Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2024 – 01:57 AM EST

PDB ID	:	1ZZH
Title	:	Structure of the fully oxidized di-heme cytochrome c peroxidase from R. capsulatus
Authors	:	De Smet, L.; Savvides, S.N.; Van Horen, E.; Pettigrew, G.; Van Beeumen, J.J.
Deposited on	:	2005-06-14
Resolution	:	2.70 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:

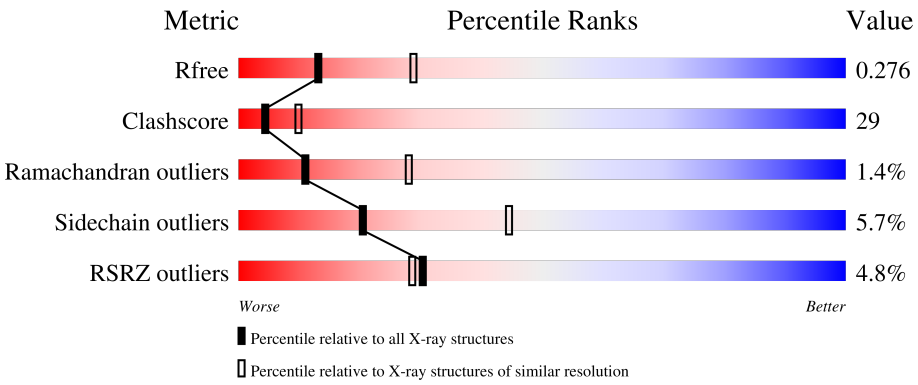
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	328	5% 54% 33% • 9%
1	B	328	6% 54% 37% • 6%
1	C	328	3% 55% 35% • 6%
1	D	328	4% 53% 34% • 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9290 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 peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	297	2172	1382	367	412	11	0	0	0
1	B	308	2277	1446	388	432	11	0	0	0
1	C	307	2251	1429	384	427	11	0	0	0
1	D	298	2198	1396	375	416	11	0	0	0

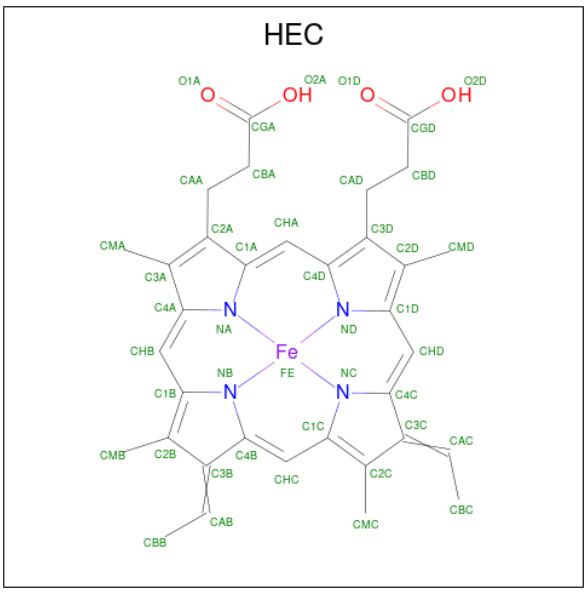
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	2	2	2	0	0
3	B	4	4	4	0	0
3	C	1	1	1	0	0
3	D	1	1	1	0	0

- Molecule 4 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	9	9	9	0	0
			Total	O		
5	B	5	5	5	0	0
			Total	O		
5	C	15	15	15	0	0

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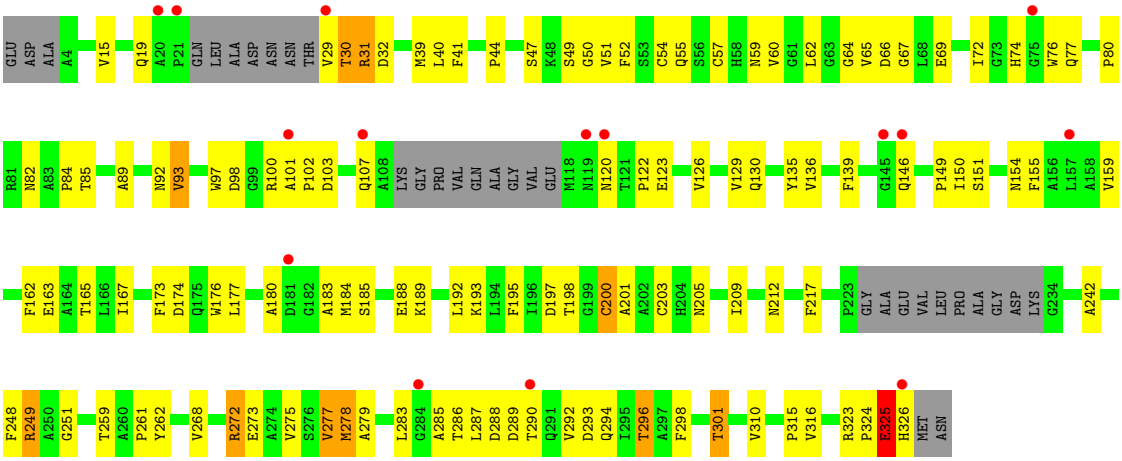
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	D	7	7	7	0	0

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.

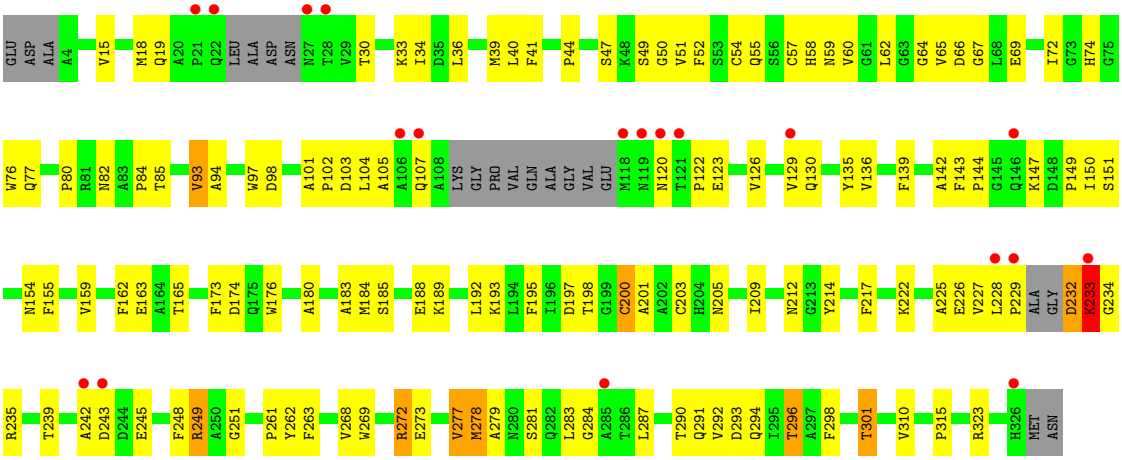
• Molecule 1: cytochrome c peroxidase

Chain A:



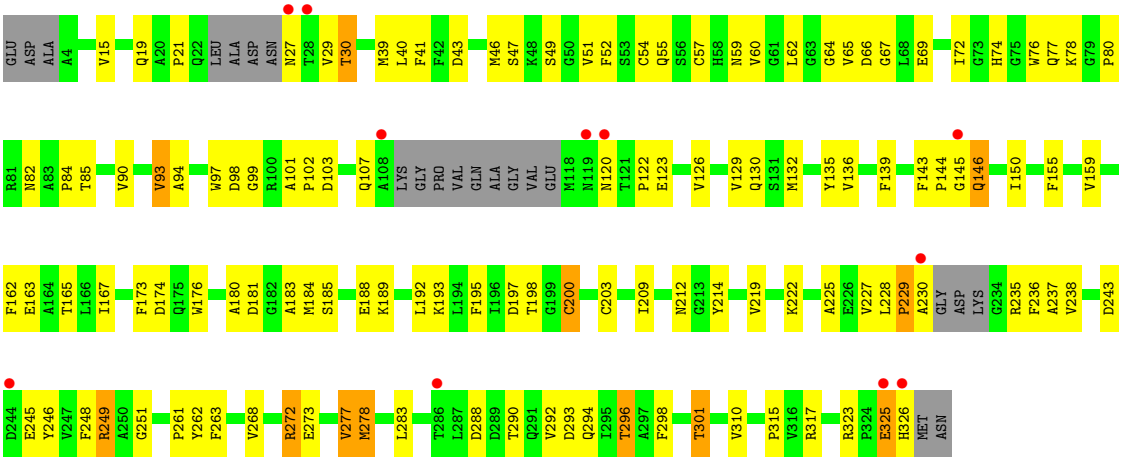
• Molecule 1: cytochrome c peroxidase

Chain B:



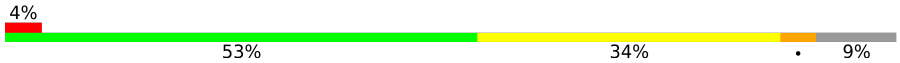
• Molecule 1: cytochrome c peroxidase

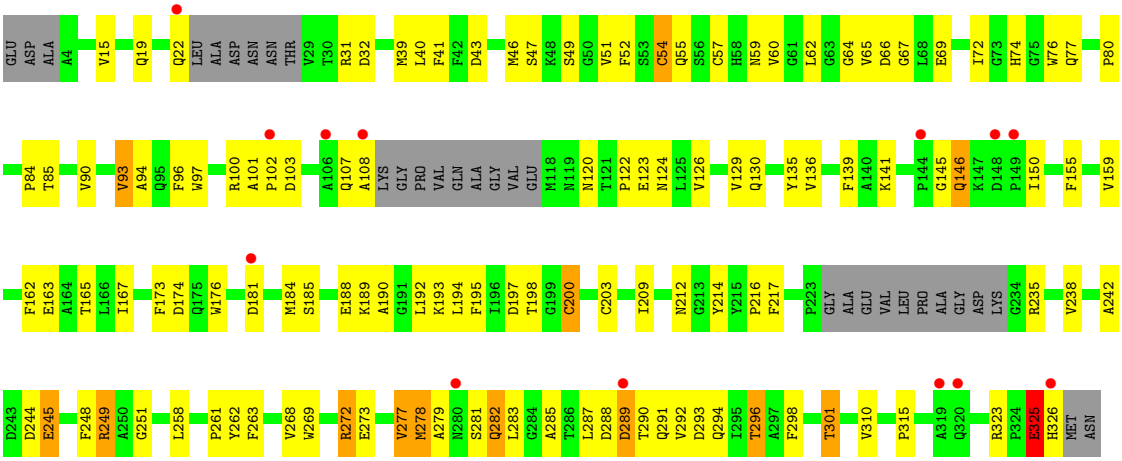
Chain C:



- Molecule 1: cytochrome c peroxidase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.63Å 132.47Å 163.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 15.01 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.0 (30.00-2.70) 96.1 (15.01-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.278 0.248 , 0.276	Depositor DCC
R_{free} test set	1877 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9290	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5940e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: HEC, CA, ZN

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	0.43	0/2225	0.65	1/3035 (0.0%)
1	B	0.45	0/2330	0.69	1/3174 (0.0%)
1	C	0.44	0/2304	0.66	1/3141 (0.0%)
1	D	0.48	1/2250 (0.0%)	0.72	2/3066 (0.1%)
All	All	0.45	1/9109 (0.0%)	0.68	5/12416 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	325	GLU	C-N	5.25	1.46	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	289	ASP	CB-CG-OD2	12.28	129.35	118.30
1	B	233	LYS	N-CA-C	8.55	134.08	111.00
1	D	181	ASP	CB-CG-OD1	7.17	124.76	118.30
1	C	181	ASP	CB-CG-OD1	6.79	124.42	118.30
1	A	325	GLU	O-C-N	-6.69	111.99	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	325	GLU	Mainchain
1	C	325	GLU	Mainchain

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	2172	0	2040	130	0
1	B	2277	0	2175	131	0
1	C	2251	0	2127	131	0
1	D	2198	0	2084	138	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	4	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	86	0	64	17	0
4	B	86	0	64	17	0
4	C	86	0	64	19	0
4	D	86	0	64	21	0
5	A	9	0	0	0	0
5	B	5	0	0	0	0
5	C	15	0	0	1	0
5	D	7	0	0	1	0
All	All	9290	0	8682	519	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 29.

