W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 06:25 AM EDT

PDB ID	:	7K5H
Title	:	1.90 A resolution structure of WT BfrB from Pseudomonas aeruginosa in complex with a protein-protein interaction inhibitor KM-5-66
Authors	:	Lovell, S.; Battaile, K.P.; Soldano, A.; Punchi-Hewage, A.; Meraz, K.; Annor-Gyamfi, J.K.; Yao, H.; Bunce, R.A.; Rivera, M.
Deposited on	:	2020-09-16
Resolution	:	1.90 Å(reported)

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

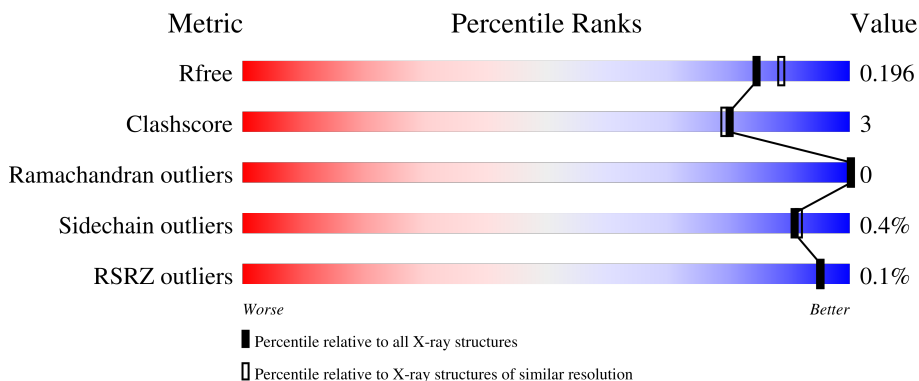|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1   Overall quality at a glance ⓘ

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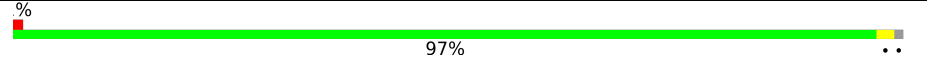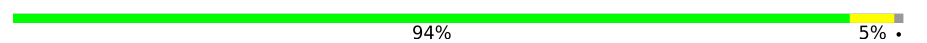*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	Percentile Ranks	Value
Rfree		0.196
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.4%
RSRZ outliers		0.1%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	158	97%
1	B	158	92% 6%
1	C	158	94% 5%
1	D	158	92% 6%

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Mol	Chain	Length	Quality of chain
1	E	158	92% 6%
1	F	158	92% 6%
1	G	158	95%
1	H	158	96%
1	I	158	94% 5%
1	J	158	92% 7%
1	K	158	92% 6%
1	L	158	96%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16725 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 Ferroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	1	0
			1272	807	218	240	7			
1	B	156	Total	C	N	O	S	0	1	0
			1266	802	216	241	7			
1	C	156	Total	C	N	O	S	0	1	0
			1267	801	216	243	7			
1	D	156	Total	C	N	O	S	0	1	0
			1263	799	216	241	7			
1	E	156	Total	C	N	O	S	0	2	0
			1272	806	216	243	7			
1	F	156	Total	C	N	O	S	0	1	0
			1261	800	215	239	7			
1	G	156	Total	C	N	O	S	0	1	0
			1266	802	215	242	7			
1	H	156	Total	C	N	O	S	0	2	0
			1275	807	217	244	7			
1	I	156	Total	C	N	O	S	0	1	0
			1269	803	215	244	7			
1	J	156	Total	C	N	O	S	0	1	0
			1268	802	216	243	7			
1	K	156	Total	C	N	O	S	0	1	0
			1264	801	214	242	7			
1	L	156	Total	C	N	O	S	0	2	0
			1270	806	216	241	7			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total K		0	0
			1 1			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
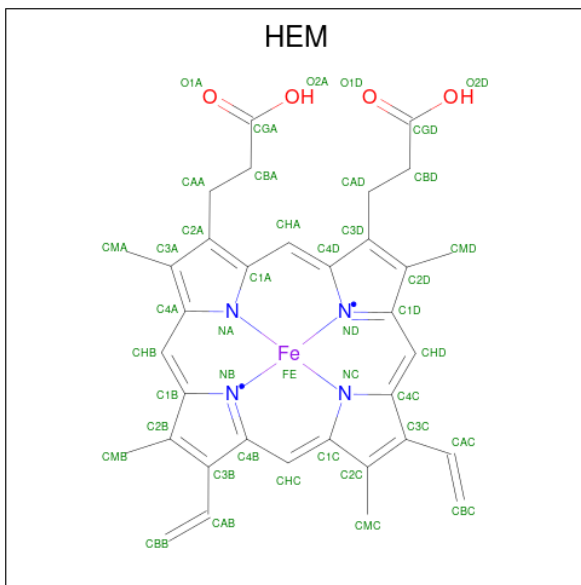
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is 4-{[3-(3-chloro-5-hydroxyphenyl)propyl]amino}-1H-isoindole-1,3(2H)-dione (three-letter code: VXV) (formula: $C_{17}H_{15}ClN_2O_3$) (labeled as "Ligand of Interest" by depositor).

VXV
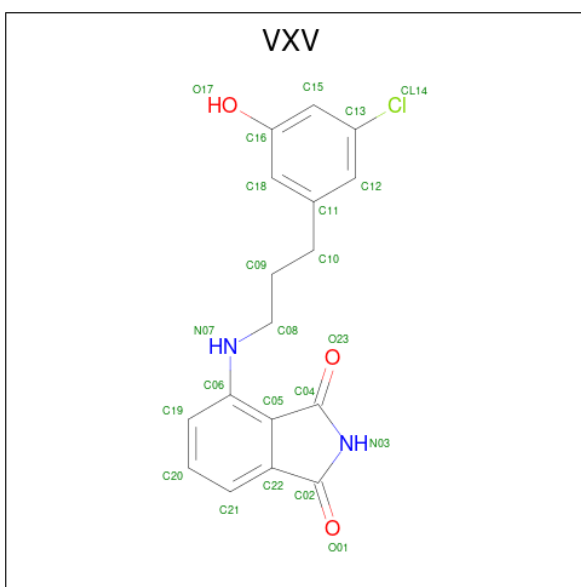
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 13	C 9	N 2	O 2		0	0
4	B	1	Total 23	C 17	Cl 1	N 2	O 3	0	0
4	C	1	Total 15	C 11	N 2	O 2		0	0
4	C	1	Total 23	C 17	Cl 1	N 2	O 3	0	0
4	D	1	Total 12	C 8	N 2	O 2		0	0
4	E	1	Total 16	C 12	N 2	O 2		0	0
4	F	1	Total 23	C 17	Cl 1	N 2	O 3	0	0
4	H	1	Total 15	C 11	N 2	O 2		0	0
4	J	1	Total 16	C 12	N 2	O 2		0	0
4	K	1	Total 23	C 17	Cl 1	N 2	O 3	0	0
4	L	1	Total 14	C 10	N 2	O 2		0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	88	Total 88	O 88	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	86	Total 86	O 86	0	0
5	C	85	Total 85	O 85	0	0
5	D	75	Total 75	O 75	0	0
5	E	83	Total 83	O 83	0	0
5	F	79	Total 79	O 79	0	0
5	G	80	Total 80	O 80	0	0
5	H	84	Total 84	O 84	0	0
5	I	79	Total 79	O 79	0	0
5	J	92	Total 92	O 92	0	0
5	K	99	Total 99	O 99	0	0
5	L	85	Total 85	O 85	0	0

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: Ferroxidase

Chain A:

- Molecule 1: Ferroxidase

Chain B:

