Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2026 – 04:19 AM EDT

PDB ID	:	9CUF / pdb_00009cuf
Title	:	Room temperature SSX structure of ccNiR
Authors	:	Malla, T.N.; Schmidt, M.
Deposited on	:	2024-07-26
Resolution	:	3.30 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 (i) 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 (i)) were used in the production of this report:

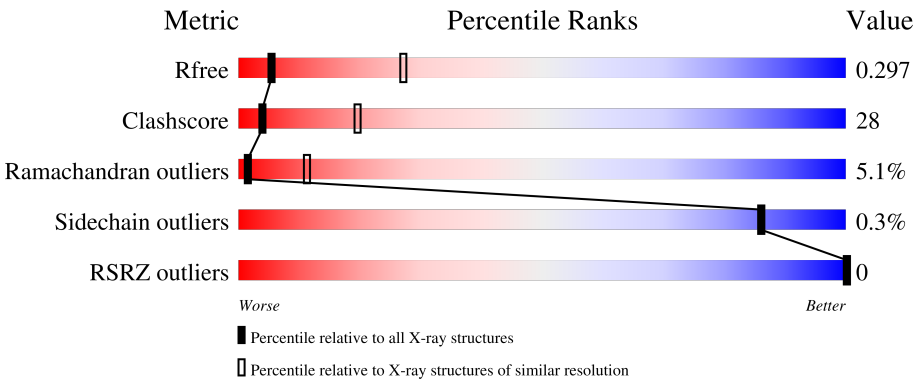
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 <=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	439	50% 47% •
1	B	439	44% 51% •

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	501	X	-	-	-
2	HEC	B	501	X	-	-	-
2	HEC	B	502	X	-	-	-
2	HEC	B	503	X	-	-	-
2	HEC	B	504	X	-	-	-

2 Entry composition (i)

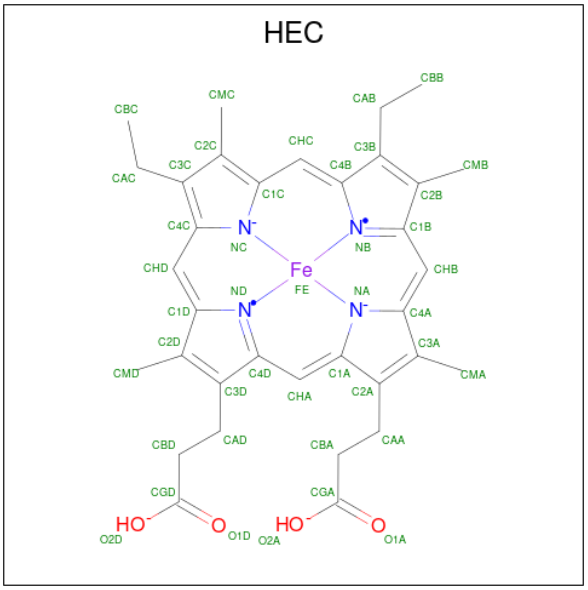
There are 4 unique types of molecules in this entry. The entry contains 7421 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome c-552.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	439	3473	2192	600	656	25	0	0	0
1	B	439	3473	2192	600	656	25	0	0	0

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

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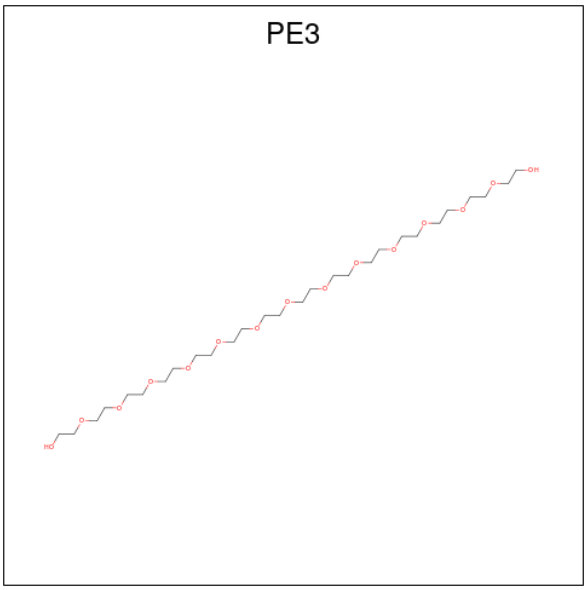
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
2	B	1	43	34	1	4	4	0	0
2	B	1	43	34	1	4	4	0	0
2	B	1	43	34	1	4	4	0	0
2	B	1	43	34	1	4	4	0	0
2	B	1	43	34	1	4	4	0	0

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

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

- Molecule 4 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDECAOXAHENTETRACONTANE-1,41-DIOL (CCD ID: PE3) (formula: $C_{28}H_{58}O_{15}$).



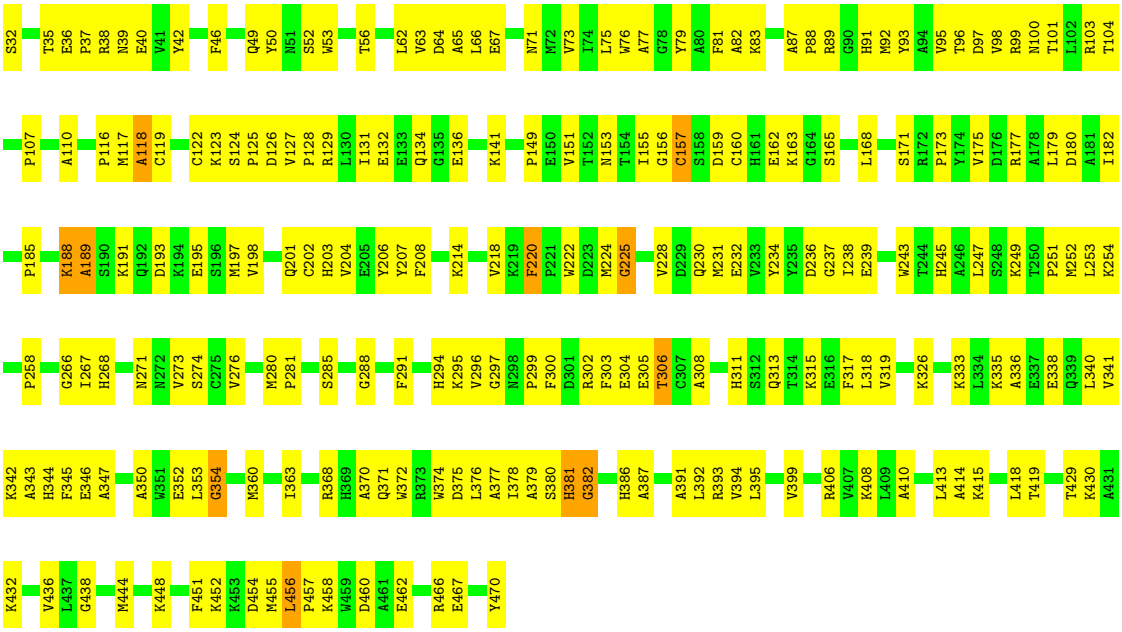
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	43	28	15	0	0

3 Residue-property plots (i)

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

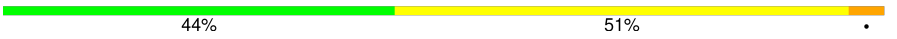
• Molecule 1: Cytochrome c-552

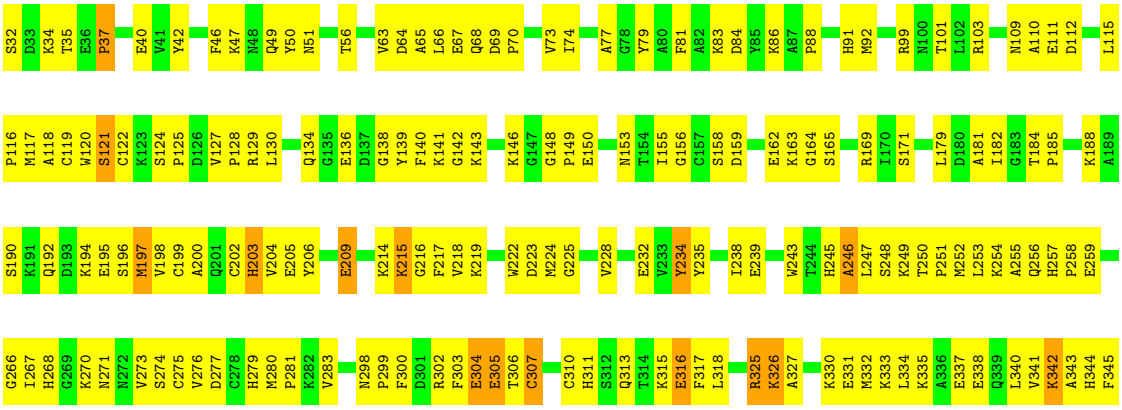
Chain A:

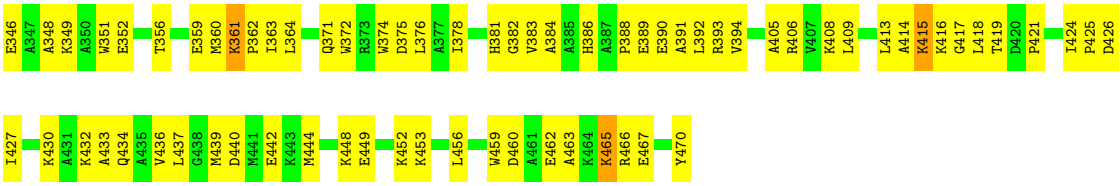


• Molecule 1: Cytochrome c-552

Chain B:






E346
A347
A348
K349
A350
W351
E352
T356
E359
M360
K361
P362
I363
L364
Q371
W372
R373
W374
D375
L376
A377
I378
H381
G382
V383
A384
A385
H386
A387
P388
E389
E390
A391
L392
R393
V394
A405
R406
V407
K408
L409
L413
A414
K415
K416
G417
L418
T419
D420
P421
I424
P425
D426
I427
K430
A431
K432
A433
Q434
A435
V436
L437
G438
M439
D440
M441
E442
K443
M444
K448
E449
K452
K453
L456
W459
D460
A461
E462
A463
K464
K465
R466
E467
Y470

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.84Å 95.47Å 228.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.49 – 3.30 59.49 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.5 (59.49-3.30) 95.5 (59.49-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.212 , 0.298 0.212 , 0.297	Depositor DCC
R_{free} test set	1749 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	113.5	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 86.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7421	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, PE3, 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	0.47	1/3558 (0.0%)	0.67	0/4801
1	B	0.44	0/3558	0.66	0/4801
All	All	0.45	1/7116 (0.0%)	0.67	0/9602

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	PHE	C-N	5.91	1.47	1.33

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	3473	0	3400	182	0
1	B	3473	0	3400	230	0
2	A	215	0	150	20	0
2	B	215	0	150	18	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	43	0	58	0	0
All	All	7421	0	7158	411	0

