W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Oct 12, 2024 – 12:26 PM EDT

PDB ID	:	6NHH
Title	:	Rhodobacter sphaeroides bc1 with azoxystrobin
Authors	:	Xia, D.; Zhou, F.; Yu, C.A.
Deposited on	:	2018-12-21
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

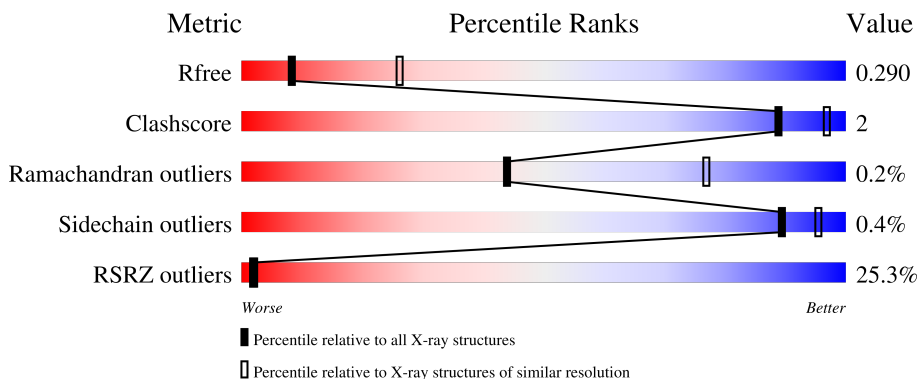|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

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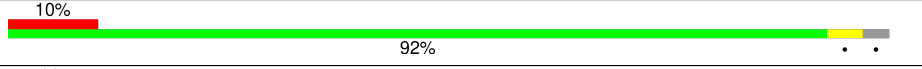*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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		0.290
Clashscore		2
Ramachandran outliers		0.2%
Sidechain outliers		0.4%
RSRZ outliers		25.3%

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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	445	7% / 92% / 5% ·
1	E	445	10% / 92% · ·
2	B	272	11% / 89% / 5% 6%
2	F	272	13% / 90% · 6%
3	C	187	80% / 91% · 6%

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Mol	Chain	Length	Quality of chain
3	G	187	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 27403 atoms, of which 13476 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	430	Total 6878	C 2334	H 3421	N 549	O 559	S 15	0	0	0
1	E	430	Total 6878	C 2334	H 3421	N 549	O 559	S 15	0	0	0

- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	256	Total 3792	C 1240	H 1839	N 326	O 374	S 13	0	0	0
2	F	256	Total 3792	C 1240	H 1839	N 326	O 374	S 13	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	264	GLY	-	expression tag	UNP A0A344Q9J2
B	265	THR	-	expression tag	UNP A0A344Q9J2
B	266	GLY	-	expression tag	UNP A0A344Q9J2
B	267	HIS	-	expression tag	UNP A0A344Q9J2
B	268	HIS	-	expression tag	UNP A0A344Q9J2
B	269	HIS	-	expression tag	UNP A0A344Q9J2
B	270	HIS	-	expression tag	UNP A0A344Q9J2
B	271	HIS	-	expression tag	UNP A0A344Q9J2
B	272	HIS	-	expression tag	UNP A0A344Q9J2
F	264	GLY	-	expression tag	UNP A0A344Q9J2
F	265	THR	-	expression tag	UNP A0A344Q9J2
F	266	GLY	-	expression tag	UNP A0A344Q9J2
F	267	HIS	-	expression tag	UNP A0A344Q9J2
F	268	HIS	-	expression tag	UNP A0A344Q9J2
F	269	HIS	-	expression tag	UNP A0A344Q9J2
F	270	HIS	-	expression tag	UNP A0A344Q9J2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	271	HIS	-	expression tag	UNP A0A344Q9J2
F	272	HIS	-	expression tag	UNP A0A344Q9J2

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	175	Total	C	H	N	O	S	0	0	0
			2576	827	1268	227	248	6			
3	G	175	Total	C	H	N	O	S	0	0	0
			2576	827	1268	227	248	6			

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

HEM
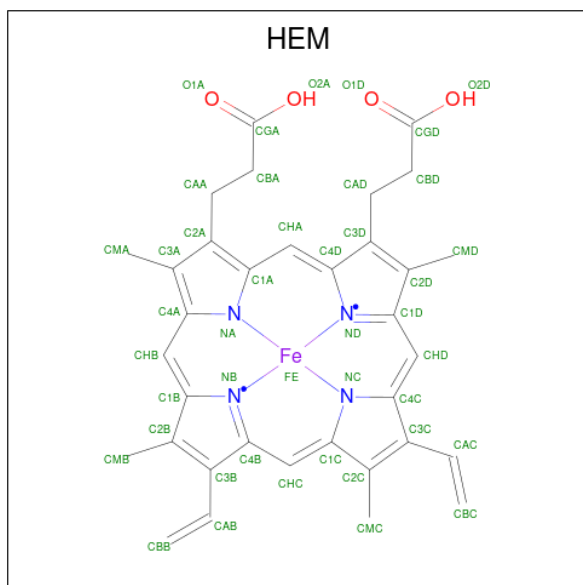
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 5 is METHYL (2Z)-2-(2-{[6-(2-CYANOPHENOXY)PYRIMIDIN-4-YL]OXY}PHENYL)-3-METHOXYACRYLATE (three-letter code: AZO) (formula: $C_{22}H_{17}N_3O_5$).
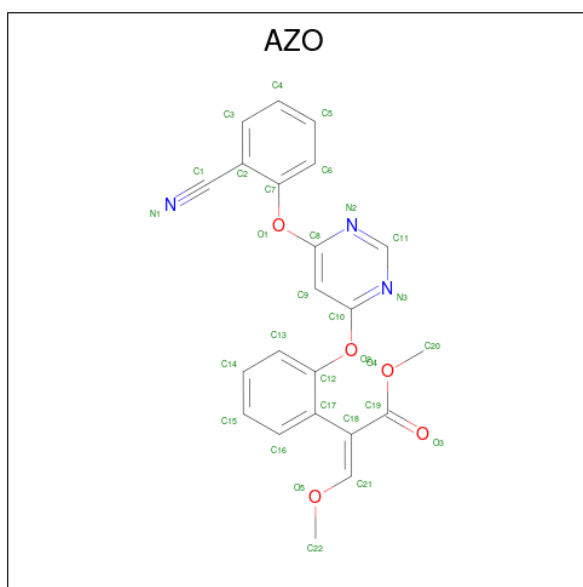
AZO

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			47	22	17	3	5		
5	E	1	Total	C	H	N	O	0	0
			47	22	17	3	5		