- Molecule 1: Ferroxidase

Chain C:

- Molecule 1: Ferroxidase
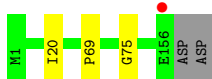
Chain D:

- Molecule 1: Ferroxidase

Chain E:

- Molecule 1: Ferroxidase

Chain F:

M1 E18 H28 E44 E51 M52 P69 I79 D90 K121 H130 E156 ASP ASP

• Molecule 1: Ferroxidase

Chain G: 95%

M1 E18 E44 E51 L65 D90 E156 ASP ASP

• Molecule 1: Ferroxidase

Chain H: 96%

M1 E18 E51 M52 P69 E156 ASP ASP

• Molecule 1: Ferroxidase

Chain I: 94% 5%

M1 H10 I14 E18 L19 I20 E51 P69 G75 K121 E156 ASP ASP

• Molecule 1: Ferroxidase

Chain J: 92% 7%

M1 E18 L19 I20 E44 E51 M52 P69 L77 N82 T83 Q84 D90 K121 E156 ASP ASP

• Molecule 1: Ferroxidase

Chain K: 92% 6%

M1 E18 L19 I20 E51 M52 L65 P69 G75 K76 L77 K121 E156 ASP ASP

• Molecule 1: Ferroxidase

Chain L: 96%

M1 E18 E51 M52 P69 E156 ASP ASP
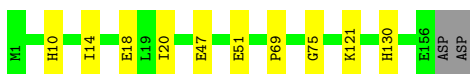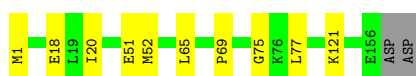
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	129.50Å　　194.50Å　　202.95Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	46.78　–　1.90 48.62　–　1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.78-1.90) 100.0 (48.62-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.19 (at 1.90Å)	Xtriage
Refinement program	PHENIX dev_3959	Depositor
R, R_{free}	0.158　,　0.189 0.167　,　0.196	Depositor DCC
R_{free} test set	10033 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.5	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16725	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, HEM, VXV

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	0.44	0/1296	0.58	0/1745
1	B	0.44	0/1290	0.55	0/1740
1	C	0.48	0/1291	0.57	0/1742
1	D	0.41	0/1287	0.56	0/1737
1	E	0.50	0/1299	0.56	0/1752
1	F	0.44	0/1285	0.55	0/1734
1	G	0.42	0/1290	0.55	0/1740
1	H	0.45	0/1302	0.55	0/1756
1	I	0.44	0/1293	0.54	0/1744
1	J	0.48	0/1292	0.57	0/1743
1	K	0.43	0/1288	0.55	0/1738
1	L	0.44	0/1297	0.54	0/1749
All	All	0.45	0/15510	0.56	0/20920

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1272	0	1254	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1266	0	1231	7	0
1	C	1267	0	1229	5	0
1	D	1263	0	1225	6	0
1	E	1272	0	1237	7	0
1	F	1261	0	1222	6	0
1	G	1266	0	1229	3	0
1	H	1275	0	1241	4	0
1	I	1269	0	1231	4	0
1	J	1268	0	1231	6	0
1	K	1264	0	1222	6	0
1	L	1270	0	1237	3	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
3	A	43	0	30	2	0
3	C	43	0	30	4	0
3	D	43	0	30	5	0
3	E	43	0	30	5	0
3	F	43	0	30	5	0
3	H	43	0	30	6	0
3	L	43	0	30	5	0
4	A	13	0	0	1	0
4	B	23	0	0	2	0
4	C	38	0	0	2	0
4	D	12	0	0	1	0
4	E	16	0	0	0	0
4	F	23	0	0	1	0
4	H	15	0	0	1	0
4	J	16	0	0	1	0
4	K	23	0	0	1	0
4	L	14	0	0	1	0
5	A	88	0	0	0	0
5	B	86	0	0	1	0
5	C	85	0	0	0	0
5	D	75	0	0	0	0
5	E	83	0	0	1	0
5	F	79	0	0	0	0
5	G	80	0	0	0	0
5	H	84	0	0	0	0
5	I	79	0	0	0	0
5	J	92	0	0	0	0
5	K	99	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	85	0	0	0	0
All	All	16725	0	14999	84	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 3.

The worst 5 of 84 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:201:HEM:HMC2	3:F:201:HEM:HBC2	1.58	0.86
3:D:202:HEM:HBC2	3:D:202:HEM:HMC2	1.62	0.80
3:E:201:HEM:HMC1	3:E:201:HEM:HBC2	1.67	0.76
3:A:202:HEM:HMC1	3:A:202:HEM:HBC2	1.73	0.71
3:F:201:HEM:HBC2	3:F:201:HEM:CMC	2.20	0.70

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	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	B	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	C	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	D	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	E	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	F	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	G	155/158 (98%)	153 (99%)	2 (1%)	0	100	100
1	H	156/158 (99%)	155 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	J	155/158 (98%)	153 (99%)	2 (1%)	0	100	100
1	K	155/158 (98%)	155 (100%)	0	0	100	100
1	L	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
All	All	1863/1896 (98%)	1850 (99%)	13 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	137/144 (95%)	137 (100%)	0	100	100
1	B	135/144 (94%)	135 (100%)	0	100	100
1	C	136/144 (94%)	135 (99%)	1 (1%)	84	84
1	D	135/144 (94%)	134 (99%)	1 (1%)	84	84
1	E	136/144 (94%)	136 (100%)	0	100	100
1	F	133/144 (92%)	132 (99%)	1 (1%)	81	82
1	G	135/144 (94%)	135 (100%)	0	100	100
1	H	137/144 (95%)	137 (100%)	0	100	100
1	I	136/144 (94%)	135 (99%)	1 (1%)	84	84
1	J	136/144 (94%)	135 (99%)	1 (1%)	84	84
1	K	134/144 (93%)	133 (99%)	1 (1%)	84	84
1	L	135/144 (94%)	135 (100%)	0	100	100
All	All	1625/1728 (94%)	1619 (100%)	6 (0%)	91	91

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	121	LYS

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Mol	Chain	Res	Type
1	J	121	LYS
1	K	121	LYS
1	D	121	LYS
1	C	121	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	130	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
4	VXV	K	201	-	25,25,25	1.58	5 (20%)	34,35,35	2.10	9 (26%)
4	VXV	D	203	-	13,13,25	1.38	2 (15%)	17,19,35	2.74	6 (35%)
4	VXV	L	202	-	15,15,25	1.35	2 (13%)	21,21,35	2.39	7 (33%)

