



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:13 AM UTC

PDB ID : 3DQS / pdb_00003dqs
Title : Structure of endothelial NOS heme domain in complex with a inhibitor (+-)-N1-{cis-4'-[(6"-amino-4"-methylpyridin-2"-yl)methyl]pyrrolidin-3'-yl}-N2-(4'-chlorobenzyl)ethane-1,2-diamine
Authors : Igarashi, J.; Li, H.; Poulos, T.L.
Deposited on : 2008-07-09
Resolution : 2.03 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (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

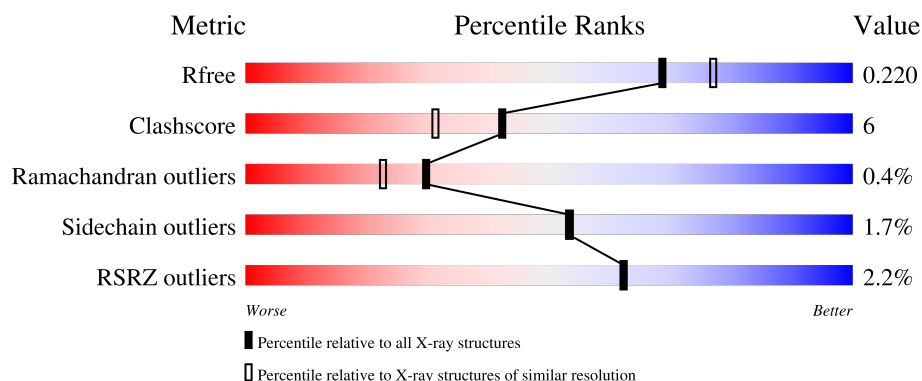
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

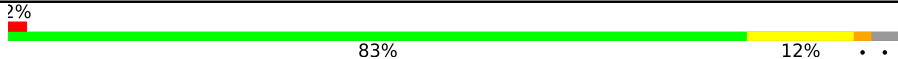
The reported resolution of this entry is 2.03 Å.

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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	416	
1	B	416	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7115 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.

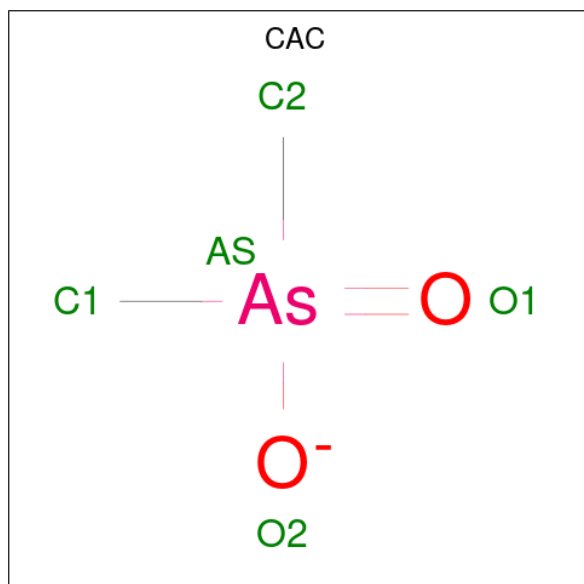
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3216	2046	565	589	16			
1	B	402	Total	C	N	O	S	0	0	0
			3202	2035	565	586	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	variant	UNP P29473
B	100	ARG	CYS	variant	UNP P29473

- Molecule 2 is CACODYLATE ION (CCD ID: CAC) (formula: $\text{C}_2\text{H}_6\text{AsO}_2$).



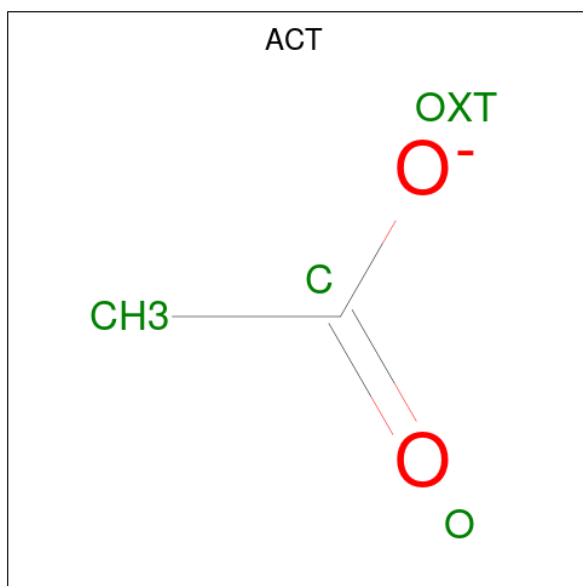
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	As C	0	0
			3	1 2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	As	C	0	0
			3	1	2		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).

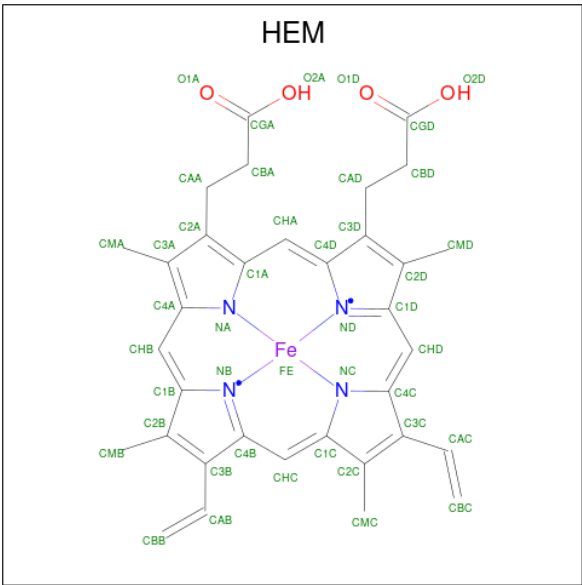


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

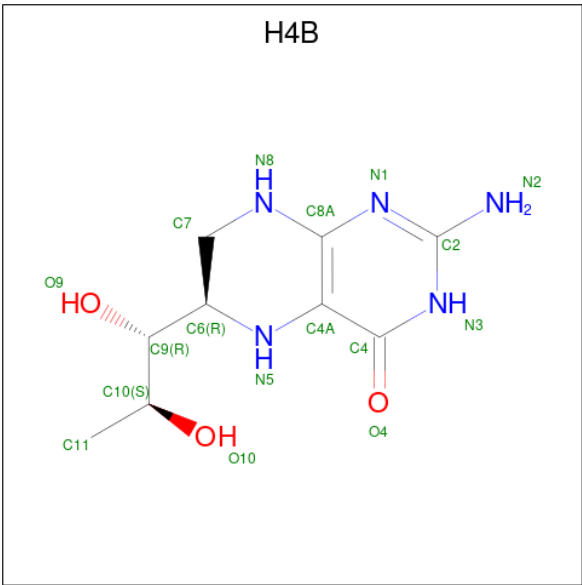
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