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

All (411) 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:B:333:LYS:HG3	1:B:378:ILE:HD13	1.46	0.96
1:A:267:ILE:HG21	2:A:505:HEC:HBA1	1.53	0.90
1:A:380:SER:O	1:A:382:GLY:N	2.08	0.86
2:A:504:HEC:HBD2	2:A:504:HEC:HHA	1.57	0.84
1:A:32:SER:N	1:A:132:GLU:O	2.15	0.80
1:B:333:LYS:HG3	1:B:378:ILE:CD1	2.13	0.79
1:B:432:LYS:O	1:B:436:VAL:HG23	1.83	0.79
1:A:363:ILE:HG12	1:A:408:LYS:HB3	1.65	0.78
1:B:69:ASP:OD2	1:B:333:LYS:NZ	2.16	0.77
1:A:36:GLU:CD	1:A:38:ARG:HH21	1.95	0.74
1:A:53:TRP:HE1	1:A:156:GLY:HA2	1.52	0.74
1:B:267:ILE:HG22	2:B:505:HEC:HBA1	1.70	0.74
1:A:273:VAL:HG13	2:A:505:HEC:HBC2	1.69	0.73
1:A:268:HIS:HB3	1:A:273:VAL:HB	1.70	0.73
1:B:245:HIS:HD2	1:B:248:SER:H	1.36	0.72
1:A:452:LYS:HA	1:A:456:LEU:HD12	1.71	0.72
1:B:120:TRP:O	1:B:122:CYS:N	2.22	0.71
1:B:333:LYS:CG	1:B:378:ILE:HD13	2.21	0.71
1:B:254:LYS:NZ	1:B:255:ALA:O	2.23	0.71
1:A:432:LYS:O	1:A:436:VAL:HG23	1.91	0.71
1:A:118:ALA:HB1	1:A:218:VAL:HG23	1.71	0.71
1:B:203:HIS:HD1	1:B:259:GLU:HG3	1.56	0.71
1:A:149:PRO:O	1:A:466:ARG:NH1	2.24	0.70
1:B:197:MET:O	1:B:200:ALA:N	2.13	0.70
1:B:414:ALA:O	1:B:417:GLY:N	2.20	0.70
1:A:245:HIS:HB2	1:A:252:MET:HG2	1.74	0.69
1:A:83:LYS:HD3	1:A:444:MET:HE1	1.75	0.69
1:A:302:ARG:O	1:A:306:THR:OG1	2.10	0.68
1:A:350:ALA:HB2	1:A:413:LEU:HG	1.75	0.68
1:B:158:SER:O	1:B:169:ARG:NH2	2.15	0.67
1:B:318:LEU:HD22	2:B:505:HEC:HMB3	1.77	0.66
1:A:39:ASN:HB3	1:A:157:CYS:SG	2.35	0.66
1:A:124:SER:OG	1:A:153:ASN:O	2.12	0.66
1:B:117:MET:O	1:B:119:CYS:N	2.28	0.66
1:B:267:ILE:CG2	2:B:505:HEC:HBA1	2.25	0.66
1:B:281:PRO:HB3	1:B:306:THR:HG22	1.76	0.66
1:A:88:PRO:HD3	1:A:381:HIS:CE1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:LYS:HB3	1:B:362:PRO:HD3	1.77	0.66
1:A:123:LYS:HZ1	2:A:501:HEC:C4C	2.08	0.65
1:A:457:PRO:HA	1:A:460:ASP:HB2	1.76	0.65
1:B:192:GLN:HA	1:B:195:GLU:HG3	1.77	0.65
1:A:377:ALA:HB2	1:A:394:VAL:HG12	1.78	0.65
1:B:110:ALA:HB1	1:B:146:LYS:HG3	1.77	0.65
1:B:326:LYS:NZ	1:B:382:GLY:HA2	2.12	0.65
1:B:437:LEU:HB2	1:B:439:MET:HG3	1.78	0.65
1:B:222:TRP:O	1:B:224:MET:N	2.29	0.65
1:A:419:THR:HB	1:B:415:LYS:HG2	1.77	0.65
1:A:228:VAL:HG11	1:A:394:VAL:HG22	1.79	0.64
1:A:311:HIS:HD2	2:A:505:HEC:NB	1.95	0.63
1:A:93:TYR:O	1:A:97:ASP:N	2.26	0.63
1:B:249:LYS:HB3	1:B:351:TRP:HE1	1.64	0.63
1:B:205:GLU:OE1	1:B:256:GLN:N	2.32	0.63
2:B:502:HEC:HBD2	2:B:502:HEC:HBA1	1.81	0.63
1:B:315:LYS:O	1:B:318:LEU:N	2.32	0.63
1:A:353:LEU:HD11	1:A:418:LEU:HD22	1.80	0.62
1:B:449:GLU:HG2	1:B:452:LYS:HD2	1.81	0.62
1:B:449:GLU:HA	1:B:452:LYS:HB2	1.82	0.62
1:B:276:VAL:HG13	1:B:280:MET:HB2	1.82	0.61
1:A:315:LYS:O	1:A:319:VAL:HG23	2.01	0.61
1:B:344:HIS:O	1:B:348:ALA:N	2.27	0.61
1:A:71:ASN:O	1:A:75:LEU:HG	2.01	0.61
1:A:95:VAL:HG23	1:A:123:LYS:O	2.02	0.60
1:B:267:ILE:HD12	1:B:270:LYS:HG3	1.82	0.60
1:B:141:LYS:HE2	1:B:215:LYS:HG2	1.83	0.60
1:B:374:TRP:NE1	1:B:378:ILE:HD11	2.15	0.60
1:B:252:MET:HE1	1:B:371:GLN:HB3	1.82	0.60
1:B:120:TRP:CZ2	1:B:148:GLY:HA2	2.37	0.60
1:A:162:GLU:O	1:A:165:SER:N	2.35	0.60
1:A:393:ARG:HB2	1:B:392:LEU:HD13	1.84	0.60
1:B:99:ARG:HD3	1:B:456:LEU:HD22	1.83	0.60
1:A:99:ARG:HE	1:A:456:LEU:HD22	1.65	0.60
1:A:168:LEU:HB3	1:A:198:VAL:HG11	1.82	0.60
1:B:49:GLN:NE2	2:B:502:HEC:O1A	2.33	0.60
1:B:129:ARG:NH2	1:B:150:GLU:OE1	2.35	0.59
1:B:345:PHE:HD2	1:B:424:ILE:HD13	1.66	0.59
1:B:363:ILE:HG21	1:B:409:LEU:HD21	1.84	0.59
1:B:203:HIS:HB3	1:B:259:GLU:HG3	1.83	0.59
1:A:276:VAL:HG13	1:A:280:MET:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LEU:HD22	1:A:418:LEU:HD23	1.84	0.59
1:B:279:HIS:CE1	1:B:299:PRO:HD3	2.38	0.59
1:B:140:PHE:HE1	1:B:218:VAL:HG23	1.67	0.59
1:A:252:MET:HE2	1:A:371:GLN:NE2	2.18	0.58
1:B:67:GLU:HA	1:B:430:LYS:HB3	1.85	0.58
1:B:65:ALA:HA	1:B:68:GLN:HB2	1.86	0.58
1:A:392:LEU:HD13	1:B:393:ARG:HB2	1.85	0.58
1:B:185:PRO:HG2	1:B:188:LYS:HB2	1.86	0.58
1:B:440:ASP:O	1:B:444:MET:HG3	2.04	0.58
1:A:180:ASP:OD1	1:A:185:PRO:HB3	2.03	0.57
1:B:427:ILE:HG22	1:B:433:ALA:HA	1.87	0.57
1:A:285:SER:OG	1:A:288:GLY:N	2.30	0.56
1:B:74:ILE:HG21	1:B:341:VAL:HG13	1.85	0.56
1:B:384:ALA:HA	1:B:388:PRO:HB3	1.87	0.56
1:B:47:LYS:O	1:B:51:ASN:ND2	2.38	0.56
1:B:67:GLU:HB2	1:B:430:LYS:HD2	1.86	0.56
1:B:245:HIS:CD2	1:B:248:SER:H	2.22	0.56
1:B:326:LYS:HZ3	1:B:382:GLY:HA2	1.70	0.56
1:A:39:ASN:HD21	1:A:125:PRO:HG3	1.71	0.56
1:A:53:TRP:CH2	1:A:92:MET:HE1	2.40	0.56
1:A:195:GLU:OE1	1:A:274:SER:OG	2.20	0.56
1:A:56:THR:HB	1:A:91:HIS:H	1.71	0.56
1:A:77:ALA:HB3	1:A:245:HIS:CE1	2.40	0.56
1:A:225:GLY:O	1:A:231:MET:HG3	2.06	0.55
1:B:274:SER:OG	1:B:277:ASP:N	2.35	0.55
1:A:193:ASP:O	1:A:197:MET:HG3	2.06	0.55
1:A:185:PRO:HG2	1:A:188:LYS:HE3	1.88	0.55
1:A:96:THR:O	1:A:100:ASN:ND2	2.40	0.55
1:B:79:TYR:HD2	1:B:81:PHE:HD2	1.54	0.55
1:B:222:TRP:O	1:B:225:GLY:N	2.41	0.54
1:B:351:TRP:CE3	1:B:351:TRP:HA	2.41	0.54
1:A:39:ASN:ND2	1:A:156:GLY:HA3	2.23	0.54
1:A:49:GLN:HG2	2:A:502:HEC:C3A	2.38	0.54
1:B:155:ILE:HG12	2:B:503:HEC:HBC2	1.89	0.54
1:A:251:PRO:O	1:A:368:ARG:NH1	2.39	0.54
1:A:162:GLU:HB2	1:A:165:SER:HB3	1.90	0.54
1:A:236:ASP:O	1:A:239:GLU:N	2.37	0.54
1:B:56:THR:HB	1:B:91:HIS:H	1.72	0.54
1:B:316:GLU:N	1:B:316:GLU:OE1	2.41	0.54
1:B:77:ALA:CB	1:B:247:LEU:HD12	2.38	0.53
1:B:184:THR:O	1:B:184:THR:OG1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:SER:HB3	1:A:151:VAL:HG13	1.90	0.53
1:B:124:SER:OG	1:B:153:ASN:O	2.16	0.53
1:B:345:PHE:HE2	1:B:425:PRO:HD2	1.74	0.53
1:B:42:TYR:CE2	1:B:164:GLY:HA2	2.43	0.53
1:B:342:LYS:O	1:B:346:GLU:HG3	2.08	0.53
1:B:349:LYS:HG3	1:B:413:LEU:HD21	1.91	0.53
1:B:203:HIS:ND1	1:B:259:GLU:HG3	2.23	0.53
1:B:361:LYS:HB3	1:B:362:PRO:CD	2.39	0.53
1:A:117:MET:O	1:A:119:CYS:N	2.42	0.52
1:A:245:HIS:CE1	1:A:344:HIS:CD2	2.97	0.52
1:B:162:GLU:HB2	1:B:165:SER:HB3	1.90	0.52
1:B:128:PRO:HB3	1:B:171:SER:HB2	1.91	0.52
1:A:258:PRO:HD2	1:A:379:ALA:HB3	1.90	0.52
1:B:150:GLU:OE1	1:B:466:ARG:NH2	2.42	0.52
1:B:194:LYS:HA	1:B:197:MET:HG3	1.90	0.52
2:A:501:HEC:HHA	2:A:501:HEC:O1D	2.09	0.52
1:A:71:ASN:HB3	1:A:341:VAL:HG21	1.91	0.52
1:A:304:GLU:HA	1:A:308:ALA:HB2	1.92	0.52
1:A:326:LYS:NZ	2:A:504:HEC:O2D	2.36	0.52
1:B:341:VAL:C	1:B:343:ALA:H	2.17	0.52
1:B:390:GLU:OE1	1:B:393:ARG:NE	2.32	0.52
1:A:206:TYR:OH	2:A:501:HEC:HHC	2.10	0.52
1:B:73:VAL:HG11	1:B:434:GLN:HG3	1.92	0.52
1:B:79:TYR:HD2	1:B:81:PHE:CD2	2.28	0.52
1:B:333:LYS:O	1:B:337:GLU:HG3	2.10	0.52
1:A:49:GLN:HG2	2:A:502:HEC:C4A	2.40	0.51
1:B:99:ARG:NH2	1:B:460:ASP:OD1	2.42	0.51
1:B:334:LEU:O	1:B:338:GLU:HG2	2.10	0.51
1:A:311:HIS:CE1	2:A:505:HEC:ND	2.75	0.51
1:B:219:LYS:NZ	1:B:234:TYR:OH	2.43	0.51
1:B:345:PHE:CD2	1:B:424:ILE:HD13	2.44	0.51
1:A:37:PRO:HD3	1:A:129:ARG:HD3	1.91	0.51
1:B:462:GLU:O	1:B:465:LYS:HB3	2.10	0.51
1:B:63:VAL:O	1:B:65:ALA:N	2.43	0.51
1:B:326:LYS:NZ	1:B:381:HIS:O	2.44	0.51
1:A:131:ILE:HD13	1:A:136:GLU:HG2	1.92	0.51
1:A:204:VAL:HG21	1:A:220:PHE:CZ	2.45	0.51
1:B:302:ARG:HB3	1:B:305:GLU:OE1	2.11	0.51
1:A:304:GLU:O	1:A:306:THR:N	2.38	0.51
1:B:182:ILE:HG21	1:B:222:TRP:HE3	1.75	0.51
1:A:46:PHE:HB3	1:A:49:GLN:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLU:HA	1:A:430:LYS:HB2	1.92	0.51
1:A:127:VAL:HB	1:A:128:PRO:HD3	1.93	0.51
1:A:267:ILE:CG2	2:A:505:HEC:HBA1	2.35	0.51
1:A:280:MET:HG2	1:A:296:VAL:HG22	1.92	0.50
1:A:415:LYS:HG2	1:B:419:THR:HB	1.92	0.50
1:B:127:VAL:H	1:B:128:PRO:HD2	1.75	0.50
1:B:206:TYR:OH	1:B:256:GLN:OE1	2.25	0.50
1:B:315:LYS:O	1:B:317:PHE:N	2.44	0.50
1:B:356:THR:OG1	1:B:359:GLU:HG3	2.11	0.50
1:A:76:TRP:O	1:A:82:ALA:HB2	2.12	0.50
1:A:126:ASP:HB2	1:A:151:VAL:HG22	1.92	0.50
1:A:122:CYS:HB3	1:A:202:CYS:HB3	1.94	0.50
1:A:160:CYS:O	1:A:168:LEU:HA	2.11	0.50
1:A:64:ASP:O	1:A:66:LEU:N	2.44	0.50
1:A:125:PRO:O	1:A:128:PRO:HD2	2.11	0.50
1:A:335:LYS:HA	1:A:338:GLU:HB2	1.94	0.50
1:A:380:SER:C	1:A:382:GLY:H	2.11	0.50
1:B:182:ILE:HG21	1:B:222:TRP:CE3	2.47	0.49
1:B:197:MET:O	1:B:199:CYS:N	2.45	0.49
1:A:49:GLN:HE22	1:A:291:PHE:HB2	1.77	0.49
1:B:121:SER:HA	1:B:127:VAL:HG11	1.94	0.49
1:A:207:TYR:HD2	1:A:208:PHE:O	1.95	0.49
1:A:333:LYS:HA	1:A:395:LEU:HD21	1.93	0.49
1:B:310:CYS:HB2	2:B:505:HEC:C2C	2.41	0.49
1:A:414:ALA:HA	1:A:418:LEU:O	2.13	0.49
1:B:111:GLU:O	1:B:143:LYS:HG3	2.13	0.49
1:A:42:TYR:HB3	1:A:46:PHE:CD2	2.48	0.49
1:B:214:LYS:HD2	1:B:217:PHE:CE2	2.48	0.49
1:B:281:PRO:O	1:B:283:VAL:HG13	2.12	0.49
2:A:502:HEC:HBD2	2:A:502:HEC:HHA	1.95	0.49
1:B:303:PHE:O	1:B:305:GLU:N	2.46	0.49
1:B:37:PRO:HG3	1:B:129:ARG:HD3	1.95	0.48
1:B:111:GLU:HA	1:B:143:LYS:HB2	1.95	0.48
1:B:245:HIS:HD2	1:B:248:SER:N	2.06	0.48
1:A:79:TYR:HB2	1:A:243:TRP:CE2	2.48	0.48
1:A:88:PRO:HD3	1:A:381:HIS:ND1	2.28	0.48
1:A:336:ALA:HA	1:A:399:VAL:HG22	1.96	0.48
1:A:107:PRO:HG2	1:A:451:PHE:HE2	1.78	0.48
1:B:88:PRO:HB3	2:B:501:HEC:HAD2	1.95	0.48
1:B:134:GLN:HB3	1:B:138:GLY:HA3	1.95	0.48
1:B:125:PRO:HA	1:B:128:PRO:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:VAL:O	1:B:343:ALA:N	2.47	0.48
1:A:66:LEU:HD22	1:A:73:VAL:HG23	1.96	0.48
1:B:125:PRO:C	1:B:128:PRO:HD2	2.38	0.48
1:A:81:PHE:CE1	1:A:254:LYS:HE3	2.49	0.48
1:A:124:SER:CB	1:A:151:VAL:HG13	2.44	0.48
1:A:224:MET:HB2	1:A:230:GLN:O	2.14	0.48
1:A:185:PRO:HD2	1:A:188:LYS:NZ	2.29	0.47
1:A:193:ASP:HB3	1:A:197:MET:HE3	1.96	0.47
1:B:47:LYS:HD2	1:B:47:LYS:HA	1.65	0.47
1:A:36:GLU:OE2	1:A:38:ARG:NH2	2.44	0.47
1:A:352:GLU:C	1:A:354:GLY:H	2.22	0.47
1:A:125:PRO:C	1:A:127:VAL:H	2.23	0.47
1:A:104:THR:OG1	1:A:448:LYS:NZ	2.48	0.47
1:B:257:HIS:O	1:B:259:GLU:HG2	2.15	0.47
1:B:405:ALA:O	1:B:408:LYS:N	2.47	0.47
1:A:271:ASN:ND2	2:A:505:HEC:HAD2	2.30	0.47
1:B:243:TRP:HZ3	1:B:254:LYS:HB2	1.79	0.47
1:B:250:THR:O	1:B:252:MET:HG2	2.15	0.47
1:B:382:GLY:O	1:B:386:HIS:ND1	2.34	0.47
1:B:232:GLU:HB2	1:B:372:TRP:NE1	2.29	0.47
1:A:281:PRO:HB2	1:A:305:GLU:HB3	1.96	0.47
1:B:254:LYS:NZ	1:B:375:ASP:OD1	2.48	0.47
1:B:426:ASP:O	1:B:432:LYS:HB3	2.15	0.46
1:A:125:PRO:HD3	1:A:155:ILE:HA	1.97	0.46
1:A:300:PHE:C	1:A:302:ARG:H	2.24	0.46
1:B:426:ASP:OD2	1:B:432:LYS:NZ	2.43	0.46
1:A:304:GLU:HA	1:A:308:ALA:CB	2.45	0.46
1:B:68:GLN:C	1:B:70:PRO:HD3	2.41	0.46
1:B:103:ARG:O	1:B:115:LEU:HD11	2.16	0.46
1:B:125:PRO:HG3	1:B:156:GLY:HA3	1.97	0.46
1:B:202:CYS:O	1:B:204:VAL:N	2.47	0.46
1:B:40:GLU:OE2	1:B:50:TYR:OH	2.26	0.46
1:A:136:GLU:OE2	1:A:177:ARG:NH1	2.34	0.46
1:A:179:LEU:HD23	1:A:182:ILE:HD11	1.98	0.46
1:B:386:HIS:NE2	2:B:504:HEC:C1C	2.78	0.46
1:A:415:LYS:HE2	1:B:419:THR:HB	1.98	0.46
1:A:303:PHE:CE1	1:A:315:LYS:HA	2.51	0.46
1:B:34:LYS:O	1:B:163:LYS:HB2	2.16	0.46
1:A:377:ALA:HB2	1:A:394:VAL:CG1	2.46	0.46
1:B:266:GLY:HA2	1:B:389:GLU:OE2	2.16	0.46
1:B:316:GLU:H	1:B:316:GLU:CD	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:PHE:CE2	1:B:425:PRO:HD2	2.50	0.46
1:A:236:ASP:O	1:A:238:ILE:N	2.49	0.46
1:A:295:LYS:O	1:A:295:LYS:HD3	2.16	0.45
1:A:83:LYS:NZ	1:A:444:MET:HE1	2.31	0.45
1:A:371:GLN:O	1:A:371:GLN:HG2	2.15	0.45
1:B:267:ILE:O	1:B:271:ASN:ND2	2.50	0.45
1:B:268:HIS:HD2	1:B:273:VAL:HG11	1.82	0.45
1:B:331:GLU:HG3	1:B:335:LYS:NZ	2.30	0.45
1:B:149:PRO:HA	1:B:459:TRP:HB3	1.98	0.45
1:B:279:HIS:CD2	2:B:504:HEC:NC	2.85	0.45
1:B:279:HIS:HD2	2:B:504:HEC:NC	2.14	0.45
1:B:352:GLU:HG2	1:B:352:GLU:O	2.16	0.45
1:B:386:HIS:CD2	2:B:504:HEC:C1C	3.00	0.45
1:A:156:GLY:O	1:A:159:ASP:HB2	2.17	0.45
1:B:92:MET:HE3	1:B:92:MET:HB3	1.84	0.45
1:B:179:LEU:C	1:B:181:ALA:H	2.24	0.45
1:B:234:TYR:O	1:B:235:TYR:C	2.59	0.45
1:B:351:TRP:CZ3	1:B:360:MET:HG3	2.52	0.45
1:A:232:GLU:HG3	1:A:372:TRP:CD1	2.52	0.45
1:A:375:ASP:O	1:A:379:ALA:HB2	2.17	0.45
1:B:109:ASN:H	1:B:112:ASP:HB2	1.81	0.45
1:B:245:HIS:C	1:B:247:LEU:H	2.25	0.45
1:B:311:HIS:HB3	1:B:313:GLN:OE1	2.16	0.45
1:A:342:LYS:HB3	1:A:406:ARG:NH2	2.33	0.44
1:B:268:HIS:CE1	2:B:505:HEC:NB	2.85	0.44
1:B:248:SER:HG	1:B:344:HIS:HD1	1.59	0.44
1:A:83:LYS:CD	1:A:444:MET:HE1	2.44	0.44
1:B:32:SER:HB3	1:B:35:THR:O	2.18	0.44
1:B:101:THR:HG21	2:B:501:HEC:HMA1	1.99	0.44
1:B:306:THR:OG1	1:B:307:CYS:N	2.48	0.44
1:A:281:PRO:HG3	1:A:302:ARG:HD2	2.00	0.44
1:B:390:GLU:O	1:B:394:VAL:HG23	2.17	0.44
1:B:430:LYS:HE2	1:B:434:GLN:HE22	1.82	0.44
1:A:35:THR:HG22	1:A:36:GLU:H	1.82	0.44
1:A:406:ARG:O	1:A:410:ALA:N	2.49	0.44
1:B:77:ALA:HB3	1:B:245:HIS:CE1	2.51	0.44
1:B:196:SER:O	1:B:199:CYS:HB2	2.17	0.44
1:A:386:HIS:NE2	2:A:504:HEC:NB	2.66	0.44
2:A:504:HEC:HMC3	2:A:504:HEC:HBC3	1.99	0.44
1:A:346:GLU:OE2	1:A:406:ARG:NH2	2.51	0.44
1:B:351:TRP:HA	1:B:351:TRP:HE3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:LEU:HA	1:A:392:LEU:HD23	1.74	0.44
1:B:81:PHE:HE2	1:B:254:LYS:HG2	1.83	0.44
1:B:84:ASP:O	1:B:103:ARG:HD3	2.18	0.44
1:B:203:HIS:HB3	1:B:259:GLU:HB2	2.00	0.44
1:B:342:LYS:HB3	1:B:406:ARG:CZ	2.48	0.44
1:B:42:TYR:HD2	1:B:46:PHE:CE1	2.36	0.44
1:B:117:MET:N	1:B:142:GLY:O	2.48	0.44
1:B:156:GLY:O	1:B:159:ASP:HB2	2.18	0.44
1:B:214:LYS:O	1:B:216:GLY:N	2.51	0.44
1:B:268:HIS:CD2	1:B:273:VAL:HG11	2.53	0.44
1:A:125:PRO:HD2	1:A:153:ASN:O	2.18	0.43
1:A:258:PRO:HG3	1:A:376:LEU:CD1	2.48	0.43
1:B:50:TYR:HA	2:B:502:HEC:HBB2	1.99	0.43
1:B:275:CYS:HA	2:B:504:HEC:HHC	1.99	0.43
1:A:49:GLN:NE2	2:A:502:HEC:HBA2	2.33	0.43
1:B:245:HIS:CD2	1:B:247:LEU:HB2	2.52	0.43
1:B:325:ARG:O	1:B:327:ALA:N	2.47	0.43
1:B:340:LEU:HD11	1:B:371:GLN:HA	2.00	0.43
1:B:448:LYS:O	1:B:452:LYS:HG3	2.18	0.43
1:A:62:LEU:HG	1:A:89:ARG:HD3	1.99	0.43
1:A:254:LYS:HA	1:A:254:LYS:HD2	1.72	0.43
1:B:117:MET:C	1:B:119:CYS:H	2.26	0.43
1:B:338:GLU:O	1:B:342:LYS:HB2	2.19	0.43
1:B:430:LYS:HB2	1:B:430:LYS:HE3	1.56	0.43
1:B:414:ALA:C	1:B:416:LYS:N	2.75	0.43
1:B:414:ALA:C	1:B:416:LYS:H	2.27	0.43
1:A:101:THR:OG1	1:A:103:ARG:HG3	2.18	0.43
1:A:299:PRO:HB2	2:A:505:HEC:HBB1	2.01	0.43
1:A:333:LYS:HA	1:A:395:LEU:CD2	2.49	0.43
1:A:418:LEU:HD12	1:A:418:LEU:HA	1.71	0.43
1:B:37:PRO:HB2	1:B:153:ASN:OD1	2.18	0.43
1:A:224:MET:HG2	1:A:234:TYR:HB2	2.01	0.43
1:A:343:ALA:HA	1:A:346:GLU:HB2	2.00	0.43
1:A:345:PHE:C	1:A:347:ALA:H	2.26	0.43
1:B:374:TRP:CE2	1:B:378:ILE:HD11	2.53	0.43
1:A:35:THR:HG22	1:A:36:GLU:N	2.34	0.43
1:A:313:GLN:HB3	1:A:317:PHE:HD2	1.84	0.43
1:A:454:ASP:HB3	1:A:458:LYS:NZ	2.34	0.43
1:B:222:TRP:CD1	1:B:222:TRP:N	2.86	0.43
1:B:266:GLY:HA3	1:B:386:HIS:O	2.19	0.43
1:A:35:THR:OG1	1:A:132:GLU:OE1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:VAL:HG21	1:A:220:PHE:CE2	2.54	0.42
1:A:266:GLY:CA	1:A:387:ALA:HB2	2.48	0.42
1:A:333:LYS:HE2	1:A:378:ILE:HD13	2.00	0.42
1:B:304:GLU:O	1:B:305:GLU:HG3	2.18	0.42
1:B:332:MET:HB3	1:B:332:MET:HE3	1.62	0.42
1:A:243:TRP:CZ3	1:A:252:MET:HB3	2.54	0.42
1:B:267:ILE:HA	1:B:270:LYS:HB2	2.01	0.42
1:B:337:GLU:O	1:B:340:LEU:N	2.51	0.42
1:B:35:THR:HG21	1:B:128:PRO:HG2	2.01	0.42
1:B:81:PHE:CE2	1:B:254:LYS:HG2	2.54	0.42
1:B:463:ALA:HA	1:B:466:ARG:NH1	2.33	0.42
1:A:75:LEU:HD12	1:A:374:TRP:CH2	2.54	0.42
1:A:95:VAL:HG21	1:A:124:SER:HB2	2.01	0.42
1:A:303:PHE:HZ	1:A:318:LEU:HD12	1.84	0.42
1:A:123:LYS:HZ1	2:A:501:HEC:C3C	2.31	0.42
1:B:140:PHE:CG	1:B:217:PHE:HD1	2.38	0.42
1:B:232:GLU:HB2	1:B:372:TRP:HE1	1.85	0.42
1:B:257:HIS:NE2	2:B:501:HEC:C1D	2.82	0.42
1:B:449:GLU:HB3	1:B:453:LYS:HE3	2.02	0.42
1:A:64:ASP:C	1:A:66:LEU:H	2.27	0.42
1:A:53:TRP:HA	1:A:294:HIS:O	2.19	0.42
1:A:222:TRP:C	1:A:225:GLY:HA3	2.45	0.42
1:A:313:GLN:CB	1:A:317:PHE:HD2	2.32	0.42
1:B:195:GLU:O	1:B:276:VAL:HG23	2.19	0.42
1:B:203:HIS:HB3	1:B:259:GLU:CG	2.47	0.42
1:B:101:THR:C	1:B:103:ARG:H	2.26	0.42
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.89	0.42
1:A:391:ALA:O	1:A:395:LEU:HB2	2.20	0.42
1:B:325:ARG:C	1:B:327:ALA:H	2.27	0.42
1:A:188:LYS:HB2	1:A:189:ALA:H	1.50	0.41
1:B:117:MET:HB2	1:B:140:PHE:O	2.20	0.41
1:B:253:LEU:HA	1:B:253:LEU:HD23	1.83	0.41
1:A:128:PRO:CG	1:A:171:SER:HB2	2.50	0.41
1:A:214:LYS:HD3	1:A:214:LYS:HA	1.85	0.41
1:A:300:PHE:C	1:A:302:ARG:N	2.78	0.41
1:B:81:PHE:C	1:B:83:LYS:H	2.28	0.41
1:B:383:VAL:HG22	1:B:391:ALA:HB2	2.01	0.41
1:B:418:LEU:HD12	1:B:419:THR:H	1.85	0.41
1:B:298:ASN:O	1:B:300:PHE:N	2.52	0.41
1:A:245:HIS:O	1:A:249:LYS:HA	2.20	0.41
1:A:63:VAL:HB	1:A:87:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:VAL:O	1:A:104:THR:HG21	2.21	0.41
1:B:136:GLU:O	1:B:139:TYR:N	2.45	0.41
1:A:40:GLU:HA	1:A:50:TYR:CE2	2.55	0.41
1:A:462:GLU:O	1:A:462:GLU:HG2	2.21	0.41
1:B:149:PRO:HB3	1:B:459:TRP:HA	2.03	0.41
1:B:206:TYR:CZ	1:B:256:GLN:OE1	2.73	0.41
1:B:414:ALA:O	1:B:416:LYS:N	2.53	0.41
1:B:440:ASP:C	1:B:442:GLU:H	2.27	0.41
1:A:415:LYS:HE2	1:B:419:THR:O	2.20	0.41
1:B:238:ILE:O	1:B:239:GLU:C	2.63	0.41
1:B:459:TRP:H	1:B:459:TRP:CD1	2.39	0.41
1:A:83:LYS:CE	1:A:444:MET:HE1	2.51	0.41
1:B:228:VAL:HG11	1:B:394:VAL:HG13	2.01	0.41
1:B:376:LEU:HD12	1:B:376:LEU:HA	1.82	0.41
1:B:430:LYS:HE2	1:B:434:GLN:NE2	2.35	0.41
1:A:63:VAL:H	1:A:87:ALA:HB3	1.86	0.41
1:A:123:LYS:HZ2	1:A:123:LYS:HG2	1.67	0.41
1:A:191:LYS:O	1:A:195:GLU:HG3	2.21	0.41
1:A:378:ILE:HD12	1:A:378:ILE:O	2.19	0.41
1:A:203:HIS:CD2	2:A:503:HEC:C1C	3.04	0.41
1:A:245:HIS:CE1	1:A:247:LEU:HB2	2.56	0.41
1:A:340:LEU:HD21	1:A:370:ALA:HB1	2.03	0.41
1:B:77:ALA:O	1:B:246:ALA:N	2.53	0.41
1:B:140:PHE:CD1	1:B:217:PHE:HA	2.56	0.41
1:B:327:ALA:HA	1:B:330:LYS:HB3	2.03	0.41
1:B:360:MET:O	1:B:364:LEU:HG	2.21	0.41
1:B:444:MET:HE2	1:B:444:MET:HB3	1.77	0.41
1:B:467:GLU:HA	1:B:470:TYR:HE1	1.86	0.41
1:A:52:SER:OG	1:A:294:HIS:HB2	2.21	0.40
1:A:467:GLU:HG2	1:A:470:TYR:CE2	2.57	0.40
1:B:116:PRO:HA	1:B:143:LYS:HA	2.04	0.40
1:B:209:GLU:HB3	1:B:214:LYS:HB2	2.02	0.40
1:B:258:PRO:HB3	1:B:376:LEU:HD11	2.03	0.40
1:A:100:ASN:O	1:A:448:LYS:HE2	2.22	0.40
1:A:159:ASP:O	1:A:171:SER:OG	2.34	0.40
1:A:201:GLN:HE21	1:A:201:GLN:HB2	1.77	0.40
1:B:84:ASP:OD2	1:B:86:LYS:NZ	2.54	0.40
1:B:311:HIS:NE2	2:B:505:HEC:NB	2.69	0.40
1:A:175:VAL:HG21	1:A:201:GLN:HG2	2.02	0.40
1:A:207:TYR:CE1	1:A:234:TYR:HE2	2.40	0.40
1:A:429:THR:HG23	1:A:432:LYS:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LEU:HD23	1:B:247:LEU:HA	1.89	0.40
1:B:66:LEU:HD11	1:B:81:PHE:O	2.21	0.40
1:B:129:ARG:CZ	1:B:130:LEU:HD21	2.52	0.40
1:B:140:PHE:CE1	1:B:218:VAL:HG23	2.52	0.40
1:B:326:LYS:HZ1	1:B:382:GLY:HA2	1.83	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	437/439 (100%)	357 (82%)	58 (13%)	22 (5%)	1 11
1	B	437/439 (100%)	333 (76%)	81 (18%)	23 (5%)	1 10
All	All	874/878 (100%)	690 (79%)	139 (16%)	45 (5%)	1 11

