



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 05:10 am GMT

PDB ID : 1GQ1  
Title : CYTOCHROME CD1 NITRITE REDUCTASE, Y25S mutant, OXIDISED FORM  
Authors : Sjogren, T.; Gordon, E.H.J.; Lofqvist, M.; Richter, C.D.; Hajdu, J.; Ferguson, S.J.  
Deposited on : 2001-11-19  
Resolution : 1.40 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

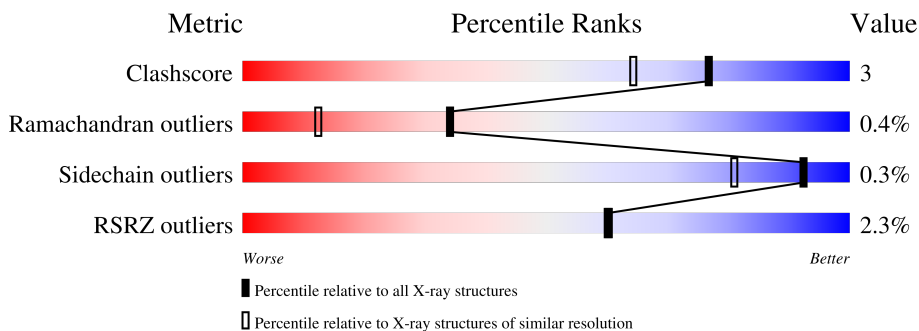
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 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))
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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  $\geq 3$ , 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	567	 2% (red), 92% (green), 6% (yellow), 0% (orange), 0% (grey)
1	B	567	 2% (red), 90% (green), 8% (yellow), 0% (orange), 0% (grey)

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DHE	A	602	X	-	-	-
3	DHE	B	602	X	-	-	-
4	SO4	A	621	-	-	-	X
5	GOL	A	611	-	X	-	-
5	GOL	A	612	-	X	-	-
5	GOL	B	611	-	X	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10317 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.

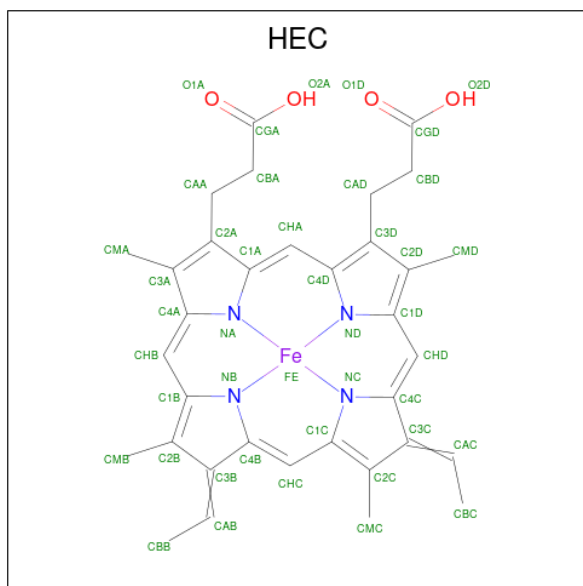
- Molecule 1 is a protein called CYTOCHROME CD1 NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	559	Total 4360	C 2750	N 731	O 863	S 16	0	5	0
1	B	559	Total 4361	C 2751	N 731	O 863	S 16	0	5	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	SER	TYR	engineered mutation	UNP Q9FCQ0
B	25	SER	TYR	engineered mutation	UNP Q9FCQ0

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



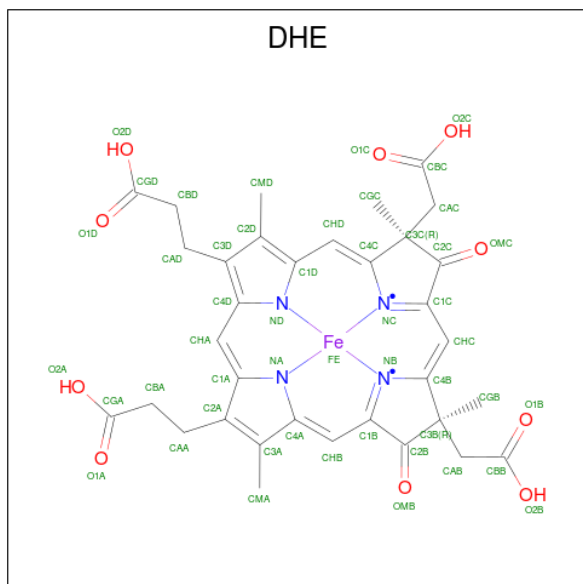
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0

- Molecule 3 is HEME D (three-letter code: DHE) (formula:  $C_{34}H_{32}FeN_4O_{10}$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	A	1	49	34	1	4	10	0	0
3	B	1	49	34	1	4	10	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

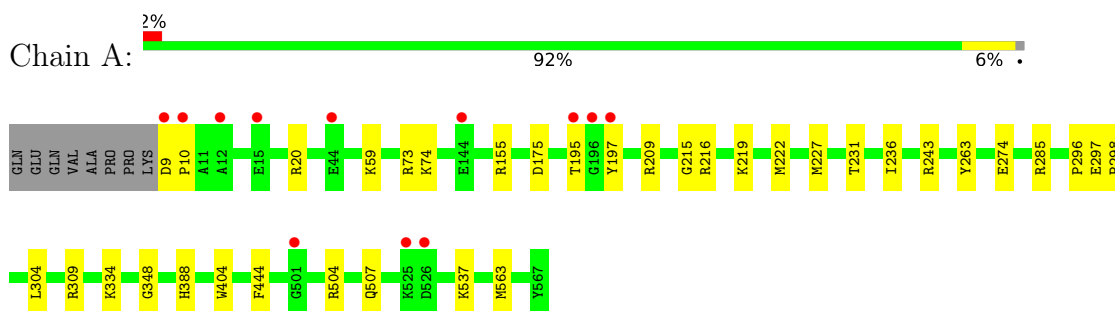
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	648	Total O 648 648	0	0
6	B	706	Total O 706 706	0	0

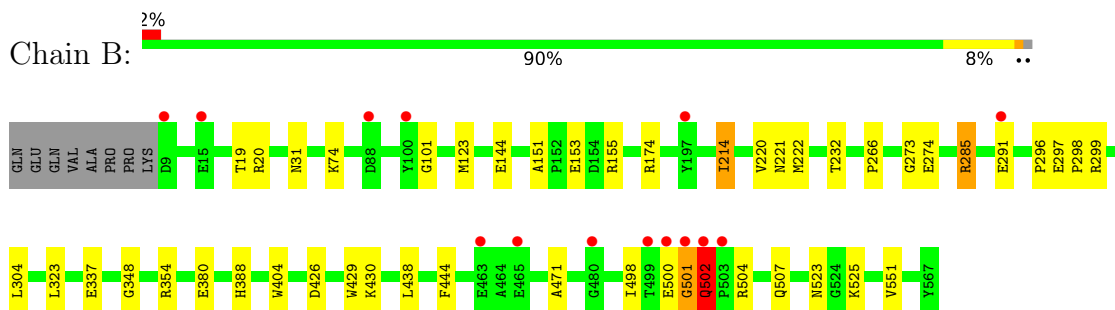
### 3 Residue-property plots [i](#)