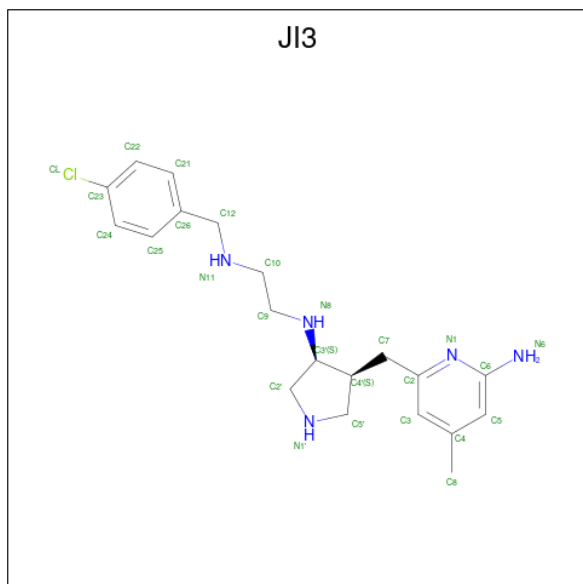
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	1
			48	37	1	4	6		
5	B	1	Total	C	Fe	N	O	0	1
			48	37	1	4	6		

- Molecule 6 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: C₉H₁₅N₅O₃).



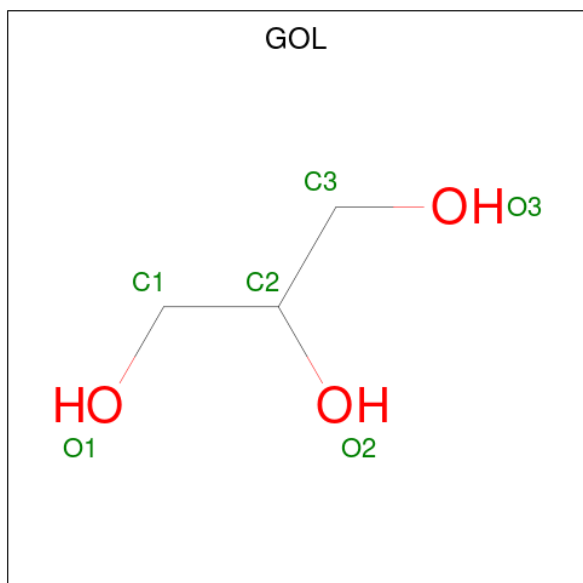
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			17	9	5	3		
6	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 7 is N-{(3S,4S)-4-[(6-AMINO-4-METHYLPYRIDIN-2-YL)METHYL]PYRROLIDIN-3-YL}-N'-(4-CHLOROBENZYL)ETHANE-1,2-DIAMINE (CCD ID: JI3) (formula: $C_{20}H_{28}ClN_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	Cl	N	0	0
			26	20	1	5		
7	B	1	Total	C	Cl	N	0	0
			26	20	1	5		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

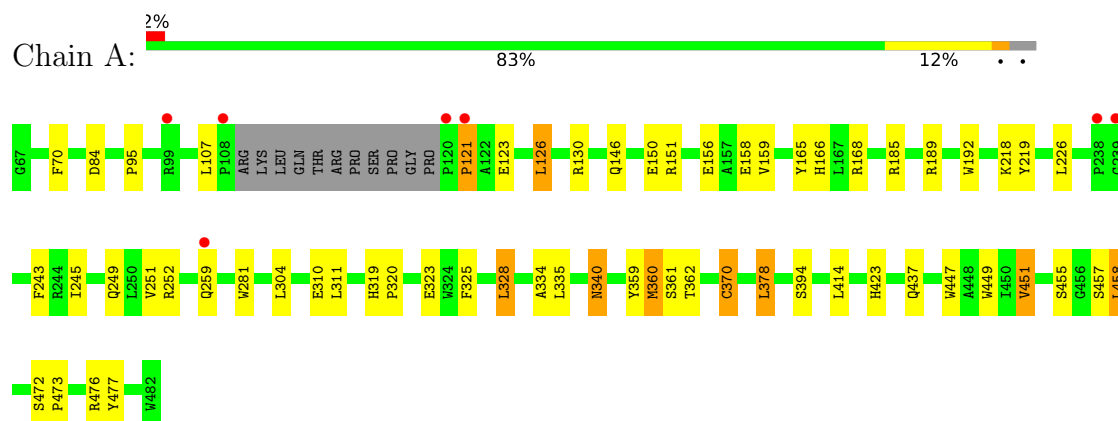
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	250	Total 250	O 250	0	0
9	B	238	Total 238	O 238	0	0

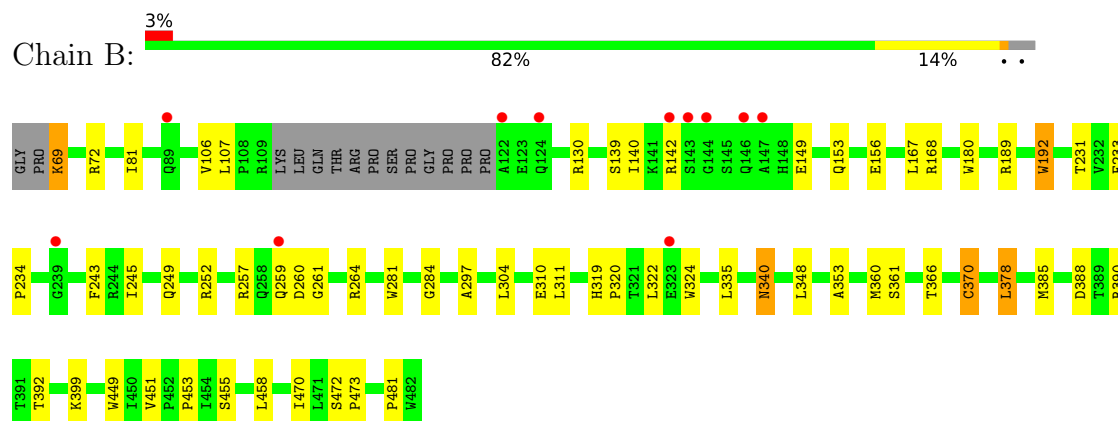
3 Residue-property plots

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: Nitric oxide synthase, endothelial



