



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 28, 2024 – 06:12 AM EDT

PDB ID : 5QJ2  
Title : CRYSTAL STRUCTURE OF MYELOPEROXIDASE SUBFORM C (MPO) COMPLEX WITH COMPOUND-20 AKA 7-((3-(1-METHYL-1H-PYRAZOL-3-YL)BENZYL)OXY)-1H-[1,2,3]TRIAZOLO[4,5-B]PYRIDIN-5-AMINE  
Authors : Khan, J.A.  
Deposited on : 2018-09-26  
Resolution : 2.82 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.

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

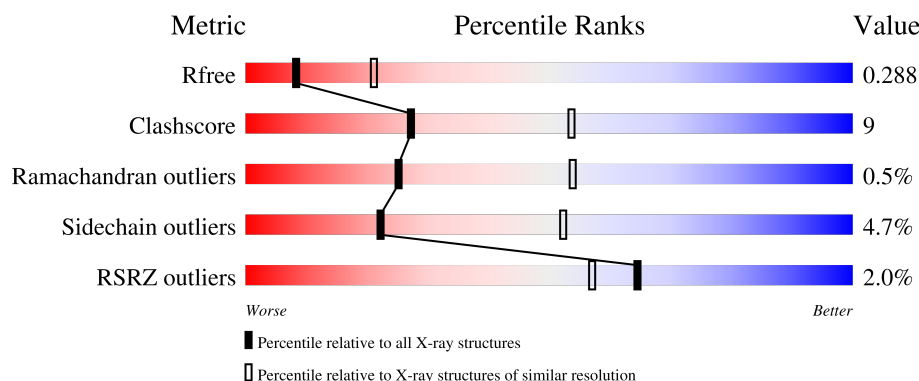
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.82 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))
$R_{free}$	164625	4293 (2.84-2.80)
Clashscore	180529	4801 (2.84-2.80)
Ramachandran outliers	177936	4739 (2.84-2.80)
Sidechain outliers	177891	4741 (2.84-2.80)
RSRZ outliers	164620	4295 (2.84-2.80)

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	105	
1	D	105	
1	F	105	
1	H	105	

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Mol	Chain	Length	Quality of chain
2	B	467	 3% 78% 21%
2	E	467	 2% 79% 20%
2	G	467	 % 81% 18% •
2	I	467	 3% 79% 19% •

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
6	BMA	G	609	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 18513 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	3	0	0
			812	515	144	148	5			
1	D	103	Total	C	N	O	S	4	0	0
			825	522	145	153	5			
1	F	103	Total	C	N	O	S	0	0	0
			813	516	144	148	5			
1	H	103	Total	C	N	O	S	3	0	0
			821	520	144	152	5			

- Molecule 2 is a protein called Myeloperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	465	Total	C	N	O	S	24	0	0
			3617	2289	648	653	27			
2	E	465	Total	C	N	O	S	19	0	0
			3619	2296	645	651	27			
2	G	465	Total	C	N	O	S	12	0	0
			3608	2290	642	650	26			
2	I	465	Total	C	N	O	S	28	0	0
			3605	2283	645	650	27			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	112	ALA	GLY	conflict	UNP P05164
E	112	ALA	GLY	conflict	UNP P05164
G	112	ALA	GLY	conflict	UNP P05164
I	112	ALA	GLY	conflict	UNP P05164

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



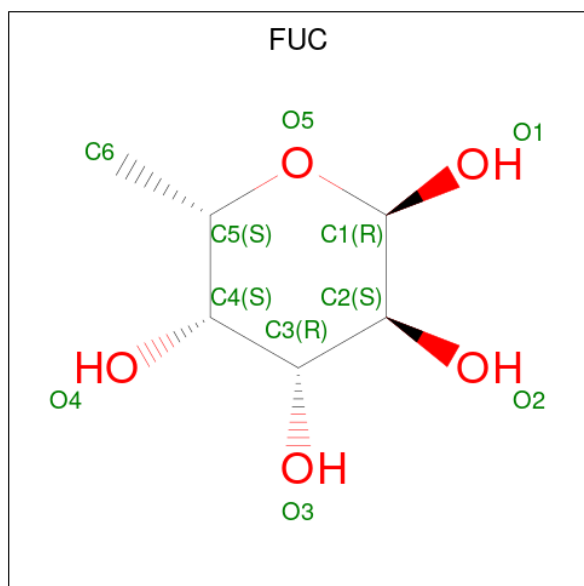
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1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

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

- Molecule 4 is alpha-L-fucopyranose (three-letter code: FUC) (formula:  $C_6H_{12}O_5$ ).



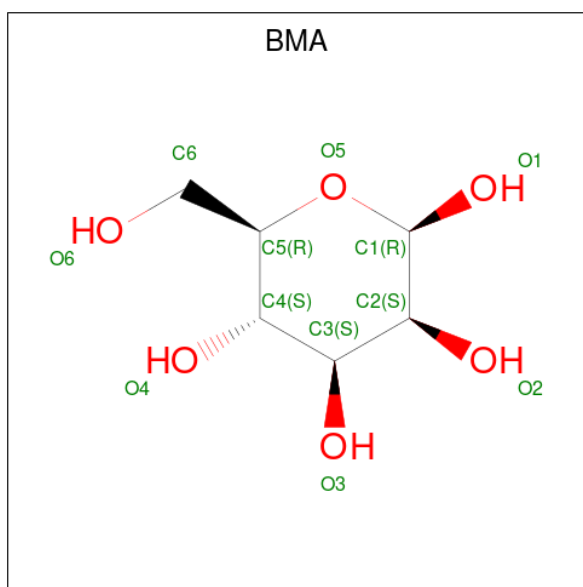
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	6	4		
4	E	1	Total	C	O	0	0
			10	6	4		
4	G	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	I	1	Total	C	O	0	0
			10	6	4		

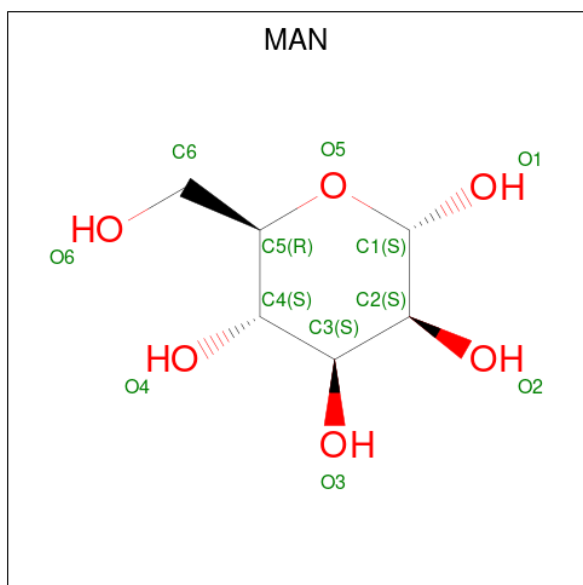
- # HEM

- Molecule 6 is beta-D-mannopyranose (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



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

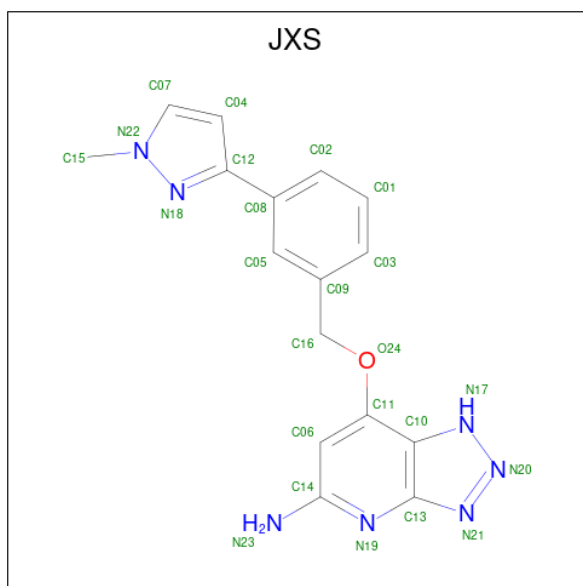
- Molecule 7 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).





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

- Molecule 8 is 7-{[3-(1-methyl-1H-pyrazol-3-yl)phenyl]methoxy}-1H-[1,2,3]triazolo[4,5-b]pyridin-5-amine (three-letter code: JXS) (formula: C<sub>16</sub>H<sub>15</sub>N<sub>7</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			24	16	7	1		
8	E	1	Total	C	N	O	0	0
			24	16	7	1		
8	G	1	Total	C	N	O	0	0
			24	16	7	1		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Cl 1 1	0	0
10	G	1	Total Cl 1 1	0	0


- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	2	Total O 2 2	0	0
11	B	11	Total O 11 11	0	0
11	D	2	Total O 2 2	0	0
11	E	10	Total O 10 10	0	0
11	F	4	Total O 4 4	0	0
11	G	21	Total O 21 21	0	0
11	H	4	Total O 4 4	0	0
11	I	9	Total O 9 9	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.

