



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 7, 2020 – 12:28 PM EDT

PDB ID : 6WYD  
Title : CRYSTAL STRUCTURE OF MYELOPEROXIDASE SUBFORM C (MPO)  
COMPLEX WITH Compound-12 (AKA; 7-benzyl-1H-[1,2,3]triazolo[4,5-b]py  
rid  
Authors : Khan, J.A.  
Deposited on : 2020-05-12  
Resolution : 2.55 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](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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
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) : 2.14.6

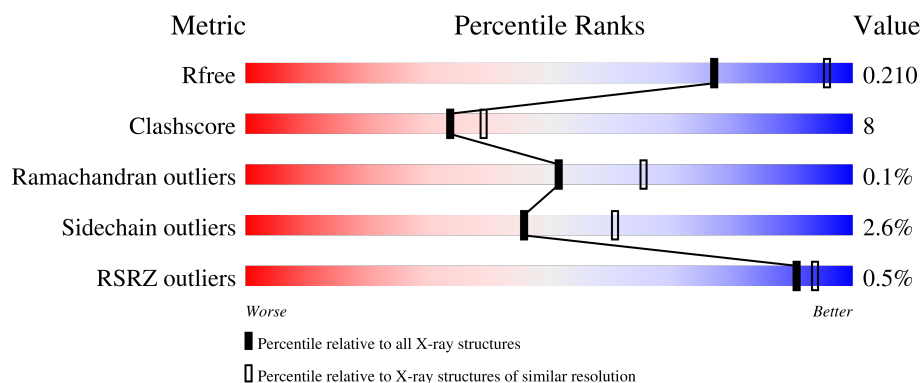
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 Å.

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



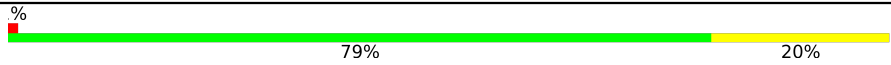


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 on 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	105	<div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	D	105	<div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	F	105	<div> <div>81%</div> <div>16%</div> <div>..</div> </div>
1	H	105	<div> <div>90%</div> <div>8%</div> <div>.</div> </div>
2	B	467	<div> <div>87%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	467	
2	G	467	
2	I	467	

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
4	NAG	B	604	-	-	X	-
4	NAG	E	608	-	-	X	-
4	NAG	G	603	-	-	X	-
4	NAG	I	608	-	-	X	-

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 18734 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 Myeloperoxidase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	0	0
			822	521	146	150	5			
1	D	103	Total	C	N	O	S	3	0	0
			820	519	145	151	5			
1	F	103	Total	C	N	O	S	3	0	0
			820	519	145	151	5			
1	H	103	Total	C	N	O	S	3	0	0
			813	516	144	148	5			

- Molecule 2 is a protein called Myeloperoxidase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	465	Total	C	N	O	S	16	0	0
			3630	2304	650	649	27			
2	E	465	Total	C	N	O	S	21	0	0
			3603	2286	643	648	26			
2	G	465	Total	C	N	O	S	32	0	0
			3639	2303	653	656	27			
2	I	465	Total	C	N	O	S	37	0	0
			3637	2306	649	655	27			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Cl	0	0
			1	1		
3	E	2	Total	Cl	0	0
			2	2		
3	H	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



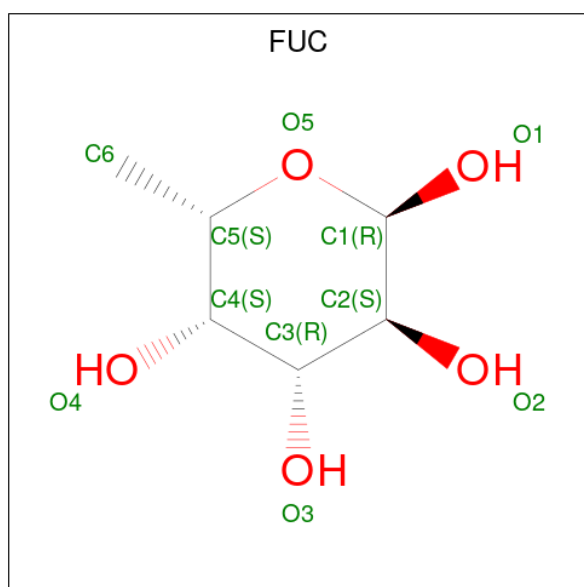
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		

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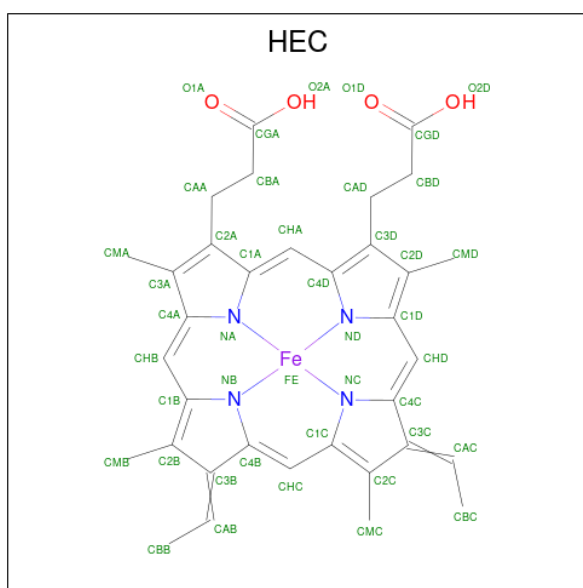
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is alpha-L-fucopyranose (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



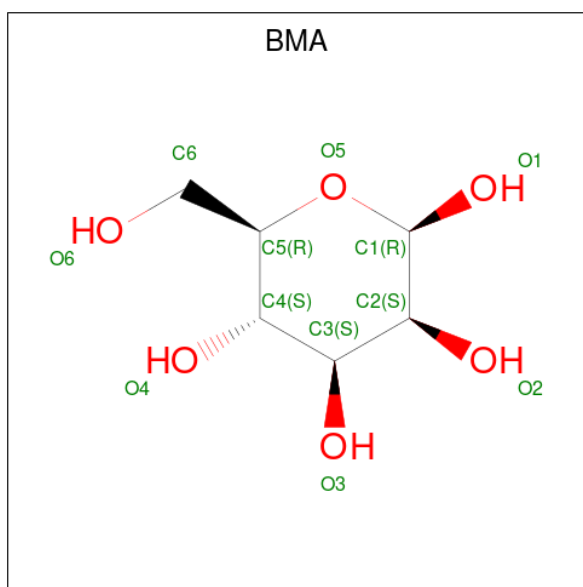
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		
5	E	1	Total	C	O	0	0
			10	6	4		
5	G	1	Total	C	O	0	0
			10	6	4		
5	I	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



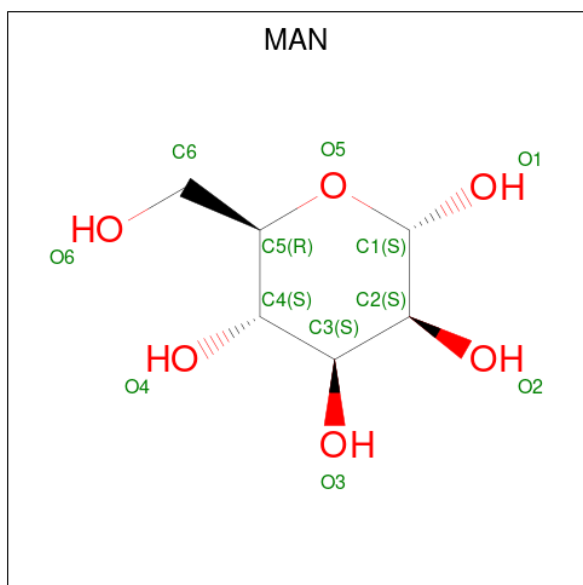
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 7 is beta-D-mannopyranose (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	I	1	Total	C	O	0	0
			11	6	5		

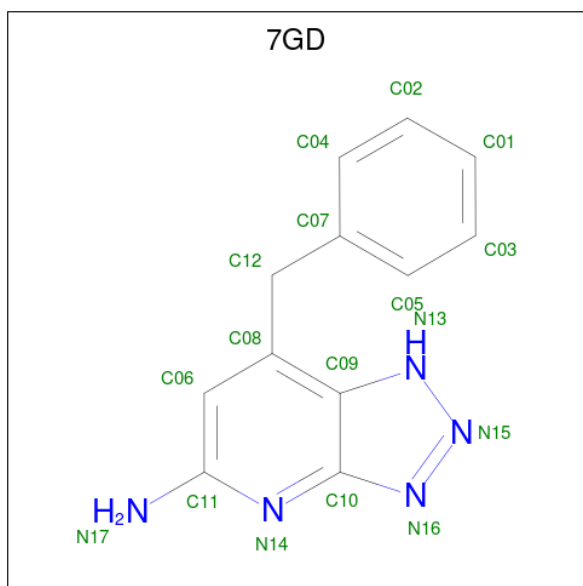
- Molecule 8 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			11	6	5		
8	B	1	Total	C	O	0	0
			11	6	5		
8	E	1	Total	C	O	0	0
			11	6	5		
8	E	1	Total	C	O	0	0
			11	6	5		
8	G	1	Total	C	O	0	0
			11	6	5		
8	G	1	Total	C	O	0	0
			11	6	5		
8	I	1	Total	C	O	0	0
			11	6	5		
8	I	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 is 7-benzyl-1H-[1,2,3]triazolo[4,5-b]pyridin-5-amine (three-letter code: 7GD) (formula: C<sub>12</sub>H<sub>11</sub>N<sub>5</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	N	0	0
			17	12	5		
9	E	1	Total	C	N	0	0
			17	12	5		
9	G	1	Total	C	N	0	0
			17	12	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	H	1	Total	C	N	0	0
			17	12	5		

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	G	1	Total	Ca	0	0
			1	1		
10	B	1	Total	Ca	0	0
			1	1		
10	I	1	Total	Ca	0	0
			1	1		
10	E	1	Total	Ca	0	0
			1	1		


- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	20	Total	O	0	0
			20	20		
11	B	66	Total	O	0	0
			66	66		
11	D	10	Total	O	0	0
			10	10		
11	E	42	Total	O	0	0
			42	42		
11	F	18	Total	O	0	0
			18	18		
11	G	43	Total	O	0	0
			43	43		
11	H	16	Total	O	0	0
			16	16		
11	I	45	Total	O	0	0
			45	45		

### 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: Myeloperoxidase light chain

Chain A:  82% 15% ..




