Full wwPDB X-ray Structure Validation Report (i)

Aug 17, 2026 – 09:39 pm BST

PDB ID	:	5C2V / pdb_00005c2v
Title	:	Kuenenia stuttgartiensis Hydrazine Synthase
Authors	:	Dietl, A.; Ferousi, C.; Maalcke, W.J.; Menzel, A.; de Vries, S.; Keltjens, J.T.; Jetten, M.S.M.; Kartal, B.; Barends, T.R.M.
Deposited on	:	2015-06-16
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:

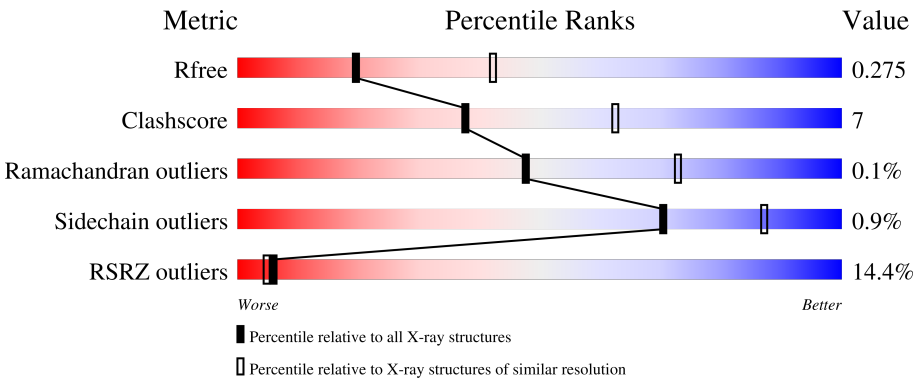
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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	782	5% 84% 13% ·
1	D	782	14% 83% 15% ·
2	B	352	9% 78% 22%
2	E	352	32% 76% 23% ·
3	C	314	7% 84% 14% ·

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Mol	Chain	Length	Quality of chain
3	F	314	32% 76% 23%

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
4	CL	A	901[A]	-	-	X	-
7	HEC	A	905	X	-	-	-
7	HEC	A	906	X	-	-	-
7	HEC	C	404	X	-	-	-
7	HEC	C	405	X	-	-	-
7	HEC	D	905	X	-	-	-
7	HEC	D	906	X	-	-	-
7	HEC	F	404	X	-	-	-
7	HEC	F	405	X	-	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 23385 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 HYDRAZINE SYNTHASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	768	6081	3867	1045	1144	25	0	0	0
1	D	770	6087	3871	1044	1147	25	0	0	0

- Molecule 2 is a protein called HYDRAZINE SYNTHASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	352	2706	1697	464	531	14	0	1	0
2	E	352	2692	1688	459	531	14	0	1	0

- Molecule 3 is a protein called HYDRAZINE SYNTHASE GAMMA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	314	2457	1543	432	472	10	0	0	0
3	F	314	2443	1534	427	472	10	0	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	2	2	0	1
4	D	1	1	1	0	0

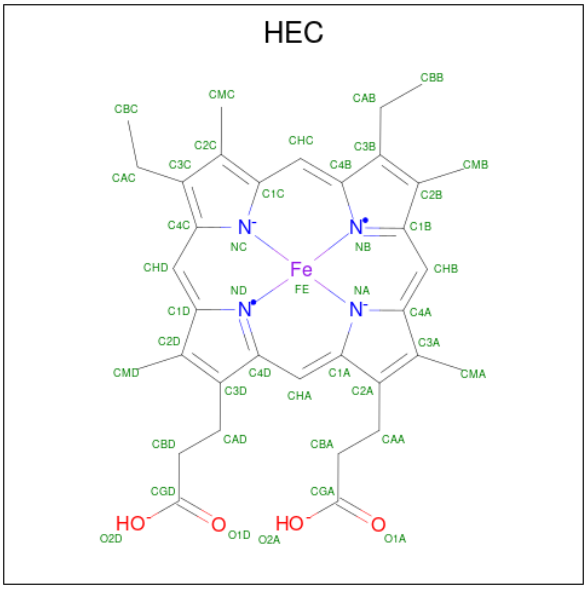
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	2	2	2	0	0
			Total	Ca		
5	B	1	1	1	0	0
			Total	Ca		
5	C	3	3	3	0	0
			Total	Ca		
5	D	2	2	2	0	0
			Total	Ca		
5	E	1	1	1	0	0
			Total	Ca		
5	F	3	3	3	0	0

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	A	1	1	1	0	0
			Total	Zn		
6	D	1	1	1	0	0

- Molecule 7 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

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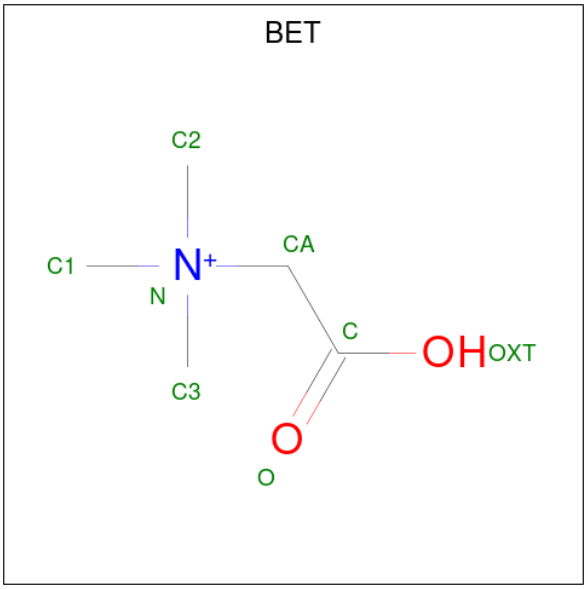
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
7	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	F	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	F	1	43	34	1	4	4	0	0

- Molecule 8 is TRIMETHYL GLYCINE (CCD ID: BET) (formula: $C_5H_{12}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	A	1	8	5	1	2	0	0
			Total	C	N	O		
8	A	1	8	5	1	2	0	0
			Total	C	N	O		
8	A	1	8	5	1	2	0	0
			Total	C	N	O		
8	B	1	8	5	1	2	0	0
			Total	C	N	O		
8	C	1	8	5	1	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	D	1	8	5	1	2	0	0
			Total	C	N	O		
8	E	1	8	5	1	2	0	0

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
9	B	1	1	1	0	0
			Total	Mg		
9	E	1	1	1	0	0

- Molecule 10 is water.

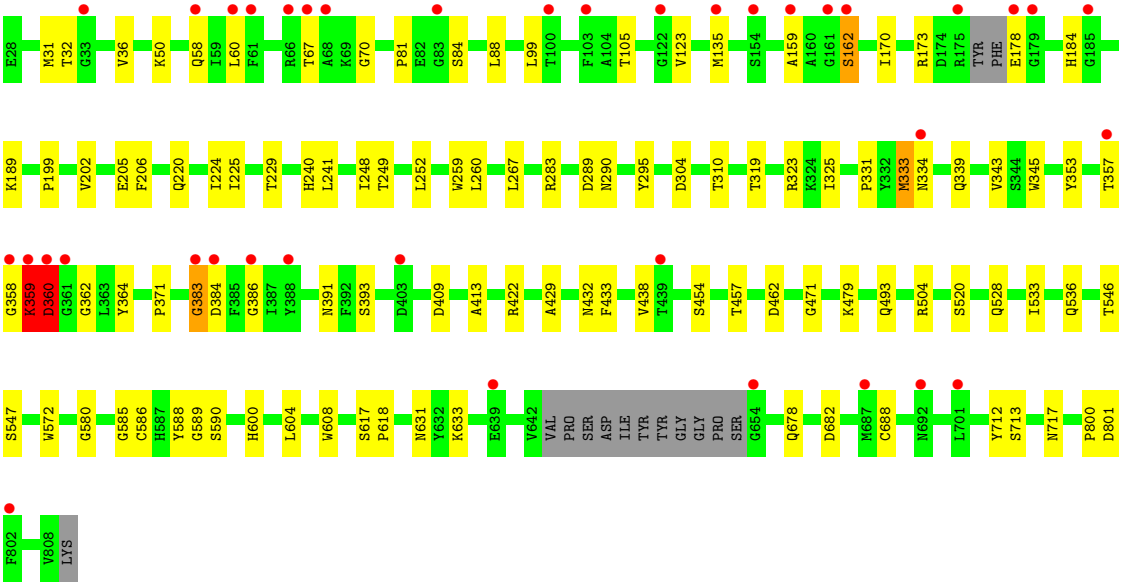
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	168	168	168	0	0
			Total	O		
10	B	60	60	60	0	0
			Total	O		
10	C	84	84	84	0	0
			Total	O		
10	D	112	112	112	0	0
			Total	O		
10	E	30	30	30	0	0
			Total	O		
10	F	46	46	46	0	0

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.

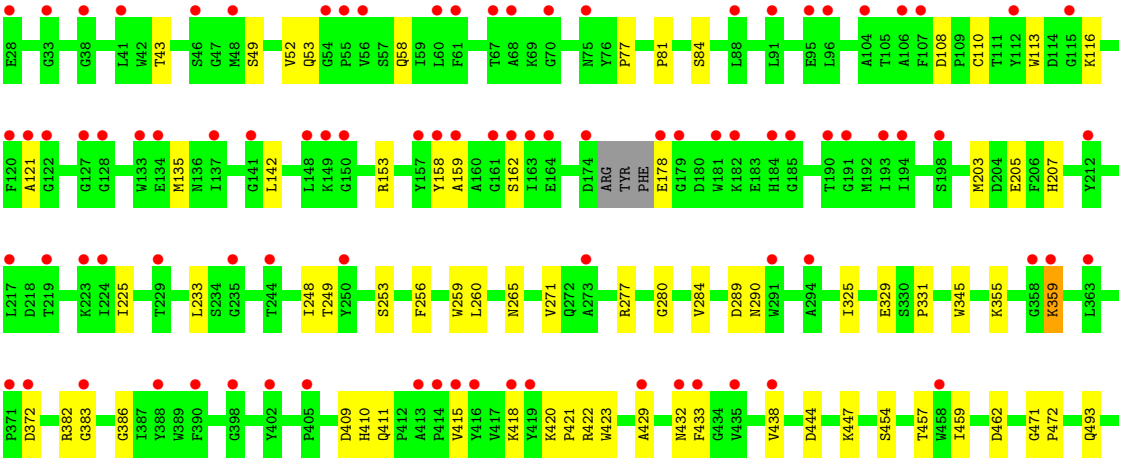
• Molecule 1: HYDRAZINE SYNTHASE ALPHA SUBUNIT

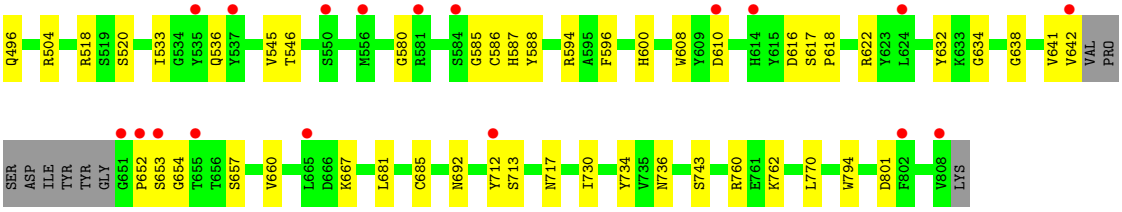
Chain A:



• Molecule 1: HYDRAZINE SYNTHASE ALPHA SUBUNIT

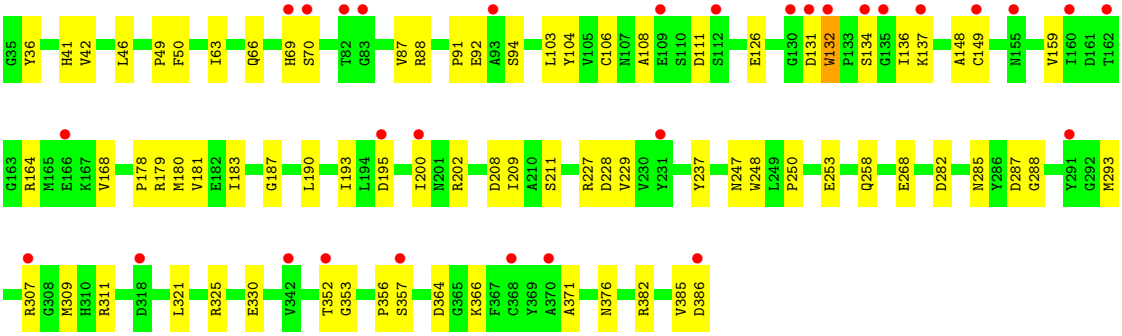
Chain D:





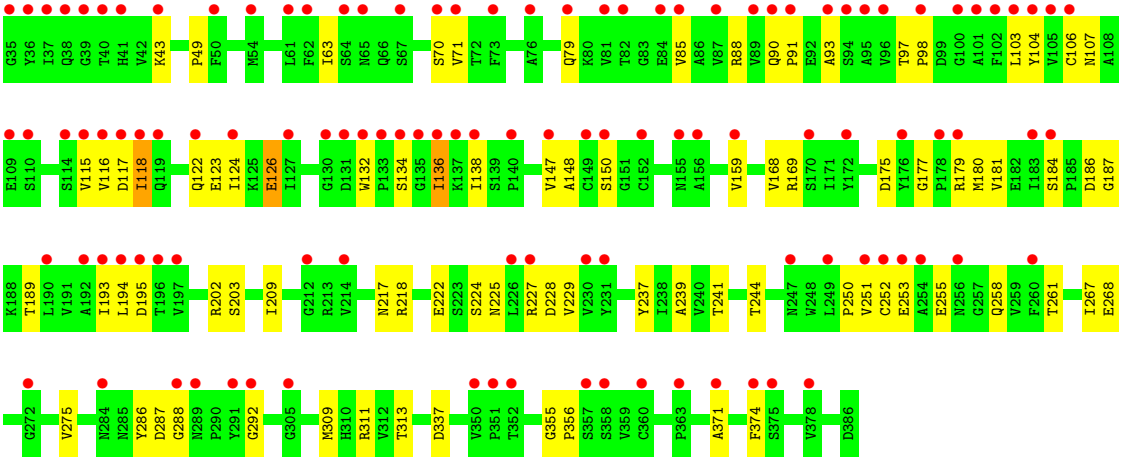
- Molecule 2: HYDRAZINE SYNTHASE BETA SUBUNIT

Chain B:



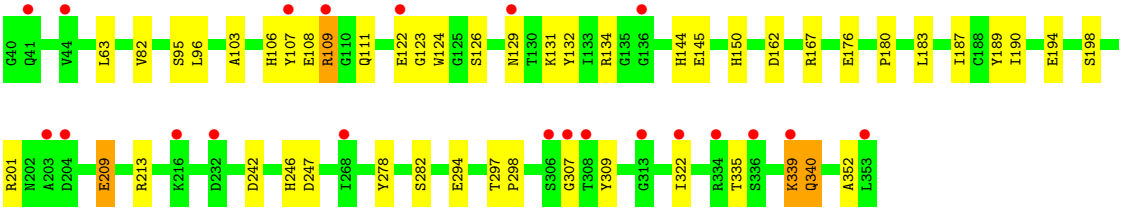
- Molecule 2: HYDRAZINE SYNTHASE BETA SUBUNIT

Chain E:



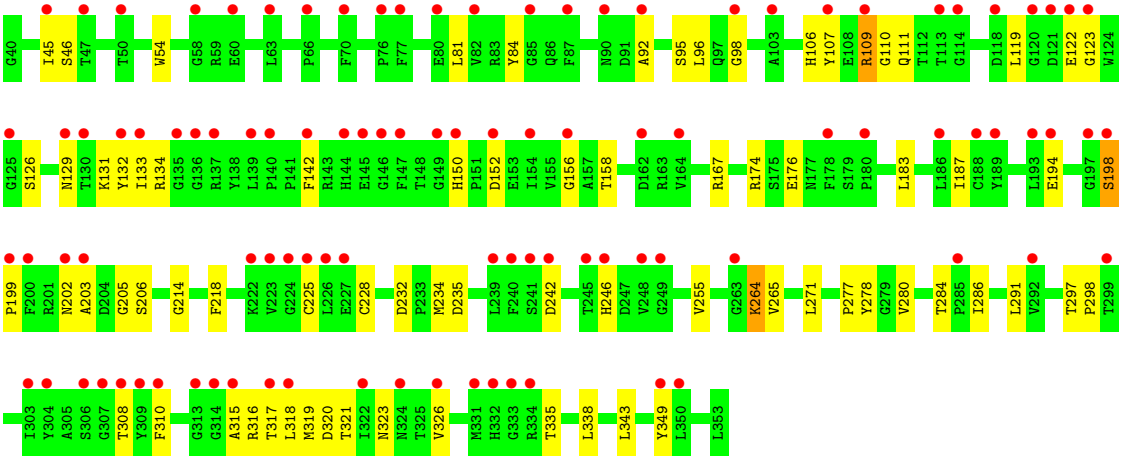
- Molecule 3: HYDRAZINE SYNTHASE GAMMA SUBUNIT

