



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:29 AM UTC

PDB ID : 5QJ2 / pdb_00005qj2
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

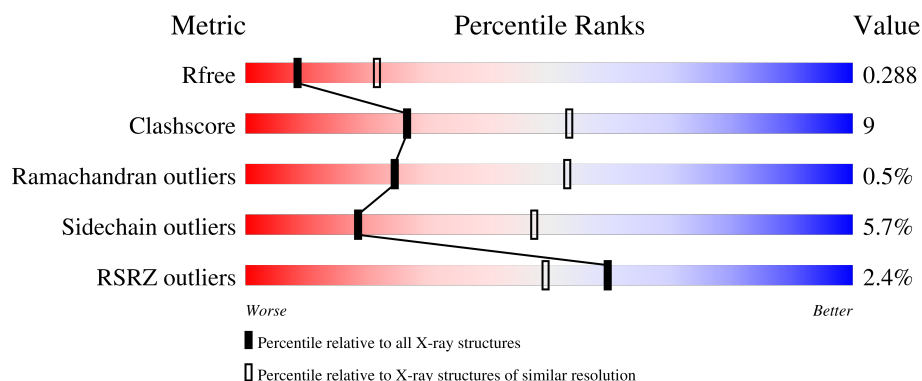
1 Overall quality at a glance

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.



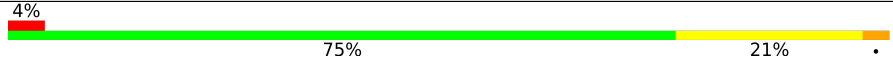
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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 ≥ 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	
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
6	BMA	G	609	-	-	X	-
8	JXS	G	612	-	X	-	-

2 Entry composition [i](#)

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			

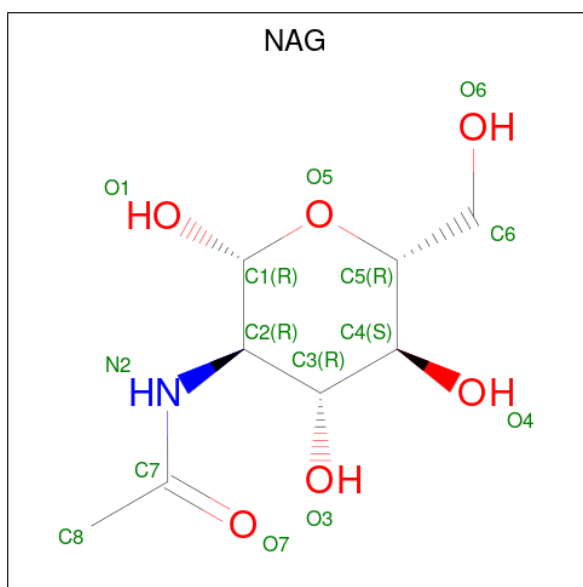
- Molecule 2 is a protein called Myeloperoxidase.

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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).



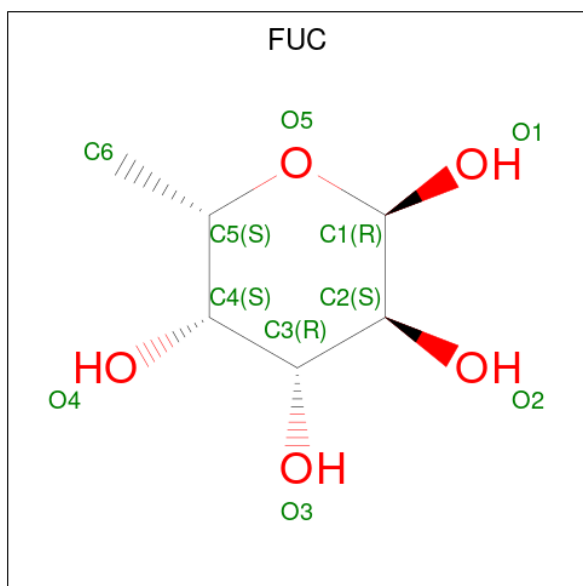
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1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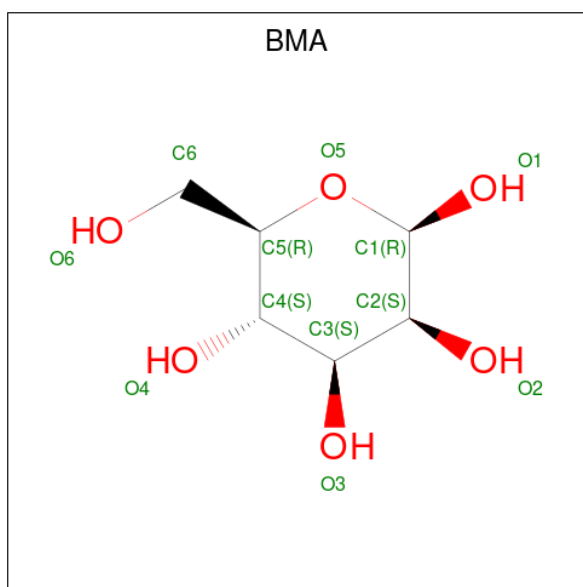
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is alpha-L-fucopyranose (CCD ID: FUC) (formula: $C_6H_{12}O_5$).



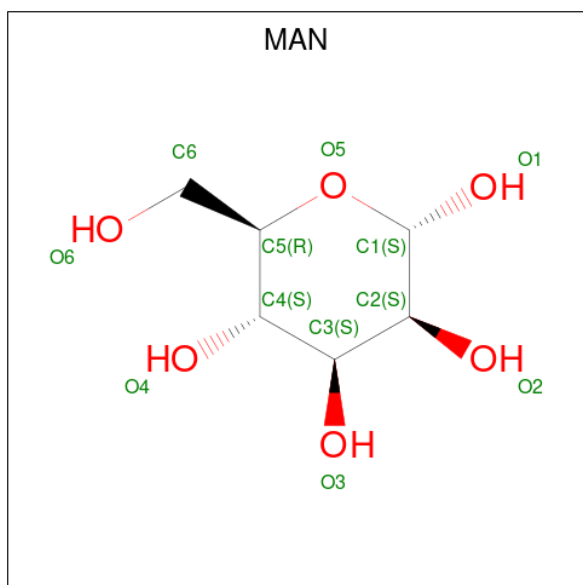
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	6	4		
4	E	1	Total	C	O	0	0
			10	6	4		
4	G	1	Total	C	O	0	0
			10	6	4		

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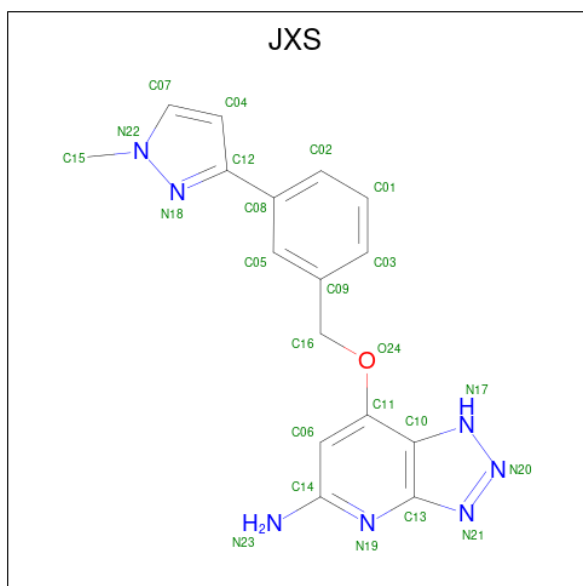
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			11	6	5		
6	E	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	I	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



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 (CCD ID: JXS) (formula: C₁₆H₁₅N₇O).



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 (CCD ID: 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 (CCD ID: 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.