- Molecule 6 is 1,2-DIHEXANOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 6PE) (formula: $C_{17}H_{33}NO_8P$).
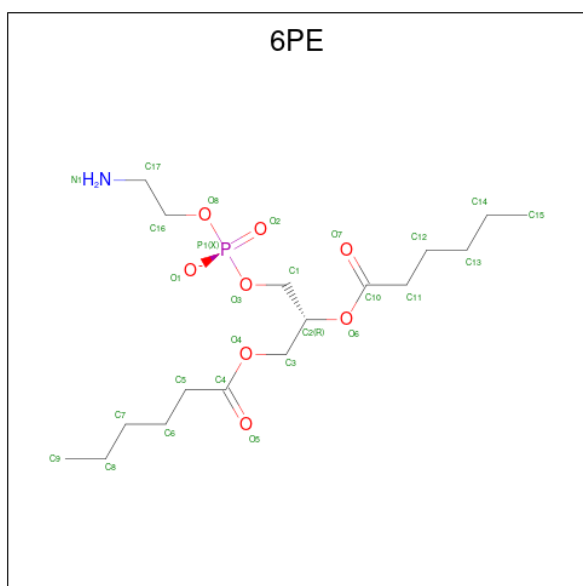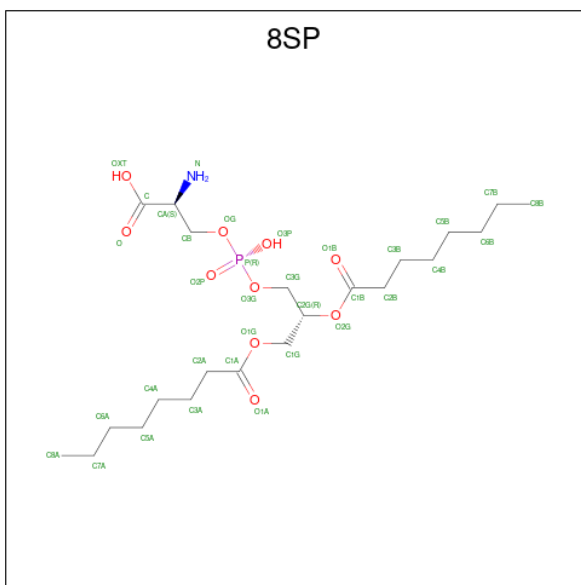

6PE

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	P	0	0
			60	17	33	1	8	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	E	1	Total	C	H	N	O	P	0	0
			60	17	33	1	8	1		

- Molecule 7 is O-[(R)-{[(2R)-2,3-bis(octanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: 8SP) (formula: $C_{22}H_{42}NO_{10}P$).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	P	0	0
			74	22	40	1	10	1		
7	F	1	Total	C	H	N	O	P	0	0
			74	22	40	1	10	1		

- Molecule 8 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Sr	0	0
			1	1		
8	B	1	Total	Sr	0	0
			1	1		
8	F	1	Total	Sr	0	0
			1	1		

- Molecule 9 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).
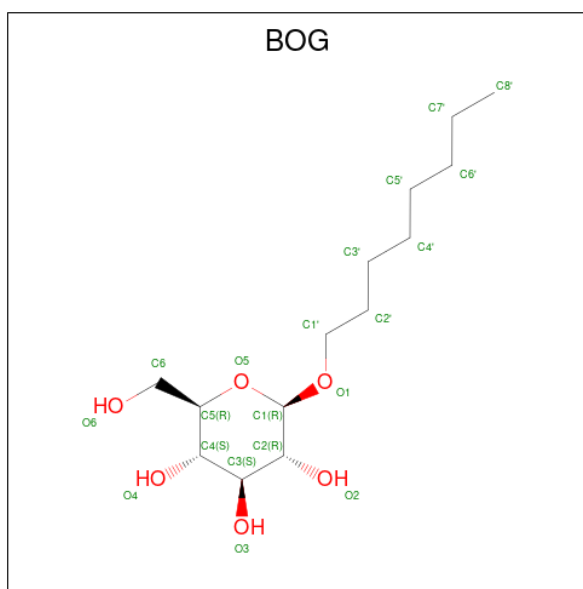
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	H	O	0	0
			48	14	28	6		
9	F	1	Total	C	H	O	0	0
			48	14	28	6		

- Molecule 10 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).
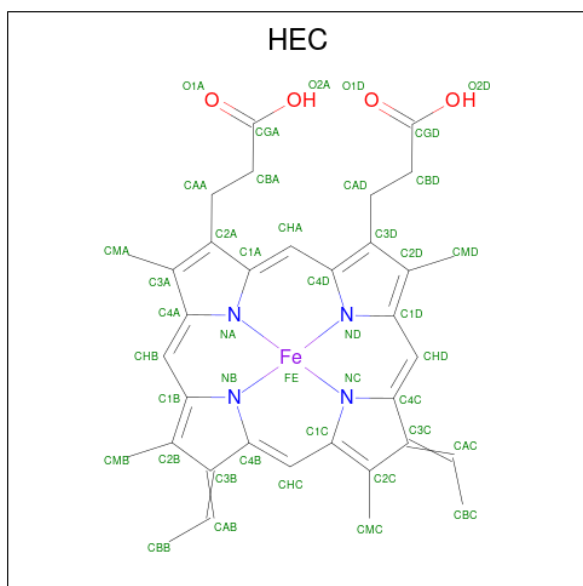
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
10	F	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).
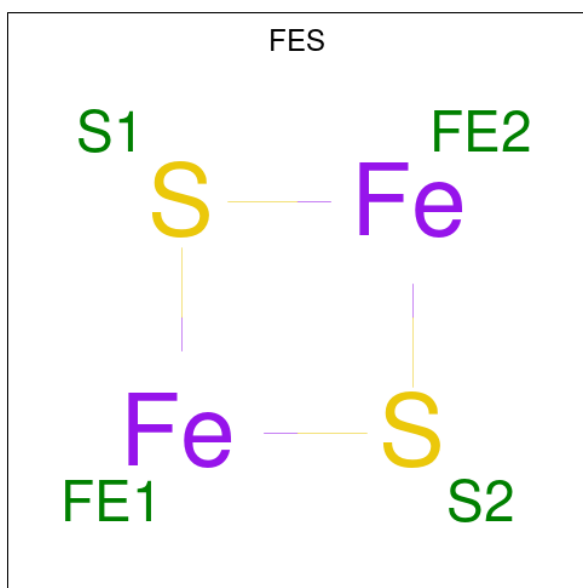
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total 4	Fe 2	S 2	0	0
11	G	1	Total 4	Fe 2	S 2	0	0

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: Cytochrome b
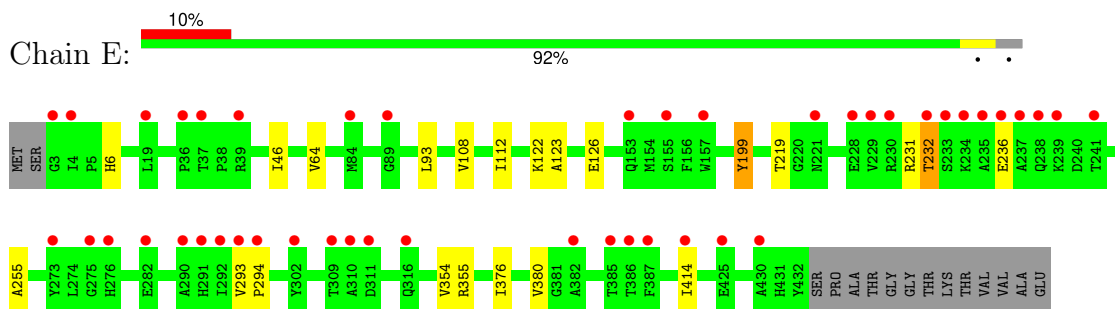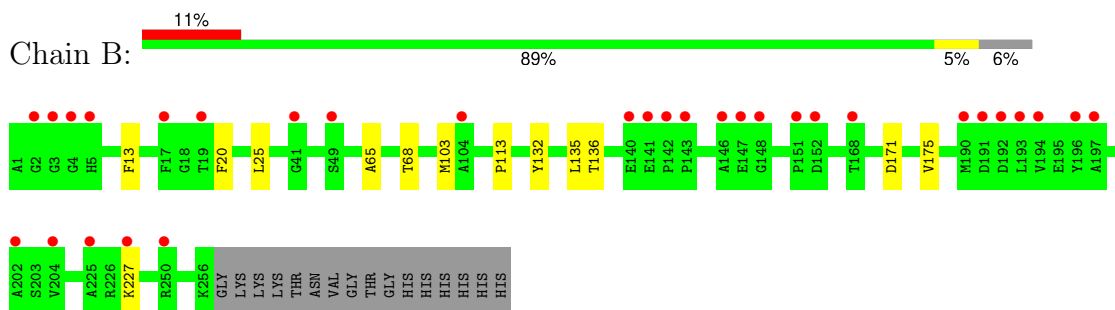
Chain A:

- Molecule 1: Cytochrome b

Chain E:

- Molecule 2: Cytochrome c1

Chain B:

- Molecule 2: Cytochrome c1

Chain F:

• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain C:

• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain G:
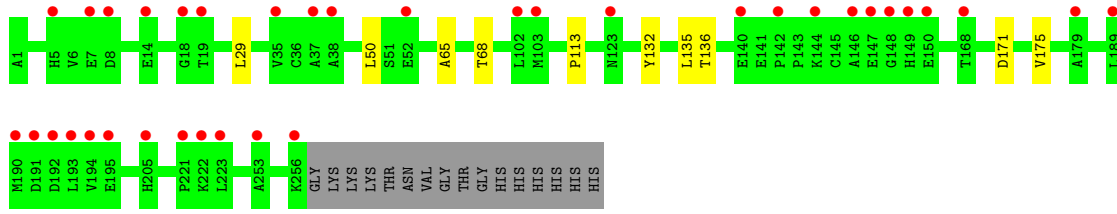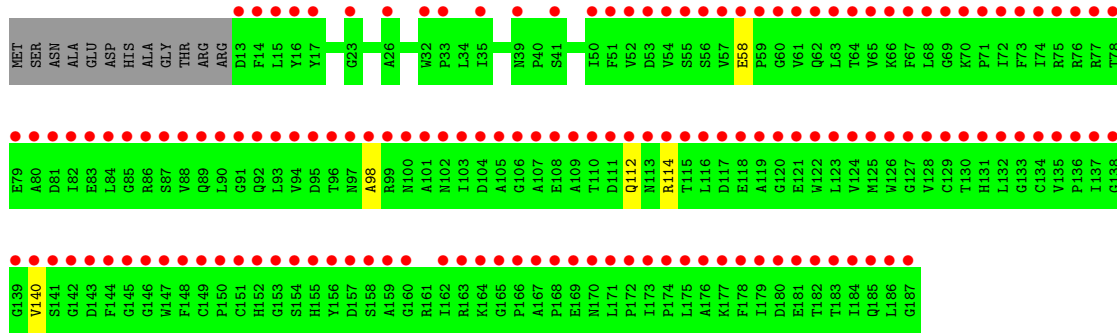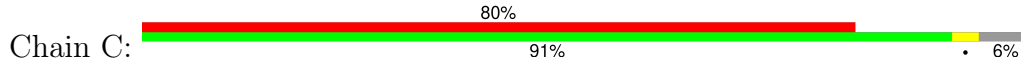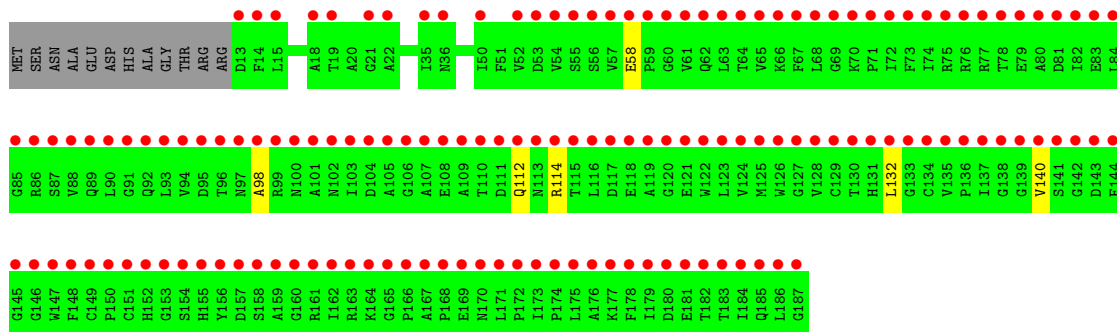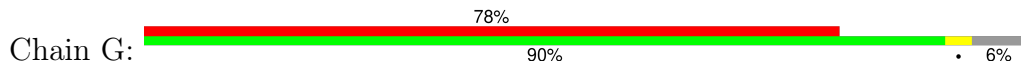
4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.31Å 154.66Å 100.94Å 90.00° 95.36° 90.00°	Depositor
Resolution (Å)	39.28 – 3.00 39.28 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.28-3.00) 93.1 (39.28-3.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 3.01Å)	Xtriage
Refinement program	PHENIX dev_3339	Depositor
R, R_{free}	0.264 , 0.282 0.275 , 0.290	Depositor DCC
R_{free} test set	52577 reflections (3.63%)	wwPDB-VP
Wilson B-factor (Å^2)	48.4	Xtriage
Anisotropy	0.935	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 46.3	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	27403	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, 6PE, SR, HEM, AZO, BOG, 8SP, 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	0.27	0/3589	0.46	0/4924
1	E	0.27	0/3589	0.46	0/4924
2	B	0.27	0/2010	0.46	0/2733
2	F	0.26	0/2010	0.45	0/2733
3	C	0.25	0/1338	0.47	0/1825
3	G	0.25	0/1338	0.47	0/1825
All	All	0.27	0/13874	0.46	0/18964

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 (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	3457	3421	3436	12	0
1	E	3457	3421	3436	11	0
2	B	1953	1839	1848	7	0
2	F	1953	1839	1848	5	0
3	C	1308	1268	1271	3	0
3	G	1308	1268	1271	4	0
4	A	86	60	60	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	86	60	60	2	0
5	A	30	17	17	0	0
5	E	30	17	17	0	0
6	A	27	33	33	0	0
6	E	27	33	33	0	0
7	A	34	40	40	0	0
7	F	34	40	40	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	F	1	0	0	0	0
9	B	20	28	28	0	0
9	F	20	28	28	0	0
10	B	43	32	30	4	0
10	F	43	32	30	3	0
11	C	4	0	0	0	0
11	G	4	0	0	0	0
All	All	13927	13476	13526	48	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 2.

The worst 5 of 48 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:E:232:THR:OG1	1:E:236:GLU:OE1	2.09	0.68
10:F:302:HEC:HBC3	10:F:302:HEC:HMC1	1.76	0.68
10:B:302:HEC:HMC1	10:B:302:HEC:HBC3	1.76	0.67
1:E:123:ALA:O	1:E:355:ARG:NH1	2.28	0.65
1:A:123:ALA:O	1:A:355:ARG:NH1	2.31	0.63

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	428/445 (96%)	416 (97%)	12 (3%)	0	100	100
1	E	428/445 (96%)	416 (97%)	12 (3%)	0	100	100
2	B	254/272 (93%)	245 (96%)	8 (3%)	1 (0%)	30	66
2	F	254/272 (93%)	245 (96%)	8 (3%)	1 (0%)	30	66
3	C	173/187 (92%)	158 (91%)	14 (8%)	1 (1%)	22	57
3	G	173/187 (92%)	158 (91%)	14 (8%)	1 (1%)	22	57
All	All	1710/1808 (95%)	1638 (96%)	68 (4%)	4 (0%)	44	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	140	VAL
3	G	140	VAL
2	B	113	PRO
2	F	113	PRO

