



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 12:58 PM EDT

PDB ID : 3PMQ / pdb_00003pmq
Title : Crystal structure of the outer membrane decaheme cytochrome MtrF
Authors : Clarke, T.A.; Edwards, M.J.; Richardson, D.J.
Deposited on : 2010-11-17
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

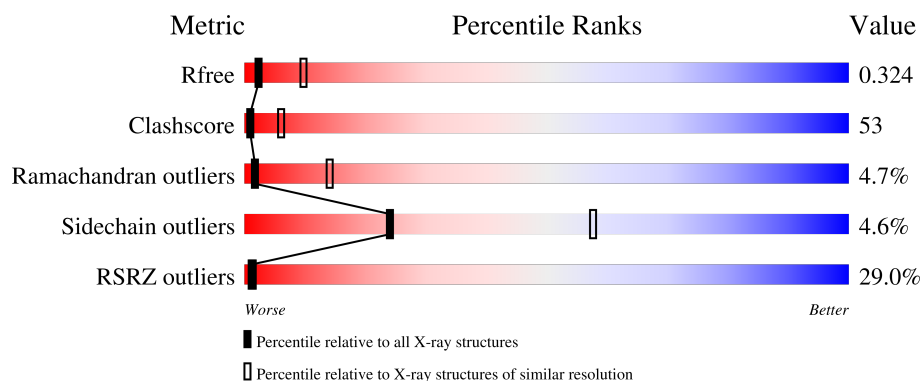
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	669	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	A	670	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	A	671	X	-	-	-
2	HEC	A	672	X	-	-	-
2	HEC	A	673	X	-	-	-
2	HEC	A	674	X	-	-	-
2	HEC	A	675	X	-	-	-
2	HEC	A	677	X	-	-	-
2	HEC	A	678	X	-	-	-
2	HEC	A	679	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4826 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 Decaheme cytochrome c MtrF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	593	Total	C	N	O	S	0	0	0
			4395	2688	791	883	33			

There are 30 discrepancies between the modelled and reference sequences:

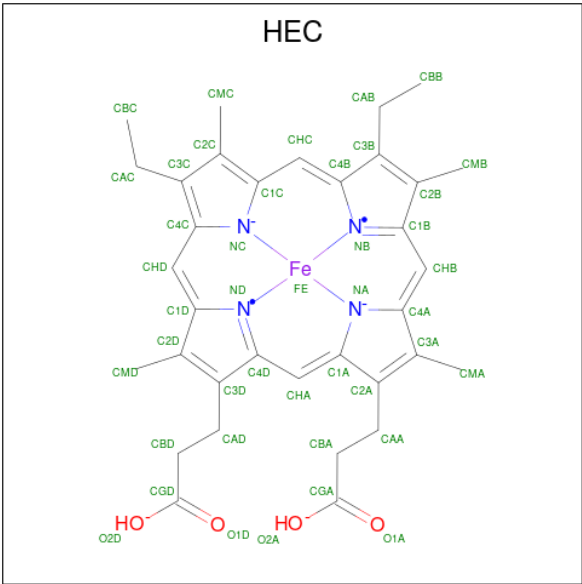
Chain	Residue	Modelled	Actual	Comment	Reference
A	640	LYS	-	expression tag	UNP Q8EG32
A	641	GLY	-	expression tag	UNP Q8EG32
A	642	GLU	-	expression tag	UNP Q8EG32
A	643	LEU	-	expression tag	UNP Q8EG32
A	644	LYS	-	expression tag	UNP Q8EG32
A	645	LEU	-	expression tag	UNP Q8EG32
A	646	GLU	-	expression tag	UNP Q8EG32
A	647	GLY	-	expression tag	UNP Q8EG32
A	648	LYS	-	expression tag	UNP Q8EG32
A	649	PRO	-	expression tag	UNP Q8EG32
A	650	ILE	-	expression tag	UNP Q8EG32
A	651	PRO	-	expression tag	UNP Q8EG32
A	652	ASN	-	expression tag	UNP Q8EG32
A	653	PRO	-	expression tag	UNP Q8EG32
A	654	LEU	-	expression tag	UNP Q8EG32
A	655	LEU	-	expression tag	UNP Q8EG32
A	656	GLY	-	expression tag	UNP Q8EG32
A	657	LEU	-	expression tag	UNP Q8EG32
A	658	ASP	-	expression tag	UNP Q8EG32
A	659	SER	-	expression tag	UNP Q8EG32
A	660	THR	-	expression tag	UNP Q8EG32
A	661	ARG	-	expression tag	UNP Q8EG32
A	662	THR	-	expression tag	UNP Q8EG32
A	663	GLY	-	expression tag	UNP Q8EG32
A	664	HIS	-	expression tag	UNP Q8EG32
A	665	HIS	-	expression tag	UNP Q8EG32
A	666	HIS	-	expression tag	UNP Q8EG32

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Chain	Residue	Modelled	Actual	Comment	Reference
A	667	HIS	-	expression tag	UNP Q8EG32
A	668	HIS	-	expression tag	UNP Q8EG32
A	669	HIS	-	expression tag	UNP Q8EG32

- Molecule 2 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



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

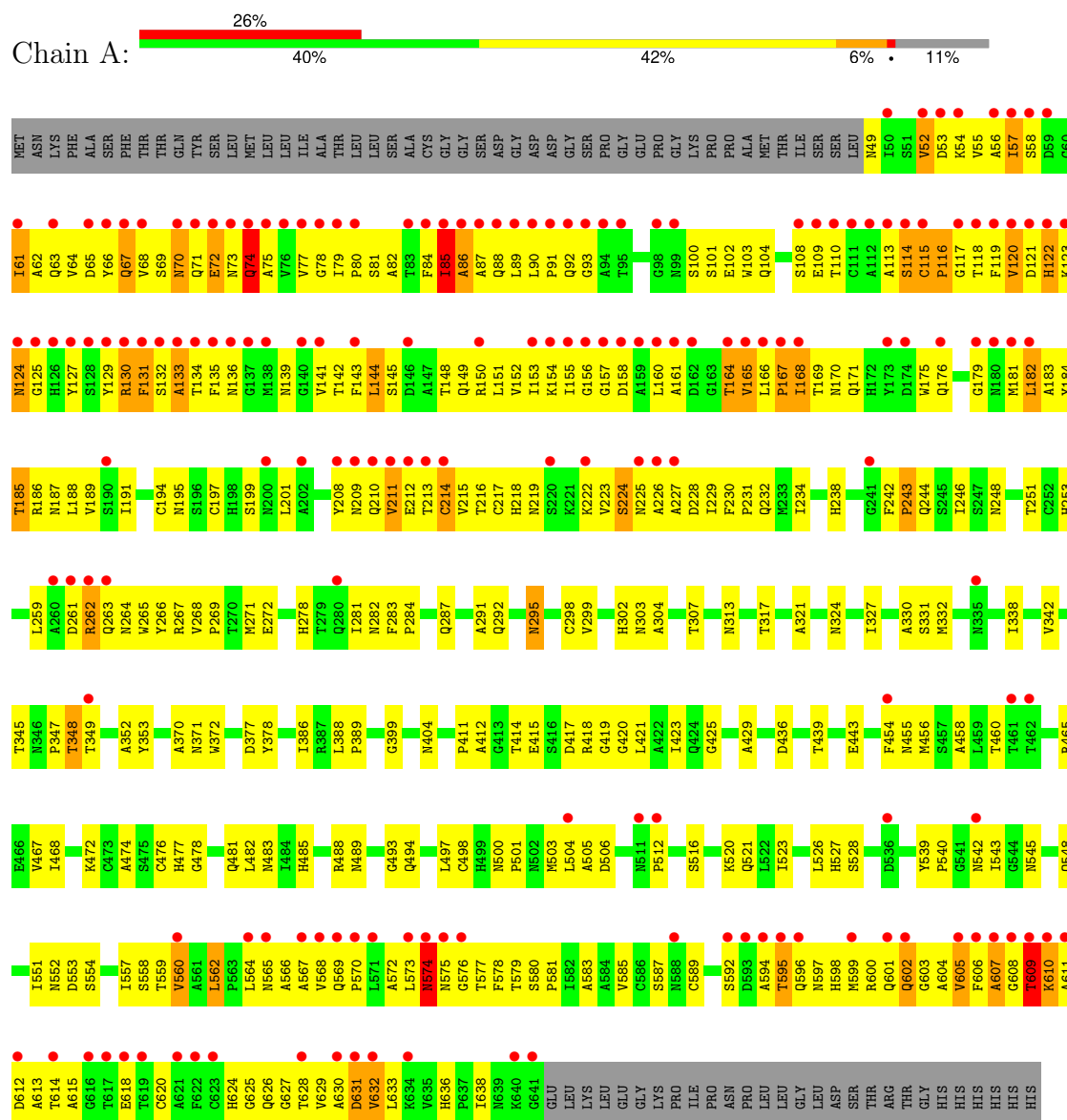
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0

3 Residue-property plots

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

• Molecule 1: Decaheme cytochrome c MtrF



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	256.64Å 256.64Å 256.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 40.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (40.00-3.20) 97.6 (40.00-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.305 , 0.321 0.304 , 0.324	Depositor DCC
R_{free} test set	2296 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	89.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 112.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	4826	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.34	0/4485	0.81	8/6111 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	SER	N-CA-C	8.34	124.69	112.94
1	A	115	CYS	N-CA-C	6.46	115.57	108.14
1	A	158	ASP	N-CA-C	5.82	118.96	109.06
1	A	69	SER	CB-CA-C	-5.67	109.04	115.79
1	A	86	ALA	N-CA-C	5.59	117.60	108.76
1	A	425	GLY	N-CA-C	5.25	119.28	110.56
1	A	189	VAL	N-CA-C	5.25	115.46	108.27
1	A	100	SER	N-CA-C	5.10	116.83	109.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4395	0	4133	477	0
2	A	430	0	300	55	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4826	0	4433	490	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 53.

