



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 09:57 pm GMT

PDB ID : 5C2W
Title : Kuenenia stuttgartiensis Hydrazine Synthase Pressurized with 20 bar Xenon
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 : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, 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

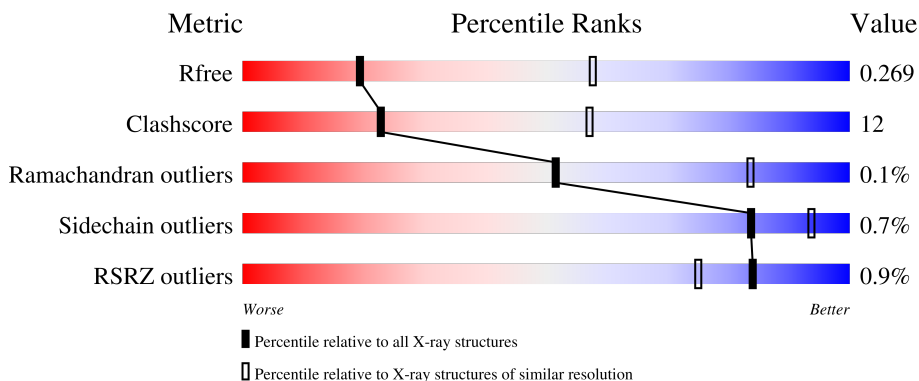
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



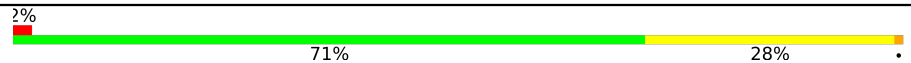
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	782	84% (green), 14% (yellow), 2% (grey), 0% (red)
1	D	782	81% (green), 17% (yellow), 2% (grey), 0% (red)
2	B	352	79% (green), 21% (yellow), 2% (grey), 0% (red)
2	E	352	61% (green), 34% (yellow), 2% (grey), 4% (red)
3	C	314	80% (green), 20% (yellow), 0% (grey), 0% (red)

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Mol	Chain	Length	Quality of chain
3	F	314	 A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a small red segment at the beginning labeled '2%', a large green segment in the middle labeled '71%', and a yellow segment at the end labeled '28%'. A small black dot is visible at the far right end of the bar.

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
5	CL	A	903[A]	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 23386 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 Hypothetical (Di heme) protein.

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 XENON (three-letter code: XE) (formula: Xe).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

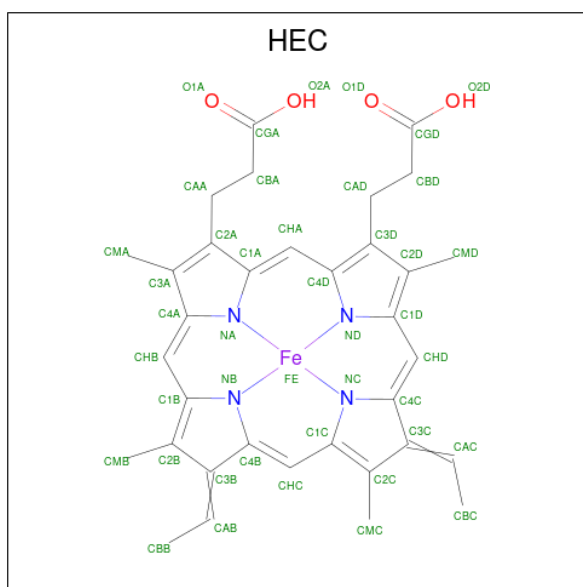
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

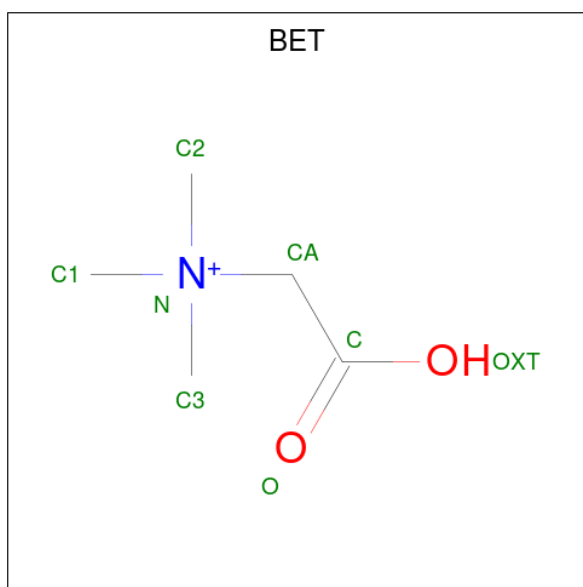
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Zn 1 1	0	0
7	D	1	Total Zn 1 1	0	0

- Molecule 8 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

- Molecule 9 is TRIMETHYL GLYCINE (three-letter code: BET) (formula: C₅H₁₂NO₂).



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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

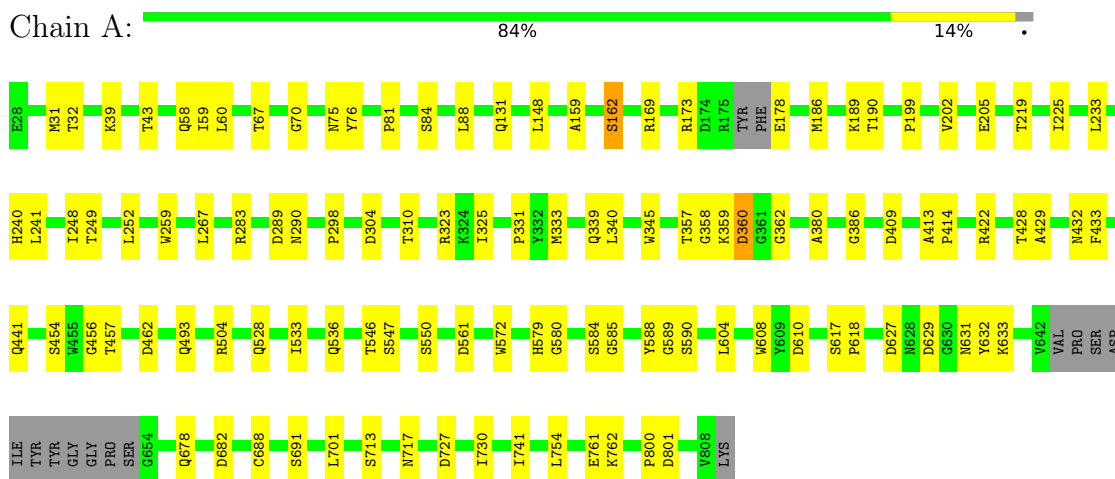
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	163	Total 163	O 163	0	0
11	B	59	Total 59	O 59	0	0
11	C	88	Total 88	O 88	0	0
11	D	112	Total 112	O 112	0	0
11	E	30	Total 30	O 30	0	0
11	F	45	Total 45	O 45	0	0

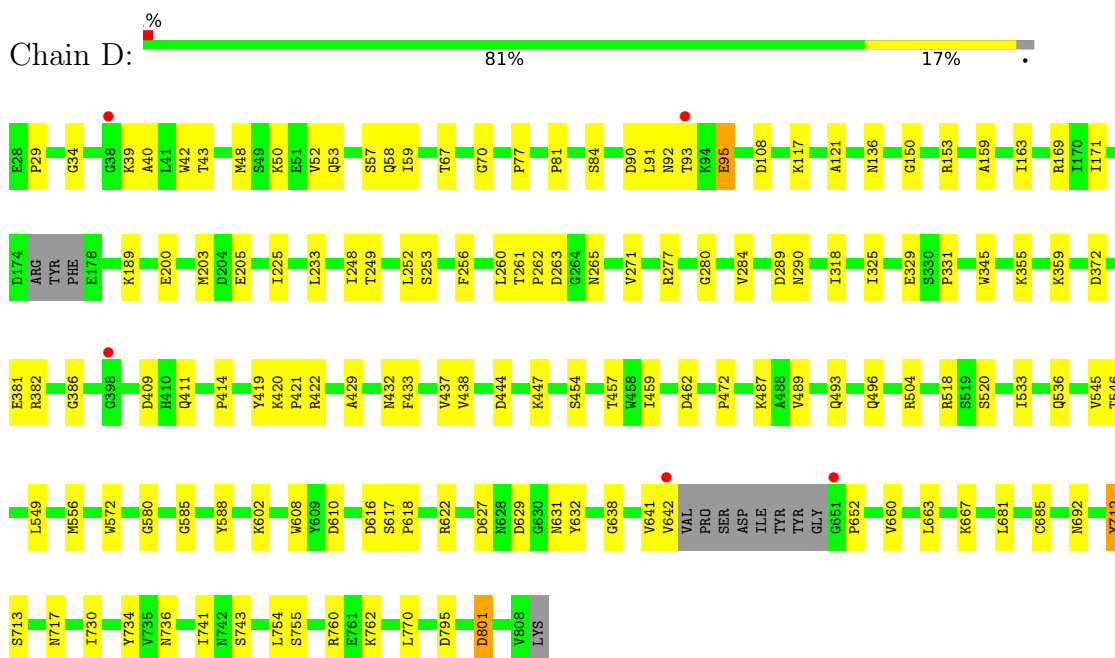
3 Residue-property plots [i](#)

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.

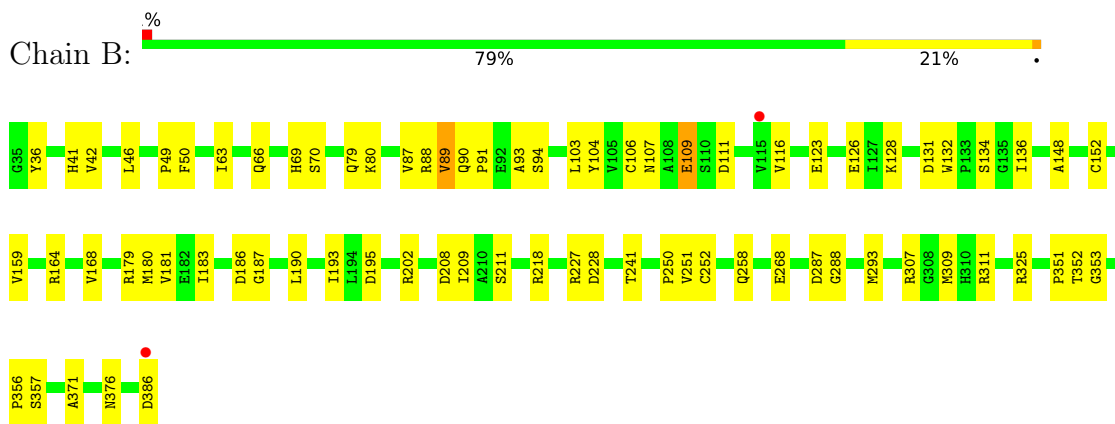
• Molecule 1: HYDRAZINE SYNTHASE ALPHA SUBUNIT



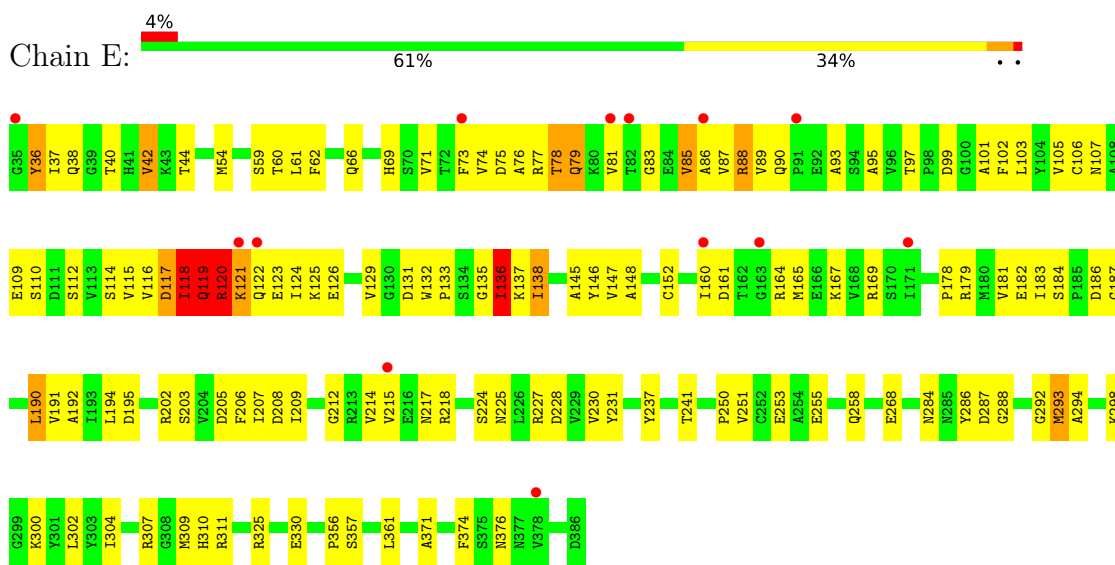
• Molecule 1: HYDRAZINE SYNTHASE ALPHA SUBUNIT



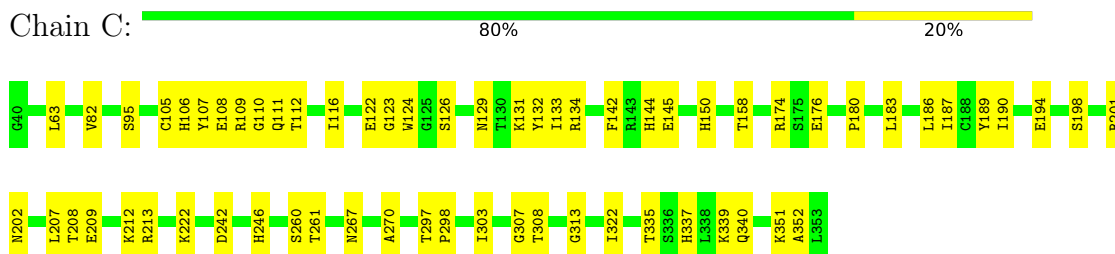
• Molecule 2: HYDRAZINE SYNTHASE BETA SUBUNIT



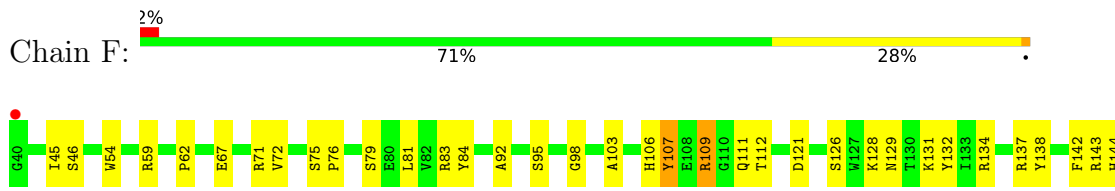
● Molecule 2: HYDRAZINE SYNTHASE BETA SUBUNIT

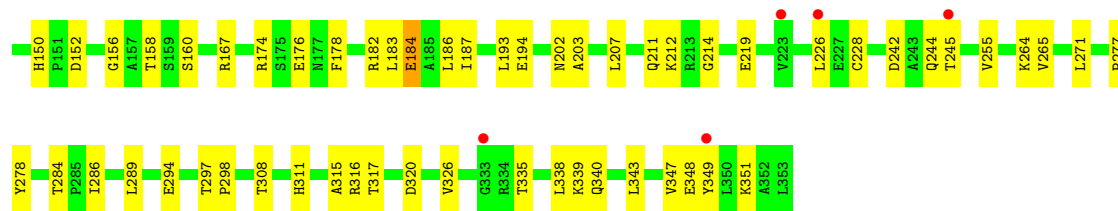


● Molecule 3: Hypothetical (Di heme) protein



● Molecule 3: Hypothetical (Di heme) protein





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	464.12Å 464.12Å 145.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.50 – 3.20 48.52 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.50-3.20) 100.0 (48.52-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.231 , 0.267 0.234 , 0.269	Depositor DCC
R_{free} test set	4865 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	67.8	Xtrriage
Anisotropy	0.505	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23386	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CL, BET, CA, XE, HEC, ZN, MG