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Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	VXV	F	202	-	25,25,25	1.47	6 (24%)	34,35,35	2.10	9 (26%)
4	VXV	C	202	-	16,16,25	1.72	5 (31%)	22,22,35	2.32	7 (31%)
3	HEM	E	201	1	41,50,50	1.50	6 (14%)	45,82,82	1.66	10 (22%)
4	VXV	B	202	-	25,25,25	1.64	5 (20%)	34,35,35	2.41	12 (35%)
3	HEM	D	202	1	41,50,50	1.42	5 (12%)	45,82,82	1.53	8 (17%)
3	HEM	H	201	1	41,50,50	1.52	5 (12%)	45,82,82	1.86	13 (28%)
4	VXV	C	203	-	25,25,25	1.87	7 (28%)	34,35,35	2.07	8 (23%)
3	HEM	C	201	1	41,50,50	1.49	6 (14%)	45,82,82	1.67	12 (26%)
3	HEM	L	201	1	41,50,50	1.41	4 (9%)	45,82,82	1.57	8 (17%)
4	VXV	A	203	-	14,14,25	1.85	2 (14%)	19,20,35	2.84	9 (47%)
4	VXV	E	202	-	17,17,25	1.54	3 (17%)	23,23,35	2.37	8 (34%)
4	VXV	J	201	-	17,17,25	1.55	3 (17%)	23,23,35	2.39	8 (34%)
4	VXV	H	202	-	16,16,25	1.90	3 (18%)	22,22,35	1.91	8 (36%)
3	HEM	A	202	1	41,50,50	1.43	5 (12%)	45,82,82	1.69	12 (26%)
3	HEM	F	201	1	41,50,50	1.41	5 (12%)	45,82,82	1.60	11 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	VXV	K	201	-	-	1/7/19/19	0/3/3/3
4	VXV	D	203	-	-	-	0/2/2/3
4	VXV	L	202	-	-	0/3/15/19	0/2/2/3
4	VXV	F	202	-	-	1/7/19/19	0/3/3/3
4	VXV	C	202	-	-	0/4/16/19	0/2/2/3
3	HEM	E	201	1	-	4/12/54/54	-
4	VXV	B	202	-	-	0/7/19/19	0/3/3/3
3	HEM	D	202	1	-	4/12/54/54	-
3	HEM	H	201	1	-	4/12/54/54	-
4	VXV	C	203	-	-	2/7/19/19	0/3/3/3
3	HEM	C	201	1	-	2/12/54/54	-
3	HEM	L	201	1	-	4/12/54/54	-
4	VXV	A	203	-	-	0/2/14/19	0/2/2/3
4	VXV	E	202	-	-	0/5/17/19	0/2/2/3
4	VXV	J	201	-	-	0/5/17/19	0/2/2/3
4	VXV	H	202	-	-	0/4/16/19	0/2/2/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	202	1	-	4/12/54/54	-
3	HEM	F	201	1	-	4/12/54/54	-

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	201	HEM	C3C-C2C	-4.80	1.33	1.40
4	A	203	VXV	C06-N07	4.79	1.46	1.37
3	E	201	HEM	C3C-C2C	-4.56	1.34	1.40
4	H	202	VXV	C02-N03	-4.50	1.32	1.38
4	C	203	VXV	C13-CL14	4.29	1.83	1.74

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	203	VXV	C04-N03-C02	-7.02	106.54	112.52
4	A	203	VXV	C04-N03-C02	-6.96	106.59	112.52
4	E	202	VXV	C04-N03-C02	-6.58	106.91	112.52
4	J	201	VXV	C04-N03-C02	-6.57	106.92	112.52
4	K	201	VXV	C04-N03-C02	-6.50	106.98	112.52

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	203	VXV	N07-C08-C09-C10
4	C	203	VXV	C08-C09-C10-C11
4	K	201	VXV	C08-C09-C10-C11
4	F	202	VXV	N07-C08-C09-C10
3	H	201	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

17 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	201	VXV	1	0
4	D	203	VXV	1	0
4	L	202	VXV	1	0
4	F	202	VXV	1	0
4	C	202	VXV	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	201	HEM	5	0
4	B	202	VXV	2	0
3	D	202	HEM	5	0
3	H	201	HEM	6	0
4	C	203	VXV	1	0
3	C	201	HEM	4	0
3	L	201	HEM	5	0
4	A	203	VXV	1	0
4	J	201	VXV	1	0
4	H	202	VXV	1	0
3	A	202	HEM	2	0
3	F	201	HEM	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand VXV K 201