All (490) 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:A:155:ILE:HG12	1:A:171:GLN:HB3	1.26	1.17
1:A:116:PRO:HB3	1:A:124:ASN:HA	1.29	1.15
1:A:133:ALA:HB1	1:A:134:THR:HB	1.15	1.15
1:A:55:VAL:HG21	1:A:61:ILE:H	1.11	1.15
1:A:527:HIS:HD1	2:A:677:HEC:HBC1	0.98	1.14
1:A:89:LEU:HD11	1:A:216:THR:HA	1.16	1.12
1:A:55:VAL:HG21	1:A:61:ILE:N	1.75	1.02
1:A:85:ILE:HG21	1:A:155:ILE:H	1.24	1.01
1:A:262:ARG:HA	1:A:263:GLN:C	1.84	1.01
1:A:632:VAL:HG22	1:A:633:LEU:HG	1.44	1.00
1:A:568:VAL:HG22	1:A:570:PRO:HD3	1.42	0.97
1:A:570:PRO:HG2	1:A:579:THR:HB	1.45	0.97
1:A:577:THR:HA	1:A:606:PHE:HB2	1.47	0.97
1:A:84:PHE:HB3	1:A:85:ILE:HB	1.45	0.96
1:A:118:THR:HG22	1:A:119:PHE:H	1.31	0.95
1:A:557:ILE:HG23	1:A:559:THR:H	1.30	0.95
1:A:527:HIS:ND1	2:A:677:HEC:HBC1	1.82	0.94
1:A:89:LEU:CD1	1:A:216:THR:HA	1.98	0.93
1:A:595:THR:C	1:A:597:ASN:HA	1.93	0.93
1:A:89:LEU:HD11	1:A:216:THR:CA	1.99	0.92
1:A:595:THR:HB	1:A:598:HIS:HB3	1.52	0.92
1:A:117:GLY:HA2	1:A:135:PHE:HD1	1.32	0.92
1:A:605:VAL:HG12	1:A:606:PHE:H	1.35	0.91
1:A:109:GLU:HG3	1:A:110:THR:H	1.37	0.90
1:A:614:THR:N	1:A:615:ALA:HA	1.84	0.90
1:A:54:LYS:HE2	1:A:179:GLY:HA2	1.55	0.89
1:A:85:ILE:HG21	1:A:155:ILE:N	1.87	0.89
1:A:117:GLY:HA3	1:A:136:ASN:OD1	1.72	0.88
1:A:139:ASN:HB2	1:A:143:PHE:HA	1.52	0.87
1:A:85:ILE:HD13	1:A:155:ILE:HB	1.56	0.87
1:A:527:HIS:HD1	2:A:677:HEC:CBC	1.86	0.87
1:A:117:GLY:HA2	1:A:135:PHE:CD1	2.11	0.85
1:A:594:ALA:HA	1:A:595:THR:O	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:TYR:HB3	1:A:67:GLN:HG3	1.57	0.84
1:A:116:PRO:CB	1:A:124:ASN:HA	2.07	0.83
1:A:527:HIS:HE1	2:A:675:HEC:NB	1.76	0.83
1:A:125:GLY:HA3	1:A:134:THR:HG22	1.59	0.83
1:A:171:GLN:NE2	1:A:209:ASN:HA	1.94	0.83
1:A:84:PHE:O	1:A:121:ASP:HB3	1.79	0.82
2:A:671:HEC:HBA1	2:A:671:HEC:HHA	1.62	0.82
1:A:559:THR:HG21	2:A:677:HEC:HMB2	1.62	0.82
1:A:91:PRO:HD2	1:A:149:GLN:O	1.78	0.81
1:A:418:ARG:HD3	1:A:460:THR:HG21	1.62	0.80
1:A:468:ILE:HD13	2:A:677:HEC:HMD2	1.62	0.80
1:A:596:GLN:N	1:A:597:ASN:HA	1.95	0.80
1:A:85:ILE:CG2	1:A:155:ILE:H	1.93	0.80
1:A:225:ASN:HB3	1:A:226:ALA:HA	1.64	0.80
1:A:246:ILE:H	1:A:246:ILE:HD12	1.46	0.79
1:A:74:GLN:HG2	1:A:75:ALA:N	1.97	0.79
1:A:543:ILE:H	1:A:543:ILE:HD12	1.48	0.78
1:A:262:ARG:HB2	1:A:264:ASN:HB2	1.66	0.78
1:A:213:THR:HG23	1:A:215:VAL:HG22	1.65	0.78
1:A:104:GLN:HB3	1:A:142:THR:HG21	1.65	0.77
1:A:55:VAL:CG2	1:A:61:ILE:H	1.95	0.77
1:A:91:PRO:HA	1:A:102:GLU:O	1.85	0.77
2:A:676:HEC:HBA1	2:A:676:HEC:HHA	1.65	0.76
1:A:85:ILE:O	1:A:85:ILE:HG23	1.86	0.76
1:A:125:GLY:HA3	1:A:134:THR:CG2	2.14	0.76
1:A:551:ILE:HG12	1:A:552:ASN:H	1.51	0.76
1:A:84:PHE:CB	1:A:85:ILE:HB	2.15	0.76
1:A:625:GLY:O	1:A:632:VAL:HB	1.86	0.75
1:A:266:TYR:HB2	1:A:307:THR:HG23	1.66	0.75
2:A:675:HEC:HBD1	2:A:675:HEC:HHA	1.68	0.75
1:A:125:GLY:CA	1:A:134:THR:HG22	2.17	0.75
1:A:133:ALA:CB	1:A:134:THR:HB	2.08	0.74
1:A:84:PHE:HB3	1:A:85:ILE:CB	2.17	0.74
1:A:208:TYR:HB3	1:A:209:ASN:HB2	1.67	0.74
1:A:89:LEU:HD12	1:A:151:LEU:HD13	1.69	0.74
1:A:85:ILE:HD12	1:A:119:PHE:CE2	2.23	0.74
1:A:570:PRO:CG	1:A:579:THR:HB	2.16	0.74
1:A:52:VAL:H	1:A:64:VAL:HG21	1.52	0.73
1:A:568:VAL:HG21	1:A:581:PRO:HA	1.71	0.72
1:A:114:SER:HB3	1:A:122:HIS:CB	2.18	0.72
1:A:214:CYS:HB3	2:A:671:HEC:CHC	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:THR:N	1:A:615:ALA:CA	2.53	0.72
1:A:133:ALA:HB1	1:A:134:THR:CB	2.09	0.72
1:A:225:ASN:HB3	1:A:226:ALA:CA	2.19	0.72
1:A:74:GLN:C	1:A:74:GLN:HE21	1.98	0.71
1:A:210:GLN:HG2	1:A:211:VAL:HG23	1.73	0.71
1:A:345:THR:HG22	1:A:352:ALA:HA	1.73	0.71
1:A:455:ASN:HB3	1:A:458:ALA:O	1.91	0.71
1:A:154:LYS:O	1:A:171:GLN:HA	1.91	0.70
1:A:632:VAL:HG13	1:A:633:LEU:H	1.55	0.70
1:A:592:SER:C	1:A:594:ALA:H	2.00	0.70
2:A:671:HEC:HH A	2:A:671:HEC:CBA	2.21	0.70
1:A:92:GLN:HE22	1:A:104:GLN:NE2	1.90	0.70
1:A:223:VAL:HG21	1:A:228:ASP:HB2	1.74	0.70
1:A:269:PRO:HD2	1:A:299:VAL:HG22	1.73	0.70
1:A:67:GLN:HG3	1:A:130:ARG:HH11	1.57	0.69
1:A:153:ILE:C	1:A:154:LYS:HG3	2.17	0.69
1:A:70:ASN:ND2	1:A:167:PRO:HB3	2.08	0.69
1:A:225:ASN:CG	1:A:228:ASP:H	2.00	0.69
1:A:191:ILE:HD11	1:A:201:LEU:HB3	1.73	0.69
1:A:217:CYS:O	1:A:222:LYS:HB3	1.92	0.69
1:A:150:ARG:HE	1:A:176:GLN:HE21	1.39	0.69
1:A:224:SER:N	1:A:225:ASN:HA	2.07	0.69
1:A:602:GLN:HB3	1:A:618:GLU:CG	2.22	0.69
1:A:171:GLN:HE21	1:A:209:ASN:HA	1.55	0.68
1:A:472:LYS:HB3	1:A:548:GLN:O	1.93	0.68
1:A:185:THR:HG22	1:A:186:ARG:H	1.58	0.68
1:A:624:HIS:HA	1:A:631:ASP:HB3	1.76	0.68
1:A:85:ILE:HD11	1:A:155:ILE:HD12	1.75	0.68
1:A:415:GLU:O	1:A:456:MET:HE2	1.93	0.68
1:A:155:ILE:HG12	1:A:171:GLN:CB	2.17	0.67
1:A:602:GLN:HB3	1:A:618:GLU:HG2	1.76	0.67
1:A:109:GLU:CG	1:A:110:THR:H	2.08	0.67
1:A:483:ASN:OD1	1:A:489:ASN:HB3	1.95	0.67
1:A:61:ILE:HA	1:A:134:THR:OG1	1.93	0.67
1:A:370:ALA:HB2	1:A:421:LEU:HD23	1.75	0.67
1:A:504:LEU:HG	1:A:572:ALA:HB1	1.76	0.67
1:A:559:THR:HG21	2:A:677:HEC:CMB	2.24	0.67
1:A:636:HIS:CE1	2:A:678:HEC:NB	2.63	0.67
1:A:52:VAL:H	1:A:64:VAL:CG2	2.06	0.67
1:A:109:GLU:H	1:A:118:THR:HG22	1.59	0.67
1:A:81:SER:HB2	1:A:82:ALA:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLN:O	1:A:72:GLU:HB3	1.96	0.66
1:A:66:TYR:HB3	1:A:67:GLN:CG	2.25	0.65
1:A:160:LEU:HD23	1:A:164:THR:HB	1.77	0.65
1:A:467:VAL:HG11	2:A:677:HEC:CGD	2.25	0.65
1:A:52:VAL:HG22	1:A:53:ASP:HB2	1.79	0.65
1:A:601:GLN:C	1:A:618:GLU:HG2	2.20	0.65
1:A:155:ILE:HD13	1:A:171:GLN:NE2	2.12	0.64
1:A:70:ASN:ND2	1:A:71:GLN:HG2	2.13	0.64
1:A:119:PHE:O	1:A:120:VAL:HB	1.97	0.64
1:A:197:CYS:O	1:A:540:PRO:HB2	1.97	0.64
1:A:595:THR:CB	1:A:598:HIS:HB3	2.26	0.64
1:A:115:CYS:HB2	1:A:116:PRO:HD2	1.78	0.64
1:A:594:ALA:HA	1:A:595:THR:C	2.20	0.64
1:A:125:GLY:N	1:A:134:THR:HG22	2.13	0.64
1:A:225:ASN:HB3	1:A:226:ALA:CB	2.29	0.63
1:A:195:ASN:O	1:A:199:SER:N	2.28	0.63
1:A:505:ALA:HB2	1:A:516:SER:HB2	1.79	0.63
1:A:151:LEU:HG	1:A:175:TRP:HE1	1.63	0.63
1:A:629:VAL:HG22	1:A:630:ALA:H	1.64	0.63
1:A:594:ALA:HB1	1:A:595:THR:HA	1.80	0.63
2:A:676:HEC:HBA1	2:A:676:HEC:CHA	2.29	0.63
1:A:139:ASN:CB	1:A:143:PHE:HA	2.28	0.62
1:A:560:VAL:HG22	1:A:562:LEU:H	1.64	0.62
1:A:608:GLY:C	1:A:610:LYS:H	2.06	0.62
1:A:73:ASN:O	1:A:74:GLN:HB3	2.00	0.62
1:A:613:ALA:C	1:A:615:ALA:HA	2.25	0.62
1:A:527:HIS:HE1	2:A:675:HEC:C4B	2.13	0.62
1:A:225:ASN:CB	1:A:226:ALA:HA	2.28	0.62
1:A:568:VAL:CG2	1:A:570:PRO:HD3	2.23	0.61
1:A:605:VAL:HG12	1:A:606:PHE:N	2.11	0.61
1:A:327:ILE:HG13	1:A:423:ILE:HD11	1.82	0.61
1:A:597:ASN:C	1:A:599:MET:N	2.56	0.61
1:A:596:GLN:N	1:A:597:ASN:CA	2.62	0.61
1:A:122:HIS:C	1:A:124:ASN:H	2.09	0.60
1:A:166:LEU:HB2	1:A:167:PRO:HA	1.83	0.60
1:A:592:SER:C	1:A:594:ALA:N	2.59	0.60
1:A:109:GLU:HG3	1:A:110:THR:N	2.12	0.60
1:A:85:ILE:HD12	1:A:119:PHE:CZ	2.37	0.60
1:A:211:VAL:HG12	1:A:212:GLU:N	2.16	0.60
2:A:678:HEC:HBD2	2:A:678:HEC:HHA	1.81	0.60
1:A:87:ALA:HB3	1:A:153:ILE:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:ARG:HE	1:A:600:ARG:HA	1.66	0.60
1:A:109:GLU:HG3	1:A:110:THR:HG22	1.84	0.60
1:A:278:HIS:ND1	2:A:674:HEC:HBA1	2.17	0.60
1:A:52:VAL:CG2	1:A:53:ASP:HB2	2.31	0.60
1:A:332:MET:HE2	1:A:338:ILE:HG12	1.83	0.59
1:A:67:GLN:OE1	1:A:77:VAL:HA	2.02	0.59
1:A:85:ILE:HD12	1:A:119:PHE:HE2	1.67	0.59
1:A:632:VAL:HG22	1:A:633:LEU:N	2.17	0.59
1:A:145:SER:O	1:A:148:THR:HG22	2.02	0.59
1:A:542:ASN:HB2	1:A:545:ASN:HB2	1.85	0.59
1:A:577:THR:CA	1:A:606:PHE:HB2	2.29	0.59
1:A:266:TYR:HD1	1:A:304:ALA:HB1	1.68	0.59
1:A:191:ILE:CG2	1:A:211:VAL:HA	2.33	0.59
1:A:181:MET:O	1:A:182:LEU:HB2	2.03	0.58
1:A:262:ARG:CB	1:A:264:ASN:HB2	2.32	0.58
1:A:88:GLN:NE2	1:A:135:PHE:CD2	2.72	0.58
1:A:225:ASN:HB3	1:A:226:ALA:HB2	1.85	0.58
1:A:271:MET:H	1:A:295:ASN:HD22	1.52	0.58
1:A:54:LYS:HG3	1:A:54:LYS:O	2.04	0.58
1:A:564:LEU:HD12	1:A:565:ASN:HB2	1.85	0.58
1:A:626:GLN:HA	1:A:632:VAL:CG2	2.34	0.58
1:A:70:ASN:HD22	1:A:166:LEU:HD13	1.69	0.58
1:A:125:GLY:H	1:A:134:THR:HG22	1.69	0.58
1:A:155:ILE:HA	1:A:170:ASN:O	2.04	0.57
1:A:88:GLN:HA	1:A:151:LEU:O	2.04	0.57
1:A:353:TYR:O	1:A:399:GLY:HA2	2.04	0.57
1:A:568:VAL:CG2	1:A:581:PRO:HA	2.34	0.57
1:A:114:SER:HB3	1:A:122:HIS:HB3	1.85	0.57
1:A:504:LEU:HG	1:A:572:ALA:CB	2.33	0.57
1:A:539:TYR:CZ	2:A:675:HEC:HBC2	2.38	0.57
1:A:85:ILE:HG21	1:A:155:ILE:O	2.04	0.57
1:A:269:PRO:HB2	1:A:298:CYS:HB3	1.87	0.57
1:A:92:GLN:HE22	1:A:104:GLN:HE22	1.52	0.57
1:A:600:ARG:HG3	2:A:679:HEC:HMC2	1.85	0.57
1:A:624:HIS:HD1	1:A:631:ASP:CG	2.12	0.57
1:A:54:LYS:HE2	1:A:179:GLY:CA	2.32	0.56
1:A:151:LEU:HG	1:A:175:TRP:NE1	2.20	0.56
1:A:85:ILE:CD1	1:A:155:ILE:HB	2.32	0.56
1:A:191:ILE:HG21	1:A:211:VAL:HA	1.86	0.56
1:A:332:MET:HE3	1:A:454:PHE:CE2	2.40	0.56
1:A:500:ASN:HB2	1:A:501:PRO:HD2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ILE:HG12	1:A:155:ILE:H	1.70	0.56
1:A:266:TYR:CD1	1:A:304:ALA:HB1	2.41	0.56
1:A:370:ALA:HA	1:A:420:GLY:O	2.06	0.56
1:A:419:GLY:CA	1:A:454:PHE:HB3	2.35	0.56
2:A:677:HEC:HBB2	2:A:678:HEC:HBC2	1.87	0.56
1:A:625:GLY:N	1:A:629:VAL:HG11	2.21	0.56
1:A:564:LEU:HD12	1:A:565:ASN:N	2.20	0.56
1:A:78:GLY:C	1:A:79:ILE:HD12	2.31	0.55
1:A:171:GLN:NE2	1:A:208:TYR:HA	2.21	0.55
1:A:225:ASN:CB	1:A:226:ALA:CA	2.84	0.55
1:A:526:LEU:HD12	1:A:527:HIS:CD2	2.40	0.55
1:A:65:ASP:O	1:A:66:TYR:CG	2.58	0.55
1:A:371:ASN:ND2	1:A:378:TYR:HB3	2.21	0.55
1:A:474:ALA:HA	1:A:478:GLY:H	1.71	0.55
1:A:261:ASP:O	1:A:262:ARG:CB	2.53	0.55
1:A:66:TYR:HB3	1:A:67:GLN:HA	1.87	0.55
1:A:225:ASN:H	1:A:226:ALA:HB2	1.71	0.55
1:A:223:VAL:HG23	2:A:671:HEC:CGD	2.37	0.55
1:A:580:SER:HB2	1:A:602:GLN:O	2.06	0.55
1:A:600:ARG:HA	1:A:600:ARG:NE	2.22	0.55
1:A:56:ALA:O	1:A:57:ILE:HB	2.07	0.55
1:A:214:CYS:HB3	2:A:671:HEC:HHC	1.89	0.55
1:A:626:GLN:HA	1:A:632:VAL:HG21	1.89	0.55
2:A:671:HEC:HHA	2:A:671:HEC:CGA	2.37	0.55
1:A:170:ASN:HA	1:A:210:GLN:NE2	2.22	0.54
1:A:632:VAL:CG2	1:A:633:LEU:HG	2.27	0.54
1:A:225:ASN:ND2	1:A:227:ALA:HA	2.23	0.54
1:A:120:VAL:HG22	1:A:122:HIS:CD2	2.42	0.54
1:A:597:ASN:O	1:A:598:HIS:C	2.50	0.54
1:A:572:ALA:O	1:A:573:LEU:C	2.49	0.54
1:A:595:THR:HB	1:A:598:HIS:CB	2.33	0.54
1:A:234:ILE:HD11	2:A:672:HEC:C1D	2.38	0.54
1:A:52:VAL:N	1:A:64:VAL:HG21	2.22	0.54
1:A:121:ASP:CG	1:A:121:ASP:O	2.48	0.54
1:A:597:ASN:O	1:A:599:MET:N	2.41	0.53
1:A:101:SER:HB2	1:A:186:ARG:HH11	1.72	0.53
1:A:603:GLY:O	1:A:604:ALA:HB2	2.09	0.53
1:A:55:VAL:HG11	1:A:61:ILE:HB	1.91	0.53
1:A:66:TYR:CB	1:A:67:GLN:HA	2.38	0.53
1:A:223:VAL:HG23	2:A:671:HEC:HBD2	1.90	0.53
1:A:155:ILE:CG1	1:A:171:GLN:HB3	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ILE:HG23	1:A:57:ILE:O	2.09	0.53
1:A:64:VAL:HA	1:A:131:PHE:HA	1.91	0.53
1:A:213:THR:CG2	1:A:215:VAL:HG22	2.37	0.53
1:A:232:GLN:CG	1:A:272:GLU:HB3	2.39	0.53
1:A:121:ASP:C	1:A:122:HIS:CG	2.87	0.52
1:A:225:ASN:HD21	1:A:229:ILE:H	1.56	0.52
1:A:214:CYS:C	1:A:216:THR:H	2.17	0.52
