



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:54 PM EDT

PDB ID : 6NHH / pdb_00006nhh
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 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:

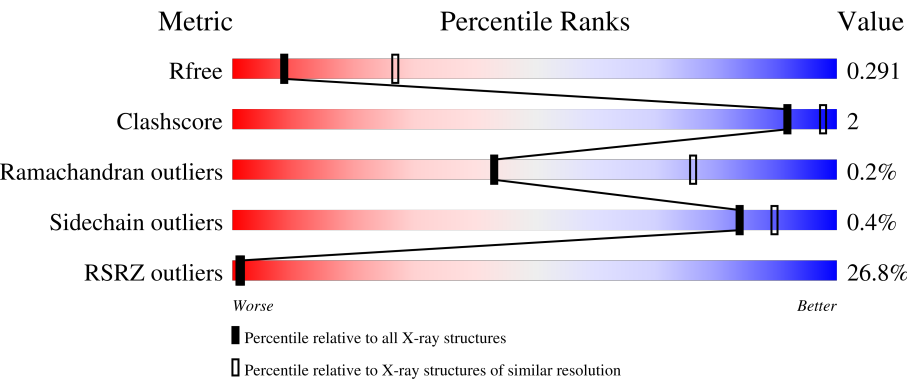
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. 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	445	8% 91% 6%
1	E	445	12% 91% 5%
2	B	272	12% 90% 6%
2	F	272	16% 90% 6%
3	C	187	81% 93% 6%

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Mol	Chain	Length	Quality of chain
3	G	187	78% 93% 6%

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
10	HEC	B	302	X	-	-	-
10	HEC	F	302	X	-	-	-

2 Entry composition

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	C	H	N	O	S	0	0	0
			6878	2334	3421	549	559	15			
1	E	430	Total	C	H	N	O	S	0	0	0
			6878	2334	3421	549	559	15			

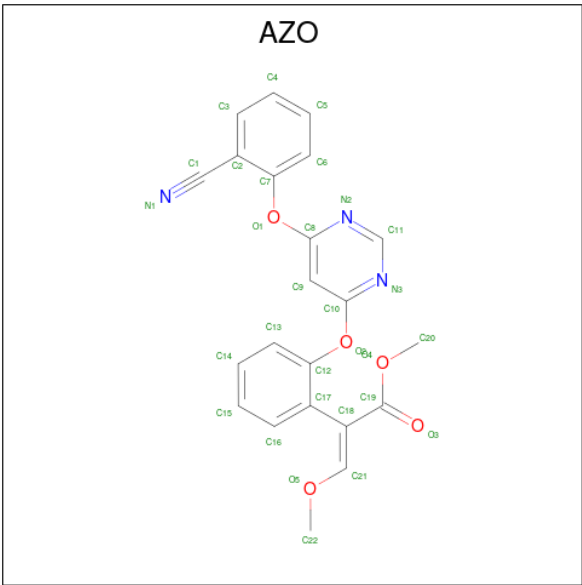
- Molecule 2 is a protein called Cytochrome c1.

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

There are 18 discrepancies between the modelled and reference sequences:

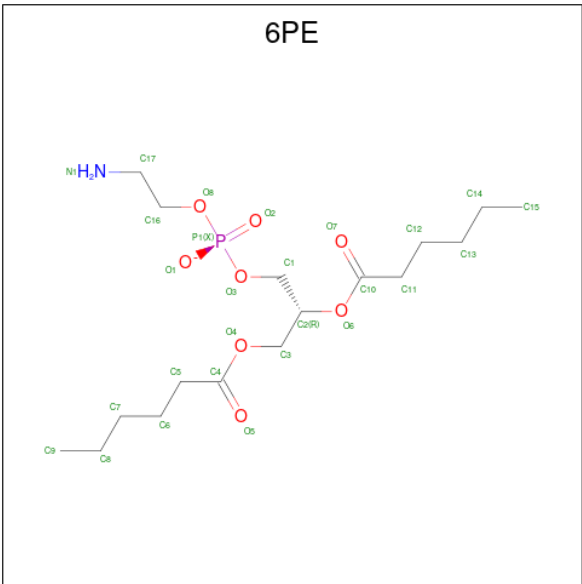
Chain	Residue	Modelled	Actual	Comment	Reference
B	264	GLY	-	expression tag	UNP A0A344Q9J2
B	265	THR	-	expression tag	UNP A0A344Q9J2
B	266	GLY	-	expression tag	UNP A0A344Q9J2
B	267	HIS	-	expression tag	UNP A0A344Q9J2
B	268	HIS	-	expression tag	UNP A0A344Q9J2
B	269	HIS	-	expression tag	UNP A0A344Q9J2
B	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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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 (CCD ID: 6PE) (formula: C₁₇H₃₃NO₈P).



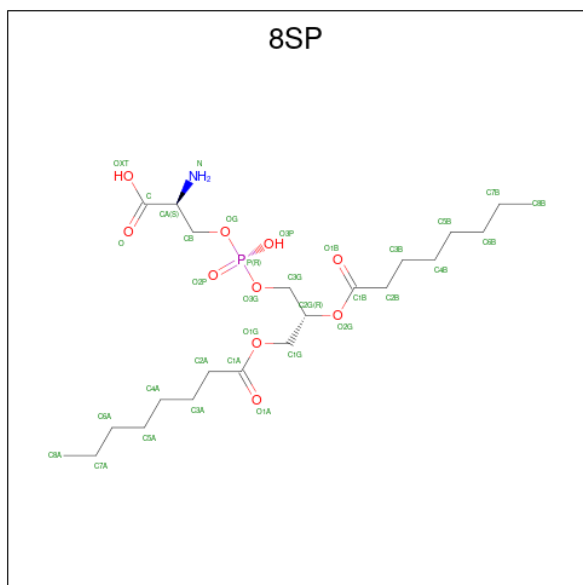
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	P	0	0
			60	17	33	1	8	1		

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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 (CCD ID: 8SP) (formula: C₂₂H₄₂NO₁₀P).

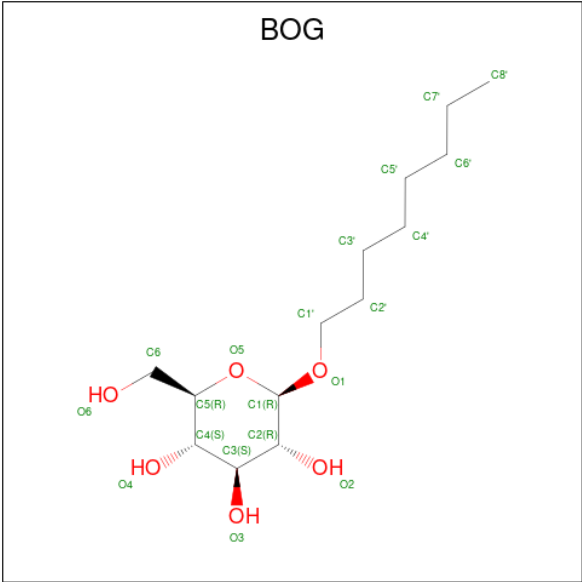


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	P	0	0
			74	22	40	1	10	1		
7	F	1	Total	C	H	N	O	P	0	0
			74	22	40	1	10	1		

- Molecule 8 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

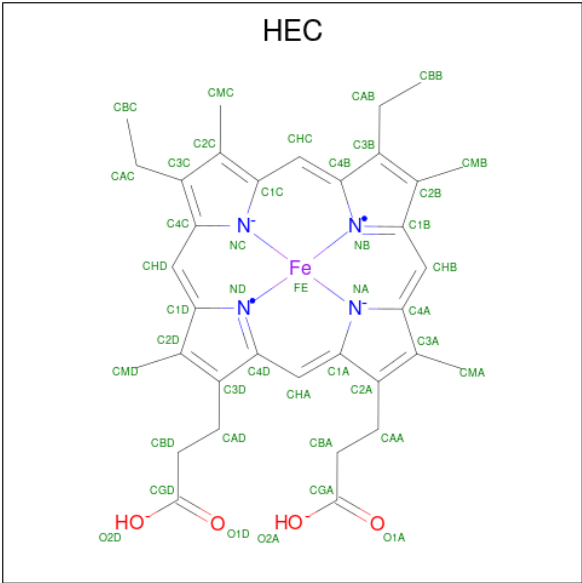
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Sr	0	0
			1	1		
8	B	1	Total	Sr	0	0
			1	1		
8	F	1	Total	Sr	0	0
			1	1		

- Molecule 9 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



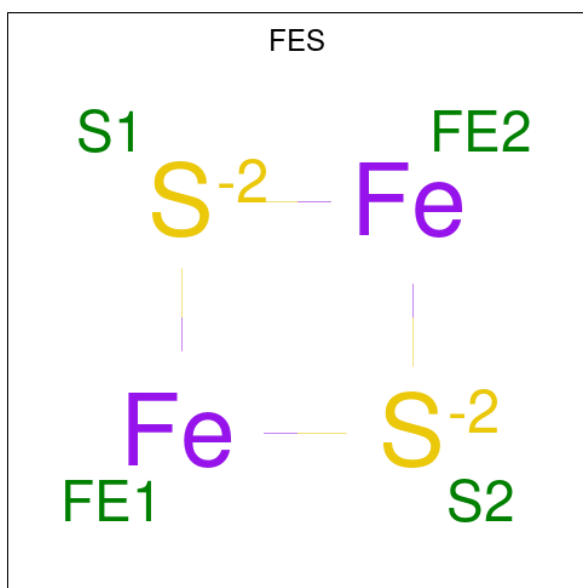
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	H	O	0	0
			48	14	28	6		
9	F	1	Total	C	H	O	0	0
			48	14	28	6		

- Molecule 10 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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 (CCD ID: FES) (formula: Fe_2S_2).

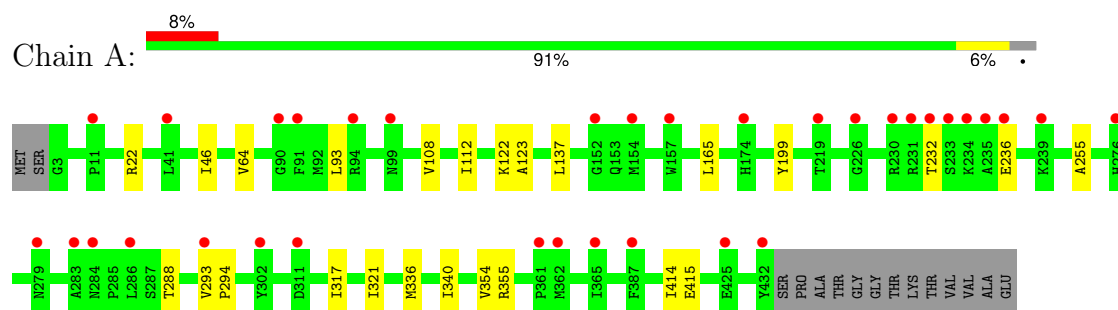


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	Fe	S	0	0
			4	2	2		
11	G	1	Total	Fe	S	0	0
			4	2	2		

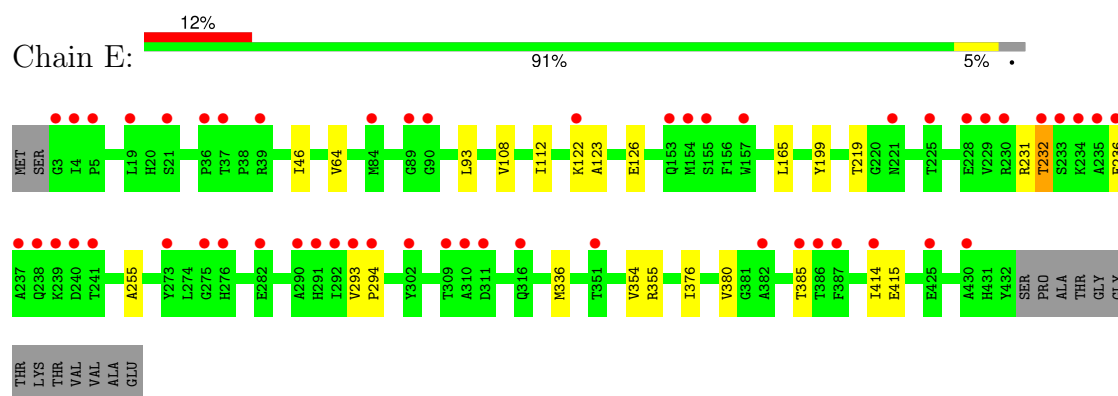
3 Residue-property plots [i](#)

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

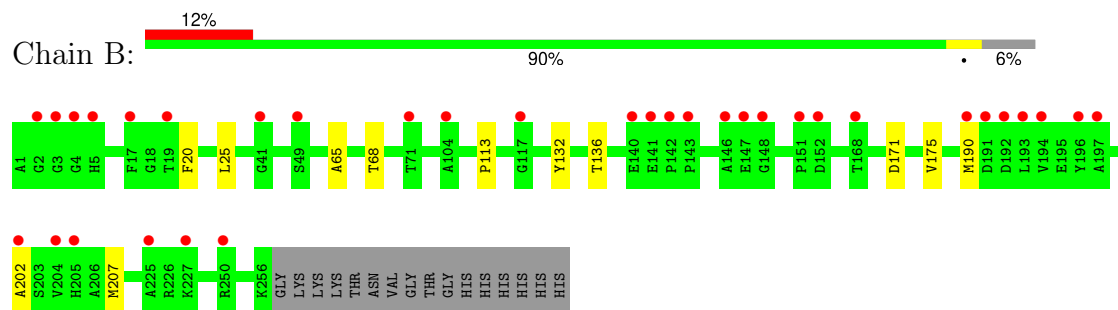
• Molecule 1: Cytochrome b



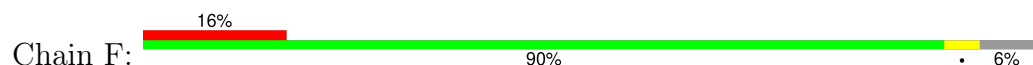
• Molecule 1: Cytochrome b

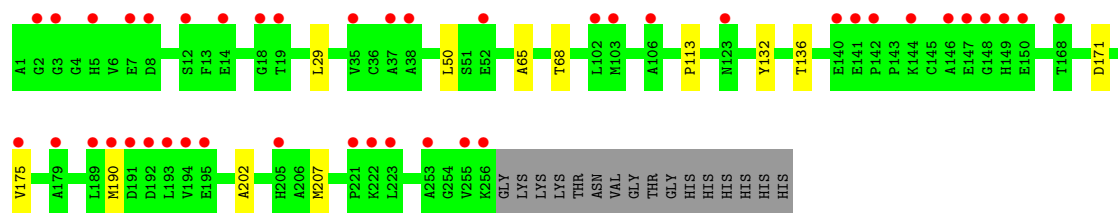


• Molecule 2: Cytochrome c1

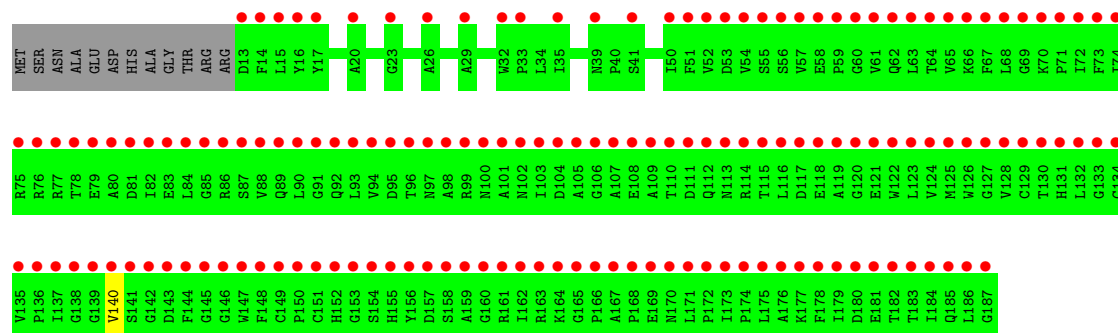
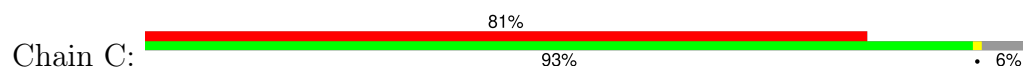