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

- Molecule 1: CYTOCHROME CD1 NITRITE REDUCTASE



- Molecule 1: CYTOCHROME CD1 NITRITE REDUCTASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.80Å 60.60Å 100.34Å 90.00° 112.33° 90.00°	Depositor
Resolution (Å)	30.00 – 1.40 29.34 – 1.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-1.40) 99.3 (29.34-1.40)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 1.39Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.159 , 0.175 0.163 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	9.9	Xtrriage
Anisotropy	0.352	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 43.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10317	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, HEC, SO4, DHE

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	0.41	0/4485	0.95	14/6099 (0.2%)
1	B	0.42	0/4486	0.95	9/6100 (0.1%)
All	All	0.42	0/8971	0.95	23/12199 (0.2%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	ARG	NE-CZ-NH2	-12.93	113.83	120.30
1	B	504	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	B	299	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	B	504	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	A	504	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	B	285[A]	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	285[B]	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	504	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	B	155	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	309	ARG	CD-NE-CZ	6.41	132.57	123.60
1	A	309	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	A	209	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	73	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	20	ARG	CD-NE-CZ	5.67	131.54	123.60
1	A	263	TYR	CB-CG-CD2	-5.64	117.62	121.00
1	A	20	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	B	404	TRP	CA-CB-CG	5.57	124.29	113.70
1	A	404	TRP	CA-CB-CG	5.42	123.99	113.70
1	B	354	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	263	TYR	CB-CG-CD1	5.20	124.12	121.00
1	A	175	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	216	ARG	NE-CZ-NH1	5.13	122.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	4360	0	4194	22	0
1	B	4361	0	4196	29	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	49	0	28	2	0
3	B	49	0	28	2	0
4	A	15	0	0	0	0
4	B	25	0	0	0	0
5	A	12	0	10	0	0
5	B	6	0	4	0	0
6	A	648	0	0	7	0
6	B	706	0	0	10	0
All	All	10317	0	8520	53	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.

All (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:GLU:HB2	1:B:523:ASN:HD21	1.39	0.88
1:A:227[B]:MET:HE1	1:A:231:THR:HG22	1.61	0.81
1:A:197:TYR:CE2	1:A:219:LYS:HB3	2.24	0.72
1:B:500:GLU:HB2	1:B:523:ASN:ND2	2.12	0.64
1:A:537:LYS:HG2	6:A:2595:HOH:O	1.96	0.64
1:A:227[B]:MET:CE	1:A:231:THR:HG22	2.28	0.63
1:B:323:LEU:HD22	1:B:337[B]:GLU:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:ASP:O	1:B:430:LYS:HD3	2.03	0.59
1:B:388:HIS:HB3	6:B:2565:HOH:O	2.03	0.59
3:B:602:DHE:HMD1	3:B:602:DHE:HBD2	1.85	0.58
1:A:197:TYR:CD1	1:A:215:GLY:HA3	2.38	0.58
1:A:388:HIS:HB3	6:A:2504:HOH:O	2.03	0.57
1:B:438:LEU:HG	1:B:471:ALA:HB2	1.87	0.57
1:B:74:LYS:HG3	1:B:296:PRO:HG3	1.88	0.56
3:A:602:DHE:HMD1	3:A:602:DHE:HBD2	1.87	0.55
1:B:380:GLU:HG3	1:B:429:TRP:O	2.07	0.53
1:B:214:ILE:HD12	1:B:220:VAL:HG22	1.90	0.53
1:B:444:PHE:CE1	3:B:602:DHE:HBD1	2.44	0.52
1:B:151:ALA:HB1	1:B:153:GLU:OE2	2.11	0.51
1:B:222[B]:MET:HE1	1:B:274:GLU:HA	1.92	0.51
1:A:155:ARG:HG2	6:A:2320:HOH:O	2.09	0.51
1:B:31:ASN:HB2	6:B:2041:HOH:O	2.11	0.49
1:A:334:LYS:NZ	1:A:334:LYS:HB3	2.29	0.48
1:A:444:PHE:CE1	3:A:602:DHE:HBD1	2.48	0.48
1:B:221:ASN:OD1	1:B:232:THR:HG21	2.13	0.48
1:B:291:GLU:HG3	6:B:2417:HOH:O	2.14	0.47
1:B:297:GLU:N	1:B:298:PRO:HD3	2.29	0.47
1:B:525:LYS:HG3	6:B:2301:HOH:O	2.14	0.47
1:B:153:GLU:H	1:B:153:GLU:CD	2.18	0.47
1:B:101:GLY:HA2	6:B:2165:HOH:O	2.14	0.47
1:B:551:VAL:HB	6:B:2305:HOH:O	2.14	0.47
1:A:222:MET:HE1	1:A:274:GLU:HA	1.97	0.46
1:A:227[B]:MET:SD	6:A:2320:HOH:O	2.61	0.46
1:A:304:LEU:HD21	1:A:348:GLY:HA2	1.99	0.45
1:A:227[B]:MET:HE2	6:A:2327:HOH:O	2.16	0.45
1:A:297:GLU:N	1:A:298:PRO:HD3	2.31	0.45
1:B:304:LEU:HD21	1:B:348:GLY:HA2	1.98	0.44
1:A:9:ASP:HB2	1:A:10:PRO:HD2	2.00	0.44
1:B:19:THR:HG23	6:B:2023:HOH:O	2.17	0.43
1:B:266:PRO:HD2	1:B:285[B]:ARG:CZ	2.48	0.43
1:A:285[B]:ARG:HD3	6:A:2367:HOH:O	2.17	0.43
1:A:195:THR:HB	1:A:197:TYR:CZ	2.53	0.43
1:A:59:LYS:HE2	6:A:2036:HOH:O	2.17	0.42
1:B:144:GLU:HG3	6:B:2228:HOH:O	2.18	0.42
1:A:74:LYS:HG3	1:A:296:PRO:HG3	2.02	0.42
1:A:219:LYS:HD3	1:A:236:ILE:O	2.20	0.42
1:B:291:GLU:HB2	6:B:2419:HOH:O	2.20	0.42
1:A:227[B]:MET:HE1	1:A:231:THR:CG2	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:ILE:HB	6:B:2612:HOH:O	2.20	0.41
1:B:222[B]:MET:HE1	1:B:273:GLY:O	2.20	0.41
1:B:501:GLY:O	1:B:502:GLN:C	2.58	0.41
1:A:9:ASP:HB2	1:A:10:PRO:CD	2.51	0.41
1:B:123:MET:HA	1:B:123:MET:HE2	2.03	0.40

There are no symmetry-related clashes.

