



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2022 – 10:04 AM EDT

PDB ID : 7TEP
Title : Crystal structure of a Cu-bound cytochrome cb562 variant in the presence of reductant
Authors : Kakkis, A.; Golub, E.
Deposited on : 2022-01-05
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 ⓘ 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
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) : 2.29

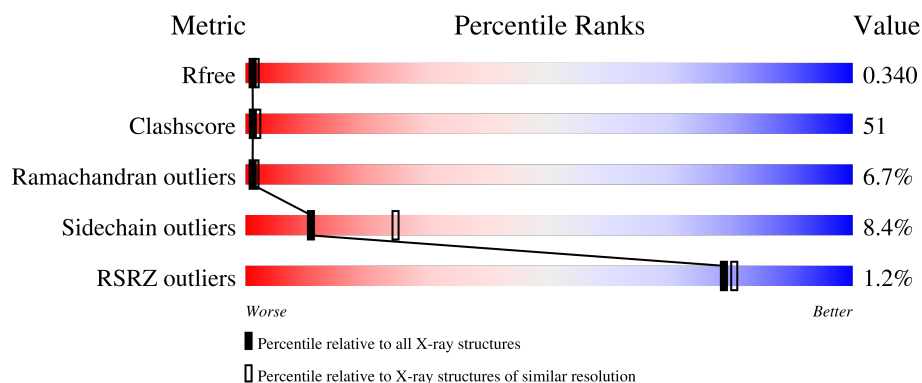
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	106	
1	B	106	
1	C	106	
1	D	106	

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
3	CU	A	203	-	-	X	-
3	CU	C	202	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6993 atoms, of which 3402 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 Soluble cytochrome b562.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	106	Total	C	H	N	O	S	0	1	0
			1619	509	797	147	160	6			
1	B	106	Total	C	H	N	O	S	0	4	0
			1663	520	829	147	161	6			
1	C	106	Total	C	H	N	O	S	0	6	0
			1703	530	853	151	162	7			
1	D	106	Total	C	H	N	O	S	0	1	0
			1618	508	797	146	161	6			

There are 52 discrepancies between the modelled and reference sequences:

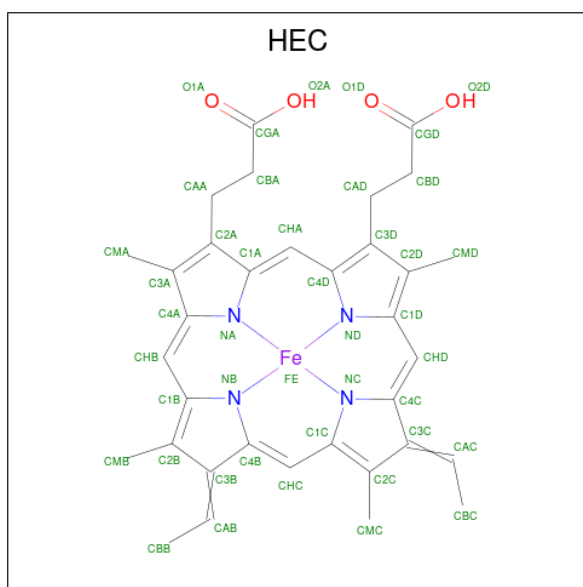
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	ALA	ARG	engineered mutation	UNP P0ABE7
A	38	ALA	LEU	engineered mutation	UNP P0ABE7
A	41	TRP	GLN	engineered mutation	UNP P0ABE7
A	42	SER	LYS	engineered mutation	UNP P0ABE7
A	59	HIS	LYS	engineered mutation	UNP P0ABE7
A	66	TRP	ASP	engineered mutation	UNP P0ABE7
A	69	ILE	VAL	engineered mutation	UNP P0ABE7
A	73	HIS	ASP	engineered mutation	UNP P0ABE7
A	74	ALA	ASP	engineered mutation	UNP P0ABE7
A	77	HIS	LYS	engineered mutation	UNP P0ABE7
A	96	CYS	THR	engineered mutation	UNP P0ABE7
A	98	CYS	ARG	engineered mutation	UNP P0ABE7
A	101	CYS	TYR	engineered mutation	UNP P0ABE7
B	34	ALA	ARG	engineered mutation	UNP P0ABE7
B	38	ALA	LEU	engineered mutation	UNP P0ABE7
B	41	TRP	GLN	engineered mutation	UNP P0ABE7
B	42	SER	LYS	engineered mutation	UNP P0ABE7
B	59	HIS	LYS	engineered mutation	UNP P0ABE7
B	66	TRP	ASP	engineered mutation	UNP P0ABE7
B	69	ILE	VAL	engineered mutation	UNP P0ABE7
B	73	HIS	ASP	engineered mutation	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	74	ALA	ASP	engineered mutation	UNP P0ABE7
B	77	HIS	LYS	engineered mutation	UNP P0ABE7
B	96	CYS	THR	engineered mutation	UNP P0ABE7
B	98	CYS	ARG	engineered mutation	UNP P0ABE7
B	101	CYS	TYR	engineered mutation	UNP P0ABE7
C	34	ALA	ARG	engineered mutation	UNP P0ABE7
C	38	ALA	LEU	engineered mutation	UNP P0ABE7
C	41	TRP	GLN	engineered mutation	UNP P0ABE7
C	42	SER	LYS	engineered mutation	UNP P0ABE7
C	59	HIS	LYS	engineered mutation	UNP P0ABE7
C	66	TRP	ASP	engineered mutation	UNP P0ABE7
C	69	ILE	VAL	engineered mutation	UNP P0ABE7
C	73	HIS	ASP	engineered mutation	UNP P0ABE7
C	74	ALA	ASP	engineered mutation	UNP P0ABE7
C	77	HIS	LYS	engineered mutation	UNP P0ABE7
C	96	CYS	THR	engineered mutation	UNP P0ABE7
C	98	CYS	ARG	engineered mutation	UNP P0ABE7
C	101	CYS	TYR	engineered mutation	UNP P0ABE7
D	34	ALA	ARG	engineered mutation	UNP P0ABE7
D	38	ALA	LEU	engineered mutation	UNP P0ABE7
D	41	TRP	GLN	engineered mutation	UNP P0ABE7
D	42	SER	LYS	engineered mutation	UNP P0ABE7
D	59	HIS	LYS	engineered mutation	UNP P0ABE7
D	66	TRP	ASP	engineered mutation	UNP P0ABE7
D	69	ILE	VAL	engineered mutation	UNP P0ABE7
D	73	HIS	ASP	engineered mutation	UNP P0ABE7
D	74	ALA	ASP	engineered mutation	UNP P0ABE7
D	77	HIS	LYS	engineered mutation	UNP P0ABE7
D	96	CYS	THR	engineered mutation	UNP P0ABE7
D	98	CYS	ARG	engineered mutation	UNP P0ABE7
D	101	CYS	TYR	engineered mutation	UNP P0ABE7

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N	O	0	0
			74	34	1	31	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
2	C	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
2	D	1	Total	C	Fe	H	N	O	0	0
			74	34	1	31	4	4		

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cu	0	0
			2	2		
3	B	1	Total	Cu	0	0
			1	1		
3	C	1	Total	Cu	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	20	Total	O	0	0
			20	20		

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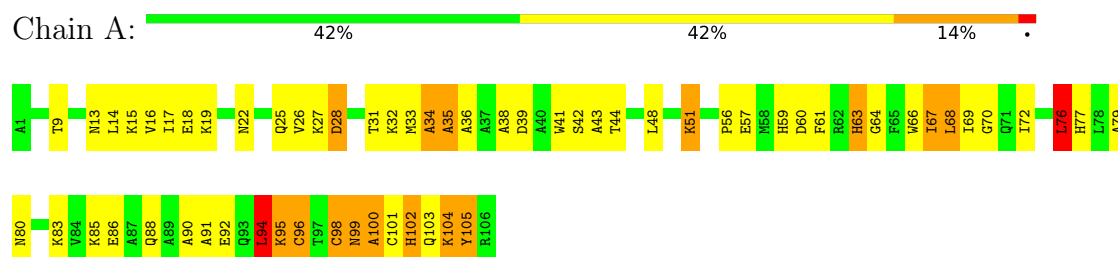
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	21	Total	O	0	0
			21	21		
4	D	21	Total	O	0	0
			21	21		

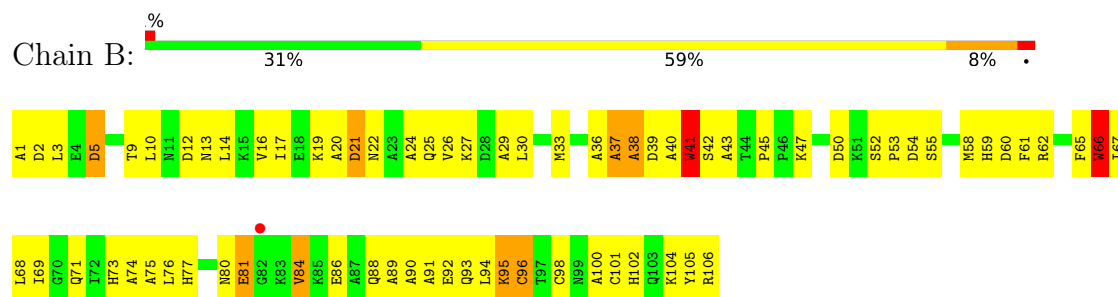
3 Residue-property plots

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

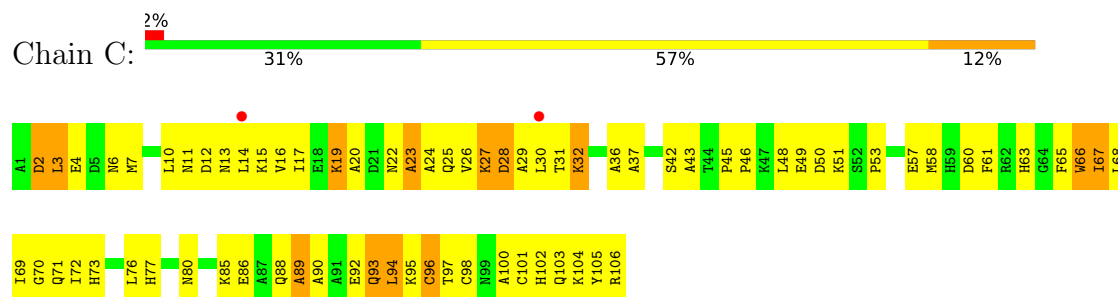
• Molecule 1: Soluble cytochrome b562



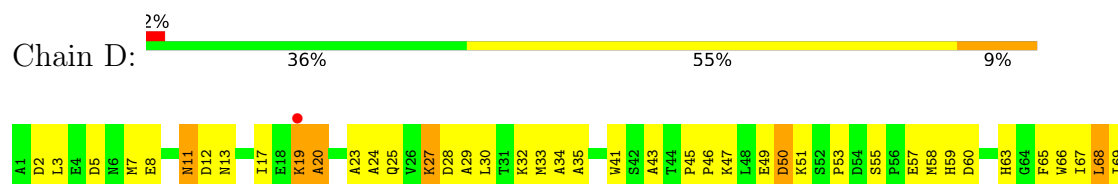
• Molecule 1: Soluble cytochrome b562



• Molecule 1: Soluble cytochrome b562



• Molecule 1: Soluble cytochrome b562



G70	Q71	I72	H73	A74	A75	L76	H77	L78	A79	N80	E81	G82	K83	V84	K85	E86	A87	Q88	E92	Q93	L94	K95	C96	N99	A100	C101	H102	Q103	K104	Y105	R106
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.08Å 80.57Å 49.44Å 90.00° 102.33° 90.00°	Depositor
Resolution (Å)	48.30 – 2.70 48.30 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.3 (48.30-2.70) 89.6 (48.30-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.63 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.253 , 0.339 0.253 , 0.340	Depositor DCC
R_{free} test set	903 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 26.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.067 for l,-k,h	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6993	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.82	2/841 (0.2%)	1.00	3/1136 (0.3%)
1	B	0.83	1/861 (0.1%)	0.93	2/1161 (0.2%)
1	C	0.74	1/893 (0.1%)	0.87	0/1200
1	D	0.67	0/839	0.86	1/1133 (0.1%)
All	All	0.77	4/3434 (0.1%)	0.91	6/4630 (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	1
1	C	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	CYS	CB-SG	-6.76	1.70	1.82
1	A	76	LEU	CG-CD2	-6.66	1.27	1.51
1	B	41	TRP	CE3-CZ3	5.62	1.48	1.38
1	C	96	CYS	CB-SG	5.48	1.91	1.82