1:A:574:ASN:C	1:A:574:ASN:OD1	2.52	0.52
1:A:86:ALA:HB1	1:A:135:PHE:CZ	2.45	0.52
1:A:185:THR:HG22	1:A:186:ARG:N	2.24	0.52
1:A:213:THR:OG1	1:A:214:CYS:N	2.42	0.52
1:A:281:ILE:CD1	2:A:674:HEC:HBA2	2.40	0.52
1:A:573:LEU:O	1:A:574:ASN:HB3	2.09	0.52
1:A:609:THR:HA	1:A:612:ASP:HB2	1.92	0.52
1:A:629:VAL:HG13	1:A:630:ALA:N	2.25	0.52
1:A:230:PHE:HB3	1:A:231:PRO:HD3	1.92	0.52
1:A:520:LYS:HD3	1:A:585:VAL:HG12	1.92	0.51
1:A:568:VAL:HG22	1:A:570:PRO:CD	2.27	0.51
1:A:85:ILE:CG2	1:A:85:ILE:O	2.57	0.51
1:A:338:ILE:HG23	1:A:454:PHE:CE1	2.45	0.51
1:A:131:PHE:N	1:A:131:PHE:CD2	2.79	0.51
1:A:332:MET:HE2	1:A:338:ILE:CG1	2.40	0.51
1:A:580:SER:OG	1:A:602:GLN:HG3	2.10	0.51
1:A:66:TYR:HB3	1:A:67:GLN:CA	2.41	0.51
1:A:72:GLU:HG3	1:A:74:GLN:H	1.75	0.51
1:A:302:HIS:CD2	2:A:674:HEC:NB	2.78	0.51
1:A:55:VAL:O	1:A:55:VAL:HG23	2.10	0.51
1:A:70:ASN:HA	1:A:170:ASN:ND2	2.26	0.51
1:A:171:GLN:HG3	1:A:209:ASN:OD1	2.10	0.51
1:A:84:PHE:C	1:A:121:ASP:HB3	2.35	0.51
1:A:149:GLN:HG2	1:A:184:TYR:O	2.12	0.50
1:A:627:GLY:O	1:A:628:THR:C	2.54	0.50
1:A:629:VAL:HG13	1:A:631:ASP:H	1.77	0.50
1:A:103:TRP:HB2	1:A:219:ASN:HD21	1.76	0.50
1:A:109:GLU:O	1:A:119:PHE:HB3	2.12	0.50
1:A:150:ARG:HE	1:A:176:GLN:NE2	2.07	0.50
1:A:234:ILE:HD11	2:A:672:HEC:CHD	2.41	0.50
1:A:208:TYR:HB3	1:A:209:ASN:CB	2.38	0.50
1:A:248:ASN:O	1:A:251:THR:HG22	2.12	0.50
1:A:223:VAL:HG22	1:A:224:SER:H	1.76	0.50
1:A:263:GLN:NE2	1:A:267:ARG:CZ	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASP:O	1:A:122:HIS:CG	2.65	0.50
1:A:212:GLU:HG3	1:A:213:THR:HB	1.92	0.50
1:A:602:GLN:HB3	1:A:618:GLU:CD	2.37	0.50
1:A:608:GLY:C	1:A:610:LYS:N	2.69	0.50
1:A:118:THR:HG22	1:A:119:PHE:N	2.11	0.50
1:A:223:VAL:HG23	2:A:671:HEC:CBD	2.42	0.50
1:A:253:HIS:HD1	1:A:262:ARG:HD2	1.76	0.50
1:A:283:PHE:O	1:A:291:ALA:HA	2.11	0.50
1:A:85:ILE:CD1	1:A:119:PHE:CE2	2.94	0.49
1:A:573:LEU:O	1:A:574:ASN:CB	2.59	0.49
1:A:625:GLY:H	1:A:629:VAL:HG11	1.73	0.49
1:A:151:LEU:C	1:A:151:LEU:HD23	2.37	0.49
1:A:263:GLN:NE2	1:A:266:TYR:OH	2.45	0.49
1:A:485:HIS:CB	1:A:488:ARG:HH21	2.25	0.49
1:A:85:ILE:HG12	1:A:155:ILE:N	2.27	0.49
1:A:101:SER:HB2	1:A:186:ARG:HD2	1.95	0.49
1:A:182:LEU:HD11	1:A:185:THR:OG1	2.13	0.49
1:A:467:VAL:HG11	2:A:677:HEC:CBD	2.43	0.49
1:A:71:GLN:O	1:A:72:GLU:CB	2.59	0.49
1:A:84:PHE:CD1	1:A:119:PHE:CZ	3.00	0.49
1:A:125:GLY:HA3	1:A:134:THR:HG21	1.94	0.49
1:A:85:ILE:CD1	1:A:119:PHE:HE2	2.24	0.48
1:A:114:SER:HB3	1:A:122:HIS:HB2	1.93	0.48
1:A:238:HIS:CD2	2:A:672:HEC:HBC1	2.47	0.48
1:A:321:ALA:O	1:A:348:THR:HG22	2.12	0.48
1:A:262:ARG:CA	1:A:263:GLN:C	2.71	0.48
1:A:332:MET:HB2	1:A:454:PHE:CZ	2.49	0.48
1:A:66:TYR:HB2	1:A:130:ARG:HD2	1.95	0.48
1:A:103:TRP:HB2	1:A:219:ASN:ND2	2.28	0.48
1:A:232:GLN:HG3	1:A:272:GLU:HB3	1.94	0.48
1:A:330:ALA:O	1:A:458:ALA:HA	2.13	0.48
1:A:338:ILE:HG23	1:A:454:PHE:HE1	1.79	0.48
1:A:569:GLN:HG3	1:A:578:PHE:HE1	1.79	0.48
1:A:213:THR:OG1	1:A:215:VAL:HG13	2.13	0.48
1:A:73:ASN:O	1:A:74:GLN:CB	2.62	0.48
1:A:467:VAL:HG11	2:A:677:HEC:HBD1	1.95	0.48
1:A:216:THR:OG1	1:A:217:CYS:N	2.46	0.48
1:A:238:HIS:HD2	1:A:242:PHE:HE1	1.62	0.48
1:A:244:GLN:HG2	1:A:477:HIS:O	2.13	0.48
1:A:253:HIS:ND1	1:A:262:ARG:HD2	2.28	0.48
1:A:494:GLN:HA	1:A:497:LEU:HD22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:LEU:HA	1:A:572:ALA:HB3	1.96	0.48
1:A:562:LEU:N	1:A:562:LEU:HD23	2.28	0.48
1:A:70:ASN:HA	1:A:170:ASN:HD22	1.78	0.48
1:A:74:GLN:CG	1:A:75:ALA:N	2.72	0.48
1:A:149:GLN:HE22	1:A:183:ALA:HB3	1.78	0.48
1:A:332:MET:HB2	1:A:454:PHE:CE2	2.49	0.48
1:A:564:LEU:HD12	1:A:565:ASN:CB	2.44	0.48
1:A:598:HIS:CG	1:A:598:HIS:O	2.67	0.47
1:A:80:PRO:HD3	1:A:129:TYR:O	2.14	0.47
2:A:672:HEC:HMD1	2:A:672:HEC:HBD1	1.95	0.47
1:A:109:GLU:H	1:A:118:THR:CG2	2.26	0.47
1:A:264:ASN:HA	1:A:267:ARG:HB2	1.96	0.47
1:A:388:LEU:N	1:A:389:PRO:HD2	2.29	0.47
1:A:494:GLN:O	1:A:497:LEU:HB2	2.14	0.47
1:A:577:THR:O	1:A:578:PHE:CD2	2.67	0.47
1:A:127:TYR:HB2	1:A:132:SER:CB	2.44	0.47
1:A:170:ASN:HA	1:A:210:GLN:HE21	1.78	0.47
1:A:242:PHE:CZ	2:A:670:HEC:HBC2	2.48	0.47
1:A:429:ALA:O	1:A:443:GLU:HG2	2.15	0.47
1:A:327:ILE:HD13	1:A:421:LEU:HD13	1.96	0.47
1:A:120:VAL:HG13	1:A:121:ASP:N	2.29	0.47
1:A:139:ASN:HB3	1:A:144:LEU:H	1.78	0.47
1:A:160:LEU:HG	1:A:161:ALA:H	1.79	0.47
1:A:283:PHE:HB2	1:A:284:PRO:HD3	1.96	0.47
1:A:540:PRO:HG3	2:A:670:HEC:C2D	2.45	0.47
1:A:607:ALA:CB	1:A:611:ALA:HB3	2.45	0.47
1:A:70:ASN:HB2	1:A:167:PRO:HG3	1.97	0.47
1:A:116:PRO:CA	1:A:124:ASN:HA	2.44	0.47
1:A:55:VAL:HG11	1:A:61:ILE:O	2.16	0.46
1:A:506:ASP:HA	1:A:573:LEU:HD13	1.96	0.46
1:A:568:VAL:HG13	1:A:568:VAL:O	2.14	0.46
1:A:580:SER:HB3	1:A:583:ALA:HB3	1.97	0.46
1:A:613:ALA:HA	1:A:614:THR:HA	1.43	0.46
1:A:61:ILE:O	1:A:62:ALA:C	2.57	0.46
1:A:103:TRP:CD1	1:A:215:VAL:HB	2.51	0.46
1:A:153:ILE:O	1:A:154:LYS:HG3	2.14	0.46
1:A:636:HIS:CE1	2:A:678:HEC:C1B	2.99	0.46
1:A:246:ILE:H	1:A:246:ILE:CD1	2.21	0.46
1:A:477:HIS:CE1	1:A:482:LEU:HD22	2.50	0.46
1:A:64:VAL:HG12	1:A:131:PHE:CD1	2.51	0.46
1:A:93:GLY:O	1:A:101:SER:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:CG	1:A:175:TRP:HE1	2.29	0.46
1:A:412:ALA:C	1:A:414:THR:H	2.24	0.46
1:A:465:ARG:HD3	1:A:564:LEU:HD11	1.97	0.46
2:A:677:HEC:HBB3	2:A:677:HEC:HMB3	1.97	0.46
1:A:636:HIS:HE1	2:A:678:HEC:C1B	2.29	0.46
1:A:212:GLU:HG3	1:A:213:THR:CG2	2.46	0.45
1:A:262:ARG:HA	1:A:264:ASN:N	2.29	0.45
1:A:67:GLN:CG	1:A:130:ARG:HH11	2.27	0.45
1:A:63:GLN:O	1:A:63:GLN:HG2	2.14	0.45
1:A:208:TYR:CZ	2:A:671:HEC:HBC3	2.52	0.45
1:A:500:ASN:HB2	1:A:501:PRO:CD	2.46	0.45
2:A:679:HEC:CMA	2:A:679:HEC:HBA1	2.46	0.45
1:A:291:ALA:C	1:A:292:GLN:HG2	2.42	0.45
1:A:523:ILE:HG22	2:A:677:HEC:HBC2	1.99	0.45
1:A:624:HIS:CD2	2:A:679:HEC:NC	2.74	0.45
2:A:678:HEC:HBD2	2:A:678:HEC:CHA	2.47	0.45
1:A:223:VAL:HG22	1:A:224:SER:N	2.31	0.45
1:A:596:GLN:O	1:A:596:GLN:HG3	2.16	0.45
1:A:115:CYS:H	1:A:120:VAL:HG11	1.81	0.45
1:A:84:PHE:HD1	1:A:119:PHE:CZ	2.35	0.45
1:A:498:CYS:O	1:A:503:MET:HE2	2.18	0.44
1:A:89:LEU:O	1:A:150:ARG:HA	2.16	0.44
1:A:303:ASN:O	1:A:307:THR:HG22	2.16	0.44
1:A:526:LEU:CD1	1:A:527:HIS:CD2	3.01	0.44
1:A:596:GLN:HB3	1:A:598:HIS:H	1.82	0.44
1:A:412:ALA:O	1:A:415:GLU:HG2	2.18	0.44
1:A:81:SER:HA	1:A:82:ALA:HA	1.72	0.44
1:A:551:ILE:O	1:A:558:SER:N	2.50	0.44
1:A:566:ALA:O	1:A:567:ALA:C	2.60	0.44
1:A:348:THR:C	1:A:349:THR:HG23	2.43	0.44
1:A:74:GLN:HG2	1:A:75:ALA:H	1.77	0.44
1:A:214:CYS:C	1:A:216:THR:N	2.71	0.44
1:A:63:GLN:O	1:A:131:PHE:HB3	2.18	0.43
1:A:130:ARG:HB3	1:A:131:PHE:CD2	2.52	0.43
1:A:265:TRP:CE2	1:A:266:TYR:HD2	2.36	0.43
1:A:417:ASP:CG	1:A:418:ARG:H	2.26	0.43
1:A:130:ARG:HB3	1:A:130:ARG:HE	1.59	0.43
1:A:160:LEU:CG	1:A:161:ALA:H	2.31	0.43
1:A:264:ASN:O	1:A:268:VAL:HG22	2.17	0.43
2:A:675:HEC:HHA	2:A:675:HEC:CBD	2.43	0.43
1:A:569:GLN:HA	1:A:578:PHE:CD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ASN:O	1:A:576:GLY:C	2.60	0.43
1:A:88:GLN:NE2	1:A:135:PHE:HD2	2.15	0.43
1:A:122:HIS:C	1:A:124:ASN:N	2.76	0.43
1:A:263:GLN:NE2	1:A:267:ARG:NH2	2.66	0.43
1:A:321:ALA:O	1:A:347:PRO:HG2	2.19	0.43
1:A:52:VAL:HA	1:A:53:ASP:HA	1.72	0.43
1:A:151:LEU:HD21	1:A:153:ILE:HG23	2.00	0.43
1:A:155:ILE:CD1	1:A:171:GLN:NE2	2.78	0.43
1:A:86:ALA:HB1	1:A:135:PHE:HZ	1.82	0.43
1:A:90:LEU:HD12	1:A:91:PRO:N	2.33	0.43
1:A:150:ARG:O	1:A:175:TRP:HA	2.19	0.43
1:A:226:ALA:HA	1:A:227:ALA:HA	1.55	0.43
1:A:313:ASN:OD1	1:A:313:ASN:C	2.61	0.43
1:A:127:TYR:HB2	1:A:132:SER:HB3	2.00	0.43
1:A:377:ASP:HB3	1:A:501:PRO:HD2	2.00	0.43
1:A:243:PRO:HG3	2:A:675:HEC:CMD	2.48	0.43
1:A:553:ASP:O	1:A:554:SER:HB2	2.18	0.43
1:A:629:VAL:HG13	1:A:631:ASP:N	2.34	0.43
1:A:268:VAL:HG23	1:A:268:VAL:O	2.19	0.43
1:A:559:THR:HG22	1:A:559:THR:O	2.19	0.43
1:A:89:LEU:HB2	1:A:151:LEU:HB3	2.00	0.42
1:A:113:ALA:O	1:A:114:SER:O	2.36	0.42
1:A:89:LEU:HD13	1:A:103:TRP:HB3	2.01	0.42
1:A:61:ILE:HG12	1:A:134:THR:OG1	2.19	0.42
1:A:73:ASN:O	1:A:74:GLN:CD	2.62	0.42
1:A:84:PHE:HB3	1:A:85:ILE:CA	2.49	0.42
1:A:155:ILE:HG22	1:A:156:GLY:N	2.34	0.42
1:A:218:HIS:HE1	2:A:671:HEC:NA	2.17	0.42
1:A:520:LYS:HG3	1:A:521:GLN:N	2.34	0.42
1:A:243:PRO:HG3	2:A:675:HEC:HMD3	2.01	0.42
1:A:577:THR:HG22	1:A:606:PHE:CB	2.50	0.42
1:A:90:LEU:HD12	1:A:90:LEU:C	2.45	0.42
1:A:165:VAL:O	1:A:166:LEU:HB3	2.20	0.42
1:A:551:ILE:HG12	1:A:552:ASN:N	2.26	0.42
1:A:589:CYS:HB3	2:A:678:HEC:C4C	2.50	0.42
1:A:606:PHE:CG	1:A:607:ALA:N	2.88	0.42
1:A:55:VAL:HG21	1:A:61:ILE:CA	2.47	0.42
1:A:89:LEU:CD1	1:A:151:LEU:HD13	2.47	0.42
1:A:324:ASN:HB2	1:A:347:PRO:HD3	2.01	0.42
1:A:101:SER:CB	1:A:186:ARG:HD2	2.50	0.42
1:A:132:SER:O	1:A:133:ALA:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:GLY:O	1:A:494:GLN:HB3	2.20	0.42
1:A:562:LEU:H	1:A:562:LEU:HD23	1.84	0.42
1:A:223:VAL:HG21	1:A:228:ASP:CB	2.48	0.42
1:A:225:ASN:ND2	1:A:228:ASP:H	2.17	0.42
1:A:600:ARG:NE	1:A:600:ARG:CA	2.83	0.42
1:A:151:LEU:HD23	1:A:152:VAL:N	2.34	0.41
1:A:168:ILE:HG22	1:A:169:THR:HG23	2.02	0.41
1:A:188:LEU:O	1:A:262:ARG:NE	2.41	0.41
1:A:49:ASN:HA	1:A:68:VAL:HG23	2.02	0.41
1:A:568:VAL:HG21	1:A:581:PRO:CA	2.45	0.41
1:A:57:ILE:HA	1:A:58:SER:HA	1.60	0.41
1:A:187:ASN:HB3	1:A:259:LEU:HD22	2.01	0.41
1:A:234:ILE:HG12	2:A:672:HEC:HMD2	2.02	0.41
1:A:242:PHE:CE1	2:A:670:HEC:HBC2	2.55	0.41
1:A:372:TRP:O	1:A:378:TYR:HA	2.21	0.41
1:A:157:GLY:HA2	1:A:168:ILE:O	2.20	0.41
1:A:229:ILE:HG22	1:A:231:PRO:HD2	2.01	0.41
1:A:436:ASP:O	1:A:439:THR:HG23	2.20	0.41
1:A:512:PRO:HG2	1:A:587:SER:O	2.19	0.41
1:A:122:HIS:O	1:A:124:ASN:N	2.53	0.41
1:A:620:CYS:HA	2:A:679:HEC:HMC3	2.01	0.41
1:A:191:ILE:O	1:A:194:CYS:HB2	2.20	0.41
1:A:338:ILE:O	1:A:404:ASN:HB2	2.21	0.41
1:A:594:ALA:CA	1:A:595:THR:O	2.58	0.41
1:A:626:GLN:O	1:A:627:GLY:C	2.63	0.41
1:A:197:CYS:HA	1:A:476:CYS:SG	2.60	0.41
1:A:212:GLU:HA	1:A:213:THR:HA	1.64	0.41
1:A:234:ILE:HD12	1:A:234:ILE:C	2.45	0.41
1:A:238:HIS:HD2	1:A:242:PHE:CE1	2.38	0.41
1:A:477:HIS:CD2	2:A:675:HEC:NB	2.88	0.41
1:A:539:TYR:HA	1:A:540:PRO:HD3	1.78	0.41
1:A:605:VAL:CG1	1:A:606:PHE:H	2.13	0.41
1:A:282:ASN:HB3	1:A:287:GLN:HB3	2.03	0.41
1:A:331:SER:O	1:A:454:PHE:HZ	2.03	0.41
1:A:342:VAL:HG21	1:A:388:LEU:HD11	2.02	0.41
1:A:175:TRP:CZ3	1:A:187:ASN:ND2	2.89	0.41
1:A:191:ILE:O	1:A:191:ILE:HG12	2.21	0.41
1:A:271:MET:HE3	1:A:283:PHE:HB2	2.02	0.41
1:A:609:THR:HA	1:A:612:ASP:CG	2.46	0.41
1:A:595:THR:HG23	2:A:679:HEC:HMA2	2.03	0.41
1:A:436:ASP:HB3	1:A:439:THR:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:HIS:HE1	2:A:678:HEC:NB	2.14	0.40
1:A:313:ASN:O	1:A:317:THR:HG23	2.22	0.40
1:A:61:ILE:O	1:A:61:ILE:HG22	2.22	0.40
1:A:411:PRO:HG2	1:A:414:THR:OG1	2.22	0.40
1:A:526:LEU:C	1:A:528:SER:H	2.29	0.40
1:A:607:ALA:HB3	1:A:611:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	591/669 (88%)	454 (77%)	109 (18%)	28 (5%)	2 14