All (519) 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:C:200:CYS:SG	4:C:402:HEC:HAB	1.88	1.14
1:D:200:CYS:SG	4:D:402:HEC:HAB	1.92	1.09
1:B:200:CYS:SG	4:B:402:HEC:HAB	1.94	1.06
1:A:200:CYS:SG	4:A:803:HEC:HAB	1.95	1.06
1:C:54:CYS:SG	4:C:401:HEC:HAB	1.98	1.03
1:B:54:CYS:SG	4:B:401:HEC:HAB	2.00	1.02
1:A:325:GLU:O	1:A:326:HIS:HB3	1.59	1.01
1:B:54:CYS:SG	4:B:401:HEC:CAB	2.49	1.00
1:B:173:PHE:HB2	1:B:301:THR:HG23	1.45	0.99
1:A:173:PHE:HB2	1:A:301:THR:HG23	1.45	0.98
1:D:54:CYS:SG	4:D:401:HEC:HAB	2.03	0.97
1:D:173:PHE:HB2	1:D:301:THR:HG23	1.44	0.97
1:B:103:ASP:O	1:B:107:GLN:HB2	1.65	0.96
1:C:173:PHE:HB2	1:C:301:THR:HG23	1.47	0.95
1:A:72:ILE:HD11	1:A:80:PRO:HG3	1.49	0.95
1:C:54:CYS:SG	4:C:401:HEC:CAB	2.55	0.94
1:C:55:GLN:HE22	1:C:60:VAL:H	1.15	0.94
1:C:200:CYS:SG	4:C:402:HEC:CAB	2.55	0.93
1:A:54:CYS:SG	4:A:802:HEC:CAB	2.57	0.92
1:D:200:CYS:SG	4:D:402:HEC:CAB	2.57	0.92
1:A:54:CYS:SG	4:A:802:HEC:HAB	2.09	0.92
1:D:282:GLN:H	1:D:282:GLN:HE21	0.96	0.90
1:B:200:CYS:SG	4:B:402:HEC:CAB	2.60	0.89
1:D:54:CYS:SG	4:D:401:HEC:CAB	2.60	0.89
1:D:72:ILE:HD11	1:D:80:PRO:HG3	1.56	0.88
1:C:143:PHE:HB3	1:C:146:GLN:HG3	1.56	0.88
1:D:282:GLN:H	1:D:282:GLN:NE2	1.70	0.87
1:A:200:CYS:SG	4:A:803:HEC:CAB	2.61	0.87
1:B:72:ILE:HD11	1:B:80:PRO:HG3	1.54	0.87
1:A:325:GLU:O	1:A:326:HIS:CB	2.17	0.87
1:B:228:LEU:O	1:B:235:ARG:HD3	1.74	0.86
1:B:55:GLN:HE22	1:B:60:VAL:H	1.21	0.86
1:A:55:GLN:HE22	1:A:60:VAL:H	1.22	0.85
1:A:40:LEU:HD22	1:A:155:PHE:CE1	2.12	0.85
1:C:72:ILE:HD11	1:C:80:PRO:HG3	1.59	0.85
1:B:40:LEU:HD22	1:B:155:PHE:CE1	2.13	0.84
1:D:40:LEU:HD22	1:D:155:PHE:CE1	2.12	0.84
1:B:323:ARG:HG2	1:B:323:ARG:HH11	1.43	0.83
1:A:279:ALA:HB1	1:A:287:LEU:HD12	1.58	0.83
1:D:282:GLN:HE21	1:D:282:GLN:N	1.76	0.83
1:C:65:VAL:HG12	1:C:66:ASP:H	1.43	0.83
1:D:325:GLU:O	1:D:326:HIS:CB	2.27	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:PHE:HB2	1:D:301:THR:CG2	2.09	0.82
1:B:65:VAL:HG12	1:B:66:ASP:H	1.42	0.82
1:D:323:ARG:HH11	1:D:323:ARG:HG2	1.45	0.82
1:A:323:ARG:HH11	1:A:323:ARG:HG2	1.43	0.81
1:D:65:VAL:HG12	1:D:66:ASP:H	1.45	0.81
1:C:40:LEU:HD22	1:C:155:PHE:CE1	2.16	0.81
1:A:173:PHE:HB2	1:A:301:THR:CG2	2.11	0.80
1:D:55:GLN:HE22	1:D:60:VAL:H	1.28	0.80
1:D:90:VAL:HG13	5:D:1013:HOH:O	1.81	0.80
1:B:65:VAL:HG12	1:B:66:ASP:N	1.96	0.80
1:A:292:VAL:O	1:A:296:THR:HG22	1.82	0.79
1:C:93:VAL:HG13	1:C:212:ASN:HA	1.65	0.79
1:B:173:PHE:HB2	1:B:301:THR:CG2	2.12	0.79
1:B:162:PHE:O	1:B:165:THR:HB	1.81	0.79
1:C:65:VAL:HG12	1:C:66:ASP:N	1.98	0.79
1:D:162:PHE:O	1:D:165:THR:HB	1.83	0.79
1:C:41:PHE:HA	1:C:54:CYS:SG	2.23	0.78
1:A:162:PHE:O	1:A:165:THR:HB	1.83	0.78
1:B:93:VAL:HG13	1:B:212:ASN:HA	1.65	0.78
1:C:323:ARG:HG2	1:C:323:ARG:HH11	1.48	0.78
1:D:41:PHE:HA	1:D:54:CYS:SG	2.25	0.77
1:A:93:VAL:HG13	1:A:212:ASN:HA	1.66	0.77
1:D:93:VAL:HG13	1:D:212:ASN:HA	1.66	0.77
1:C:162:PHE:O	1:C:165:THR:HB	1.85	0.76
1:A:41:PHE:HA	1:A:54:CYS:SG	2.25	0.76
1:D:65:VAL:HG12	1:D:66:ASP:N	1.99	0.76
1:C:173:PHE:HB2	1:C:301:THR:CG2	2.15	0.75
1:D:19:GLN:NE2	1:D:22:GLN:HE22	1.85	0.74
1:A:65:VAL:HG12	1:A:66:ASP:N	2.04	0.73
1:A:65:VAL:HG12	1:A:66:ASP:H	1.54	0.73
1:D:122:PRO:O	1:D:126:VAL:HG23	1.89	0.73
1:A:324:PRO:HD2	1:D:269:TRP:CH2	2.24	0.72
1:D:100:ARG:CZ	1:D:245:GLU:HG2	2.18	0.72
1:C:222:LYS:HE3	1:C:237:ALA:HB2	1.73	0.71
1:D:129:VAL:HG11	1:D:139:PHE:CE1	2.26	0.71
1:A:283:LEU:HD22	4:A:803:HEC:HBC2	1.73	0.71
1:D:283:LEU:HD22	4:D:402:HEC:HBC2	1.73	0.71
1:C:203:CYS:SG	4:C:402:HEC:CAC	2.79	0.70
1:D:272:ARG:NH2	1:D:289:ASP:OD1	2.22	0.70
1:B:129:VAL:HG21	1:B:155:PHE:CE1	2.26	0.70
1:B:209:ILE:N	1:B:209:ILE:HD12	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:VAL:HG11	1:B:139:PHE:CE1	2.27	0.69
1:C:15:VAL:HG23	1:C:174:ASP:HB3	1.74	0.69
1:A:57:CYS:HA	1:A:66:ASP:HB3	1.74	0.69
1:B:41:PHE:HA	1:B:54:CYS:SG	2.31	0.69
1:B:292:VAL:O	1:B:296:THR:HG22	1.92	0.69
1:D:203:CYS:SG	4:D:402:HEC:CAC	2.81	0.69
1:C:129:VAL:HG21	1:C:155:PHE:CE1	2.28	0.68
1:B:57:CYS:SG	4:B:401:HEC:CAC	2.82	0.68
1:A:310:VAL:HA	1:D:310:VAL:HA	1.76	0.68
1:A:129:VAL:HG11	1:A:139:PHE:CE1	2.28	0.68
1:B:101:ALA:HB3	1:B:102:PRO:HD3	1.74	0.68
1:D:290:THR:O	1:D:294:GLN:HG3	1.94	0.68
1:C:283:LEU:HD13	4:C:402:HEC:HBC2	1.75	0.68
1:D:235:ARG:HG3	1:D:235:ARG:HH11	1.59	0.67
1:B:65:VAL:CG1	1:B:66:ASP:H	2.07	0.67
1:A:129:VAL:HG21	1:A:155:PHE:CE1	2.28	0.67
1:A:203:CYS:SG	4:A:803:HEC:CAC	2.82	0.67
1:C:227:VAL:HG11	1:D:100:ARG:NH1	2.10	0.67
1:C:122:PRO:O	1:C:126:VAL:HG23	1.94	0.67
1:D:292:VAL:O	1:D:296:THR:HG22	1.94	0.67
1:D:15:VAL:HG23	1:D:174:ASP:HB3	1.77	0.67
1:D:273:GLU:O	1:D:277:VAL:HG13	1.95	0.66
1:C:209:ILE:HD12	1:C:209:ILE:N	2.11	0.66
1:A:273:GLU:O	1:A:277:VAL:HG13	1.95	0.66
1:D:298:PHE:O	1:D:301:THR:HB	1.96	0.65
1:D:57:CYS:HA	1:D:66:ASP:HB3	1.77	0.65
1:C:57:CYS:SG	4:C:401:HEC:CAC	2.84	0.65
1:B:15:VAL:HG23	1:B:174:ASP:HB3	1.79	0.65
1:C:65:VAL:CG1	1:C:66:ASP:H	2.09	0.65
1:B:273:GLU:O	1:B:277:VAL:HG13	1.96	0.64
1:D:57:CYS:SG	4:D:401:HEC:CAC	2.84	0.64
1:B:159:VAL:O	1:B:163:GLU:HG3	1.97	0.64
1:A:209:ILE:HD12	1:A:209:ILE:N	2.13	0.64
1:B:203:CYS:SG	4:B:402:HEC:CAC	2.85	0.64
1:D:101:ALA:HB3	1:D:102:PRO:HD3	1.79	0.64
1:A:122:PRO:O	1:A:126:VAL:HG23	1.98	0.64
1:D:129:VAL:HG21	1:D:155:PHE:CE1	2.32	0.64
1:C:101:ALA:HB3	1:C:102:PRO:HD3	1.78	0.64
1:C:143:PHE:CB	1:C:146:GLN:HG3	2.27	0.64
1:C:290:THR:O	1:C:294:GLN:HG3	1.98	0.64
1:B:122:PRO:O	1:B:126:VAL:HG23	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:ILE:N	1:D:209:ILE:HD12	2.13	0.63
1:C:273:GLU:O	1:C:277:VAL:HG13	1.98	0.63
1:A:159:VAL:O	1:A:163:GLU:HG3	1.99	0.63
1:B:57:CYS:HA	1:B:66:ASP:HB3	1.79	0.63
1:D:65:VAL:CG1	1:D:66:ASP:H	2.11	0.62
1:C:57:CYS:HA	1:C:66:ASP:HB3	1.81	0.62
1:C:159:VAL:O	1:C:163:GLU:HG3	2.00	0.62
1:C:185:SER:OG	1:C:188:GLU:HG3	1.98	0.62
1:C:129:VAL:HG11	1:C:139:PHE:CE1	2.33	0.62
1:C:292:VAL:O	1:C:296:THR:HG22	1.99	0.62
1:B:193:LYS:HE2	1:B:197:ASP:OD1	2.00	0.62
1:C:228:LEU:O	1:C:235:ARG:HD3	1.99	0.62
1:C:193:LYS:HE2	1:C:197:ASP:OD1	2.00	0.62
1:B:49:SER:OG	1:B:51:VAL:HG13	2.01	0.61
1:C:249:ARG:HH22	4:C:401:HEC:CGA	2.14	0.61
1:B:65:VAL:CG1	1:B:66:ASP:N	2.63	0.60
1:D:193:LYS:HE2	1:D:197:ASP:OD1	2.01	0.60
1:D:249:ARG:HH22	4:D:401:HEC:CGA	2.13	0.60
1:A:310:VAL:HG22	1:D:310:VAL:HG22	1.84	0.60
1:A:193:LYS:HE2	1:A:197:ASP:OD1	2.02	0.60
1:D:100:ARG:NH2	1:D:245:GLU:HG2	2.17	0.59
1:B:243:ASP:OD2	1:B:245:GLU:HB2	2.02	0.59
1:C:227:VAL:HG11	1:D:100:ARG:HH12	1.67	0.59
1:B:129:VAL:HG21	1:B:155:PHE:CD1	2.36	0.59
1:B:225:ALA:HB1	1:B:235:ARG:HB3	1.84	0.59
1:C:65:VAL:CG1	1:C:66:ASP:N	2.65	0.59
1:D:159:VAL:O	1:D:163:GLU:HG3	2.03	0.59
1:B:278:MET:HG2	4:B:402:HEC:NB	2.17	0.59
1:A:15:VAL:HG23	1:A:174:ASP:HB3	1.84	0.59
1:A:129:VAL:HG21	1:A:155:PHE:CD1	2.38	0.59
1:A:290:THR:O	1:A:294:GLN:HG3	2.03	0.59
1:A:249:ARG:HH22	4:A:802:HEC:CGA	2.15	0.59
1:B:287:LEU:HD22	1:B:291:GLN:HB3	1.84	0.59
1:B:249:ARG:HH22	4:B:401:HEC:CGA	2.16	0.59
1:C:298:PHE:O	1:C:301:THR:HB	2.03	0.59
1:C:323:ARG:HH11	1:C:323:ARG:CG	2.16	0.59
1:B:323:ARG:HH11	1:B:323:ARG:CG	2.13	0.58
1:A:65:VAL:CG1	1:A:66:ASP:H	2.16	0.58
1:B:209:ILE:HG22	1:B:209:ILE:O	2.04	0.58
1:C:272:ARG:HG3	1:C:272:ARG:HH11	1.68	0.58
1:A:185:SER:OG	1:A:188:GLU:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:CYS:SG	4:A:802:HEC:CAC	2.92	0.58
1:D:19:GLN:HE22	1:D:22:GLN:HE22	1.50	0.58
1:B:278:MET:HG2	4:B:402:HEC:C4B	2.34	0.58
1:C:27:ASN:CB	1:C:30:THR:HG22	2.33	0.58
1:D:192:LEU:HD13	1:D:298:PHE:CE1	2.38	0.58
1:A:65:VAL:HG12	1:A:67:GLY:H	1.69	0.58
1:B:39:MET:CE	1:B:315:PRO:HD3	2.34	0.58
1:D:103:ASP:O	1:D:107:GLN:HB2	2.04	0.58
1:D:65:VAL:HG12	1:D:67:GLY:H	1.70	0.57
1:B:298:PHE:O	1:B:301:THR:HB	2.04	0.57
1:A:298:PHE:O	1:A:301:THR:HB	2.05	0.57
1:A:323:ARG:HH11	1:A:323:ARG:CG	2.14	0.57
1:D:279:ALA:HB1	1:D:287:LEU:HD12	1.85	0.57
1:B:147:LYS:O	1:B:149:PRO:HD3	2.05	0.57
1:D:283:LEU:HD22	4:D:402:HEC:CBC	2.33	0.57
1:A:101:ALA:HB3	1:A:102:PRO:HD3	1.85	0.57
1:B:290:THR:O	1:B:294:GLN:HG3	2.05	0.57
1:D:272:ARG:HG3	1:D:272:ARG:HH11	1.70	0.57
1:A:285:ALA:O	1:A:287:LEU:HG	2.04	0.57
1:D:190:ALA:O	1:D:194:LEU:HG	2.04	0.57
1:B:195:PHE:O	1:B:200:CYS:SG	2.62	0.56
1:B:129:VAL:CG2	1:B:155:PHE:CE1	2.88	0.56
1:C:129:VAL:HG21	1:C:155:PHE:CD1	2.41	0.56
1:D:65:VAL:CG1	1:D:66:ASP:N	2.67	0.56
1:B:69:GLU:HA	1:B:261:PRO:HG3	1.88	0.56
1:D:198:THR:HG23	1:D:285:ALA:HB3	1.88	0.56
1:A:129:VAL:CG2	1:A:155:PHE:CE1	2.89	0.56
1:B:195:PHE:HA	1:B:200:CYS:SG	2.46	0.56
1:C:278:MET:HG2	4:C:402:HEC:C4B	2.36	0.55
1:D:209:ILE:O	1:D:209:ILE:HG22	2.06	0.55
1:B:292:VAL:O	1:B:296:THR:CG2	2.54	0.55
1:C:278:MET:HG2	4:C:402:HEC:NB	2.22	0.55
1:D:49:SER:HA	1:D:325:GLU:CB	2.36	0.55
1:C:15:VAL:HG23	1:C:174:ASP:CB	2.36	0.55
1:B:65:VAL:HG12	1:B:67:GLY:H	1.71	0.55
1:A:278:MET:HG2	4:A:803:HEC:NB	2.22	0.55
1:B:228:LEU:HD12	1:B:229:PRO:HD2	1.89	0.55
1:D:15:VAL:HG23	1:D:174:ASP:CG	2.27	0.55
1:A:65:VAL:CG1	1:A:66:ASP:N	2.70	0.55
1:A:100:ARG:NH1	1:B:227:VAL:HG11	2.22	0.54
1:B:176:TRP:HB2	1:B:184:MET:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ALA:HB1	1:B:287:LEU:HD12	1.88	0.54
1:D:15:VAL:HG23	1:D:174:ASP:CB	2.37	0.54
1:D:195:PHE:HA	1:D:200:CYS:SG	2.48	0.54
1:A:316:VAL:HG22	1:D:258:LEU:HD22	1.89	0.54
1:C:203:CYS:SG	4:C:402:HEC:HAC	2.48	0.54
1:D:323:ARG:HH11	1:D:323:ARG:CG	2.16	0.54
1:D:129:VAL:HG21	1:D:155:PHE:CD1	2.41	0.54
1:D:185:SER:O	1:D:189:LYS:HG3	2.06	0.54
1:A:278:MET:HG2	4:A:803:HEC:C4B	2.37	0.54
1:A:103:ASP:O	1:A:107:GLN:HB2	2.08	0.54
1:A:262:TYR:HB2	1:A:268:VAL:CG2	2.38	0.54
1:B:268:VAL:O	1:B:268:VAL:HG23	2.07	0.54
1:C:65:VAL:HG12	1:C:67:GLY:H	1.74	0.53
1:C:129:VAL:CG2	1:C:155:PHE:CE1	2.91	0.53
1:C:145:GLY:O	1:C:146:GLN:HG2	2.08	0.53
1:B:129:VAL:CG2	1:B:155:PHE:HE1	2.21	0.53
1:D:292:VAL:O	1:D:296:THR:CG2	2.55	0.53
1:A:209:ILE:O	1:A:209:ILE:HG22	2.08	0.53
1:A:272:ARG:HG3	1:A:272:ARG:HH11	1.72	0.53
1:A:126:VAL:O	1:A:130:GLN:HB2	2.09	0.53
1:D:126:VAL:O	1:D:130:GLN:HB2	2.09	0.53
1:A:47:SER:HB3	1:A:52:PHE:O	2.09	0.53
1:C:129:VAL:CG2	1:C:155:PHE:HE1	2.22	0.53
1:D:216:PRO:HB3	1:D:244:ASP:HA	1.91	0.53
1:A:129:VAL:CG2	1:A:155:PHE:HE1	2.22	0.53
1:C:15:VAL:HG23	1:C:174:ASP:CG	2.29	0.53
1:C:55:GLN:NE2	1:C:60:VAL:H	1.96	0.52
1:A:185:SER:O	1:A:189:LYS:HG3	2.09	0.52
1:C:292:VAL:O	1:C:296:THR:CG2	2.57	0.52
1:D:59:ASN:HB3	1:D:62:LEU:HB2	1.91	0.52
1:D:129:VAL:CG2	1:D:155:PHE:CE1	2.92	0.52
1:D:195:PHE:O	1:D:200:CYS:SG	2.66	0.52
1:B:272:ARG:HG3	1:B:272:ARG:HH11	1.75	0.52
1:C:268:VAL:HG23	1:C:268:VAL:O	2.09	0.52
1:B:209:ILE:N	1:B:209:ILE:CD1	2.73	0.52
1:A:195:PHE:HA	1:A:200:CYS:SG	2.49	0.52
1:A:49:SER:OG	1:A:51:VAL:HG13	2.10	0.52
1:B:126:VAL:O	1:B:130:GLN:HB2	2.10	0.51
1:C:126:VAL:O	1:C:130:GLN:HB2	2.10	0.51
1:C:209:ILE:HG22	1:C:209:ILE:O	2.10	0.51
1:A:69:GLU:HA	1:A:261:PRO:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:PHE:O	1:A:200:CYS:SG	2.65	0.51
1:B:151:SER:OG	1:B:154:ASN:ND2	2.44	0.51
1:C:262:TYR:HB2	1:C:268:VAL:CG2	2.40	0.51
1:D:74:HIS:O	1:D:77:GLN:HB2	2.11	0.51
1:D:278:MET:HG2	4:D:402:HEC:C4B	2.40	0.51
1:B:15:VAL:HG23	1:B:174:ASP:CB	2.40	0.51
1:C:103:ASP:O	1:C:107:GLN:HB2	2.11	0.51
1:D:129:VAL:HG13	1:D:135:TYR:HB3	1.92	0.51
1:D:200:CYS:CB	4:D:402:HEC:HAB	2.39	0.51
1:D:268:VAL:HG23	1:D:268:VAL:O	2.11	0.51
1:B:185:SER:OG	1:B:188:GLU:HG3	2.10	0.51
1:A:323:ARG:HG2	1:A:323:ARG:NH1	2.22	0.50
1:B:104:LEU:O	1:B:107:GLN:HB3	2.11	0.50
1:B:262:TYR:HB2	1:B:268:VAL:CG2	2.41	0.50
1:D:49:SER:OG	1:D:51:VAL:HG13	2.11	0.50