• Molecule 2: Cytochrome c1

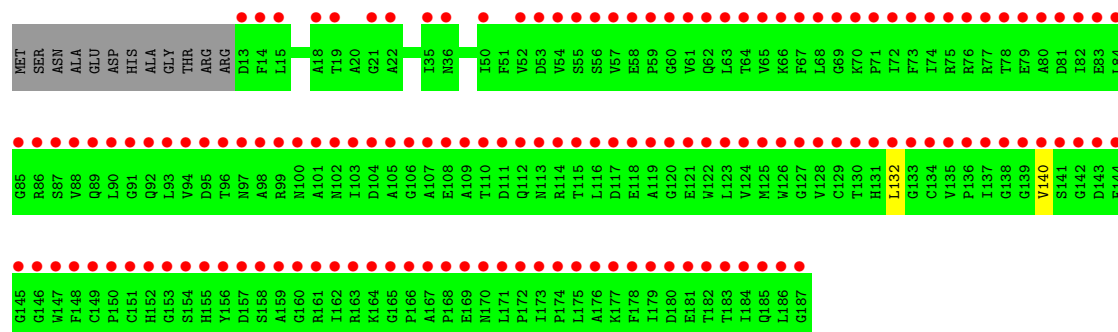
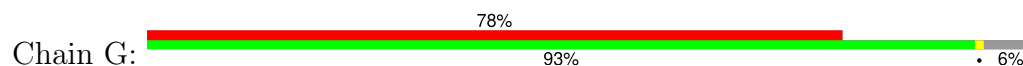




● Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



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



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
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.01Å)	Xtriage
Refinement program	PHENIX dev_3339	Depositor
R, R_{free}	0.264 , 0.282 0.275 , 0.291	Depositor DCC
R_{free} test set	1991 reflections (3.64%)	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	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SR, AZO, HEC, 6PE, HEM, FES, 8SP, BOG

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	0.18	0/3589	0.34	0/4924
1	E	0.17	0/3589	0.33	0/4924
2	B	0.15	0/2010	0.31	0/2733
2	F	0.14	0/2010	0.29	0/2733
3	C	0.15	0/1338	0.27	0/1825
3	G	0.15	0/1338	0.27	0/1825
All	All	0.16	0/13874	0.32	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	13	0
1	E	3457	3421	3436	12	0
2	B	1953	1839	1848	6	0
2	F	1953	1839	1848	6	0
3	C	1308	1268	1271	0	0
3	G	1308	1268	1271	1	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	2	0
10	F	43	32	30	1	0
11	C	4	0	0	0	0
11	G	4	0	0	0	0
All	All	13927	13476	13526	43	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.

All (43) 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:B:302:HEC:HBB3	10:B:302:HEC:HMB3	1.76	0.68
10:B:302:HEC:HMC1	10:B:302:HEC:HBC3	1.76	0.67
10:F:302:HEC:HBB3	10:F:302:HEC:HMB3	1.75	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
1:E:122:LYS:NZ	1:E:354:VAL:O	2.32	0.61
1:E:64:VAL:HG11	1:E:93:LEU:HD13	1.85	0.57
1:E:219:THR:O	1:E:231:ARG:NH2	2.39	0.56
4:A:1001:HEM:HBB2	4:A:1001:HEM:HHC	1.91	0.52
1:A:64:VAL:HG11	1:A:93:LEU:HD13	1.92	0.52
2:F:65:ALA:O	2:F:68:THR:OG1	2.28	0.52
2:B:202:ALA:O	2:B:207:MET:HE2	2.12	0.50
1:A:108:VAL:O	1:A:112:ILE:N	2.43	0.49
1:E:199:TYR:CZ	4:E:1001:HEM:HBC1	2.48	0.49
4:E:1001:HEM:HBC2	4:E:1001:HEM:HMC1	1.94	0.49
2:F:171:ASP:OD1	2:F:175:VAL:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:THR:OG1	1:A:236:GLU:OE1	2.32	0.48
1:A:122:LYS:NZ	1:A:354:VAL:O	2.25	0.47
2:B:171:ASP:OD1	2:B:175:VAL:N	2.47	0.47
1:E:376:ILE:O	1:E:380:VAL:HG22	2.15	0.47
4:A:1002:HEM:HBB2	4:A:1002:HEM:HMB2	1.96	0.47
2:B:132:TYR:O	2:B:136:THR:HG22	2.15	0.47
1:A:288:THR:HB	3:G:132:LEU:HD22	1.96	0.47
2:F:202:ALA:O	2:F:207:MET:HE2	2.14	0.46
2:B:65:ALA:O	2:B:68:THR:OG1	2.34	0.45
1:E:46:ILE:HD12	1:E:255:ALA:HB1	1.98	0.45
2:F:132:TYR:O	2:F:136:THR:HG22	2.17	0.45
1:A:199:TYR:CE2	4:A:1001:HEM:HBC1	2.52	0.45
2:B:20:PHE:HB3	2:B:25:LEU:HD11	2.00	0.44
1:E:108:VAL:O	1:E:112:ILE:N	2.46	0.43
4:A:1001:HEM:HHD	4:A:1001:HEM:HBC2	1.99	0.43
2:B:190:MET:O	2:B:207:MET:HE1	2.18	0.43
1:A:22:ARG:NE	1:E:126:GLU:OE1	2.47	0.43
1:A:165:LEU:CD1	1:A:336:MET:HE1	2.48	0.43
2:F:190:MET:O	2:F:207:MET:HE1	2.19	0.42
1:A:46:ILE:HD12	1:A:255:ALA:HB1	2.01	0.42
1:A:137:LEU:HD21	1:A:340:ILE:HG21	2.01	0.42
1:A:293:VAL:HG12	1:A:294:PRO:O	2.19	0.42
1:A:317:ILE:HG22	1:A:321:ILE:HD12	2.03	0.41
2:F:29:LEU:HD22	2:F:50:LEU:HD22	2.02	0.41
1:E:165:LEU:CD1	1:E:336:MET:HE1	2.51	0.41
1:E:293:VAL:HG12	1:E:294:PRO:O	2.21	0.41

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	65
2	F	254/272 (93%)	245 (96%)	8 (3%)	1 (0%)	30	65
3	C	173/187 (92%)	158 (91%)	14 (8%)	1 (1%)	21	56
3	G	173/187 (92%)	158 (91%)	14 (8%)	1 (1%)	21	56
All	All	1710/1808 (95%)	1638 (96%)	68 (4%)	4 (0%)	43	76

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%)	78	88
1	E	355/366 (97%)	351 (99%)	4 (1%)	65	83
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%)	84	90

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	414	ILE

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Mol	Chain	Res	Type
1	A	415	GLU
1	E	232	THR
1	E	385	THR
1	E	414	ILE
1	E	415	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	192	ASN
1	A	319	ASN
2	B	200	HIS
3	C	113	ASN
1	E	6	HIS
1	E	86	ASN
1	E	319	ASN
3	G	113	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
6	6PE	A	1004	-	26,26,26	0.88	2 (7%)	29,31,31	0.69	0
7	8SP	A	1005	-	32,33,33	0.90	1 (3%)	34,40,40	0.92	2 (5%)
7	8SP	F	303	-	32,33,33	0.90	1 (3%)	34,40,40	1.33	3 (8%)
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	-	-	-	-	-
10	HEC	F	302	2	50,50,50	1.80	7 (14%)	68,82,82	1.25	4 (5%)
4	HEM	A	1002	1	50,50,50	1.56	9 (18%)	67,82,82	1.04	3 (4%)
11	FES	C	1001	3	0,4,4	-	-	-	-	-
6	6PE	E	1004	-	26,26,26	0.89	2 (7%)	29,31,31	0.68	1 (3%)
9	BOG	B	301	-	20,20,20	0.88	0	25,25,25	1.24	4 (16%)
5	AZO	E	1003	-	32,32,32	0.62	0	42,42,42	1.62	8 (19%)
4	HEM	E	1002	1	50,50,50	1.48	9 (18%)	67,82,82	1.08	4 (5%)
10	HEC	B	302	2	50,50,50	1.79	7 (14%)	68,82,82	1.24	2 (2%)
5	AZO	A	1003	-	32,32,32	0.58	0	42,42,42	1.58	7 (16%)
4	HEM	A	1001	1	50,50,50	1.46	9 (18%)	67,82,82	1.29	6 (8%)
4	HEM	E	1001	1	50,50,50	1.42	9 (18%)	67,82,82	1.10	4 (5%)

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
6	6PE	A	1004	-	-	11/30/30/30	-
7	8SP	A	1005	-	-	20/39/39/39	-
7	8SP	F	303	-	-	16/39/39/39	-
9	BOG	F	301	-	-	3/11/31/31	0/1/1/1
11	FES	G	1001	3	-	-	0/1/1/1
10	HEC	F	302	2	1/1/7/7	6/14/54/54	-
4	HEM	A	1002	1	-	5/14/54/54	-
11	FES	C	1001	3	-	-	0/1/1/1
6	6PE	E	1004	-	-	20/30/30/30	-
9	BOG	B	301	-	-	6/11/31/31	0/1/1/1
5	AZO	E	1003	-	-	0/23/23/23	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	E	1002	1	-	0/14/54/54	-
10	HEC	B	302	2	1/1/7/7	6/14/54/54	-
5	AZO	A	1003	-	-	1/23/23/23	0/3/3/3
4	HEM	A	1001	1	-	4/14/54/54	-
4	HEM	E	1001	1	-	4/14/54/54	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	302	HEC	C3D-C2D	7.72	1.53	1.36
10	F	302	HEC	C3D-C2D	7.71	1.53	1.36
4	A	1002	HEM	FE-NB	5.93	2.13	1.94
10	B	302	HEC	FE-ND	5.12	2.10	1.94
10	F	302	HEC	FE-ND	4.85	2.09	1.94
4	E	1002	HEM	FE-NB	4.74	2.09	1.94
4	E	1001	HEM	FE-NA	4.32	2.09	1.95
4	A	1001	HEM	FE-NB	4.09	2.07	1.94
4	A	1002	HEM	FE-NC	4.00	2.08	1.95
4	E	1002	HEM	FE-NC	3.64	2.07	1.95
4	E	1002	HEM	FE-NA	3.57	2.07	1.95
10	F	302	HEC	FE-NB	3.56	2.05	1.94
4	E	1001	HEM	FE-NB	3.35	2.05	1.94
10	F	302	HEC	FE-NC	3.29	2.06	1.95
4	E	1001	HEM	FE-ND	3.25	2.04	1.94
4	A	1002	HEM	CAB-C3B	3.20	1.55	1.47
4	A	1001	HEM	CAB-C3B	3.18	1.55	1.47
4	A	1001	HEM	FE-NA	3.18	2.05	1.95
10	B	302	HEC	FE-NA	3.18	2.05	1.95
10	B	302	HEC	FE-NB	3.18	2.04	1.94
4	E	1002	HEM	CAC-C3C	3.11	1.55	1.47
4	A	1002	HEM	CAC-C3C	3.06	1.55	1.47
10	B	302	HEC	FE-NC	3.05	2.05	1.95
4	E	1002	HEM	CAB-C3B	2.99	1.55	1.47
4	A	1001	HEM	CAC-C3C	2.98	1.55	1.47
4	A	1001	HEM	FE-NC	2.95	2.04	1.95
4	E	1001	HEM	CAB-C3B	2.92	1.55	1.47
10	F	302	HEC	FE-NA	2.91	2.04	1.95
6	E	1004	6PE	P1-O3	2.71	1.70	1.59
4	A	1001	HEM	FE-ND	2.71	2.03	1.94
4	A	1002	HEM	FE-NA	2.62	2.03	1.95
4	E	1001	HEM	CAC-C3C	2.62	1.54	1.47
7	F	303	8SP	P-O3G	2.54	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	302	HEC	CMC-C2C	2.44	1.55	1.50
6	A	1004	6PE	P1-O3	2.42	1.68	1.59
7	A	1005	8SP	P-O3G	2.39	1.68	1.59
4	A	1002	HEM	CMB-C2B	2.33	1.55	1.50
10	B	302	HEC	CMC-C2C	2.24	1.55	1.50
4	A	1002	HEM	CMC-C2C	2.23	1.55	1.50
4	E	1002	HEM	CMB-C2B	2.22	1.55	1.50
10	F	302	HEC	CMB-C2B	2.20	1.55	1.50
6	A	1004	6PE	P1-O8	2.18	1.67	1.59
4	E	1002	HEM	CMC-C2C	2.17	1.55	1.50
4	E	1001	HEM	CMD-C2D	2.16	1.55	1.50
4	E	1001	HEM	CMB-C2B	2.14	1.55	1.50
10	B	302	HEC	CMB-C2B	2.14	1.55	1.50
4	A	1002	HEM	CMA-C3A	2.13	1.55	1.50
4	E	1001	HEM	CMC-C2C	2.11	1.55	1.50
4	A	1001	HEM	CMC-C2C	2.10	1.55	1.50
4	A	1001	HEM	CMB-C2B	2.10	1.55	1.50
4	E	1002	HEM	CMA-C3A	2.10	1.55	1.50
4	E	1001	HEM	CMA-C3A	2.09	1.55	1.50
4	A	1001	HEM	CMA-C3A	2.05	1.55	1.50
6	E	1004	6PE	P1-O8	2.01	1.67	1.59
4	A	1002	HEM	CMD-C2D	2.01	1.54	1.50
4	E	1002	HEM	CMD-C2D	2.00	1.54	1.50

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	C1D-ND-C4D	5.16	111.32	105.21
10	B	302	HEC	C1D-ND-C4D	5.05	111.19	105.21
7	F	303	8SP	OG-CB-CA	-4.69	103.97	108.06
7	F	303	8SP	C2G-O2G-C1B	4.12	127.65	117.80
9	F	301	BOG	C1-C2-C3	-3.29	103.08	110.01
5	A	1003	AZO	C12-O2-C10	3.18	124.88	118.43
5	E	1003	AZO	C11-N2-C8	3.14	116.89	114.50
5	A	1003	AZO	C11-N2-C8	3.10	116.86	114.50
5	E	1003	AZO	C12-O2-C10	3.00	124.50	118.43
5	E	1003	AZO	N2-C11-N3	-2.99	124.06	128.58
5	A	1003	AZO	N2-C11-N3	-2.96	124.09	128.58
4	A	1001	HEM	C3B-C2B-C1B	2.96	108.64	106.41
5	E	1003	AZO	C9-C10-N3	-2.93	120.32	124.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	HEM	C4D-ND-C1D	2.89	108.62	105.21
4	A	1001	HEM	C1B-NB-C4B	2.82	108.55	105.21
4	E	1002	HEM	C4D-ND-C1D	2.80	108.52	105.21
5	A	1003	AZO	C9-C10-N3	-2.79	120.53	124.47
4	A	1001	HEM	C3B-C4B-NB	-2.77	107.47	109.47
5	A	1003	AZO	C20-O4-C19	2.64	120.74	115.85
9	F	301	BOG	O3-C3-C4	-2.54	104.40	110.38
4	E	1001	HEM	CHD-C4C-NC	2.45	127.12	124.45
5	E	1003	AZO	C20-O4-C19	2.45	120.38	115.85
7	A	1005	8SP	OG-CB-CA	-2.42	105.94	108.06
7	F	303	8SP	OXT-C-O	2.39	129.51	124.08
4	A	1002	HEM	C3D-C4D-ND	-2.39	107.55	110.17
10	F	302	HEC	C2A-C1A-NA	-2.39	108.02	110.32
4	A	1001	HEM	CAC-C3C-C4C	2.37	130.47	124.82
5	A	1003	AZO	C21-C18-C19	2.36	121.39	117.16
4	E	1002	HEM	C3D-C4D-ND	-2.36	107.58	110.17
10	B	302	HEC	C4B-NB-C1B	2.33	107.96	105.21
5	E	1003	AZO	C21-C18-C19	2.31	121.29	117.16
4	A	1001	HEM	C4D-ND-C1D	2.31	107.94	105.21
4	E	1001	HEM	C1B-NB-C4B	2.29	107.91	105.21
9	B	301	BOG	C1-C2-C3	-2.24	105.30	110.01
10	F	302	HEC	C4B-NB-C1B	2.24	107.86	105.21
4	E	1001	HEM	C4C-C3C-C2C	2.20	108.72	106.81
9	B	301	BOG	O3-C3-C4	-2.19	105.22	110.38
6	E	1004	6PE	O1-P1-O2	2.10	122.20	112.44
4	A	1001	HEM	CAC-C3C-C2C	-2.08	121.67	128.43
4	E	1001	HEM	C4D-ND-C1D	2.08	107.67	105.21
7	A	1005	8SP	OXT-C-O	2.07	128.79	124.08
4	E	1002	HEM	C2D-C1D-ND	-2.06	107.52	109.90
4	E	1002	HEM	CHA-C4D-ND	2.06	126.92	124.37
9	B	301	BOG	O2-C2-C3	-2.04	105.57	110.38
9	B	301	BOG	O5-C5-C4	-2.04	106.03	109.70
10	F	302	HEC	CAA-CBA-CGA	-2.03	108.28	113.67
4	A	1002	HEM	C2D-C1D-ND	-2.02	107.57	109.90
5	E	1003	AZO	C17-C18-C21	-2.02	119.22	122.09