- Molecule 1: Myeloperoxidase light chain

Chain D:  82% 16% .



- Molecule 1: Myeloperoxidase light chain

Chain F:  81% 16% ..



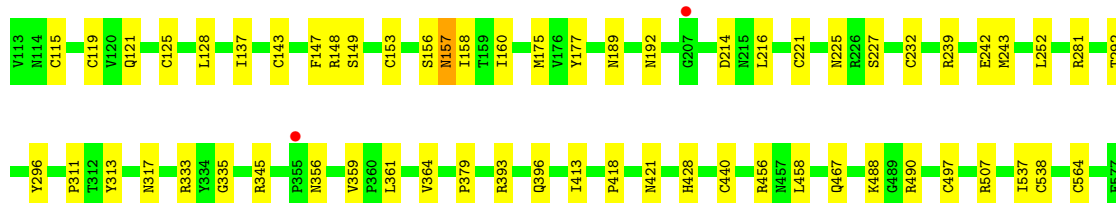
- Molecule 1: Myeloperoxidase light chain

Chain H:  90% 8% .



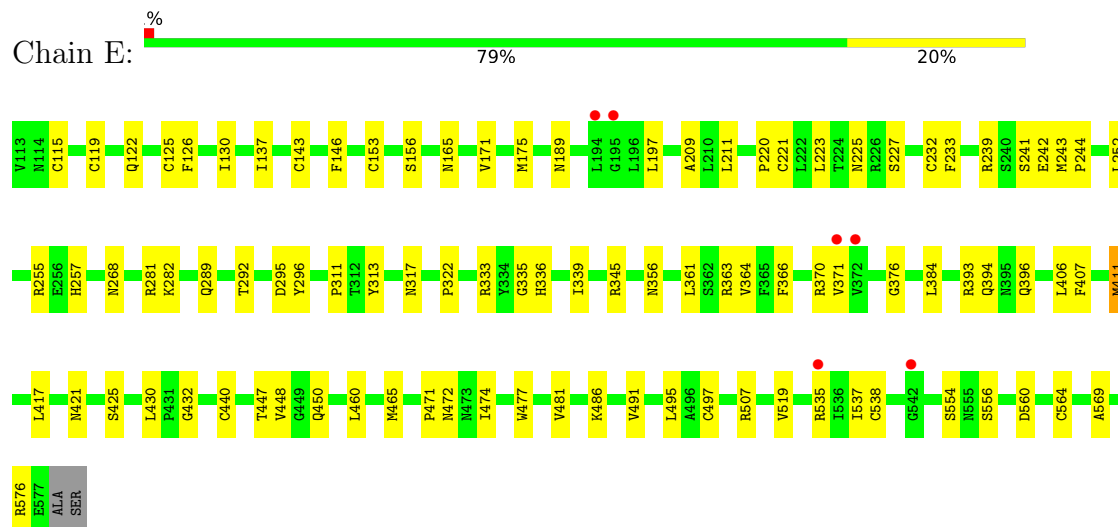
- Molecule 2: Myeloperoxidase heavy chain

Chain B:  87% 13%

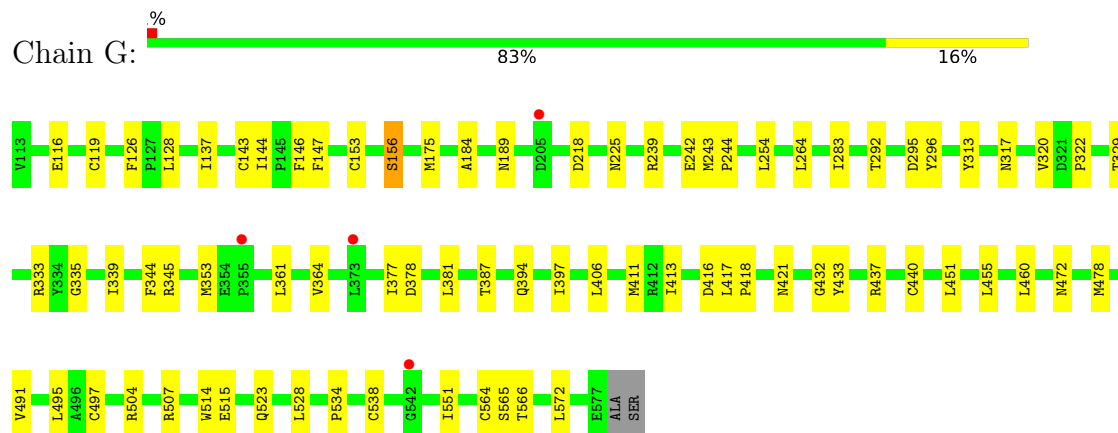


ALA  
SER

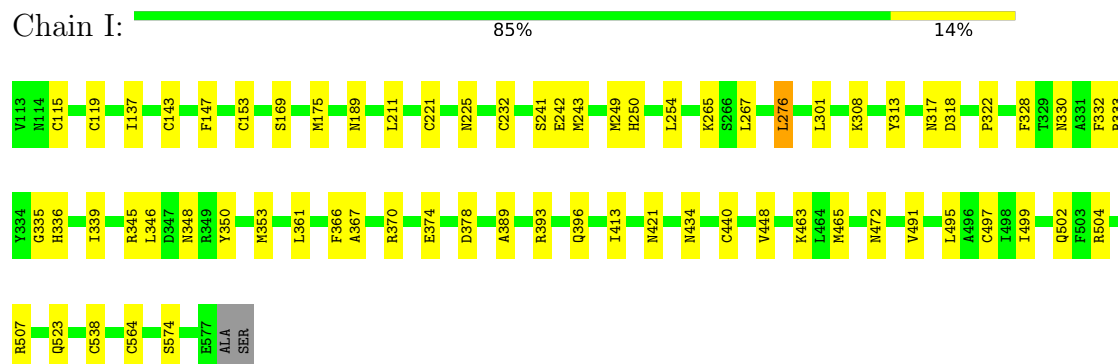
- Molecule 2: Myeloperoxidase heavy chain



- Molecule 2: Myeloperoxidase heavy chain



- Molecule 2: Myeloperoxidase heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.68Å 150.65Å 231.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.53 – 2.55 115.53 – 2.41	Depositor EDS
% Data completeness (in resolution range)	100.0 (115.53-2.55) 98.1 (115.53-2.41)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.42Å)	Xtriage
Refinement program	BUSTER 2.9.6	Depositor
R, $R_{free}$	0.194 , 0.254 0.206 , 0.210	Depositor DCC
$R_{free}$ test set	4654 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.0	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18734	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: 7GD, BMA, NAG, CL, CA, FUC, HEC, MAN

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	0.49	0/847	0.72	0/1155
1	D	0.50	0/845	0.74	0/1153
1	F	0.48	0/845	0.72	0/1153
1	H	0.47	0/838	0.73	0/1144
2	B	0.50	0/3715	0.70	0/5054
2	E	0.51	0/3688	0.70	0/5022
2	G	0.49	0/3725	0.68	0/5069
2	I	0.49	0/3722	0.68	0/5064
All	All	0.49	0/18225	0.70	0/24814

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	822	0	780	17	0
1	D	820	0	774	14	0
1	F	820	0	774	13	0
1	H	813	0	766	8	0
2	B	3630	0	3570	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3603	0	3515	68	0
2	G	3639	0	3571	53	0
2	I	3637	0	3579	52	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
4	B	70	0	65	16	0
4	E	70	0	65	16	0
4	G	56	0	52	17	0
4	I	70	0	65	15	0
5	B	10	0	10	1	0
5	E	10	0	10	2	0
5	G	10	0	10	1	0
5	I	10	0	10	2	0
6	B	43	0	32	17	0
6	E	43	0	32	14	0
6	G	43	0	32	12	0
6	I	43	0	32	17	0
7	B	11	0	9	4	0
7	E	11	0	10	2	0
7	G	11	0	10	4	0
7	I	11	0	10	3	0
8	B	22	0	20	2	0
8	E	22	0	20	1	0
8	G	22	0	20	2	0
8	I	22	0	20	2	0
9	B	17	0	0	0	0
9	E	17	0	0	2	0
9	G	17	0	0	1	0
9	H	17	0	0	0	0
10	B	1	0	0	0	0
10	E	1	0	0	0	0
10	G	1	0	0	0	0
10	I	1	0	0	0	0
11	A	20	0	0	0	0
11	B	66	0	0	0	0
11	D	10	0	0	0	0
11	E	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	F	18	0	0	0	0
11	G	43	0	0	0	0
11	H	16	0	0	0	0
11	I	45	0	0	0	0
All	All	18734	0	17863	288	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 8.