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	355/366 (97%)	353 (99%)	2 (1%)	84	93
1	E	355/366 (97%)	351 (99%)	4 (1%)	70	87
2	B	203/216 (94%)	203 (100%)	0	100	100
2	F	203/216 (94%)	203 (100%)	0	100	100
3	C	135/144 (94%)	135 (100%)	0	100	100
3	G	135/144 (94%)	135 (100%)	0	100	100
All	All	1386/1452 (96%)	1380 (100%)	6 (0%)	89	95

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

Mol	Chain	Res	Type
1	E	199	TYR
1	E	232	THR
1	E	414	ILE
1	A	414	ILE
1	A	199	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	113	ASN
3	G	113	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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	#$|Z| > 2$
7	8SP	F	303	-	32,33,33	0.90	1 (3%)	34,40,40	1.33	3 (8%)
6	6PE	E	1004	-	26,26,26	0.89	2 (7%)	29,31,31	0.68	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	AZO	A	1003	-	32,32,32	0.58	0	42,42,42	1.58	7 (16%)
4	HEM	E	1001	1	42,50,50	1.44	6 (14%)	46,82,82	1.36	6 (13%)
4	HEM	E	1002	1	42,50,50	1.48	7 (16%)	46,82,82	1.36	7 (15%)
9	BOG	B	301	-	20,20,20	0.88	0	25,25,25	1.24	4 (16%)
6	6PE	A	1004	-	26,26,26	0.88	2 (7%)	29,31,31	0.69	0
9	BOG	F	301	-	20,20,20	0.81	0	25,25,25	1.33	2 (8%)
11	FES	G	1001	3	0,4,4	-	-	-		
4	HEM	A	1002	1	42,50,50	1.54	7 (16%)	46,82,82	1.35	7 (15%)
5	AZO	E	1003	-	32,32,32	0.62	0	42,42,42	1.62	8 (19%)
11	FES	C	1001	3	0,4,4	-	-	-		
4	HEM	A	1001	1	42,50,50	1.59	5 (11%)	46,82,82	1.55	8 (17%)
7	8SP	A	1005	-	32,33,33	0.90	1 (3%)	34,40,40	0.92	2 (5%)
10	HEC	F	302	2	32,50,50	2.02	3 (9%)	30,82,82	2.09	6 (20%)
10	HEC	B	302	2	32,50,50	2.00	3 (9%)	30,82,82	2.12	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	8SP	F	303	-	-	16/39/39/39	-
6	6PE	E	1004	-	-	20/30/30/30	-
5	AZO	A	1003	-	-	1/23/23/23	0/3/3/3
4	HEM	E	1001	1	-	4/12/54/54	-
4	HEM	E	1002	1	-	0/12/54/54	-
9	BOG	B	301	-	-	6/11/31/31	0/1/1/1
6	6PE	A	1004	-	-	11/30/30/30	-
9	BOG	F	301	-	-	3/11/31/31	0/1/1/1
11	FES	G	1001	3	-	-	0/1/1/1
4	HEM	A	1002	1	-	5/12/54/54	-
5	AZO	E	1003	-	-	0/23/23/23	0/3/3/3
11	FES	C	1001	3	-	-	0/1/1/1
4	HEM	A	1001	1	-	4/12/54/54	-
7	8SP	A	1005	-	-	20/39/39/39	-
10	HEC	F	302	2	-	2/10/54/54	-
10	HEC	B	302	2	-	2/10/54/54	-

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	302	HEC	C2B-C3B	-5.84	1.34	1.40
10	B	302	HEC	C2B-C3B	-5.81	1.34	1.40
10	B	302	HEC	C3D-C2D	5.32	1.53	1.37
10	F	302	HEC	C3D-C2D	5.31	1.53	1.37
10	B	302	HEC	C3C-C2C	-4.81	1.35	1.40

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	302	HEC	CBB-CAB-C3B	-6.61	112.02	127.49
10	F	302	HEC	CBB-CAB-C3B	-6.48	112.33	127.49
5	E	1003	AZO	C11-N3-C10	6.09	119.14	114.50
5	A	1003	AZO	C11-N3-C10	5.85	118.96	114.50
10	F	302	HEC	CBC-CAC-C3C	-5.84	113.82	127.49

There are no chirality outliers.

5 of 94 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	1004	6PE	C1-O3-P1-O1
6	E	1004	6PE	C1-O3-P1-O8
6	E	1004	6PE	C16-O8-P1-O2
6	E	1004	6PE	O8-C16-C17-N1
7	A	1005	8SP	CB-OG-P-O3G

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1001	HEM	2	0
4	A	1002	HEM	1	0
4	A	1001	HEM	3	0
10	F	302	HEC	3	0
10	B	302	HEC	4	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 8SP F 303

Bond lengths

Bond angles

Torsions

Rings

Ligand 6PE E 1004

Bond lengths

Bond angles

Torsions

Rings

Ligand AZO A 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM E 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM E 1002

Bond lengths

Bond angles

Torsions

Rings

Ligand BOG B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 6PE A 1004

Bond lengths

Bond angles

Torsions

Rings

Ligand BOG F 301

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 1002

Bond lengths

Bond angles

Torsions

Rings

Ligand AZO E 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand 8SP A 1005

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC F 302

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC B 302

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(Å^2)	Q<0.9
1	A	430/445 (96%)	0.50	29 (6%)	25	14	37, 55, 107, 136	0
1	E	430/445 (96%)	0.69	45 (10%)	13	7	18, 64, 114, 178	0
2	B	256/272 (94%)	0.76	31 (12%)	10	6	50, 73, 134, 188	0
2	F	256/272 (94%)	0.98	36 (14%)	7	4	51, 87, 160, 206	0
3	C	175/187 (93%)	6.84	149 (85%)	0	0	23, 34, 92, 107	136 (77%)
3	G	175/187 (93%)	6.53	146 (83%)	0	0	23, 29, 104, 153	136 (77%)
All	All	1722/1808 (95%)	1.92	436 (25%)	2	2	18, 63, 126, 206	272 (15%)

The worst 5 of 436 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	133	GLY	28.3
3	C	124	VAL	22.1
3	C	87	SER	22.1
3	C	119	ALA	21.1
3	C	78	THR	20.5