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	LYS
1	A	381	HIS
1	B	121	SER
1	B	190	SER
1	B	209	GLU
1	B	223	ASP
1	B	305	GLU
1	A	65	ALA
1	A	189	ALA
1	A	237	GLY
1	A	438	GLY
1	A	455	MET
1	B	64	ASP

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Mol	Chain	Res	Type
1	B	118	ALA
1	B	197	MET
1	B	215	LYS
1	B	304	GLU
1	B	316	GLU
1	B	326	LYS
1	B	342	LYS
1	A	118	ALA
1	A	134	GLN
1	A	163	LYS
1	A	173	PRO
1	A	225	GLY
1	A	306	THR
1	B	203	HIS
1	B	246	ALA
1	B	421	PRO
1	B	465	LYS
1	A	157	CYS
1	A	360	MET
1	A	110	ALA
1	A	116	PRO
1	A	354	GLY
1	A	456	LEU
1	B	37	PRO
1	B	234	TYR
1	B	415	LYS
1	A	141	LYS
1	B	361	LYS
1	A	382	GLY
1	B	198	VAL
1	B	251	PRO
1	A	297	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	367/367 (100%)	367 (100%)	0	100	100
1	B	367/367 (100%)	365 (100%)	2 (0%)	81	83
All	All	734/734 (100%)	732 (100%)	2 (0%)	86	86

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	307	CYS
1	B	325	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	51	ASN
1	A	201	GLN
1	B	192	GLN
1	B	245	HIS
1	B	272	ASN
1	B	371	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	502	1	50,50,50	2.06	7 (14%)	68,82,82	1.53	10 (14%)
2	HEC	A	503	1	50,50,50	1.91	6 (12%)	68,82,82	1.63	11 (16%)
2	HEC	A	505	1	50,50,50	2.01	3 (6%)	68,82,82	1.43	10 (14%)
2	HEC	B	503	1	50,50,50	1.82	6 (12%)	68,82,82	1.59	10 (14%)
4	PE3	B	507	-	42,42,42	0.32	0	41,41,41	0.26	0
2	HEC	B	505	1	50,50,50	1.75	5 (10%)	68,82,82	1.57	13 (19%)
2	HEC	A	501	1	50,50,50	2.06	6 (12%)	68,82,82	1.58	12 (17%)
2	HEC	B	501	1	50,50,50	1.99	3 (6%)	68,82,82	1.31	4 (5%)
2	HEC	B	504	1	50,50,50	1.84	4 (8%)	68,82,82	1.67	14 (20%)
2	HEC	B	502	1	50,50,50	1.78	6 (12%)	68,82,82	1.57	11 (16%)
2	HEC	A	504	1	50,50,50	2.00	8 (16%)	68,82,82	1.47	10 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	502	1	-	7/14/54/54	-
2	HEC	A	503	1	-	2/14/54/54	-
2	HEC	A	505	1	-	6/14/54/54	-
2	HEC	B	503	1	1/1/3/7	5/14/54/54	-
4	PE3	B	507	-	-	22/40/40/40	-
2	HEC	B	505	1	-	5/14/54/54	-
2	HEC	B	504	1	1/1/3/7	5/14/54/54	-
2	HEC	A	501	1	1/1/3/7	4/14/54/54	-
2	HEC	B	501	1	1/1/3/7	6/14/54/54	-
2	HEC	B	502	1	1/1/3/7	7/14/54/54	-
2	HEC	A	504	1	-	8/14/54/54	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	505	HEC	FE-NA	8.52	2.23	1.95
2	B	502	HEC	C3D-C2D	8.50	1.55	1.36
2	A	504	HEC	C3D-C2D	8.31	1.54	1.36
2	A	501	HEC	C3D-C2D	8.18	1.54	1.36
2	B	501	HEC	C3D-C2D	8.12	1.54	1.36
2	A	503	HEC	C3D-C2D	7.93	1.53	1.36
2	B	504	HEC	C3D-C2D	7.78	1.53	1.36
2	B	505	HEC	C3D-C2D	7.74	1.53	1.36
2	A	502	HEC	C3D-C2D	7.74	1.53	1.36
2	A	505	HEC	C3D-C2D	7.72	1.53	1.36
2	B	503	HEC	C3D-C2D	7.19	1.52	1.36
2	A	504	HEC	FE-NC	6.60	2.16	1.95
2	B	501	HEC	FE-NB	6.47	2.14	1.94
2	A	502	HEC	FE-ND	6.39	2.14	1.94
2	A	503	HEC	FE-NB	6.21	2.14	1.94
2	B	501	HEC	FE-NC	6.09	2.15	1.95
2	B	503	HEC	FE-NB	5.77	2.12	1.94
2	A	501	HEC	FE-ND	5.60	2.12	1.94
2	A	501	HEC	FE-NA	5.54	2.13	1.95
2	A	503	HEC	FE-NA	5.44	2.13	1.95
2	B	503	HEC	FE-NA	5.41	2.13	1.95
2	B	504	HEC	FE-NC	5.40	2.13	1.95
2	A	502	HEC	FE-NC	5.08	2.11	1.95
2	A	501	HEC	FE-NC	4.84	2.11	1.95
2	B	505	HEC	FE-NB	4.58	2.09	1.94
2	B	504	HEC	FE-NB	4.57	2.09	1.94
2	A	504	HEC	FE-ND	4.48	2.08	1.94
2	A	502	HEC	FE-NA	4.38	2.09	1.95
2	B	502	HEC	FE-ND	4.25	2.08	1.94
2	A	502	HEC	FE-NB	3.91	2.06	1.94
2	B	504	HEC	FE-ND	3.64	2.06	1.94
2	B	502	HEC	FE-NC	3.39	2.06	1.95
2	B	503	HEC	FE-ND	3.13	2.04	1.94
2	A	503	HEC	FE-ND	2.94	2.04	1.94
2	B	505	HEC	FE-NC	2.92	2.04	1.95
2	A	505	HEC	FE-ND	2.77	2.03	1.94
2	A	504	HEC	FE-NB	2.61	2.02	1.94
2	A	501	HEC	CMC-C2C	2.36	1.55	1.50
2	A	504	HEC	C3B-C2B	-2.36	1.31	1.36
2	B	503	HEC	CMB-C2B	2.34	1.55	1.50
2	A	504	HEC	CMA-C3A	2.27	1.55	1.50
2	B	503	HEC	CMC-C2C	2.22	1.55	1.50
2	A	501	HEC	CMB-C2B	2.21	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	HEC	FE-NA	2.19	2.02	1.95
2	A	503	HEC	CMB-C2B	2.19	1.55	1.50
2	A	503	HEC	CMC-C2C	2.19	1.55	1.50
2	A	504	HEC	CMC-C2C	2.17	1.55	1.50
2	B	505	HEC	CMD-C2D	2.15	1.55	1.50
2	A	502	HEC	CMB-C2B	2.15	1.55	1.50
2	A	504	HEC	CMD-C2D	2.11	1.55	1.50
2	B	502	HEC	CAC-C3C	2.11	1.56	1.51
2	B	505	HEC	CMC-C2C	2.07	1.55	1.50
2	A	502	HEC	CMC-C2C	2.04	1.55	1.50
2	B	502	HEC	CMC-C2C	2.00	1.54	1.50