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	72	GLU
1	A	114	SER
1	A	120	VAL
1	A	262	ARG
1	A	74	GLN
1	A	85	ILE
1	A	124	ASN
1	A	182	LEU
1	A	211	VAL
1	A	574	ASN
1	A	595	THR
1	A	607	ALA
1	A	631	ASP
1	A	632	VAL

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Mol	Chain	Res	Type
1	A	116	PRO
1	A	123	LYS
1	A	609	THR
1	A	133	ALA
1	A	122	HIS
1	A	168	ILE
1	A	605	VAL
1	A	164	THR
1	A	165	VAL
1	A	243	PRO
1	A	52	VAL
1	A	61	ILE
1	A	167	PRO

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	479/542 (88%)	457 (95%)	22 (5%)	24 58

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	70	ASN
1	A	74	GLN
1	A	85	ILE
1	A	108	SER
1	A	130	ARG
1	A	131	PHE
1	A	141	VAL
1	A	144	LEU
1	A	185	THR
1	A	214	CYS
1	A	295	ASN
1	A	348	THR

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Mol	Chain	Res	Type
1	A	386	ILE
1	A	481	GLN
1	A	560	VAL
1	A	562	LEU
1	A	574	ASN
1	A	602	GLN
1	A	609	THR
1	A	610	LYS
1	A	638	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	70	ASN
1	A	71	GLN
1	A	73	ASN
1	A	74	GLN
1	A	88	GLN
1	A	104	GLN
1	A	149	GLN
1	A	176	GLN
1	A	210	GLN
1	A	219	ASN
1	A	263	GLN
1	A	280	GLN
1	A	292	GLN
1	A	297	ASN
1	A	322	GLN
1	A	324	ASN
1	A	502	ASN
1	A	548	GLN
1	A	552	ASN
1	A	588	ASN
1	A	602	GLN
1	A	626	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEC	A	676	1	50,50,50	1.83	7 (14%)	68,82,82	1.23	3 (4%)
2	HEC	A	677	1	50,50,50	1.81	6 (12%)	68,82,82	1.40	7 (10%)
2	HEC	A	672	1	50,50,50	1.83	8 (16%)	68,82,82	1.26	4 (5%)
2	HEC	A	679	1	50,50,50	1.76	5 (10%)	68,82,82	1.33	8 (11%)
2	HEC	A	673	1	50,50,50	1.78	5 (10%)	68,82,82	1.28	3 (4%)
2	HEC	A	674	1	50,50,50	1.82	8 (16%)	68,82,82	1.27	5 (7%)
2	HEC	A	675	1	50,50,50	1.81	7 (14%)	68,82,82	1.35	6 (8%)
2	HEC	A	671	1	50,50,50	1.85	6 (12%)	68,82,82	1.27	5 (7%)
2	HEC	A	670	1	50,50,50	1.84	7 (14%)	68,82,82	1.25	5 (7%)
2	HEC	A	678	1	50,50,50	1.91	7 (14%)	68,82,82	1.27	4 (5%)

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
2	HEC	A	676	1	-	14/14/54/54	-
2	HEC	A	677	1	1/1/3/7	11/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	672	1	1/1/3/7	5/14/54/54	-
2	HEC	A	679	1	1/1/3/7	5/14/54/54	-
2	HEC	A	673	1	1/1/3/7	6/14/54/54	-
2	HEC	A	674	1	1/1/3/7	9/14/54/54	-
2	HEC	A	675	1	1/1/3/7	7/14/54/54	-
2	HEC	A	671	1	1/1/3/7	7/14/54/54	-
2	HEC	A	670	1	1/1/3/7	5/14/54/54	-
2	HEC	A	678	1	1/1/3/7	7/14/54/54	-

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	671	HEC	C3D-C2D	8.16	1.54	1.36
2	A	674	HEC	C3D-C2D	8.08	1.54	1.36
2	A	672	HEC	C3D-C2D	8.05	1.54	1.36
2	A	670	HEC	C3D-C2D	8.01	1.54	1.36
2	A	676	HEC	C3D-C2D	7.98	1.54	1.36
2	A	679	HEC	C3D-C2D	7.88	1.53	1.36
2	A	678	HEC	C3D-C2D	7.83	1.53	1.36
2	A	673	HEC	C3D-C2D	7.81	1.53	1.36
2	A	677	HEC	C3D-C2D	7.76	1.53	1.36
2	A	675	HEC	C3D-C2D	7.74	1.53	1.36
2	A	678	HEC	FE-ND	5.78	2.12	1.94
2	A	677	HEC	FE-ND	4.95	2.10	1.94
2	A	674	HEC	FE-ND	4.76	2.09	1.94
2	A	673	HEC	FE-NB	4.73	2.09	1.94
2	A	675	HEC	FE-ND	4.65	2.09	1.94
2	A	672	HEC	FE-ND	4.57	2.09	1.94
2	A	671	HEC	FE-NA	4.52	2.10	1.95
2	A	675	HEC	FE-NB	4.44	2.08	1.94
2	A	670	HEC	FE-ND	4.40	2.08	1.94
2	A	679	HEC	FE-ND	4.36	2.08	1.94
2	A	678	HEC	FE-NB	4.35	2.08	1.94
2	A	676	HEC	FE-ND	4.30	2.08	1.94
2	A	676	HEC	FE-NC	4.25	2.09	1.95
2	A	671	HEC	FE-NB	4.18	2.07	1.94
2	A	670	HEC	FE-NB	4.17	2.07	1.94
2	A	674	HEC	FE-NC	4.13	2.08	1.95
2	A	670	HEC	FE-NC	4.06	2.08	1.95
2	A	672	HEC	FE-NB	4.04	2.07	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	671	HEC	FE-ND	3.95	2.07	1.94
2	A	677	HEC	FE-NB	3.95	2.07	1.94
2	A	677	HEC	FE-NC	3.80	2.07	1.95
2	A	679	HEC	FE-NA	3.74	2.07	1.95
2	A	676	HEC	FE-NB	3.71	2.06	1.94
2	A	678	HEC	FE-NC	3.70	2.07	1.95
2	A	673	HEC	FE-ND	3.69	2.06	1.94
2	A	672	HEC	FE-NC	3.58	2.07	1.95
2	A	679	HEC	FE-NB	3.54	2.05	1.94
2	A	674	HEC	FE-NB	3.47	2.05	1.94
2	A	673	HEC	FE-NC	3.38	2.06	1.95
2	A	678	HEC	FE-NA	3.22	2.05	1.95
2	A	675	HEC	FE-NC	3.08	2.05	1.95
2	A	675	HEC	FE-NA	2.97	2.05	1.95
2	A	676	HEC	FE-NA	2.91	2.04	1.95
2	A	670	HEC	FE-NA	2.90	2.04	1.95
2	A	673	HEC	FE-NA	2.79	2.04	1.95
2	A	672	HEC	FE-NA	2.73	2.04	1.95
2	A	672	HEC	CMC-C2C	2.17	1.55	1.50
2	A	674	HEC	CMC-C2C	2.16	1.55	1.50
2	A	674	HEC	FE-NA	2.16	2.02	1.95
2	A	671	HEC	FE-NC	2.14	2.02	1.95
2	A	671	HEC	CMA-C3A	2.11	1.55	1.50
2	A	677	HEC	CMC-C2C	2.11	1.55	1.50
2	A	676	HEC	CMC-C2C	2.10	1.55	1.50
2	A	679	HEC	CMB-C2B	2.08	1.55	1.50
2	A	674	HEC	CMB-C2B	2.07	1.55	1.50
2	A	675	HEC	CMA-C3A	2.07	1.55	1.50
2	A	675	HEC	CMC-C2C	2.06	1.55	1.50
2	A	677	HEC	FE-NA	2.05	2.01	1.95
2	A	674	HEC	CMA-C3A	2.04	1.55	1.50
2	A	670	HEC	CMB-C2B	2.04	1.55	1.50
2	A	672	HEC	CMD-C2D	2.03	1.54	1.50
2	A	670	HEC	CMA-C3A	2.01	1.54	1.50
2	A	678	HEC	CMB-C2B	2.01	1.54	1.50
2	A	672	HEC	CMB-C2B	2.01	1.54	1.50
2	A	676	HEC	CMB-C2B	2.00	1.54	1.50
2	A	678	HEC	CMC-C2C	2.00	1.54	1.50

All (50) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	679	HEC	C1D-ND-C4D	5.72	111.98	105.21
2	A	674	HEC	C1D-ND-C4D	5.71	111.97	105.21
2	A	677	HEC	C1D-ND-C4D	5.51	111.73	105.21
2	A	672	HEC	C1D-ND-C4D	5.48	111.69	105.21
2	A	673	HEC	C1D-ND-C4D	5.48	111.69	105.21
2	A	675	HEC	C1D-ND-C4D	5.45	111.66	105.21
2	A	671	HEC	C1D-ND-C4D	5.26	111.44	105.21
2	A	670	HEC	C1D-ND-C4D	5.24	111.42	105.21
2	A	676	HEC	C1D-ND-C4D	5.22	111.39	105.21
2	A	678	HEC	C1D-ND-C4D	5.18	111.35	105.21
2	A	675	HEC	CAD-C3D-C4D	3.70	131.15	124.70
2	A	677	HEC	CAD-C3D-C4D	3.54	130.86	124.70
2	A	678	HEC	CAD-C3D-C4D	3.10	130.09	124.70
2	A	677	HEC	C2A-C1A-NA	-2.81	107.61	110.32
2	A	672	HEC	C2A-C1A-NA	-2.69	107.73	110.32
2	A	679	HEC	C2A-C1A-NA	-2.62	107.79	110.32
2	A	676	HEC	C2A-C1A-NA	-2.61	107.81	110.32
2	A	679	HEC	C4B-NB-C1B	2.56	108.23	105.21
2	A	677	HEC	CBC-CAC-C3C	-2.56	105.49	112.42
2	A	674	HEC	C4B-NB-C1B	2.51	108.18	105.21
2	A	670	HEC	C4B-NB-C1B	2.47	108.13	105.21
2	A	671	HEC	C2A-C1A-NA	-2.41	108.00	110.32
2	A	675	HEC	C2A-C1A-NA	-2.39	108.02	110.32
2	A	673	HEC	C2A-C1A-NA	-2.36	108.04	110.32
2	A	678	HEC	C2A-C1A-NA	-2.29	108.12	110.32
2	A	678	HEC	C4B-NB-C1B	2.28	107.90	105.21
2	A	670	HEC	C3B-C4B-NB	-2.25	107.70	110.17
2	A	675	HEC	CAD-CBD-CGD	-2.24	107.73	113.67
2	A	679	HEC	CAD-C3D-C4D	2.23	128.59	124.70
2	A	679	HEC	C3B-C4B-NB	-2.23	107.73	110.17
2	A	673	HEC	CAD-C3D-C4D	2.22	128.57	124.70
2	A	674	HEC	C2A-C1A-NA	-2.22	108.18	110.32
2	A	679	HEC	C3C-C4C-NC	-2.20	107.71	110.15
2	A	671	HEC	CHA-C4D-ND	2.18	126.77	124.42
2	A	679	HEC	C3D-C4D-ND	-2.16	108.26	110.35
2	A	670	HEC	C2A-C1A-NA	-2.15	108.24	110.32
2	A	675	HEC	C4B-NB-C1B	2.15	107.76	105.21
2	A	675	HEC	CAD-C3D-C2D	-2.14	123.86	127.87
2	A	677	HEC	CAD-CBD-CGD	-2.13	108.02	113.67
2	A	672	HEC	C3C-C4C-NC	-2.11	107.81	110.15
2	A	676	HEC	C4B-NB-C1B	2.10	107.69	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	671	HEC	CAD-CBD-CGD	-2.09	108.12	113.67
2	A	677	HEC	C3C-C4C-NC	-2.07	107.85	110.15
2	A	674	HEC	CAD-CBD-CGD	-2.07	108.18	113.67
2	A	674	HEC	C3B-C4B-NB	-2.06	107.91	110.17
2	A	677	HEC	CAD-C3D-C2D	-2.05	124.02	127.87
2	A	670	HEC	CMC-C2C-C1C	-2.05	122.31	125.42
2	A	679	HEC	CAD-CBD-CGD	-2.04	108.27	113.67
2	A	671	HEC	C4B-NB-C1B	2.01	107.59	105.21
2	A	672	HEC	C4B-NB-C1B	2.01	107.58	105.21

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	670	HEC	NA
2	A	671	HEC	NA
2	A	672	HEC	NA
2	A	673	HEC	NA
2	A	674	HEC	NA
2	A	675	HEC	NA
2	A	677	HEC	NA
2	A	678	HEC	NA
2	A	679	HEC	NA

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	670	HEC	C2D-C3D-CAD-CBD
2	A	670	HEC	C4D-C3D-CAD-CBD
2	A	671	HEC	C1A-C2A-CAA-CBA
2	A	671	HEC	C3A-C2A-CAA-CBA
2	A	671	HEC	C2D-C3D-CAD-CBD
2	A	674	HEC	C1A-C2A-CAA-CBA
2	A	674	HEC	C3A-C2A-CAA-CBA
2	A	675	HEC	C2D-C3D-CAD-CBD
2	A	675	HEC	C4D-C3D-CAD-CBD
2	A	678	HEC	C2D-C3D-CAD-CBD
2	A	678	HEC	C4D-C3D-CAD-CBD
2	A	671	HEC	C4D-C3D-CAD-CBD
2	A	676	HEC	C1A-C2A-CAA-CBA
2	A	677	HEC	C4D-C3D-CAD-CBD
2	A	676	HEC	C3D-CAD-CBD-CGD
2	A	672	HEC	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
2	A	677	HEC	C2D-C3D-CAD-CBD
2	A	676	HEC	C2B-C3B-CAB-CBB
2	A	676	HEC	C3A-C2A-CAA-CBA
2	A	676	HEC	C4C-C3C-CAC-CBC
2	A	676	HEC	C2D-C3D-CAD-CBD
2	A	672	HEC	C4D-C3D-CAD-CBD
2	A	676	HEC	C2C-C3C-CAC-CBC
2	A	679	HEC	C4D-C3D-CAD-CBD
2	A	674	HEC	C2C-C3C-CAC-CBC
2	A	673	HEC	C4D-C3D-CAD-CBD
2	A	676	HEC	C4D-C3D-CAD-CBD
2	A	677	HEC	C1A-C2A-CAA-CBA
2	A	679	HEC	C1A-C2A-CAA-CBA
2	A	673	HEC	C2B-C3B-CAB-CBB
2	A	673	HEC	C2C-C3C-CAC-CBC
2	A	675	HEC	C2C-C3C-CAC-CBC
2	A	677	HEC	C3A-C2A-CAA-CBA
2	A	679	HEC	C3A-C2A-CAA-CBA
2	A	672	HEC	C2C-C3C-CAC-CBC
2	A	679	HEC	C2D-C3D-CAD-CBD
2	A	670	HEC	C2C-C3C-CAC-CBC
2	A	676	HEC	C4B-C3B-CAB-CBB
2	A	673	HEC	C2D-C3D-CAD-CBD
2	A	676	HEC	C2A-CAA-CBA-CGA
2	A	677	HEC	C3D-CAD-CBD-CGD
2	A	677	HEC	C2C-C3C-CAC-CBC
2	A	675	HEC	C2B-C3B-CAB-CBB
2	A	673	HEC	C4B-C3B-CAB-CBB
2	A	675	HEC	C1A-C2A-CAA-CBA
2	A	673	HEC	C4C-C3C-CAC-CBC
2	A	670	HEC	C2B-C3B-CAB-CBB
2	A	675	HEC	C3A-C2A-CAA-CBA
2	A	678	HEC	C2B-C3B-CAB-CBB
2	A	674	HEC	C4C-C3C-CAC-CBC
2	A	674	HEC	C2B-C3B-CAB-CBB
2	A	671	HEC	C2B-C3B-CAB-CBB
2	A	678	HEC	C2C-C3C-CAC-CBC
2	A	676	HEC	CAA-CBA-CGA-O1A
2	A	678	HEC	C3A-C2A-CAA-CBA
2	A	678	HEC	C1A-C2A-CAA-CBA
2	A	672	HEC	C2B-C3B-CAB-CBB
2	A	676	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
2	A	677	HEC	C2B-C3B-CAB-CBB
2	A	671	HEC	C3D-CAD-CBD-CGD
2	A	677	HEC	C2A-CAA-CBA-CGA
2	A	676	HEC	CAD-CBD-CGD-O2D
2	A	675	HEC	C4B-C3B-CAB-CBB
2	A	676	HEC	CAD-CBD-CGD-O1D
2	A	678	HEC	C4B-C3B-CAB-CBB
2	A	674	HEC	CAA-CBA-CGA-O2A
2	A	671	HEC	C4B-C3B-CAB-CBB
2	A	670	HEC	C4B-C3B-CAB-CBB
2	A	677	HEC	C4B-C3B-CAB-CBB
2	A	677	HEC	CAA-CBA-CGA-O2A
2	A	674	HEC	CAA-CBA-CGA-O1A
2	A	674	HEC	C4B-C3B-CAB-CBB
2	A	672	HEC	C4B-C3B-CAB-CBB
2	A	679	HEC	C2B-C3B-CAB-CBB
2	A	674	HEC	C4D-C3D-CAD-CBD
2	A	677	HEC	CAA-CBA-CGA-O1A