- Molecule 1: Nitric oxide synthase, endothelial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.96Å 106.84Å 156.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.45 – 2.03 48.45 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.45-2.03) 99.9 (48.45-2.03)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.227 0.191 , 0.220	Depositor DCC
R_{free} test set	3211 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7115	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: JI3, H4B, ACT, ZN, GOL, HEM, CAC

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	0.51	0/3307	0.97	17/4506 (0.4%)
1	B	0.50	0/3290	0.97	15/4480 (0.3%)
All	All	0.51	0/6597	0.97	32/8986 (0.4%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	MET	N-CA-C	-9.09	94.43	109.07
1	B	243	PHE	N-CA-C	-8.73	96.40	110.20
1	A	360	MET	N-CA-C	-8.70	95.06	109.24
1	A	335	LEU	N-CA-C	7.20	121.64	108.69
1	B	451	VAL	CA-C-N	7.16	124.89	119.66
1	B	451	VAL	C-N-CA	7.16	124.89	119.66
1	B	335	LEU	N-CA-C	7.05	121.39	108.69
1	B	361	SER	N-CA-C	6.96	119.75	111.33
1	A	243	PHE	N-CA-C	-6.80	98.53	109.96
1	B	284	GLY	N-CA-C	-6.69	104.76	112.79
1	A	361	SER	N-CA-C	6.63	120.24	111.75
1	B	245	ILE	N-CA-C	-6.23	98.76	107.80
1	B	192	TRP	N-CA-C	6.08	119.53	111.75
1	B	470	ILE	N-CA-C	5.88	116.58	107.99
1	A	226	LEU	N-CA-C	5.82	118.45	110.24
1	A	192	TRP	N-CA-C	5.74	119.10	111.75
1	A	245	ILE	N-CA-C	-5.74	99.48	107.80
1	A	359	TYR	N-CA-C	5.65	118.47	110.50
1	B	168	ARG	N-CA-C	-5.65	102.92	110.55
1	B	370	CYS	N-CA-C	5.49	120.14	113.38
1	A	334	ALA	N-CA-C	5.47	117.33	111.36
1	B	189	ARG	N-CA-C	5.46	119.42	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	ALA	N-CA-C	-5.40	103.13	110.36
1	A	451	VAL	CA-C-N	5.31	123.53	119.66
1	A	451	VAL	C-N-CA	5.31	123.53	119.66
1	A	458	LEU	N-CA-C	-5.27	106.85	113.28
1	A	189	ARG	N-CA-C	5.19	119.24	113.01
1	A	370	CYS	N-CA-C	5.17	119.74	113.38
1	A	394	SER	N-CA-C	-5.15	106.95	113.18
1	A	323	GLU	N-CA-C	5.13	117.61	111.71
1	A	437	GLN	N-CA-C	-5.10	105.72	111.28
1	B	385	MET	N-CA-C	-5.06	106.89	113.16

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3216	0	3121	40	0
1	B	3202	0	3109	40	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	1	0	0	0	0
5	A	48	0	8	2	0
5	B	48	0	8	1	0
6	A	17	0	15	1	0
6	B	17	0	15	1	0
7	A	26	0	28	2	0
7	B	26	0	28	4	0
8	A	6	0	8	0	0
8	B	6	0	8	1	0
9	A	250	0	0	4	0
9	B	238	0	0	3	0
All	All	7115	0	6354	81	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 6.