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	0.22	0/6259	0.42	0/8503
1	D	0.23	0/6266	0.44	0/8514
2	B	0.24	0/2758	0.47	0/3752
2	E	0.47	1/2744 (0.0%)	0.86	18/3737 (0.5%)
3	C	0.23	0/2522	0.44	0/3421
3	F	0.25	0/2508	0.50	2/3406 (0.1%)
All	All	0.27	1/23057 (0.0%)	0.51	20/31333 (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
2	E	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	36	TYR	CD1-CE1	-5.77	1.30	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	79	GLN	N-CA-C	9.03	135.39	111.00
2	E	120	ARG	CA-CB-CG	8.95	133.08	113.40
2	E	120	ARG	N-CA-CB	-7.52	97.07	110.60
2	E	118	ILE	CG1-CB-CG2	-6.98	96.04	111.40
2	E	117	ASP	CB-CG-OD2	-6.88	112.11	118.30
2	E	120	ARG	N-CA-C	6.48	128.49	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	190	LEU	CA-CB-CG	6.46	130.15	115.30
2	E	136	ILE	N-CA-C	6.38	128.22	111.00
2	E	121	LYS	C-N-CA	6.24	137.30	121.70
2	E	85	VAL	CA-CB-CG2	-5.78	102.22	110.90
3	F	107	TYR	CA-CB-CG	5.77	124.37	113.40
2	E	79	GLN	CA-C-N	-5.77	104.50	117.20
2	E	117	ASP	CB-CG-OD1	5.68	123.41	118.30
2	E	136	ILE	CB-CA-C	-5.58	100.43	111.60
3	F	109	ARG	NE-CZ-NH1	5.42	123.01	120.30
2	E	79	GLN	CB-CA-C	-5.38	99.65	110.40
2	E	36	TYR	CB-CG-CD1	-5.32	117.81	121.00
2	E	136	ILE	CG1-CB-CG2	5.24	122.93	111.40
2	E	85	VAL	N-CA-C	5.23	125.12	111.00
2	E	119	GLN	N-CA-C	5.16	124.93	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	118	ILE	Peptide
2	E	119	GLN	Peptide
2	E	120	ARG	Peptide
2	E	42	VAL	Peptide
2	E	78	THR	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	5782	76	0
1	D	6087	0	5784	100	0
2	B	2706	0	2675	53	0
2	E	2692	0	2642	182	0
3	C	2457	0	2324	52	0
3	F	2443	0	2290	86	0
4	A	2	0	0	1	0
4	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	2	0	0	3	0
5	D	1	0	0	1	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	3	0	0	0	0
6	D	2	0	0	0	0
6	E	1	0	0	0	0
6	F	3	0	0	0	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0
8	A	86	0	60	4	0
8	C	86	0	59	8	0
8	D	86	0	60	7	0
8	F	86	0	59	8	0
9	A	24	0	33	0	0
9	B	8	0	11	0	0
9	C	8	0	11	0	0
9	D	8	0	11	0	0
9	E	8	0	11	0	0
10	B	1	0	0	0	0
10	E	1	0	0	0	0
11	A	163	0	0	2	0
11	B	59	0	0	2	0
11	C	88	0	0	6	0
11	D	112	0	0	4	0
11	E	30	0	0	1	0
11	F	45	0	0	5	0
All	All	23386	0	21812	514	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 12.