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	562/567 (99%)	543 (97%)	18 (3%)	1 (0%)	47 21
1	B	562/567 (99%)	538 (96%)	20 (4%)	4 (1%)	22 5
All	All	1124/1134 (99%)	1081 (96%)	38 (3%)	5 (0%)	34 12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	507	GLN
1	B	507	GLN
1	B	174	ARG
1	B	501	GLY
1	B	502	GLN

#### 5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	467/469 (100%)	465 (100%)	2 (0%)	91	78
1	B	467/469 (100%)	465 (100%)	2 (0%)	91	78
All	All	934/938 (100%)	930 (100%)	4 (0%)	92	78

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	563[A]	MET
1	A	563[B]	MET
1	B	214	ILE
1	B	502	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	A	502	GLN
1	B	282	GLN
1	B	523	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

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
3	DHE	B	602	4,1	50,56,56	4.26	7 (14%)	44,94,94	1.73	12 (27%)
4	SO4	B	603	3	4,4,4	0.62	0	6,6,6	0.25	0
4	SO4	B	623	-	4,4,4	0.70	0	6,6,6	0.69	0
4	SO4	B	622	-	4,4,4	0.63	0	6,6,6	0.21	0
4	SO4	A	603	3	4,4,4	0.62	0	6,6,6	0.34	0
5	GOL	B	611	-	5,5,5	4.42	5 (100%)	5,5,5	2.36	2 (40%)
4	SO4	A	622	-	4,4,4	0.61	0	6,6,6	0.19	0
4	SO4	B	624	-	4,4,4	0.61	0	6,6,6	0.17	0
5	GOL	A	611	-	5,5,5	4.50	5 (100%)	5,5,5	2.73	3 (60%)
3	DHE	A	602	4,1	50,56,56	4.37	8 (16%)	44,94,94	1.81	13 (29%)
2	HEC	A	601	1	32,50,50	2.04	4 (12%)	24,82,82	1.92	10 (41%)
4	SO4	A	621	-	4,4,4	0.61	0	6,6,6	0.15	0
4	SO4	B	621	-	4,4,4	0.60	0	6,6,6	0.14	0
5	GOL	A	612	-	5,5,5	3.94	4 (80%)	5,5,5	1.83	2 (40%)
2	HEC	B	601	1	32,50,50	2.04	4 (12%)	24,82,82	2.03	10 (41%)

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
3	DHE	B	602	4,1	1/1/15/19	7/20/108/108	-
5	GOL	B	611	-	-	2/4/4/4	-
5	GOL	A	611	-	-	3/4/4/4	-
3	DHE	A	602	4,1	1/1/15/19	7/20/108/108	-
2	HEC	A	601	1	-	2/10/54/54	-
5	GOL	A	612	-	-	0/4/4/4	-
2	HEC	B	601	1	-	2/10/54/54	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	DHE	OMC-C2C	16.84	1.52	1.22
3	A	602	DHE	OMB-C2B	16.54	1.51	1.22
3	B	602	DHE	OMC-C2C	16.20	1.51	1.22
3	B	602	DHE	OMB-C2B	16.15	1.51	1.22
3	A	602	DHE	C3C-C2C	-12.34	1.33	1.52
3	B	602	DHE	C3C-C2C	-11.97	1.34	1.52
3	B	602	DHE	C3B-C2B	-11.65	1.35	1.52
3	A	602	DHE	C3B-C2B	-11.56	1.35	1.52
2	A	601	HEC	C3C-C2C	-6.77	1.33	1.40
5	A	611	GOL	C3-C2	-6.71	1.24	1.51
5	B	611	GOL	C3-C2	-6.66	1.24	1.51
2	B	601	HEC	C3C-C2C	-6.44	1.34	1.40
2	B	601	HEC	C2B-C3B	-6.14	1.34	1.40
2	A	601	HEC	C2B-C3B	-6.02	1.34	1.40
5	A	612	GOL	C3-C2	-5.91	1.27	1.51
3	A	602	DHE	CAC-CBC	-5.89	1.32	1.50
3	A	602	DHE	CAB-CBB	-5.72	1.33	1.50
3	B	602	DHE	CAB-CBB	-5.69	1.33	1.50
3	B	602	DHE	CAC-CBC	-5.48	1.33	1.50
5	B	611	GOL	O1-C1	4.63	1.61	1.42
5	A	611	GOL	O1-C1	4.50	1.61	1.42
5	A	612	GOL	O1-C1	4.47	1.61	1.42
5	B	611	GOL	O3-C3	3.87	1.58	1.42
5	A	612	GOL	O3-C3	3.86	1.58	1.42
5	A	611	GOL	O3-C3	3.84	1.58	1.42
5	A	611	GOL	C1-C2	-3.49	1.37	1.51
2	B	601	HEC	CBC-CAC	-3.41	1.36	1.49
5	B	611	GOL	C1-C2	-3.24	1.38	1.51
2	A	601	HEC	CBC-CAC	-3.18	1.37	1.49
5	A	611	GOL	O2-C2	-2.96	1.34	1.43
5	B	611	GOL	O2-C2	-2.56	1.35	1.43
5	A	612	GOL	C1-C2	-2.28	1.42	1.51
2	B	601	HEC	CBB-CAB	-2.20	1.41	1.49
3	A	602	DHE	CMA-C3A	2.13	1.55	1.50
3	A	602	DHE	CHA-C1A	2.08	1.38	1.35
2	A	601	HEC	CBB-CAB	-2.08	1.41	1.49
3	B	602	DHE	CMA-C3A	2.05	1.55	1.50