All (81) 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:A:126:LEU:HD11	1:A:156:GLU:HG2	1.45	0.98
1:B:140:ILE:HD12	1:B:142:ARG:HD2	1.68	0.75
1:B:249:GLN:HB2	1:B:252:ARG:HD3	1.71	0.72
1:A:126:LEU:HD12	1:A:130:ARG:NE	2.08	0.69
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.78	0.66
1:A:249:GLN:HB2	1:A:252:ARG:HG3	1.83	0.61
1:A:310:GLU:HB2	9:A:1027:HOH:O	1.99	0.61
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.42	0.60
1:B:340:ASN:HD22	1:B:340:ASN:H	1.49	0.60
5:A:700[A]:HEM:O2D	7:A:800:JI3:H101	2.01	0.59
1:A:126:LEU:HD12	1:A:130:ARG:HE	1.66	0.59
5:B:700[A]:HEM:O2D	7:B:800:JI3:H101	2.04	0.58
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.45	0.57
1:A:340:ASN:H	1:A:340:ASN:HD22	1.52	0.57
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.87	0.57
1:B:106:VAL:HG21	8:B:880:GOL:H12	1.85	0.57
1:B:130:ARG:HH21	1:B:156:GLU:CD	2.12	0.56
1:A:146:GLN:O	1:A:150:GLU:HG3	2.07	0.55
1:A:249:GLN:HB2	1:A:252:ARG:CG	2.37	0.54
1:B:455:SER:HB3	1:B:458:LEU:HD12	1.89	0.53
1:B:69:LYS:N	1:B:69:LYS:HZ3	2.06	0.52
1:A:259:GLN:HB2	9:A:1113:HOH:O	2.10	0.52
1:A:378:LEU:HB2	9:A:910:HOH:O	2.10	0.52
1:A:472:SER:HA	1:A:473:PRO:C	2.35	0.52
1:B:107:LEU:HD21	7:B:800:JI3:H24	1.92	0.52
1:A:360:MET:HE3	1:A:362:THR:OG1	2.11	0.51
1:A:126:LEU:HD11	1:A:156:GLU:CG	2.31	0.51
1:B:340:ASN:HD22	1:B:340:ASN:N	2.07	0.51
1:B:264:ARG:HH11	1:B:264:ARG:HG3	1.76	0.50
1:B:366:THR:O	1:B:370:CYS:HB2	2.12	0.50
1:A:158:GLU:HG2	1:A:165:TYR:HA	1.94	0.49
1:B:149:GLU:O	1:B:153:GLN:HG3	2.12	0.49
1:A:449:TRP:HA	6:A:760:H4B:N1	2.27	0.49
1:B:449:TRP:HA	6:B:760:H4B:N1	2.27	0.48
1:B:340:ASN:H	1:B:340:ASN:ND2	2.11	0.48
1:A:107:LEU:HD21	7:A:800:JI3:H24	1.96	0.48
1:A:126:LEU:O	1:A:130:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ASN:HD22	1:A:340:ASN:N	2.11	0.47
1:B:231:THR:O	1:B:353:ALA:HA	2.14	0.47
1:B:249:GLN:HB2	1:B:252:ARG:CD	2.42	0.47
1:A:218:LYS:HG2	1:A:311:LEU:HD22	1.97	0.46
1:B:107:LEU:HD21	7:B:800:JI3:C24	2.45	0.46
1:B:130:ARG:NH2	1:B:156:GLU:CD	2.74	0.46
1:A:251:VAL:O	1:A:252:ARG:HG2	2.16	0.45
1:A:447:TRP:CZ2	1:A:451:VAL:HG21	2.52	0.45
1:B:257:ARG:NH1	1:B:261:GLY:O	2.49	0.45
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.52	0.45
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.47	0.44
1:A:151:ARG:HD3	1:A:168:ARG:CZ	2.48	0.44
1:A:477:TYR:OH	5:A:700[A]:HEM:O1D	2.25	0.44
1:B:378:LEU:HB2	9:B:909:HOH:O	2.18	0.44
1:A:423:HIS:HB2	1:B:392:THR:HB	2.00	0.43
1:A:130:ARG:NH1	1:A:156:GLU:OE1	2.51	0.43
1:A:166:HIS:HD2	9:A:1092:HOH:O	1.99	0.43
1:A:325:PHE:O	1:A:328:LEU:HB2	2.17	0.43
1:B:69:LYS:N	1:B:69:LYS:HE2	2.34	0.43
1:B:310:GLU:H	1:B:310:GLU:CD	2.21	0.43
1:A:126:LEU:HD12	1:A:130:ARG:CZ	2.48	0.43
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.53	0.43
1:A:447:TRP:CE2	1:A:451:VAL:HG21	2.53	0.42
1:B:264:ARG:HG3	1:B:264:ARG:NH1	2.34	0.42
1:B:399:LYS:NZ	9:B:1114:HOH:O	2.52	0.42
1:A:70:PHE:HB3	1:A:84:ASP:O	2.19	0.42
1:A:340:ASN:H	1:A:340:ASN:ND2	2.17	0.42
1:A:121:PRO:C	1:A:123:GLU:N	2.76	0.42
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.55	0.42
1:A:126:LEU:HD23	1:A:159:VAL:HG11	2.02	0.42
1:B:259:GLN:H	1:B:259:GLN:HG3	1.57	0.42
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.55	0.41
1:B:140:ILE:CD1	1:B:142:ARG:HD2	2.45	0.41
1:B:72:ARG:NH1	9:B:945:HOH:O	2.53	0.41
1:A:185:ARG:HD3	1:A:449:TRP:CD2	2.55	0.41
1:B:472:SER:HA	1:B:473:PRO:C	2.46	0.41
1:B:69:LYS:N	1:B:69:LYS:CE	2.84	0.41
1:B:72:ARG:NE	1:B:81:ILE:HD13	2.36	0.41
1:B:388:ASP:OD1	1:B:390:ARG:HB2	2.21	0.41
1:A:455:SER:HB3	1:A:458:LEU:HD12	2.02	0.41
1:A:457:SER:OG	1:B:453:PRO:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:TYR:CD1	1:A:219:TYR:C	2.98	0.40
1:B:281:TRP:HB2	1:B:304:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	401/416 (96%)	388 (97%)	12 (3%)	1 (0%)	43	40
1	B	398/416 (96%)	386 (97%)	10 (2%)	2 (0%)	24	17
All	All	799/832 (96%)	774 (97%)	22 (3%)	3 (0%)	30	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	PRO
1	B	260	ASP
1	B	481	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/354 (97%)	337 (98%)	7 (2%)	48	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	342/354 (97%)	337 (98%)	5 (2%)	57	59
All	All	686/708 (97%)	674 (98%)	12 (2%)	53	53

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	PRO
1	A	126	LEU
1	A	328	LEU
1	A	340	ASN
1	A	378	LEU
1	A	414	LEU
1	A	476	ARG
1	B	69	LYS
1	B	139	SER
1	B	311	LEU
1	B	340	ASN
1	B	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	153	GLN
1	A	191	GLN
1	A	259	GLN
1	A	279	HIS
1	A	340	ASN
1	A	413	GLN
1	A	468	ASN
1	A	478	GLN
1	B	124	GLN
1	B	146	GLN
1	B	178	GLN
1	B	222	ASN
1	B	278	GLN
1	B	340	ASN
1	B	410	HIS
1	B	413	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	JI3	B	800	-	27,28,28	2.42	11 (40%)	29,37,37	2.01	5 (17%)
5	HEM	B	700[A]	-	50,50,50	1.23	4 (8%)	67,82,82	1.10	1 (1%)
8	GOL	B	880	-	5,5,5	0.16	0	5,5,5	0.23	0
6	H4B	A	760	-	17,18,18	1.50	4 (23%)	14,26,26	2.10	4 (28%)
6	H4B	B	760	-	17,18,18	1.39	2 (11%)	14,26,26	2.00	3 (21%)
3	ACT	A	860	-	3,3,3	1.02	0	3,3,3	0.78	0
2	CAC	A	850	-	0,2,4	-	-	0,1,6	-	-
5	HEM	B	700[B]	-	50,50,50	1.24	4 (8%)	67,82,82	1.23	3 (4%)
5	HEM	A	700[B]	-	50,50,50	1.42	8 (16%)	67,82,82	1.20	5 (7%)
7	JI3	A	800	-	27,28,28	2.57	10 (37%)	29,37,37	1.99	4 (13%)
8	GOL	A	880	-	5,5,5	0.22	0	5,5,5	0.29	0
2	CAC	B	850	-	0,2,4	-	-	0,1,6	-	-
5	HEM	A	700[A]	-	50,50,50	1.42	8 (16%)	67,82,82	1.11	4 (5%)
3	ACT	B	860	-	3,3,3	0.99	0	3,3,3	0.80	0

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	JI3	B	800	-	-	4/12/22/22	0/3/3/3
5	HEM	B	700[A]	-	-	3/14/54/54	-
8	GOL	B	880	-	-	2/4/4/4	-
6	H4B	B	760	-	-	0/8/17/17	0/2/2/2
7	JI3	A	800	-	-	0/12/22/22	0/3/3/3
5	HEM	A	700[B]	-	-	1/14/54/54	-
5	HEM	A	700[A]	-	-	0/14/54/54	-
8	GOL	A	880	-	-	1/4/4/4	-
5	HEM	B	700[B]	-	-	6/14/54/54	-
6	H4B	A	760	-	-	0/8/17/17	0/2/2/2