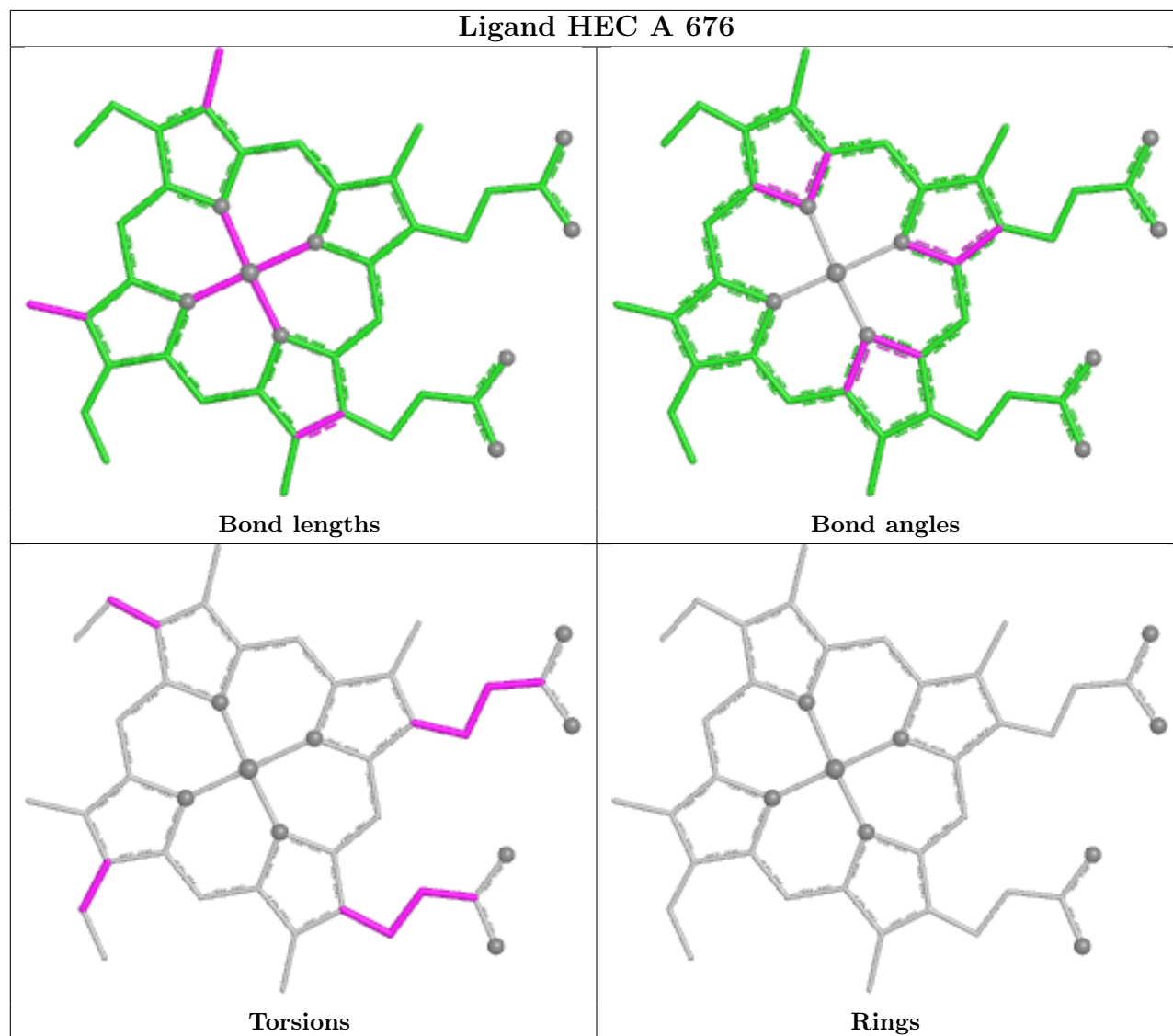
There are no ring outliers.

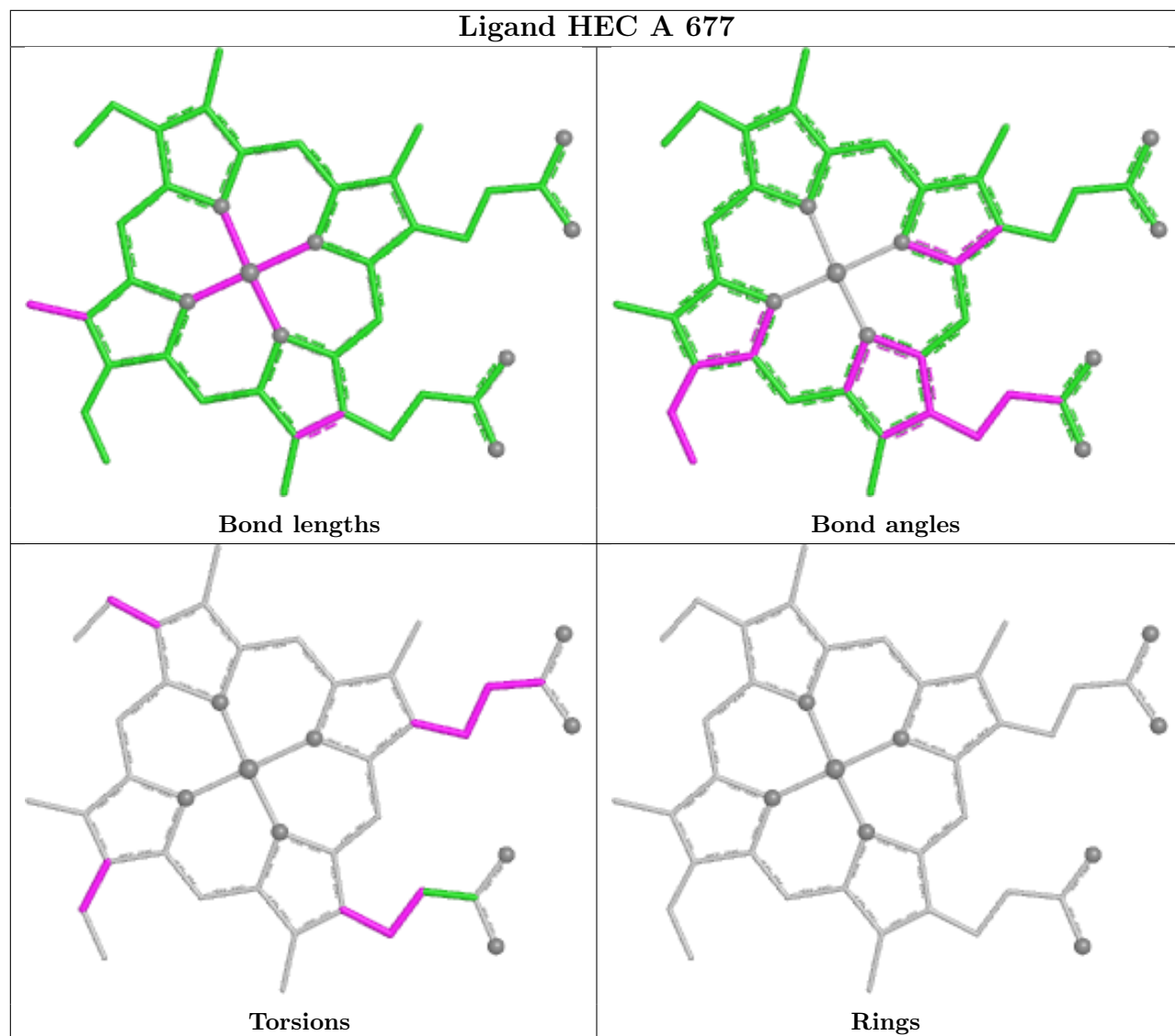
9 monomers are involved in 55 short contacts:

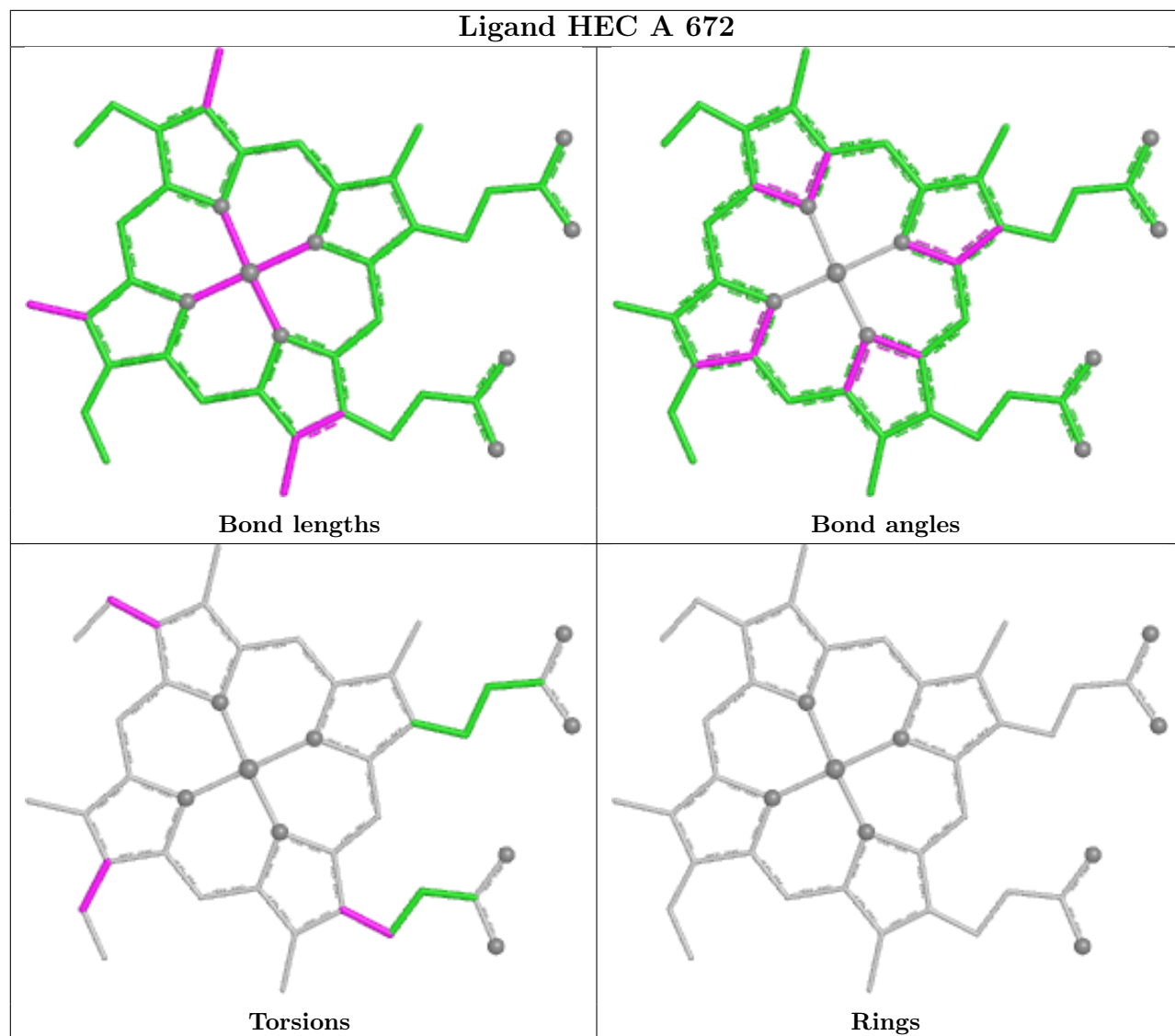
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	676	HEC	2	0
2	A	677	HEC	12	0
2	A	672	HEC	5	0
2	A	679	HEC	5	0
2	A	674	HEC	3	0
2	A	675	HEC	8	0
2	A	671	HEC	10	0
2	A	670	HEC	3	0
2	A	678	HEC	8	0

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

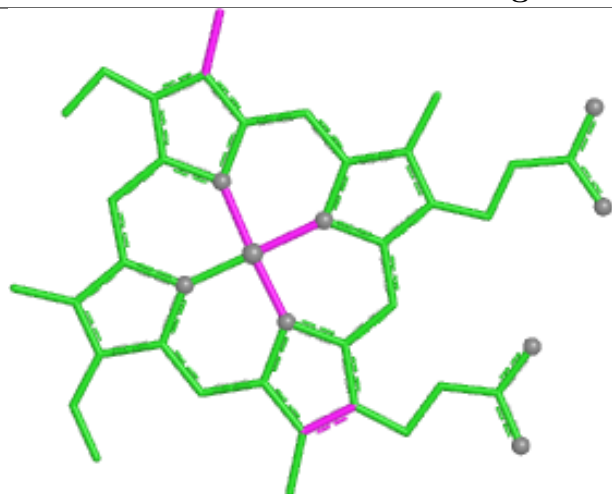
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