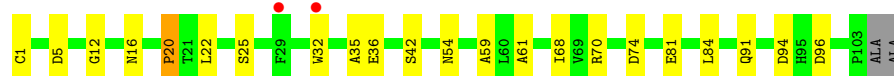
- Molecule 1: Myeloperoxidase

Chain A: 



- Molecule 1: Myeloperoxidase

Chain D: 



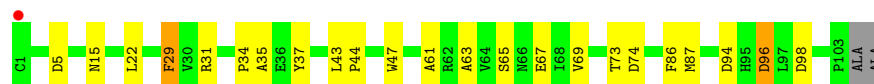
- Molecule 1: Myeloperoxidase

Chain F: 



- Molecule 1: Myeloperoxidase

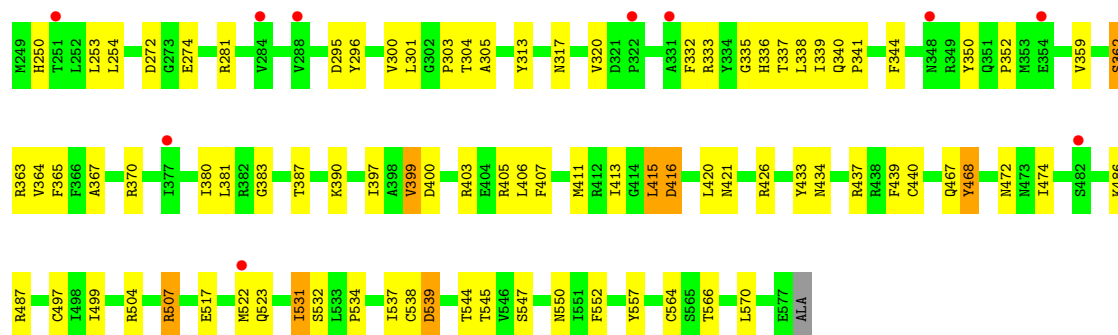
Chain H: 



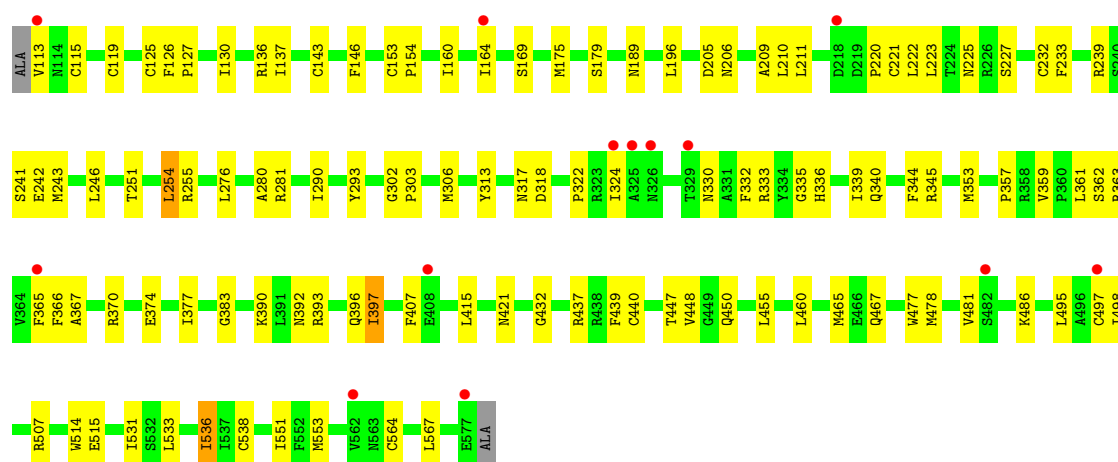
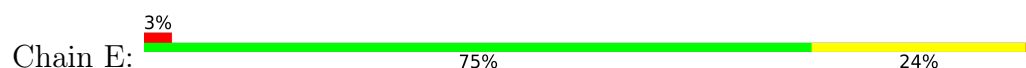
- Molecule 2: Myeloperoxidase

Chain B: 

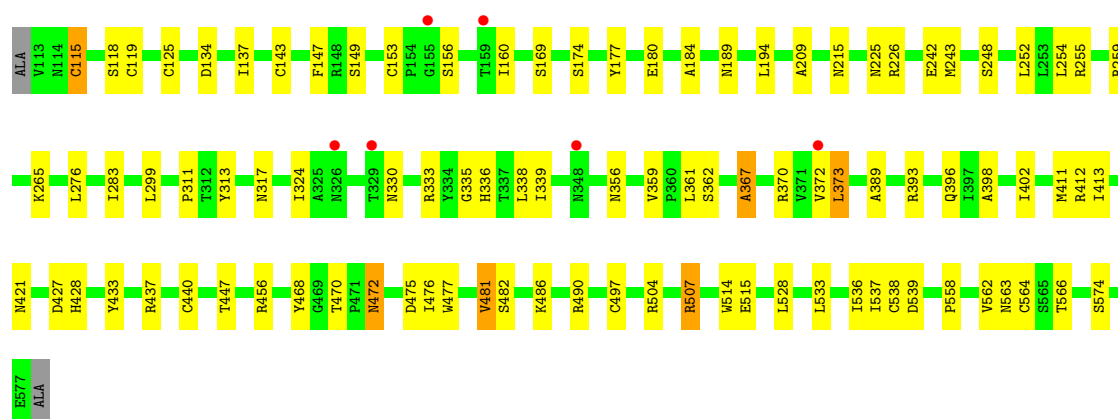
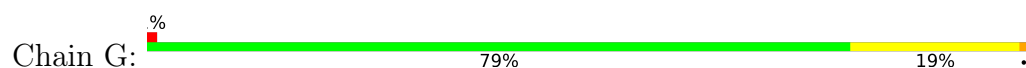




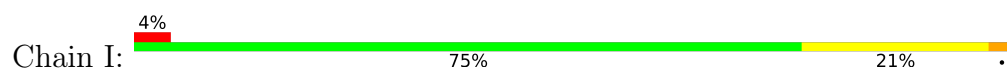
• Molecule 2: Myeloperoxidase

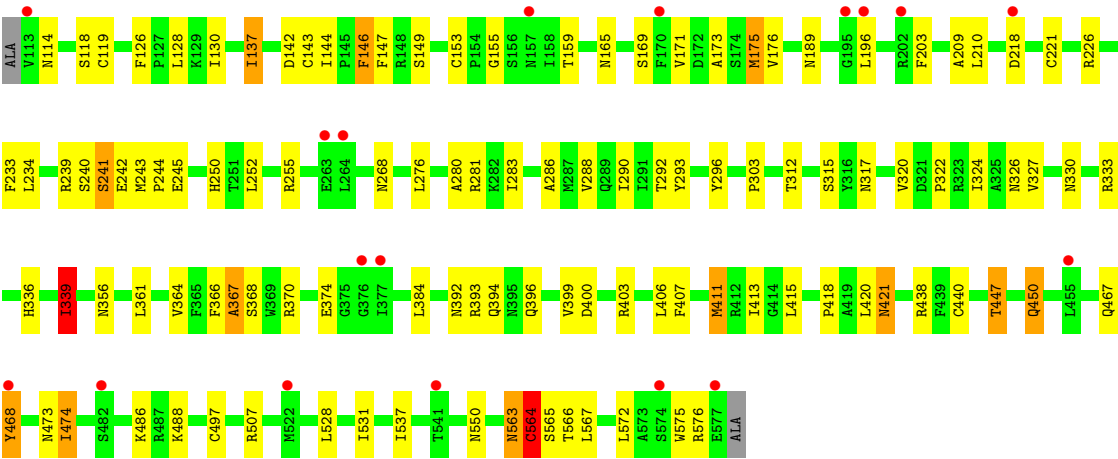


• Molecule 2: Myeloperoxidase



• Molecule 2: Myeloperoxidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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	3114 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, CL, HEM, BMA, MAN, JXS, CA, NAG

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	0.80	0/837	1.38	6/1143 (0.5%)
1	D	0.81	0/850	1.38	9/1159 (0.8%)
1	F	0.83	0/838	1.40	11/1144 (1.0%)
1	H	0.84	0/846	1.39	9/1154 (0.8%)
2	B	0.86	0/3703	1.39	26/5043 (0.5%)
2	E	0.85	0/3704	1.36	21/5043 (0.4%)
2	G	0.90	0/3693	1.38	20/5030 (0.4%)
2	I	0.86	0/3690	1.42	33/5026 (0.7%)
All	All	0.86	0/18161	1.39	135/24742 (0.5%)

There are no bond length outliers.