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
11	FES	C	1001	4/4	0.71	0.24	128,129,132,132	4
7	8SP	F	303	34/34	0.81	0.14	11,17,48,49	0
11	FES	G	1001	4/4	0.81	0.28	106,107,109,109	4
7	8SP	A	1005	34/34	0.83	0.14	6,12,35,35	0
6	6PE	E	1004	27/27	0.85	0.13	7,14,19,20	0
6	6PE	A	1004	27/27	0.87	0.13	9,15,19,21	0
5	AZO	A	1003	30/30	0.87	0.15	32,35,43,44	0
9	BOG	B	301	20/20	0.90	0.16	9,12,15,19	0
9	BOG	F	301	20/20	0.90	0.18	12,16,21,25	0
5	AZO	E	1003	30/30	0.91	0.14	39,39,47,49	0
8	SR	A	1006	1/1	0.93	0.08	103,103,103,103	0
10	HEC	F	302	43/43	0.94	0.13	43,48,58,58	0
4	HEM	E	1002	43/43	0.94	0.16	48,54,65,66	0
4	HEM	A	1002	43/43	0.94	0.17	49,54,66,66	0
4	HEM	E	1001	43/43	0.95	0.17	46,52,63,63	0
4	HEM	A	1001	43/43	0.95	0.17	47,53,64,64	0
10	HEC	B	302	43/43	0.96	0.13	43,48,58,58	0
8	SR	F	304	1/1	0.98	0.07	108,108,108,108	0
8	SR	B	303	1/1	0.99	0.08	102,102,102,102	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.
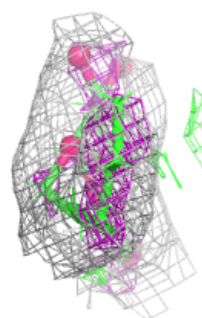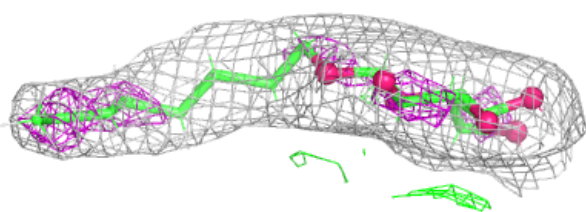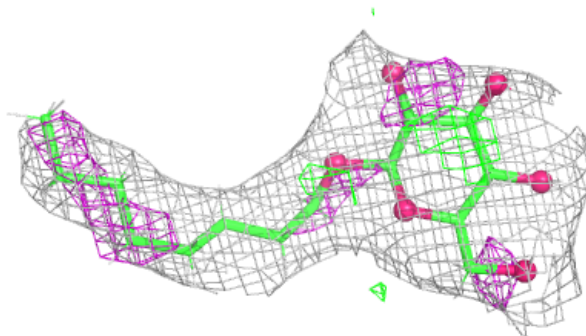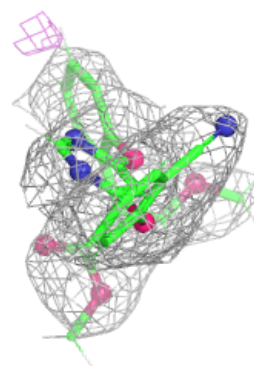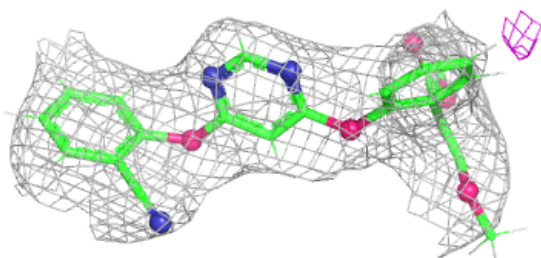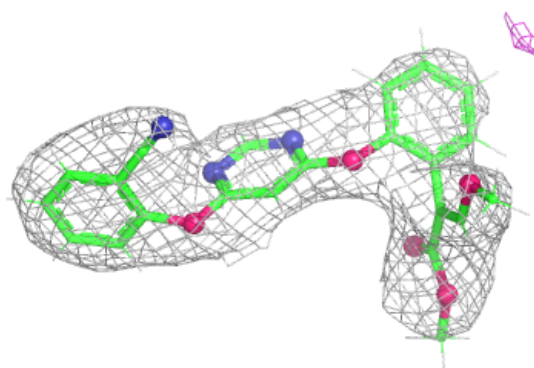
Electron density around 8SP F 303:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
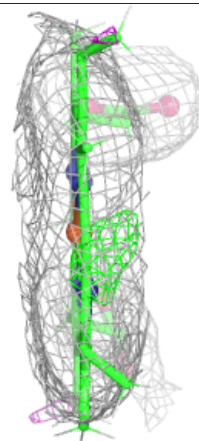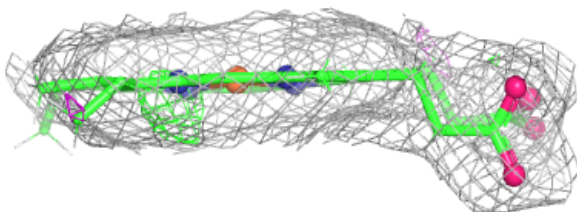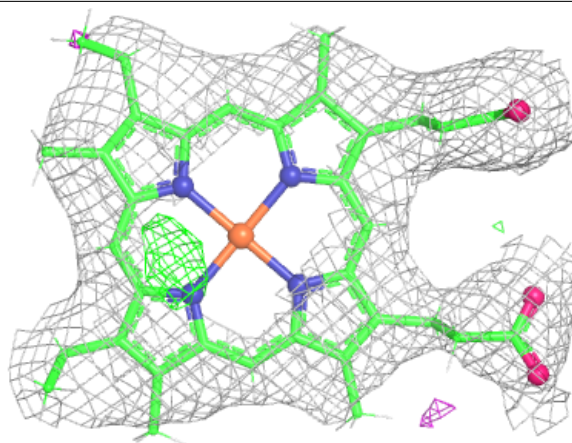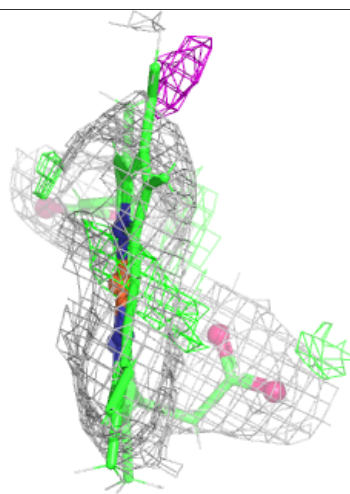and green (positive)