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	LEU	CA-CB-CG	8.03	133.76	115.30
1	A	28	ASP	CB-CG-OD1	7.96	125.46	118.30
1	D	101	CYS	CA-CB-SG	-6.41	102.46	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	GLU	CG-CD-OE1	5.87	130.04	118.30
1	A	96	CYS	CA-CB-SG	5.83	124.50	114.00
1	B	96	CYS	CA-CB-SG	5.54	123.98	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	TYR	Mainchain
1	C	93	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	822	797	797	85	0
1	B	834	829	832	108	2
1	C	850	853	837	96	0
1	D	821	797	799	80	2
2	A	43	31	30	7	0
2	B	43	32	32	14	0
2	C	43	32	32	20	0
2	D	43	31	31	12	0
3	A	2	0	0	2	0
3	B	1	0	0	1	0
3	C	1	0	0	2	0
4	A	26	0	0	11	0
4	B	20	0	0	6	0
4	C	21	0	0	7	0
4	D	21	0	0	11	0
All	All	3591	3402	3390	352	2

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 51.

All (352) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:CYS:SG	2:B:201:HEC:HAB	1.89	1.12
1:C:61:PHE:O	2:C:201:HEC:HBC1	1.62	1.00
1:D:101:CYS:SG	2:D:201:HEC:HAC	2.03	0.99
1:B:89:ALA:O	1:B:93:GLN:HG2	1.64	0.95
1:B:101:CYS:SG	2:B:201:HEC:HAC	2.06	0.95
1:D:103:GLN:O	1:D:103:GLN:NE2	1.99	0.94
1:A:14:LEU:O	4:A:301:HOH:O	1.85	0.94
2:B:201:HEC:HMB1	2:B:201:HEC:HBB3	1.53	0.91
1:B:96:CYS:HG	3:C:202:CU:CU	0.83	0.88
1:A:96:CYS:HG	3:A:203:CU:CU	0.57	0.88
1:B:101:CYS:SG	2:B:201:HEC:CAC	2.65	0.85
1:A:96:CYS:SG	3:A:203:CU:CU	1.68	0.84
1:B:59:HIS:O	4:B:301:HOH:O	1.95	0.83
1:D:74:ALA:O	4:D:301:HOH:O	1.96	0.83
1:A:92:GLU:OE2	4:A:302:HOH:O	1.99	0.81
1:A:14:LEU:HD12	2:A:201:HEC:HMB1	1.62	0.81
1:D:76:LEU:O	1:D:80:ASN:ND2	2.14	0.80
1:B:22:ASN:OD1	1:B:24:ALA:N	2.15	0.79
1:C:10:LEU:HD13	2:C:201:HEC:HBB2	1.64	0.78
1:D:41:TRP:CZ3	1:D:69:ILE:HD11	2.20	0.77
1:B:5:ASP:OD1	1:B:5:ASP:N	2.19	0.76
1:C:65:PHE:CE2	2:C:201:HEC:HBC2	2.21	0.76
1:A:99:ASN:O	1:A:101:CYS:N	2.18	0.75
1:B:59:HIS:HD2	1:C:96:CYS:HB3	1.52	0.74
1:D:101:CYS:SG	2:D:201:HEC:CAC	2.74	0.74
1:D:8:GLU:O	1:D:12:ASP:N	2.19	0.74
1:B:13:ASN:HB3	1:B:29:ALA:HB1	1.68	0.74
1:B:106:ARG:HD2	2:B:201:HEC:HHA	1.69	0.74
1:B:59:HIS:CD2	1:C:96:CYS:HB3	2.22	0.73
1:C:102:HIS:NE2	2:C:201:HEC:NB	2.36	0.73
1:D:53:PRO:HA	1:D:58:MET:HG2	1.70	0.73
2:D:201:HEC:HMC1	2:D:201:HEC:HBC3	1.69	0.72
1:B:21:ASP:HB2	1:B:25:GLN:OE1	1.90	0.71
1:C:98:CYS:SG	2:C:201:HEC:CAB	2.79	0.70
1:B:96:CYS:SG	3:C:202:CU:CU	1.82	0.70
1:B:26:VAL:HG21	1:B:84[B]:VAL:CG1	2.22	0.69
1:B:37:ALA:O	1:B:39:ASP:N	2.24	0.69
1:D:55:SER:OG	1:D:58:MET:N	2.24	0.69
1:D:20:ALA:HB1	1:D:25:GLN:HG2	1.73	0.69
1:A:76:LEU:CD2	1:B:41:TRP:CZ3	2.75	0.69
2:A:201:HEC:HMC1	2:A:201:HEC:CBC	2.23	0.68
1:A:14:LEU:CD1	2:A:201:HEC:HMB1	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:VAL:HG21	1:B:84[A]:VAL:CG1	2.22	0.68
1:C:31:THR:HG22	1:C:32[B]:LYS:HE2	1.76	0.68
1:C:65:PHE:CZ	2:C:201:HEC:HBC2	2.29	0.68
1:D:5:ASP:OD2	4:D:303:HOH:O	2.11	0.68
1:B:37:ALA:O	1:B:40:ALA:N	2.28	0.67
2:D:201:HEC:HBD2	2:D:201:HEC:HHA	1.76	0.67
1:B:65:PHE:CD1	2:B:201:HEC:HBC2	2.30	0.67
1:C:67:ILE:O	1:C:70:GLY:N	2.28	0.66
1:C:80:ASN:O	4:C:302:HOH:O	2.14	0.66
1:A:86:GLU:OE1	1:A:86:GLU:N	2.21	0.66
1:B:41:TRP:CZ3	1:B:69:ILE:HD12	2.30	0.66
1:A:76:LEU:HD23	1:B:41:TRP:CH2	2.31	0.66
1:D:3:LEU:CD2	1:D:43:ALA:HB1	2.26	0.66
2:A:201:HEC:HMC1	2:A:201:HEC:HBC3	1.77	0.66
1:A:66:TRP:HD1	1:B:77:HIS:HB2	1.60	0.65
1:D:57:GLU:O	4:D:304:HOH:O	2.14	0.65
1:B:10:LEU:HB3	2:B:201:HEC:HBB2	1.77	0.65
1:C:17:ILE:HG23	1:C:26:VAL:HG23	1.79	0.65
1:D:78:LEU:HB2	1:D:87:ALA:HB2	1.79	0.65
1:A:60:ASP:O	1:A:63[A]:HIS:CD2	2.50	0.64
1:A:76:LEU:HD23	1:B:41:TRP:CZ3	2.32	0.64
1:B:65:PHE:O	1:B:69:ILE:HG13	1.98	0.64
1:D:27:LYS:NZ	4:D:305:HOH:O	2.22	0.63
1:B:41:TRP:HZ3	1:B:69:ILE:HD12	1.62	0.63
1:A:76:LEU:HD21	1:B:41:TRP:CE3	2.34	0.62
2:B:201:HEC:HMC1	2:B:201:HEC:HBC3	1.80	0.62
1:A:44:THR:OG1	4:A:303:HOH:O	2.15	0.61
1:A:77:HIS:HB2	1:B:66:TRP:CD1	2.35	0.61
1:A:90:ALA:O	1:A:94:LEU:HD23	1.99	0.61
1:C:48:LEU:HD12	1:C:51:LYS:HB2	1.83	0.61
2:C:201:HEC:HBC3	2:C:201:HEC:HMC1	1.83	0.61
1:C:24:ALA:O	1:C:28:ASP:N	2.27	0.61
1:D:72:ILE:HG12	1:D:94:LEU:HD11	1.81	0.61
1:D:65:PHE:O	1:D:69:ILE:HG12	2.00	0.61
1:B:101:CYS:HA	1:B:104:LYS:HE3	1.83	0.61
1:B:98:CYS:SG	2:B:201:HEC:CAB	2.79	0.61
1:B:58:MET:O	1:B:62:ARG:HB2	2.01	0.61
2:B:201:HEC:HBB3	2:B:201:HEC:CMB	2.30	0.60
1:C:24:ALA:HA	1:C:27[A]:LYS:HB3	1.83	0.60
1:D:32:LYS:HG3	4:D:302:HOH:O	2.00	0.60
1:C:95:LYS:HE2	1:C:96:CYS:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLU:OE1	3:B:202:CU:CU	1.51	0.60
1:B:106:ARG:NH2	4:B:306:HOH:O	2.34	0.60
1:C:98:CYS:SG	2:C:201:HEC:HAB	2.42	0.59
1:D:13:ASN:HB3	1:D:29:ALA:HB1	1.85	0.59
1:B:9:THR:O	1:B:13:ASN:ND2	2.36	0.59
1:C:13:ASN:HA	1:C:16:VAL:HG12	1.83	0.58
1:D:102:HIS:NE2	2:D:201:HEC:NC	2.51	0.58
1:B:41:TRP:CE3	1:B:69:ILE:HD11	2.39	0.58
1:A:33:MET:O	1:A:36:ALA:HB3	2.03	0.58
1:B:93:GLN:HE22	1:D:86:GLU:HB3	1.68	0.58
1:A:76:LEU:CD2	1:B:41:TRP:CE3	2.86	0.58
1:A:88:GLN:O	1:A:91:ALA:HB3	2.04	0.57
1:D:96:CYS:HA	1:D:99:ASN:HB2	1.87	0.57
1:B:26:VAL:HG21	1:B:84[B]:VAL:HG12	1.86	0.57
1:C:95:LYS:HE2	1:C:96:CYS:CA	2.34	0.57
1:D:3:LEU:HD23	1:D:43:ALA:HB1	1.85	0.57
1:A:83:LYS:HB3	1:A:86:GLU:HG2	1.87	0.56
1:A:83:LYS:HB3	1:A:86:GLU:CG	2.35	0.56
1:D:60:ASP:HB3	4:D:304:HOH:O	2.05	0.56
1:C:12:ASP:O	1:C:15:LYS:N	2.39	0.56
1:C:67:ILE:O	1:C:68:LEU:C	2.44	0.56
1:A:68:LEU:HD13	2:A:201:HEC:HMC3	1.88	0.56
1:B:77:HIS:CD2	1:B:77:HIS:O	2.59	0.55
1:C:68:LEU:HD11	1:C:94:LEU:HD21	1.87	0.55
1:D:3:LEU:HD13	1:D:45:PRO:HA	1.89	0.55
1:A:85:LYS:O	1:A:88:GLN:HB2	2.06	0.55
1:B:41:TRP:HA	1:B:65:PHE:CD2	2.42	0.55
1:D:47:LYS:HE3	1:D:106:ARG:O	2.07	0.55
1:D:32:LYS:N	4:D:302:HOH:O	2.40	0.55
1:C:45:PRO:HB2	1:C:46:PRO:HD2	1.89	0.54
1:D:69:ILE:HA	1:D:72:ILE:HG13	1.89	0.54
1:C:28:ASP:O	1:C:31:THR:HB	2.07	0.54
1:A:38:ALA:O	1:A:41:TRP:HB2	2.06	0.54
1:B:95[A]:LYS:HA	1:B:98:CYS:SG	2.48	0.54
1:C:12:ASP:O	1:C:15:LYS:HB2	2.08	0.54
1:D:33:MET:HB3	1:D:72:ILE:HD13	1.90	0.54
1:A:41:TRP:CE3	1:B:76:LEU:HD23	2.43	0.54
1:D:11:ASN:OD1	2:D:201:HEC:HMA1	2.09	0.53
1:A:98:CYS:HB3	2:A:201:HEC:C4B	2.39	0.53
2:D:201:HEC:CBB	2:D:201:HEC:HHC	2.39	0.53
1:B:13:ASN:HB3	1:B:29:ALA:CB	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:CYS:SG	1:C:63:HIS:CE1	3.01	0.53
1:D:28:ASP:O	1:D:32:LYS:HG3	2.09	0.53
1:A:16:VAL:O	1:A:19:LYS:N	2.40	0.53
1:A:18:GLU:N	4:A:301:HOH:O	2.04	0.53
1:D:3:LEU:HD21	1:D:43:ALA:HB1	1.91	0.53
2:D:201:HEC:HMC1	2:D:201:HEC:CBC	2.38	0.53
1:A:51:LYS:HD2	1:A:51:LYS:N	2.24	0.53
1:D:11:ASN:O	1:D:11:ASN:ND2	2.38	0.53
1:D:99:ASN:O	1:D:100:ALA:C	2.46	0.52
1:B:41:TRP:CZ3	1:B:69:ILE:CD1	2.92	0.52
1:C:89:ALA:HB2	4:C:301:HOH:O	2.09	0.52
2:D:201:HEC:HHA	2:D:201:HEC:CBD	2.39	0.52
2:D:201:HEC:HHC	2:D:201:HEC:HBB3	1.90	0.52
1:A:67:ILE:HG12	1:D:67:ILE:HD11	1.92	0.52
1:C:71:GLN:HB2	1:C:94:LEU:HD12	1.91	0.52
1:B:100:ALA:HB1	1:C:60:ASP:HB2	1.91	0.52
1:C:93:GLN:C	1:C:95:LYS:N	2.63	0.52
1:D:60:ASP:OD2	1:D:105:TYR:OH	2.22	0.51
1:D:71[A]:GLN:HG3	1:D:94:LEU:HD12	1.91	0.51
1:D:102:HIS:CD2	1:D:106:ARG:NH1	2.78	0.51
1:B:59:HIS:HD2	1:C:96:CYS:CB	2.21	0.51
1:A:27:LYS:HD3	1:A:80:ASN:CG	2.30	0.51
1:B:92:GLU:O	1:B:94:LEU:N	2.43	0.51
1:B:14:LEU:HD11	1:B:91:ALA:O	2.11	0.51
1:B:22:ASN:OD1	1:B:25:GLN:N	2.36	0.51
1:B:26:VAL:HG21	1:B:84[A]:VAL:HG12	1.86	0.51
1:C:58[B]:MET:HE2	1:C:58[B]:MET:HA	1.92	0.51
1:A:63[A]:HIS:CD2	1:A:64:GLY:N	2.78	0.51
1:C:28:ASP:O	1:C:31:THR:N	2.44	0.51
1:C:51:LYS:HD3	1:C:57:GLU:CD	2.32	0.51
1:D:41:TRP:HD1	1:D:41:TRP:O	1.94	0.51
1:A:28:ASP:O	1:A:32:LYS:HG3	2.11	0.50
1:A:67:ILE:O	1:A:70:GLY:N	2.29	0.50
1:B:77:HIS:CD2	1:B:81:GLU:OE2	2.64	0.50
1:D:13:ASN:O	1:D:17:ILE:HG12	2.11	0.50
1:A:22:ASN:CG	1:A:25:GLN:OE1	2.50	0.50
1:A:85:LYS:O	1:A:88:GLN:N	2.44	0.50
1:B:98:CYS:O	1:B:102:HIS:CD2	2.64	0.50