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	503	HEC	C1D-ND-C4D	6.49	112.90	105.21
2	A	501	HEC	C1D-ND-C4D	6.18	112.52	105.21
2	B	501	HEC	C1D-ND-C4D	6.07	112.40	105.21
2	B	503	HEC	C1D-ND-C4D	5.80	112.07	105.21
2	A	502	HEC	C1D-ND-C4D	5.76	112.03	105.21
2	A	505	HEC	C1D-ND-C4D	5.49	111.70	105.21
2	B	502	HEC	C1D-ND-C4D	5.43	111.64	105.21
2	A	504	HEC	C1D-ND-C4D	5.20	111.36	105.21
2	B	505	HEC	CHB-C4A-NA	5.14	130.05	124.45
2	B	504	HEC	C1D-ND-C4D	5.01	111.14	105.21
2	B	505	HEC	C1D-ND-C4D	4.98	111.10	105.21
2	B	504	HEC	CAA-CBA-CGA	-4.76	101.04	113.67
2	A	502	HEC	CAD-C3D-C4D	4.65	132.80	124.70
2	B	502	HEC	C1A-CHA-C4D	-4.02	117.47	126.02
2	B	503	HEC	CAD-C3D-C4D	4.00	131.66	124.70
2	A	504	HEC	CAD-C3D-C4D	3.77	131.26	124.70
2	A	505	HEC	CHA-C1A-C2A	3.70	130.71	124.86
2	A	503	HEC	CBA-CAA-C2A	-3.70	102.32	112.53
2	A	504	HEC	CHC-C4B-NB	3.66	128.90	124.37
2	A	503	HEC	C2A-C1A-NA	-3.65	106.80	110.32
2	B	504	HEC	CAD-C3D-C4D	3.59	130.95	124.70
2	A	503	HEC	C3C-C4C-NC	-3.48	106.29	110.15
2	B	503	HEC	CBA-CAA-C2A	-3.42	103.09	112.53
2	B	502	HEC	CHA-C1A-C2A	3.23	129.96	124.86
2	A	501	HEC	CHD-C1D-ND	3.19	128.32	124.37
2	A	501	HEC	C4B-NB-C1B	3.16	108.95	105.21
2	A	505	HEC	CHA-C1A-NA	-3.09	121.09	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	504	HEC	CHA-C4D-C3D	3.07	129.26	124.77
2	A	501	HEC	CHB-C1B-C2B	3.06	129.86	125.03
2	A	505	HEC	CAA-C2A-C3A	-3.04	122.18	127.87
2	B	504	HEC	CHA-C4D-ND	-2.98	121.22	124.42
2	A	502	HEC	CAD-C3D-C2D	-2.93	122.39	127.87
2	A	505	HEC	CAA-C2A-C1A	2.87	130.69	124.85
2	B	504	HEC	C3B-C4B-NB	-2.87	107.03	110.17
2	A	504	HEC	C2A-C1A-NA	-2.81	107.61	110.32
2	A	505	HEC	CHD-C1D-ND	2.79	127.82	124.37
2	B	502	HEC	C4B-NB-C1B	2.77	108.48	105.21
2	A	502	HEC	C2A-C1A-NA	-2.77	107.66	110.32
2	B	503	HEC	CHB-C1B-NB	2.73	127.36	124.42
2	A	501	HEC	C2B-C1B-NB	-2.69	106.80	109.90
2	A	504	HEC	C1A-CHA-C4D	2.69	131.73	126.02
2	A	503	HEC	CAA-CBA-CGA	-2.68	106.56	113.67
2	B	504	HEC	C4B-NB-C1B	2.61	108.30	105.21
2	B	502	HEC	CHA-C1A-NA	-2.57	121.65	124.45
2	B	505	HEC	CAA-CBA-CGA	2.54	120.41	113.67
2	A	504	HEC	CHA-C1A-NA	2.52	127.20	124.45
2	A	501	HEC	C2D-C1D-ND	-2.52	106.94	109.84
2	B	503	HEC	C2A-C1A-NA	-2.51	107.91	110.32
2	A	505	HEC	CHA-C4D-ND	2.49	127.11	124.42
2	A	505	HEC	CAD-C3D-C4D	2.49	129.03	124.70
2	B	505	HEC	CBD-CAD-C3D	-2.47	105.69	112.53
2	B	505	HEC	CMA-C3A-C4A	-2.47	120.37	124.73
2	B	503	HEC	CBB-CAB-C3B	-2.46	105.74	112.42
2	A	502	HEC	CAD-CBD-CGD	-2.46	107.15	113.67
2	A	501	HEC	CAD-C3D-C4D	2.46	128.98	124.70
2	B	502	HEC	C1C-CHC-C4B	-2.44	120.51	126.25
2	A	505	HEC	C3D-C4D-ND	-2.43	108.00	110.35
2	B	504	HEC	CAC-C3C-C4C	-2.41	121.60	124.91
2	B	501	HEC	CHB-C4A-NA	2.40	127.07	124.45
2	A	502	HEC	C4B-NB-C1B	2.38	108.02	105.21
2	B	504	HEC	C2B-C1B-NB	-2.35	107.18	109.90
2	B	504	HEC	CAC-C3C-C2C	2.34	130.59	126.89
2	B	503	HEC	CAD-C3D-C2D	-2.33	123.50	127.87
2	A	501	HEC	CHA-C1A-C2A	2.32	128.52	124.86
2	B	504	HEC	C2A-C1A-NA	-2.31	108.09	110.32
2	B	505	HEC	O1D-CGD-CBD	-2.30	115.78	123.09
2	A	504	HEC	C4A-CHB-C1B	-2.30	121.14	126.02
2	A	501	HEC	C3C-C4C-NC	-2.26	107.64	110.15
2	B	505	HEC	CHA-C1A-C2A	2.25	128.42	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	505	HEC	CAA-C2A-C1A	2.24	129.40	124.85
2	A	503	HEC	CMC-C2C-C1C	-2.23	122.03	125.42
2	A	502	HEC	CHD-C1D-ND	2.22	127.12	124.37
2	B	502	HEC	C3B-C4B-NB	-2.22	107.73	110.17
2	B	505	HEC	CHC-C1C-NC	2.22	127.89	123.86
2	A	501	HEC	CHD-C4C-C3C	2.21	130.15	125.30
2	A	505	HEC	C2A-C1A-NA	-2.20	108.20	110.32
2	B	503	HEC	C3D-C4D-ND	-2.20	108.23	110.35
2	A	503	HEC	C2D-C1D-ND	-2.19	107.32	109.84
2	A	504	HEC	CHA-C4D-C3D	2.18	127.96	124.77
2	B	502	HEC	CHC-C4B-C3B	2.18	129.24	125.23
2	A	501	HEC	CBB-CAB-C3B	-2.17	106.55	112.42
2	B	501	HEC	C2A-C1A-NA	-2.16	108.24	110.32
2	B	505	HEC	CHB-C4A-C3A	-2.15	121.02	125.49
2	B	502	HEC	CAB-C3B-C4B	2.14	127.58	124.79
2	B	505	HEC	C1D-C2D-C3D	-2.13	104.74	106.98
2	A	502	HEC	C3D-C4D-ND	-2.12	108.30	110.35
2	A	503	HEC	CAD-C3D-C4D	2.10	128.36	124.70
2	A	502	HEC	C3B-C4B-NB	-2.09	107.88	110.17
2	B	502	HEC	CAD-CBD-CGD	-2.08	108.14	113.67
2	A	501	HEC	C2A-C1A-NA	-2.08	108.31	110.32
2	B	503	HEC	C3B-C4B-NB	-2.08	107.89	110.17
2	A	504	HEC	CAD-C3D-C2D	-2.08	123.98	127.87
2	B	503	HEC	C4B-NB-C1B	2.07	107.66	105.21
2	A	503	HEC	C4C-NC-C1C	2.07	109.20	105.82
2	B	501	HEC	CAC-C3C-C4C	2.06	127.75	124.91
2	B	504	HEC	CBA-CAA-C2A	-2.06	106.84	112.53
2	A	503	HEC	CHC-C1C-NC	2.06	127.59	123.86
2	B	502	HEC	C2A-C1A-NA	-2.06	108.34	110.32
2	B	505	HEC	CMC-C2C-C3C	2.05	129.97	125.62
2	B	504	HEC	CHA-C1A-NA	2.03	126.67	124.45
2	A	504	HEC	CAD-CBD-CGD	-2.03	108.29	113.67
2	B	505	HEC	CAD-CBD-CGD	-2.03	108.29	113.67
2	A	502	HEC	CBD-CAD-C3D	2.02	118.11	112.53
2	B	504	HEC	CHB-C1B-NB	2.02	126.59	124.42
2	A	503	HEC	CMC-C2C-C3C	2.01	129.88	125.62

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	HEC	NA
2	B	501	HEC	NA

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Mol	Chain	Res	Type	Atom
2	B	502	HEC	NA
2	B	503	HEC	NA
2	B	504	HEC	NA

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	504	HEC	C2D-C3D-CAD-CBD
2	A	504	HEC	C4D-C3D-CAD-CBD
2	A	502	HEC	C4D-C3D-CAD-CBD
2	B	502	HEC	C1A-C2A-CAA-CBA
2	B	502	HEC	C2A-CAA-CBA-CGA
2	B	504	HEC	C2A-CAA-CBA-CGA
4	B	507	PE3	O34-C35-C36-O37
4	B	507	PE3	O10-C11-C12-O13
2	A	502	HEC	C2D-C3D-CAD-CBD
2	A	501	HEC	C2A-CAA-CBA-CGA
4	B	507	PE3	O16-C17-C18-O19
4	B	507	PE3	O25-C26-C27-O28
4	B	507	PE3	O19-C20-C21-O22
2	B	502	HEC	C3A-C2A-CAA-CBA
4	B	507	PE3	O37-C38-C39-O40
4	B	507	PE3	C39-C38-O37-C36
2	B	503	HEC	C2D-C3D-CAD-CBD
4	B	507	PE3	O28-C29-C30-O31
2	A	502	HEC	C2B-C3B-CAB-CBB
2	B	503	HEC	C4D-C3D-CAD-CBD
2	A	504	HEC	C2C-C3C-CAC-CBC
4	B	507	PE3	O7-C8-C9-O10
2	B	502	HEC	C4D-C3D-CAD-CBD
2	B	504	HEC	C4D-C3D-CAD-CBD
2	A	504	HEC	C2A-CAA-CBA-CGA
4	B	507	PE3	C26-C27-O28-C29
2	B	501	HEC	C2C-C3C-CAC-CBC
2	A	503	HEC	C2B-C3B-CAB-CBB
2	B	502	HEC	C2D-C3D-CAD-CBD
2	B	504	HEC	C2D-C3D-CAD-CBD
2	A	504	HEC	C4C-C3C-CAC-CBC
4	B	507	PE3	O1-C2-C3-O4
2	A	502	HEC	C4B-C3B-CAB-CBB
4	B	507	PE3	C5-C6-O7-C8
2	A	502	HEC	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
2	B	501	HEC	C3D-CAD-CBD-CGD
4	B	507	PE3	C15-C14-O13-C12
2	B	501	HEC	C4C-C3C-CAC-CBC
4	B	507	PE3	C29-C30-O31-C32
4	B	507	PE3	C21-C20-O19-C18
2	B	505	HEC	C2A-CAA-CBA-CGA
2	A	503	HEC	C4B-C3B-CAB-CBB
2	A	505	HEC	C2C-C3C-CAC-CBC
2	A	504	HEC	C1A-C2A-CAA-CBA
4	B	507	PE3	C14-C15-O16-C17
2	B	505	HEC	C2C-C3C-CAC-CBC
2	B	501	HEC	CAA-CBA-CGA-O2A
2	A	501	HEC	CAA-CBA-CGA-O1A
4	B	507	PE3	C17-C18-O19-C20
2	B	501	HEC	CAA-CBA-CGA-O1A
2	A	504	HEC	CAD-CBD-CGD-O1D
4	B	507	PE3	C30-C29-O28-C27
2	A	505	HEC	C4C-C3C-CAC-CBC
2	A	502	HEC	CAA-CBA-CGA-O1A
2	B	505	HEC	CAA-CBA-CGA-O1A
2	A	502	HEC	CAA-CBA-CGA-O2A
2	A	505	HEC	CAA-CBA-CGA-O1A
2	B	502	HEC	CAD-CBD-CGD-O1D
2	B	502	HEC	CAD-CBD-CGD-O2D
2	A	501	HEC	CAA-CBA-CGA-O2A
2	A	504	HEC	CAD-CBD-CGD-O2D
2	B	505	HEC	CAA-CBA-CGA-O2A
2	A	505	HEC	CAD-CBD-CGD-O2D
2	B	505	HEC	C4C-C3C-CAC-CBC
4	B	507	PE3	C33-C32-O31-C30
2	A	505	HEC	CAA-CBA-CGA-O2A
2	A	505	HEC	CAD-CBD-CGD-O1D
2	B	503	HEC	CAD-CBD-CGD-O2D
2	B	503	HEC	CAD-CBD-CGD-O1D
2	B	503	HEC	C3D-CAD-CBD-CGD
2	B	504	HEC	CAA-CBA-CGA-O2A
4	B	507	PE3	C35-C36-O37-C38
2	A	501	HEC	C2C-C3C-CAC-CBC
4	B	507	PE3	C11-C12-O13-C14
2	B	501	HEC	C2D-C3D-CAD-CBD
2	B	504	HEC	CAA-CBA-CGA-O1A
4	B	507	PE3	C38-C39-O40-C41

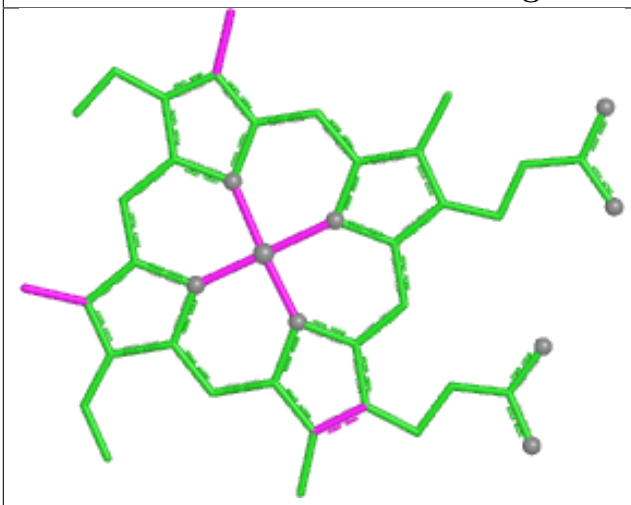
There are no ring outliers.