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	302	HEC	NA
10	F	302	HEC	NA

All (102) 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
7	A	1005	8SP	CB-OG-P-O3P
7	A	1005	8SP	C3G-O3G-P-OG
7	A	1005	8SP	C3G-O3G-P-O2P
7	A	1005	8SP	C2B-C1B-O2G-C2G
7	A	1005	8SP	O-C-CA-CB
7	A	1005	8SP	OXT-C-CA-CB
7	F	303	8SP	CB-OG-P-O2P
7	F	303	8SP	N-CA-CB-OG
7	F	303	8SP	C-CA-CB-OG
9	F	301	BOG	C2'-C1'-O1-C1
10	F	302	HEC	C4C-C3C-CAC-CBC
7	A	1005	8SP	O1A-C1A-O1G-C1G
10	B	302	HEC	C4C-C3C-CAC-CBC
7	A	1005	8SP	O1B-C1B-O2G-C2G
10	B	302	HEC	C2C-C3C-CAC-CBC
7	A	1005	8SP	C2A-C1A-O1G-C1G
7	F	303	8SP	C2A-C1A-O1G-C1G
9	B	301	BOG	C4-C5-C6-O6
7	F	303	8SP	O1A-C1A-O1G-C1G
10	F	302	HEC	C2C-C3C-CAC-CBC
9	B	301	BOG	O5-C5-C6-O6
4	A	1002	HEM	C2A-CAA-CBA-CGA
10	F	302	HEC	C2B-C3B-CAB-CBB
10	B	302	HEC	C2B-C3B-CAB-CBB
6	E	1004	6PE	C10-C11-C12-C13
6	A	1004	6PE	C5-C4-O4-C3
6	E	1004	6PE	C5-C4-O4-C3
6	A	1004	6PE	C10-C11-C12-C13
9	F	301	BOG	O1-C1'-C2'-C3'
6	A	1004	6PE	O5-C4-O4-C3
6	E	1004	6PE	C1-C2-C3-O4
6	E	1004	6PE	O5-C4-O4-C3
7	A	1005	8SP	C1A-C2A-C3A-C4A
7	A	1005	8SP	C2A-C3A-C4A-C5A
7	F	303	8SP	C2B-C1B-O2G-C2G
4	A	1001	HEM	C4B-C3B-CAB-CBB
9	F	301	BOG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	F	302	HEC	C4B-C3B-CAB-CBB
6	A	1004	6PE	O3-C1-C2-C3
10	B	302	HEC	C4B-C3B-CAB-CBB
7	F	303	8SP	O1G-C1G-C2G-C3G
7	A	1005	8SP	C3B-C4B-C5B-C6B
6	E	1004	6PE	C11-C10-O6-C2
7	F	303	8SP	O1B-C1B-O2G-C2G
9	B	301	BOG	C4'-C5'-C6'-C7'
6	E	1004	6PE	O6-C2-C3-O4
6	E	1004	6PE	C5-C6-C7-C8
6	E	1004	6PE	O3-C1-C2-C3
9	B	301	BOG	C2'-C3'-C4'-C5'
7	A	1005	8SP	O2G-C2G-C3G-O3G
7	A	1005	8SP	C1G-C2G-C3G-O3G
7	F	303	8SP	C1G-C2G-C3G-O3G
4	A	1002	HEM	C1A-C2A-CAA-CBA
6	E	1004	6PE	O7-C10-O6-C2
6	E	1004	6PE	C12-C13-C14-C15
7	A	1005	8SP	C1G-C2G-O2G-C1B
7	F	303	8SP	C3G-C2G-O2G-C1B
6	A	1004	6PE	O3-C1-C2-O6
6	A	1004	6PE	C1-C2-C3-O4
7	F	303	8SP	O1G-C1G-C2G-O2G
7	F	303	8SP	C3B-C4B-C5B-C6B
6	E	1004	6PE	O3-C1-C2-O6
7	F	303	8SP	O2G-C2G-C3G-O3G
6	E	1004	6PE	C1-O3-P1-O2
7	A	1005	8SP	CB-OG-P-O2P
7	F	303	8SP	CB-OG-P-O3G
7	F	303	8SP	CB-OG-P-O3P
7	F	303	8SP	C1A-C2A-C3A-C4A
7	A	1005	8SP	C4A-C5A-C6A-C7A
4	A	1001	HEM	CAA-CBA-CGA-O1A
6	A	1004	6PE	O6-C2-C3-O4
10	F	302	HEC	CAA-CBA-CGA-O2A
4	A	1001	HEM	CAA-CBA-CGA-O2A
4	A	1002	HEM	CAA-CBA-CGA-O2A
9	B	301	BOG	O1-C1'-C2'-C3'
5	A	1003	AZO	N1-C1-C2-C7
4	A	1002	HEM	C3A-C2A-CAA-CBA
10	F	302	HEC	CAA-CBA-CGA-O1A
4	A	1002	HEM	CAA-CBA-CGA-O1A

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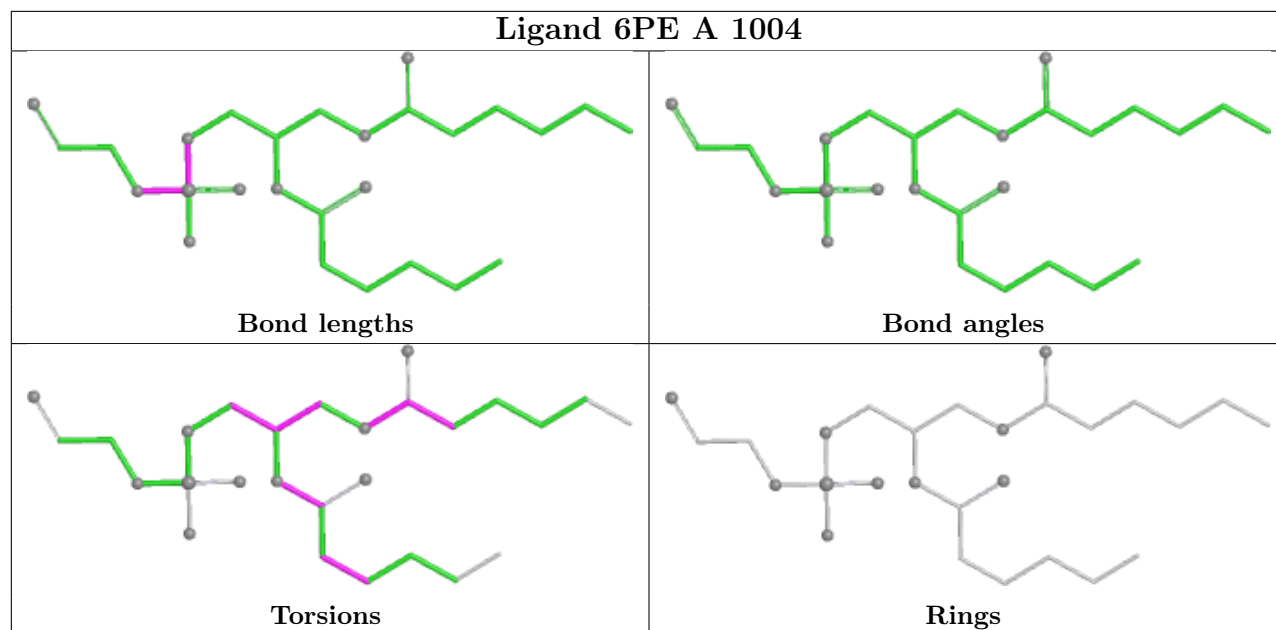
Mol	Chain	Res	Type	Atoms
6	A	1004	6PE	O7-C10-O6-C2
4	E	1001	HEM	CAD-CBD-CGD-O1D
4	A	1001	HEM	C3D-CAD-CBD-CGD
6	A	1004	6PE	O4-C4-C5-C6
6	E	1004	6PE	O4-C4-C5-C6
6	E	1004	6PE	O6-C10-C11-C12
9	B	301	BOG	C3'-C4'-C5'-C6'
7	A	1005	8SP	C4B-C5B-C6B-C7B
10	B	302	HEC	CAA-CBA-CGA-O2A
6	E	1004	6PE	O5-C4-C5-C6
4	E	1001	HEM	CAD-CBD-CGD-O2D
6	A	1004	6PE	O5-C4-C5-C6
7	A	1005	8SP	O1G-C1G-C2G-C3G
4	E	1001	HEM	CAA-CBA-CGA-O2A
6	E	1004	6PE	O7-C10-C11-C12
10	B	302	HEC	CAA-CBA-CGA-O1A
4	E	1001	HEM	CAA-CBA-CGA-O1A
6	A	1004	6PE	C11-C10-O6-C2

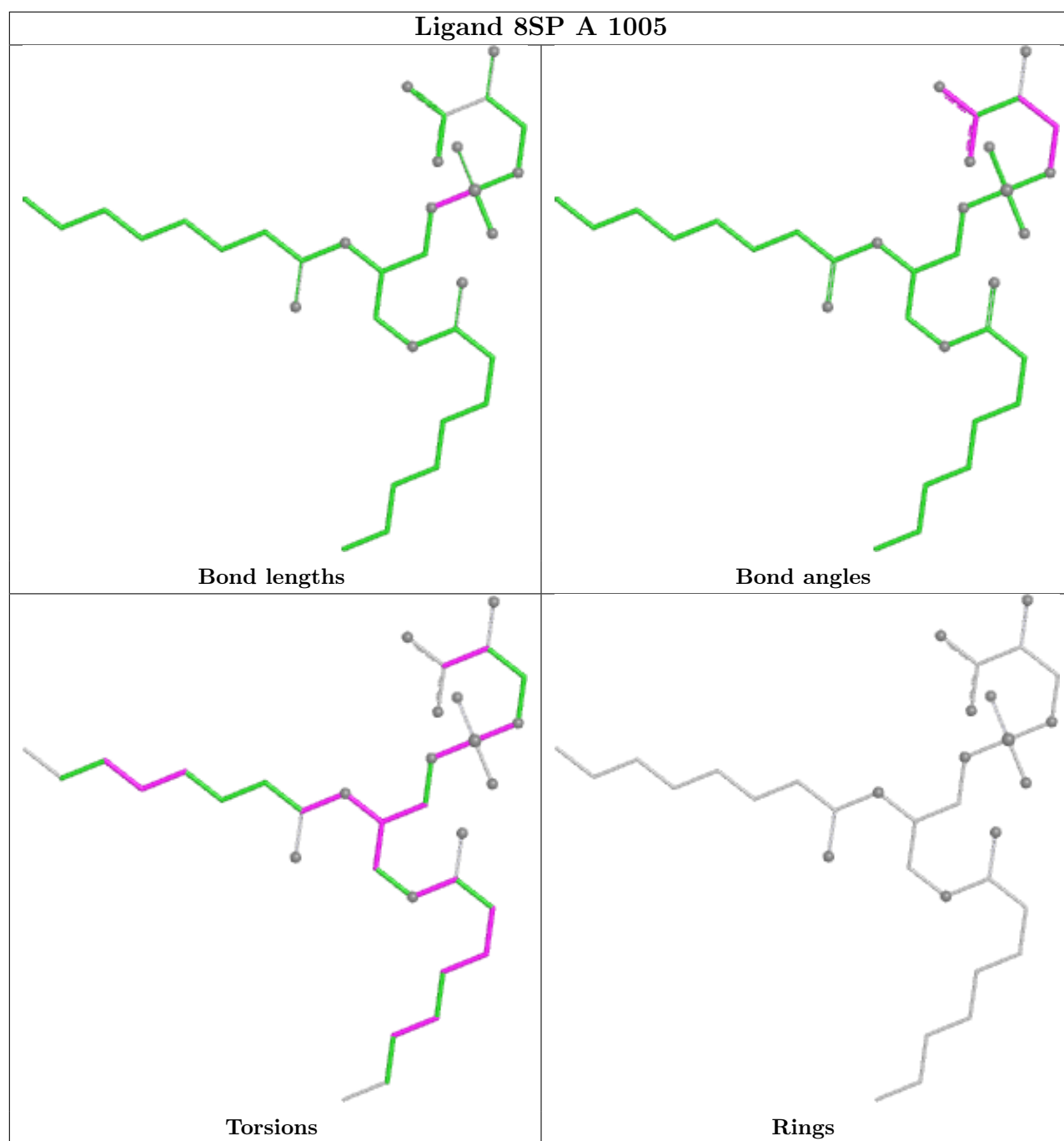
There are no ring outliers.

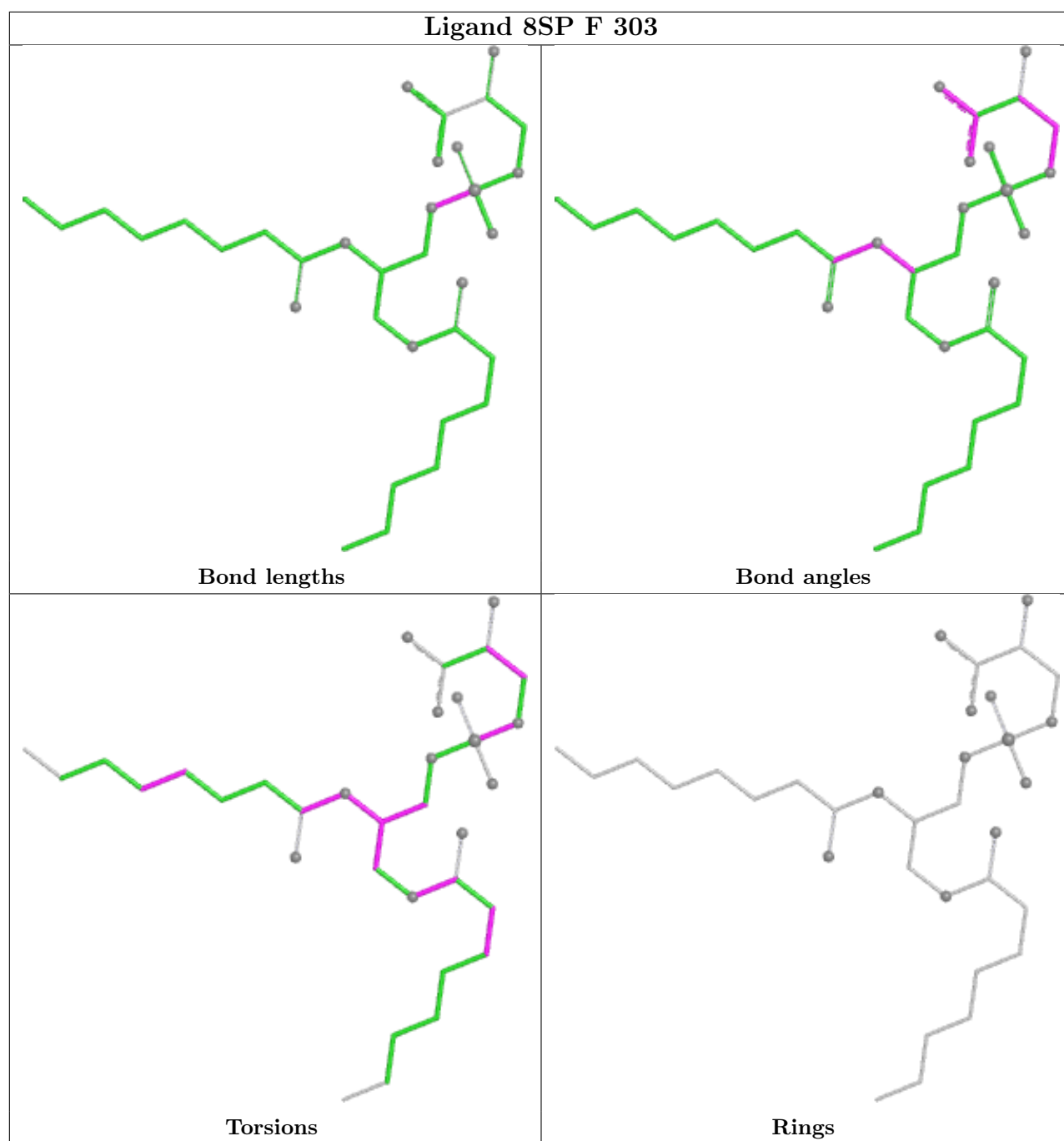
5 monomers are involved in 9 short contacts:

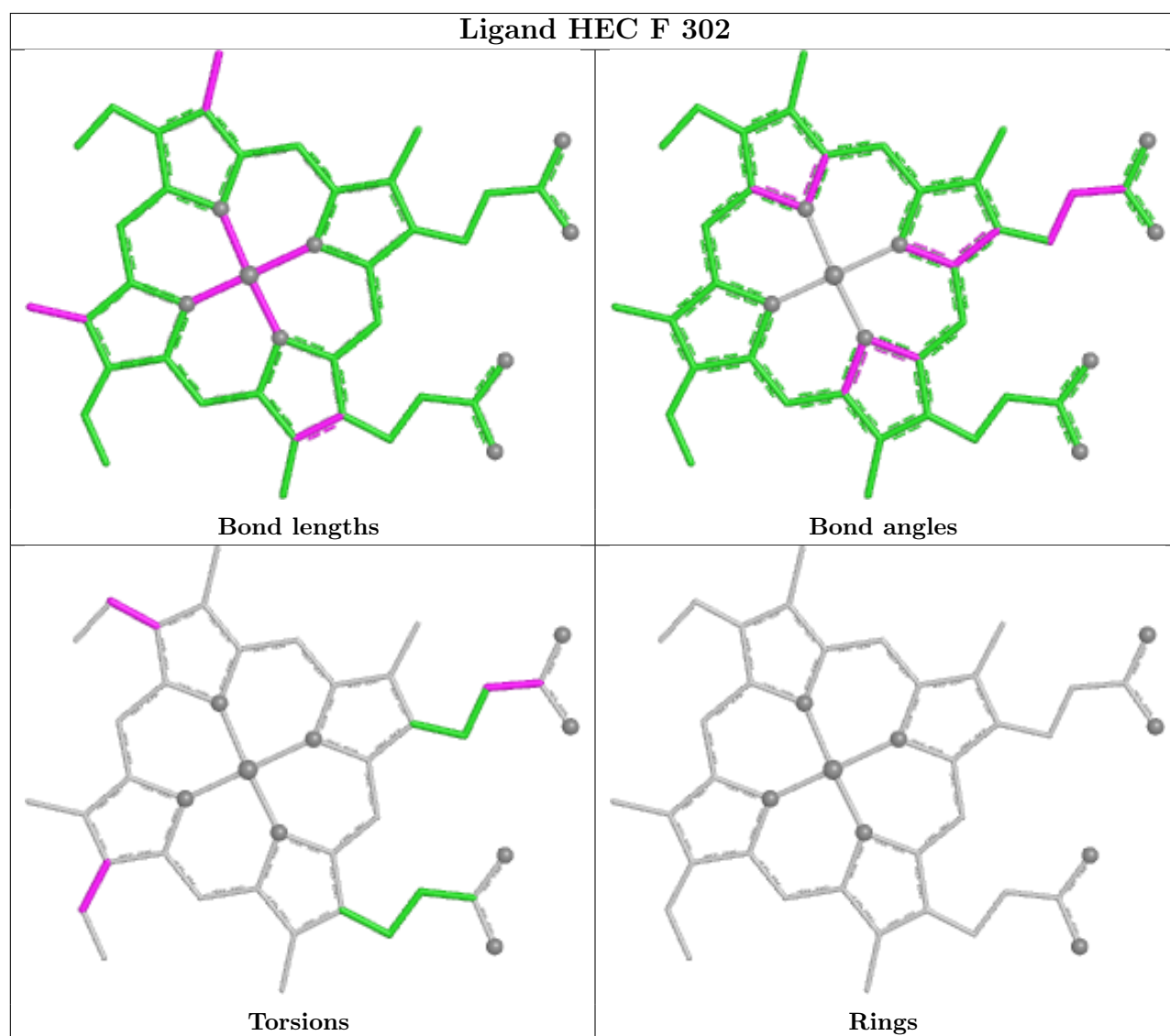
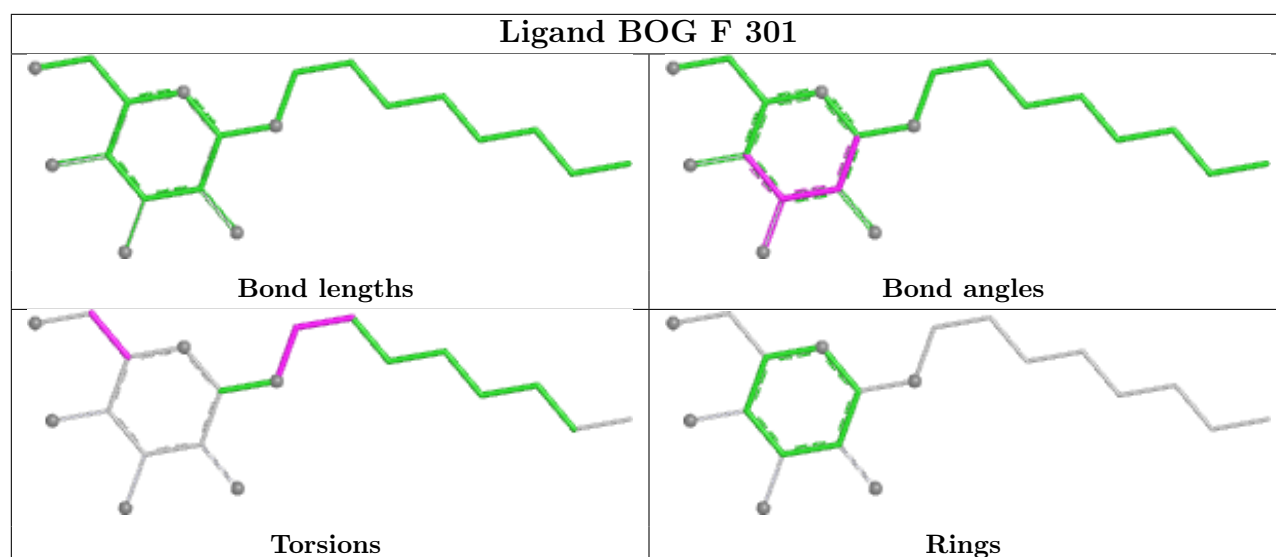
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	F	302	HEC	1	0
4	A	1002	HEM	1	0
10	B	302	HEC	2	0
4	A	1001	HEM	3	0
4	E	1001	HEM	2	0

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.

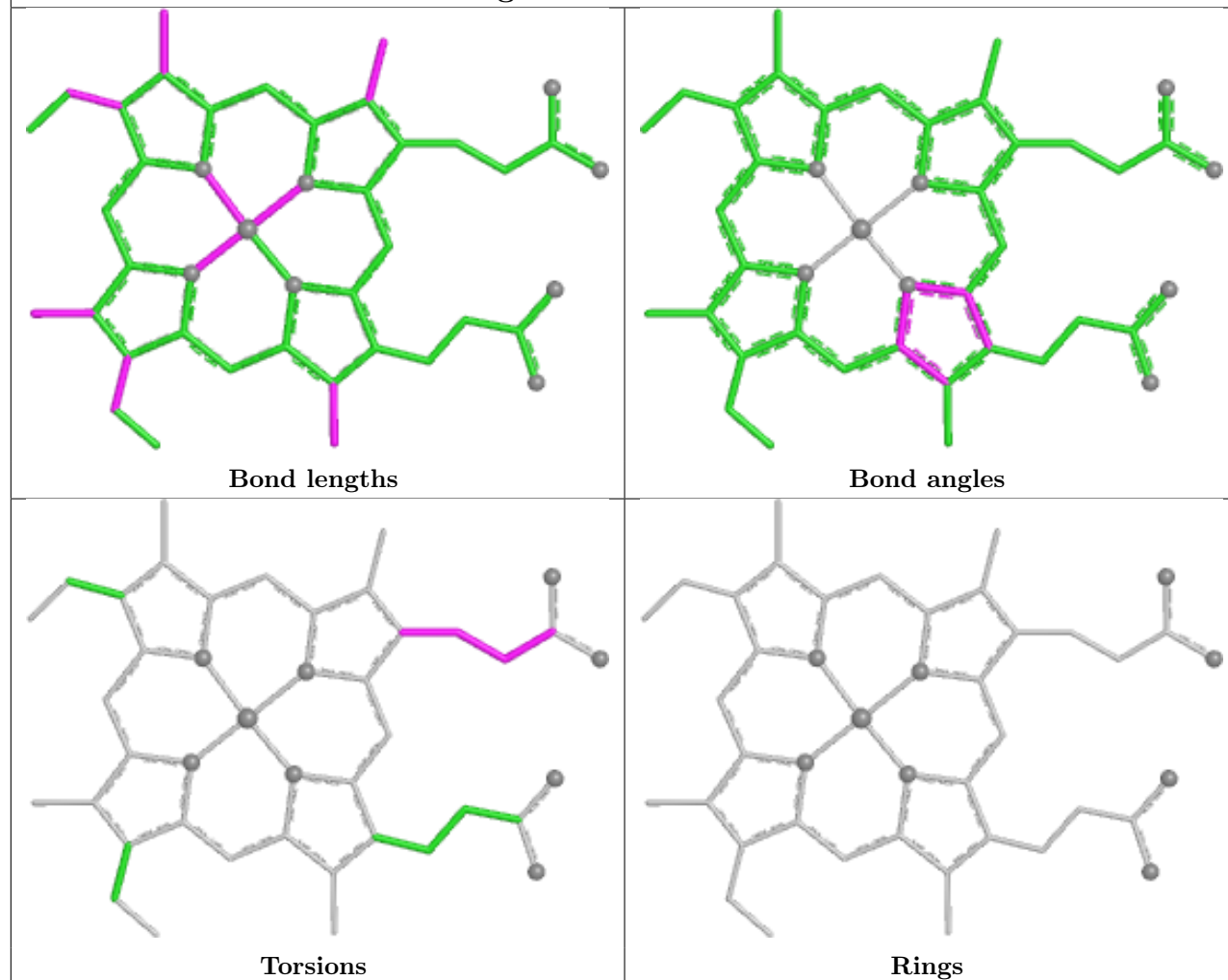




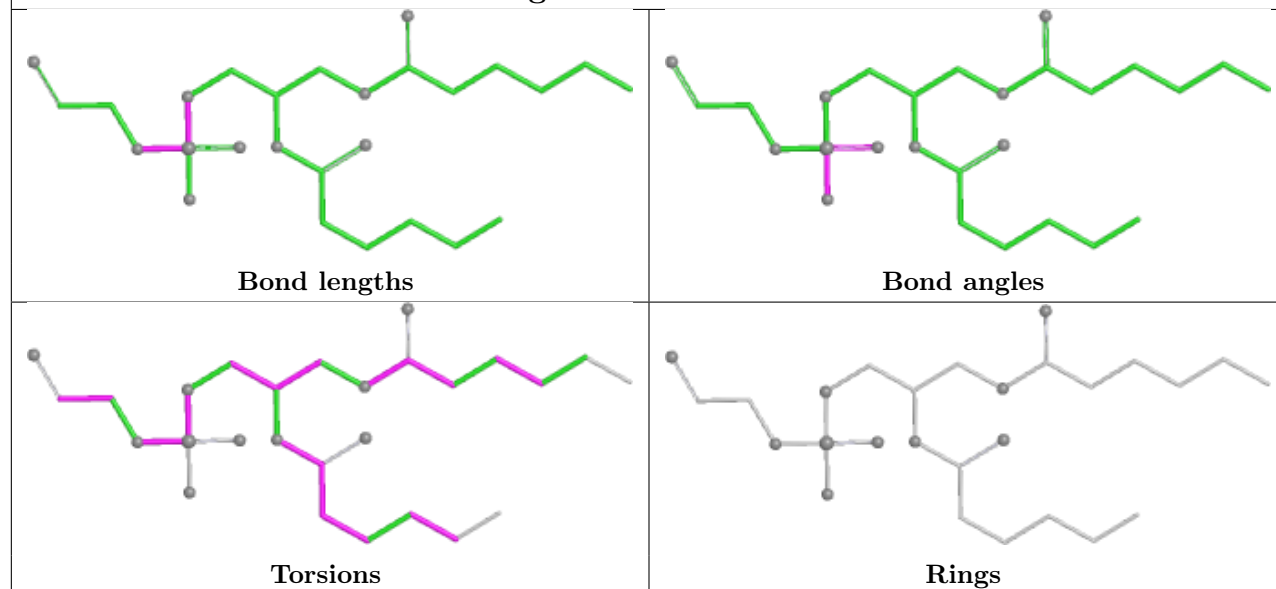


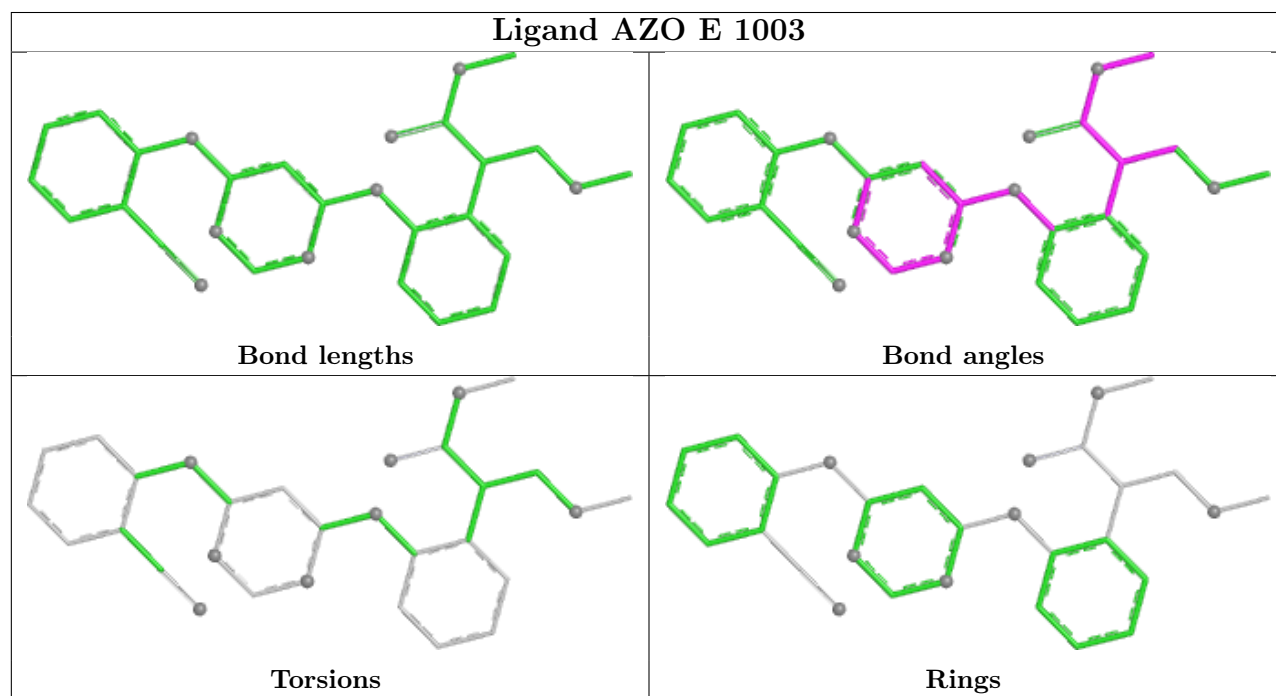
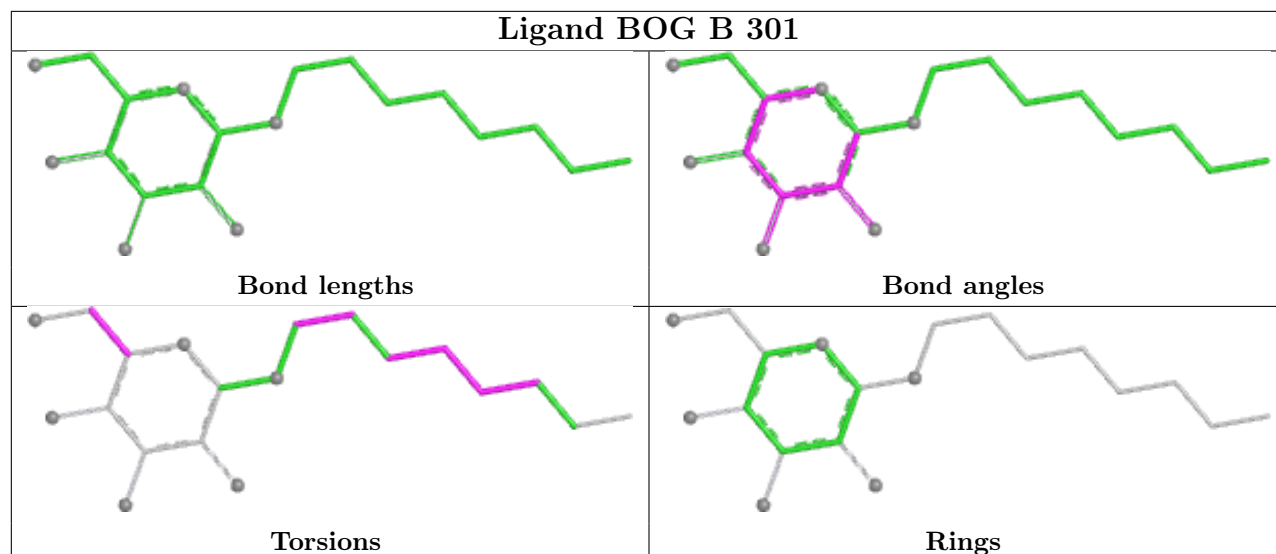