1:C:15:LYS:O	1:C:19:LYS:HE3	2.12	0.50
1:B:55:SER:O	1:B:59:HIS:ND1	2.40	0.50
1:B:65:PHE:CE1	2:B:201:HEC:HBC2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ASP:O	1:C:29:ALA:C	2.50	0.50
1:D:13:ASN:HD21	1:D:32:LYS:HE3	1.76	0.50
1:D:45:PRO:HB3	1:D:46:PRO:HD2	1.94	0.50
1:D:72:ILE:O	1:D:75:ALA:HB3	2.11	0.50
1:B:96:CYS:SG	1:C:63:HIS:NE2	2.82	0.50
1:D:23:ALA:O	1:D:27:LYS:HG3	2.11	0.50
1:D:86:GLU:N	1:D:86:GLU:CD	2.64	0.50
1:B:50:ASP:OD1	1:B:50:ASP:N	2.43	0.50
1:B:86:GLU:N	1:B:86:GLU:OE1	2.44	0.50
1:A:60:ASP:O	1:A:63[A]:HIS:HD2	1.93	0.49
1:B:104:LYS:HB2	1:B:105:TYR:CD2	2.47	0.49
4:B:303:HOH:O	1:C:100:ALA:HB1	2.10	0.49
1:C:73:HIS:HE1	1:D:73:HIS:CE1	2.30	0.49
1:B:41:TRP:HD1	1:B:41:TRP:O	1.96	0.49
1:B:104:LYS:HD2	1:B:105:TYR:CE2	2.46	0.49
1:C:94:LEU:O	1:C:95:LYS:C	2.51	0.49
1:D:67:ILE:HG22	1:D:71[A]:GLN:OE1	2.12	0.49
1:A:91:ALA:HA	1:A:94:LEU:HD23	1.95	0.49
1:A:76:LEU:HG	1:A:80:ASN:HD22	1.78	0.49
1:C:23:ALA:O	1:C:26:VAL:N	2.45	0.49
1:C:65:PHE:CD2	2:C:201:HEC:HBC2	2.47	0.49
1:C:69:ILE:HD12	1:D:73:HIS:CD2	2.47	0.49
1:A:14:LEU:C	4:A:301:HOH:O	2.41	0.49
1:B:33:MET:O	1:B:37:ALA:N	2.47	0.48
1:D:106:ARG:NH2	4:D:308:HOH:O	2.45	0.48
4:A:321:HOH:O	1:D:66:TRP:HZ2	1.95	0.48
1:C:2:ASP:OD2	1:C:4:GLU:HB2	2.13	0.48
1:D:84:VAL:O	1:D:88:GLN:HG3	2.14	0.48
1:A:34:ALA:HB3	4:A:307:HOH:O	2.12	0.48
1:A:9:THR:O	1:A:13:ASN:ND2	2.47	0.48
1:B:13:ASN:O	1:B:16:VAL:HG22	2.13	0.48
1:D:51:LYS:HD3	1:D:57:GLU:OE1	2.14	0.48
1:D:102:HIS:NE2	2:D:201:HEC:NB	2.62	0.48
1:C:68:LEU:O	1:C:72:ILE:HG13	2.13	0.48
1:C:69:ILE:HG22	1:C:73:HIS:CE1	2.49	0.48
1:B:68:LEU:HD12	1:B:71:GLN:OE1	2.14	0.48
1:C:26:VAL:O	1:C:30:LEU:HD12	2.14	0.48
1:B:77:HIS:NE2	1:B:81:GLU:OE1	2.47	0.47
1:A:17:ILE:N	4:A:301:HOH:O	2.46	0.47
1:A:48:LEU:HD21	1:A:105:TYR:CD1	2.49	0.47
1:A:63[B]:HIS:CD2	1:B:81:GLU:OE2	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ILE:O	1:B:20:ALA:HB2	2.14	0.47
1:C:43:ALA:HB2	4:C:304:HOH:O	2.15	0.47
1:A:18:GLU:O	4:A:304:HOH:O	2.20	0.47
1:A:57:GLU:OE2	1:D:103:GLN:HG3	2.14	0.47
1:A:66:TRP:CD1	1:B:77:HIS:HB2	2.44	0.47
1:A:72:ILE:HG13	1:A:94:LEU:HD11	1.95	0.47
1:A:90:ALA:O	1:A:94:LEU:CD2	2.62	0.47
1:A:15:LYS:HG2	1:A:19:LYS:HD3	1.97	0.47
1:A:67:ILE:HG23	1:D:66:TRP:CE3	2.49	0.47
1:B:1:ALA:N	1:B:39:ASP:OD2	2.39	0.47
1:D:45:PRO:CB	1:D:46:PRO:HD2	2.44	0.47
1:D:27:LYS:O	1:D:30:LEU:N	2.47	0.47
1:B:2:ASP:HB3	1:B:5:ASP:OD1	2.15	0.47
1:B:41:TRP:CE3	1:B:69:ILE:CD1	2.97	0.47
1:B:54:ASP:O	1:B:59:HIS:HE1	1.98	0.47
1:C:72:ILE:HG12	1:C:94:LEU:HD11	1.96	0.47
1:A:48:LEU:HA	1:A:51:LYS:HD3	1.96	0.47
1:A:91:ALA:CA	1:A:94:LEU:HD23	2.44	0.47
1:C:45:PRO:HB3	2:C:201:HEC:CMD	2.45	0.47
1:B:37:ALA:O	1:B:38:ALA:C	2.53	0.46
1:A:99:ASN:O	1:A:100:ALA:C	2.54	0.46
1:B:67:ILE:HA	4:B:317:HOH:O	2.14	0.46
1:D:59:HIS:O	1:D:63:HIS:CD2	2.69	0.46
1:A:14:LEU:HD12	2:A:201:HEC:CMB	2.40	0.46
1:B:53:PRO:HA	1:B:58:MET:HG2	1.96	0.46
1:C:20:ALA:HB2	1:C:25:GLN:HB3	1.97	0.46
1:C:31:THR:HG22	1:C:32[B]:LYS:CE	2.45	0.46
1:C:101:CYS:HB3	2:C:201:HEC:CAC	2.45	0.46
1:C:42:SER:OG	1:D:27:LYS:HD3	2.16	0.46
1:C:104:LYS:HE2	1:C:105:TYR:CE2	2.51	0.46
4:C:311:HOH:O	1:D:74:ALA:HB2	2.15	0.46
1:B:33:MET:HA	1:B:36:ALA:HB3	1.97	0.46
1:B:96:CYS:HG	1:C:63:HIS:CE1	2.33	0.46
1:C:68:LEU:HD22	2:C:201:HEC:HMC2	1.98	0.46
1:A:22:ASN:OD1	1:A:25:GLN:OE1	2.33	0.45
1:A:60:ASP:HB2	1:D:100:ALA:HB1	1.97	0.45
1:A:101:CYS:O	1:A:103:GLN:N	2.49	0.45
1:C:3:LEU:O	1:C:4:GLU:C	2.55	0.45
1:A:66:TRP:HZ2	4:D:321:HOH:O	1.99	0.45
1:C:95:LYS:HE2	1:C:96:CYS:N	2.31	0.45
1:A:59:HIS:ND1	1:B:81:GLU:HG2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ALA:O	1:B:94:LEU:HD13	2.17	0.45
1:B:77:HIS:HD2	1:B:81:GLU:OE2	2.00	0.45
1:C:43:ALA:HB1	4:C:317:HOH:O	2.17	0.45
1:D:41:TRP:O	1:D:41:TRP:CD1	2.70	0.45
1:B:66:TRP:O	1:B:67:ILE:C	2.55	0.45
1:C:37:ALA:HB3	1:C:69:ILE:HD11	1.97	0.45
1:C:50:ASP:OD1	1:C:51:LYS:N	2.50	0.45
1:A:95:LYS:HE2	4:A:322:HOH:O	2.17	0.45
1:B:40:ALA:HB1	1:B:65:PHE:CZ	2.52	0.45
1:A:17:ILE:HB	4:A:301:HOH:O	2.17	0.45
1:B:47:LYS:HE2	1:B:47:LYS:HA	1.98	0.44
1:C:97:THR:HG22	1:C:97:THR:O	2.17	0.44
1:A:91:ALA:HA	1:A:94:LEU:CD2	2.47	0.44
1:D:46:PRO:HD2	4:D:311:HOH:O	2.17	0.44
1:D:85:LYS:HD2	1:D:88:GLN:OE1	2.17	0.44
1:A:34:ALA:O	1:A:35:ALA:C	2.55	0.44
1:B:77:HIS:CD2	1:B:81:GLU:CD	2.91	0.44
1:C:86:GLU:OE1	1:C:86:GLU:N	2.46	0.44
1:B:101:CYS:O	1:B:102:HIS:C	2.56	0.44
1:C:102:HIS:NE2	2:C:201:HEC:NA	2.64	0.44
1:D:83:LYS:HD3	1:D:83:LYS:N	2.33	0.44
1:B:27:LYS:HD3	1:B:80:ASN:OD1	2.18	0.44
1:A:27:LYS:HD3	1:A:80:ASN:OD1	2.17	0.44
1:B:17:ILE:O	1:B:20:ALA:CB	2.66	0.44
1:D:67:ILE:O	1:D:70:GLY:N	2.50	0.44
1:D:68:LEU:O	1:D:70:GLY:N	2.51	0.44
1:C:24:ALA:HA	1:C:27[B]:LYS:HB3	2.00	0.43
1:C:102:HIS:CE1	2:C:201:HEC:C1B	3.01	0.43
1:B:67:ILE:O	1:B:68:LEU:C	2.54	0.43
1:C:17:ILE:HD11	1:C:30:LEU:HG	2.00	0.43
1:C:66:TRP:O	1:C:67:ILE:C	2.56	0.43
1:D:3:LEU:CD1	1:D:45:PRO:HA	2.48	0.43
1:B:69:ILE:HG22	1:B:73:HIS:CD2	2.52	0.43
1:C:15:LYS:O	1:C:19:LYS:HB2	2.19	0.43
1:C:50:ASP:OD1	1:C:50:ASP:C	2.57	0.43
1:A:56:PRO:HG2	1:D:103:GLN:HG2	2.00	0.43
1:A:104:LYS:O	1:A:105:TYR:CD1	2.72	0.43
1:C:102:HIS:CE1	2:C:201:HEC:NB	2.86	0.43
1:A:17:ILE:O	1:A:88:GLN:HG2	2.18	0.42
1:B:69:ILE:HG13	1:B:69:ILE:H	1.58	0.42
1:B:106:ARG:HD2	2:B:201:HEC:CHA	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:HIS:HA	1:B:41:TRP:CZ2	2.54	0.42
1:B:43:ALA:O	1:B:61:PHE:HE2	2.02	0.42
4:B:303:HOH:O	1:C:100:ALA:CB	2.65	0.42
1:A:31:THR:O	1:A:34:ALA:HB3	2.19	0.42
1:D:101:CYS:CB	2:D:201:HEC:CAC	2.98	0.42
1:A:48:LEU:HA	1:A:51:LYS:CD	2.50	0.42
1:A:66:TRP:HZ3	1:D:66:TRP:CZ3	2.37	0.42
1:B:95[B]:LYS:HA	1:B:98:CYS:SG	2.60	0.42
1:C:24:ALA:HA	1:C:27[C]:LYS:HB3	2.01	0.42
1:C:88:GLN:C	1:C:90:ALA:N	2.74	0.42
1:B:40:ALA:O	1:B:41:TRP:C	2.56	0.41
1:C:30:LEU:HD22	1:C:72:ILE:HG23	2.02	0.41
1:D:63:HIS:O	1:D:67:ILE:HG12	2.19	0.41
1:B:59:HIS:HD1	1:B:59:HIS:H	1.67	0.41
1:C:85[A]:LYS:HG2	4:C:316:HOH:O	2.19	0.41
1:A:61:PHE:HD1	1:A:105:TYR:CD2	2.39	0.41
1:B:30:LEU:HD22	1:B:75:ALA:HB3	2.02	0.41
1:C:73:HIS:O	1:C:76:LEU:N	2.48	0.41
1:D:46:PRO:HG2	4:D:311:HOH:O	2.21	0.41
1:D:68:LEU:O	1:D:71[A]:GLN:HG2	2.20	0.41
1:C:106:ARG:HH11	2:C:201:HEC:C2A	2.33	0.41
1:D:41:TRP:HA	1:D:65:PHE:CD2	2.56	0.41
1:A:66:TRP:HE1	1:B:74:ALA:HA	1.85	0.41
1:B:60:ASP:CG	1:C:104:LYS:HD2	2.41	0.41
1:D:24:ALA:HA	1:D:27:LYS:HE2	2.03	0.41
1:B:3:LEU:HD23	1:B:45:PRO:HA	2.01	0.41
1:B:3:LEU:HD22	1:B:43:ALA:HB3	2.03	0.41
1:D:3:LEU:O	1:D:7:MET:HG2	2.20	0.41
1:A:91:ALA:C	1:A:94:LEU:HD23	2.40	0.41
1:A:67:ILE:HB	1:A:68:LEU:H	1.60	0.41
1:A:14:LEU:HG	1:A:33:MET:HE3	2.03	0.41
1:B:41:TRP:O	1:B:41:TRP:CD1	2.72	0.41
1:B:45:PRO:HB3	2:B:201:HEC:CMD	2.51	0.41
1:B:65:PHE:O	1:B:66:TRP:C	2.59	0.41
1:C:3:LEU:O	1:C:6:ASN:HB2	2.21	0.41
1:C:7:MET:HE3	2:C:201:HEC:NC	2.36	0.41
1:C:11:ASN:HD22	2:C:201:HEC:HHB	1.86	0.41
1:C:68:LEU:O	1:C:71:GLN:N	2.54	0.41
1:C:106:ARG:HH11	2:C:201:HEC:C1A	2.32	0.41
1:C:20:ALA:CB	1:C:25:GLN:HB3	2.51	0.41
1:D:34:ALA:O	1:D:35:ALA:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:PRO:HA	1:C:58[A]:MET:CE	2.50	0.40
1:C:73:HIS:O	1:C:76:LEU:HB3	2.21	0.40
1:A:48:LEU:HD21	1:A:105:TYR:HD1	1.85	0.40
1:A:64:GLY:HA2	1:A:67:ILE:HG13	2.02	0.40
1:A:69:ILE:O	1:A:69:ILE:CG2	2.67	0.40
1:C:68:LEU:HD12	1:C:68:LEU:HA	1.95	0.40
2:B:201:HEC:HMC1	2:B:201:HEC:CBC	2.48	0.40
1:C:3:LEU:HB2	1:C:43:ALA:HB3	2.04	0.40
1:C:98:CYS:CB	2:C:201:HEC:CAB	2.98	0.40
1:A:99:ASN:O	1:A:102:HIS:N	2.55	0.40
1:B:102:HIS:CE1	4:B:313:HOH:O	2.75	0.40
1:D:49:GLU:O	1:D:50:ASP:C	2.60	0.40
1:A:26:VAL:HG12	1:A:79:ALA:HB2	2.04	0.40
1:C:22:ASN:O	1:C:26:VAL:HG12	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ARG:OXT	1:D:19:LYS:NZ[2_555]	1.69	0.51
1:B:106:ARG:OXT	1:D:19:LYS:HZ3[2_555]	1.41	0.19