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	800	JI3	C7-C4'	5.53	1.60	1.53
7	A	800	JI3	C3-C4	5.24	1.47	1.39
7	A	800	JI3	C5-C4	5.11	1.46	1.39
7	B	800	JI3	C7-C4'	5.07	1.60	1.53
7	B	800	JI3	C5-C4	4.89	1.46	1.39
7	B	800	JI3	C3-C4	4.57	1.46	1.39
7	A	800	JI3	C5-C6	4.36	1.46	1.40
7	B	800	JI3	C5-C6	4.24	1.46	1.40
7	A	800	JI3	C3-C2	4.05	1.45	1.38
6	B	760	H4B	C4A-N5	3.82	1.46	1.37
7	B	800	JI3	C3-C2	3.58	1.44	1.38
7	A	800	JI3	C2-N1	3.56	1.40	1.34
6	A	760	H4B	C4A-N5	3.44	1.45	1.37
5	A	700[A]	HEM	CAB-C3B	-3.16	1.39	1.47
5	A	700[B]	HEM	CAB-C3B	-3.16	1.39	1.47
5	B	700[A]	HEM	FE-NC	3.06	2.05	1.95
5	B	700[B]	HEM	FE-NC	3.06	2.05	1.95
7	B	800	JI3	C24-C23	3.01	1.43	1.38
5	B	700[A]	HEM	FE-NA	2.98	2.05	1.95
5	B	700[B]	HEM	FE-NA	2.98	2.05	1.95
5	B	700[A]	HEM	FE-NB	2.97	2.04	1.94
5	B	700[B]	HEM	FE-NB	2.97	2.04	1.94
5	A	700[A]	HEM	FE-NC	2.96	2.04	1.95
5	A	700[B]	HEM	FE-NC	2.96	2.04	1.95
5	A	700[A]	HEM	FE-NA	2.83	2.04	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	700[B]	HEM	FE-NA	2.83	2.04	1.95
7	B	800	JI3	C25-C24	2.80	1.43	1.38
7	B	800	JI3	C2-N1	2.77	1.39	1.34
7	A	800	JI3	C22-C23	2.67	1.43	1.38
5	A	700[A]	HEM	FE-NB	2.59	2.02	1.94
5	A	700[B]	HEM	FE-NB	2.59	2.02	1.94
7	A	800	JI3	C24-C23	2.54	1.42	1.38
5	B	700[A]	HEM	CHC-C4B	2.52	1.44	1.39
5	B	700[B]	HEM	CHC-C4B	2.52	1.44	1.39
6	B	760	H4B	C6-N5	2.51	1.51	1.47
7	B	800	JI3	C22-C21	2.47	1.42	1.38
7	A	800	JI3	C25-C24	2.45	1.42	1.38
5	A	700[A]	HEM	FE-ND	2.43	2.02	1.94
5	A	700[B]	HEM	FE-ND	2.43	2.02	1.94
7	B	800	JI3	C22-C23	2.38	1.42	1.38
6	A	760	H4B	C6-N5	2.34	1.51	1.47
5	A	700[A]	HEM	CAC-C3C	-2.24	1.41	1.47
5	A	700[B]	HEM	CAC-C3C	-2.24	1.41	1.47
7	A	800	JI3	C22-C21	2.15	1.42	1.38
5	A	700[A]	HEM	CMA-C3A	2.14	1.55	1.50
5	A	700[B]	HEM	CMA-C3A	2.14	1.55	1.50
7	B	800	JI3	C21-C26	2.13	1.43	1.38
6	A	760	H4B	C4-N3	2.13	1.42	1.38
6	A	760	H4B	C7-N8	2.07	1.48	1.46
5	A	700[A]	HEM	CHA-C4D	2.04	1.42	1.38
5	A	700[B]	HEM	CHA-C4D	2.04	1.42	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	800	JI3	C6-N1-C2	8.09	124.12	118.07
7	B	800	JI3	C6-N1-C2	7.98	124.04	118.07
5	B	700[A]	HEM	CBA-CAA-C2A	-6.03	95.87	112.53
5	B	700[B]	HEM	CBA-CAA-C2A	-6.03	95.87	112.53
6	A	760	H4B	C2-N1-C8A	5.16	122.47	113.36
6	B	760	H4B	C2-N1-C8A	5.09	122.34	113.36
5	A	700[A]	HEM	CBA-CAA-C2A	-4.51	100.05	112.53
5	A	700[B]	HEM	CBA-CAA-C2A	-4.51	100.05	112.53
6	A	760	H4B	O10-C10-C9	-3.74	103.58	109.77
6	B	760	H4B	O10-C10-C9	-3.50	103.97	109.77
5	B	700[B]	HEM	CAD-C3D-C4D	3.44	130.69	124.70
6	A	760	H4B	N3-C2-N1	-3.18	117.50	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	700[B]	HEM	CAD-C3D-C2D	-2.96	122.32	127.87
6	B	760	H4B	N3-C2-N1	-2.95	117.92	123.32
7	A	800	JI3	C3-C4-C5	2.94	121.38	118.11
7	B	800	JI3	C3-C4-C5	2.93	121.37	118.11
5	A	700[A]	HEM	CMD-C2D-C1D	2.90	129.57	125.03
5	A	700[B]	HEM	CMD-C2D-C1D	2.90	129.57	125.03
5	A	700[B]	HEM	CBD-CAD-C3D	2.81	120.31	112.53
7	B	800	JI3	C2'-C3'-N8	-2.72	108.89	113.73
7	A	800	JI3	C5'-C4'-C3'	-2.46	99.70	103.97
7	A	800	JI3	C2'-C3'-N8	-2.42	109.42	113.73
5	A	700[A]	HEM	CMC-C2C-C1C	2.27	128.72	124.73
5	A	700[B]	HEM	CMC-C2C-C1C	2.27	128.72	124.73
6	A	760	H4B	O9-C9-C6	2.27	114.71	109.28
7	B	800	JI3	C5'-C4'-C3'	-2.23	100.11	103.97
7	B	800	JI3	N6-C6-N1	2.16	120.07	116.59
5	A	700[A]	HEM	CHC-C1C-NC	-2.15	122.12	124.45
5	A	700[B]	HEM	CHC-C1C-NC	-2.15	122.12	124.45

There are no chirality outliers.