Chain C:



• Molecule 3: HYDRAZINE SYNTHASE GAMMA SUBUNIT

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	464.54Å 464.54Å 145.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 40.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.70) 99.8 (40.00-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.234 , 0.271 0.240 , 0.275	Depositor DCC
R_{free} test set	8147 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	57.0	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 45.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	23385	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% 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, BET, HEC, MG, CL, 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	0.30	0/6259	0.76	7/8503 (0.1%)
1	D	0.29	0/6266	0.74	2/8514 (0.0%)
2	B	0.30	0/2758	0.83	2/3752 (0.1%)
2	E	0.32	0/2744	0.86	8/3737 (0.2%)
3	C	0.32	0/2522	0.81	5/3421 (0.1%)
3	F	0.30	0/2508	0.79	4/3406 (0.1%)
All	All	0.30	0/23057	0.78	28/31333 (0.1%)

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	2
3	C	0	1
All	All	0	3

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	359	LYS	CB-CA-C	-8.56	105.58	117.23
2	B	132	TRP	CA-C-N	-8.26	110.40	119.98
2	B	132	TRP	C-N-CA	-8.26	110.40	119.98
2	E	132	TRP	CA-C-N	-7.27	111.98	119.83
2	E	132	TRP	C-N-CA	-7.27	111.98	119.83
3	C	198	SER	CA-C-N	7.24	126.88	119.56
3	C	198	SER	C-N-CA	7.24	126.88	119.56
3	C	109	ARG	N-CA-C	-6.51	105.09	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	109	ARG	N-CA-C	-6.51	105.09	113.16
3	C	340	GLN	N-CA-C	6.45	119.13	111.33
3	C	309	TYR	N-CA-C	6.30	119.24	109.60
3	F	205	GLY	N-CA-C	-6.29	107.20	114.69
1	A	360	ASP	N-CA-C	6.18	119.97	110.20
1	A	359	LYS	N-CA-C	6.04	118.75	108.67
1	A	471	GLY	CA-C-N	5.59	125.21	119.56
1	A	471	GLY	C-N-CA	5.59	125.21	119.56
2	E	90	GLN	CA-C-N	-5.53	113.57	119.98
2	E	90	GLN	C-N-CA	-5.53	113.57	119.98
1	A	362	GLY	N-CA-C	5.41	120.34	112.60
2	E	177	GLY	CA-C-N	-5.36	114.05	119.83
2	E	177	GLY	C-N-CA	-5.36	114.05	119.83
3	F	198	SER	CA-C-N	5.25	124.86	119.56
3	F	198	SER	C-N-CA	5.25	124.86	119.56
2	E	355	GLY	CA-C-N	-5.12	114.31	119.83
2	E	355	GLY	C-N-CA	-5.12	114.31	119.83
1	D	471	GLY	CA-C-N	5.05	124.55	119.19
1	D	471	GLY	C-N-CA	5.05	124.55	119.19
1	A	383	GLY	N-CA-C	5.03	122.23	115.59

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	LYS	Peptide
1	A	360	ASP	Peptide
3	C	339	LYS	Peptide

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	6081	0	5783	74	0
1	D	6087	0	5784	77	0
2	B	2706	0	2675	50	0
2	E	2692	0	2642	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2457	0	2324	38	0
3	F	2443	0	2291	48	0
4	A	2	0	0	3	0
4	D	1	0	0	1	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
5	F	3	0	0	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	A	86	0	61	9	0
7	C	86	0	59	3	0
7	D	86	0	60	7	0
7	F	86	0	59	3	0
8	A	24	0	33	0	0
8	B	8	0	11	0	0
8	C	8	0	11	0	0
8	D	8	0	11	0	0
8	E	8	0	11	0	0
9	B	1	0	0	0	0
9	E	1	0	0	0	0
10	A	168	0	0	2	0
10	B	60	0	0	1	0
10	C	84	0	0	3	0
10	D	112	0	0	5	0
10	E	30	0	0	1	0
10	F	46	0	0	2	0
All	All	23385	0	21815	314	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 7.