The worst 5 of 288 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:F:94:ASP:OD2	6:G:605:HEC:HMD3	1.25	1.37
2:I:242:GLU:OE2	6:I:610:HEC:HMB3	1.22	1.32
1:H:94:ASP:OD2	6:I:610:HEC:HMD3	1.31	1.30
2:G:242:GLU:OE2	6:G:605:HEC:HMB3	1.25	1.26
1:A:94:ASP:OD2	6:B:606:HEC:HMD3	1.31	1.25

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	101/105 (96%)	97 (96%)	4 (4%)	0	100	100
1	D	101/105 (96%)	96 (95%)	5 (5%)	0	100	100
1	F	101/105 (96%)	97 (96%)	4 (4%)	0	100	100
1	H	101/105 (96%)	100 (99%)	1 (1%)	0	100	100
2	B	463/467 (99%)	442 (96%)	20 (4%)	1 (0%)	47	60
2	E	463/467 (99%)	442 (96%)	21 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	463/467 (99%)	437 (94%)	26 (6%)	0	100	100
2	I	463/467 (99%)	442 (96%)	20 (4%)	1 (0%)	47	60
All	All	2256/2288 (99%)	2153 (95%)	101 (4%)	2 (0%)	51	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	348	ASN
2	B	158	ILE

### 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	87/90 (97%)	86 (99%)	1 (1%)	73	83
1	D	87/90 (97%)	85 (98%)	2 (2%)	50	65
1	F	87/90 (97%)	86 (99%)	1 (1%)	73	83
1	H	85/90 (94%)	84 (99%)	1 (1%)	71	81
2	B	385/412 (93%)	377 (98%)	8 (2%)	53	68
2	E	380/412 (92%)	366 (96%)	14 (4%)	34	46
2	G	390/412 (95%)	376 (96%)	14 (4%)	35	47
2	I	390/412 (95%)	381 (98%)	9 (2%)	50	65
All	All	1891/2008 (94%)	1841 (97%)	50 (3%)	46	61

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	486	LYS
2	G	156	SER
2	I	318	ASP
2	E	556	SER
1	F	19	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	421	ASN
2	B	467	GLN
2	G	121	GLN
2	B	317	ASN
2	E	450	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 12 are monoatomic - leaving 43 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	$\# Z  > 2$
9	7GD	H	201	-	17,19,19	4.73	13 (76%)	17,26,26	1.07	1 (5%)
4	NAG	B	601	-	14,14,15	1.88	5 (35%)	17,19,21	2.31	5 (29%)
8	MAN	I	603	-	11,11,12	1.23	1 (9%)	15,15,17	2.28	5 (33%)
5	FUC	B	605	-	10,10,11	1.48	3 (30%)	14,14,16	2.55	6 (42%)
6	HEC	I	610	2	26,50,50	2.08	3 (11%)	18,82,82	2.58	6 (33%)
5	FUC	I	609	-	10,10,11	1.34	0	14,14,16	2.69	7 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	FUC	G	604	-	10,10,11	1.20	1 (10%)	14,14,16	2.37	7 (50%)
4	NAG	G	606	-	14,14,15	1.23	2 (14%)	17,19,21	2.12	5 (29%)
7	BMA	E	602	-	11,11,12	1.57	3 (27%)	15,15,17	3.11	10 (66%)
5	FUC	E	609	-	10,10,11	1.11	0	14,14,16	1.98	5 (35%)
8	MAN	G	608	-	11,11,12	1.12	0	15,15,17	2.10	5 (33%)
6	HEC	G	605	2	26,50,50	2.23	5 (19%)	18,82,82	1.83	6 (33%)
4	NAG	I	601	-	14,14,15	1.20	1 (7%)	17,19,21	1.94	4 (23%)
8	MAN	G	609	-	11,11,12	1.55	3 (27%)	15,15,17	2.51	6 (40%)
4	NAG	E	608	-	14,14,15	0.98	0	17,19,21	3.86	5 (29%)
9	7GD	E	611	-	17,19,19	4.88	13 (76%)	17,26,26	1.14	1 (5%)
4	NAG	E	606	-	14,14,15	1.08	1 (7%)	17,19,21	2.72	9 (52%)
4	NAG	E	605	-	14,14,15	1.63	3 (21%)	17,19,21	2.33	6 (35%)
4	NAG	B	604	-	14,14,15	1.04	1 (7%)	17,19,21	3.64	9 (52%)
4	NAG	I	606	-	14,14,15	1.36	2 (14%)	17,19,21	2.61	8 (47%)
9	7GD	B	611	-	17,19,19	4.74	13 (76%)	17,26,26	0.84	1 (5%)
8	MAN	E	604	-	11,11,12	1.29	1 (9%)	15,15,17	2.20	5 (33%)
4	NAG	E	601	-	14,14,15	1.25	1 (7%)	17,19,21	2.59	7 (41%)
9	7GD	G	610	-	17,19,19	4.55	12 (70%)	17,26,26	0.99	2 (11%)
4	NAG	B	602	-	14,14,15	1.33	3 (21%)	17,19,21	3.27	8 (47%)
7	BMA	B	608	-	11,11,12	1.15	0	15,15,17	2.71	4 (26%)
4	NAG	I	605	-	14,14,15	1.37	2 (14%)	17,19,21	1.76	5 (29%)
7	BMA	G	607	-	11,11,12	1.17	2 (18%)	15,15,17	2.23	3 (20%)
4	NAG	G	602	-	14,14,15	1.39	4 (28%)	17,19,21	2.05	4 (23%)
4	NAG	G	603	-	14,14,15	1.41	2 (14%)	17,19,21	3.06	8 (47%)
4	NAG	B	603	-	14,14,15	1.27	1 (7%)	17,19,21	2.47	5 (29%)
7	BMA	I	602	-	11,11,12	0.99	0	15,15,17	3.36	4 (26%)
8	MAN	B	610	-	11,11,12	1.66	3 (27%)	15,15,17	2.66	5 (33%)
4	NAG	B	607	-	14,14,15	1.20	1 (7%)	17,19,21	2.32	9 (52%)
6	HEC	E	610	2	26,50,50	1.87	6 (23%)	18,82,82	2.19	7 (38%)
4	NAG	I	608	-	14,14,15	1.57	3 (21%)	17,19,21	3.26	6 (35%)
6	HEC	B	606	2	26,50,50	2.20	6 (23%)	18,82,82	2.13	7 (38%)
8	MAN	I	604	-	11,11,12	1.91	4 (36%)	15,15,17	3.16	4 (26%)
8	MAN	E	603	-	11,11,12	1.15	1 (9%)	15,15,17	2.18	6 (40%)
4	NAG	I	607	-	14,14,15	1.56	3 (21%)	17,19,21	1.93	6 (35%)
4	NAG	E	607	-	14,14,15	1.43	3 (21%)	17,19,21	1.93	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	MAN	B	609	-	11,11,12	1.40	2 (18%)	15,15,17	1.99	3 (20%)
4	NAG	G	601	-	14,14,15	1.47	1 (7%)	17,19,21	2.31	8 (47%)

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
9	7GD	H	201	-	-	0/4/4/4	0/3/3/3
8	MAN	E	604	-	-	1/2/19/22	1/1/1/1
8	MAN	I	603	-	-	2/2/19/22	0/1/1/1
5	FUC	B	605	-	-	-	0/1/1/1
6	HEC	I	610	2	-	0/6/54/54	-
8	MAN	E	603	-	-	0/2/19/22	0/1/1/1
5	FUC	G	604	-	-	-	0/1/1/1
4	NAG	G	606	-	-	0/6/23/26	0/1/1/1
7	BMA	E	602	-	-	2/2/19/22	0/1/1/1
5	FUC	E	609	-	-	-	0/1/1/1
8	MAN	G	608	-	-	1/2/19/22	0/1/1/1
6	HEC	G	605	2	-	0/6/54/54	-
4	NAG	E	605	-	-	1/6/23/26	0/1/1/1
8	MAN	G	609	-	-	2/2/19/22	0/1/1/1
4	NAG	E	608	-	-	0/6/23/26	0/1/1/1
9	7GD	E	611	-	-	0/4/4/4	0/3/3/3
4	NAG	E	606	-	-	1/6/23/26	0/1/1/1
9	7GD	B	611	-	-	0/4/4/4	0/3/3/3
4	NAG	B	604	-	-	2/6/23/26	0/1/1/1
4	NAG	I	606	-	-	1/6/23/26	0/1/1/1
4	NAG	I	601	-	-	2/6/23/26	0/1/1/1
4	NAG	B	601	-	-	0/6/23/26	0/1/1/1
4	NAG	E	601	-	-	0/6/23/26	0/1/1/1
9	7GD	G	610	-	-	1/4/4/4	0/3/3/3
4	NAG	B	602	-	-	1/6/23/26	0/1/1/1
7	BMA	B	608	-	-	0/2/19/22	0/1/1/1
4	NAG	I	605	-	-	0/6/23/26	0/1/1/1
7	BMA	G	607	-	-	2/2/19/22	0/1/1/1
4	NAG	G	602	-	-	0/6/23/26	0/1/1/1
4	NAG	G	603	-	-	2/6/23/26	0/1/1/1
4	NAG	B	603	-	-	1/6/23/26	0/1/1/1
7	BMA	I	602	-	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	B	610	-	-	0/2/19/22	0/1/1/1
4	NAG	B	607	-	-	2/6/23/26	0/1/1/1
6	HEC	E	610	2	-	0/6/54/54	-
4	NAG	I	608	-	-	2/6/23/26	0/1/1/1
6	HEC	B	606	2	-	0/6/54/54	-
8	MAN	I	604	-	-	1/2/19/22	0/1/1/1
5	FUC	I	609	-	-	-	0/1/1/1
4	NAG	I	607	-	-	2/6/23/26	0/1/1/1
4	NAG	E	607	-	-	2/6/23/26	0/1/1/1
8	MAN	B	609	-	-	2/2/19/22	0/1/1/1
4	NAG	G	601	-	-	1/6/23/26	0/1/1/1

The worst 5 of 134 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	611	7GD	C11-N14	10.14	1.45	1.33
9	H	201	7GD	C11-N14	9.62	1.44	1.33
9	B	611	7GD	C11-N14	9.48	1.44	1.33
9	G	610	7GD	C11-N14	8.79	1.43	1.33
9	E	611	7GD	C10-N14	7.96	1.52	1.36

The worst 5 of 239 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	608	NAG	C1-O5-C5	-11.15	97.08	112.19
4	I	608	NAG	C1-O5-C5	-10.28	98.27	112.19
4	B	602	NAG	C1-O5-C5	-9.81	98.91	112.19
4	B	604	NAG	C1-O5-C5	-9.67	99.09	112.19
7	I	602	BMA	C1-C2-C3	-9.17	98.39	109.67

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	607	BMA	C4-C5-C6-O6
7	E	602	BMA	O5-C5-C6-O6
8	B	609	MAN	O5-C5-C6-O6
4	G	603	NAG	O5-C5-C6-O6
4	G	603	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