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	43	LEU	N-CA-C	8.30	120.10	109.72
2	B	177	TYR	N-CA-C	7.14	120.11	111.40
2	I	550	ASN	CA-CB-CG	6.96	119.56	112.60
2	B	550	ASN	CA-CB-CG	6.93	119.53	112.60
2	I	147	PHE	CA-CB-CG	6.67	120.47	113.80

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	21	0
1	D	825	0	780	13	0
1	F	813	0	766	12	0
1	H	821	0	774	14	0
2	B	3617	0	3529	72	0
2	E	3619	0	3555	71	0
2	G	3608	0	3526	57	0
2	I	3605	0	3513	62	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	12	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	H	4	0	0	0	0
11	I	9	0	0	0	0
All	All	18513	0	17773	318	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 318 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
1:F:94:ASP:OD2	5:G:607:HEM:HMD1	1.46	1.15

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%)	12	36
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	58
2	E	463/467 (99%)	433 (94%)	27 (6%)	3 (1%)	21	48
2	G	463/467 (99%)	426 (92%)	36 (8%)	1 (0%)	43	71
2	I	463/467 (99%)	428 (92%)	31 (7%)	4 (1%)	14	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2256/2288 (99%)	2090 (93%)	155 (7%)	11 (0%)	24 53

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	367	ALA
1	D	74	ASP
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%)	79 (93%)	6 (7%)	13 38
1	D	88/90 (98%)	83 (94%)	5 (6%)	18 47
1	F	85/90 (94%)	80 (94%)	5 (6%)	18 46
1	H	87/90 (97%)	85 (98%)	2 (2%)	44 76
2	B	386/411 (94%)	364 (94%)	22 (6%)	18 47
2	E	387/411 (94%)	367 (95%)	20 (5%)	21 51
2	G	382/411 (93%)	362 (95%)	20 (5%)	21 51
2	I	382/411 (93%)	354 (93%)	28 (7%)	13 36
All	All	1882/2004 (94%)	1774 (94%)	108 (6%)	18 47

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	88	GLN
2	G	447	THR
2	I	361	LEU
2	G	149	SER
2	G	330	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	317	ASN
2	I	450	GLN
2	I	549	ASN
2	E	121	GLN
2	E	114	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	$\# Z > 2$
7	MAN	E	603	-	11,11,12	1.27	1 (9%)	15,15,17	3.23	6 (40%)
3	NAG	I	606	-	14,14,15	1.50	3 (21%)	17,19,21	2.08	5 (29%)
3	NAG	B	603	-	14,14,15	1.80	5 (35%)	17,19,21	2.29	8 (47%)
3	NAG	G	606	-	14,14,15	1.59	2 (14%)	17,19,21	1.70	6 (35%)
4	FUC	G	605	-	10,10,11	1.46	1 (10%)	14,14,16	2.26	5 (35%)
3	NAG	B	605	-	14,14,15	0.88	0	17,19,21	2.14	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	609	-	14,14,15	1.02	1 (7%)	17,19,21	2.90	8 (47%)
3	NAG	E	606	-	14,14,15	1.41	3 (21%)	17,19,21	1.81	5 (29%)
7	MAN	G	610	-	11,11,12	1.07	1 (9%)	15,15,17	2.07	3 (20%)
3	NAG	G	601	-	14,14,15	2.03	6 (42%)	17,19,21	2.13	6 (35%)
5	HEM	E	609	2	50,50,50	1.33	7 (14%)	67,82,82	1.45	13 (19%)
6	BMA	I	602	-	11,11,12	1.36	2 (18%)	15,15,17	2.32	7 (46%)
7	MAN	E	602	-	11,11,12	1.32	2 (18%)	15,15,17	1.78	4 (26%)
4	FUC	I	609	-	10,10,11	1.60	3 (30%)	14,14,16	2.37	5 (35%)
3	NAG	I	608	-	14,14,15	1.49	2 (14%)	17,19,21	4.17	10 (58%)
8	JXS	G	612	-	27,27,27	5.12	19 (70%)	33,38,38	2.49	13 (39%)
4	FUC	E	608	-	10,10,11	2.01	3 (30%)	14,14,16	2.53	7 (50%)
6	BMA	G	609	-	11,11,12	1.22	1 (9%)	15,15,17	2.93	5 (33%)
3	NAG	G	602	-	14,14,15	1.67	2 (14%)	17,19,21	2.44	5 (29%)
7	MAN	B	611	-	11,11,12	1.04	0	15,15,17	1.15	1 (6%)
3	NAG	B	604	-	14,14,15	1.08	0	17,19,21	2.37	7 (41%)
8	JXS	B	613	-	27,27,27	5.03	19 (70%)	33,38,38	2.35	9 (27%)
3	NAG	E	604	-	14,14,15	1.65	3 (21%)	17,19,21	2.24	7 (41%)
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	B	602	-	14,14,15	1.33	2 (14%)	17,19,21	2.59	6 (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%)
7	MAN	B	612	-	11,11,12	1.79	5 (45%)	15,15,17	1.95	5 (33%)
6	BMA	B	610	-	11,11,12	1.16	1 (9%)	15,15,17	2.19	6 (40%)
6	BMA	E	601	-	11,11,12	1.35	1 (9%)	15,15,17	2.46	5 (33%)
5	HEM	B	608	2	50,50,50	1.64	13 (26%)	67,82,82	1.66	18 (26%)
3	NAG	I	605	-	14,14,15	1.41	2 (14%)	17,19,21	1.44	3 (17%)
5	HEM	G	607	2	50,50,50	1.38	8 (16%)	67,82,82	1.75	16 (23%)
3	NAG	B	601	-	14,14,15	1.89	4 (28%)	17,19,21	2.37	7 (41%)
7	MAN	I	603	-	11,11,12	1.34	0	15,15,17	1.67	2 (13%)
7	MAN	G	611	-	11,11,12	1.26	2 (18%)	15,15,17	1.62	4 (26%)
7	MAN	I	604	-	11,11,12	1.44	2 (18%)	15,15,17	1.58	3 (20%)
8	JXS	E	610	-	27,27,27	4.99	18 (66%)	33,38,38	2.41	9 (27%)
3	NAG	E	605	-	14,14,15	1.18	1 (7%)	17,19,21	1.64	3 (17%)
5	HEM	I	610	2	50,50,50	1.53	9 (18%)	67,82,82	1.71	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	G	608	-	14,14,15	1.09	1 (7%)	17,19,21	2.24	7 (41%)
4	FUC	B	606	-	10,10,11	1.98	3 (30%)	14,14,16	2.37	5 (35%)
3	NAG	G	604	-	14,14,15	1.37	2 (14%)	17,19,21	3.87	9 (52%)
3	NAG	I	607	-	14,14,15	1.17	1 (7%)	17,19,21	2.20	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	E	603	-	-	2/2/19/22	0/1/1/1
3	NAG	I	606	-	-	2/6/23/26	0/1/1/1
3	NAG	B	603	-	-	0/6/23/26	0/1/1/1
3	NAG	G	606	-	-	0/6/23/26	0/1/1/1
4	FUC	G	605	-	-	-	0/1/1/1
3	NAG	B	605	-	-	2/6/23/26	0/1/1/1
3	NAG	B	609	-	-	3/6/23/26	0/1/1/1
3	NAG	E	606	-	-	2/6/23/26	0/1/1/1
7	MAN	G	610	-	-	2/2/19/22	1/1/1/1
3	NAG	G	601	-	-	2/6/23/26	0/1/1/1
5	HEM	E	609	2	-	7/14/54/54	-
6	BMA	I	602	-	-	2/2/19/22	0/1/1/1
7	MAN	E	602	-	-	1/2/19/22	0/1/1/1
4	FUC	I	609	-	-	-	0/1/1/1
3	NAG	I	608	-	-	0/6/23/26	0/1/1/1
8	JXS	G	612	-	-	0/9/9/9	0/4/4/4
6	BMA	G	609	-	-	1/2/19/22	0/1/1/1
7	MAN	B	611	-	-	2/2/19/22	0/1/1/1
3	NAG	G	602	-	-	0/6/23/26	0/1/1/1
4	FUC	E	608	-	-	-	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
3	NAG	E	604	-	-	0/6/23/26	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	B	602	-	-	2/6/23/26	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	B	612	-	-	2/2/19/22	0/1/1/1
6	BMA	B	610	-	-	2/2/19/22	0/1/1/1
6	BMA	E	601	-	-	2/2/19/22	0/1/1/1
5	HEM	B	608	2	-	6/14/54/54	-
3	NAG	I	605	-	-	2/6/23/26	0/1/1/1
5	HEM	G	607	2	-	6/14/54/54	-
3	NAG	B	601	-	-	1/6/23/26	0/1/1/1
7	MAN	I	603	-	-	2/2/19/22	0/1/1/1
7	MAN	G	611	-	-	2/2/19/22	0/1/1/1
7	MAN	I	604	-	-	2/2/19/22	1/1/1/1
8	JXS	E	610	-	-	0/9/9/9	0/4/4/4
3	NAG	E	605	-	-	3/6/23/26	0/1/1/1
5	HEM	I	610	2	-	3/14/54/54	-
3	NAG	G	608	-	-	2/6/23/26	0/1/1/1
4	FUC	B	606	-	-	-	0/1/1/1
3	NAG	G	604	-	-	0/6/23/26	0/1/1/1
3	NAG	I	607	-	-	1/6/23/26	0/1/1/1

