



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:54 AM UTC

PDB ID : 8HKJ / pdb_00008hkj
Title : Crystal structure of the CYP102A5 haem Domain isolated from *Bacillus cereus*
Authors : Stanfield, J.K.; Onoda, H.; Sugimoto, H.; Shoji, O.
Deposited on : 2022-11-27
Resolution : 2.80 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:

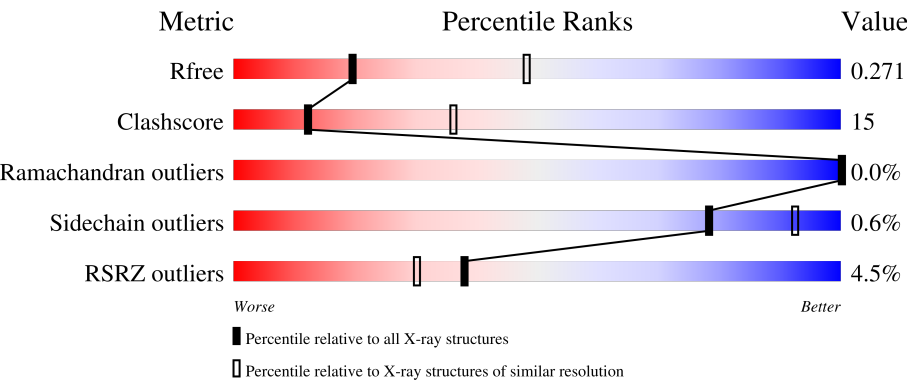
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	458	% 71% 22% 6%
1	B	458	% 66% 28% 6%
1	C	458	% 67% 24% 8%
1	D	458	67% 24% 9%
1	E	458	66% 26% 8%

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Mol	Chain	Length	Quality of chain
1	F	458	% 66% 26% 9%
1	G	458	3% 60% 27% 12%
1	H	458	3% 60% 30% 9%
1	I	458	9% 50% 37% 13%
1	J	458	9% 54% 36% 9%
1	K	458	8% 54% 37% 9%
1	L	458	12% 55% 35% 10%

2 Entry composition

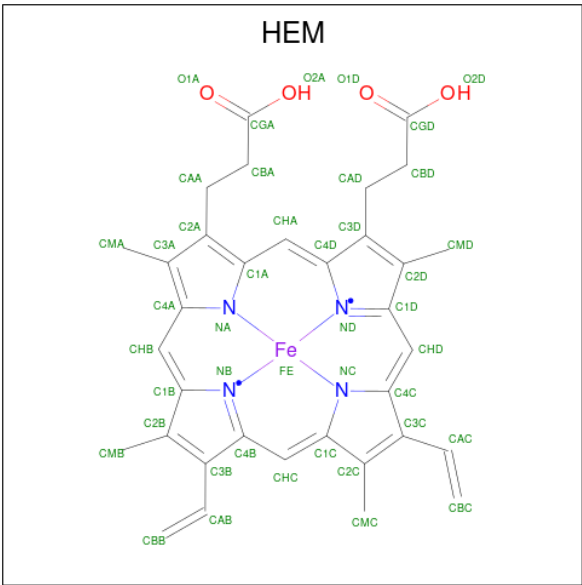
There are 3 unique types of molecules in this entry. The entry contains 41062 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional cytochrome P450/NADPH-P450 reductase.

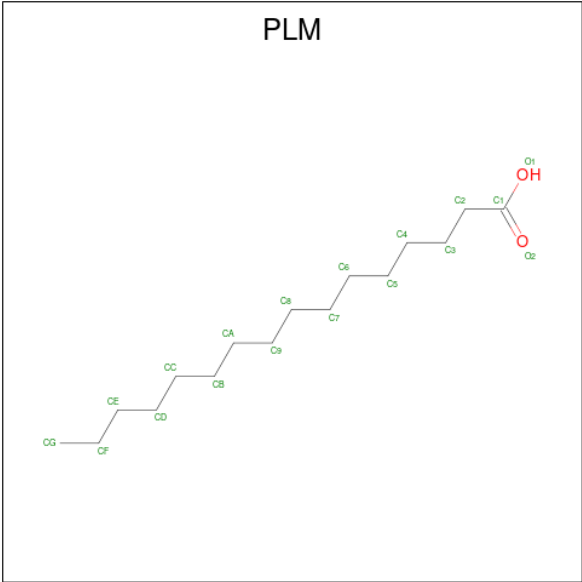
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3460	2213	582	648	17			
1	B	430	Total	C	N	O	S	0	0	0
			3473	2221	585	649	18			
1	C	421	Total	C	N	O	S	0	0	0
			3400	2180	569	634	17			
1	D	419	Total	C	N	O	S	0	0	0
			3380	2170	566	627	17			
1	E	422	Total	C	N	O	S	0	0	0
			3406	2183	574	632	17			
1	F	419	Total	C	N	O	S	0	0	0
			3382	2171	569	625	17			
1	G	401	Total	C	N	O	S	0	0	0
			3238	2084	542	595	17			
1	H	415	Total	C	N	O	S	0	0	0
			3354	2154	563	620	17			
1	I	399	Total	C	N	O	S	0	0	0
			3223	2075	538	594	16			
1	J	415	Total	C	N	O	S	0	0	0
			3351	2153	562	619	17			
1	K	416	Total	C	N	O	S	0	0	0
			3357	2154	564	622	17			
1	L	410	Total	C	N	O	S	0	0	0
			3306	2126	551	612	17			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).

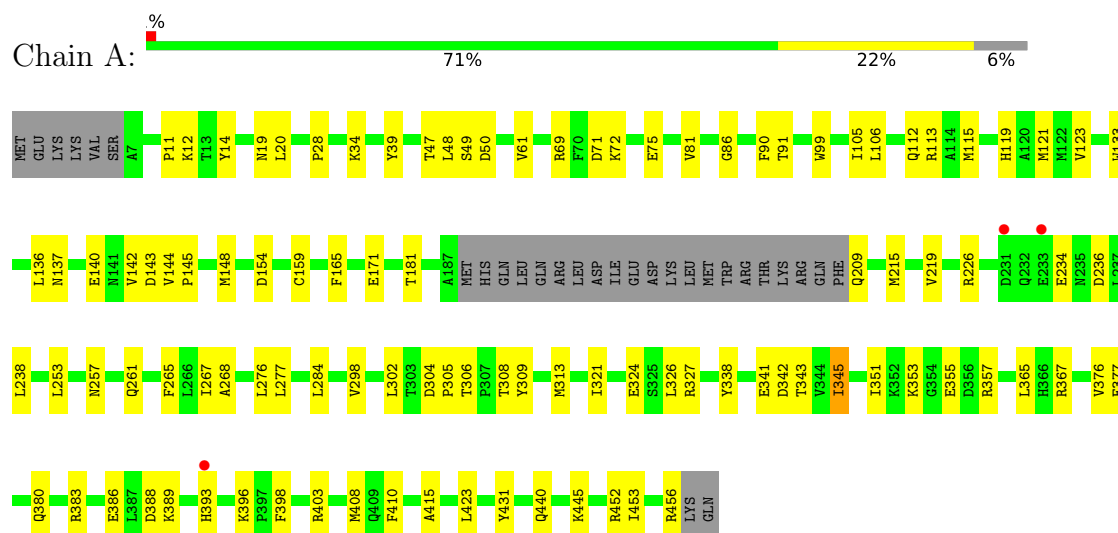


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			18	16	2		
3	B	1	Total	C	O	0	0
			18	16	2		
3	C	1	Total	C	O	0	0
			18	16	2		
3	D	1	Total	C	O	0	0
			18	16	2		
3	D	1	Total	C	O	0	0
			18	16	2		
3	E	1	Total	C	O	0	0
			18	16	2		
3	G	1	Total	C	O	0	0
			18	16	2		
3	H	1	Total	C	O	0	0
			18	16	2		
3	I	1	Total	C	O	0	0
			18	16	2		
3	J	1	Total	C	O	0	0
			18	16	2		
3	K	1	Total	C	O	0	0
			18	16	2		
3	L	1	Total	C	O	0	0
			18	16	2		

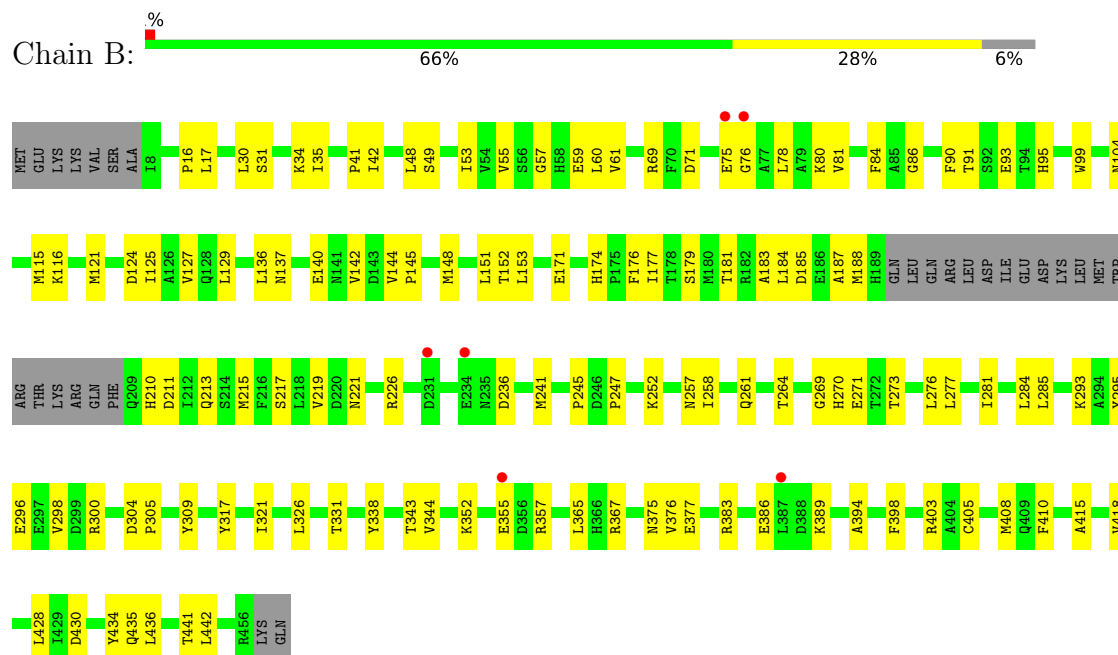
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

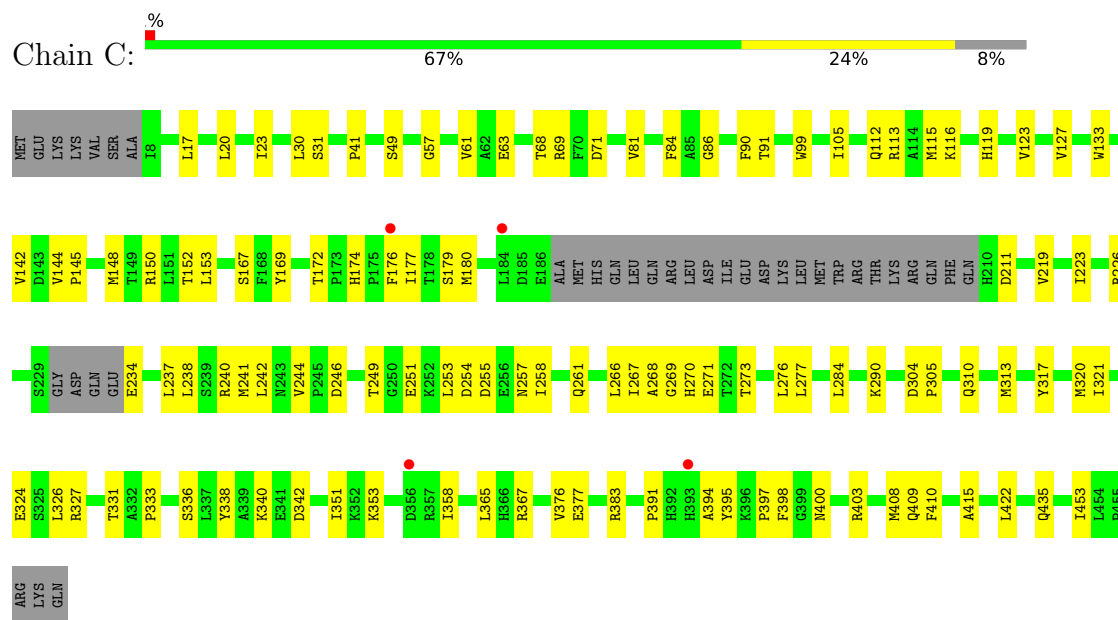
- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



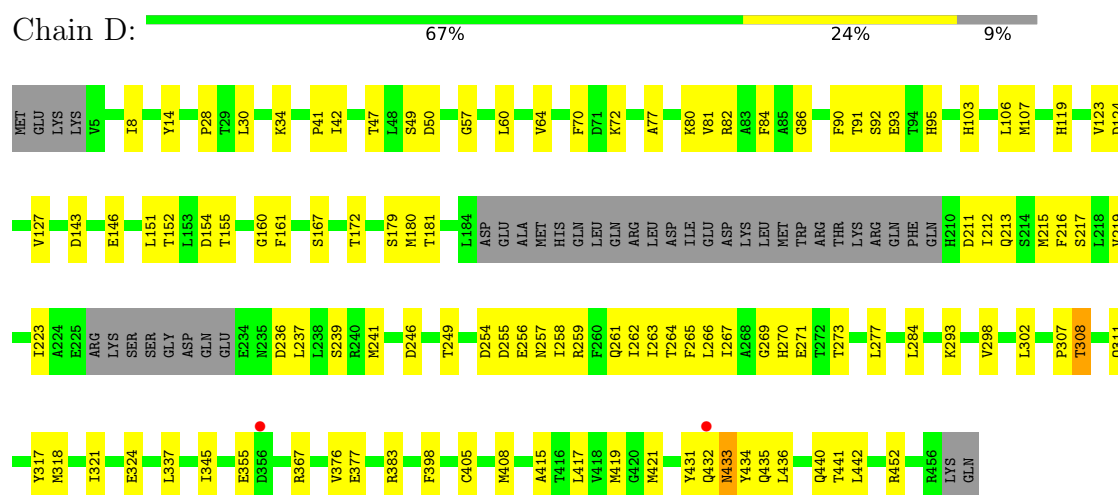
- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



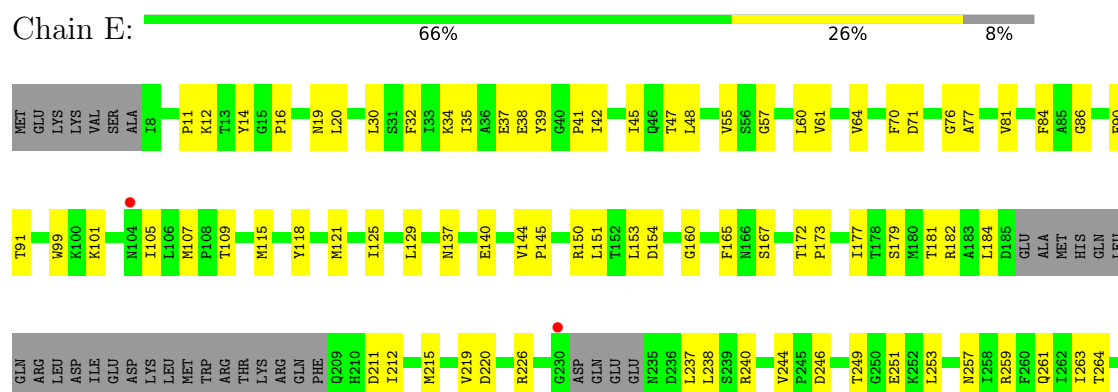
• Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

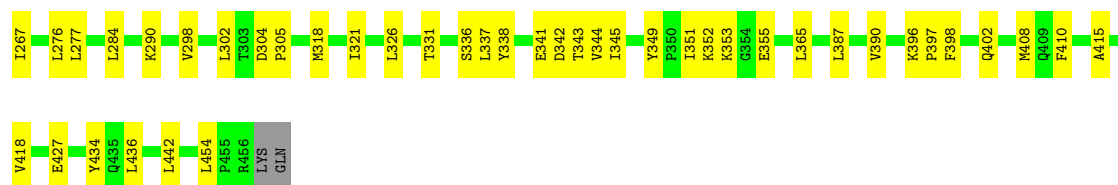


• Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

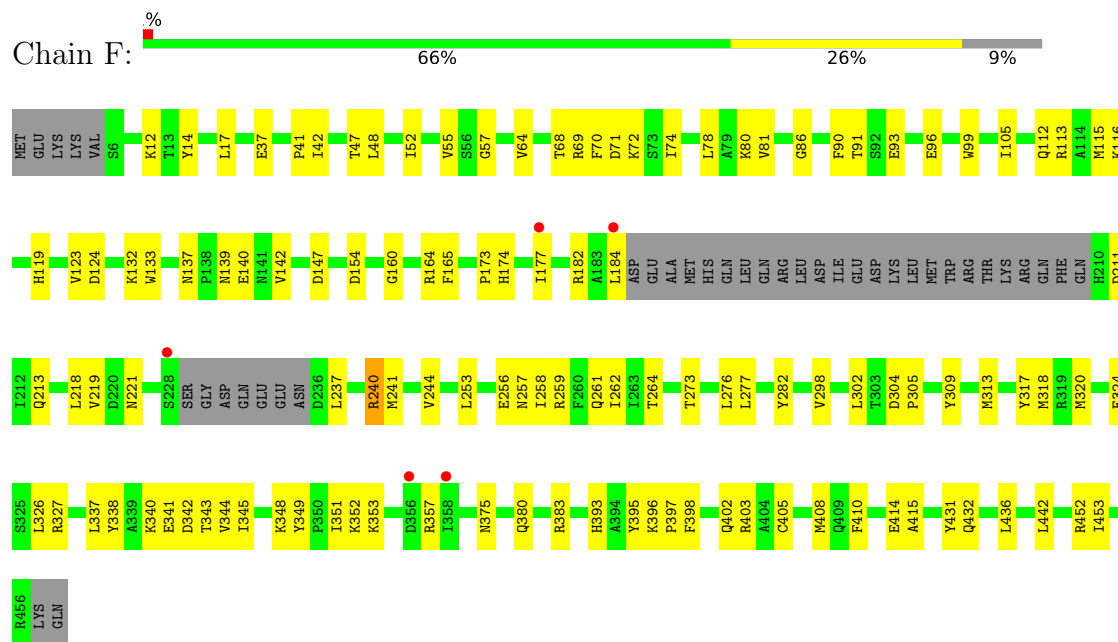


• Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

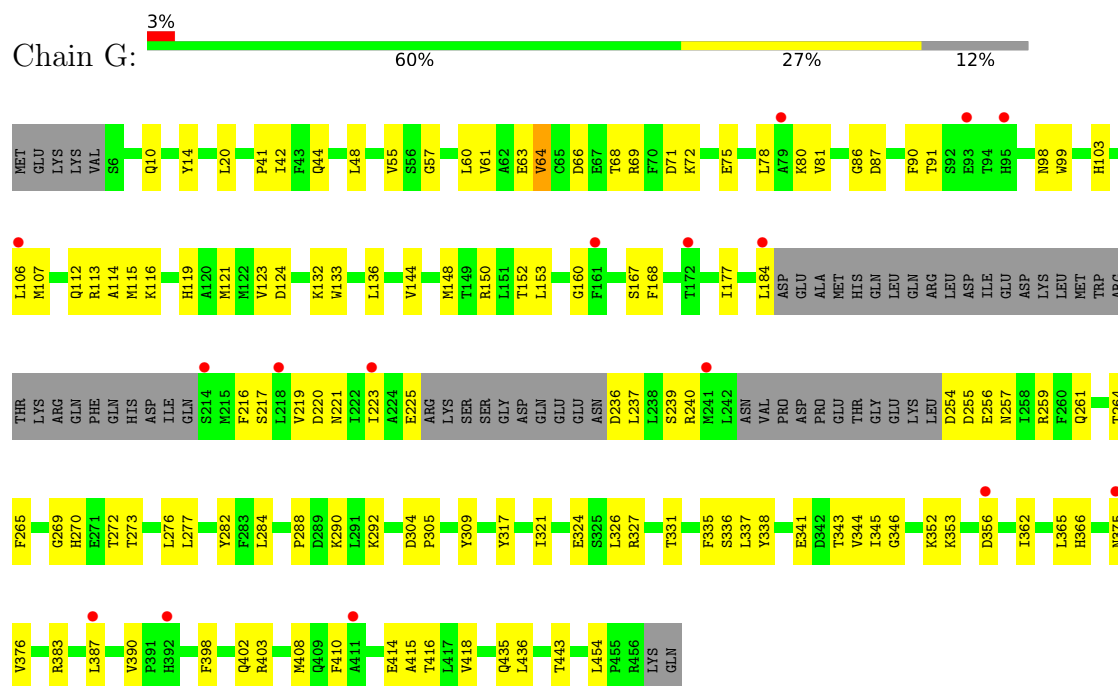




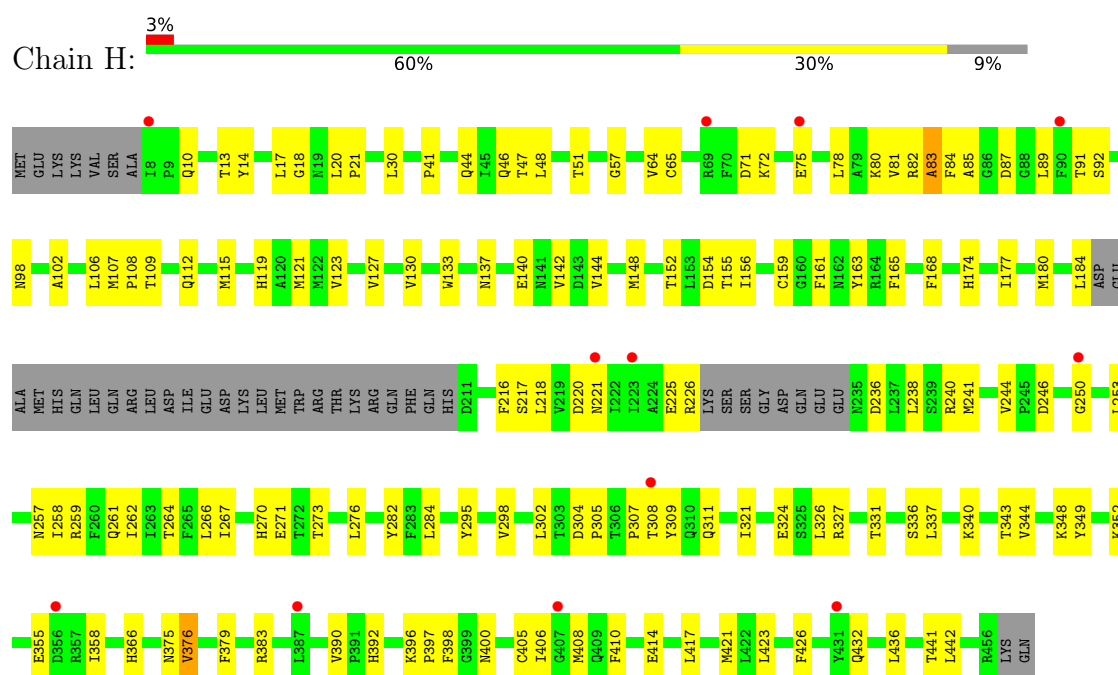
- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



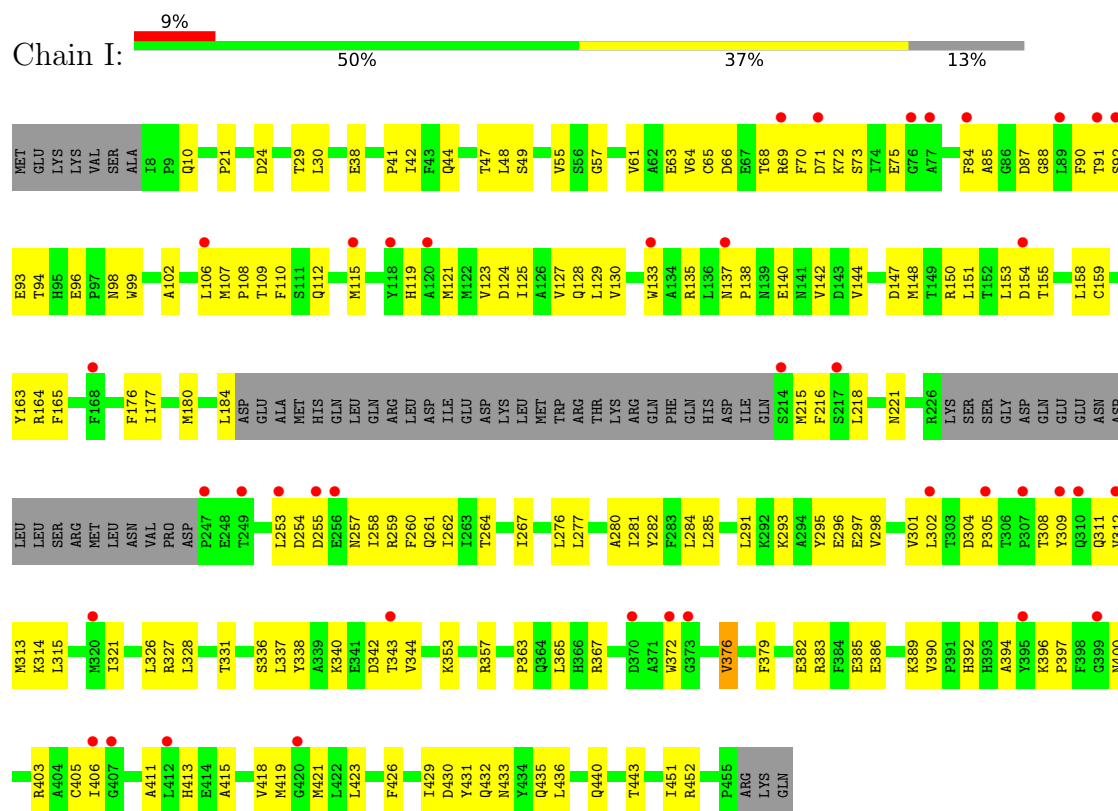
- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

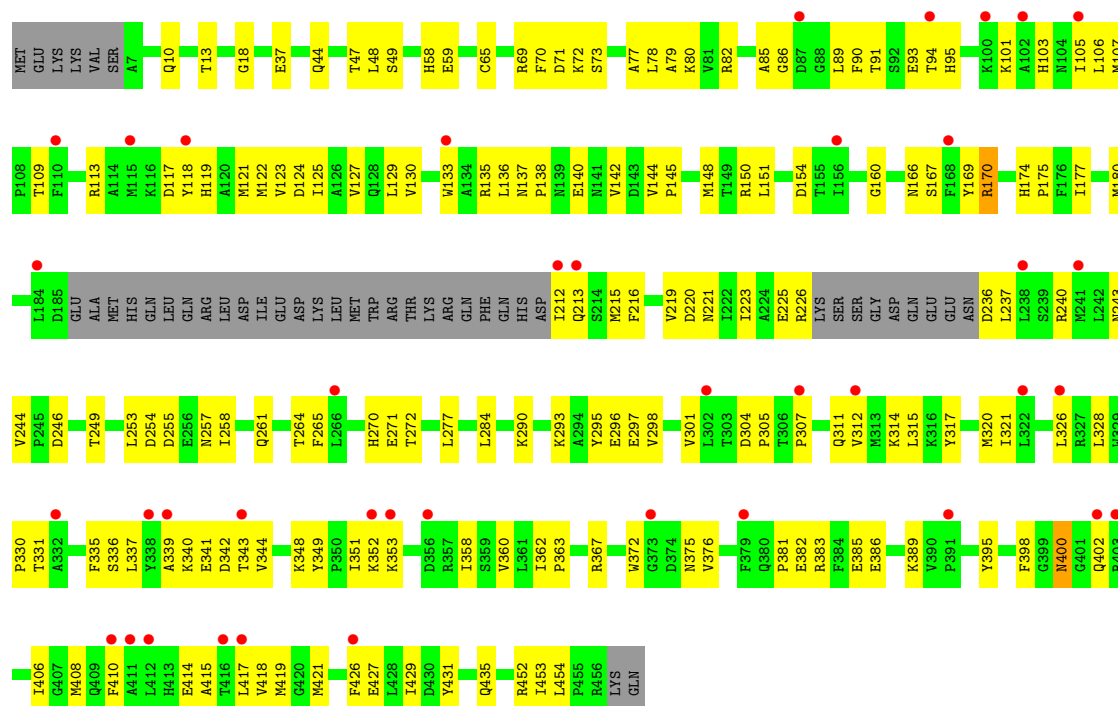


- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

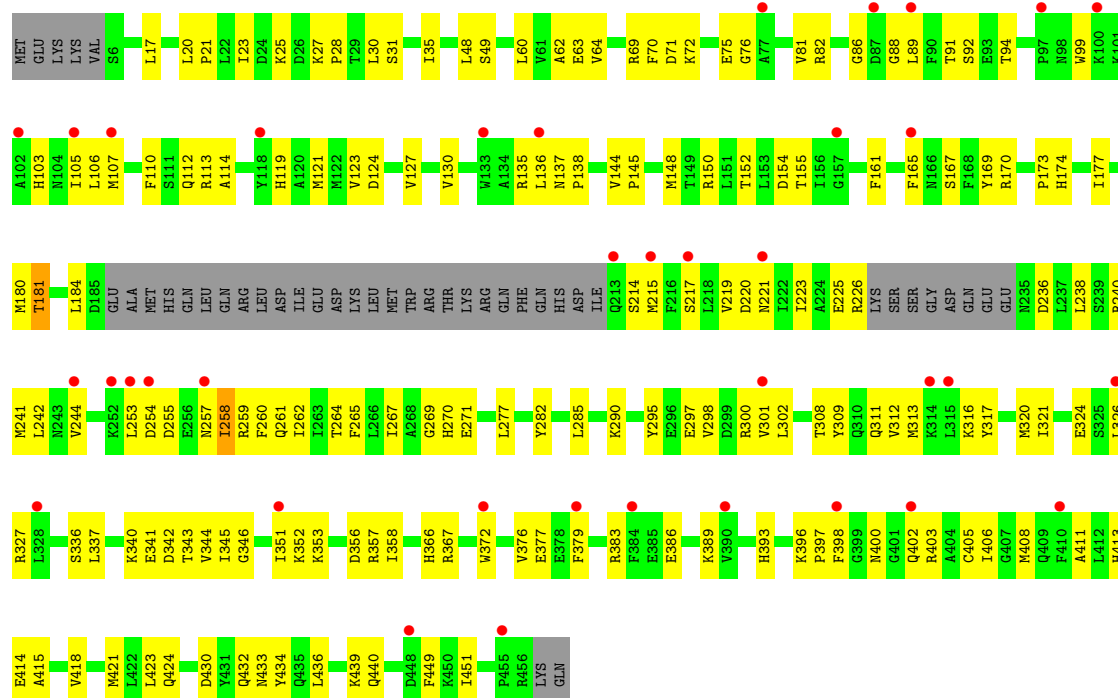


- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase





• Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



• Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	96.62Å 126.06Å 141.44Å 86.66° 79.47° 84.97°	Depositor
Resolution (Å)	19.96 – 2.80 19.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.5 (19.96-2.80) 97.8 (19.96-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.239 , 0.270 0.241 , 0.271	Depositor DCC
R_{free} test set	7977 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	41062	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.25	0/3540	0.50	0/4794
1	B	0.26	0/3554	0.51	0/4812
1	C	0.23	0/3479	0.49	0/4711
1	D	0.27	0/3459	0.54	0/4686
1	E	0.26	0/3485	0.52	0/4718
1	F	0.25	0/3461	0.50	0/4686
1	G	0.26	0/3313	0.55	0/4484
1	H	0.24	0/3432	0.51	0/4648
1	I	0.27	0/3300	0.57	0/4468
1	J	0.27	0/3429	0.56	0/4644
1	K	0.24	0/3435	0.52	0/4652
1	L	0.25	0/3383	0.57	0/4582
All	All	0.25	0/41270	0.53	0/55885

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3460	0	3435	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3473	0	3446	87	0
1	C	3400	0	3382	81	0
1	D	3380	0	3368	79	0
1	E	3406	0	3394	83	0
1	F	3382	0	3378	91	0
1	G	3238	0	3237	92	0
1	H	3354	0	3349	110	0
1	I	3223	0	3218	147	0
1	J	3351	0	3348	149	0
1	K	3357	0	3348	141	0
1	L	3306	0	3297	140	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0
2	C	43	0	30	4	0
2	D	43	0	30	4	0
2	E	43	0	30	2	0
2	F	43	0	30	3	0
2	G	43	0	30	4	0
2	H	43	0	30	6	0
2	I	43	0	30	10	0
2	J	43	0	30	3	0
2	K	43	0	30	6	0
2	L	43	0	30	4	0
3	A	18	0	31	4	0
3	B	18	0	31	4	0
3	C	18	0	31	3	0
3	D	36	0	62	4	0
3	E	18	0	31	2	0
3	G	18	0	31	3	0
3	H	18	0	31	5	0
3	I	18	0	31	3	0
3	J	18	0	31	1	0
3	K	18	0	31	1	0
3	L	18	0	31	5	0
All	All	41062	0	40932	1270	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 15.