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	611	GOL	O2-C2-C3	4.60	129.38	109.12
3	A	602	DHE	CBD-CAD-C3D	4.36	120.06	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	611	GOL	O2-C2-C3	4.14	127.36	109.12
3	B	602	DHE	CMD-C2D-C1D	-3.52	123.06	128.46
3	A	602	DHE	CAA-CBA-CGA	3.46	121.06	113.60
3	B	602	DHE	CBD-CAD-C3D	3.43	118.47	112.62
2	B	601	HEC	CMC-C2C-C1C	-3.42	123.22	128.46
2	A	601	HEC	CMD-C2D-C1D	-3.37	123.28	128.46
3	B	602	DHE	CAA-CBA-CGA	3.29	120.69	113.60
3	A	602	DHE	O1D-CGD-CBD	-3.29	112.50	123.08
3	A	602	DHE	OMC-C2C-C3C	3.29	130.03	125.92
3	A	602	DHE	CMD-C2D-C1D	-3.24	123.48	128.46
2	B	601	HEC	CMB-C2B-C1B	-3.23	123.50	128.46
2	A	601	HEC	CMB-C2B-C1B	-3.22	123.51	128.46
2	B	601	HEC	CMB-C2B-C3B	3.16	129.54	125.82
3	B	602	DHE	OMC-C2C-C3C	3.13	129.84	125.92
3	A	602	DHE	O2C-CBC-O1C	-3.11	115.56	123.30
2	B	601	HEC	CMD-C2D-C1D	-3.10	123.70	128.46
2	A	601	HEC	CMC-C2C-C1C	-3.06	123.76	128.46
3	B	602	DHE	O2B-CBB-O1B	-3.03	115.75	123.30
3	B	602	DHE	O1D-CGD-CBD	-2.95	113.59	123.08
2	B	601	HEC	CMC-C2C-C3C	2.94	129.28	125.82
2	A	601	HEC	CMB-C2B-C3B	2.93	129.27	125.82
3	B	602	DHE	O2C-CBC-O1C	-2.92	116.02	123.30
3	A	602	DHE	OMB-C2B-C3B	2.91	129.55	125.92
5	A	612	GOL	O3-C3-C2	2.88	124.00	110.20
3	A	602	DHE	O2B-CBB-O1B	-2.87	116.16	123.30
2	A	601	HEC	CMC-C2C-C3C	2.86	129.19	125.82
5	A	611	GOL	O3-C3-C2	2.84	123.83	110.20
2	B	601	HEC	O2A-CGA-O1A	2.72	130.09	123.30
3	B	602	DHE	CMD-C2D-C3D	2.70	130.03	124.94
2	B	601	HEC	C2B-C3B-C4B	2.56	109.11	106.35
3	A	602	DHE	C1C-CHC-C4B	2.55	128.87	124.98
3	A	602	DHE	C1D-CHD-C4C	-2.50	125.16	130.12
5	B	611	GOL	O3-C3-C2	2.48	122.10	110.20
3	A	602	DHE	O2D-CGD-O1D	2.45	129.40	123.30
3	A	602	DHE	O2C-CBC-CAC	2.43	122.16	114.35
2	A	601	HEC	C4C-C3C-C2C	2.40	108.95	106.35
3	B	602	DHE	CHA-C1A-NA	2.29	126.91	124.43
2	B	601	HEC	O1A-CGA-CBA	-2.26	115.83	123.08
3	A	602	DHE	CMD-C2D-C3D	2.25	129.18	124.94
2	B	601	HEC	CMA-C3A-C2A	2.25	129.18	124.94
5	A	612	GOL	C3-C2-C1	-2.20	103.16	111.70
3	B	602	DHE	OMB-C2B-C3B	2.17	128.63	125.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	611	GOL	O1-C1-C2	2.14	120.47	110.20
2	B	601	HEC	C4C-C3C-C2C	2.09	108.60	106.35
3	B	602	DHE	C1D-CHD-C4C	-2.07	126.02	130.12
2	A	601	HEC	CMA-C3A-C2A	2.07	128.84	124.94
3	B	602	DHE	O2C-CBC-CAC	2.06	120.96	114.35
2	A	601	HEC	O1A-CGA-CBA	-2.05	116.48	123.08
2	A	601	HEC	CMD-C2D-C3D	2.05	128.81	124.94
2	A	601	HEC	O2A-CGA-O1A	2.02	128.33	123.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	602	DHE	NA
3	B	602	DHE	NA

All (23) torsion outliers are listed below:

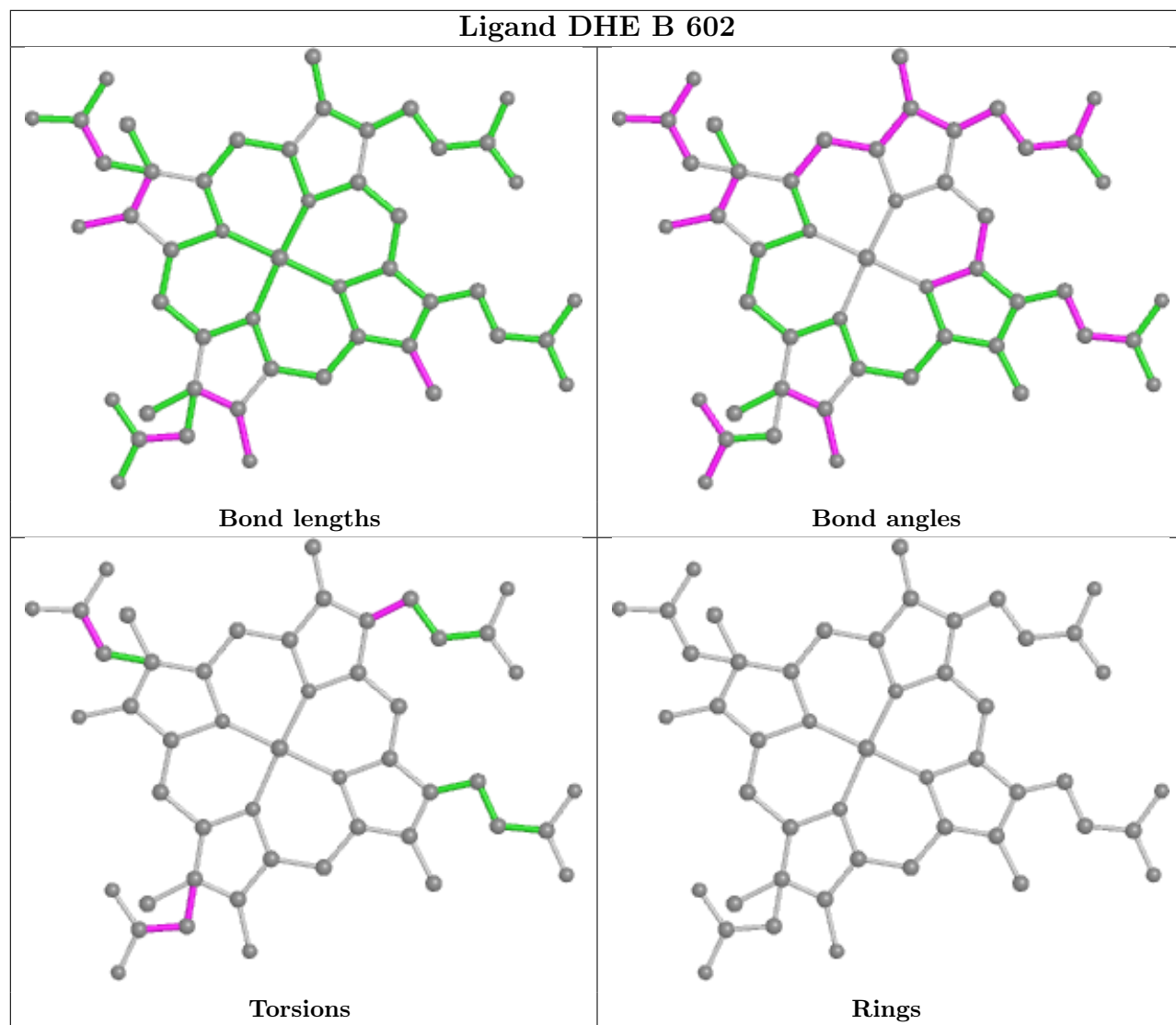
Mol	Chain	Res	Type	Atoms
3	A	602	DHE	C2D-C3D-CAD-CBD
3	A	602	DHE	C4D-C3D-CAD-CBD
3	B	602	DHE	C2D-C3D-CAD-CBD
3	B	602	DHE	C4D-C3D-CAD-CBD
5	A	611	GOL	O1-C1-C2-O2
3	A	602	DHE	C3B-CAB-CBB-O2B
3	A	602	DHE	C3C-CAC-CBC-O2C
3	B	602	DHE	C3B-CAB-CBB-O2B
3	B	602	DHE	C3C-CAC-CBC-O2C
5	A	611	GOL	O2-C2-C3-O3
3	B	602	DHE	C4B-C3B-CAB-CBB
5	B	611	GOL	O2-C2-C3-O3
3	A	602	DHE	C3B-CAB-CBB-O1B
3	A	602	DHE	C3C-CAC-CBC-O1C
3	B	602	DHE	C3B-CAB-CBB-O1B
3	B	602	DHE	C3C-CAC-CBC-O1C
2	A	601	HEC	CAD-CBD-CGD-O2D
2	B	601	HEC	CAD-CBD-CGD-O2D
2	A	601	HEC	CAD-CBD-CGD-O1D
2	B	601	HEC	CAD-CBD-CGD-O1D
5	B	611	GOL	O1-C1-C2-O2
3	A	602	DHE	C4B-C3B-CAB-CBB
5	A	611	GOL	C1-C2-C3-O3