All (514) 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)
3:F:228:CYS:SG	8:F:405:HEC:CAC	2.02	1.47
3:C:105:CYS:SG	8:C:404:HEC:CAC	2.04	1.46
2:E:120:ARG:HD3	2:E:122:GLN:H	1.00	1.09
2:E:88:ARG:HD2	2:E:110:SER:HB2	1.34	1.09
3:C:107:TYR:HD2	3:C:108:GLU:H	1.14	0.92
2:E:120:ARG:HD3	2:E:122:GLN:N	1.84	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:182:GLU:HG2	2:E:230:VAL:HA	1.50	0.92
3:C:105:CYS:SG	8:C:404:HEC:C3C	2.57	0.92
2:E:88:ARG:NH2	2:E:109:GLU:OE1	2.04	0.91
2:E:118:ILE:HB	2:E:119:GLN:HG2	1.51	0.90
3:F:228:CYS:SG	8:F:405:HEC:C3C	2.59	0.90
2:E:36:TYR:HH	2:E:40:THR:HG1	1.03	0.90
1:A:359:LYS:HG3	1:A:360:ASP:H	1.37	0.89
2:E:88:ARG:HG2	2:E:89:VAL:H	1.37	0.88
2:E:120:ARG:NH2	2:E:122:GLN:OE1	2.09	0.84
2:E:136:ILE:HG21	2:E:147:VAL:HA	1.61	0.82
2:E:120:ARG:HG3	2:E:121:LYS:H	1.43	0.81
2:E:88:ARG:HG2	2:E:89:VAL:N	1.95	0.81
1:D:163:ILE:HG13	3:F:62:PRO:HD2	1.63	0.81
2:E:88:ARG:CZ	2:E:107:ASN:HB2	2.10	0.80
3:F:107:TYR:CE2	3:F:111:GLN:HB2	2.17	0.80
3:F:107:TYR:HE2	3:F:111:GLN:HB2	1.45	0.80
2:E:183:ILE:HG13	2:E:190:LEU:HD22	1.63	0.80
2:B:36:TYR:H	2:B:69:HIS:HE2	1.31	0.79
2:E:69:HIS:CE1	2:E:89:VAL:HG23	2.17	0.78
2:E:120:ARG:CD	2:E:122:GLN:H	1.90	0.78
2:B:90:GLN:HB3	2:B:109:GLU:HG2	1.66	0.77
2:E:145:ALA:HB3	2:E:160:ILE:HB	1.66	0.77
1:D:429:ALA:HB3	1:D:433:PHE:HB3	1.67	0.76
1:A:359:LYS:CG	1:A:360:ASP:H	1.99	0.75
2:E:135:GLY:O	2:E:136:ILE:HG23	1.86	0.75
1:D:92:ASN:CG	1:D:93:THR:H	1.90	0.75
2:E:88:ARG:NH2	2:E:89:VAL:O	2.20	0.75
2:E:288:GLY:H	2:E:309:MET:HG2	1.52	0.74
2:E:125:LYS:HD2	2:E:126:GLU:N	2.02	0.74
2:E:88:ARG:HH22	2:E:109:GLU:H	1.36	0.74
2:E:183:ILE:HD12	2:E:191:VAL:H	1.51	0.74
3:F:109:ARG:HG2	3:F:109:ARG:HH11	1.53	0.73
2:E:120:ARG:CG	2:E:121:LYS:H	1.97	0.73
3:C:307:GLY:O	11:C:501:HOH:O	2.06	0.73
1:D:608:TRP:NE1	1:D:610:ASP:O	2.21	0.73
2:E:88:ARG:HD2	2:E:110:SER:CB	2.17	0.72
2:E:125:LYS:HD2	2:E:126:GLU:H	1.55	0.72
2:E:38:GLN:HB2	2:E:90:GLN:NE2	2.06	0.71
2:E:36:TYR:OH	2:E:42:VAL:N	2.23	0.71
2:E:119:GLN:CG	2:E:120:ARG:HB3	2.21	0.71
2:B:288:GLY:H	2:B:309:MET:HG2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:77:ARG:N	2:E:79:GLN:HE22	1.89	0.70
2:E:101:ALA:HA	2:E:118:ILE:HD11	1.72	0.70
2:E:88:ARG:NH1	2:E:110:SER:H	1.88	0.70
2:E:62:PHE:HD1	2:E:73:PHE:CE1	2.10	0.70
1:D:150:GLY:HA2	1:D:200:GLU:HG3	1.74	0.70
3:F:71:ARG:HH21	3:F:184:GLU:HG3	1.57	0.70
3:C:122:GLU:OE2	11:C:502:HOH:O	2.09	0.69
2:E:66:GLN:HG3	2:E:90:GLN:HG2	1.74	0.69
1:A:422:ARG:NH1	3:C:95:SER:O	2.25	0.69
1:D:438:VAL:O	3:F:167:ARG:NH2	2.26	0.69
2:E:85:VAL:HB	2:E:121:LYS:HE2	1.74	0.69
1:D:642:VAL:HG12	1:D:652:PRO:HG3	1.74	0.69
1:D:58:GLN:HG2	1:D:90:ASP:OD1	1.93	0.68
2:E:74:VAL:HG12	2:E:79:GLN:HG2	1.74	0.68
2:E:119:GLN:HG3	2:E:120:ARG:HG2	1.74	0.68
2:E:78:THR:H	2:E:79:GLN:NE2	1.92	0.68
2:E:182:GLU:C	2:E:183:ILE:HD13	2.15	0.68
3:F:111:GLN:HB3	3:F:132:TYR:CE1	2.29	0.67
1:A:173:ARG:NH2	1:A:178:GLU:OE2	2.27	0.67
2:E:101:ALA:HA	2:E:118:ILE:CD1	2.24	0.67
2:E:190:LEU:HB3	2:E:207:ILE:HB	1.75	0.67
2:E:136:ILE:HG22	2:E:181:VAL:HG22	1.77	0.67
3:C:129:ASN:ND2	11:C:505:HOH:O	2.28	0.66
1:A:422:ARG:HB2	3:C:176:GLU:HB2	1.76	0.66
2:B:307:ARG:HE	2:B:357:SER:HB3	1.61	0.66
1:A:386:GLY:HA2	1:A:409:ASP:HB2	1.77	0.65
3:C:109:ARG:HG2	3:C:109:ARG:HH11	1.61	0.65
1:D:159:ALA:HB3	1:D:420:LYS:HD2	1.79	0.65
3:F:131:LYS:NZ	11:F:505:HOH:O	2.29	0.65
1:D:280:GLY:O	1:D:518:ARG:NH1	2.29	0.65
2:E:136:ILE:HG21	2:E:147:VAL:CA	2.25	0.65
1:A:429:ALA:HB3	1:A:433:PHE:HB3	1.78	0.64
3:F:137:ARG:NH2	3:F:194:GLU:OE2	2.31	0.64
2:E:40:THR:HG22	3:F:193:LEU:HA	1.77	0.64
2:E:118:ILE:HG22	2:E:119:GLN:H	1.63	0.64
1:D:108:ASP:OD1	1:D:411:GLN:NE2	2.31	0.63
2:B:250:PRO:O	2:B:258:GLN:NE2	2.31	0.63
2:E:87:VAL:HG11	2:E:105:VAL:HG21	1.79	0.63
1:A:589:GLY:N	5:A:903[B]:CL:CL	2.64	0.63
2:E:36:TYR:HE2	2:E:40:THR:O	1.82	0.63
2:B:195:ASP:OD1	2:B:202:ARG:NH1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:119:GLN:HG3	2:E:120:ARG:HB3	1.79	0.63
2:B:126:GLU:OE1	2:B:128:LYS:NZ	2.29	0.63
2:E:85:VAL:HG23	2:E:121:LYS:HG3	1.81	0.62
2:E:202:ARG:HD2	2:E:224:SER:HA	1.81	0.62
1:A:588:TYR:HB3	5:A:903[A]:CL:CL	2.38	0.61
1:D:386:GLY:HA2	1:D:409:ASP:HB2	1.82	0.61
2:E:97:THR:OG1	2:E:102:PHE:N	2.32	0.61
2:E:138:ILE:HB	2:E:145:ALA:HA	1.83	0.61
2:E:120:ARG:HE	2:E:122:GLN:HB3	1.66	0.60
1:D:225:ILE:HG13	1:D:233:LEU:HB2	1.83	0.60
1:D:622:ARG:HD2	1:D:638:GLY:HA3	1.82	0.60
1:A:713:SER:O	1:A:717:ASN:ND2	2.28	0.60
1:D:39:LYS:HD2	1:D:40:ALA:N	2.17	0.60
1:D:248:ILE:HG13	1:D:249:THR:HG23	1.83	0.60
1:D:496:GLN:NE2	11:D:1004:HOH:O	2.35	0.60
1:D:265:ASN:OD1	1:D:290:ASN:ND2	2.35	0.60
2:E:169:ARG:HH22	2:E:212:GLY:HA3	1.67	0.59
2:E:73:PHE:CE1	2:E:121:LYS:HE3	2.38	0.59
1:D:271:VAL:HG22	1:D:284:VAL:HG22	1.85	0.59
2:E:119:GLN:HG3	2:E:120:ARG:CG	2.32	0.59
2:E:136:ILE:HG22	2:E:181:VAL:CG2	2.32	0.59
3:C:107:TYR:OH	11:C:503:HOH:O	2.16	0.58
2:E:207:ILE:HD13	2:E:214:VAL:HG12	1.84	0.58
3:F:129:ASN:ND2	11:F:507:HOH:O	2.35	0.58
3:C:297:THR:HG22	8:C:405:HEC:HMD3	1.85	0.58
1:D:422:ARG:HB3	3:F:176:GLU:HB2	1.85	0.58
1:A:536:GLN:HG2	1:A:546:THR:HB	1.84	0.58
3:F:265:VAL:HB	3:F:271:LEU:HD12	1.86	0.58
2:E:112:SER:HA	2:E:129:VAL:HG22	1.86	0.58
3:F:132:TYR:CE2	3:F:134:ARG:HB2	2.38	0.58
1:D:29:PRO:HA	1:D:40:ALA:HB2	1.86	0.57
3:F:207:LEU:HB2	3:F:212:LYS:HG3	1.85	0.57
1:D:741:ILE:HG12	1:D:755:SER:HB3	1.86	0.57
3:F:75:SER:HB2	3:F:184:GLU:OE2	2.04	0.57
1:D:536:GLN:HG2	1:D:546:THR:HB	1.87	0.57
2:E:136:ILE:HB	2:E:146:TYR:O	2.05	0.57
2:E:59:SER:O	2:E:76:ALA:N	2.38	0.57
1:A:359:LYS:CG	1:A:360:ASP:N	2.67	0.57
3:C:63:LEU:HD21	3:C:180:PRO:HG3	1.86	0.57
3:C:222:LYS:HE2	3:C:337:HIS:CD2	2.39	0.57
1:A:75:ASN:ND2	11:A:1006:HOH:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:ARG:NH1	2:B:268:GLU:O	2.35	0.56
3:C:242:ASP:OD2	3:C:246:HIS:NE2	2.38	0.56
3:C:107:TYR:HD2	3:C:108:GLU:N	1.95	0.56
3:C:339:LYS:HG3	3:C:340:GLN:H	1.70	0.56
1:D:736:ASN:HD22	1:D:743:SER:HA	1.70	0.56
2:E:137:LYS:HD2	2:E:181:VAL:O	2.04	0.56
2:E:186:ASP:OD1	2:E:187:GLY:N	2.38	0.56
2:E:206:PHE:O	2:E:215:VAL:N	2.39	0.56
3:F:131:LYS:NZ	3:F:143:ARG:O	2.19	0.56
3:F:202:ASN:OD1	3:F:203:ALA:N	2.39	0.56
1:A:688:CYS:SG	8:A:908:HEC:C2C	2.79	0.56
1:D:203:MET:O	1:D:496:GLN:NE2	2.38	0.56
3:C:107:TYR:CD2	3:C:109:ARG:HG3	2.41	0.56
2:E:287:ASP:OD1	2:E:311:ARG:NH2	2.37	0.56
1:D:622:ARG:NH2	1:D:667:LYS:O	2.39	0.55
2:E:191:VAL:HA	2:E:205:ASP:O	2.05	0.55
2:B:88:ARG:NE	2:B:126:GLU:OE2	2.40	0.55
2:E:81:VAL:HG12	2:E:83:GLY:H	1.70	0.55
2:E:88:ARG:CD	2:E:110:SER:HB2	2.22	0.55
2:E:102:PHE:HA	2:E:117:ASP:HB3	1.88	0.55
2:E:89:VAL:HG22	2:E:109:GLU:OE2	2.06	0.55
1:A:190:THR:OG1	1:A:219:THR:OG1	2.22	0.55
1:D:169:ARG:HH21	1:D:171:ILE:HD11	1.72	0.55
2:B:90:GLN:HB3	2:B:109:GLU:CG	2.37	0.55
3:C:145:GLU:OE1	3:C:150:HIS:NE2	2.32	0.55
2:B:111:ASP:OD2	2:B:131:ASP:HA	2.06	0.55
2:B:183:ILE:HG12	2:B:190:LEU:HD23	1.88	0.55
1:D:90:ASP:HB3	1:D:95:GLU:OE2	2.06	0.55
2:E:228:ASP:HB2	2:E:292:GLY:HA2	1.88	0.55
2:E:250:PRO:O	2:E:258:GLN:NE2	2.40	0.55
1:A:67:THR:HB	1:A:70:GLY:H	1.70	0.54
1:D:422:ARG:NH1	3:F:95:SER:O	2.40	0.54
3:F:214:GLY:HA3	3:F:349:TYR:HB2	1.89	0.54
3:C:187:ILE:HA	3:C:190:ILE:HD12	1.90	0.54
2:E:36:TYR:HE1	2:E:42:VAL:O	1.90	0.54
3:C:116:ILE:HD11	3:C:308:THR:HG21	1.88	0.54
2:B:287:ASP:OD1	2:B:311:ARG:NH2	2.39	0.54
2:E:78:THR:H	2:E:79:GLN:HE22	1.54	0.54
1:D:42:TRP:HA	1:D:48:MET:SD	2.48	0.54
2:E:79:GLN:N	2:E:79:GLN:OE1	2.41	0.54
2:E:106:CYS:SG	2:E:133:PRO:HB2	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:208:ASP:O	2:E:212:GLY:N	2.41	0.54
3:C:132:TYR:CE2	3:C:134:ARG:HB2	2.42	0.54
1:D:325:ILE:HD11	1:D:345:TRP:HE3	1.73	0.54
1:A:31:MET:O	2:B:311:ARG:NH1	2.40	0.54
2:E:119:GLN:NE2	2:E:120:ARG:HG2	2.22	0.54
1:D:329:GLU:OE2	1:D:355:LYS:NZ	2.27	0.53
1:D:493:GLN:HB2	1:D:533:ILE:HG13	1.90	0.53
3:C:82:VAL:HG23	3:C:189:TYR:HA	1.90	0.53
2:E:105:VAL:HB	2:E:114:SER:HB2	1.91	0.53
2:E:101:ALA:O	2:E:117:ASP:HB2	2.08	0.53
1:A:762:LYS:NZ	2:E:330:GLU:OE2	2.38	0.53
2:B:179:ARG:NH1	3:C:107:TYR:OH	2.42	0.53
3:F:255:VAL:HA	3:F:264:LYS:HG3	1.91	0.53
1:A:283:ARG:NH2	1:A:304:ASP:OD1	2.42	0.53
2:B:46:LEU:HD13	2:B:376:ASN:HD21	1.74	0.53
3:F:128:LYS:NZ	8:F:404:HEC:O2D	2.42	0.53
1:A:631:ASN:ND2	11:A:1009:HOH:O	2.41	0.53
2:E:90:GLN:HB2	2:E:109:GLU:OE1	2.09	0.53
1:A:604:LEU:HD13	2:B:250:PRO:HG3	1.89	0.52
3:C:107:TYR:CE2	3:C:109:ARG:HG3	2.44	0.52
1:A:590:SER:OG	5:A:903[A]:CL:CL	2.55	0.52
2:E:120:ARG:CG	2:E:121:LYS:N	2.69	0.52
1:A:691:SER:OG	2:E:325:ARG:NH1	2.42	0.52
1:A:741:ILE:HG13	1:A:754:LEU:HB3	1.91	0.52
2:E:88:ARG:CZ	2:E:110:SER:H	2.22	0.52
1:D:345:TRP:O	2:E:284:ASN:ND2	2.42	0.52
2:E:131:ASP:OD1	2:E:132:TRP:N	2.43	0.52
3:F:109:ARG:HH11	3:F:109:ARG:CG	2.23	0.52
1:D:52:VAL:HG11	1:D:419:TYR:HB2	1.92	0.52
2:B:208:ASP:HB3	2:B:211:SER:HB3	1.92	0.52
3:C:322:ILE:HG23	3:C:335:THR:HG21	1.91	0.52
2:E:62:PHE:CD1	2:E:73:PHE:CE1	2.97	0.52
2:E:195:ASP:OD2	2:E:227:ARG:NH2	2.43	0.52
2:B:152:CYS:SG	11:C:574:HOH:O	2.59	0.52
2:B:79:GLN:C	2:B:80:LYS:HD3	2.31	0.51
2:E:118:ILE:CB	2:E:119:GLN:HG2	2.34	0.51
1:D:520:SER:O	1:D:712:TYR:OH	2.25	0.51
2:E:38:GLN:NE2	3:F:109:ARG:HA	2.26	0.51
2:E:75:ASP:CG	2:E:79:GLN:HE21	2.13	0.51
2:E:93:ALA:CB	2:E:135:GLY:HA2	2.41	0.51
2:E:38:GLN:HE21	3:F:109:ARG:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:201:ARG:HD3	3:C:352:ALA:HB1	1.92	0.51
1:D:205:GLU:OE1	1:D:253:SER:OG	2.23	0.51
2:E:184:SER:HB3	2:E:231:TYR:HE2	1.76	0.51
2:B:148:ALA:HB2	2:B:181:VAL:HG13	1.93	0.51
2:E:181:VAL:HG12	2:E:192:ALA:HB2	1.93	0.51
1:D:762:LYS:O	1:D:762:LYS:HG3	2.11	0.50
3:F:311:HIS:ND1	8:F:405:HEC:O2D	2.38	0.50
1:A:678:GLN:NE2	1:A:682:ASP:OD1	2.44	0.50
2:B:90:GLN:CB	2:B:109:GLU:HG2	2.40	0.50
2:E:60:THR:HA	2:E:75:ASP:HA	1.93	0.50
2:E:69:HIS:CD2	2:E:90:GLN:H	2.29	0.50
2:E:88:ARG:HH22	2:E:109:GLU:N	2.05	0.50
3:C:198:SER:OG	3:C:351:LYS:O	2.24	0.50
2:B:227:ARG:NH2	11:B:509:HOH:O	2.44	0.50
2:E:78:THR:N	2:E:79:GLN:NE2	2.58	0.50
3:F:81:LEU:HA	3:F:84:TYR:HD2	1.76	0.50
2:E:152:CYS:SG	3:F:107:TYR:OH	2.70	0.50
1:A:248:ILE:HG13	1:A:249:THR:HG23	1.93	0.50
1:A:462:ASP:O	1:A:585:GLY:HA2	2.12	0.50
1:A:608:TRP:NE1	1:A:610:ASP:O	2.42	0.50
1:D:770:LEU:HD21	8:D:908:HEC:HBC2	1.94	0.50
2:E:120:ARG:HH12	2:E:124:ILE:HD12	1.76	0.50
2:E:169:ARG:NH2	2:E:212:GLY:HA3	2.26	0.50
1:D:260:LEU:HD13	1:D:421:PRO:HG2	1.93	0.50
1:D:277:ARG:HG3	8:D:907:HEC:O1D	2.12	0.50
1:D:444:ASP:OD1	1:D:447:LYS:N	2.44	0.49
1:D:457:THR:O	1:D:580:GLY:HA2	2.12	0.49
2:E:71:VAL:O	2:E:121:LYS:NZ	2.32	0.49
1:A:432:ASN:ND2	1:A:454:SER:OG	2.39	0.49
2:B:42:VAL:HG11	3:C:82:VAL:HG11	1.94	0.49
3:C:202:ASN:ND2	3:C:207:LEU:O	2.43	0.49
3:F:150:HIS:CD2	3:F:156:GLY:H	2.30	0.49
2:B:104:TYR:HB3	2:B:136:ILE:HD13	1.95	0.49
3:F:317:THR:OG1	3:F:320:ASP:OD2	2.26	0.49
3:F:335:THR:HA	3:F:338:LEU:HD13	1.95	0.49
1:A:547:SER:OG	1:A:617:SER:OG	2.26	0.49
3:C:186:LEU:HD21	8:C:404:HEC:HMB1	1.95	0.49
1:A:340:LEU:HB2	1:A:357:THR:HG22	1.95	0.49
1:D:34:GLY:HA3	1:D:39:LYS:O	2.12	0.49
1:D:57:SER:O	1:D:91:LEU:HG	2.13	0.49
2:E:115:VAL:HG11	2:E:165:MET:SD	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:241:THR:HG23	2:E:293:MET:SD	2.53	0.49
1:D:419:TYR:OH	3:F:59:ARG:NH1	2.46	0.49
1:D:734:TYR:HE1	8:D:908:HEC:HBA2	1.78	0.49
3:F:219:GLU:HG2	3:F:226:LEU:HD21	1.94	0.49
2:E:38:GLN:HB2	2:E:90:GLN:HE22	1.78	0.49
2:E:218:ARG:NH1	2:E:268:GLU:O	2.38	0.49
3:F:107:TYR:CB	3:F:109:ARG:H	2.26	0.49
1:D:77:PRO:HB3	1:D:256:PHE:CG	2.47	0.48
1:D:90:ASP:OD2	1:D:92:ASN:ND2	2.46	0.48