1:B:129:VAL:HG13	1:B:135:TYR:HB3	1.94	0.50
1:B:249:ARG:O	4:B:402:HEC:HAD1	2.11	0.50
1:A:39:MET:CE	1:A:315:PRO:HD3	2.41	0.50
1:B:143:PHE:N	1:B:144:PRO:HD3	2.27	0.50
1:A:129:VAL:HG13	1:A:135:TYR:HB3	1.93	0.50
1:C:69:GLU:HA	1:C:261:PRO:HG3	1.93	0.50
1:C:195:PHE:HA	1:C:200:CYS:SG	2.52	0.50
1:C:27:ASN:C	1:C:29:VAL:H	2.15	0.50
1:A:324:PRO:CD	1:D:269:TRP:CH2	2.95	0.50
1:D:40:LEU:HD22	1:D:155:PHE:CZ	2.47	0.50
1:D:283:LEU:HD13	4:D:402:HEC:HBC2	1.94	0.50
1:C:185:SER:O	1:C:189:LYS:HG3	2.12	0.49
1:D:129:VAL:CG2	1:D:155:PHE:HE1	2.24	0.49
1:B:15:VAL:HG23	1:B:174:ASP:CG	2.32	0.49
1:B:47:SER:HB3	1:B:52:PHE:O	2.13	0.49
1:C:249:ARG:O	4:C:402:HEC:HAD1	2.12	0.49
1:B:200:CYS:CB	4:B:402:HEC:HAB	2.42	0.49
1:A:184:MET:HE3	1:A:189:LYS:HG2	1.94	0.49
1:C:99:GLY:HA2	1:C:246:TYR:CE1	2.48	0.49
1:C:184:MET:HE3	1:C:189:LYS:HG2	1.95	0.49
1:C:229:PRO:O	1:C:230:ALA:C	2.51	0.49
1:A:200:CYS:CB	4:A:803:HEC:HAB	2.42	0.49
1:B:279:ALA:O	1:B:284:GLY:HA3	2.13	0.49
1:C:209:ILE:N	1:C:209:ILE:CD1	2.76	0.49
1:D:69:GLU:HA	1:D:261:PRO:HG3	1.94	0.49
1:D:278:MET:HG2	4:D:402:HEC:NB	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:SER:O	1:B:189:LYS:HG3	2.13	0.49
1:C:15:VAL:CG2	1:C:174:ASP:HB3	2.41	0.49
1:C:135:TYR:O	1:C:139:PHE:HD1	1.96	0.49
1:C:200:CYS:CB	4:C:402:HEC:HAB	2.43	0.49
1:D:185:SER:OG	1:D:188:GLU:HG3	2.11	0.49
1:A:15:VAL:HG23	1:A:174:ASP:CG	2.33	0.49
1:B:193:LYS:HE2	1:B:197:ASP:CG	2.33	0.49
1:C:235:ARG:NH2	1:C:236:PHE:HE1	2.11	0.49
1:D:100:ARG:NH2	1:D:245:GLU:OE2	2.46	0.49
1:B:323:ARG:CG	1:B:323:ARG:NH1	2.74	0.49
1:C:39:MET:CE	1:C:315:PRO:HD3	2.43	0.49
1:C:176:TRP:HB2	1:C:184:MET:HG3	1.95	0.49
1:D:203:CYS:SG	4:D:402:HEC:HAC	2.51	0.49
1:A:323:ARG:HD3	1:D:269:TRP:CD1	2.48	0.48
1:D:193:LYS:HG3	1:D:197:ASP:OD2	2.13	0.48
1:A:192:LEU:HD13	1:A:298:PHE:CE1	2.48	0.48
1:C:193:LYS:HE2	1:C:197:ASP:CG	2.34	0.48
1:A:176:TRP:HB2	1:A:184:MET:HG3	1.95	0.48
1:B:203:CYS:SG	4:B:402:HEC:HAC	2.53	0.48
1:C:195:PHE:O	1:C:200:CYS:SG	2.69	0.48
1:A:40:LEU:HD22	1:A:155:PHE:CZ	2.49	0.48
1:B:222:LYS:O	1:B:225:ALA:HB2	2.13	0.48
1:C:47:SER:HB3	1:C:52:PHE:O	2.14	0.48
1:B:59:ASN:HB3	1:B:62:LEU:HB2	1.94	0.48
1:B:281:SER:C	1:B:283:LEU:H	2.15	0.48
1:C:84:PRO:HD3	4:C:401:HEC:HAD1	1.95	0.48
1:B:40:LEU:HD22	1:B:155:PHE:CZ	2.48	0.48
1:B:233:LYS:NZ	1:B:233:LYS:CB	2.77	0.48
1:C:55:GLN:NE2	1:C:60:VAL:HG13	2.28	0.48
1:C:143:PHE:HB3	1:C:146:GLN:CG	2.38	0.48
1:A:203:CYS:SG	4:A:803:HEC:HAC	2.53	0.48
1:A:268:VAL:HG23	1:A:268:VAL:O	2.13	0.48
1:A:279:ALA:CB	1:A:287:LEU:HD12	2.38	0.48
1:B:228:LEU:HG	1:B:232:ASP:CG	2.34	0.48
1:C:129:VAL:HG13	1:C:135:TYR:HB3	1.95	0.48
1:D:262:TYR:HB2	1:D:268:VAL:CG2	2.44	0.48
1:A:323:ARG:CG	1:A:323:ARG:NH1	2.75	0.47
1:D:209:ILE:N	1:D:209:ILE:CD1	2.77	0.47
1:B:82:ASN:ND2	1:B:261:PRO:HG2	2.27	0.47
1:B:193:LYS:HE2	1:B:197:ASP:OD2	2.15	0.47
1:B:272:ARG:NH1	1:B:293:ASP:OD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:HIS:O	1:A:77:GLN:HB2	2.14	0.47
1:D:135:TYR:O	1:D:139:PHE:HD1	1.97	0.47
1:A:84:PRO:HD3	4:A:802:HEC:HAD1	1.97	0.47
1:C:19:GLN:HA	1:C:167:ILE:HD11	1.96	0.47
1:A:30:THR:O	1:A:31:ARG:CB	2.62	0.47
1:A:242:ALA:CB	1:B:225:ALA:HA	2.44	0.47
1:B:269:TRP:NE1	1:C:323:ARG:HD3	2.28	0.47
1:B:310:VAL:HA	1:C:310:VAL:HA	1.97	0.47
1:C:225:ALA:O	1:C:235:ARG:HD2	2.15	0.47
1:D:323:ARG:CG	1:D:323:ARG:NH1	2.77	0.47
1:A:59:ASN:HB3	1:A:62:LEU:HB2	1.97	0.47
1:C:283:LEU:HD22	4:C:402:HEC:HBC2	1.97	0.47
1:D:176:TRP:HB2	1:D:184:MET:HG3	1.95	0.47
1:C:78:LYS:HG3	1:C:246:TYR:OH	2.15	0.47
4:C:401:HEC:HMC1	4:C:401:HEC:HBC3	1.96	0.47
1:A:249:ARG:O	4:A:803:HEC:HAD1	2.15	0.47
1:C:27:ASN:N	1:C:30:THR:CG2	2.78	0.47
1:D:15:VAL:CG2	1:D:174:ASP:HB3	2.43	0.47
1:D:272:ARG:NH1	1:D:293:ASP:OD1	2.48	0.47
1:C:198:THR:HG22	1:C:198:THR:O	2.16	0.46
1:A:15:VAL:HG23	1:A:174:ASP:CB	2.44	0.46
1:C:76:TRP:CD1	1:C:76:TRP:C	2.89	0.46
1:D:40:LEU:CD2	1:D:155:PHE:CE1	2.93	0.46
1:A:180:ALA:HB3	1:A:183:ALA:HB2	1.97	0.46
1:C:84:PRO:CD	4:C:401:HEC:HAD1	2.46	0.46
1:C:193:LYS:HE2	1:C:197:ASP:OD2	2.16	0.46
1:D:262:TYR:O	1:D:263:PHE:HB2	2.15	0.46
1:A:272:ARG:NH1	1:A:293:ASP:OD1	2.48	0.46
1:B:262:TYR:O	1:B:263:PHE:HB2	2.15	0.46
1:C:55:GLN:HE22	1:C:60:VAL:HG13	1.80	0.46
1:C:59:ASN:HB3	1:C:62:LEU:HB2	1.97	0.46
1:C:272:ARG:NH1	1:C:293:ASP:OD1	2.49	0.46
1:A:209:ILE:N	1:A:209:ILE:CD1	2.77	0.46
1:A:184:MET:CE	1:A:189:LYS:HG2	2.46	0.46
1:A:193:LYS:HE2	1:A:197:ASP:CG	2.36	0.46
1:B:84:PRO:HG2	4:B:401:HEC:HBA1	1.98	0.46
1:C:49:SER:OG	1:C:51:VAL:HG13	2.16	0.46
1:C:225:ALA:HA	1:D:242:ALA:CB	2.46	0.46
1:B:193:LYS:HG3	1:B:197:ASP:OD2	2.16	0.46
1:B:198:THR:HG22	1:B:198:THR:O	2.15	0.46
1:D:76:TRP:CD1	1:D:76:TRP:C	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:TYR:HB2	1:A:268:VAL:HG23	1.98	0.46
1:A:316:VAL:HG22	1:D:258:LEU:CD2	2.46	0.46
1:B:84:PRO:HD3	4:B:401:HEC:HAD1	1.97	0.46
1:A:29:VAL:O	1:A:30:THR:C	2.55	0.46
1:A:217:PHE:O	1:A:248:PHE:HB2	2.17	0.45
1:A:29:VAL:O	1:A:31:ARG:N	2.49	0.45
1:A:136:VAL:HA	1:A:150:ILE:HD11	1.99	0.45
1:B:33:LYS:HB2	1:B:33:LYS:HE3	1.84	0.45
1:A:64:GLY:O	1:A:85:THR:HA	2.16	0.45
1:A:129:VAL:CG1	1:A:139:PHE:CE1	3.00	0.45
1:B:249:ARG:HD3	1:B:251:GLY:HA2	1.98	0.45
1:C:136:VAL:HA	1:C:150:ILE:HD11	1.98	0.45
1:D:84:PRO:HG2	4:D:401:HEC:HBA1	1.99	0.45
1:A:146:GLN:O	1:A:149:PRO:HD3	2.17	0.45
1:A:151:SER:OG	1:A:154:ASN:ND2	2.49	0.45
1:D:84:PRO:HD3	4:D:401:HEC:HAD1	1.97	0.45
1:C:288:ASP:OD1	1:C:290:THR:N	2.50	0.45
1:A:29:VAL:O	1:A:32:ASP:N	2.49	0.45
1:A:49:SER:HA	1:A:325:GLU:CB	2.46	0.45
1:B:129:VAL:CG1	1:B:139:PHE:CE1	2.98	0.45
1:B:287:LEU:HA	1:B:291:GLN:OE1	2.17	0.45
1:C:219:VAL:HG22	1:C:238:VAL:HG22	1.99	0.45
1:A:249:ARG:HD3	1:A:251:GLY:HA2	1.99	0.44
1:C:193:LYS:HG3	1:C:197:ASP:OD2	2.17	0.44
1:D:129:VAL:CG1	1:D:139:PHE:CE1	2.98	0.44
1:D:193:LYS:HE2	1:D:197:ASP:CG	2.37	0.44
1:A:40:LEU:HD22	1:A:155:PHE:HE1	1.75	0.44
1:A:198:THR:O	1:A:198:THR:HG22	2.18	0.44
1:D:249:ARG:O	4:D:402:HEC:HAD1	2.17	0.44
1:D:323:ARG:HG2	1:D:323:ARG:NH1	2.22	0.44
4:A:802:HEC:HBC3	4:A:802:HEC:HMC1	1.99	0.44
1:C:82:ASN:ND2	1:C:261:PRO:HG2	2.32	0.44
1:D:41:PHE:HA	1:D:54:CYS:HG	1.79	0.44
1:D:198:THR:O	1:D:198:THR:HG22	2.18	0.44
1:A:76:TRP:CD1	1:A:76:TRP:C	2.89	0.44
1:C:40:LEU:HD22	1:C:155:PHE:CZ	2.50	0.44
1:C:272:ARG:HG3	1:C:272:ARG:NH1	2.32	0.44
1:C:74:HIS:O	1:C:77:GLN:HB2	2.16	0.44
1:C:132:MET:HG2	1:C:317:ARG:HA	1.99	0.44
1:D:136:VAL:HA	1:D:150:ILE:HD11	2.00	0.44
1:A:19:GLN:HA	1:A:167:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:PRO:HG2	4:C:401:HEC:HBA1	1.99	0.44
1:C:192:LEU:HD13	1:C:298:PHE:CE1	2.54	0.43
1:B:39:MET:HE2	1:B:315:PRO:HD3	2.00	0.43
1:B:74:HIS:O	1:B:77:GLN:HB2	2.18	0.43
1:C:243:ASP:OD1	1:C:245:GLU:CD	2.57	0.43
1:D:39:MET:CE	1:D:315:PRO:HD3	2.47	0.43
1:B:233:LYS:HE3	1:B:233:LYS:HB2	1.73	0.43
1:C:98:ASP:HB3	1:C:248:PHE:CD2	2.52	0.43
1:D:145:GLY:O	1:D:146:GLN:CB	2.67	0.43
1:B:102:PRO:C	1:B:104:LEU:N	2.70	0.43
1:D:22:GLN:OE1	1:D:22:GLN:N	2.51	0.43
1:D:40:LEU:HD22	1:D:155:PHE:HE1	1.76	0.43
1:B:102:PRO:O	1:B:105:ALA:N	2.51	0.43
1:D:288:ASP:C	1:D:288:ASP:OD1	2.56	0.43
1:C:64:GLY:O	1:C:85:THR:HA	2.19	0.43
1:C:262:TYR:O	1:C:263:PHE:HB2	2.18	0.43
1:D:47:SER:HB3	1:D:52:PHE:O	2.19	0.43
1:A:84:PRO:CD	4:A:802:HEC:HAD1	2.49	0.43
1:B:44:PRO:O	1:B:50:GLY:HA2	2.19	0.43
1:B:84:PRO:CD	4:B:401:HEC:HAD1	2.49	0.43
1:B:40:LEU:HD22	1:B:155:PHE:HE1	1.76	0.43
1:B:142:ALA:C	1:B:144:PRO:HD3	2.39	0.43
1:B:228:LEU:O	1:B:232:ASP:HB2	2.19	0.43
1:C:94:ALA:HB1	1:C:214:TYR:CZ	2.54	0.43
1:D:19:GLN:HA	1:D:167:ILE:HD11	2.01	0.43
1:D:235:ARG:HH11	1:D:235:ARG:CG	2.26	0.43
1:D:288:ASP:OD1	1:D:291:GLN:HG3	2.19	0.43
4:B:401:HEC:HBC3	4:B:401:HEC:HMC1	2.01	0.42
1:D:84:PRO:CD	4:D:401:HEC:HAD1	2.49	0.42
1:D:283:LEU:CD2	4:D:402:HEC:HBC2	2.46	0.42
1:B:15:VAL:CG2	1:B:174:ASP:HB3	2.46	0.42
1:B:30:THR:O	1:B:34:ILE:HG13	2.19	0.42
1:B:192:LEU:HD13	1:B:298:PHE:CE1	2.55	0.42
1:B:222:LYS:HA	1:B:222:LYS:HD3	1.85	0.42
1:A:217:PHE:CD2	1:A:283:LEU:HD21	2.54	0.42
1:B:58:HIS:HA	1:B:64:GLY:O	2.20	0.42
1:C:325:GLU:O	1:C:326:HIS:CB	2.65	0.42
1:D:96:PHE:O	1:D:214:TYR:HE2	2.02	0.42
1:D:217:PHE:O	1:D:248:PHE:HB2	2.20	0.42
1:D:238:VAL:HG11	1:D:283:LEU:HG	2.01	0.42
1:B:180:ALA:HB3	1:B:183:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ALA:O	1:B:205:ASN:HB3	2.20	0.42
1:C:84:PRO:HD2	4:C:401:HEC:C3D	2.49	0.42
1:C:184:MET:CE	1:C:189:LYS:HG2	2.49	0.42
1:A:44:PRO:O	1:A:50:GLY:HA2	2.19	0.42
1:A:76:TRP:HB2	1:A:107:GLN:NE2	2.35	0.42
1:A:288:ASP:CG	1:A:289:ASP:N	2.73	0.42
1:A:324:PRO:HD2	1:D:269:TRP:CZ2	2.55	0.42
1:B:176:TRP:CB	1:B:184:MET:HG3	2.50	0.42
1:A:65:VAL:HG21	1:A:259:THR:HB	2.02	0.42
1:B:98:ASP:HB3	1:B:248:PHE:CD2	2.55	0.42
1:B:262:TYR:HB2	1:B:268:VAL:HG23	2.02	0.42
1:B:301:THR:HG23	1:B:301:THR:O	2.18	0.42
1:D:214:TYR:CD2	1:D:249:ARG:HB2	2.54	0.42
1:C:43:ASP:HB3	1:C:46:MET:HG2	2.01	0.42
4:D:401:HEC:HBC3	4:D:401:HEC:HMC1	2.02	0.42
1:A:293:ASP:O	1:A:296:THR:HG23	2.20	0.41
1:B:184:MET:CE	1:B:189:LYS:HG2	2.50	0.41
1:C:249:ARG:HD3	1:C:251:GLY:HA2	2.02	0.41
1:A:275:VAL:HG21	1:A:296:THR:HB	2.02	0.41
1:B:136:VAL:HA	1:B:150:ILE:HD11	2.02	0.41
1:B:268:VAL:O	1:B:268:VAL:CG2	2.68	0.41
1:D:84:PRO:HD2	4:D:401:HEC:C3D	2.50	0.41
1:A:135:TYR:O	1:A:139:PHE:HD1	2.03	0.41
1:A:193:LYS:HE2	1:A:197:ASP:OD2	2.21	0.41
1:A:193:LYS:HG3	1:A:197:ASP:OD2	2.20	0.41
1:D:96:PHE:HE1	1:D:108:ALA:HB2	1.84	0.41
1:A:198:THR:HG21	1:A:287:LEU:HD11	2.02	0.41
1:A:201:ALA:O	1:A:205:ASN:HB3	2.21	0.41
1:B:36:LEU:HD11	1:B:139:PHE:CE1	2.56	0.41
1:B:76:TRP:CD1	1:B:76:TRP:C	2.93	0.41
1:B:217:PHE:O	1:B:248:PHE:HB2	2.19	0.41
1:D:43:ASP:HB3	1:D:46:MET:HG2	2.02	0.41
1:A:98:ASP:HB3	1:A:248:PHE:CD2	2.55	0.41
1:C:41:PHE:HA	1:C:54:CYS:HG	1.82	0.41
1:D:32:ASP:OD2	1:D:141:LYS:HB3	2.20	0.41
1:D:192:LEU:HD13	1:D:298:PHE:CZ	2.54	0.41
1:D:214:TYR:CE2	1:D:249:ARG:HB2	2.55	0.41
1:D:94:ALA:HB1	1:D:214:TYR:CZ	2.55	0.41
1:D:235:ARG:CG	1:D:235:ARG:NH1	2.84	0.41
1:A:40:LEU:CD2	1:A:155:PHE:CE1	2.95	0.41
1:B:64:GLY:O	1:B:85:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ASN:ND2	1:A:261:PRO:HG2	2.35	0.41
1:B:40:LEU:CD2	1:B:155:PHE:CE1	2.95	0.41
1:B:283:LEU:HD13	4:B:402:HEC:HBC2	2.03	0.41
1:D:249:ARG:HD3	1:D:251:GLY:HA2	2.03	0.41
1:A:292:VAL:O	1:A:296:THR:CG2	2.61	0.41
1:C:40:LEU:CD2	1:C:155:PHE:CE1	2.98	0.41
1:C:90:VAL:HG13	5:C:1017:HOH:O	2.21	0.40
1:C:243:ASP:C	1:C:245:GLU:H	2.24	0.40
1:C:262:TYR:HB2	1:C:268:VAL:HG23	2.03	0.40
1:C:272:ARG:HD3	1:C:272:ARG:C	2.41	0.40
1:A:55:GLN:HE22	1:A:60:VAL:HG13	1.87	0.40
1:A:55:GLN:NE2	1:A:60:VAL:HG13	2.36	0.40
1:A:84:PRO:HD2	4:A:802:HEC:C3D	2.51	0.40
1:C:146:GLN:HE21	1:C:146:GLN:HA	1.85	0.40
1:C:301:THR:HG23	1:C:301:THR:O	2.21	0.40
1:D:64:GLY:O	1:D:85:THR:HA	2.20	0.40
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.96	0.40
1:B:18:MET:O	1:B:19:GLN:HG3	2.21	0.40
1:B:94:ALA:HB1	1:B:214:TYR:CZ	2.55	0.40
1:B:135:TYR:O	1:B:139:PHE:HD1	2.04	0.40
1:C:180:ALA:HB3	1:C:183:ALA:HB2	2.04	0.40
1:A:217:PHE:CG	1:A:283:LEU:HD21	2.56	0.40
1:C:323:ARG:CG	1:C:323:ARG:NH1	2.77	0.40
1:A:89:ALA:HA	1:A:92:ASN:ND2	2.36	0.40
1:C:129:VAL:CG1	1:C:139:PHE:CE1	3.03	0.40
1:D:238:VAL:HB	1:D:281:SER:HB2	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	289/328 (88%)	272 (94%)	14 (5%)	3 (1%)	15	37
1	B	300/328 (92%)	276 (92%)	19 (6%)	5 (2%)	9	23
1	C	299/328 (91%)	278 (93%)	17 (6%)	4 (1%)	12	30
1	D	290/328 (88%)	272 (94%)	14 (5%)	4 (1%)	11	28
All	All	1178/1312 (90%)	1098 (93%)	64 (5%)	16 (1%)	11	28