Bond lengths　　Bond angles

Torsions　　Rings

Ligand VXV D 203

Bond lengths

Bond angles

Torsions

Rings

Ligand VXV L 202

Bond lengths

Bond angles

Torsions

Rings

Ligand VXV F 202

Bond lengths

Bond angles

Torsions

Rings

Ligand VXV C 202

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM E 201

Bond lengths

Bond angles

Torsions

Rings

Ligand VXV B 202

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM D 202

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM H 201

Bond lengths

Bond angles

Torsions

Rings

Ligand VXV C 203

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 201

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM L 201

Bond lengths

Bond angles

Torsions

Rings

Ligand VXV A 203

Bond lengths

Bond angles

Torsions

Rings

Ligand VXV E 202

Bond lengths

Bond angles

Torsions

Rings

Ligand VXV J 201

Bond lengths

Bond angles

Torsions

Rings

Ligand VXV H 202

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 202

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM F 201

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	156/158 (98%)	-0.47	1 (0%)	89	90	20, 25, 36, 55	0
1	B	156/158 (98%)	-0.50	0	100	100	20, 25, 38, 55	0
1	C	156/158 (98%)	-0.45	0	100	100	19, 25, 36, 56	0
1	D	156/158 (98%)	-0.46	0	100	100	22, 27, 38, 59	0
1	E	156/158 (98%)	-0.48	0	100	100	19, 23, 34, 56	0
1	F	156/158 (98%)	-0.46	0	100	100	20, 26, 36, 58	0
1	G	156/158 (98%)	-0.50	0	100	100	21, 25, 36, 58	0
1	H	156/158 (98%)	-0.42	0	100	100	21, 26, 37, 58	0
1	I	156/158 (98%)	-0.52	0	100	100	21, 26, 37, 60	0
1	J	156/158 (98%)	-0.46	0	100	100	21, 25, 35, 58	0
1	K	156/158 (98%)	-0.46	0	100	100	20, 26, 35, 61	0
1	L	156/158 (98%)	-0.40	0	100	100	21, 25, 35, 61	0
All	All	1872/1896 (98%)	-0.47	1 (0%)	95	95	19, 25, 36, 61	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	GLU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	VXV	C	202	15/23	0.73	0.23	29,46,51,52	0
4	VXV	H	202	15/23	0.79	0.27	34,44,52,52	0
4	VXV	E	202	16/23	0.81	0.25	33,46,54,63	0
4	VXV	A	203	13/23	0.85	0.23	29,41,51,52	0