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	105/106 (99%)	76 (72%)	19 (18%)	10 (10%)	0	0
1	B	108/106 (102%)	88 (82%)	15 (14%)	5 (5%)	2	4
1	C	111/106 (105%)	86 (78%)	19 (17%)	6 (5%)	2	3
1	D	105/106 (99%)	85 (81%)	13 (12%)	7 (7%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	429/424 (101%)	335 (78%)	66 (15%)	28 (6%)	1 2

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ALA
1	A	68	LEU
1	A	102	HIS
1	B	38	ALA
1	C	23	ALA
1	C	94	LEU
1	A	43	ALA
1	A	100	ALA
1	C	67	ILE
1	C	89	ALA
1	D	99	ASN
1	D	100	ALA
1	A	35	ALA
1	A	104	LYS
1	B	37	ALA
1	B	41	TRP
1	B	66	TRP
1	C	77	HIS
1	D	2	ASP
1	D	27	LYS
1	D	68	LEU
1	A	94	LEU
1	A	99	ASN
1	D	20	ALA
1	A	67	ILE
1	B	12	ASP
1	C	66	TRP
1	D	94	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/83 (101%)	77 (92%)	7 (8%)	11	25
1	B	87/83 (105%)	76 (87%)	11 (13%)	4	10
1	C	90/83 (108%)	78 (87%)	12 (13%)	4	9
1	D	84/83 (101%)	79 (94%)	5 (6%)	19	42
All	All	345/332 (104%)	310 (90%)	35 (10%)	11	17

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	42	SER
1	A	51	LYS
1	A	63[A]	HIS
1	A	63[B]	HIS
1	A	76	LEU
1	A	95	LYS
1	B	5	ASP
1	B	19	LYS
1	B	21	ASP
1	B	42[A]	SER
1	B	42[B]	SER
1	B	52	SER
1	B	66	TRP
1	B	84[A]	VAL
1	B	84[B]	VAL
1	B	95[A]	LYS
1	B	95[B]	LYS
1	C	2	ASP
1	C	3	LEU
1	C	19	LYS
1	C	27[A]	LYS
1	C	27[B]	LYS
1	C	27[C]	LYS
1	C	28	ASP
1	C	32[A]	LYS
1	C	32[B]	LYS
1	C	49	GLU
1	C	92	GLU
1	C	103	GLN
1	D	11	ASN
1	D	19	LYS
1	D	50	ASP