All (1270) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:302:LEU:HD11	1:K:424:GLN:HG3	1.25	1.15
1:H:65:CYS:HB3	1:H:400:ASN:ND2	1.71	1.06
1:I:65:CYS:HB2	1:I:400:ASN:ND2	1.77	1.00
1:J:10:GLN:HB3	1:J:44:GLN:HG3	1.48	0.94
1:K:302:LEU:HD11	1:K:424:GLN:CG	1.98	0.93
1:I:386:GLU:HB2	1:I:389:LYS:HG2	1.54	0.90
3:D:503:PLM:H22	3:K:502:PLM:HA1	1.50	0.90
1:I:257:ASN:O	1:I:261:GLN:HG2	1.72	0.89
3:B:502:PLM:H92	3:I:502:PLM:H62	1.57	0.86
1:I:125:ILE:HG22	1:I:151:LEU:HD12	1.56	0.86
1:L:219:VAL:HG13	1:L:262:ILE:HD11	1.57	0.85
1:I:163:TYR:HE1	1:L:137:ASN:HD21	1.21	0.85
1:J:339:ALA:HB3	1:J:353:LYS:HD3	1.58	0.85
1:F:219:VAL:HG13	1:F:262:ILE:HD11	1.59	0.85
1:G:216:PHE:HB3	1:G:259:ARG:HH21	1.42	0.85
1:I:216:PHE:HD1	1:I:259:ARG:HD2	1.40	0.84
1:G:63:GLU:OE2	1:G:345:ILE:HA	1.77	0.83
1:H:65:CYS:HB3	1:H:400:ASN:HD21	1.43	0.83
1:E:35:ILE:HD11	1:E:45:ILE:HD11	1.62	0.82
1:J:124:ASP:OD1	1:J:125:ILE:N	2.13	0.81
1:D:219:VAL:HB	1:D:262:ILE:HD11	1.62	0.81
1:F:139:ASN:HB3	1:F:452:ARG:HH21	1.44	0.81
1:G:324:GLU:OE2	1:G:383:ARG:NH1	2.13	0.81
1:L:125:ILE:HG22	1:L:151:LEU:HD12	1.61	0.81
1:L:19:ASN:HD21	1:L:45:ILE:HA	1.44	0.81
1:I:281:ILE:HG13	1:I:419:MET:HE1	1.60	0.81
1:C:153:LEU:HD21	1:C:177:ILE:HG13	1.63	0.81
1:J:340:LYS:HG3	1:J:341:GLU:HG2	1.61	0.81
1:J:386:GLU:HB3	1:J:389:LYS:HB3	1.61	0.81
1:L:254:ASP:HB3	1:L:257:ASN:HB2	1.60	0.80
1:A:393:HIS:HA	1:A:396:LYS:HE2	1.63	0.80
1:J:307:PRO:HD2	1:J:421:MET:HE2	1.61	0.80
1:C:180:MET:HE2	1:C:267:ILE:HG23	1.63	0.80
1:L:276:LEU:HD13	1:L:326:LEU:HG	1.64	0.80
1:A:386:GLU:HG3	1:A:388:ASP:OD1	1.82	0.79
1:L:137:ASN:HB2	1:L:140:GLU:HG3	1.64	0.79
1:I:328:LEU:O	1:I:367:ARG:NH2	2.15	0.79
1:H:216:PHE:HB3	1:H:259:ARG:HH21	1.46	0.78
1:H:273:THR:HG22	2:H:501:HEM:HAB	1.63	0.78
1:E:173:PRO:HB3	1:E:177:ILE:HD11	1.64	0.78
1:G:341:GLU:HA	1:G:353:LYS:HD2	1.65	0.77
1:B:151:LEU:HD21	1:B:418:VAL:HG21	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:71:ASP:OD1	1:J:94:THR:HG23	1.85	0.76
1:B:241:MET:HE2	1:B:258:ILE:HG12	1.68	0.76
1:H:375:ASN:O	1:H:383:ARG:NH2	2.19	0.75
1:J:124:ASP:OD1	1:J:125:ILE:HG13	1.86	0.75
1:F:375:ASN:O	1:F:383:ARG:NH2	2.19	0.75
1:C:174:HIS:HB3	1:C:177:ILE:HG12	1.66	0.75
1:L:29:THR:H	1:L:440:GLN:HE22	1.35	0.75
1:C:112:GLN:HE22	1:C:313:MET:HE1	1.51	0.75
1:F:113:ARG:HH12	1:F:116:LYS:HD2	1.52	0.75
1:I:93:GLU:HB2	1:I:96:GLU:HG3	1.69	0.74
1:L:372:TRP:O	1:L:383:ARG:NH1	2.21	0.74
1:H:155:THR:HG21	1:H:414:GLU:OE2	1.87	0.74
1:I:64:VAL:HG12	1:I:337:LEU:HD22	1.68	0.74
1:B:125:ILE:HG22	1:B:151:LEU:HD12	1.68	0.74
1:B:153:LEU:HD21	1:B:177:ILE:HG13	1.68	0.74
1:L:131:GLN:HB3	1:L:135:ARG:HH12	1.52	0.74
3:E:502:PLM:H72	3:L:502:PLM:H62	1.69	0.73
1:E:151:LEU:HD21	1:E:418:VAL:HG21	1.70	0.73
1:J:144:VAL:HG23	1:J:145:PRO:HD3	1.71	0.73
1:I:285:LEU:HD21	1:I:430:ASP:HB2	1.72	0.72
1:L:307:PRO:HD2	1:L:421:MET:HE2	1.71	0.72
1:B:269:GLY:O	1:B:273:THR:HG22	1.89	0.71
1:J:427:GLU:HG2	1:J:454:LEU:HB2	1.72	0.71
1:I:276:LEU:HD13	1:I:326:LEU:HG	1.72	0.71
1:A:12:LYS:O	1:A:19:ASN:ND2	2.22	0.71
1:A:355:GLU:O	1:A:357:ARG:NH1	2.22	0.71
1:E:182:ARG:HD2	1:E:211:ASP:OD2	1.89	0.71
1:G:236:ASP:N	1:G:239:SER:HG	1.89	0.71
1:J:71:ASP:OD1	1:J:94:THR:CG2	2.39	0.71
1:J:10:GLN:HB3	1:J:44:GLN:CG	2.20	0.71
1:A:388:ASP:OD1	1:A:389:LYS:HG2	1.91	0.70
1:C:249:THR:HG23	1:C:251:GLU:H	1.56	0.70
1:F:213:GLN:HG2	1:J:221:ASN:HD21	1.56	0.70
1:G:352:LYS:H	1:G:352:LYS:HD2	1.56	0.70
1:H:65:CYS:CB	1:H:400:ASN:ND2	2.53	0.70
1:K:430:ASP:OD2	1:K:433:ASN:HA	1.91	0.70
1:G:219:VAL:O	1:G:223:ILE:HG23	1.91	0.70
1:K:64:VAL:HG12	1:K:337:LEU:HD21	1.73	0.70
1:J:339:ALA:CB	1:J:353:LYS:HD3	2.21	0.70
1:I:312:VAL:HG11	1:I:413:HIS:HE2	1.56	0.70
1:E:125:ILE:HG22	1:E:151:LEU:HD12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:216:PHE:HA	1:J:219:VAL:HG22	1.74	0.69
1:G:116:LYS:HE2	1:G:309:TYR:CE2	2.27	0.69
3:H:502:PLM:H42	3:L:502:PLM:H92	1.74	0.69
1:I:180:MET:HB2	1:I:215:MET:HE1	1.74	0.69
1:D:217:SER:HA	1:G:217:SER:OG	1.93	0.69
1:I:280:ALA:HB3	1:I:419:MET:HE3	1.74	0.69
1:J:79:ALA:O	1:J:82:ARG:HB3	1.92	0.69
1:J:106:LEU:HD13	1:J:265:PHE:HZ	1.56	0.69
1:J:177:ILE:HA	1:J:180:MET:HG2	1.73	0.69
1:J:85:ALA:HB1	1:J:264:THR:HG22	1.75	0.69
1:H:307:PRO:HD2	1:H:421:MET:HE2	1.76	0.68
1:J:290:LYS:HZ3	1:J:381:PRO:HD2	1.58	0.68
1:L:58:HIS:NE2	1:L:370:ASP:OD2	2.24	0.68
1:K:75:GLU:OE1	1:K:357:ARG:HD2	1.93	0.68
1:K:137:ASN:HB3	1:K:138:PRO:HD2	1.76	0.68
1:L:148:MET:HE3	1:L:277:LEU:HD13	1.76	0.68
1:J:151:LEU:HD21	1:J:418:VAL:HG11	1.76	0.67
1:K:148:MET:HE2	1:K:277:LEU:HB3	1.76	0.67
1:G:256:GLU:HA	1:G:259:ARG:HD3	1.75	0.67
1:J:169:TYR:OH	1:K:135:ARG:NH1	2.27	0.67
1:L:238:LEU:O	1:L:242:LEU:HB2	1.94	0.67
1:I:65:CYS:CB	1:I:400:ASN:ND2	2.56	0.67
1:F:68:THR:C	1:F:340:LYS:HZ1	2.02	0.67
1:I:254:ASP:OD1	1:I:255:ASP:N	2.27	0.67
1:K:155:THR:HG21	1:K:414:GLU:OE2	1.95	0.67
1:L:154:ASP:OD1	1:L:165:PHE:HB2	1.93	0.67
1:I:127:VAL:HA	1:I:130:VAL:HG12	1.76	0.67
1:B:80:LYS:HD3	1:B:187:ALA:HA	1.75	0.67
1:G:87:ASP:OD2	1:G:98:ASN:ND2	2.28	0.67
1:K:173:PRO:HB3	1:K:177:ILE:HD11	1.76	0.67
1:I:216:PHE:CD1	1:I:259:ARG:HD2	2.28	0.67
1:L:176:PHE:O	1:L:179:SER:HB3	1.94	0.67
1:K:72:LYS:HB2	1:K:403:ARG:HD3	1.77	0.66
1:G:152:THR:HG21	1:G:273:THR:HB	1.77	0.66
1:D:179:SER:HB2	1:D:211:ASP:HB3	1.76	0.66
1:J:125:ILE:HG22	1:J:151:LEU:HD12	1.78	0.66
1:L:143:ASP:OD1	1:L:146:GLU:HG2	1.94	0.66
1:D:367:ARG:NE	1:D:377:GLU:OE2	2.29	0.66
1:K:89:LEU:HG	1:K:261:GLN:HE22	1.60	0.66
1:L:307:PRO:HA	1:L:311:GLN:NE2	2.11	0.66
1:G:352:LYS:HD3	1:G:356:ASP:OD2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:290:LYS:NZ	1:J:382:GLU:OE1	2.29	0.66
1:C:241:MET:HE2	1:C:258:ILE:HG12	1.76	0.65
1:F:182:ARG:HD3	1:F:211:ASP:OD2	1.96	0.65
1:K:345:ILE:HG12	1:K:351:ILE:HD13	1.77	0.65
1:H:327:ARG:NH2	1:H:376:VAL:O	2.29	0.65
1:K:215:MET:O	1:K:219:VAL:HG22	1.96	0.65
1:K:254:ASP:O	1:K:258:ILE:HG12	1.96	0.65
1:C:324:GLU:OE2	1:C:383:ARG:NH1	2.30	0.65
2:C:501:HEM:HMB1	2:C:501:HEM:HBB2	1.78	0.65
1:E:99:TRP:HH2	1:E:402:GLN:HG2	1.62	0.65
1:F:341:GLU:HA	1:F:353:LYS:HG3	1.78	0.65
1:K:70:PHE:HB3	1:K:337:LEU:HD13	1.79	0.65
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.78	0.65
1:H:216:PHE:HB3	1:H:259:ARG:NH2	2.12	0.65
1:G:220:ASP:O	1:G:223:ILE:HG12	1.97	0.65
1:G:327:ARG:NH2	1:G:376:VAL:O	2.29	0.65
1:J:317:TYR:HA	1:J:320:MET:HE2	1.78	0.65
1:K:121:MET:O	1:K:124:ASP:HB3	1.97	0.65
1:D:432:GLN:O	1:D:433:ASN:C	2.40	0.64
1:E:226:ARG:HH11	1:E:238:LEU:HD23	1.63	0.64
1:B:42:ILE:HD13	1:B:55:VAL:HG12	1.79	0.64
1:D:241:MET:HE3	1:D:258:ILE:HG23	1.79	0.64
1:G:236:ASP:N	1:G:239:SER:OG	2.30	0.64
1:G:254:ASP:OD1	1:G:255:ASP:N	2.30	0.64
1:H:81:VAL:HG12	1:H:91:THR:HG21	1.79	0.64
1:H:417:LEU:HD11	1:H:421:MET:HE3	1.78	0.64
1:F:68:THR:O	1:F:340:LYS:NZ	2.30	0.64
1:H:87:ASP:OD2	1:H:98:ASN:ND2	2.30	0.64
1:I:137:ASN:HB2	1:I:140:GLU:HG3	1.80	0.64
1:H:152:THR:CG2	1:H:270:HIS:HA	2.28	0.64
1:I:124:ASP:O	1:I:127:VAL:HG22	1.98	0.64
1:G:150:ARG:HG2	1:G:167:SER:HB3	1.78	0.64
1:I:125:ILE:HD11	1:I:158:LEU:HD13	1.80	0.64
1:L:132:LYS:NZ	1:L:147:ASP:OD1	2.24	0.64
1:I:129:LEU:HD22	1:I:151:LEU:HD22	1.80	0.63
1:C:176:PHE:HD1	1:C:177:ILE:HD13	1.63	0.63
1:F:393:HIS:HA	1:F:396:LYS:HE2	1.80	0.63
1:L:131:GLN:HB3	1:L:135:ARG:NH1	2.13	0.63
1:A:388:ASP:OD1	1:A:389:LYS:N	2.31	0.63
1:H:127:VAL:HA	1:H:130:VAL:HG12	1.80	0.63
1:I:135:ARG:NH1	1:L:169:TYR:OH	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:137:ASN:HB2	1:J:140:GLU:HG3	1.81	0.63
1:J:137:ASN:HB3	1:J:138:PRO:HD2	1.79	0.63
1:K:220:ASP:O	1:K:223:ILE:HG12	1.99	0.63
1:A:345:ILE:HD11	1:A:351:ILE:CG1	2.28	0.63
1:F:298:VAL:HG13	1:F:302:LEU:HD12	1.80	0.63
1:A:345:ILE:HD11	1:A:351:ILE:HG12	1.80	0.63
1:D:398:PHE:CD2	1:D:408:MET:HE3	2.33	0.63
2:K:501:HEM:HMB1	2:K:501:HEM:HBB2	1.81	0.63
1:J:69:ARG:O	1:J:339:ALA:HB1	1.98	0.63
1:B:174:HIS:HB3	1:B:177:ILE:HG12	1.81	0.62
1:C:113:ARG:HG2	1:C:116:LYS:HE3	1.81	0.62
1:F:52:ILE:HG12	1:F:357:ARG:HE	1.64	0.62
1:K:161:PHE:HD1	1:K:238:LEU:HB2	1.64	0.62
1:J:127:VAL:HA	1:J:130:VAL:HG12	1.81	0.62
1:L:245:PRO:HA	1:L:252:LYS:HA	1.81	0.62
1:B:78:LEU:HA	1:B:81:VAL:HG12	1.82	0.62
1:E:341:GLU:HA	1:E:353:LYS:HG3	1.81	0.62
1:C:398:PHE:CD2	1:C:408:MET:HE3	2.35	0.62
1:J:255:ASP:O	1:J:258:ILE:HG12	1.99	0.62
1:K:20:LEU:HD12	1:K:48:LEU:HD13	1.81	0.62
1:C:219:VAL:O	1:C:223:ILE:HG12	1.99	0.62
1:E:343:THR:HG22	1:E:344:VAL:H	1.63	0.62
1:F:174:HIS:H	1:F:177:ILE:HD12	1.64	0.62
1:G:72:LYS:HE2	2:G:501:HEM:CGA	2.30	0.62
1:L:396:LYS:HD2	1:L:400:ASN:HB2	1.80	0.62
1:A:324:GLU:OE2	1:A:327:ARG:NH2	2.33	0.62
1:K:277:LEU:HD21	1:K:415:ALA:HA	1.80	0.62
1:L:428:LEU:HD22	1:L:451:ILE:HD12	1.81	0.62
2:E:501:HEM:HBC2	2:E:501:HEM:HMC2	1.82	0.62
1:K:69:ARG:HE	1:K:343:THR:HG21	1.65	0.62
1:H:308:THR:N	1:H:311:GLN:OE1	2.25	0.62
1:J:341:GLU:O	1:J:353:LYS:HD2	1.99	0.62
1:K:217:SER:O	1:K:221:ASN:ND2	2.33	0.62
1:F:213:GLN:HG2	1:J:221:ASN:ND2	2.15	0.61
1:L:98:ASN:ND2	1:L:257:ASN:HD21	1.97	0.61
2:L:501:HEM:HMC1	2:L:501:HEM:HBC2	1.82	0.61
1:D:82:ARG:HH12	1:D:92:SER:HA	1.65	0.61
1:D:257:ASN:O	1:D:261:GLN:HG2	2.00	0.61
1:E:42:ILE:HG23	1:E:60:LEU:HD13	1.81	0.61
1:I:47:THR:HG22	1:I:48:LEU:H	1.65	0.61
1:H:284:LEU:HD21	1:H:321:ILE:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:336:SER:HA	1:K:358:ILE:O	2.00	0.61
1:K:386:GLU:HG3	1:K:389:LYS:HB2	1.82	0.61
1:L:343:THR:HG22	1:L:344:VAL:H	1.65	0.61
1:K:62:ALA:HA	1:K:393:HIS:NE2	2.14	0.61
1:C:284:LEU:HD21	1:C:321:ILE:HD13	1.81	0.61
1:F:219:VAL:CG1	1:F:262:ILE:HD11	2.31	0.61
1:K:264:THR:HA	1:K:267:ILE:HG12	1.83	0.61
1:A:81:VAL:HG12	1:A:91:THR:HG21	1.83	0.61
1:G:240:ARG:NE	1:G:240:ARG:O	2.34	0.61
1:K:144:VAL:O	1:K:148:MET:HG2	1.99	0.61
1:D:60:LEU:HD22	1:D:345:ILE:HG22	1.81	0.61
1:J:212:ILE:N	1:J:215:MET:HG3	2.15	0.61
1:L:341:GLU:HA	1:L:353:LYS:HD3	1.83	0.61
1:I:309:TYR:O	1:I:312:VAL:HG12	2.00	0.61
1:G:331:THR:HG22	1:G:443:THR:HG23	1.83	0.61
1:L:284:LEU:HB3	1:L:291:LEU:HD13	1.83	0.61
1:L:437:ASP:OD2	1:L:439:LYS:NZ	2.34	0.61
3:B:502:PLM:H31	3:C:502:PLM:H81	1.82	0.60
1:K:161:PHE:CE1	1:K:262:ILE:HG12	2.36	0.60
1:J:47:THR:HG22	1:J:48:LEU:H	1.67	0.60
1:J:82:ARG:NH1	1:J:91:THR:O	2.34	0.60
1:L:220:ASP:HA	1:L:223:ILE:HD12	1.83	0.60
1:A:298:VAL:HG13	1:A:302:LEU:HD12	1.81	0.60
1:G:398:PHE:CD2	1:G:408:MET:HE3	2.36	0.60
1:H:41:PRO:HB3	1:H:57:GLY:HA3	1.84	0.60
1:I:69:ARG:HH21	1:I:343:THR:HB	1.66	0.60
1:J:375:ASN:O	1:J:383:ARG:NH2	2.31	0.60
1:B:375:ASN:O	1:B:383:ARG:NH2	2.32	0.60
1:F:12:LYS:HG2	1:F:14:TYR:CZ	2.36	0.60
1:L:254:ASP:OD1	1:L:255:ASP:N	2.35	0.60
1:D:82:ARG:NH1	1:D:91:THR:O	2.33	0.60
1:I:147:ASP:OD1	1:I:150:ARG:NH1	2.35	0.60
1:J:72:LYS:HA	1:J:337:LEU:HD23	1.82	0.60
1:I:124:ASP:OD2	1:I:164:ARG:NH2	2.30	0.60
1:J:133:TRP:NE1	1:J:142:VAL:HG21	2.17	0.60
1:L:74:ILE:HG12	1:L:93:GLU:OE2	2.02	0.60
1:F:273:THR:HG21	1:F:414:GLU:OE2	2.01	0.60
3:A:502:PLM:HA1	3:G:502:PLM:H51	1.83	0.60
1:D:30:LEU:HD22	1:K:17:LEU:HD21	1.84	0.60
1:H:87:ASP:HA	1:H:92:SER:HB3	1.83	0.59
1:L:98:ASN:HA	1:L:101:LYS:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:181:THR:HA	1:K:184:LEU:HG	1.85	0.59
1:A:367:ARG:NE	1:A:377:GLU:OE2	2.31	0.59
1:B:398:PHE:CD2	1:B:408:MET:HE3	2.38	0.59
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.85	0.59
1:K:219:VAL:O	1:K:223:ILE:HG23	2.03	0.59
1:G:106:LEU:HD13	1:G:265:PHE:HZ	1.68	0.59
1:A:47:THR:HG23	1:A:49:SER:H	1.68	0.59
1:C:105:ILE:HD12	1:C:253:LEU:HG	1.85	0.59
1:G:113:ARG:O	1:G:116:LYS:HG2	2.02	0.59
1:H:226:ARG:HE	1:H:238:LEU:HD23	1.68	0.59
1:K:308:THR:HG22	1:K:311:GLN:OE1	2.03	0.59
1:K:386:GLU:HG3	1:K:389:LYS:HE3	1.83	0.59
1:F:380:GLN:HB2	1:F:383:ARG:HG3	1.85	0.59
1:F:398:PHE:CD2	1:F:408:MET:HE3	2.38	0.59
1:G:216:PHE:HB3	1:G:259:ARG:NH2	2.14	0.59
1:I:87:ASP:OD2	1:I:98:ASN:ND2	2.35	0.59
1:L:241:MET:O	1:L:253:LEU:HD22	2.01	0.59
1:B:90:PHE:HB2	1:B:264:THR:HG23	1.84	0.58
1:K:341:GLU:HA	1:K:353:LYS:HG3	1.85	0.58
1:K:71:ASP:HB2	1:K:340:LYS:HE3	1.84	0.58
1:D:47:THR:HG23	1:D:49:SER:H	1.69	0.58
1:I:98:ASN:OD1	1:I:257:ASN:ND2	2.36	0.58
1:I:106:LEU:HD12	1:I:406:ILE:HD13	1.86	0.58
1:I:293:LYS:O	1:I:296:GLU:HG3	2.03	0.58
2:I:501:HEM:HMC2	2:I:501:HEM:HBC2	1.85	0.58
1:B:30:LEU:HD23	3:B:502:PLM:HE1	1.86	0.58
1:E:42:ILE:HG22	1:E:55:VAL:HA	1.86	0.58
1:H:154:ASP:OD1	1:H:165:PHE:HB2	2.04	0.58
1:F:139:ASN:HA	1:F:452:ARG:HE	1.69	0.58
1:B:93:GLU:OE1	1:B:95:HIS:NE2	2.33	0.58
1:E:34:LYS:HD2	1:H:21:PRO:HB3	1.86	0.58
1:I:284:LEU:HB3	1:I:291:LEU:HD13	1.84	0.58
1:L:411:ALA:HB2	2:L:501:HEM:HMC2	1.84	0.58
1:K:297:GLU:OE1	1:K:317:TYR:HB3	2.03	0.58
1:G:69:ARG:HE	1:G:343:THR:HG21	1.69	0.58
1:L:47:THR:HG23	1:L:49:SER:H	1.68	0.58
1:D:81:VAL:HG12	1:D:91:THR:HG21	1.85	0.57
1:D:298:VAL:HG13	1:D:302:LEU:HD12	1.86	0.57
1:B:75:GLU:HG2	1:B:76:GLY:H	1.69	0.57
1:E:398:PHE:CD2	1:E:408:MET:HE3	2.38	0.57
1:G:81:VAL:HG12	1:G:91:THR:HG21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:312:VAL:HG11	1:I:413:HIS:NE2	2.18	0.57
1:H:102:ALA:O	1:H:106:LEU:HG	2.04	0.57
1:E:246:ASP:OD2	1:E:249:THR:HG22	2.04	0.57
1:F:42:ILE:HD13	1:F:55:VAL:HG22	1.86	0.57
1:G:72:LYS:HD2	1:G:403:ARG:HB3	1.86	0.57
1:G:257:ASN:O	1:G:261:GLN:HG2	2.05	0.57
1:G:352:LYS:HD3	1:G:356:ASP:CG	2.30	0.57
1:J:257:ASN:O	1:J:261:GLN:HG2	2.05	0.57
1:L:285:LEU:HD12	1:L:449:PHE:HZ	1.70	0.57
1:B:34:LYS:HD2	1:I:21:PRO:HB3	1.85	0.57
1:C:269:GLY:O	1:C:273:THR:HG22	2.05	0.57
1:C:123:VAL:O	1:C:127:VAL:HG23	2.05	0.57
1:G:63:GLU:CD	1:G:345:ILE:HA	2.29	0.57
1:J:312:VAL:HG23	1:J:315:LEU:HD12	1.86	0.57
1:D:269:GLY:O	1:D:273:THR:HG22	2.04	0.56
1:I:99:TRP:NE1	2:I:501:HEM:O1D	2.37	0.56
2:G:501:HEM:HMC2	2:G:501:HEM:HBC2	1.85	0.56
1:J:106:LEU:HD13	1:J:265:PHE:CZ	2.39	0.56
1:A:75:GLU:HG2	1:A:357:ARG:HG3	1.88	0.56
3:E:502:PLM:O2	3:H:502:PLM:H91	2.04	0.56
1:F:80:LYS:HE3	1:K:432:GLN:HB2	1.87	0.56
1:L:98:ASN:CG	1:L:257:ASN:HD21	2.13	0.56
1:D:307:PRO:HD2	1:D:421:MET:HE2	1.87	0.56
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.87	0.56
1:J:284:LEU:HD21	1:J:321:ILE:HD13	1.88	0.56
1:K:343:THR:HG22	1:K:344:VAL:H	1.69	0.56
1:H:321:ILE:HG23	1:H:379:PHE:HZ	1.71	0.56
1:J:375:ASN:HB3	1:J:383:ARG:NH2	2.20	0.56
2:K:501:HEM:HBC2	2:K:501:HEM:HMC2	1.86	0.56
1:H:152:THR:HG21	1:H:270:HIS:HA	1.88	0.56
1:J:220:ASP:HA	1:J:223:ILE:HG12	1.86	0.56
1:E:336:SER:C	1:E:337:LEU:HD12	2.31	0.56
1:L:69:ARG:HE	1:L:343:THR:HG21	1.71	0.56
1:D:441:THR:OG1	1:D:442:LEU:N	2.39	0.56
1:F:240:ARG:CZ	1:F:244:VAL:HG21	2.36	0.56
1:J:123:VAL:O	1:J:127:VAL:HG23	2.06	0.56
1:J:340:LYS:HE3	1:J:341:GLU:OE2	2.05	0.56
1:K:181:THR:HG23	1:K:184:LEU:HD12	1.87	0.56
1:K:398:PHE:CD2	1:K:408:MET:HE3	2.41	0.56
1:B:129:LEU:HD22	1:B:151:LEU:HD22	1.87	0.56
1:C:81:VAL:HG12	1:C:91:THR:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:LEU:HD21	1:E:177:ILE:HG21	1.87	0.56
1:K:94:THR:OG1	1:K:403:ARG:HD2	2.06	0.56
2:F:501:HEM:HMC2	2:F:501:HEM:HBC2	1.86	0.55
1:D:277:LEU:HD21	1:D:415:ALA:HA	1.88	0.55
1:H:257:ASN:O	1:H:261:GLN:HG2	2.06	0.55
1:G:133:TRP:HA	1:G:136:LEU:HD13	1.87	0.55
1:H:119:HIS:O	1:H:123:VAL:HG23	2.06	0.55
1:K:161:PHE:CE2	1:K:262:ILE:HG23	2.42	0.55
1:B:61:VAL:HG11	1:B:365:LEU:HD22	1.87	0.55
1:I:277:LEU:HD21	1:I:415:ALA:HA	1.89	0.55
1:L:178:THR:HA	1:L:181:THR:OG1	2.07	0.55
1:E:144:VAL:HB	1:E:145:PRO:HD3	1.88	0.55
1:G:284:LEU:HD21	1:G:321:ILE:HD13	1.88	0.55
1:J:277:LEU:HD21	1:J:415:ALA:HA	1.88	0.55
1:A:106:LEU:HD13	1:A:265:PHE:HZ	1.72	0.55
1:F:219:VAL:HG13	1:F:262:ILE:CD1	2.34	0.55
1:G:414:GLU:O	1:G:418:VAL:HG23	2.05	0.55
1:H:75:GLU:HG2	1:H:336:SER:HB2	1.88	0.55
1:A:226:ARG:HH22	1:A:236:ASP:CG	2.15	0.55
1:I:69:ARG:NH2	1:I:343:THR:HB	2.22	0.55
1:A:226:ARG:NE	1:A:234:GLU:OE1	2.40	0.55
1:F:174:HIS:HB3	1:F:177:ILE:HG13	1.87	0.55
1:I:121:MET:HE2	1:I:159:CYS:HA	1.89	0.55
1:K:60:LEU:HD22	1:K:345:ILE:HG22	1.88	0.55
1:C:246:ASP:OD2	1:C:249:THR:HG22	2.06	0.55
1:F:219:VAL:HG22	1:F:262:ILE:HD11	1.89	0.55
1:G:220:ASP:OD1	1:G:259:ARG:NE	2.39	0.55
1:J:130:VAL:HG23	1:J:426:PHE:CE2	2.41	0.55
1:H:240:ARG:HD3	1:H:244:VAL:HG21	1.87	0.55
1:L:174:HIS:CG	1:L:175:PRO:HD2	2.42	0.55
1:B:71:ASP:HB3	1:B:338:TYR:CE1	2.41	0.54
1:D:216:PHE:HA	1:D:219:VAL:HG22	1.89	0.54
1:F:343:THR:HG22	1:F:344:VAL:H	1.72	0.54
1:G:327:ARG:HG2	1:G:366:HIS:HB3	1.88	0.54
1:H:258:ILE:O	1:H:262:ILE:HG13	2.08	0.54
1:H:348:LYS:HE3	1:H:349:TYR:CZ	2.41	0.54
1:J:103:HIS:CE1	1:J:107:MET:CG	2.90	0.54
1:K:106:LEU:HD11	1:K:241:MET:HE1	1.89	0.54
1:A:11:PRO:HA	1:A:39:TYR:CZ	2.41	0.54
1:E:99:TRP:CH2	1:E:402:GLN:HG2	2.41	0.54
1:F:304:ASP:HB3	1:F:305:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:405:CYS:HB2	2:H:501:HEM:NA	2.21	0.54
1:J:216:PHE:HA	1:J:219:VAL:CG2	2.37	0.54
1:E:11:PRO:HA	1:E:39:TYR:CZ	2.43	0.54
1:D:28:PRO:HD2	1:D:440:GLN:OE1	2.08	0.54
1:D:302:LEU:HD22	1:D:307:PRO:HB3	1.89	0.54
1:J:13:THR:HG23	1:J:18:GLY:HA2	1.88	0.54
1:C:180:MET:HE1	1:C:266:LEU:HB2	1.88	0.54
1:J:342:ASP:HA	1:J:353:LYS:HG3	1.88	0.54
1:L:137:ASN:HB3	1:L:138:PRO:HD2	1.89	0.54
1:L:144:VAL:O	1:L:148:MET:HG2	2.07	0.54
1:C:342:ASP:OD1	1:C:353:LYS:N	2.38	0.54
1:E:257:ASN:O	1:E:261:GLN:HG2	2.06	0.54
1:F:213:GLN:HG2	1:J:221:ASN:OD1	2.08	0.54
1:H:152:THR:HG21	1:H:273:THR:OG1	2.07	0.54
1:J:166:ASN:HB3	1:J:169:TYR:CD2	2.43	0.54
1:K:112:GLN:NE2	1:K:313:MET:SD	2.81	0.54
1:G:256:GLU:HA	1:G:259:ARG:CD	2.37	0.54
1:G:352:LYS:H	1:G:352:LYS:CD	2.21	0.54
1:I:284:LEU:HD21	1:I:321:ILE:HD13	1.89	0.54
1:I:311:GLN:O	1:I:314:LYS:HB3	2.07	0.54
1:J:138:PRO:HG3	1:K:225:GLU:OE2	2.07	0.54
1:J:328:LEU:O	1:J:367:ARG:NH2	2.41	0.54
1:J:417:LEU:HD11	1:J:421:MET:HE3	1.89	0.54
1:B:293:LYS:O	1:B:296:GLU:HG3	2.07	0.54
1:I:297:GLU:HG2	1:I:315:LEU:HD23	1.90	0.54
1:I:336:SER:HB3	1:I:357:ARG:NH1	2.23	0.54
1:L:302:LEU:HD21	1:L:311:GLN:HB2	1.89	0.54
1:G:66:ASP:OD2	1:G:68:THR:HB	2.08	0.54
1:I:282:TYR:CZ	1:I:436:LEU:HB2	2.43	0.54
1:I:295:TYR:HA	1:I:298:VAL:HG12	1.90	0.54
1:J:103:HIS:CE1	1:J:107:MET:SD	3.00	0.54
1:K:352:LYS:HG2	1:K:356:ASP:OD2	2.08	0.54
1:C:20:LEU:HD23	1:C:23:ILE:HD11	1.90	0.54
1:E:153:LEU:CD2	1:E:177:ILE:HG21	2.38	0.54
1:J:343:THR:HG22	1:J:344:VAL:H	1.73	0.54
1:B:441:THR:OG1	1:B:442:LEU:N	2.39	0.53
1:G:343:THR:HG22	1:G:344:VAL:H	1.71	0.53
1:H:85:ALA:HB1	1:H:264:THR:HG22	1.90	0.53
1:D:318:MET:HE2	1:D:419:MET:HB3	1.91	0.53
1:E:118:TYR:HA	1:E:121:MET:HE3	1.89	0.53
1:H:65:CYS:HB3	1:H:400:ASN:HD22	1.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:101:LYS:HG2	1:J:246:ASP:OD2	2.09	0.53
1:J:293:LYS:HE3	1:J:317:TYR:CE1	2.43	0.53
1:K:372:TRP:CE3	1:K:383:ARG:HD3	2.43	0.53
1:L:266:LEU:O	1:L:270:HIS:ND1	2.30	0.53
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.90	0.53
1:D:124:ASP:O	1:D:127:VAL:HG22	2.07	0.53
1:I:106:LEU:O	1:I:109:THR:OG1	2.24	0.53
1:J:107:MET:SD	1:J:406:ILE:HG23	2.48	0.53
1:J:123:VAL:HG13	1:J:421:MET:HE1	1.90	0.53
1:J:342:ASP:HB3	1:J:352:LYS:HA	1.90	0.53
1:K:312:VAL:HG11	1:K:413:HIS:NE2	2.24	0.53
1:L:136:LEU:HD12	1:L:453:ILE:HD11	1.89	0.53
1:E:20:LEU:HD21	1:E:47:THR:HG22	1.90	0.53
1:E:427:GLU:HB3	1:E:454:LEU:HB2	1.90	0.53
1:K:103:HIS:NE2	1:K:107:MET:HE2	2.23	0.53
1:L:284:LEU:HD21	1:L:321:ILE:HD13	1.89	0.53
1:D:106:LEU:HD13	1:D:265:PHE:HZ	1.74	0.53
1:I:61:VAL:O	1:I:65:CYS:HB3	2.09	0.53
1:I:137:ASN:HB3	1:I:138:PRO:HD2	1.90	0.53
1:I:342:ASP:OD1	1:I:353:LYS:N	2.32	0.53
3:C:502:PLM:O2	3:I:502:PLM:HD1	2.08	0.53
1:D:103:HIS:O	1:D:107:MET:HG2	2.08	0.53
1:F:317:TYR:HA	1:F:320:MET:HE3	1.90	0.53
1:H:343:THR:HG22	1:H:344:VAL:H	1.73	0.53
1:J:398:PHE:CD2	1:J:408:MET:HE3	2.43	0.53
2:J:501:HEM:HBC2	2:J:501:HEM:HMC2	1.90	0.53
1:A:137:ASN:H	1:A:140:GLU:CD	2.17	0.53
1:F:124:ASP:OD2	1:F:164:ARG:NH2	2.40	0.53
1:F:218:LEU:O	1:F:221:ASN:HB2	2.09	0.53
1:H:20:LEU:HD12	1:H:48:LEU:HG	1.89	0.53
1:H:71:ASP:HB2	1:H:340:LYS:HE3	1.90	0.53
1:H:352:LYS:HG3	1:H:355:GLU:HB3	1.91	0.53
1:J:136:LEU:HD12	1:J:453:ILE:HD13	1.90	0.53
1:D:256:GLU:O	1:D:259:ARG:HG2	2.08	0.53
1:F:90:PHE:HB2	1:F:264:THR:HG23	1.91	0.53
1:H:308:THR:HG22	1:H:311:GLN:OE1	2.08	0.53
1:I:254:ASP:O	1:I:258:ILE:HG13	2.08	0.53
1:J:144:VAL:CG2	1:J:145:PRO:HD3	2.39	0.53
1:D:123:VAL:HG13	1:D:421:MET:HE1	1.90	0.53
1:E:81:VAL:HG12	1:E:91:THR:HG21	1.90	0.53
1:F:276:LEU:HD13	1:F:326:LEU:HG	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:PHE:HB2	1:D:264:THR:HG23	1.90	0.53
1:D:435:GLN:OE1	1:K:49:SER:HB2	2.09	0.53
1:E:276:LEU:HD13	1:E:326:LEU:HG	1.90	0.52
1:H:253:LEU:HD22	1:H:257:ASN:HD22	1.74	0.52
1:K:366:HIS:CE1	1:K:397:PRO:HG3	2.44	0.52
1:D:72:LYS:HA	1:D:337:LEU:HD23	1.92	0.52
1:F:93:GLU:HB2	1:F:96:GLU:HG3	1.91	0.52
1:G:63:GLU:OE1	1:G:346:GLY:N	2.28	0.52
1:G:220:ASP:OD2	1:G:259:ARG:NH2	2.41	0.52
1:K:155:THR:HG21	1:K:414:GLU:CD	2.34	0.52
1:B:343:THR:HG22	1:B:344:VAL:H	1.73	0.52
1:G:221:ASN:O	1:G:225:GLU:HG3	2.09	0.52
2:H:501:HEM:HMC2	2:H:501:HEM:HBC2	1.91	0.52
1:L:20:LEU:HD23	1:L:23:ILE:HD12	1.92	0.52
1:L:81:VAL:HG12	1:L:91:THR:HG21	1.90	0.52
1:A:14:TYR:HA	1:J:37:GLU:HG2	1.92	0.52
1:A:226:ARG:NH2	1:A:236:ASP:OD1	2.42	0.52
3:B:502:PLM:C3	3:C:502:PLM:H81	2.40	0.52
1:D:308:THR:N	1:D:311:GLN:OE1	2.32	0.52
1:I:321:ILE:HG23	1:I:379:PHE:HZ	1.75	0.52
1:J:254:ASP:O	1:J:258:ILE:HG23	2.09	0.52
1:J:326:LEU:HD12	1:J:330:PRO:HA	1.91	0.52
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	1.92	0.52
1:I:64:VAL:HA	1:I:70:PHE:CD2	2.45	0.52
1:L:72:LYS:HD3	1:L:336:SER:O	2.09	0.52
1:D:219:VAL:O	1:D:223:ILE:HG12	2.10	0.52
1:I:102:ALA:HB2	1:I:253:LEU:HD11	1.91	0.52
1:L:123:VAL:HG12	1:L:417:LEU:HD11	1.92	0.52
1:J:119:HIS:O	1:J:123:VAL:HG23	2.10	0.52
1:A:276:LEU:HD13	1:A:326:LEU:HG	1.92	0.52
1:B:210:HIS:O	1:B:213:GLN:HG2	2.09	0.52
1:G:336:SER:C	1:G:337:LEU:HD12	2.35	0.52
1:J:78:LEU:HD21	1:J:90:PHE:HE1	1.75	0.52
1:K:297:GLU:HG3	1:K:300:ARG:NH2	2.25	0.52
1:L:105:ILE:HG22	1:L:106:LEU:HG	1.92	0.52
1:L:258:ILE:O	1:L:262:ILE:HG23	2.09	0.52
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.91	0.52
1:B:257:ASN:O	1:B:261:GLN:HG2	2.09	0.52
1:B:304:ASP:HB3	1:B:305:PRO:HD2	1.92	0.52
1:H:270:HIS:CE1	1:H:271:GLU:HG3	2.45	0.52
1:I:85:ALA:HB1	1:I:264:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:429:ILE:HB	1:J:452:ARG:HB2	1.92	0.52
1:E:284:LEU:HD21	1:E:321:ILE:HD13	1.90	0.51
1:F:47:THR:HG22	1:F:48:LEU:N	2.25	0.51
1:H:84:PHE:HE1	1:H:267:ILE:HD13	1.74	0.51
1:A:20:LEU:HD12	1:A:48:LEU:HD13	1.92	0.51
1:B:152:THR:HG21	1:B:273:THR:HG23	1.92	0.51
1:F:241:MET:HE2	1:F:258:ILE:HG12	1.92	0.51
1:G:61:VAL:HG11	1:G:365:LEU:HD22	1.92	0.51
1:I:308:THR:HG23	1:I:311:GLN:HB2	1.92	0.51
1:L:74:ILE:O	1:L:74:ILE:HG13	2.09	0.51
1:L:302:LEU:HD11	1:L:315:LEU:HD11	1.92	0.51
1:L:331:THR:O	1:L:443:THR:HG23	2.09	0.51
1:A:69:ARG:NH2	1:A:343:THR:OG1	2.39	0.51
1:G:375:ASN:O	1:G:383:ARG:NH2	2.42	0.51
1:I:47:THR:HG22	1:I:48:LEU:N	2.25	0.51
1:C:86:GLY:O	1:C:91:THR:OG1	2.29	0.51
1:I:276:LEU:N	1:I:331:THR:HG21	2.26	0.51
1:F:241:MET:HE1	1:F:261:GLN:HB2	1.92	0.51
1:F:309:TYR:CZ	1:F:313:MET:HE2	2.46	0.51
1:I:65:CYS:HB2	1:I:400:ASN:HD21	1.68	0.51
1:A:121:MET:SD	1:A:159:CYS:HA	2.50	0.51
1:B:152:THR:CG2	1:B:273:THR:HG23	2.41	0.51
1:C:254:ASP:O	1:C:258:ILE:HG13	2.11	0.51
1:D:324:GLU:OE2	1:D:383:ARG:NH1	2.44	0.51
1:K:63:GLU:OE1	1:K:346:GLY:N	2.36	0.51
1:B:213:GLN:HB2	1:H:221:ASN:OD1	2.11	0.51
1:D:284:LEU:HD21	1:D:321:ILE:HD13	1.92	0.51
1:E:101:LYS:HG3	1:E:246:ASP:HB2	1.91	0.51
1:I:84:PHE:HZ	1:I:184:LEU:HD21	1.75	0.51
1:J:47:THR:HG22	1:J:48:LEU:N	2.25	0.51
1:L:136:LEU:HD11	1:L:142:VAL:HG22	1.93	0.51
2:E:501:HEM:HBB2	2:E:501:HEM:HMB2	1.93	0.51
1:H:72:LYS:HA	1:H:337:LEU:HD23	1.92	0.51
2:I:501:HEM:HMB2	2:I:501:HEM:HBB2	1.91	0.51
1:L:212:ILE:HG23	1:L:213:GLN:H	1.76	0.51
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.92	0.51
1:E:298:VAL:HG13	1:E:302:LEU:HD12	1.92	0.51
1:K:406:ILE:HG12	2:K:501:HEM:HBD2	1.92	0.51
1:L:126:ALA:O	1:L:130:VAL:HG23	2.11	0.51
1:G:343:THR:HG22	1:G:344:VAL:N	2.26	0.51
1:I:42:ILE:HD13	1:I:55:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:336:SER:C	1:I:337:LEU:HD12	2.36	0.51
1:J:135:ARG:NH1	1:K:169:TYR:OH	2.41	0.51
1:J:342:ASP:HA	1:J:351:ILE:O	2.11	0.51
1:A:123:VAL:HG11	1:A:306:THR:HG23	1.93	0.50
1:B:355:GLU:O	1:B:357:ARG:NH1	2.44	0.50
1:C:267:ILE:HG13	1:C:268:ALA:H	1.75	0.50
1:F:72:LYS:HD3	1:F:403:ARG:CZ	2.42	0.50
1:F:282:TYR:CZ	1:F:436:LEU:HB2	2.46	0.50
1:H:298:VAL:HG13	1:H:302:LEU:HD12	1.92	0.50
1:B:177:ILE:O	1:B:181:THR:HG23	2.11	0.50
1:G:144:VAL:O	1:G:148:MET:HG2	2.12	0.50
1:L:101:LYS:O	1:L:105:ILE:HG13	2.11	0.50
1:A:11:PRO:HA	1:A:39:TYR:CE2	2.46	0.50
1:C:241:MET:HE1	1:C:258:ILE:HA	1.92	0.50
1:E:32:PHE:CE1	1:E:45:ILE:HD12	2.46	0.50
1:E:387:LEU:O	1:E:390:VAL:HG22	2.10	0.50
1:I:102:ALA:O	1:I:106:LEU:HG	2.11	0.50
1:J:58:HIS:CE1	1:J:59:GLU:HG3	2.45	0.50
1:K:82:ARG:HG3	1:K:86:GLY:O	2.12	0.50
1:L:295:TYR:CE1	1:L:423:LEU:HD22	2.47	0.50
1:C:254:ASP:OD1	1:C:255:ASP:N	2.44	0.50
1:F:133:TRP:HB3	1:F:453:ILE:CD1	2.41	0.50
1:C:112:GLN:NE2	1:C:313:MET:HE1	2.24	0.50
1:D:154:ASP:OD1	1:D:167:SER:OG	2.25	0.50
2:G:501:HEM:HMB2	2:G:501:HEM:HBB2	1.94	0.50
1:J:72:LYS:HE3	1:J:73:SER:O	2.12	0.50
1:K:81:VAL:HG12	1:K:91:THR:HG21	1.93	0.50
1:L:47:THR:HG23	1:L:50:ASP:H	1.77	0.50
2:L:501:HEM:HBB2	2:L:501:HEM:HMB2	1.94	0.50
1:A:209:GLN:HE22	1:J:140:GLU:HA	1.76	0.50
1:A:267:ILE:HG13	1:A:268:ALA:N	2.26	0.50
1:C:304:ASP:HB3	1:C:305:PRO:HD2	1.93	0.50
1:D:77:ALA:O	1:D:80:LYS:HG2	2.11	0.50
1:E:342:ASP:OD1	1:E:353:LYS:N	2.45	0.50
1:F:237:LEU:O	1:F:241:MET:HG3	2.11	0.50
1:H:276:LEU:HD13	1:H:326:LEU:HG	1.93	0.50
1:I:133:TRP:NE1	1:I:142:VAL:HG21	2.27	0.50
1:I:340:LYS:O	1:I:353:LYS:HD2	2.12	0.50
1:B:69:ARG:HE	1:B:343:THR:HG21	1.77	0.50
1:C:277:LEU:HD21	1:C:415:ALA:HA	1.93	0.50
1:D:293:LYS:HB3	1:D:317:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:352:LYS:NZ	1:E:355:GLU:OE2	2.35	0.50
1:H:130:VAL:HG23	1:H:426:PHE:CE2	2.46	0.50
1:I:308:THR:CG2	1:I:311:GLN:HB2	2.41	0.50
1:J:336:SER:HA	1:J:358:ILE:O	2.11	0.50
1:A:20:LEU:HD11	1:A:47:THR:OG1	2.11	0.49
1:B:124:ASP:O	1:B:127:VAL:HG22	2.12	0.49
1:K:113:ARG:HG3	1:K:114:ALA:H	1.76	0.49
1:K:127:VAL:HA	1:K:130:VAL:HG12	1.93	0.49
1:K:219:VAL:CG2	1:K:259:ARG:HG3	2.43	0.49
1:K:342:ASP:OD1	1:K:353:LYS:N	2.45	0.49
1:A:119:HIS:O	1:A:123:VAL:HG23	2.12	0.49
1:B:171:GLU:OE1	1:E:172:THR:HG22	2.11	0.49
1:E:37:GLU:HG2	1:H:14:TYR:HA	1.94	0.49
1:F:41:PRO:HB3	1:F:57:GLY:HA3	1.93	0.49
1:G:71:ASP:HB3	1:G:338:TYR:CE1	2.48	0.49
1:I:135:ARG:HD2	1:L:169:TYR:OH	2.13	0.49
1:A:257:ASN:O	1:A:261:GLN:HG2	2.12	0.49
2:H:501:HEM:HMB2	2:H:501:HEM:HBB2	1.93	0.49
1:I:163:TYR:HE1	1:L:137:ASN:ND2	2.01	0.49
2:J:501:HEM:HBB2	2:J:501:HEM:HMB2	1.95	0.49
1:A:72:LYS:NZ	1:A:90:PHE:O	2.44	0.49
1:C:267:ILE:HG13	1:C:268:ALA:N	2.28	0.49
1:D:84:PHE:HE2	1:D:267:ILE:HD13	1.77	0.49
1:F:342:ASP:OD1	1:F:352:LYS:HA	2.13	0.49
1:G:113:ARG:HG3	1:G:114:ALA:N	2.27	0.49
1:J:240:ARG:O	1:J:244:VAL:HG22	2.12	0.49
1:A:112:GLN:NE2	1:A:313:MET:HE2	2.28	0.49
1:D:151:LEU:O	1:D:155:THR:OG1	2.28	0.49
1:J:363:PRO:O	1:J:367:ARG:HG3	2.13	0.49
1:F:99:TRP:CH2	1:F:402:GLN:HG2	2.47	0.49
1:F:431:TYR:CE2	1:F:432:GLN:HG3	2.47	0.49
1:I:327:ARG:NH2	1:I:376:VAL:HA	2.27	0.49
1:K:226:ARG:HH12	1:K:236:ASP:CG	2.20	0.49
1:K:302:LEU:HD11	1:K:424:GLN:CD	2.38	0.49
1:J:144:VAL:O	1:J:148:MET:HG2	2.13	0.49
1:J:297:GLU:HG2	1:J:315:LEU:HD23	1.94	0.49
1:B:293:LYS:HB3	1:B:317:TYR:CE2	2.47	0.49
1:L:129:LEU:HD22	1:L:151:LEU:HD22	1.94	0.49
1:D:47:THR:HG22	1:D:50:ASP:O	2.12	0.49
1:J:301:VAL:O	1:J:311:GLN:NE2	2.41	0.49
1:K:161:PHE:HZ	1:K:265:PHE:HD2	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ASP:OD1	1:A:145:PRO:HD2	2.12	0.49
1:B:86:GLY:O	1:B:91:THR:OG1	2.30	0.49
1:D:70:PHE:CZ	1:D:345:ILE:HD11	2.47	0.49
1:D:215:MET:O	1:D:219:VAL:HG13	2.12	0.49
1:D:417:LEU:HD11	1:D:421:MET:HE3	1.94	0.49
1:F:240:ARG:NH1	1:F:244:VAL:HG11	2.27	0.49
1:H:216:PHE:HD1	1:H:259:ARG:NE	2.11	0.48
1:H:241:MET:HE2	1:H:258:ILE:HG23	1.94	0.48
1:J:129:LEU:HD22	1:J:151:LEU:HD22	1.95	0.48
1:J:293:LYS:HE3	1:J:317:TYR:CZ	2.47	0.48
1:K:75:GLU:HG3	1:K:76:GLY:N	2.28	0.48
1:L:86:GLY:O	1:L:91:THR:OG1	2.22	0.48
1:C:71:ASP:HB3	1:C:338:TYR:CE1	2.48	0.48
1:E:160:GLY:HA2	1:E:237:LEU:HD12	1.93	0.48
1:F:213:GLN:HG2	1:J:221:ASN:CG	2.39	0.48
1:G:41:PRO:HB3	1:G:57:GLY:HA3	1.95	0.48
1:H:152:THR:HG22	1:H:270:HIS:HA	1.93	0.48
1:H:304:ASP:HB3	1:H:305:PRO:HD2	1.95	0.48
1:I:382:GLU:O	1:I:385:GLU:HG3	2.13	0.48
1:E:249:THR:HG23	1:E:251:GLU:H	1.77	0.48
1:F:47:THR:HG22	1:F:48:LEU:H	1.77	0.48
1:G:387:LEU:O	1:G:390:VAL:HG22	2.14	0.48
1:I:90:PHE:CE1	2:I:501:HEM:HBA1	2.48	0.48
1:B:136:LEU:HD11	1:B:142:VAL:CG1	2.43	0.48
1:C:351:ILE:HD13	1:C:358:ILE:HD11	1.95	0.48
1:D:8:ILE:HD11	1:D:42:ILE:HD11	1.93	0.48
1:E:84:PHE:HB3	1:E:212:ILE:HG12	1.93	0.48
1:F:256:GLU:HG3	1:F:259:ARG:NH2	2.28	0.48
1:F:318:MET:HE3	1:F:318:MET:O	2.13	0.48