10 monomers are involved in 38 short contacts:

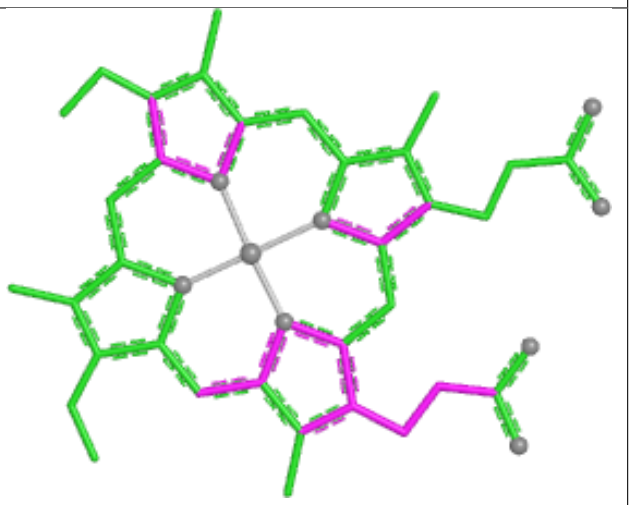
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	HEC	4	0
2	A	503	HEC	1	0
2	A	505	HEC	7	0
2	B	503	HEC	1	0
2	B	505	HEC	6	0
2	A	501	HEC	4	0
2	B	501	HEC	3	0
2	B	504	HEC	5	0
2	B	502	HEC	3	0
2	A	504	HEC	4	0

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 then 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.

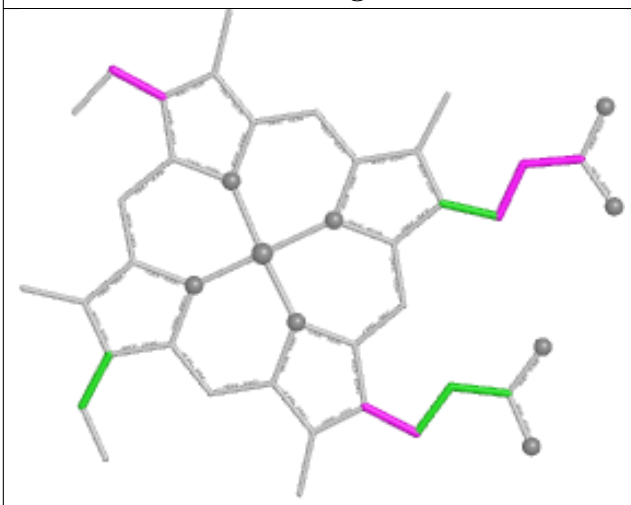
Ligand HEC A 502



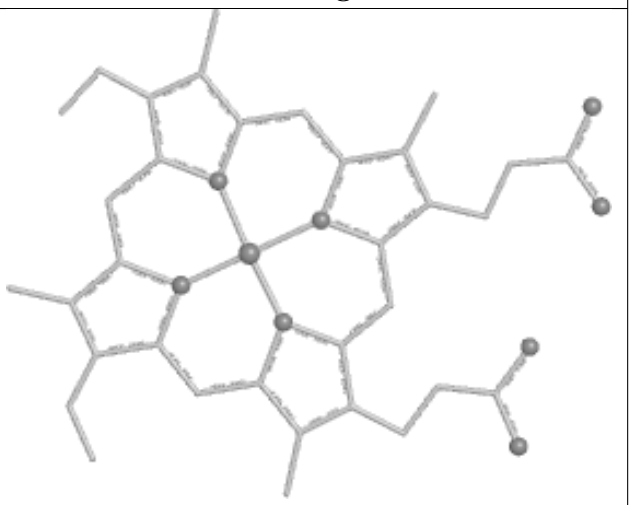
Bond lengths



Bond angles

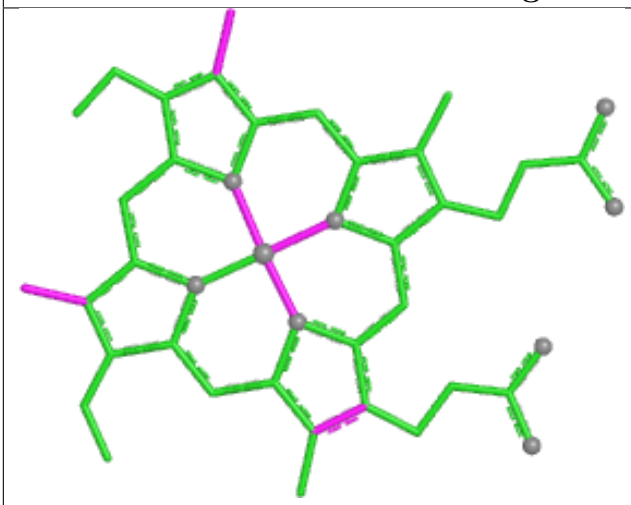


Torsions

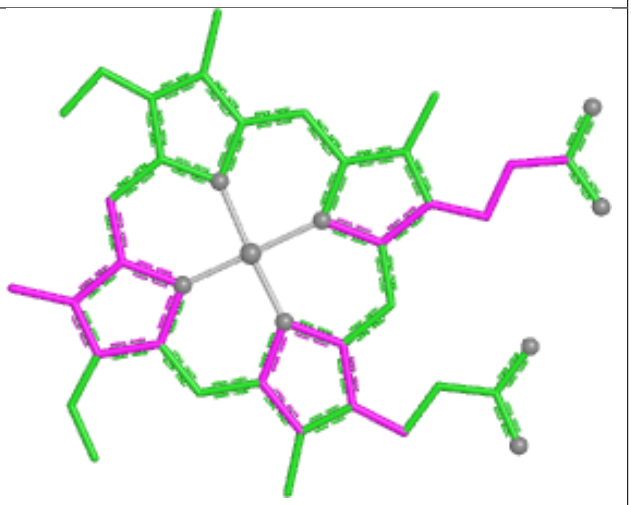


Rings

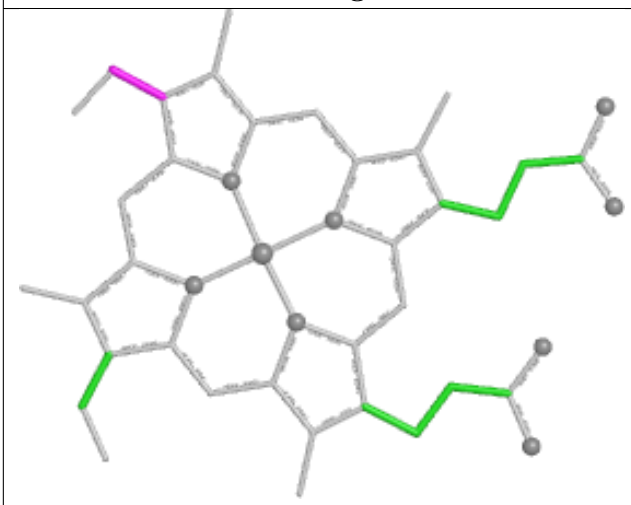
Ligand HEC A 503



Bond lengths



Bond angles



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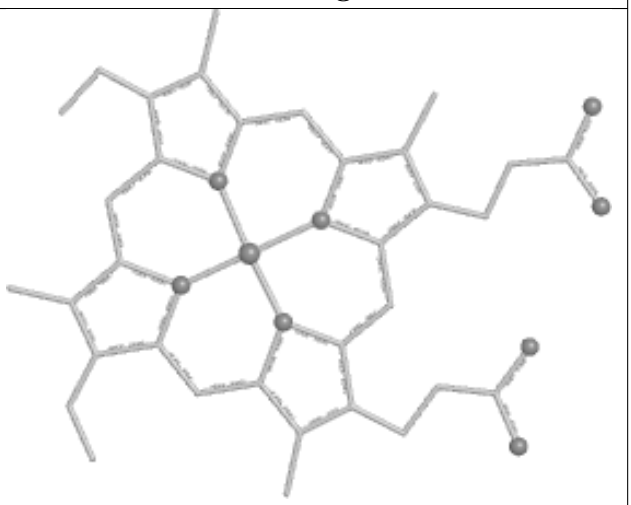
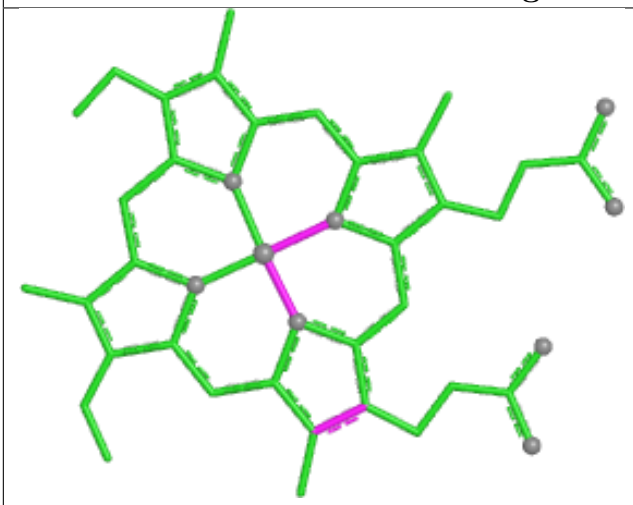


Rings

Ligand HEC A 505



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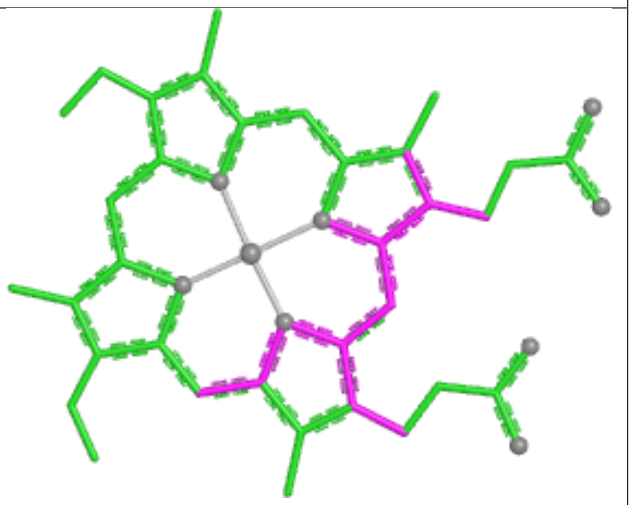
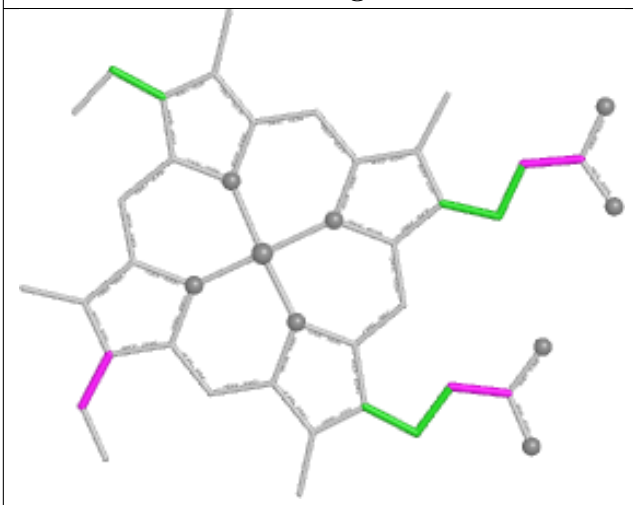
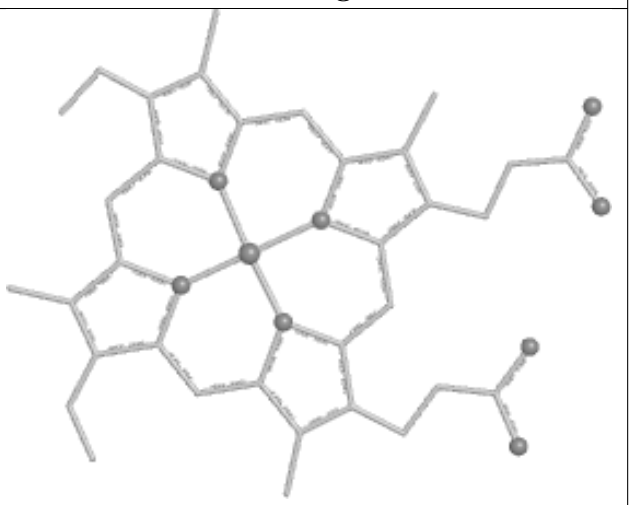


Bond angles

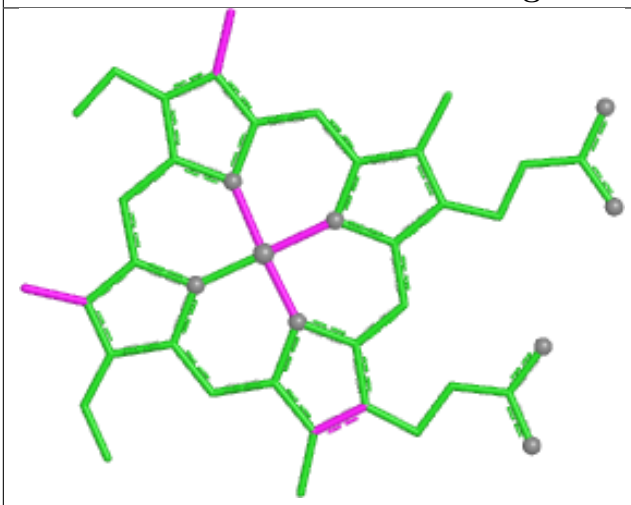


Torsions

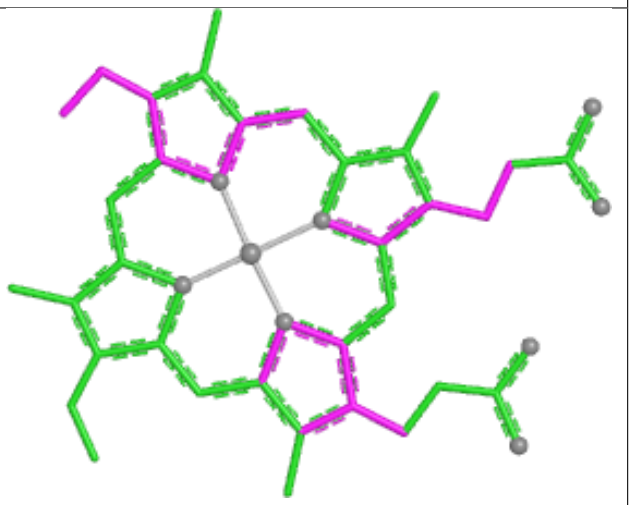


Rings

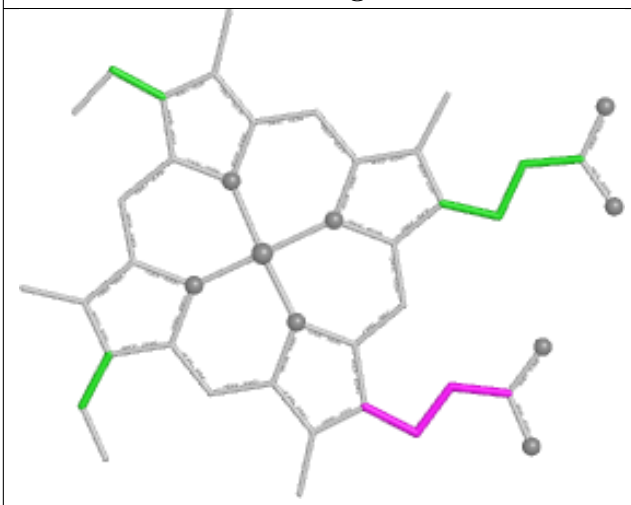
Ligand HEC B 503



Bond lengths



Bond angles



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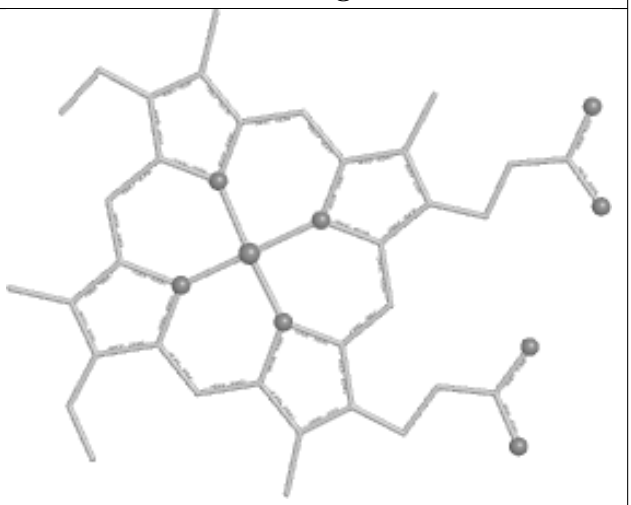
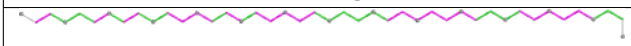