All (314) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:CYS:SG	7:A:906:HEC:CAC	2.16	1.32
1:A:688:CYS:SG	7:A:906:HEC:HBC1	1.83	1.07
1:A:688:CYS:CB	7:A:906:HEC:HBC2	1.84	1.06
1:A:688:CYS:SG	7:A:906:HEC:HBC2	0.51	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:CYS:SG	7:A:906:HEC:CBC	1.04	1.03
3:C:339:LYS:HG3	3:C:340:GLN:H	1.34	0.93
1:A:688:CYS:HG	7:A:906:HEC:HBC3	1.18	0.90
1:A:688:CYS:SG	7:A:906:HEC:C3C	2.61	0.88
1:D:520:SER:O	1:D:712:TYR:OH	2.01	0.78
2:B:288:GLY:H	2:B:309:MET:HG2	1.49	0.76
3:F:122:GLU:OE2	3:F:126:SER:OG	2.03	0.76
3:F:123:GLY:O	3:F:126:SER:OG	2.03	0.75
1:D:429:ALA:HB3	1:D:433:PHE:HB3	1.67	0.75
2:E:288:GLY:H	2:E:309:MET:HG2	1.53	0.74
1:A:688:CYS:SG	7:A:906:HEC:HBC3	1.32	0.73
3:C:122:GLU:OE2	10:C:501:HOH:O	2.06	0.73
2:E:122:GLN:NE2	2:E:123:GLU:O	2.24	0.71
3:C:339:LYS:HG3	3:C:340:GLN:N	2.06	0.71
1:D:642:VAL:HG12	1:D:652:PRO:HG3	1.71	0.70
1:D:608:TRP:NE1	1:D:610:ASP:O	2.24	0.70
1:D:438:VAL:O	3:F:167:ARG:NH2	2.24	0.69
3:F:129:ASN:ND2	10:F:501:HOH:O	2.26	0.69
1:A:422:ARG:NH1	3:C:95:SER:O	2.26	0.68
3:C:129:ASN:ND2	10:C:504:HOH:O	2.27	0.67
1:D:280:GLY:O	1:D:518:ARG:NH1	2.26	0.67
1:A:386:GLY:HA2	1:A:409:ASP:HB2	1.77	0.67
1:A:429:ALA:HB3	1:A:433:PHE:HB3	1.76	0.67
2:E:195:ASP:OD1	2:E:202:ARG:NH1	2.27	0.66
1:A:589:GLY:N	4:A:901[B]:CL:CL	2.66	0.66
2:B:250:PRO:O	2:B:258:GLN:NE2	2.29	0.66
3:C:307:GLY:O	10:C:502:HOH:O	2.12	0.65
1:A:32:THR:OG1	2:B:309:MET:O	2.12	0.64
1:D:418:LYS:NZ	10:D:1002:HOH:O	2.30	0.64
2:B:36:TYR:H	2:B:69:HIS:HE2	1.44	0.64
2:E:252:CYS:H	2:E:258:GLN:HE22	1.45	0.64
1:D:496:GLN:NE2	10:D:1003:HOH:O	2.31	0.64
1:D:622:ARG:NH2	1:D:667:LYS:O	2.31	0.63
1:A:422:ARG:HB2	3:C:176:GLU:HB2	1.80	0.62
1:D:386:GLY:HA2	1:D:409:ASP:HB2	1.80	0.62
1:D:248:ILE:HG13	1:D:249:THR:HG23	1.82	0.61
2:E:98:PRO:HD3	2:E:138:ILE:HD11	1.81	0.61
2:B:195:ASP:OD1	2:B:202:ARG:NH1	2.33	0.61
3:C:322:ILE:HG23	3:C:335:THR:HG21	1.82	0.61
1:D:203:MET:O	1:D:496:GLN:NE2	2.33	0.61
1:D:108:ASP:OD1	1:D:411:GLN:NE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:622:ARG:HD2	1:D:638:GLY:HA3	1.83	0.60
2:B:227:ARG:NH2	3:C:107:TYR:HE1	2.00	0.60
3:C:106:HIS:CD2	7:C:404:HEC:NB	2.70	0.60
1:D:422:ARG:HB3	3:F:176:GLU:HB2	1.84	0.59
1:D:760:ARG:NE	1:D:762:LYS:O	2.24	0.59
1:A:438:VAL:O	3:C:167:ARG:NH2	2.36	0.59
2:E:228:ASP:HB2	2:E:292:GLY:HA2	1.85	0.58
2:E:287:ASP:OD1	2:E:311:ARG:NH2	2.31	0.58
1:D:359:LYS:NZ	10:D:1005:HOH:O	2.35	0.58
1:D:207:HIS:NE2	10:D:1004:HOH:O	2.32	0.58
2:E:218:ARG:NH1	2:E:268:GLU:O	2.37	0.57
1:A:162:SER:HB3	1:A:189:LYS:HB3	1.86	0.56
2:B:134:SER:OG	2:B:179:ARG:O	2.19	0.56
1:A:432:ASN:ND2	1:A:454:SER:OG	2.34	0.56
2:B:159:VAL:HG23	2:B:168:VAL:HB	1.87	0.56
3:F:106:HIS:CD2	7:F:404:HEC:NB	2.74	0.56
1:D:504:ARG:NH2	1:D:801:ASP:O	2.38	0.56
1:D:457:THR:O	1:D:580:GLY:HA2	2.06	0.55
1:A:248:ILE:HG13	1:A:249:THR:HG23	1.88	0.55
2:B:183:ILE:HG12	2:B:190:LEU:HD23	1.88	0.55
3:C:111:GLN:HB3	3:C:132:TYR:CE1	2.42	0.55
2:E:70:SER:OG	2:E:71:VAL:N	2.39	0.55
1:A:588:TYR:HB3	4:A:901[A]:CL:CL	2.45	0.54
3:F:142:PHE:HB2	3:F:158:THR:HB	1.88	0.54
3:F:206:SER:HA	3:F:234:MET:HE1	1.90	0.54
1:A:283:ARG:NH2	1:A:304:ASP:OD1	2.40	0.54
1:A:162:SER:CB	1:A:189:LYS:HB3	2.38	0.54
1:A:462:ASP:O	1:A:585:GLY:HA2	2.08	0.54
3:F:315:ALA:HB2	3:F:326:VAL:HG21	1.90	0.54
1:D:770:LEU:HD21	7:D:906:HEC:HBC2	1.90	0.54
2:B:287:ASP:OD1	2:B:311:ARG:NH2	2.35	0.54
2:B:111:ASP:OD2	2:B:131:ASP:HA	2.07	0.54
1:A:631:ASN:ND2	10:A:1007:HOH:O	2.40	0.54
3:F:317:THR:OG1	3:F:320:ASP:OD2	2.26	0.54
3:F:335:THR:HA	3:F:338:LEU:HD13	1.88	0.54
1:D:159:ALA:HB1	1:D:162:SER:O	2.07	0.54
3:C:145:GLU:OE1	3:C:150:HIS:NE2	2.32	0.53
3:C:82:VAL:HG23	3:C:189:TYR:HA	1.89	0.53
3:F:318:LEU:O	3:F:321:THR:OG1	2.19	0.53
2:E:148:ALA:HB2	2:E:181:VAL:HG13	1.89	0.53
1:A:170:ILE:HB	1:A:184:HIS:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:SER:O	1:A:712:TYR:OH	2.22	0.52
3:F:132:TYR:CE2	3:F:134:ARG:HB2	2.44	0.52
1:A:590:SER:OG	4:A:901[A]:CL:CL	2.60	0.52
3:C:144:HIS:ND1	7:C:404:HEC:O2D	2.34	0.52
3:C:132:TYR:CE2	3:C:134:ARG:HB2	2.45	0.52
7:D:906:HEC:HBD2	7:D:906:HEC:HHA	1.91	0.52
3:F:319:MET:HE3	3:F:323:ASN:HB3	1.91	0.52
2:B:42:VAL:HG11	3:C:82:VAL:HG11	1.92	0.51
1:A:159:ALA:HB1	1:A:162:SER:O	2.10	0.51
3:C:63:LEU:HD21	3:C:180:PRO:HG3	1.92	0.51
1:D:325:ILE:HD11	1:D:345:TRP:HE3	1.75	0.51
1:D:493:GLN:HB2	1:D:533:ILE:HG13	1.93	0.51
1:D:462:ASP:O	1:D:585:GLY:HA2	2.11	0.51
3:F:202:ASN:OD1	3:F:203:ALA:N	2.43	0.51
2:B:70:SER:HA	2:B:87:VAL:HG22	1.92	0.51
2:B:307:ARG:HE	2:B:357:SER:HB3	1.75	0.51
2:B:88:ARG:NE	2:B:126:GLU:OE2	2.44	0.51
1:D:265:ASN:OD1	1:D:290:ASN:ND2	2.44	0.51
1:D:713:SER:O	1:D:717:ASN:ND2	2.39	0.51
1:A:678:GLN:NE2	1:A:682:ASP:OD1	2.44	0.50
1:D:422:ARG:NH1	3:F:95:SER:O	2.43	0.50
3:F:81:LEU:HA	3:F:84:TYR:HD2	1.76	0.50
1:D:329:GLU:OE2	1:D:355:LYS:NZ	2.31	0.50
1:D:608:TRP:CE3	3:F:123:GLY:HA2	2.47	0.50
2:B:49:PRO:HB3	2:B:63:ILE:CG2	2.41	0.50
2:E:251:VAL:HG12	10:F:518:HOH:O	2.10	0.50
2:B:94:SER:HB2	2:B:103:LEU:HD11	1.94	0.50
2:E:71:VAL:HG23	2:E:85:VAL:HB	1.92	0.50
1:A:339:GLN:HB3	1:A:357:THR:O	2.12	0.50
2:E:168:VAL:HG12	2:E:169:ARG:HG3	1.94	0.50
2:E:91:PRO:HA	2:E:106:CYS:O	2.11	0.49
3:F:109:ARG:HG2	3:F:109:ARG:HH11	1.77	0.49
1:D:536:GLN:HG2	1:D:546:THR:HB	1.93	0.49
3:F:284:THR:HG21	3:F:308:THR:HG21	1.93	0.49
3:C:242:ASP:OD2	3:C:246:HIS:NE2	2.41	0.49
1:A:604:LEU:HD13	2:B:250:PRO:HG3	1.93	0.49
1:D:225:ILE:HG13	1:D:233:LEU:HB2	1.94	0.49
1:A:504:ARG:NH1	1:A:801:ASP:O	2.40	0.49
1:D:205:GLU:OE1	1:D:253:SER:OG	2.27	0.49
2:E:88:ARG:NE	2:E:126:GLU:OE1	2.45	0.49
1:A:359:LYS:HE3	1:A:360:ASP:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:88:ARG:HB2	2:E:107:ASN:CG	2.38	0.49
1:A:713:SER:O	1:A:717:ASN:ND2	2.35	0.49
2:E:202:ARG:HD2	2:E:224:SER:HA	1.93	0.49
2:E:225:ASN:HA	2:E:227:ARG:NH2	2.28	0.48
3:F:228:CYS:HA	3:F:242:ASP:HB2	1.94	0.48
1:D:432:ASN:HD22	1:D:454:SER:HB3	1.76	0.48
2:E:134:SER:OG	2:E:150:SER:OG	2.22	0.48
3:F:255:VAL:HA	3:F:264:LYS:HG3	1.95	0.48
1:A:608:TRP:CE3	3:C:123:GLY:HA2	2.49	0.48
2:B:92:GLU:OE1	2:B:132:TRP:NE1	2.42	0.48
1:A:58:GLN:HB3	1:A:88:LEU:HD11	1.95	0.48
2:E:203:SER:HB3	2:E:217:ASN:OD1	2.13	0.48
3:F:277:PRO:HA	3:F:286:ILE:HD11	1.95	0.48
1:A:81:PRO:HB2	1:A:84:SER:OG	2.14	0.48
1:A:383:GLY:HA3	1:D:383:GLY:HA3	1.96	0.48
2:B:46:LEU:HD13	2:B:376:ASN:HD21	1.78	0.48
1:D:444:ASP:OD1	1:D:447:LYS:N	2.46	0.48
2:B:91:PRO:HA	2:B:106:CYS:O	2.14	0.48
1:A:358:GLY:C	1:A:359:LYS:HG3	2.39	0.47
1:D:736:ASN:HD22	1:D:743:SER:HA	1.79	0.47
2:E:97:THR:HA	2:E:138:ILE:HD11	1.96	0.47
2:B:352:THR:HG22	2:B:353:GLY:H	1.79	0.47
2:B:382:ARG:NH1	2:B:385:VAL:O	2.41	0.47
3:C:131:LYS:HB3	7:C:404:HEC:HBA1	1.97	0.47
2:E:356:PRO:HA	2:E:371:ALA:O	2.15	0.47
3:F:111:GLN:HB3	3:F:132:TYR:CE1	2.50	0.47
3:C:107:TYR:CG	3:C:108:GLU:N	2.83	0.47
1:A:325:ILE:HD11	1:A:345:TRP:HE3	1.78	0.46
3:F:92:ALA:O	3:F:98:GLY:HA2	2.15	0.46
2:E:159:VAL:HG22	2:E:169:ARG:H	1.79	0.46
2:B:208:ASP:HB3	2:B:211:SER:HB3	1.97	0.46
1:D:260:LEU:HD13	1:D:421:PRO:HG2	1.97	0.46
2:E:93:ALA:HB3	2:E:106:CYS:HB2	1.98	0.46
3:F:119:LEU:HB2	3:F:122:GLU:OE1	2.15	0.46
1:D:81:PRO:HB2	1:D:84:SER:OG	2.16	0.46
2:B:228:ASP:HB3	2:B:293:MET:HE2	1.98	0.46
1:D:110:CYS:SG	10:D:1002:HOH:O	2.61	0.46
1:D:382:ARG:HA	1:D:382:ARG:HD3	1.42	0.46
1:D:472:PRO:HB2	1:D:730:ILE:HD13	1.97	0.46
3:F:319:MET:HE1	3:F:343:LEU:HD13	1.98	0.46
1:A:31:MET:O	2:B:311:ARG:NH1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:MET:HE2	1:D:142:LEU:HD23	1.97	0.46
3:F:45:ILE:HG23	3:F:46:SER:H	1.80	0.46
3:F:214:GLY:HA3	3:F:349:TYR:HB2	1.98	0.46
1:A:173:ARG:HH21	1:A:178:GLU:HG3	1.81	0.46
2:B:50:PHE:HB2	2:B:66:GLN:HB2	1.97	0.46
1:A:99:LEU:HB3	1:A:135:MET:HE1	1.98	0.46
2:B:227:ARG:NH2	3:C:107:TYR:CE1	2.82	0.46
1:A:310:THR:O	1:A:333:MET:HG3	2.16	0.46
1:A:391:ASN:OD1	1:A:393:SER:OG	2.27	0.46
2:B:364:ASP:CG	2:B:366:LYS:HG3	2.41	0.46
2:E:186:ASP:OD1	2:E:187:GLY:N	2.48	0.46
1:D:653:SER:OG	1:D:654:GLY:N	2.48	0.45
2:E:116:VAL:HG22	2:E:123:GLU:HA	1.97	0.45
2:E:287:ASP:OD2	2:E:313:THR:OG1	2.30	0.45
1:A:60:LEU:O	1:A:413:ALA:N	2.43	0.45
1:A:240:HIS:CD2	1:A:241:LEU:HG	2.51	0.45
1:A:225:ILE:O	1:A:229:THR:OG1	2.18	0.45
2:B:108:ALA:HB1	2:B:132:TRP:CE2	2.51	0.45
2:E:134:SER:CB	2:E:150:SER:HG	2.26	0.45
1:D:432:ASN:HA	1:D:454:SER:HB3	1.99	0.45
2:E:49:PRO:HB3	2:E:63:ILE:CG2	2.47	0.45
1:A:319:THR:O	1:A:323:ARG:HA	2.16	0.45
1:A:331:PRO:HB2	1:D:331:PRO:HB3	1.98	0.45
1:A:586:CYS:SG	7:A:905:HEC:HHD	2.57	0.45
2:B:200:ILE:HD12	3:C:282:SER:O	2.17	0.45
1:A:504:ARG:HD3	1:A:800:PRO:HB3	1.99	0.45
2:B:187:GLY:O	2:B:209:ILE:HD12	2.17	0.45
3:C:209:GLU:O	3:C:213:ARG:HB2	2.16	0.45
2:E:253[B]:GLU:HA	3:F:174:ARG:HG3	1.98	0.45
3:F:150:HIS:CD2	3:F:156:GLY:H	2.34	0.45
1:D:77:PRO:HB3	1:D:256:PHE:CG	2.52	0.45
1:A:536:GLN:HG2	1:A:546:THR:HB	1.97	0.44
2:B:227:ARG:NH2	10:B:507:HOH:O	2.50	0.44
1:D:271:VAL:HG22	1:D:284:VAL:HG22	1.99	0.44
2:E:267:ILE:HG12	2:E:275:VAL:HG13	1.98	0.44
3:C:183:LEU:O	3:C:187:ILE:HG12	2.17	0.44
3:F:134:ARG:NH1	3:F:194:GLU:O	2.44	0.44
2:E:103:LEU:HD23	2:E:104:TYR:N	2.32	0.44
1:A:259:TRP:CG	1:A:260:LEU:H	2.35	0.44
2:B:149:CYS:O	2:B:178:PRO:HD2	2.18	0.44
2:E:286:TYR:O	2:E:311:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:GLN:HB2	1:A:533:ILE:HG13	1.99	0.44
2:B:247:ASN:HD21	2:B:248:TRP:NE1	2.16	0.44
1:D:681:LEU:O	1:D:685:CYS:HB2	2.17	0.44
2:B:104:TYR:HB3	2:B:136:ILE:HD13	2.00	0.44
2:B:227:ARG:NH1	3:C:108:GLU:OE2	2.51	0.44
2:B:250:PRO:HB3	3:C:124:TRP:CZ3	2.52	0.44
3:F:297:THR:HA	3:F:298:PRO:HD3	1.80	0.44
1:A:633:LYS:HD2	1:A:633:LYS:HA	1.73	0.44
1:D:586:CYS:SG	7:D:905:HEC:HHD	2.58	0.44
1:D:641:VAL:HA	1:D:660:VAL:O	2.17	0.44
3:F:131:LYS:HB3	7:F:404:HEC:HBA1	1.99	0.44
1:D:53:GLN:NE2	1:D:372:ASP:OD1	2.51	0.43
1:D:113:TRP:CG	1:D:420:LYS:HE2	2.53	0.43
1:A:50:LYS:HG2	1:A:371:PRO:O	2.18	0.43
3:C:297:THR:HA	3:C:298:PRO:HD3	1.80	0.43
3:C:247:ASP:HB2	3:C:294:GLU:HG2	2.01	0.43
2:E:374:PHE:HB3	3:F:54:TRP:CZ3	2.53	0.43
3:F:232:ASP:HB3	3:F:235:ASP:HB2	2.00	0.43
1:A:479:LYS:NZ	10:A:1019:HOH:O	2.51	0.43
3:C:103:ALA:O	3:C:107:TYR:HA	2.18	0.43
3:C:187:ILE:HA	3:C:190:ILE:HD12	2.00	0.43
1:D:289:ASP:OD1	1:D:290:ASN:N	2.51	0.43
2:E:244:THR:HB	2:E:261:THR:OG1	2.19	0.43
1:A:547:SER:OG	1:A:617:SER:OG	2.32	0.43
1:D:43:THR:O	1:D:422:ARG:NH2	2.46	0.43
1:A:289:ASP:OD1	1:A:290:ASN:N	2.52	0.43
1:A:457:THR:O	1:A:580:GLY:HA2	2.19	0.43
1:D:734:TYR:HE1	7:D:906:HEC:HBA2	1.84	0.43
2:E:180:MET:HB3	2:E:193:ILE:HD11	2.01	0.43
1:D:616:ASP:OD1	1:D:657:SER:OG	2.34	0.43
2:E:237:TYR:CE1	2:E:268:GLU:HG2	2.54	0.43
1:A:259:TRP:N	1:A:267:LEU:O	2.50	0.42
1:D:121:ALA:HB2	1:D:153:ARG:HA	2.00	0.42
3:C:107:TYR:HE2	3:C:109:ARG:CG	2.33	0.42
3:F:242:ASP:OD2	3:F:246:HIS:NE2	2.42	0.42
2:B:41:HIS:CD2	3:C:194:GLU:HG3	2.55	0.42
1:D:158:TYR:OH	1:D:423:TRP:HA	2.20	0.42
1:D:459:ILE:HB	1:D:545:VAL:HG23	2.01	0.42
1:D:587:HIS:HB2	7:D:905:HEC:C1D	2.49	0.42
1:D:617:SER:HA	1:D:618:PRO:HD3	1.90	0.42
2:E:237:TYR:HE1	2:E:268:GLU:HG2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:VAL:HG12	1:A:353:TYR:HA	2.01	0.42
3:C:201:ARG:HD3	3:C:352:ALA:HB1	2.01	0.42
1:D:712:TYR:HD1	1:D:794:TRP:CG	2.38	0.42
2:E:184:SER:OG	2:E:189:THR:OG1	2.24	0.42
3:F:265:VAL:HB	3:F:271:LEU:HD12	2.02	0.42
2:B:164:ARG:HG2	2:B:164:ARG:HH11	1.84	0.42
1:D:277:ARG:HG3	7:D:905:HEC:O1D	2.20	0.42
3:F:111:GLN:O	3:F:132:TYR:HA	2.19	0.42
1:A:357:THR:HG21	1:A:364:TYR:CE2	2.55	0.42
2:B:136:ILE:O	2:B:137:LYS:HG3	2.20	0.42
3:F:310:PHE:N	7:F:405:HEC:O1A	2.53	0.42
1:A:67:THR:HB	1:A:70:GLY:H	1.85	0.42
1:D:49:SER:HA	1:D:52:VAL:HG12	2.02	0.42
1:D:588:TYR:HB3	4:D:901:CL:CL	2.57	0.41
1:D:632:TYR:CZ	1:D:634:GLY:HA2	2.55	0.41
2:B:180:MET:HB3	2:B:193:ILE:HD11	2.02	0.41
2:E:228:ASP:CB	2:E:292:GLY:HA2	2.50	0.41
2:E:115:VAL:O	2:E:124:ILE:N	2.50	0.41
2:E:288:GLY:H	2:E:309:MET:CG	2.27	0.41
2:B:325:ARG:HD3	1:D:692:ASN:HA	2.02	0.41
2:B:386:ASP:N	2:B:386:ASP:OD1	2.54	0.41
2:E:117:ASP:OD1	2:E:118:ILE:N	2.53	0.41
2:E:136:ILE:HG22	2:E:147:VAL:HG22	2.03	0.41
2:E:175:ASP:H	2:E:194:LEU:HD13	1.85	0.41
3:F:183:LEU:O	3:F:187:ILE:HG12	2.20	0.41
3:F:218:PHE:O	3:F:225:CYS:HB2	2.21	0.41
1:A:173:ARG:NH2	1:A:178:GLU:OE2	2.54	0.41
1:A:252:LEU:HD12	1:A:572:TRP:CZ2	2.55	0.41
1:D:600:HIS:HB3	3:F:278:TYR:O	2.21	0.41
1:D:596:PHE:HB2	2:E:258:GLN:HA	2.02	0.41
2:E:179:ARG:NH1	3:F:107:TYR:OH	2.54	0.41
3:F:198:SER:HA	3:F:199:PRO:HD3	1.85	0.41
1:A:205:GLU:HA	1:A:528:GLN:NE2	2.35	0.41
3:C:123:GLY:O	3:C:126:SER:OG	2.32	0.41
1:D:116:LYS:HA	1:D:116:LYS:HD3	1.89	0.41
1:D:259:TRP:CG	1:D:260:LEU:H	2.38	0.41
1:D:410:HIS:CD2	1:D:411:GLN:HG3	2.56	0.41
2:E:255:GLU:OE1	2:E:255:GLU:N	2.54	0.41
2:B:237:TYR:CE1	2:B:268:GLU:HG2	2.55	0.41
1:D:58:GLN:O	1:D:415:VAL:HG22	2.20	0.41
2:E:134:SER:OG	2:E:179:ARG:O	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:229:VAL:HA	2:E:239:ALA:O	2.21	0.41
3:F:122:GLU:O	3:F:291:LEU:HD22	2.20	0.41
1:A:600:HIS:HB3	3:C:278:TYR:O	2.21	0.41
1:A:617:SER:HA	1:A:618:PRO:HD3	1.93	0.41
2:B:148:ALA:HB2	2:B:181:VAL:HG13	2.03	0.41
2:B:282:ASP:N	2:B:285:ASN:O	2.50	0.41
2:B:356:PRO:HA	2:B:371:ALA:O	2.21	0.41
1:D:594:ARG:NH2	2:E:337:ASP:HB2	2.36	0.41
2:E:253[A]:GLU:HB3	2:E:255:GLU:OE1	2.20	0.41
2:E:222:GLU:OE2	10:E:501:HOH:O	2.22	0.41
2:E:250:PRO:O	2:E:258:GLN:NE2	2.54	0.41
1:A:105:THR:HB	1:A:123:VAL:HG12	2.02	0.40
2:E:187:GLY:O	2:E:209:ILE:HD12	2.21	0.40
1:A:199:PRO:HG2	1:A:202:VAL:HG21	2.03	0.40
1:A:295:TYR:CE1	2:B:253[A]:GLU:HG3	2.56	0.40
3:C:131:LYS:HE2	3:C:144:HIS:CE1	2.57	0.40
3:F:110:GLY:HA2	3:F:133:ILE:HD11	2.03	0.40
1:A:206:PHE:CZ	1:A:333:MET:HE1	2.56	0.40
3:F:308:THR:HG23	3:F:316:ARG:HA	2.03	0.40
1:A:220:GLN:HB2	1:A:224:ILE:HG12	2.03	0.40
2:B:321:LEU:O	2:B:325:ARG:HG3	2.22	0.40
1:D:277:ARG:NH1	7:D:905:HEC:O2D	2.55	0.40
1:D:608:TRP:HD1	1:D:616:ASP:OD2	2.05	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	762/782 (97%)	731 (96%)	31 (4%)	0	100	100
1	D	764/782 (98%)	739 (97%)	25 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	351/352 (100%)	343 (98%)	8 (2%)	0	100	100
2	E	351/352 (100%)	342 (97%)	9 (3%)	0	100	100
3	C	312/314 (99%)	295 (95%)	16 (5%)	1 (0%)	36	60
3	F	312/314 (99%)	298 (96%)	13 (4%)	1 (0%)	36	60
All	All	2852/2896 (98%)	2748 (96%)	102 (4%)	2 (0%)	48	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	96	LEU
3	F	96	LEU

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	641/653 (98%)	635 (99%)	6 (1%)	70	87
1	D	642/653 (98%)	640 (100%)	2 (0%)	86	94
2	B	303/302 (100%)	301 (99%)	2 (1%)	76	90
2	E	300/302 (99%)	294 (98%)	6 (2%)	48	76
3	C	262/264 (99%)	260 (99%)	2 (1%)	73	88
3	F	259/264 (98%)	256 (99%)	3 (1%)	63	84
All	All	2407/2438 (99%)	2386 (99%)	21 (1%)	70	87

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	162	SER
1	A	333	MET
1	A	334	ASN
1	A	359	LYS

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Mol	Chain	Res	Type
1	A	384	ASP
2	B	229	VAL
2	B	330	GLU
3	C	162	ASP
3	C	209	GLU
1	D	178	GLU
1	D	359	LYS
2	E	43	LYS
2	E	79	GLN
2	E	118	ILE
2	E	126	GLU
2	E	136	ILE
2	E	241	THR
3	F	152	ASP
3	F	264	LYS
3	F	280	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	207	HIS
1	A	213	ASN
1	A	265	ASN
1	A	441	GLN
1	A	475	HIS
1	A	528	GLN
1	A	678	GLN
2	B	41	HIS
2	B	247	ASN
2	B	376	ASN
3	C	111	GLN
3	C	202	ASN
3	C	327	ASN
3	C	337	HIS
3	C	340	GLN
3	C	344	GLN
1	D	75	ASN
1	D	184	HIS
1	D	207	HIS
1	D	208	ASN
1	D	290	ASN

