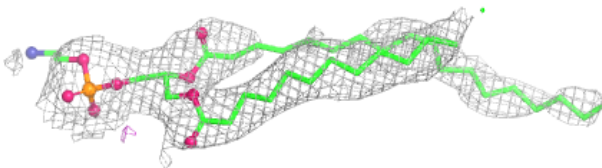
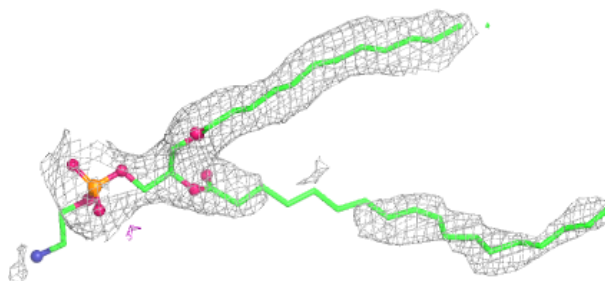


Electron density around ANJ G 505:

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

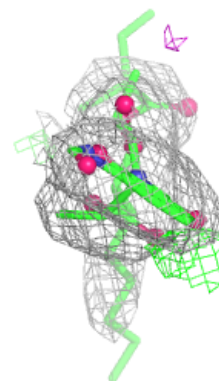
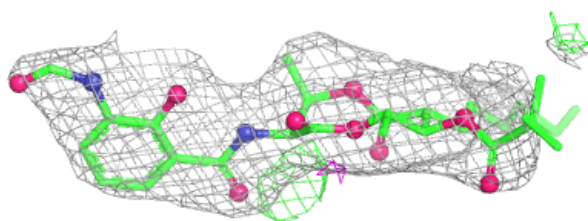
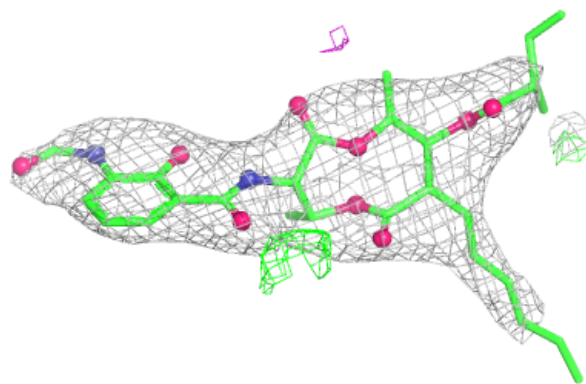
**Electron density around LOP D 503:**

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

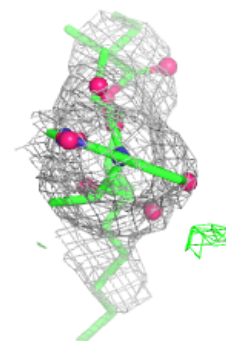
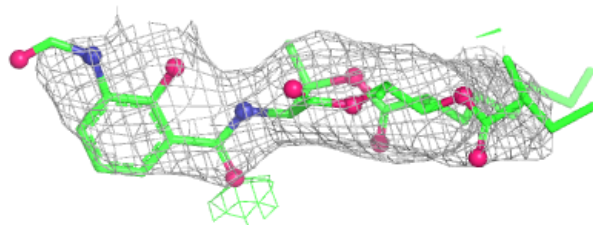
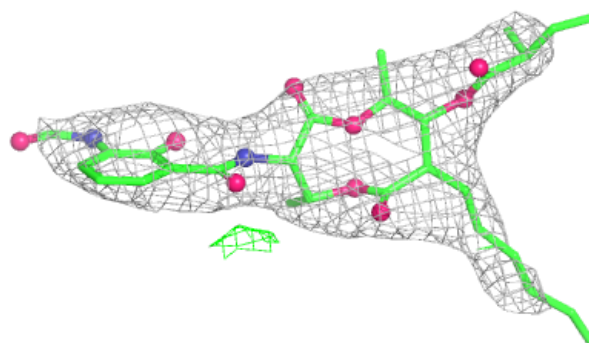


Electron density around ANJ P 505:

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

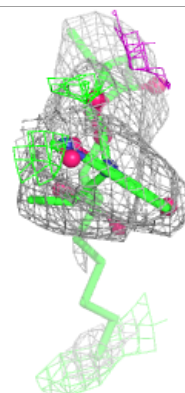
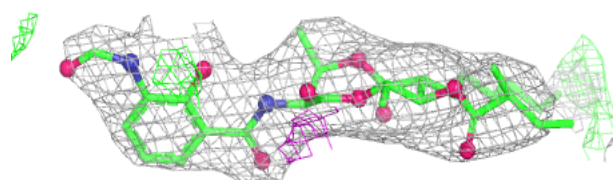
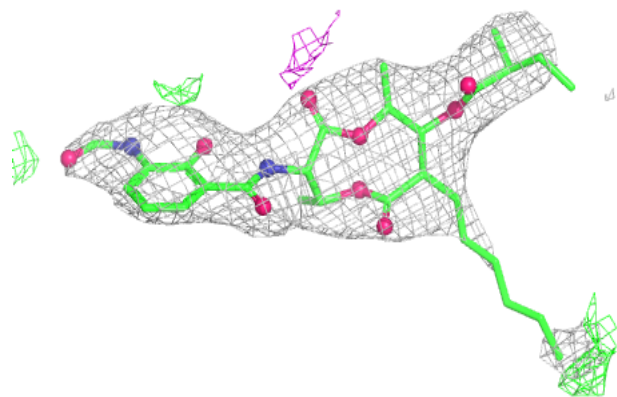
**Electron density around ANJ M 505:**

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

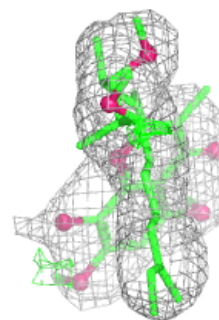
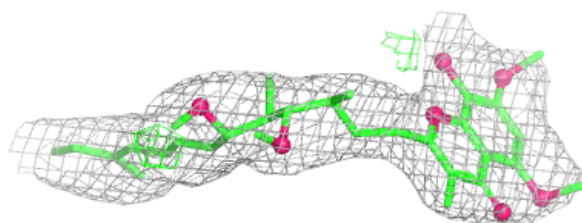


Electron density around ANJ D 504:

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

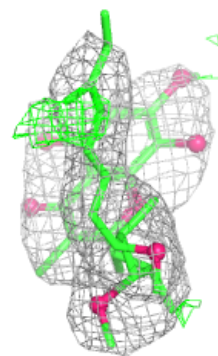
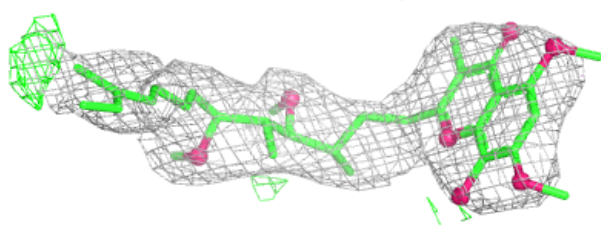
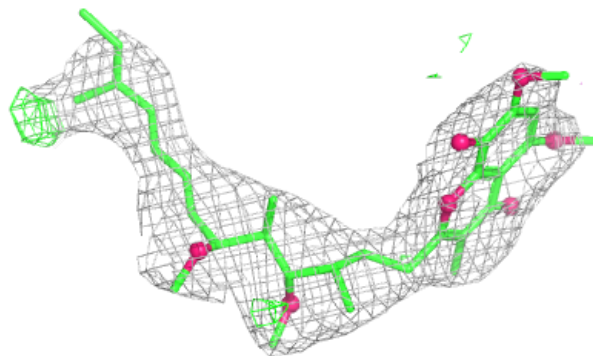
**Electron density around SMA A 1:**

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



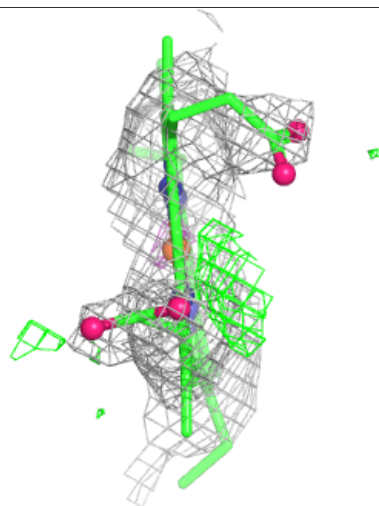
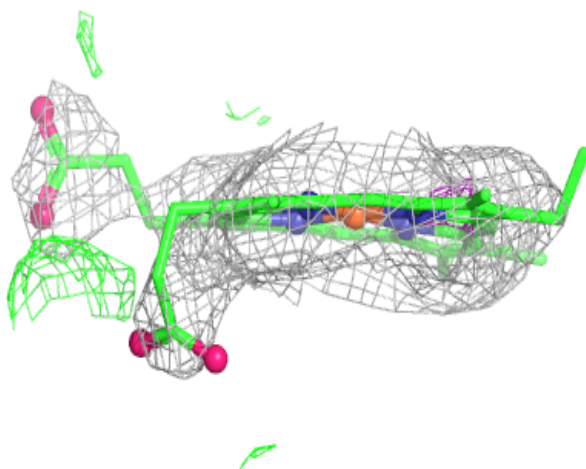
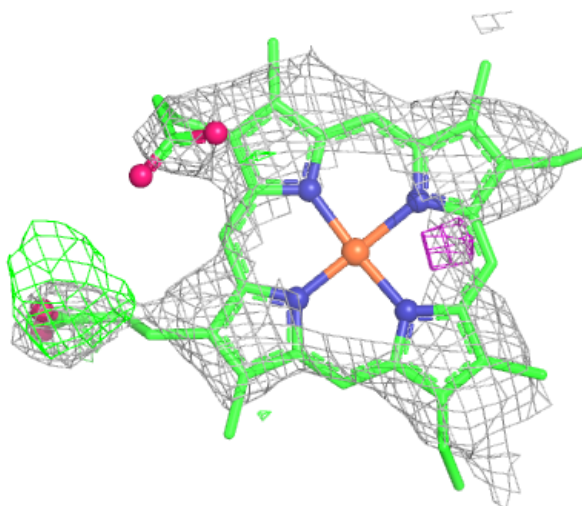
Electron density around SMA M 503:

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



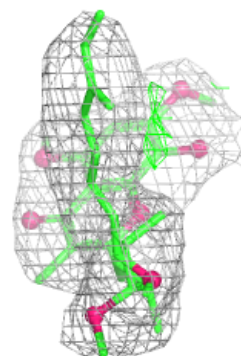
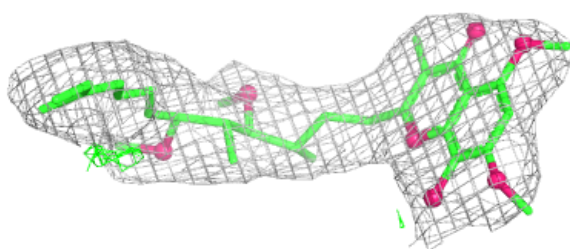
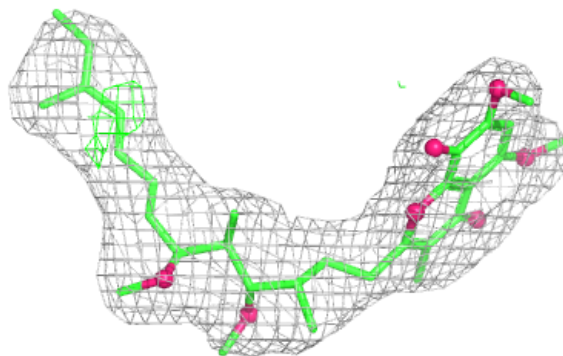
Electron density around HEM J 501:

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

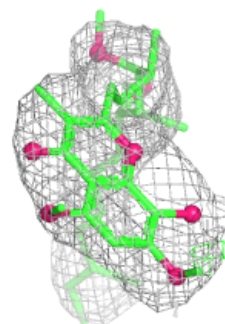
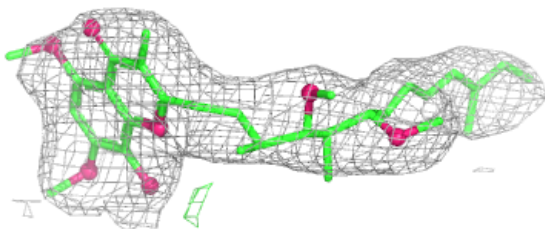
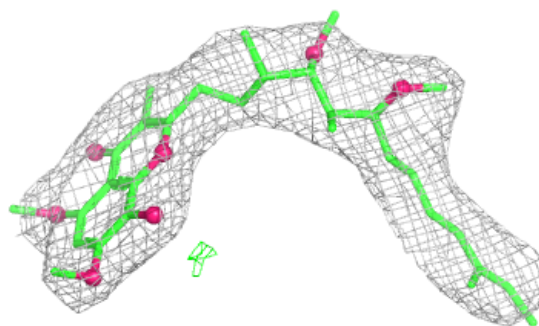


Electron density around SMA D 2:

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

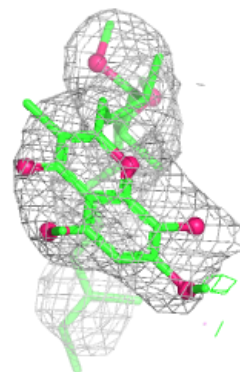
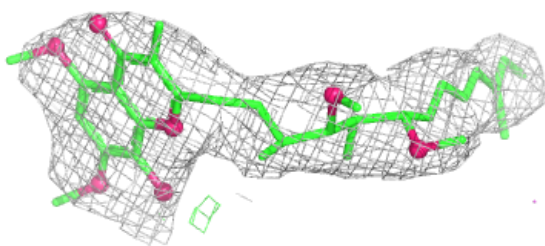
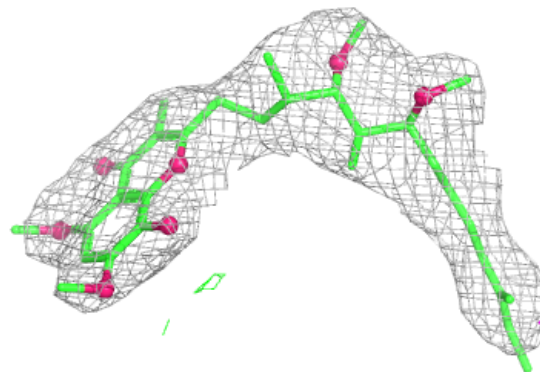
**Electron density around SMA G 503:**

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



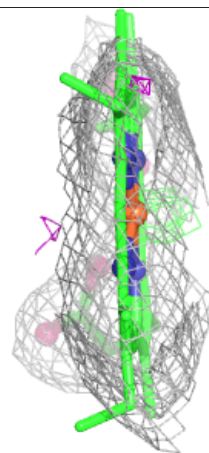
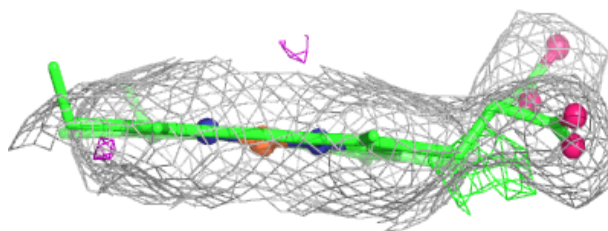
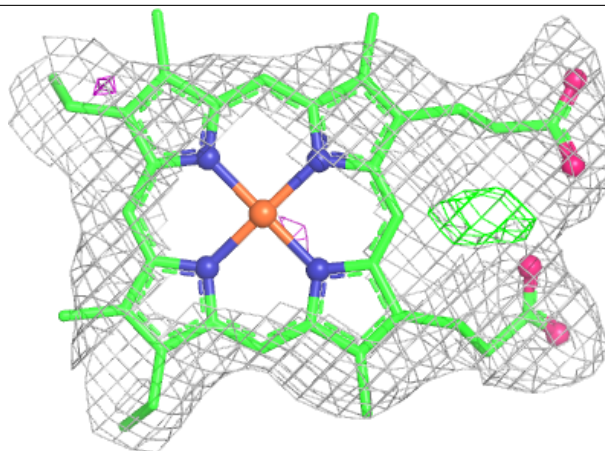
Electron density around SMA J 503:

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



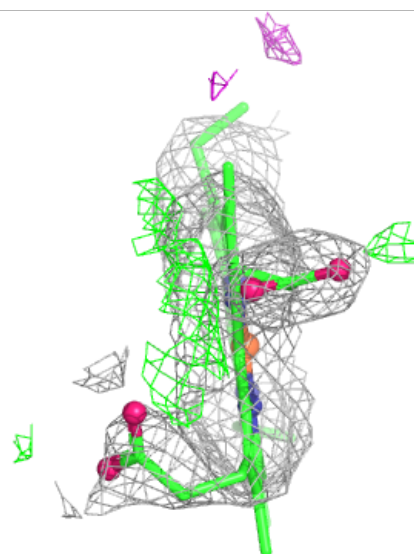
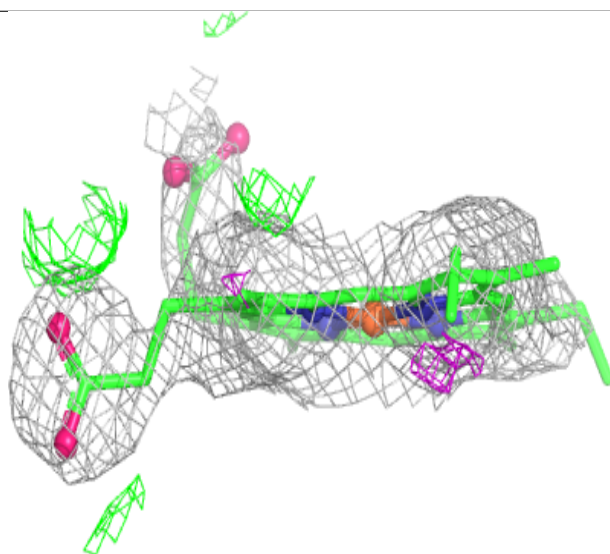
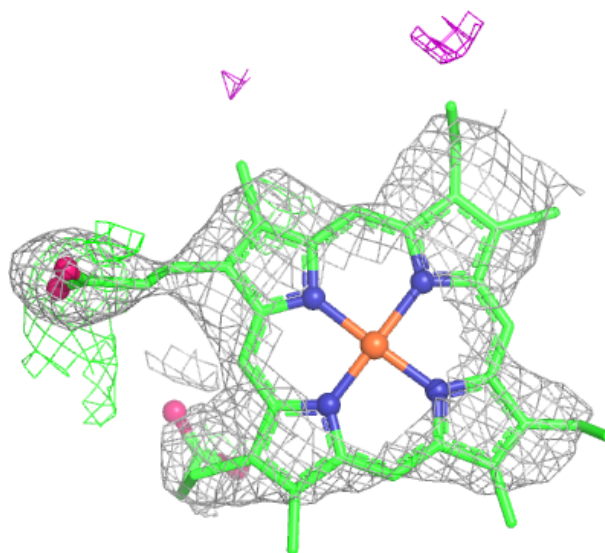
Electron density around HEM N 301:

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



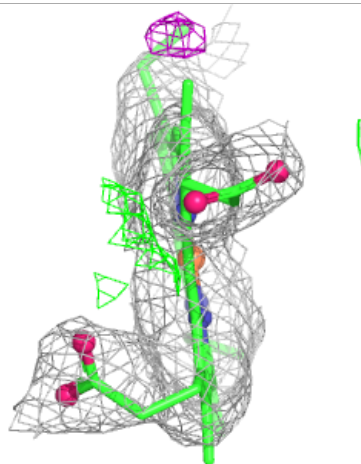
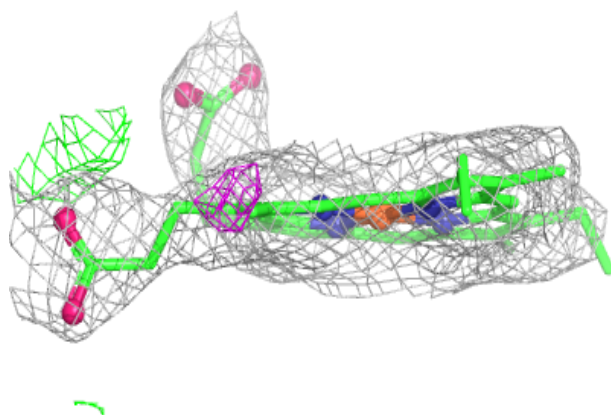
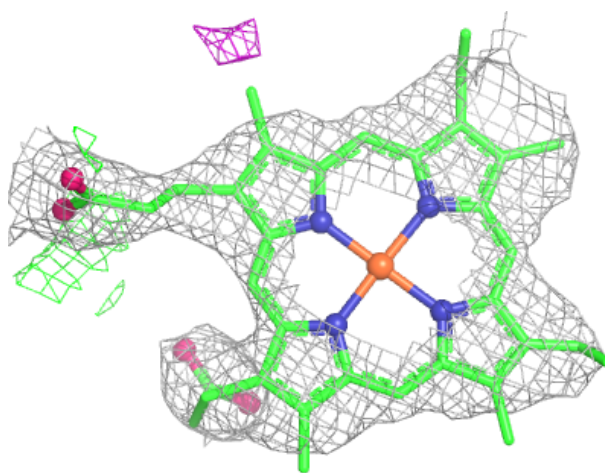
Electron density around HEM G 501:

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



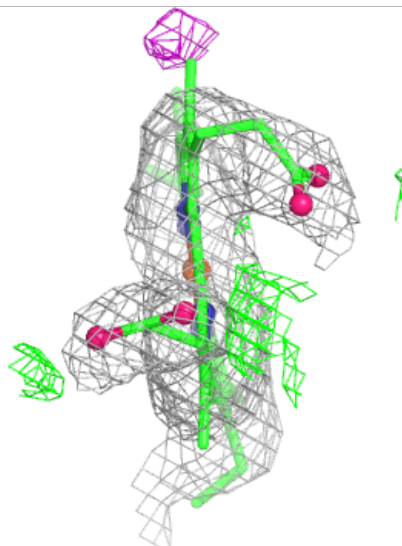
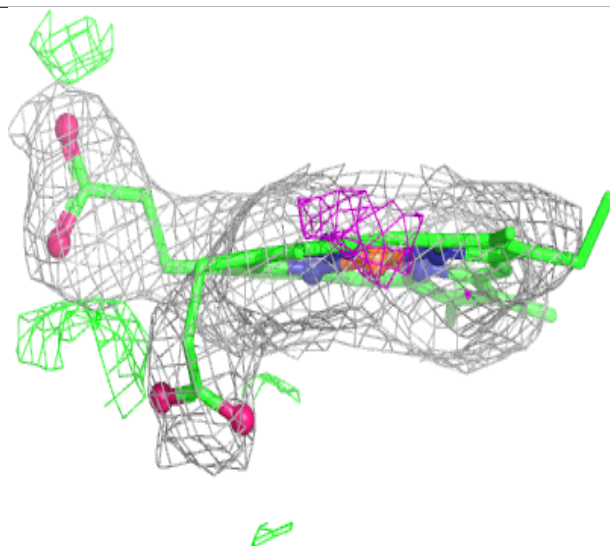
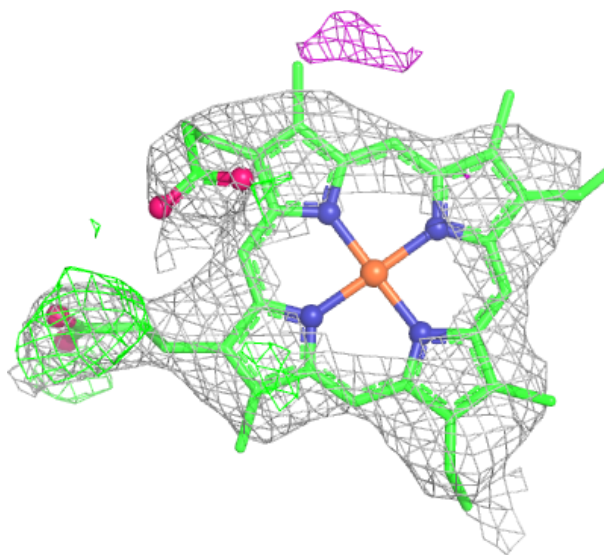
Electron density around HEM A 501:

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



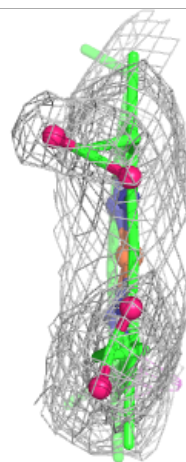
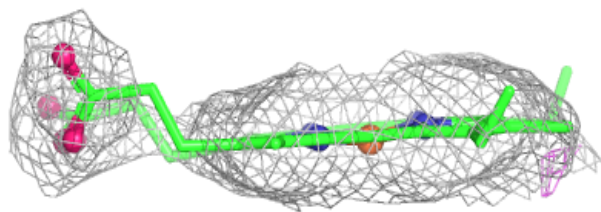
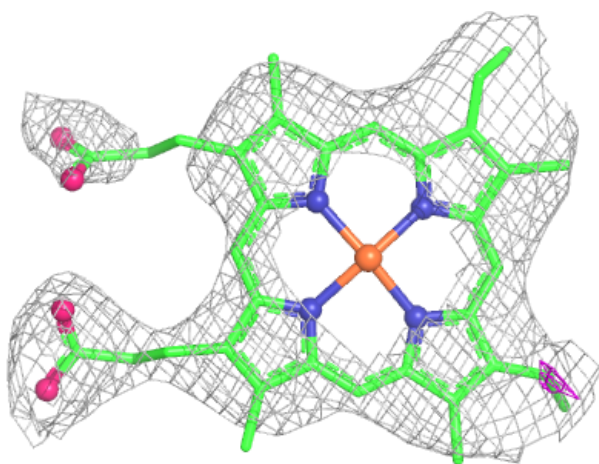
Electron density around HEM D 501:

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



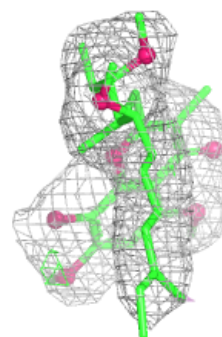
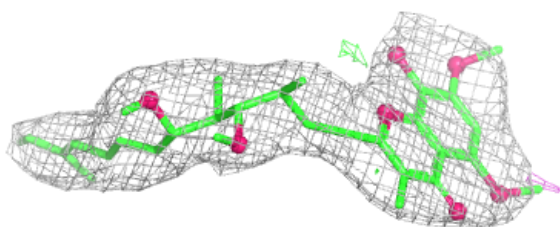
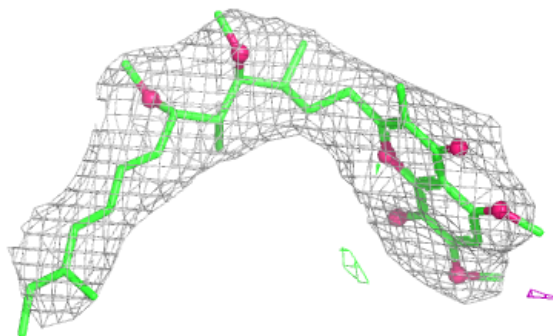
Electron density around HEM E 301:

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



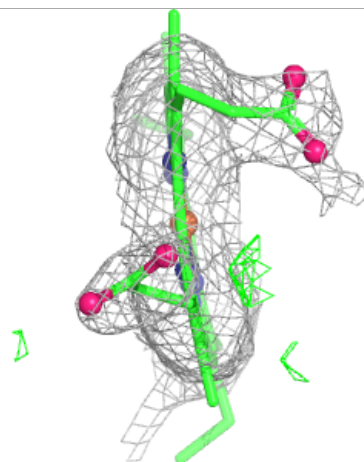
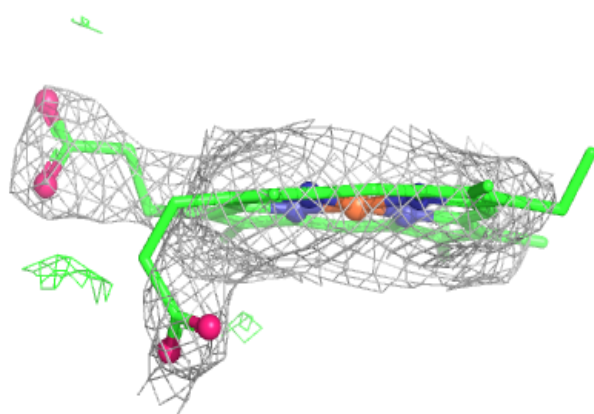
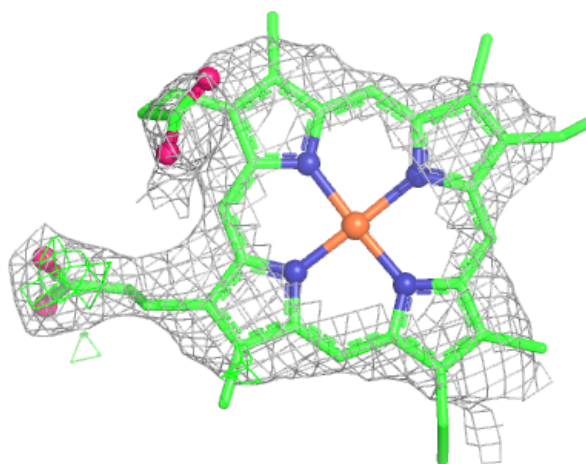
Electron density around SMA P 503:

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



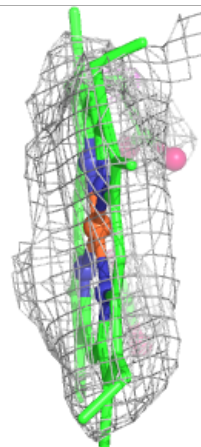
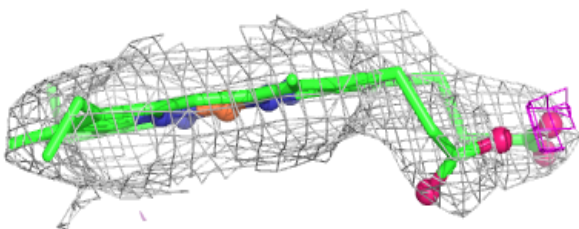
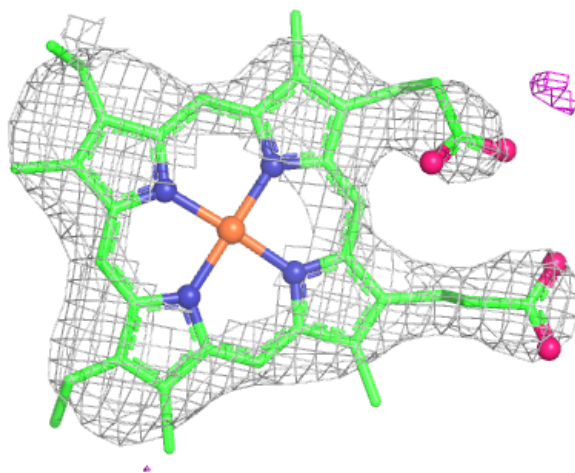
Electron density around HEM M 501:

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



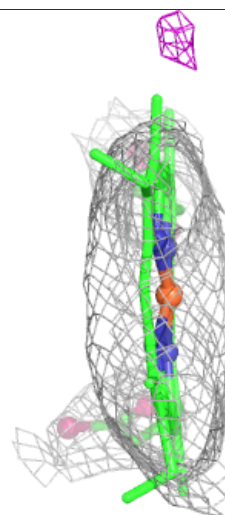
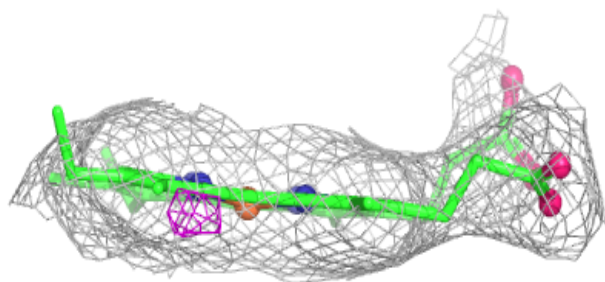
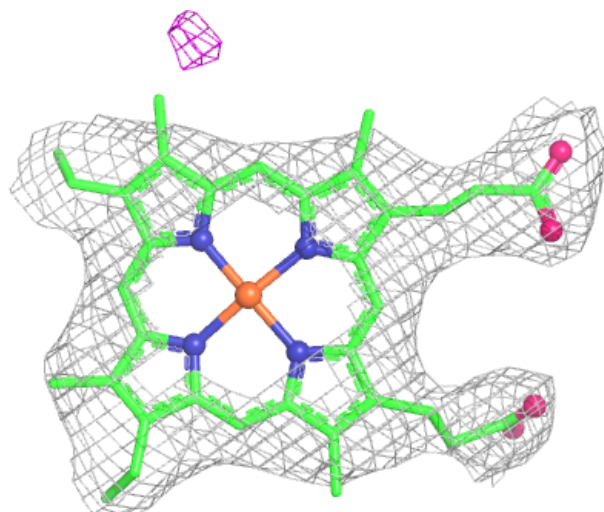
Electron density around HEM M 502:

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



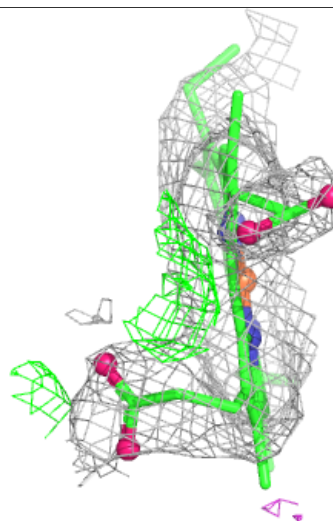
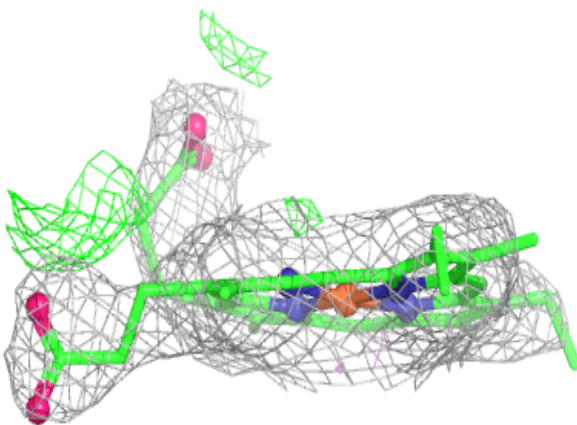
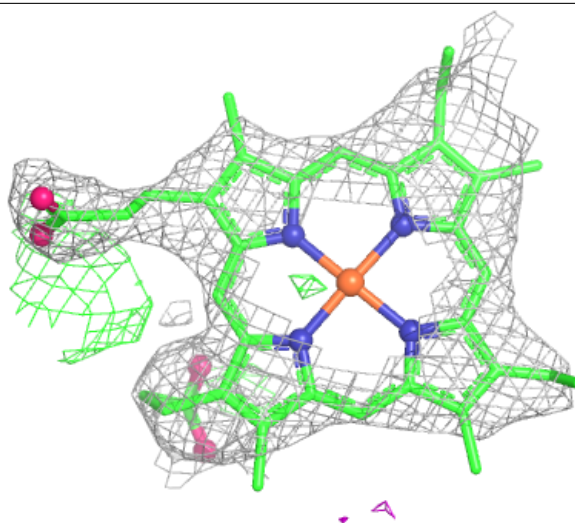
Electron density around HEM B 301:

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



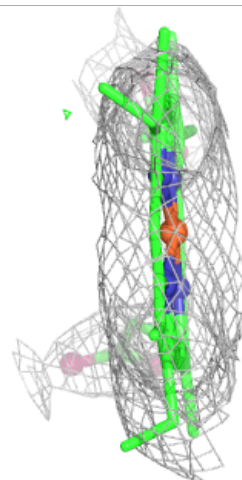
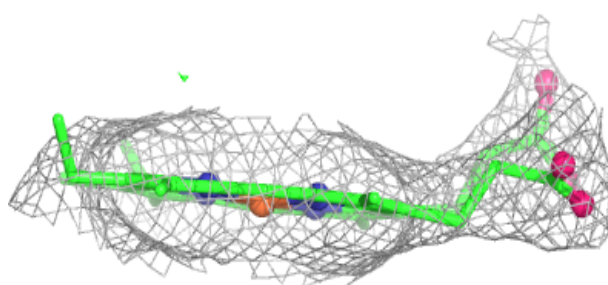
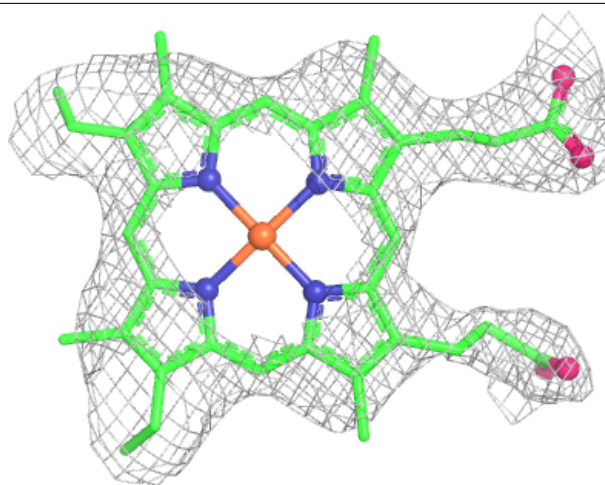
Electron density around HEM P 501:

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



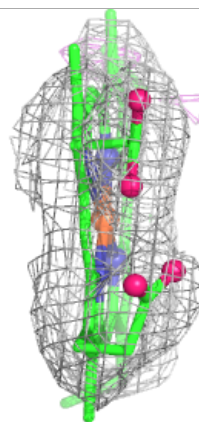
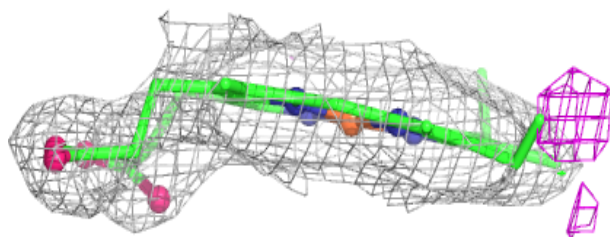
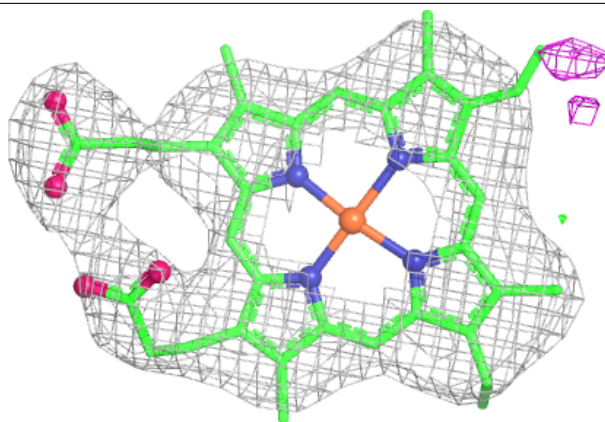
Electron density around HEM Q 301:

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



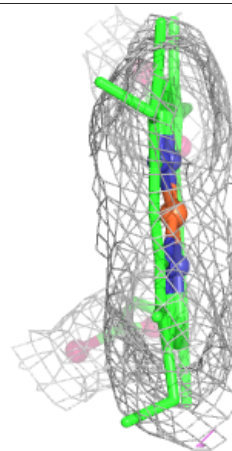
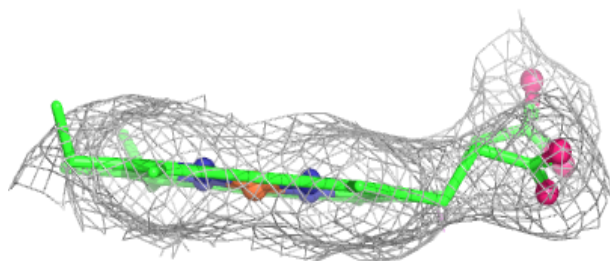
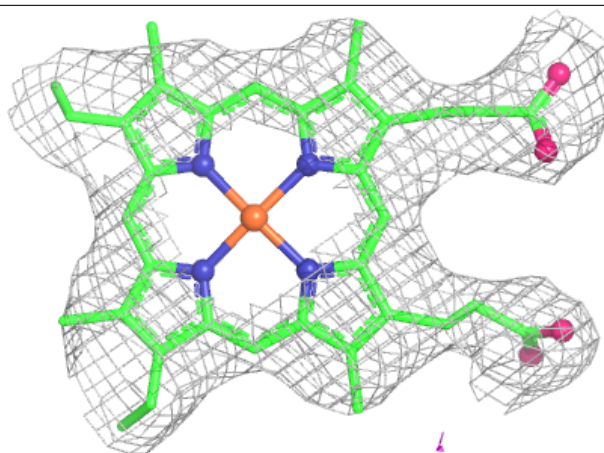
Electron density around HEM A 502:

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



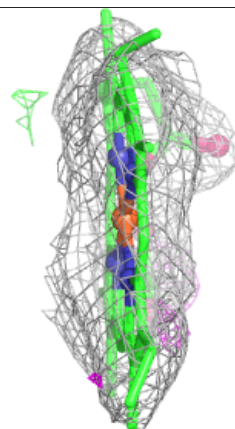
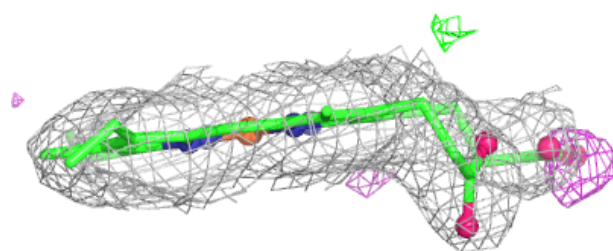
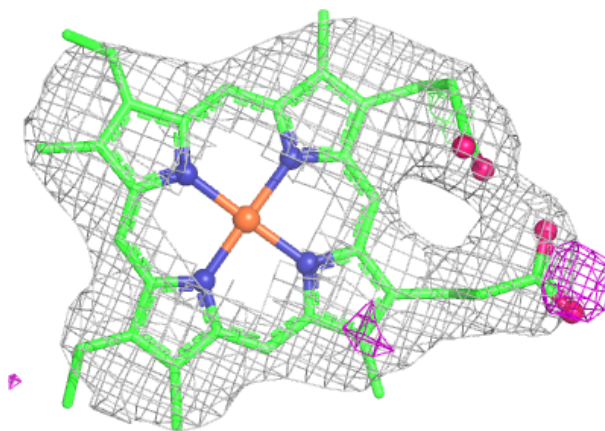
Electron density around HEM H 301:

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



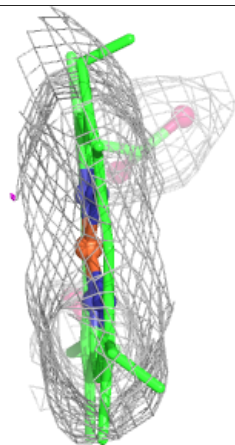
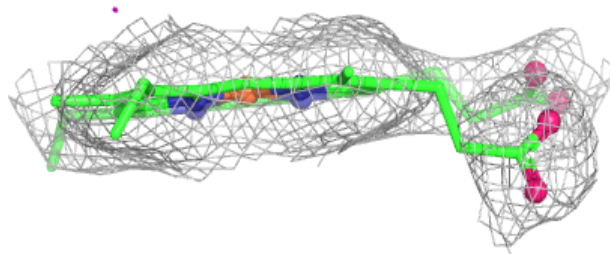
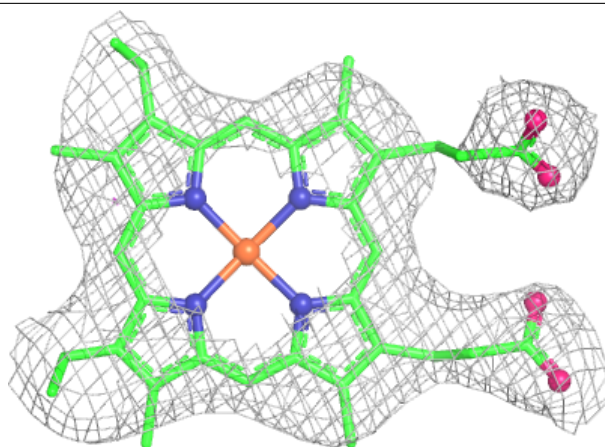
Electron density around HEM D 502:

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



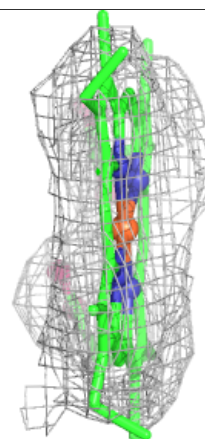
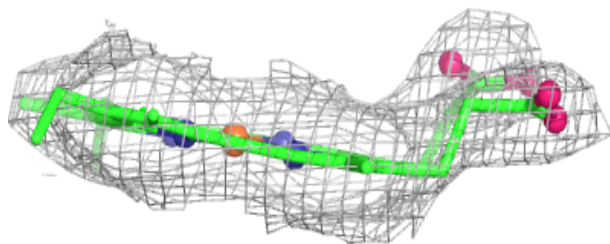
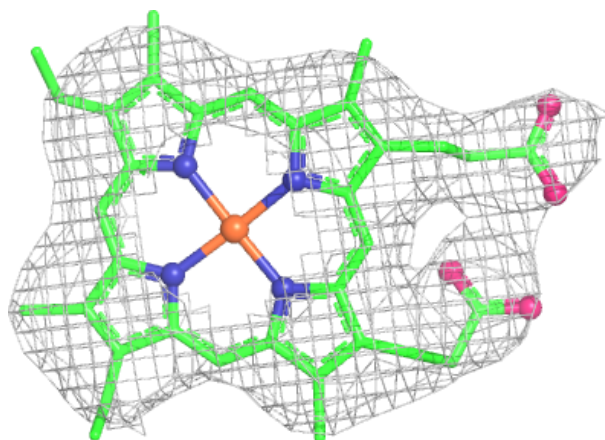
Electron density around HEM K 301:

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



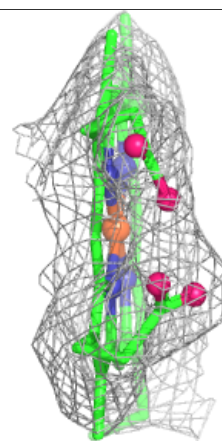
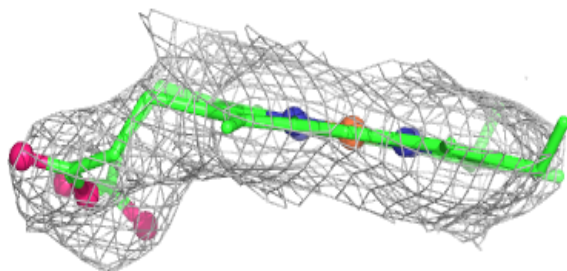
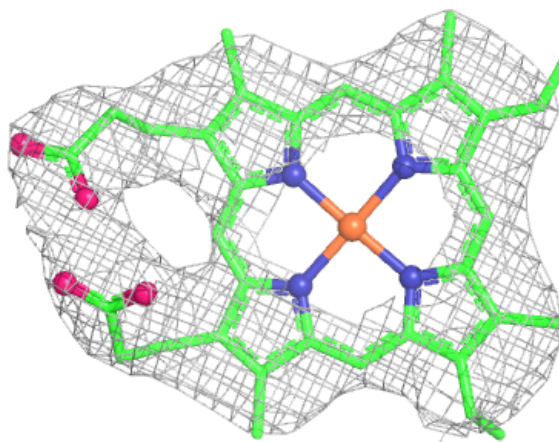
Electron density around HEM G 502:

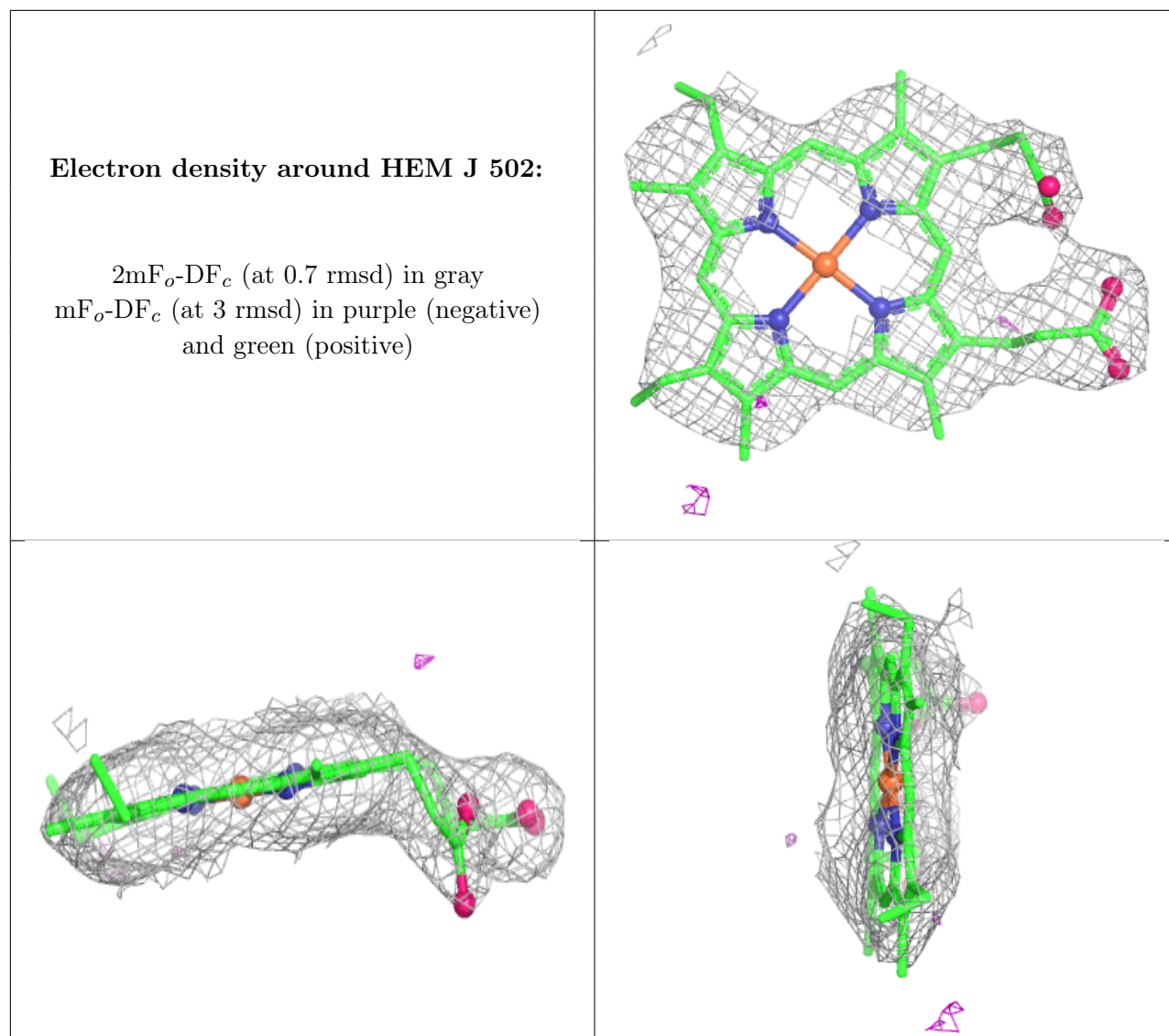
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM P 502:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.