The worst 5 of 168 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	610	JXS	C13-N19	13.18	1.52	1.34
8	B	613	JXS	C13-N19	13.14	1.52	1.34
8	G	612	JXS	C13-N19	13.08	1.52	1.34
8	B	613	JXS	C02-C08	9.33	1.53	1.39
8	G	612	JXS	C02-C08	9.17	1.53	1.39

The worst 5 of 300 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 74 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
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 100 short contacts:

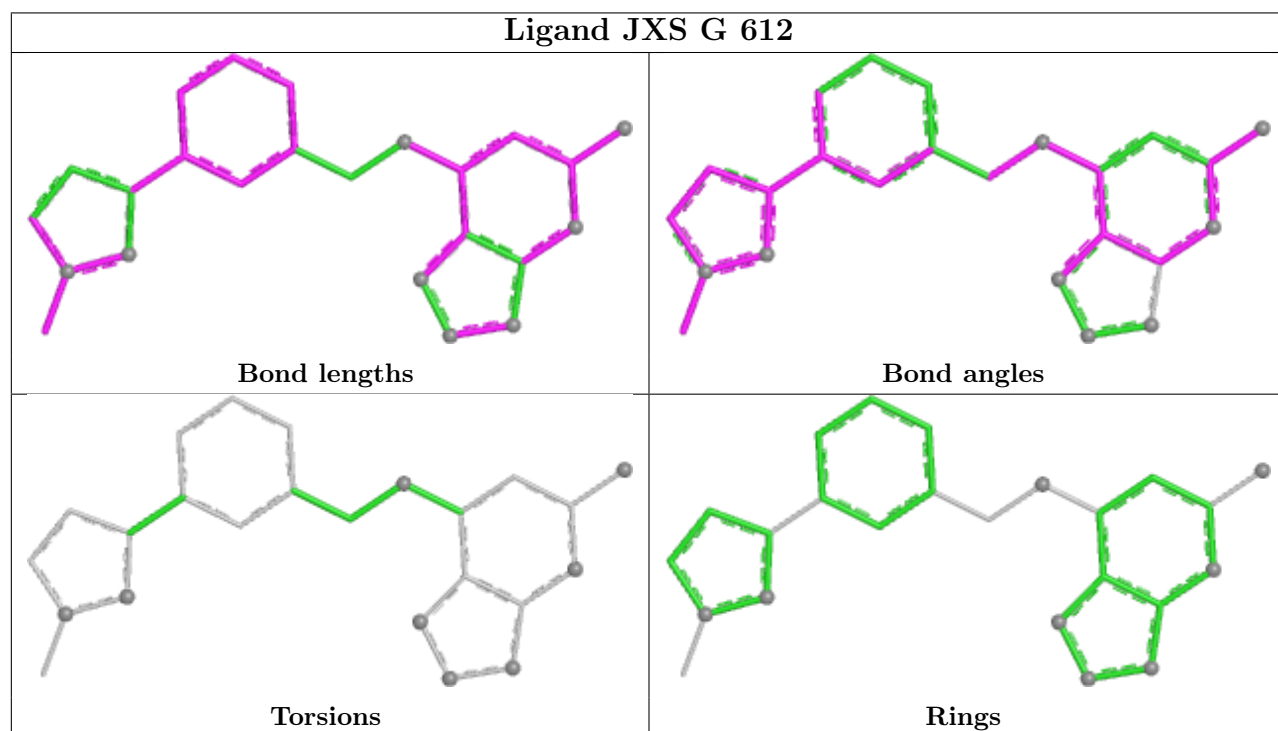
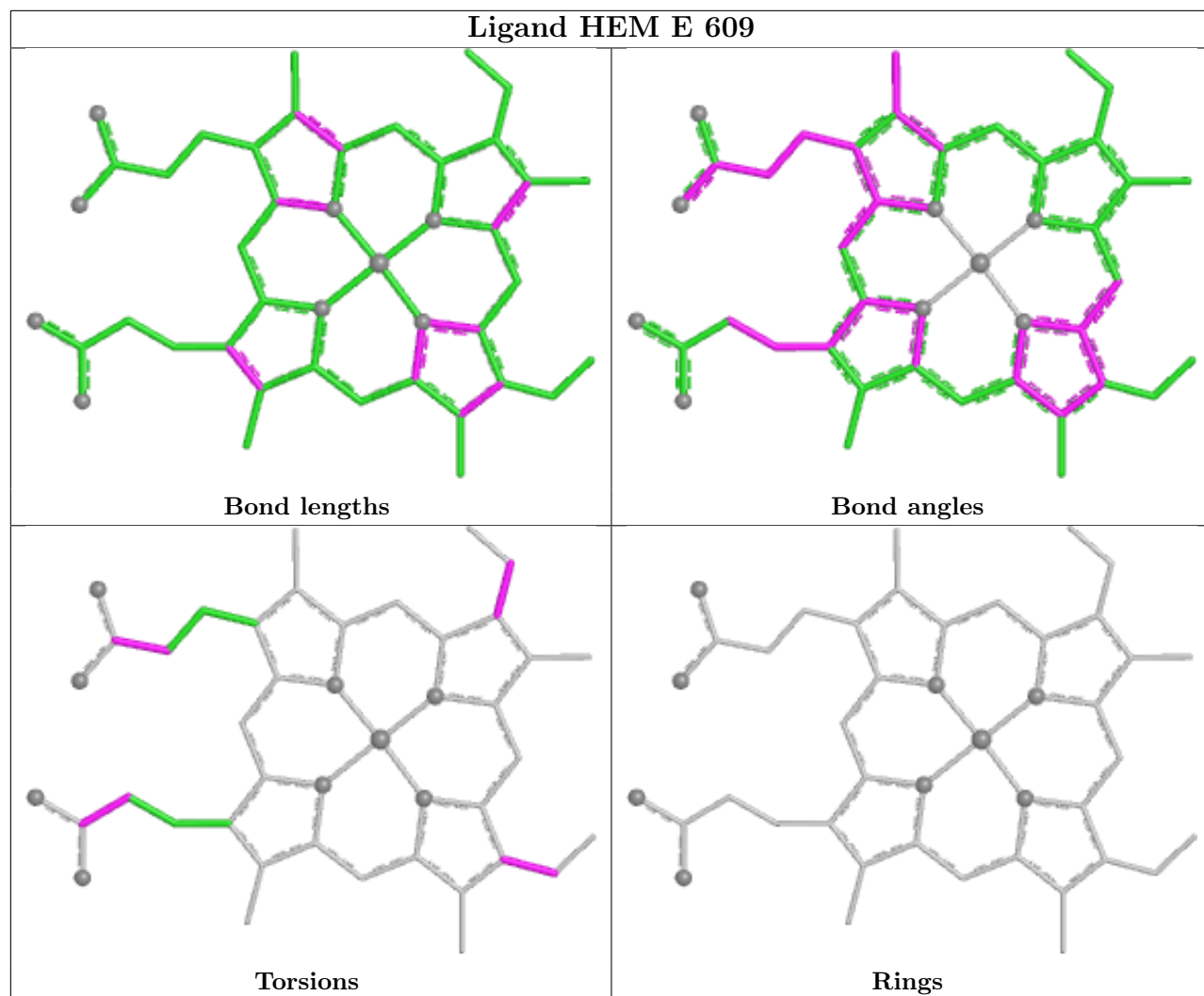
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	606	NAG	1	0
3	B	603	NAG	3	0
3	B	605	NAG	4	0
3	B	609	NAG	3	0
3	E	606	NAG	1	0
7	G	610	MAN	1	0
3	G	601	NAG	1	0
5	E	609	HEM	8	0
6	I	602	BMA	2	0
7	E	602	MAN	4	0
4	I	609	FUC	1	0
3	I	608	NAG	4	0
6	G	609	BMA	8	0
3	G	602	NAG	5	0
3	B	604	NAG	6	0
3	B	607	NAG	1	0
3	E	607	NAG	4	0
3	B	602	NAG	5	0
3	G	603	NAG	2	0
3	I	601	NAG	4	0
6	B	610	BMA	3	0
6	E	601	BMA	5	0
5	B	608	HEM	12	0
3	I	605	NAG	1	0
5	G	607	HEM	11	0
3	B	601	NAG	1	0
7	G	611	MAN	4	0
7	I	604	MAN	1	0