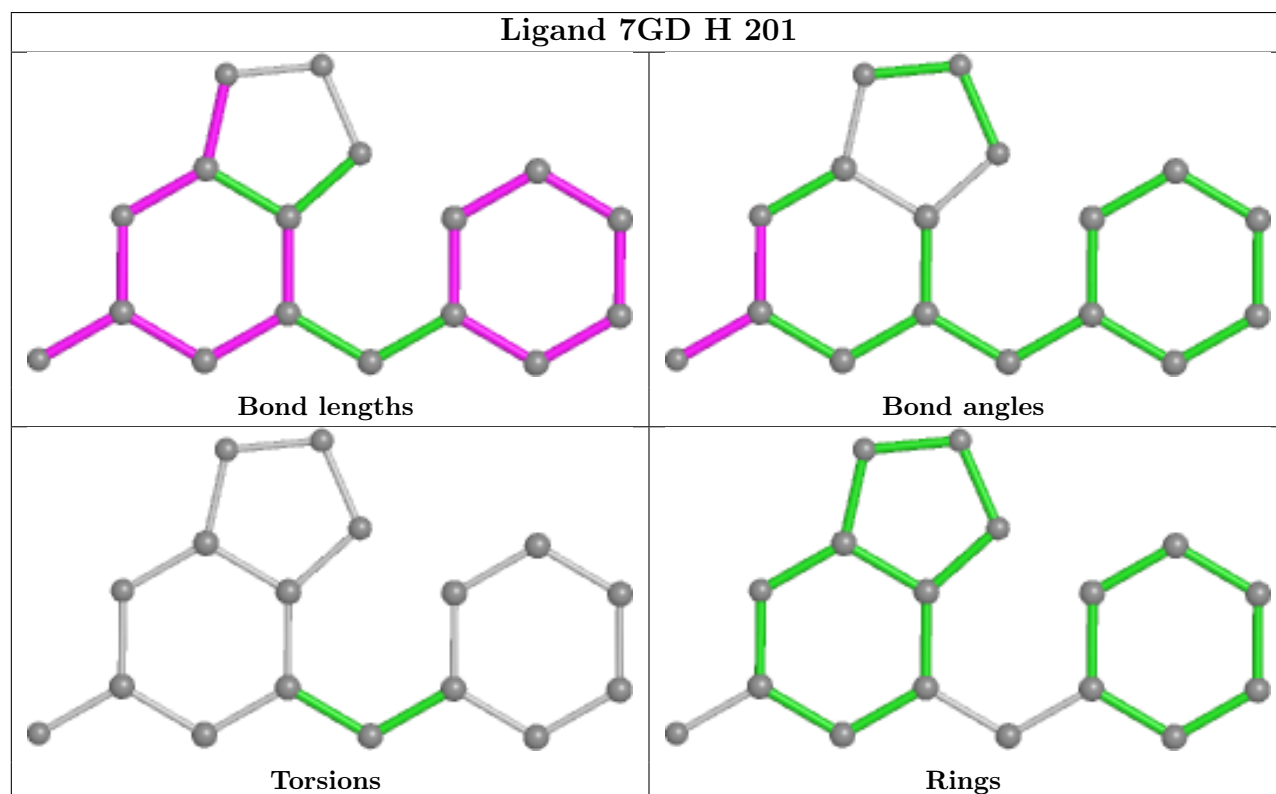
Mol	Chain	Res	Type	Atoms
8	E	604	MAN	C1-C2-C3-C4-C5-O5

35 monomers are involved in 124 short contacts:

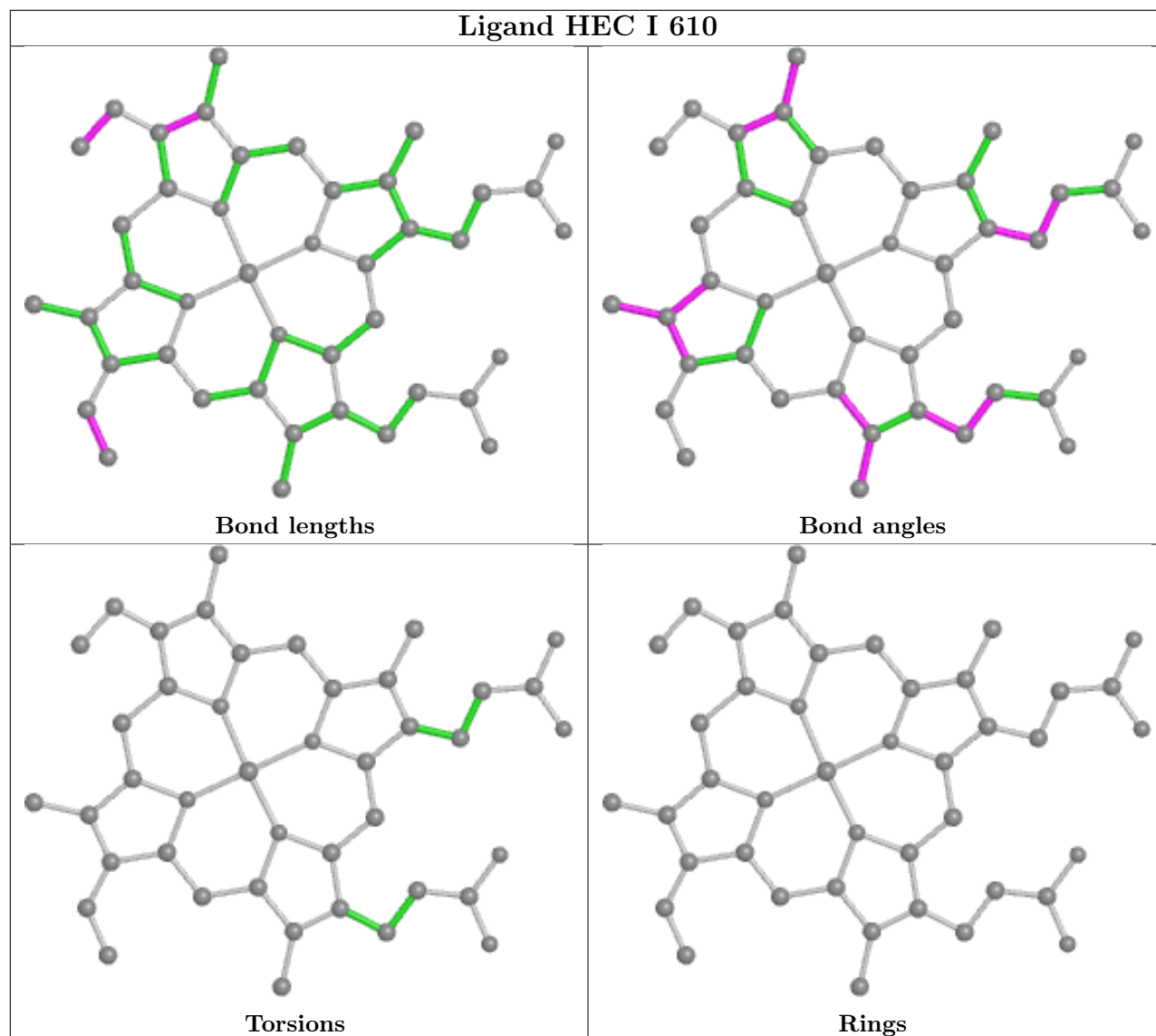
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	603	MAN	1	0
5	B	605	FUC	1	0
6	I	610	HEC	17	0
5	I	609	FUC	2	0
5	G	604	FUC	1	0
4	G	606	NAG	5	0
7	E	602	BMA	2	0
5	E	609	FUC	2	0
8	G	608	MAN	1	0
6	G	605	HEC	12	0
4	I	601	NAG	5	0
8	G	609	MAN	1	0
4	E	608	NAG	9	0
9	E	611	7GD	2	0
4	E	606	NAG	2	0
4	E	605	NAG	1	0
4	B	604	NAG	9	0
4	I	606	NAG	2	0
8	E	604	MAN	1	0
4	E	601	NAG	4	0
9	G	610	7GD	1	0
4	B	602	NAG	3	0
7	B	608	BMA	4	0
4	I	605	NAG	1	0
7	G	607	BMA	4	0
4	G	602	NAG	2	0
4	G	603	NAG	9	0
7	I	602	BMA	3	0
8	B	610	MAN	2	0
4	B	607	NAG	4	0
6	E	610	HEC	14	0
4	I	608	NAG	7	0
6	B	606	HEC	17	0
8	I	604	MAN	1	0
4	G	601	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