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Mol	Chain	Res	Type
1	D	432	ASN
1	D	496	GLN
1	D	606	ASN
1	D	678	GLN
2	E	51	HIS
2	E	65	ASN
2	E	90	GLN
2	E	225	ASN
2	E	243	GLN
3	F	150	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 19 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
8	BET	A	909	-	7,7,7	2.49	1 (14%)	10,10,10	1.96	2 (20%)
7	HEC	D	905	6,1	50,50,50	1.85	5 (10%)	68,82,82	1.38	7 (10%)
7	HEC	C	404	10,3	50,50,50	1.83	7 (14%)	68,82,82	1.37	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	HEC	A	906	1	50,50,50	1.79	5 (10%)	68,82,82	1.41	6 (8%)
8	BET	C	406	-	7,7,7	2.57	1 (14%)	10,10,10	1.86	2 (20%)
8	BET	B	403	-	7,7,7	2.51	1 (14%)	10,10,10	1.96	2 (20%)
7	HEC	F	405	3	50,50,50	1.82	5 (10%)	68,82,82	1.37	5 (7%)
7	HEC	D	906	1	50,50,50	1.84	5 (10%)	68,82,82	1.47	7 (10%)
7	HEC	F	404	10,3	50,50,50	1.82	5 (10%)	68,82,82	1.38	6 (8%)
7	HEC	A	905	6,1	50,50,50	1.88	5 (10%)	68,82,82	1.37	7 (10%)
8	BET	A	908	-	7,7,7	2.52	1 (14%)	10,10,10	1.96	2 (20%)
8	BET	D	907	-	7,7,7	2.47	1 (14%)	10,10,10	1.98	2 (20%)
7	HEC	C	405	3	50,50,50	1.81	5 (10%)	68,82,82	1.40	5 (7%)
8	BET	A	907	-	7,7,7	2.49	1 (14%)	10,10,10	1.88	2 (20%)
8	BET	E	403	-	7,7,7	2.47	1 (14%)	10,10,10	1.96	2 (20%)

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
8	BET	A	909	-	-	5/5/5/5	-
7	HEC	D	905	6,1	1/1/3/7	2/14/54/54	-
7	HEC	C	404	10,3	1/1/3/7	4/14/54/54	-
7	HEC	A	906	1	1/1/3/7	1/14/54/54	-
8	BET	C	406	-	-	5/5/5/5	-
8	BET	B	403	-	-	5/5/5/5	-
7	HEC	F	405	3	1/1/3/7	1/14/54/54	-
7	HEC	D	906	1	1/1/3/7	7/14/54/54	-
7	HEC	F	404	10,3	1/1/3/7	0/14/54/54	-
7	HEC	A	905	6,1	1/1/3/7	5/14/54/54	-
8	BET	A	908	-	-	5/5/5/5	-
8	BET	D	907	-	-	5/5/5/5	-
7	HEC	C	405	3	1/1/3/7	3/14/54/54	-
8	BET	A	907	-	-	5/5/5/5	-
8	BET	E	403	-	-	5/5/5/5	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	405	HEC	C3D-C2D	8.15	1.54	1.36
7	F	404	HEC	C3D-C2D	8.10	1.54	1.36
7	A	906	HEC	C3D-C2D	8.09	1.54	1.36
7	F	405	HEC	C3D-C2D	8.09	1.53	1.36
7	D	906	HEC	C3D-C2D	8.07	1.53	1.36
7	C	404	HEC	C3D-C2D	8.07	1.53	1.36
7	A	905	HEC	C3D-C2D	8.02	1.53	1.36
7	D	905	HEC	C3D-C2D	7.98	1.53	1.36
8	C	406	BET	CA-C	6.21	1.63	1.52
8	A	908	BET	CA-C	6.05	1.62	1.52
8	A	909	BET	CA-C	6.05	1.62	1.52
8	B	403	BET	CA-C	6.04	1.62	1.52
8	A	907	BET	CA-C	6.02	1.62	1.52
8	E	403	BET	CA-C	5.99	1.62	1.52
8	D	907	BET	CA-C	5.96	1.62	1.52
7	A	905	HEC	FE-ND	5.17	2.10	1.94
7	D	906	HEC	FE-ND	5.02	2.10	1.94
7	D	905	HEC	FE-ND	4.91	2.10	1.94
7	F	405	HEC	FE-ND	4.87	2.09	1.94
7	C	405	HEC	FE-ND	4.75	2.09	1.94
7	A	905	HEC	FE-NB	4.72	2.09	1.94
7	D	905	HEC	FE-NB	4.48	2.08	1.94
7	C	404	HEC	FE-ND	4.45	2.08	1.94
7	A	906	HEC	FE-ND	4.39	2.08	1.94
7	F	404	HEC	FE-ND	4.35	2.08	1.94
7	F	404	HEC	FE-NB	4.26	2.08	1.94
7	F	405	HEC	FE-NB	4.17	2.07	1.94
7	C	404	HEC	FE-NB	4.01	2.07	1.94
7	D	906	HEC	FE-NB	3.86	2.06	1.94
7	C	405	HEC	FE-NB	3.78	2.06	1.94
7	A	906	HEC	FE-NB	3.64	2.06	1.94
7	D	905	HEC	FE-NC	3.50	2.07	1.95
7	C	404	HEC	FE-NC	3.46	2.06	1.95
7	D	906	HEC	FE-NC	3.44	2.06	1.95
7	A	905	HEC	FE-NA	3.38	2.06	1.95
7	C	404	HEC	FE-NA	3.33	2.06	1.95
7	A	906	HEC	FE-NC	3.26	2.06	1.95
7	F	404	HEC	FE-NC	3.24	2.06	1.95
7	F	404	HEC	FE-NA	3.18	2.05	1.95
7	A	905	HEC	FE-NC	3.16	2.05	1.95
7	F	405	HEC	FE-NC	3.12	2.05	1.95
7	D	905	HEC	FE-NA	3.07	2.05	1.95
7	A	906	HEC	FE-NA	3.00	2.05	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	405	HEC	FE-NA	2.98	2.05	1.95
7	C	405	HEC	FE-NC	2.98	2.05	1.95
7	F	405	HEC	FE-NA	2.87	2.04	1.95
7	D	906	HEC	FE-NA	2.73	2.04	1.95
7	C	404	HEC	CMC-C2C	2.03	1.55	1.50
7	C	404	HEC	CMA-C3A	2.02	1.55	1.50

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	906	HEC	C1D-ND-C4D	6.57	111.86	105.07
7	F	404	HEC	C1D-ND-C4D	6.56	111.85	105.07
7	C	404	HEC	C1D-ND-C4D	6.50	111.79	105.07
7	C	405	HEC	C1D-ND-C4D	6.35	111.64	105.07
7	A	906	HEC	C1D-ND-C4D	6.33	111.61	105.07
7	F	405	HEC	C1D-ND-C4D	6.29	111.57	105.07
7	A	905	HEC	C1D-ND-C4D	5.93	111.20	105.07
7	D	905	HEC	C1D-ND-C4D	5.87	111.14	105.07
8	D	907	BET	C-CA-N	-4.85	109.67	116.34
8	A	909	BET	C-CA-N	-4.85	109.68	116.34
8	E	403	BET	C-CA-N	-4.81	109.73	116.34
8	A	908	BET	C-CA-N	-4.79	109.75	116.34
8	B	403	BET	C-CA-N	-4.75	109.80	116.34
8	A	907	BET	C-CA-N	-4.58	110.04	116.34
8	C	406	BET	C-CA-N	-4.48	110.19	116.34
8	E	403	BET	OXT-C-O	3.32	131.57	123.30
8	D	907	BET	OXT-C-O	3.31	131.55	123.30
8	A	909	BET	OXT-C-O	3.31	131.54	123.30
8	C	406	BET	OXT-C-O	3.29	131.51	123.30
8	A	907	BET	OXT-C-O	3.28	131.48	123.30
8	B	403	BET	OXT-C-O	3.28	131.47	123.30
8	A	908	BET	OXT-C-O	3.28	131.47	123.30
7	D	906	HEC	CAD-C3D-C4D	3.25	130.34	124.66
7	C	405	HEC	C4A-NA-C1A	2.86	108.15	105.35
7	C	405	HEC	C4B-NB-C1B	2.85	108.02	105.07
7	D	906	HEC	C4A-NA-C1A	2.84	108.13	105.35
7	A	906	HEC	C4B-NB-C1B	2.79	107.96	105.07
7	F	405	HEC	C4A-NA-C1A	2.77	108.06	105.35
7	D	905	HEC	C4B-NB-C1B	2.75	107.92	105.07
7	A	905	HEC	C4B-NB-C1B	2.73	107.89	105.07
7	D	906	HEC	C4B-NB-C1B	2.69	107.85	105.07
7	C	405	HEC	C4C-NC-C1C	2.67	107.97	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	906	HEC	C4A-NA-C1A	2.66	107.95	105.35
7	A	906	HEC	C4C-NC-C1C	2.66	107.95	105.35
7	C	404	HEC	C4B-NB-C1B	2.64	107.80	105.07
7	F	404	HEC	C4A-NA-C1A	2.63	107.92	105.35
7	C	405	HEC	C2A-C1A-NA	-2.61	107.79	110.32
7	A	905	HEC	C4C-NC-C1C	2.60	107.90	105.35
7	F	404	HEC	C4B-NB-C1B	2.60	107.76	105.07
7	F	405	HEC	C2A-C1A-NA	-2.60	107.80	110.32
7	C	404	HEC	C4A-NA-C1A	2.60	107.89	105.35
7	D	906	HEC	C2A-C1A-NA	-2.59	107.81	110.32
7	D	905	HEC	C4A-NA-C1A	2.57	107.86	105.35
7	F	405	HEC	C4B-NB-C1B	2.55	107.71	105.07
7	C	404	HEC	C4C-NC-C1C	2.53	107.83	105.35
7	F	404	HEC	C4C-NC-C1C	2.53	107.83	105.35
7	F	405	HEC	C4C-NC-C1C	2.52	107.82	105.35
7	A	905	HEC	C4A-NA-C1A	2.51	107.81	105.35
7	D	905	HEC	C4C-NC-C1C	2.48	107.78	105.35
7	A	906	HEC	C2A-C1A-NA	-2.40	107.99	110.32
7	D	906	HEC	C4C-NC-C1C	2.30	107.60	105.35
7	F	404	HEC	C2A-C1A-NA	-2.30	108.08	110.32
7	D	905	HEC	C2A-C1A-NA	-2.23	108.16	110.32
7	A	905	HEC	CAD-CBD-CGD	-2.21	108.85	113.60
7	C	404	HEC	C2A-C1A-NA	-2.20	108.18	110.32
7	A	905	HEC	C3C-C4C-NC	-2.19	107.70	110.15
7	F	404	HEC	C3C-C4C-NC	-2.14	107.76	110.15
7	A	905	HEC	C2A-C1A-NA	-2.11	108.27	110.32
7	C	404	HEC	C3C-C4C-NC	-2.10	107.80	110.15
7	A	906	HEC	C3C-C4C-NC	-2.02	107.89	110.15
7	D	905	HEC	C3C-C4C-NC	-2.02	107.89	110.15
7	D	906	HEC	CHD-C1D-ND	2.00	126.84	124.37
7	D	905	HEC	C3B-C4B-NB	-2.00	107.94	110.17

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	905	HEC	NA
7	A	906	HEC	NA
7	C	404	HEC	NA
7	C	405	HEC	NA
7	D	905	HEC	NA
7	D	906	HEC	NA
7	F	404	HEC	NA

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Mol	Chain	Res	Type	Atom
7	F	405	HEC	NA

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	907	BET	C-CA-N-C2
8	A	907	BET	O-C-CA-N
8	A	907	BET	OXT-C-CA-N
8	A	908	BET	O-C-CA-N
8	A	908	BET	OXT-C-CA-N
8	A	909	BET	O-C-CA-N
8	A	909	BET	OXT-C-CA-N
8	B	403	BET	O-C-CA-N
8	B	403	BET	OXT-C-CA-N
8	C	406	BET	O-C-CA-N
8	C	406	BET	OXT-C-CA-N
8	D	907	BET	O-C-CA-N
8	D	907	BET	OXT-C-CA-N
8	E	403	BET	O-C-CA-N
8	E	403	BET	OXT-C-CA-N
7	D	906	HEC	C4D-C3D-CAD-CBD
8	B	403	BET	C-CA-N-C1
8	B	403	BET	C-CA-N-C3
8	D	907	BET	C-CA-N-C1
8	D	907	BET	C-CA-N-C3
8	A	908	BET	C-CA-N-C1
8	C	406	BET	C-CA-N-C2
8	E	403	BET	C-CA-N-C1
8	A	907	BET	C-CA-N-C1
8	B	403	BET	C-CA-N-C2
8	D	907	BET	C-CA-N-C2
7	D	906	HEC	C2D-C3D-CAD-CBD
8	A	907	BET	C-CA-N-C3
8	A	908	BET	C-CA-N-C2
8	A	908	BET	C-CA-N-C3
8	A	909	BET	C-CA-N-C1
8	C	406	BET	C-CA-N-C1
8	E	403	BET	C-CA-N-C2
8	E	403	BET	C-CA-N-C3
8	A	909	BET	C-CA-N-C2
8	A	909	BET	C-CA-N-C3
7	A	906	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
8	C	406	BET	C-CA-N-C3
7	D	905	HEC	CAA-CBA-CGA-O1A
7	A	905	HEC	CAA-CBA-CGA-O1A
7	D	906	HEC	C2C-C3C-CAC-CBC
7	A	905	HEC	CAA-CBA-CGA-O2A
7	D	905	HEC	CAA-CBA-CGA-O2A
7	C	404	HEC	CAD-CBD-CGD-O2D
7	A	905	HEC	CAD-CBD-CGD-O2D
7	C	404	HEC	CAD-CBD-CGD-O1D
7	A	905	HEC	CAD-CBD-CGD-O1D
7	F	405	HEC	C2C-C3C-CAC-CBC
7	C	404	HEC	C3A-C2A-CAA-CBA
7	C	404	HEC	C1A-C2A-CAA-CBA
7	C	405	HEC	CAD-CBD-CGD-O2D
7	C	405	HEC	CAD-CBD-CGD-O1D
7	C	405	HEC	C2C-C3C-CAC-CBC
7	A	905	HEC	C2C-C3C-CAC-CBC
7	D	906	HEC	CAA-CBA-CGA-O2A
7	D	906	HEC	CAD-CBD-CGD-O2D
7	D	906	HEC	CAA-CBA-CGA-O1A
7	D	906	HEC	CAD-CBD-CGD-O1D

There are no ring outliers.