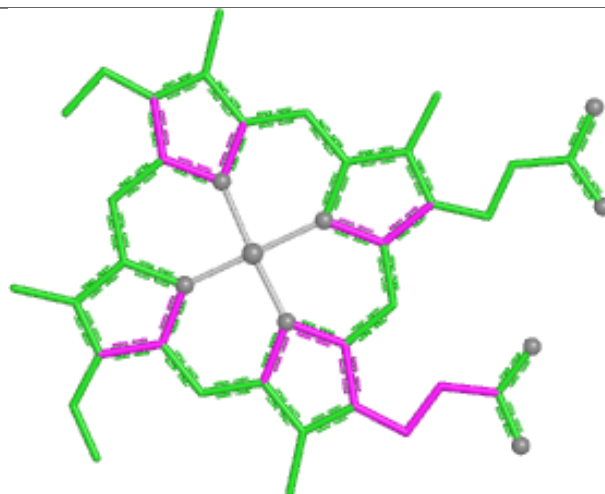




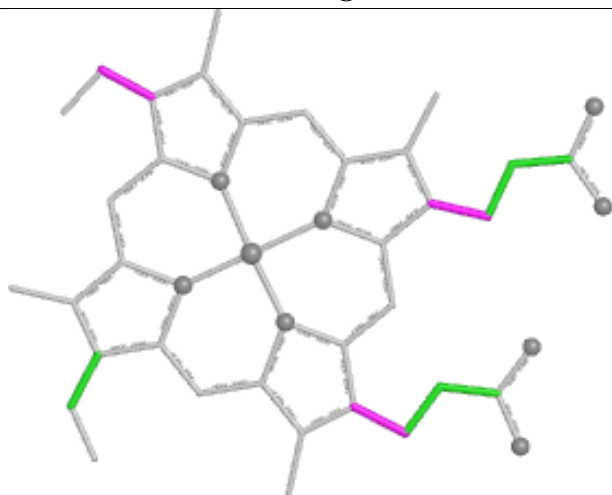
Ligand HEC A 679



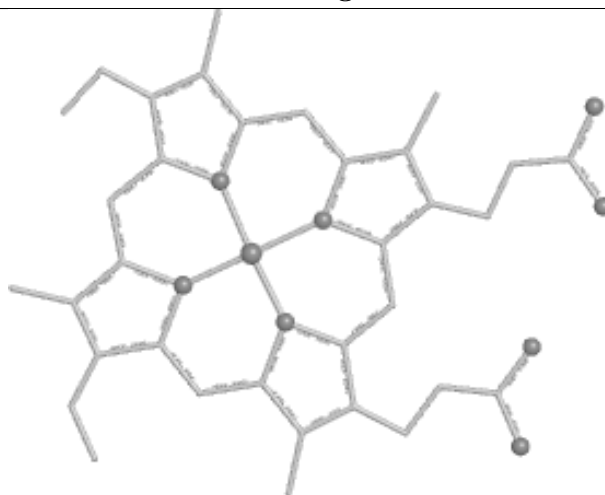
Bond lengths



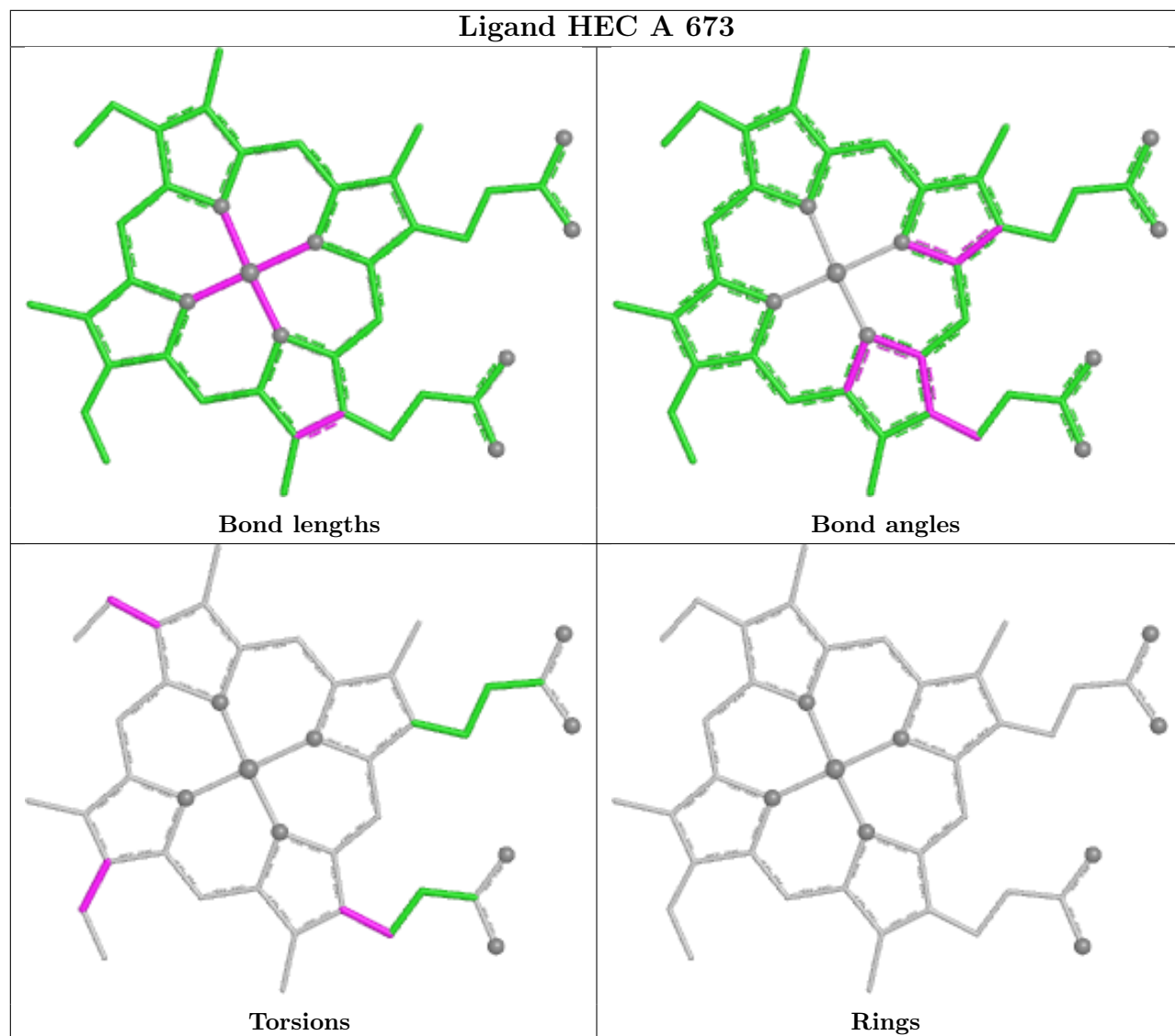
Bond angles

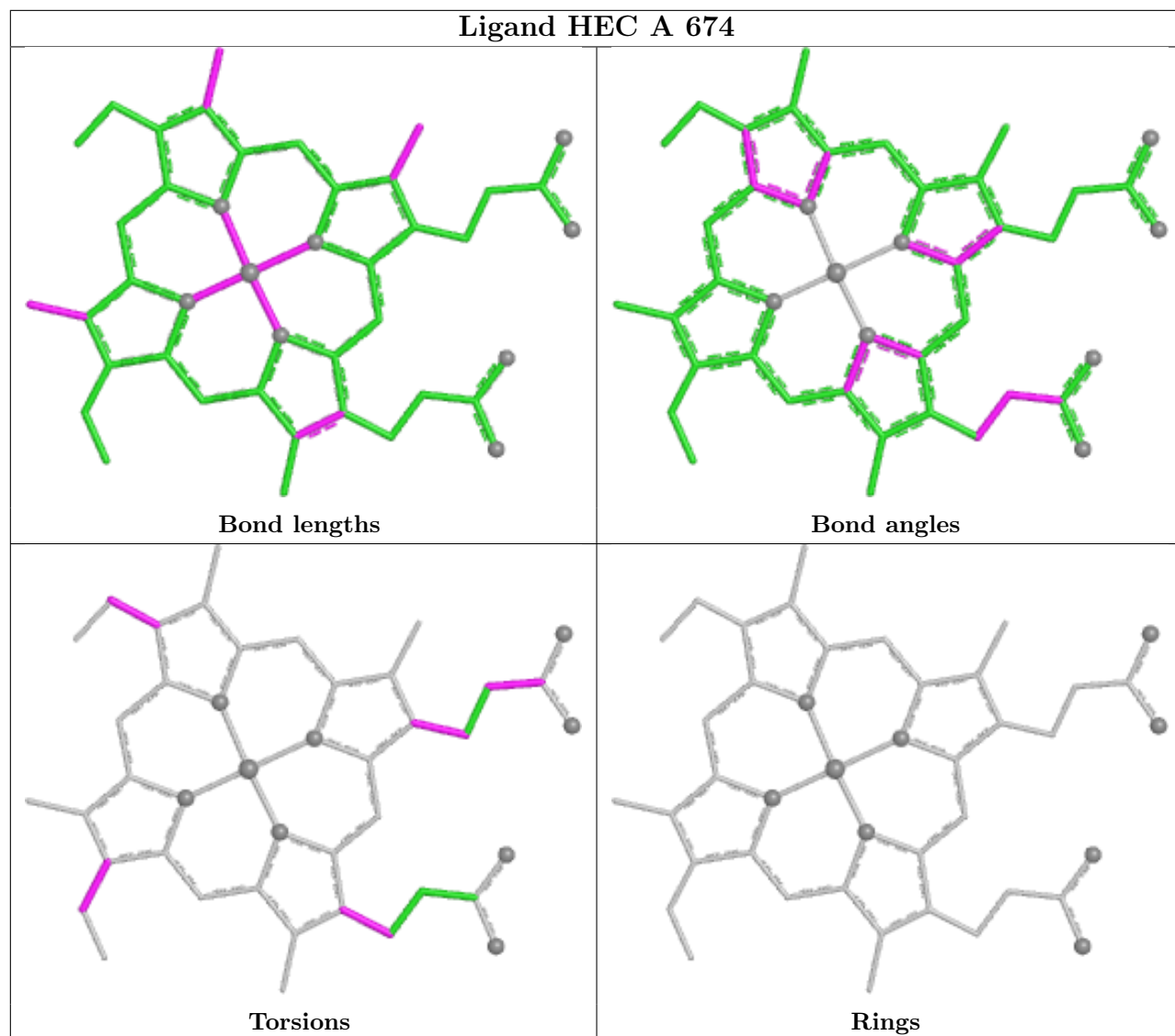


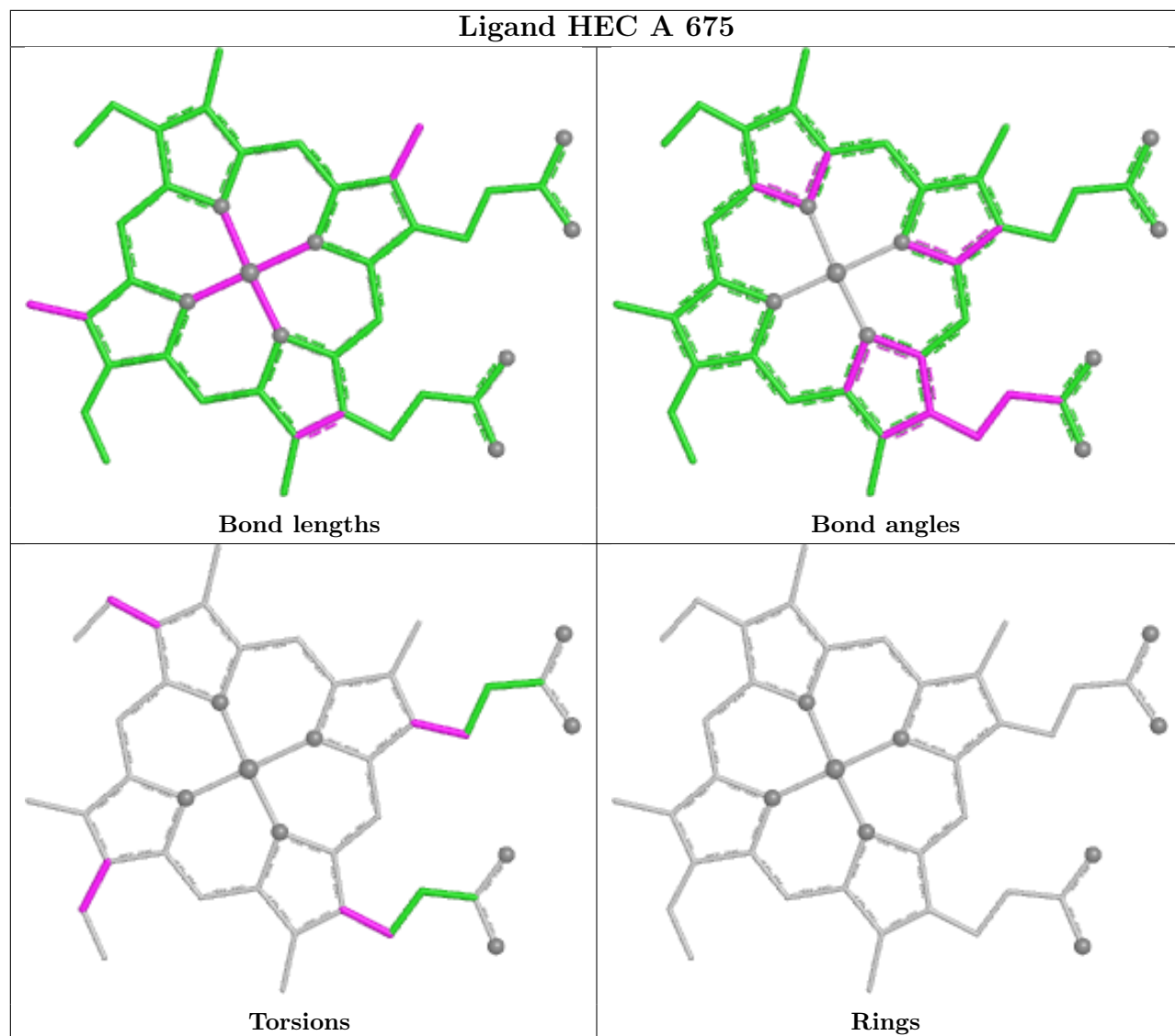
Torsions



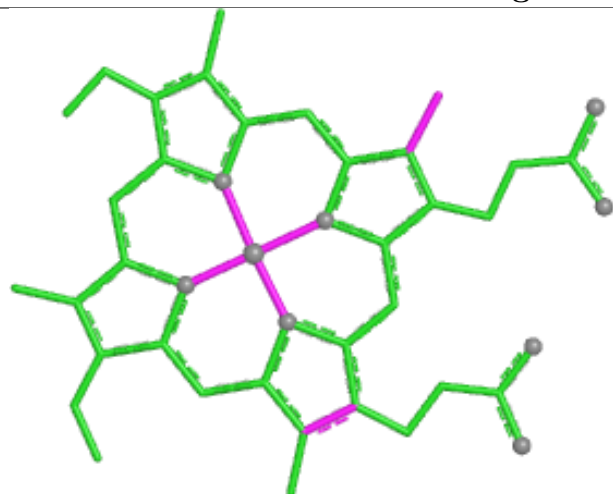
Rings



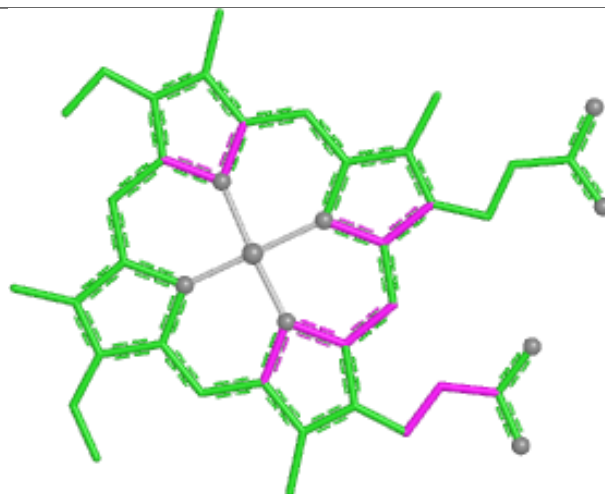




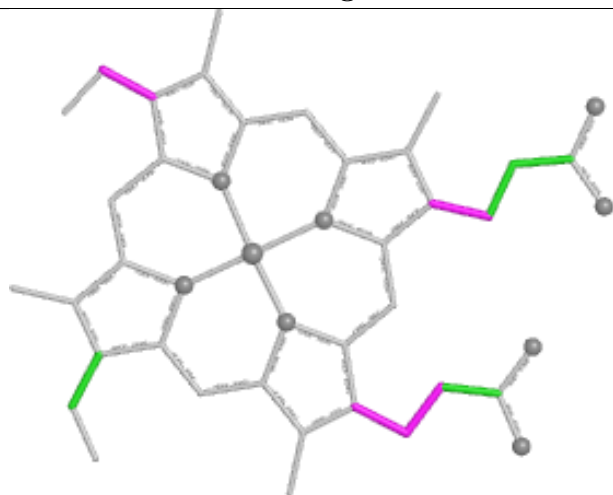
Ligand HEC A 671



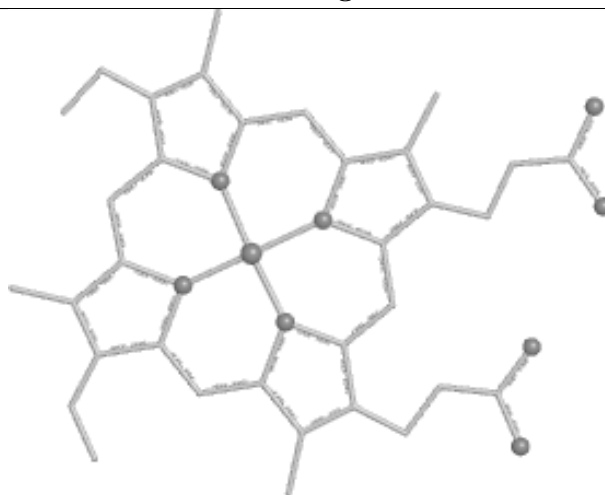
Bond lengths



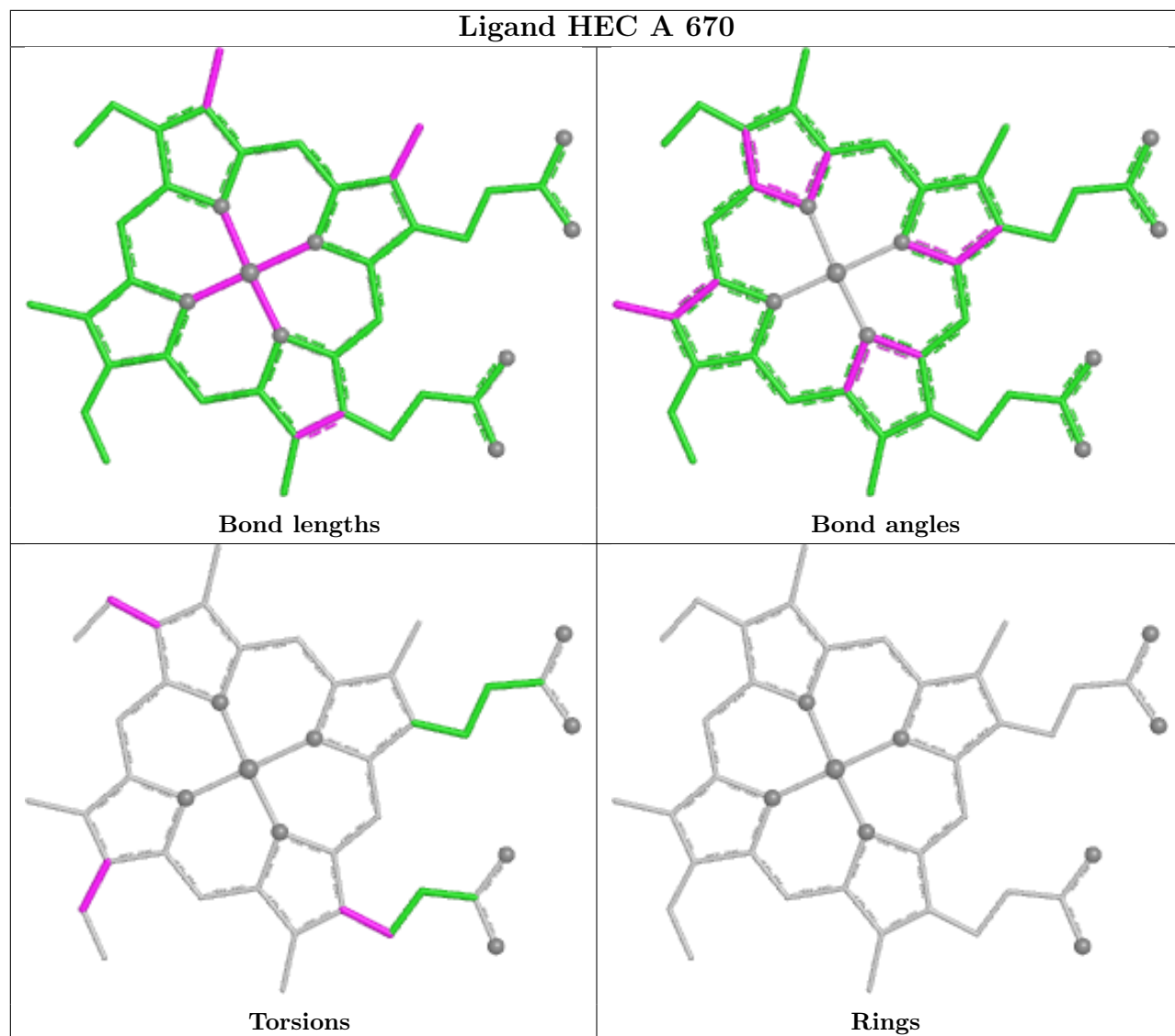
Bond angles

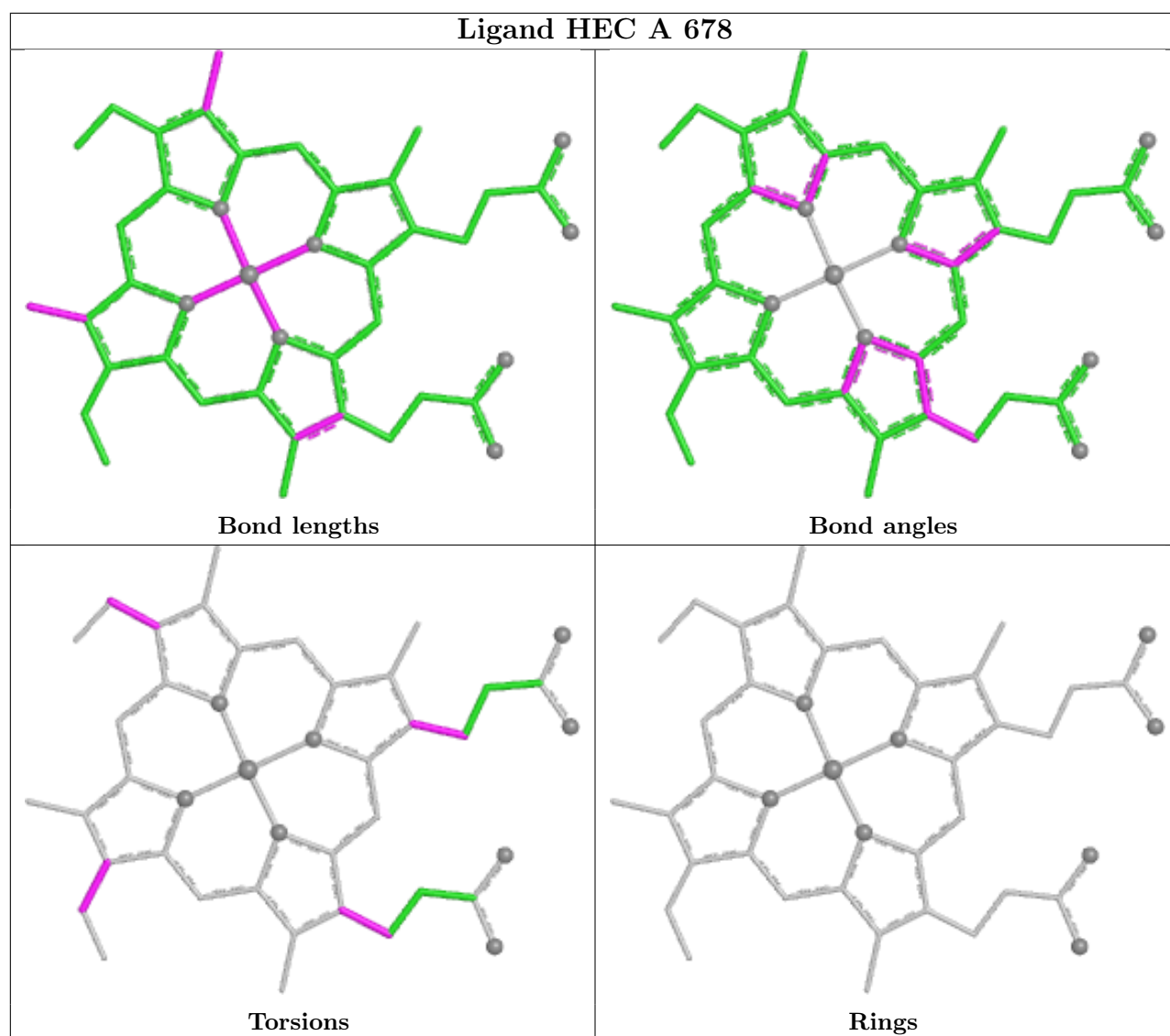


Torsions



Rings





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	593/669 (88%)	1.36	172 (29%) 1 1	46, 99, 206, 272	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	ALA	11.2
1	A	84	PHE	10.8
1	A	126	HIS	10.5
1	A	628	THR	8.3
1	A	158	ASP	7.9
1	A	127	TYR	7.4
1	A	134	THR	7.3
1	A	619	THR	6.8
1	A	118	THR	6.7
1	A	161	ALA	6.6
1	A	95	THR	6.6
1	A	168	ILE	6.4
1	A	166	LEU	6.2
1	A	113	ALA	6.1
1	A	80	PRO	6.0
1	A	121	ASP	6.0
1	A	129	TYR	5.8
1	A	88	GLN	5.8
1	A	601	GLN	5.8
1	A	641	GLY	5.8
1	A	213	THR	5.7
1	A	212	GLU	5.6
1	A	94	ALA	5.6
1	A	125	GLY	5.6
1	A	57	ILE	5.6
1	A	77	VAL	5.5
1	A	226	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	111	CYS	5.4
1	A	617	THR	5.4
1	A	594	ALA	5.3
1	A	138	MET	5.3
1	A	83	THR	5.2
1	A	109	GLU	5.2
1	A	122	HIS	5.2
1	A	560	VAL	5.1
1	A	92	GLN	5.0
1	A	131	PHE	4.9
1	A	76	VAL	4.9
1	A	98	GLY	4.8
1	A	606	PHE	4.8
1	A	280	GLN	4.7
1	A	162	ASP	4.7
1	A	119	PHE	4.7
1	A	593	ASP	4.7
1	A	573	LEU	4.7
1	A	67	GLN	4.6
1	A	54	LYS	4.6
1	A	74	GLN	4.6
1	A	110	THR	4.5
1	A	124	ASN	4.5
1	A	225	ASN	4.5
1	A	576	GLY	4.5
1	A	85	ILE	4.4
1	A	133	ALA	4.4
1	A	112	ALA	4.2
1	A	622	PHE	4.2
1	A	93	GLY	4.1
1	A	66	TYR	4.1
1	A	164	THR	4.1
1	A	608	GLY	4.1
1	A	108	SER	4.0
1	A	614	THR	4.0
1	A	157	GLY	4.0
1	A	61	ILE	3.9
1	A	595	THR	3.9
1	A	165	VAL	3.9
1	A	141	VAL	3.9
1	A	140	GLY	3.9
1	A	58	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	211	VAL	3.8
1	A	50	ILE	3.8
1	A	569	GLN	3.8
1	A	607	ALA	3.7
1	A	136	ASN	3.7
1	A	575	ASN	3.7
1	A	73	ASN	3.6
1	A	159	ALA	3.6
1	A	99	ASN	3.6
1	A	120	VAL	3.6
1	A	596	GLN	3.5
1	A	87	ALA	3.5
1	A	210	GLN	3.5
1	A	65	ASP	3.4
1	A	150	ARG	3.4
1	A	75	ALA	3.4
1	A	616	GLY	3.3
1	A	182	LEU	3.3