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	B	233	LYS
1	D	325	GLU
1	A	120	ASN
1	B	120	ASN
1	B	242	ALA
1	C	120	ASN
1	D	31	ARG
1	D	120	ASN
1	D	146	GLN
1	A	30	THR
1	B	226	GLU
1	C	144	PRO
1	B	234	GLY
1	C	21	PRO
1	C	229	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	214/254 (84%)	203 (95%)	11 (5%)	24	50
1	B	229/254 (90%)	216 (94%)	13 (6%)	20	44
1	C	222/254 (87%)	210 (95%)	12 (5%)	22	47
1	D	219/254 (86%)	205 (94%)	14 (6%)	17	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	884/1016 (87%)	834 (94%)	50 (6%)	20 44

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	VAL
1	A	97	TRP
1	A	123	GLU
1	A	200	CYS
1	A	249	ARG
1	A	272	ARG
1	A	277	VAL
1	A	278	MET
1	A	286	THR
1	A	296	THR
1	A	301	THR
1	B	93	VAL
1	B	97	TRP
1	B	123	GLU
1	B	200	CYS
1	B	232	ASP
1	B	233	LYS
1	B	239	THR
1	B	249	ARG
1	B	272	ARG
1	B	277	VAL
1	B	278	MET
1	B	296	THR
1	B	301	THR
1	C	30	THR
1	C	93	VAL
1	C	97	TRP
1	C	123	GLU
1	C	146	GLN
1	C	200	CYS
1	C	249	ARG
1	C	272	ARG
1	C	277	VAL
1	C	278	MET
1	C	296	THR
1	C	301	THR
1	D	54	CYS

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Mol	Chain	Res	Type
1	D	93	VAL
1	D	97	TRP
1	D	123	GLU
1	D	124	ASN
1	D	200	CYS
1	D	245	GLU
1	D	249	ARG
1	D	272	ARG
1	D	277	VAL
1	D	278	MET
1	D	282	GLN
1	D	296	THR
1	D	301	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	107	GLN
1	A	154	ASN
1	A	311	HIS
1	B	55	GLN
1	B	154	ASN
1	B	311	HIS
1	C	55	GLN
1	C	107	GLN
1	C	146	GLN
1	C	154	ASN
1	C	311	HIS
1	D	19	GLN
1	D	55	GLN
1	D	107	GLN
1	D	124	ASN
1	D	154	ASN
1	D	282	GLN
1	D	311	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	HEC	B	402	1	32,50,50	1.45	3 (9%)	24,82,82	1.49	5 (20%)
4	HEC	D	402	1	32,50,50	1.36	1 (3%)	24,82,82	1.50	4 (16%)
4	HEC	D	401	1	32,50,50	1.49	4 (12%)	24,82,82	1.79	5 (20%)
4	HEC	A	802	1	32,50,50	1.40	3 (9%)	24,82,82	1.76	6 (25%)
4	HEC	C	402	1	32,50,50	1.42	3 (9%)	24,82,82	1.49	4 (16%)
4	HEC	B	401	1	32,50,50	1.44	4 (12%)	24,82,82	1.74	5 (20%)
4	HEC	C	401	1	32,50,50	1.47	4 (12%)	24,82,82	1.64	5 (20%)
4	HEC	A	803	1	32,50,50	1.42	2 (6%)	24,82,82	1.47	4 (16%)

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
4	HEC	B	402	1	-	1/10/54/54	-
4	HEC	D	402	1	-	1/10/54/54	-
4	HEC	D	401	1	-	3/10/54/54	-
4	HEC	A	802	1	-	3/10/54/54	-
4	HEC	C	402	1	-	1/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEC	B	401	1	-	3/10/54/54	-
4	HEC	C	401	1	-	3/10/54/54	-
4	HEC	A	803	1	-	1/10/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	HEC	C3C-C2C	-4.74	1.35	1.40
4	A	803	HEC	C3C-C2C	-4.48	1.36	1.40
4	D	402	HEC	C3C-C2C	-4.43	1.36	1.40
4	C	402	HEC	C3C-C2C	-4.39	1.36	1.40
4	C	401	HEC	C3C-C2C	-3.67	1.36	1.40
4	D	401	HEC	C3C-C2C	-3.39	1.37	1.40
4	A	802	HEC	C3C-C2C	-3.12	1.37	1.40
4	D	401	HEC	C2A-C1A	2.92	1.49	1.42
4	B	401	HEC	CAD-C3D	2.80	1.56	1.52
4	D	401	HEC	CAD-C3D	2.79	1.56	1.52
4	A	802	HEC	C2A-C1A	2.72	1.48	1.42
4	C	401	HEC	C2A-C1A	2.63	1.48	1.42
4	B	401	HEC	C3C-C2C	-2.62	1.38	1.40
4	A	802	HEC	CAD-C3D	2.59	1.55	1.52
4	B	401	HEC	C2A-C1A	2.52	1.48	1.42
4	D	401	HEC	C2B-C3B	-2.48	1.38	1.40
4	B	402	HEC	C1B-NB	2.18	1.40	1.36
4	C	401	HEC	CAD-C3D	2.16	1.55	1.52
4	B	401	HEC	C2B-C3B	-2.13	1.38	1.40
4	A	803	HEC	C4B-C3B	2.08	1.46	1.43
4	C	401	HEC	C2B-C3B	-2.07	1.38	1.40
4	B	402	HEC	C2A-C1A	2.05	1.47	1.42
4	C	402	HEC	C1B-NB	2.04	1.40	1.36
4	C	402	HEC	C4B-C3B	2.01	1.46	1.43