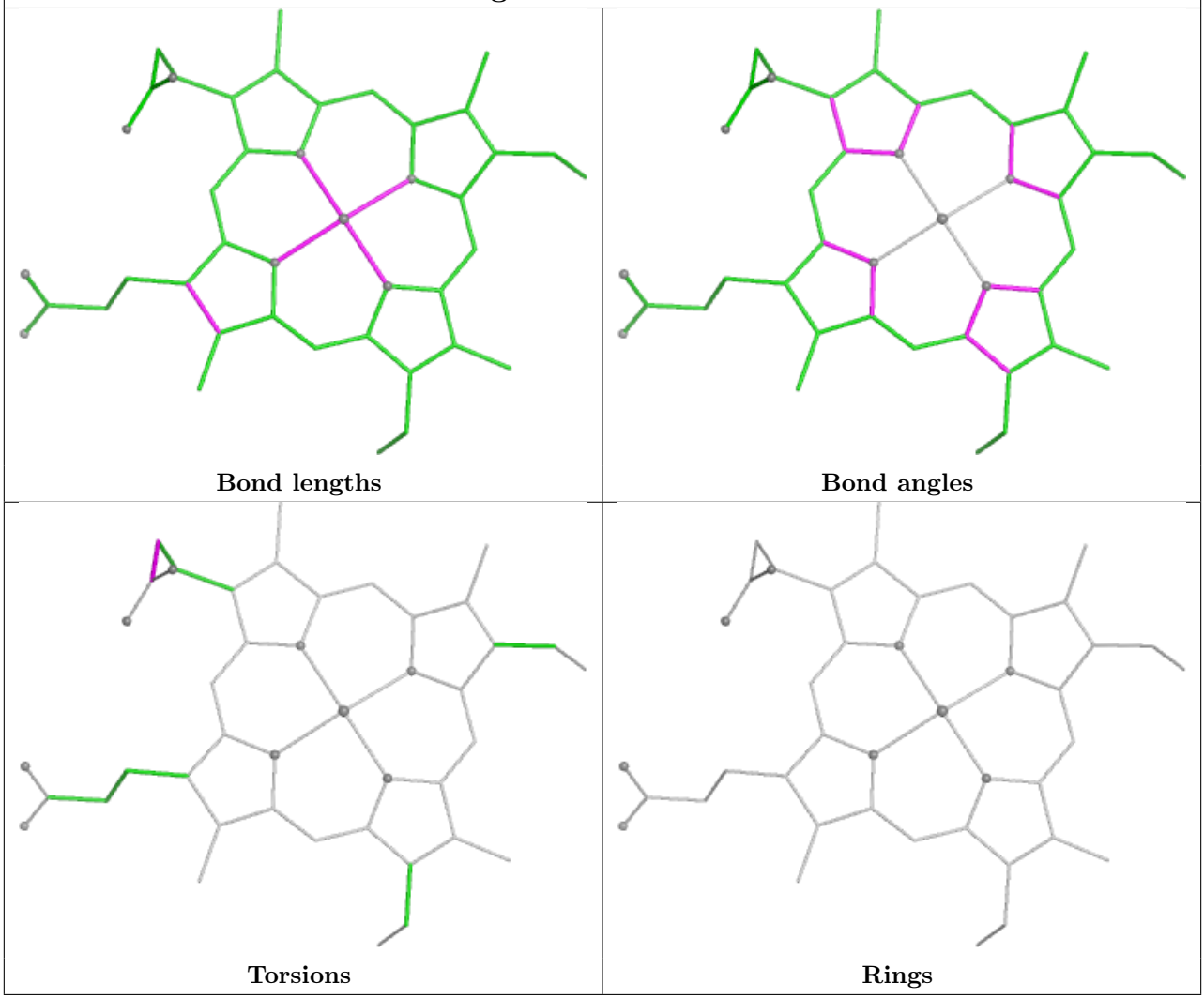
7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	905	HEC	4	0
7	C	404	HEC	3	0
7	A	906	HEC	8	0
7	F	405	HEC	1	0
7	D	906	HEC	3	0
7	F	404	HEC	2	0
7	A	905	HEC	1	0

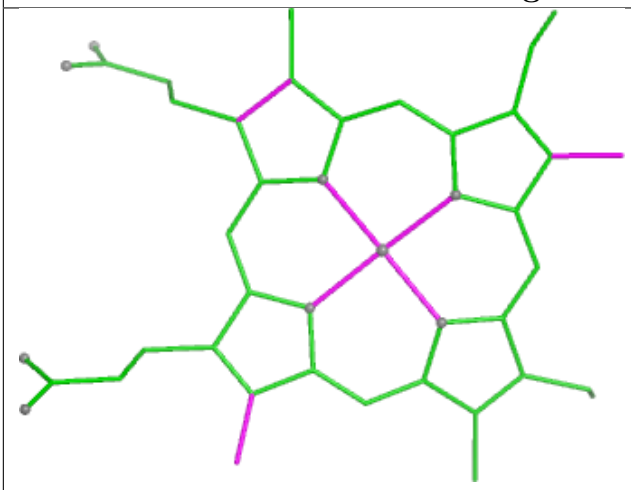
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