4	VXV	F	202	23/23	0.85	0.29	33,48,70,95	0
4	VXV	C	203	23/23	0.85	0.25	33,47,64,71	0
4	VXV	J	201	16/23	0.85	0.20	36,47,54,54	0
4	VXV	K	201	23/23	0.86	0.28	37,51,77,88	0
4	VXV	B	202	23/23	0.87	0.30	29,48,68,94	0
4	VXV	L	202	14/23	0.87	0.18	29,40,47,53	0
4	VXV	D	203	12/23	0.92	0.17	37,43,50,51	0
3	HEM	L	201	43/43	0.93	0.16	24,28,39,46	43
3	HEM	D	202	43/43	0.94	0.13	28,34,50,53	43
3	HEM	F	201	43/43	0.94	0.14	23,28,47,53	0
3	HEM	E	201	43/43	0.95	0.13	21,27,48,57	0
3	HEM	C	201	43/43	0.95	0.14	25,28,46,64	0
3	HEM	H	201	43/43	0.95	0.14	23,29,51,62	0
3	HEM	A	202	43/43	0.96	0.12	24,28,50,56	0
2	K	A	201	1/1	1.00	0.08	17,17,17,17	0
2	K	B	201	1/1	1.00	0.09	18,18,18,18	0
2	K	D	201	1/1	1.00	0.08	20,20,20,20	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.
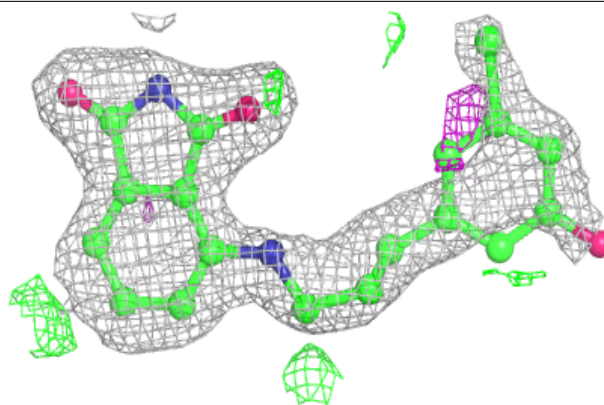
Electron density around VXV C 202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
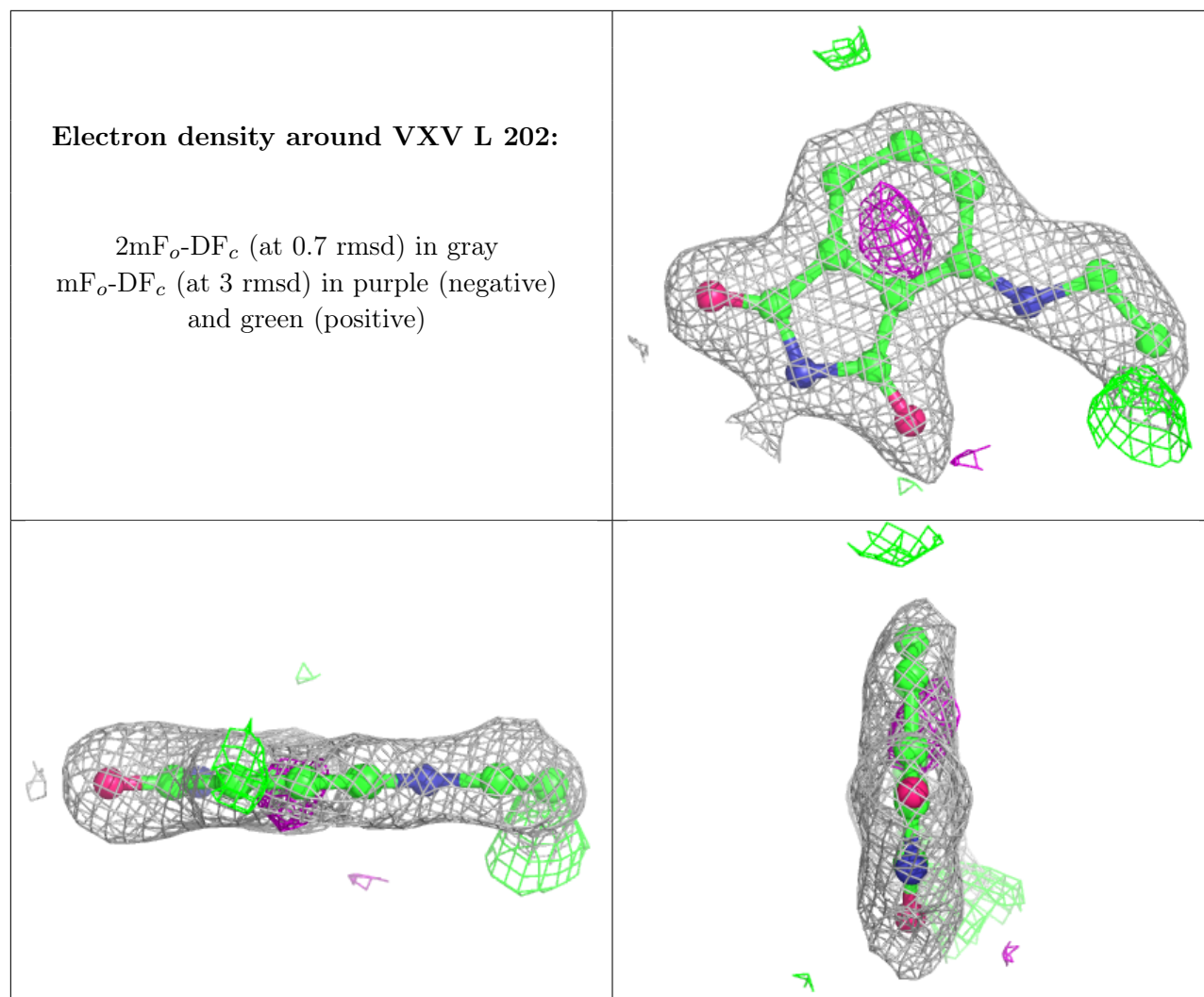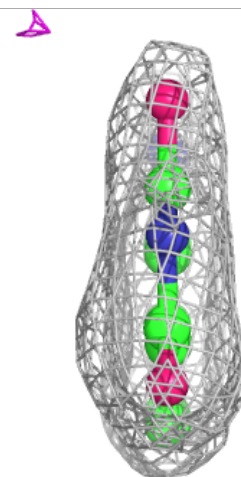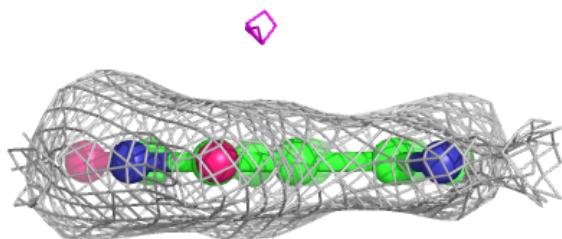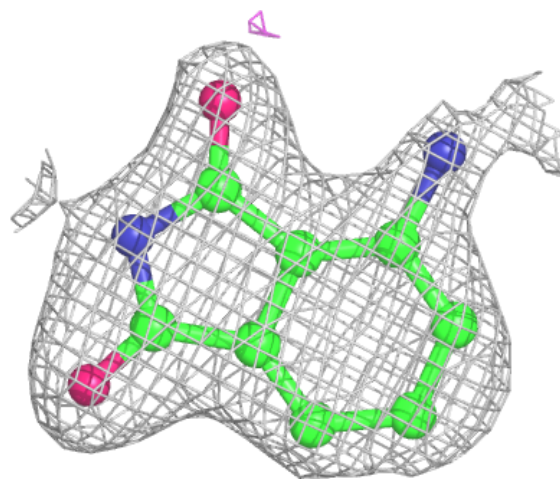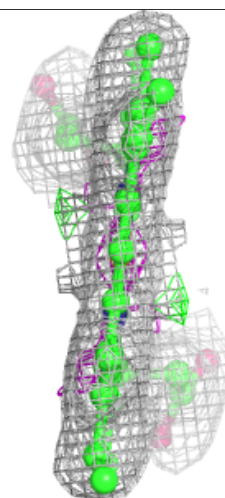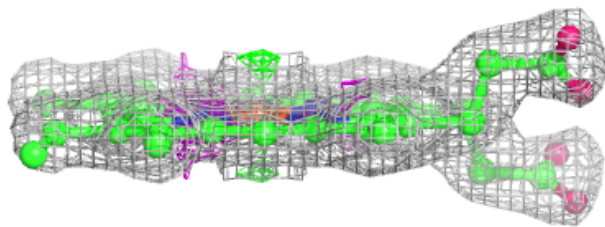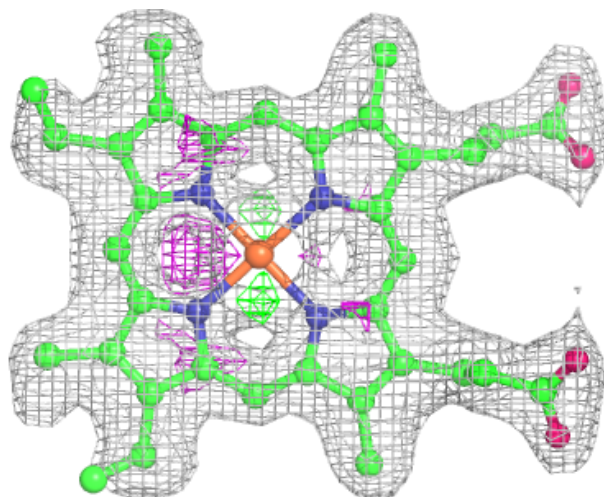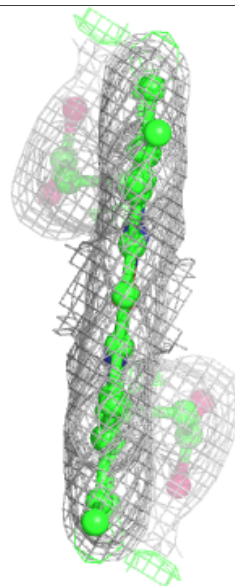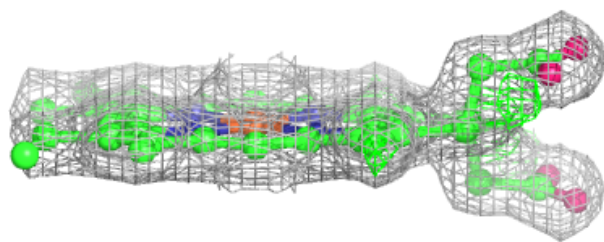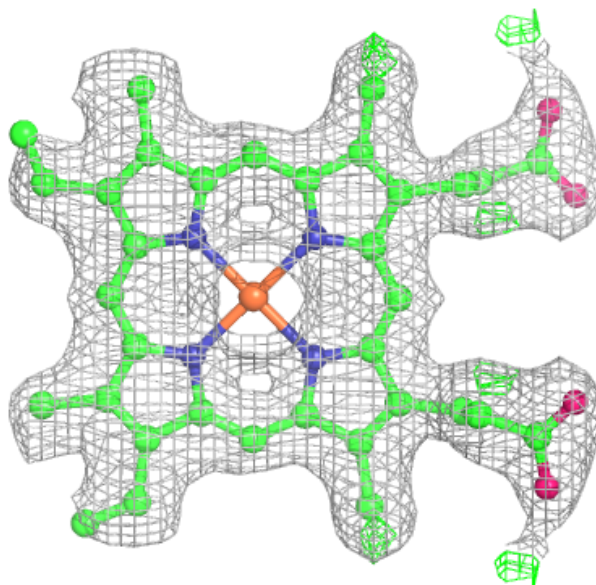and green (positive)
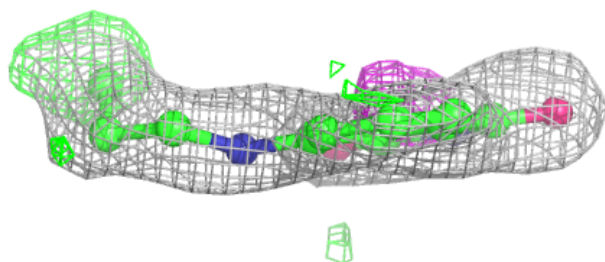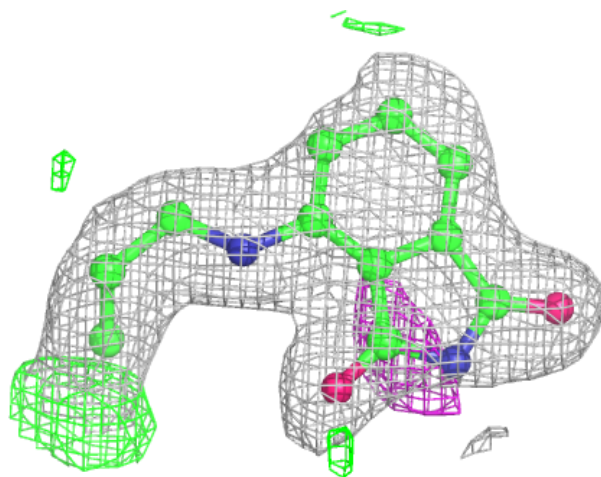
Electron density around VXV H 202:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
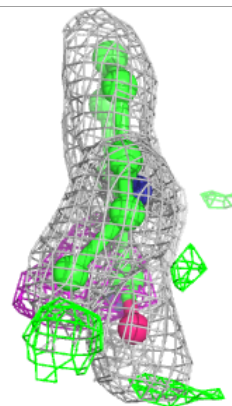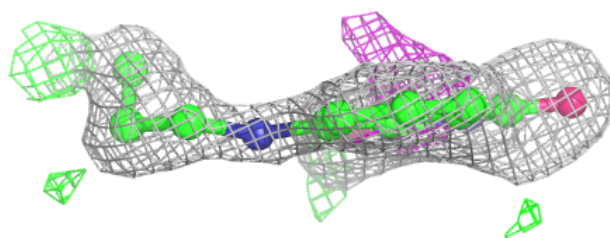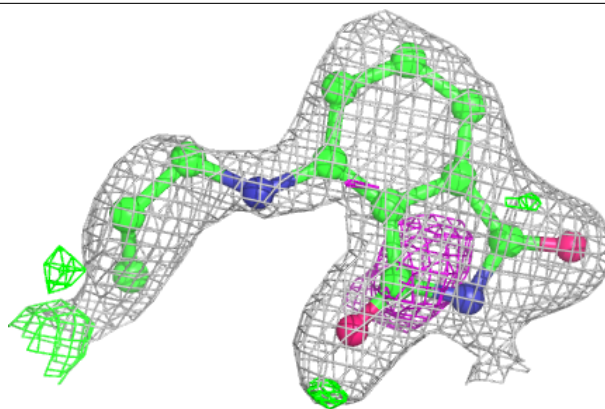
Electron density around VXV E 202:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
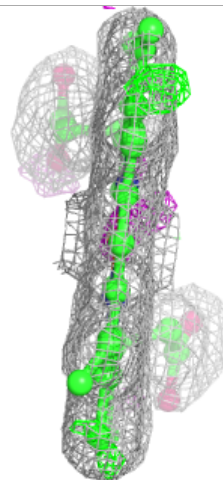$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
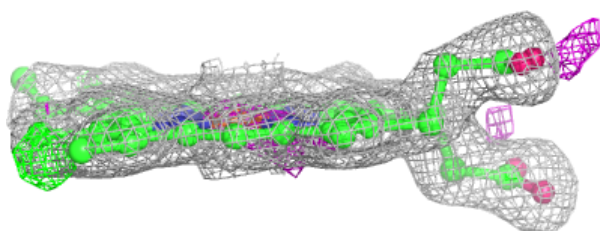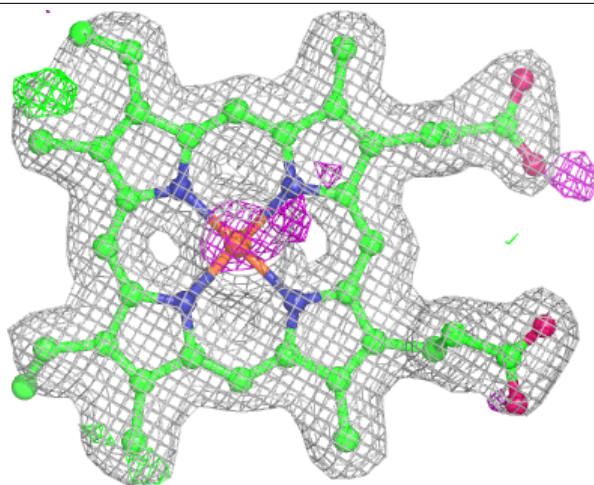and green (positive)
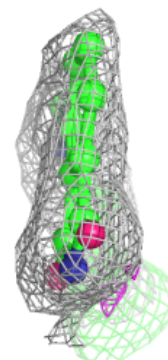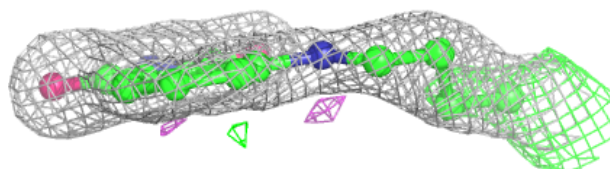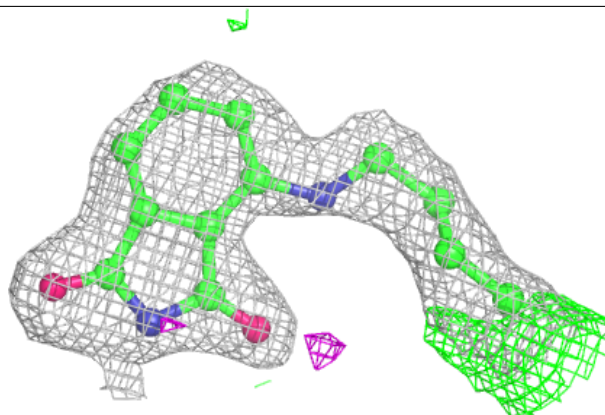
Electron density around VXV A 203:

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 VXV F 202:

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

Electron density around VXV C 203:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
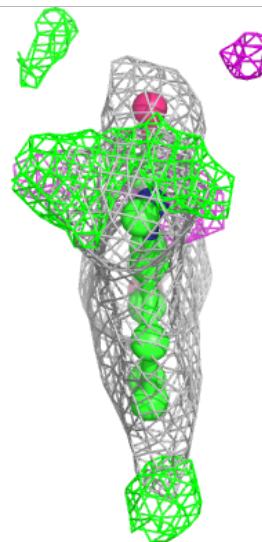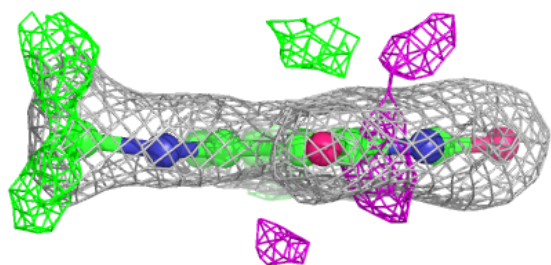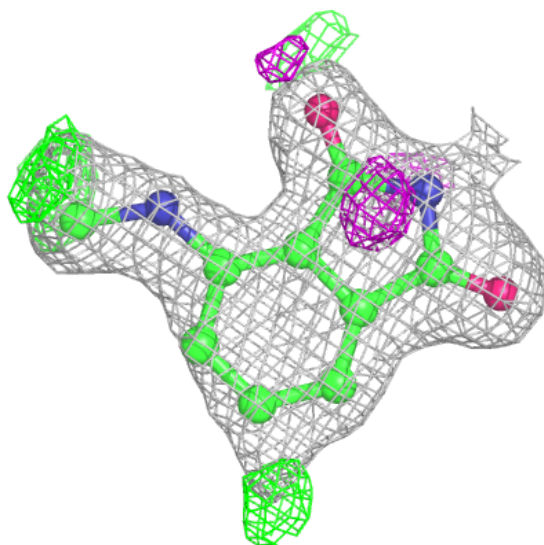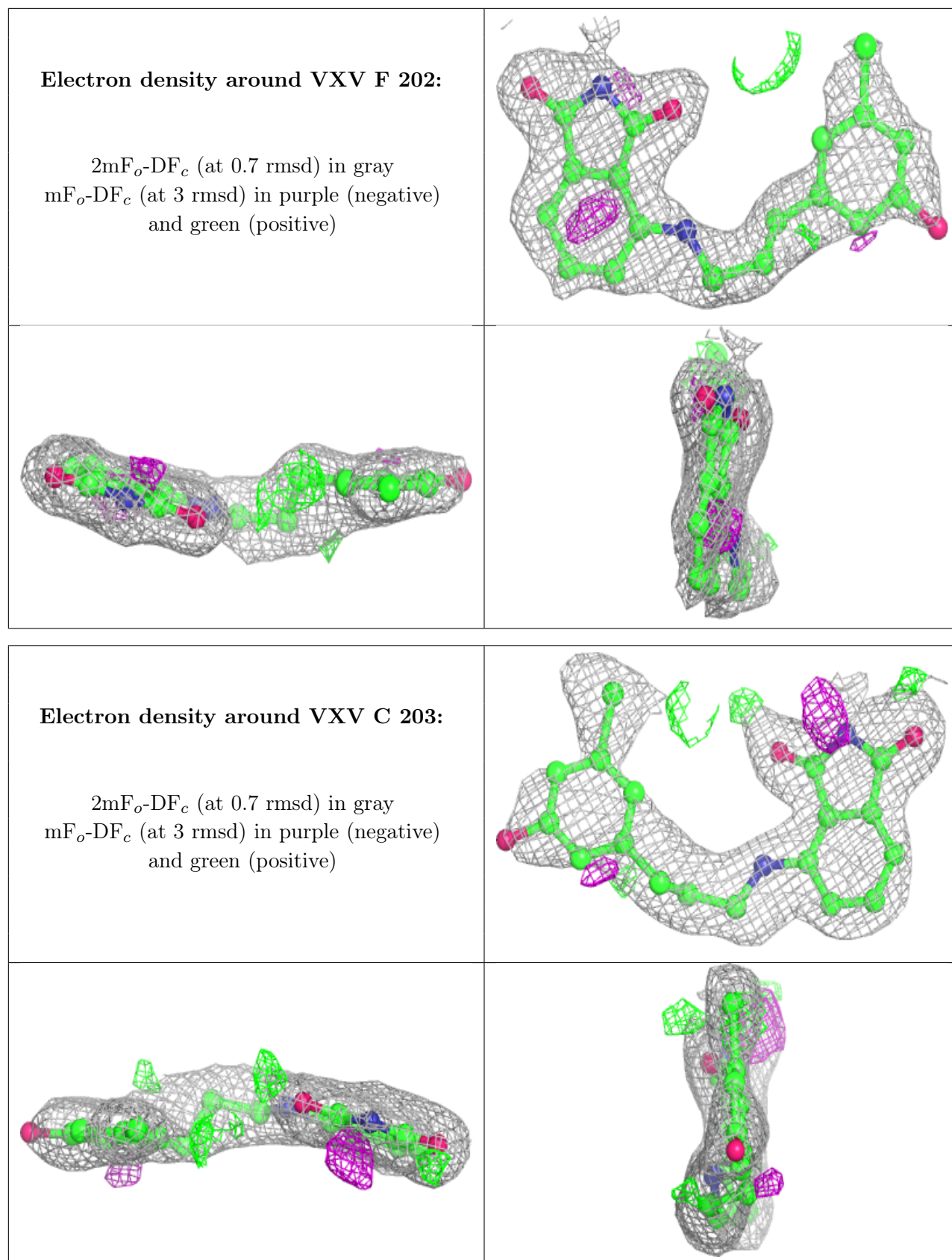
Electron density around VXV J 201:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
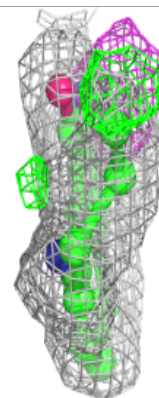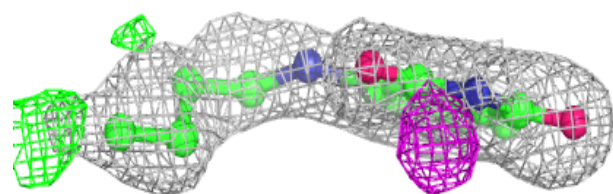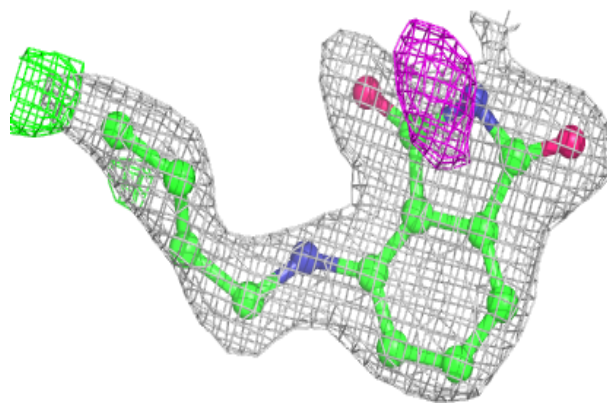
Electron density around VXV K 201:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
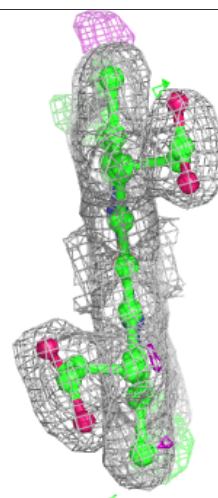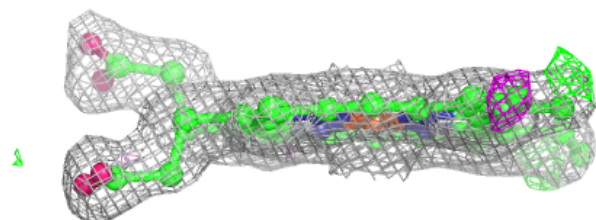$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
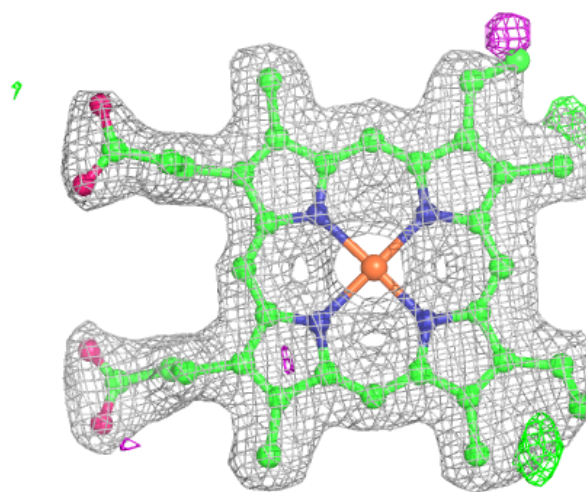and green (positive)
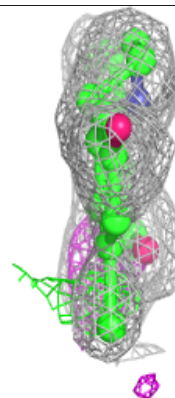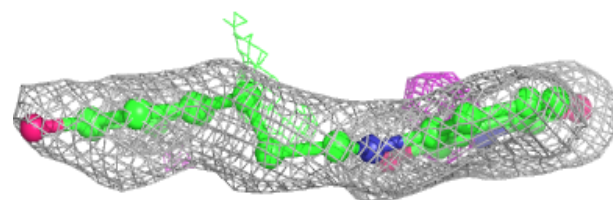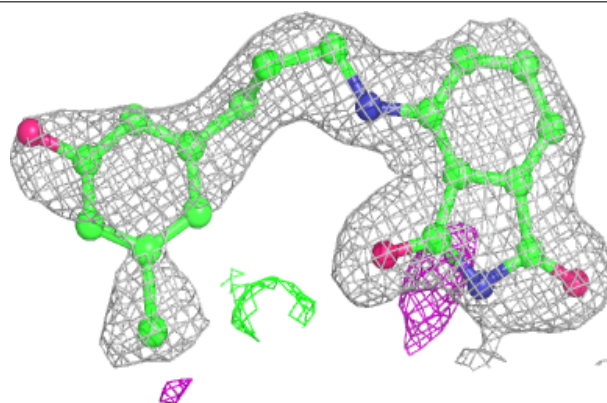
Electron density around VXV B 202:

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

Electron density around VXV L 202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
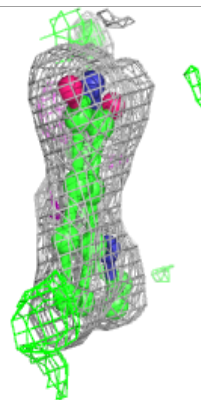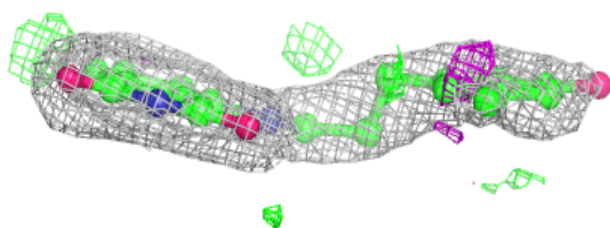
Electron density around VXV D 203:

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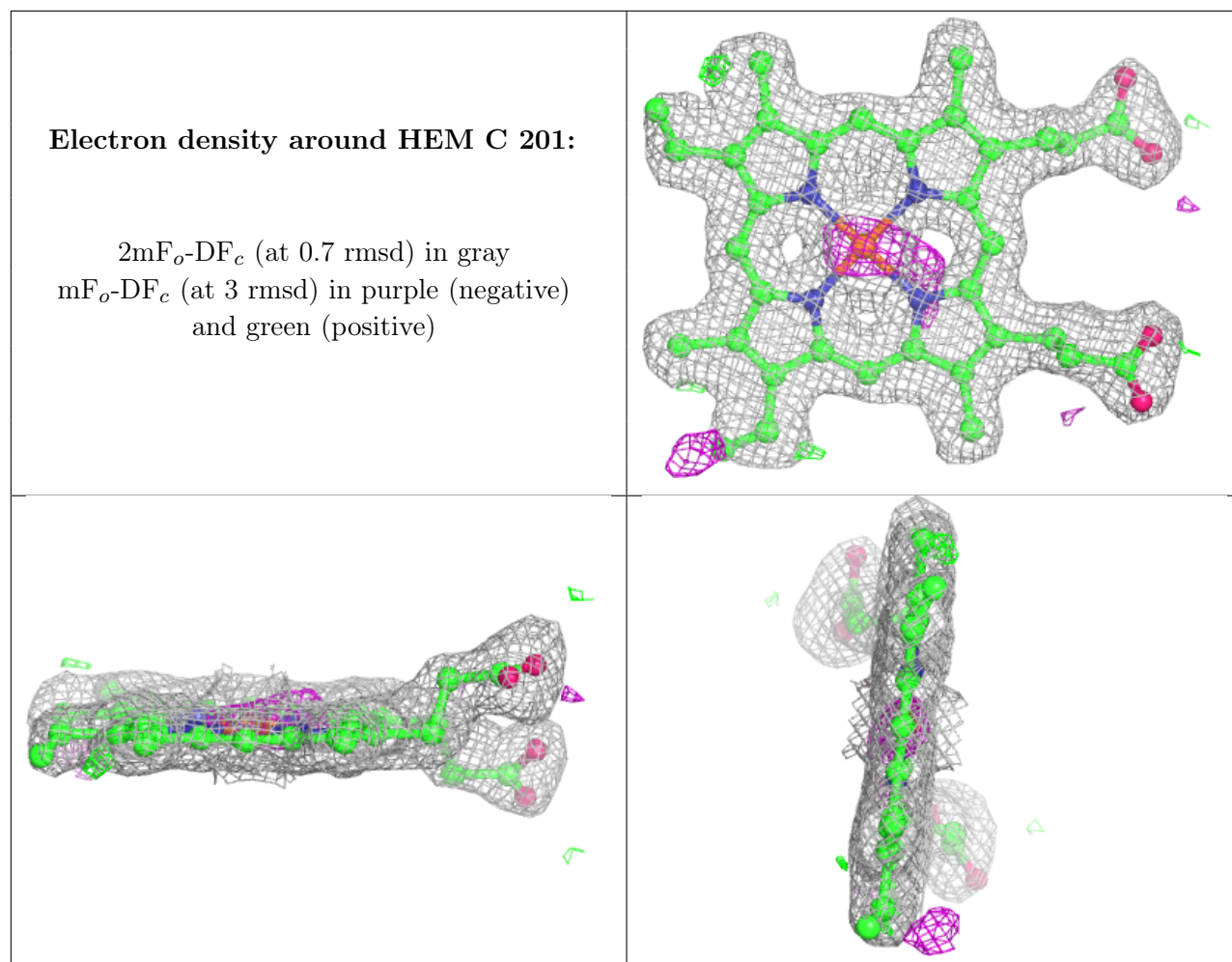and green (positive)