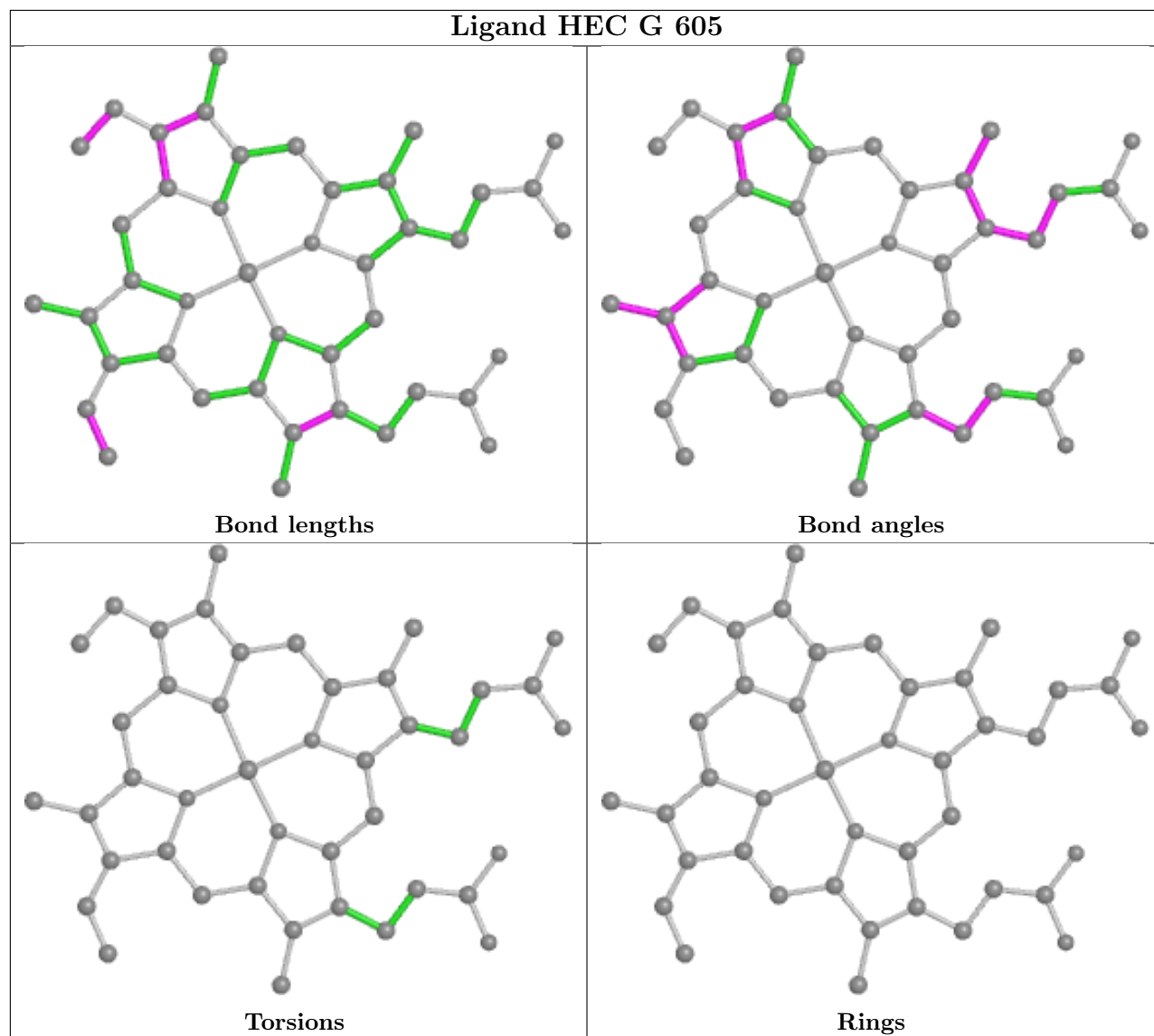
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