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	401	HEC	CMC-C2C-C3C	4.36	130.94	125.82
4	B	401	HEC	CMC-C2C-C3C	4.25	130.81	125.82
4	A	802	HEC	CMC-C2C-C3C	4.20	130.76	125.82
4	C	401	HEC	CMC-C2C-C3C	3.82	130.31	125.82
4	B	402	HEC	C1D-C2D-C3D	-3.63	104.47	107.00
4	D	402	HEC	C1D-C2D-C3D	-3.63	104.47	107.00
4	C	402	HEC	C1D-C2D-C3D	-3.52	104.55	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	803	HEC	C1D-C2D-C3D	-3.39	104.64	107.00
4	D	401	HEC	C1D-C2D-C3D	-3.33	104.68	107.00
4	A	802	HEC	C1D-C2D-C3D	-3.31	104.69	107.00
4	B	402	HEC	CMB-C2B-C3B	3.24	129.63	125.82
4	C	402	HEC	CMB-C2B-C3B	3.21	129.60	125.82
4	D	402	HEC	CMB-C2B-C3B	3.18	129.56	125.82
4	A	802	HEC	CMB-C2B-C3B	3.13	129.50	125.82
4	A	803	HEC	CMB-C2B-C3B	3.11	129.47	125.82
4	B	401	HEC	C1D-C2D-C3D	-3.09	104.84	107.00
4	C	401	HEC	C1D-C2D-C3D	-3.00	104.91	107.00
4	D	401	HEC	CMB-C2B-C3B	2.98	129.33	125.82
4	B	401	HEC	CMB-C2B-C3B	2.94	129.28	125.82
4	D	402	HEC	CMC-C2C-C3C	2.90	129.23	125.82
4	A	802	HEC	CMC-C2C-C1C	-2.88	124.05	128.46
4	D	401	HEC	CMC-C2C-C1C	-2.86	124.07	128.46
4	C	401	HEC	CMB-C2B-C3B	2.82	129.14	125.82
4	B	402	HEC	CMC-C2C-C3C	2.81	129.13	125.82
4	B	401	HEC	CMC-C2C-C1C	-2.81	124.15	128.46
4	C	402	HEC	CMC-C2C-C3C	2.80	129.12	125.82
4	A	803	HEC	CMC-C2C-C3C	2.70	128.99	125.82
4	C	401	HEC	CMC-C2C-C1C	-2.53	124.57	128.46
4	D	401	HEC	CMD-C2D-C3D	2.47	129.60	124.94
4	B	401	HEC	CMD-C2D-C3D	2.39	129.45	124.94
4	A	802	HEC	CMD-C2D-C3D	2.38	129.43	124.94
4	C	401	HEC	CMD-C2D-C3D	2.38	129.43	124.94
4	B	402	HEC	CMD-C2D-C3D	2.13	128.97	124.94
4	C	402	HEC	CMD-C2D-C3D	2.10	128.91	124.94
4	D	402	HEC	CMD-C2D-C3D	2.06	128.83	124.94
4	B	402	HEC	CMC-C2C-C1C	-2.05	125.31	128.46
4	A	803	HEC	CMD-C2D-C3D	2.04	128.80	124.94
4	A	802	HEC	O2D-CGD-CBD	2.02	120.53	114.03

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	802	HEC	C2D-C3D-CAD-CBD
4	A	802	HEC	C4D-C3D-CAD-CBD
4	A	802	HEC	C3D-CAD-CBD-CGD
4	A	803	HEC	C3D-CAD-CBD-CGD
4	B	401	HEC	C2D-C3D-CAD-CBD
4	B	401	HEC	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
4	B	401	HEC	C3D-CAD-CBD-CGD
4	B	402	HEC	C3D-CAD-CBD-CGD
4	C	401	HEC	C2D-C3D-CAD-CBD
4	C	401	HEC	C4D-C3D-CAD-CBD
4	C	401	HEC	C3D-CAD-CBD-CGD
4	C	402	HEC	C3D-CAD-CBD-CGD
4	D	401	HEC	C2D-C3D-CAD-CBD
4	D	401	HEC	C4D-C3D-CAD-CBD
4	D	401	HEC	C3D-CAD-CBD-CGD
4	D	402	HEC	C3D-CAD-CBD-CGD

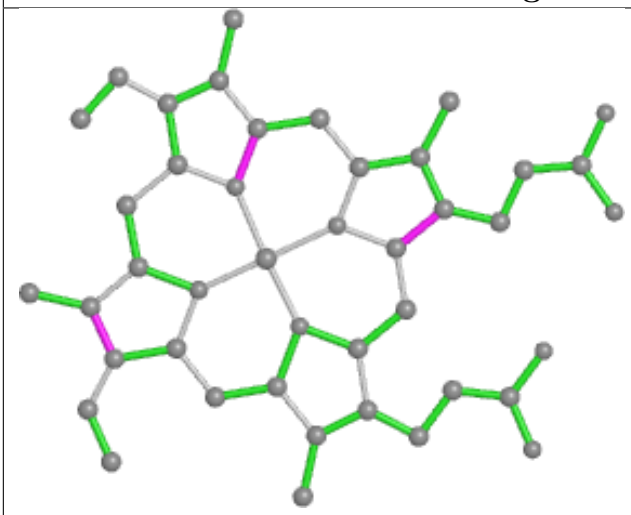
There are no ring outliers.

8 monomers are involved in 74 short contacts:

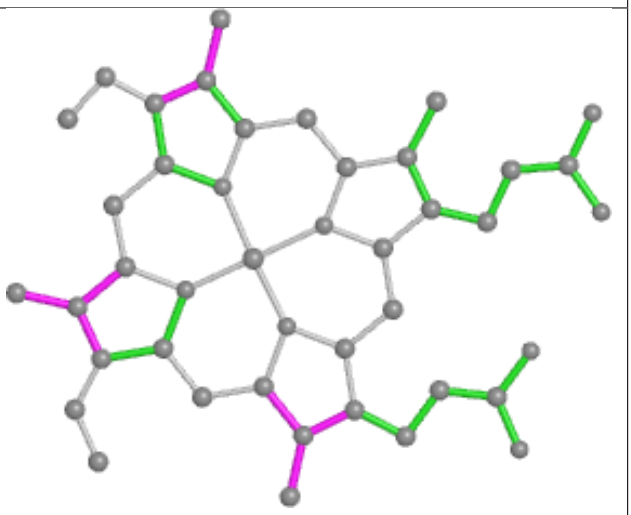
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	402	HEC	9	0
4	D	402	HEC	12	0
4	D	401	HEC	9	0
4	A	802	HEC	8	0
4	C	402	HEC	10	0
4	B	401	HEC	8	0
4	C	401	HEC	9	0
4	A	803	HEC	9	0

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.