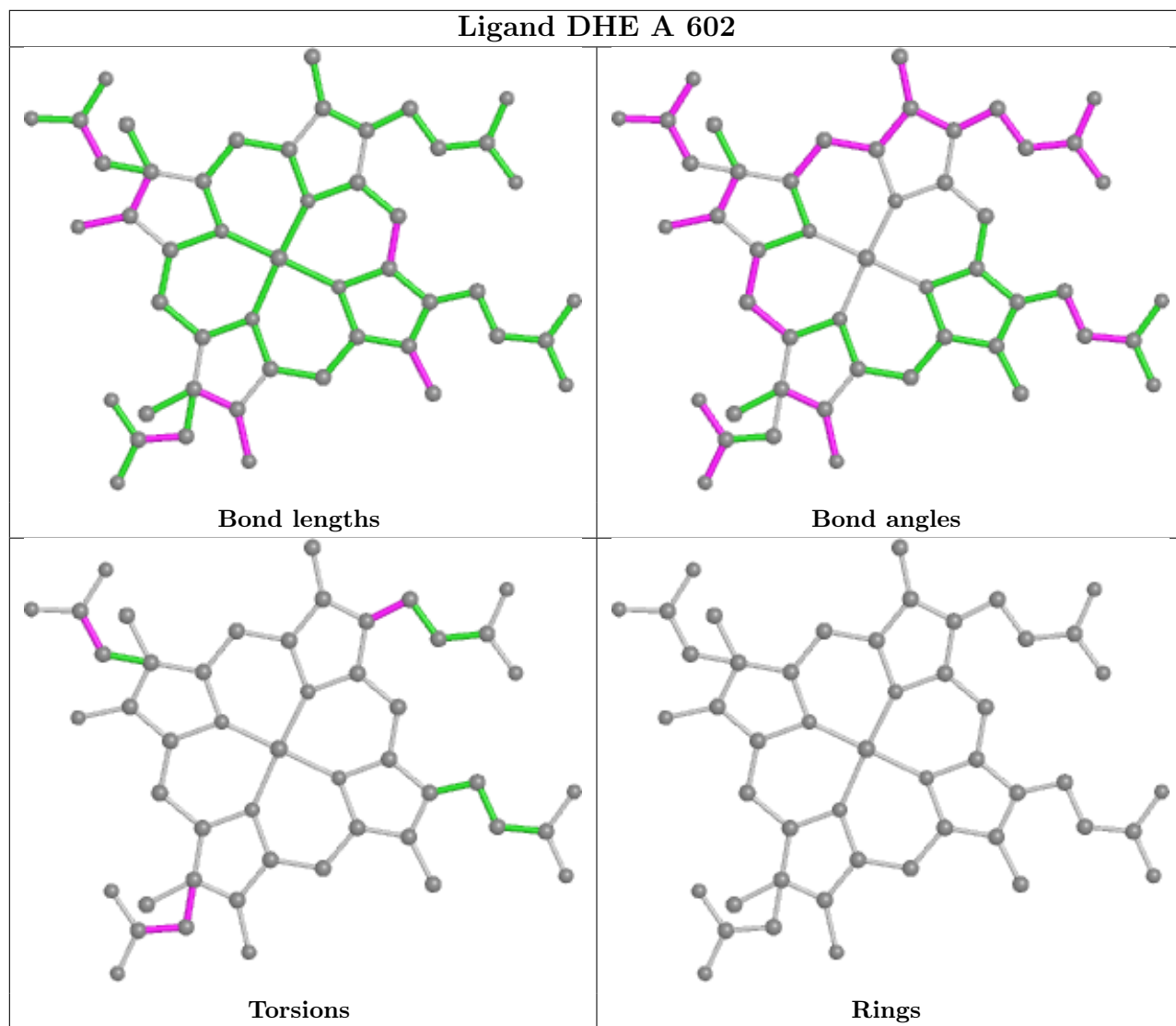
There are no ring outliers.