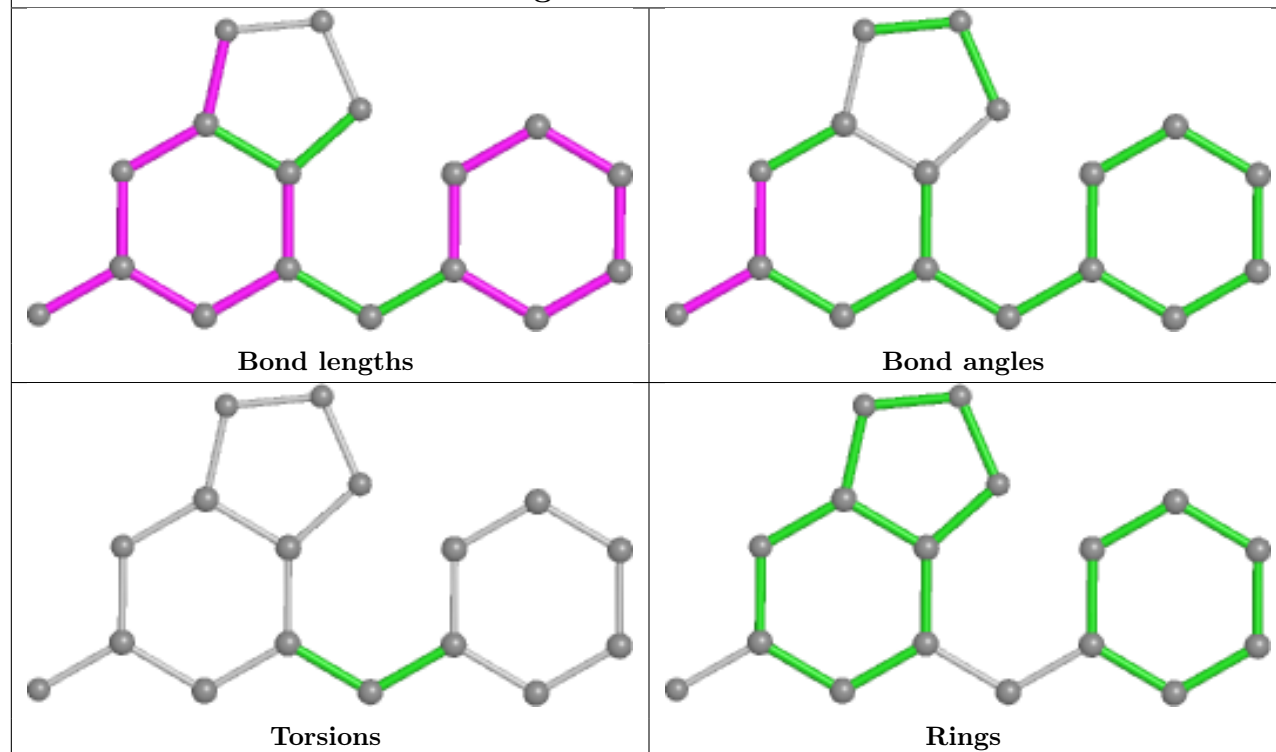
## Ligand HEC I 610



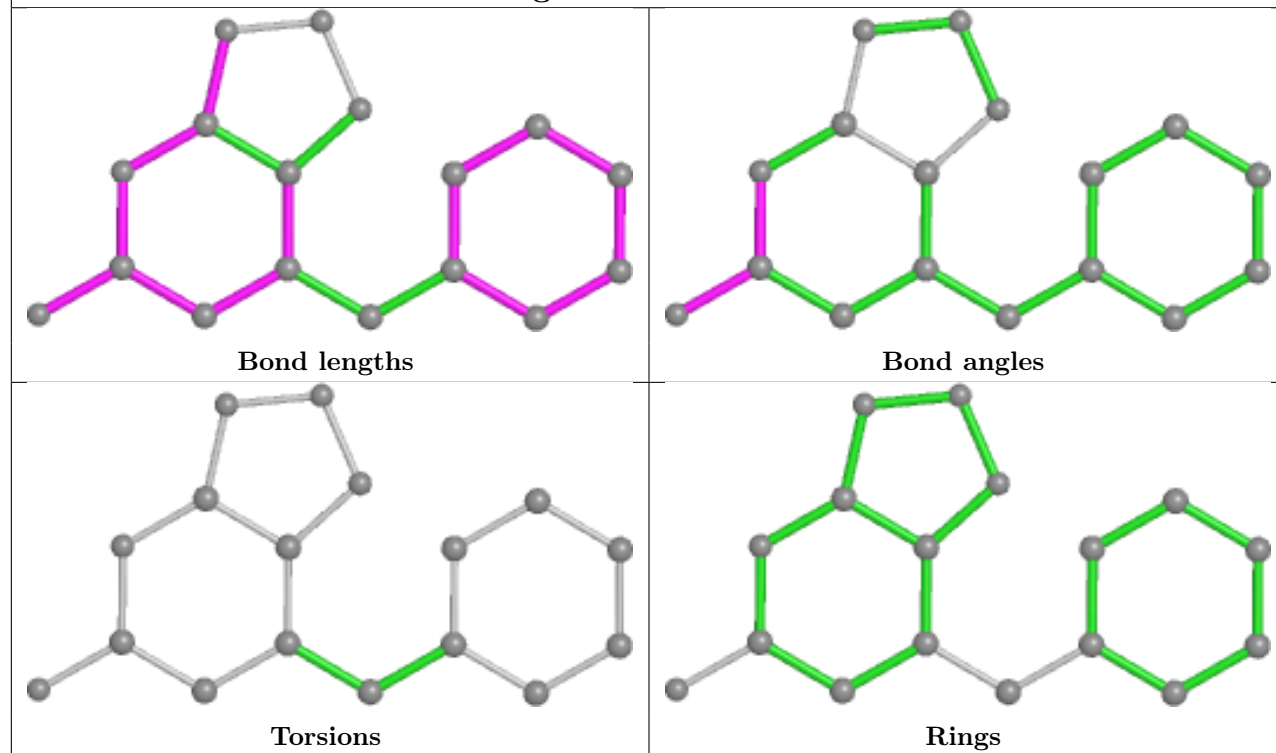


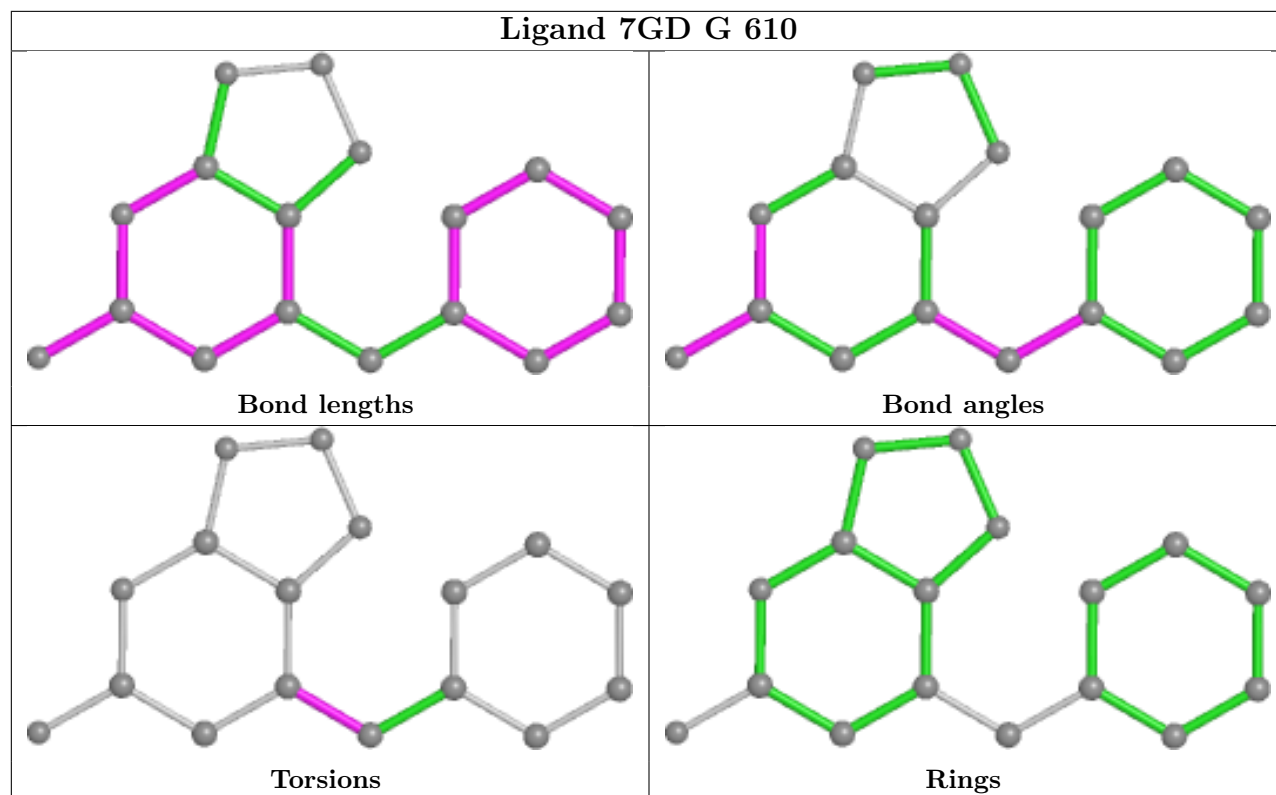


## Ligand 7GD E 611

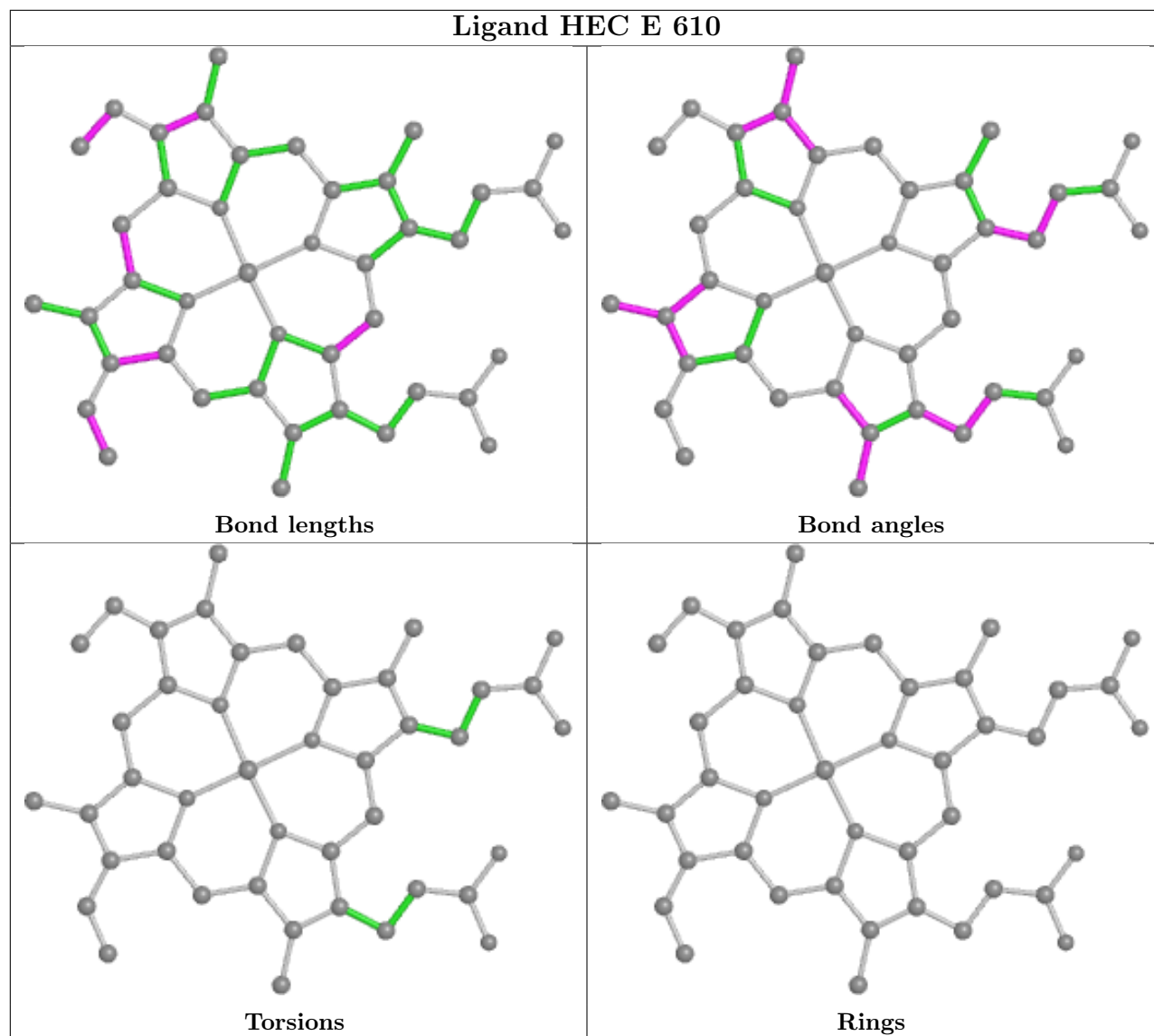


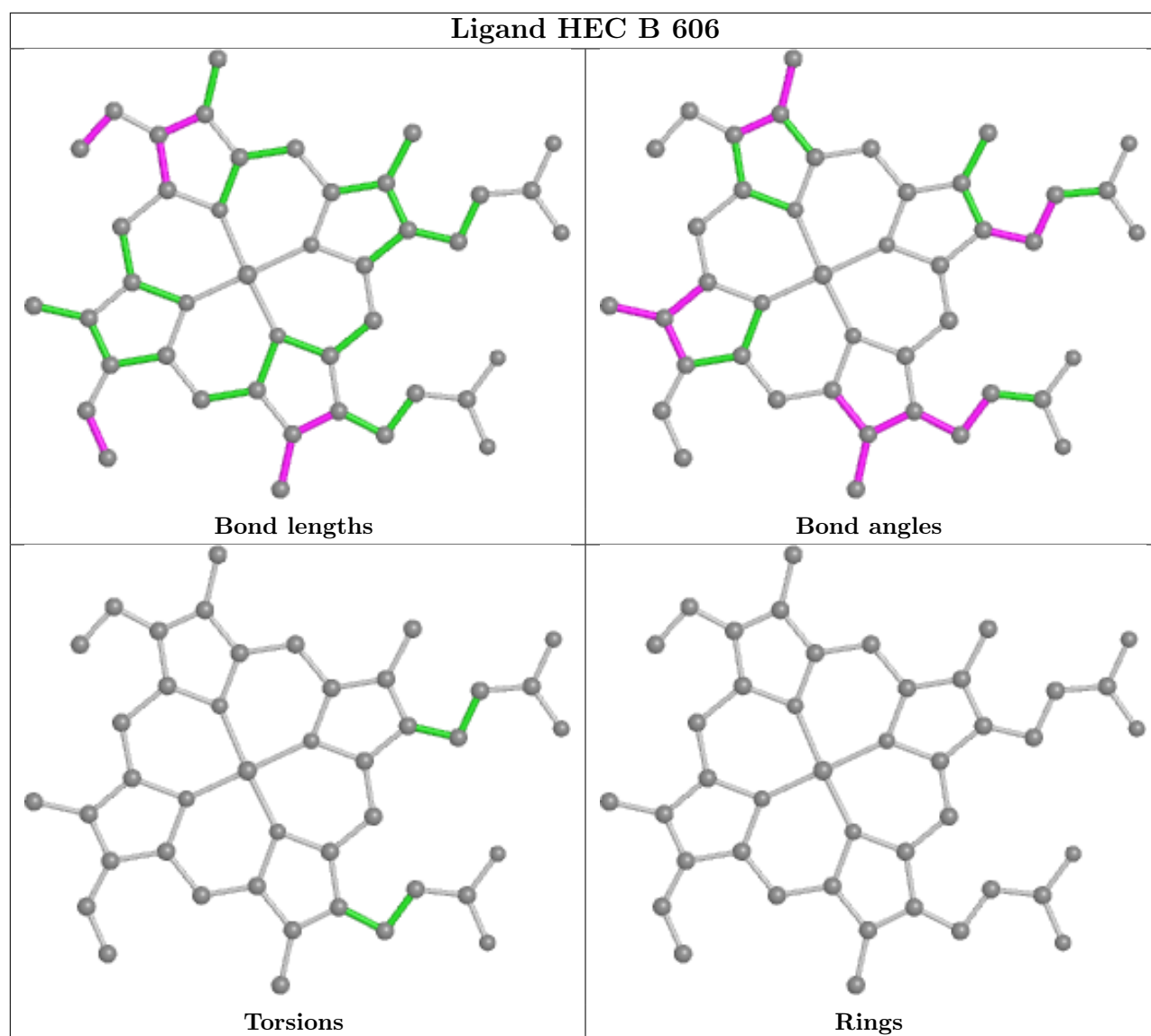
## Ligand 7GD B 611





## Ligand HEC E 610





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	103/105 (98%)	-0.10	0 100 100	28, 43, 62, 84	0
1	D	103/105 (98%)	0.01	0 100 100	28, 46, 65, 88	1 (0%)
1	F	103/105 (98%)	0.00	0 100 100	28, 44, 66, 77	1 (0%)
1	H	103/105 (98%)	-0.05	0 100 100	32, 47, 70, 83	1 (0%)
2	B	465/467 (99%)	-0.11	2 (0%) 92 96	27, 45, 68, 92	6 (1%)
2	E	465/467 (99%)	0.09	6 (1%) 77 82	27, 53, 80, 102	7 (1%)
2	G	465/467 (99%)	0.03	4 (0%) 84 88	26, 51, 73, 104	9 (1%)
2	I	465/467 (99%)	0.01	0 100 100	26, 51, 72, 82	12 (2%)
All	All	2272/2288 (99%)	-0.01	12 (0%) 91 94	26, 49, 73, 104	37 (1%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	355	PRO	3.1
2	E	371	VAL	3.0
2	G	373	LEU	2.9
2	E	195	GLY	2.9
2	B	207	GLY	2.9