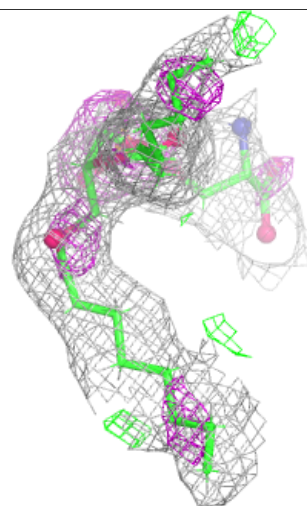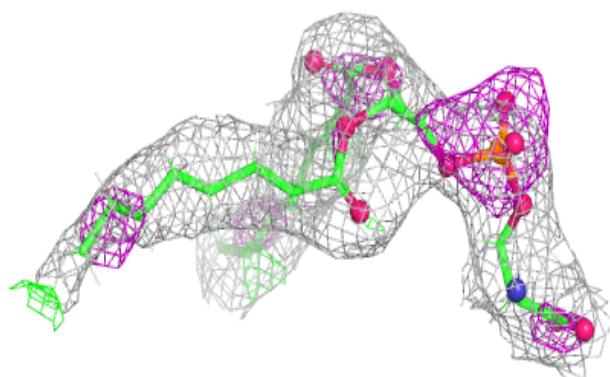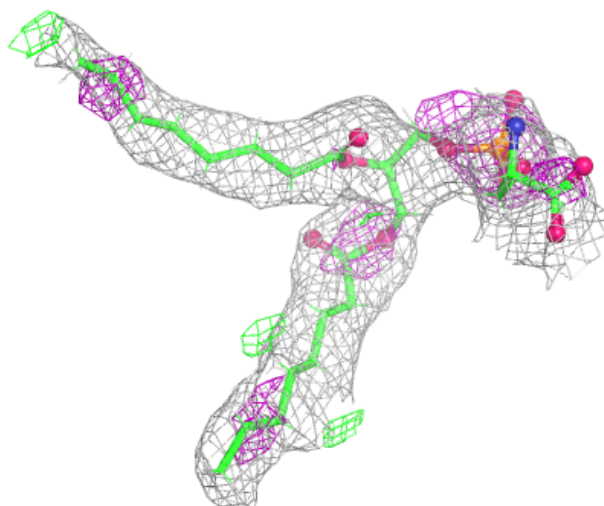
Electron density around 8SP A 1005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
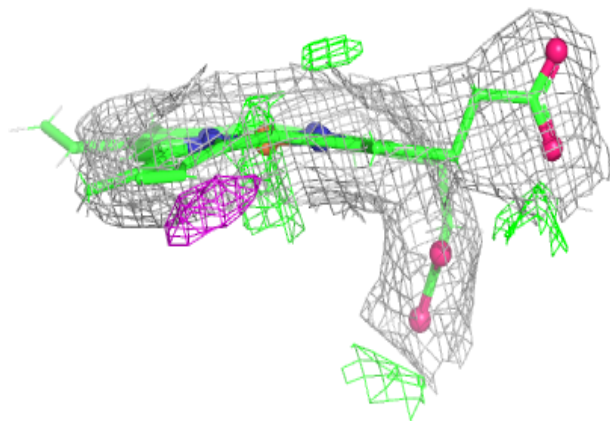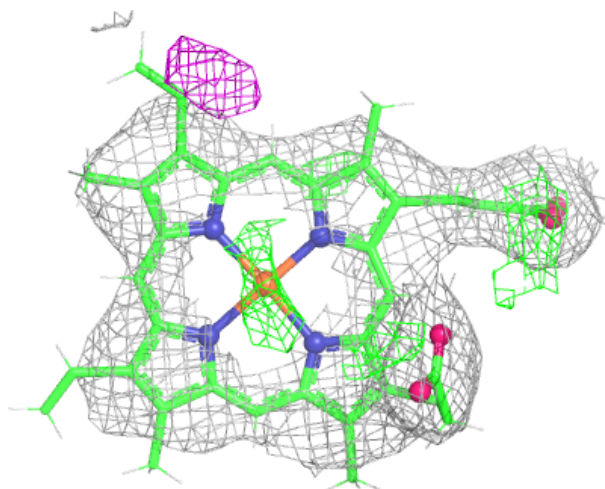mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
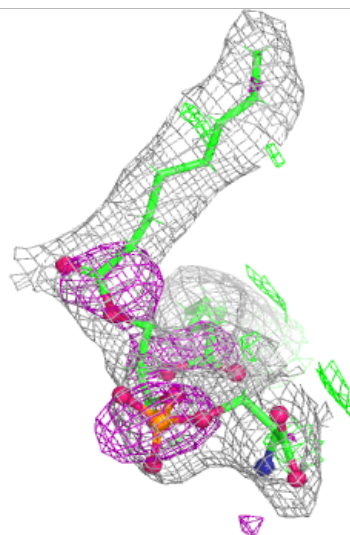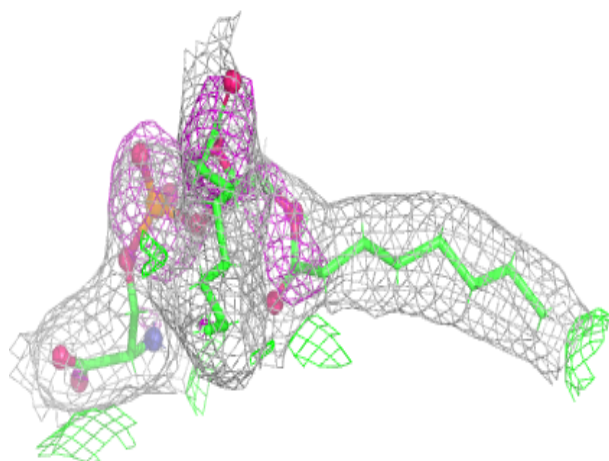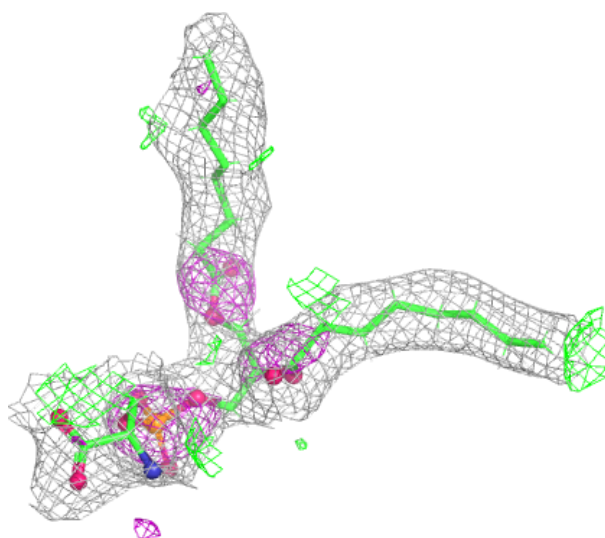
Electron density around 6PE E 1004:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
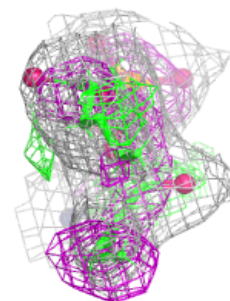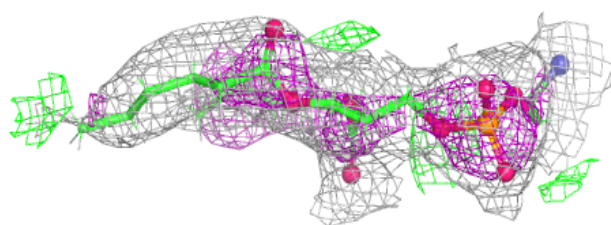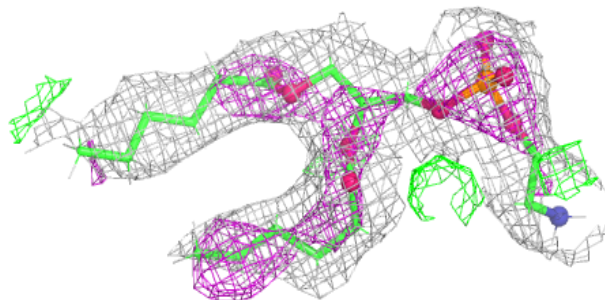
Electron density around 6PE A 1004:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
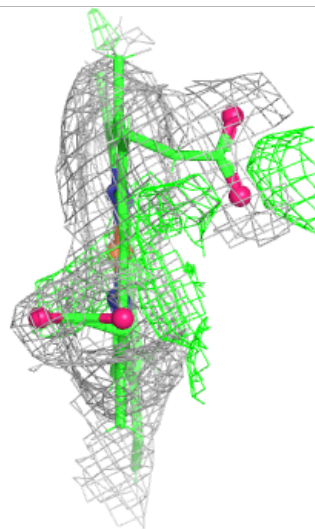$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
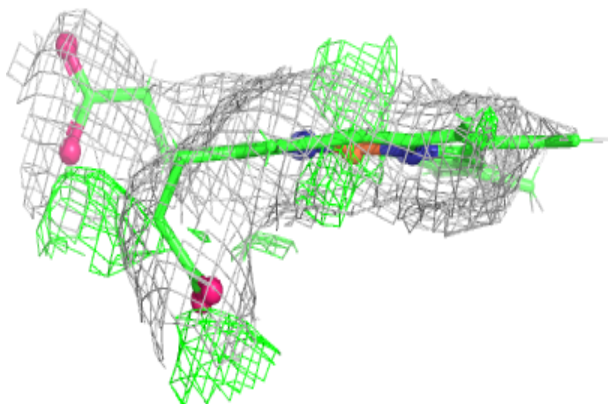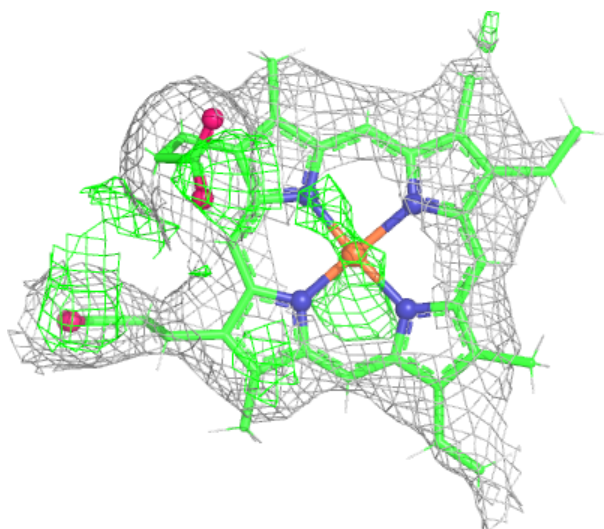and green (positive)
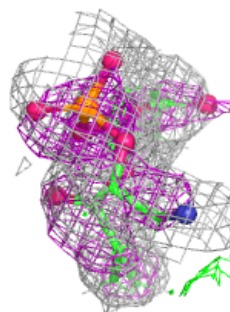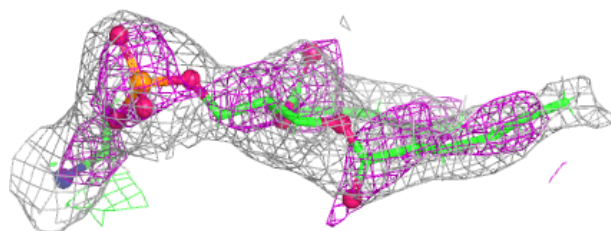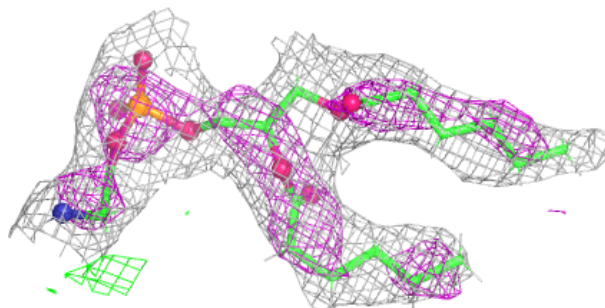
Electron density around AZO A 1003:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
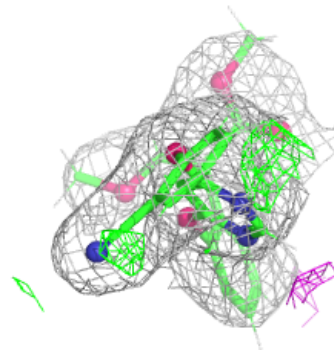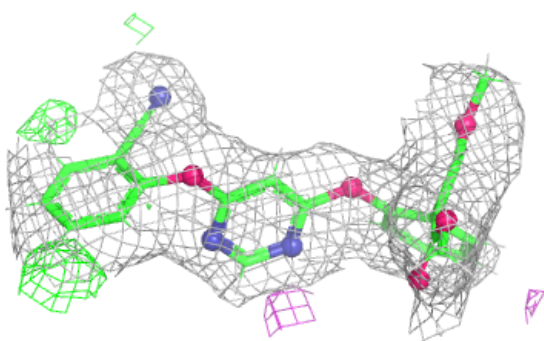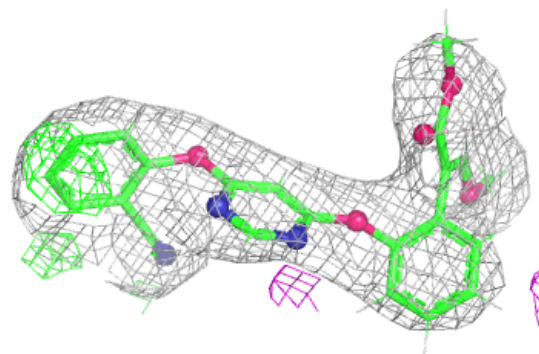
Electron density around BOG B 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
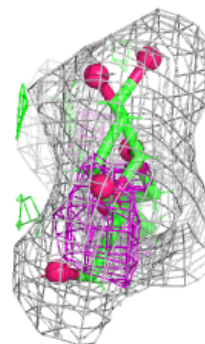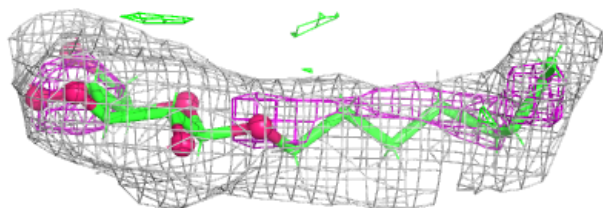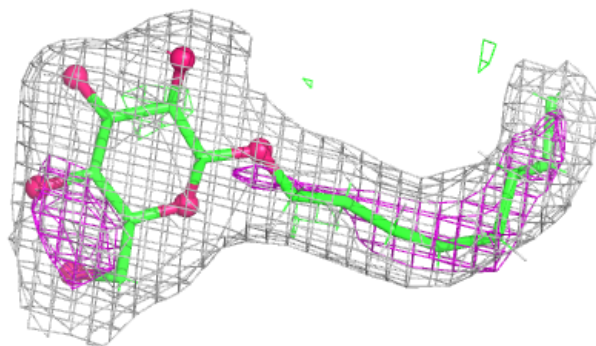
Electron density around BOG F 301:

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

Electron density around AZO E 1003:

$2mF_o$-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 302:

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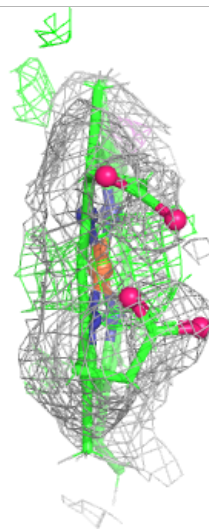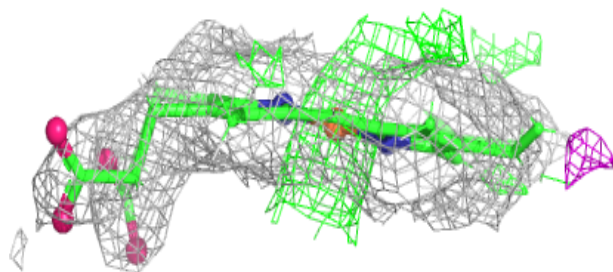mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around HEM E 1002:

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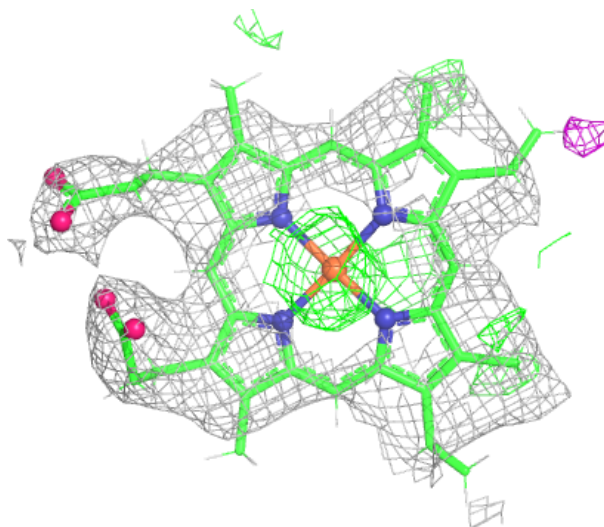and green (positive)