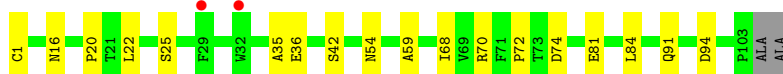
- Molecule 1: Myeloperoxidase

Chain A: 




- Molecule 1: Myeloperoxidase

Chain D: 




- Molecule 1: Myeloperoxidase

Chain F: 




- Molecule 1: Myeloperoxidase

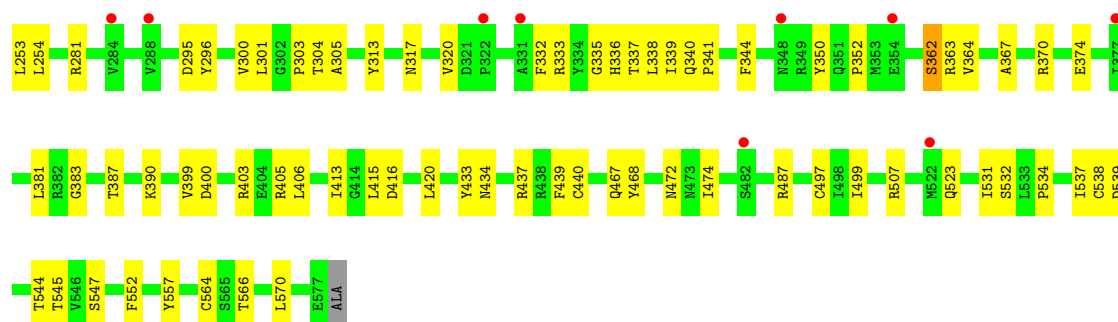
Chain H: 



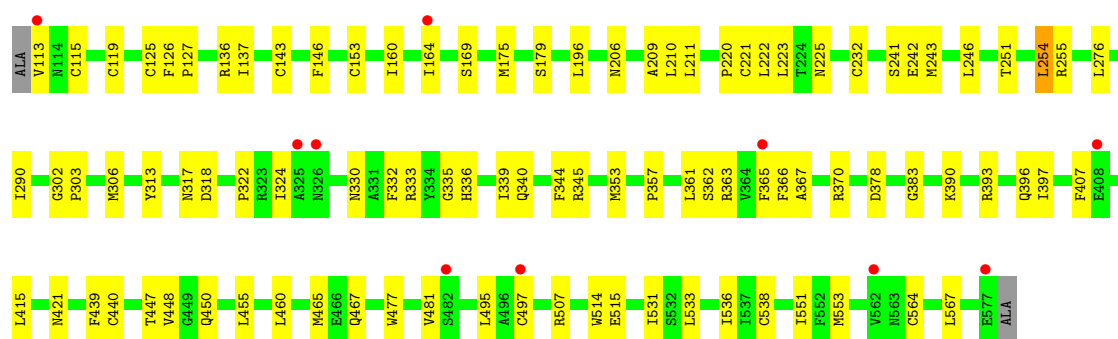
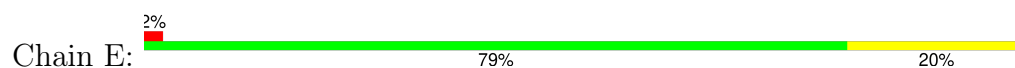
- Molecule 2: Myeloperoxidase

Chain B: 

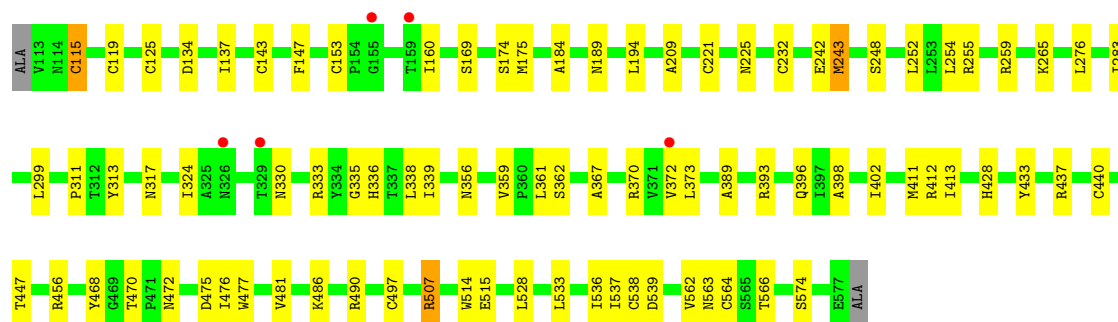
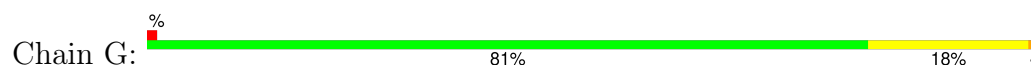




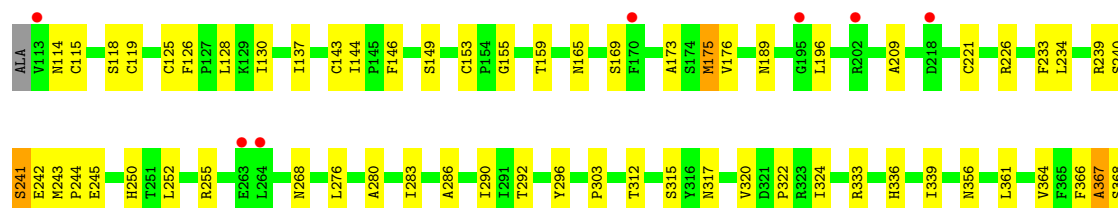
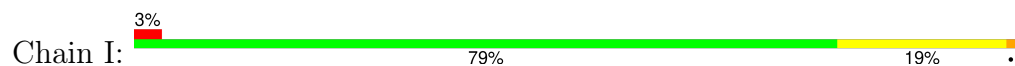
• Molecule 2: Myeloperoxidase

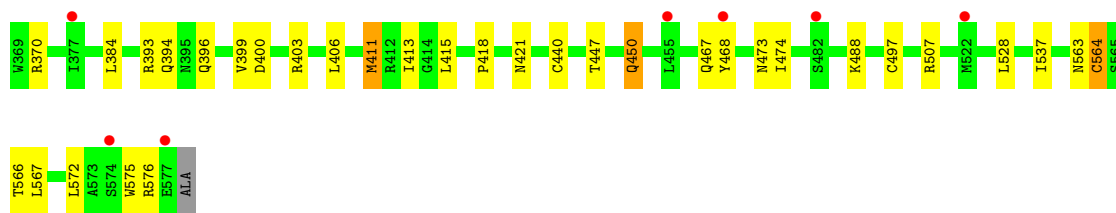


• Molecule 2: Myeloperoxidase



• Molecule 2: Myeloperoxidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.82Å 150.95Å 233.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	116.55 – 2.82 116.55 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.7 (116.55-2.82) 99.7 (116.55-2.82)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 2.82Å)	Xtriage
Refinement program	BUSTER 2.9.6	Depositor
R, $R_{free}$	0.206 , 0.272 0.218 , 0.288	Depositor DCC
$R_{free}$ test set	3100 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.1	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 71.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.056 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	18513	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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: CL, CA, MAN, NAG, HEM, JXS, FUC, BMA

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	0.47	0/837	0.75	0/1143
1	D	0.47	0/850	0.74	0/1159
1	F	0.49	0/838	0.75	0/1144
1	H	0.49	0/846	0.76	0/1154
2	B	0.50	0/3703	0.71	0/5043
2	E	0.49	0/3704	0.71	0/5043
2	G	0.52	0/3693	0.72	0/5030
2	I	0.50	0/3690	0.71	0/5026
All	All	0.50	0/18161	0.72	0/24742

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	812	0	764	20	0
1	D	825	0	780	13	0
1	F	813	0	766	11	0
1	H	821	0	774	13	0
2	B	3617	0	3529	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3619	0	3555	69	0
2	G	3608	0	3526	56	0
2	I	3605	0	3513	61	0
3	B	98	0	91	18	0
3	E	56	0	52	8	0
3	G	84	0	78	17	0
3	I	70	0	65	10	0
4	B	10	0	10	1	0
4	E	10	0	10	0	0
4	G	10	0	10	0	0
4	I	10	0	10	1	0
5	B	43	0	30	10	0
5	E	43	0	30	8	0
5	G	43	0	30	11	0
5	I	43	0	30	9	0
6	B	11	0	10	3	0
6	E	11	0	10	5	0
6	G	11	0	10	8	0
6	I	11	0	10	2	0
7	B	22	0	20	0	0
7	E	22	0	20	4	0
7	G	22	0	20	5	0
7	I	22	0	20	1	0
8	B	24	0	0	0	0
8	E	24	0	0	0	0
8	G	24	0	0	0	0
9	B	1	0	0	0	0
9	E	1	0	0	0	0
9	G	1	0	0	0	0
9	I	1	0	0	0	0
10	B	1	0	0	0	0
10	G	1	0	0	0	0
11	A	2	0	0	0	0
11	B	11	0	0	0	0
11	D	2	0	0	1	0
11	E	10	0	0	0	0
11	F	4	0	0	0	0
11	G	21	0	0	2	0
11	H	4	0	0	0	0
11	I	9	0	0	0	0
All	All	18513	0	17773	309	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 9.