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Mol	Chain	Res	Type
1	D	81	GLU
1	D	92	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	13	ASN
1	B	102	HIS
1	C	73	HIS
1	D	13	ASN
1	D	63	HIS
1	D	80	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEC	C	201	1	32,50,50	2.23	6 (18%)	24,82,82	2.01	8 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	A	201	1	32,50,50	2.47	9 (28%)	24,82,82	1.93	8 (33%)
2	HEC	B	201	1	32,50,50	2.56	6 (18%)	24,82,82	2.26	9 (37%)
2	HEC	D	201	1	32,50,50	2.68	8 (25%)	24,82,82	2.13	6 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	C	201	1	-	4/10/54/54	-
2	HEC	A	201	1	-	5/10/54/54	-
2	HEC	B	201	1	-	2/10/54/54	-
2	HEC	D	201	1	-	7/10/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	HEC	C2B-C3B	-8.72	1.31	1.40
2	D	201	HEC	C2B-C3B	-8.38	1.32	1.40
2	B	201	HEC	C3C-C2C	-7.59	1.32	1.40
2	D	201	HEC	C3C-C2C	-7.32	1.33	1.40
2	C	201	HEC	C3C-C2C	-7.23	1.33	1.40
2	A	201	HEC	C3C-C2C	-7.15	1.33	1.40
2	A	201	HEC	C3D-C2D	6.02	1.55	1.37
2	D	201	HEC	C3D-C2D	5.68	1.54	1.37
2	C	201	HEC	C2B-C3B	-5.50	1.35	1.40
2	C	201	HEC	C3D-C2D	5.37	1.53	1.37
2	A	201	HEC	C2B-C3B	-4.61	1.35	1.40
2	B	201	HEC	C3D-C2D	4.61	1.51	1.37
2	D	201	HEC	CAA-C2A	4.17	1.59	1.52
2	A	201	HEC	CAD-C3D	4.10	1.58	1.52
2	A	201	HEC	CAA-C2A	3.34	1.58	1.52
2	A	201	HEC	C4D-ND	3.21	1.42	1.36
2	A	201	HEC	C3C-C4C	3.00	1.48	1.43
2	D	201	HEC	C2A-C1A	2.76	1.48	1.42
2	D	201	HEC	C4D-ND	2.52	1.41	1.36
2	D	201	HEC	CAD-C3D	2.47	1.55	1.52
2	A	201	HEC	C2A-C1A	2.45	1.48	1.42
2	B	201	HEC	C2A-C1A	2.30	1.47	1.42
2	A	201	HEC	CMD-C2D	2.30	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	HEC	CAD-C3D	2.27	1.55	1.52
2	C	201	HEC	C1C-CHC	-2.21	1.34	1.41
2	B	201	HEC	C3C-C4C	2.21	1.47	1.43
2	C	201	HEC	C1B-CHB	-2.19	1.34	1.41
2	D	201	HEC	C3A-C4A	2.13	1.47	1.42
2	B	201	HEC	CAA-C2A	2.01	1.55	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	HEC	CMC-C2C-C1C	-5.94	119.34	128.46
2	C	201	HEC	CMC-C2C-C1C	-5.91	119.38	128.46
2	D	201	HEC	CMC-C2C-C1C	-5.61	119.84	128.46
2	B	201	HEC	CBD-CAD-C3D	-4.63	104.72	112.62
2	A	201	HEC	CMC-C2C-C1C	-4.53	121.50	128.46
2	D	201	HEC	CBA-CAA-C2A	4.04	119.41	112.60
2	A	201	HEC	CMC-C2C-C3C	-3.77	121.39	125.82
2	D	201	HEC	CMD-C2D-C1D	-3.72	122.75	128.46
2	D	201	HEC	CMC-C2C-C3C	-3.16	122.11	125.82
2	B	201	HEC	C1D-C2D-C3D	-3.07	104.86	107.00
2	A	201	HEC	CBD-CAD-C3D	2.95	117.65	112.62
2	D	201	HEC	CMD-C2D-C3D	2.89	130.39	124.94
2	B	201	HEC	O2A-CGA-CBA	2.89	123.31	114.03
2	C	201	HEC	CMB-C2B-C3B	2.76	129.07	125.82
2	B	201	HEC	C2B-C3B-C4B	2.65	109.22	106.35
2	B	201	HEC	CMC-C2C-C3C	-2.62	122.74	125.82
2	C	201	HEC	CMC-C2C-C3C	2.57	128.84	125.82
2	C	201	HEC	CMD-C2D-C1D	-2.53	124.57	128.46
2	A	201	HEC	CAD-CBD-CGD	-2.46	106.86	113.76
2	C	201	HEC	C2B-C3B-C4B	2.45	109.00	106.35
2	C	201	HEC	CMA-C3A-C2A	2.42	129.50	124.94
2	B	201	HEC	CMA-C3A-C2A	2.34	129.36	124.94
2	B	201	HEC	O1A-CGA-CBA	-2.31	115.67	123.08
2	A	201	HEC	C3C-C4C-NC	-2.29	106.61	110.94
2	A	201	HEC	CMB-C2B-C3B	2.18	128.38	125.82
2	D	201	HEC	CBD-CAD-C3D	2.14	116.27	112.62
2	C	201	HEC	CMB-C2B-C1B	-2.12	125.20	128.46
2	B	201	HEC	O1D-CGD-CBD	-2.08	116.41	123.08
2	C	201	HEC	O1A-CGA-CBA	-2.06	116.46	123.08
2	A	201	HEC	CMB-C2B-C1B	-2.06	125.30	128.46
2	A	201	HEC	CBA-CAA-C2A	2.01	115.99	112.60

There are no chirality outliers.

All (18) torsion outliers are listed below:

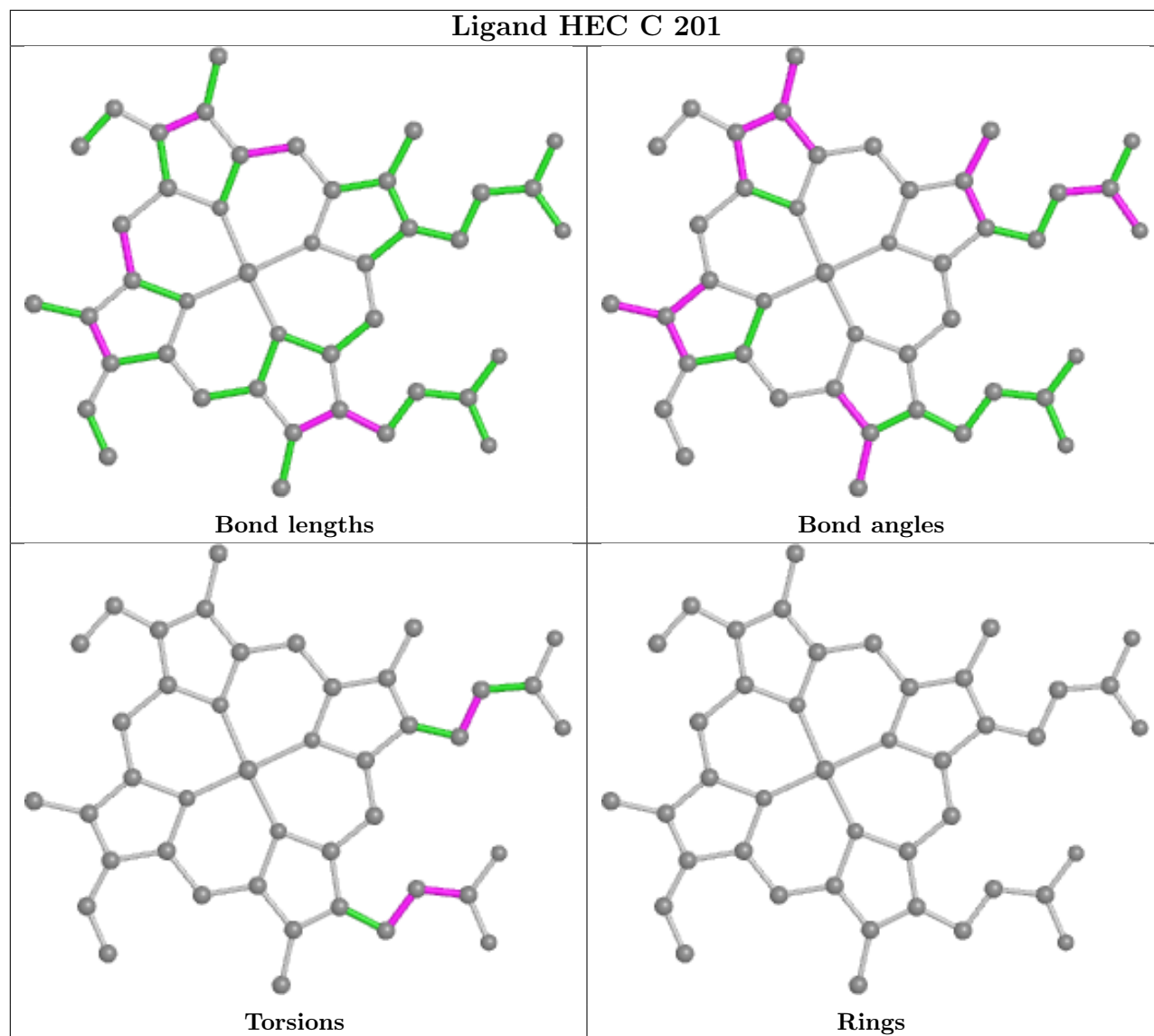
Mol	Chain	Res	Type	Atoms
2	A	201	HEC	C1A-C2A-CAA-CBA
2	A	201	HEC	C3A-C2A-CAA-CBA
2	A	201	HEC	C2D-C3D-CAD-CBD
2	A	201	HEC	C4D-C3D-CAD-CBD
2	D	201	HEC	C2D-C3D-CAD-CBD
2	D	201	HEC	C4D-C3D-CAD-CBD
2	A	201	HEC	C3D-CAD-CBD-CGD
2	C	201	HEC	C2A-CAA-CBA-CGA
2	D	201	HEC	C3D-CAD-CBD-CGD
2	B	201	HEC	C1A-C2A-CAA-CBA
2	B	201	HEC	C3A-C2A-CAA-CBA
2	C	201	HEC	C3D-CAD-CBD-CGD
2	D	201	HEC	CAD-CBD-CGD-O1D
2	D	201	HEC	CAA-CBA-CGA-O1A
2	D	201	HEC	CAD-CBD-CGD-O2D
2	C	201	HEC	CAD-CBD-CGD-O2D
2	C	201	HEC	CAD-CBD-CGD-O1D
2	D	201	HEC	CAA-CBA-CGA-O2A