Electron density around HEM A 1002:

$2mF_o$-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 E 1001:

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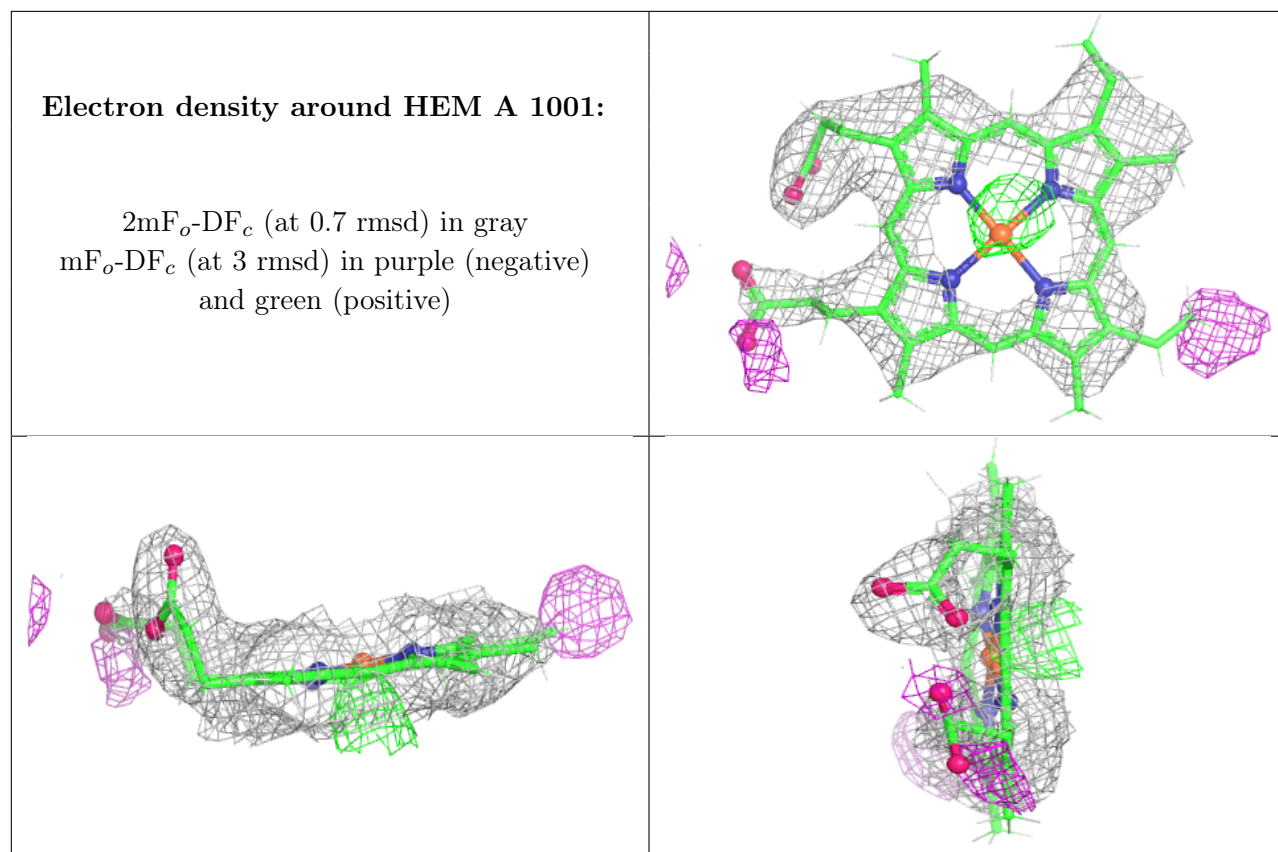and green (positive)

Electron density around HEM A 1001:

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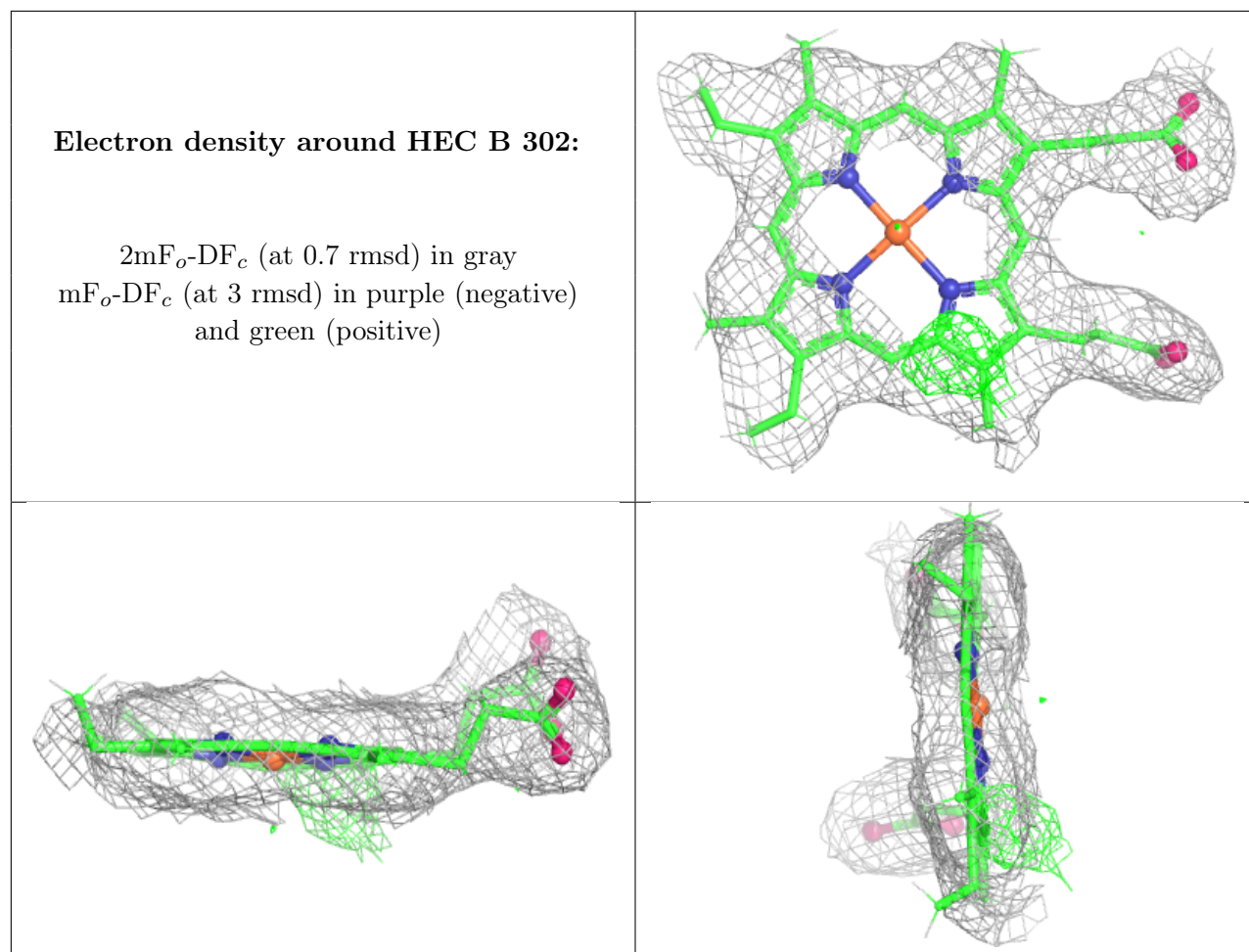and green (positive)

Electron density around HEC B 302:

$2mF_o$-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.