The worst 5 of 309 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)
2:G:317:ASN:HD21	3:G:604:NAG:C1	1.35	1.37
2:E:115:CYS:SG	2:E:125:CYS:SG	1.35	1.28
2:E:115:CYS:CB	2:E:125:CYS:SG	2.25	1.23
1:A:94:ASP:OD2	5:B:608:HEM:HMD1	1.41	1.17
2:I:173:ALA:HA	2:I:175:MET:HE1	1.18	1.17

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	101/105 (96%)	94 (93%)	7 (7%)	0	100	100
1	D	101/105 (96%)	93 (92%)	7 (7%)	1 (1%)	13	37
1	F	101/105 (96%)	94 (93%)	7 (7%)	0	100	100
1	H	101/105 (96%)	94 (93%)	7 (7%)	0	100	100
2	B	463/467 (99%)	428 (92%)	33 (7%)	2 (0%)	30	59
2	E	463/467 (99%)	433 (94%)	27 (6%)	3 (1%)	22	49
2	G	463/467 (99%)	426 (92%)	36 (8%)	1 (0%)	44	71
2	I	463/467 (99%)	428 (92%)	31 (7%)	4 (1%)	14	39
All	All	2256/2288 (99%)	2090 (93%)	155 (7%)	11 (0%)	25	54

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	367	ALA
1	D	74	ASP

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Mol	Chain	Res	Type
2	I	155	GLY
2	I	572	LEU
2	B	352	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	85/90 (94%)	82 (96%)	3 (4%)	31	63
1	D	88/90 (98%)	82 (93%)	6 (7%)	13	36
1	F	85/90 (94%)	82 (96%)	3 (4%)	31	63
1	H	87/90 (97%)	83 (95%)	4 (5%)	23	53
2	B	386/411 (94%)	373 (97%)	13 (3%)	32	64
2	E	387/411 (94%)	370 (96%)	17 (4%)	24	55
2	G	382/411 (93%)	362 (95%)	20 (5%)	19	48
2	I	382/411 (93%)	360 (94%)	22 (6%)	17	43
All	All	1882/2004 (94%)	1794 (95%)	88 (5%)	22	52

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	486	LYS
2	I	196	LEU
2	G	562	VAL
1	H	74	ASP
2	I	240	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	75	GLN
2	I	250	HIS

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Mol	Chain	Res	Type
2	I	467	GLN
2	I	317	ASN
2	I	189	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 51 ligands modelled in this entry, 6 are monoatomic - leaving 45 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	FUC	G	605	-	10,10,11	1.46	1 (10%)	14,14,16	2.26	5 (35%)
3	NAG	G	603	-	14,14,15	1.16	1 (7%)	17,19,21	1.89	5 (29%)
3	NAG	I	601	-	14,14,15	1.43	2 (14%)	17,19,21	2.64	8 (47%)
8	JXS	E	610	-	23,27,27	5.03	16 (69%)	28,38,38	2.20	8 (28%)
7	MAN	I	604	-	11,11,12	1.44	2 (18%)	15,15,17	1.58	3 (20%)
3	NAG	E	604	-	14,14,15	1.65	3 (21%)	17,19,21	2.24	7 (41%)
4	FUC	E	608	-	10,10,11	2.01	3 (30%)	14,14,16	2.53	7 (50%)
3	NAG	I	607	-	14,14,15	1.17	1 (7%)	17,19,21	2.20	5 (29%)
3	NAG	G	606	-	14,14,15	1.59	2 (14%)	17,19,21	1.70	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	MAN	E	602	-	11,11,12	1.32	2 (18%)	15,15,17	1.78	4 (26%)
7	MAN	E	603	-	11,11,12	1.27	1 (9%)	15,15,17	3.23	6 (40%)
3	NAG	B	604	-	14,14,15	1.08	0	17,19,21	2.37	7 (41%)
4	FUC	I	609	-	10,10,11	1.60	3 (30%)	14,14,16	2.37	5 (35%)
8	JXS	B	613	-	23,27,27	5.04	15 (65%)	28,38,38	2.08	8 (28%)
8	JXS	G	612	-	23,27,27	5.11	15 (65%)	28,38,38	2.19	8 (28%)
7	MAN	B	612	-	11,11,12	1.79	5 (45%)	15,15,17	1.95	5 (33%)
3	NAG	B	607	-	14,14,15	1.50	2 (14%)	17,19,21	1.63	3 (17%)
3	NAG	E	607	-	14,14,15	1.10	2 (14%)	17,19,21	2.62	6 (35%)
3	NAG	G	601	-	14,14,15	2.03	6 (42%)	17,19,21	2.13	6 (35%)
3	NAG	I	606	-	14,14,15	1.50	3 (21%)	17,19,21	2.08	5 (29%)
7	MAN	G	610	-	11,11,12	1.07	1 (9%)	15,15,17	2.07	3 (20%)
5	HEM	G	607	2	42,50,50	1.50	7 (16%)	46,82,82	2.04	13 (28%)
3	NAG	B	603	-	14,14,15	1.80	5 (35%)	17,19,21	2.29	8 (47%)
7	MAN	I	603	-	11,11,12	1.34	0	15,15,17	1.67	2 (13%)
6	BMA	I	602	-	11,11,12	1.36	2 (18%)	15,15,17	2.32	7 (46%)
3	NAG	G	604	-	14,14,15	1.37	2 (14%)	17,19,21	3.87	9 (52%)
3	NAG	B	609	-	14,14,15	1.02	1 (7%)	17,19,21	2.90	8 (47%)
3	NAG	B	602	-	14,14,15	1.33	2 (14%)	17,19,21	2.59	6 (35%)
4	FUC	B	606	-	10,10,11	1.98	3 (30%)	14,14,16	2.37	5 (35%)
3	NAG	G	608	-	14,14,15	1.09	1 (7%)	17,19,21	2.24	7 (41%)
3	NAG	E	606	-	14,14,15	1.41	3 (21%)	17,19,21	1.81	5 (29%)
3	NAG	E	605	-	14,14,15	1.18	1 (7%)	17,19,21	1.64	3 (17%)
5	HEM	B	608	2	42,50,50	1.69	12 (28%)	46,82,82	1.95	15 (32%)
6	BMA	E	601	-	11,11,12	1.35	1 (9%)	15,15,17	2.46	5 (33%)
6	BMA	G	609	-	11,11,12	1.22	1 (9%)	15,15,17	2.93	5 (33%)
5	HEM	I	610	2	42,50,50	1.51	7 (16%)	46,82,82	2.11	16 (34%)
7	MAN	G	611	-	11,11,12	1.26	2 (18%)	15,15,17	1.62	4 (26%)
3	NAG	I	605	-	14,14,15	1.41	2 (14%)	17,19,21	1.44	3 (17%)
7	MAN	B	611	-	11,11,12	1.04	0	15,15,17	1.15	1 (6%)
3	NAG	I	608	-	14,14,15	1.49	2 (14%)	17,19,21	4.17	10 (58%)
6	BMA	B	610	-	11,11,12	1.16	1 (9%)	15,15,17	2.19	6 (40%)
3	NAG	B	605	-	14,14,15	0.88	0	17,19,21	2.14	6 (35%)
3	NAG	B	601	-	14,14,15	1.89	4 (28%)	17,19,21	2.37	7 (41%)
3	NAG	G	602	-	14,14,15	1.67	2 (14%)	17,19,21	2.44	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	HEM	E	609	2	42,50,50	1.49	8 (19%)	46,82,82	1.76	11 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUC	G	605	-	-	-	0/1/1/1
3	NAG	G	603	-	-	1/6/23/26	0/1/1/1
3	NAG	I	601	-	-	2/6/23/26	0/1/1/1
8	JXS	E	610	-	-	0/9/9/9	0/4/4/4
7	MAN	I	604	-	-	2/2/19/22	1/1/1/1
3	NAG	E	604	-	-	0/6/23/26	0/1/1/1
4	FUC	E	608	-	-	-	0/1/1/1
3	NAG	I	607	-	-	1/6/23/26	0/1/1/1
3	NAG	G	606	-	-	0/6/23/26	0/1/1/1
7	MAN	E	602	-	-	1/2/19/22	0/1/1/1
7	MAN	E	603	-	-	2/2/19/22	0/1/1/1
3	NAG	B	604	-	-	3/6/23/26	0/1/1/1
8	JXS	B	613	-	-	0/9/9/9	0/4/4/4
4	FUC	I	609	-	-	-	0/1/1/1
8	JXS	G	612	-	-	0/9/9/9	0/4/4/4
7	MAN	B	612	-	-	2/2/19/22	0/1/1/1
3	NAG	B	607	-	-	2/6/23/26	0/1/1/1
3	NAG	E	607	-	-	0/6/23/26	0/1/1/1
3	NAG	G	601	-	-	2/6/23/26	0/1/1/1
3	NAG	I	606	-	-	2/6/23/26	0/1/1/1
7	MAN	G	610	-	-	2/2/19/22	1/1/1/1
5	HEM	G	607	2	-	6/12/54/54	-
3	NAG	B	603	-	-	0/6/23/26	0/1/1/1
7	MAN	I	603	-	-	2/2/19/22	0/1/1/1
6	BMA	I	602	-	-	2/2/19/22	0/1/1/1
3	NAG	G	604	-	-	0/6/23/26	0/1/1/1
3	NAG	B	609	-	-	3/6/23/26	0/1/1/1
3	NAG	B	602	-	-	2/6/23/26	0/1/1/1
4	FUC	B	606	-	-	-	0/1/1/1
3	NAG	G	608	-	-	2/6/23/26	0/1/1/1
3	NAG	E	606	-	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	605	-	-	3/6/23/26	0/1/1/1
5	HEM	B	608	2	-	6/12/54/54	-
6	BMA	E	601	-	-	2/2/19/22	0/1/1/1
6	BMA	G	609	-	-	1/2/19/22	0/1/1/1
5	HEM	I	610	2	-	3/12/54/54	-
7	MAN	G	611	-	-	2/2/19/22	0/1/1/1
3	NAG	I	605	-	-	2/6/23/26	0/1/1/1
7	MAN	B	611	-	-	2/2/19/22	0/1/1/1
3	NAG	I	608	-	-	0/6/23/26	0/1/1/1
6	BMA	B	610	-	-	2/2/19/22	0/1/1/1
3	NAG	B	605	-	-	2/6/23/26	0/1/1/1
3	NAG	B	601	-	-	1/6/23/26	0/1/1/1
3	NAG	G	602	-	-	0/6/23/26	0/1/1/1
5	HEM	E	609	2	-	6/12/54/54	-