1:G:80:LYS:HD2	1:G:184:LEU:HA	1.95	0.48
1:H:327:ARG:HG2	1:H:366:HIS:HB3	1.95	0.48
1:I:405:CYS:HB2	2:I:501:HEM:NA	2.28	0.48
1:J:72:LYS:NZ	1:J:336:SER:H	2.11	0.48
1:J:169:TYR:OH	1:K:135:ARG:HD2	2.13	0.48
1:K:99:TRP:HH2	1:K:402:GLN:HG2	1.78	0.48
1:L:291:LEU:HG	1:L:295:TYR:CE2	2.48	0.48
1:C:180:MET:HE1	1:C:266:LEU:CB	2.44	0.48
1:I:66:ASP:CG	1:I:68:THR:HG22	2.39	0.48
1:K:238:LEU:HG	1:K:242:LEU:HD23	1.96	0.48
1:C:112:GLN:HG2	1:C:409:GLN:OE1	2.13	0.48
1:C:336:SER:HA	1:C:358:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:TYR:HA	1:F:37:GLU:HG2	1.95	0.48
1:K:99:TRP:CH2	1:K:402:GLN:HG2	2.48	0.48
1:A:113:ARG:HD2	1:I:38:GLU:O	2.14	0.48
1:C:327:ARG:NH2	1:C:376:VAL:O	2.29	0.48
1:F:72:LYS:HA	1:F:337:LEU:HD23	1.95	0.48
1:H:10:GLN:HB3	1:H:44:GLN:HG3	1.95	0.48
1:J:174:HIS:O	1:J:177:ILE:HG22	2.14	0.48
1:L:155:THR:HG21	1:L:414:GLU:OE2	2.14	0.48
1:A:115:MET:SD	1:A:410:PHE:HA	2.54	0.48
1:F:105:ILE:HD12	1:F:253:LEU:HG	1.95	0.48
1:I:218:LEU:O	1:I:221:ASN:HB2	2.13	0.48
1:L:142:VAL:HG13	1:L:147:ASP:OD2	2.14	0.48
1:D:47:THR:CG2	1:D:50:ASP:H	2.27	0.48
1:E:35:ILE:CD1	1:E:45:ILE:HD11	2.38	0.48
1:H:144:VAL:O	1:H:148:MET:HG2	2.13	0.48
1:H:270:HIS:NE2	1:H:271:GLU:HG3	2.28	0.48
1:J:293:LYS:O	1:J:296:GLU:HG3	2.13	0.48
1:K:366:HIS:HE1	1:K:397:PRO:HG3	1.77	0.48
1:L:58:HIS:HD2	1:L:368:ASP:OD2	1.97	0.48
1:C:276:LEU:HD13	1:C:326:LEU:HG	1.96	0.47
1:C:391:PRO:HB2	1:C:394:ALA:HB3	1.96	0.47
1:D:41:PRO:HB3	1:D:57:GLY:HA3	1.96	0.47
1:D:219:VAL:HG11	1:D:263:ILE:HG13	1.96	0.47
1:D:431:TYR:CD1	1:D:452:ARG:HG3	2.48	0.47
1:G:42:ILE:HB	1:G:60:LEU:HD13	1.96	0.47
1:J:105:ILE:HD12	1:J:253:LEU:HG	1.96	0.47
1:J:301:VAL:HG11	1:J:314:LYS:HB2	1.95	0.47
1:K:82:ARG:O	1:K:86:GLY:N	2.35	0.47
1:A:34:LYS:HG2	1:G:14:TYR:CD2	2.49	0.47
1:H:82:ARG:HD2	1:H:91:THR:O	2.13	0.47
1:J:431:TYR:HB3	1:J:452:ARG:HG3	1.96	0.47
1:K:285:LEU:HD11	1:K:451:ILE:HG21	1.95	0.47
1:L:336:SER:HA	1:L:358:ILE:O	2.14	0.47
1:C:133:TRP:HB3	1:C:453:ILE:CD1	2.44	0.47
1:C:257:ASN:O	1:C:261:GLN:HG2	2.14	0.47
1:E:277:LEU:HD21	1:E:415:ALA:HA	1.96	0.47
1:H:441:THR:OG1	1:H:442:LEU:N	2.47	0.47
1:K:64:VAL:HG13	1:K:337:LEU:HD11	1.97	0.47
1:B:343:THR:HG22	1:B:344:VAL:N	2.29	0.47
1:F:257:ASN:O	1:F:261:GLN:HG2	2.15	0.47
3:G:502:PLM:H91	3:J:502:PLM:H21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:19:ASN:OD1	1:L:45:ILE:HG23	2.15	0.47
1:A:309:TYR:CZ	1:A:313:MET:HE1	2.50	0.47
1:C:84:PHE:HE2	1:C:267:ILE:HG21	1.80	0.47
1:E:30:LEU:HD22	1:H:17:LEU:HD21	1.97	0.47
2:F:501:HEM:HMB2	2:F:501:HEM:HBB2	1.95	0.47
1:H:30:LEU:HD22	1:L:17:LEU:HD21	1.97	0.47
1:H:161:PHE:HA	1:H:236:ASP:OD2	2.14	0.47
1:I:72:LYS:HB2	1:I:403:ARG:HG3	1.95	0.47
1:L:100:LYS:HE3	1:L:104:ASN:HD21	1.79	0.47
1:B:42:ILE:HD11	1:B:53:ILE:HG23	1.96	0.47
1:E:184:LEU:HD22	1:E:442:LEU:HD11	1.96	0.47
1:K:88:GLY:H	1:K:92:SER:HB3	1.80	0.47
1:L:72:LYS:HB2	1:L:403:ARG:HG3	1.97	0.47
1:A:342:ASP:OD1	1:A:353:LYS:N	2.45	0.47
1:E:41:PRO:HB3	1:E:57:GLY:HA3	1.97	0.47
1:F:174:HIS:N	1:F:177:ILE:HD12	2.29	0.47
1:F:240:ARG:HD3	1:F:244:VAL:HB	1.97	0.47
1:G:20:LEU:HD12	1:G:48:LEU:CD1	2.45	0.47
1:G:115:MET:SD	1:G:410:PHE:HA	2.55	0.47
1:I:176:PHE:CE2	1:I:215:MET:HE2	2.49	0.47
1:J:122:MET:HE2	1:J:410:PHE:CE1	2.50	0.47
1:A:105:ILE:HD12	1:A:253:LEU:HG	1.96	0.47
1:B:277:LEU:HD21	1:B:415:ALA:HA	1.96	0.47
1:H:65:CYS:CB	1:H:400:ASN:HD22	2.26	0.47
1:H:89:LEU:HD21	1:H:106:LEU:HD11	1.95	0.47
1:H:123:VAL:HG13	1:H:421:MET:HE1	1.95	0.47
1:H:217:SER:O	1:H:220:ASP:HB2	2.14	0.47
1:J:225:GLU:OE2	1:J:226:ARG:HG3	2.14	0.47
1:J:351:ILE:HG22	1:J:353:LYS:HG2	1.97	0.47
1:K:31:SER:O	1:K:35:ILE:HG13	2.15	0.47
1:A:171:GLU:OE2	1:D:172:THR:HG23	2.15	0.47
3:A:502:PLM:H61	3:A:502:PLM:H32	1.65	0.47
1:B:435:GLN:OE1	1:I:49:SER:HB2	2.15	0.47
1:J:86:GLY:O	1:J:91:THR:OG1	2.31	0.47
1:L:65:CYS:HB2	1:L:400:ASN:CG	2.40	0.47
1:A:341:GLU:HA	1:A:353:LYS:HD3	1.97	0.47
1:E:129:LEU:HD22	1:E:151:LEU:HD22	1.97	0.47
1:F:115:MET:SD	1:F:410:PHE:HA	2.55	0.47
1:F:139:ASN:O	1:F:452:ARG:NH2	2.48	0.47
1:F:343:THR:HG22	1:F:344:VAL:N	2.30	0.47
1:H:396:LYS:N	1:H:397:PRO:HD3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:246:ASP:OD1	1:J:249:THR:N	2.47	0.47
1:J:312:VAL:HG21	1:J:417:LEU:HA	1.97	0.47
1:K:180:MET:HE3	1:K:180:MET:HB3	1.70	0.47
1:K:285:LEU:HD12	1:K:449:PHE:HZ	1.78	0.47
1:L:156:ILE:HD11	1:L:269:GLY:HA3	1.97	0.47
1:L:302:LEU:CD2	1:L:311:GLN:HB2	2.45	0.47
1:D:119:HIS:O	1:D:123:VAL:HG23	2.15	0.46
3:D:502:PLM:H61	3:D:503:PLM:H81	1.97	0.46
1:F:64:VAL:HG12	1:F:337:LEU:HD13	1.97	0.46
1:F:99:TRP:HH2	1:F:402:GLN:HG2	1.80	0.46
1:H:398:PHE:CE2	1:H:408:MET:HE3	2.50	0.46
1:I:123:VAL:O	1:I:127:VAL:HG13	2.14	0.46
1:I:130:VAL:HG23	1:I:426:PHE:CE2	2.50	0.46
1:I:430:ASP:OD2	1:I:433:ASN:HA	2.15	0.46
1:L:8:ILE:HG12	1:L:349:TYR:HD1	1.79	0.46
1:C:290:LYS:HD2	1:C:290:LYS:N	2.30	0.46
1:F:133:TRP:CZ2	1:F:142:VAL:HG11	2.51	0.46
1:I:94:THR:HA	1:I:403:ARG:NH1	2.30	0.46
1:L:302:LEU:HD22	1:L:311:GLN:NE2	2.31	0.46
1:A:12:LYS:H	1:A:19:ASN:HD21	1.62	0.46
1:C:115:MET:SD	1:C:410:PHE:HA	2.55	0.46
1:C:119:HIS:O	1:C:123:VAL:HG23	2.15	0.46
1:C:367:ARG:NE	1:C:377:GLU:OE2	2.40	0.46
1:E:11:PRO:HA	1:E:39:TYR:CE2	2.51	0.46
1:L:163:TYR:CZ	1:L:218:LEU:HD11	2.51	0.46
1:L:253:LEU:HD21	1:L:258:ILE:HG12	1.96	0.46
1:C:41:PRO:HB3	1:C:57:GLY:HA3	1.97	0.46
1:E:64:VAL:HA	1:E:70:PHE:CD2	2.50	0.46
1:G:78:LEU:HD23	1:G:78:LEU:HA	1.67	0.46
1:J:170:ARG:NH2	1:J:175:PRO:HD3	2.30	0.46
1:K:309:TYR:O	1:K:312:VAL:HG12	2.15	0.46
1:B:59:GLU:H	1:B:59:GLU:CD	2.24	0.46
1:B:185:ASP:HA	1:B:188:MET:HG2	1.98	0.46
1:E:76:GLY:O	1:E:77:ALA:C	2.59	0.46
1:G:99:TRP:CH2	1:G:402:GLN:HG2	2.50	0.46
1:G:119:HIS:O	1:G:123:VAL:HG23	2.15	0.46
1:I:84:PHE:HA	1:I:216:PHE:CZ	2.50	0.46
1:J:335:PHE:CD1	1:J:362:ILE:HD11	2.50	0.46
1:L:120:ALA:O	1:L:123:VAL:HG22	2.16	0.46
1:C:226:ARG:NH1	1:C:234:GLU:HB3	2.30	0.46
1:H:390:VAL:O	1:H:392:HIS:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:127:VAL:O	1:I:130:VAL:HG12	2.15	0.46
1:K:290:LYS:HG3	1:K:317:TYR:OH	2.15	0.46
1:K:367:ARG:NE	1:K:377:GLU:OE2	2.38	0.46
1:E:109:THR:HG21	1:E:237:LEU:HD23	1.97	0.46
1:E:290:LYS:HD2	1:E:290:LYS:N	2.31	0.46
1:H:174:HIS:O	1:H:177:ILE:HG22	2.16	0.46
1:I:84:PHE:HA	1:I:216:PHE:HZ	1.80	0.46
1:K:241:MET:HG2	1:K:258:ILE:HG23	1.98	0.46
1:K:301:VAL:HG12	1:K:301:VAL:O	2.15	0.46
1:L:47:THR:CG2	1:L:50:ASP:H	2.28	0.46
1:B:296:GLU:OE2	1:B:300:ARG:NH2	2.48	0.46
1:E:220:ASP:OD1	1:E:259:ARG:HD3	2.16	0.46
1:G:288:PRO:O	1:G:292:LYS:HG2	2.16	0.46
1:I:99:TRP:HE1	2:I:501:HEM:CGD	2.26	0.46
1:J:65:CYS:HB3	1:J:400:ASN:OD1	2.16	0.46
1:J:272:THR:HA	1:J:331:THR:HG21	1.96	0.46
1:B:184:LEU:HA	1:B:187:ALA:HB3	1.98	0.46
1:C:240:ARG:HH11	1:C:244:VAL:HG11	1.81	0.46
1:I:154:ASP:OD1	1:I:165:PHE:HB2	2.16	0.46
1:J:89:LEU:HD23	1:J:406:ILE:HG13	1.97	0.46
3:A:502:PLM:H42	3:G:502:PLM:H61	1.98	0.46
1:B:84:PHE:HZ	1:B:184:LEU:HD23	1.81	0.46
1:D:161:PHE:CZ	1:D:266:LEU:HD21	2.51	0.46
1:G:276:LEU:HD13	1:G:326:LEU:HG	1.97	0.46
1:I:119:HIS:O	1:I:123:VAL:HG23	2.16	0.46
1:I:121:MET:HB3	1:I:158:LEU:CD2	2.46	0.46
1:J:348:LYS:HE2	1:J:349:TYR:CZ	2.51	0.46
1:K:154:ASP:OD1	1:K:165:PHE:HB2	2.16	0.46
1:L:238:LEU:O	1:L:242:LEU:CB	2.62	0.46
1:H:273:THR:CG2	2:H:501:HEM:HAB	2.40	0.45
1:K:240:ARG:O	1:K:244:VAL:HG22	2.15	0.45
1:C:133:TRP:HB3	1:C:453:ILE:HD13	1.97	0.45
1:E:12:LYS:O	1:E:19:ASN:ND2	2.48	0.45
1:E:61:VAL:HG11	1:E:365:LEU:HD22	1.98	0.45
1:A:72:LYS:HE3	2:A:501:HEM:O1A	2.16	0.45
1:C:90:PHE:HE1	2:C:501:HEM:HBA1	1.82	0.45
1:C:133:TRP:NE1	1:C:142:VAL:HG21	2.32	0.45
1:E:290:LYS:HD2	1:E:290:LYS:H	1.82	0.45
1:E:318:MET:HE3	1:E:321:ILE:HB	1.97	0.45
1:F:74:ILE:HG22	1:F:78:LEU:HD13	1.98	0.45
1:G:255:ASP:O	1:G:259:ARG:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:80:LYS:HE2	1:H:184:LEU:HA	1.98	0.45
1:J:160:GLY:HA2	1:J:237:LEU:HB2	1.99	0.45
1:A:284:LEU:HD21	1:A:321:ILE:HD13	1.97	0.45
1:B:285:LEU:HG	1:B:430:ASP:HB2	1.99	0.45
1:E:150:ARG:HG2	1:E:167:SER:HB3	1.98	0.45
1:E:304:ASP:HB3	1:E:305:PRO:HD2	1.97	0.45
1:F:112:GLN:CD	1:F:313:MET:HE1	2.41	0.45
1:H:253:LEU:HD22	1:H:257:ASN:ND2	2.31	0.45
1:I:304:ASP:HB3	1:I:305:PRO:HD2	1.96	0.45
1:K:69:ARG:NH2	1:K:345:ILE:HD13	2.31	0.45
1:K:145:PRO:HD3	1:K:449:PHE:HB3	1.97	0.45
1:L:61:VAL:HA	1:L:64:VAL:HG22	1.99	0.45
1:L:133:TRP:CZ3	1:L:422:LEU:HD22	2.52	0.45
1:B:81:VAL:HG23	1:B:84:PHE:CE2	2.51	0.45
1:C:226:ARG:HH12	1:C:234:GLU:HB3	1.82	0.45
1:C:237:LEU:O	1:C:241:MET:HG3	2.16	0.45
1:G:115:MET:HE2	1:G:115:MET:HA	1.99	0.45
1:H:295:TYR:CE1	1:H:423:LEU:HD22	2.51	0.45
1:L:148:MET:HE2	1:L:277:LEU:HB3	1.97	0.45
1:F:86:GLY:O	1:F:91:THR:OG1	2.35	0.45
1:I:88:GLY:HA3	1:I:264:THR:HG21	1.99	0.45
1:I:301:VAL:CG1	1:I:311:GLN:HG2	2.47	0.45
1:J:150:ARG:HG2	1:J:167:SER:HB3	1.98	0.45
1:K:411:ALA:HB2	2:K:501:HEM:HHC	1.99	0.45
1:B:179:SER:HB3	1:B:211:ASP:HB3	1.98	0.45
1:C:133:TRP:O	1:C:453:ILE:HD11	2.17	0.45
1:E:86:GLY:O	1:E:91:THR:OG1	2.33	0.45
1:E:396:LYS:N	1:E:397:PRO:HD3	2.32	0.45
1:E:434:TYR:CE2	1:E:436:LEU:HA	2.52	0.45
1:I:153:LEU:HD22	1:I:177:ILE:HD11	1.99	0.45
1:I:405:CYS:HA	2:I:501:HEM:C4D	2.52	0.45
1:K:110:PHE:HB3	1:K:406:ILE:O	2.16	0.45
1:B:151:LEU:HD21	1:B:418:VAL:CG2	2.42	0.45
1:C:61:VAL:HG11	1:C:365:LEU:HD22	1.98	0.45
1:E:16:PRO:HG3	1:L:367:ARG:NE	2.32	0.45
1:I:115:MET:HE2	1:I:413:HIS:HB3	1.97	0.45
1:L:16:PRO:O	1:L:48:LEU:HD23	2.17	0.45
1:A:69:ARG:HH21	1:A:343:THR:HG1	1.65	0.45
1:D:161:PHE:HZ	1:D:266:LEU:HD21	1.81	0.45
1:D:254:ASP:OD1	1:D:255:ASP:N	2.49	0.45
1:E:42:ILE:HD11	1:E:349:TYR:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:ARG:O	1:H:83:ALA:C	2.59	0.45
1:J:246:ASP:OD1	1:J:246:ASP:C	2.60	0.45
1:K:180:MET:HA	1:K:215:MET:CE	2.47	0.45
1:B:144:VAL:HB	1:B:145:PRO:HD3	1.98	0.45
1:B:226:ARG:HH12	1:B:236:ASP:CG	2.20	0.45
1:E:38:GLU:OE2	1:H:14:TYR:HE2	2.00	0.45
1:F:71:ASP:HB3	1:F:338:TYR:CE2	2.52	0.45
1:K:321:ILE:HG23	1:K:379:PHE:HZ	1.82	0.45
1:K:405:CYS:HB2	2:K:501:HEM:NA	2.32	0.45
1:A:380:GLN:O	1:A:383:ARG:HG3	2.16	0.44
1:B:42:ILE:HB	1:B:60:LEU:HD13	1.99	0.44
1:D:82:ARG:NH1	1:D:92:SER:HA	2.31	0.44
1:F:71:ASP:OD1	1:F:72:LYS:N	2.50	0.44
3:H:502:PLM:H22	3:L:502:PLM:HB2	1.99	0.44
1:K:302:LEU:CD1	1:K:424:GLN:HG3	2.18	0.44
1:B:41:PRO:HB3	1:B:57:GLY:HA3	1.99	0.44
1:B:276:LEU:HD13	1:B:326:LEU:HG	2.00	0.44
1:F:105:ILE:O	1:F:240:ARG:HD2	2.17	0.44
1:G:103:HIS:O	1:G:107:MET:HG2	2.17	0.44
1:I:295:TYR:CZ	1:I:423:LEU:HD22	2.52	0.44
1:I:396:LYS:N	1:I:397:PRO:HD3	2.32	0.44
1:L:90:PHE:HE1	2:L:501:HEM:HBA1	1.81	0.44
1:L:219:VAL:O	1:L:223:ILE:HG13	2.18	0.44
1:L:398:PHE:CD2	1:L:408:MET:HE3	2.52	0.44
1:I:75:GLU:HB3	1:I:357:ARG:NH1	2.32	0.44
1:J:372:TRP:CZ2	1:J:395:TYR:HB2	2.53	0.44
1:K:181:THR:O	1:K:184:LEU:HB2	2.17	0.44
1:K:260:PHE:O	1:K:264:THR:HG23	2.17	0.44
1:K:414:GLU:O	1:K:418:VAL:HG23	2.17	0.44
1:A:61:VAL:HG21	1:A:365:LEU:HD13	2.00	0.44
1:B:217:SER:O	1:B:221:ASN:ND2	2.47	0.44
1:C:152:THR:CG2	1:C:273:THR:HG23	2.47	0.44
1:C:169:TYR:HD1	1:H:168:PHE:O	2.01	0.44
1:D:93:GLU:OE1	1:D:95:HIS:NE2	2.50	0.44
1:C:179:SER:HB2	1:C:211:ASP:HB3	2.00	0.44
1:E:105:ILE:HD12	1:E:253:LEU:HG	1.99	0.44
1:F:345:ILE:HG12	1:F:351:ILE:HD11	1.98	0.44
1:G:86:GLY:O	1:G:91:THR:OG1	2.35	0.44
1:J:335:PHE:HD1	1:J:362:ILE:HD11	1.82	0.44
1:K:396:LYS:N	1:K:397:PRO:HD3	2.33	0.44
1:L:398:PHE:CE2	1:L:408:MET:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:163:TYR:CZ	1:H:218:LEU:HD21	2.53	0.44
1:K:282:TYR:CZ	1:K:436:LEU:HB2	2.53	0.44
1:A:47:THR:HG23	1:A:50:ASP:H	1.81	0.44
1:B:281:ILE:HG23	1:B:428:LEU:HD23	1.98	0.44
1:D:30:LEU:HB3	3:D:503:PLM:HC1	1.99	0.44
1:D:246:ASP:HB3	1:D:249:THR:HG22	2.00	0.44
1:E:42:ILE:CG2	1:E:60:LEU:HD13	2.48	0.44
1:H:405:CYS:HB2	2:H:501:HEM:C4A	2.52	0.44
1:K:253:LEU:HD22	1:K:257:ASN:OD1	2.18	0.44
1:K:386:GLU:CG	1:K:389:LYS:HB2	2.46	0.44
1:B:241:MET:HE1	1:B:261:GLN:HB2	2.00	0.44
1:E:115:MET:SD	1:E:410:PHE:HA	2.58	0.44
1:G:75:GLU:HG2	1:G:336:SER:HB2	2.00	0.44
1:I:65:CYS:CB	1:I:400:ASN:HD21	2.24	0.44
1:I:363:PRO:HB3	1:I:367:ARG:HH12	1.83	0.44
1:A:71:ASP:HB3	1:A:338:TYR:CE1	2.53	0.44
1:B:226:ARG:NH1	1:B:236:ASP:OD2	2.27	0.44
1:G:272:THR:O	1:G:331:THR:HG21	2.17	0.44
1:H:115:MET:SD	1:H:410:PHE:HA	2.58	0.44
1:I:112:GLN:HE22	1:I:313:MET:HE3	1.83	0.44
1:I:125:ILE:HD12	1:I:154:ASP:HB3	1.99	0.44
1:J:136:LEU:HB2	1:J:453:ILE:HD11	2.00	0.44
1:K:398:PHE:CE2	1:K:408:MET:HE3	2.52	0.44
1:L:109:THR:HG22	1:L:118:TYR:OH	2.18	0.44
1:L:161:PHE:CE1	1:L:262:ILE:HG22	2.53	0.44
1:A:133:TRP:HB3	1:A:453:ILE:CD1	2.48	0.43
1:A:136:LEU:HD11	1:A:142:VAL:CG1	2.48	0.43
1:B:17:LEU:HD21	1:C:30:LEU:HD22	1.98	0.43
1:C:144:VAL:HB	1:C:145:PRO:HD3	2.00	0.43
1:D:84:PHE:CE2	1:D:267:ILE:HD13	2.53	0.43
1:F:154:ASP:OD1	1:F:165:PHE:HB2	2.18	0.43
1:I:133:TRP:CE2	1:I:142:VAL:HG21	2.53	0.43
1:I:258:ILE:O	1:I:262:ILE:HG12	2.18	0.43
1:J:270:HIS:NE2	1:J:271:GLU:HG3	2.32	0.43
1:L:70:PHE:HZ	1:L:345:ILE:HD11	1.83	0.43
1:A:47:THR:CG2	1:A:50:ASP:H	2.31	0.43
1:H:121:MET:SD	1:H:159:CYS:HA	2.58	0.43
1:J:71:ASP:OD1	1:J:94:THR:HG21	2.15	0.43
1:J:212:ILE:HG23	1:J:213:GLN:N	2.33	0.43
1:J:320:MET:HE1	1:J:385:GLU:OE1	2.18	0.43
1:A:423:LEU:O	1:A:456:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:LYS:HB3	1:A:445:LYS:HE2	1.77	0.43
1:H:398:PHE:CD2	1:H:408:MET:HE3	2.54	0.43
1:K:119:HIS:O	1:K:123:VAL:HG23	2.18	0.43
1:K:219:VAL:HG21	1:K:259:ARG:HG3	1.99	0.43
1:L:21:PRO:HA	3:L:502:PLM:HD2	2.01	0.43
1:L:109:THR:OG1	1:L:240:ARG:HG2	2.18	0.43
1:A:86:GLY:O	1:A:91:THR:OG1	2.34	0.43
1:B:352:LYS:HG3	1:B:355:GLU:HB3	2.00	0.43
1:B:367:ARG:NE	1:B:377:GLU:OE2	2.44	0.43
1:H:13:THR:HG23	1:H:18:GLY:HA2	2.01	0.43
1:I:121:MET:O	1:I:124:ASP:HB3	2.19	0.43
1:J:243:ASN:OD1	1:J:244:VAL:HG13	2.18	0.43
1:K:324:GLU:CD	1:K:327:ARG:HH21	2.24	0.43
1:L:47:THR:HG22	1:L:50:ASP:O	2.18	0.43
1:L:414:GLU:O	1:L:418:VAL:HG23	2.19	0.43
1:A:215:MET:O	1:A:219:VAL:HG23	2.19	0.43
1:C:226:ARG:HD2	1:C:238:LEU:HG	2.00	0.43
1:E:345:ILE:HG12	1:E:351:ILE:HD11	1.99	0.43
1:F:173:PRO:HB2	1:F:177:ILE:HB	2.00	0.43
1:I:107:MET:N	1:I:108:PRO:HD2	2.34	0.43
1:I:180:MET:CB	1:I:215:MET:HE1	2.44	0.43
1:I:390:VAL:O	1:I:392:HIS:N	2.51	0.43
1:K:177:ILE:O	1:K:181:THR:OG1	2.33	0.43
1:L:254:ASP:HB3	1:L:257:ASN:CB	2.42	0.43
1:L:362:ILE:N	1:L:363:PRO:HD2	2.33	0.43
1:B:42:ILE:HD11	1:B:53:ILE:CG2	2.48	0.43
1:B:176:PHE:HD1	1:B:177:ILE:HD13	1.82	0.43
1:H:221:ASN:O	1:H:225:GLU:HG2	2.18	0.43
1:H:276:LEU:N	1:H:331:THR:HG21	2.34	0.43
1:I:29:THR:OG1	1:I:440:GLN:NE2	2.51	0.43
1:I:63:GLU:OE2	1:I:69:ARG:NH1	2.47	0.43
1:K:69:ARG:NE	1:K:343:THR:HG21	2.33	0.43
1:K:421:MET:O	1:K:424:GLN:HB3	2.17	0.43
1:L:353:LYS:HE3	1:L:353:LYS:HB3	1.84	0.43
1:A:226:ARG:HG3	1:A:238:LEU:HD23	2.00	0.43
3:A:502:PLM:H61	3:A:502:PLM:H91	1.83	0.43
1:B:137:ASN:HB2	1:B:140:GLU:CD	2.43	0.43
1:B:284:LEU:HD21	1:B:321:ILE:HD13	2.00	0.43
1:D:160:GLY:HA2	1:D:237:LEU:HG	1.99	0.43
1:D:236:ASP:O	1:D:239:SER:OG	2.29	0.43
1:F:69:ARG:HE	1:F:343:THR:HG21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:161:PHE:CZ	1:H:266:LEU:HD21	2.53	0.43
1:K:28:PRO:HD2	1:K:440:GLN:OE1	2.18	0.43
1:K:69:ARG:NH2	1:K:344:VAL:O	2.51	0.43
1:K:255:ASP:HA	1:K:258:ILE:HG13	2.01	0.43
1:K:295:TYR:CZ	1:K:423:LEU:HD22	2.53	0.43
1:K:386:GLU:O	1:K:386:GLU:HG2	2.18	0.43
1:D:236:ASP:N	1:D:239:SER:OG	2.47	0.43
1:E:12:LYS:HD3	1:E:14:TYR:OH	2.19	0.43
1:F:277:LEU:HD21	1:F:415:ALA:HA	2.00	0.43
1:K:148:MET:O	1:K:152:THR:HG23	2.18	0.43
1:L:345:ILE:HD12	1:L:345:ILE:HG23	1.76	0.43
1:A:304:ASP:HB3	1:A:305:PRO:HD2	2.01	0.43
1:B:49:SER:HB2	1:C:435:GLN:OE1	2.19	0.43
1:C:310:GLN:O	1:C:313:MET:HB2	2.19	0.43
1:F:17:LEU:HD21	1:K:30:LEU:HD22	2.00	0.43
1:H:123:VAL:O	1:H:127:VAL:HG23	2.18	0.43
1:I:72:LYS:HD3	1:I:403:ARG:NE	2.34	0.43
1:J:169:TYR:HD1	1:J:169:TYR:HA	1.58	0.43
1:J:414:GLU:O	1:J:418:VAL:HG22	2.19	0.43
1:L:61:VAL:HG21	1:L:365:LEU:HD13	2.00	0.43
1:C:68:THR:O	1:C:340:LYS:HD3	2.18	0.43
1:D:152:THR:HG21	1:D:273:THR:HG23	2.00	0.43
1:D:405:CYS:HB2	2:D:501:HEM:NA	2.34	0.43
1:F:184:LEU:HD22	1:F:442:LEU:HD11	2.00	0.43
1:G:20:LEU:HD12	1:G:48:LEU:HD12	2.01	0.43
1:I:24:ASP:OD2	3:I:502:PLM:H22	2.19	0.43
1:I:41:PRO:HB3	1:I:57:GLY:HA3	2.01	0.43
1:I:429:ILE:HG23	1:I:452:ARG:HB2	2.00	0.43
1:J:253:LEU:HD22	1:J:257:ASN:ND2	2.34	0.43
1:K:106:LEU:HD11	1:K:241:MET:CE	2.48	0.43
1:L:133:TRP:CE2	1:L:142:VAL:HG11	2.54	0.43
1:L:143:ASP:OD1	1:L:145:PRO:HD2	2.19	0.43
1:D:254:ASP:O	1:D:258:ILE:HG13	2.19	0.42
3:D:502:PLM:H62	3:D:502:PLM:H32	1.83	0.42
1:E:71:ASP:HB3	1:E:338:TYR:CZ	2.54	0.42
1:E:179:SER:HB3	1:E:211:ASP:HB3	2.01	0.42
3:H:502:PLM:H22	3:L:502:PLM:H92	2.00	0.42
1:I:431:TYR:HD2	1:I:432:GLN:HG2	1.84	0.42
1:J:243:ASN:OD1	1:J:244:VAL:N	2.52	0.42
1:J:398:PHE:CE2	1:J:408:MET:HE3	2.54	0.42
1:K:92:SER:O	1:K:403:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:212:ILE:N	1:L:214:SER:HG	2.17	0.42
1:L:276:LEU:HD22	1:L:326:LEU:HD11	2.00	0.42
1:L:285:LEU:HD21	1:L:428:LEU:HB3	2.00	0.42
1:F:113:ARG:HD2	1:F:113:ARG:HA	1.85	0.42
1:F:324:GLU:CD	1:F:327:ARG:HE	2.27	0.42
1:G:121:MET:O	1:G:124:ASP:HB3	2.18	0.42
1:J:415:ALA:O	1:J:419:MET:HG2	2.19	0.42
1:L:418:VAL:O	1:L:422:LEU:HG	2.18	0.42
1:C:395:TYR:CZ	1:C:397:PRO:HG3	2.54	0.42
1:E:71:ASP:HB3	1:E:338:TYR:CE2	2.54	0.42
1:G:112:GLN:O	1:G:309:TYR:OH	2.37	0.42
1:G:282:TYR:CZ	1:G:436:LEU:HB2	2.55	0.42
1:I:69:ARG:NH2	1:I:344:VAL:O	2.45	0.42
1:J:70:PHE:CD1	1:J:339:ALA:HB2	2.54	0.42
1:K:72:LYS:NZ	1:K:400:ASN:HD22	2.16	0.42
1:K:170:ARG:HH11	1:K:174:HIS:CD2	2.37	0.42
1:K:269:GLY:HA2	2:K:501:HEM:C2C	2.53	0.42
1:L:160:GLY:O	1:L:237:LEU:HB3	2.19	0.42
1:A:49:SER:HB2	1:J:435:GLN:OE1	2.18	0.42
1:B:405:CYS:HB2	2:B:501:HEM:NA	2.33	0.42
1:H:156:ILE:HG22	1:H:266:LEU:HD23	2.00	0.42
1:I:260:PHE:O	1:I:264:THR:HG23	2.20	0.42
1:J:219:VAL:O	1:J:223:ILE:HG23	2.19	0.42
1:K:270:HIS:CG	1:K:271:GLU:N	2.88	0.42
1:L:70:PHE:CZ	1:L:345:ILE:HD11	2.54	0.42
1:L:335:PHE:CE1	1:L:360:VAL:HG21	2.54	0.42
1:D:70:PHE:CE2	1:D:345:ILE:HD11	2.54	0.42
1:F:132:LYS:NZ	1:F:147:ASP:OD1	2.37	0.42
1:G:72:LYS:HD3	1:G:403:ARG:CZ	2.49	0.42
1:G:90:PHE:HB2	1:G:264:THR:HG23	2.00	0.42
1:G:277:LEU:HD21	1:G:415:ALA:HA	2.00	0.42
1:G:335:PHE:CD1	1:G:362:ILE:HD11	2.54	0.42
1:H:133:TRP:CE2	1:H:142:VAL:HG11	2.54	0.42
1:I:90:PHE:HE1	2:I:501:HEM:HBA1	1.85	0.42
1:I:93:GLU:HB2	1:I:96:GLU:CG	2.46	0.42
1:J:335:PHE:O	1:J:360:VAL:HG22	2.19	0.42
1:B:121:MET:O	1:B:124:ASP:HB3	2.20	0.42
1:B:434:TYR:CE2	1:B:436:LEU:HA	2.55	0.42
1:C:152:THR:HG21	1:C:273:THR:HG23	2.00	0.42
1:D:86:GLY:O	1:D:91:THR:OG1	2.37	0.42
1:D:405:CYS:HA	2:D:501:HEM:CHA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:436:LEU:O	1:L:48:LEU:HD12	2.19	0.42
1:J:125:ILE:HD13	1:J:154:ASP:C	2.44	0.42
1:J:170:ARG:HH21	1:J:174:HIS:HA	1.84	0.42
1:K:316:LYS:O	1:K:320:MET:HG3	2.19	0.42
1:L:277:LEU:HD21	1:L:415:ALA:HA	2.02	0.42
1:L:307:PRO:HA	1:L:311:GLN:HE21	1.83	0.42
1:A:28:PRO:HD2	1:A:440:GLN:OE1	2.20	0.42
1:B:104:ASN:HB3	1:B:247:PRO:HD2	2.01	0.42
1:B:116:LYS:HE2	1:B:309:TYR:CE2	2.55	0.42
2:C:501:HEM:HBC2	2:C:501:HEM:CMC	2.47	0.42
1:H:46:GLN:HB2	1:H:51:THR:HG22	2.01	0.42
1:H:137:ASN:HB2	1:H:140:GLU:CD	2.45	0.42
1:I:10:GLN:OE1	1:I:44:GLN:NE2	2.51	0.42
1:I:405:CYS:HA	2:I:501:HEM:CHA	2.49	0.42
1:B:144:VAL:O	1:B:148:MET:HG2	2.20	0.42
1:C:290:LYS:HD2	1:C:290:LYS:H	1.84	0.42
1:D:434:TYR:CE2	1:D:436:LEU:HA	2.55	0.42
1:E:48:LEU:HD12	1:L:436:LEU:O	2.19	0.42
1:I:125:ILE:O	1:I:128:GLN:HB2	2.20	0.42
1:I:301:VAL:HG12	1:I:311:GLN:HG2	2.00	0.42
1:A:75:GLU:OE1	1:A:75:GLU:HA	2.19	0.42
1:A:123:VAL:HG11	1:A:306:THR:CG2	2.48	0.42
1:A:398:PHE:CE2	1:A:408:MET:HG3	2.55	0.42
1:B:386:GLU:HB2	1:B:389:LYS:HB3	2.01	0.42
1:C:150:ARG:HG2	1:C:167:SER:HB3	2.01	0.42
1:D:246:ASP:OD2	1:D:249:THR:HG22	2.20	0.42
1:G:304:ASP:HB3	1:G:305:PRO:HD2	2.02	0.42
1:H:155:THR:HG21	1:H:414:GLU:CD	2.43	0.42
3:H:502:PLM:H41	1:L:21:PRO:O	2.19	0.42
1:J:254:ASP:OD1	1:J:255:ASP:N	2.42	0.42
1:K:150:ARG:HG2	1:K:167:SER:OG	2.19	0.42
1:A:144:VAL:HB	1:A:145:PRO:HD3	2.02	0.42
1:C:49:SER:HB2	1:I:435:GLN:OE1	2.18	0.42
1:C:153:LEU:HD11	1:C:177:ILE:HD12	2.02	0.42
1:C:238:LEU:O	1:C:242:LEU:HG	2.20	0.42
1:C:240:ARG:NH1	1:C:244:VAL:HG11	2.35	0.42
1:E:19:ASN:HB2	1:E:45:ILE:HG23	2.02	0.42
1:H:107:MET:N	1:H:108:PRO:HD2	2.35	0.42
1:I:115:MET:HB3	1:I:115:MET:HE3	1.79	0.42
1:I:142:VAL:HG12	1:I:451:ILE:O	2.20	0.42
1:K:214:SER:O	1:K:217:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:240:ARG:H	1:K:240:ARG:HG2	1.54	0.42
1:F:119:HIS:O	1:F:123:VAL:HG23	2.20	0.41
1:I:144:VAL:O	1:I:148:MET:HG2	2.19	0.41
1:J:77:ALA:O	1:J:80:LYS:HG2	2.20	0.41
1:J:90:PHE:HA	2:J:501:HEM:HAD2	2.01	0.41
1:L:442:LEU:HD23	1:L:442:LEU:HA	1.87	0.41
1:A:20:LEU:HD12	1:A:48:LEU:CD1	2.50	0.41
1:F:405:CYS:HB2	2:F:501:HEM:NA	2.35	0.41
1:H:20:LEU:HD21	1:H:47:THR:HG22	2.02	0.41
1:H:324:GLU:OE1	1:H:383:ARG:HD2	2.20	0.41
1:J:113:ARG:HD3	1:J:113:ARG:HA	1.73	0.41
1:J:117:ASP:O	1:J:121:MET:HE3	2.21	0.41
1:K:372:TRP:CZ3	1:K:383:ARG:HD3	2.55	0.41
1:L:136:LEU:HD11	1:L:142:VAL:CG2	2.50	0.41
1:L:174:HIS:ND1	1:L:175:PRO:HD2	2.35	0.41
1:C:148:MET:HE1	1:C:422:LEU:HD11	2.03	0.41
1:D:212:ILE:HG13	1:D:213:GLN:N	2.35	0.41
1:F:395:TYR:CZ	1:F:397:PRO:HG3	2.56	0.41
1:H:112:GLN:HG3	1:H:309:TYR:OH	2.20	0.41
1:H:282:TYR:CZ	1:H:436:LEU:HB2	2.55	0.41
1:I:92:SER:OG	1:I:99:TRP:HD1	2.03	0.41
1:K:25:LYS:HD2	1:K:25:LYS:HA	1.83	0.41
1:B:16:PRO:O	1:B:48:LEU:HD23	2.20	0.41
1:B:84:PHE:CE1	1:B:183:ALA:HB1	2.56	0.41
1:B:115:MET:SD	1:B:410:PHE:HA	2.60	0.41
1:F:345:ILE:HG23	1:F:351:ILE:HD13	2.02	0.41
1:G:290:LYS:HD2	1:G:317:TYR:OH	2.19	0.41
1:H:180:MET:HE3	1:H:180:MET:HB3	1.98	0.41
1:I:106:LEU:HD13	1:I:110:PHE:HE2	1.85	0.41
1:J:293:LYS:HG2	1:J:317:TYR:CE2	2.55	0.41
1:A:144:VAL:O	1:A:148:MET:HG2	2.21	0.41
1:B:31:SER:O	1:B:35:ILE:HG13	2.19	0.41
1:B:213:GLN:HB2	1:H:221:ASN:CG	2.44	0.41
1:B:398:PHE:HD2	1:B:408:MET:HE3	1.84	0.41
1:D:143:ASP:OD1	1:D:146:GLU:HB2	2.20	0.41
1:E:107:MET:HE3	1:E:107:MET:HB3	1.86	0.41
1:G:72:LYS:HB2	1:G:403:ARG:HG3	2.03	0.41
1:H:106:LEU:O	1:H:109:THR:OG1	2.35	0.41
1:I:372:TRP:CE3	1:I:383:ARG:HD3	2.55	0.41
1:J:180:MET:HB3	1:J:215:MET:HE3	2.03	0.41
1:D:123:VAL:O	1:D:127:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:ILE:O	1:E:267:ILE:HG22	2.21	0.41
1:F:64:VAL:HA	1:F:70:PHE:CD2	2.55	0.41
1:H:75:GLU:HG3	1:H:78:LEU:HD13	2.02	0.41
1:I:282:TYR:CE2	1:I:436:LEU:HD22	2.56	0.41
1:I:327:ARG:HH22	1:I:376:VAL:HA	1.85	0.41
1:I:331:THR:O	1:I:443:THR:HG23	2.21	0.41
1:L:60:LEU:O	1:L:64:VAL:HG13	2.21	0.41
1:A:431:TYR:CD1	1:A:452:ARG:HG3	2.56	0.41
1:C:270:HIS:CG	1:C:271:GLU:N	2.88	0.41
1:C:317:TYR:CD1	1:C:320:MET:HE2	2.56	0.41
1:D:50:ASP:OD1	1:D:355:GLU:OE2	2.39	0.41
1:E:90:PHE:HB2	1:E:264:THR:HG23	2.03	0.41
1:G:341:GLU:CA	1:G:353:LYS:HD2	2.41	0.41
1:H:432:GLN:N	1:H:432:GLN:OE1	2.53	0.41
1:I:73:SER:HB2	1:I:338:TYR:HB2	2.01	0.41
1:I:85:ALA:CB	1:I:91:THR:HG21	2.50	0.41
1:I:411:ALA:HB2	2:I:501:HEM:HHC	2.02	0.41
1:J:72:LYS:NZ	1:J:335:PHE:HB2	2.36	0.41
1:K:238:LEU:HA	1:K:241:MET:HB3	2.02	0.41
1:L:343:THR:HG22	1:L:344:VAL:N	2.33	0.41
1:B:245:PRO:HB3	1:B:252:LYS:HG3	2.03	0.41
1:E:64:VAL:HA	1:E:70:PHE:CE2	2.55	0.41
1:F:81:VAL:HG12	1:F:91:THR:HG21	2.03	0.41
1:G:153:LEU:HD22	1:G:177:ILE:HD11	2.03	0.41
1:H:115:MET:HE2	1:H:115:MET:HA	2.02	0.41
1:J:402:GLN:H	1:J:402:GLN:CD	2.24	0.41
1:K:241:MET:SD	1:K:258:ILE:HD13	2.61	0.41
1:L:143:ASP:CG	1:L:146:GLU:HG2	2.45	0.41
1:A:154:ASP:OD1	1:A:165:PHE:HB2	2.21	0.41
1:B:270:HIS:CG	1:B:271:GLU:N	2.89	0.41
1:B:295:TYR:HA	1:B:298:VAL:HG12	2.02	0.41
1:B:365:LEU:HD11	1:B:394:ALA:HA	2.03	0.41
1:C:23:ILE:HG22	1:C:31:SER:HB3	2.02	0.41
1:C:63:GLU:HG2	1:C:69:ARG:HH12	1.86	0.41
1:C:99:TRP:CZ2	1:C:403:ARG:HD2	2.56	0.41
1:D:180:MET:HE3	1:D:180:MET:HB3	2.01	0.41
1:D:270:HIS:CG	1:D:271:GLU:N	2.88	0.41
1:E:42:ILE:HG22	1:E:55:VAL:HG12	2.03	0.41
1:E:154:ASP:OD1	1:E:165:PHE:HB2	2.21	0.41
1:E:240:ARG:CZ	1:E:244:VAL:HG21	2.50	0.41
1:E:246:ASP:HB3	1:E:249:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:ILE:HG12	1:F:357:ARG:NE	2.31	0.41
1:G:10:GLN:HG3	1:G:44:GLN:O	2.20	0.41
1:G:61:VAL:O	1:G:64:VAL:HG12	2.21	0.41
1:H:107:MET:HA	1:H:406:ILE:HD11	2.03	0.41
1:I:137:ASN:HB2	1:I:140:GLU:CG	2.50	0.41
1:I:151:LEU:HD21	1:I:418:VAL:HG21	2.03	0.41
1:I:180:MET:SD	1:I:267:ILE:HG12	2.61	0.41
1:I:365:LEU:HD11	1:I:394:ALA:HA	2.03	0.41
1:I:421:MET:HE3	1:I:421:MET:HB2	1.79	0.41
1:J:174:HIS:CG	1:J:175:PRO:HD2	2.56	0.41
1:J:295:TYR:O	1:J:298:VAL:HG12	2.21	0.41
1:J:304:ASP:HB3	1:J:305:PRO:HD2	2.02	0.41
1:K:27:LYS:HE2	1:K:439:LYS:NZ	2.35	0.41
1:L:20:LEU:HG	1:L:47:THR:HA	2.01	0.41
1:L:161:PHE:HE1	1:L:262:ILE:HG22	1.86	0.41
1:L:307:PRO:CD	1:L:421:MET:HE2	2.47	0.41
1:B:241:MET:HE1	1:B:258:ILE:HA	2.03	0.41
1:C:17:LEU:HD21	1:I:30:LEU:HD22	2.03	0.41
1:C:365:LEU:HD11	1:C:394:ALA:HA	2.03	0.41
1:F:348:LYS:HD2	1:F:349:TYR:CZ	2.56	0.41
1:G:454:LEU:HD23	1:G:454:LEU:HA	1.92	0.41
1:H:89:LEU:CD2	1:H:106:LEU:HD11	2.51	0.41
1:H:246:ASP:O	1:H:250:GLY:N	2.41	0.41
1:I:327:ARG:HH22	1:I:376:VAL:CA	2.33	0.41
1:J:169:TYR:C	1:J:170:ARG:HG2	2.46	0.41
1:K:113:ARG:HG3	1:K:114:ALA:N	2.36	0.41
1:K:136:LEU:HD23	1:K:136:LEU:HA	1.86	0.41
1:L:133:TRP:HB3	1:L:453:ILE:CD1	2.51	0.41
1:L:154:ASP:OD1	1:L:167:SER:OG	2.30	0.41
1:A:277:LEU:HD21	1:A:415:ALA:HA	2.03	0.40
1:F:160:GLY:HA2	1:F:237:LEU:HD12	2.02	0.40
1:G:132:LYS:HD2	1:G:168:PHE:HD1	1.86	0.40
1:H:336:SER:HA	1:H:358:ILE:O	2.21	0.40
1:I:298:VAL:O	1:I:302:LEU:N	2.54	0.40
1:I:327:ARG:HH22	1:I:376:VAL:C	2.29	0.40
1:L:175:PRO:C	1:L:177:ILE:N	2.78	0.40
1:B:215:MET:O	1:B:219:VAL:HG23	2.20	0.40
1:C:234:GLU:OE1	1:C:234:GLU:HA	2.21	0.40
1:E:276:LEU:N	1:E:331:THR:HG21	2.36	0.40
1:F:137:ASN:HB2	1:F:140:GLU:CD	2.46	0.40
1:F:240:ARG:HE	1:F:240:ARG:HB2	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:269:GLY:HA2	2:G:501:HEM:C1C	2.56	0.40
1:G:435:GLN:OE1	1:J:49:SER:HB2	2.21	0.40
1:H:152:THR:HG21	1:H:273:THR:HG1	1.85	0.40
1:H:302:LEU:HD22	1:H:307:PRO:HG3	2.03	0.40
1:K:298:VAL:O	1:K:302:LEU:HB2	2.22	0.40
1:L:72:LYS:CB	1:L:403:ARG:HG3	2.51	0.40
1:B:78:LEU:HA	1:B:78:LEU:HD23	1.82	0.40
1:B:99:TRP:CZ2	1:B:403:ARG:HD2	2.57	0.40
1:C:331:THR:O	1:C:333:PRO:HD3	2.22	0.40
1:D:34:LYS:HD2	1:K:21:PRO:HB3	2.03	0.40
1:D:60:LEU:O	1:D:64:VAL:HG23	2.21	0.40
1:E:215:MET:O	1:E:219:VAL:HG23	2.21	0.40
1:G:160:GLY:O	1:G:237:LEU:HB2	2.21	0.40
1:J:79:ALA:O	1:J:82:ARG:CB	2.63	0.40
1:K:324:GLU:OE2	1:K:383:ARG:NH1	2.55	0.40
1:K:434:TYR:CE2	1:K:436:LEU:HA	2.57	0.40
1:E:137:ASN:HB2	1:E:140:GLU:CD	2.46	0.40
1:G:10:GLN:OE1	1:G:44:GLN:NE2	2.54	0.40
1:G:78:LEU:HD21	1:G:90:PHE:CE2	2.57	0.40
1:G:99:TRP:HH2	1:G:402:GLN:HG2	1.86	0.40
1:I:71:ASP:O	1:I:338:TYR:N	2.52	0.40
1:J:93:GLU:OE1	1:J:95:HIS:NE2	2.54	0.40
1:J:109:THR:HG23	1:J:118:TYR:OH	2.21	0.40
1:J:226:ARG:HH12	1:J:236:ASP:CG	2.28	0.40
1:K:20:LEU:HD23	1:K:23:ILE:HD12	2.03	0.40
1:L:107:MET:N	1:L:108:PRO:HD2	2.36	0.40
1:L:352:LYS:HG2	1:L:356:ASP:OD2	2.22	0.40
1:L:402:GLN:OE1	1:L:402:GLN:N	2.54	0.40
1:A:99:TRP:CZ2	1:A:403:ARG:HD2	2.56	0.40
1:G:152:THR:CG2	1:G:270:HIS:HA	2.52	0.40
1:I:125:ILE:HG13	1:I:155:THR:HA	2.02	0.40
1:J:109:THR:HG21	1:J:237:LEU:HD23	2.04	0.40
1:K:105:ILE:HD12	1:K:253:LEU:HG	2.03	0.40
1:K:297:GLU:HG3	1:K:300:ARG:HH21	1.85	0.40
1:K:326:LEU:HG	1:K:397:PRO:HB3	2.04	0.40
1:L:13:THR:HG23	1:L:18:GLY:HA2	2.03	0.40
1:L:89:LEU:HD13	1:L:261:GLN:OE1	2.20	0.40
1:L:151:LEU:HD21	1:L:418:VAL:CG2	2.52	0.40
1:L:241:MET:SD	1:L:258:ILE:HG23	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	425/458 (93%)	411 (97%)	14 (3%)	0	100	100
1	B	426/458 (93%)	414 (97%)	12 (3%)	0	100	100
1	C	415/458 (91%)	401 (97%)	14 (3%)	0	100	100
1	D	413/458 (90%)	401 (97%)	11 (3%)	1 (0%)	43	72
1	E	416/458 (91%)	398 (96%)	18 (4%)	0	100	100
1	F	413/458 (90%)	399 (97%)	14 (3%)	0	100	100
1	G	393/458 (86%)	382 (97%)	11 (3%)	0	100	100
1	H	409/458 (89%)	394 (96%)	14 (3%)	1 (0%)	43	72
1	I	393/458 (86%)	381 (97%)	12 (3%)	0	100	100
1	J	409/458 (89%)	394 (96%)	15 (4%)	0	100	100
1	K	410/458 (90%)	397 (97%)	13 (3%)	0	100	100
1	L	404/458 (88%)	383 (95%)	21 (5%)	0	100	100
All	All	4926/5496 (90%)	4755 (96%)	169 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	433	ASN
1	H	83	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	381/410 (93%)	377 (99%)	4 (1%)	68	88
1	B	383/410 (93%)	381 (100%)	2 (0%)	81	93
1	C	376/410 (92%)	374 (100%)	2 (0%)	81	93
1	D	373/410 (91%)	370 (99%)	3 (1%)	73	90
1	E	376/410 (92%)	375 (100%)	1 (0%)	86	95
1	F	373/410 (91%)	372 (100%)	1 (0%)	86	95
1	G	356/410 (87%)	353 (99%)	3 (1%)	73	90
1	H	370/410 (90%)	368 (100%)	2 (0%)	81	93
1	I	354/410 (86%)	353 (100%)	1 (0%)	86	95
1	J	369/410 (90%)	366 (99%)	3 (1%)	73	90
1	K	370/410 (90%)	367 (99%)	3 (1%)	73	90
1	L	364/410 (89%)	362 (100%)	2 (0%)	81	93
All	All	4445/4920 (90%)	4418 (99%)	27 (1%)	78	92