2:E:191:VAL:HG13	2:E:231:TYR:OH	2.14	0.48
3:F:71:ARG:NH2	3:F:184:GLU:HG3	2.27	0.48
3:F:245:THR:HG22	3:F:294:GLU:HB3	1.96	0.48
2:B:41:HIS:CD2	3:C:194:GLU:HG3	2.49	0.48
2:B:94:SER:HB2	2:B:103:LEU:HD11	1.94	0.48
3:F:59:ARG:NH2	3:F:176:GLU:OE2	2.38	0.48
2:E:286:TYR:O	2:E:311:ARG:NH2	2.47	0.48
2:E:119:GLN:CB	2:E:120:ARG:HB3	2.43	0.48
1:D:169:ARG:HE	1:D:171:ILE:HD11	1.78	0.48
1:D:432:ASN:HA	1:D:454:SER:HB3	1.95	0.48
2:E:119:GLN:CG	2:E:120:ARG:HG2	2.43	0.48
2:E:294:ALA:HB1	2:E:361:LEU:HG	1.95	0.48
2:B:352:THR:HG22	2:B:353:GLY:H	1.79	0.48
2:E:202:ARG:NH1	2:E:225:ASN:H	2.12	0.48
1:A:225:ILE:HG13	1:A:233:LEU:HB2	1.95	0.48
3:C:142:PHE:HB2	3:C:158:THR:HB	1.95	0.48
2:E:36:TYR:CD1	2:E:37:ILE:N	2.82	0.47
2:E:74:VAL:HG12	2:E:79:GLN:CG	2.44	0.47
2:E:376:ASN:HD21	3:F:83:ARG:NH2	2.12	0.47
1:A:58:GLN:HB3	1:A:88:LEU:HD11	1.95	0.47
1:A:504:ARG:HD3	1:A:800:PRO:HB3	1.96	0.47
2:B:228:ASP:HB3	2:B:293:MET:HE2	1.96	0.47
8:D:908:HEC:HBD2	8:D:908:HEC:HHA	1.96	0.47
2:E:88:ARG:NH1	2:E:110:SER:N	2.60	0.47
3:F:106:HIS:CD2	8:F:404:HEC:NB	2.82	0.47
3:F:137:ARG:NH2	3:F:138:TYR:OH	2.48	0.47
1:A:357:THR:HA	1:A:358:GLY:HA3	1.44	0.47
1:D:67:THR:HB	1:D:70:GLY:H	1.80	0.47
2:E:187:GLY:O	2:E:209:ILE:HD12	2.13	0.47
3:F:111:GLN:O	3:F:132:TYR:HA	2.14	0.47
8:A:908:HEC:HBC3	8:A:908:HEC:HHD	1.94	0.47
3:C:209:GLU:O	3:C:213:ARG:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:ASN:CG	1:D:93:THR:N	2.63	0.47
2:E:85:VAL:HB	2:E:121:LYS:CE	2.43	0.47
2:E:109:GLU:HA	11:E:511:HOH:O	2.14	0.47
2:E:117:ASP:OD1	2:E:118:ILE:HG12	2.13	0.47
1:A:240:HIS:CD2	1:A:241:LEU:HG	2.49	0.47
3:C:260:SER:OG	3:C:261:THR:N	2.47	0.47
2:E:119:GLN:HG3	2:E:120:ARG:CB	2.43	0.47
3:C:131:LYS:HB3	8:C:404:HEC:HBA1	1.97	0.47
2:E:182:GLU:O	2:E:183:ILE:HD13	2.15	0.47
1:A:688:CYS:SG	8:A:908:HEC:C4C	2.89	0.47
2:E:183:ILE:CG1	2:E:190:LEU:HD22	2.41	0.47
1:A:289:ASP:OD1	1:A:290:ASN:N	2.48	0.46
3:C:106:HIS:HA	3:C:112:THR:HA	1.97	0.46
1:D:81:PRO:HB2	1:D:84:SER:OG	2.15	0.46
2:E:88:ARG:NH2	2:E:109:GLU:H	2.07	0.46
1:A:259:TRP:N	1:A:267:LEU:O	2.48	0.46
1:A:339:GLN:HB3	1:A:357:THR:O	2.15	0.46
3:C:110:GLY:HA2	3:C:133:ILE:HD11	1.98	0.46
2:E:307:ARG:NE	2:E:357:SER:OG	2.41	0.46
3:F:316:ARG:H	3:F:316:ARG:HG2	1.50	0.46
1:A:60:LEU:O	1:A:413:ALA:N	2.43	0.46
3:C:208:THR:O	3:C:212:LYS:HG3	2.16	0.46
1:D:289:ASP:OD1	1:D:290:ASN:N	2.48	0.46
1:D:504:ARG:NH2	1:D:801:ASP:O	2.48	0.46
2:E:116:VAL:HA	2:E:120:ARG:NH1	2.31	0.46
2:B:50:PHE:HB2	2:B:66:GLN:HB2	1.98	0.46
1:D:462:ASP:O	1:D:585:GLY:HA2	2.16	0.46
2:E:117:ASP:C	2:E:119:GLN:HE21	2.19	0.46
3:F:142:PHE:HB2	3:F:158:THR:HB	1.98	0.46
1:A:504:ARG:NH1	1:A:801:ASP:O	2.45	0.46
2:E:109:GLU:OE1	2:E:109:GLU:N	2.40	0.46
1:A:169:ARG:HA	1:A:186:MET:HG2	1.98	0.46
1:D:795:ASP:OD2	11:D:1001:HOH:O	2.21	0.46
2:B:307:ARG:HA	2:B:356:PRO:HD2	1.97	0.45
1:D:472:PRO:HB2	1:D:730:ILE:HD13	1.98	0.45
1:D:760:ARG:NE	1:D:762:LYS:O	2.47	0.45
2:E:40:THR:HG22	3:F:193:LEU:CA	2.46	0.45
1:A:131:GLN:HE22	1:A:148:LEU:H	1.64	0.45
2:B:159:VAL:HG23	2:B:168:VAL:HB	1.98	0.45
1:D:741:ILE:HG13	1:D:754:LEU:HB3	1.99	0.45
2:E:54:MET:HG3	2:E:61:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:251:VAL:HG12	11:F:504:HOH:O	2.16	0.45
1:A:81:PRO:HB2	1:A:84:SER:OG	2.16	0.45
1:D:588:TYR:HB3	5:D:903:CL:CL	2.53	0.45
3:F:186:LEU:HD21	8:F:404:HEC:HMB1	1.99	0.45
1:A:627:ASP:HB3	1:A:633:LYS:HD3	1.99	0.45
2:B:70:SER:HA	2:B:87:VAL:HG22	1.99	0.45
2:B:325:ARG:HD3	1:D:692:ASN:HA	1.99	0.45
2:E:37:ILE:HD11	2:E:44:THR:HG23	1.99	0.45
3:F:207:LEU:HB3	3:F:211:GLN:HB2	1.97	0.45
1:A:362:GLY:HA3	1:A:380:ALA:O	2.17	0.45
3:F:134:ARG:NH1	3:F:194:GLU:O	2.37	0.45
1:A:162:SER:OG	1:A:189:LYS:HB3	2.16	0.45
1:A:608:TRP:CE3	3:C:123:GLY:HA2	2.52	0.45
2:B:93:ALA:HB3	2:B:106:CYS:HB2	1.99	0.45
3:F:228:CYS:HA	3:F:242:ASP:HB2	1.99	0.45
1:A:493:GLN:HB2	1:A:533:ILE:HG13	1.98	0.45
3:C:303:ILE:HG12	8:C:405:HEC:HMA3	1.99	0.45
1:D:549:LEU:HD21	1:D:663:LEU:HA	1.99	0.45
2:E:121:LYS:HD2	2:E:121:LYS:HA	1.71	0.45
1:A:43:THR:O	1:A:422:ARG:NH2	2.50	0.45
2:E:69:HIS:CG	2:E:89:VAL:HA	2.51	0.45
2:E:203:SER:HB3	2:E:217:ASN:OD1	2.16	0.44
3:C:123:GLY:O	3:C:126:SER:OG	2.27	0.44
1:D:627:ASP:OD2	1:D:631:ASN:HB2	2.18	0.44
2:E:75:ASP:C	2:E:79:GLN:NE2	2.71	0.44
3:F:315:ALA:HB2	3:F:326:VAL:HG21	1.99	0.44
1:A:173:ARG:HB3	1:A:441:GLN:NE2	2.33	0.44
2:E:190:LEU:HD12	2:E:207:ILE:HG13	1.98	0.44
3:F:126:SER:HB3	3:F:289:LEU:O	2.18	0.44
1:D:43:THR:O	1:D:422:ARG:NH2	2.43	0.44
1:D:760:ARG:NH2	8:D:908:HEC:O2A	2.47	0.44
2:E:117:ASP:CG	2:E:119:GLN:NE2	2.71	0.44
3:F:297:THR:HA	3:F:298:PRO:HD3	1.79	0.44
3:C:106:HIS:CD2	8:C:404:HEC:NB	2.86	0.44
3:C:111:GLN:HB3	3:C:132:TYR:CE1	2.52	0.44
1:D:153:ARG:NH1	11:D:1020:HOH:O	2.50	0.44
1:D:169:ARG:HG3	3:F:67:GLU:OE2	2.17	0.44
1:D:382:ARG:HA	1:D:382:ARG:HD3	1.55	0.44
2:E:81:VAL:HG12	2:E:83:GLY:N	2.32	0.44
3:F:45:ILE:HG23	3:F:46:SER:H	1.83	0.44
2:E:93:ALA:HB3	2:E:135:GLY:HA2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:93:ALA:HB3	2:E:106:CYS:HB3	2.00	0.44
3:F:112:THR:HB	3:F:131:LYS:O	2.18	0.44
2:B:241:THR:HG23	2:B:293:MET:SD	2.57	0.44
3:F:178:PHE:HA	3:F:182:ARG:HH12	1.82	0.44
2:E:85:VAL:HG21	2:E:122:GLN:N	2.33	0.43
2:E:160:ILE:HG12	2:E:167:LYS:HA	1.99	0.43
1:A:331:PRO:HB2	1:D:331:PRO:HB3	1.99	0.43
1:A:428:THR:HB	1:A:579:HIS:HE1	1.81	0.43
1:A:629:ASP:OD1	1:A:629:ASP:N	2.51	0.43
2:B:116:VAL:HA	2:B:123:GLU:HA	2.00	0.43
1:A:310:THR:O	1:A:333:MET:HG3	2.19	0.43
1:D:556:MET:SD	8:D:907:HEC:HMC3	2.58	0.43
3:F:143:ARG:HB3	3:F:144:HIS:H	1.54	0.43
2:B:164:ARG:NH2	11:B:512:HOH:O	2.51	0.43
1:D:53:GLN:NE2	1:D:372:ASP:OD1	2.51	0.43
1:D:489:VAL:HG22	1:D:536:GLN:O	2.18	0.43
2:E:36:TYR:CE2	2:E:40:THR:O	2.68	0.43
1:A:159:ALA:HB1	1:A:162:SER:O	2.19	0.43
1:D:117:LYS:HA	1:D:136:ASN:HA	2.01	0.43
1:D:432:ASN:ND2	11:D:1015:HOH:O	2.47	0.43
2:E:102:PHE:CD1	2:E:117:ASP:HB3	2.54	0.43
2:E:133:PRO:HA	2:E:148:ALA:O	2.19	0.43
2:E:183:ILE:HG22	2:E:184:SER:N	2.34	0.43
2:E:253[B]:GLU:HA	3:F:174:ARG:HG3	2.01	0.43
1:A:561:ASP:O	1:A:632:TYR:N	2.42	0.43
2:B:187:GLY:O	2:B:209:ILE:HD12	2.19	0.43
1:D:713:SER:O	1:D:717:ASN:ND2	2.38	0.43
2:E:374:PHE:HB3	3:F:54:TRP:CZ3	2.54	0.43
3:F:107:TYR:HB3	3:F:109:ARG:H	1.83	0.43
3:F:244:GLN:OE1	3:F:244:GLN:N	2.52	0.43
1:A:633:LYS:HD2	1:A:633:LYS:HA	1.88	0.43
2:E:42:VAL:HG13	3:F:79:SER:HB2	2.00	0.43
2:E:293:MET:HE2	2:E:302:LEU:HD11	1.99	0.43
3:F:143:ARG:NH2	8:F:404:HEC:O2D	2.51	0.43
1:A:428:THR:HB	1:A:579:HIS:CE1	2.53	0.43
1:D:252:LEU:HD12	1:D:572:TRP:CZ2	2.54	0.43
2:E:69:HIS:ND1	2:E:89:VAL:HA	2.34	0.43
3:F:75:SER:HB3	3:F:76:PRO:HD2	2.00	0.43
1:D:163:ILE:HD13	1:D:420:LYS:HE2	2.00	0.43
2:E:137:LYS:HD3	2:E:182:GLU:OE1	2.19	0.43
3:F:284:THR:HG21	3:F:308:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:HIS:CE1	2:B:89:VAL:HG12	2.54	0.42
2:B:356:PRO:HA	2:B:371:ALA:O	2.19	0.42
1:D:617:SER:HA	1:D:618:PRO:HD3	1.87	0.42
2:B:132:TRP:CH2	3:C:109:ARG:HD3	2.54	0.42
3:C:183:LEU:O	3:C:187:ILE:HG12	2.19	0.42
3:F:72:VAL:O	3:F:160:SER:HB2	2.20	0.42
1:A:727:ASP:HB3	1:A:730:ILE:HG13	2.02	0.42
1:D:359:LYS:HA	1:D:359:LYS:HD2	1.72	0.42
1:A:59:ILE:HG22	1:A:414:PRO:HA	2.02	0.42
2:B:180:MET:HB3	2:B:193:ILE:HD11	2.02	0.42
1:D:189:LYS:HE3	1:D:189:LYS:HB2	1.87	0.42
2:E:298:LYS:HD3	2:E:300:LYS:HE2	2.02	0.42
2:B:252:CYS:O	3:C:174:ARG:NE	2.52	0.42
1:D:629:ASP:OD1	1:D:629:ASP:N	2.52	0.42
2:E:184:SER:HB3	2:E:231:TYR:CE2	2.55	0.42
3:C:107:TYR:CD2	3:C:108:GLU:N	2.75	0.42
1:D:437:VAL:HG13	3:F:121:ASP:HA	2.02	0.42
1:D:459:ILE:HB	1:D:545:VAL:HG23	2.00	0.42
2:E:42:VAL:CG1	3:F:79:SER:HB2	2.50	0.42
2:E:120:ARG:HH22	2:E:124:ILE:HD12	1.85	0.42
2:E:179:ARG:O	2:E:179:ARG:HG3	2.19	0.42
3:F:339:LYS:O	3:F:343:LEU:HG	2.19	0.42
1:A:325:ILE:HD11	1:A:345:TRP:HE3	1.85	0.42
2:B:250:PRO:HB3	3:C:124:TRP:CZ3	2.55	0.42
2:B:251:VAL:HG12	11:C:511:HOH:O	2.19	0.42
3:C:297:THR:HA	3:C:298:PRO:HD3	1.81	0.42
1:D:641:VAL:HA	1:D:660:VAL:O	2.19	0.42
2:E:40:THR:CG2	3:F:193:LEU:HD23	2.50	0.42
2:E:85:VAL:HB	2:E:121:LYS:CD	2.50	0.42
2:E:85:VAL:HG13	2:E:86:ALA:N	2.35	0.42
2:E:118:ILE:HD12	2:E:118:ILE:HG23	1.58	0.42
2:E:161:ASP:HB3	2:E:164:ARG:HB3	2.02	0.42
2:E:146:TYR:OH	2:E:209:ILE:HG23	2.20	0.42
3:F:103:ALA:HA	3:F:107:TYR:O	2.19	0.42
3:F:183:LEU:O	3:F:187:ILE:HG12	2.20	0.42
1:A:298:PRO:HD3	8:A:907:HEC:HMA2	2.02	0.41
1:A:617:SER:HA	1:A:618:PRO:HD3	1.90	0.41
1:D:261:THR:OG1	1:D:263:ASP:OD1	2.31	0.41
2:E:95:ALA:O	2:E:103:LEU:HA	2.20	0.41
3:F:128:LYS:HG3	8:F:404:HEC:O2D	2.20	0.41
1:D:381:GLU:O	1:D:382:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:97:THR:HG23	2:E:102:PHE:O	2.20	0.41
2:E:293:MET:HE3	2:E:304:ILE:HG12	2.02	0.41
1:A:31:MET:SD	1:A:323:ARG:NH2	2.93	0.41
3:C:267:ASN:HB3	3:C:270:ALA:HB3	2.02	0.41
3:C:308:THR:HG22	3:C:313:GLY:CA	2.50	0.41
1:D:602:LYS:HG2	3:F:278:TYR:CZ	2.55	0.41
2:E:88:ARG:NH1	2:E:107:ASN:HB2	2.34	0.41
1:A:131:GLN:NE2	1:A:148:LEU:H	2.18	0.41
1:A:584:SER:HB2	1:A:590:SER:HB3	2.02	0.41
2:B:91:PRO:HA	2:B:106:CYS:O	2.20	0.41
3:C:144:HIS:ND1	8:C:404:HEC:O2D	2.39	0.41
1:D:121:ALA:HB2	1:D:153:ARG:HA	2.02	0.41
2:E:178:PRO:HB3	2:E:194:LEU:HD23	2.02	0.41
2:E:237:TYR:CE1	2:E:268:GLU:HG2	2.55	0.41
2:E:253[B]:GLU:HB3	2:E:255:GLU:OE1	2.19	0.41
3:F:134:ARG:HD2	3:F:194:GLU:O	2.20	0.41
1:A:32:THR:OG1	2:B:309:MET:O	2.22	0.41
4:A:902:XE:XE	2:B:351:PRO:HG3	2.98	0.41
1:D:159:ALA:O	1:D:420:LYS:NZ	2.37	0.41
1:A:199:PRO:HG2	1:A:202:VAL:HG21	2.02	0.41
2:E:310:HIS:HA	2:E:356:PRO:HD2	2.02	0.41
3:F:348:GLU:O	3:F:351:LYS:HB2	2.21	0.41
2:B:88:ARG:HB2	2:B:107:ASN:CG	2.41	0.41
2:B:386:ASP:N	2:B:386:ASP:OD1	2.54	0.41
1:D:163:ILE:HG13	3:F:62:PRO:CD	2.41	0.41
2:E:119:GLN:CD	2:E:120:ARG:HG2	2.42	0.41
2:E:136:ILE:HG23	2:E:148:ALA:H	1.85	0.41
2:B:49:PRO:HB3	2:B:63:ILE:CG2	2.51	0.41
1:D:487:LYS:HB3	1:D:632:TYR:CD1	2.55	0.41
3:F:320:ASP:O	11:F:501:HOH:O	2.21	0.41
3:F:347:VAL:HG13	3:F:351:LYS:NZ	2.35	0.41
1:A:252:LEU:HD12	1:A:572:TRP:CZ2	2.56	0.40
1:A:456:GLY:N	1:A:550:SER:OG	2.54	0.40
1:D:59:ILE:HA	1:D:414:PRO:HA	2.03	0.40
1:D:608:TRP:HD1	1:D:616:ASP:OD2	2.05	0.40
3:F:150:HIS:HD2	3:F:156:GLY:H	1.69	0.40
3:F:228:CYS:O	3:F:242:ASP:HB2	2.20	0.40
1:D:277:ARG:NH1	8:D:907:HEC:O2D	2.53	0.40
1:D:681:LEU:O	1:D:685:CYS:HB2	2.21	0.40
2:E:136:ILE:CG2	2:E:146:TYR:O	2.69	0.40
3:F:92:ALA:O	3:F:98:GLY:HA2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:112:THR:HG21	11:F:519:HOH:O	2.22	0.40
1:A:205:GLU:HA	1:A:528:GLN:NE2	2.36	0.40
1:A:457:THR:O	1:A:580:GLY:HA2	2.22	0.40
1:A:678:GLN:HG2	1:A:701:LEU:HG	2.03	0.40
2:B:134:SER:OG	2:B:179:ARG:O	2.18	0.40
2:E:99:ASP:OD1	2:E:99:ASP:N	2.52	0.40
3:F:277:PRO:HA	3:F:286:ILE:HD11	2.02	0.40
1:A:761:GLU:H	1:A:761:GLU:CD	2.23	0.40
1:D:262:PRO:HD3	1:D:318:ILE:HD12	2.03	0.40
1:D:432:ASN:HD22	1:D:454:SER:HB3	1.85	0.40
3:F:81:LEU:O	3:F:84:TYR:HB2	2.22	0.40
1:D:252:LEU:HD23	1:D:252:LEU:HA	1.94	0.40
2:E:118:ILE:HB	2:E:119:GLN:CG	2.37	0.40
2:E:122:GLN:OE1	2:E:123:GLU:N	2.54	0.40
2:E:183:ILE:HG22	2:E:184:SER:H	1.86	0.40
2:E:356:PRO:HA	2:E:371:ALA:O	2.21	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%)	728 (96%)	34 (4%)	0	100	100
1	D	764/782 (98%)	740 (97%)	24 (3%)	0	100	100
2	B	351/352 (100%)	344 (98%)	7 (2%)	0	100	100
2	E	351/352 (100%)	332 (95%)	16 (5%)	3 (1%)	17	56
3	C	312/314 (99%)	296 (95%)	16 (5%)	0	100	100
3	F	312/314 (99%)	294 (94%)	18 (6%)	0	100	100
All	All	2852/2896 (98%)	2734 (96%)	115 (4%)	3 (0%)	51	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	118	ILE
2	E	136	ILE
2	E	119	GLN