Ligand HEM A 1002

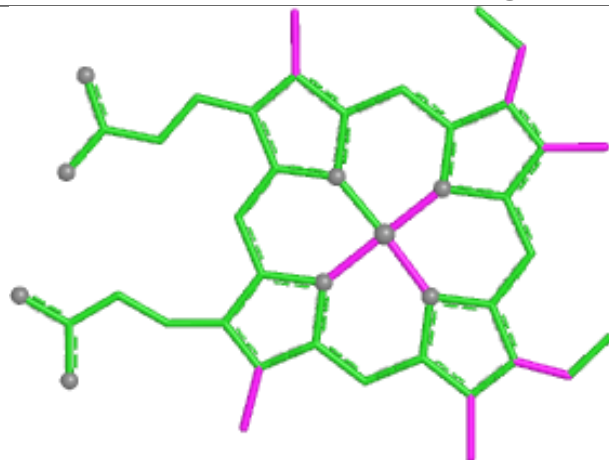


Ligand 6PE E 1004

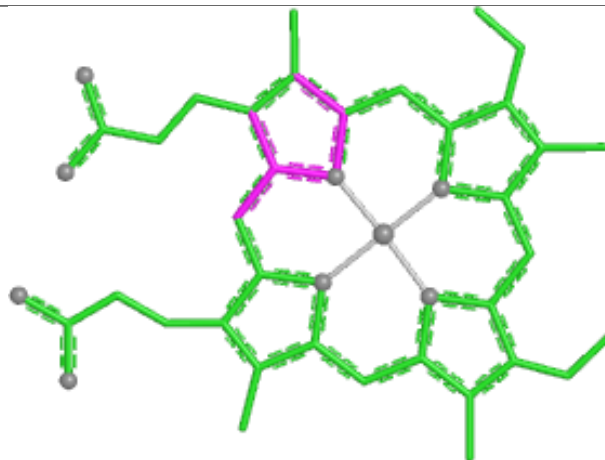




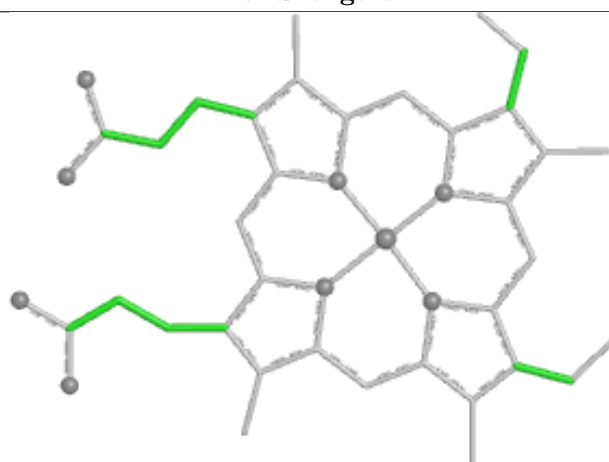
Ligand HEM E 1002



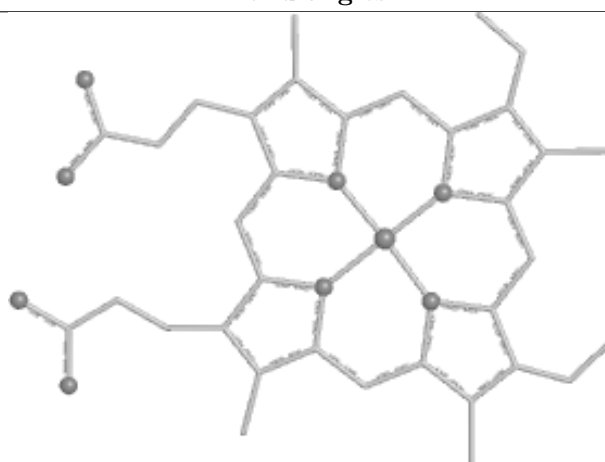
Bond lengths



Bond angles

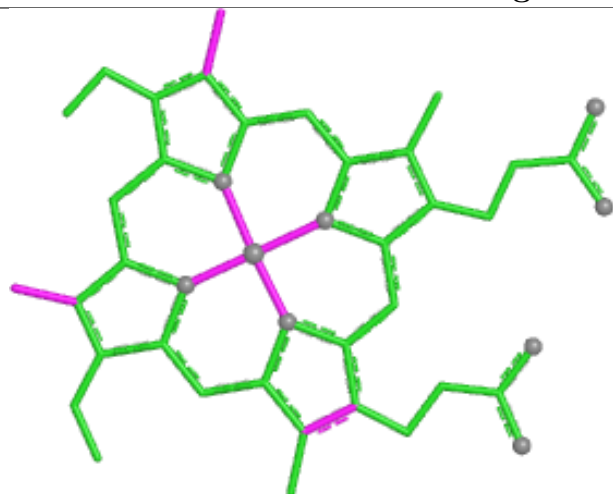


Torsions

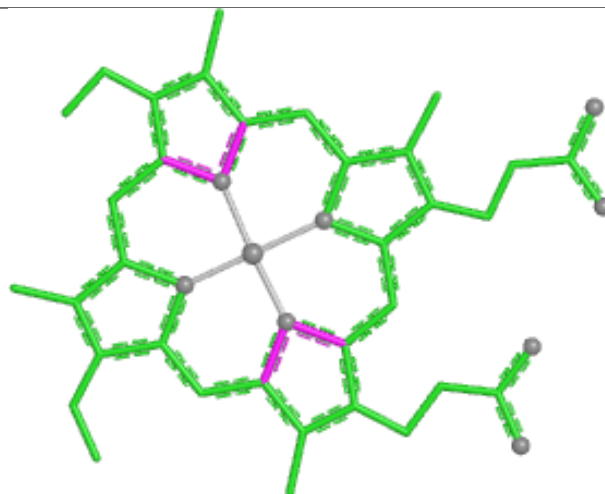


Rings

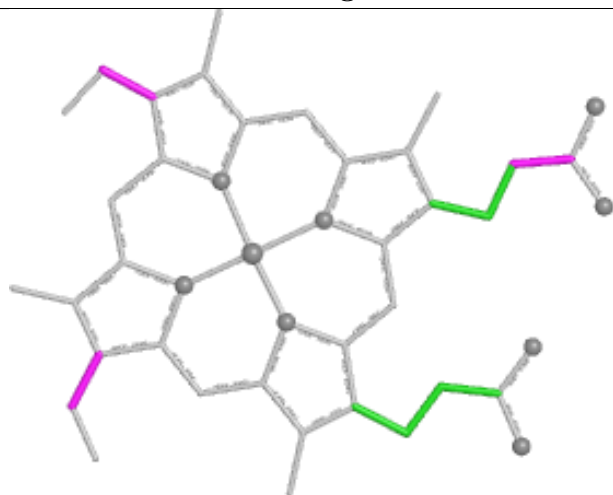
Ligand HEC B 302



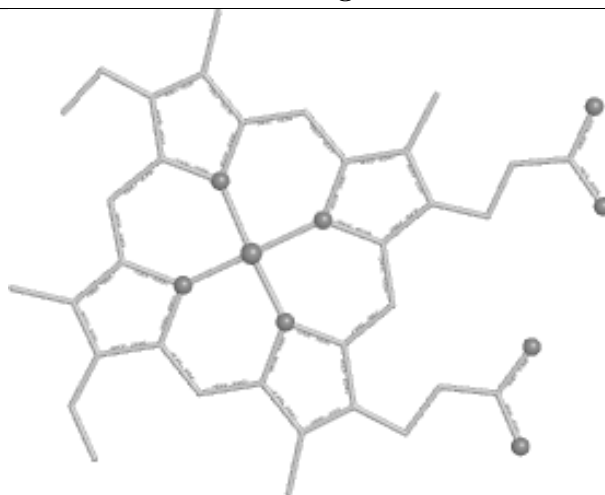
Bond lengths



Bond angles

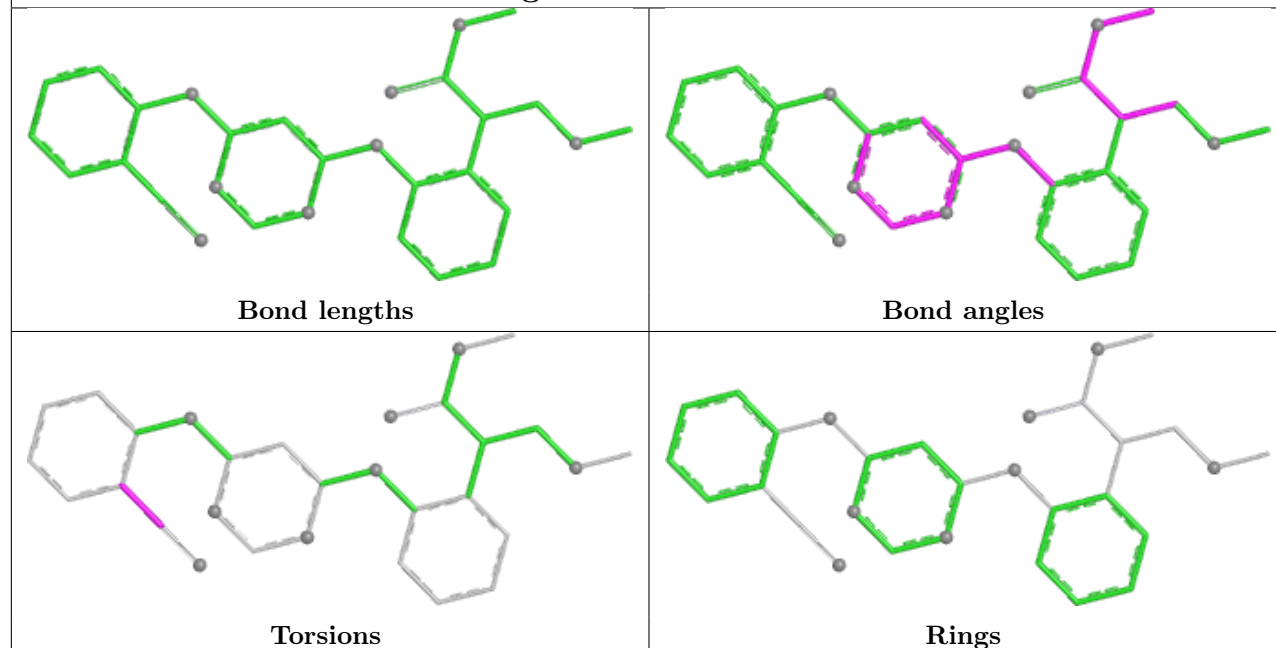


Torsions

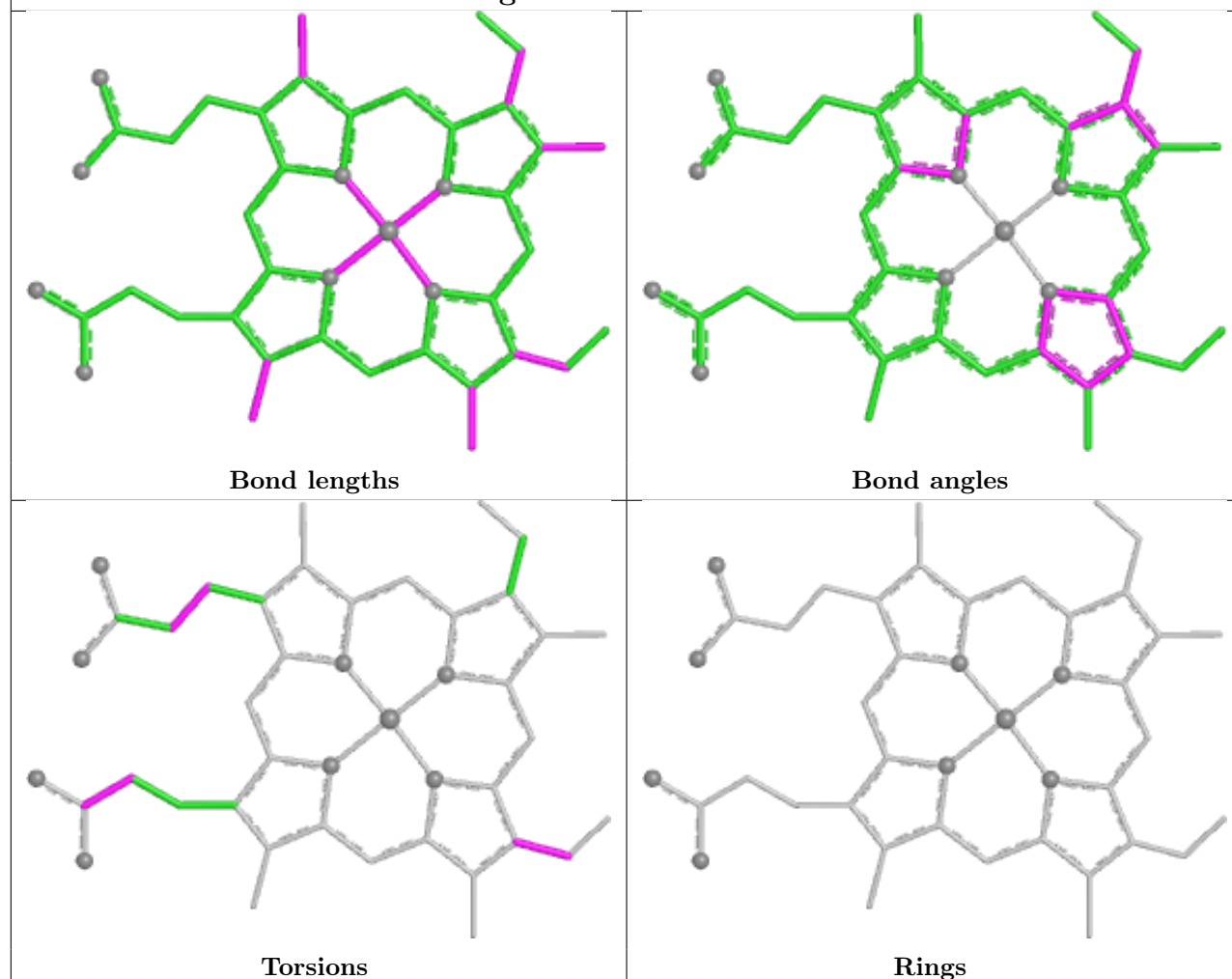


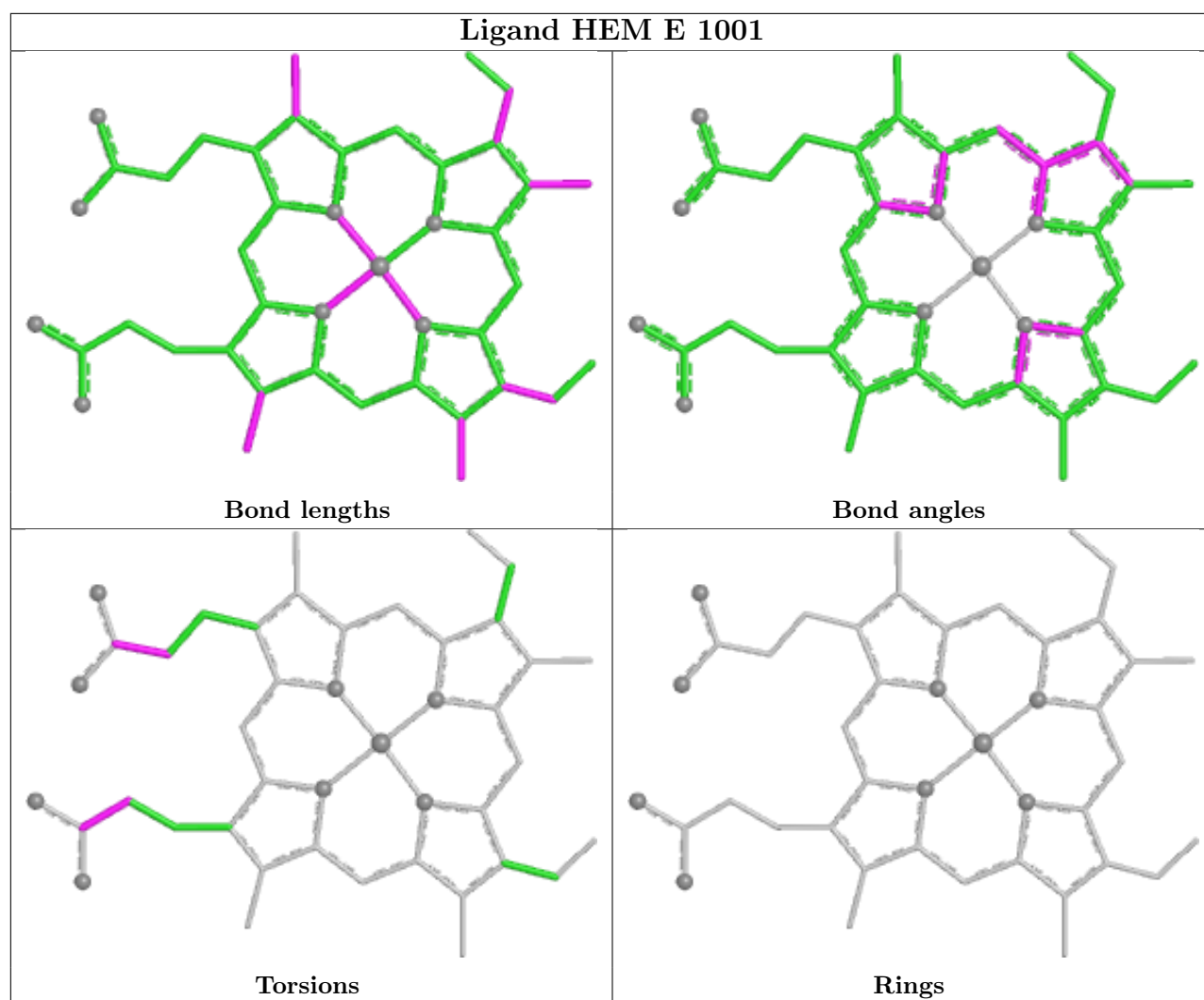
Rings

Ligand AZO A 1003



Ligand HEM A 1001





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	430/445 (96%)	0.65	34 (7%) 18 10	37, 55, 107, 136	0
1	E	430/445 (96%)	0.84	53 (12%) 8 5	18, 64, 114, 178	0
2	B	256/272 (94%)	0.91	34 (13%) 7 4	50, 73, 134, 188	0
2	F	256/272 (94%)	1.13	43 (16%) 4 3	51, 87, 160, 206	0
3	C	175/187 (93%)	7.00	152 (86%) 0 0	23, 34, 92, 107	136 (77%)
3	G	175/187 (93%)	6.69	146 (83%) 0 0	23, 29, 104, 153	136 (77%)
All	All	1722/1808 (95%)	2.07	462 (26%) 1 1	18, 63, 126, 206	272 (15%)

All (462) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	133	GLY	28.6
3	C	87	SER	22.4
3	C	124	VAL	22.3
3	C	119	ALA	21.3
3	C	78	THR	20.7
3	C	120	GLY	20.1
3	C	116	LEU	19.5
3	C	178	PHE	19.0
3	G	88	VAL	17.8
3	G	171	LEU	17.6
3	G	74	ILE	17.1
3	G	116	LEU	16.9
3	C	68	LEU	15.8
3	C	80	ALA	15.5
3	C	118	GLU	15.4
3	C	187	GLY	15.2
3	C	69	GLY	14.6
3	G	118	GLU	14.5
3	C	176	ALA	14.3

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Mol	Chain	Res	Type	RSRZ
3	G	114	ARG	14.2
3	C	115	THR	14.1
3	G	68	LEU	14.0
3	C	74	ILE	13.8
3	G	77	ARG	13.2
3	C	79	GLU	13.2
3	G	150	PRO	13.0
3	C	152	HIS	13.0
3	G	87	SER	12.9
3	C	104	ASP	12.9
3	C	143	ASP	12.9
3	C	150	PRO	12.9
3	G	141	SER	12.8
3	G	128	VAL	12.8
3	G	61	VAL	12.5
3	C	181	GLU	12.4
3	C	151	CYS	12.4
3	G	89	GLN	12.3
3	G	178	PHE	12.1
3	G	151	CYS	11.9
3	C	113	ASN	11.9
3	G	125	MET	11.7
3	C	83	GLU	11.5
3	C	140	VAL	11.3
3	G	53	ASP	11.3
3	C	186	LEU	11.3
3	G	55	SER	11.3
3	G	143	ASP	11.3
3	G	166	PRO	11.2
3	G	111	ASP	11.2
3	C	122	TRP	11.2
3	C	184	ILE	11.1
3	G	173	ILE	11.1
3	G	56	SER	11.1
3	G	105	ALA	11.0
3	C	166	PRO	11.0
3	G	174	PRO	11.0
3	G	119	ALA	11.0
3	G	127	GLY	11.0
3	C	133	GLY	11.0
3	G	140	VAL	11.0
3	G	152	HIS	10.9

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Mol	Chain	Res	Type	RSRZ
3	C	180	ASP	10.8
3	G	187	GLY	10.6
3	C	84	LEU	10.6
3	G	134	CYS	10.5
3	G	142	GLY	10.5
3	G	124	VAL	10.4
3	C	177	LYS	10.3
3	C	65	VAL	10.3
3	C	105	ALA	10.3
3	G	139	GLY	10.2
3	G	69	GLY	10.2
3	C	112	GLN	10.1
3	C	182	THR	10.1
3	G	186	LEU	10.0
3	G	126	TRP	10.0
3	G	67	PHE	10.0
3	G	122	TRP	9.9
3	G	104	ASP	9.9
3	C	81	ASP	9.9
3	C	114	ARG	9.8
3	C	138	GLY	9.8
3	C	56	SER	9.8
3	G	160	GLY	9.5
3	C	58	GLU	9.5
3	C	67	PHE	9.5
3	G	113	ASN	9.5
3	C	185	GLN	9.4
3	C	108	GLU	9.4
2	F	148	GLY	9.2
3	C	66	LYS	9.1
3	G	66	LYS	9.0
3	C	60	GLY	8.9
3	G	54	VAL	8.9
3	C	168	PRO	8.8
3	G	110	THR	8.7
3	C	77	ARG	8.7
3	G	132	LEU	8.7