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	THR
1	A	308	THR
1	A	345	ILE
1	A	376	VAL
1	B	331	THR
1	B	376	VAL
1	C	172	THR
1	C	400	ASN
1	D	181	THR
1	D	308	THR
1	D	376	VAL
1	E	181	THR
1	F	240	ARG
1	G	55	VAL
1	G	64	VAL
1	G	416	THR
1	H	64	VAL
1	H	376	VAL
1	I	376	VAL
1	J	170	ARG
1	J	376	VAL
1	J	400	ASN

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Mol	Chain	Res	Type
1	K	181	THR
1	K	258	ILE
1	K	376	VAL
1	L	259	ARG
1	L	400	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	HIS
1	A	104	ASN
1	A	209	GLN
1	A	425	HIS
1	B	131	GLN
1	B	287	ASN
1	C	287	ASN
1	C	393	HIS
1	D	213	GLN
1	D	221	ASN
1	E	58	HIS
1	E	95	HIS
1	E	103	HIS
1	E	287	ASN
1	E	392	HIS
1	F	287	ASN
1	F	380	GLN
1	F	432	GLN
1	G	44	GLN
1	G	323	ASN
1	G	424	GLN
1	H	44	GLN
1	H	257	ASN
1	I	257	ASN
1	I	287	ASN
1	I	424	GLN
1	J	98	ASN
1	J	103	HIS
1	J	131	GLN
1	J	323	ASN
1	J	380	GLN
1	J	432	GLN
1	K	98	ASN