1	A	209	ASN	3.2
1	A	542	ASN	3.2
1	A	181	MET	3.2
1	A	79	ILE	3.1
1	A	602	GLN	3.1
1	A	70	ASN	3.1
1	A	220	SER	3.1
1	A	52	VAL	3.1
1	A	260	ALA	3.1
1	A	454	PHE	3.1
1	A	462	THR	3.0
1	A	263	GLN	3.0
1	A	180	ASN	3.0
1	A	200	ASN	3.0
1	A	588	ASN	2.9
1	A	91	PRO	2.9
1	A	611	ALA	2.9
1	A	78	GLY	2.9
1	A	156	GLY	2.9
1	A	634	LYS	2.9
1	A	135	PHE	2.9
1	A	143	PHE	2.9
1	A	72	GLU	2.9
1	A	567	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	123	LYS	2.8
1	A	511	ASN	2.8
1	A	117	GLY	2.8
1	A	564	LEU	2.8
1	A	176	GLN	2.8
1	A	190	SER	2.8
1	A	89	LEU	2.8
1	A	241	GLY	2.8
1	A	154	LYS	2.8
1	A	173	TYR	2.7
1	A	571	LEU	2.7
1	A	146	ASP	2.7
1	A	174	ASP	2.7
1	A	114	SER	2.7
1	A	631	ASP	2.7
1	A	153	ILE	2.7
1	A	609	THR	2.6
1	A	262	ARG	2.6
1	A	208	TYR	2.6
1	A	565	ASN	2.6
1	A	160	LEU	2.5
1	A	130	ARG	2.5
1	A	574	ASN	2.5
1	A	570	PRO	2.5
1	A	610	LYS	2.5
1	A	137	GLY	2.5
1	A	53	ASP	2.5
1	A	63	GLN	2.4
1	A	261	ASP	2.4
1	A	630	ALA	2.4
1	A	68	VAL	2.4
1	A	536	ASP	2.4
1	A	349	THR	2.3
1	A	335	ASN	2.3
1	A	605	VAL	2.3
1	A	227	ALA	2.3
1	A	461	THR	2.3
1	A	592	SER	2.3
1	A	155	ILE	2.3
1	A	115	CYS	2.3
1	A	214	CYS	2.3
1	A	56	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	179	GLY	2.2
1	A	621	ALA	2.2
1	A	632	VAL	2.2
1	A	128	SER	2.2
1	A	623	CYS	2.2
1	A	612	ASP	2.1
1	A	59	ASP	2.1
1	A	90	LEU	2.1
1	A	599	MET	2.1
1	A	71	GLN	2.1
1	A	167	PRO	2.1
1	A	202	ALA	2.1
1	A	132	SER	2.1
1	A	568	VAL	2.1
1	A	512	PRO	2.1
1	A	618	GLU	2.1
1	A	222	LYS	2.0
1	A	504	LEU	2.0
1	A	640	LYS	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
2	HEC	A	679	43/43	0.85	0.26	106,176,195,203	0
3	CA	A	680	1/1	0.94	0.09	101,101,101,101	0
2	HEC	A	678	43/43	0.96	0.17	114,162,187,202	0
2	HEC	A	671	43/43	0.97	0.12	63,86,140,148	0

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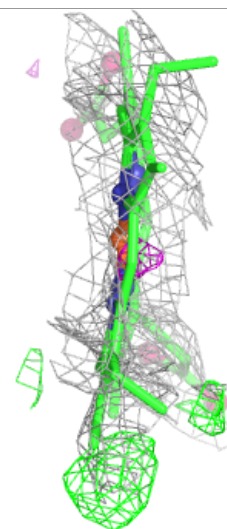
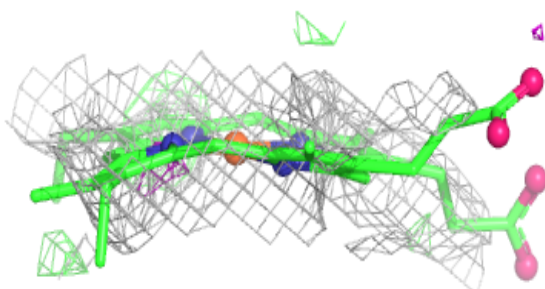
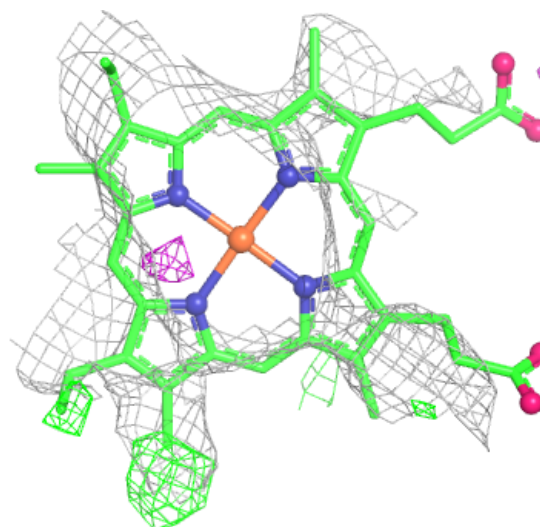
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEC	A	672	43/43	0.97	0.11	40,69,89,104	0
2	HEC	A	676	43/43	0.97	0.12	39,73,127,151	0
2	HEC	A	677	43/43	0.98	0.12	73,103,115,122	0
2	HEC	A	673	43/43	0.98	0.10	29,61,98,106	0
2	HEC	A	675	43/43	0.98	0.10	53,83,105,143	0
2	HEC	A	670	43/43	0.98	0.10	55,90,118,129	0
2	HEC	A	674	43/43	0.99	0.08	31,52,83,105	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.