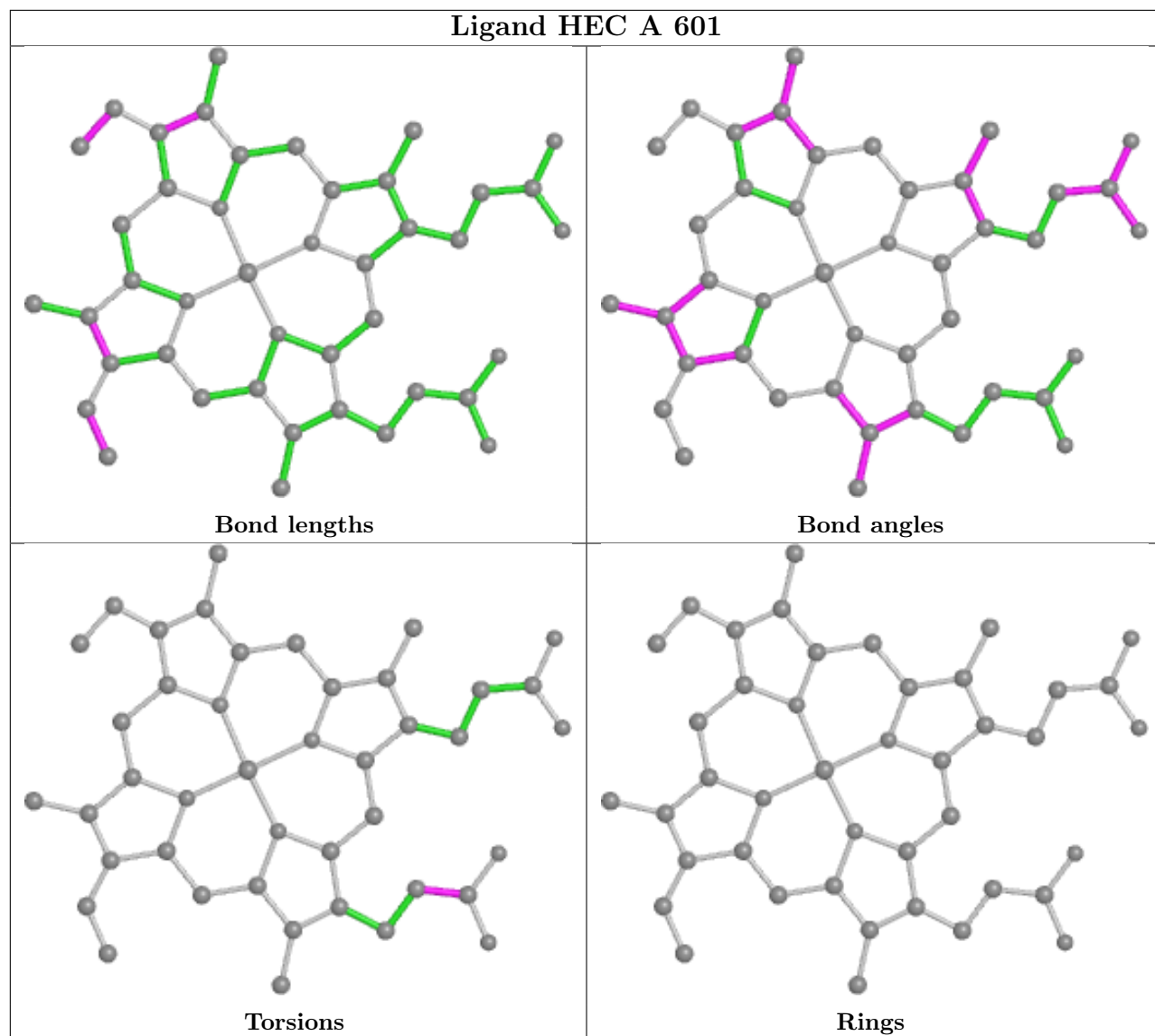
2 monomers are involved in 4 short contacts:

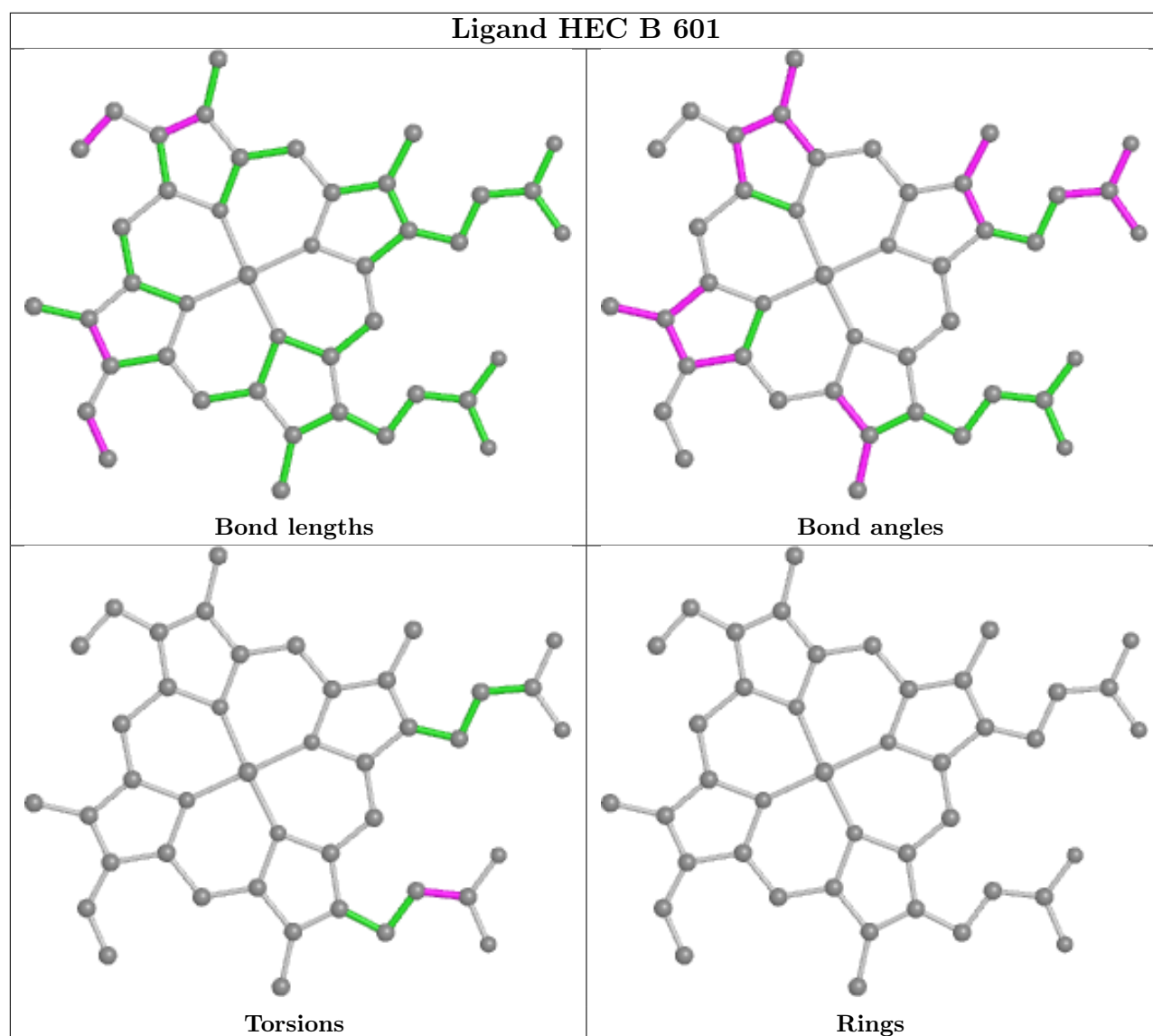
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	DHE	2	0
3	A	602	DHE	2	0

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.









## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	559/567 (98%)	-0.15	12 (2%) 63 63	6, 10, 19, 35	0
1	B	559/567 (98%)	-0.15	14 (2%) 57 57	6, 10, 19, 37	0
All	All	1118/1134 (98%)	-0.15	26 (2%) 60 60	6, 10, 19, 37	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	499	THR	8.8
1	A	197	TYR	8.8
1	B	501	GLY	8.4
1	B	197	TYR	7.9
1	A	196	GLY	6.3
1	B	502	GLN	4.8
1	A	9	ASP	4.7
1	B	480	GLY	4.3
1	B	500	GLU	3.7
1	A	526	ASP	3.7
1	A	15	GLU	3.2
1	B	465	GLU	2.6
1	B	291	GLU	2.6
1	A	44	GLU	2.5
1	B	15	GLU	2.4
1	B	100	TYR	2.4
1	B	88	ASP	2.3
1	A	144	GLU	2.3
1	A	195	THR	2.2
1	B	463	GLU	2.2
1	B	9	ASP	2.2
1	A	10	PRO	2.1
1	A	501	GLY	2.1
1	A	525	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	503	PRO	2.1
1	A	12	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