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Mol	Chain	Res	Type
1	K	287	ASN
1	K	402	GLN
1	L	10	GLN
1	L	98	ASN
1	L	104	ASN
1	L	137	ASN
1	L	139	ASN
1	L	166	ASN
1	L	257	ASN
1	L	311	GLN
1	L	323	ASN
1	L	380	GLN
1	L	413	HIS
1	L	440	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](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLM	B	502	-	17,17,17	0.92	1 (5%)	17,17,17	0.76	1 (5%)
2	HEM	A	501	1	50,50,50	1.45	7 (14%)	67,82,82	1.15	4 (5%)
3	PLM	D	503	-	17,17,17	0.72	0	17,17,17	0.85	2 (11%)
2	HEM	J	501	1	50,50,50	1.43	7 (14%)	67,82,82	1.24	10 (14%)
3	PLM	L	502	-	17,17,17	1.22	1 (5%)	17,17,17	0.69	0
2	HEM	E	501	1	50,50,50	1.50	8 (16%)	67,82,82	1.10	5 (7%)
2	HEM	F	501	1	50,50,50	1.37	8 (16%)	67,82,82	1.14	5 (7%)
2	HEM	H	501	1	50,50,50	1.52	9 (18%)	67,82,82	1.18	5 (7%)
3	PLM	C	502	-	17,17,17	0.99	1 (5%)	17,17,17	0.71	1 (5%)
3	PLM	H	502	-	17,17,17	0.63	0	17,17,17	0.83	2 (11%)
3	PLM	G	502	-	17,17,17	1.16	1 (5%)	17,17,17	0.75	1 (5%)
3	PLM	E	502	-	17,17,17	0.84	1 (5%)	17,17,17	0.80	2 (11%)
3	PLM	A	502	-	17,17,17	0.92	1 (5%)	17,17,17	0.71	1 (5%)
2	HEM	K	501	1	50,50,50	1.39	10 (20%)	67,82,82	1.12	6 (8%)
3	PLM	K	502	-	17,17,17	1.16	1 (5%)	17,17,17	0.72	1 (5%)
2	HEM	B	501	1	50,50,50	1.43	9 (18%)	67,82,82	1.09	5 (7%)
2	HEM	D	501	1	50,50,50	1.48	9 (18%)	67,82,82	1.18	4 (5%)
3	PLM	D	502	-	17,17,17	1.10	1 (5%)	17,17,17	0.80	2 (11%)
3	PLM	J	502	-	17,17,17	0.79	1 (5%)	17,17,17	0.83	2 (11%)
2	HEM	G	501	1	50,50,50	1.44	9 (18%)	67,82,82	1.22	6 (8%)
2	HEM	I	501	1	50,50,50	1.49	8 (16%)	67,82,82	1.22	5 (7%)
2	HEM	C	501	1	50,50,50	1.40	9 (18%)	67,82,82	1.11	2 (2%)
3	PLM	I	502	-	17,17,17	1.14	1 (5%)	17,17,17	0.73	0
2	HEM	L	501	1	50,50,50	1.42	9 (18%)	67,82,82	1.15	6 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLM	B	502	-	-	7/15/15/15	-
2	HEM	A	501	1	-	3/14/54/54	-
3	PLM	D	503	-	-	4/15/15/15	-
2	HEM	J	501	1	-	5/14/54/54	-
3	PLM	L	502	-	-	5/15/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	E	501	1	-	3/14/54/54	-
2	HEM	F	501	1	-	2/14/54/54	-
2	HEM	H	501	1	-	2/14/54/54	-
3	PLM	C	502	-	-	7/15/15/15	-
3	PLM	H	502	-	-	4/15/15/15	-
3	PLM	G	502	-	-	2/15/15/15	-
3	PLM	E	502	-	-	7/15/15/15	-
3	PLM	A	502	-	-	8/15/15/15	-
2	HEM	K	501	1	-	0/14/54/54	-
3	PLM	K	502	-	-	6/15/15/15	-
2	HEM	B	501	1	-	4/14/54/54	-
2	HEM	D	501	1	-	2/14/54/54	-
3	PLM	D	502	-	-	7/15/15/15	-
3	PLM	J	502	-	-	6/15/15/15	-
2	HEM	G	501	1	-	2/14/54/54	-
2	HEM	I	501	1	-	2/14/54/54	-
2	HEM	C	501	1	-	2/14/54/54	-
3	PLM	I	502	-	-	7/15/15/15	-
2	HEM	L	501	1	-	2/14/54/54	-

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	501	HEM	FE-NB	5.35	2.11	1.94
2	A	501	HEM	FE-NB	5.08	2.10	1.94
2	H	501	HEM	FE-NB	4.99	2.10	1.94
2	J	501	HEM	FE-NA	4.63	2.10	1.95
2	E	501	HEM	FE-NB	4.55	2.08	1.94
2	H	501	HEM	FE-NA	4.34	2.09	1.95
2	G	501	HEM	FE-NC	4.32	2.09	1.95
3	K	502	PLM	C2-C1	4.17	1.60	1.50
3	L	502	PLM	C2-C1	4.15	1.60	1.50
2	B	501	HEM	FE-NA	4.15	2.08	1.95
2	D	501	HEM	FE-NA	4.02	2.08	1.95
2	E	501	HEM	FE-NC	3.92	2.08	1.95
3	G	502	PLM	C2-C1	3.87	1.59	1.50
2	J	501	HEM	FE-NB	3.86	2.06	1.94
3	I	502	PLM	C2-C1	3.83	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	FE-NB	3.63	2.06	1.94
2	L	501	HEM	FE-NA	3.58	2.07	1.95
2	K	501	HEM	FE-NB	3.52	2.05	1.94
2	C	501	HEM	FE-NB	3.48	2.05	1.94
2	G	501	HEM	FE-ND	3.48	2.05	1.94
3	C	502	PLM	C2-C1	3.42	1.58	1.50
2	D	501	HEM	FE-NC	3.40	2.06	1.95
3	D	502	PLM	C2-C1	3.35	1.58	1.50
2	L	501	HEM	FE-NB	3.34	2.05	1.94
2	H	501	HEM	CAC-C3C	3.26	1.56	1.47
2	E	501	HEM	CAB-C3B	3.24	1.56	1.47
2	A	501	HEM	CAB-C3B	3.21	1.55	1.47
2	L	501	HEM	CAC-C3C	3.21	1.55	1.47
2	C	501	HEM	FE-ND	3.18	2.04	1.94
2	I	501	HEM	CAB-C3B	3.18	1.55	1.47
2	G	501	HEM	CAC-C3C	3.18	1.55	1.47
2	D	501	HEM	CAB-C3B	3.18	1.55	1.47
2	B	501	HEM	CAC-C3C	3.17	1.55	1.47
2	I	501	HEM	CAC-C3C	3.16	1.55	1.47
2	K	501	HEM	CAC-C3C	3.16	1.55	1.47
2	K	501	HEM	FE-NA	3.15	2.05	1.95
3	B	502	PLM	C2-C1	3.14	1.57	1.50
2	C	501	HEM	CAB-C3B	3.13	1.55	1.47
2	E	501	HEM	CAC-C3C	3.11	1.55	1.47
2	C	501	HEM	FE-NC	3.11	2.05	1.95
2	L	501	HEM	CAB-C3B	3.10	1.55	1.47
2	F	501	HEM	CAC-C3C	3.08	1.55	1.47
2	J	501	HEM	CAB-C3B	3.08	1.55	1.47
2	K	501	HEM	CAB-C3B	3.08	1.55	1.47
2	F	501	HEM	CAB-C3B	3.07	1.55	1.47
2	H	501	HEM	CAB-C3B	3.07	1.55	1.47
2	I	501	HEM	FE-NC	3.06	2.05	1.95
2	F	501	HEM	FE-NB	3.04	2.04	1.94
2	G	501	HEM	CAB-C3B	3.04	1.55	1.47
2	D	501	HEM	CAC-C3C	3.02	1.55	1.47
2	A	501	HEM	CAC-C3C	3.02	1.55	1.47
2	A	501	HEM	FE-NA	3.01	2.05	1.95
3	A	502	PLM	C2-C1	3.00	1.57	1.50
2	J	501	HEM	CAC-C3C	2.98	1.55	1.47
2	B	501	HEM	FE-NB	2.94	2.03	1.94
2	B	501	HEM	CAB-C3B	2.88	1.55	1.47
2	F	501	HEM	FE-NC	2.85	2.04	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	CAC-C3C	2.84	1.55	1.47
2	B	501	HEM	FE-NC	2.83	2.04	1.95
2	G	501	HEM	FE-NA	2.80	2.04	1.95
2	A	501	HEM	FE-NC	2.78	2.04	1.95
2	E	501	HEM	FE-NA	2.73	2.04	1.95
2	H	501	HEM	FE-NC	2.65	2.03	1.95
2	K	501	HEM	FE-NC	2.65	2.03	1.95
2	F	501	HEM	FE-NA	2.61	2.03	1.95
2	L	501	HEM	FE-NC	2.60	2.03	1.95
2	F	501	HEM	FE-ND	2.59	2.02	1.94
2	C	501	HEM	FE-NA	2.49	2.03	1.95
2	B	501	HEM	FE-ND	2.48	2.02	1.94
2	L	501	HEM	FE-ND	2.43	2.02	1.94
2	I	501	HEM	FE-ND	2.37	2.02	1.94
2	B	501	HEM	CMB-C2B	2.32	1.55	1.50
3	E	502	PLM	C2-C1	2.32	1.55	1.50
2	D	501	HEM	CMC-C2C	2.31	1.55	1.50
2	F	501	HEM	CMC-C2C	2.29	1.55	1.50
2	D	501	HEM	CMB-C2B	2.28	1.55	1.50
2	A	501	HEM	CMC-C2C	2.26	1.55	1.50
2	B	501	HEM	CMC-C2C	2.26	1.55	1.50
2	K	501	HEM	FE-ND	2.24	2.01	1.94
2	H	501	HEM	CMB-C2B	2.22	1.55	1.50
2	D	501	HEM	FE-ND	2.20	2.01	1.94
2	H	501	HEM	CMC-C2C	2.18	1.55	1.50
2	I	501	HEM	CMB-C2B	2.17	1.55	1.50
2	J	501	HEM	CMB-C2B	2.17	1.55	1.50
2	K	501	HEM	CMC-C2C	2.16	1.55	1.50
2	G	501	HEM	CMC-C2C	2.15	1.55	1.50
3	J	502	PLM	C2-C1	2.15	1.55	1.50
2	L	501	HEM	CMD-C2D	2.15	1.55	1.50
2	G	501	HEM	CMB-C2B	2.14	1.55	1.50
2	L	501	HEM	C2A-C3A	-2.14	1.33	1.38
2	F	501	HEM	C2A-C3A	-2.14	1.33	1.38
2	E	501	HEM	CMC-C2C	2.14	1.55	1.50
2	E	501	HEM	CMB-C2B	2.12	1.55	1.50
2	H	501	HEM	C2A-C3A	-2.12	1.33	1.38
2	L	501	HEM	CMB-C2B	2.12	1.55	1.50
2	D	501	HEM	CMD-C2D	2.09	1.55	1.50
2	H	501	HEM	CMD-C2D	2.08	1.55	1.50
2	I	501	HEM	CMC-C2C	2.07	1.55	1.50
2	C	501	HEM	C2A-C3A	-2.06	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	CMC-C2C	2.06	1.55	1.50
2	G	501	HEM	CMD-C2D	2.05	1.55	1.50
2	I	501	HEM	CAD-C3D	2.05	1.56	1.51
2	K	501	HEM	CMB-C2B	2.05	1.55	1.50
2	B	501	HEM	CMD-C2D	2.04	1.55	1.50
2	K	501	HEM	C2A-C3A	-2.04	1.33	1.38
2	J	501	HEM	FE-ND	2.03	2.01	1.94
2	K	501	HEM	CMD-C2D	2.01	1.54	1.50
2	G	501	HEM	C2A-C3A	-2.01	1.33	1.38
2	E	501	HEM	CMD-C2D	2.01	1.54	1.50
2	J	501	HEM	CMA-C3A	2.01	1.54	1.50
2	A	501	HEM	CMA-C3A	2.01	1.54	1.50
2	C	501	HEM	CMD-C2D	2.00	1.54	1.50

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	C3D-C4D-ND	-3.07	106.80	110.17
2	H	501	HEM	C4D-ND-C1D	3.01	108.77	105.21
2	D	501	HEM	C4D-ND-C1D	3.00	108.76	105.21
2	I	501	HEM	C4D-ND-C1D	2.95	108.70	105.21
2	H	501	HEM	C3D-C4D-ND	-2.78	107.12	110.17
2	A	501	HEM	C4D-ND-C1D	2.73	108.44	105.21
2	E	501	HEM	C4D-ND-C1D	2.70	108.41	105.21
2	K	501	HEM	CBD-CAD-C3D	-2.67	105.14	112.53
2	I	501	HEM	C2D-C1D-ND	-2.67	106.82	109.90
2	J	501	HEM	CAA-CBA-CGA	-2.65	106.63	113.67
2	K	501	HEM	C4D-ND-C1D	2.62	108.31	105.21
2	J	501	HEM	O1D-CGD-CBD	-2.61	114.81	123.09
2	G	501	HEM	C2A-C1A-NA	-2.60	107.27	110.15
3	D	503	PLM	O1-C1-O2	2.58	129.96	123.33
2	F	501	HEM	C4D-ND-C1D	2.57	108.25	105.21
2	I	501	HEM	C2A-C1A-NA	-2.52	107.36	110.15
2	G	501	HEM	C4D-ND-C1D	2.50	108.17	105.21
2	L	501	HEM	CAA-CBA-CGA	-2.49	107.06	113.67
2	A	501	HEM	C2A-C1A-NA	-2.48	107.40	110.15
3	H	502	PLM	O1-C1-O2	2.48	129.70	123.33
2	I	501	HEM	O2D-CGD-CBD	2.47	121.81	114.00
2	G	501	HEM	C3D-C4D-ND	-2.47	107.47	110.17
2	A	501	HEM	C3D-C4D-ND	-2.44	107.49	110.17
2	F	501	HEM	C2A-C1A-NA	-2.43	107.46	110.15
3	J	502	PLM	O1-C1-O2	2.42	129.55	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	501	HEM	CHC-C1C-NC	2.40	127.06	124.45
2	I	501	HEM	C1D-C2D-C3D	2.38	109.48	106.98
2	D	501	HEM	C2A-C1A-NA	-2.36	107.53	110.15
2	E	501	HEM	C2A-C1A-NA	-2.36	107.53	110.15
3	E	502	PLM	O1-C1-O2	2.34	129.35	123.33
2	L	501	HEM	C4D-ND-C1D	2.32	107.95	105.21
2	G	501	HEM	C1B-NB-C4B	2.31	107.95	105.21
2	K	501	HEM	C3D-C4D-ND	-2.31	107.64	110.17
3	J	502	PLM	O2-C1-C2	-2.29	115.83	123.09
2	J	501	HEM	CBD-CAD-C3D	-2.28	106.23	112.53
2	D	501	HEM	CHA-C4D-ND	2.26	127.17	124.37
2	B	501	HEM	C3D-C4D-ND	-2.25	107.70	110.17
2	H	501	HEM	C2A-C1A-NA	-2.24	107.67	110.15
2	F	501	HEM	C3D-C4D-ND	-2.23	107.72	110.17
2	G	501	HEM	CHD-C1D-ND	2.23	126.83	124.42
2	L	501	HEM	C1B-NB-C4B	2.23	107.84	105.21
2	E	501	HEM	C2D-C1D-ND	-2.22	107.33	109.90
3	D	503	PLM	O2-C1-C2	-2.22	116.04	123.09
2	K	501	HEM	C3B-C2B-C1B	2.22	108.08	106.41
2	B	501	HEM	C1B-NB-C4B	2.22	107.83	105.21
2	B	501	HEM	C4D-ND-C1D	2.20	107.81	105.21
2	J	501	HEM	C3D-C4D-ND	-2.19	107.77	110.17
2	K	501	HEM	C1B-NB-C4B	2.19	107.80	105.21
2	E	501	HEM	CHD-C1D-ND	2.17	126.75	124.42
2	C	501	HEM	C2A-C1A-NA	-2.17	107.75	110.15
3	G	502	PLM	O2-C1-C2	-2.16	116.23	123.09
2	L	501	HEM	CAD-C3D-C4D	-2.16	120.94	124.70
3	H	502	PLM	O2-C1-C2	-2.15	116.28	123.09
2	A	501	HEM	CHD-C1D-ND	2.15	126.73	124.42
2	E	501	HEM	C3D-C4D-ND	-2.14	107.82	110.17
2	J	501	HEM	C4D-ND-C1D	2.12	107.72	105.21
2	G	501	HEM	CAA-CBA-CGA	-2.12	108.06	113.67
2	L	501	HEM	CHA-C4D-ND	2.10	126.97	124.37
2	J	501	HEM	O2D-CGD-CBD	2.10	120.64	114.00
3	D	502	PLM	O2-C1-C2	-2.09	116.46	123.09
3	B	502	PLM	O1-C1-O2	2.08	128.69	123.33
2	B	501	HEM	C2A-C1A-NA	-2.08	107.84	110.15
3	E	502	PLM	O2-C1-C2	-2.08	116.49	123.09
2	J	501	HEM	C3B-C2B-C1B	2.08	107.97	106.41
3	K	502	PLM	O2-C1-C2	-2.07	116.53	123.09
2	H	501	HEM	C2D-C1D-ND	-2.06	107.53	109.90
3	D	502	PLM	O1-C1-O2	2.06	128.62	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	501	HEM	C3D-C4D-ND	-2.06	107.92	110.17
2	K	501	HEM	C2A-C1A-NA	-2.05	107.87	110.15
2	F	501	HEM	C2D-C1D-ND	-2.05	107.53	109.90
3	A	502	PLM	O1-C1-O2	2.05	128.61	123.33
2	J	501	HEM	C1B-NB-C4B	2.05	107.63	105.21
3	C	502	PLM	O1-C1-O2	2.04	128.59	123.33
2	C	501	HEM	C4D-ND-C1D	2.03	107.61	105.21
2	F	501	HEM	C3B-C2B-C1B	2.02	107.93	106.41
2	J	501	HEM	CAD-CBD-CGD	-2.02	108.30	113.67
2	H	501	HEM	CBD-CAD-C3D	-2.02	106.96	112.53
2	B	501	HEM	C3B-C2B-C1B	2.01	107.92	106.41

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	502	PLM	C1-C2-C3-C4
3	A	502	PLM	C3-C4-C5-C6
3	C	502	PLM	C5-C6-C7-C8
3	D	503	PLM	C1-C2-C3-C4
3	I	502	PLM	CA-CB-CC-CD
3	H	502	PLM	C9-CA-CB-CC
3	B	502	PLM	C4-C5-C6-C7
3	D	502	PLM	C8-C9-CA-CB
3	D	503	PLM	C9-CA-CB-CC
3	D	502	PLM	C4-C5-C6-C7
3	B	502	PLM	C5-C6-C7-C8
3	D	502	PLM	C9-CA-CB-CC
3	I	502	PLM	C5-C6-C7-C8
3	E	502	PLM	C4-C5-C6-C7
3	A	502	PLM	C9-CA-CB-CC
3	A	502	PLM	CA-CB-CC-CD
3	G	502	PLM	C4-C5-C6-C7
3	I	502	PLM	C8-C9-CA-CB
3	G	502	PLM	C9-CA-CB-CC
3	H	502	PLM	C7-C8-C9-CA
3	B	502	PLM	C1-C2-C3-C4
3	C	502	PLM	C3-C4-C5-C6
3	C	502	PLM	C4-C5-C6-C7
3	E	502	PLM	C1-C2-C3-C4
3	D	503	PLM	CA-CB-CC-CD
3	L	502	PLM	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	A	502	PLM	C6-C7-C8-C9
3	B	502	PLM	C8-C9-CA-CB
3	C	502	PLM	C8-C9-CA-CB
3	D	503	PLM	C2-C3-C4-C5
3	J	502	PLM	C7-C8-C9-CA
3	L	502	PLM	C7-C8-C9-CA
3	D	502	PLM	CD-CE-CF-CG
3	A	502	PLM	C2-C3-C4-C5
3	K	502	PLM	C4-C5-C6-C7
3	K	502	PLM	C2-C3-C4-C5
3	E	502	PLM	C6-C7-C8-C9
3	J	502	PLM	CA-CB-CC-CD
3	B	502	PLM	C9-CA-CB-CC
3	J	502	PLM	C2-C3-C4-C5
3	J	502	PLM	C6-C7-C8-C9
3	C	502	PLM	C7-C8-C9-CA
3	C	502	PLM	C9-CA-CB-CC
3	H	502	PLM	C6-C7-C8-C9
3	I	502	PLM	C6-C7-C8-C9
3	K	502	PLM	C8-C9-CA-CB
3	A	502	PLM	CB-CC-CD-CE
3	L	502	PLM	CC-CD-CE-CF
3	J	502	PLM	O1-C1-C2-C3
3	D	502	PLM	CB-CC-CD-CE
3	A	502	PLM	C4-C5-C6-C7
3	I	502	PLM	C2-C3-C4-C5
3	J	502	PLM	O2-C1-C2-C3
3	E	502	PLM	C5-C6-C7-C8
2	I	501	HEM	CAD-CBD-CGD-O1D
3	I	502	PLM	O2-C1-C2-C3
3	K	502	PLM	O2-C1-C2-C3
3	A	502	PLM	C8-C9-CA-CB
3	H	502	PLM	CA-CB-CC-CD
3	D	502	PLM	C7-C8-C9-CA
2	J	501	HEM	CAA-CBA-CGA-O2A
3	K	502	PLM	O1-C1-C2-C3
2	D	501	HEM	CAD-CBD-CGD-O1D
2	I	501	HEM	CAD-CBD-CGD-O2D
3	E	502	PLM	C2-C3-C4-C5
3	E	502	PLM	O1-C1-C2-C3
2	A	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
2	B	501	HEM	CAA-CBA-CGA-O1A
2	J	501	HEM	CAA-CBA-CGA-O1A
3	I	502	PLM	O1-C1-C2-C3
2	F	501	HEM	CAD-CBD-CGD-O1D
3	E	502	PLM	O2-C1-C2-C3
3	D	502	PLM	C3-C4-C5-C6
2	D	501	HEM	CAD-CBD-CGD-O2D
2	C	501	HEM	CAD-CBD-CGD-O1D
2	H	501	HEM	CAD-CBD-CGD-O1D
2	G	501	HEM	CAD-CBD-CGD-O1D
3	C	502	PLM	C2-C3-C4-C5
2	E	501	HEM	CAD-CBD-CGD-O1D
2	E	501	HEM	CAD-CBD-CGD-O2D
2	L	501	HEM	CAD-CBD-CGD-O1D
2	L	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O2D
2	G	501	HEM	CAD-CBD-CGD-O2D
2	J	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O2D
2	C	501	HEM	CAD-CBD-CGD-O2D
2	F	501	HEM	CAD-CBD-CGD-O2D
3	L	502	PLM	C4-C5-C6-C7
2	J	501	HEM	CAD-CBD-CGD-O1D
3	B	502	PLM	O2-C1-C2-C3
3	B	502	PLM	O1-C1-C2-C3
2	H	501	HEM	CAD-CBD-CGD-O2D
2	J	501	HEM	C3D-CAD-CBD-CGD
2	B	501	HEM	CAA-CBA-CGA-O2A
3	L	502	PLM	C5-C6-C7-C8
2	A	501	HEM	C2C-C3C-CAC-CBC
2	E	501	HEM	C2C-C3C-CAC-CBC

There are no ring outliers.

24 monomers are involved in 74 short contacts:

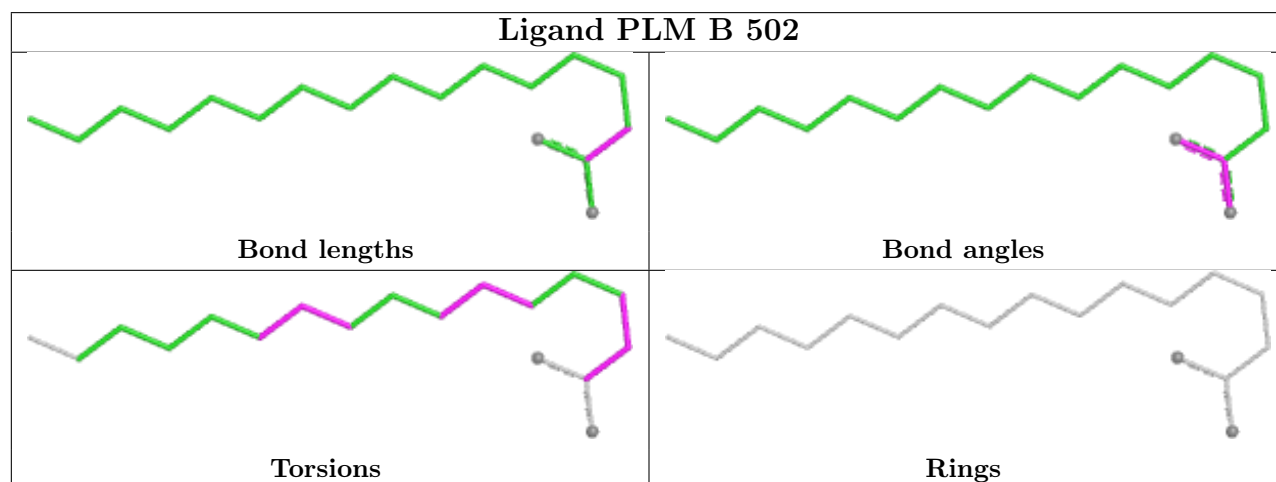
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	PLM	4	0
2	A	501	HEM	3	0
3	D	503	PLM	3	0
2	J	501	HEM	3	0
3	L	502	PLM	5	0
2	E	501	HEM	2	0

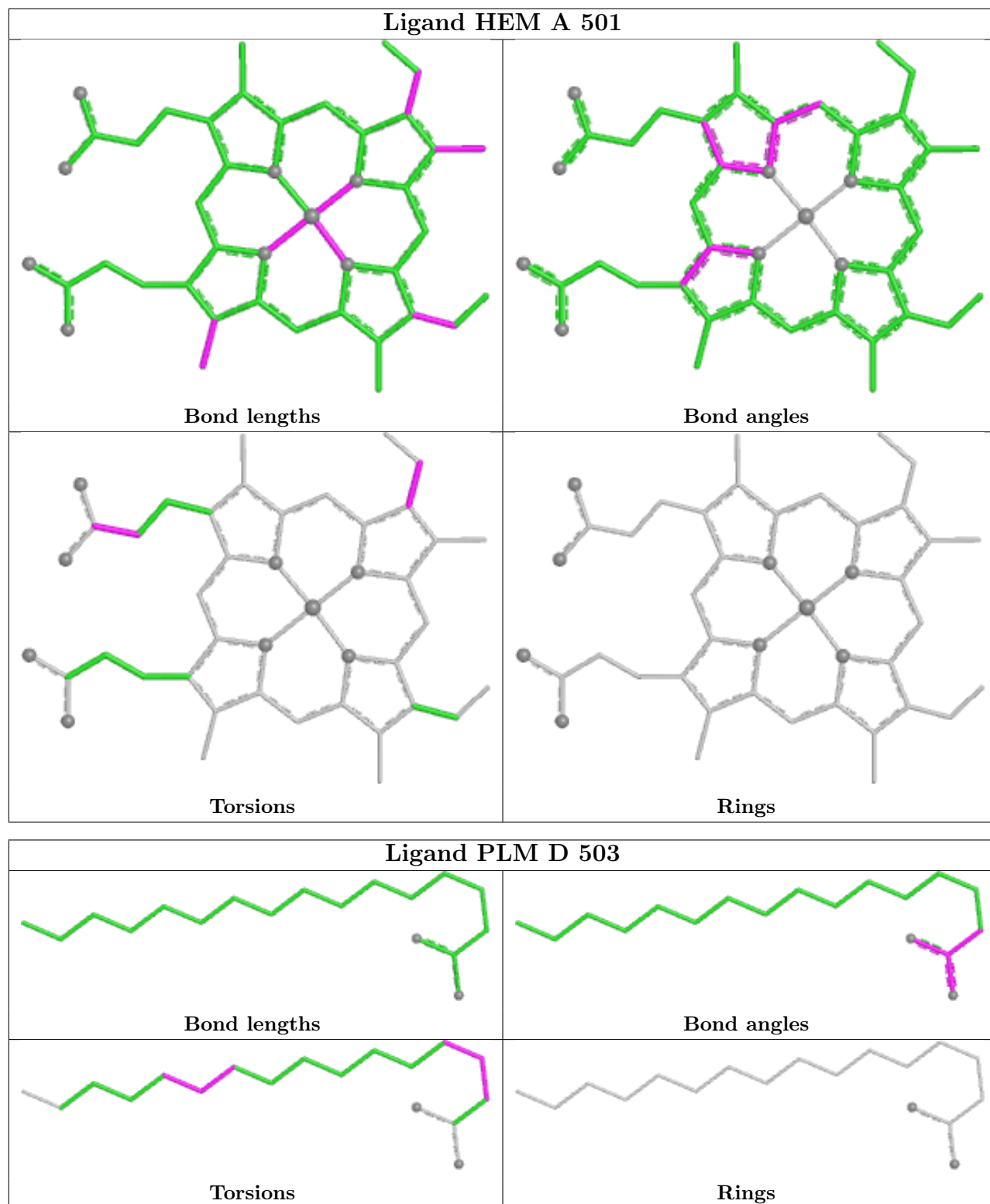
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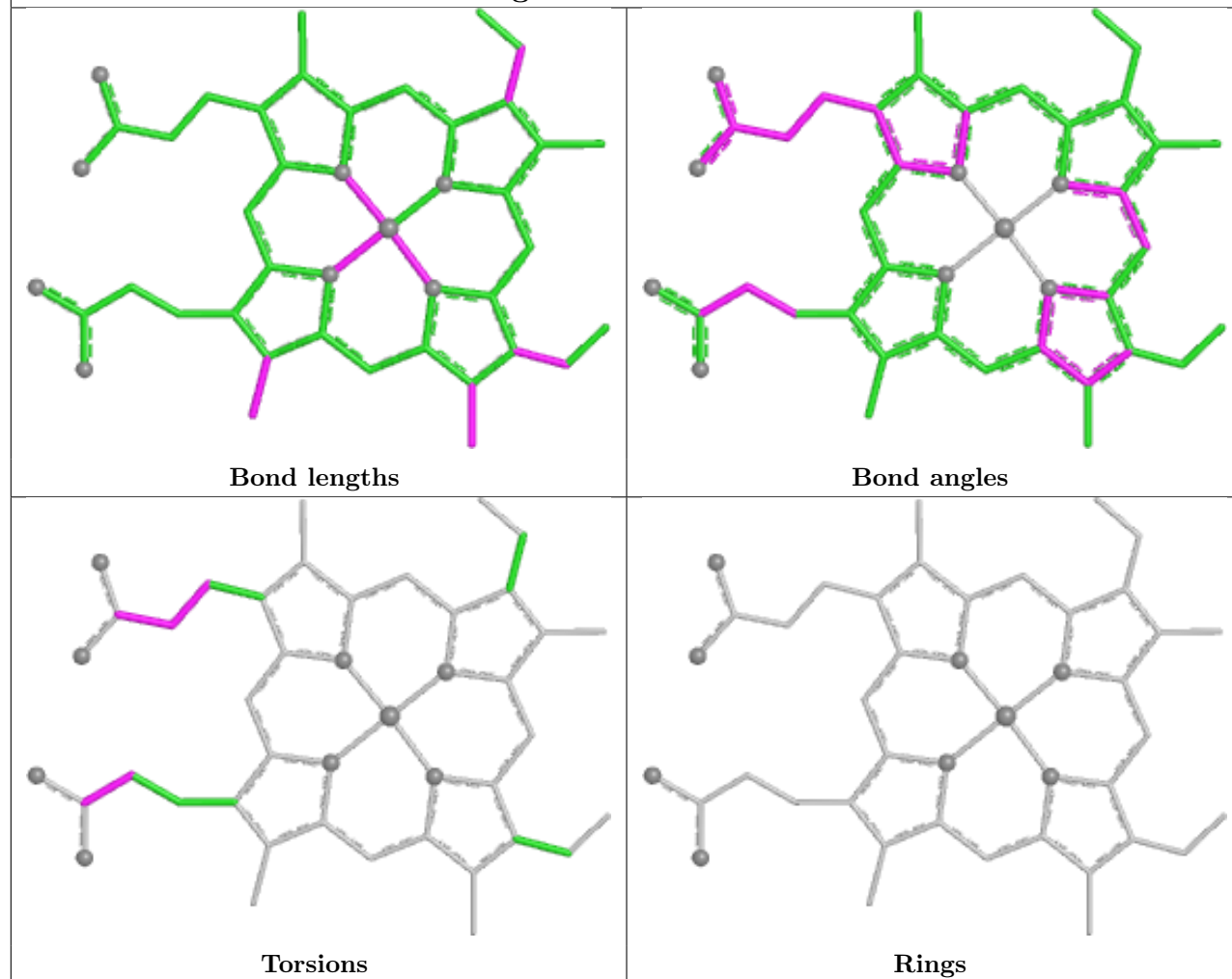
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	HEM	3	0
2	H	501	HEM	6	0
3	C	502	PLM	3	0
3	H	502	PLM	5	0
3	G	502	PLM	3	0
3	E	502	PLM	2	0
3	A	502	PLM	4	0
2	K	501	HEM	6	0
3	K	502	PLM	1	0
2	B	501	HEM	3	0
2	D	501	HEM	4	0
3	D	502	PLM	2	0
3	J	502	PLM	1	0
2	G	501	HEM	4	0
2	I	501	HEM	10	0
2	C	501	HEM	4	0
3	I	502	PLM	3	0
2	L	501	HEM	4	0