The worst 5 of 155 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	612	JXS	C14-N19	11.52	1.47	1.33
8	E	610	JXS	C14-N19	11.48	1.47	1.33
8	B	613	JXS	C14-N19	11.24	1.46	1.33
8	G	612	JXS	C05-C09	8.68	1.54	1.39
8	E	610	JXS	C05-C09	8.40	1.53	1.39

The worst 5 of 287 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	604	NAG	C1-C2-N2	-12.53	90.70	110.43
3	I	608	NAG	C1-O5-C5	-12.43	95.52	112.19
7	E	603	MAN	C1-O5-C5	9.25	124.58	112.19
3	B	609	NAG	C1-O5-C5	7.59	122.36	112.19
3	G	602	NAG	C1-O5-C5	-7.49	102.14	112.19

There are no chirality outliers.

5 of 73 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	608	HEM	C2B-C3B-CAB-CBB
5	B	608	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
6	I	602	BMA	C4-C5-C6-O6
6	B	610	BMA	C4-C5-C6-O6
3	G	608	NAG	O5-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	610	MAN	C1-C2-C3-C4-C5-O5
7	I	604	MAN	C1-C2-C3-C4-C5-O5

34 monomers are involved in 98 short contacts:

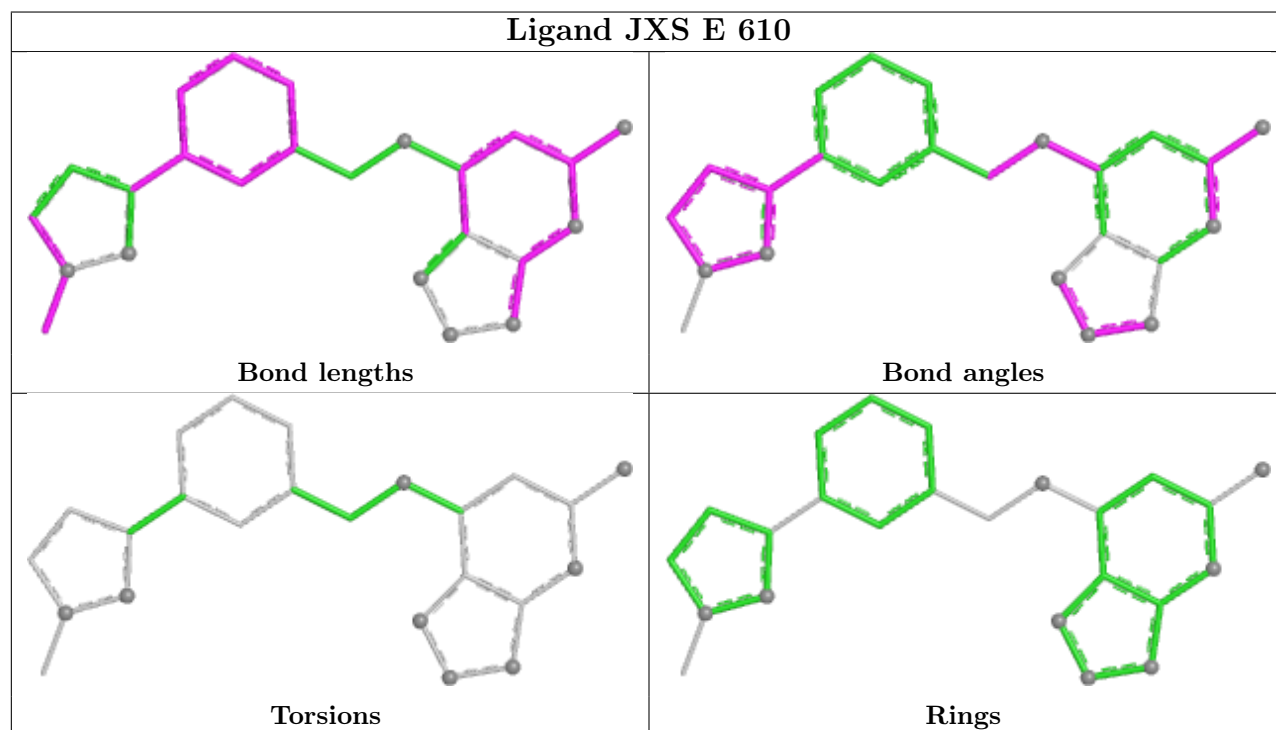
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	603	NAG	2	0
3	I	601	NAG	4	0
7	I	604	MAN	1	0
3	I	607	NAG	1	0
7	E	602	MAN	4	0
3	B	604	NAG	6	0
4	I	609	FUC	1	0
3	B	607	NAG	1	0
3	E	607	NAG	4	0
3	G	601	NAG	1	0
3	I	606	NAG	1	0
7	G	610	MAN	1	0
5	G	607	HEM	11	0
3	B	603	NAG	3	0
6	I	602	BMA	2	0
3	G	604	NAG	6	0
3	B	609	NAG	3	0
3	B	602	NAG	5	0
4	B	606	FUC	1	0
3	G	608	NAG	5	0
3	E	606	NAG	1	0
3	E	605	NAG	4	0
5	B	608	HEM	10	0
6	E	601	BMA	5	0
6	G	609	BMA	8	0
5	I	610	HEM	9	0
7	G	611	MAN	4	0
3	I	605	NAG	1	0
3	I	608	NAG	4	0

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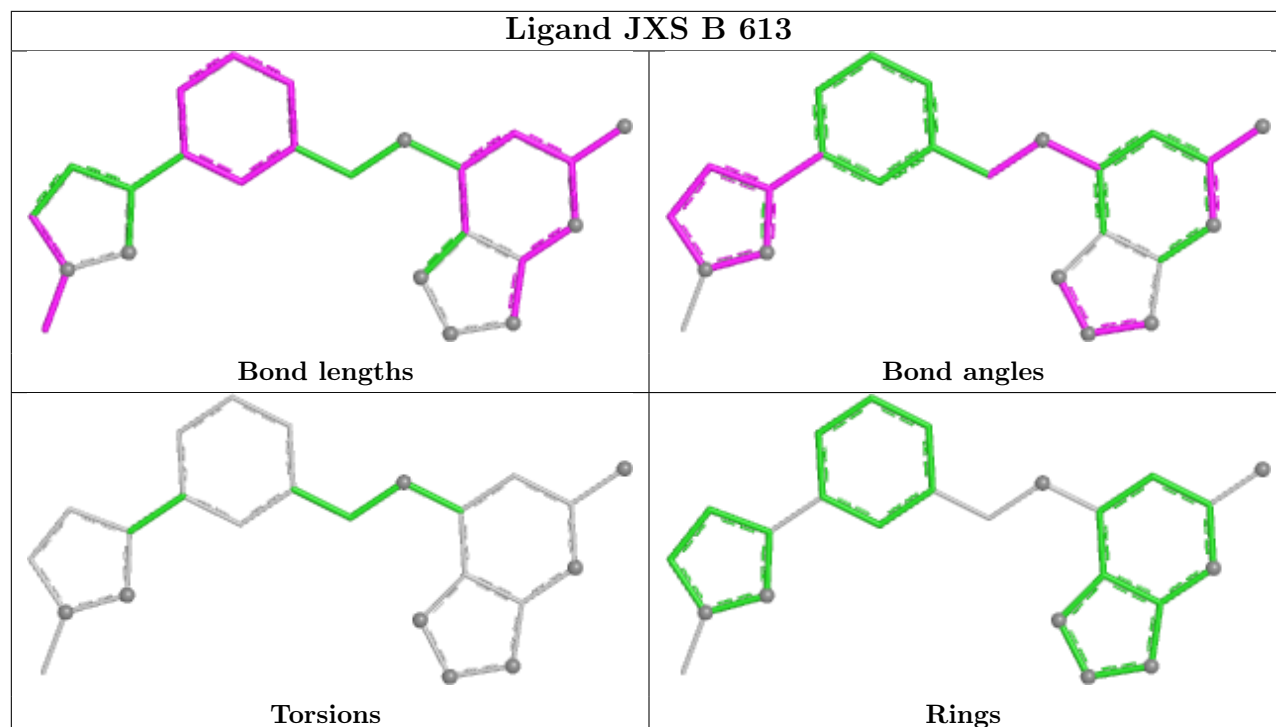
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	610	BMA	3	0
3	B	605	NAG	4	0
3	B	601	NAG	1	0
3	G	602	NAG	5	0
5	E	609	HEM	8	0

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.