Electron density around HEM L 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
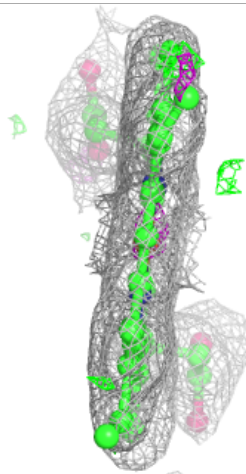
Electron density around HEM D 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
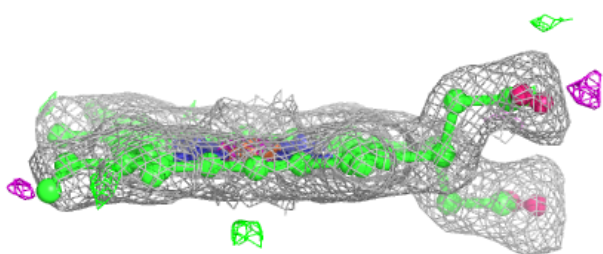
Electron density around HEM F 201:

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

Electron density around HEM E 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
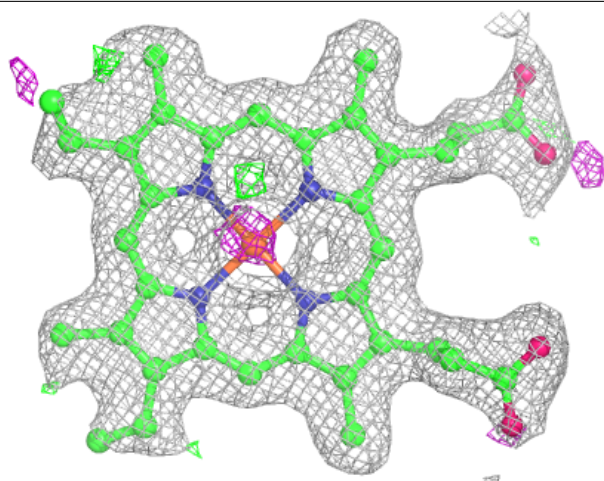
Electron density around HEM C 201:

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

Electron density around HEM H 201:

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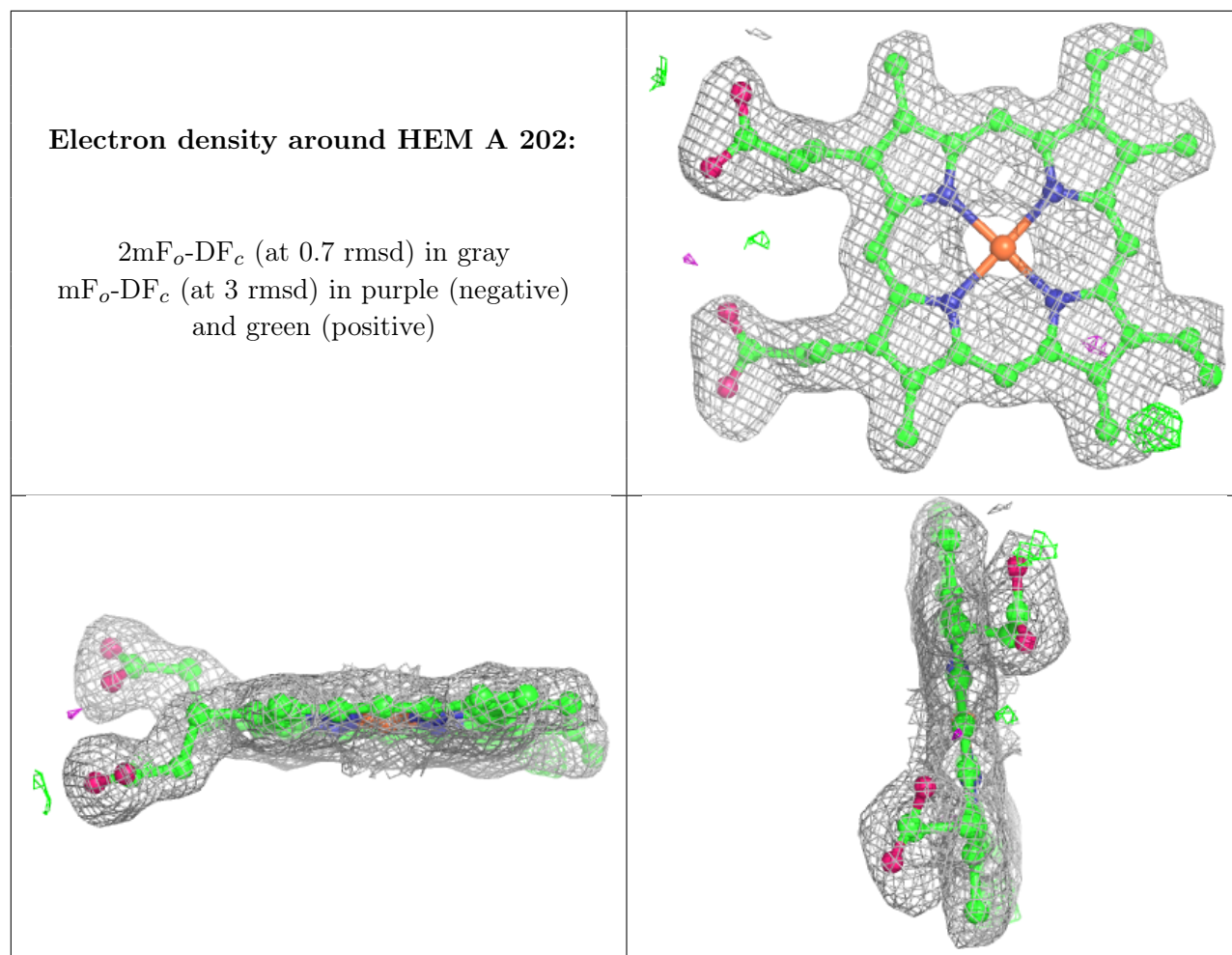and green (positive)

Electron density around HEM A 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.