Rings

Ligand PE3 B 507

Bond lengths

Bond angles



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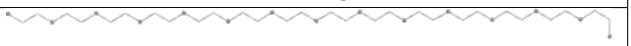

Rings

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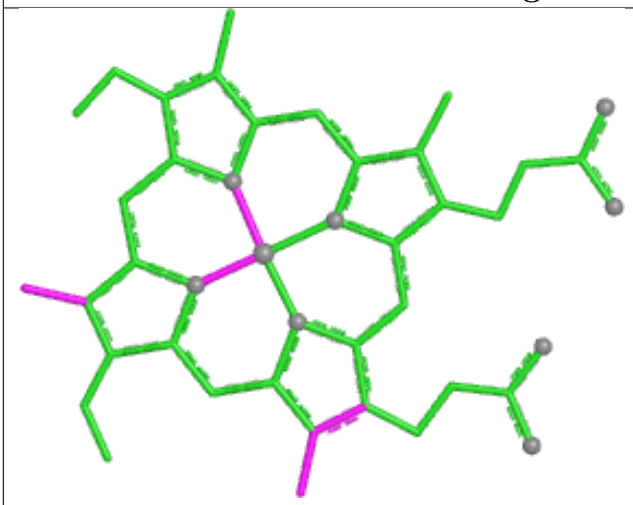

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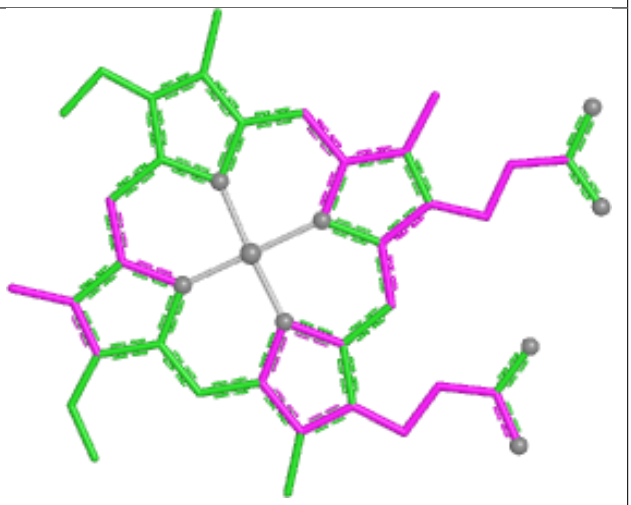

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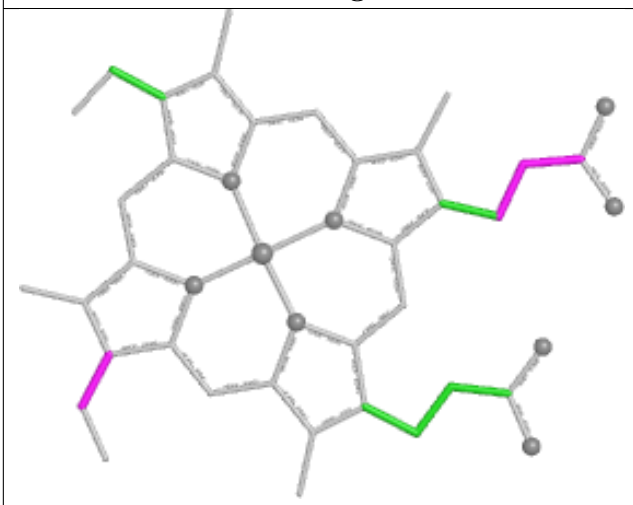

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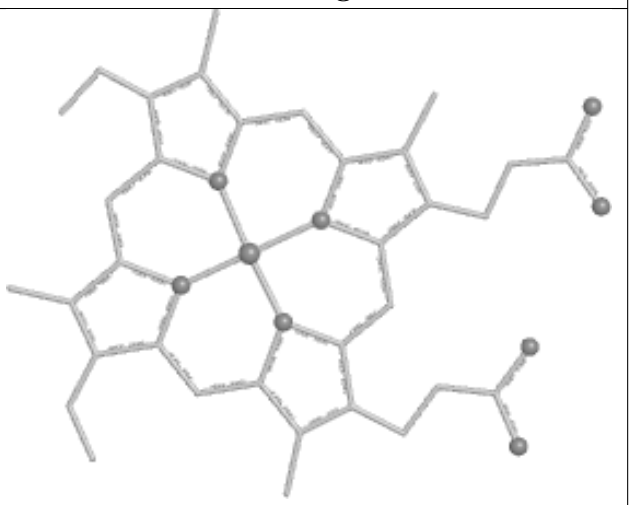
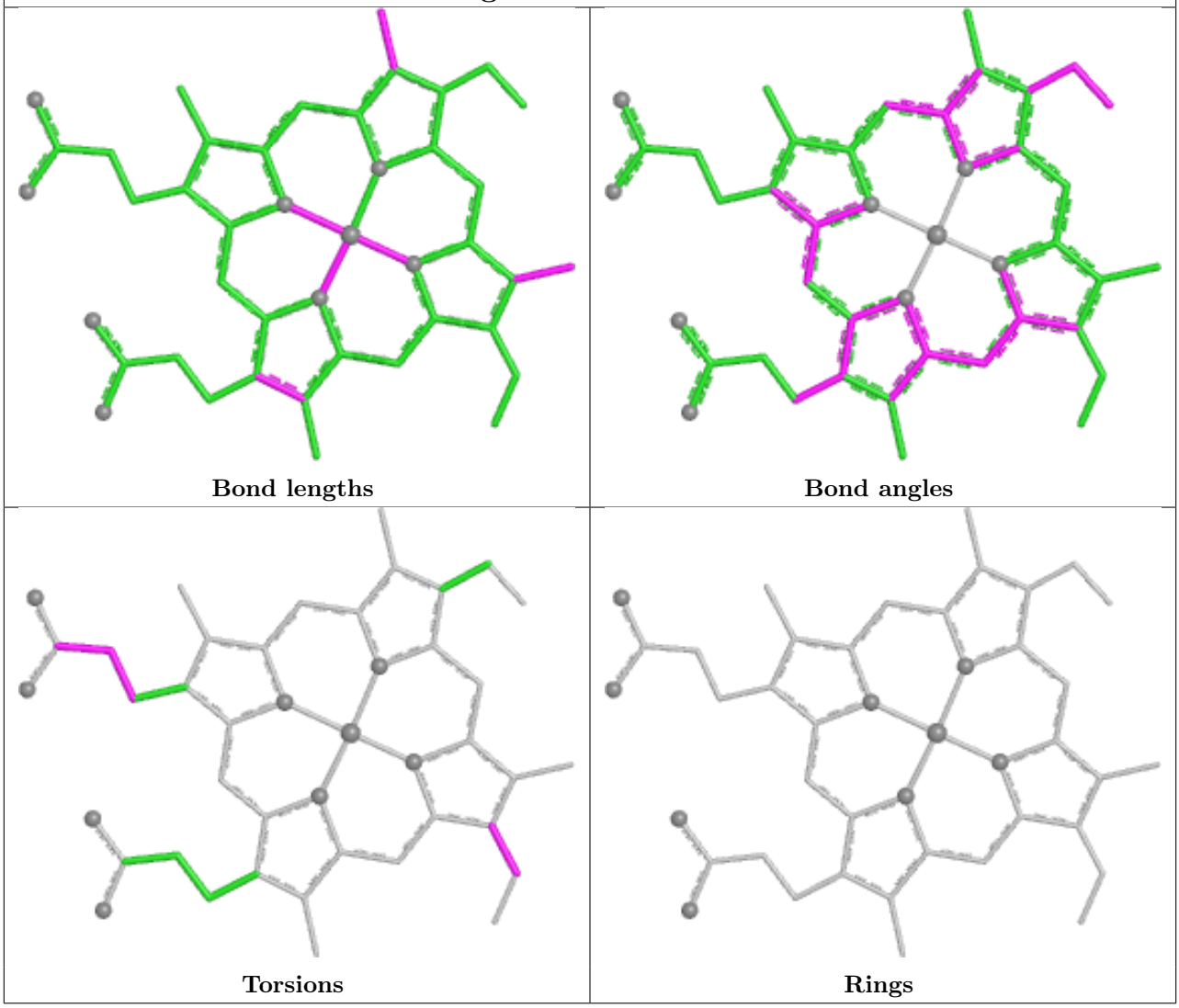


Rings

Ligand HEC A 501



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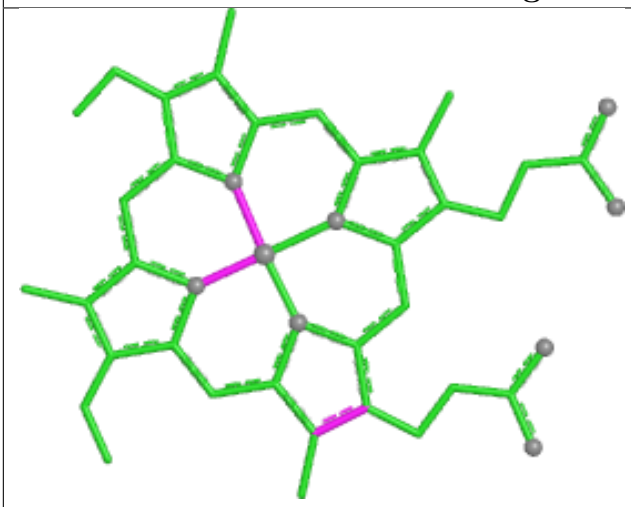

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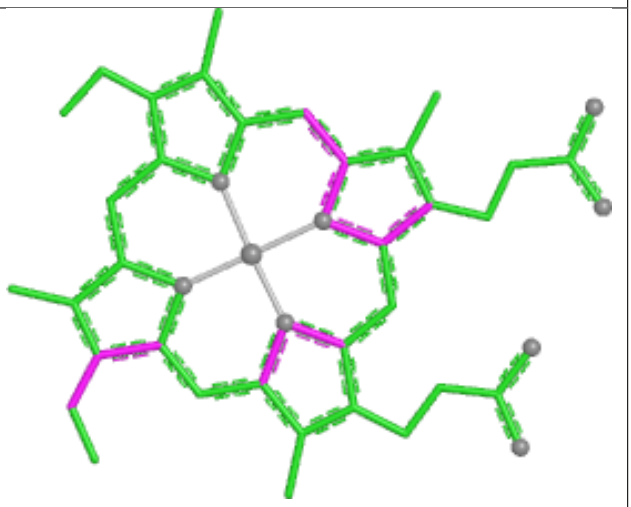
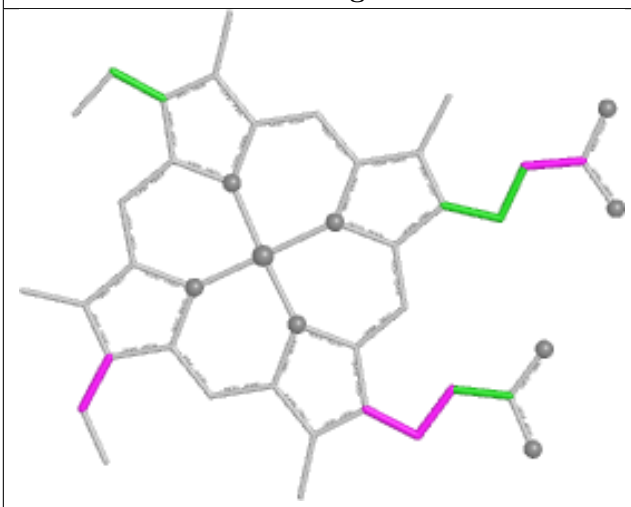


Bond angles



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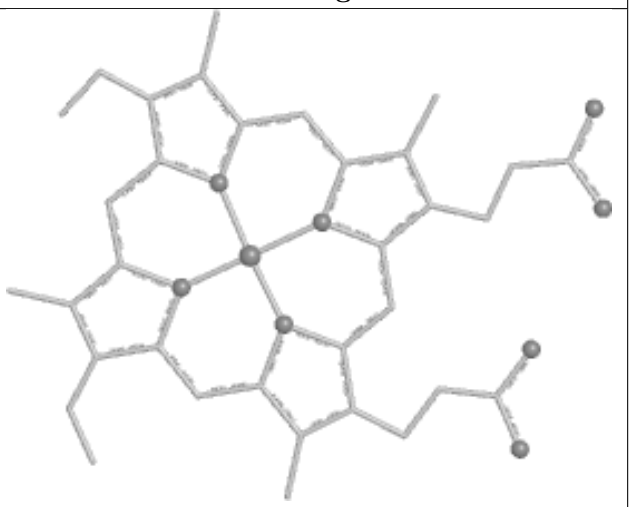

Rings

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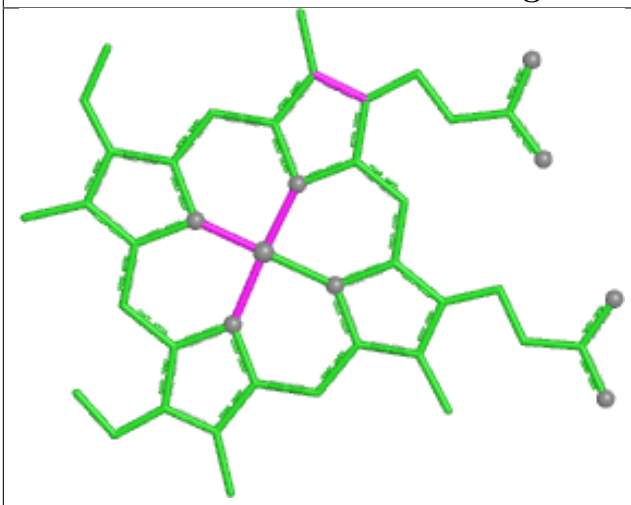

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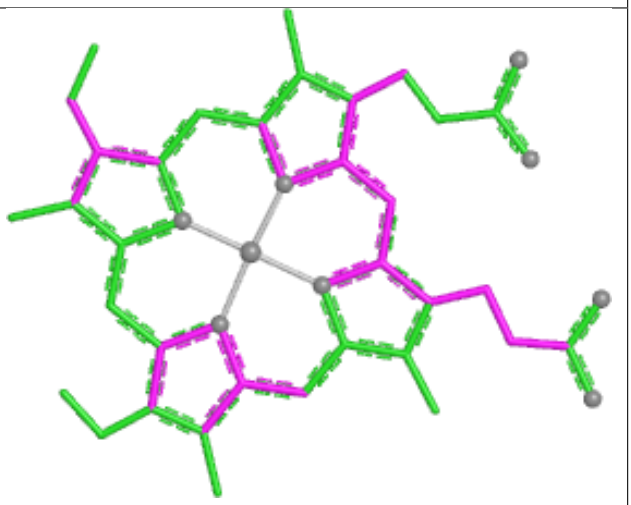
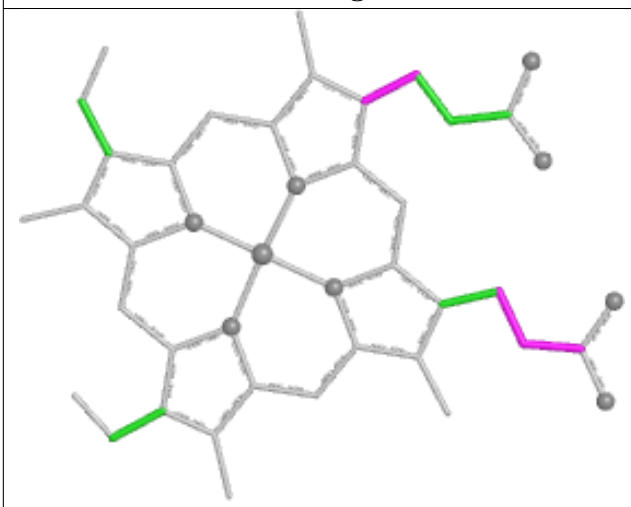