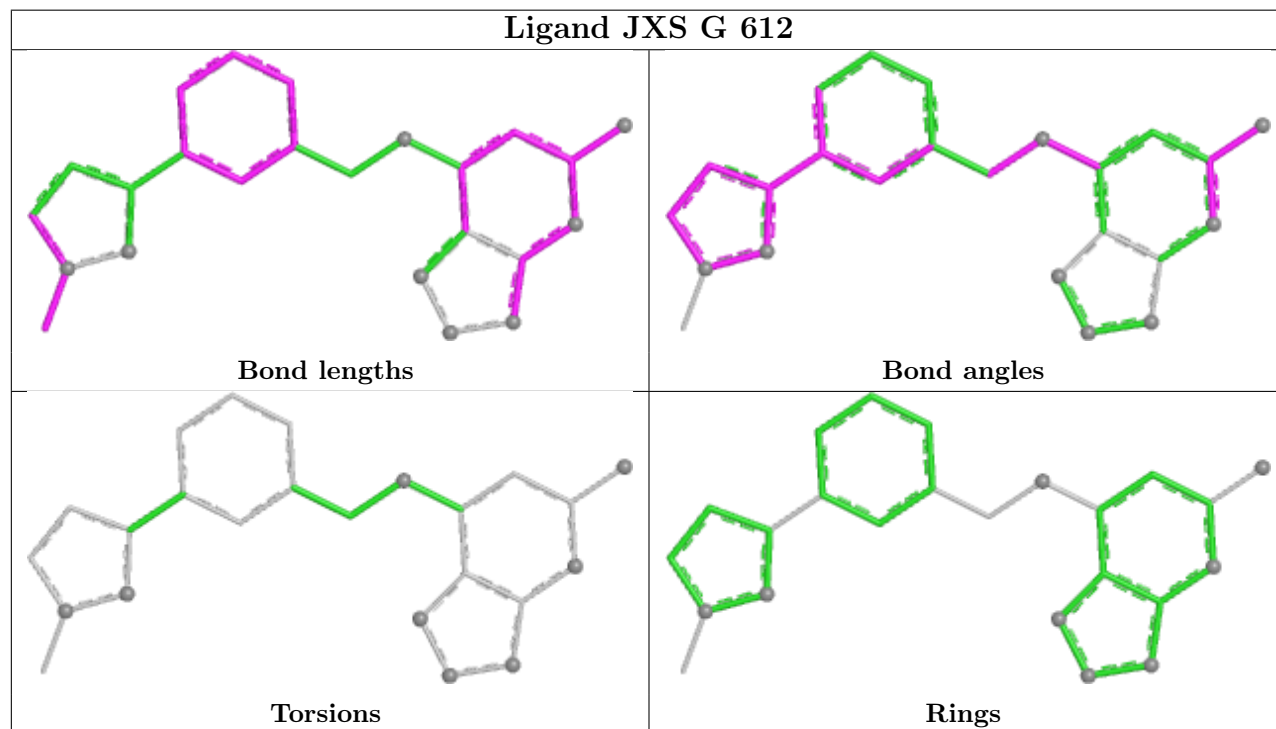




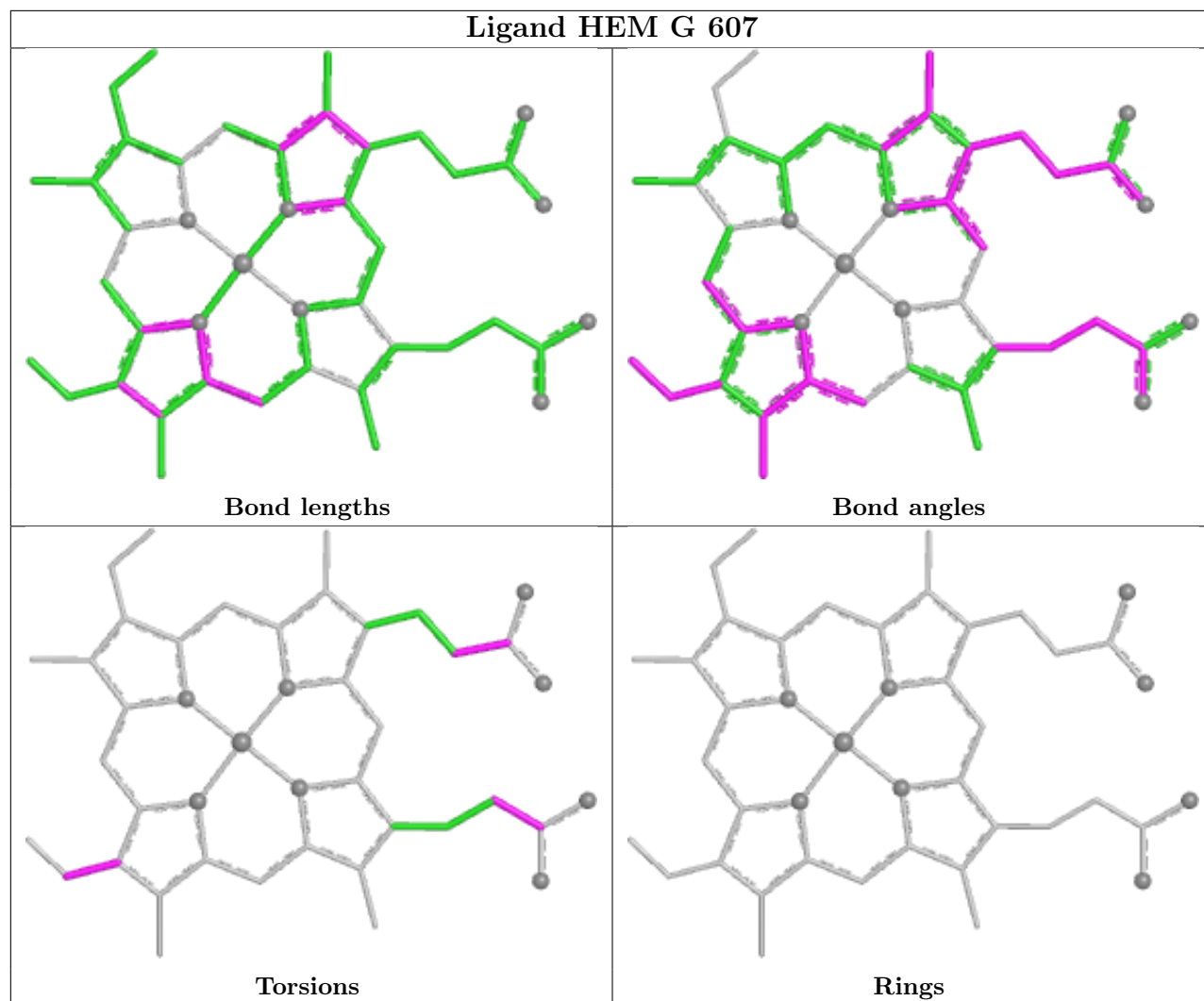
## Ligand JXS B 613

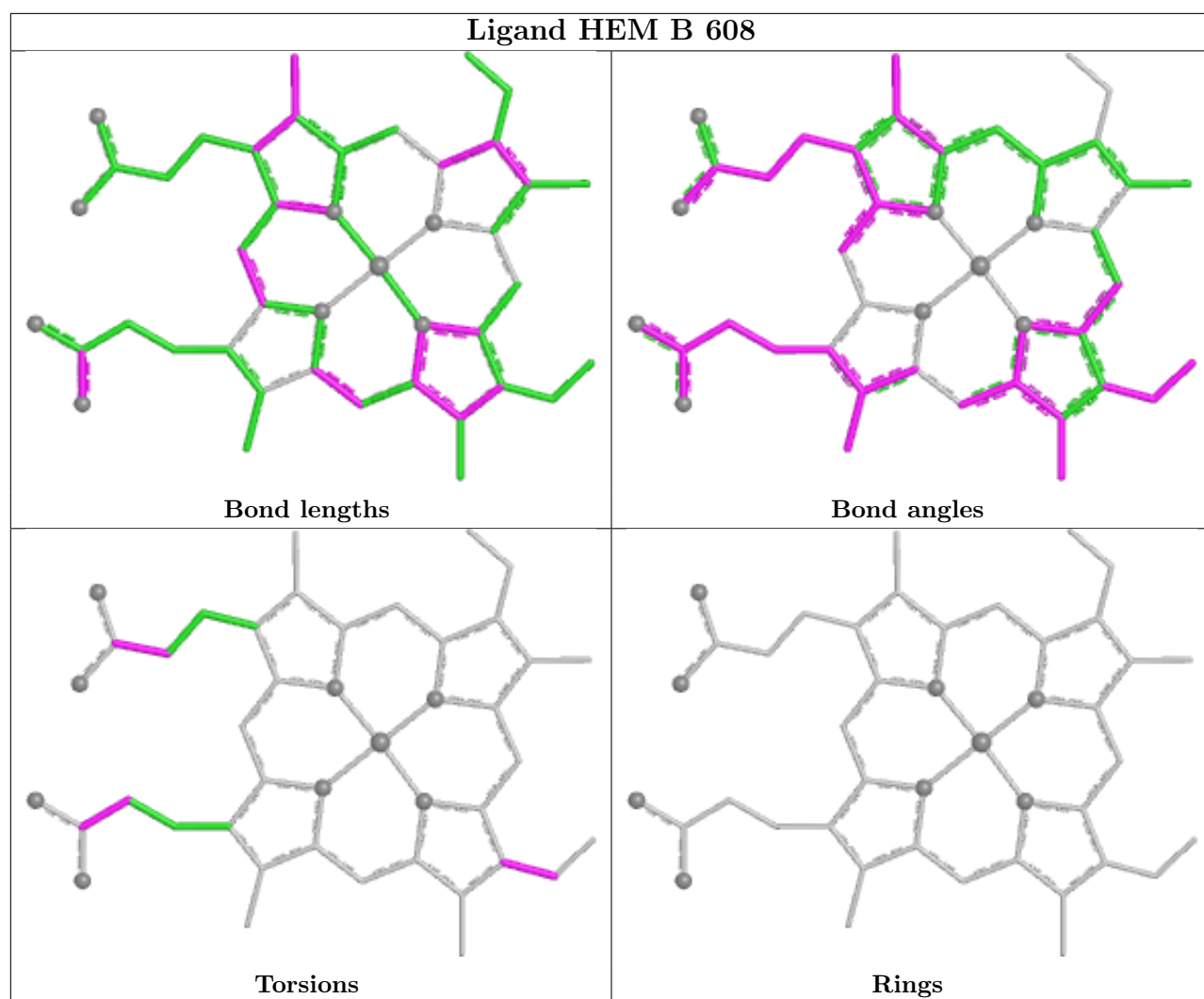


## Ligand JXS G 612

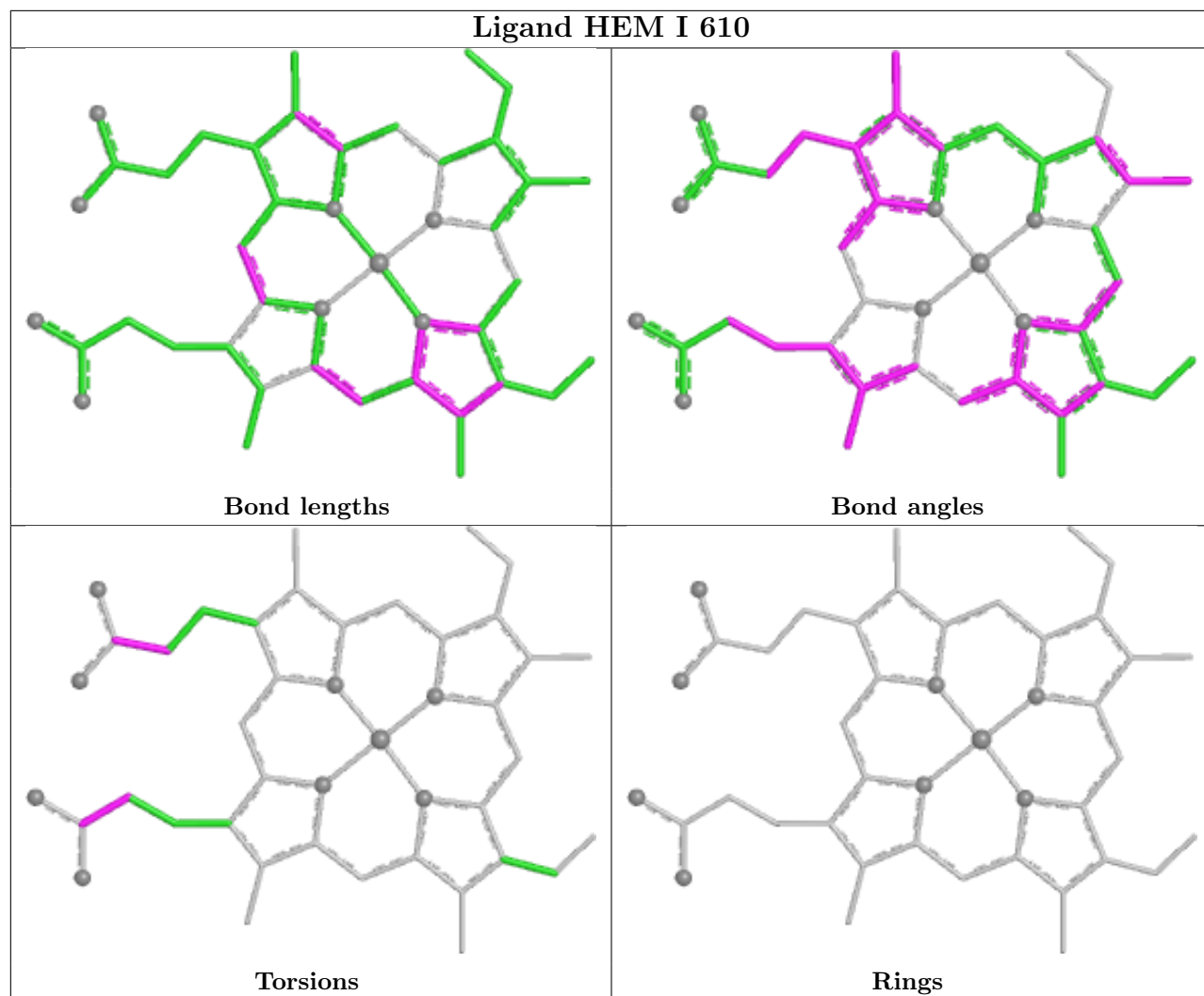


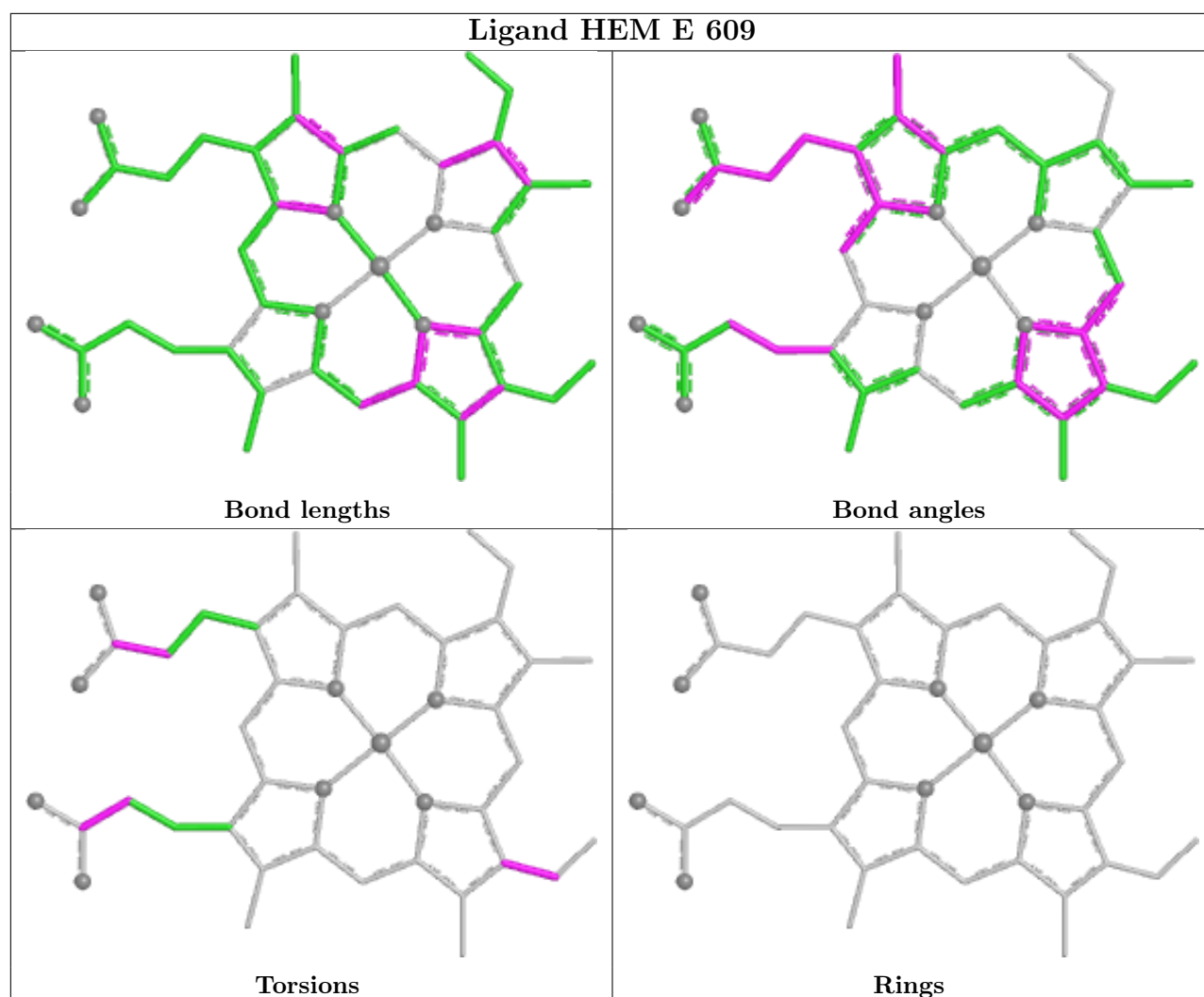
## Ligand HEM G 607





## Ligand HEM I 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%)	-0.04	0 <b>100</b> <b>100</b>	29, 51, 77, 85	1 (0%)
1	D	103/105 (98%)	0.17	2 (1%) 66 59	38, 54, 74, 90	2 (1%)
1	F	103/105 (98%)	0.19	1 (0%) 79 73	35, 52, 70, 86	0
1	H	103/105 (98%)	0.03	1 (0%) 79 73	29, 52, 80, 95	1 (0%)
2	B	465/467 (99%)	0.29	13 (2%) 55 47	27, 58, 86, 112	7 (1%)
2	E	465/467 (99%)	0.28	10 (2%) 62 54	32, 58, 79, 90	6 (1%)
2	G	465/467 (99%)	0.11	5 (1%) 77 72	26, 54, 75, 94	7 (1%)
2	I	465/467 (99%)	0.39	14 (3%) 52 44	29, 62, 94, 111	10 (2%)
All	All	2272/2288 (99%)	0.24	46 (2%) 64 57	26, 56, 84, 112	34 (1%)