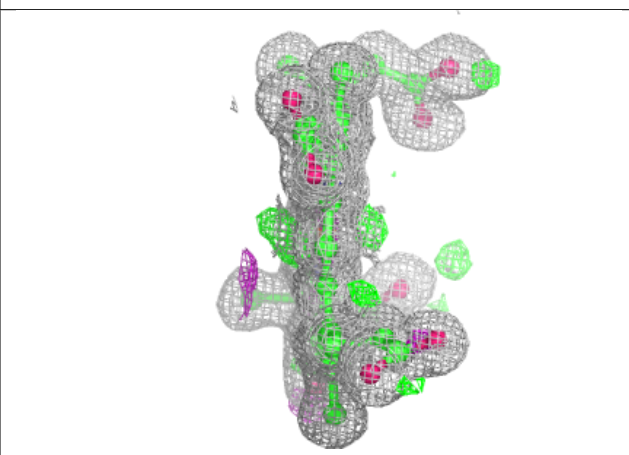
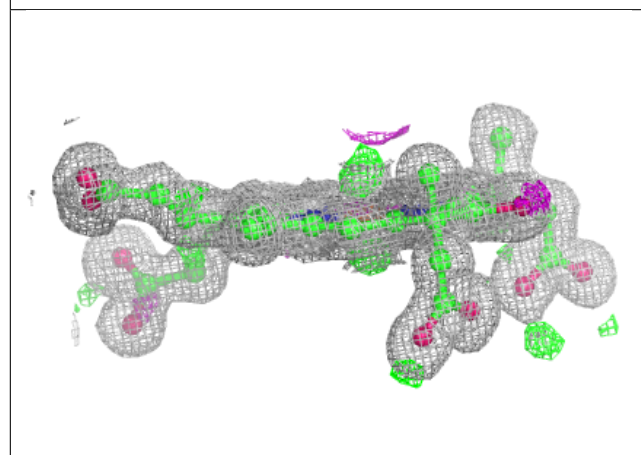
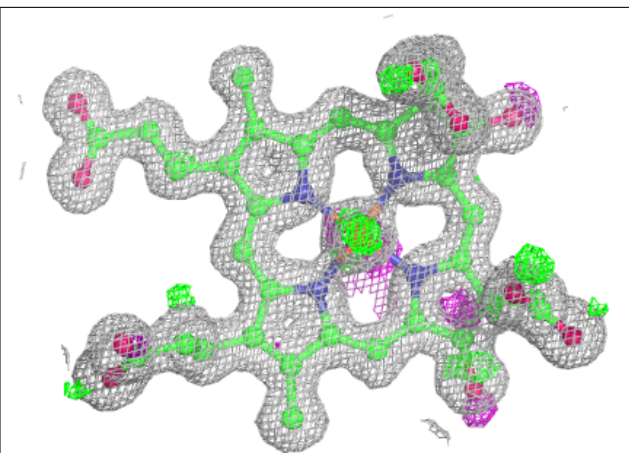
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	A	621	5/5	0.60	0.43	41,41,41,42	0
4	SO4	B	623	5/5	0.68	0.34	20,20,23,24	0
4	SO4	B	621	5/5	0.80	0.20	32,32,33,33	0
4	SO4	A	603	5/5	0.83	0.21	18,20,22,22	0
4	SO4	B	603	5/5	0.83	0.21	17,19,21,21	0
5	GOL	A	611	6/6	0.88	0.12	12,13,14,15	0
4	SO4	A	622	5/5	0.91	0.24	27,27,28,28	0
5	GOL	B	611	6/6	0.92	0.11	12,13,13,14	0
5	GOL	A	612	6/6	0.93	0.11	9,10,11,11	0
4	SO4	B	622	5/5	0.95	0.19	26,26,27,27	0
4	SO4	B	624	5/5	0.96	0.20	29,29,30,30	0
3	DHE	A	602	49/49	0.97	0.08	6,8,11,12	0
3	DHE	B	602	49/49	0.98	0.08	6,7,10,11	0
2	HEC	B	601	43/43	0.98	0.08	8,9,14,18	0
2	HEC	A	601	43/43	0.98	0.08	8,9,15,16	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.

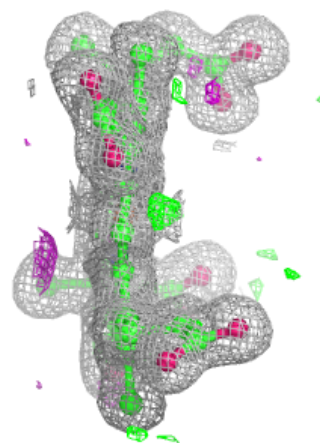
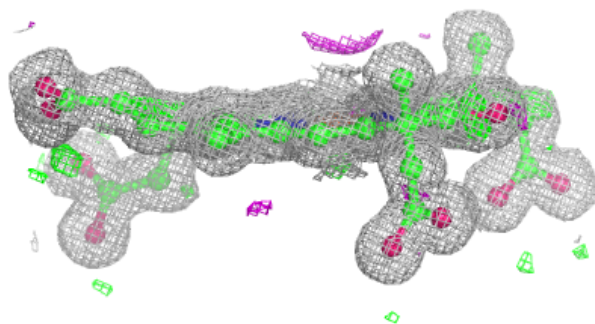
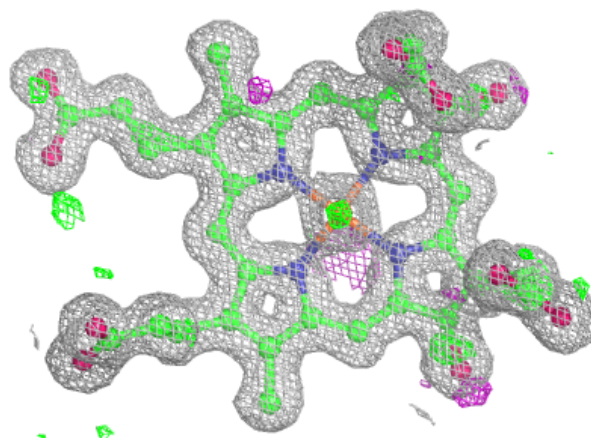
**Electron density around DHE A 602:**