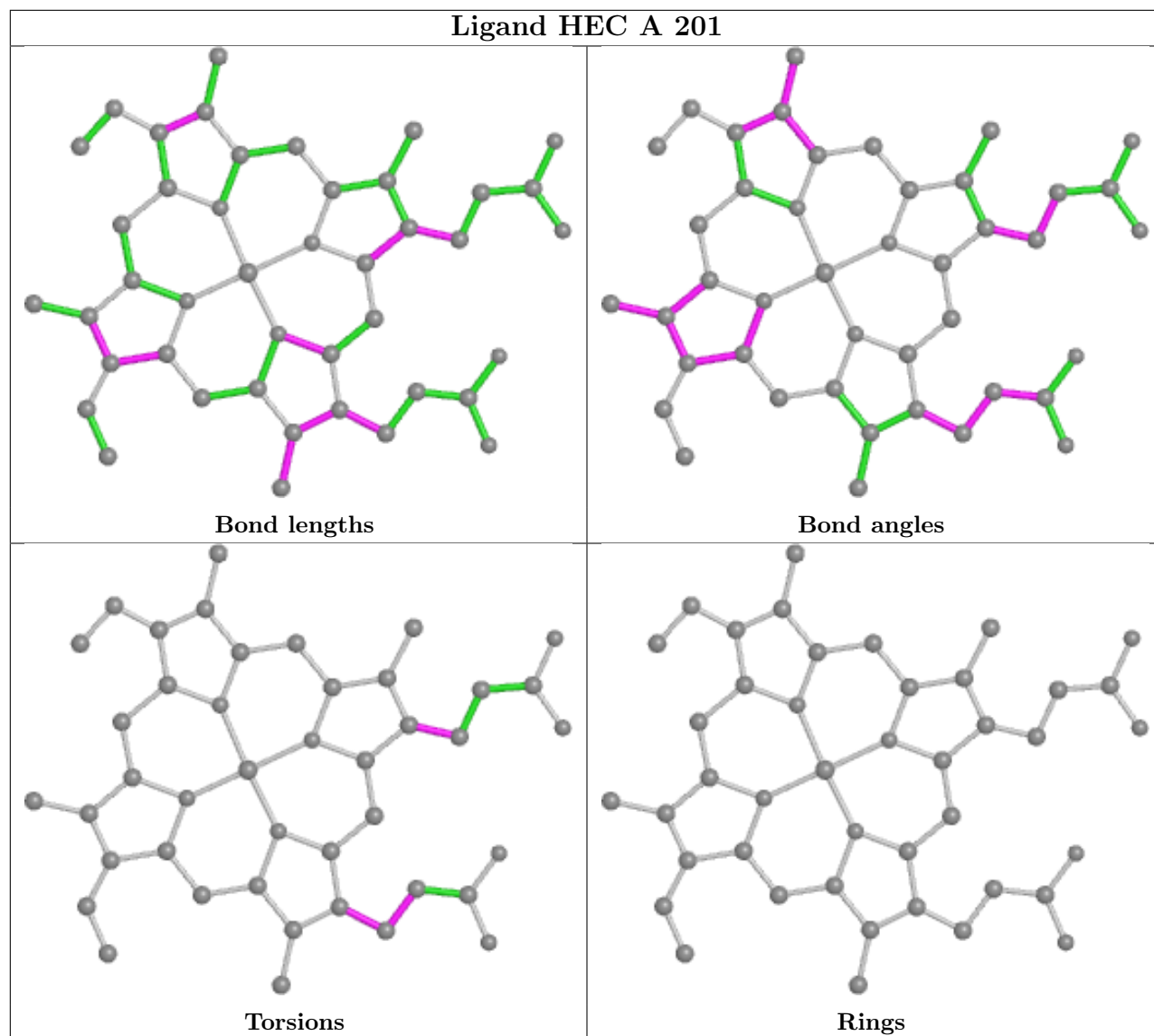
There are no ring outliers.

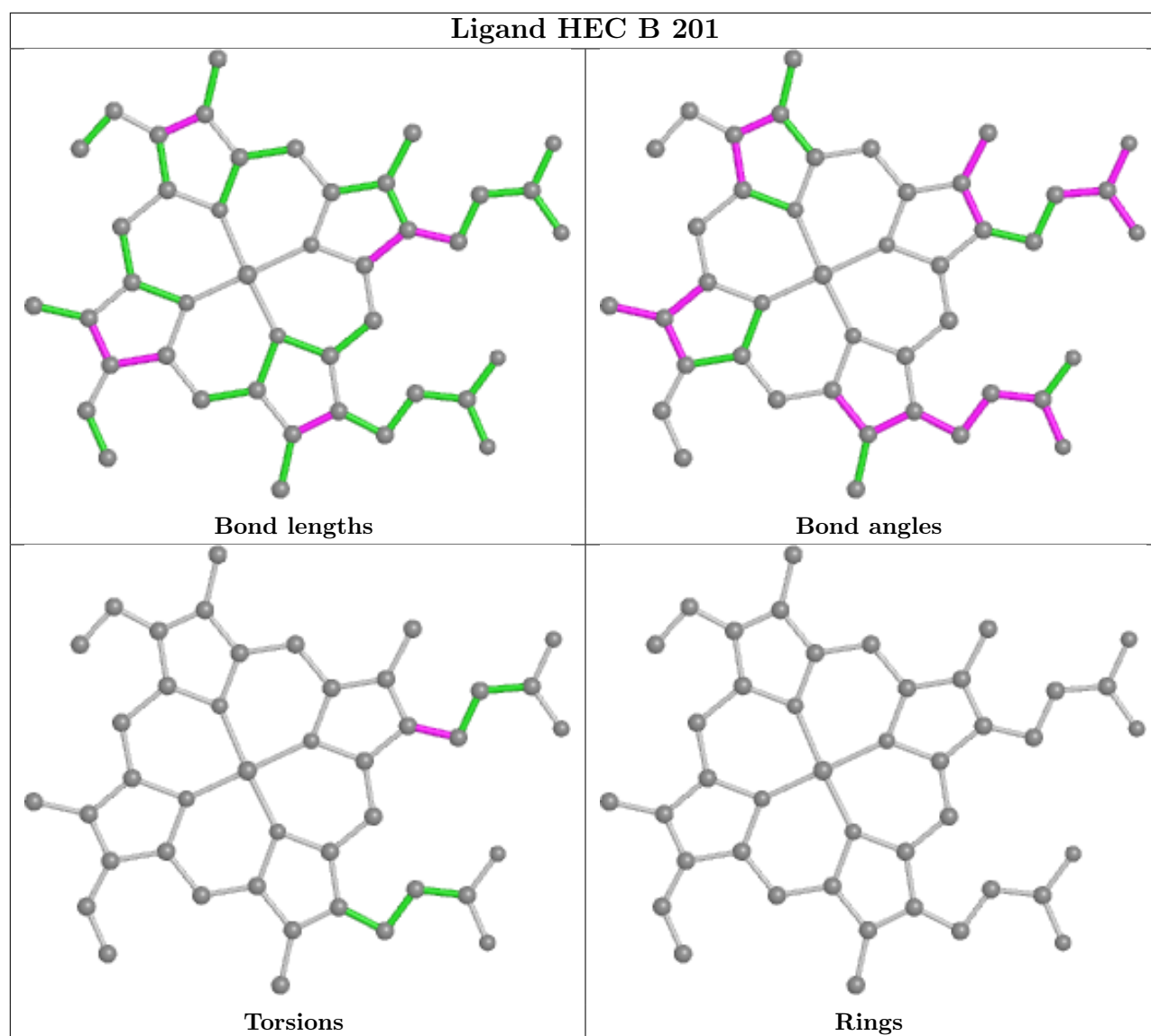
4 monomers are involved in 53 short contacts:

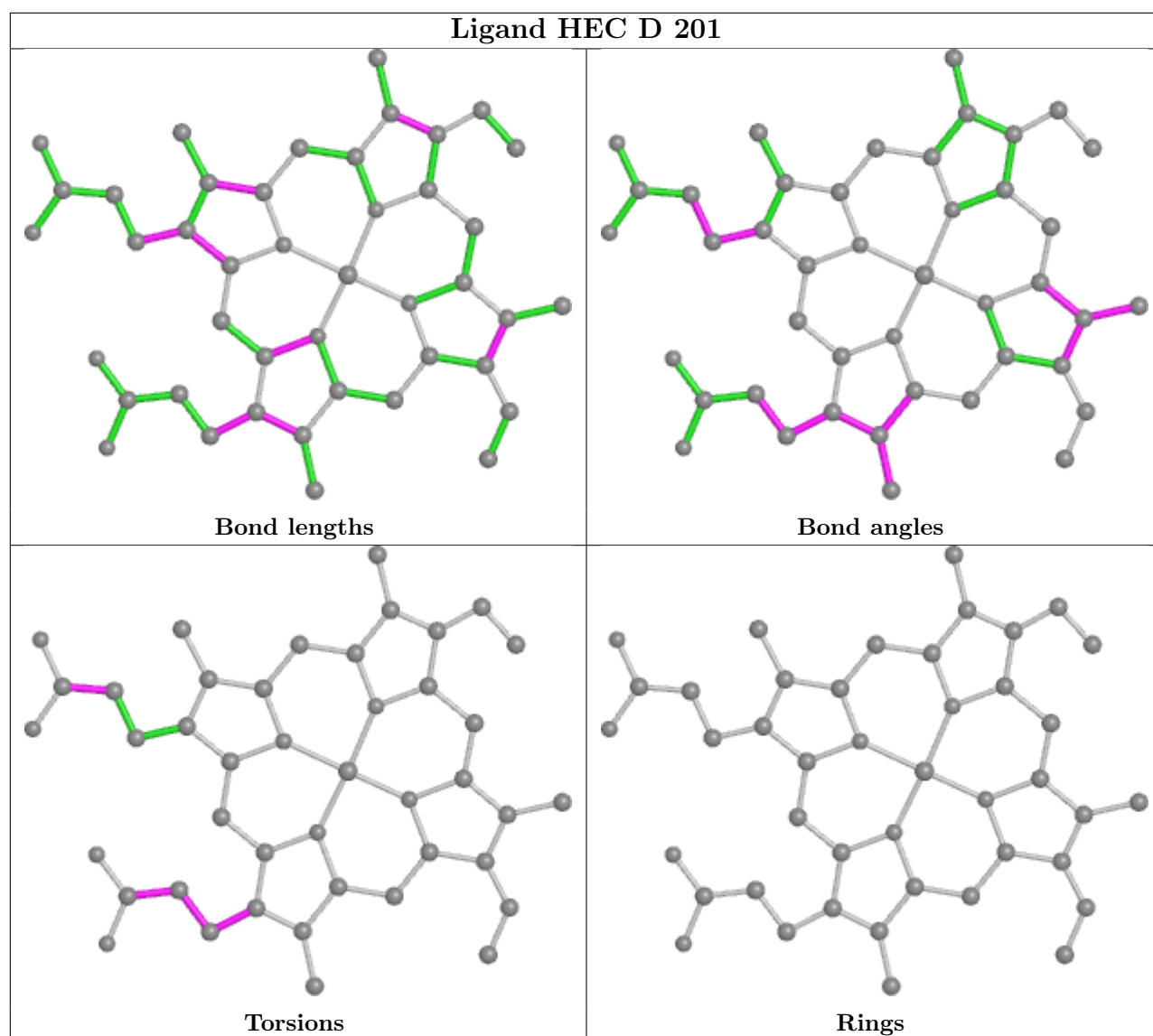
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201	HEC	20	0
2	A	201	HEC	7	0
2	B	201	HEC	14	0
2	D	201	HEC	12	0

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 [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	106/106 (100%)	-0.02	0 100 100	18, 23, 33, 37	0
1	B	106/106 (100%)	0.21	1 (0%) 84 85	20, 27, 34, 36	0
1	C	106/106 (100%)	0.26	2 (1%) 66 69	23, 31, 35, 38	0
1	D	106/106 (100%)	0.26	2 (1%) 66 69	27, 32, 37, 38	0
All	All	424/424 (100%)	0.18	5 (1%) 79 80	18, 29, 36, 38	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	19	LYS	2.8
1	C	14	LEU	2.6
1	B	82	GLY	2.4
1	C	30	LEU	2.2
1	D	85	LYS	2.2

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.