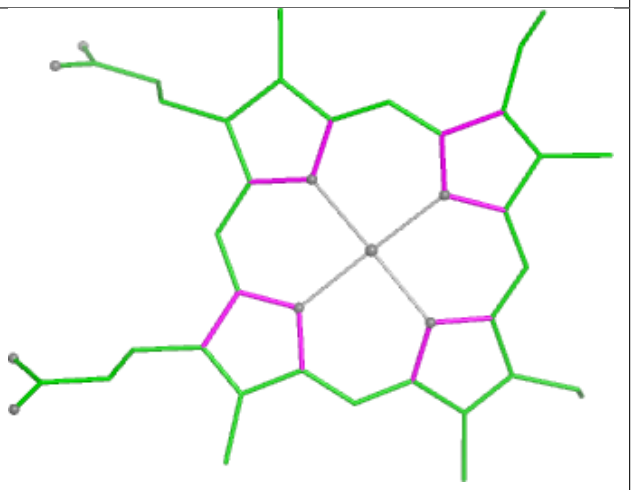
Ligand HEC D 905



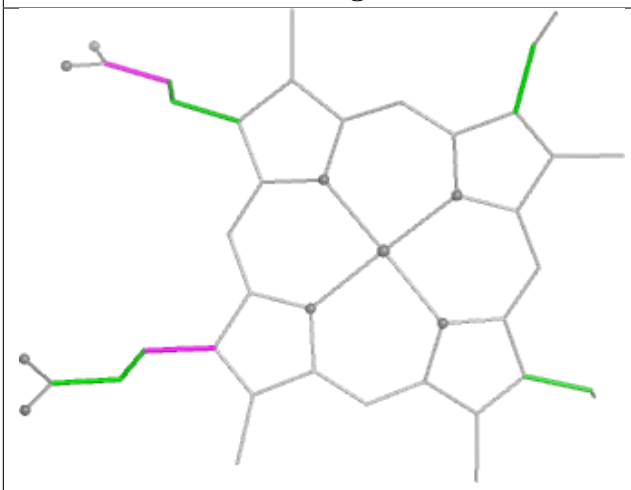
Ligand HEC C 404



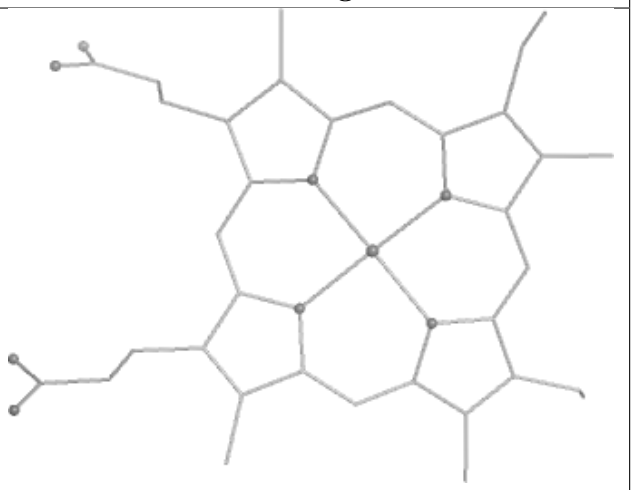
Bond lengths



Bond angles

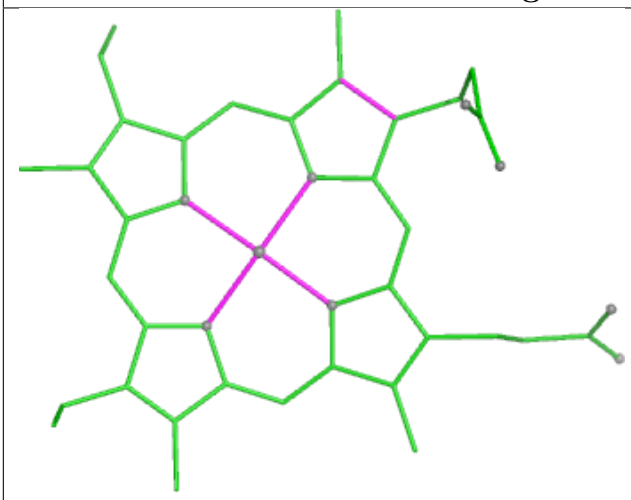


Torsions

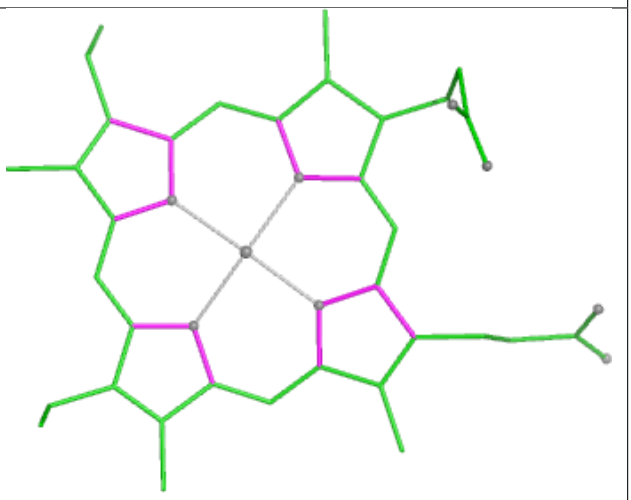


Rings

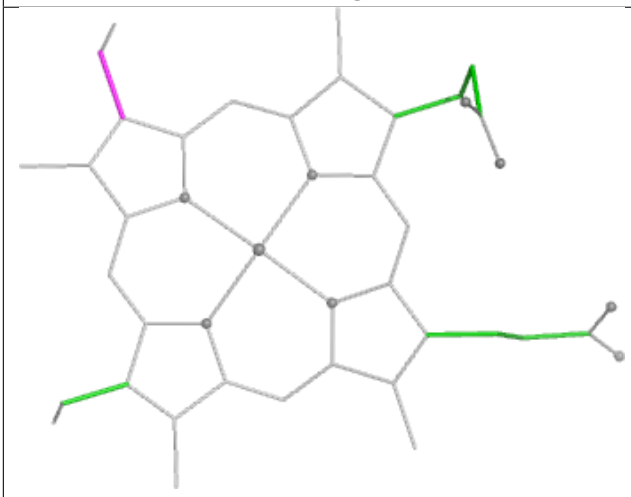
Ligand HEC A 906



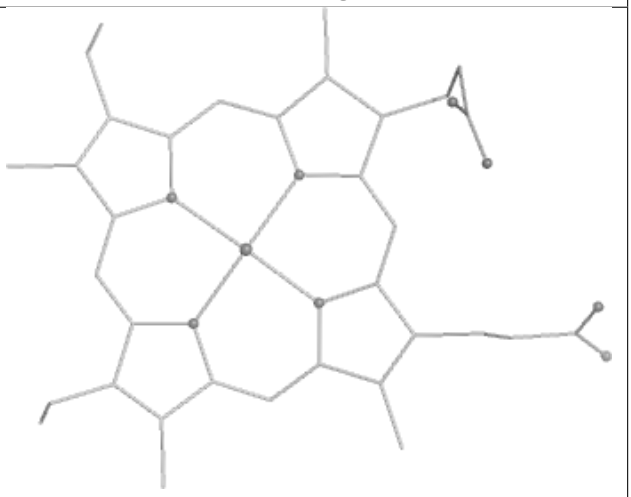
Bond lengths



Bond angles

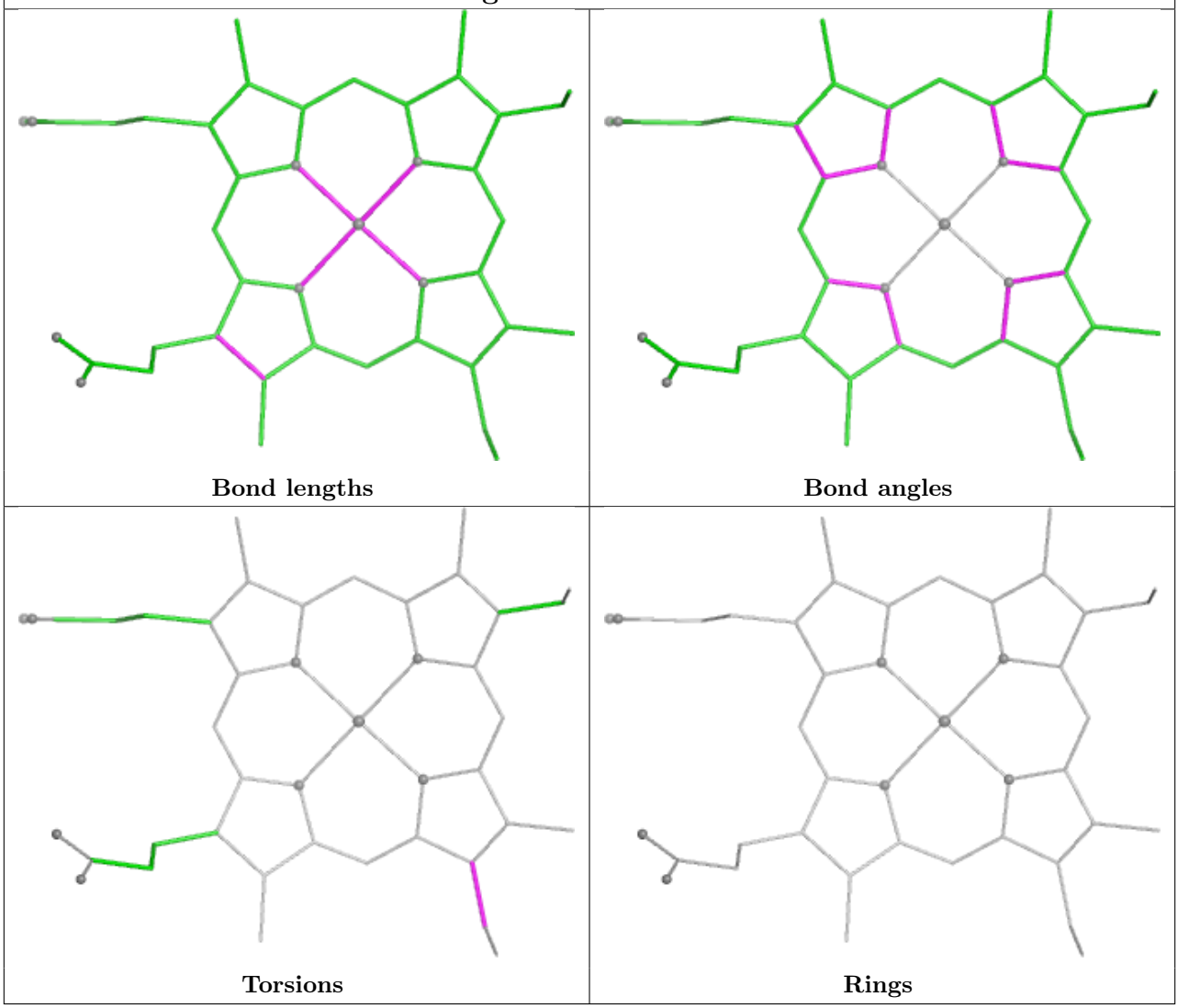


Torsions

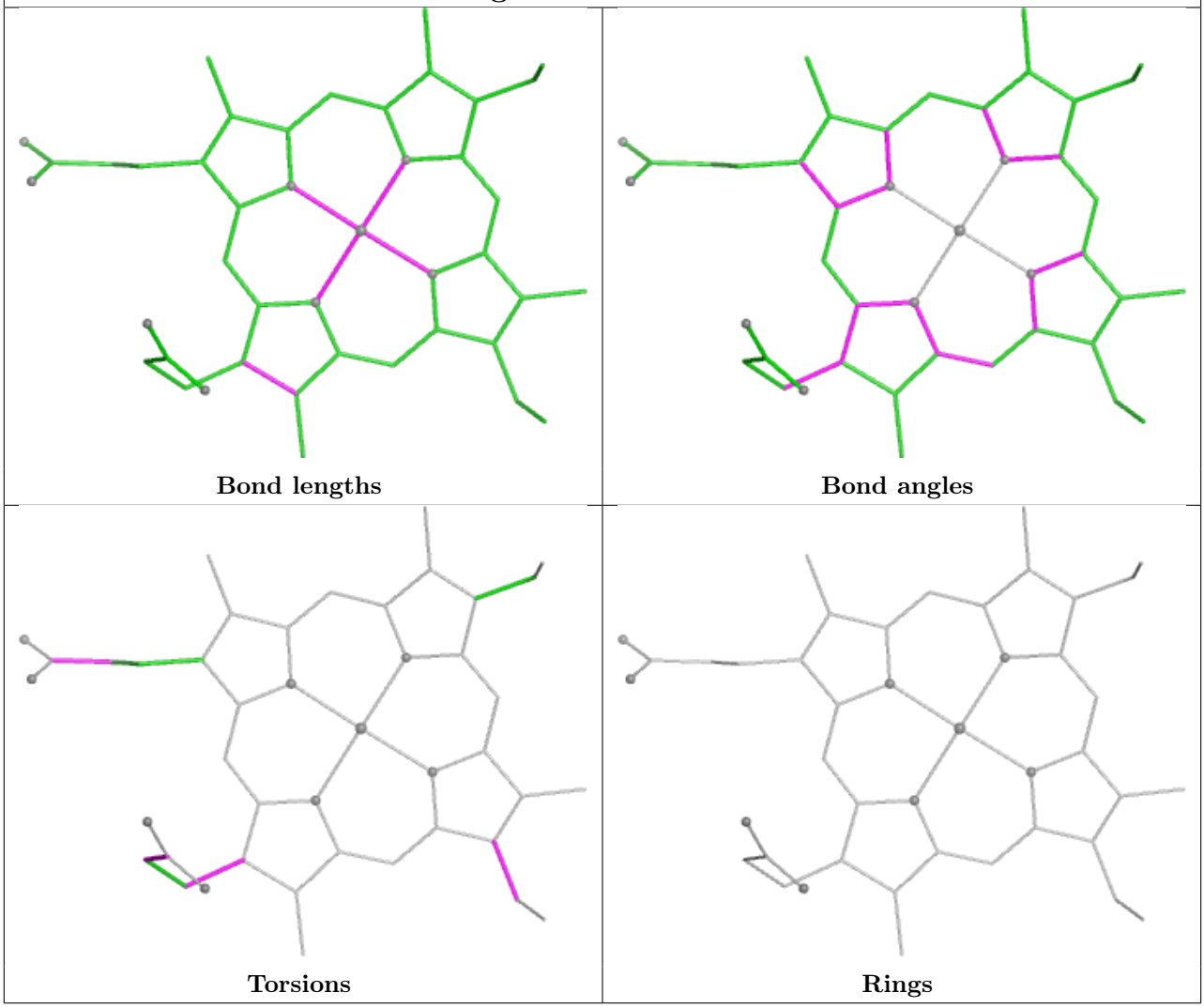


Rings

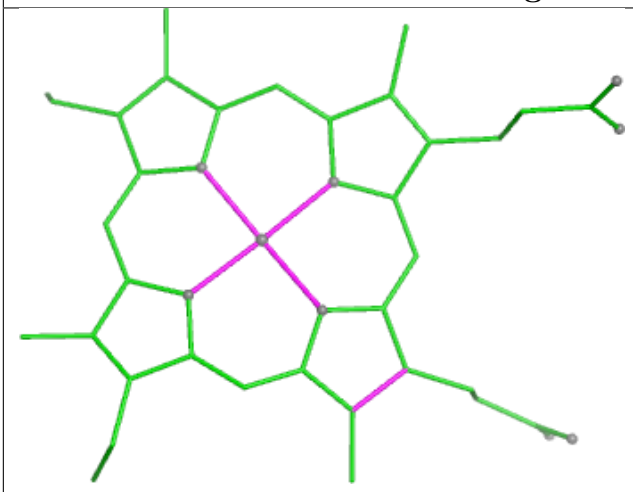
Ligand HEC F 405



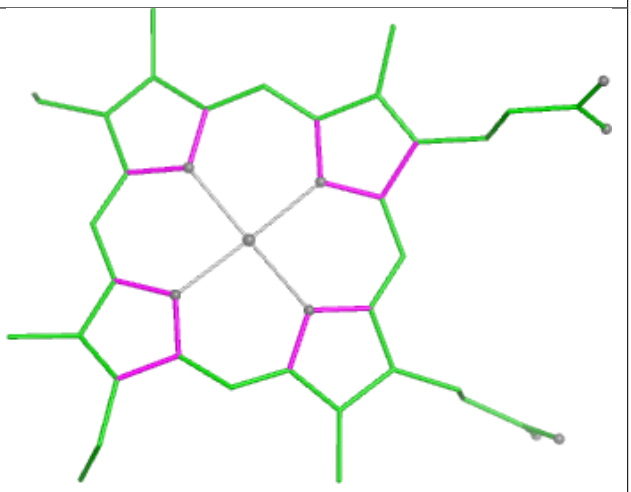
Ligand HEC D 906



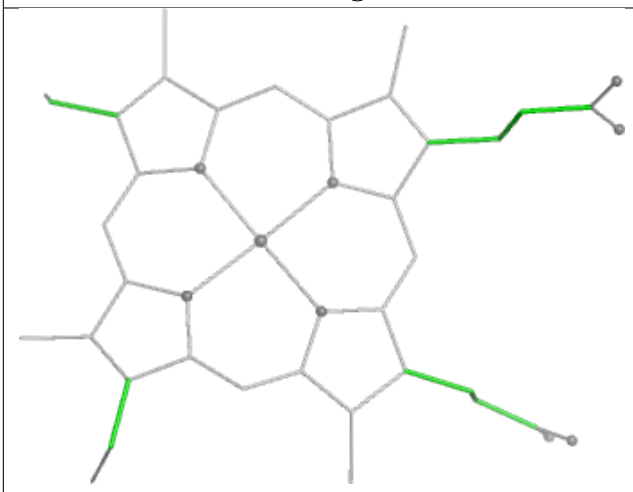
Ligand HEC F 404



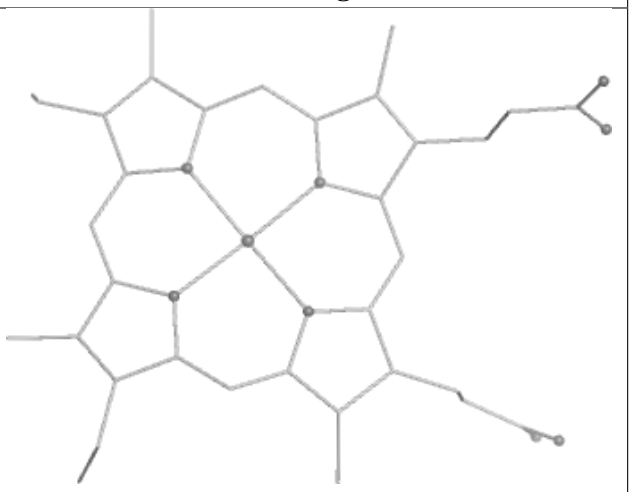
Bond lengths



Bond angles

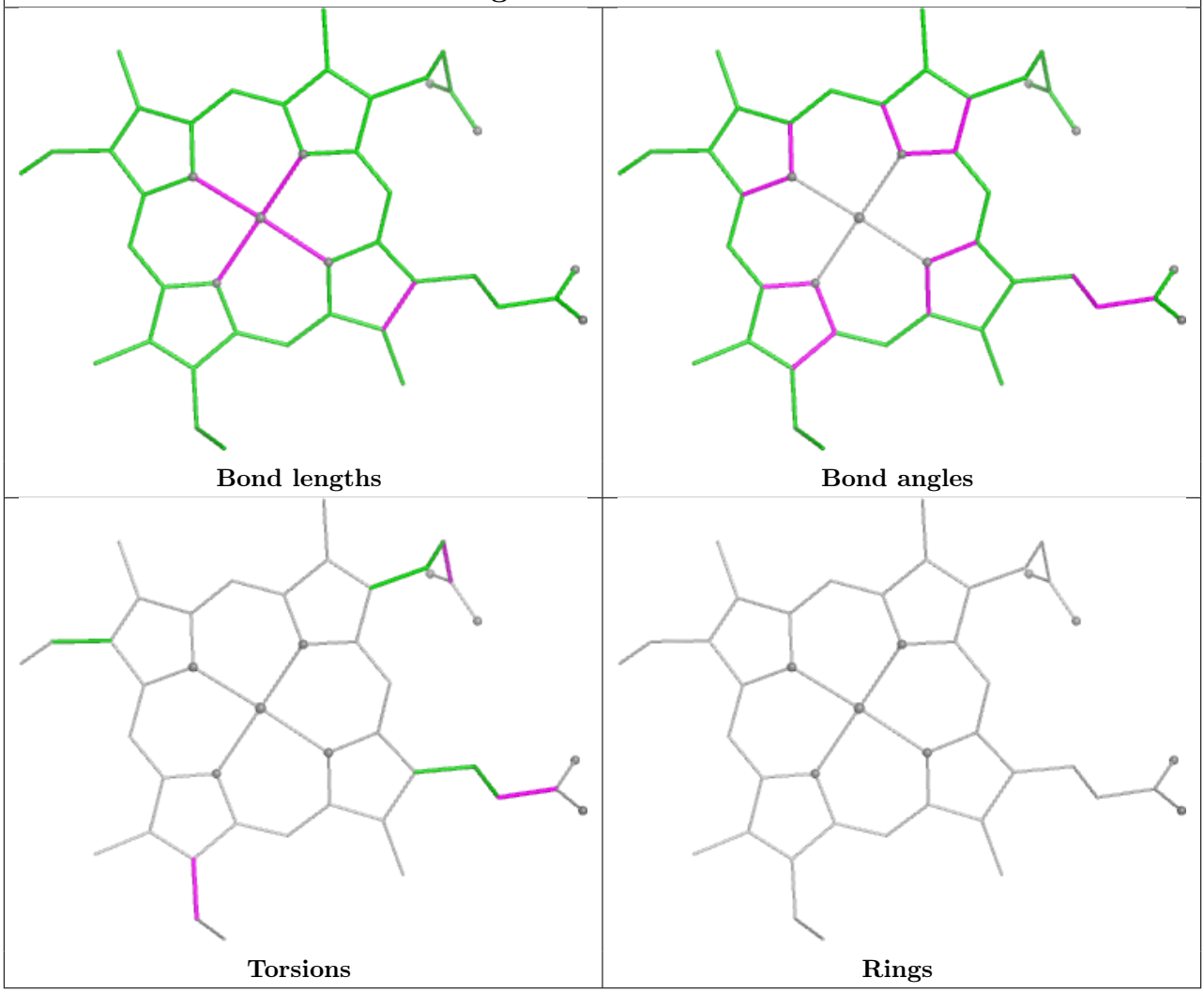


Torsions

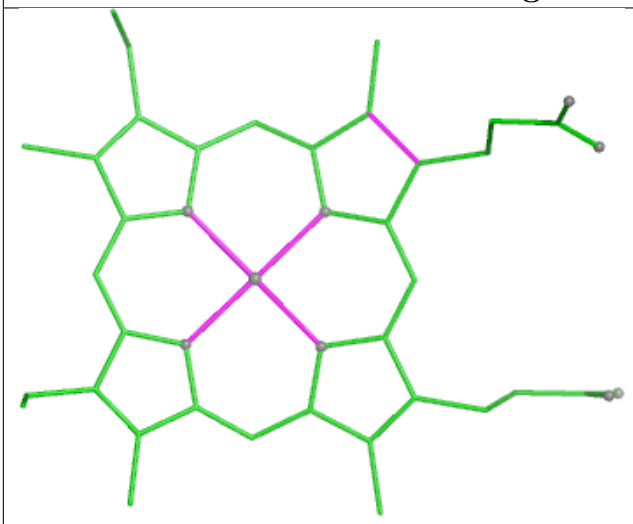


Rings

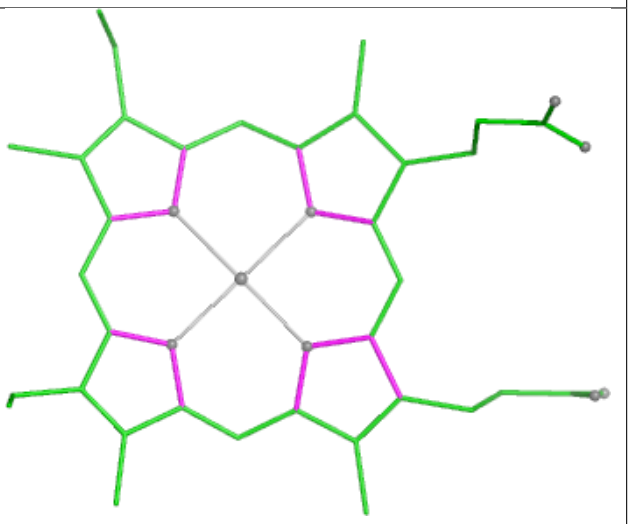
Ligand HEC A 905



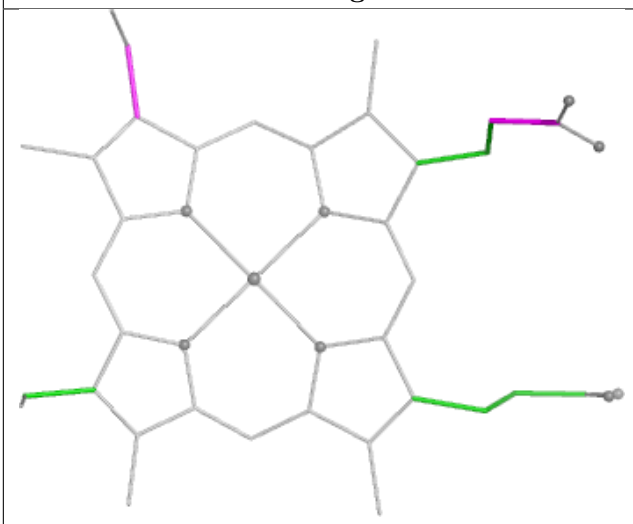
Ligand HEC C 405



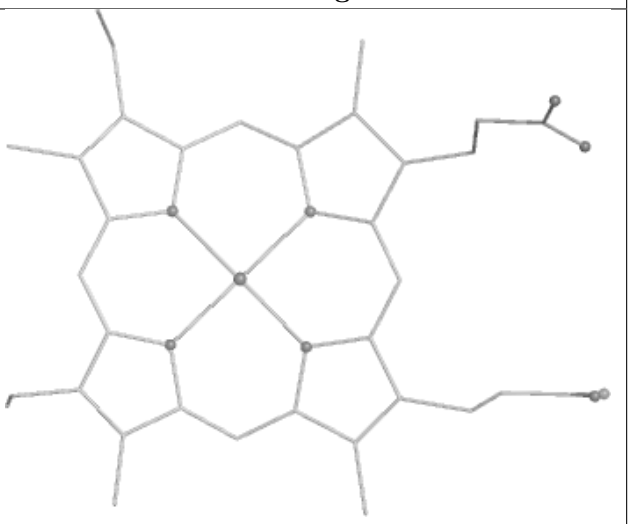
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	768/782 (98%)	0.49	38 (4%) 35 31	32, 54, 77, 111	0
1	D	770/782 (98%)	1.03	108 (14%) 6 5	37, 61, 83, 119	0
2	B	352/352 (100%)	0.93	30 (8%) 16 14	19, 60, 80, 96	1 (0%)
2	E	352/352 (100%)	1.60	114 (32%) 1 1	23, 77, 99, 113	1 (0%)
3	C	314/314 (100%)	0.77	21 (6%) 24 21	36, 57, 79, 97	0
3	F	314/314 (100%)	1.75	101 (32%) 1 1	46, 74, 91, 103	0
All	All	2870/2896 (99%)	1.00	412 (14%) 6 5	19, 62, 87, 119	2 (0%)

All (412) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	107	TYR	8.3
3	F	107	TYR	8.0
3	F	307	GLY	7.2
3	F	149	GLY	5.1
3	C	109	ARG	4.7
3	F	308	THR	4.5
2	B	132	TRP	4.4
3	F	224	GLY	4.3
1	D	652	PRO	4.2
1	A	359	LYS	4.1
2	E	132	TRP	4.1
3	F	313	GLY	4.0
2	E	352	THR	4.0
3	C	308	THR	4.0
3	F	333	GLY	4.0
1	D	383	GLY	4.0
2	E	292	GLY	4.0
1	D	159	ALA	3.9
2	E	134	SER	3.9