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%)	637 (99%)	4 (1%)	86 94
1	D	642/653 (98%)	638 (99%)	4 (1%)	86 94
2	B	303/302 (100%)	300 (99%)	3 (1%)	76 90
2	E	300/302 (99%)	296 (99%)	4 (1%)	69 87
3	C	262/264 (99%)	262 (100%)	0	100 100
3	F	259/264 (98%)	256 (99%)	3 (1%)	71 88
All	All	2407/2438 (99%)	2389 (99%)	18 (1%)	84 94

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	76	TYR
1	A	162	SER
1	A	360	ASP
2	B	89	VAL
2	B	109	GLU
2	B	186	ASP
1	D	50	LYS
1	D	95	GLU
1	D	712	TYR
1	D	801	ASP
2	E	88	ARG
2	E	120	ARG
2	E	138	ILE

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Mol	Chain	Res	Type
2	E	293	MET
3	F	152	ASP
3	F	184	GLU
3	F	340	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	441	GLN
2	B	41	HIS
2	B	107	ASN
3	C	337	HIS
1	D	184	HIS
1	D	290	ASN
1	D	410	HIS
1	D	432	ASN
1	D	468	GLN
1	D	496	GLN
1	D	606	ASN
1	D	631	ASN
1	D	736	ASN
2	E	38	GLN
2	E	66	GLN
2	E	79	GLN
2	E	119	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 38 ligands modelled in this entry, 23 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	HEC	F	404	3,11	32,50,50	2.18	3 (9%)	24,82,82	1.58	4 (16%)
9	BET	D	909	-	7,7,7	2.57	1 (14%)	10,10,10	1.94	2 (20%)
9	BET	E	403	-	7,7,7	2.47	1 (14%)	10,10,10	1.96	2 (20%)
8	HEC	C	405	3	32,50,50	2.17	3 (9%)	24,82,82	1.43	3 (12%)
9	BET	A	909	-	7,7,7	2.55	1 (14%)	10,10,10	1.87	2 (20%)
9	BET	A	910	-	7,7,7	2.53	1 (14%)	10,10,10	1.95	2 (20%)
9	BET	A	911	-	7,7,7	2.51	1 (14%)	10,10,10	1.93	2 (20%)
9	BET	B	403	-	7,7,7	2.52	1 (14%)	10,10,10	1.98	2 (20%)
8	HEC	D	908	1	32,50,50	2.19	4 (12%)	24,82,82	1.33	1 (4%)
8	HEC	A	907	1,7	32,50,50	2.24	3 (9%)	24,82,82	1.33	2 (8%)
8	HEC	F	405	3	32,50,50	2.19	3 (9%)	24,82,82	1.49	4 (16%)
8	HEC	D	907	1,7	32,50,50	2.26	3 (9%)	24,82,82	1.37	2 (8%)
8	HEC	C	404	3,11	32,50,50	2.18	3 (9%)	24,82,82	1.46	4 (16%)
8	HEC	A	908	1	32,50,50	2.22	3 (9%)	24,82,82	1.44	4 (16%)
9	BET	C	406	-	7,7,7	2.54	1 (14%)	10,10,10	1.87	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	HEC	F	404	3,11	-	2/10/54/54	-
9	BET	D	909	-	-	5/5/5/5	-
9	BET	E	403	-	-	5/5/5/5	-
8	HEC	C	405	3	-	2/10/54/54	-
9	BET	A	909	-	-	5/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BET	A	910	-	-	5/5/5/5	-
9	BET	A	911	-	-	5/5/5/5	-
9	BET	B	403	-	-	5/5/5/5	-
8	HEC	D	908	1	-	5/10/54/54	-
8	HEC	A	907	1,7	-	4/10/54/54	-
8	HEC	F	405	3	-	0/10/54/54	-
8	HEC	D	907	1,7	-	2/10/54/54	-
8	HEC	C	404	3,11	-	2/10/54/54	-
8	HEC	A	908	1	-	2/10/54/54	-
9	BET	C	406	-	-	5/5/5/5	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	907	HEC	C2B-C3B	-6.69	1.33	1.40
8	D	907	HEC	C3C-C2C	-6.66	1.33	1.40
8	A	907	HEC	C3C-C2C	-6.57	1.33	1.40
8	A	907	HEC	C2B-C3B	-6.53	1.33	1.40
8	A	908	HEC	C3C-C2C	-6.48	1.34	1.40
8	F	405	HEC	C3C-C2C	-6.34	1.34	1.40
8	A	908	HEC	C2B-C3B	-6.32	1.34	1.40
8	D	908	HEC	C2B-C3B	-6.21	1.34	1.40
8	F	404	HEC	C2B-C3B	-6.19	1.34	1.40
8	F	404	HEC	C3C-C2C	-6.18	1.34	1.40
8	C	404	HEC	C2B-C3B	-6.17	1.34	1.40
9	D	909	BET	CA-C	6.17	1.63	1.52
9	C	406	BET	CA-C	6.16	1.62	1.52
9	A	909	BET	CA-C	6.15	1.62	1.52
8	C	405	HEC	C3C-C2C	-6.15	1.34	1.40
8	C	404	HEC	C3C-C2C	-6.12	1.34	1.40
8	D	908	HEC	C3C-C2C	-6.12	1.34	1.40
9	B	403	BET	CA-C	6.10	1.62	1.52
9	A	911	BET	CA-C	6.07	1.62	1.52
8	F	405	HEC	C2B-C3B	-6.07	1.34	1.40
9	A	910	BET	CA-C	6.06	1.62	1.52
8	C	405	HEC	C2B-C3B	-6.03	1.34	1.40
9	E	403	BET	CA-C	5.98	1.62	1.52
8	F	404	HEC	C3D-C2D	5.54	1.54	1.37
8	C	405	HEC	C3D-C2D	5.49	1.53	1.37
8	D	908	HEC	C3D-C2D	5.48	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	405	HEC	C3D-C2D	5.48	1.53	1.37
8	D	907	HEC	C3D-C2D	5.45	1.53	1.37
8	C	404	HEC	C3D-C2D	5.45	1.53	1.37
8	A	908	HEC	C3D-C2D	5.44	1.53	1.37
8	A	907	HEC	C3D-C2D	5.42	1.53	1.37
8	D	908	HEC	CAD-C3D	2.34	1.55	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	403	BET	C-CA-N	-4.83	109.70	116.34
9	E	403	BET	C-CA-N	-4.80	109.74	116.34
9	A	910	BET	C-CA-N	-4.76	109.79	116.34
9	A	911	BET	C-CA-N	-4.76	109.80	116.34
9	D	909	BET	C-CA-N	-4.72	109.85	116.34
9	C	406	BET	C-CA-N	-4.53	110.11	116.34
9	A	909	BET	C-CA-N	-4.52	110.12	116.34
9	A	909	BET	OXT-C-O	3.33	131.59	123.30
9	E	403	BET	OXT-C-O	3.31	131.56	123.30
9	A	910	BET	OXT-C-O	3.30	131.52	123.30
9	C	406	BET	OXT-C-O	3.30	131.51	123.30
9	B	403	BET	OXT-C-O	3.29	131.50	123.30
9	A	911	BET	OXT-C-O	3.29	131.50	123.30
9	D	909	BET	OXT-C-O	3.28	131.46	123.30
8	D	908	HEC	CMC-C2C-C1C	-3.02	123.83	128.46
8	F	404	HEC	CMC-C2C-C1C	-2.90	124.00	128.46
8	C	404	HEC	CMC-C2C-C1C	-2.89	124.03	128.46
8	F	404	HEC	CBD-CAD-C3D	-2.82	107.81	112.62
8	F	405	HEC	CMC-C2C-C1C	-2.74	124.25	128.46
8	C	405	HEC	C1D-C2D-C3D	-2.60	105.19	107.00
8	C	405	HEC	CMC-C2C-C1C	-2.58	124.50	128.46
8	F	405	HEC	C1D-C2D-C3D	-2.55	105.22	107.00
8	C	404	HEC	CBD-CAD-C3D	-2.53	108.30	112.62
8	F	404	HEC	C1D-C2D-C3D	-2.52	105.24	107.00
8	D	907	HEC	C1D-C2D-C3D	-2.43	105.30	107.00
8	A	907	HEC	C1D-C2D-C3D	-2.42	105.31	107.00
8	C	404	HEC	CMB-C2B-C1B	-2.38	124.81	128.46
8	F	404	HEC	CMB-C2B-C1B	-2.38	124.81	128.46
8	C	405	HEC	CMB-C2B-C1B	-2.29	124.94	128.46
8	A	908	HEC	CBD-CAD-C3D	-2.29	108.72	112.62
8	A	908	HEC	C1D-C2D-C3D	-2.24	105.44	107.00
8	F	405	HEC	CBA-CAA-C2A	-2.24	108.83	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	404	HEC	C1D-C2D-C3D	-2.23	105.44	107.00
8	F	405	HEC	CMB-C2B-C1B	-2.22	125.05	128.46
8	A	908	HEC	CMB-C2B-C1B	-2.17	125.13	128.46
8	D	907	HEC	CBD-CAD-C3D	-2.06	109.10	112.62
8	A	908	HEC	CBA-CAA-C2A	-2.06	109.12	112.60
8	A	907	HEC	CBD-CAD-C3D	-2.02	109.18	112.62

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	908	HEC	C2D-C3D-CAD-CBD
8	D	908	HEC	C4D-C3D-CAD-CBD
9	A	909	BET	C-CA-N-C2
9	A	909	BET	O-C-CA-N
9	A	909	BET	OXT-C-CA-N
9	A	910	BET	O-C-CA-N
9	A	910	BET	OXT-C-CA-N
9	A	911	BET	O-C-CA-N
9	A	911	BET	OXT-C-CA-N
9	B	403	BET	O-C-CA-N
9	B	403	BET	OXT-C-CA-N
9	C	406	BET	O-C-CA-N
9	C	406	BET	OXT-C-CA-N
9	D	909	BET	O-C-CA-N
9	D	909	BET	OXT-C-CA-N
9	E	403	BET	O-C-CA-N
9	E	403	BET	OXT-C-CA-N
9	E	403	BET	C-CA-N-C1
9	A	910	BET	C-CA-N-C1
9	A	911	BET	C-CA-N-C1
9	B	403	BET	C-CA-N-C1
9	B	403	BET	C-CA-N-C3
9	C	406	BET	C-CA-N-C2
9	D	909	BET	C-CA-N-C1
9	D	909	BET	C-CA-N-C3
9	E	403	BET	C-CA-N-C2
9	A	909	BET	C-CA-N-C1
9	A	909	BET	C-CA-N-C3
9	A	910	BET	C-CA-N-C2
9	A	910	BET	C-CA-N-C3
9	A	911	BET	C-CA-N-C2

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Mol	Chain	Res	Type	Atoms
9	A	911	BET	C-CA-N-C3
9	B	403	BET	C-CA-N-C2
9	C	406	BET	C-CA-N-C1
9	D	909	BET	C-CA-N-C2
9	E	403	BET	C-CA-N-C3
9	C	406	BET	C-CA-N-C3
8	F	404	HEC	C2D-C3D-CAD-CBD
8	F	404	HEC	C4D-C3D-CAD-CBD
8	D	907	HEC	CAA-CBA-CGA-O1A
8	C	404	HEC	CAD-CBD-CGD-O2D
8	C	405	HEC	CAD-CBD-CGD-O2D
8	D	907	HEC	CAA-CBA-CGA-O2A
8	A	907	HEC	CAA-CBA-CGA-O1A
8	A	907	HEC	CAD-CBD-CGD-O2D
8	C	404	HEC	CAD-CBD-CGD-O1D
8	C	405	HEC	CAD-CBD-CGD-O1D
8	A	907	HEC	CAD-CBD-CGD-O1D
8	A	907	HEC	CAA-CBA-CGA-O2A
8	A	908	HEC	CAD-CBD-CGD-O2D
8	D	908	HEC	CAD-CBD-CGD-O2D
8	D	908	HEC	CAA-CBA-CGA-O2A
8	A	908	HEC	CAD-CBD-CGD-O1D
8	D	908	HEC	CAD-CBD-CGD-O1D

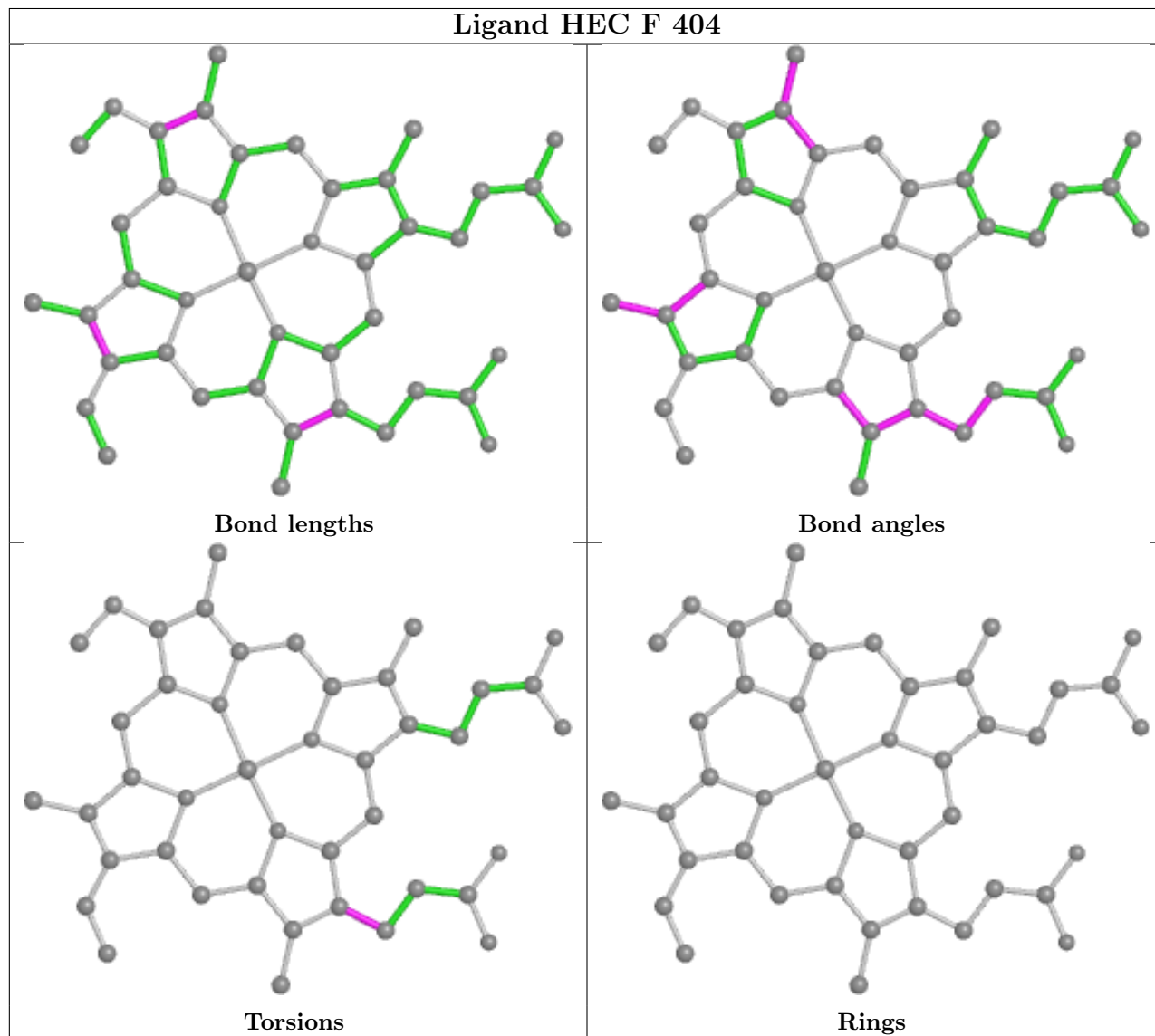
There are no ring outliers.

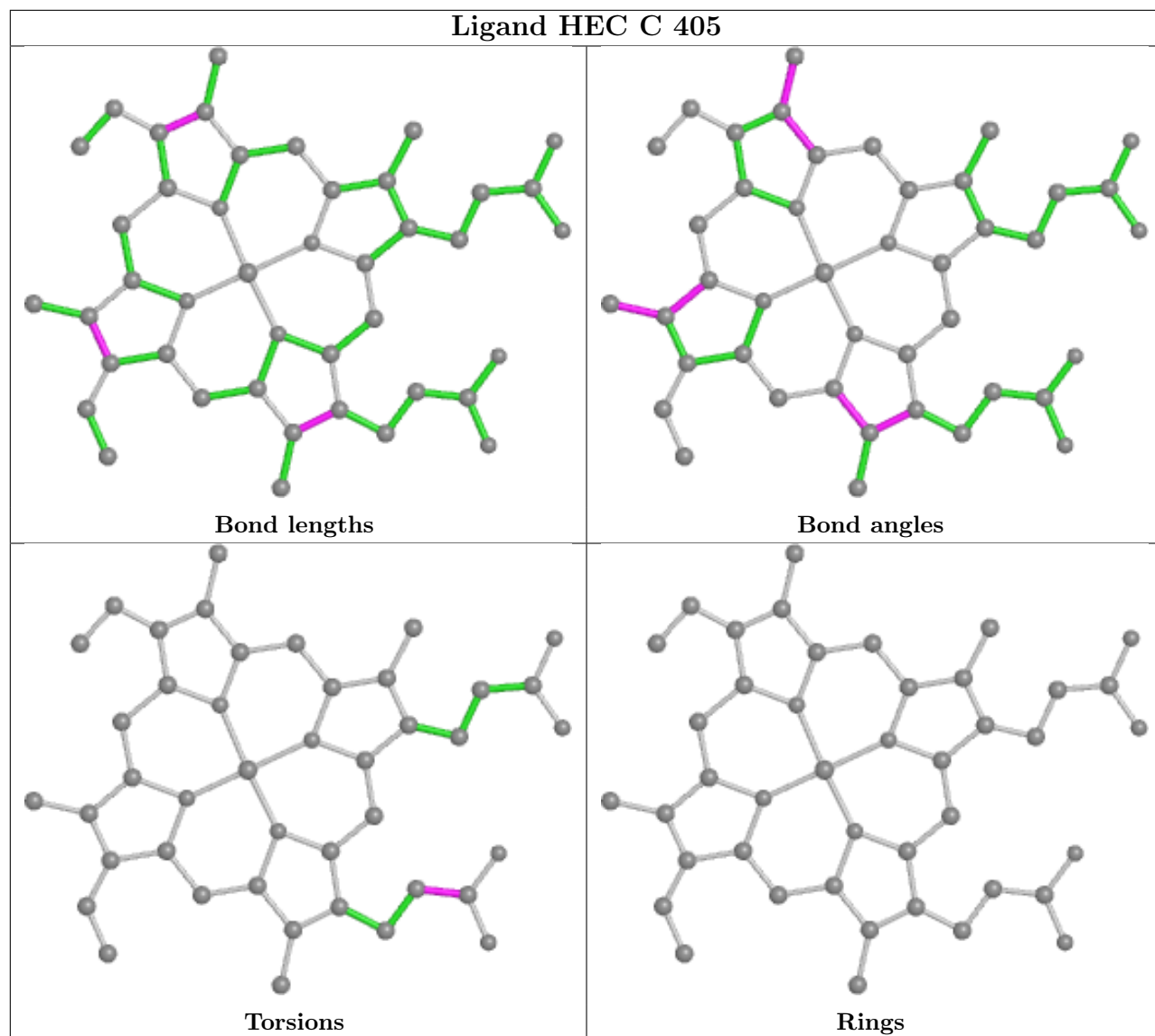
8 monomers are involved in 27 short contacts:

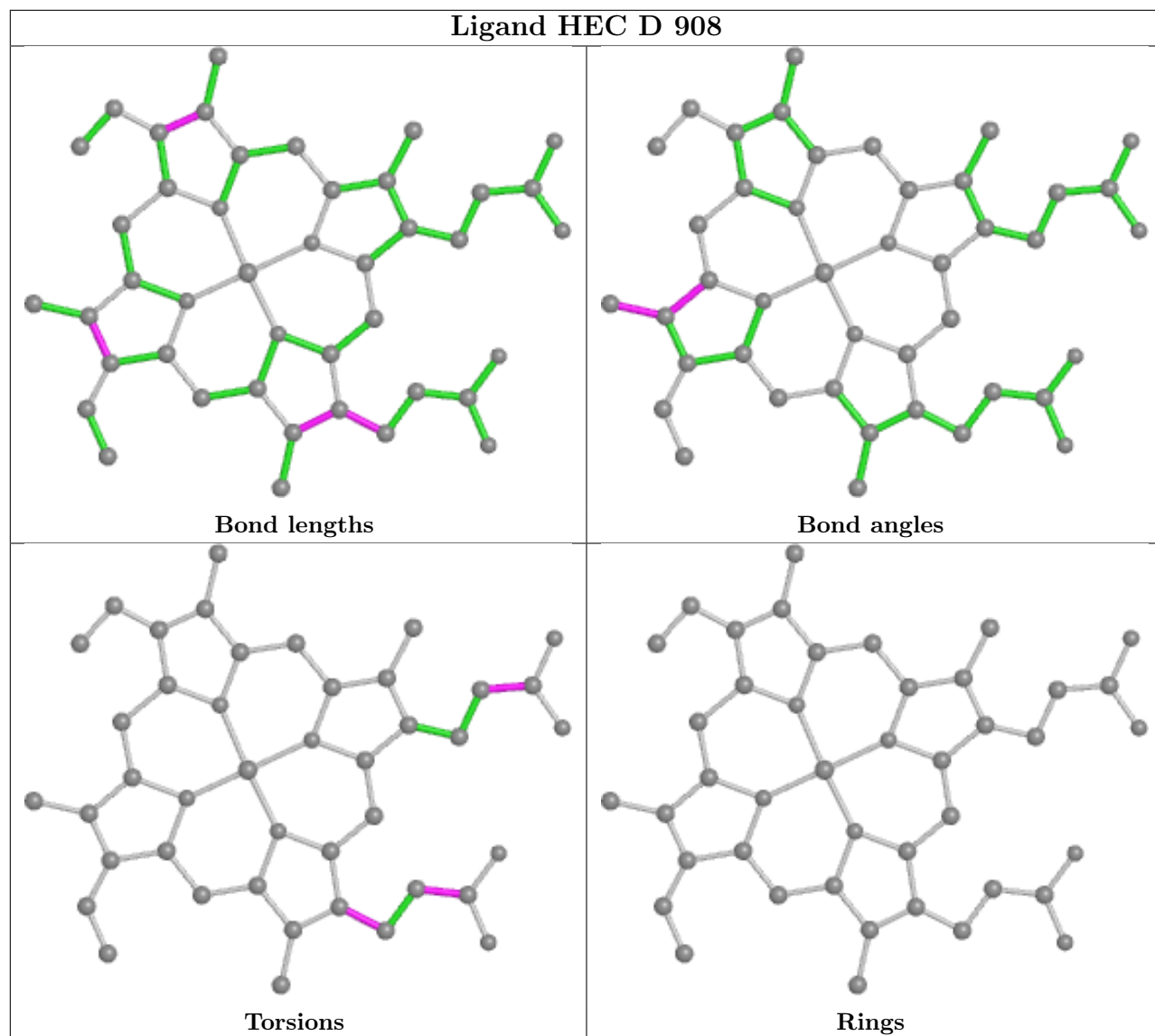
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	404	HEC	5	0
8	C	405	HEC	2	0
8	D	908	HEC	4	0
8	A	907	HEC	1	0
8	F	405	HEC	3	0
8	D	907	HEC	3	0
8	C	404	HEC	6	0
8	A	908	HEC	3	0

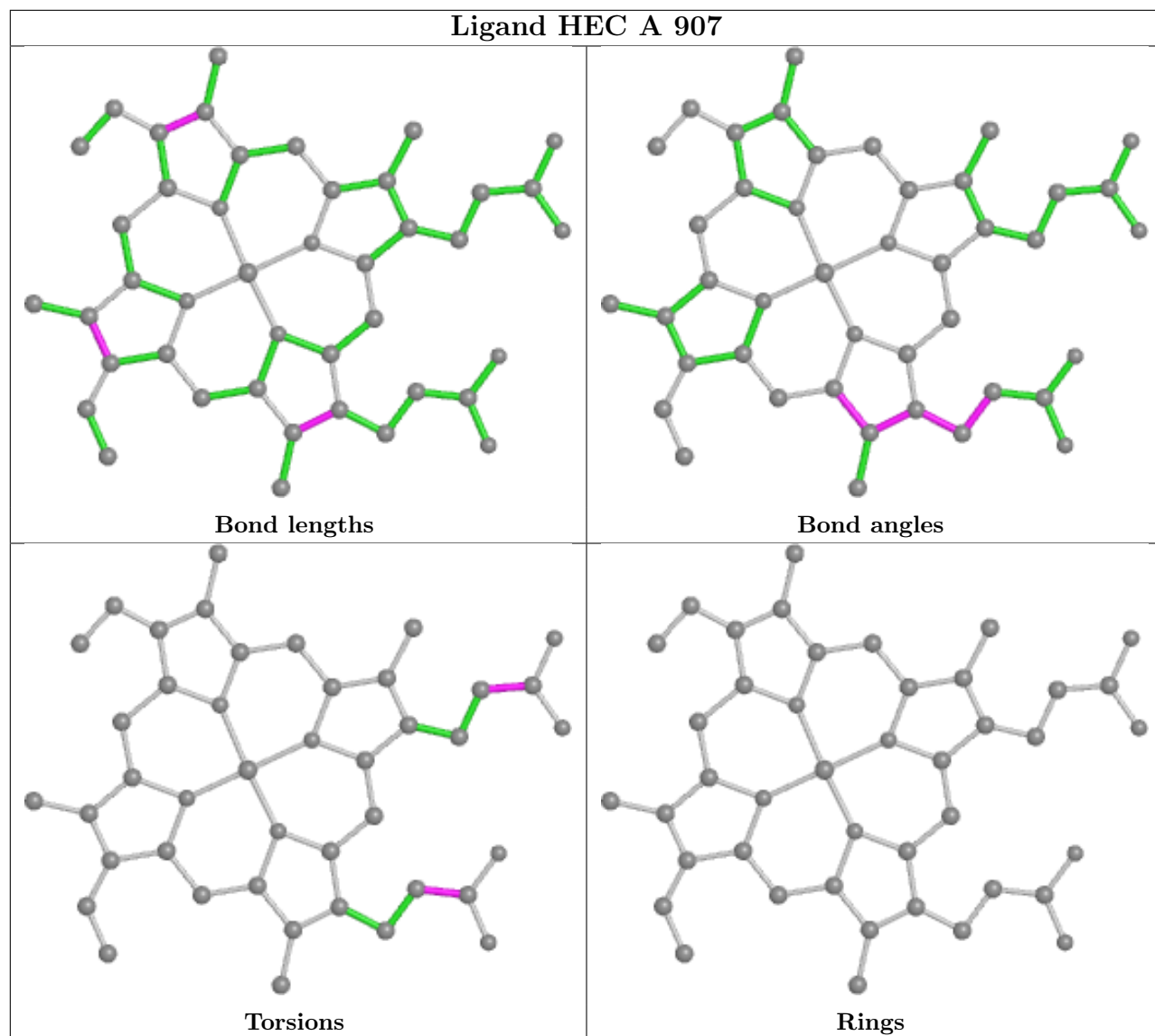
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

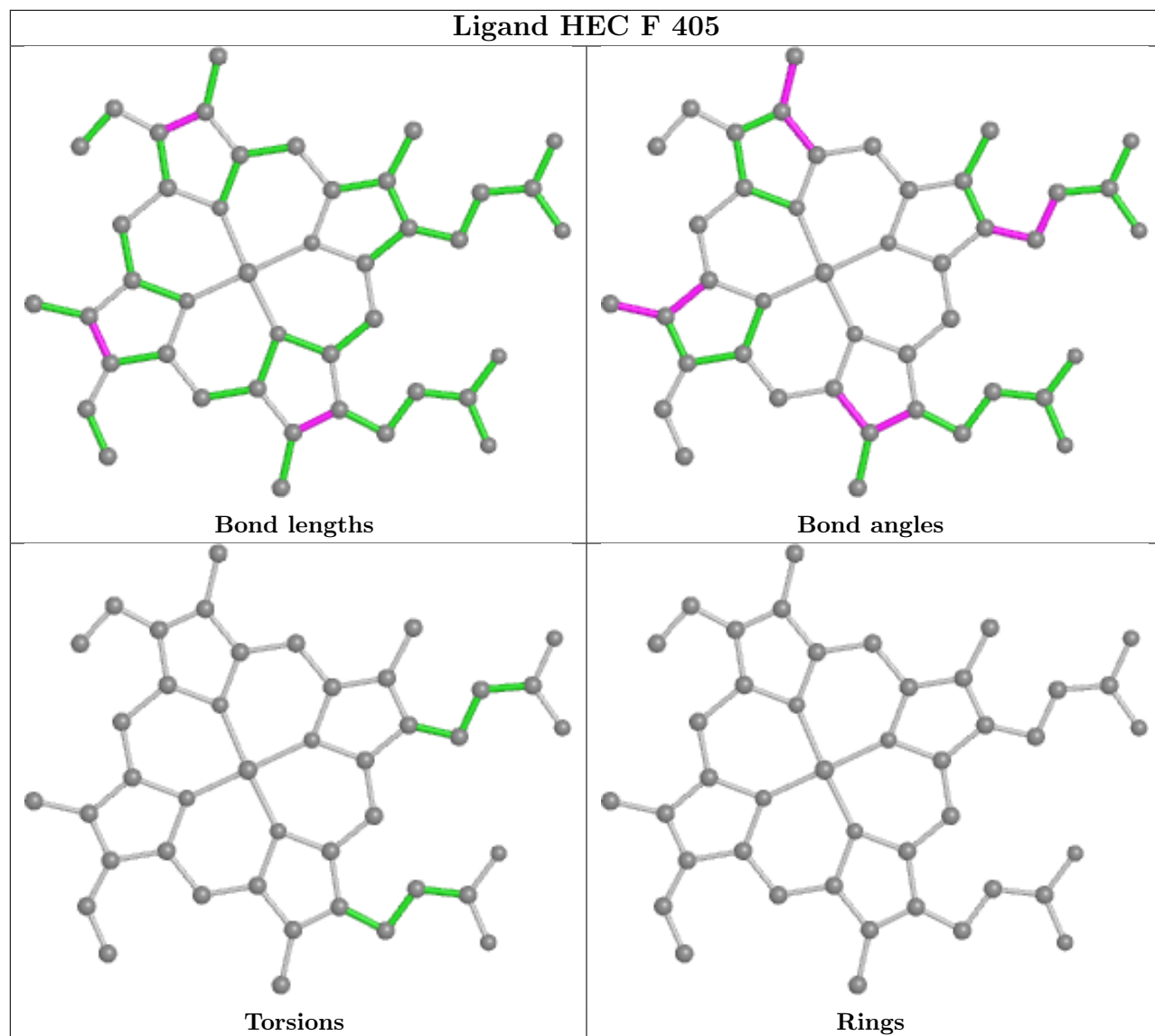
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