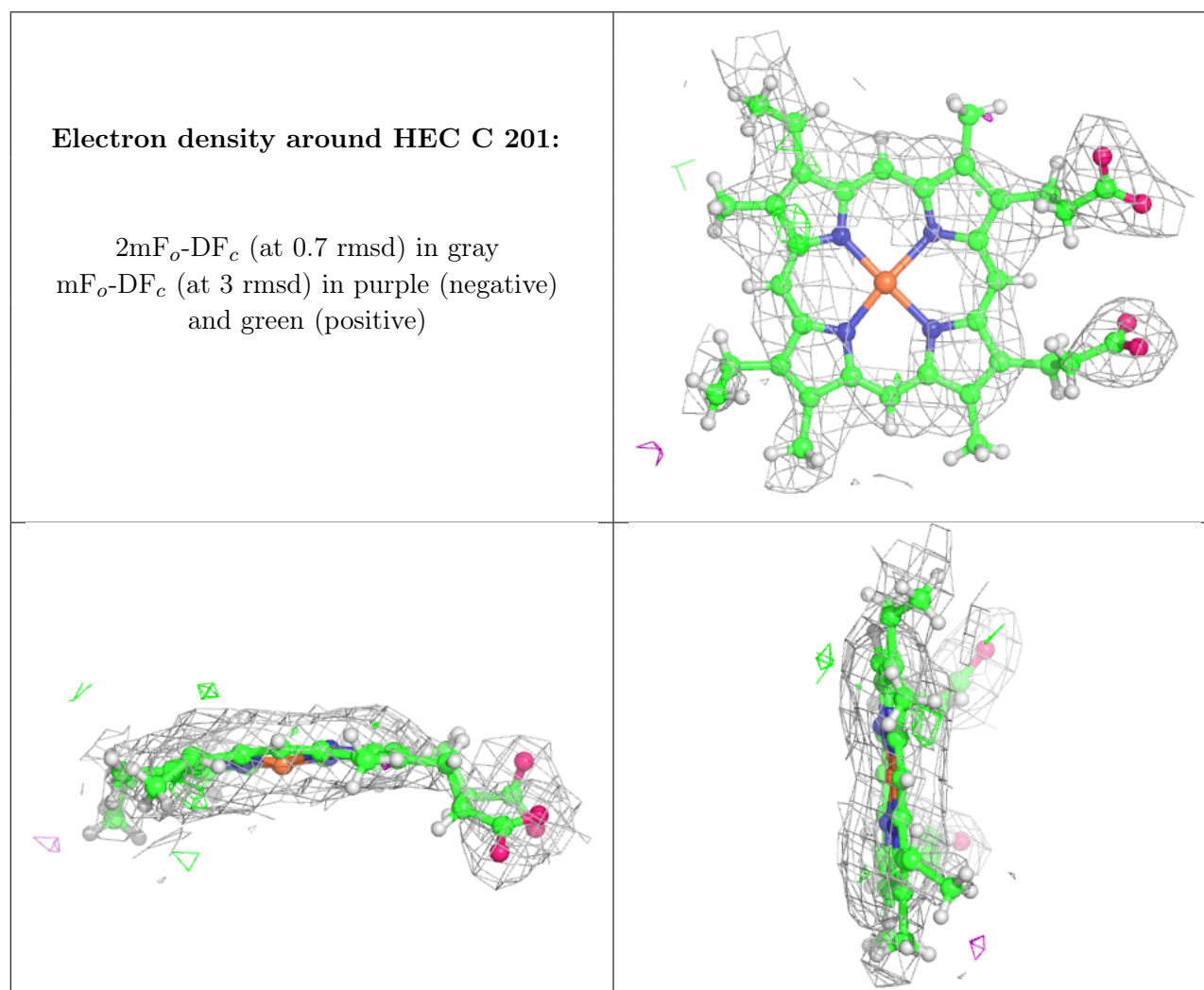
6.4 Ligands [i](#)

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.

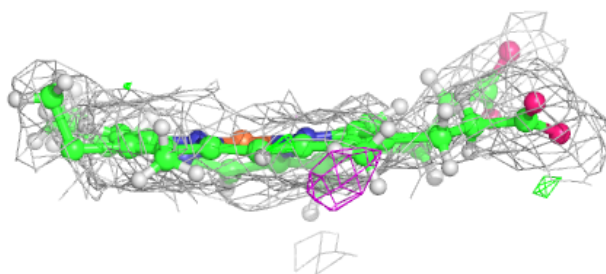
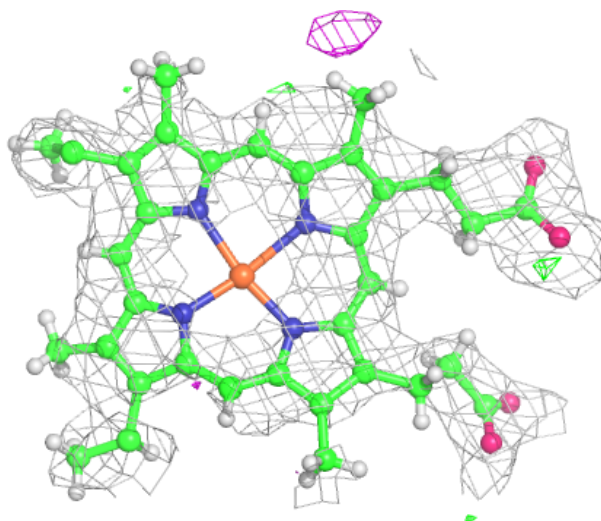
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEC	C	201	43/43	0.90	0.22	28,34,42,43	0
2	HEC	A	201	43/43	0.91	0.22	20,26,32,33	0
2	HEC	B	201	43/43	0.92	0.21	23,27,34,35	0
2	HEC	D	201	43/43	0.93	0.22	28,33,40,42	0
3	CU	C	202	1/1	0.95	0.12	46,46,46,46	0
3	CU	A	203	1/1	0.96	0.04	39,39,39,39	0
3	CU	B	202	1/1	0.98	0.04	35,35,35,35	0
3	CU	A	202	1/1	0.99	0.13	21,21,21,21	0

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



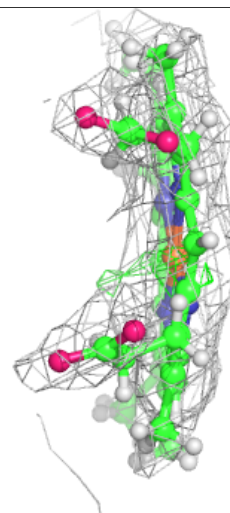
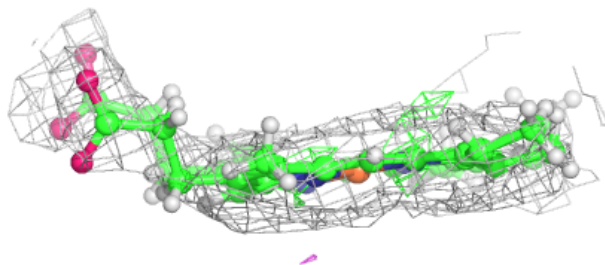
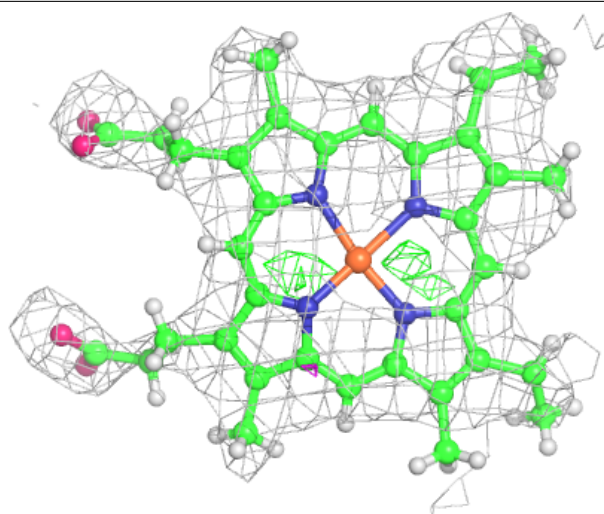
Electron density around HEC A 201:

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



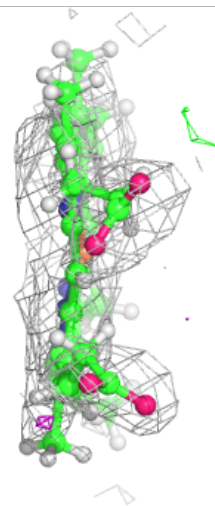
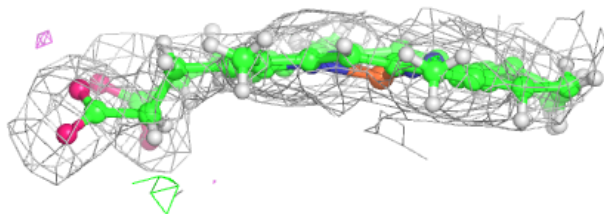
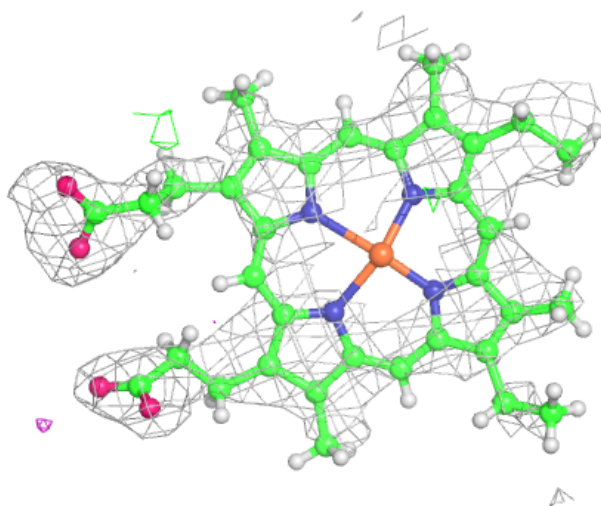
Electron density around HEC B 201:

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



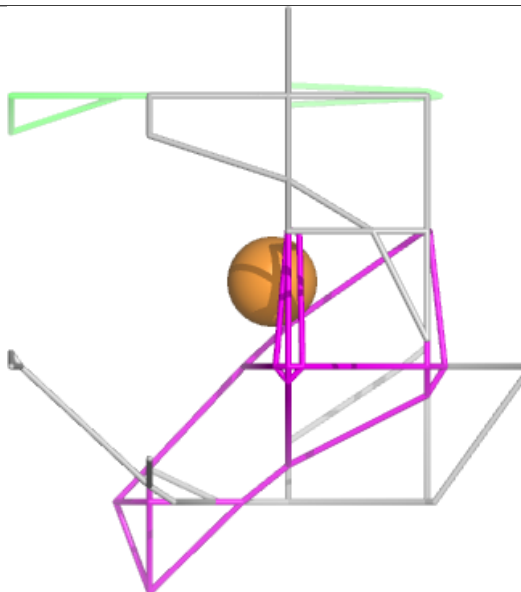
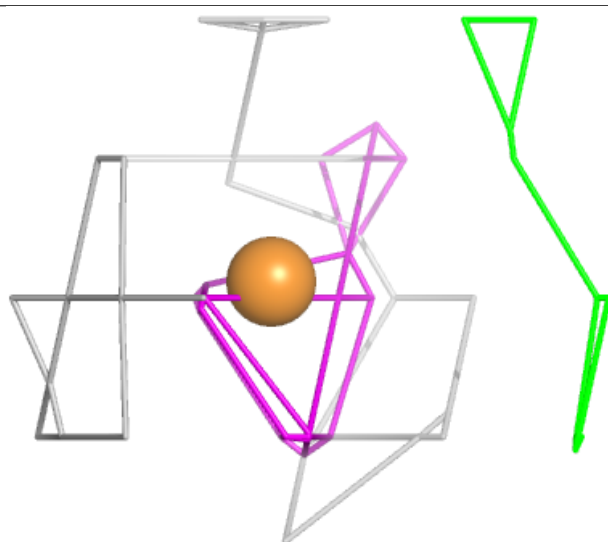
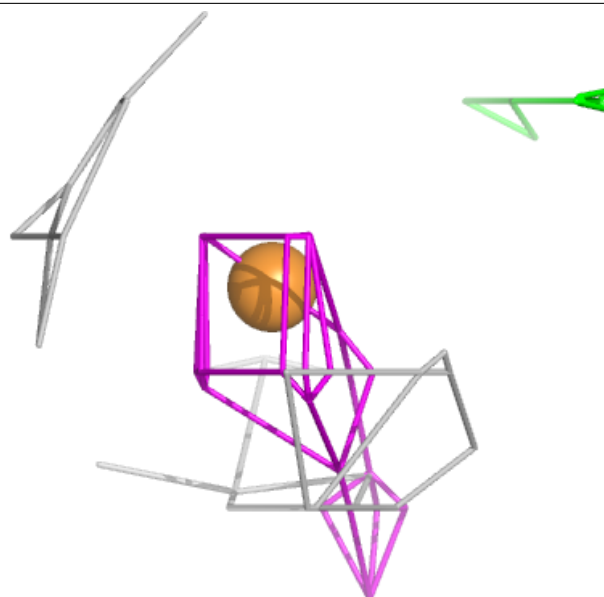
Electron density around HEC D 201:

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



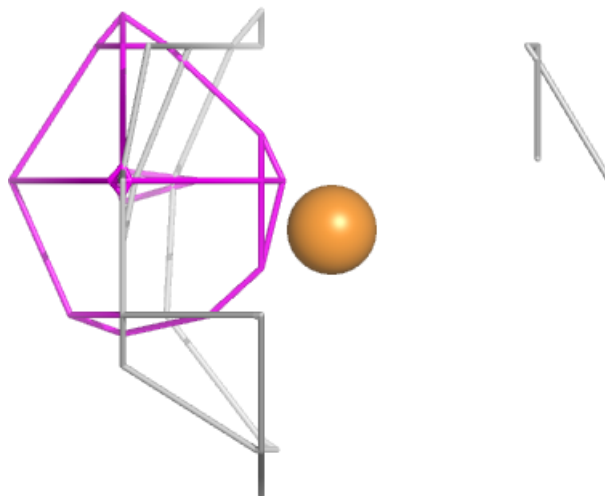
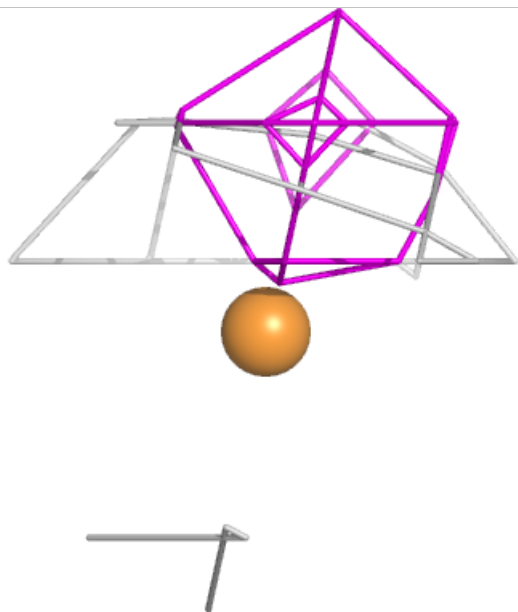
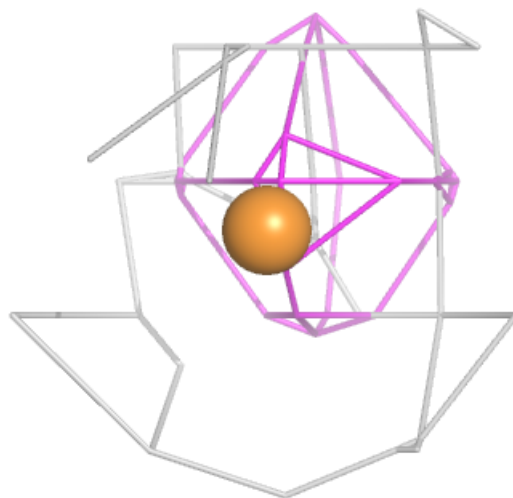
Electron density around CU C 202:

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



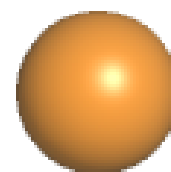
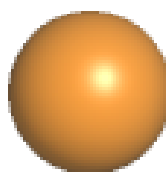
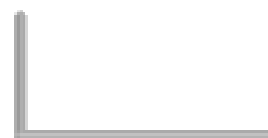
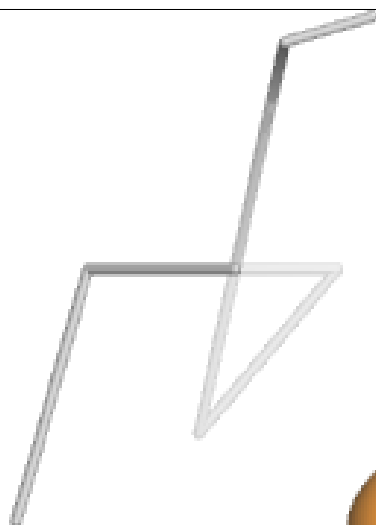
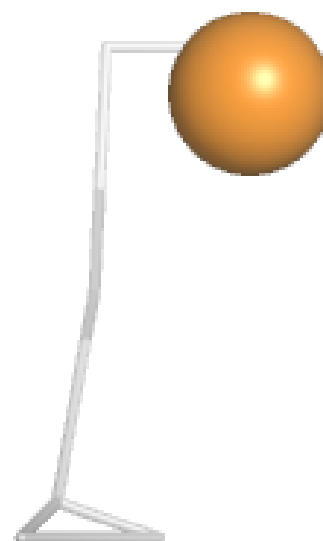
Electron density around CU A 203:

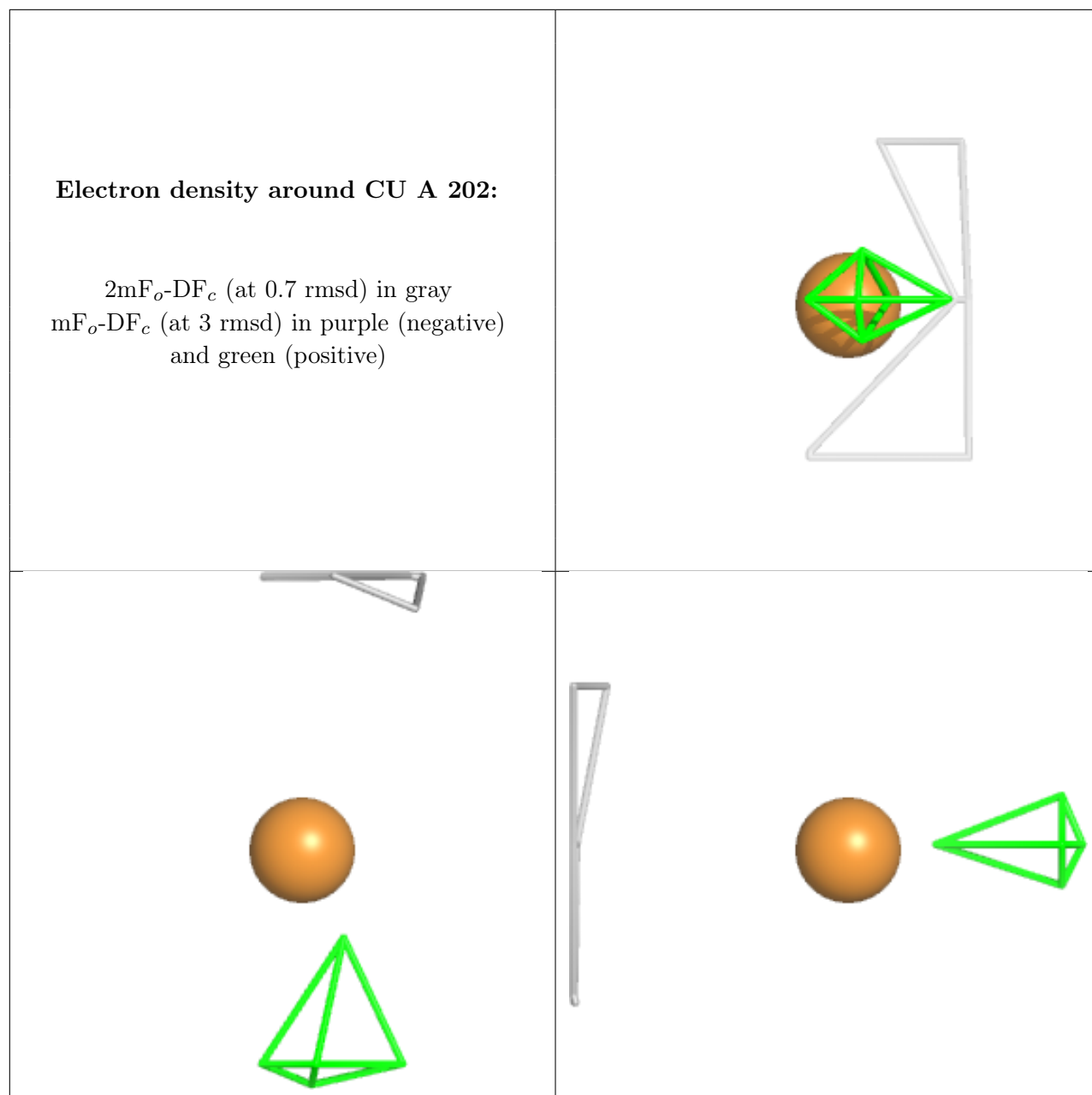
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CU B 202:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.