All (17) torsion outliers are listed below:

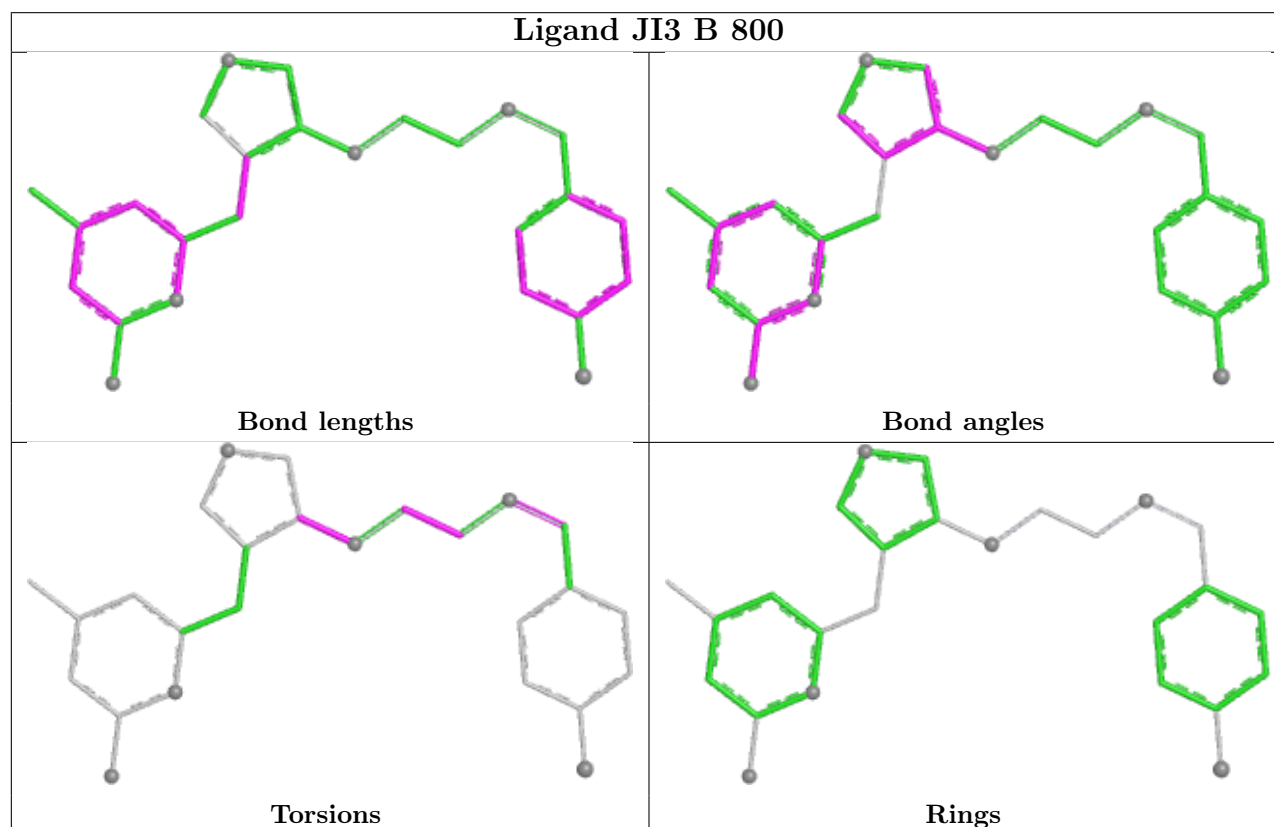
Mol	Chain	Res	Type	Atoms
8	B	880	GOL	O1-C1-C2-C3
8	B	880	GOL	O1-C1-C2-O2
8	A	880	GOL	O1-C1-C2-O2
7	B	800	JI3	C26-C12-N11-C10
7	B	800	JI3	N11-C10-C9-N8
5	B	700[A]	HEM	C4B-C3B-CAB-CBB
5	B	700[B]	HEM	C4B-C3B-CAB-CBB
7	B	800	JI3	C2'-C3'-N8-C9
5	B	700[B]	HEM	CAD-CBD-CGD-O2D
5	B	700[B]	HEM	CAD-CBD-CGD-O1D
5	B	700[A]	HEM	CAA-CBA-CGA-O2A
5	B	700[B]	HEM	CAA-CBA-CGA-O2A
5	B	700[A]	HEM	CAA-CBA-CGA-O1A
5	B	700[B]	HEM	CAA-CBA-CGA-O1A
7	B	800	JI3	C4'-C3'-N8-C9
5	B	700[B]	HEM	C3D-CAD-CBD-CGD
5	A	700[B]	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

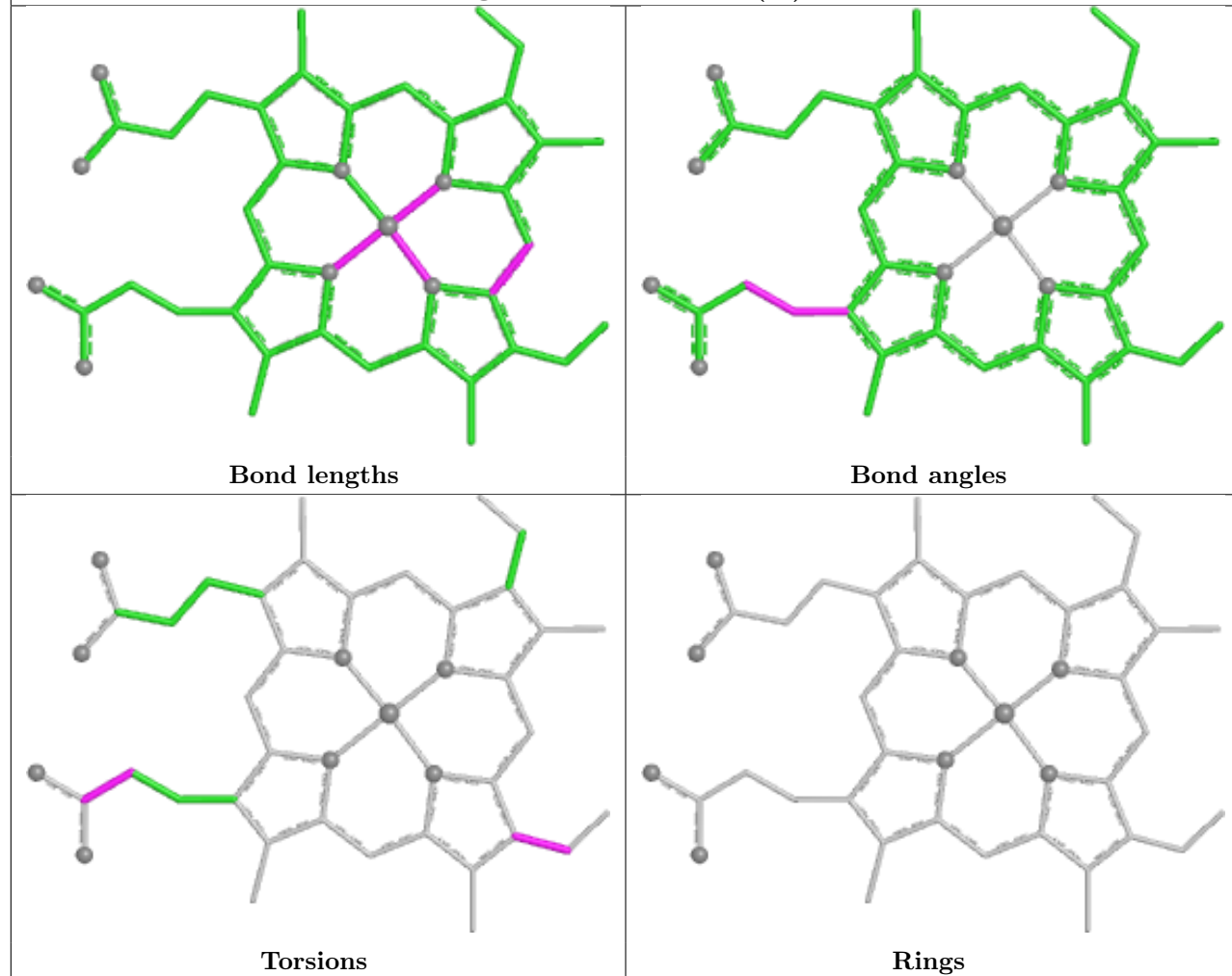
7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	800	JI3	4	0
5	B	700[A]	HEM	1	0
8	B	880	GOL	1	0
6	A	760	H4B	1	0
6	B	760	H4B	1	0
7	A	800	JI3	2	0
5	A	700[A]	HEM	2	0