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	482	SER	7.0
2	I	482	SER	3.4
2	I	522	MET	3.1
2	B	348	ASN	2.9
2	B	354	GLU	2.8

### 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
3	NAG	B	603	14/15	0.30	0.18	120,124,126,126	0
3	NAG	G	603	14/15	0.51	0.16	112,115,118,118	0
3	NAG	B	607	14/15	0.53	0.18	114,117,120,120	0
3	NAG	G	606	14/15	0.53	0.17	117,121,123,123	0
3	NAG	E	606	14/15	0.74	0.12	81,85,88,88	0
7	MAN	I	603	11/12	0.75	0.16	85,88,90,90	0
3	NAG	I	605	14/15	0.77	0.13	90,94,96,96	0
7	MAN	E	602	11/12	0.78	0.13	70,72,74,76	0
3	NAG	B	601	14/15	0.78	0.14	73,77,79,79	0
7	MAN	G	610	11/12	0.80	0.13	76,78,80,82	0
3	NAG	E	604	14/15	0.80	0.13	77,81,83,83	0
3	NAG	I	607	14/15	0.81	0.12	91,95,97,97	0
3	NAG	B	602	14/15	0.83	0.14	96,100,102,103	0
3	NAG	I	606	14/15	0.83	0.13	80,84,86,86	0
3	NAG	G	602	14/15	0.84	0.14	74,78,80,80	0
3	NAG	E	605	14/15	0.84	0.14	87,90,93,93	0
7	MAN	B	611	11/12	0.84	0.11	54,57,59,60	0
8	JXS	B	613	24/24	0.85	0.15	70,76,84,85	0
3	NAG	G	601	14/15	0.86	0.11	61,64,67,67	0
7	MAN	I	604	11/12	0.87	0.12	46,48,51,51	0
6	BMA	G	609	11/12	0.87	0.13	45,47,49,49	0
8	JXS	E	610	24/24	0.87	0.14	66,70,72,74	0
7	MAN	B	612	11/12	0.88	0.11	51,54,56,56	0
7	MAN	G	611	11/12	0.88	0.09	37,39,41,41	0
4	FUC	B	606	10/11	0.88	0.12	47,48,49,49	0
3	NAG	I	608	14/15	0.89	0.11	46,49,52,52	0
4	FUC	I	609	10/11	0.90	0.11	53,53,54,55	0
6	BMA	E	601	11/12	0.90	0.17	63,65,67,68	0
3	NAG	E	607	14/15	0.90	0.10	58,62,64,64	0
8	JXS	G	612	24/24	0.90	0.11	46,54,64,68	0
3	NAG	B	609	14/15	0.91	0.09	40,44,47,47	0
6	BMA	I	602	11/12	0.91	0.14	62,65,66,67	0
6	BMA	B	610	11/12	0.91	0.12	52,54,55,57	0
3	NAG	B	604	14/15	0.91	0.11	48,52,54,55	0
3	NAG	G	604	14/15	0.92	0.09	40,44,46,47	0
7	MAN	E	603	11/12	0.93	0.08	36,39,41,41	0
4	FUC	E	608	10/11	0.93	0.10	49,49,51,51	0

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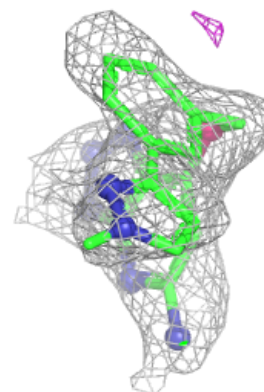
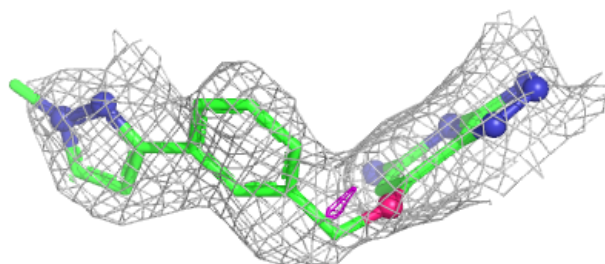
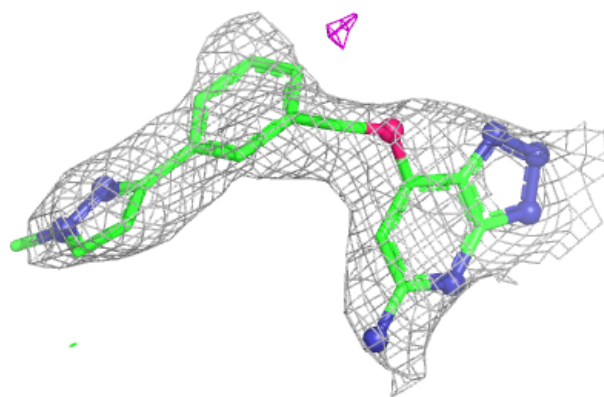
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	HEM	B	608	43/43	0.94	0.11	49,50,54,56	0
3	NAG	G	608	14/15	0.94	0.10	51,54,57,57	0
3	NAG	B	605	14/15	0.95	0.07	35,38,41,42	0
3	NAG	I	601	14/15	0.95	0.08	30,35,37,38	0
5	HEM	E	609	43/43	0.95	0.11	59,60,64,67	0
5	HEM	G	607	43/43	0.95	0.10	44,45,49,50	0
5	HEM	I	610	43/43	0.95	0.10	45,46,49,55	0
10	CL	G	614	1/1	0.95	0.12	50,50,50,50	0
10	CL	B	615	1/1	0.96	0.26	62,62,62,62	0
4	FUC	G	605	10/11	0.96	0.09	41,41,42,42	0
9	CA	E	611	1/1	0.97	0.04	44,44,44,44	0
9	CA	I	611	1/1	0.99	0.07	51,51,51,51	0
9	CA	B	614	1/1	0.99	0.05	43,43,43,43	0
9	CA	G	613	1/1	0.99	0.03	40,40,40,40	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 JXS B 613:

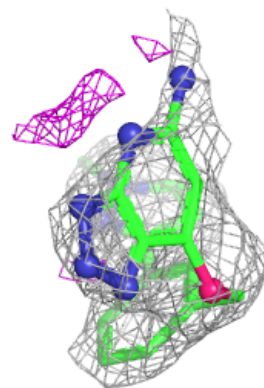
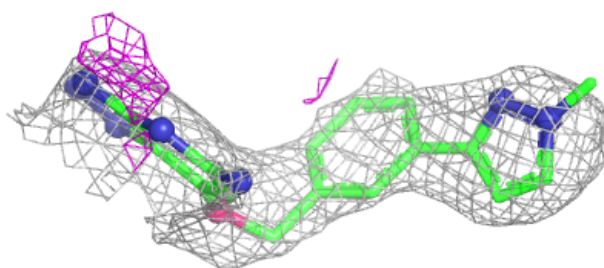
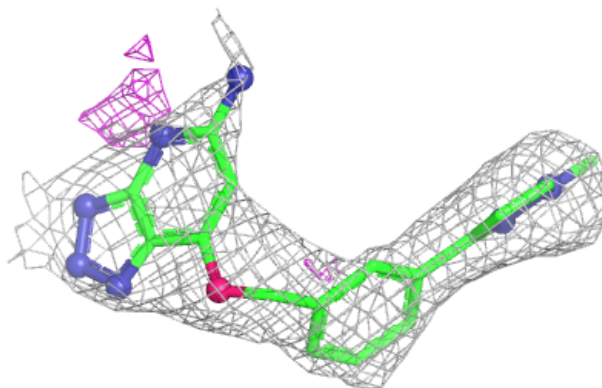
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