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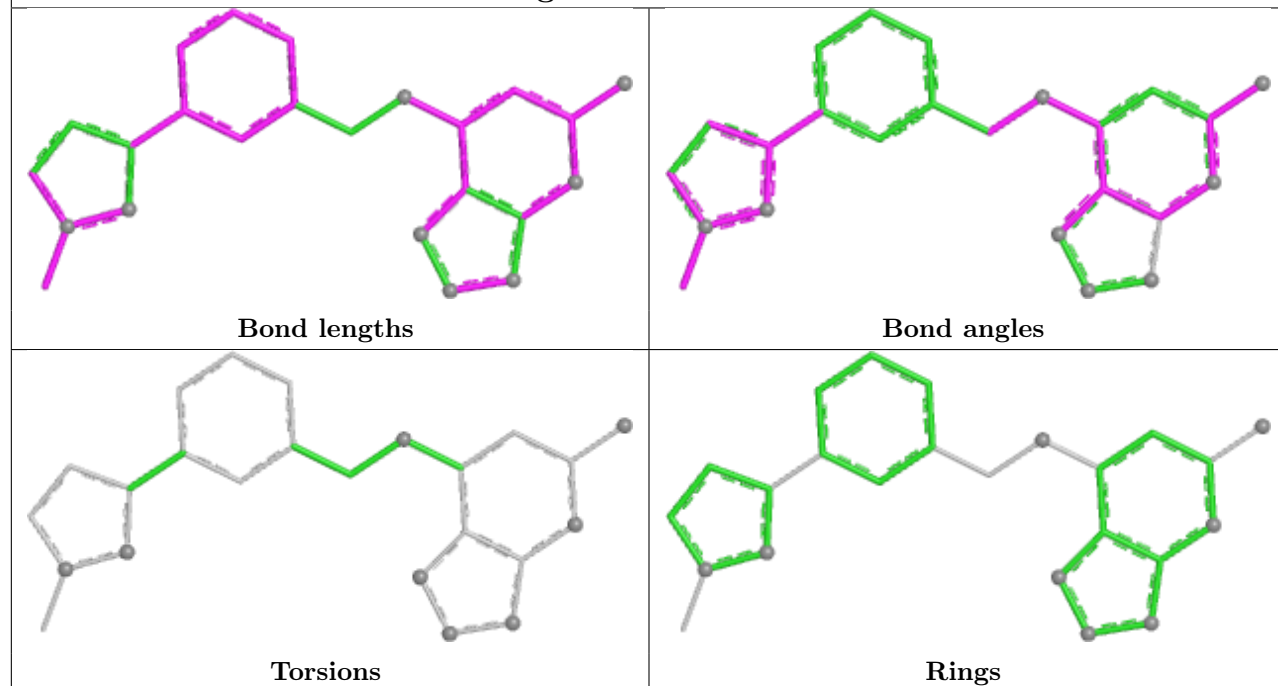
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	605	NAG	4	0
5	I	610	HEM	9	0
3	G	608	NAG	5	0
4	B	606	FUC	1	0
3	G	604	NAG	6	0
3	I	607	NAG	1	0

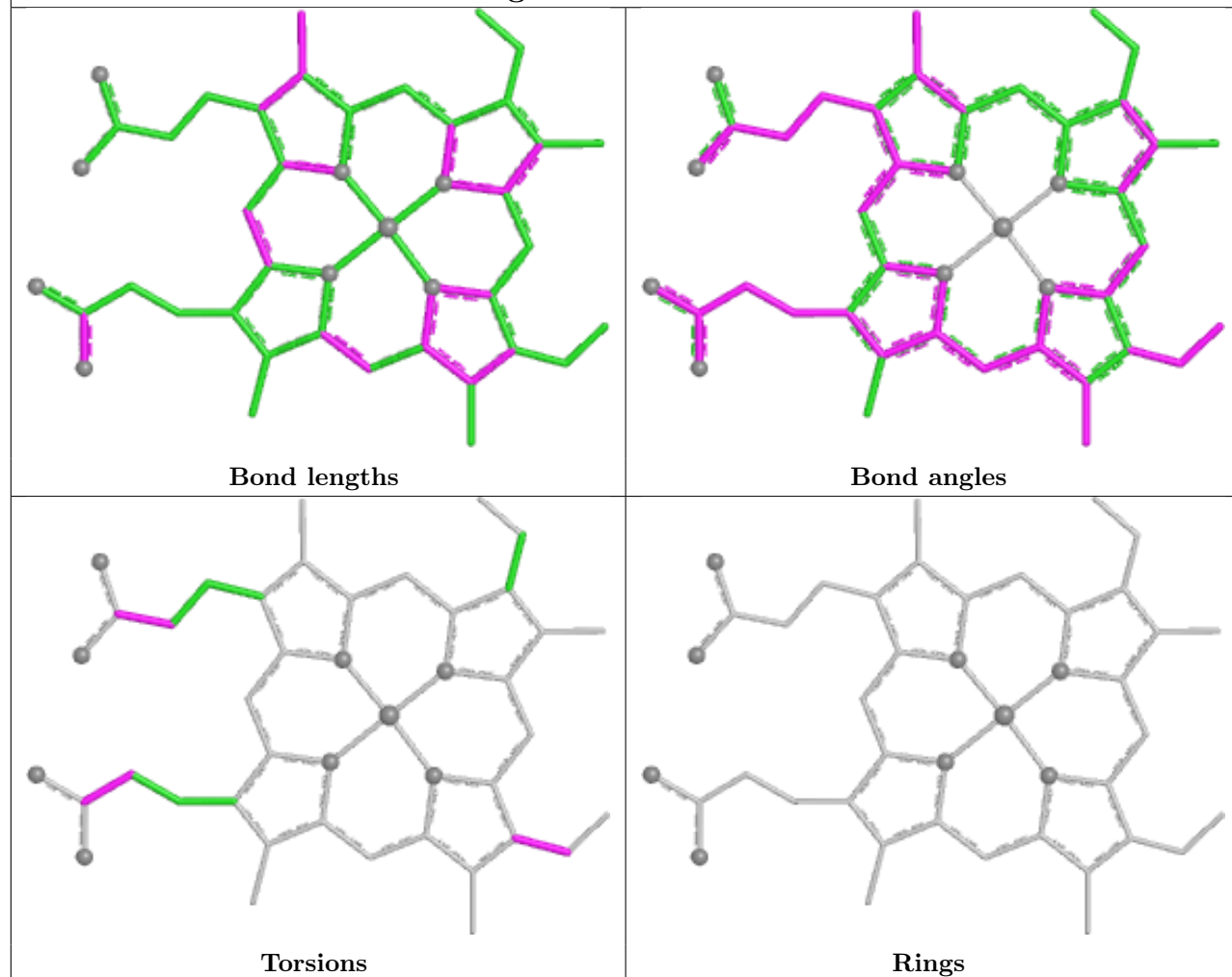
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