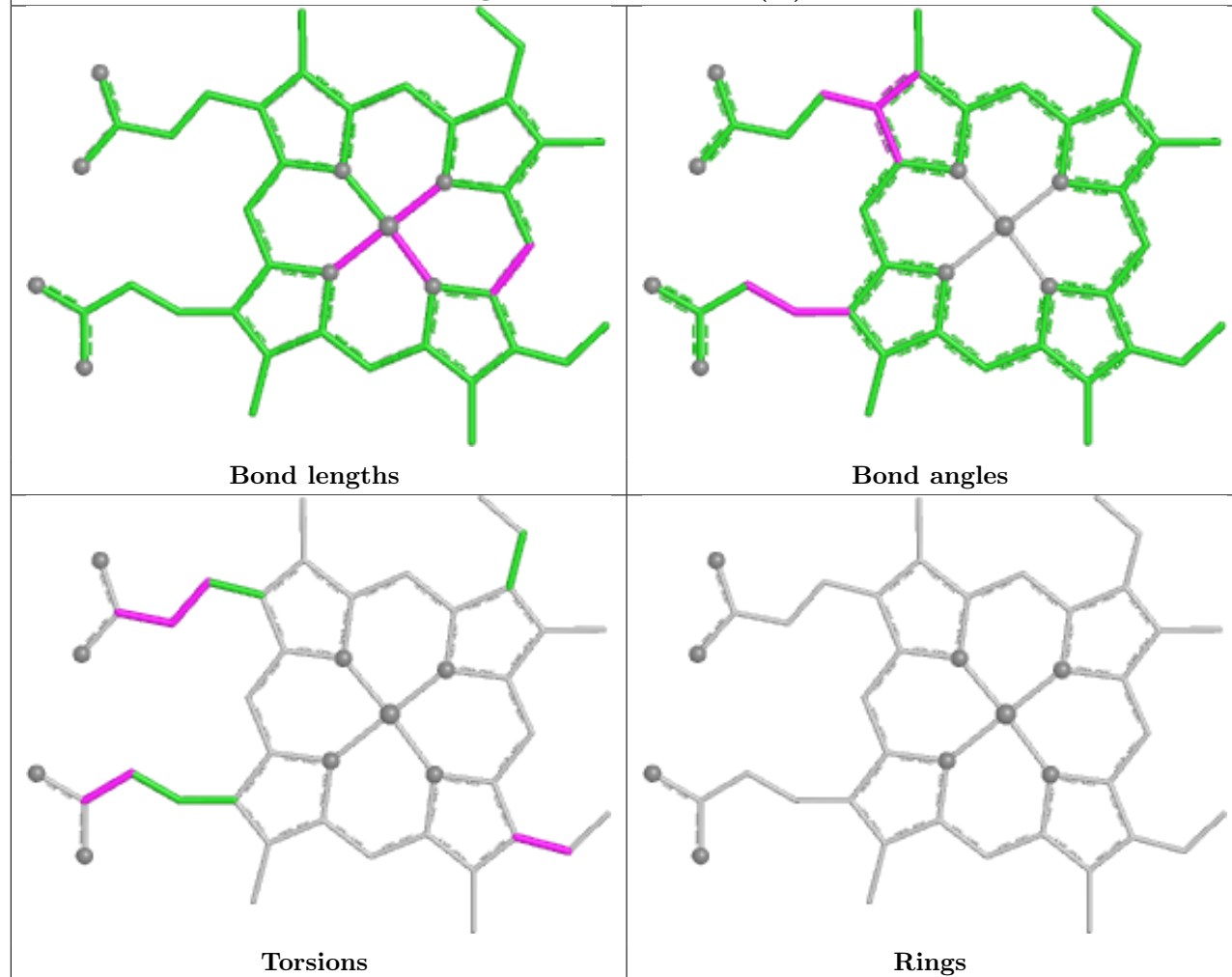
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