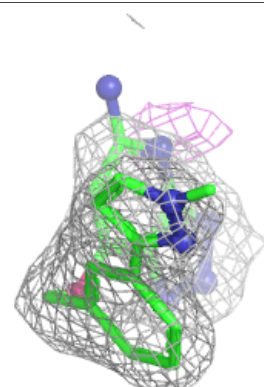
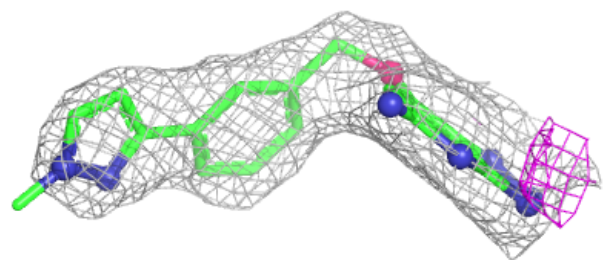
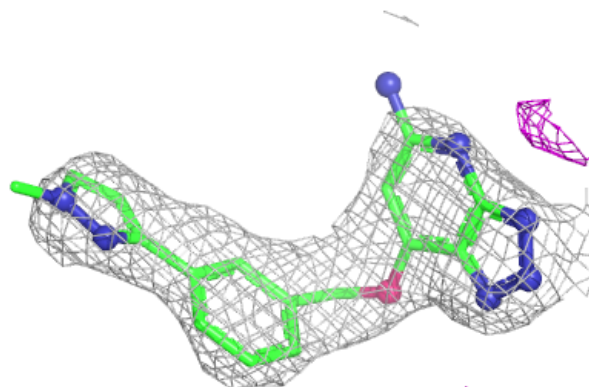


**Electron density around JXS E 610:**

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

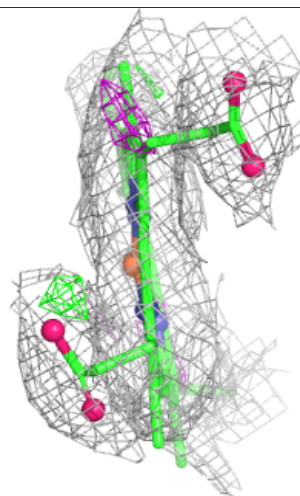
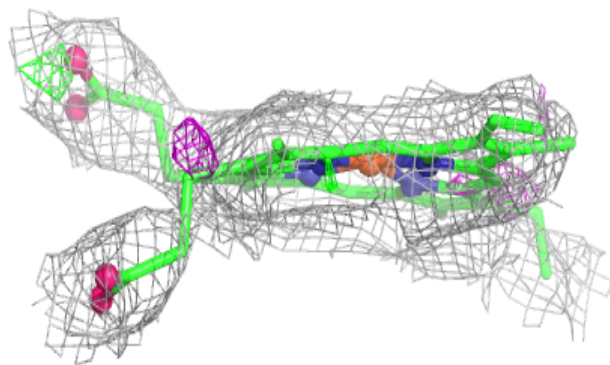
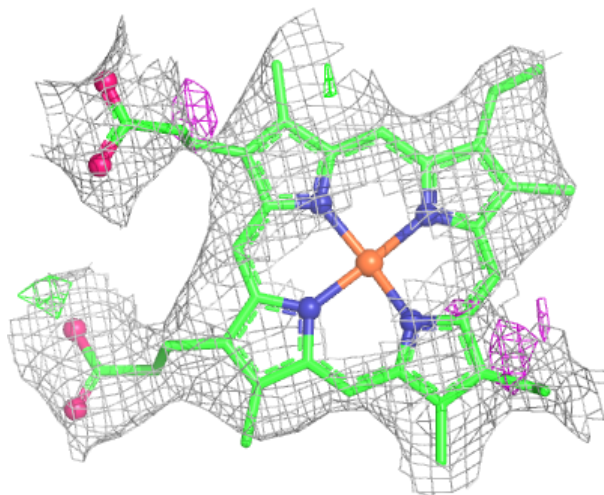
**Electron density around JXS G 612:**

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



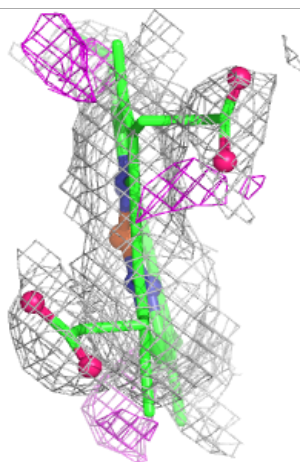
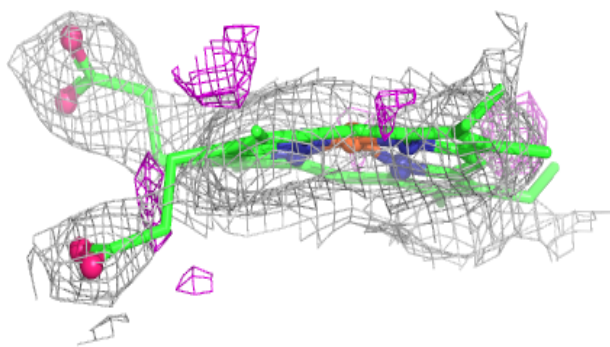
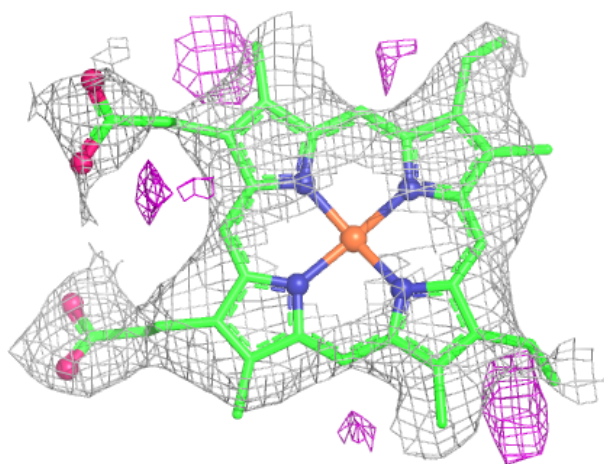
**Electron density around HEM B 608:**

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



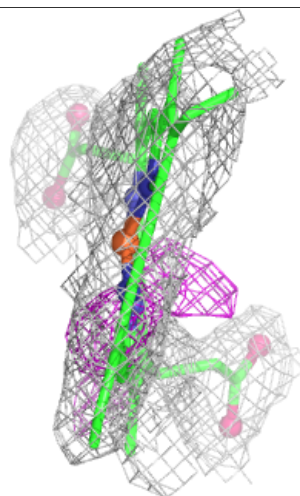
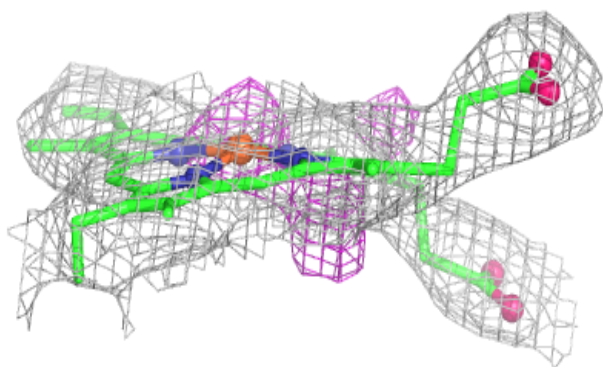
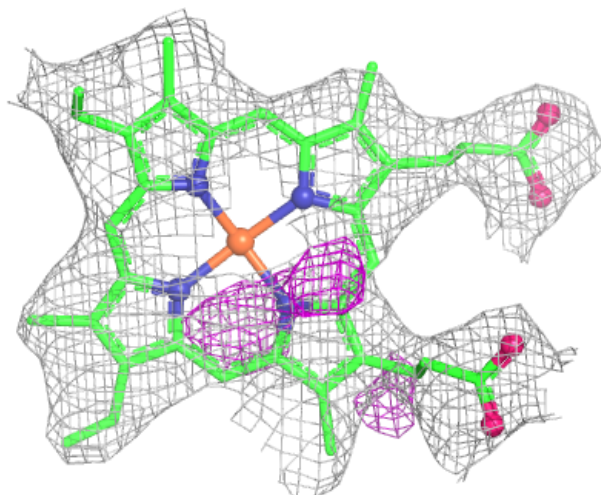
**Electron density around HEM E 609:**

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



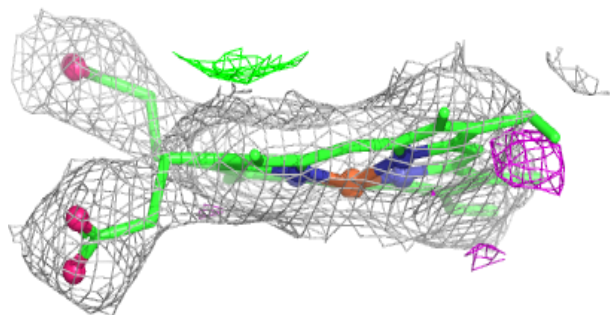
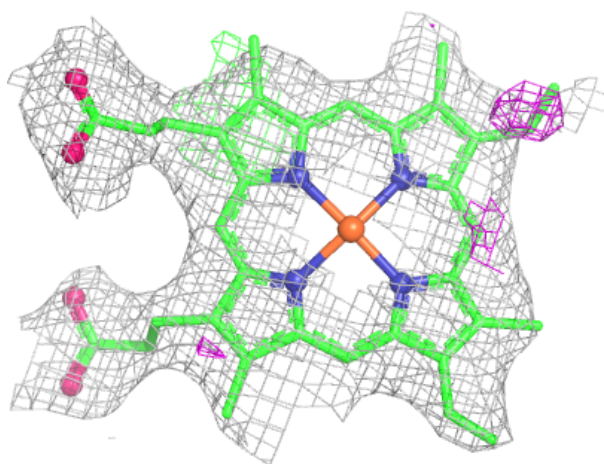
**Electron density around HEM G 607:**

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



**Electron density around HEM 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.