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

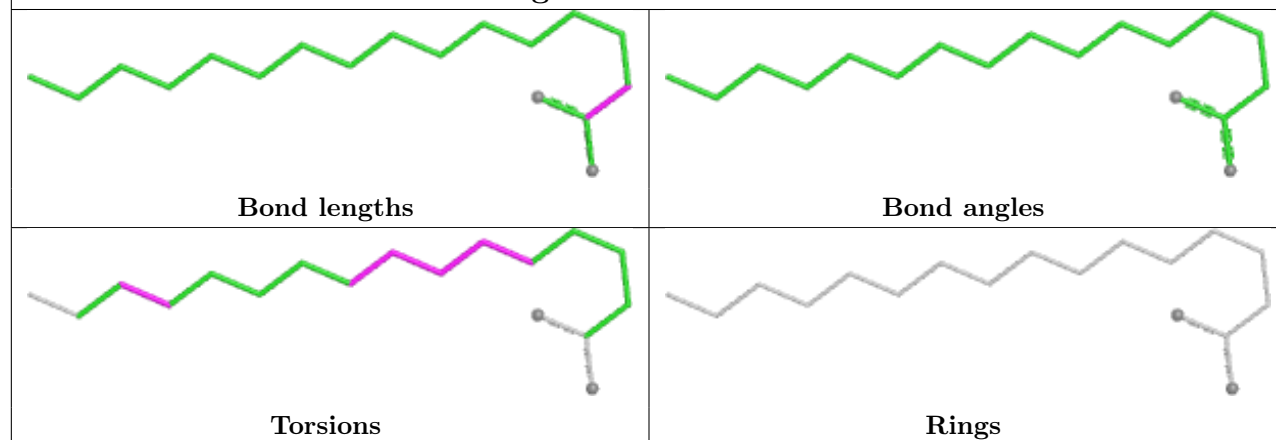


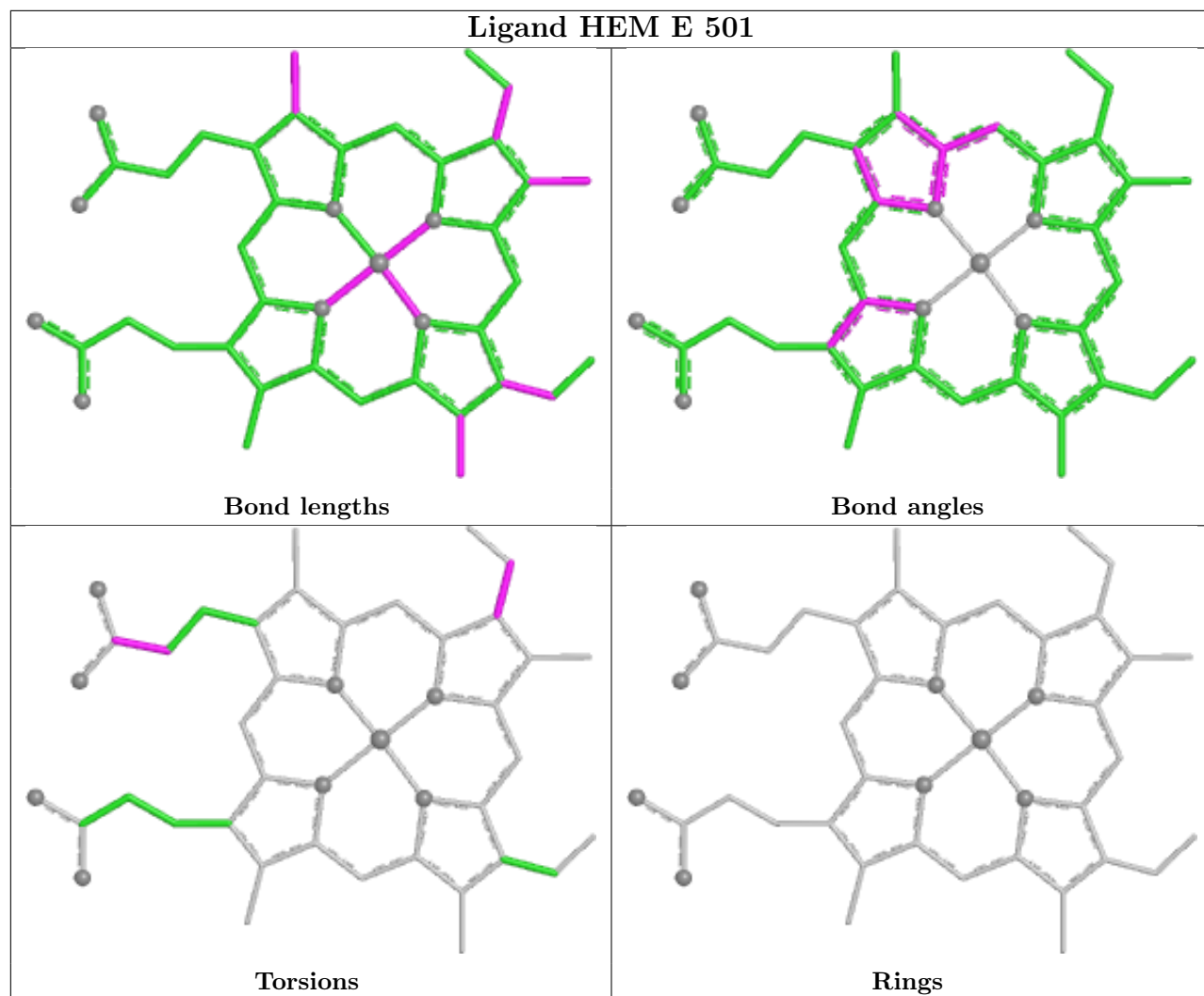


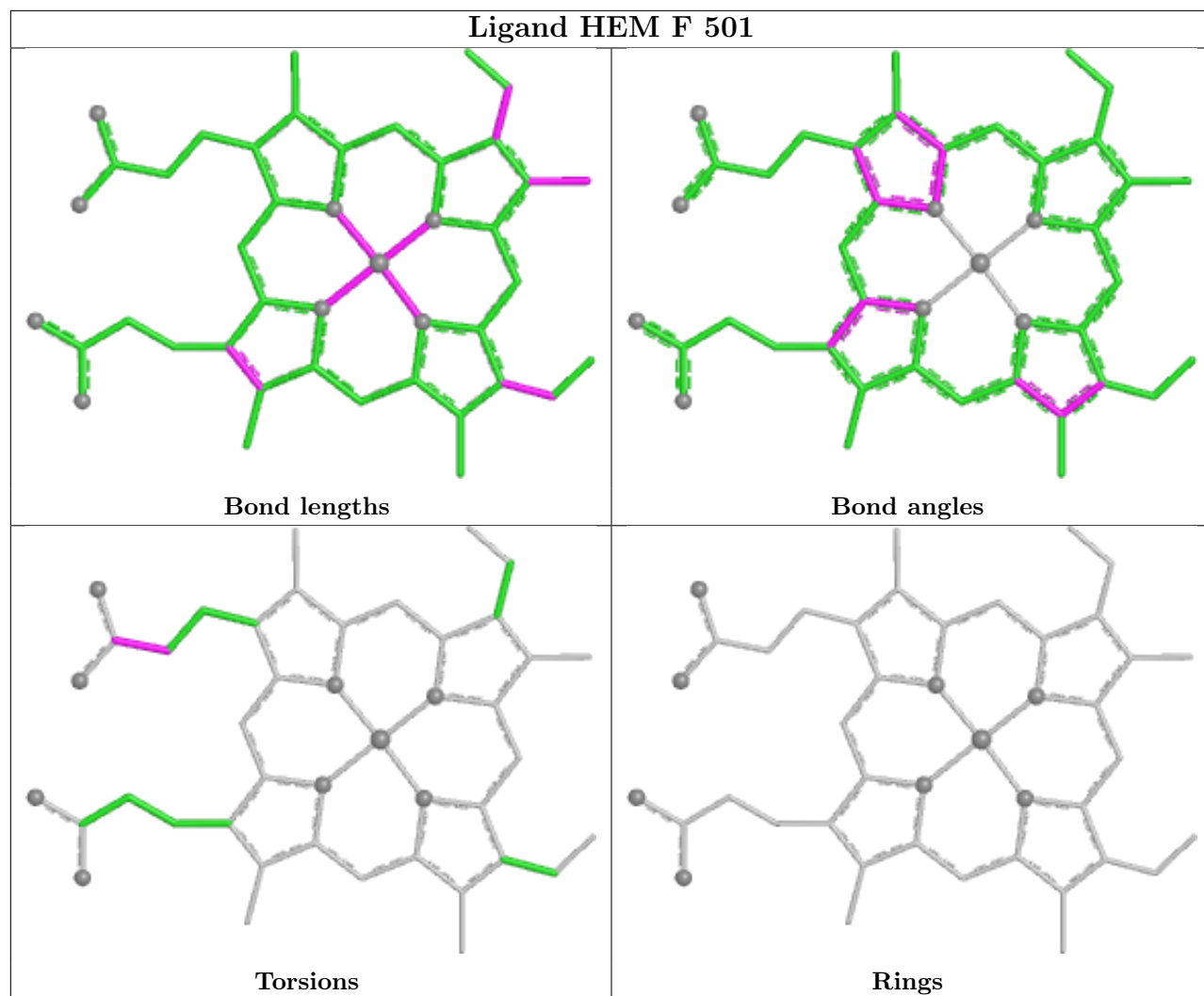
Ligand HEM J 501

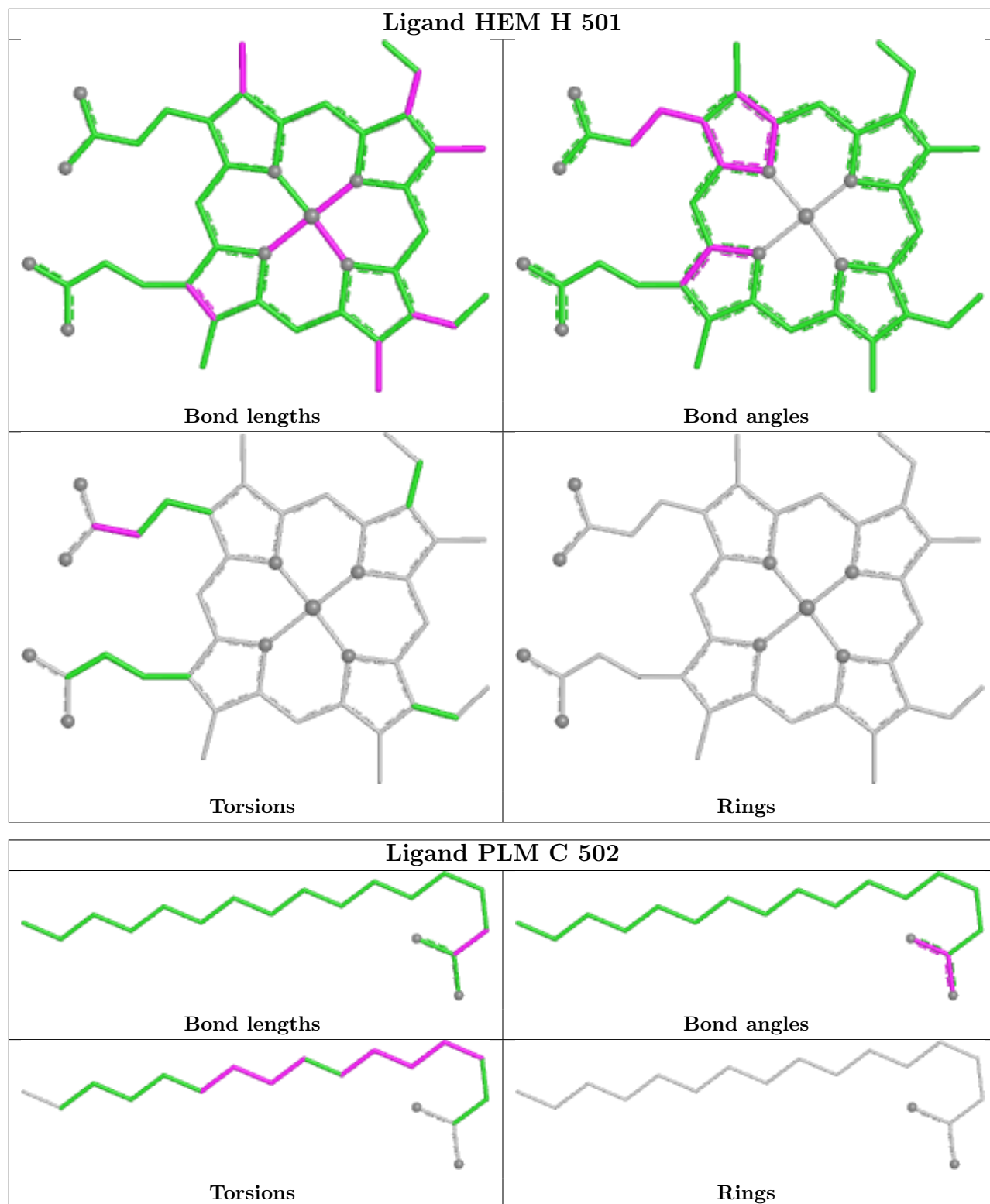


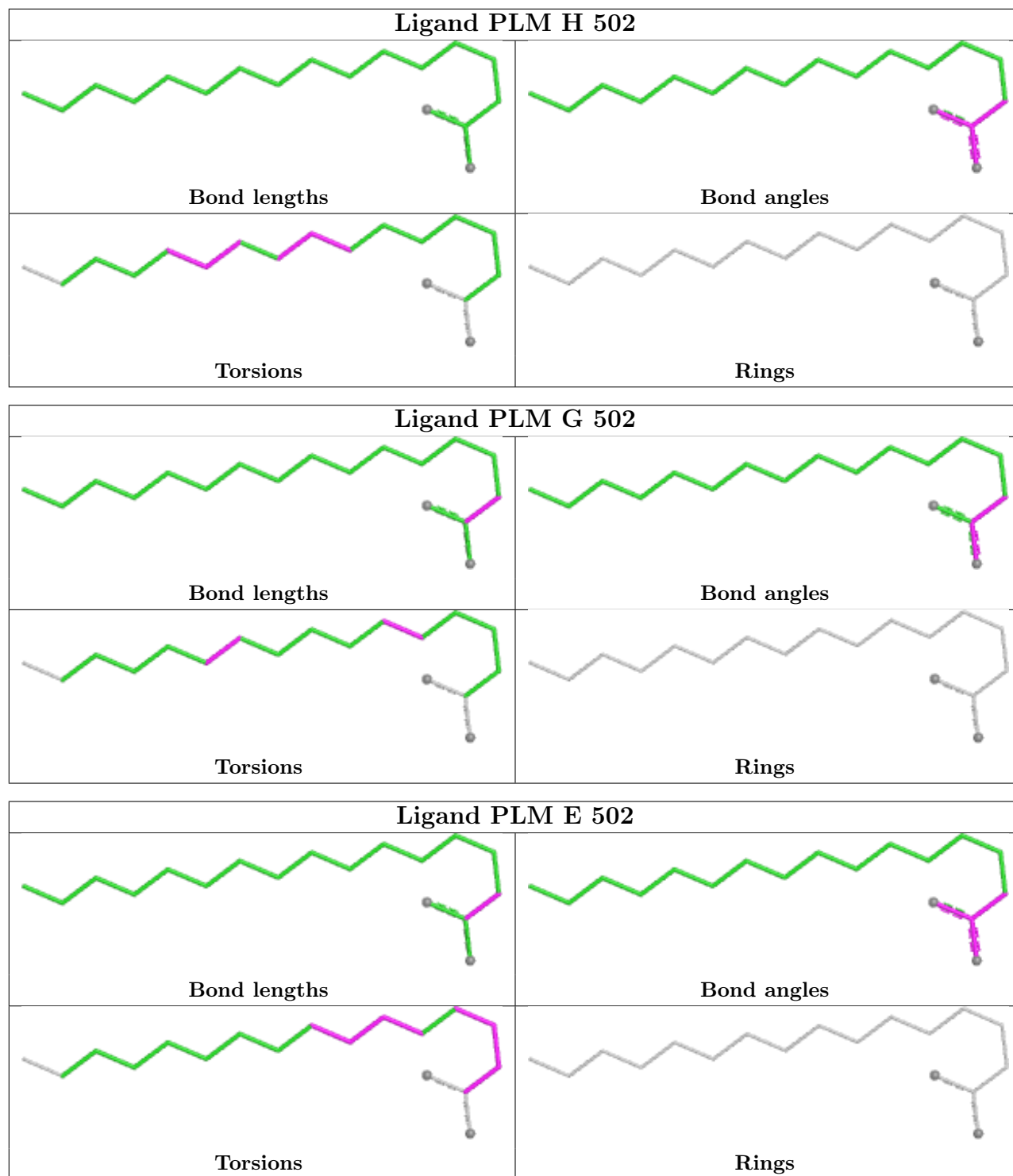
Ligand PLM L 502

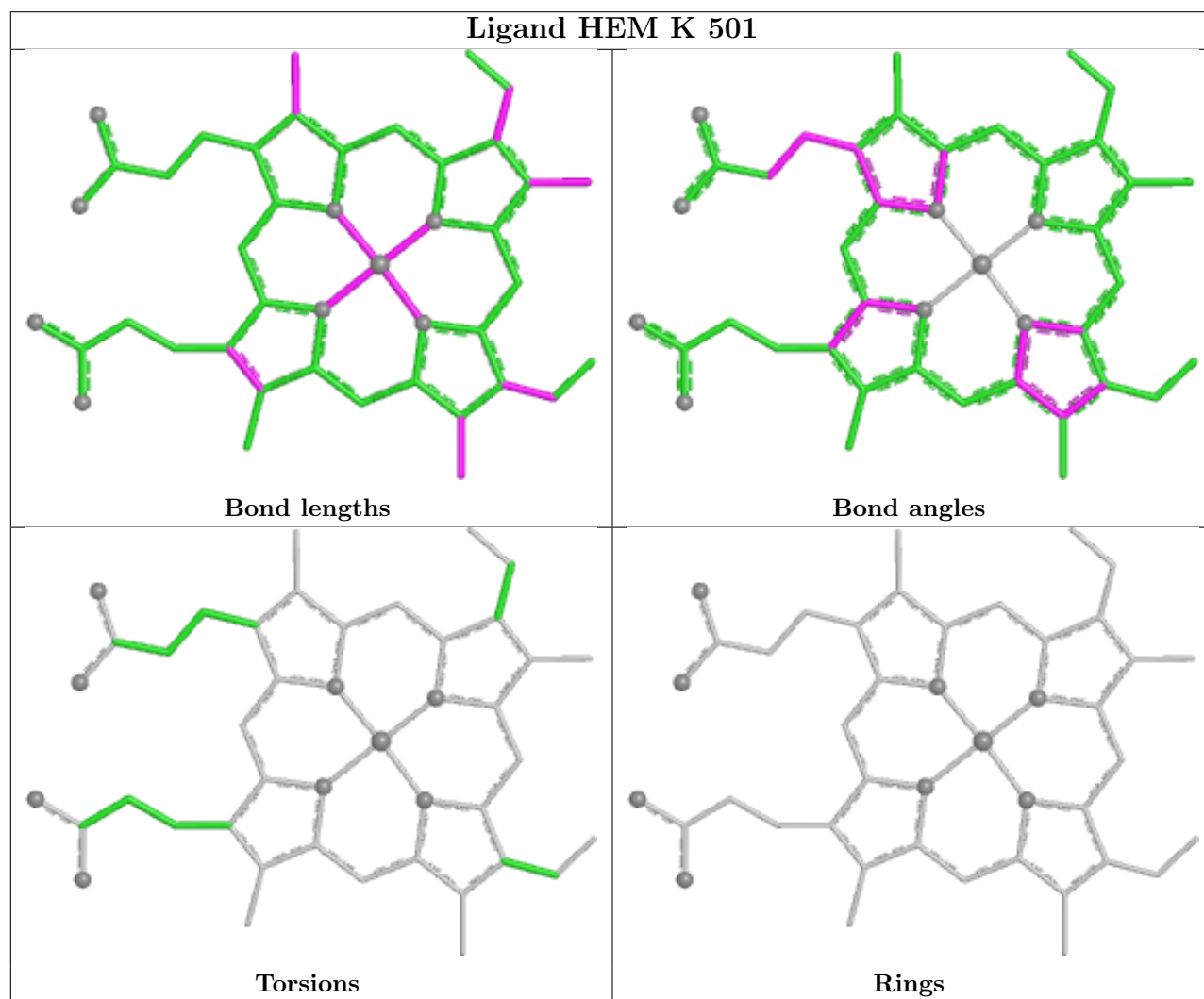
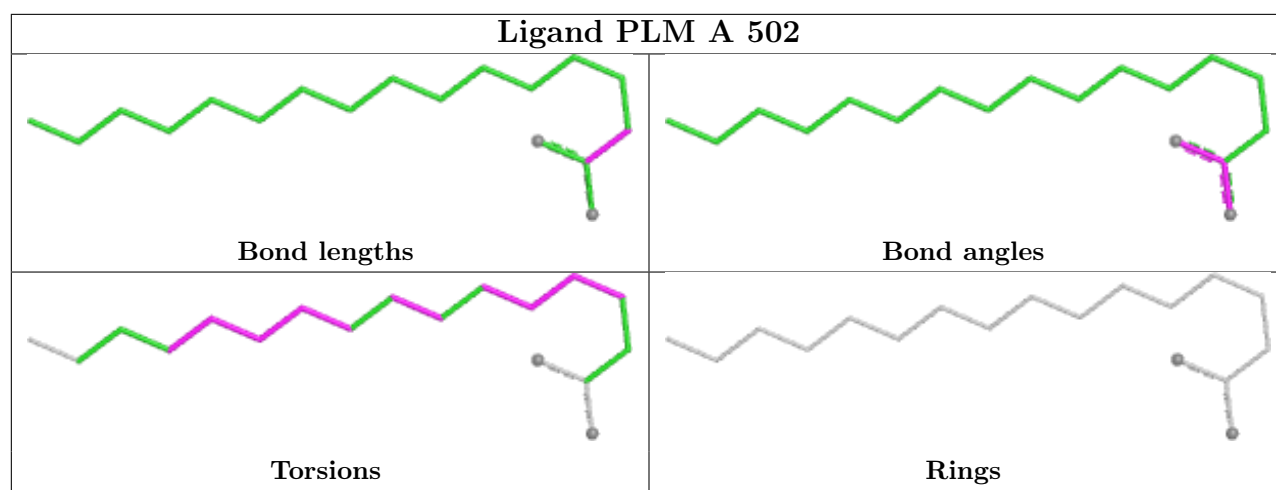


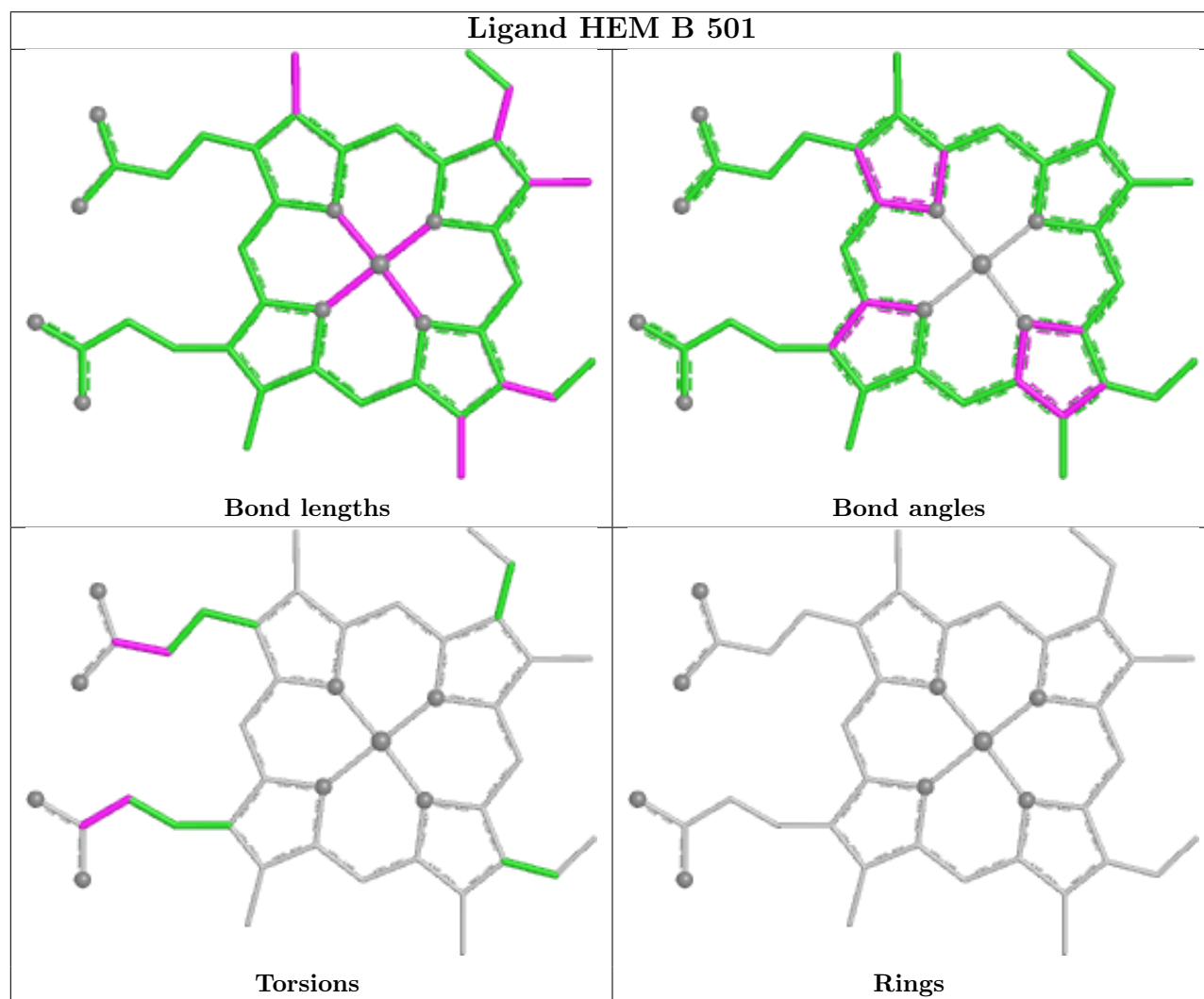
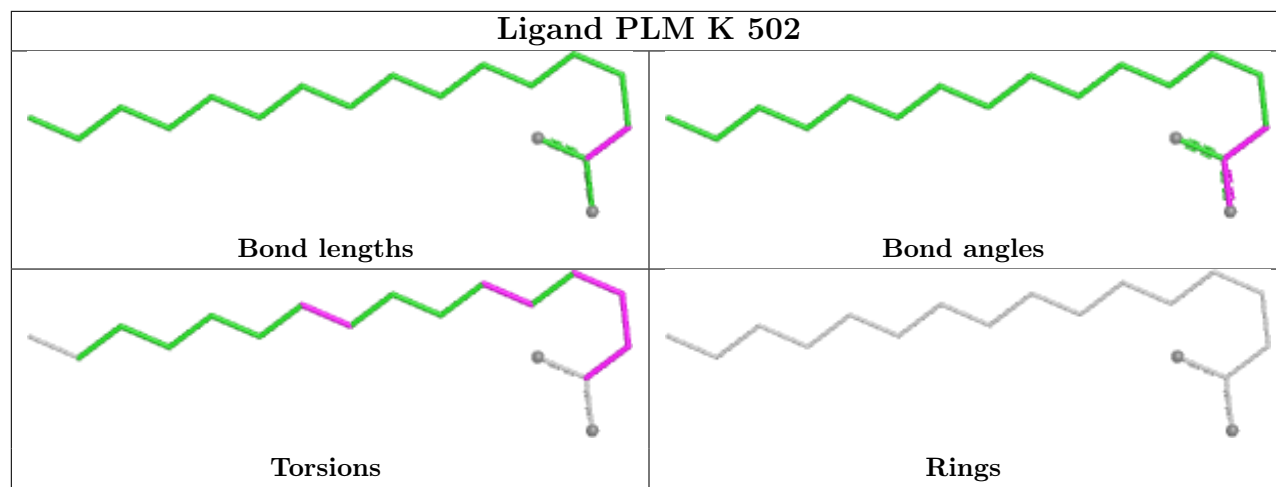


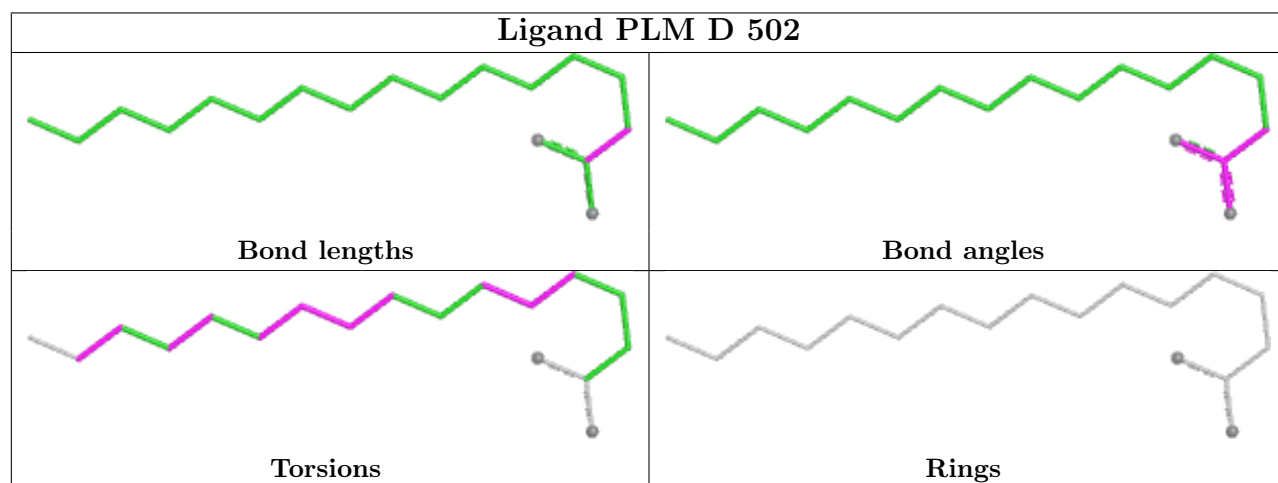
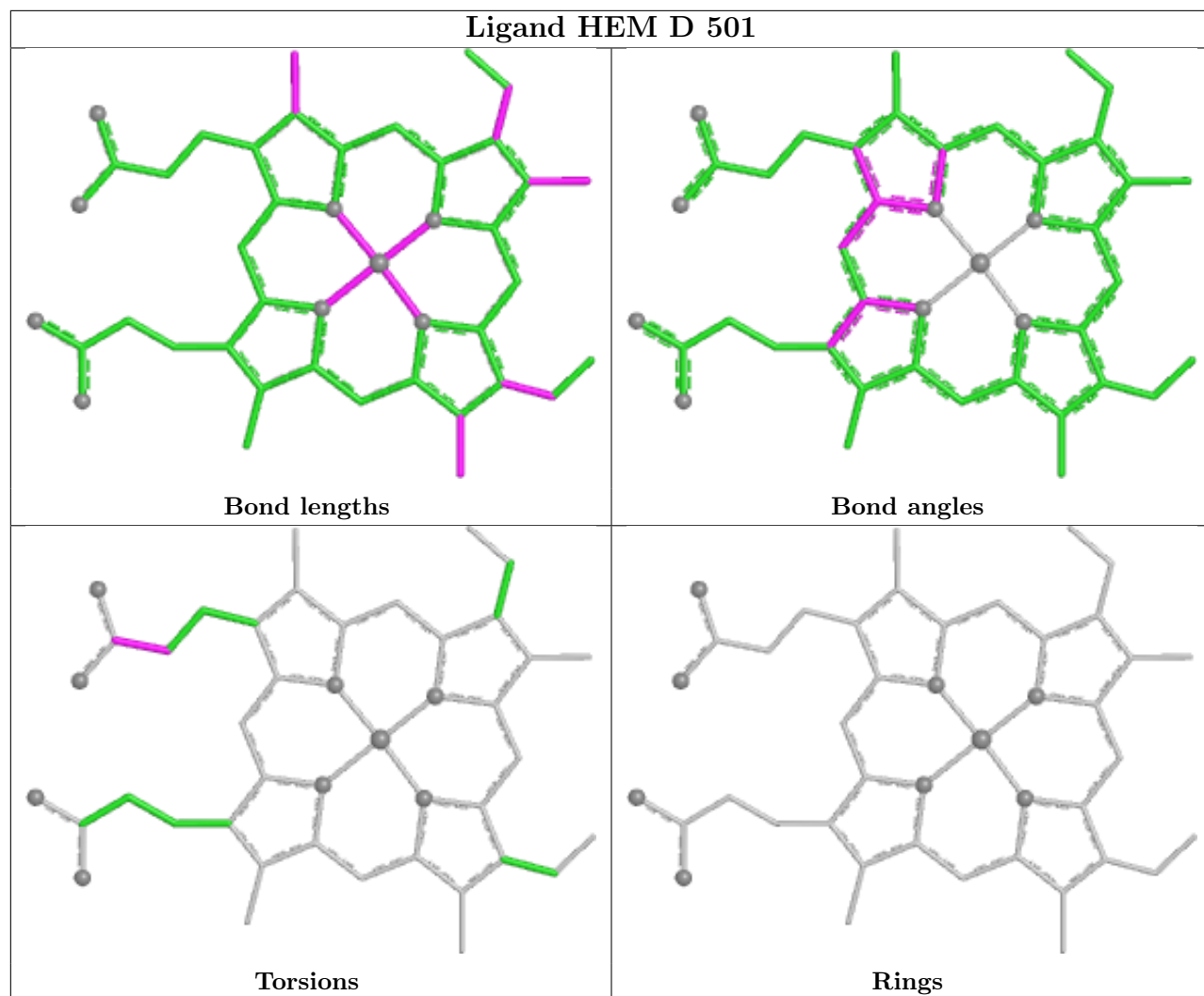