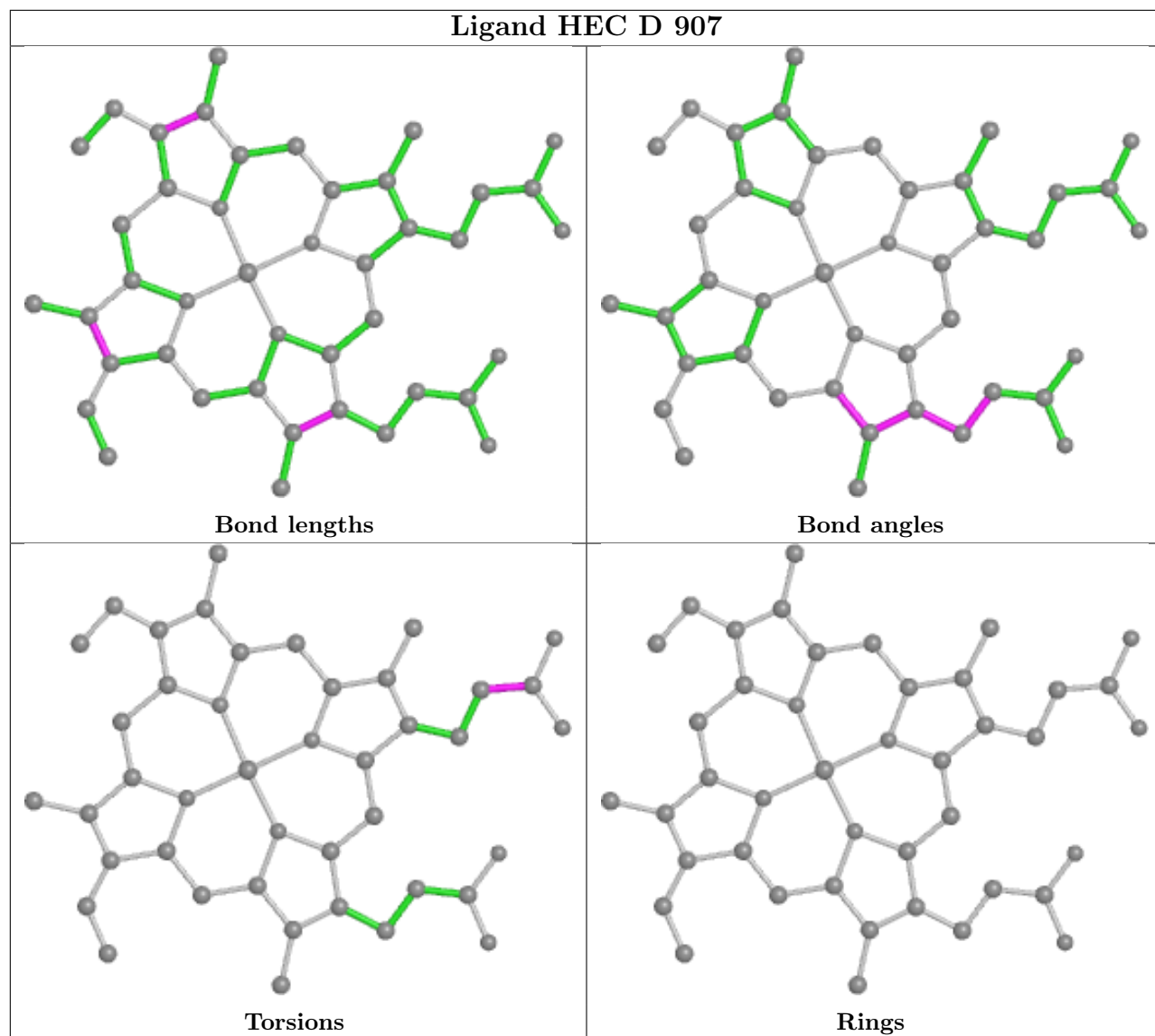


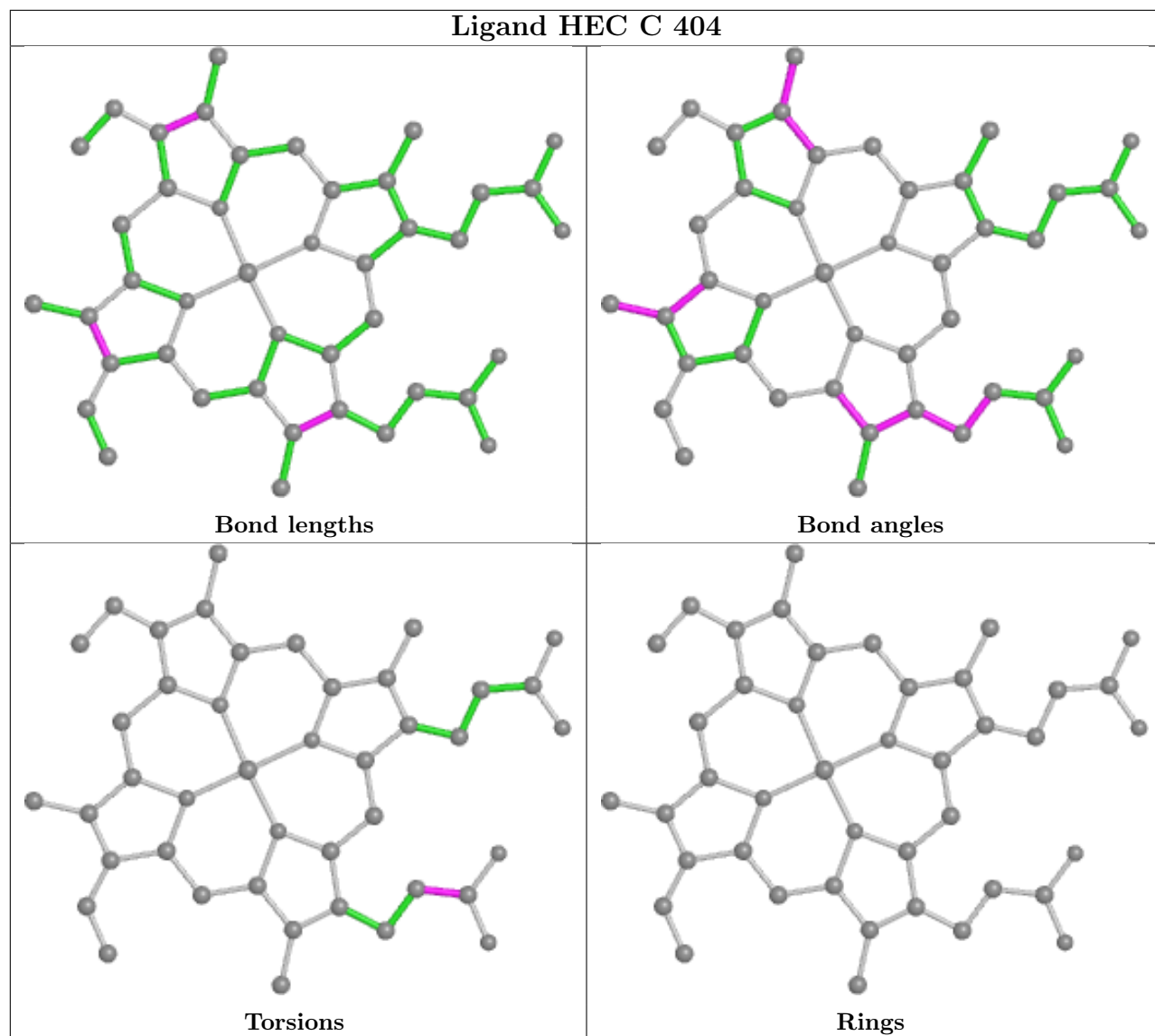


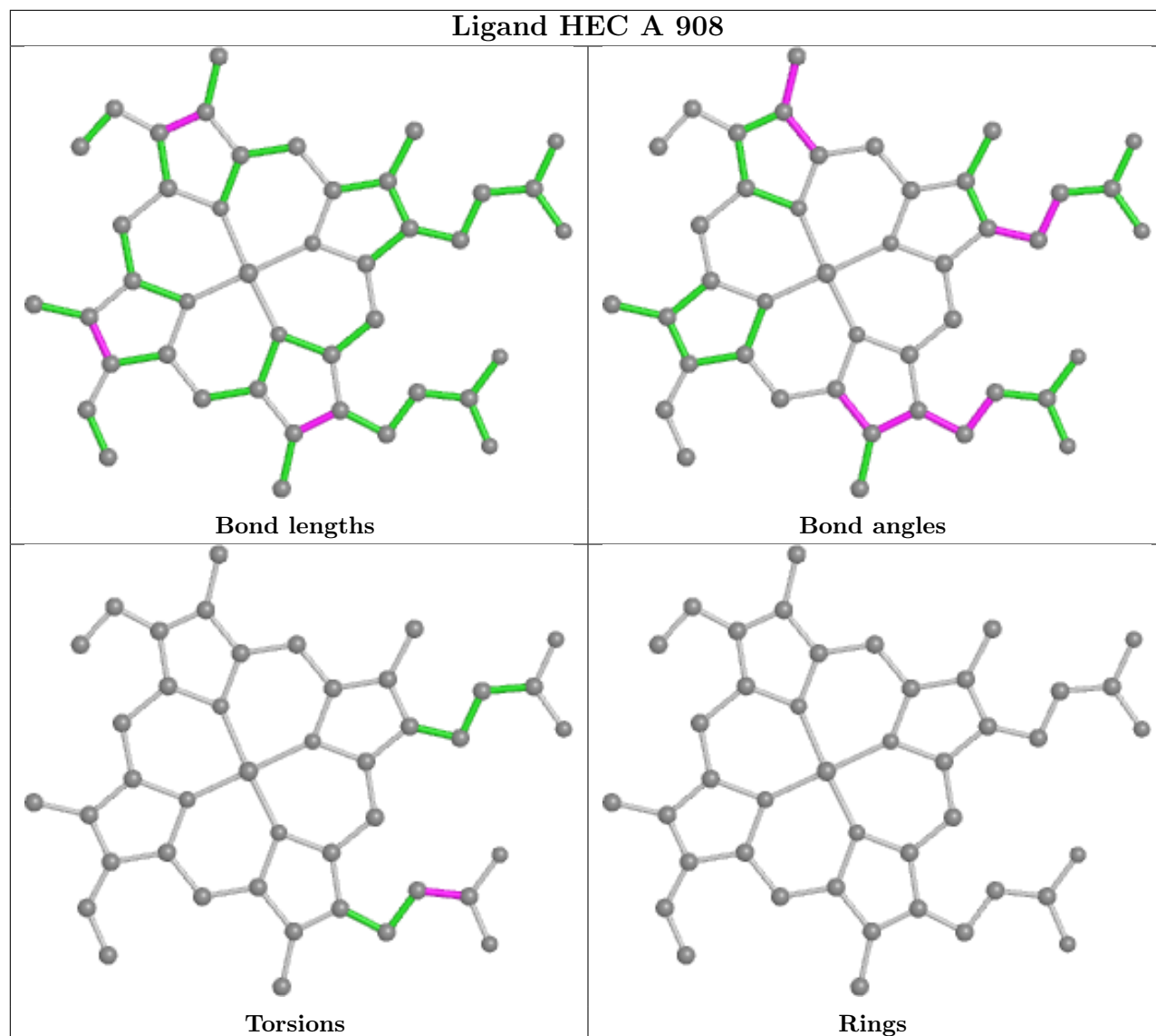












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	768/782 (98%)	-0.28	0 100 100	35, 60, 83, 111	0
1	D	770/782 (98%)	-0.06	5 (0%) 89 83	42, 70, 94, 113	0
2	B	352/352 (100%)	-0.08	2 (0%) 89 83	34, 65, 85, 102	0
2	E	352/352 (100%)	0.36	13 (3%) 41 26	49, 90, 117, 136	0
3	C	314/314 (100%)	-0.13	0 100 100	41, 63, 85, 95	0
3	F	314/314 (100%)	0.26	6 (1%) 66 53	60, 86, 105, 116	0
All	All	2870/2896 (99%)	-0.04	26 (0%) 84 75	34, 70, 100, 136	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	35	GLY	4.9
2	E	82	THR	3.8
3	F	223	VAL	3.6
2	E	91	PRO	3.6
2	E	121	LYS	3.5
3	F	333	GLY	3.0
2	E	378	VAL	3.0
2	E	81	VAL	2.6
2	E	122	GLN	2.6
3	F	349	TYR	2.6
1	D	398	GLY	2.5
2	E	163	GLY	2.4
1	D	93	THR	2.4
1	D	642	VAL	2.3
3	F	40	GLY	2.3
1	D	38	GLY	2.2
2	E	160	ILE	2.2
2	B	115	VAL	2.2
1	D	651	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	386	ASP	2.1
2	E	73	PHE	2.0
2	E	86	ALA	2.0
2	E	171	ILE	2.0
3	F	226	LEU	2.0
2	E	215	VAL	2.0
3	F	245	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
6	CA	F	401	1/1	0.62	0.17	91,91,91,91	0
10	MG	E	401	1/1	0.73	0.37	53,53,53,53	0
6	CA	B	402	1/1	0.78	0.10	68,68,68,68	0
6	CA	C	401	1/1	0.85	0.13	57,57,57,57	0
6	CA	F	403	1/1	0.86	0.12	73,73,73,73	0
4	XE	D	901	1/1	0.86	0.77	250,250,250,250	0
9	BET	C	406	8/8	0.88	0.54	58,70,75,78	0
6	CA	A	905	1/1	0.88	0.09	80,80,80,80	0
9	BET	A	909	8/8	0.89	0.31	40,72,83,91	0
9	BET	D	909	8/8	0.91	0.46	76,85,90,93	0
10	MG	B	401	1/1	0.91	0.26	30,30,30,30	0
9	BET	A	911	8/8	0.91	0.53	68,75,85,90	0
5	CL	D	903	1/1	0.92	0.18	61,61,61,61	0
6	CA	C	402	1/1	0.92	0.11	70,70,70,70	0
6	CA	C	403	1/1	0.93	0.15	54,54,54,54	0
6	CA	E	402	1/1	0.93	0.07	90,90,90,90	0

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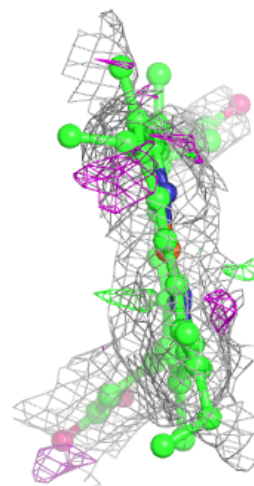
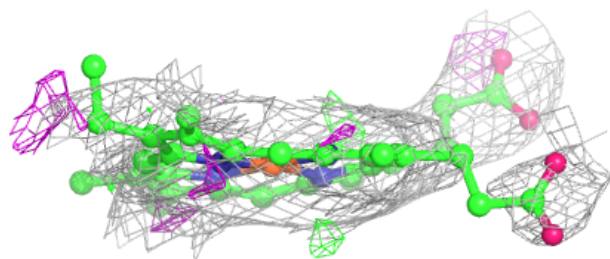
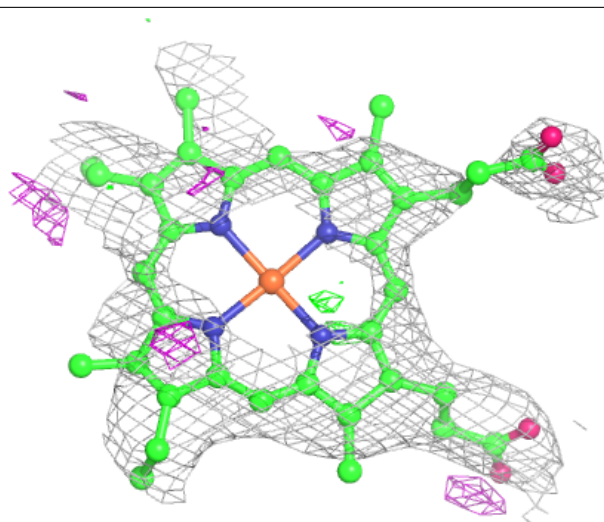
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CL	A	903[A]	1/1	0.93	0.39	17,17,17,17	1
6	CA	A	904	1/1	0.93	0.04	75,75,75,75	0
5	CL	A	903[B]	1/1	0.93	0.39	39,39,39,39	1
6	CA	D	905	1/1	0.94	0.07	84,84,84,84	0
8	HEC	F	404	43/43	0.94	0.24	52,77,99,100	0
8	HEC	F	405	43/43	0.94	0.28	62,90,103,105	0
6	CA	F	402	1/1	0.95	0.11	82,82,82,82	0
9	BET	A	910	8/8	0.95	0.33	68,71,78,85	0
9	BET	E	403	8/8	0.95	0.21	58,69,81,81	0
4	XE	A	901	1/1	0.95	0.20	127,127,127,127	0
9	BET	B	403	8/8	0.95	0.19	40,46,59,70	0
8	HEC	C	405	43/43	0.96	0.26	48,69,77,82	0
6	CA	D	904	1/1	0.96	0.05	70,70,70,70	0
8	HEC	C	404	43/43	0.96	0.21	37,52,69,77	0
8	HEC	D	907	43/43	0.97	0.19	41,62,80,82	0
8	HEC	D	908	43/43	0.98	0.22	35,54,67,77	0
4	XE	D	902	1/1	0.98	0.31	178,178,178,178	0
8	HEC	A	907	43/43	0.98	0.17	31,45,55,56	0
8	HEC	A	908	43/43	0.98	0.22	39,57,68,71	0
7	ZN	A	906	1/1	0.99	0.15	54,54,54,54	0
4	XE	A	902	1/1	0.99	0.09	81,81,81,81	0
7	ZN	D	906	1/1	1.00	0.17	55,55,55,55	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.