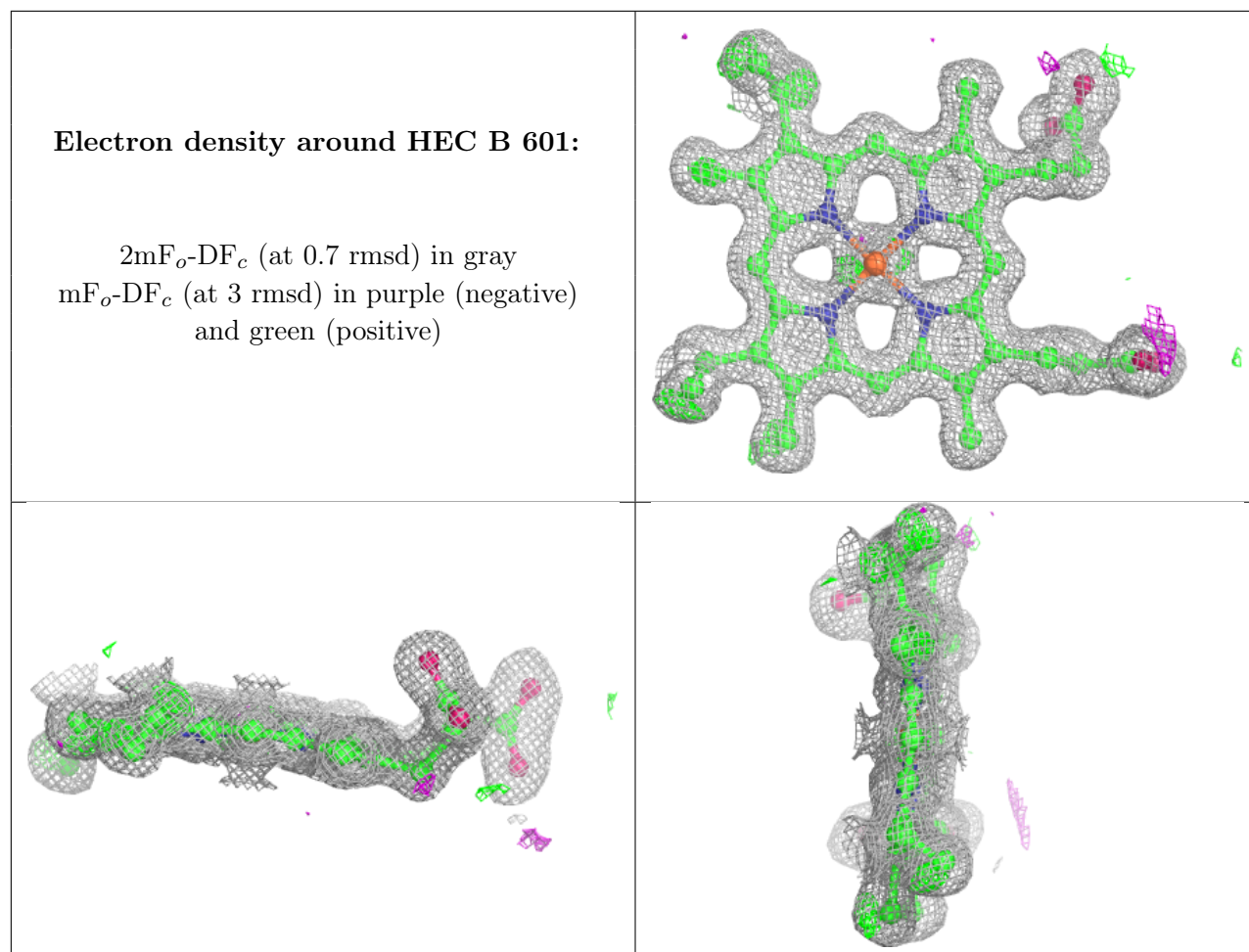
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

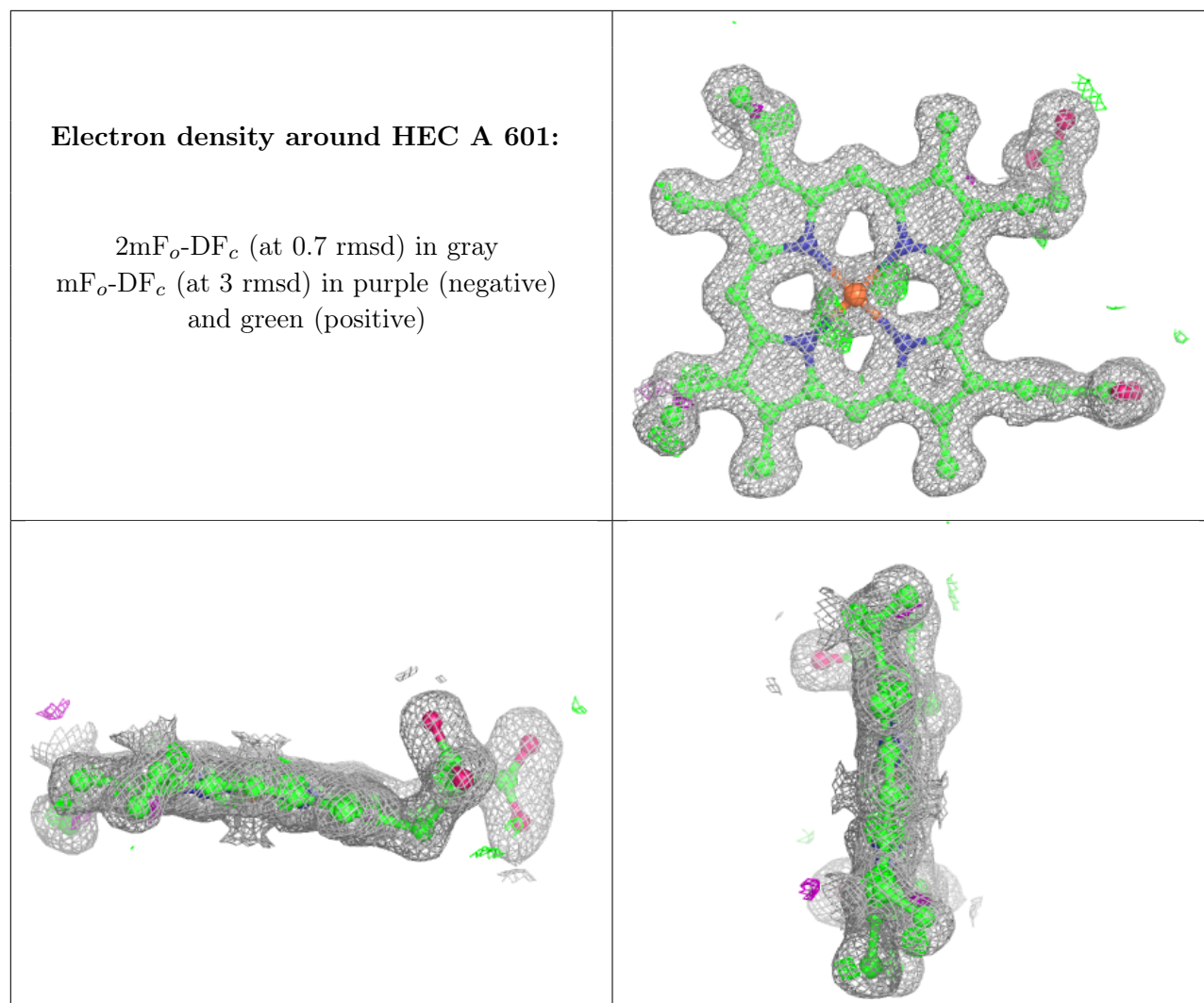


**Electron density around DHE B 602:**

$2mF_o-DF_c$  (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.