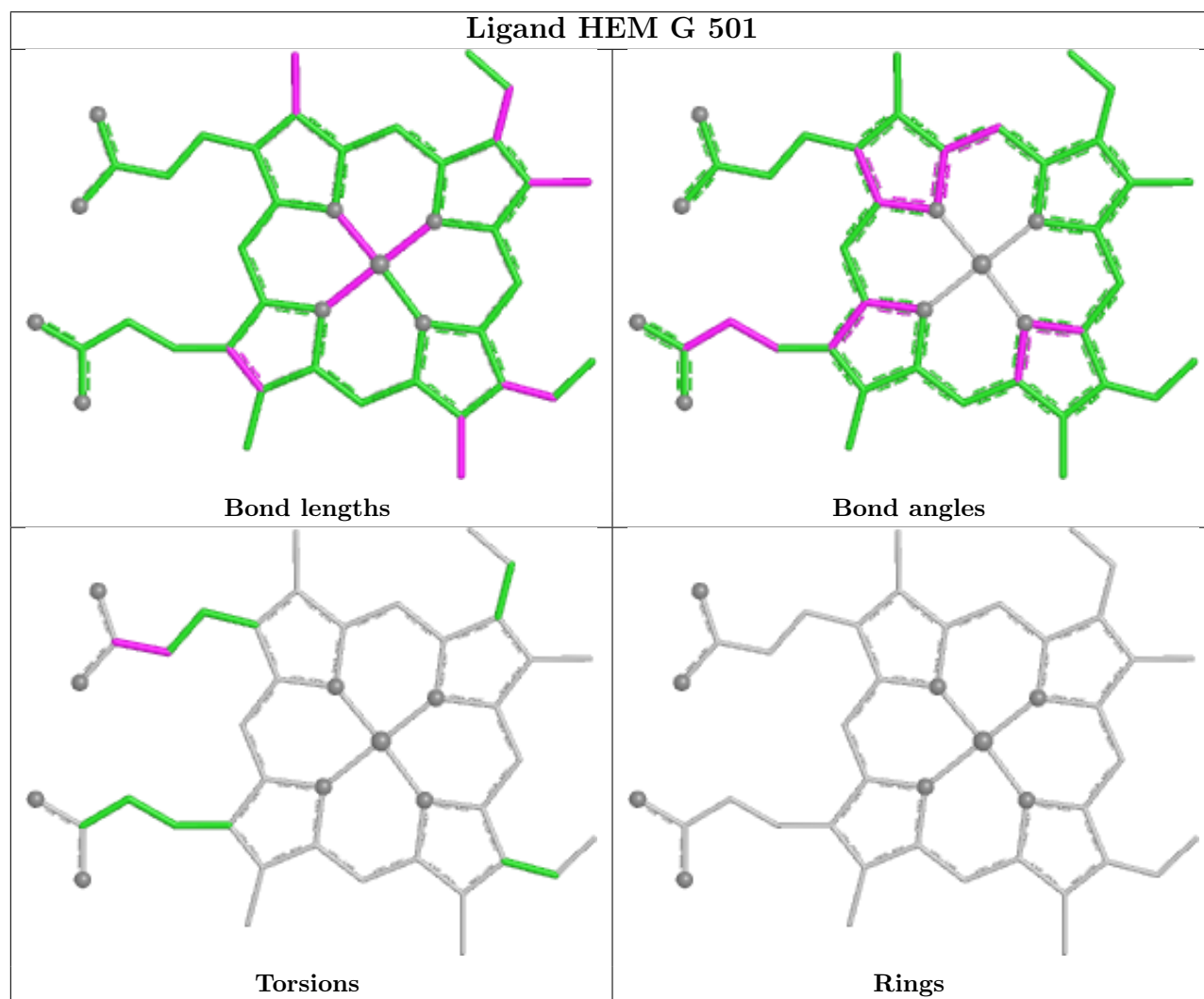
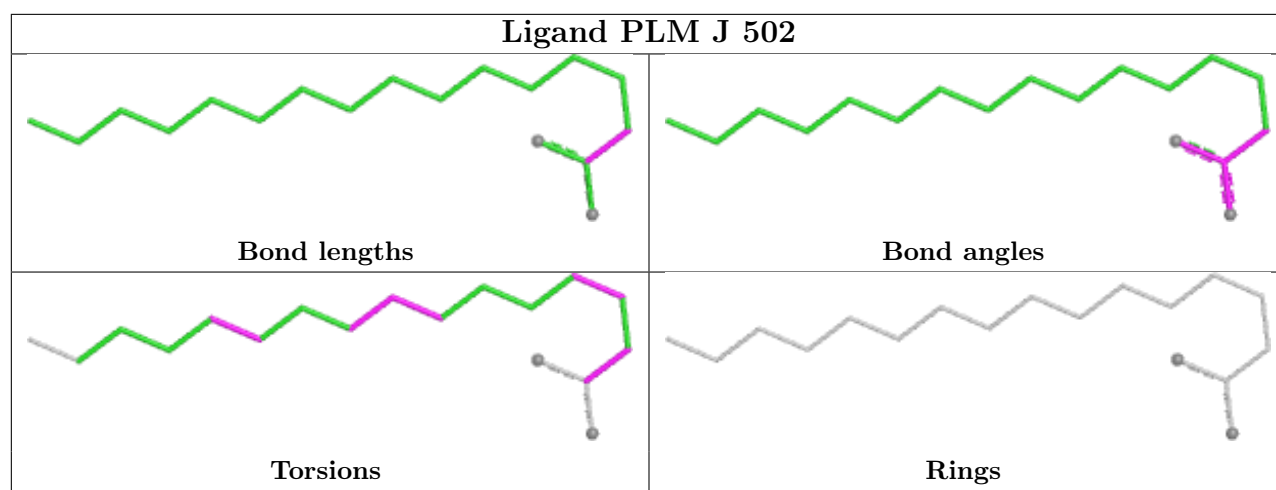




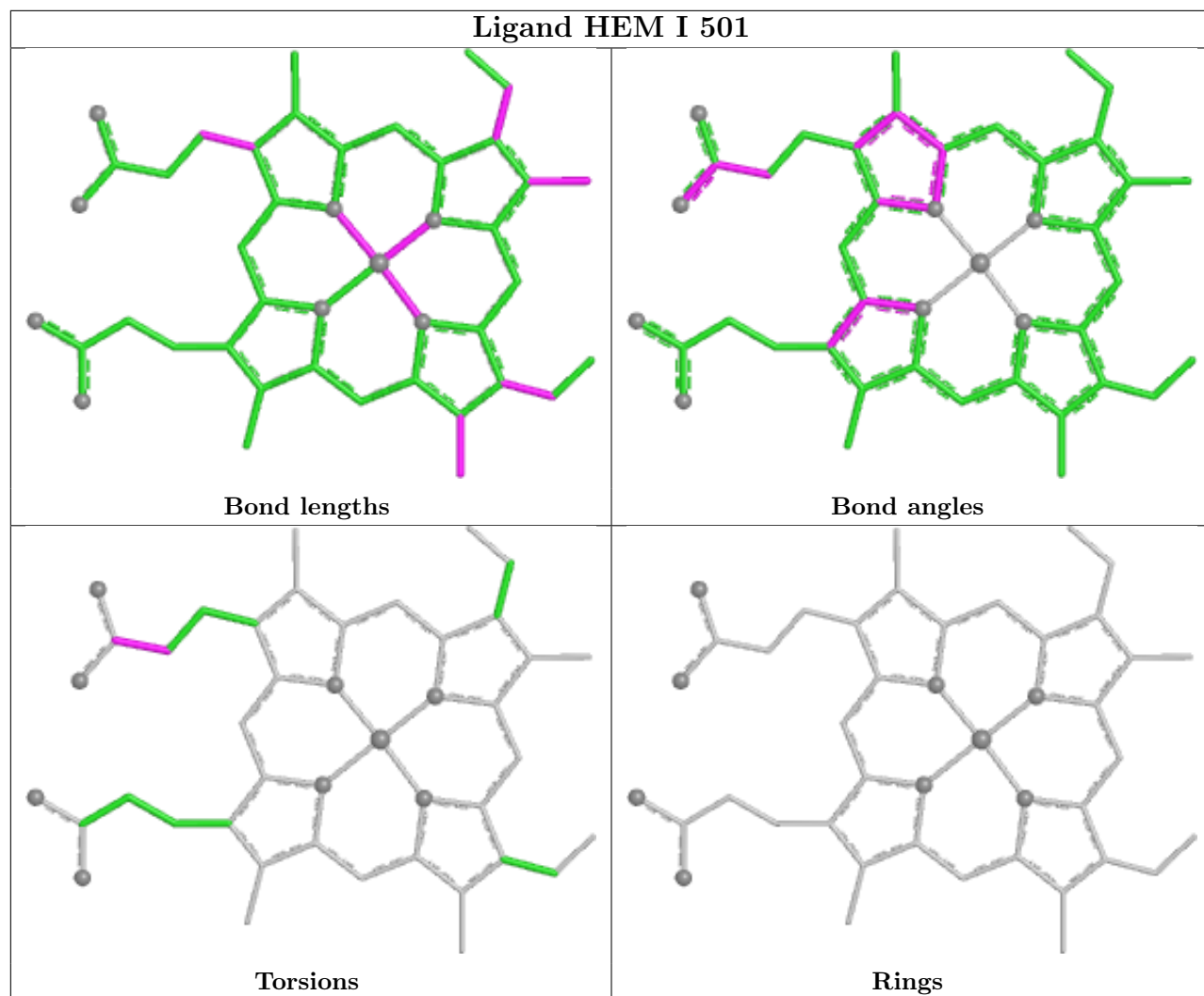


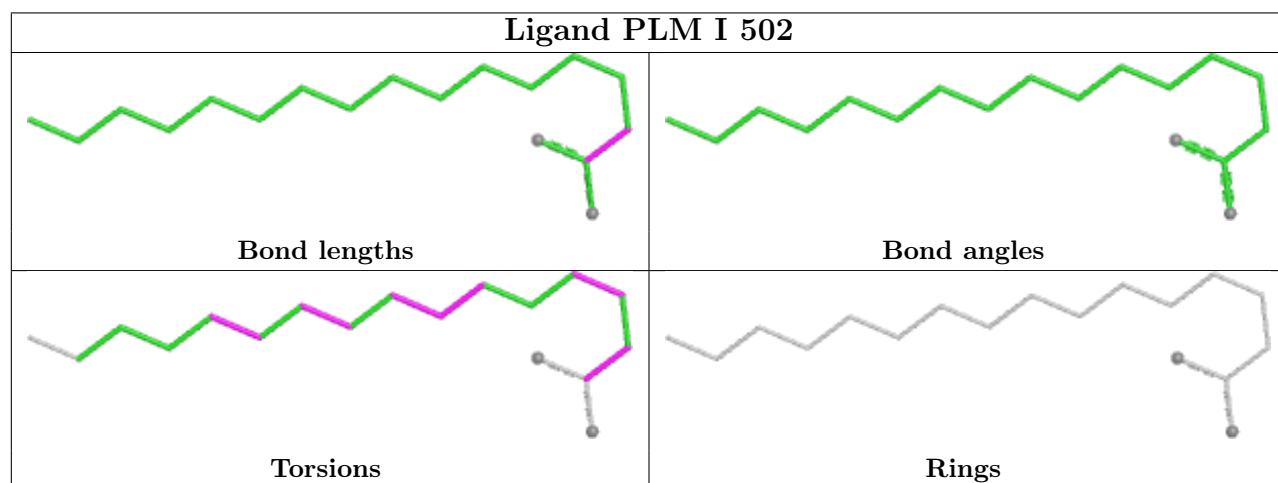
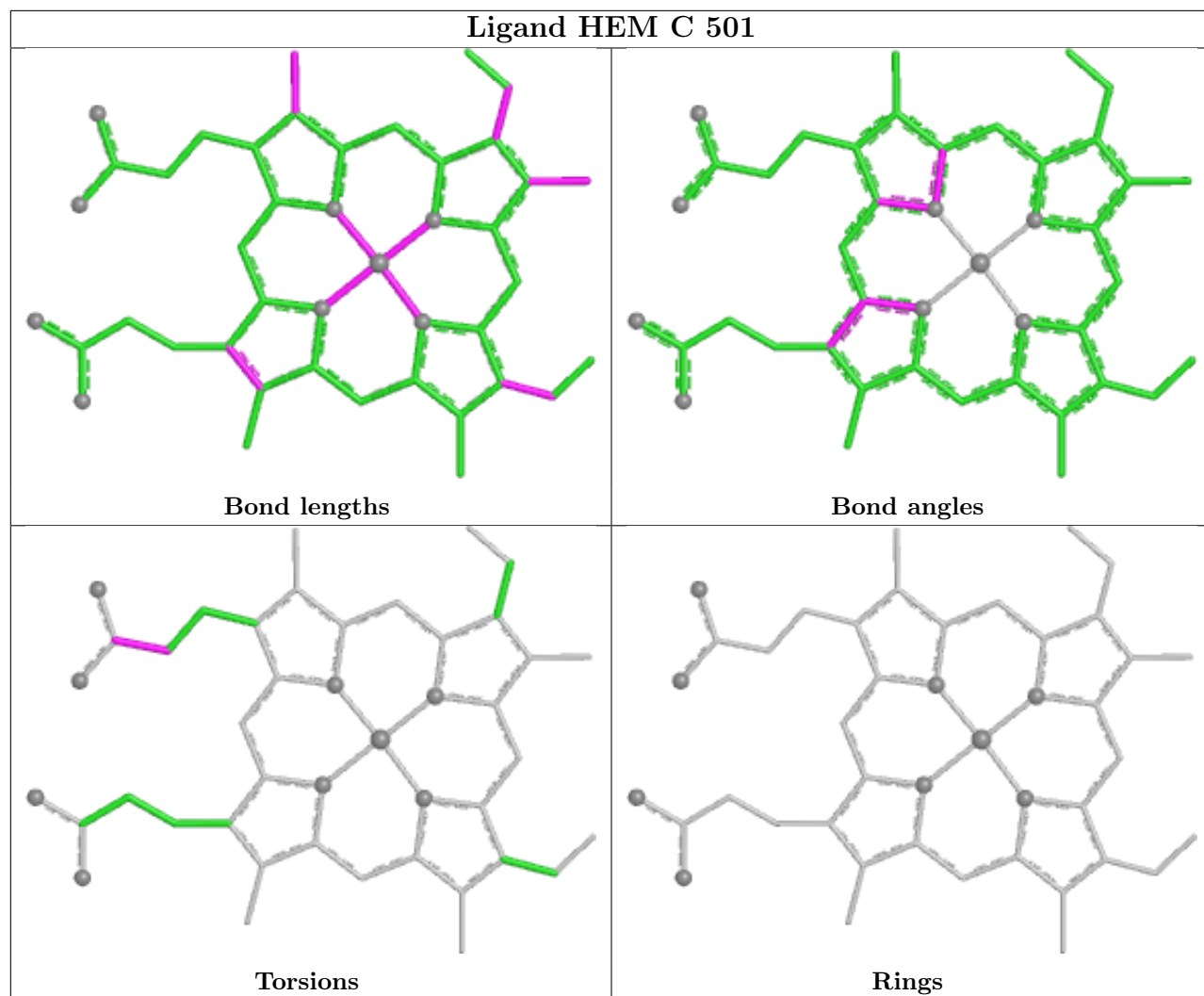


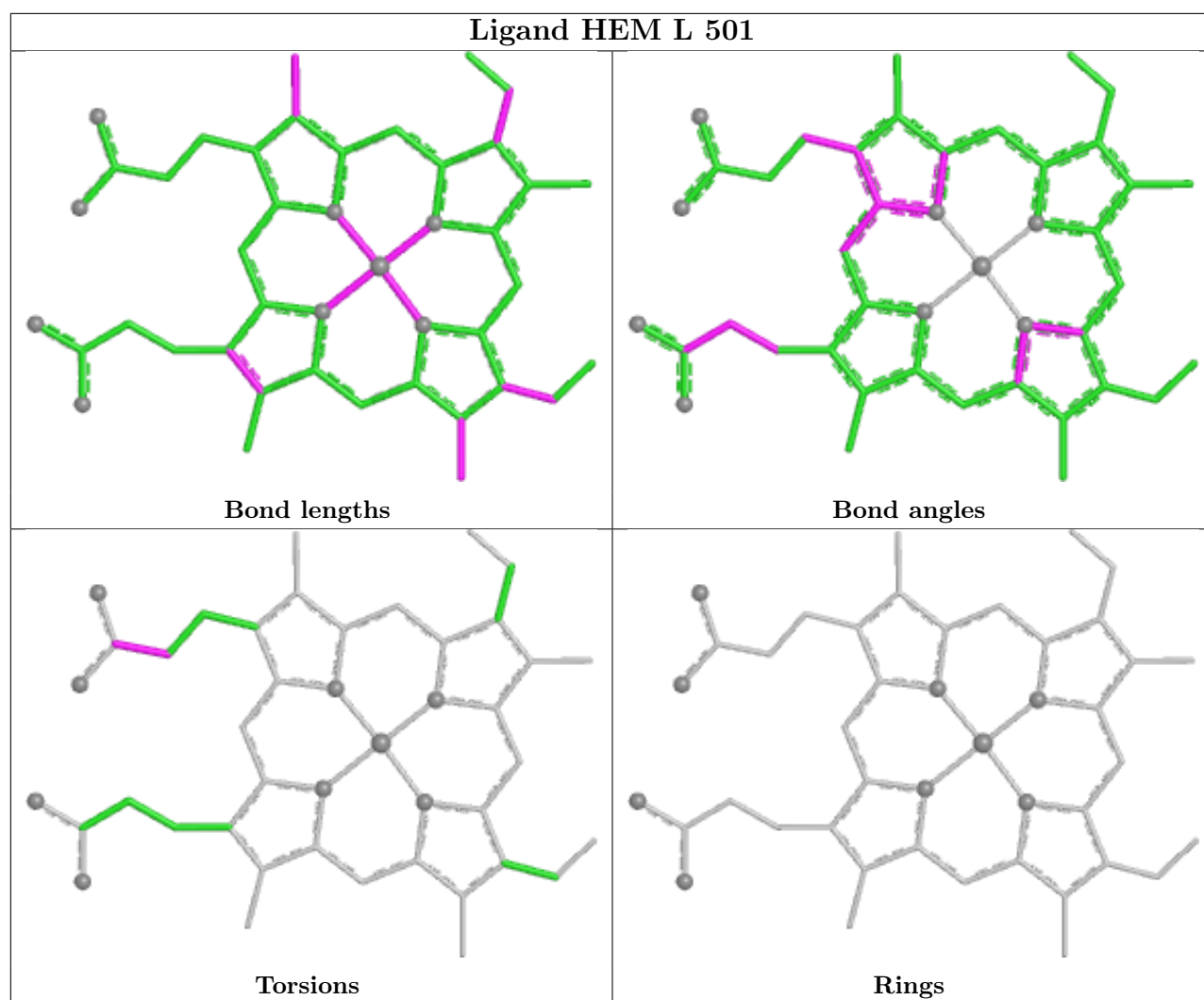




Ligand HEM I 501







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	429/458 (93%)	-0.05	3 (0%) 84 77	43, 64, 103, 154	0
1	B	430/458 (93%)	-0.12	6 (1%) 73 64	41, 61, 95, 136	0
1	C	421/458 (91%)	0.04	4 (0%) 79 72	43, 67, 100, 117	0
1	D	419/458 (91%)	-0.00	2 (0%) 87 82	38, 63, 107, 124	0
1	E	422/458 (92%)	0.07	2 (0%) 87 82	47, 69, 104, 126	0
1	F	419/458 (91%)	0.20	5 (1%) 76 68	47, 74, 106, 123	0
1	G	401/458 (87%)	0.42	16 (3%) 42 33	49, 83, 120, 136	0
1	H	415/458 (90%)	0.42	12 (2%) 53 43	58, 87, 122, 151	0
1	I	399/458 (87%)	0.95	40 (10%) 12 9	51, 113, 147, 168	0
1	J	415/458 (90%)	0.97	40 (9%) 13 10	55, 113, 150, 168	0
1	K	416/458 (90%)	0.95	37 (8%) 15 11	54, 112, 151, 174	0
1	L	410/458 (89%)	1.11	56 (13%) 6 5	65, 119, 156, 178	0
All	All	4996/5496 (90%)	0.41	223 (4%) 38 30	38, 81, 139, 178	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	356	ASP	4.0
1	G	375	ASN	3.8
1	I	255	ASP	3.7
1	L	180	MET	3.6
1	G	214	SER	3.6
1	K	213	GLN	3.5
1	K	217	SER	3.5
1	J	94	THR	3.5
1	K	221	ASN	3.5
1	L	77	ALA	3.4
1	A	231	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	J	87	ASP	3.4
1	I	77	ALA	3.3
1	I	168	PHE	3.3
1	I	154	ASP	3.3
1	L	212	ILE	3.3
1	C	184	LEU	3.2
1	J	168	PHE	3.2
1	I	214	SER	3.2
1	D	432	GLN	3.2
1	B	76	GLY	3.2
1	E	230	GLY	3.2
1	L	347	GLY	3.2
1	G	172	THR	3.2
1	H	431	TYR	3.2
1	K	77	ALA	3.2
1	J	115	MET	3.2
1	L	338	TYR	3.1
1	I	76	GLY	3.1
1	I	249	THR	3.1
1	J	353	LYS	3.1
1	L	178	THR	3.1
1	K	301	VAL	3.1
1	L	402	GLN	3.1
1	L	372	TRP	3.1
1	K	402	GLN	3.0
1	G	93	GLU	3.0
1	K	118	TYR	3.0
1	G	223	ILE	3.0
1	J	312	VAL	3.0
1	H	8	ILE	3.0
1	L	75	GLU	3.0
1	L	310	GLN	2.9
1	L	146	GLU	2.9
1	L	217	SER	2.9
1	I	84	PHE	2.9
1	J	410	PHE	2.9
1	H	308	THR	2.9
1	J	379	PHE	2.8
1	K	136	LEU	2.8
1	H	250	GLY	2.8
1	I	247	PRO	2.8
1	J	356	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	181	THR	2.8
1	L	387	LEU	2.8
1	J	212	ILE	2.8
1	L	345	ILE	2.7
1	J	343	THR	2.7
1	L	413	HIS	2.7
1	I	69	ARG	2.7
1	J	391	PRO	2.7
1	K	351	ILE	2.7
1	L	412	LEU	2.7
1	L	307	PRO	2.7
1	J	302	LEU	2.7
1	L	398	PHE	2.6
1	I	217	SER	2.6
1	L	107	MET	2.6
1	L	309	TYR	2.6
1	F	184	LEU	2.6
1	J	322	LEU	2.6
1	B	234	GLU	2.6
1	G	79	ALA	2.6
1	K	398	PHE	2.6
1	L	302	LEU	2.5
1	J	156	ILE	2.5
1	J	241	MET	2.5
1	I	395	TYR	2.5
1	I	91	THR	2.5
1	G	184	LEU	2.5
1	L	237	LEU	2.5
1	K	372	TRP	2.5
1	L	395	TYR	2.5
1	B	75	GLU	2.5
1	J	100	LYS	2.5
1	H	356	ASP	2.5
1	K	89	LEU	2.5
1	L	106	LEU	2.5
1	L	381	PRO	2.5
1	I	406	ILE	2.5
1	K	254	ASP	2.4
1	L	138	PRO	2.4
1	J	373	GLY	2.4
1	J	133	TRP	2.4
1	J	118	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	183	ALA	2.4
1	I	343	THR	2.4
1	L	110	PHE	2.4
1	J	102	ALA	2.4
1	J	213	GLN	2.4
1	F	356	ASP	2.4
1	L	379	PHE	2.4
1	I	120	ALA	2.4
1	H	387	LEU	2.4
1	K	105	ILE	2.4
1	L	420	GLY	2.4
1	L	120	ALA	2.4
1	K	107	MET	2.4
1	K	97	PRO	2.4
1	J	352	LYS	2.3
1	K	410	PHE	2.3
1	K	448	ASP	2.3
1	C	393	HIS	2.3
1	K	252	LYS	2.3
1	E	104	ASN	2.3
1	C	176	PHE	2.3
1	J	326	LEU	2.3
1	L	179	SER	2.3
1	K	314	LYS	2.3
1	I	420	GLY	2.3
1	H	75	GLU	2.3
1	G	95	HIS	2.3
1	G	392	HIS	2.3
1	K	100	LYS	2.3
1	L	177	ILE	2.3
1	J	338	TYR	2.3
1	J	110	PHE	2.3
1	G	356	ASP	2.3
1	L	454	LEU	2.3
1	L	100	LYS	2.3
1	I	92	SER	2.3
1	I	118	TYR	2.3
1	H	90	PHE	2.2
1	I	302	LEU	2.2
1	L	253	LEU	2.2
1	L	244	VAL	2.2
1	I	373	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	332	ALA	2.2
1	I	106	LEU	2.2
1	I	137	ASN	2.2
1	J	266	LEU	2.2
1	L	400	ASN	2.2
1	J	105	ILE	2.2
1	I	370	ASP	2.2
1	I	309	TYR	2.2
1	I	407	GLY	2.2
1	I	412	LEU	2.2
1	L	409	GLN	2.2
1	A	233	GLU	2.2
1	L	102	ALA	2.2
1	H	69	ARG	2.2
1	H	221	ASN	2.2
1	L	104	ASN	2.2
1	B	231	ASP	2.2
1	K	390	VAL	2.2
1	L	64	VAL	2.2
1	L	314	LYS	2.2
1	K	384	PHE	2.2
1	G	218	LEU	2.2
1	K	326	LEU	2.2
1	G	411	ALA	2.2
1	L	383	ARG	2.1
1	A	393	HIS	2.1
1	I	307	PRO	2.1
1	K	315	LEU	2.1
1	L	260	PHE	2.1
1	G	241	MET	2.1
1	I	115	MET	2.1
1	K	215	MET	2.1
1	L	97	PRO	2.1
1	J	416	THR	2.1
1	L	249	THR	2.1
1	G	161	PHE	2.1
1	J	417	LEU	2.1
1	J	339	ALA	2.1
1	J	403	ARG	2.1
1	F	228	SER	2.1
1	L	93	GLU	2.1
1	J	402	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	305	PRO	2.1
1	J	307	PRO	2.1
1	L	247	PRO	2.1
1	G	387	LEU	2.1
1	H	407	GLY	2.1
1	I	89	LEU	2.1
1	J	238	LEU	2.1
1	J	412	LEU	2.1
1	J	426	PHE	2.1
1	K	87	ASP	2.1
1	L	129	LEU	2.1
1	K	379	PHE	2.1
1	F	358	ILE	2.1
1	H	223	ILE	2.1
1	I	310	GLN	2.1
1	I	320	MET	2.1
1	G	106	LEU	2.1
1	I	399	GLY	2.1
1	K	157	GLY	2.1
1	K	165	PHE	2.1
1	D	356	ASP	2.1
1	I	71	ASP	2.1
1	F	177	ILE	2.1
1	J	411	ALA	2.1
1	K	133	TRP	2.1
1	B	355	GLU	2.1
1	I	312	VAL	2.0
1	K	455	PRO	2.0
1	B	387	LEU	2.0
1	I	253	LEU	2.0
1	L	78	LEU	2.0
1	I	133	TRP	2.0
1	L	101	LYS	2.0
1	L	312	VAL	2.0
1	J	184	LEU	2.0
1	K	253	LEU	2.0
1	K	328	LEU	2.0
1	K	257	ASN	2.0
1	L	265	PHE	2.0
1	K	102	ALA	2.0
1	C	356	ASP	2.0
1	I	256	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	372	TRP	2.0
1	K	244	VAL	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($\text{\AA}^2$)	Q<0.9
3	PLM	G	502	18/18	0.75	0.19	46,61,69,72	0
3	PLM	L	502	18/18	0.77	0.20	50,67,75,75	0
3	PLM	D	502	18/18	0.79	0.21	36,56,81,87	0
3	PLM	K	502	18/18	0.79	0.17	35,51,77,79	0
3	PLM	D	503	18/18	0.79	0.19	44,58,62,62	0
3	PLM	H	502	18/18	0.81	0.18	59,66,73,76	0
3	PLM	E	502	18/18	0.81	0.17	45,61,71,71	0
3	PLM	B	502	18/18	0.81	0.19	41,57,61,65	0
3	PLM	A	502	18/18	0.84	0.16	40,53,62,64	0
3	PLM	C	502	18/18	0.85	0.16	38,49,55,57	0
3	PLM	I	502	18/18	0.85	0.15	32,57,72,75	0
3	PLM	J	502	18/18	0.87	0.14	37,60,74,77	0
2	HEM	J	501	43/43	0.93	0.15	86,95,113,117	0
2	HEM	L	501	43/43	0.93	0.15	94,101,119,123	0
2	HEM	K	501	43/43	0.94	0.13	83,97,113,124	0
2	HEM	I	501	43/43	0.95	0.13	93,107,118,120	0
2	HEM	F	501	43/43	0.96	0.09	43,52,65,70	0
2	HEM	G	501	43/43	0.96	0.10	63,74,88,89	0
2	HEM	E	501	43/43	0.96	0.08	33,38,63,69	0
2	HEM	B	501	43/43	0.97	0.07	36,46,56,68	0
2	HEM	H	501	43/43	0.97	0.09	57,76,99,102	0

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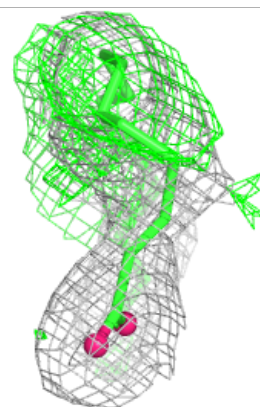
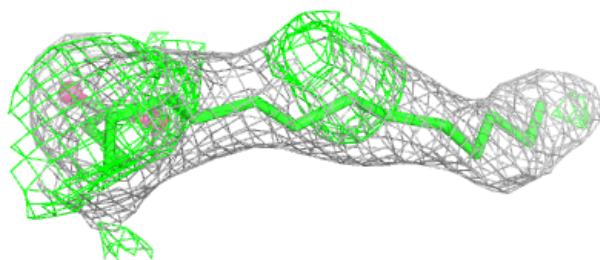
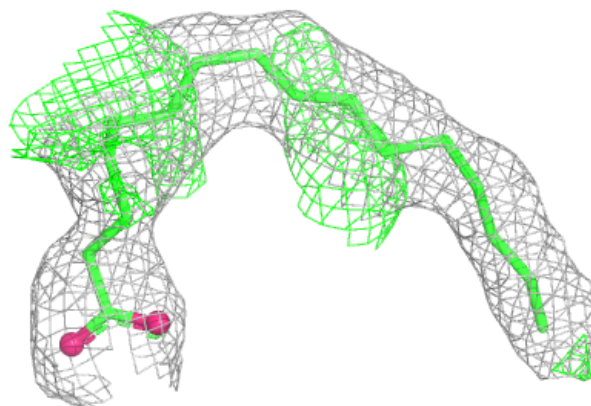
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	C	501	43/43	0.97	0.08	26,37,59,61	0
2	HEM	A	501	43/43	0.98	0.06	34,42,52,58	0
2	HEM	D	501	43/43	0.98	0.07	40,51,60,62	0

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.