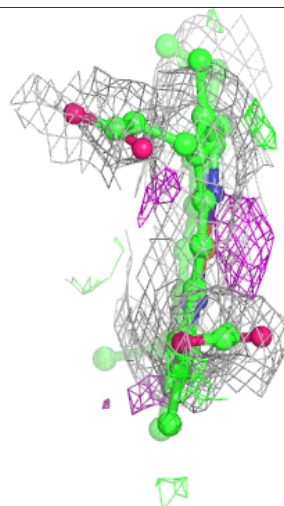
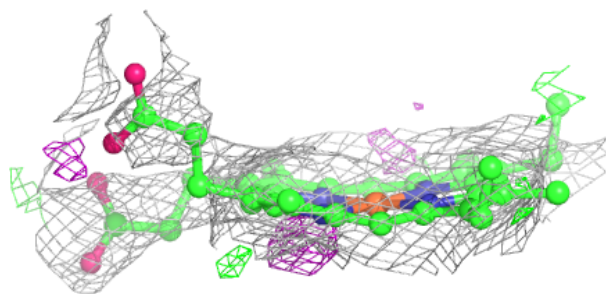
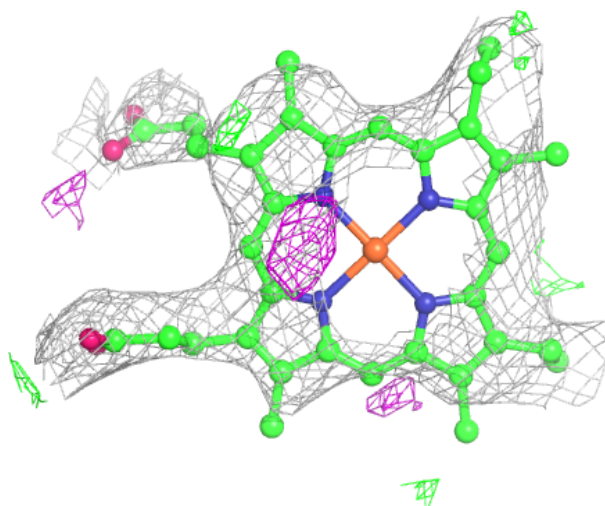
Electron density around HEC F 404:

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



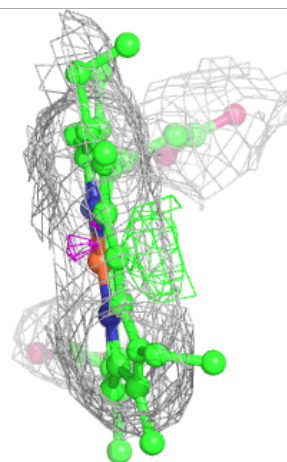
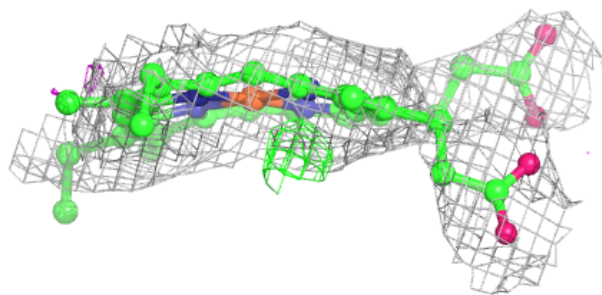
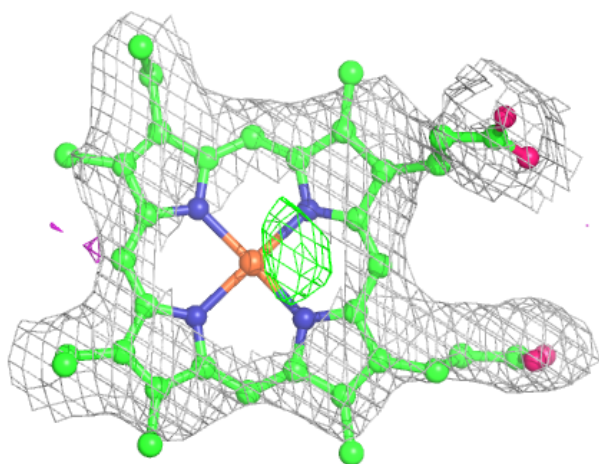
Electron density around HEC F 405:

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



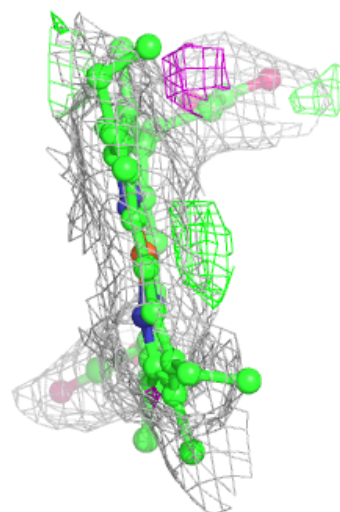
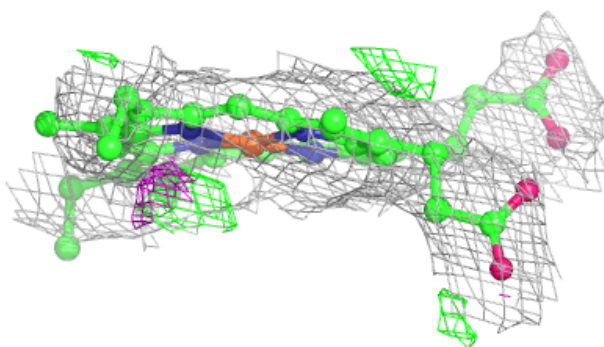
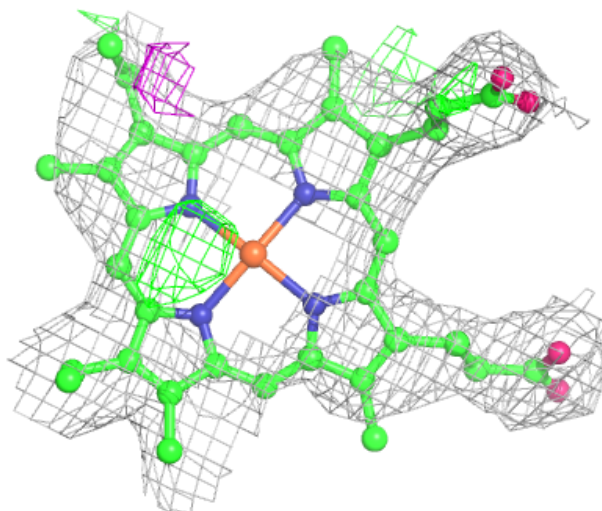
Electron density around HEC C 405:

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



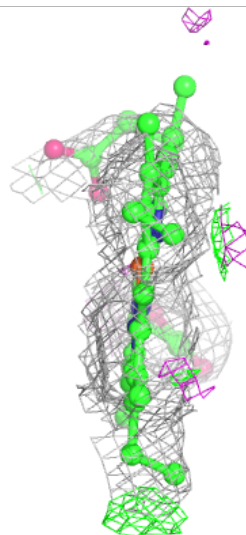
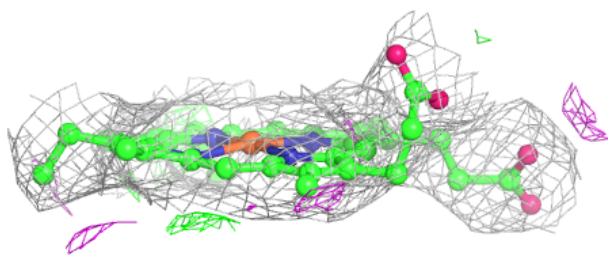
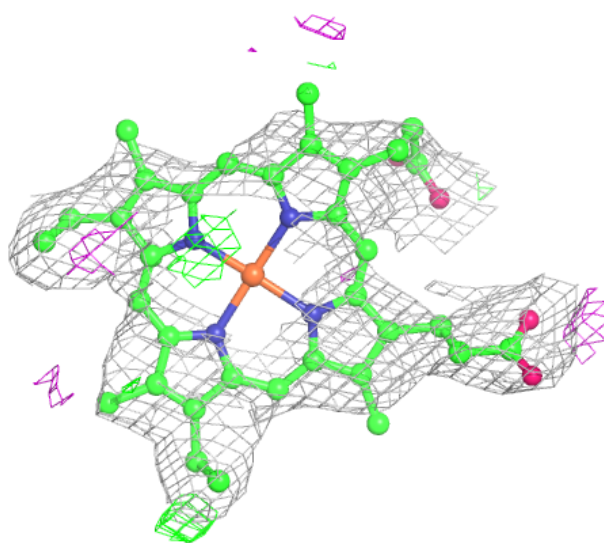
Electron density around HEC C 404:

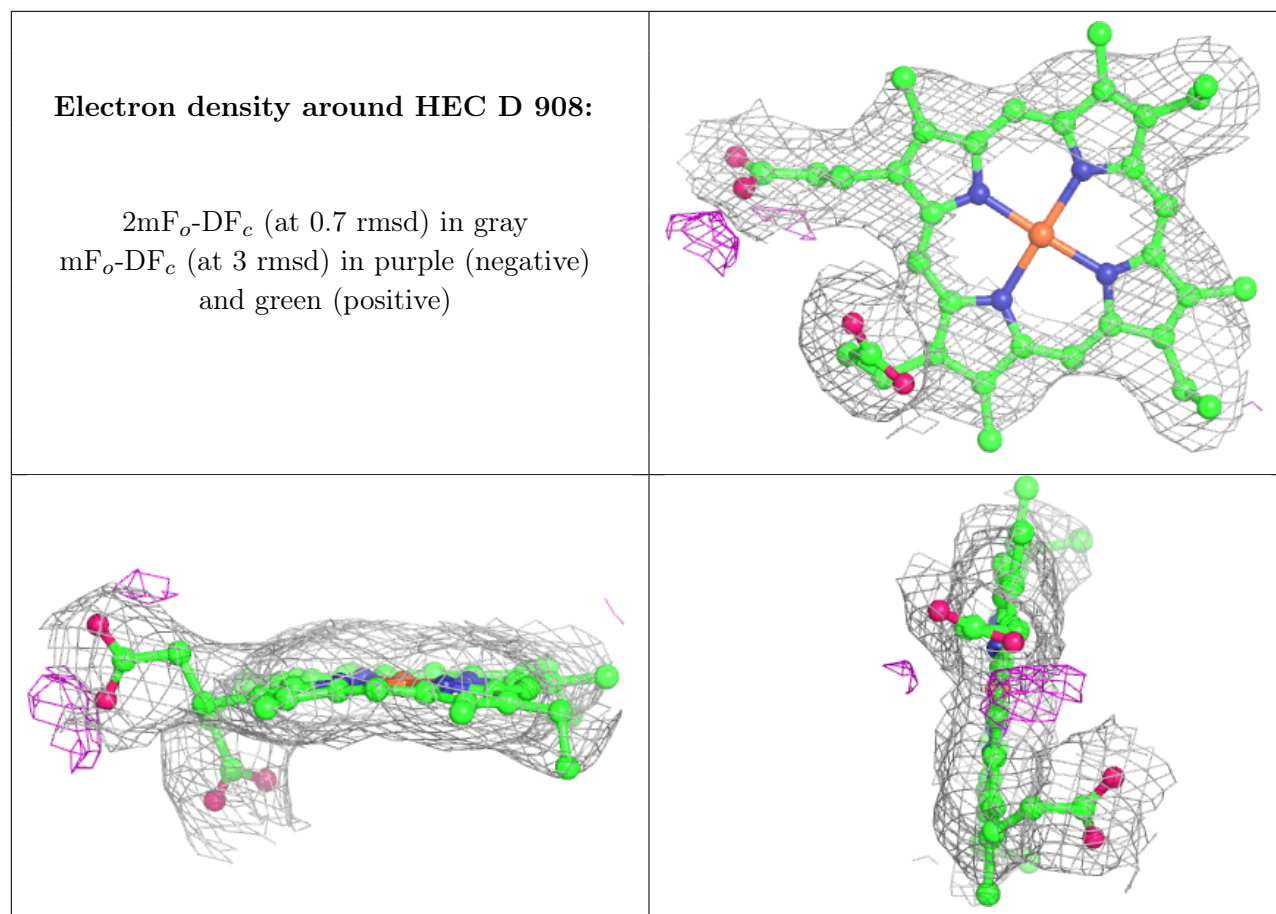
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC D 907:

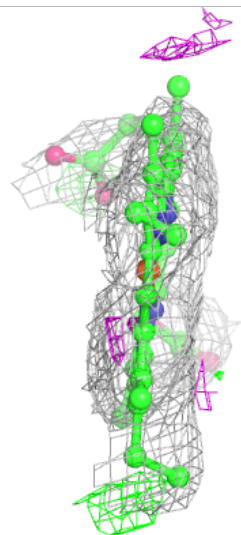
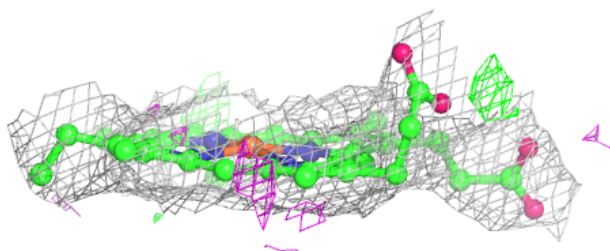
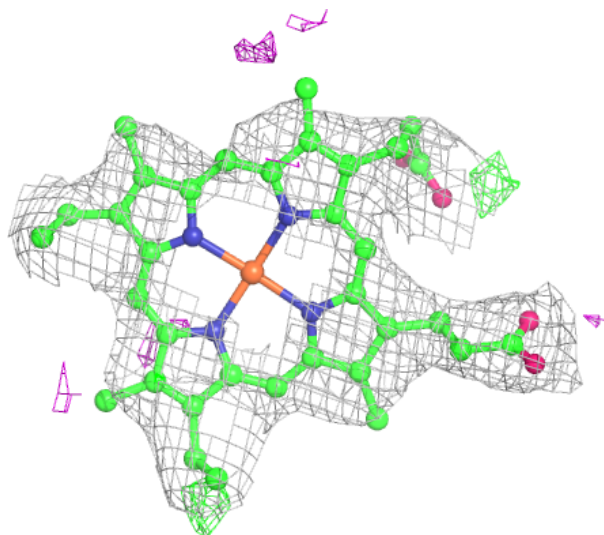
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

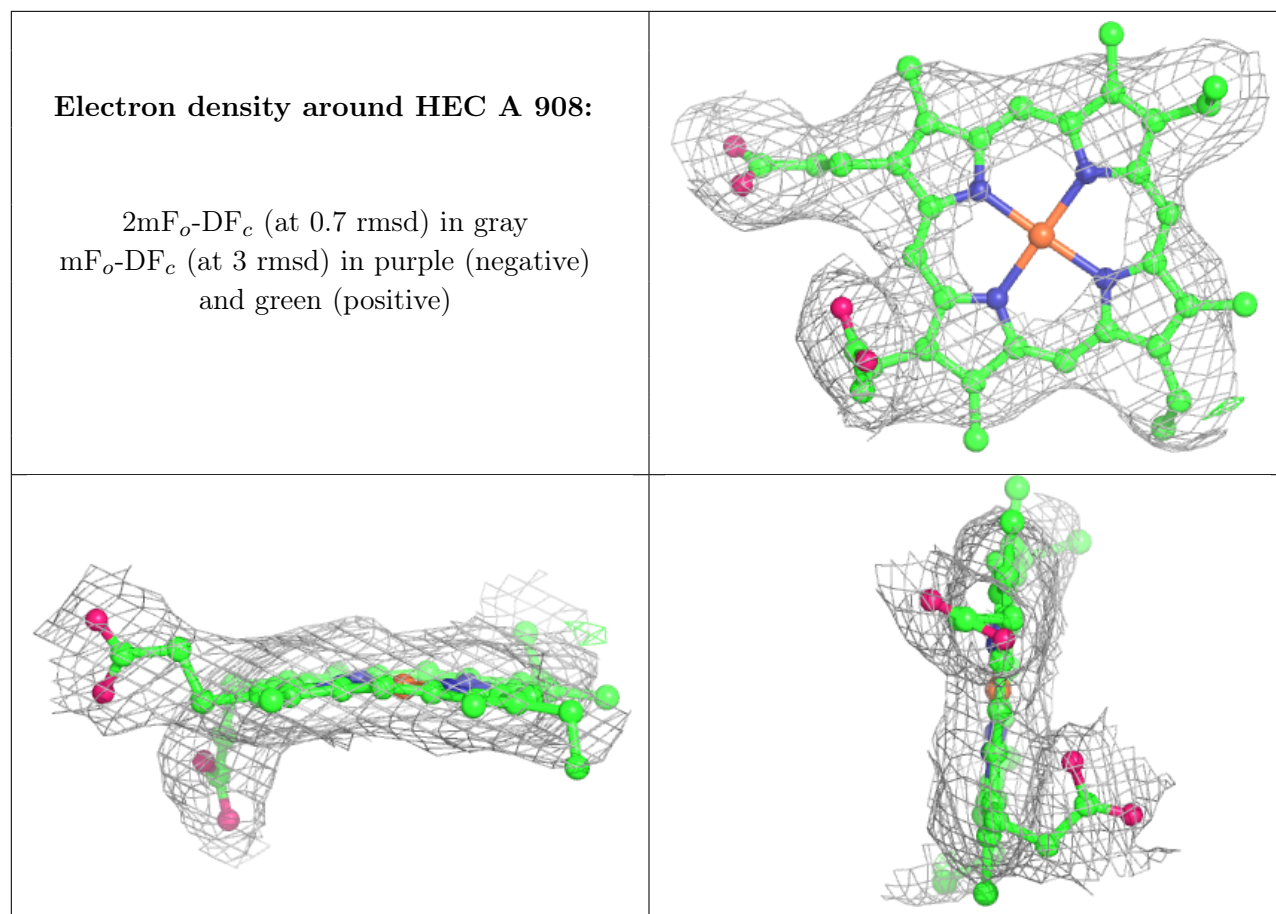




Electron density around HEC A 907:

$2mF_o-DF_c$ (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.