### 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

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	NAG	B	603	14/15	0.66	0.28	106,110,113,113	0
4	NAG	I	607	14/15	0.72	0.22	82,85,88,88	0
4	NAG	G	602	14/15	0.74	0.26	101,105,107,107	0
4	NAG	E	607	14/15	0.79	0.22	96,99,102,102	0
4	NAG	G	601	14/15	0.82	0.18	70,74,77,77	0
4	NAG	E	605	14/15	0.83	0.18	63,67,69,69	0
4	NAG	I	605	14/15	0.84	0.21	78,81,84,84	0
4	NAG	B	601	14/15	0.85	0.16	55,58,60,61	0
7	BMA	G	607	11/12	0.87	0.20	49,52,53,54	0
8	MAN	E	603	11/12	0.87	0.15	77,79,82,83	0
4	NAG	E	606	14/15	0.87	0.21	91,95,98,98	0
8	MAN	I	603	11/12	0.87	0.21	75,77,79,81	0
8	MAN	B	609	11/12	0.88	0.24	79,81,84,85	0
3	CL	E	613	1/1	0.88	0.28	62,62,62,62	0
8	MAN	G	609	11/12	0.89	0.20	41,43,45,46	0
7	BMA	I	602	11/12	0.90	0.15	44,47,48,49	0
7	BMA	E	602	11/12	0.90	0.17	53,55,56,56	0
5	FUC	B	605	10/11	0.92	0.19	44,44,45,45	0
4	NAG	I	606	14/15	0.92	0.21	67,71,73,74	0
9	7GD	E	611	17/17	0.92	0.19	42,45,48,51	0
8	MAN	G	608	11/12	0.92	0.17	75,77,80,81	0
9	7GD	G	610	17/17	0.93	0.18	40,43,46,49	0
7	BMA	B	608	11/12	0.93	0.14	34,37,39,39	0
8	MAN	I	604	11/12	0.93	0.14	40,42,44,46	0
3	CL	I	612	1/1	0.93	0.28	57,57,57,57	0
8	MAN	E	604	11/12	0.93	0.17	48,50,52,53	0
4	NAG	B	604	14/15	0.93	0.13	37,41,43,44	0
4	NAG	G	603	14/15	0.93	0.14	42,46,48,49	0
4	NAG	B	602	14/15	0.94	0.16	67,71,73,74	0
4	NAG	I	601	14/15	0.94	0.17	32,36,38,40	0
5	FUC	I	609	10/11	0.94	0.15	39,40,41,41	0
5	FUC	G	604	10/11	0.94	0.14	50,50,51,52	0
9	7GD	H	201	17/17	0.94	0.19	42,44,47,48	0
4	NAG	I	608	14/15	0.94	0.16	38,42,44,45	0
4	NAG	E	601	14/15	0.95	0.14	31,34,37,38	0
4	NAG	E	608	14/15	0.95	0.16	37,41,43,45	0
9	7GD	B	611	17/17	0.95	0.18	36,40,44,46	0

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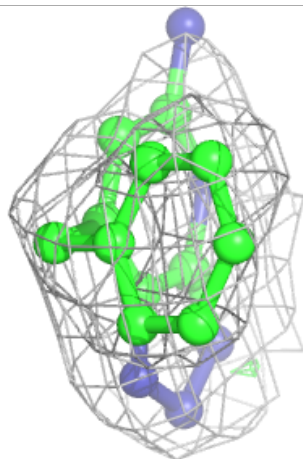
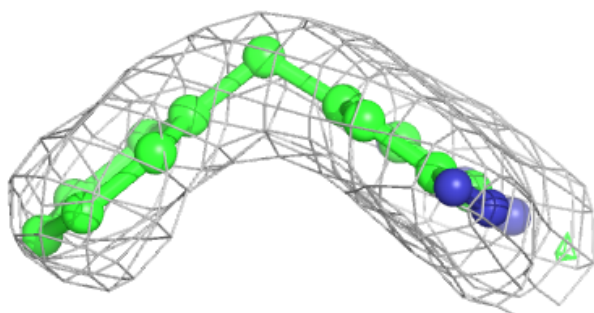
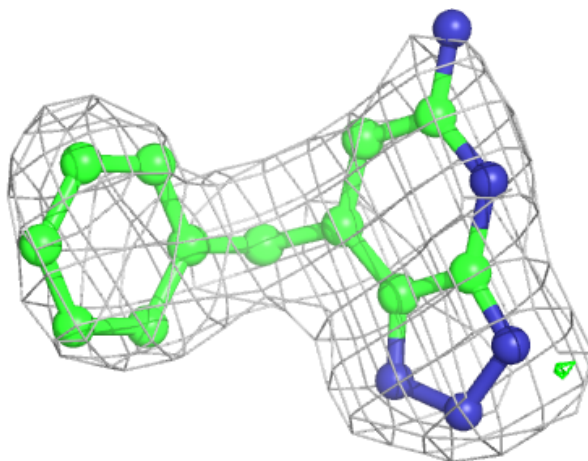
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	G	612	1/1	0.95	0.32	54,54,54,54	0
5	FUC	E	609	10/11	0.95	0.16	55,56,57,57	0
8	MAN	B	610	11/12	0.95	0.18	41,43,45,46	0
4	NAG	B	607	14/15	0.95	0.16	35,39,42,43	0
3	CL	B	613	1/1	0.96	0.30	51,51,51,51	0
6	HEC	E	610	43/43	0.96	0.16	39,40,44,51	0
6	HEC	G	605	43/43	0.96	0.16	40,41,43,48	0
6	HEC	B	606	43/43	0.96	0.16	38,39,43,47	0
6	HEC	I	610	43/43	0.96	0.17	44,45,49,58	0
4	NAG	G	606	14/15	0.97	0.14	29,32,35,36	0
10	CA	E	612	1/1	0.97	0.11	41,41,41,41	0
3	CL	E	614	1/1	0.97	0.12	37,37,37,37	0
3	CL	F	201	1/1	0.98	0.12	35,35,35,35	0
10	CA	G	611	1/1	0.98	0.07	39,39,39,39	0
3	CL	A	201	1/1	0.98	0.09	35,35,35,35	0
3	CL	H	202	1/1	0.99	0.12	36,36,36,36	0
10	CA	B	612	1/1	0.99	0.10	32,32,32,32	0
10	CA	I	611	1/1	0.99	0.14	39,39,39,39	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.



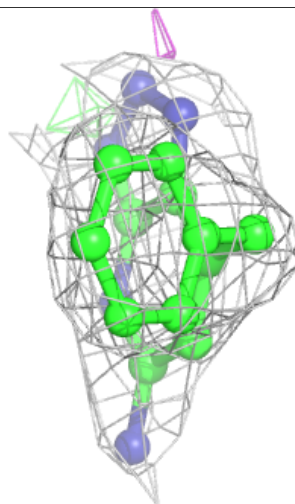
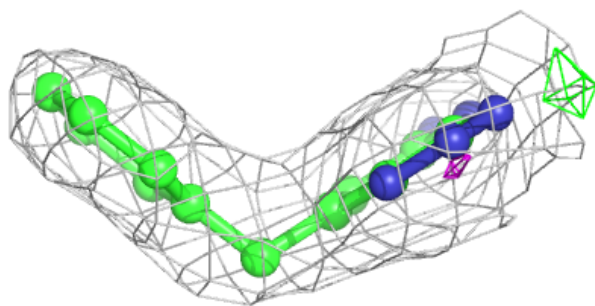
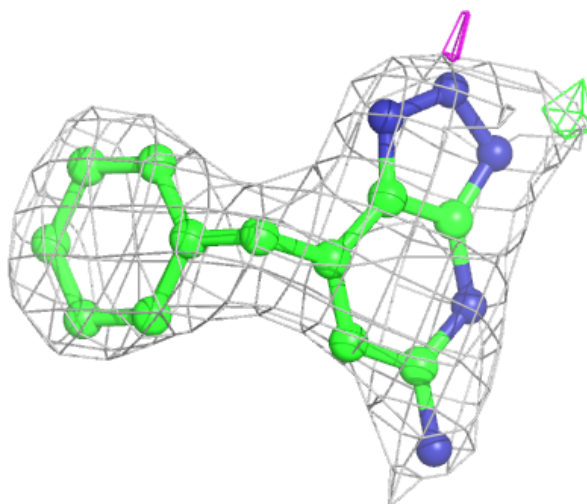
**Electron density around 7GD E 611:**

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



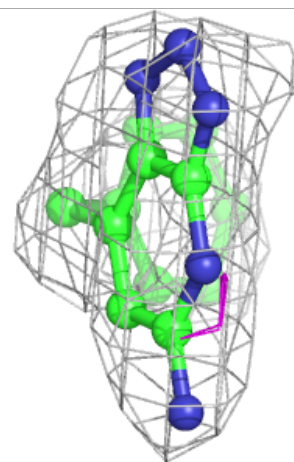
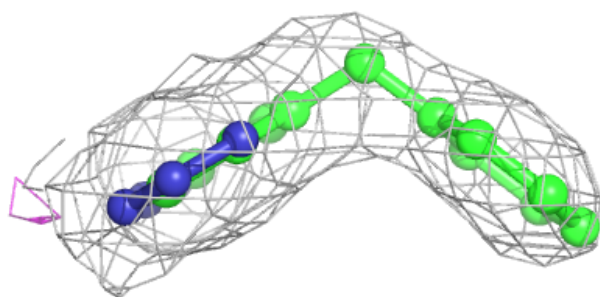
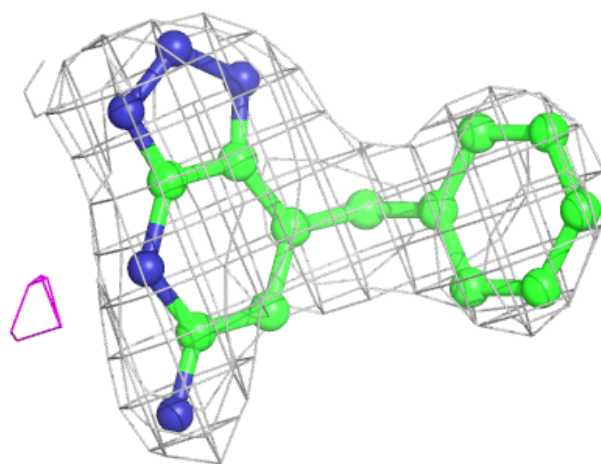
**Electron density around 7GD G 610:**