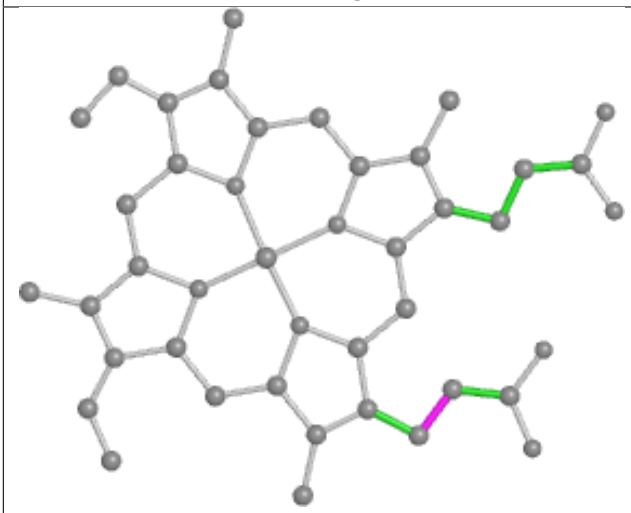
Ligand HEC B 402



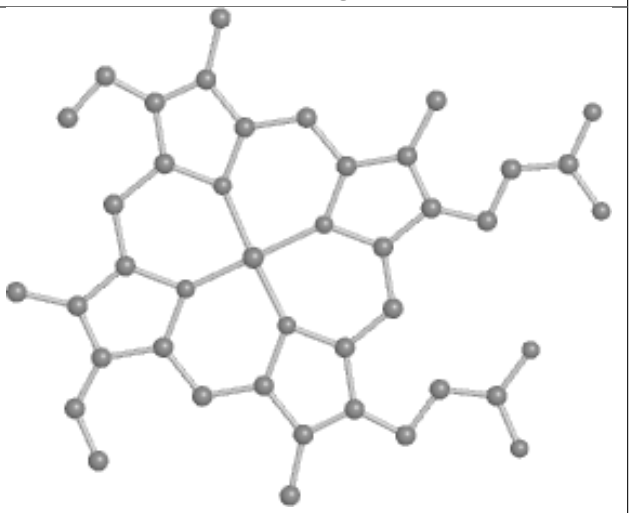
Bond lengths



Bond angles

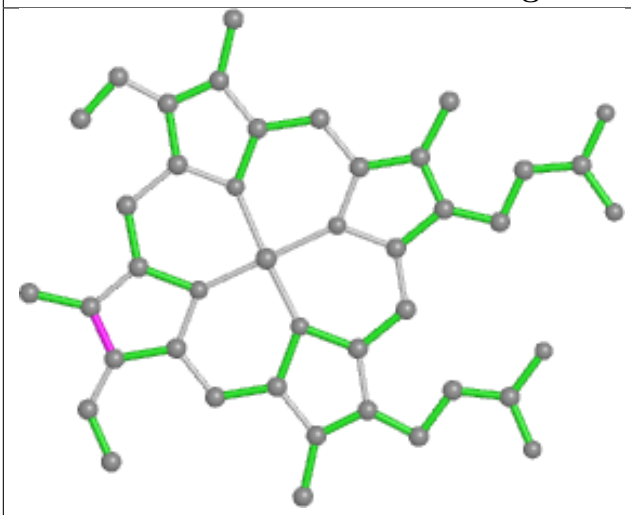


Torsions

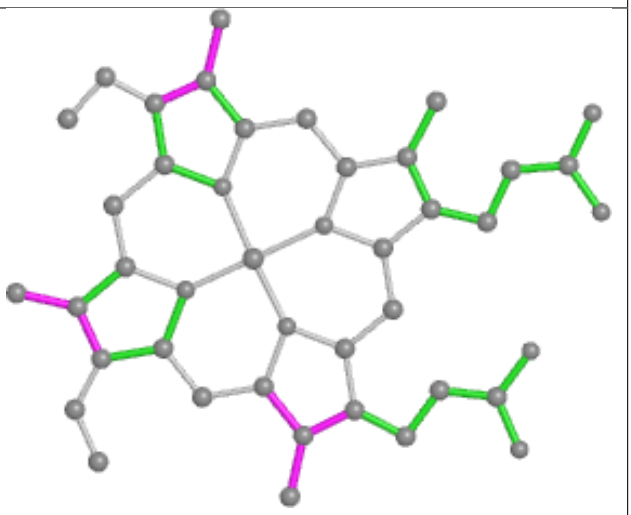


Rings

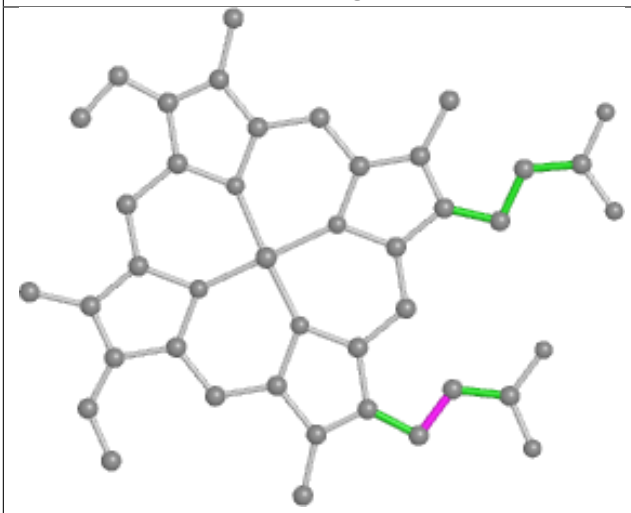
Ligand HEC D 402



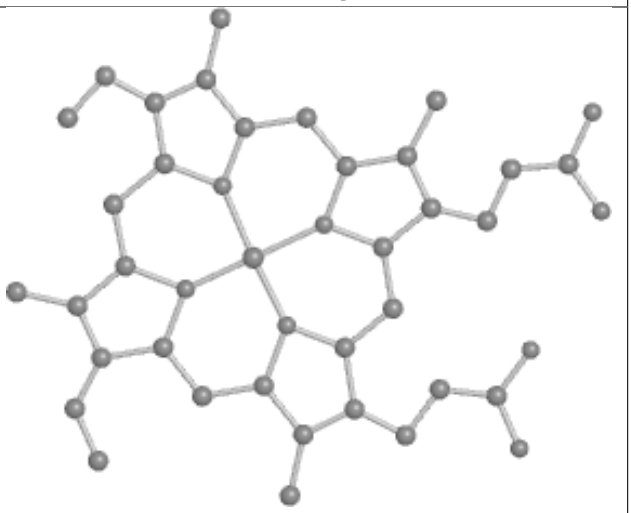
Bond lengths



Bond angles

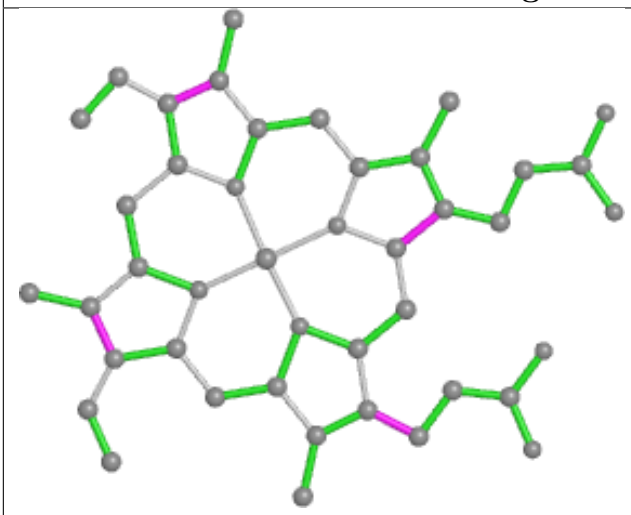


Torsions

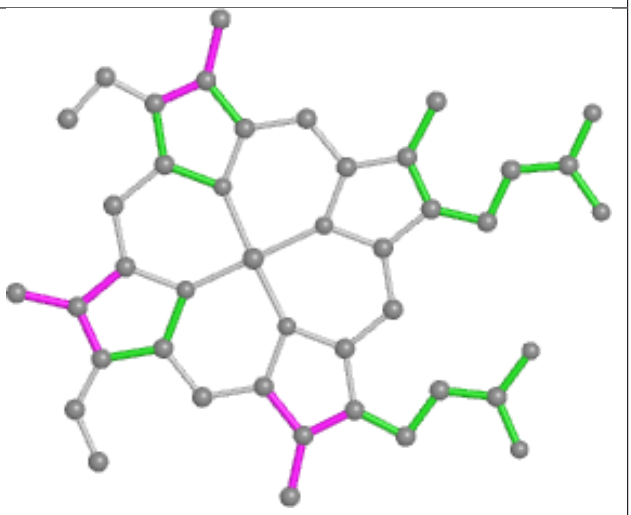


Rings

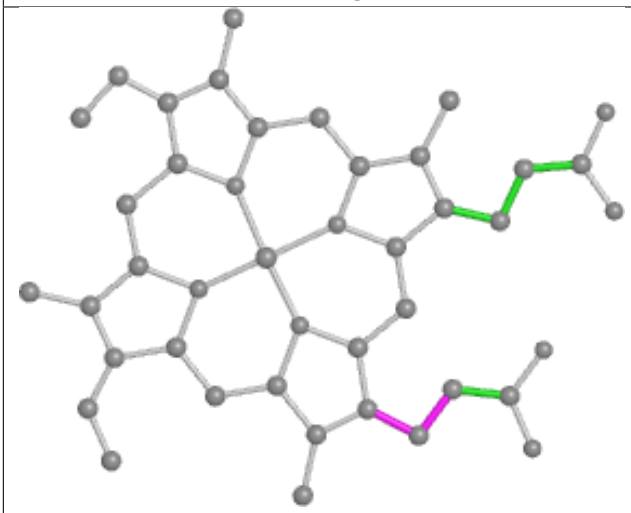
Ligand HEC D 401



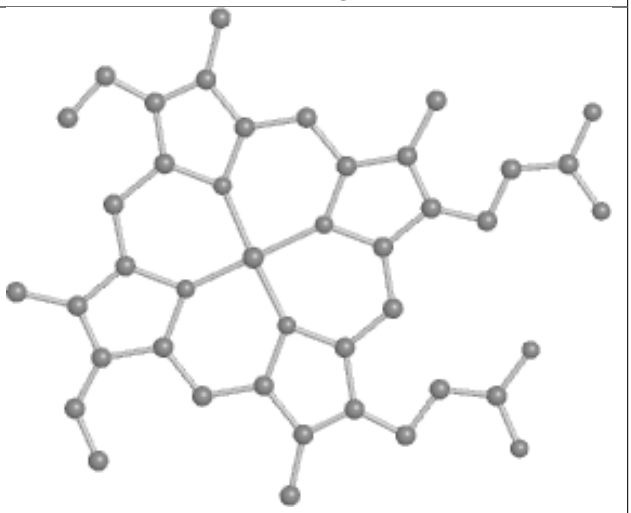
Bond lengths



Bond angles

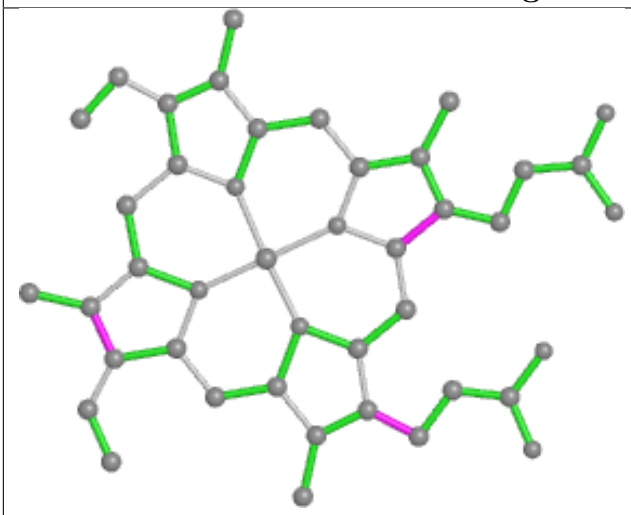


Torsions

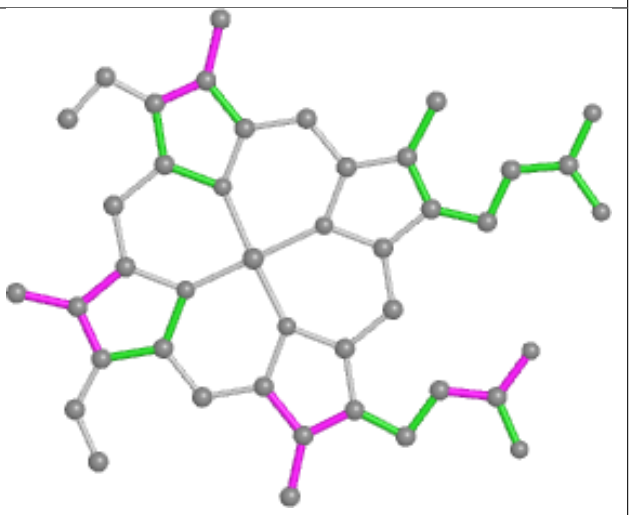


Rings

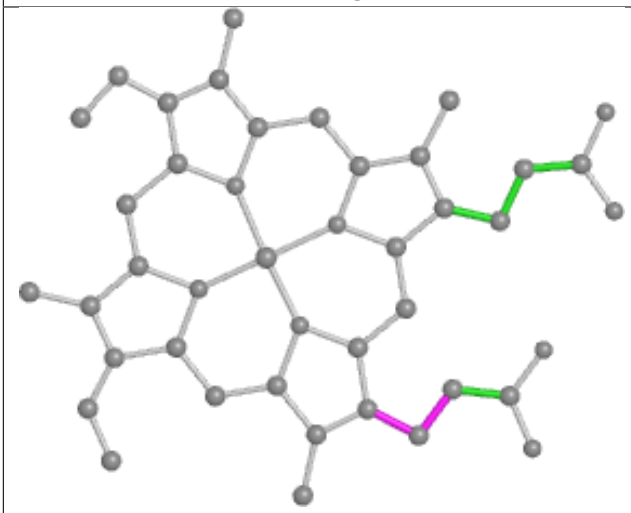
Ligand HEC A 802



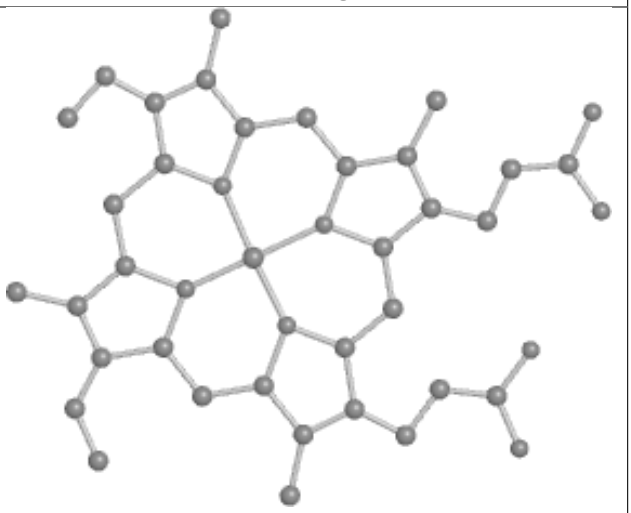
Bond lengths



Bond angles

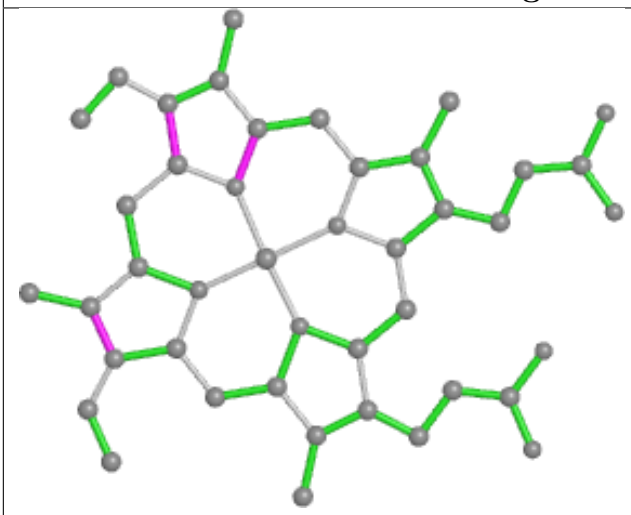


Torsions

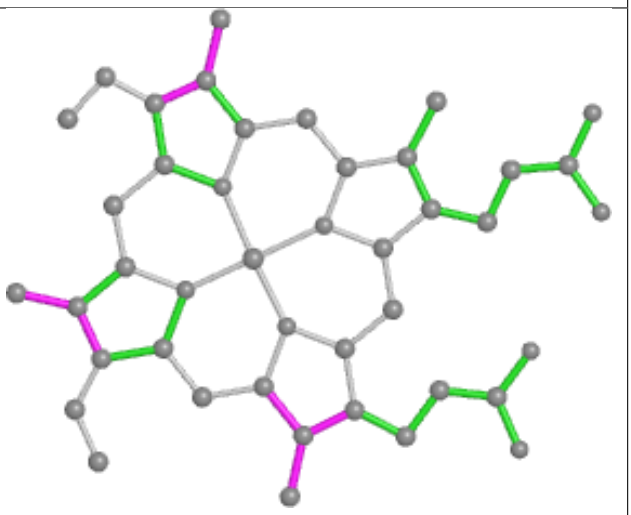


Rings

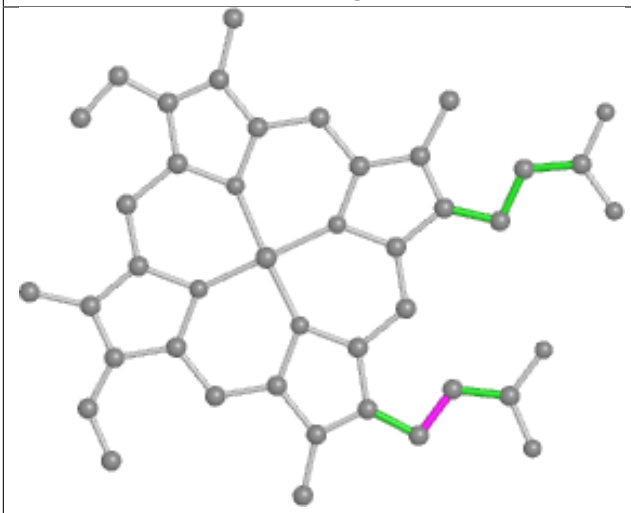
Ligand HEC C 402



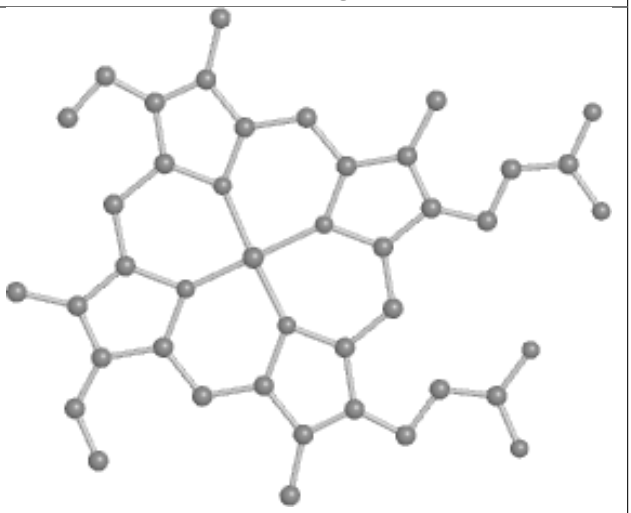
Bond lengths



Bond angles

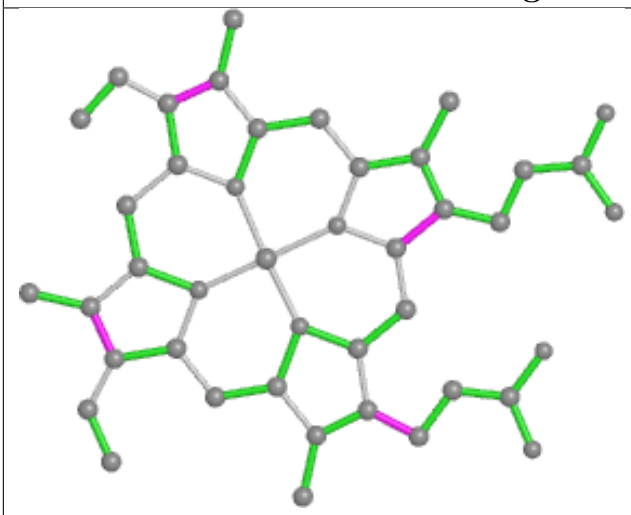


Torsions



Rings

Ligand HEC B 401



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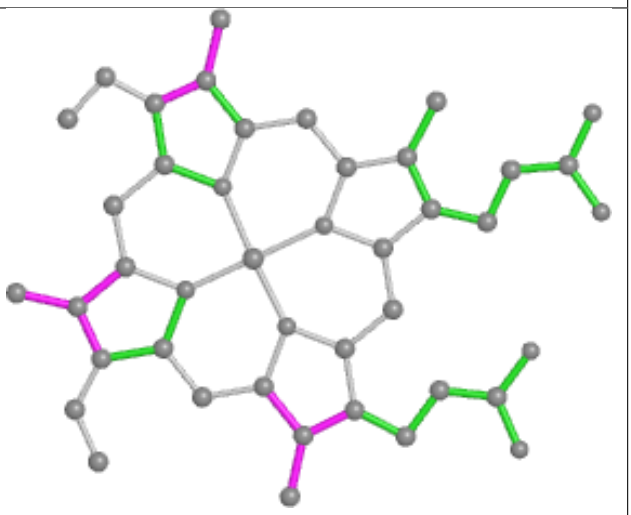
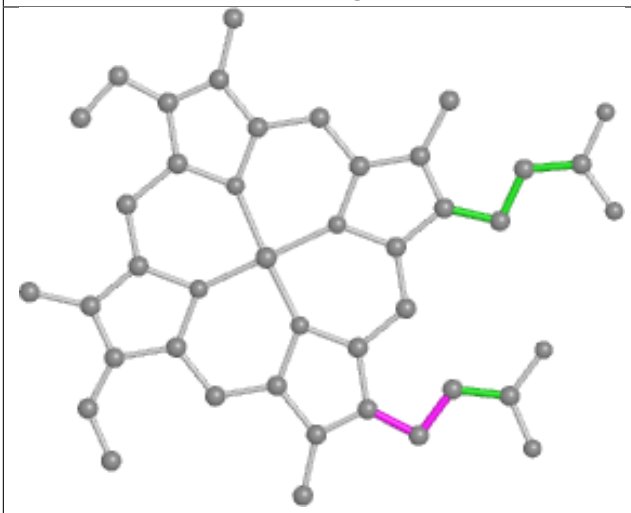


Bond angles



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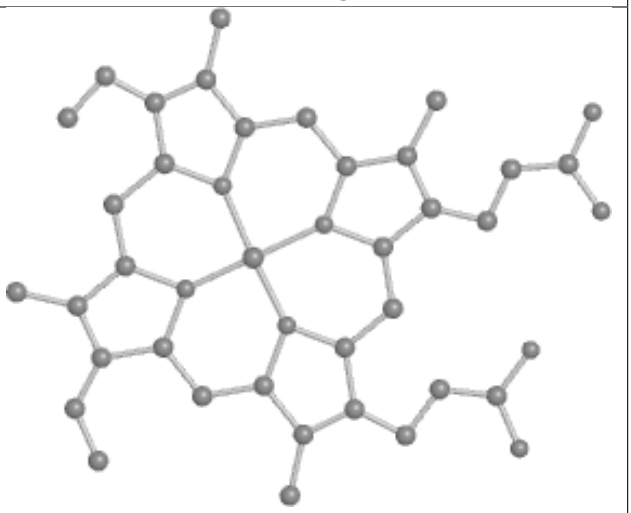
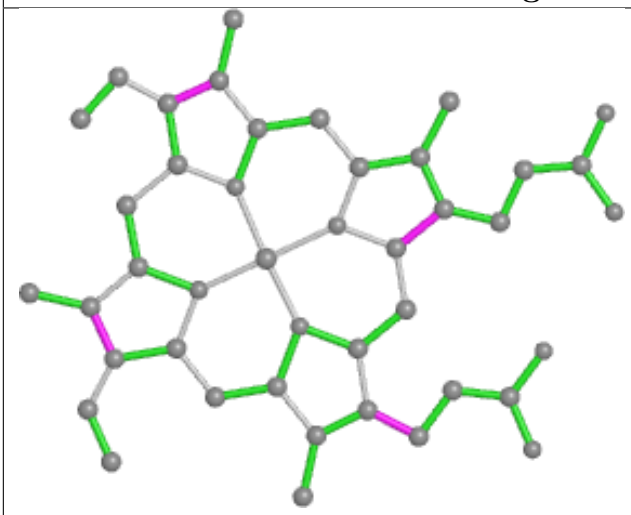
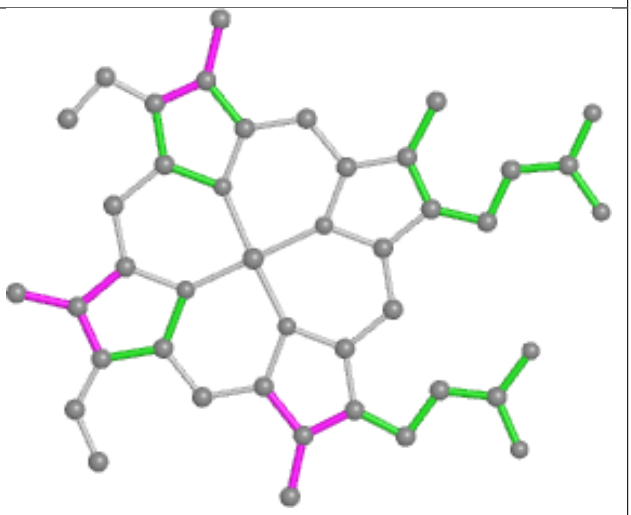