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Mol	Chain	Res	Type	RSRZ
2	E	288	GLY	3.9
1	A	360	ASP	3.9
2	E	117	ASP	3.9
1	A	358	GLY	3.8
1	A	361	GLY	3.8
2	E	122	GLN	3.8
3	C	307	GLY	3.8
3	F	152	ASP	3.8
3	F	109	ARG	3.8
2	E	95	ALA	3.7
2	E	156	ALA	3.7
3	F	249	GLY	3.7
3	F	334	ARG	3.6
3	F	240	PHE	3.6
2	E	71	VAL	3.6
3	C	306	SER	3.6
2	E	138	ILE	3.5
2	E	109	GLU	3.5
2	E	214	VAL	3.5
2	E	94	SER	3.5
2	E	254	ALA	3.5
2	B	231	TYR	3.5
2	E	183	ILE	3.5
2	E	130	GLY	3.5
2	E	135	GLY	3.5
3	F	146	GLY	3.5
2	E	212	GLY	3.4
3	F	120	GLY	3.4
2	E	103	LEU	3.4
2	E	87	VAL	3.4
1	D	181	TRP	3.4
3	F	77	PHE	3.4
2	E	253[A]	GLU	3.4
2	E	149	CYS	3.4
2	B	318	ASP	3.4
1	D	416	TYR	3.3
1	D	712	TYR	3.3
1	D	54	GLY	3.3
2	E	96	VAL	3.3
1	A	357	THR	3.3
1	A	178	GLU	3.3
1	D	235	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	131	ASP	3.3
2	E	152	CYS	3.3
1	A	175	ARG	3.3
2	E	115	VAL	3.3
2	E	89	VAL	3.2
3	F	223	VAL	3.2
3	F	63	LEU	3.2
3	C	313	GLY	3.2
2	E	155	ASN	3.2
1	D	60	LEU	3.2
1	D	162	SER	3.2
2	E	93	ALA	3.2
1	A	687	MET	3.2
3	F	92	ALA	3.2
1	D	174	ASP	3.1
2	E	195	ASP	3.1
2	E	194	LEU	3.1
2	B	109	GLU	3.1
2	E	272	GLY	3.1
3	F	45	ILE	3.1
1	D	191	GLY	3.1
1	D	413	ALA	3.1
2	E	81	VAL	3.1
3	F	226	LEU	3.1
2	E	41	HIS	3.1
2	E	114	SER	3.1
1	D	624	LEU	3.1
1	D	359	LYS	3.1
3	F	306	SER	3.0
2	B	69	HIS	3.0
2	E	178	PRO	3.0
3	F	180	PRO	3.0
2	B	131	ASP	3.0
1	A	383	GLY	3.0
3	F	58	GLY	3.0
2	E	170	SER	3.0
2	E	360	CYS	3.0
2	E	36	TYR	3.0
3	F	132	TYR	3.0
1	D	193	ILE	3.0
1	D	358	GLY	3.0
1	A	403	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	E	124	ILE	3.0
1	A	67	THR	3.0
1	A	802	PHE	3.0
3	F	200	PHE	3.0
2	E	150	SER	2.9
2	E	118	ILE	2.9
1	D	190	THR	2.9
3	F	318	LEU	2.9
1	D	122	GLY	2.9
2	E	363	PRO	2.9
3	F	322	ILE	2.9
1	D	651	GLY	2.9
2	B	82	THR	2.9
2	E	76	ALA	2.9
2	E	116	VAL	2.9
2	B	386	ASP	2.9
2	E	102	PHE	2.9
2	E	105	VAL	2.9
2	E	38	GLN	2.8
2	E	357	SER	2.8
2	B	200	ILE	2.8
1	D	402	TYR	2.8
2	E	82	THR	2.8
3	F	130	THR	2.8
2	E	136	ILE	2.8
3	C	129	ASN	2.8
1	D	415	VAL	2.8
2	B	149	CYS	2.8
2	E	291	TYR	2.8
3	F	113	THR	2.8
3	F	87	PHE	2.8
1	D	653	SER	2.8
1	D	418	LYS	2.8
2	E	37	ILE	2.8
1	D	133	TRP	2.8
3	C	136	GLY	2.8
3	F	263	GLY	2.8
1	D	802	PHE	2.8
3	F	122	GLU	2.8
3	F	154	ILE	2.7
3	F	303	ILE	2.7
2	E	64	SER	2.7

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Mol	Chain	Res	Type	RSRZ
3	F	156	GLY	2.7
1	D	106	ALA	2.7
1	D	372	ASP	2.7
2	B	166	GLU	2.7
3	F	194	GLU	2.7
3	F	186	LEU	2.7
1	D	291	TRP	2.7
2	E	110	SER	2.7
3	F	314	GLY	2.7
1	D	178	GLU	2.7
3	F	202	ASN	2.7
1	D	61	PHE	2.7
1	D	219	THR	2.7
1	D	435	VAL	2.7
2	E	371	ALA	2.7
3	F	103	ALA	2.7
2	E	79	GLN	2.7
3	F	70	PHE	2.7
2	E	106	CYS	2.6
2	E	100	GLY	2.6
3	F	197	GLY	2.6
1	A	68	ALA	2.6
1	A	159	ALA	2.6
1	D	273	ALA	2.6
3	F	203	ALA	2.6
2	E	98	PRO	2.6
3	F	162	ASP	2.6
1	D	179	GLY	2.6
2	E	305	GLY	2.6
3	F	136	GLY	2.6
3	F	147	PHE	2.6
3	F	248	VAL	2.6
1	D	244	THR	2.6
1	D	556	MET	2.6
3	C	353	LEU	2.6
2	E	252	CYS	2.6
1	D	67	THR	2.6
1	D	137	ILE	2.6
2	E	104	TYR	2.6
1	D	182	LYS	2.6
3	F	114	GLY	2.6
2	B	155	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	133	PRO	2.5
3	F	178	PHE	2.5
2	E	256	ASN	2.5
3	C	232	ASP	2.5
1	D	91	LEU	2.5
2	B	307	ARG	2.5
2	E	43	LYS	2.5
1	D	642	VAL	2.5
2	E	251	VAL	2.5
3	F	310	PHE	2.5
3	F	193	LEU	2.5
1	D	75	ASN	2.5
3	F	188	CYS	2.5
3	C	336	SER	2.5
1	D	157	TYR	2.5
2	E	176	TYR	2.5
3	F	285	PRO	2.5
3	F	349	TYR	2.5
1	A	66	ARG	2.4
3	F	129	ASN	2.4
3	F	324	ASN	2.4
2	B	368	CYS	2.4
2	E	67	SER	2.4
2	E	375	SER	2.4
3	F	198	SER	2.4
3	F	225	CYS	2.4
1	A	384	ASP	2.4
1	D	33	GLY	2.4
1	D	161	GLY	2.4
2	E	35	GLY	2.4
3	F	331	MET	2.4
1	D	537	TYR	2.4
2	E	90	GLN	2.4
3	C	41	GLN	2.4
1	A	61	PHE	2.4
2	B	134	SER	2.4
3	F	241	SER	2.4
3	F	121	ASP	2.4
1	D	95	GLU	2.4
1	A	33	GLY	2.4
1	A	122	GLY	2.4
1	D	115	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	388	TYR	2.4
1	D	808	VAL	2.4
1	D	429	ALA	2.4
3	C	322	ILE	2.4
2	B	70	SER	2.4
2	E	70	SER	2.4
1	D	55	PRO	2.4
3	F	82	VAL	2.4
2	E	172	TYR	2.4
3	C	203	ALA	2.4
1	D	363	LEU	2.4
2	B	160	ILE	2.4
2	E	61	LEU	2.4
3	F	350	LEU	2.4
1	D	584	SER	2.4
3	F	227	GLU	2.4
2	E	91	PRO	2.4
1	A	654	GLY	2.4
1	D	185	GLY	2.4
3	F	98	GLY	2.4
3	F	164	VAL	2.4
1	A	103	PHE	2.4
1	D	107	PHE	2.4
3	F	142	PHE	2.4
1	D	184	HIS	2.3
2	E	85	VAL	2.3
1	D	148	LEU	2.3
1	D	112	TYR	2.3
1	D	419	TYR	2.3
3	F	317	THR	2.3
1	A	334	ASN	2.3
2	E	137	LYS	2.3
1	D	198	SER	2.3
1	D	550	SER	2.3
2	B	112	SER	2.3
2	E	358	SER	2.3
3	C	204	ASP	2.3
1	D	371	PRO	2.3
1	D	141	GLY	2.3
2	E	350	VAL	2.3
1	A	60	LEU	2.3
1	D	250	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	291	TYR	2.3
1	D	610	ASP	2.3
3	F	118	ASP	2.3
1	A	179	GLY	2.3
1	A	701	LEU	2.3
2	B	135	GLY	2.3
2	E	230	VAL	2.3
2	E	378	VAL	2.3
1	D	120	PHE	2.3
2	E	73	PHE	2.3
1	D	224	ILE	2.2
1	D	294	ALA	2.2
2	B	370	ALA	2.2
3	F	246	HIS	2.2
3	F	222	LYS	2.2
1	D	164	GLU	2.2
1	D	535	TYR	2.2
3	F	90	ASN	2.2
1	D	581	ARG	2.2
2	B	357	SER	2.2
1	A	83	GLY	2.2
3	C	44	VAL	2.2
2	E	50	PHE	2.2
2	B	93	ALA	2.2
3	C	339	LYS	2.2
2	E	54	MET	2.2
1	D	414	PRO	2.2
1	A	154	SER	2.2
1	A	161	GLY	2.2
1	D	70	GLY	2.2
3	F	85	GLY	2.2
3	F	123	GLY	2.2
2	E	101	ALA	2.2
3	F	137	ARG	2.2
3	F	66	PRO	2.2
3	F	76	PRO	2.2
3	F	135	GLY	2.2
1	D	46	SER	2.2
2	E	147	VAL	2.2
1	D	163	ILE	2.2
1	D	614	HIS	2.2
2	E	62	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	127	ILE	2.2
1	D	104	ALA	2.2
1	D	229	THR	2.2
2	E	196	THR	2.2
2	E	227	ARG	2.2
2	E	140	PRO	2.2
2	E	284	ASN	2.2
1	D	149	LYS	2.2
1	D	223	LYS	2.2
1	A	185	GLY	2.2
1	D	88	LEU	2.2
1	D	96	LEU	2.2
1	A	135	MET	2.2
3	F	242	ASP	2.2
1	D	56	VAL	2.2
2	E	184	SER	2.2
3	F	144	HIS	2.2
3	F	292	VAL	2.2
1	D	458	TRP	2.1
3	F	315	ALA	2.1
1	A	639	GLU	2.1
3	F	80	GLU	2.1
3	F	139	LEU	2.1
1	D	398	GLY	2.1
2	B	83	GLY	2.1
2	B	195	ASP	2.1
1	A	162	SER	2.1
2	E	193	ILE	2.1
3	F	133	ILE	2.1
1	D	433	PHE	2.1
3	C	334	ARG	2.1
1	D	655	THR	2.1
2	B	352	THR	2.1
3	C	216	LYS	2.1
3	F	140	PRO	2.1
1	A	58	GLN	2.1
1	D	158	TYR	2.1
1	D	665	LEU	2.1
1	D	150	GLY	2.1
3	F	125	GLY	2.1
1	D	194	ILE	2.1
2	E	84	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	122	GLU	2.1
3	F	60	GLU	2.1
3	F	145	GLU	2.1
3	F	245	THR	2.1
3	F	299	THR	2.1
3	F	199	PRO	2.1
1	D	128	GLY	2.1
2	E	39	GLY	2.1
2	B	342	VAL	2.1
1	D	390	PHE	2.1
1	D	28	GLU	2.1
1	D	121	ALA	2.1
1	D	134	GLU	2.1
2	B	137	LYS	2.1
1	A	100	THR	2.1
3	F	47	THR	2.1
1	D	405	PRO	2.1
2	E	190	LEU	2.1
1	A	386	GLY	2.1
3	F	332	HIS	2.1
3	F	309	TYR	2.1
2	E	197	VAL	2.1
2	E	260	PHE	2.1
1	A	439	THR	2.0
2	E	40	THR	2.0
3	F	50	THR	2.0
1	D	48	MET	2.0
2	E	351	PRO	2.0
1	D	41	LEU	2.0
1	D	217	LEU	2.0
2	E	226	LEU	2.0
2	E	249	LEU	2.0
1	A	692	ASN	2.0
1	D	432	ASN	2.0
2	E	247	ASN	2.0
2	E	289	ASN	2.0
1	D	38	GLY	2.0
2	E	159	VAL	2.0
2	E	231	TYR	2.0
3	F	304	TYR	2.0
2	E	374	PHE	2.0
1	D	68	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	192	ALA	2.0
2	B	162	THR	2.0
2	E	119	GLN	2.0
3	F	239	LEU	2.0
3	F	150	HIS	2.0
1	D	127	GLY	2.0
2	B	130	GLY	2.0
2	E	65	ASN	2.0
3	C	268	ILE	2.0
1	D	438	VAL	2.0
2	E	179	ARG	2.0
3	F	326	VAL	2.0
1	D	212	TYR	2.0
1	D	388	TYR	2.0
3	F	189	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	C	401	1/1	0.78	0.14	54,54,54,54	0
5	CA	F	401	1/1	0.82	0.15	79,79,79,79	0
8	BET	A	907	8/8	0.82	0.24	62,75,83,86	0
5	CA	C	403	1/1	0.84	0.11	48,48,48,48	0
8	BET	A	909	8/8	0.85	0.21	72,80,84,89	0
8	BET	C	406	8/8	0.86	0.18	65,74,80,81	0
8	BET	D	907	8/8	0.86	0.22	64,72,84,86	0
8	BET	A	908	8/8	0.88	0.18	62,69,72,77	0

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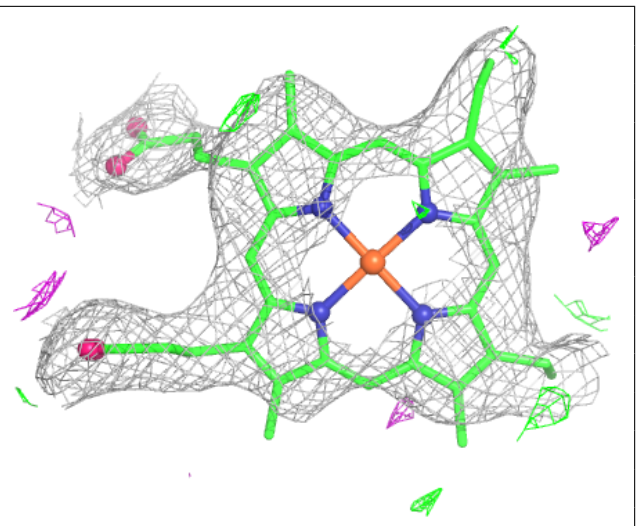
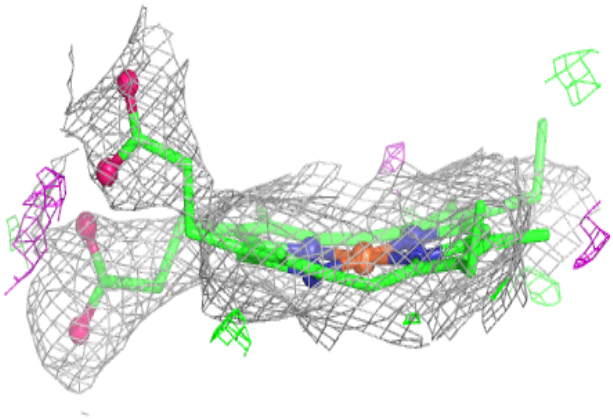
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	D	901	1/1	0.90	0.14	60,60,60,60	0
8	BET	B	403	8/8	0.90	0.15	52,58,69,69	0
5	CA	F	403	1/1	0.92	0.08	88,88,88,88	0
9	MG	E	401	1/1	0.92	0.11	47,47,47,47	0
9	MG	B	401	1/1	0.93	0.09	33,33,33,33	0
8	BET	E	403	8/8	0.93	0.14	63,66,71,74	0
5	CA	A	903	1/1	0.94	0.07	68,68,68,68	0
5	CA	F	402	1/1	0.94	0.09	70,70,70,70	0
7	HEC	F	405	43/43	0.95	0.14	64,77,87,93	0
7	HEC	F	404	43/43	0.95	0.14	47,62,77,82	0
7	HEC	D	905	43/43	0.96	0.11	38,53,67,71	0
4	CL	A	901[B]	1/1	0.96	0.21	40,40,40,40	1
5	CA	B	402	1/1	0.96	0.06	68,68,68,68	0
4	CL	A	901[A]	1/1	0.96	0.21	14,14,14,14	1
5	CA	C	402	1/1	0.96	0.05	59,59,59,59	0
7	HEC	C	405	43/43	0.96	0.11	42,61,70,75	0
7	HEC	C	404	43/43	0.97	0.11	26,44,61,66	0
5	CA	E	402	1/1	0.97	0.06	76,76,76,76	0
5	CA	D	903	1/1	0.97	0.05	65,65,65,65	0
7	HEC	D	906	43/43	0.97	0.09	36,46,58,74	0
7	HEC	A	906	43/43	0.97	0.10	37,55,69,94	0
6	ZN	D	904	1/1	0.98	0.07	53,53,53,53	0
7	HEC	A	905	43/43	0.98	0.08	23,37,49,54	0
5	CA	D	902	1/1	0.98	0.05	68,68,68,68	0
5	CA	A	902	1/1	0.99	0.05	59,59,59,59	0
6	ZN	A	904	1/1	0.99	0.06	46,46,46,46	0

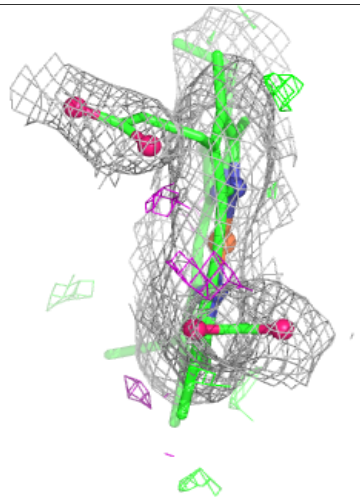
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC F 405:

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

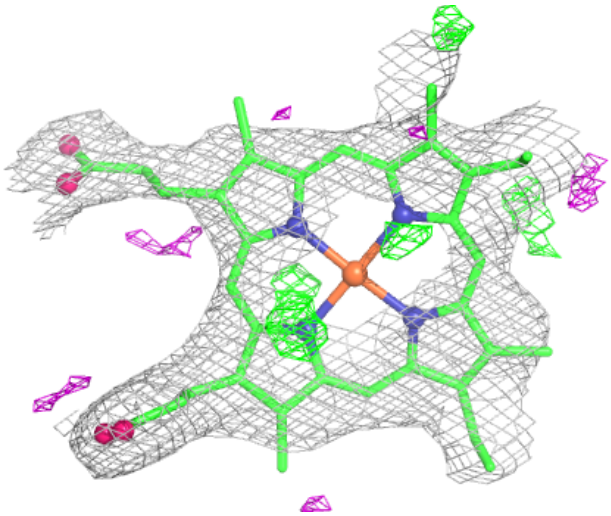


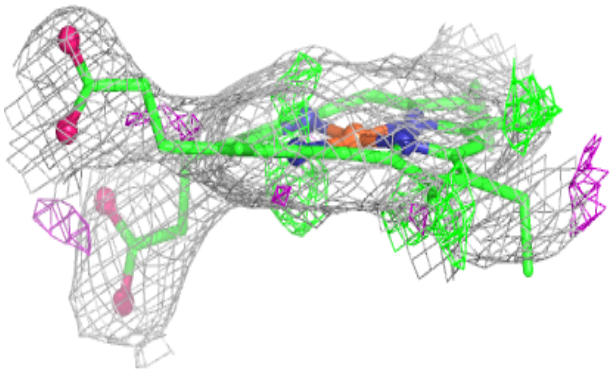


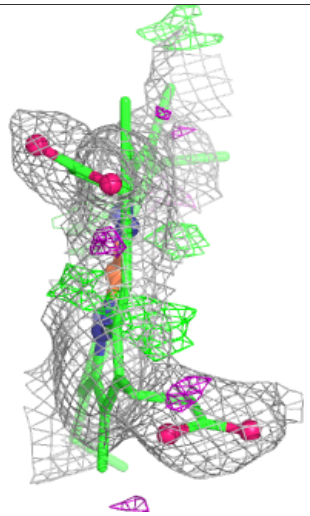


Electron density around HEC F 404:

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

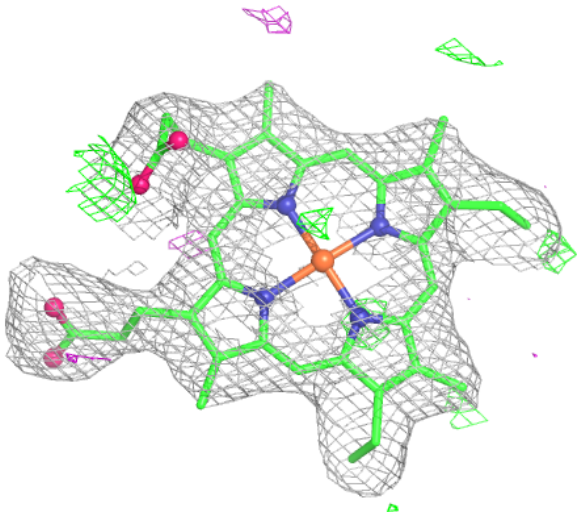


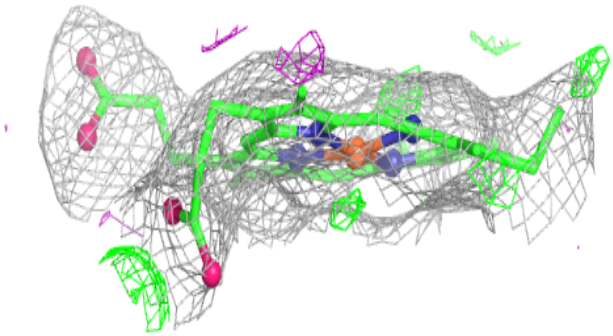


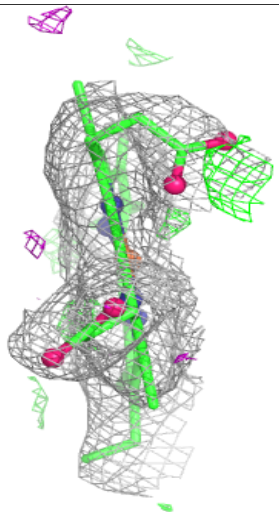


Electron density around HEC D 905:

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

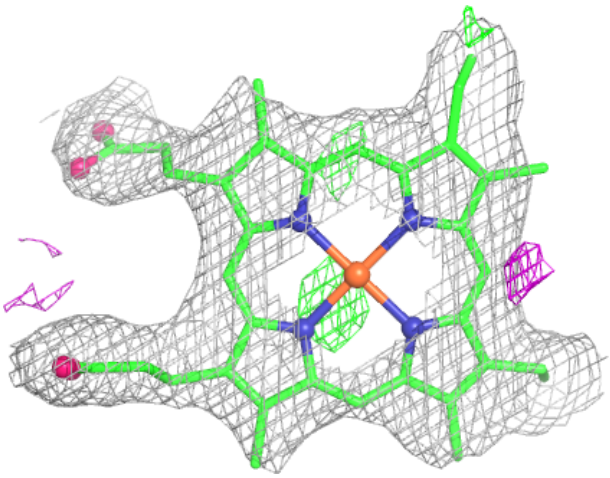


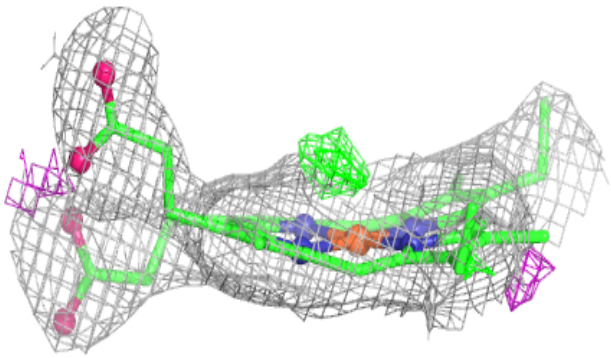


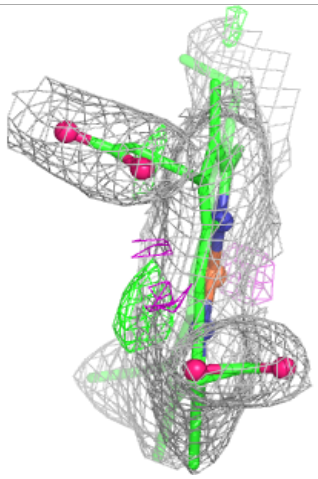


Electron density around HEC C 405:

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

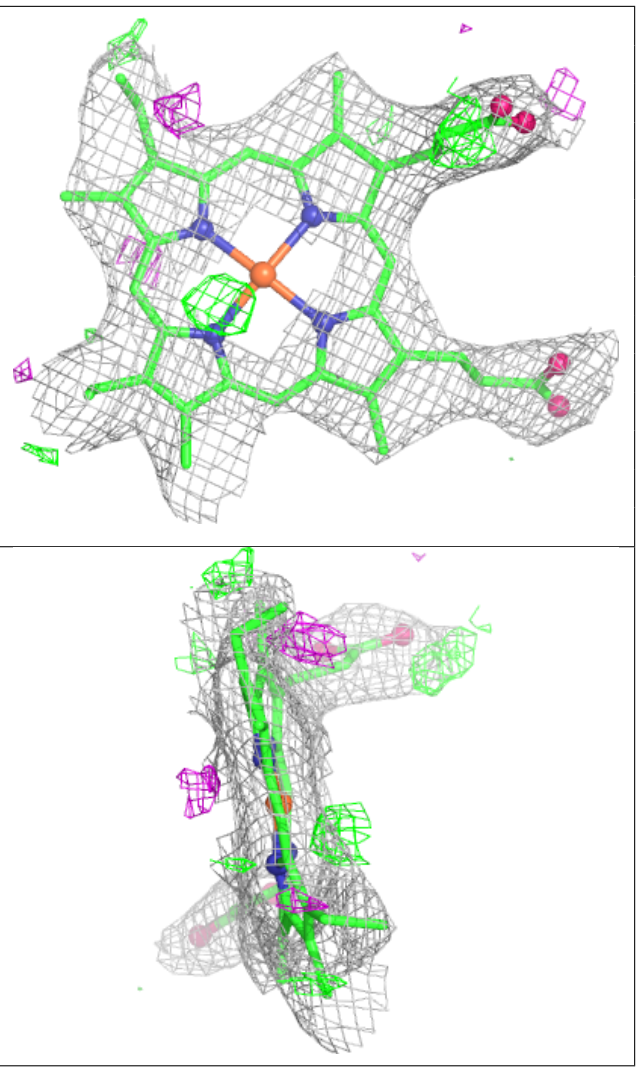






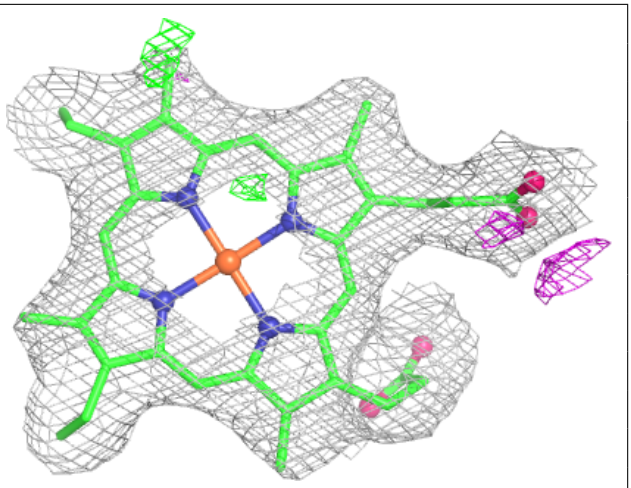
Electron density around HEC C 404:

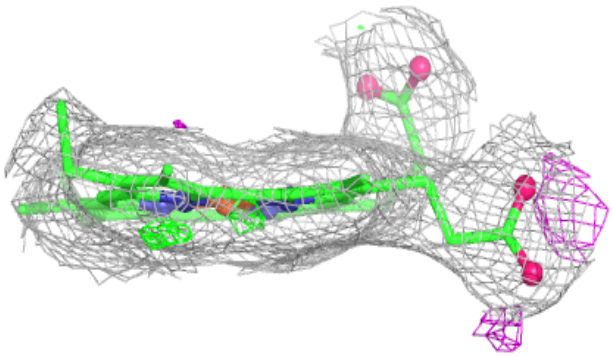
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC D 906:

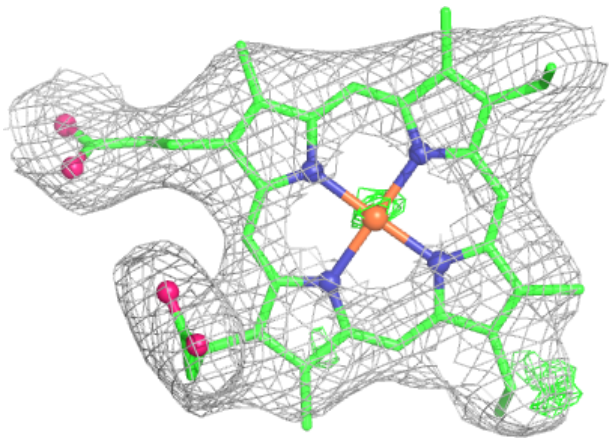
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

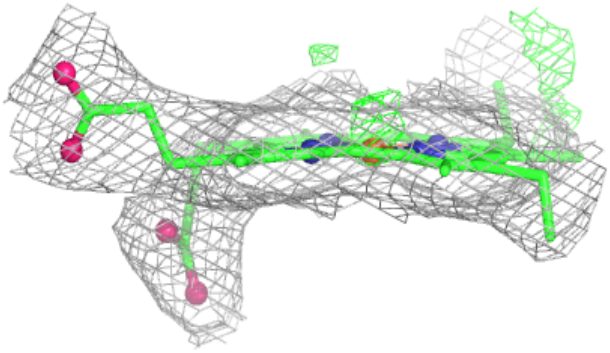


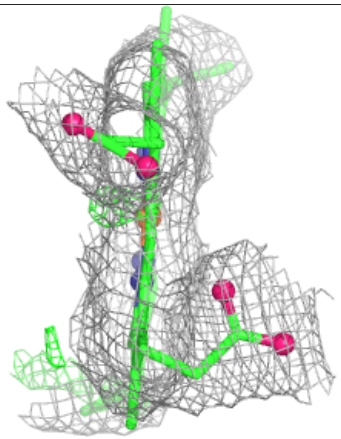


Electron density around HEC A 906:

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

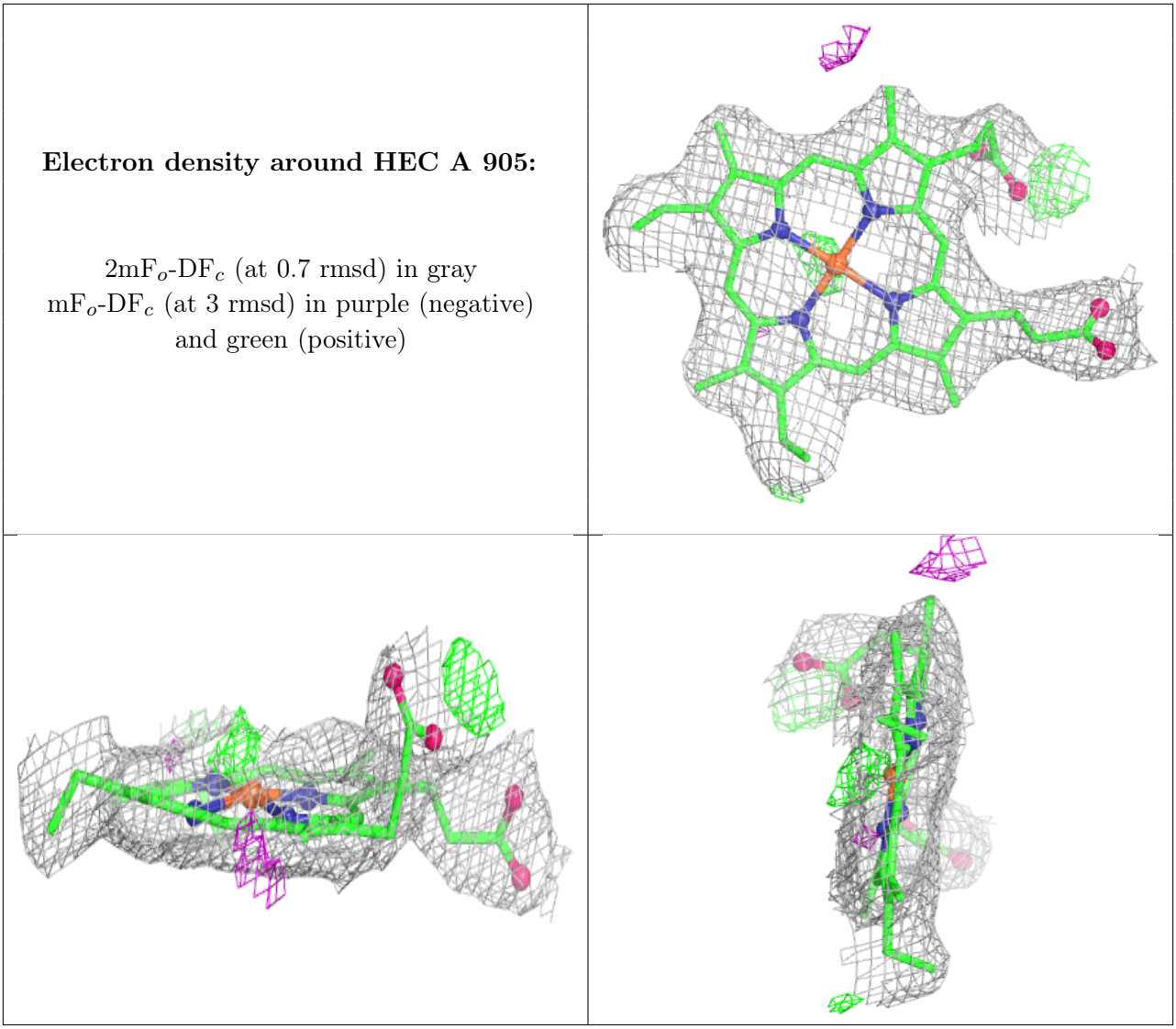






Electron density around HEC A 905:

$2mF_o$-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.