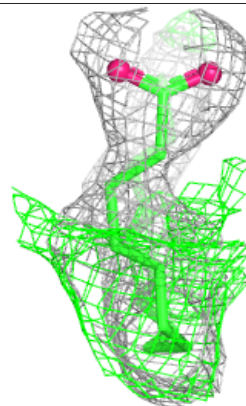
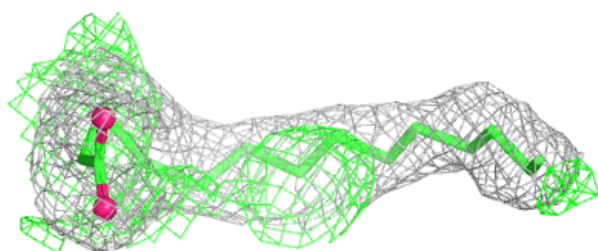
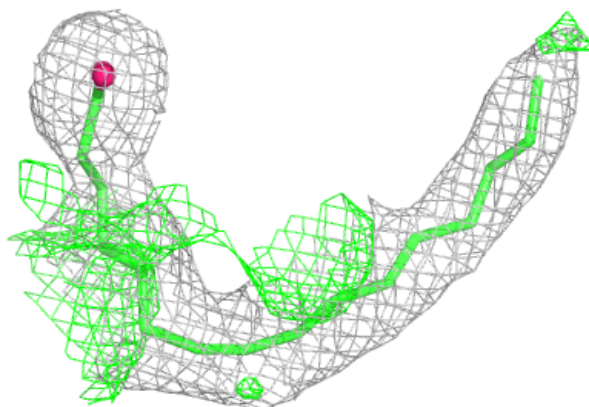
Electron density around PLM G 502:

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



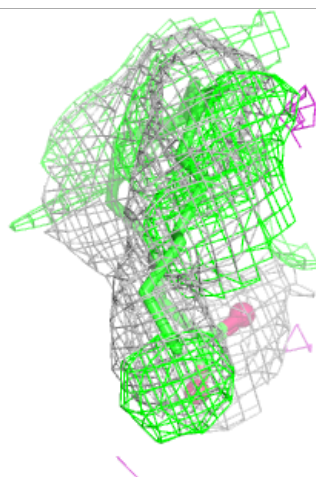
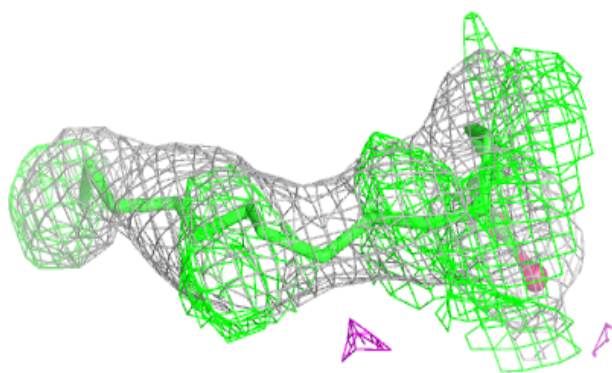
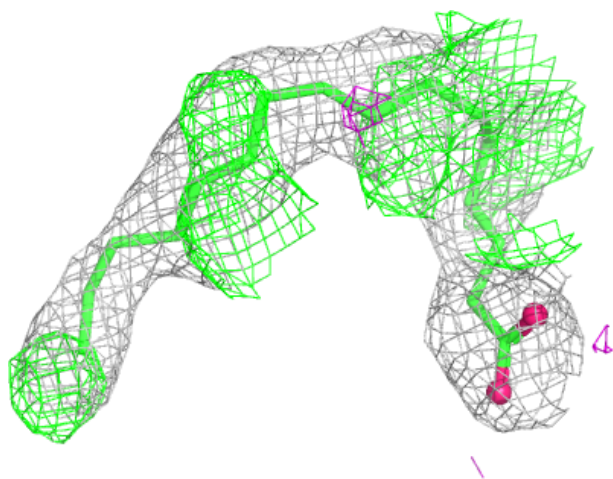
Electron density around PLM L 502:

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and green (positive)



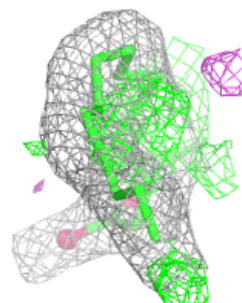
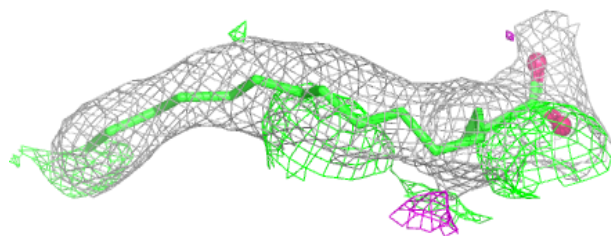
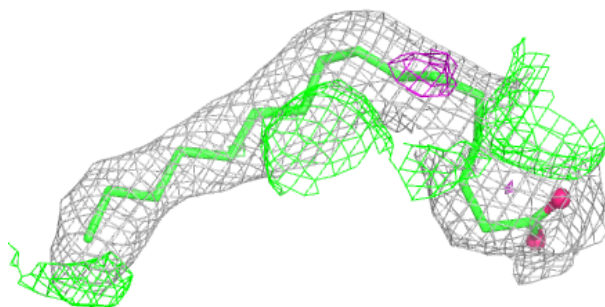
Electron density around PLM D 502:

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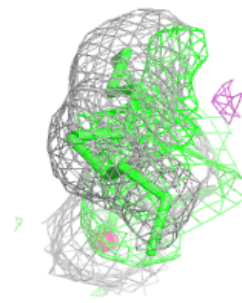
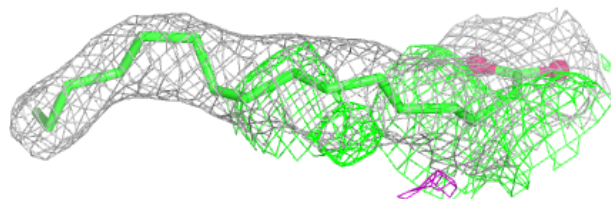
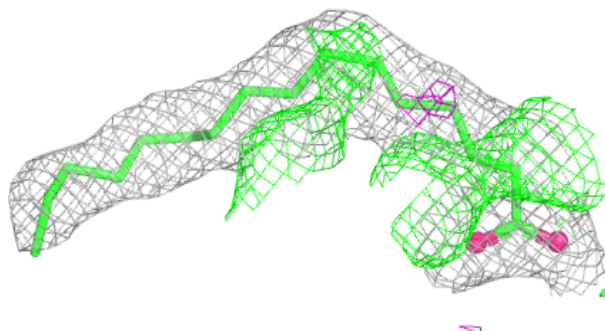


Electron density around PLM K 502:

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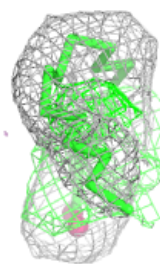
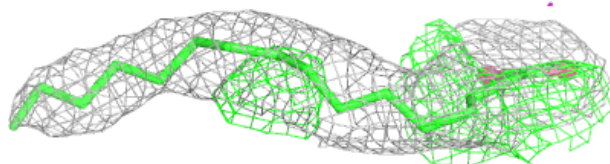
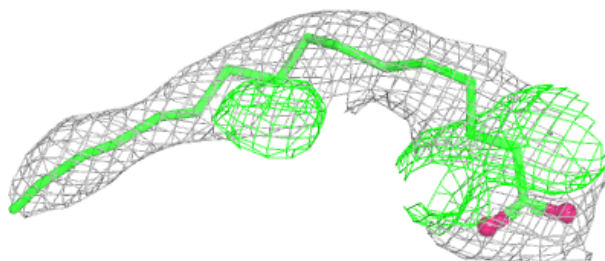
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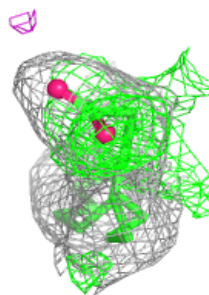
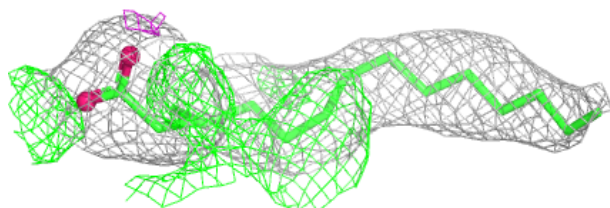
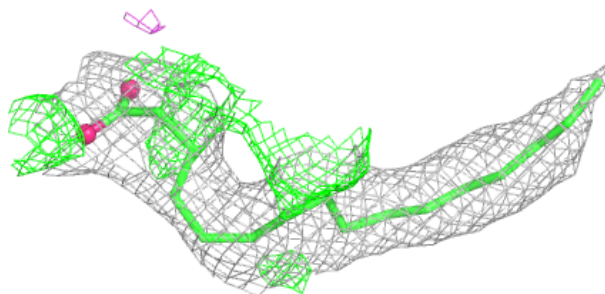


Electron density around PLM H 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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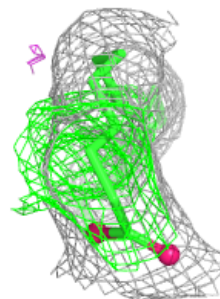
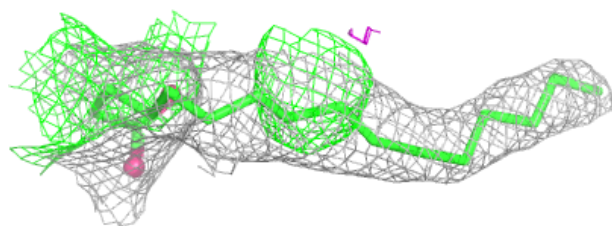
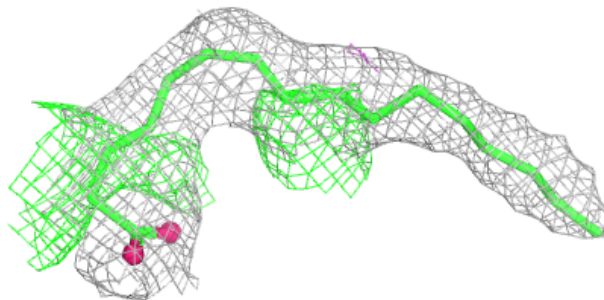
**Electron density around PLM E 502:**

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

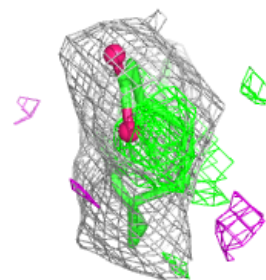
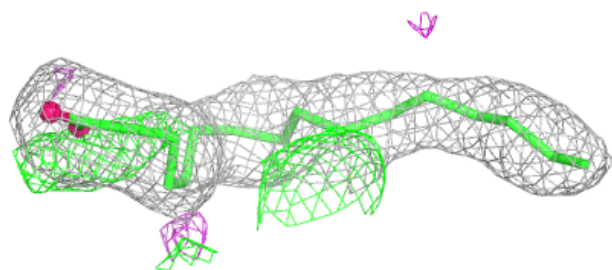
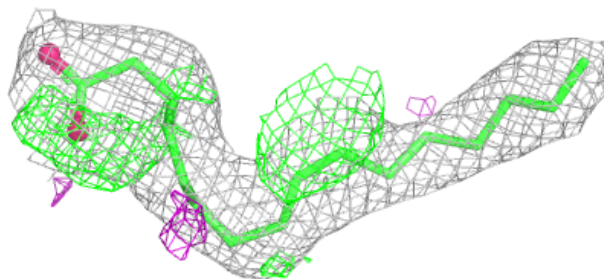


Electron density around PLM B 502:

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and green (positive)

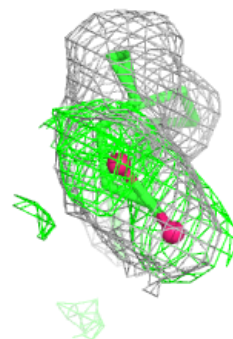
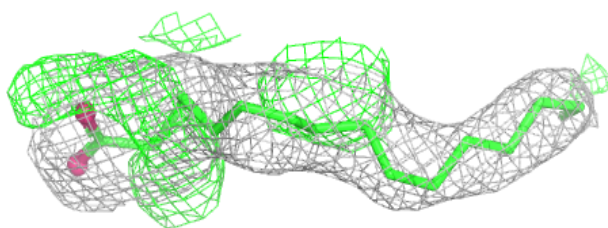
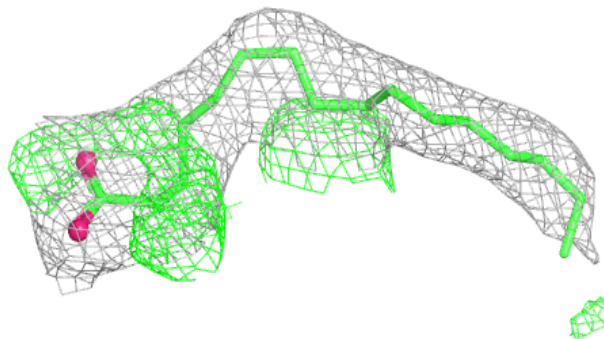
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and green (positive)



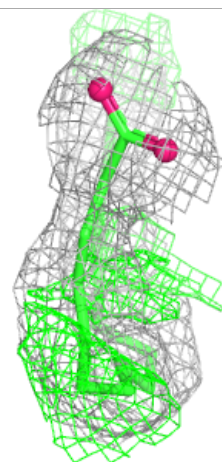
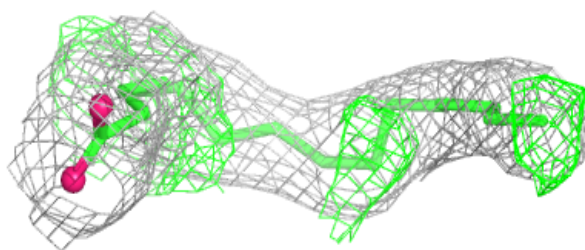
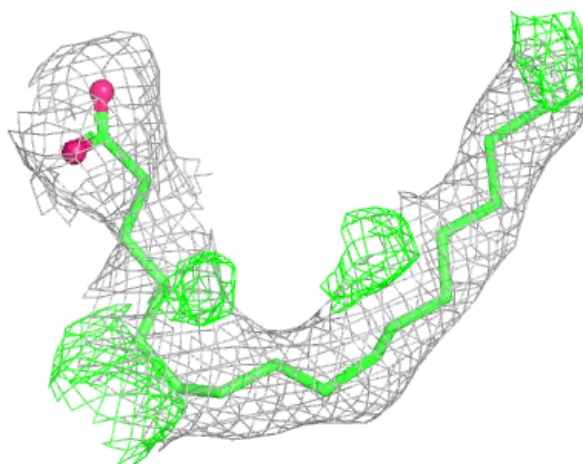
Electron density around PLM C 502:

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and green (positive)



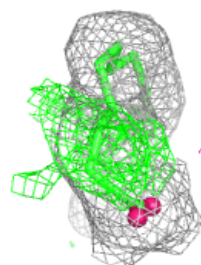
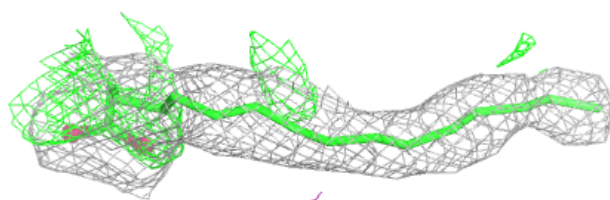
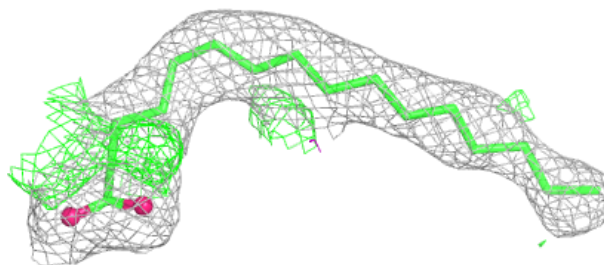
Electron density around PLM I 502:

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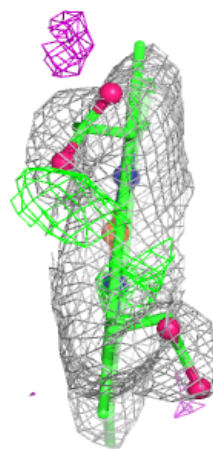
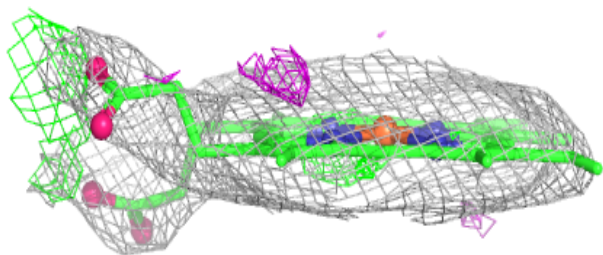
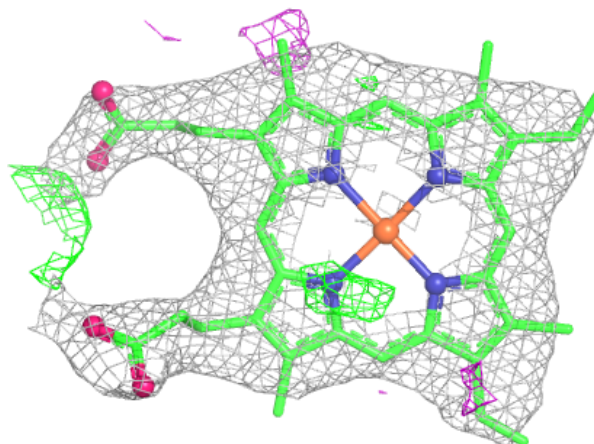
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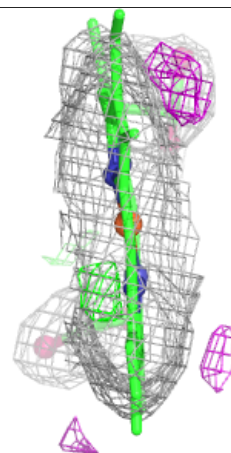
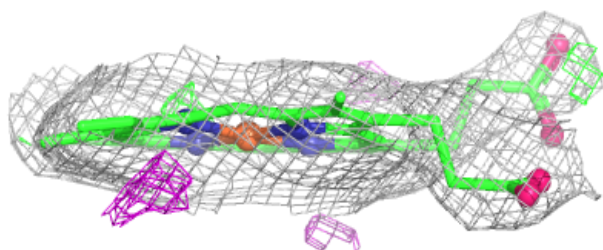
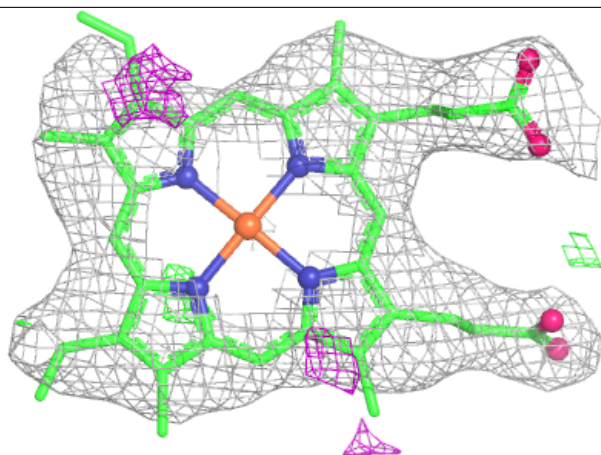
Electron density around HEM J 501:

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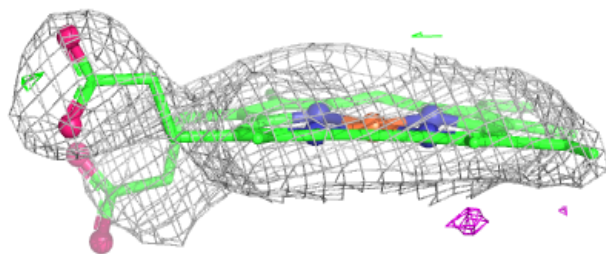
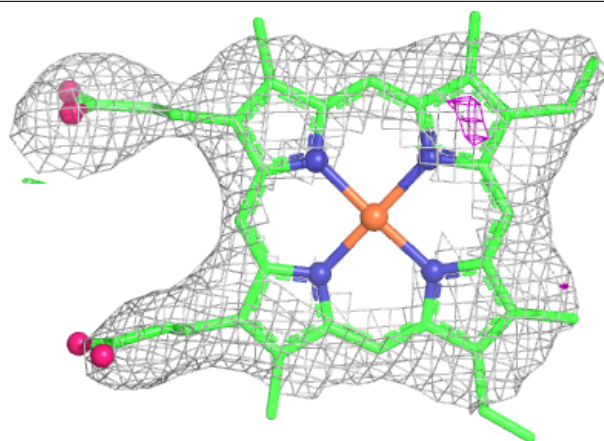
Electron density around HEM L 501:

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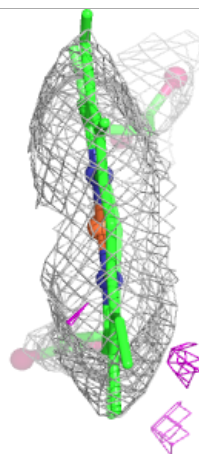
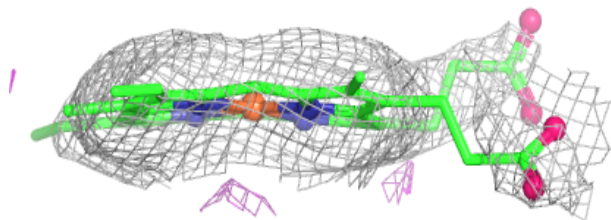
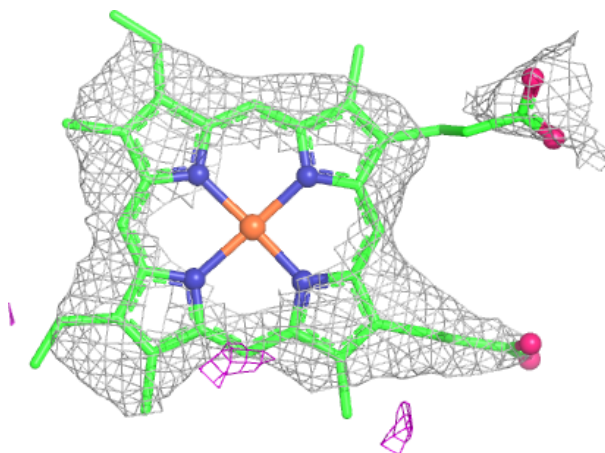
Electron density around HEM K 501:

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and green (positive)



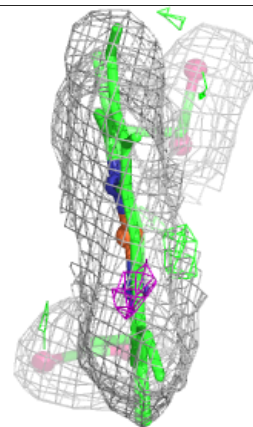
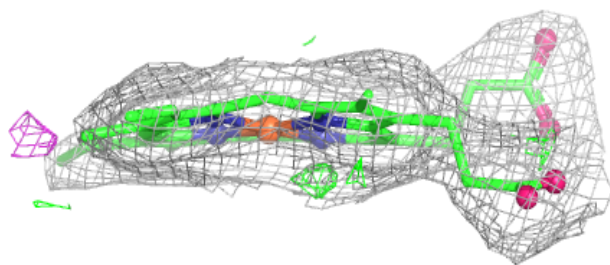
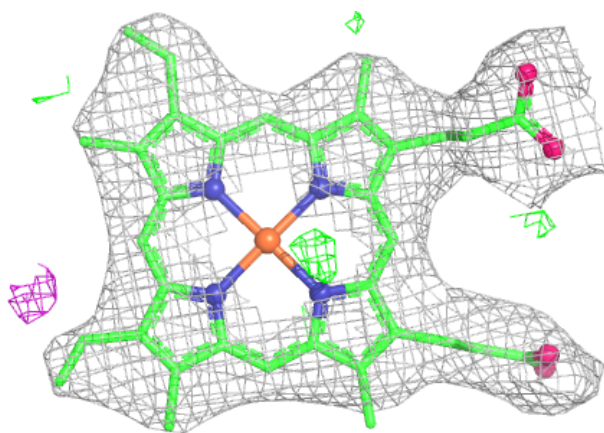
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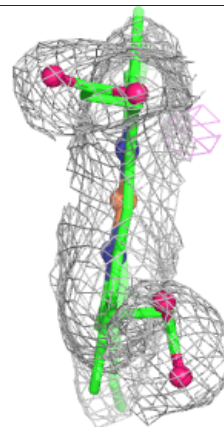
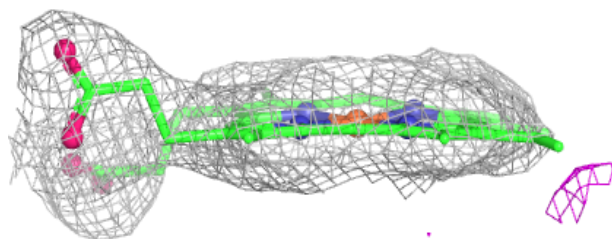
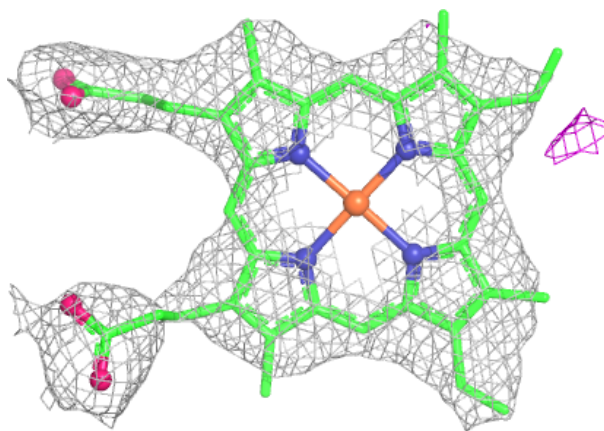
Electron density around HEM F 501:

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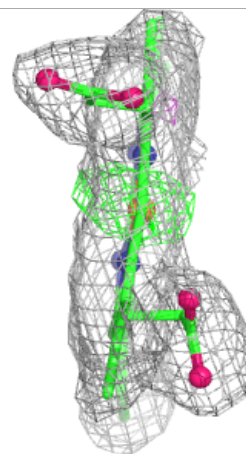
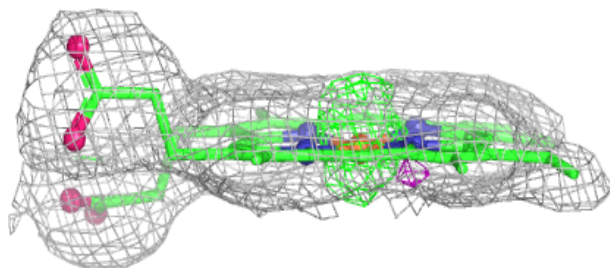
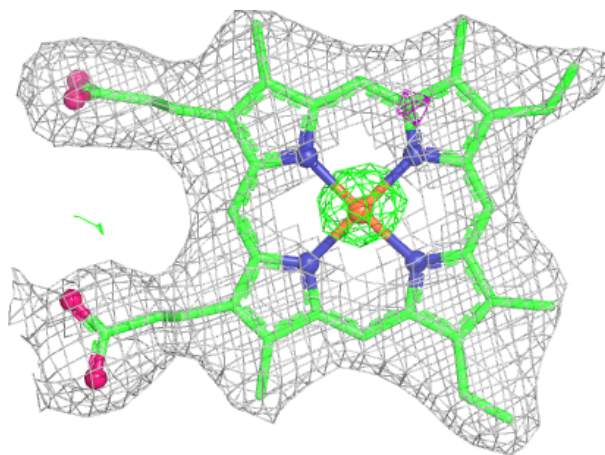
Electron density around HEM G 501:

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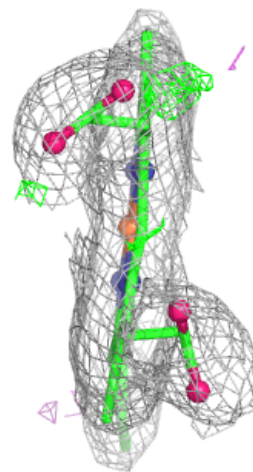
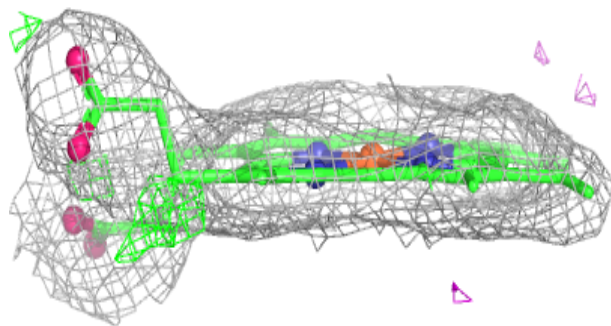
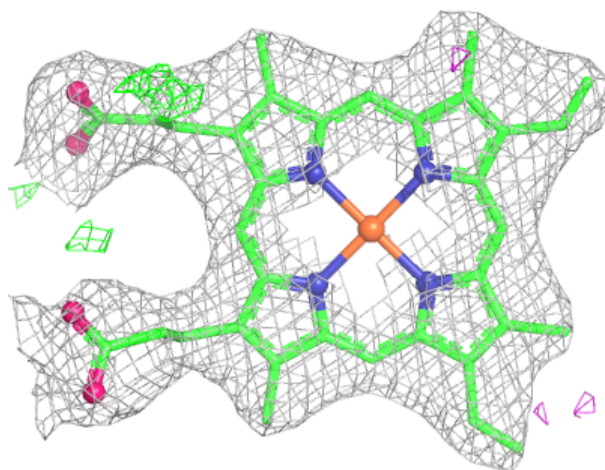
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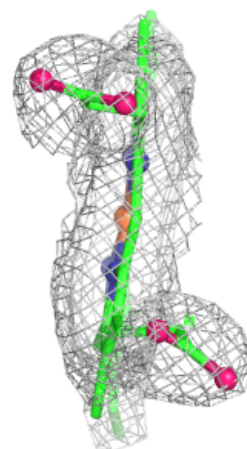
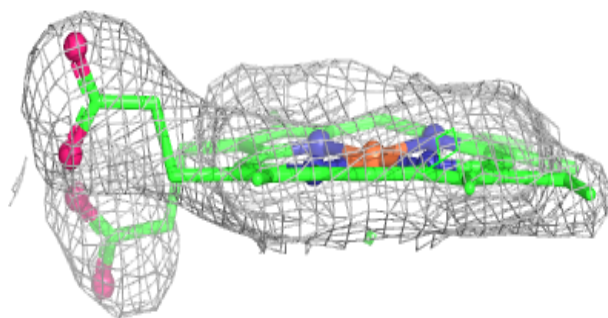
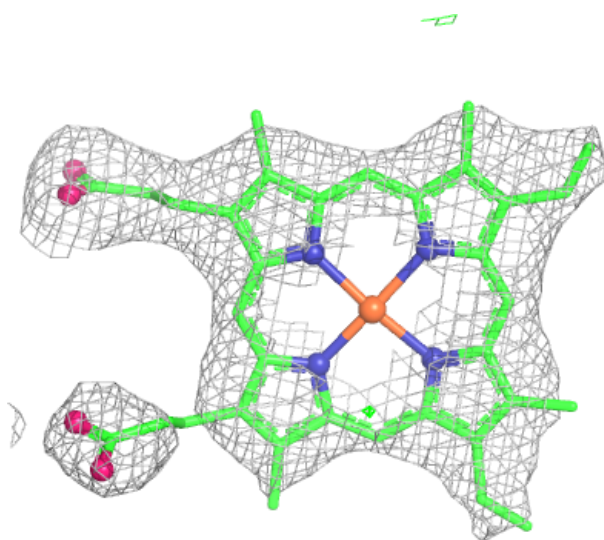
Electron density around HEM B 501:

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



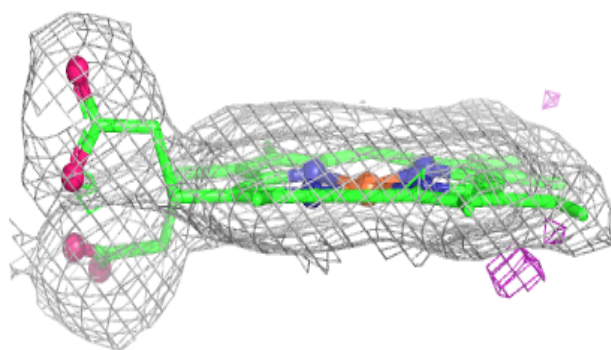
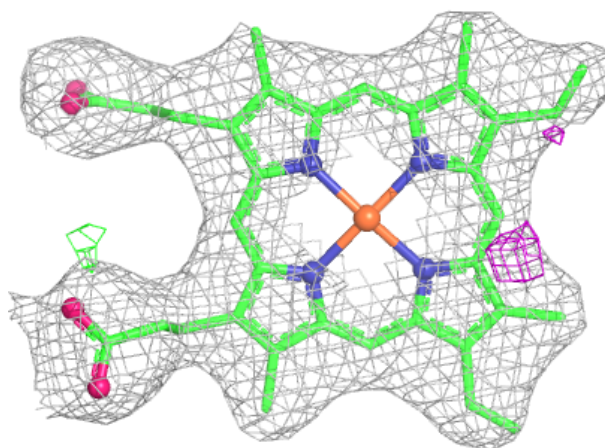
Electron density around HEM H 501:

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



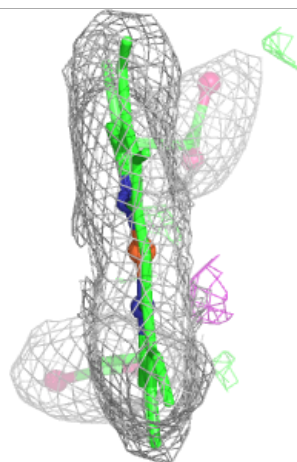
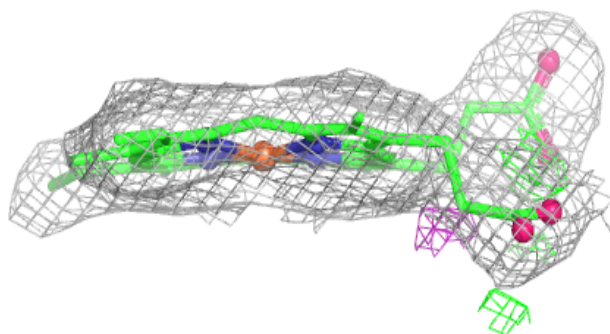
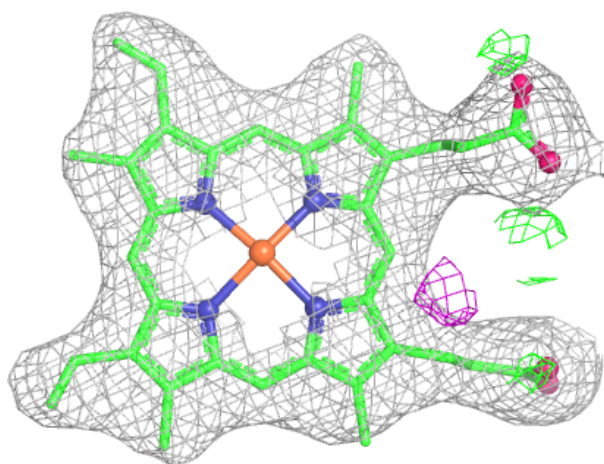
Electron density around HEM C 501:

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



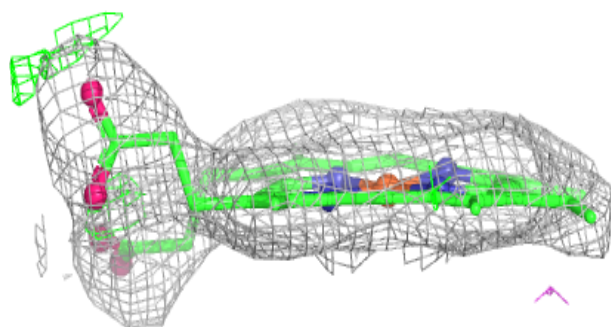
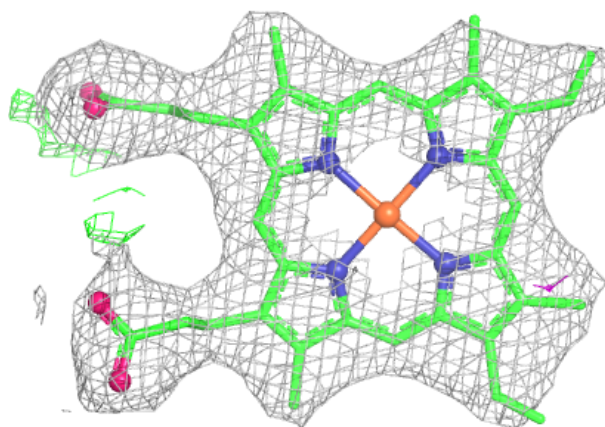
Electron density around HEM A 501:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.