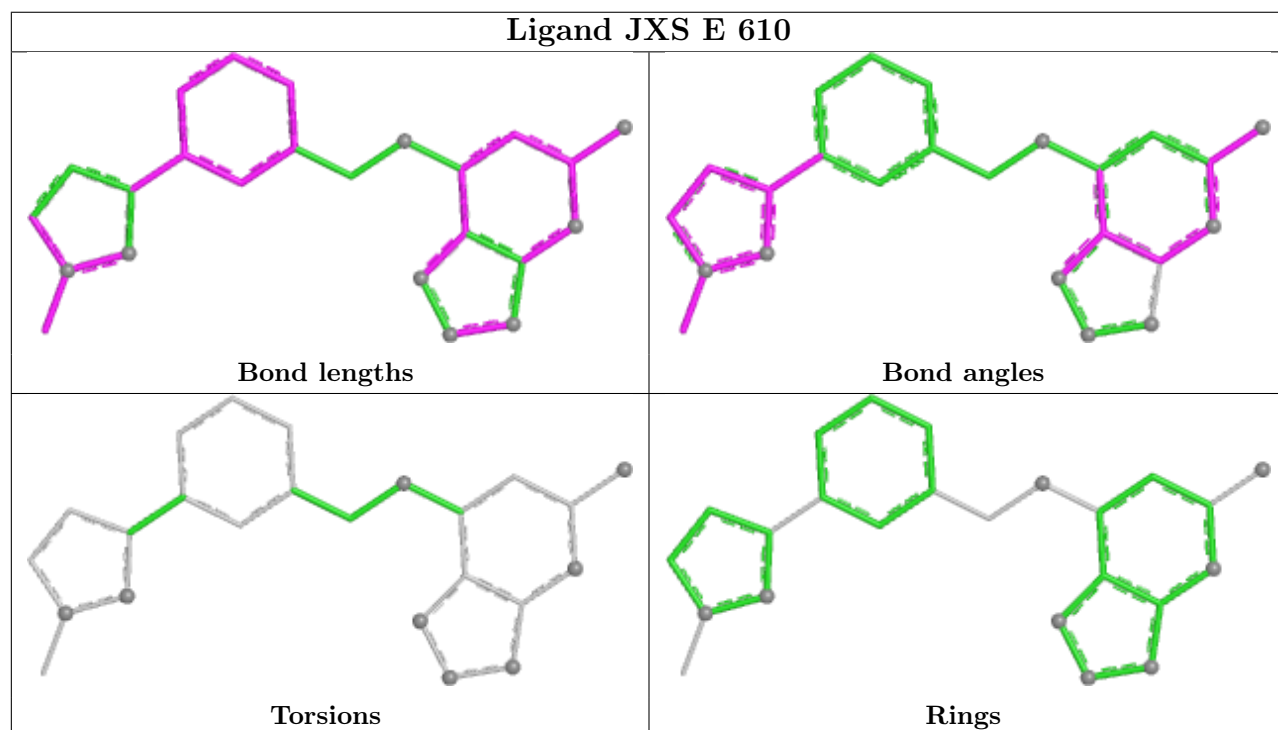
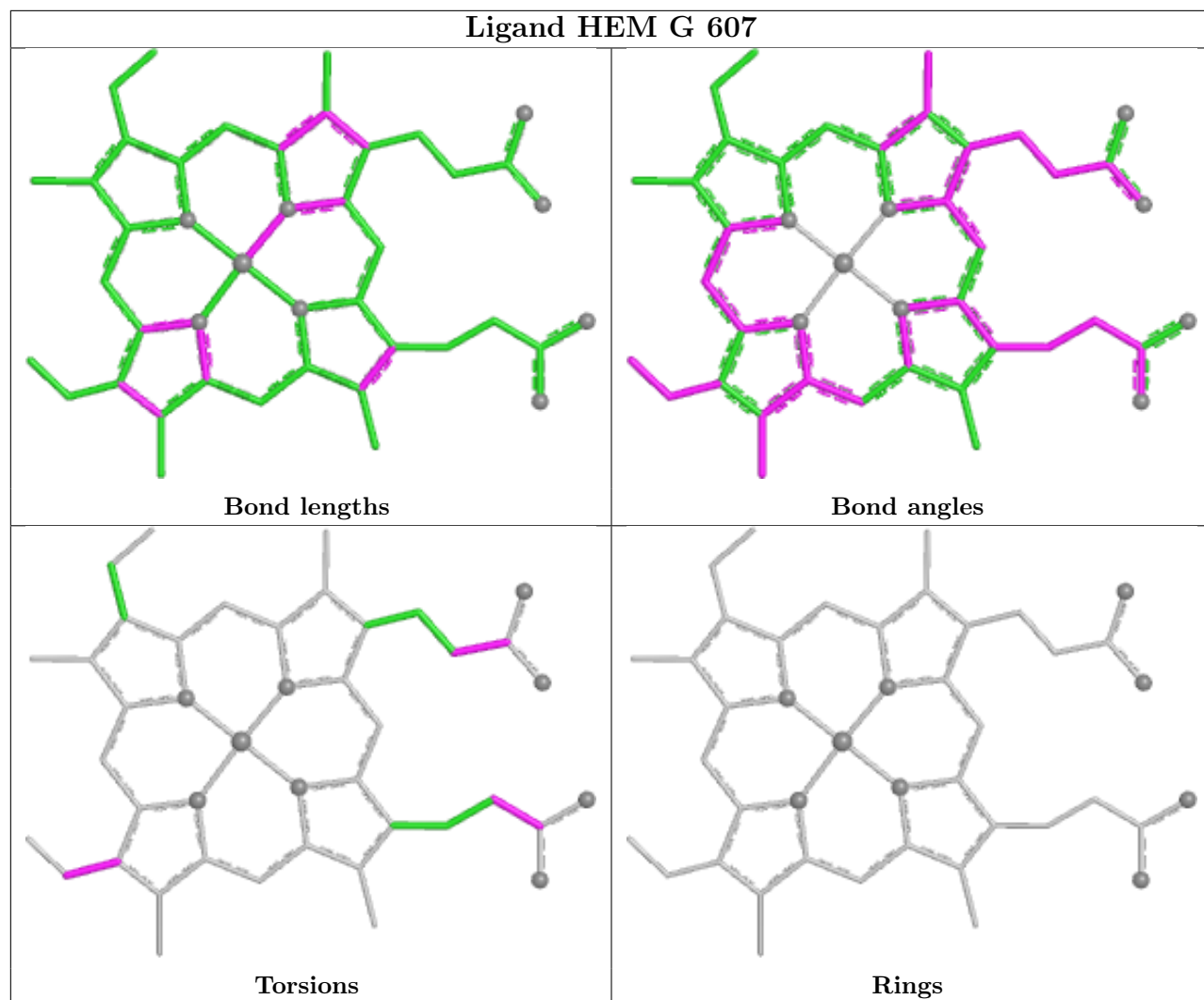