Bond angles



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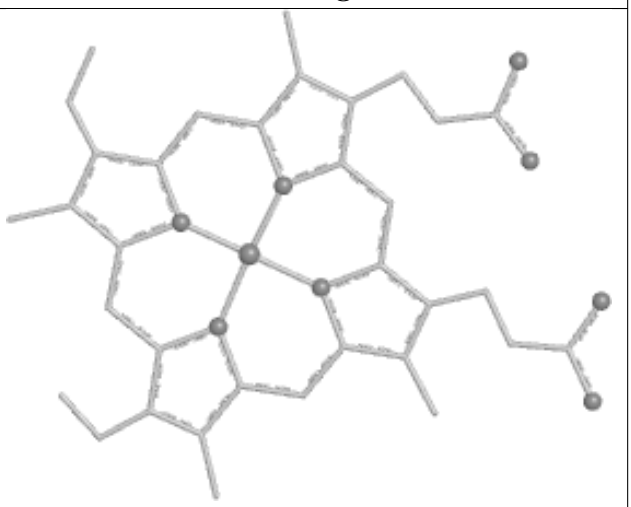
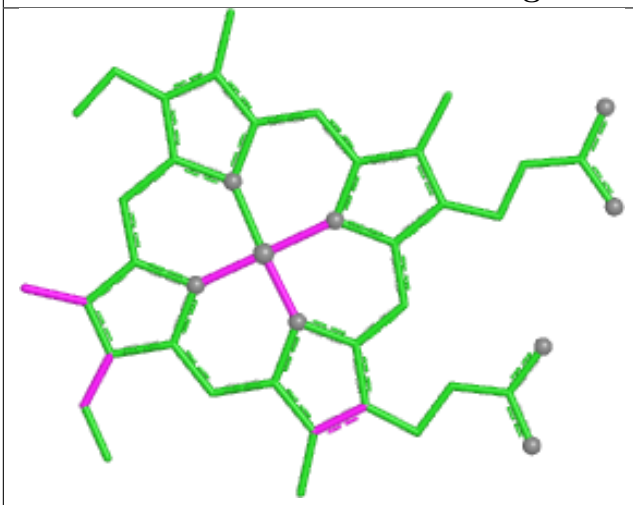


Rings

Ligand HEC B 502



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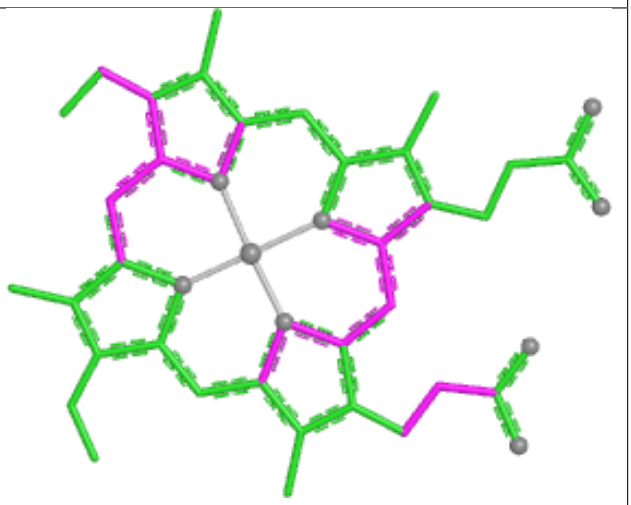
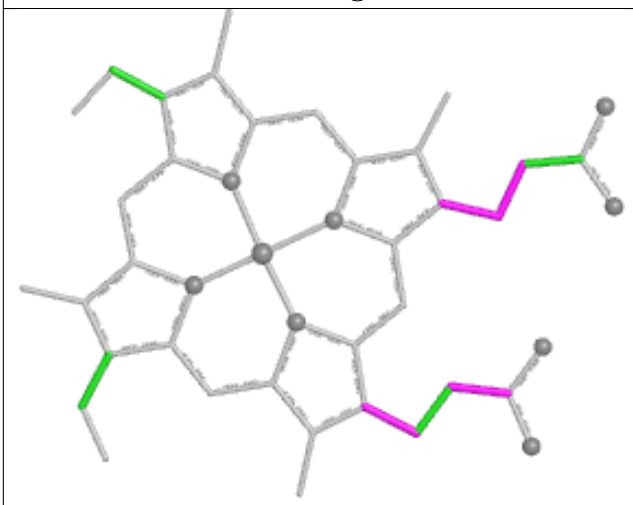
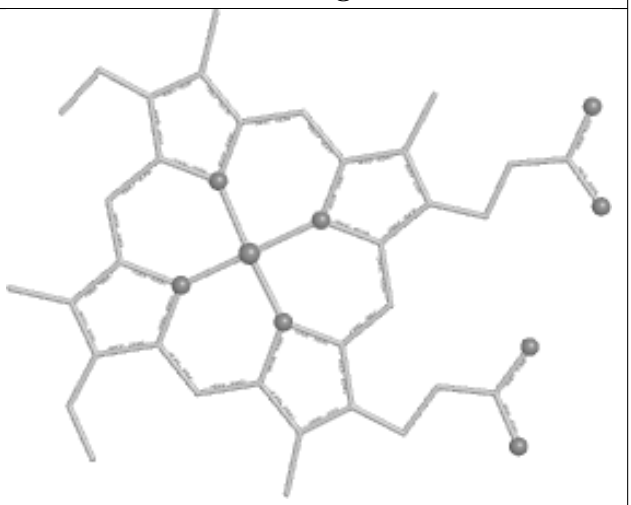


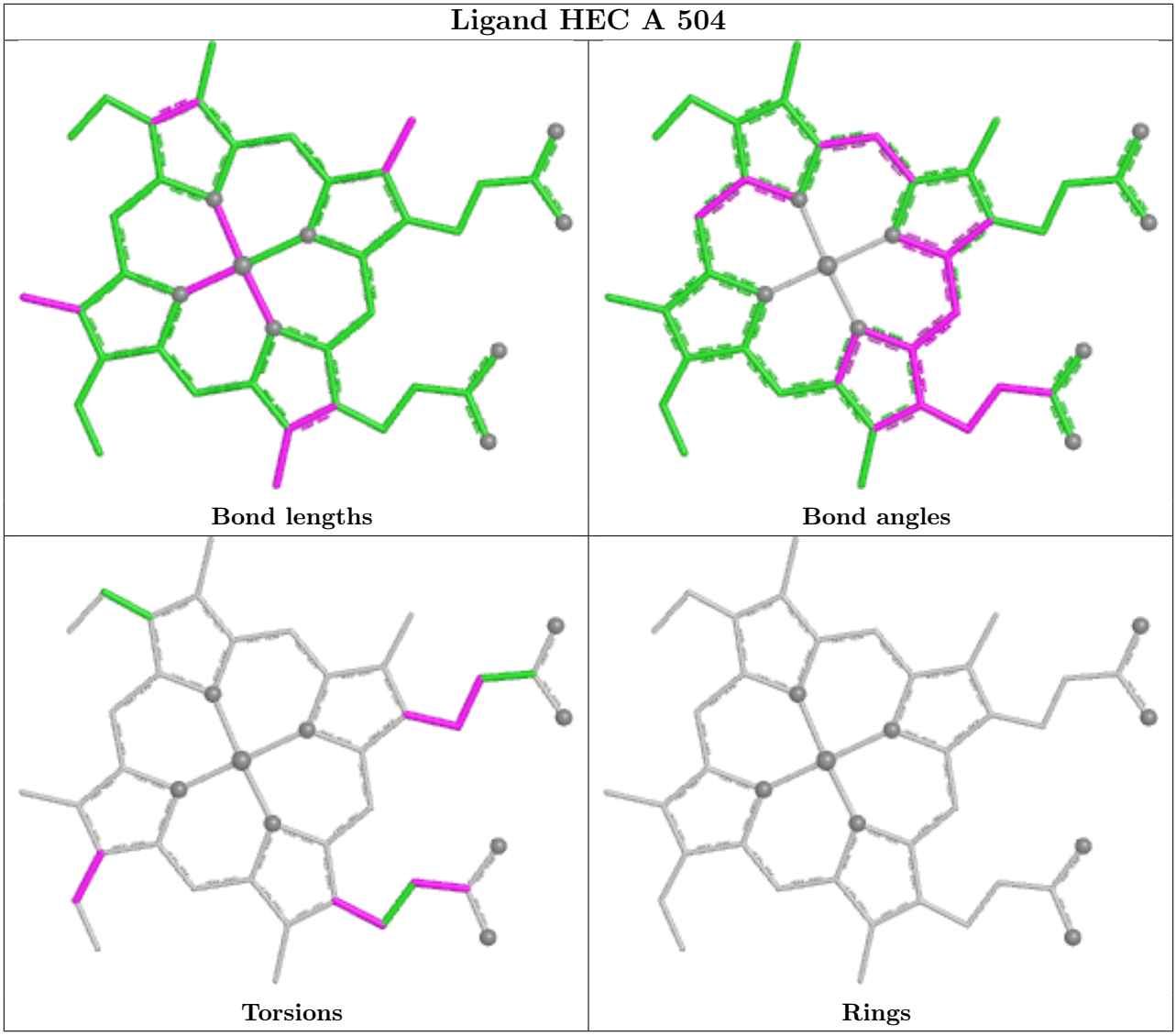
Bond angles



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	439/439 (100%)	-0.79	0	100	100	83, 95, 110, 117	0
1	B	439/439 (100%)	-0.83	0	100	100	83, 99, 119, 124	0
All	All	878/878 (100%)	-0.81	0	100	100	83, 97, 116, 124	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PE3	B	507	43/43	0.67	0.09	139,143,145,145	0
2	HEC	B	502	43/43	0.95	0.08	108,112,113,114	0
3	CA	B	506	1/1	0.96	0.07	93,93,93,93	0
2	HEC	A	501	43/43	0.96	0.07	95,97,99,100	0
2	HEC	A	505	43/43	0.97	0.08	89,90,92,93	0
2	HEC	B	501	43/43	0.97	0.07	100,102,104,104	0
2	HEC	A	502	43/43	0.97	0.07	99,101,102,102	0

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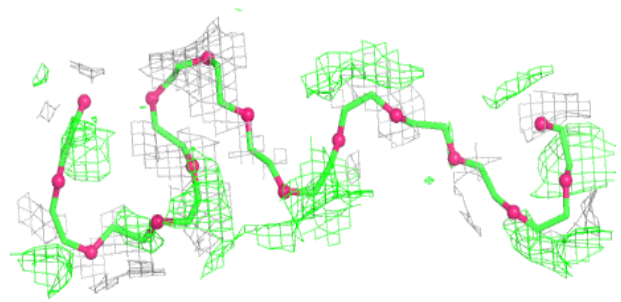
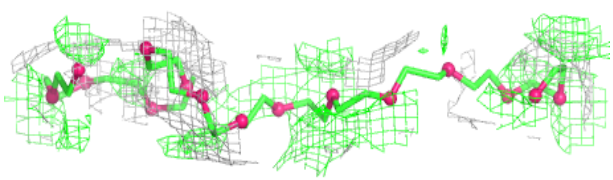
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEC	B	503	43/43	0.97	0.07	101,103,105,107	0
2	HEC	B	504	43/43	0.97	0.07	96,98,100,101	0
2	HEC	B	505	43/43	0.97	0.09	91,93,96,97	0
2	HEC	A	503	43/43	0.97	0.07	94,96,98,99	0
2	HEC	A	504	43/43	0.97	0.07	89,92,93,94	0
3	CA	A	506	1/1	0.98	0.03	91,91,91,91	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 PE3 B 507:

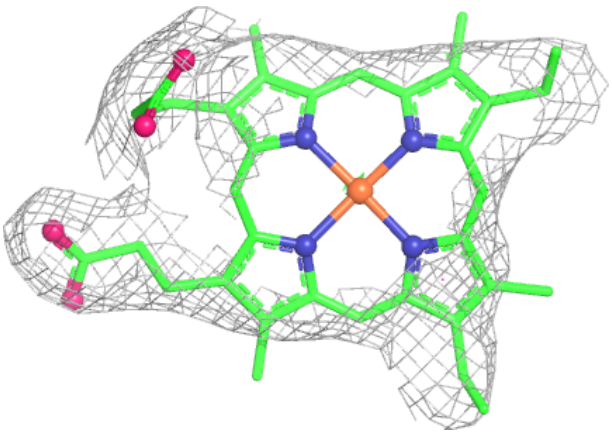
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

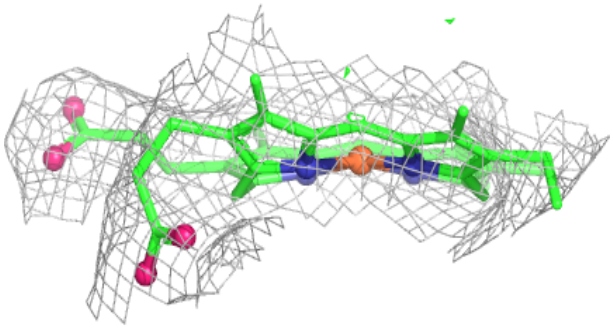


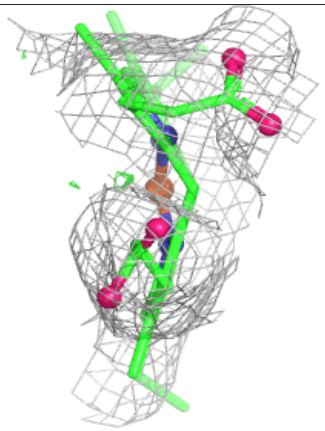


Electron density around HEC B 502:

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

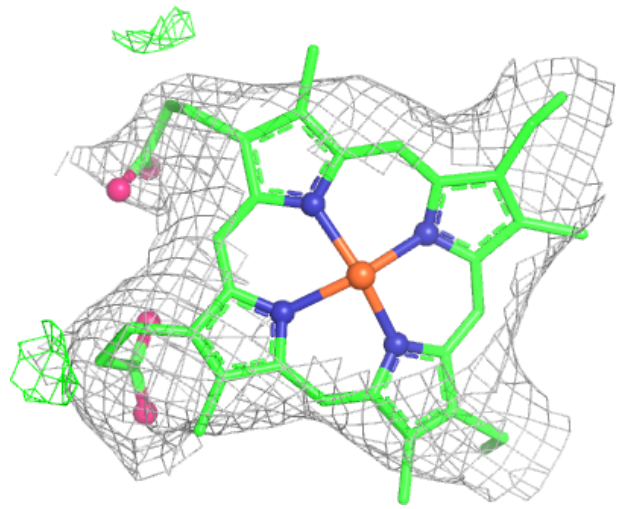


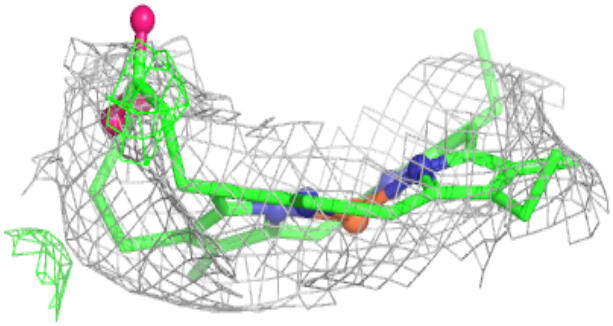


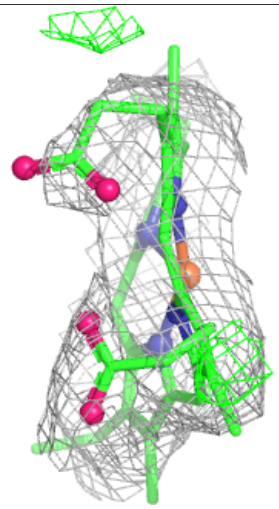


Electron density around HEC A 501:

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

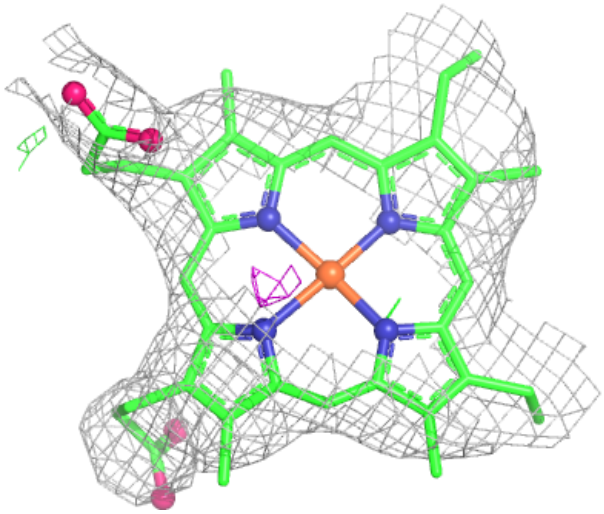


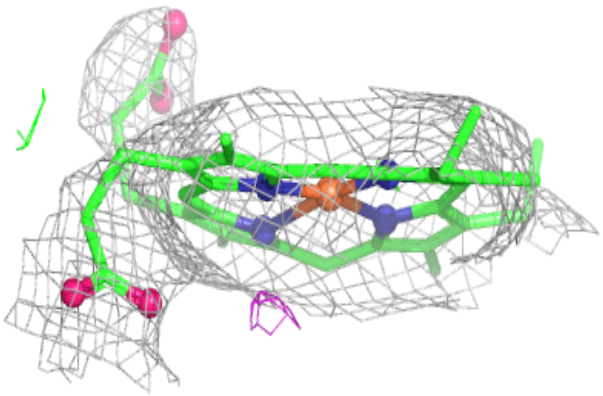


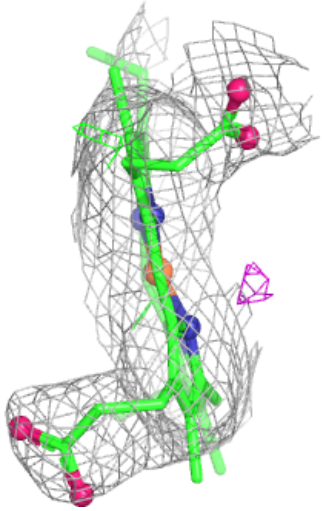


Electron density around HEC A 505:

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

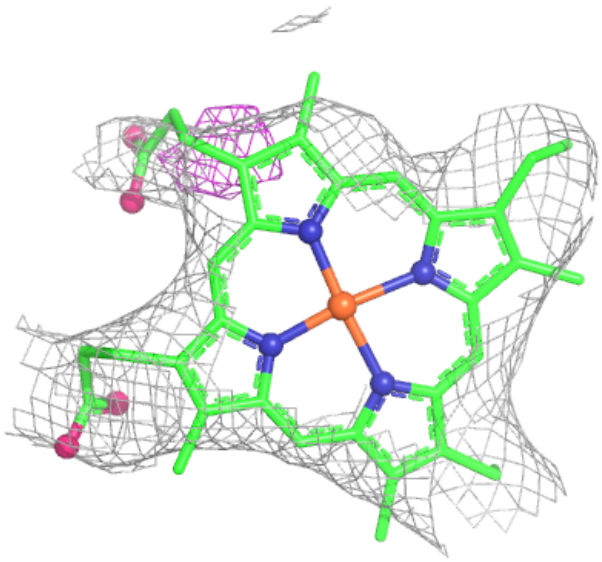


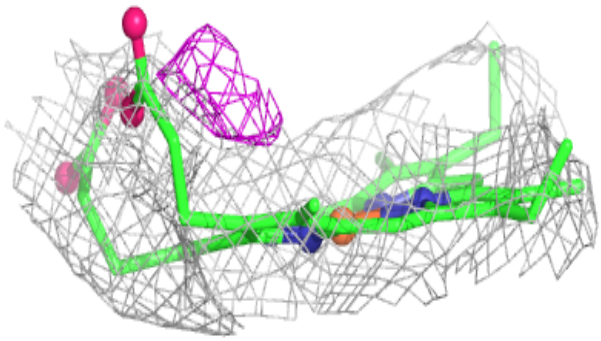


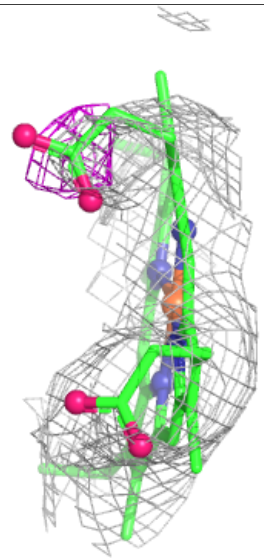


Electron density around HEC B 501:

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

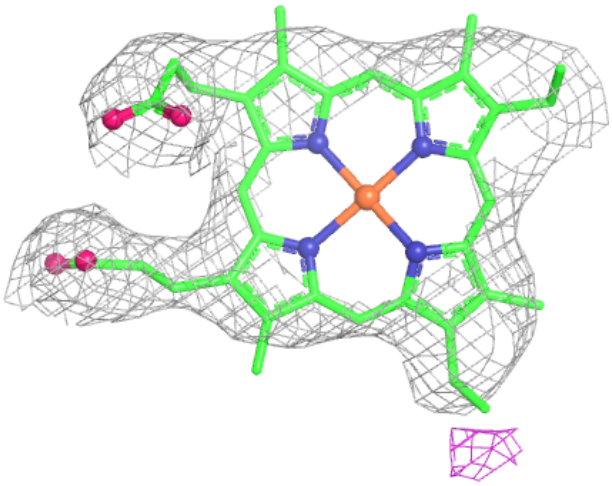


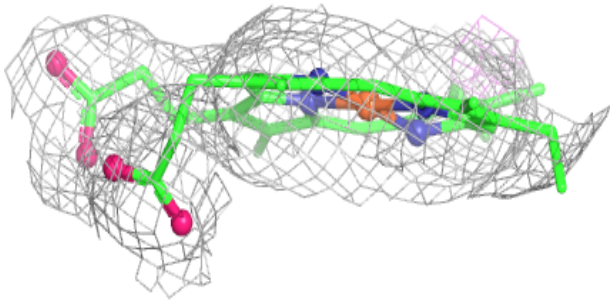


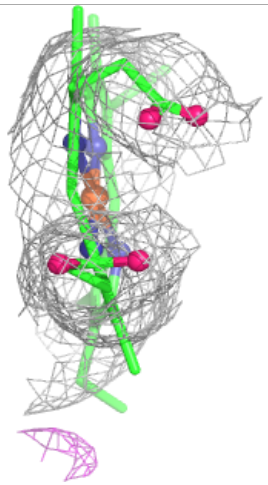


Electron density around HEC A 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

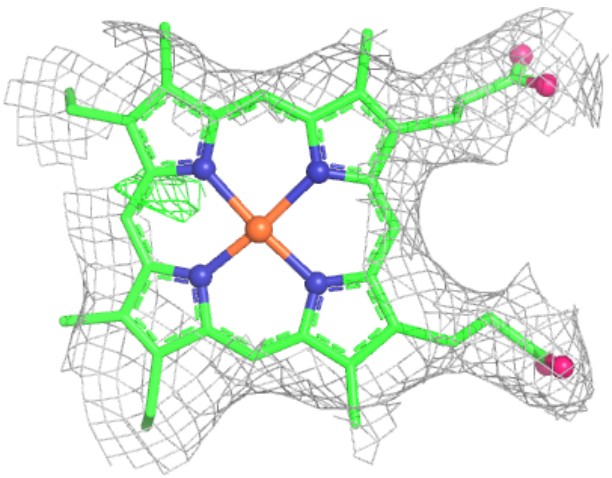


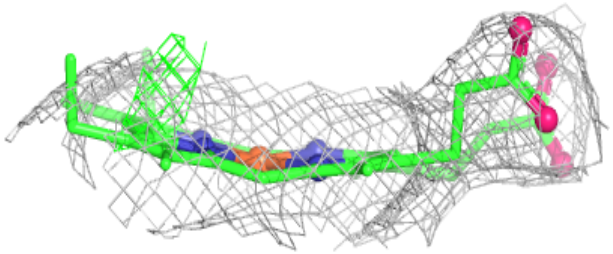


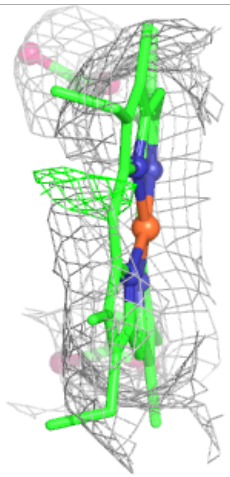


Electron density around HEC B 503:

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

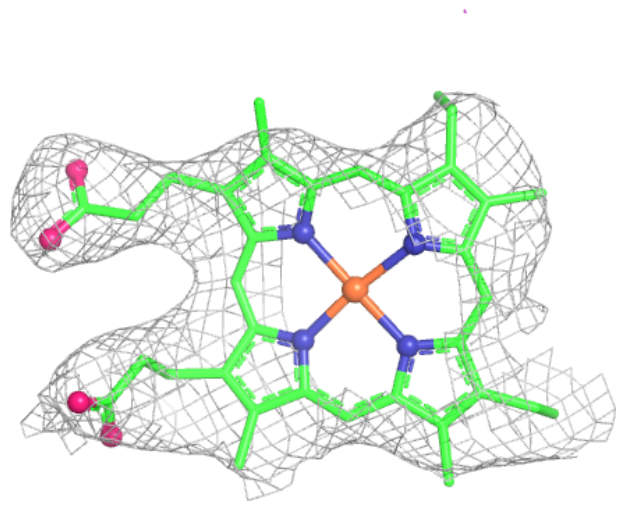


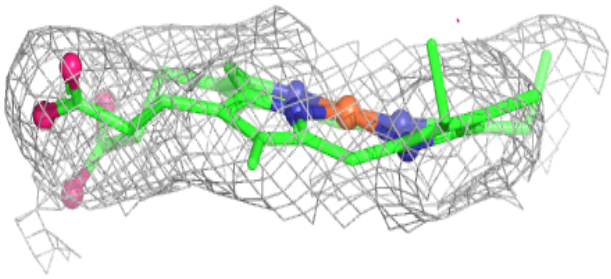


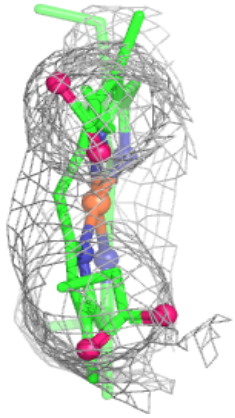


Electron density around HEC B 504:

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

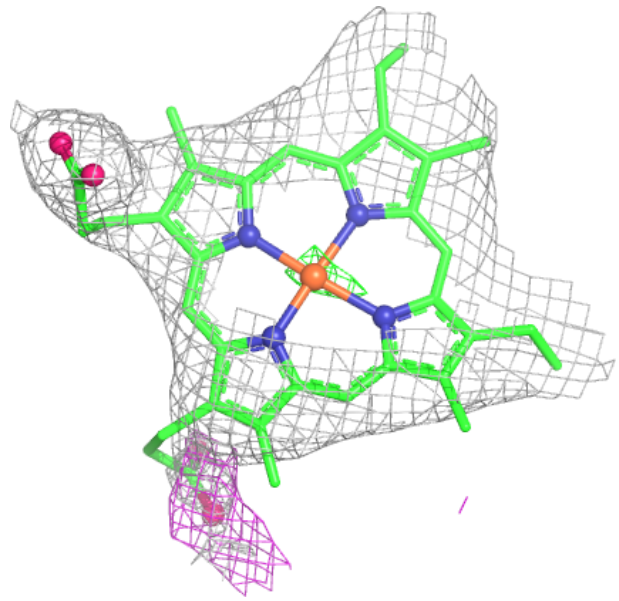


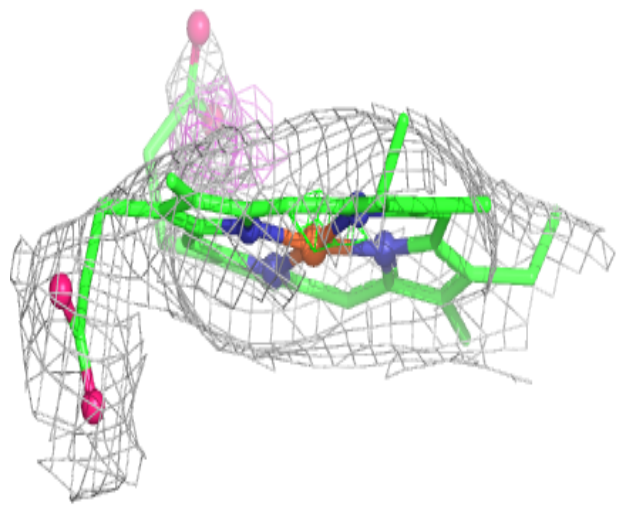


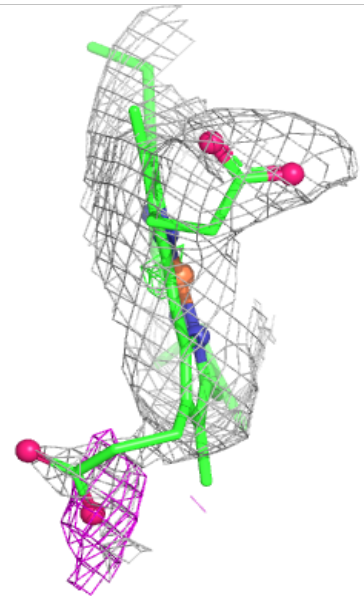


Electron density around HEC B 505:

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

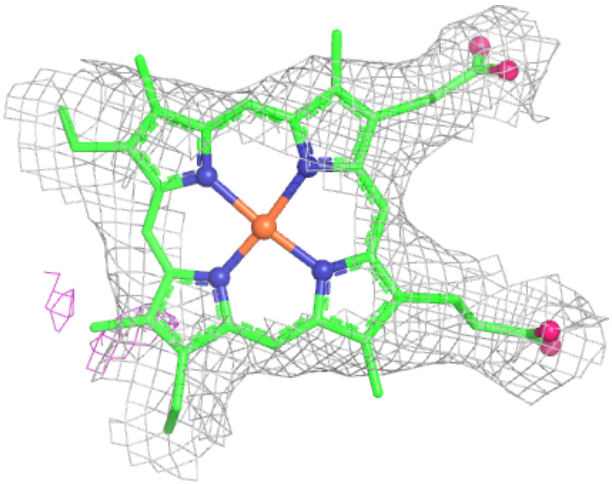


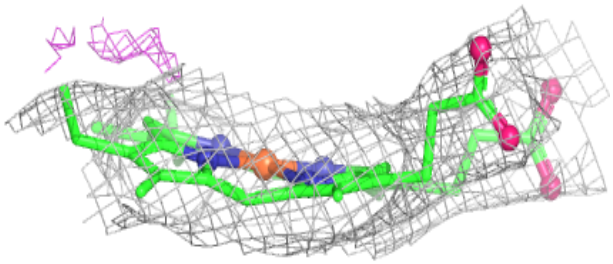


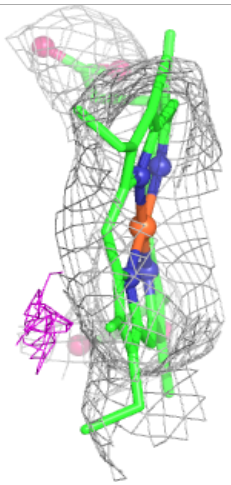


Electron density around HEC A 503:

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

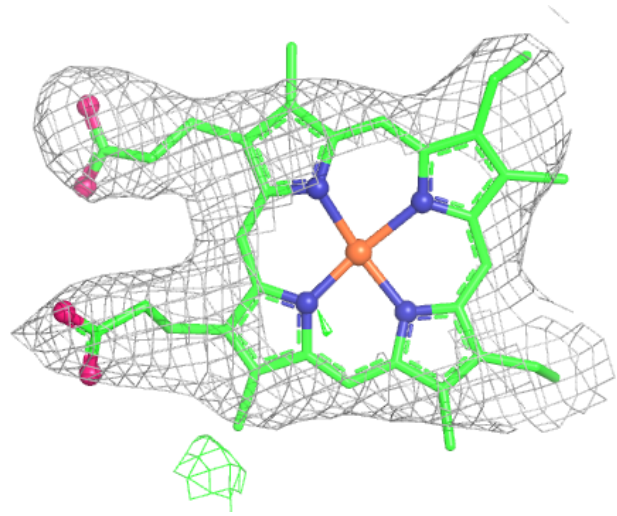


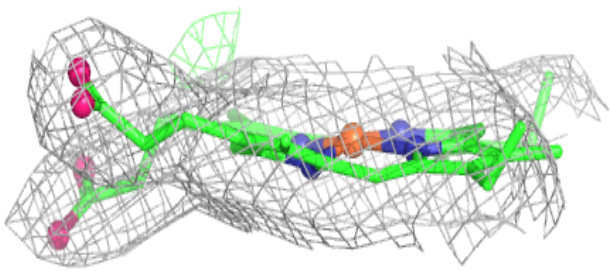


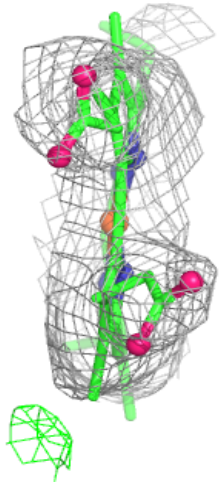


Electron density around HEC A 504:

$2mF_o$-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.