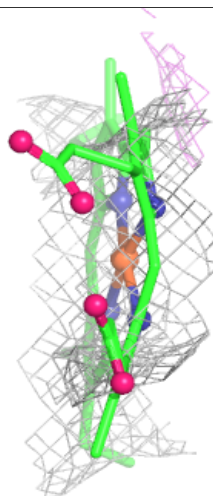
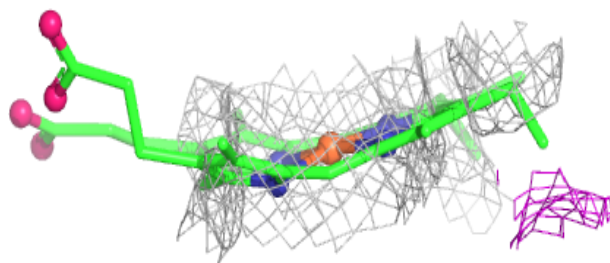
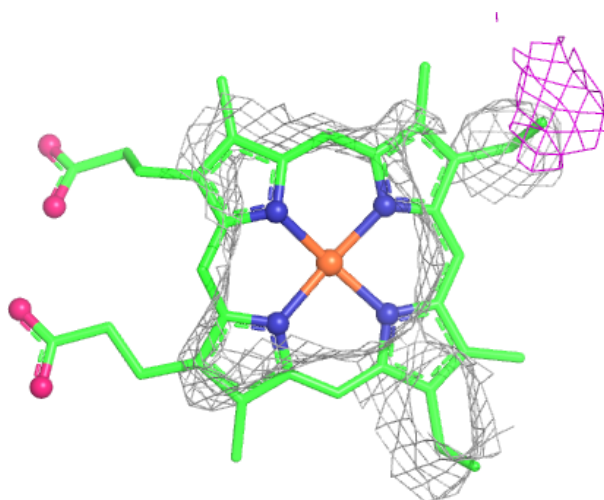
Electron density around HEC A 679:

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



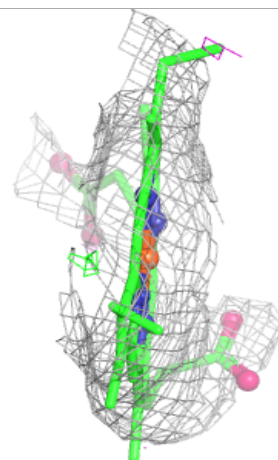
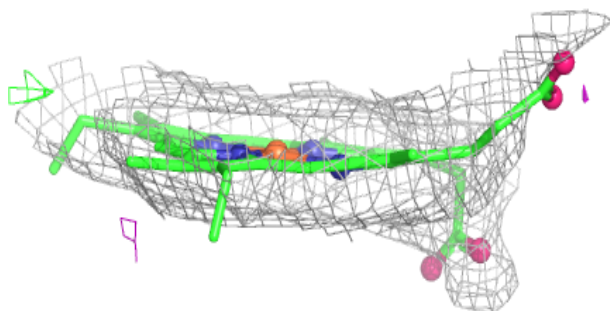
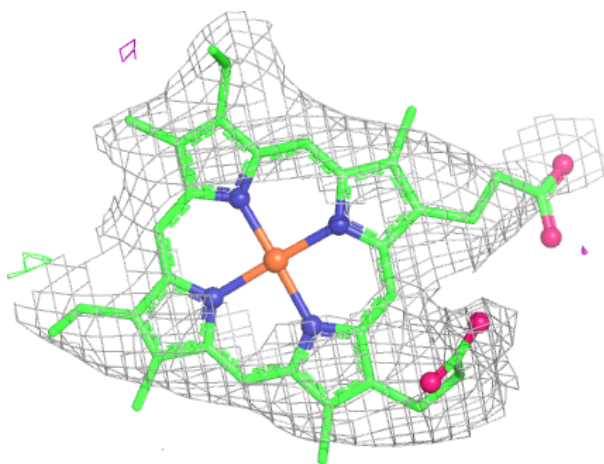
Electron density around HEC A 678:

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



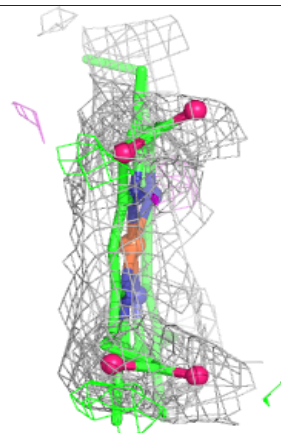
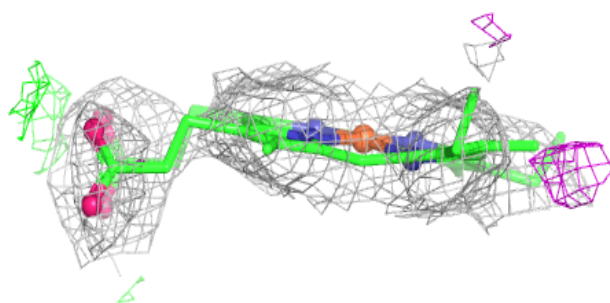
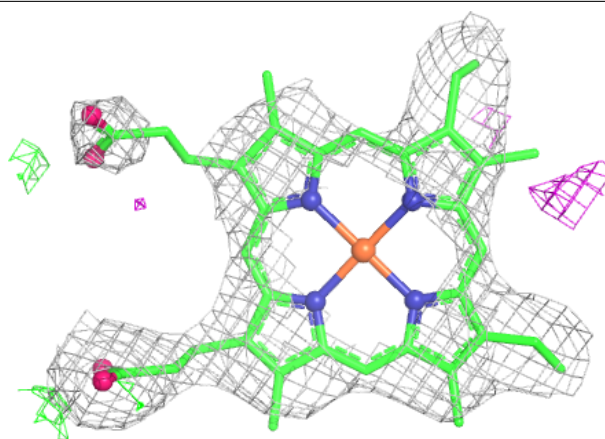
Electron density around HEC A 671:

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



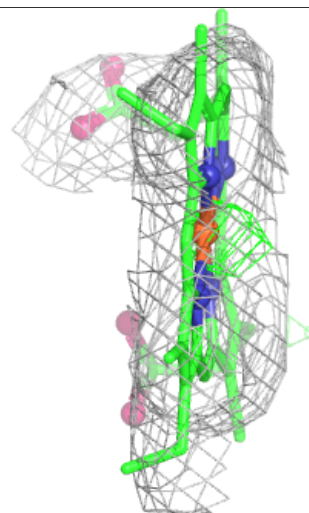
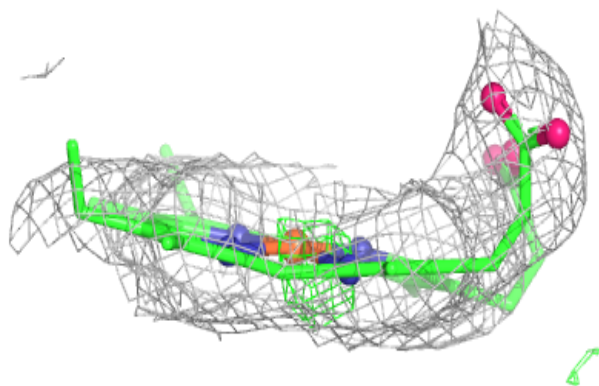
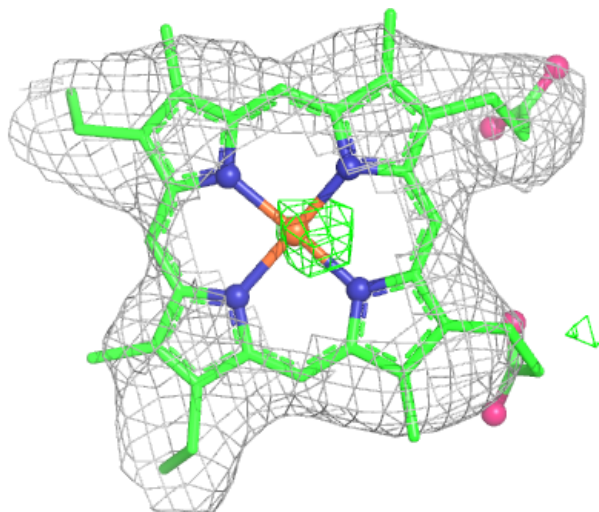
Electron density around HEC A 672:

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



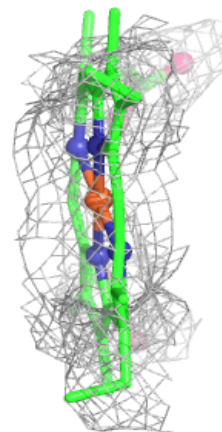
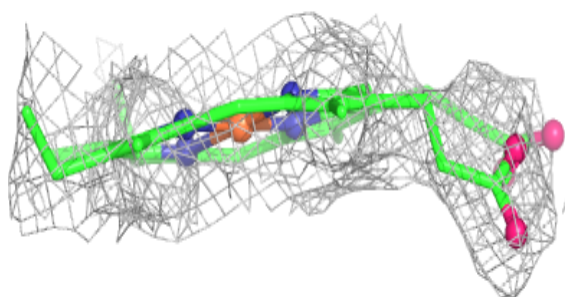
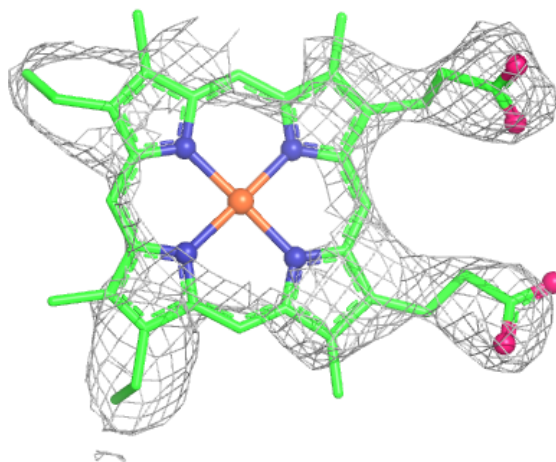
Electron density around HEC A 676:

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



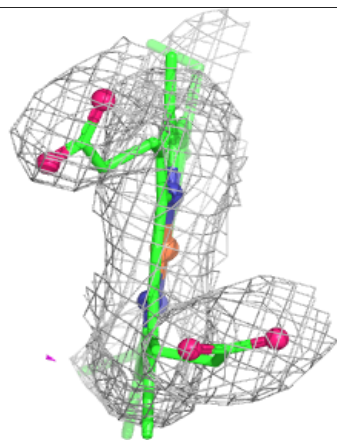
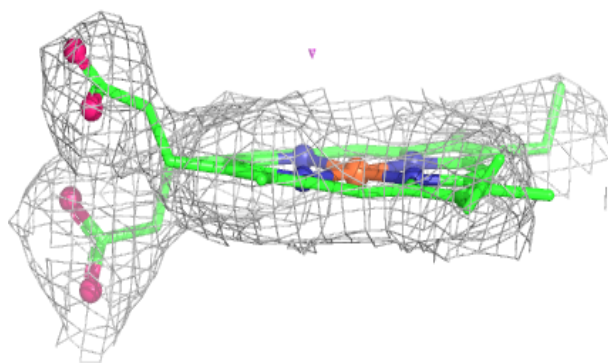
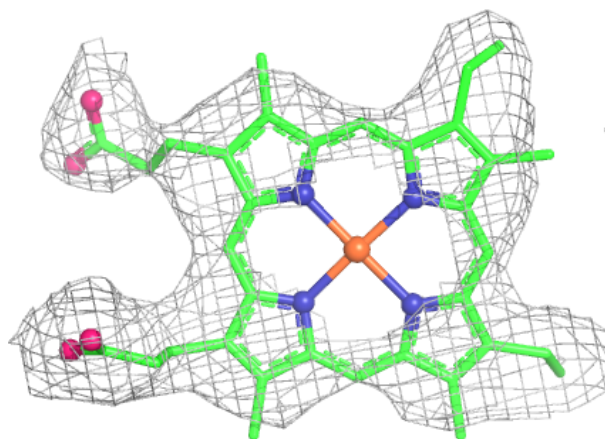
Electron density around HEC A 677:

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



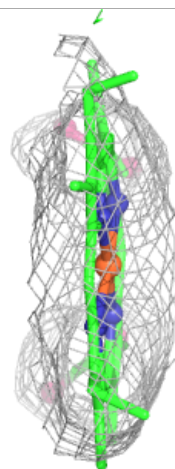
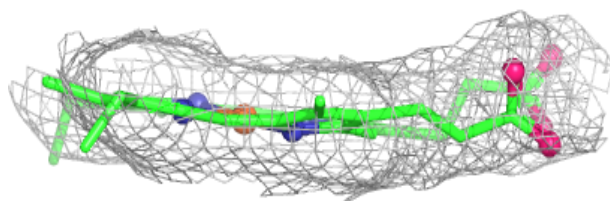
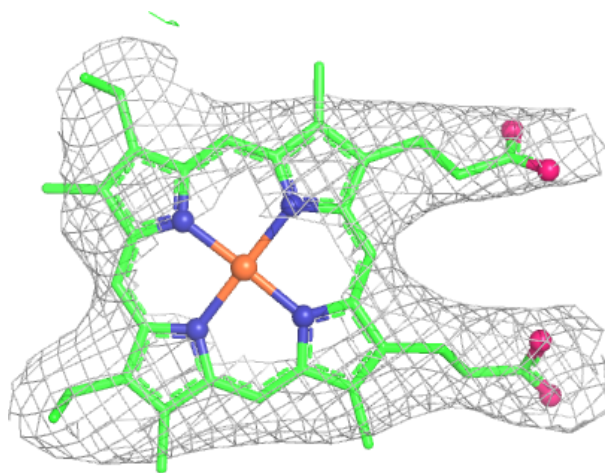
Electron density around HEC A 673:

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



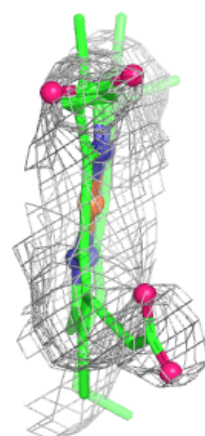
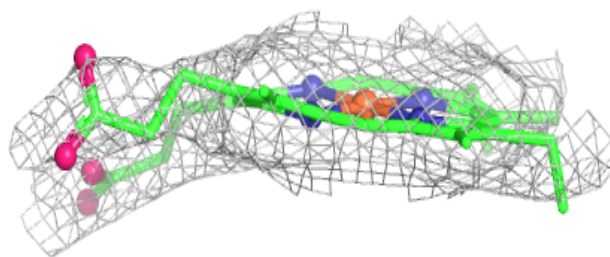
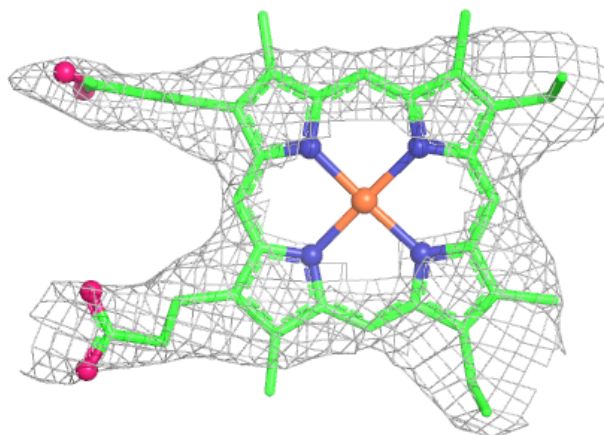
Electron density around HEC A 675:

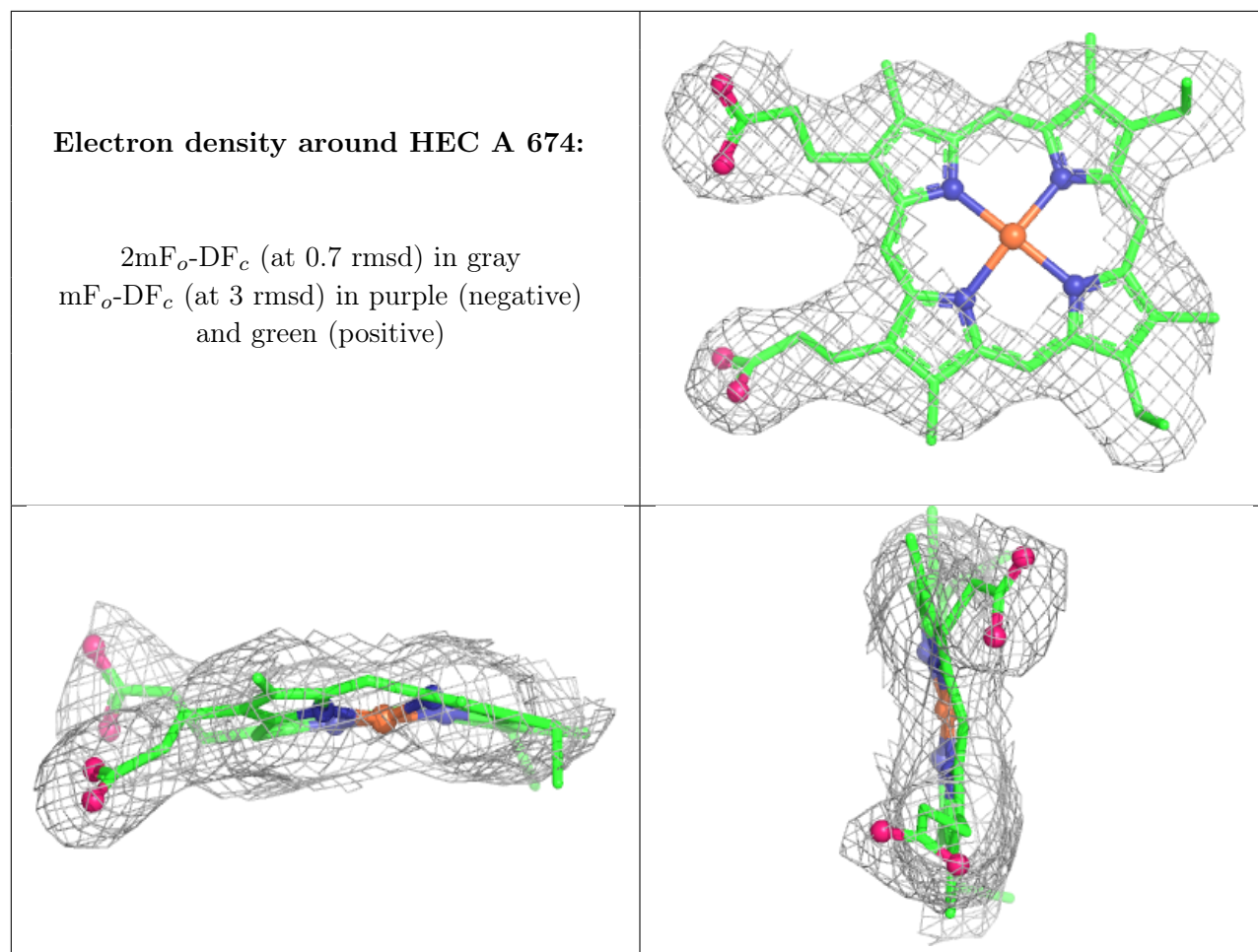
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC A 670:

$2mF_o-DF_c$ (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.