3	G	120	GLY	8.7
3	C	89	GLN	8.6
3	G	108	GLU	8.6
3	G	180	ASP	8.6
3	C	59	PRO	8.5

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Mol	Chain	Res	Type	RSRZ
3	C	179	ILE	8.5
3	C	131	HIS	8.5
3	C	111	ASP	8.5
3	C	53	ASP	8.4
3	G	182	THR	8.4
3	C	171	LEU	8.4
3	C	160	GLY	8.4
3	C	174	PRO	8.4
3	G	168	PRO	8.3
3	C	183	THR	8.3
3	G	112	GLN	8.3
3	C	57	VAL	8.3
3	G	63	LEU	8.2
3	C	61	VAL	8.2
3	C	102	ASN	8.2
3	G	103	ILE	8.2
3	G	144	PHE	8.2
3	C	103	ILE	8.2
3	C	85	GLY	8.1
3	G	72	ILE	8.1
3	G	181	GLU	8.1
3	C	107	ALA	8.1
3	C	144	PHE	8.1
3	G	83	GLU	8.1
3	G	164	LYS	8.0
3	G	79	GLU	7.9
3	C	110	THR	7.9
3	G	58	GLU	7.9
3	G	93	LEU	7.9
3	G	115	THR	7.9
3	G	153	GLY	7.9
3	C	117	ASP	7.8
3	C	175	LEU	7.8
3	G	107	ALA	7.8
3	G	90	LEU	7.7
3	G	57	VAL	7.7
3	C	13	ASP	7.7
3	G	148	PHE	7.6
3	C	92	GLN	7.6
3	C	106	GLY	7.6
3	G	131	HIS	7.6
3	C	125	MET	7.6

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Mol	Chain	Res	Type	RSRZ
3	G	71	PRO	7.6
3	G	175	LEU	7.5
3	G	86	ARG	7.5
3	G	84	LEU	7.4
3	G	185	GLN	7.4
2	F	8	ASP	7.4
3	C	137	ILE	7.3
3	G	91	GLY	7.3
3	C	164	LYS	7.3
3	G	106	GLY	7.2
3	C	52	VAL	7.2
3	G	123	LEU	7.2
3	G	179	ILE	7.2
3	C	70	LYS	7.1
3	G	52	VAL	7.1
3	C	123	LEU	7.1
3	G	94	VAL	7.0
3	G	59	PRO	7.0
3	C	64	THR	7.0
3	G	64	THR	7.0
3	G	130	THR	7.0
3	C	55	SER	7.0
3	C	132	LEU	7.0
3	C	86	ARG	6.9
3	G	184	ILE	6.9
3	G	78	THR	6.9
3	G	176	ALA	6.9
3	C	54	VAL	6.9
3	C	173	ILE	6.9
3	G	82	ILE	6.8
3	G	177	LYS	6.8
3	G	70	LYS	6.8
3	G	159	ALA	6.8
3	C	142	GLY	6.8
3	G	172	PRO	6.8
3	C	141	SER	6.8
3	G	137	ILE	6.7
3	C	82	ILE	6.7
2	F	256	LYS	6.6
3	C	91	GLY	6.6
3	G	65	VAL	6.5
3	G	102	ASN	6.5

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Mol	Chain	Res	Type	RSRZ
3	G	101	ALA	6.4
3	C	149	CYS	6.3
3	C	139	GLY	6.2
3	G	109	ALA	6.2
3	C	155	HIS	6.0
3	C	148	PHE	6.0
3	G	169	GLU	6.0
3	C	167	ALA	6.0
3	C	63	LEU	5.9
2	F	147	GLU	5.9
3	G	73	PHE	5.9
3	G	117	ASP	5.9
3	C	128	VAL	5.8
3	G	81	ASP	5.8
3	C	51	PHE	5.8
1	A	286	LEU	5.8
3	C	126	TRP	5.8
3	G	80	ALA	5.7
2	B	190	MET	5.7
3	C	165	GLY	5.7
3	C	169	GLU	5.7
3	C	88	VAL	5.6
3	G	98	ALA	5.6
3	C	130	THR	5.6
2	F	193	LEU	5.5
3	C	135	VAL	5.5
3	C	94	VAL	5.5
3	G	167	ALA	5.5
1	E	309	THR	5.5
3	G	100	ASN	5.4
3	G	165	GLY	5.4
3	C	101	ALA	5.4
1	E	228	GLU	5.3
3	G	155	HIS	5.3
3	C	159	ALA	5.3
3	G	95	ASP	5.3
3	G	75	ARG	5.2
3	C	153	GLY	5.2
3	C	90	LEU	5.1
3	C	145	GLY	5.1
3	G	96	THR	5.1
3	G	121	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
2	F	205	HIS	5.1
3	C	32	TRP	5.1
3	C	172	PRO	5.0
3	C	100	ASN	5.0
3	G	92	GLN	5.0
3	G	135	VAL	5.0
3	C	93	LEU	5.0
3	C	72	ILE	5.0
3	C	109	ALA	5.0
1	A	232	THR	4.9
3	G	60	GLY	4.9
3	C	134	CYS	4.9
3	C	98	ALA	4.8
2	B	2	GLY	4.7
3	G	85	GLY	4.7
1	E	153	GLN	4.7
1	A	230	ARG	4.6
3	C	73	PHE	4.6
3	C	97	ASN	4.6
3	G	149	CYS	4.6
1	E	293	VAL	4.6
3	C	50	ILE	4.6
1	A	233	SER	4.6
1	A	239	LYS	4.5
3	G	183	THR	4.5
1	E	239	LYS	4.5
2	F	103	MET	4.5
3	G	163	ARG	4.4
3	G	158	SER	4.4
1	A	311	ASP	4.4
3	C	154	SER	4.3
3	C	62	GLN	4.3
3	C	75	ARG	4.2
3	C	16	TYR	4.2
2	F	195	GLU	4.2
3	C	127	GLY	4.2
3	G	62	GLN	4.2
1	A	387	PHE	4.2
3	G	35	ILE	4.2
3	G	129	CYS	4.1
3	G	99	ARG	4.1
3	C	147	TRP	4.1