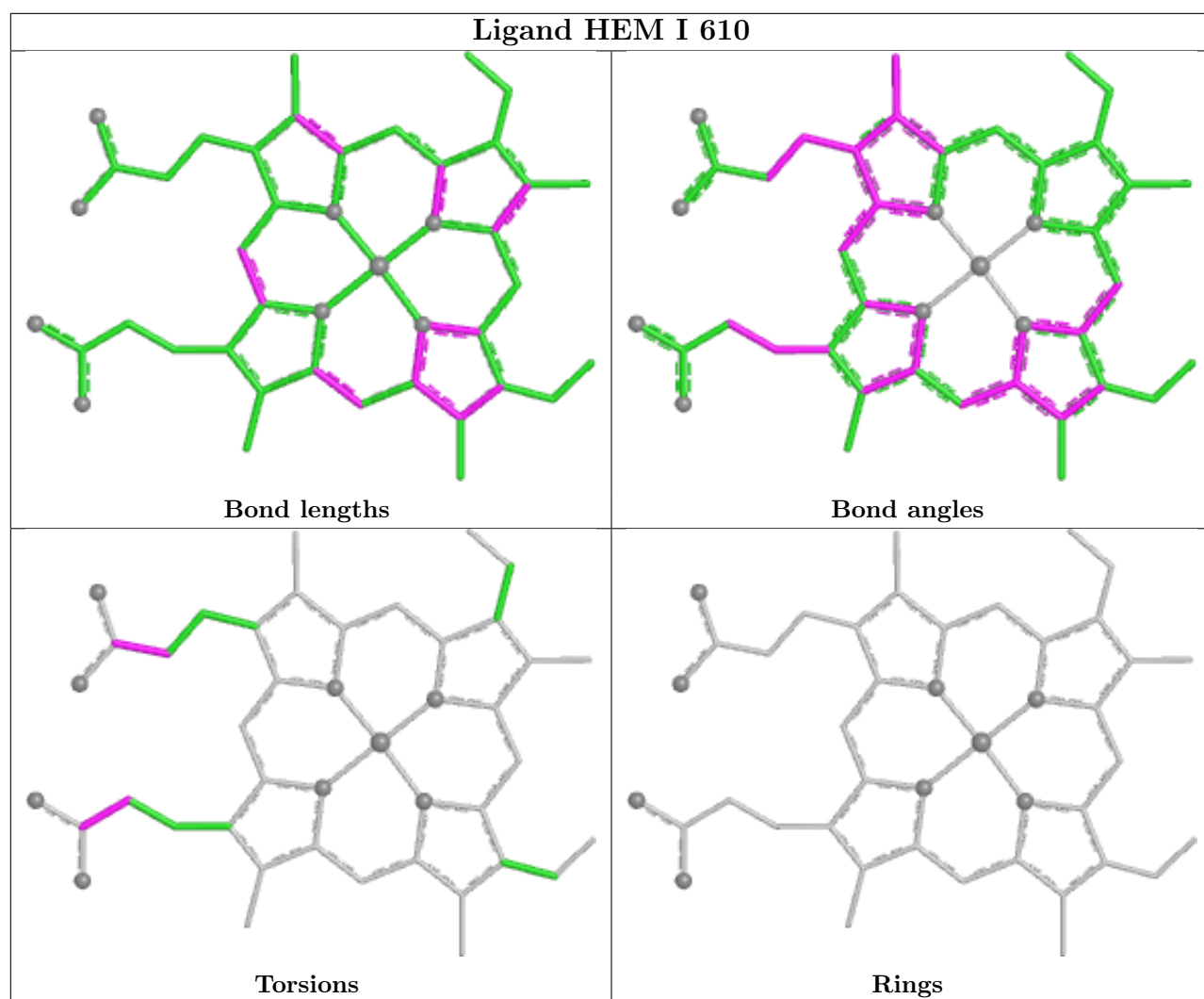
Ligand JXS B 613



Ligand HEM B 608







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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	103/105 (98%)	0.11	0 100 100	29, 51, 77, 85	1 (0%)
1	D	103/105 (98%)	0.31	2 (1%) 66 57	38, 54, 74, 90	2 (1%)
1	F	103/105 (98%)	0.34	2 (1%) 66 57	35, 52, 70, 86	0
1	H	103/105 (98%)	0.17	1 (0%) 79 72	29, 52, 80, 95	1 (0%)
2	B	465/467 (99%)	0.43	13 (2%) 55 44	27, 58, 86, 112	7 (1%)
2	E	465/467 (99%)	0.43	13 (2%) 55 44	32, 58, 79, 90	6 (1%)
2	G	465/467 (99%)	0.26	6 (1%) 75 66	26, 54, 75, 94	7 (1%)
2	I	465/467 (99%)	0.53	18 (3%) 43 34	29, 62, 94, 111	10 (2%)
All	All	2272/2288 (99%)	0.38	55 (2%) 59 49	26, 56, 84, 112	34 (1%)

The worst 5 of 55 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	3.2
2	B	348	ASN	3.0
2	B	248	SER	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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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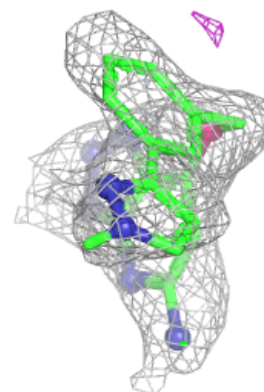
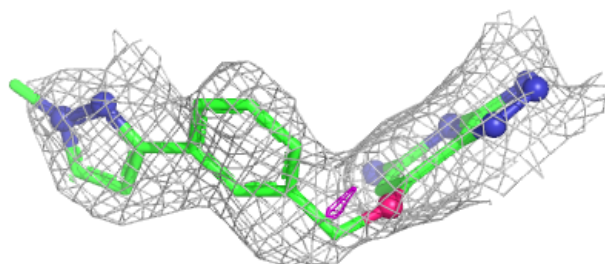
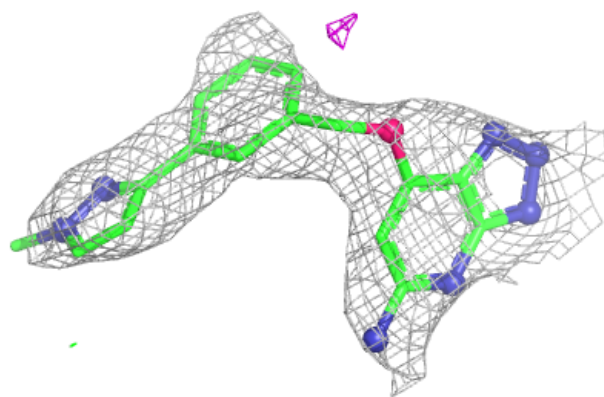
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	HEM	B	608	43/43	0.94	0.11	49,50,54,56	0
3	NAG	G	608	14/15	0.94	0.10	51,54,57,57	0
3	NAG	B	605	14/15	0.95	0.07	35,38,41,42	0
3	NAG	I	601	14/15	0.95	0.08	30,35,37,38	0
5	HEM	E	609	43/43	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
4	FUC	G	605	10/11	0.96	0.09	41,41,42,42	0
10	CL	B	615	1/1	0.97	0.27	62,62,62,62	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.

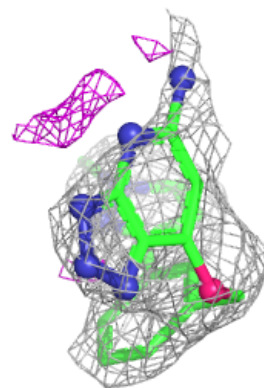
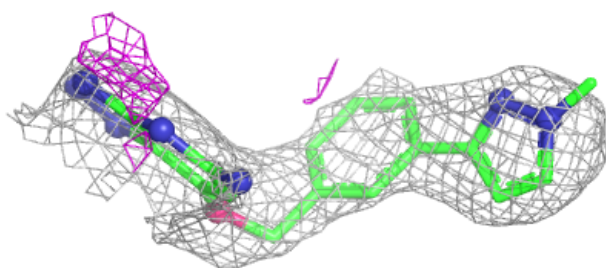
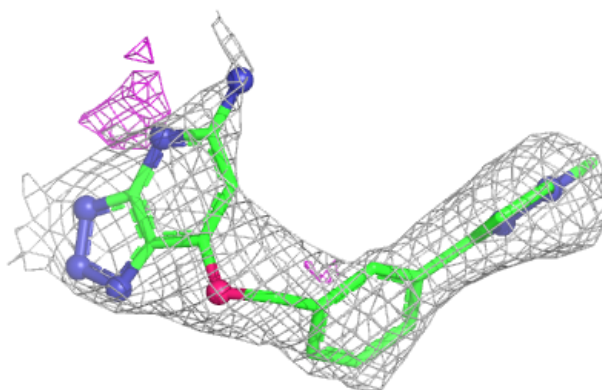
Electron density around JXS B 613:

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

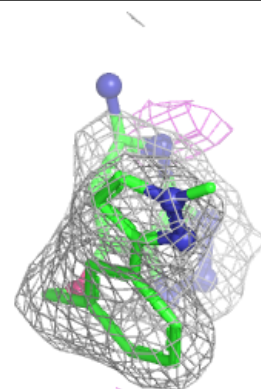
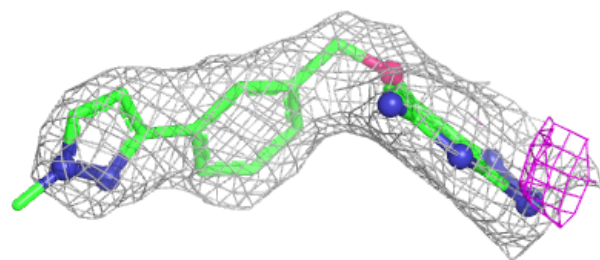
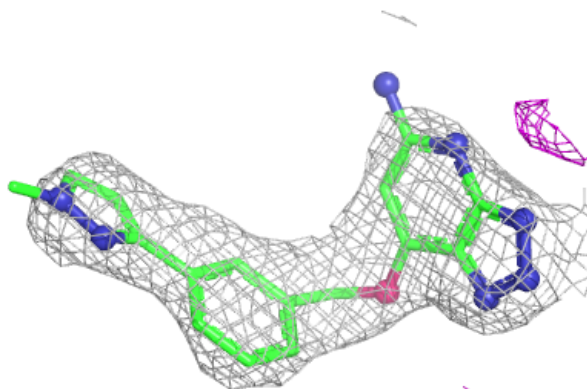


Electron density around JXS E 610:

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

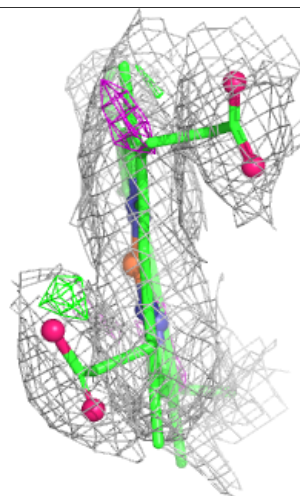
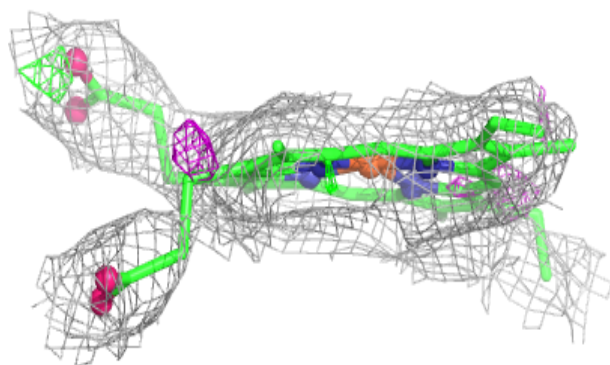
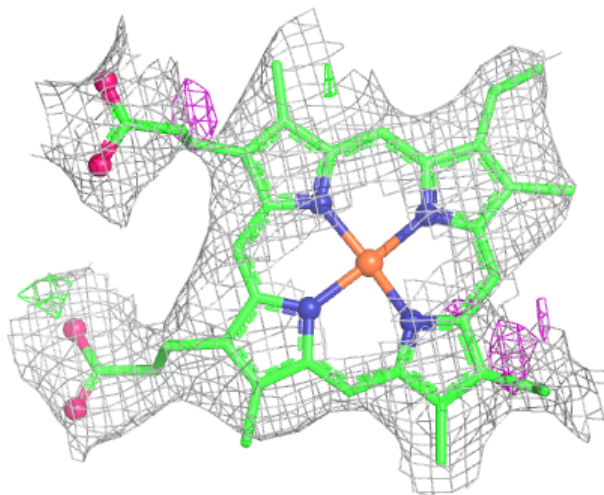
**Electron density around JXS G 612:**

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



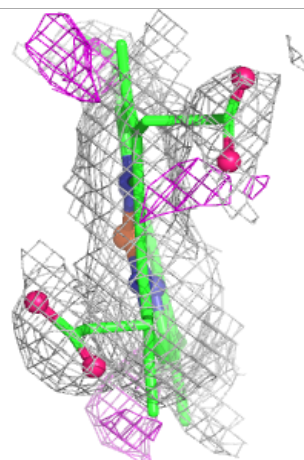
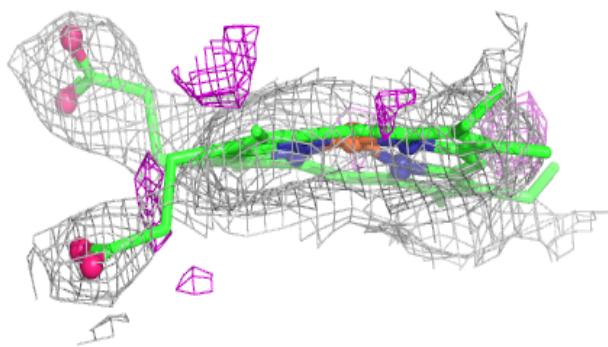
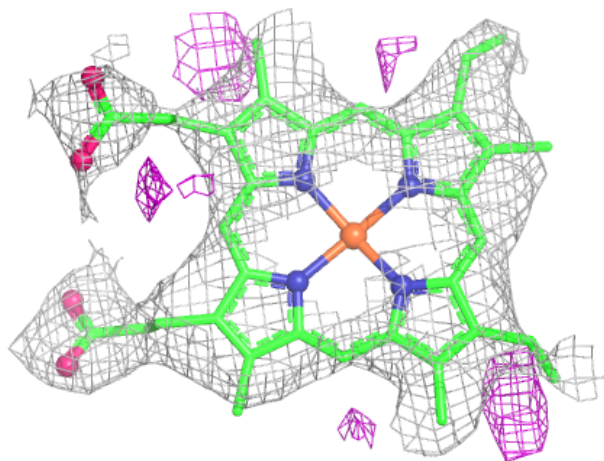
Electron density around HEM B 608:

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



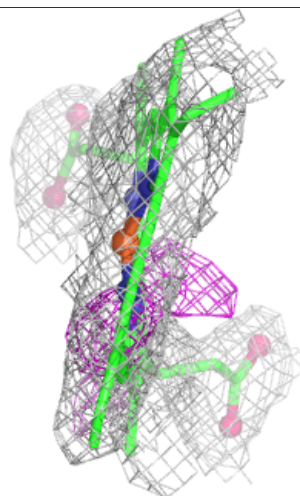
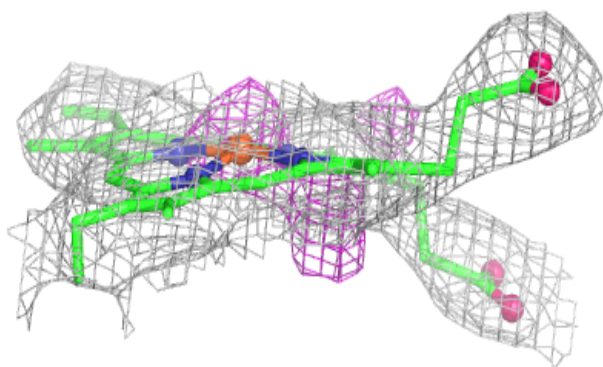
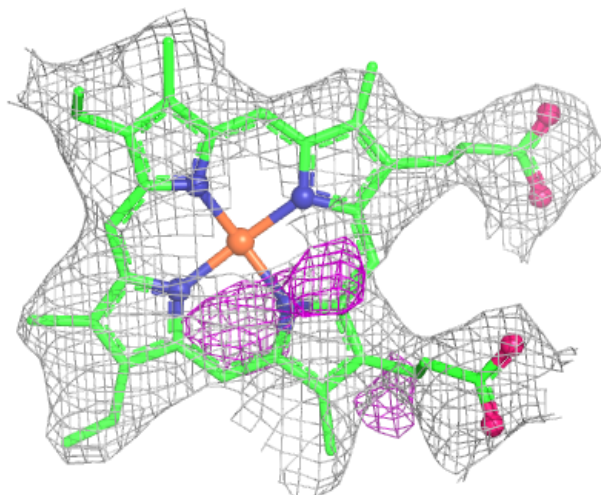
Electron density around HEM E 609:

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



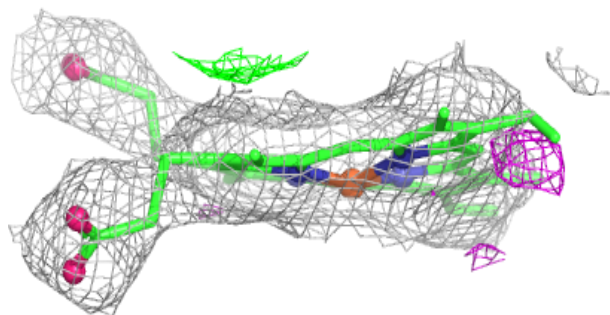
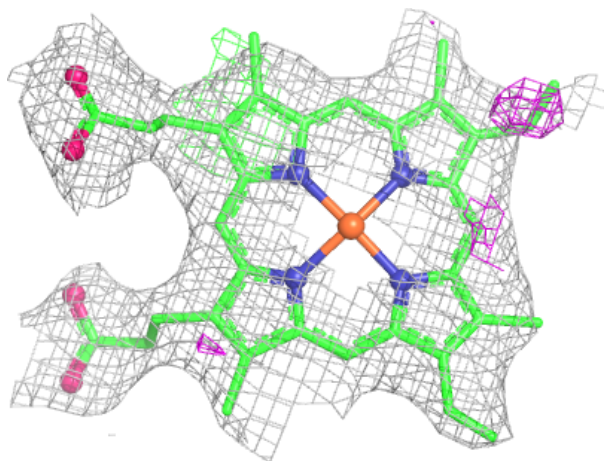
Electron density around HEM G 607:

$2mF_o-DF_c$ (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.