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



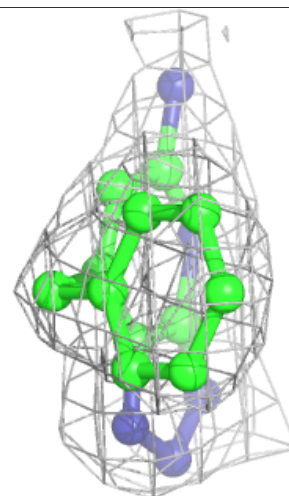
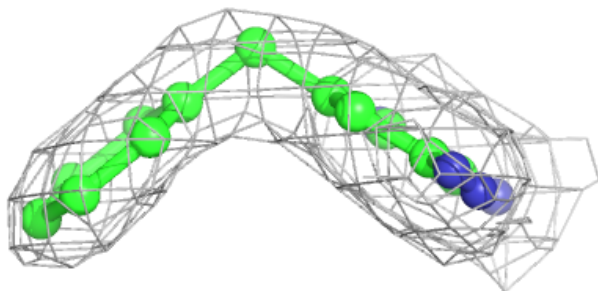
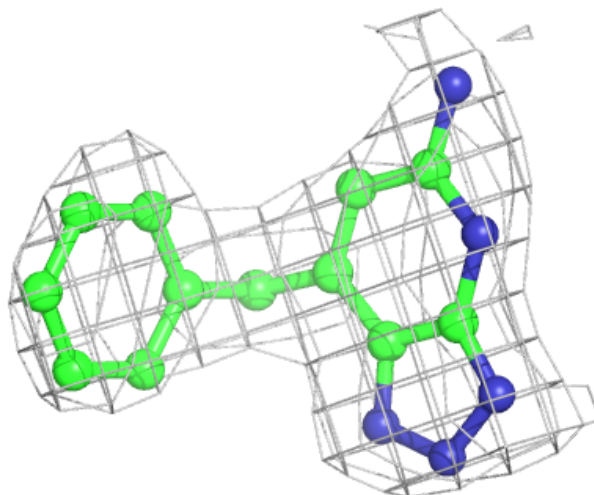
**Electron density around 7GD H 201:**

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



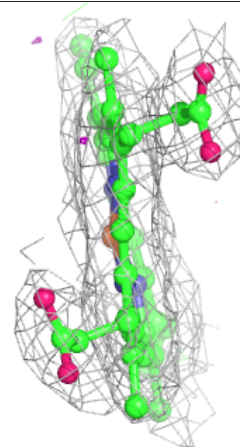
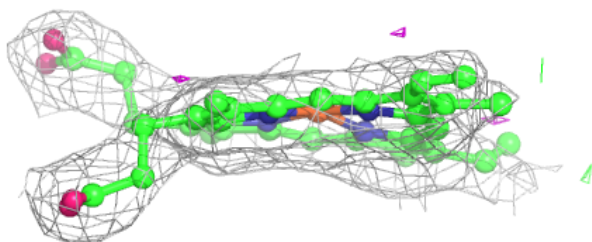
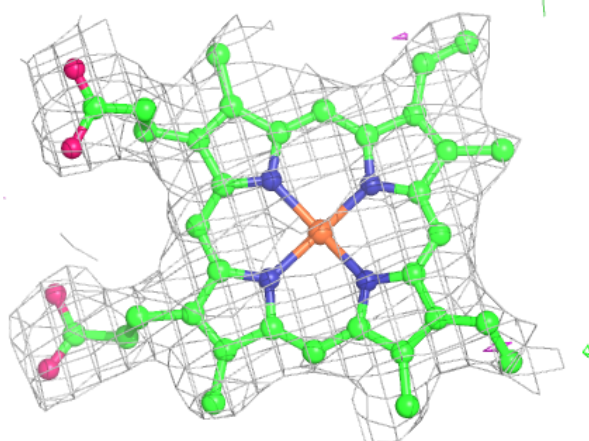
**Electron density around 7GD B 611:**

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



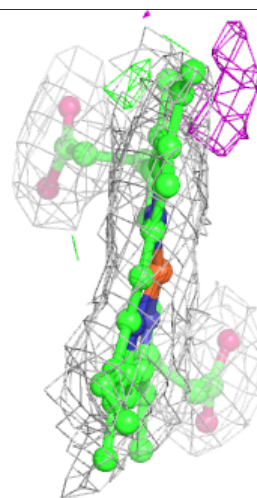
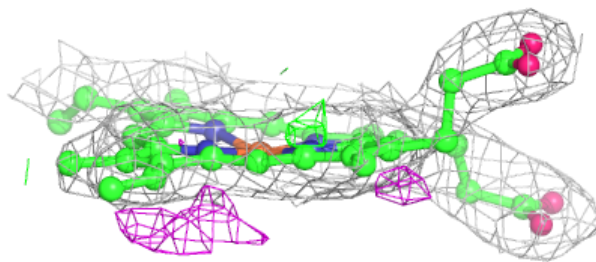
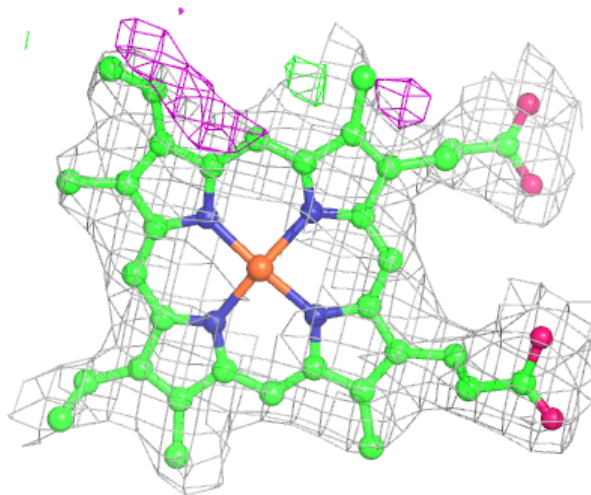
**Electron density around HEC E 610:**

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



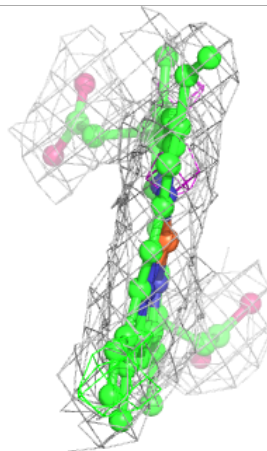
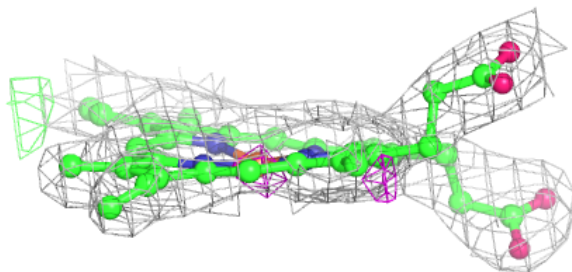
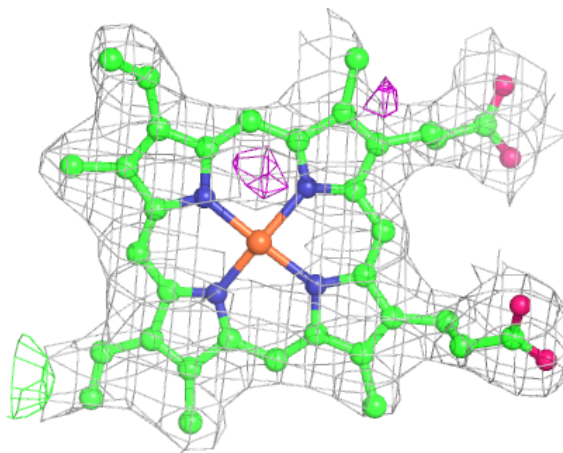
**Electron density around HEC G 605:**

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



**Electron density around HEC B 606:**

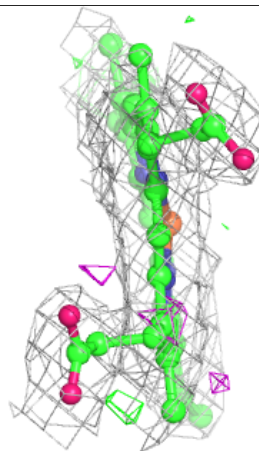
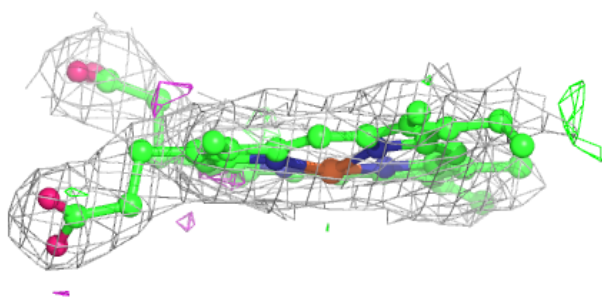
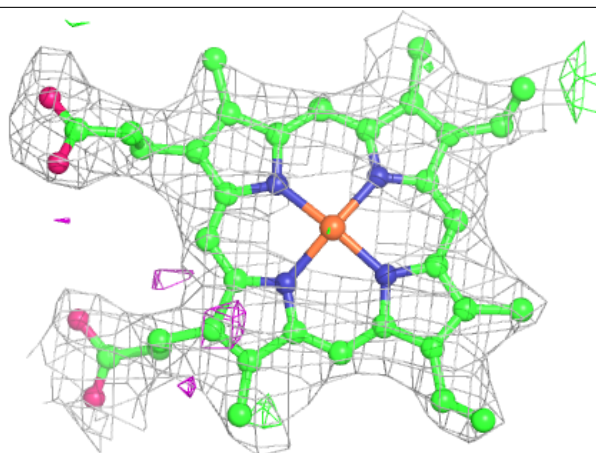
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC I 610:**

$2mF_o-DF_c$  (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.