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Mol	Chain	Res	Type	RSRZ
3	G	154	SER	4.1
3	G	138	GLY	4.1
1	E	233	SER	4.0
3	G	97	ASN	4.0
3	C	33	PRO	4.0
3	C	95	ASP	4.0
2	F	18	GLY	4.0
1	E	235	ALA	4.0
3	C	121	GLU	4.0
1	A	235	ALA	3.9
3	G	161	ARG	3.9
3	C	96	THR	3.9
1	A	234	LYS	3.9
1	E	232	THR	3.8
2	F	19	THR	3.8
3	C	14	PHE	3.8
3	C	156	TYR	3.7
1	A	293	VAL	3.7
3	C	170	ASN	3.7
3	C	163	ARG	3.7
2	B	250	ARG	3.6
2	B	197	ALA	3.6
2	B	225	ALA	3.6
2	F	38	ALA	3.6
2	F	144	LYS	3.6
2	F	190	MET	3.6
1	A	276	HIS	3.6
2	B	202	ALA	3.6
3	C	129	CYS	3.6
1	A	231	ARG	3.5
1	E	387	PHE	3.5
2	B	141	GLU	3.5
1	E	37	THR	3.5
2	B	147	GLU	3.5
2	F	168	THR	3.5
1	A	226	GLY	3.5
2	F	223	LEU	3.5
3	C	99	ARG	3.5
1	E	221	ASN	3.4
1	E	382	ALA	3.4
3	G	76	ARG	3.4
3	C	71	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	230	ARG	3.3
3	C	15	LEU	3.3
1	A	90	GLY	3.3
3	C	136	PRO	3.3
3	G	14	PHE	3.3
1	E	425	GLU	3.3
2	B	146	ALA	3.3
3	C	158	SER	3.3
3	G	170	ASN	3.3
1	A	236	GLU	3.2
2	F	150	GLU	3.2
3	G	157	ASP	3.2
1	A	362	MET	3.2
2	B	148	GLY	3.2
3	G	19	THR	3.2
2	F	191	ASP	3.2
2	B	193	LEU	3.1
1	E	430	ALA	3.1
2	B	104	ALA	3.1
2	F	146	ALA	3.1
2	B	227	LYS	3.1
1	E	237	ALA	3.1
3	C	41	SER	3.1
1	A	425	GLU	3.1
3	G	156	TYR	3.1
2	F	222	LYS	3.0
3	G	136	PRO	3.0
1	E	311	ASP	3.0
2	F	7	GLU	3.0
3	C	17	TYR	3.0
3	C	162	ILE	3.0
3	G	146	GLY	3.0
3	G	36	ASN	3.0
1	A	94	ARG	2.9
1	E	36	PRO	2.9
1	E	39	ARG	2.9
2	F	102	LEU	2.9
2	B	142	PRO	2.9
1	A	283	ALA	2.9
1	E	310	ALA	2.9
1	E	89	GLY	2.9
3	G	162	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
3	G	50	ILE	2.9
1	E	238	GLN	2.9
3	G	15	LEU	2.9
2	F	142	PRO	2.9
2	B	194	VAL	2.9
3	C	76	ARG	2.9
1	A	219	THR	2.9
3	C	146	GLY	2.8
2	B	196	TYR	2.8
3	G	145	GLY	2.8
1	E	155	SER	2.8
3	G	147	TRP	2.8
1	E	3	GLY	2.8
1	E	157	TRP	2.8
2	F	35	VAL	2.8
1	E	386	THR	2.8
3	G	18	ALA	2.7
2	B	143	PRO	2.7
1	E	236	GLU	2.7
2	B	4	GLY	2.7
1	E	19	LEU	2.7
2	B	3	GLY	2.7
1	E	273	TYR	2.7
3	G	13	ASP	2.7
1	E	316	GLN	2.7
1	A	152	GLY	2.6
2	B	191	ASP	2.6
2	F	189	LEU	2.6
2	F	192	ASP	2.6
1	A	174	HIS	2.6
2	F	149	HIS	2.6
2	B	19	THR	2.6
1	E	292	ILE	2.5
3	C	35	ILE	2.5
1	E	302	TYR	2.5
3	G	21	GLY	2.5
2	F	5	HIS	2.5
3	C	23	GLY	2.5
1	E	84	MET	2.5
1	E	385	THR	2.5
2	F	194	VAL	2.5
1	E	414	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	302	TYR	2.5
1	E	234	LYS	2.5
1	E	294	PRO	2.5
1	E	275	GLY	2.5
3	C	26	ALA	2.4
2	F	123	ASN	2.4
3	G	22	ALA	2.4
2	F	52	GLU	2.4
3	C	39	ASN	2.4
3	C	157	ASP	2.4
1	A	432	TYR	2.4
1	A	91	PHE	2.4
2	B	49	SER	2.4
2	B	41	GLY	2.4
2	F	221	PRO	2.4
1	A	365	ILE	2.3
2	B	140	GLU	2.3
2	F	140	GLU	2.3
2	B	152	ASP	2.3
2	F	253	ALA	2.3
1	E	276	HIS	2.3
1	A	361	PRO	2.3
1	E	4	ILE	2.3
1	A	154	MET	2.3
1	E	229	VAL	2.3
2	F	14	GLU	2.3
1	E	290	ALA	2.3
1	E	241	THR	2.3
2	B	192	ASP	2.3
2	B	17	PHE	2.2
2	B	168	THR	2.2
2	F	37	ALA	2.2
1	E	291	HIS	2.2
2	B	204	VAL	2.2
1	E	282	GLU	2.2
2	B	151	PRO	2.2
1	A	99	ASN	2.2
2	B	5	HIS	2.2
2	F	12	SER	2.2
2	F	179	ALA	2.1
1	E	5	PRO	2.1
2	F	2	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	240	ASP	2.1
2	B	205	HIS	2.1
1	A	41	LEU	2.1
1	E	154	MET	2.1
1	A	279	ASN	2.1
1	A	157	TRP	2.1
1	E	351	THR	2.1
2	B	71	THR	2.1
3	C	20	ALA	2.1
1	A	11	PRO	2.1
1	E	122	LYS	2.1
1	E	225	THR	2.1
2	F	3	GLY	2.1
1	E	21	SER	2.0
1	A	284	ASN	2.0
3	C	161	ARG	2.0
3	C	29	ALA	2.0
1	E	90	GLY	2.0
2	F	141	GLU	2.0
2	F	175	VAL	2.0
2	F	106	ALA	2.0
2	B	117	GLY	2.0
2	F	255	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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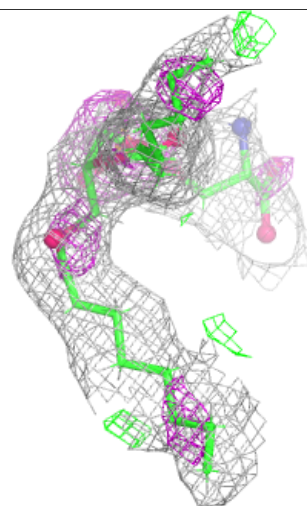
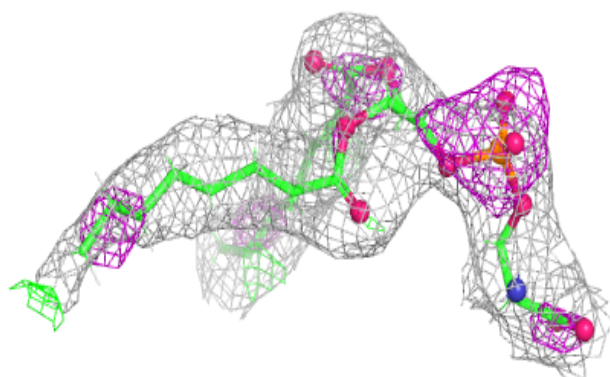
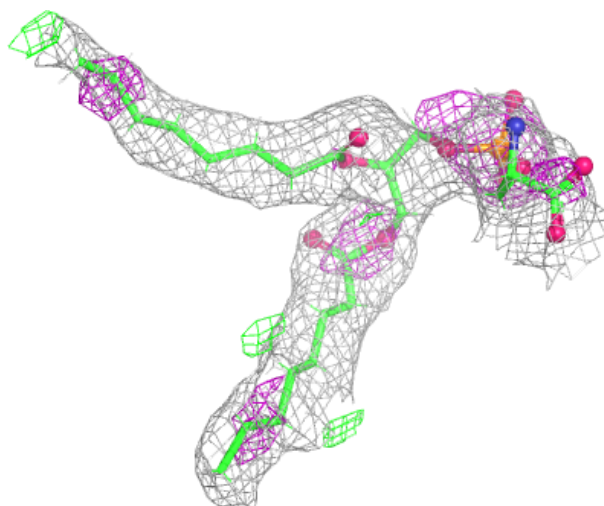
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	FES	C	1001	4/4	0.71	0.24	128,129,132,132	4
7	8SP	F	303	34/34	0.81	0.14	11,17,48,49	0
11	FES	G	1001	4/4	0.81	0.28	106,107,109,109	4
7	8SP	A	1005	34/34	0.83	0.14	6,12,35,35	0
6	6PE	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	0.07	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.

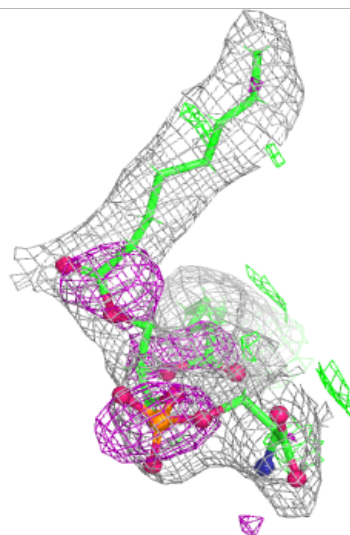
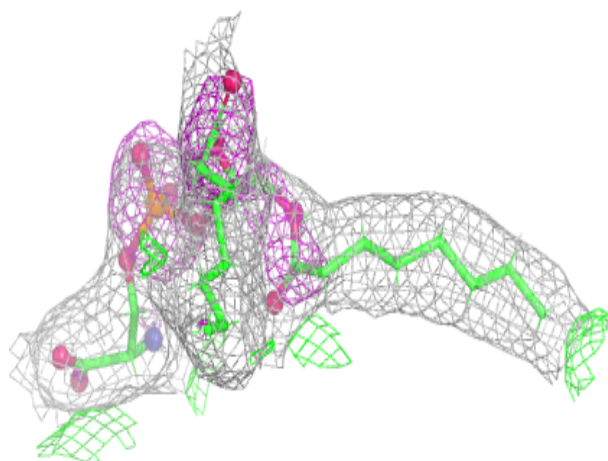
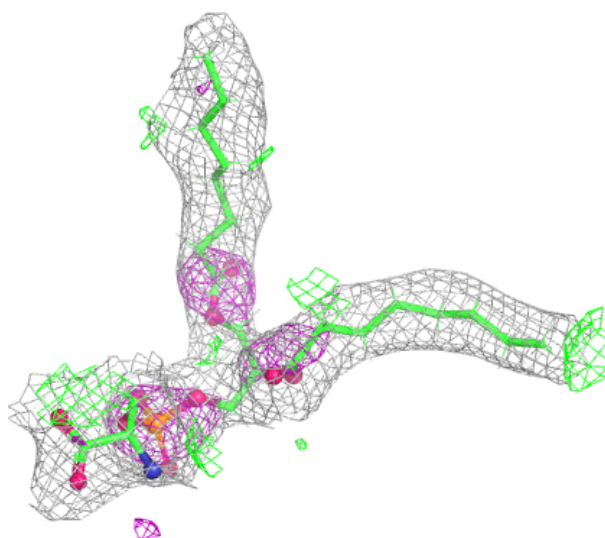
Electron density around 8SP F 303:

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



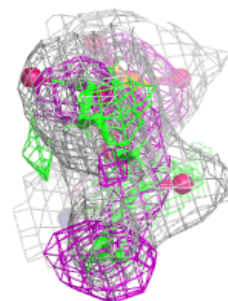
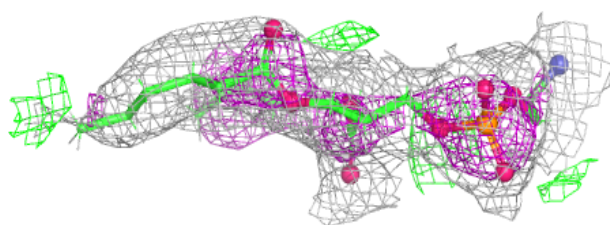
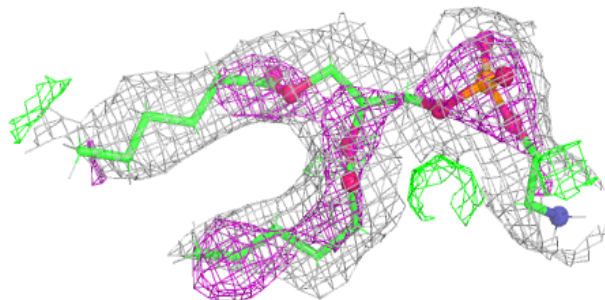
Electron density around 8SP A 1005:

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

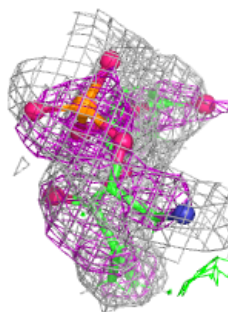
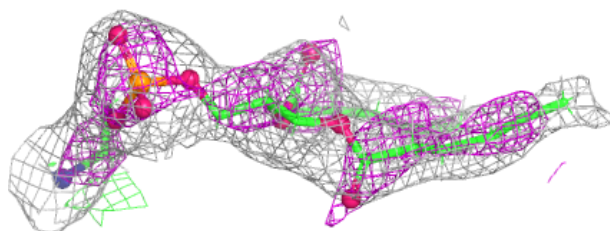
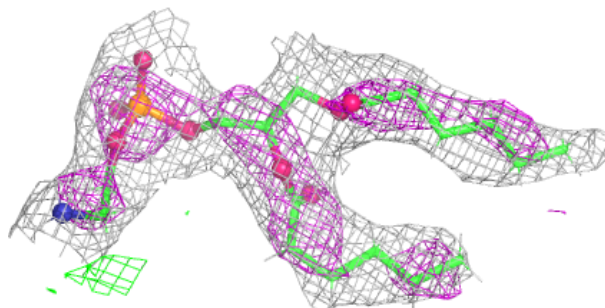


Electron density around 6PE E 1004:

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

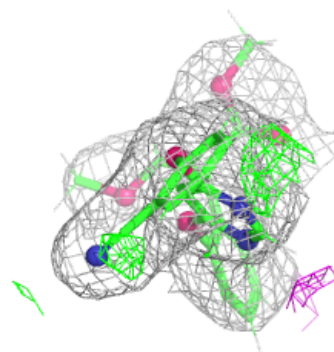
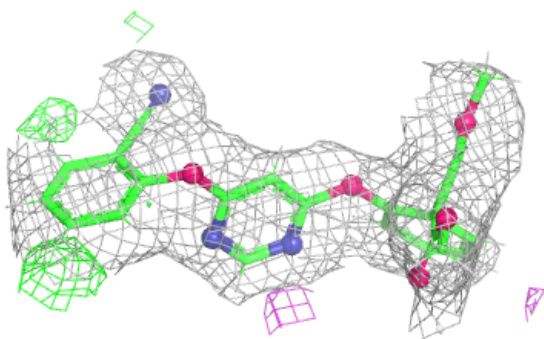
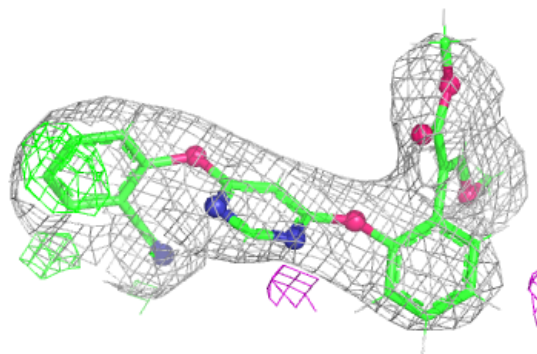
**Electron density around 6PE A 1004:**

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

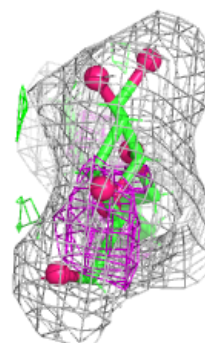
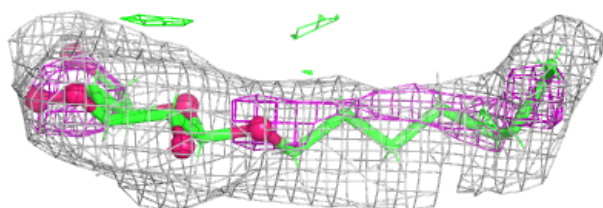
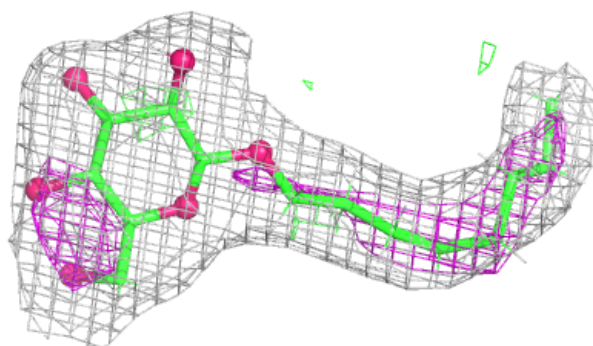


Electron density around AZO A 1003:

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

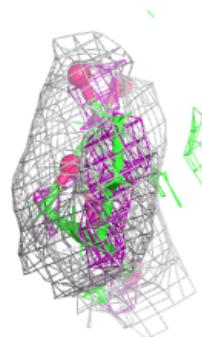
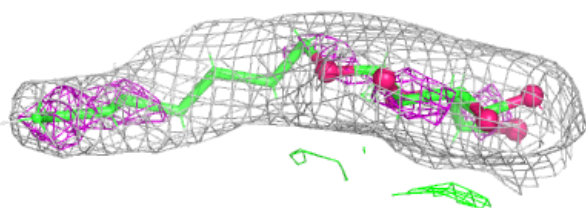
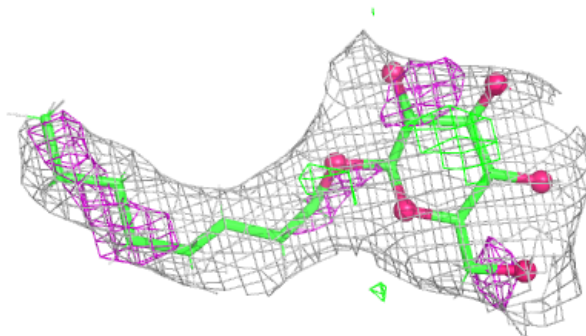
**Electron density around BOG B 301:**

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

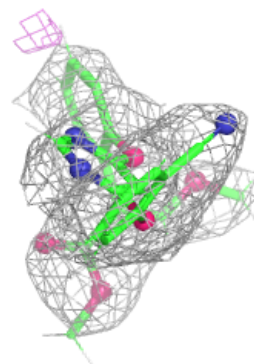
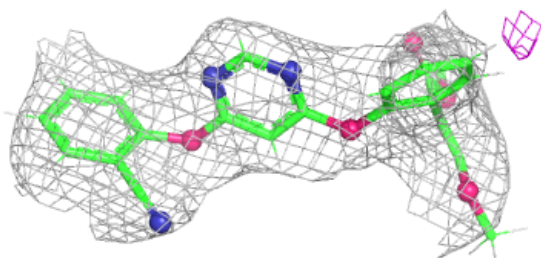
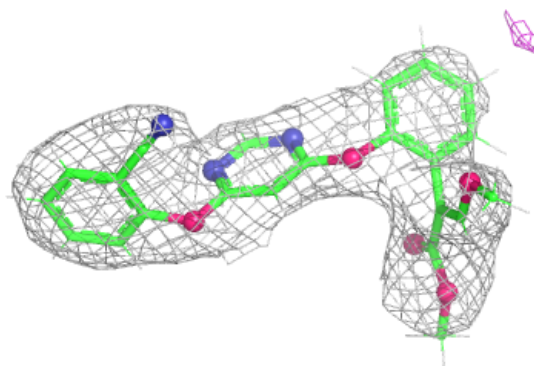


Electron density around BOG F 301:

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

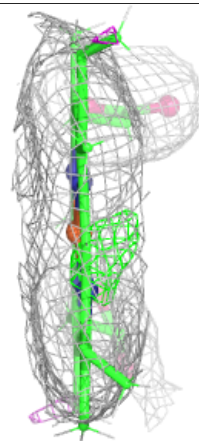
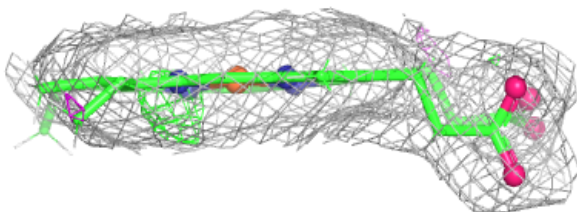
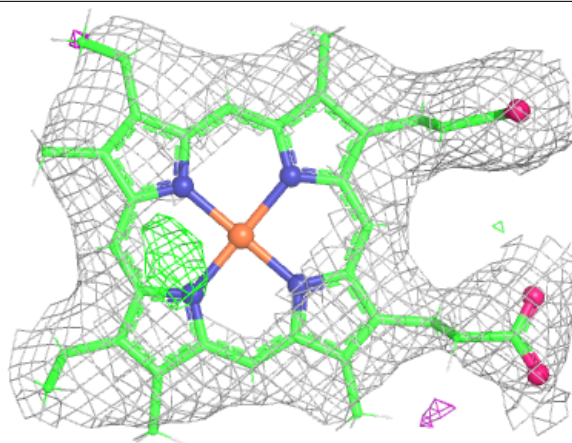
**Electron density around AZO E 1003:**

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



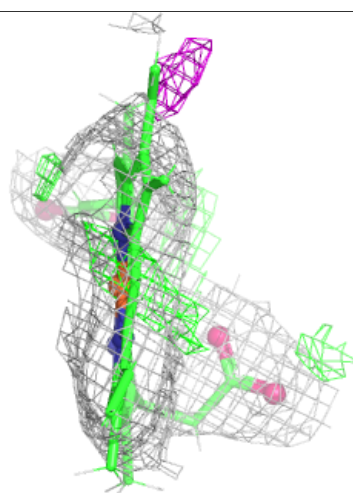
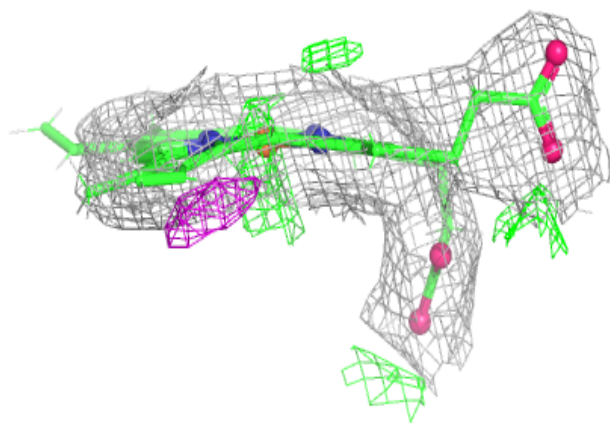
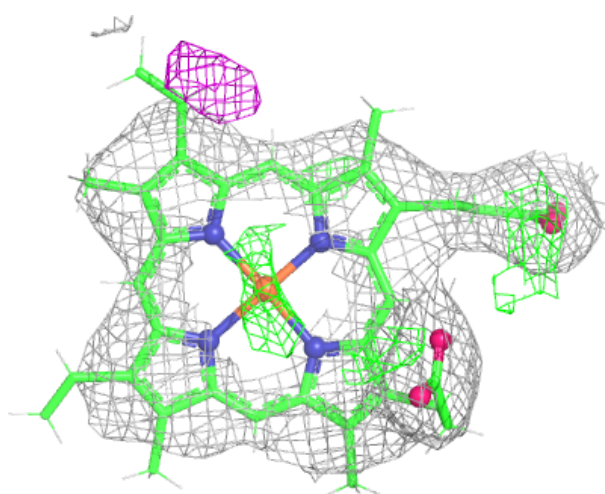
Electron density around HEC F 302:

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



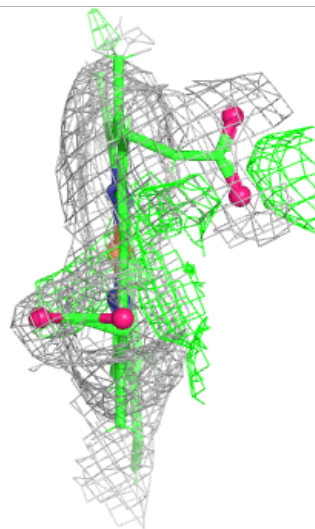
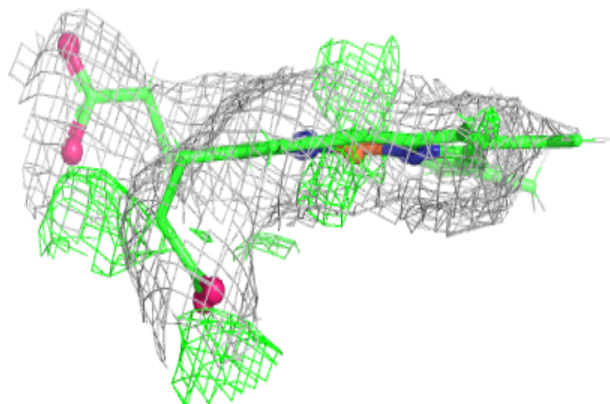
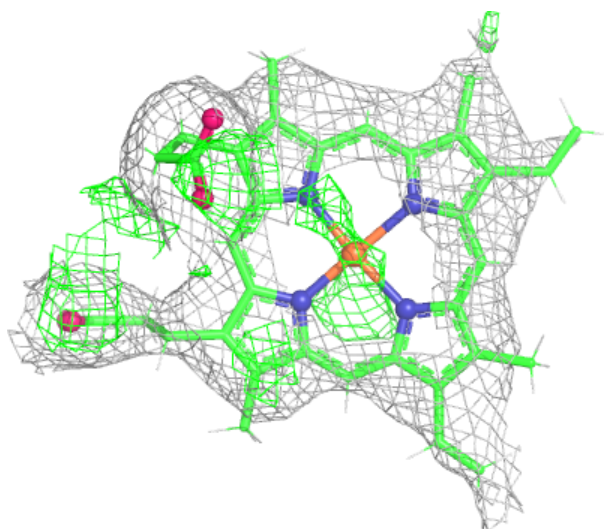
Electron density around HEM E 1002:

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



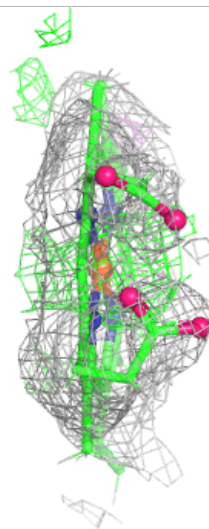
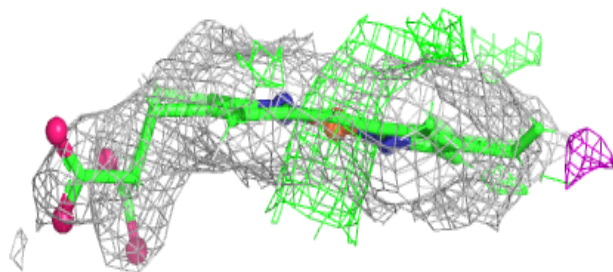
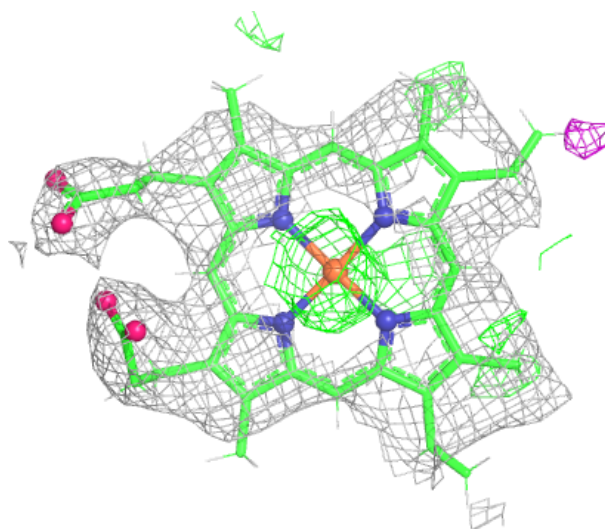
Electron density around HEM A 1002:

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



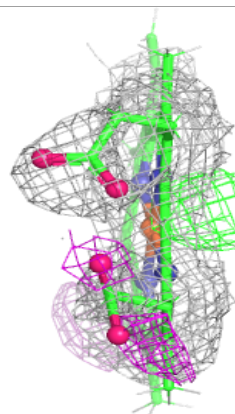
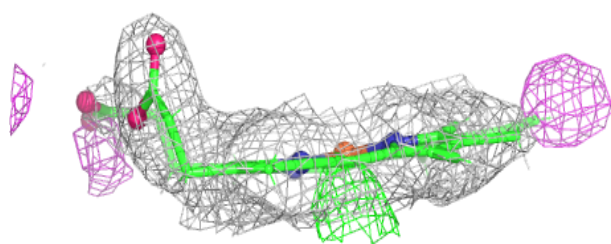
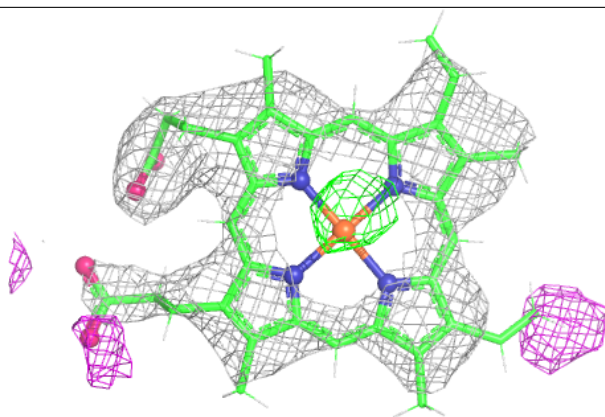
Electron density around HEM E 1001:

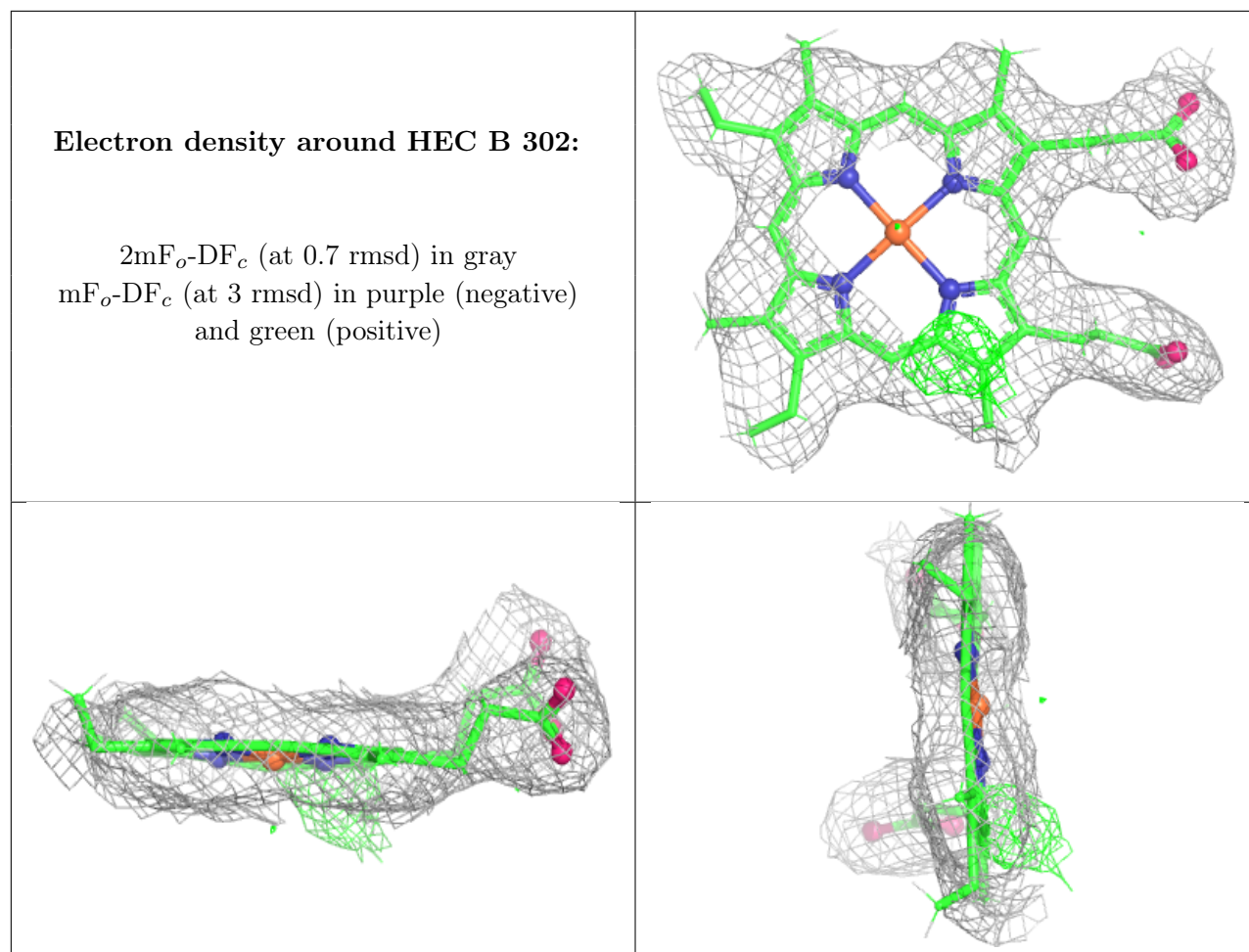
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 1001:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.