Rings

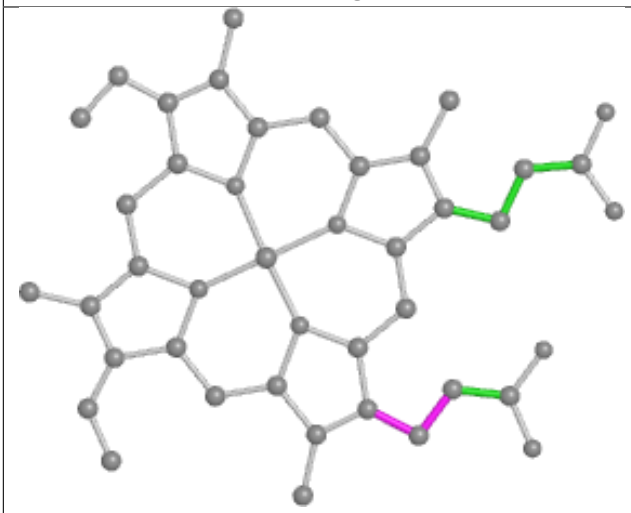
Ligand HEC C 401



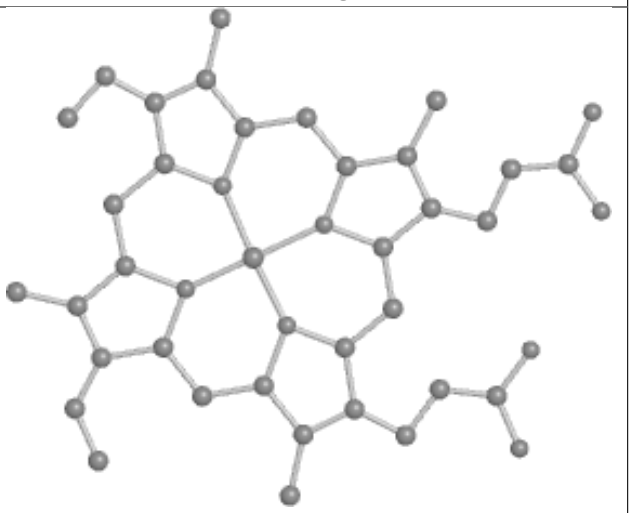
Bond lengths



Bond angles

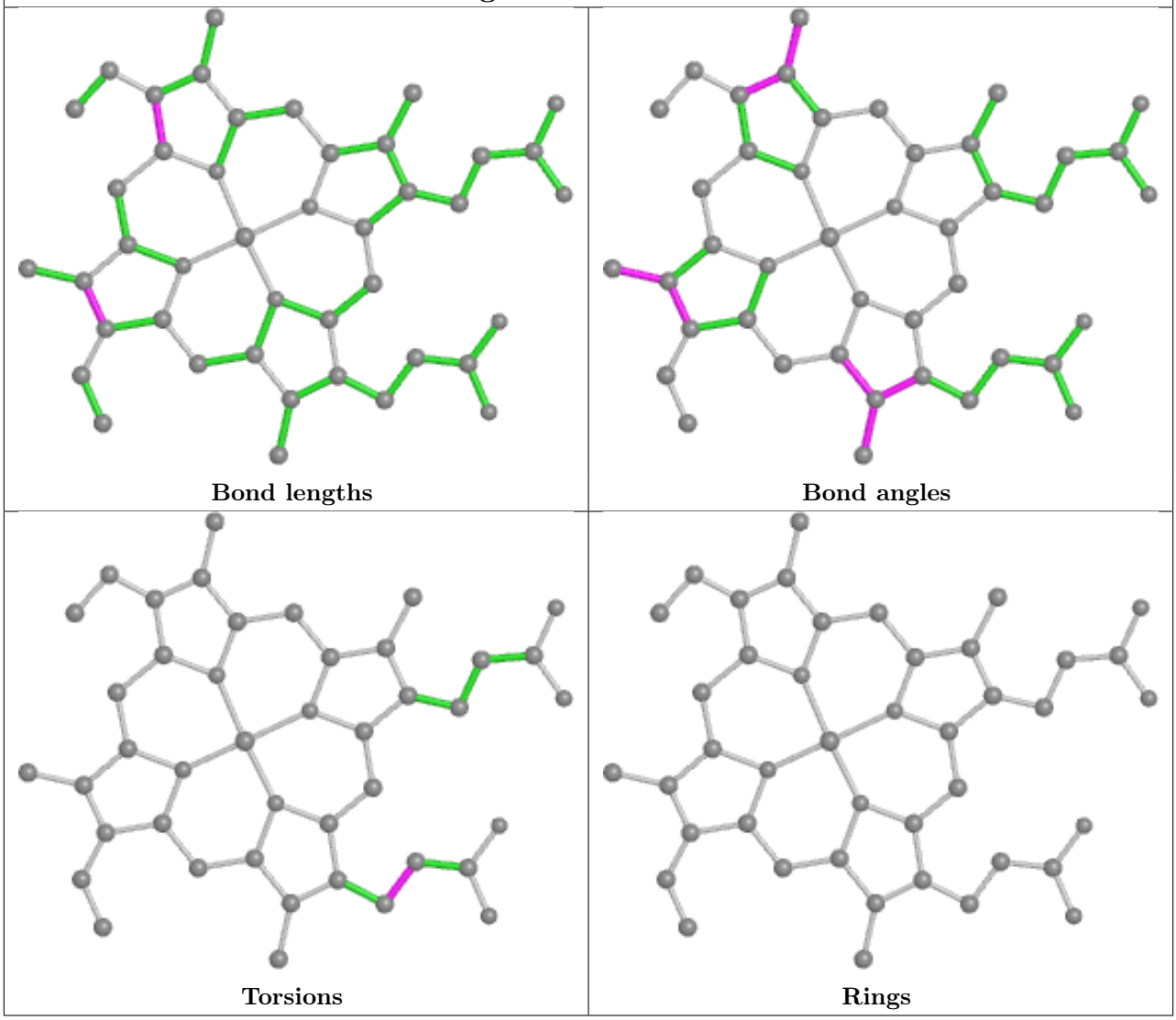


Torsions



Rings

Ligand HEC A 803



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	297/328 (90%)	0.19	15 (5%)	28	26	30, 49, 76, 91	0
1	B	308/328 (93%)	0.16	19 (6%)	20	19	27, 43, 73, 93	0
1	C	307/328 (93%)	0.04	11 (3%)	42	42	27, 42, 72, 80	0
1	D	298/328 (90%)	0.12	13 (4%)	34	33	31, 43, 73, 89	0
All	All	1210/1312 (92%)	0.13	58 (4%)	30	28	27, 45, 74, 93	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	118	MET	6.2
1	B	120	ASN	5.8
1	B	229	PRO	5.5
1	B	326	HIS	5.5
1	C	120	ASN	5.0
1	D	326	HIS	4.8
1	C	27	ASN	4.8
1	B	22	GLN	4.8
1	A	120	ASN	4.4
1	A	21	PRO	4.2
1	D	289	ASP	4.0
1	B	119	ASN	4.0
1	C	326	HIS	3.9
1	B	106	ALA	3.8
1	D	102	PRO	3.5
1	B	233	LYS	3.2
1	D	22	GLN	3.0
1	C	28	THR	3.0
1	A	145	GLY	3.0
1	B	121	THR	2.9
1	D	106	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	320	GLN	2.8
1	B	242	ALA	2.7
1	A	29	VAL	2.7
1	B	129	VAL	2.7
1	B	228	LEU	2.7
1	D	108	ALA	2.6
1	A	326	HIS	2.5
1	B	285	ALA	2.5
1	A	119	ASN	2.5
1	A	157	LEU	2.5
1	B	243	ASP	2.4
1	C	119	ASN	2.4
1	A	75	GLY	2.4
1	B	27	ASN	2.4
1	D	148	ASP	2.4
1	D	319	ALA	2.4
1	A	146	GLN	2.3
1	D	149	PRO	2.3
1	C	244	ASP	2.3
1	B	21	PRO	2.2
1	B	107	GLN	2.2
1	A	20	ALA	2.2
1	A	101	ALA	2.2
1	C	230	ALA	2.2
1	B	146	GLN	2.2
1	D	144	PRO	2.2
1	C	325	GLU	2.2
1	C	145	GLY	2.2
1	A	107	GLN	2.1
1	D	280	ASN	2.1
1	B	28	THR	2.1
1	C	108	ALA	2.1
1	A	284	GLY	2.1
1	A	181	ASP	2.1
1	A	290	THR	2.0
1	D	181	ASP	2.0
1	C	286	THR	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 monosaccharides in this entry.

6.4 Ligands (i)

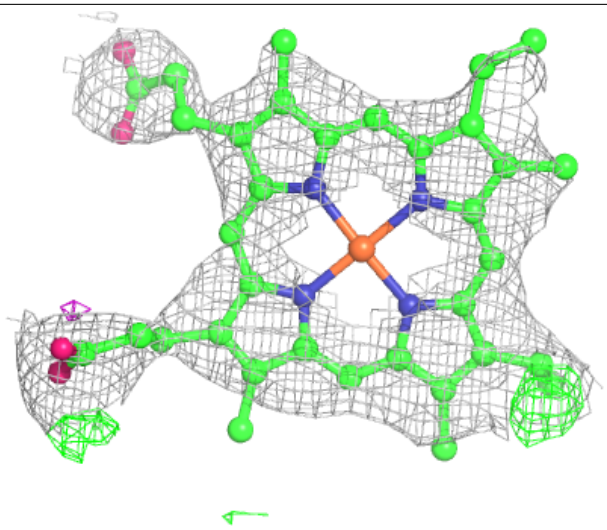
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

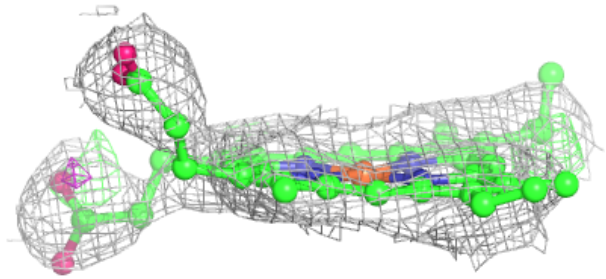
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	B	502	1/1	0.93	0.08	83,83,83,83	0
3	ZN	D	702	1/1	0.93	0.10	83,83,83,83	0
4	HEC	A	802	43/43	0.93	0.20	43,47,54,60	0
2	CA	C	601	1/1	0.94	0.19	45,45,45,45	0
3	ZN	B	503	1/1	0.94	0.04	74,74,74,74	0
4	HEC	A	803	43/43	0.94	0.18	38,44,50,53	0
4	HEC	B	402	43/43	0.94	0.20	32,42,48,53	0
4	HEC	C	402	43/43	0.94	0.19	33,39,46,49	0
4	HEC	D	401	43/43	0.94	0.21	36,41,49,52	0
4	HEC	D	402	43/43	0.94	0.20	34,39,50,53	0
2	CA	D	701	1/1	0.95	0.19	53,53,53,53	0
4	HEC	B	401	43/43	0.95	0.18	31,35,40,42	0
4	HEC	C	401	43/43	0.96	0.17	34,39,50,55	0
3	ZN	B	504	1/1	0.96	0.04	66,66,66,66	0
2	CA	A	401	1/1	0.97	0.08	46,46,46,46	0
3	ZN	B	802	1/1	0.97	0.04	52,52,52,52	0
3	ZN	C	602	1/1	0.97	0.04	72,72,72,72	0
2	CA	B	501	1/1	0.97	0.20	40,40,40,40	0
3	ZN	A	402	1/1	0.98	0.06	67,67,67,67	0
3	ZN	A	801	1/1	0.99	0.03	44,44,44,44	0

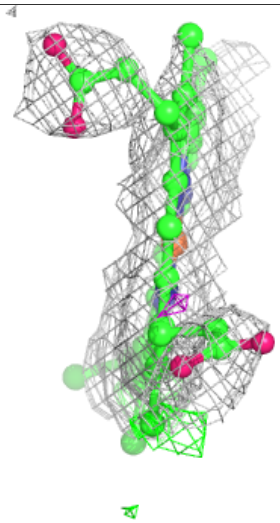
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC A 802:

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

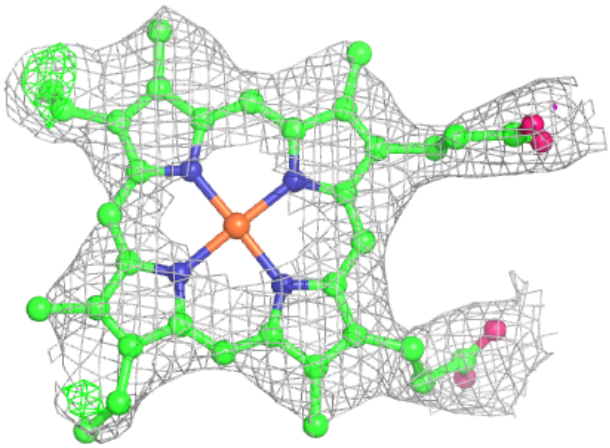


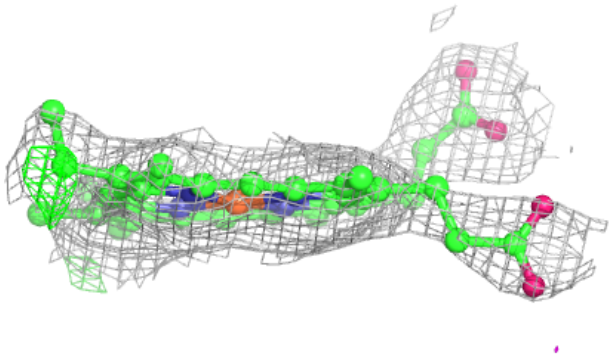


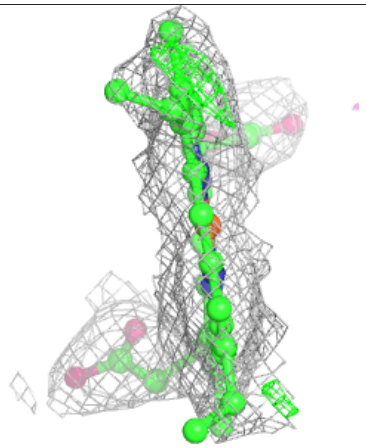


Electron density around HEC A 803:

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

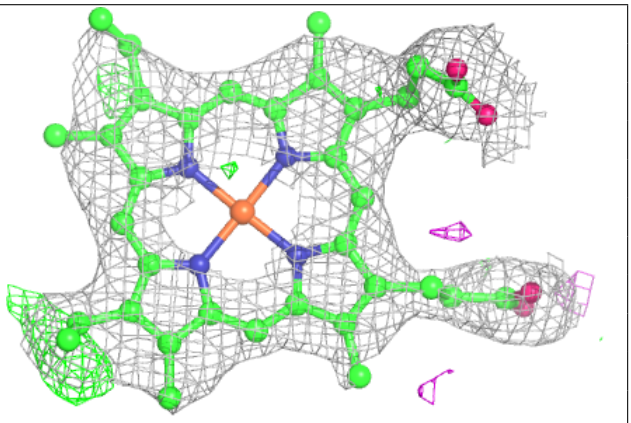


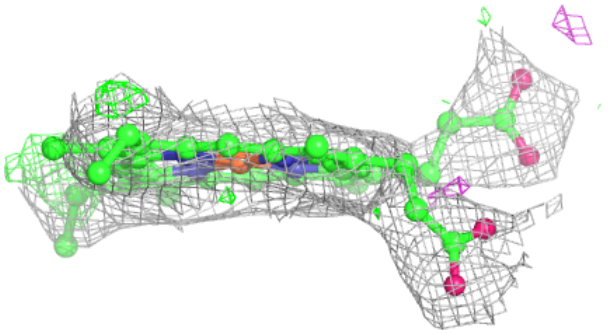


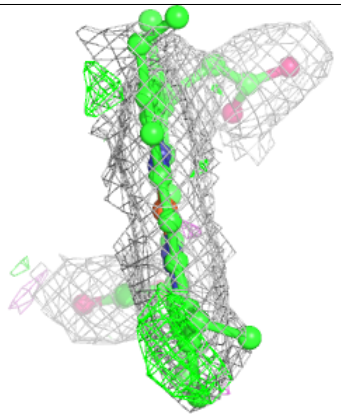


Electron density around HEC B 402:

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

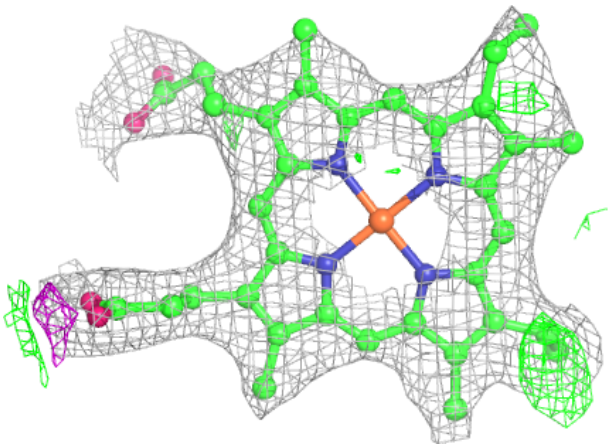


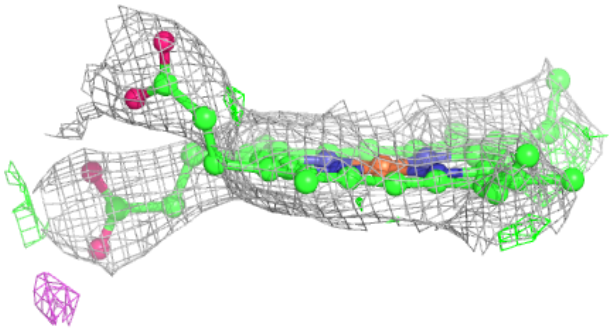


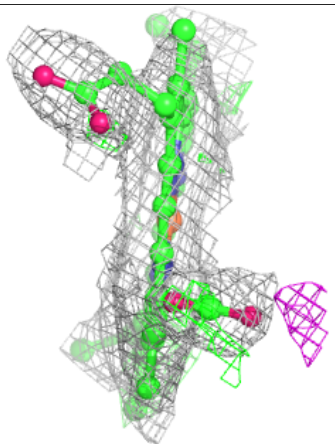


Electron density around HEC C 402:

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

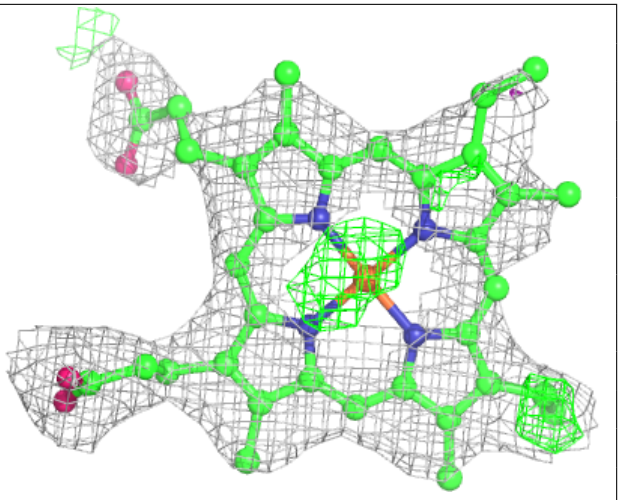


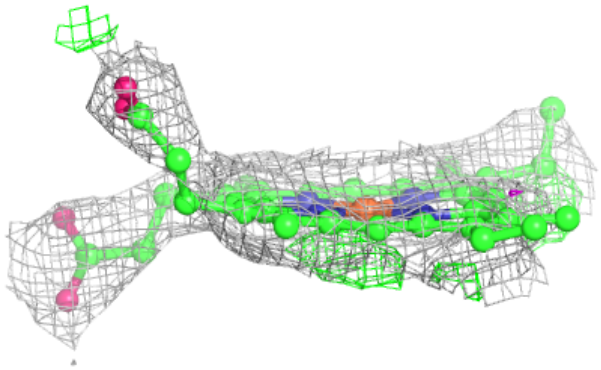


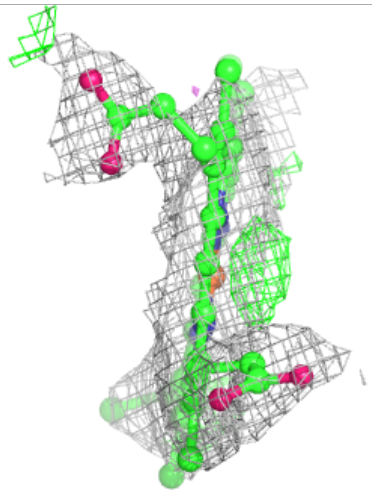


Electron density around HEC D 401:

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

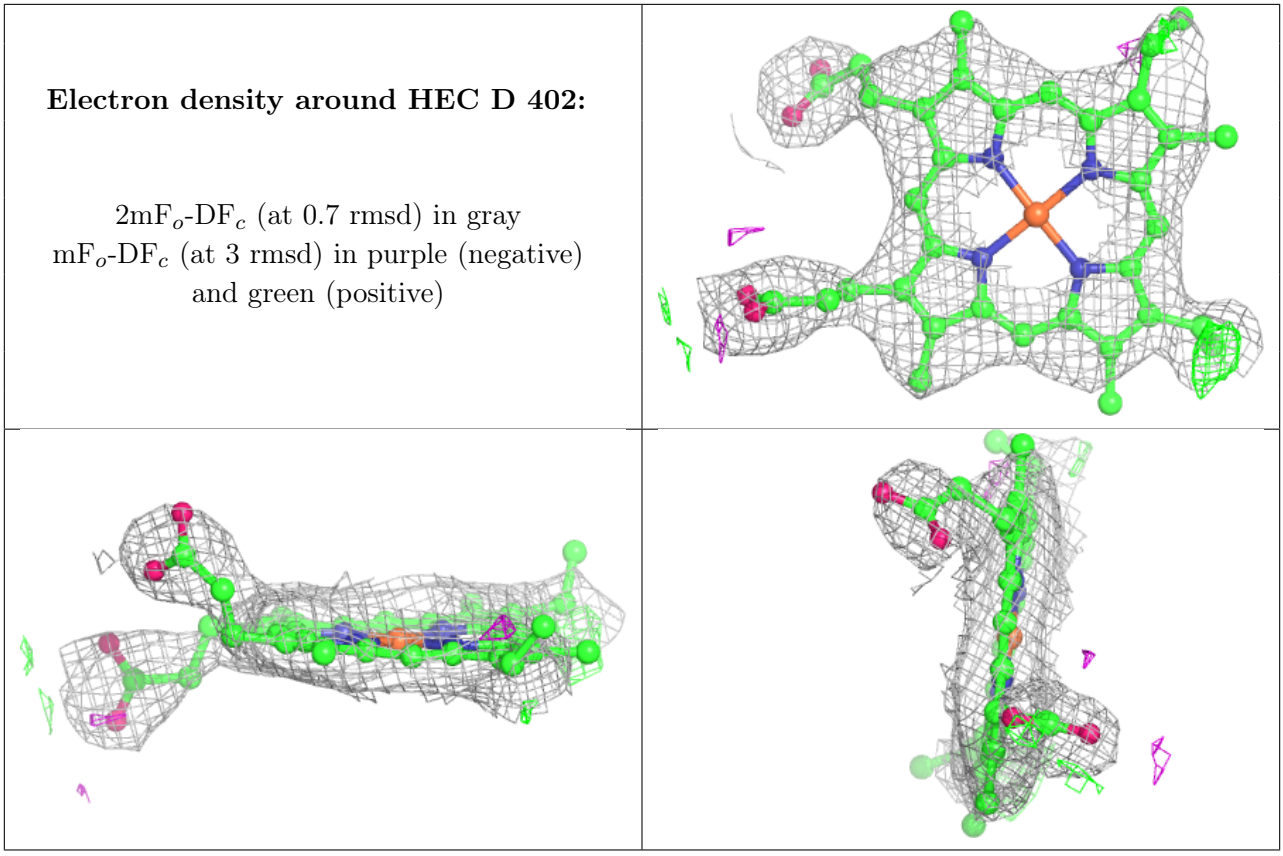






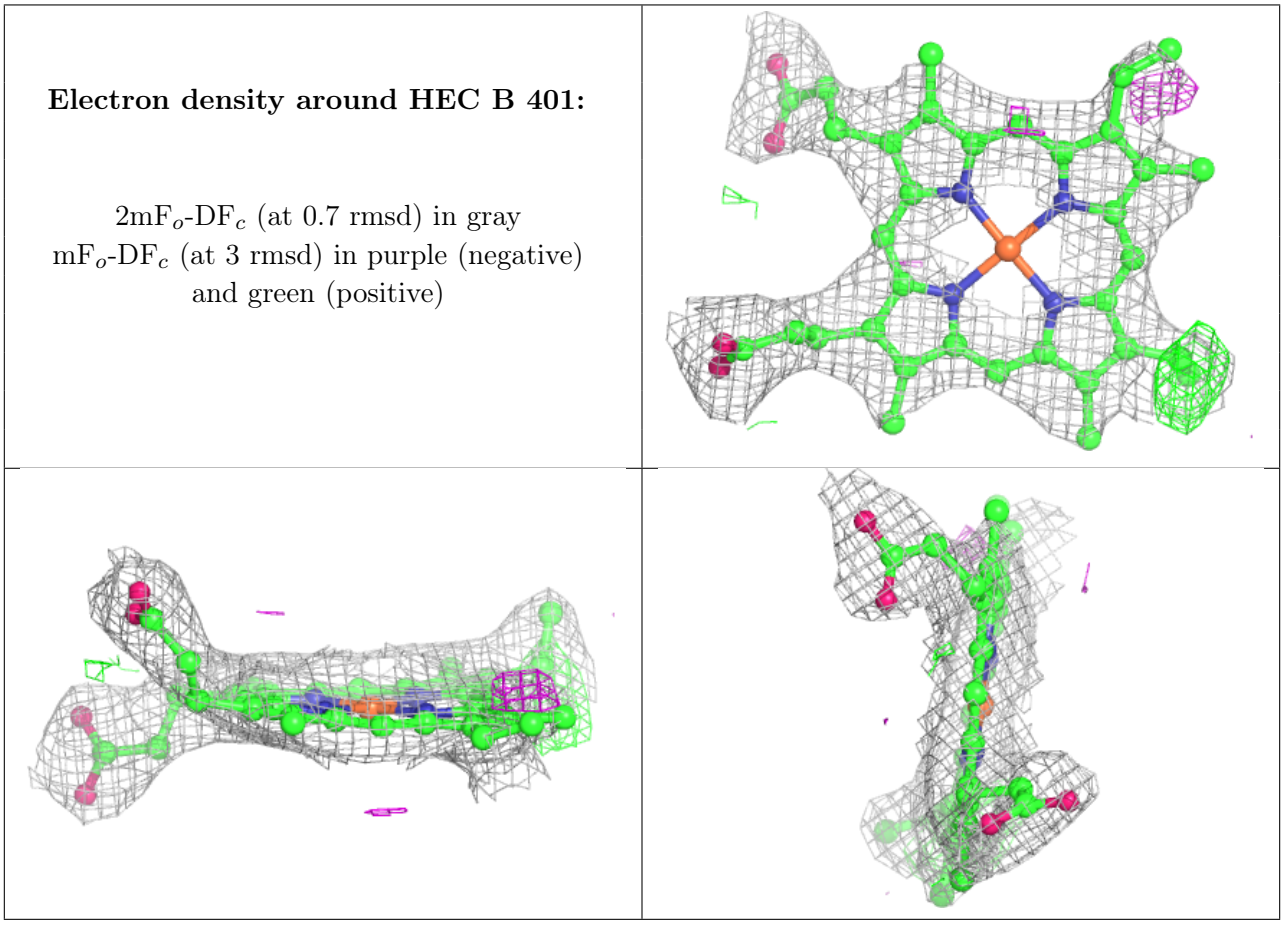
Electron density around HEC D 402:

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



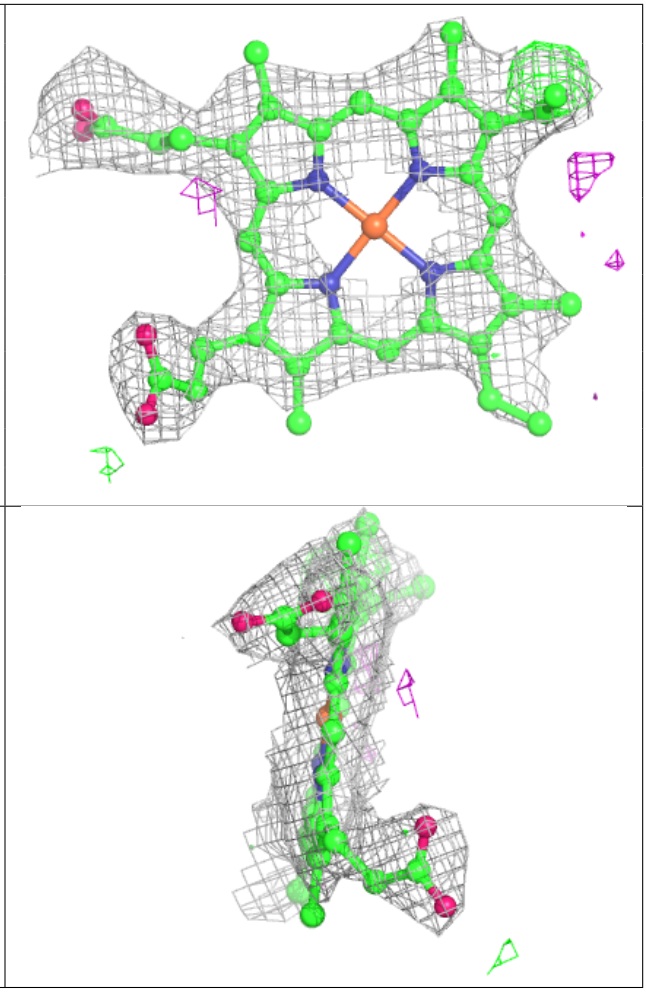
Electron density around HEC B 401:

$2mF_o$-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 C 401:

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.