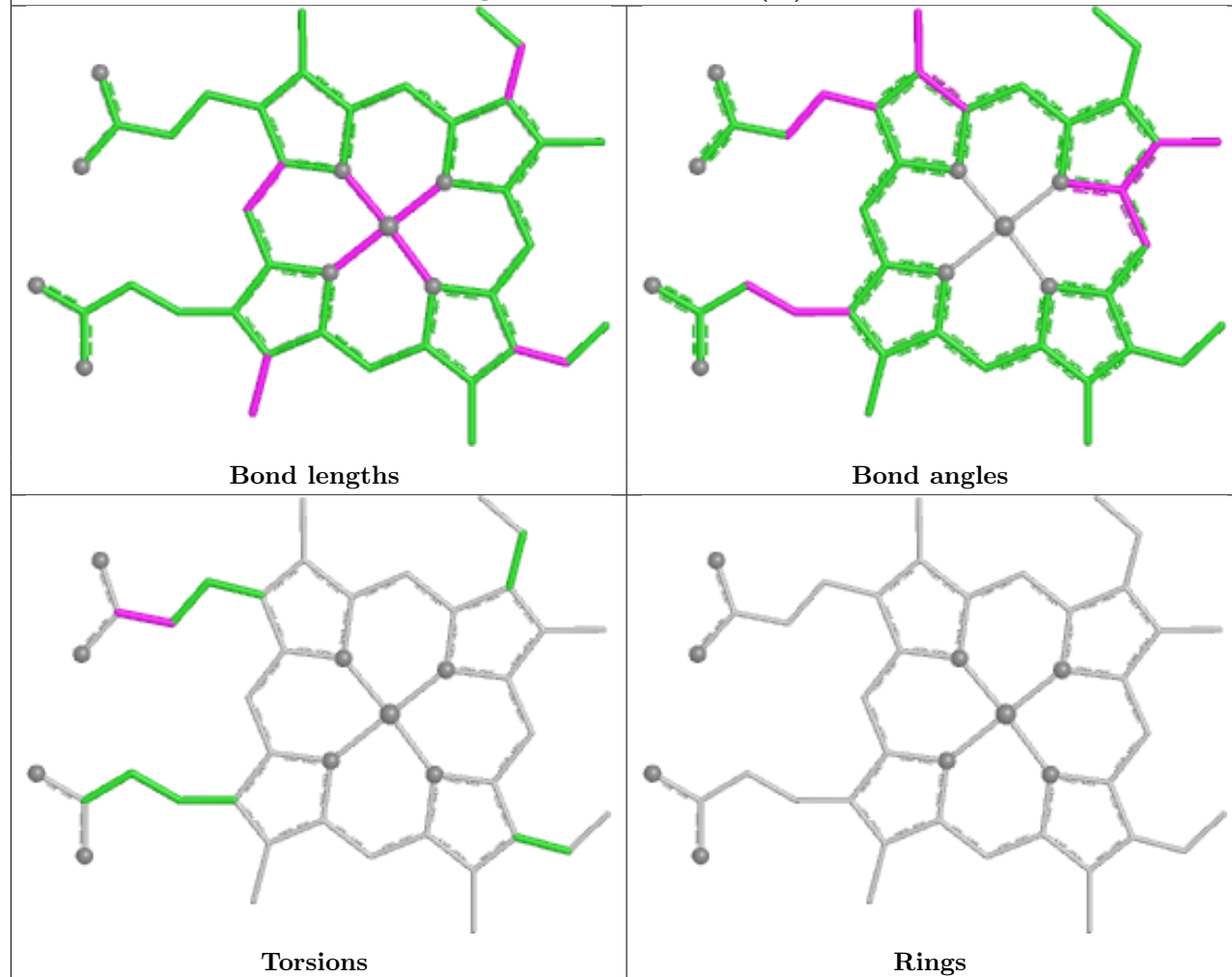
Ligand HEM B 700 (A)

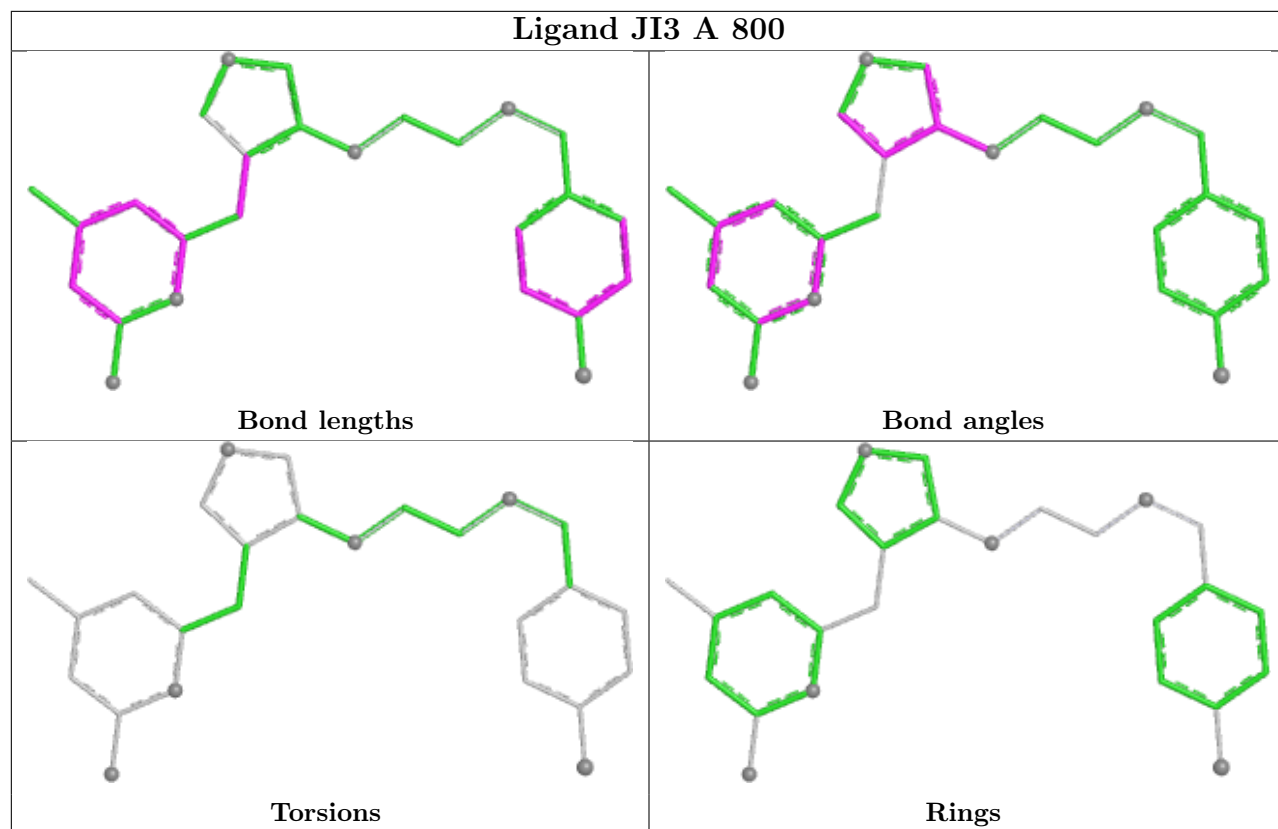


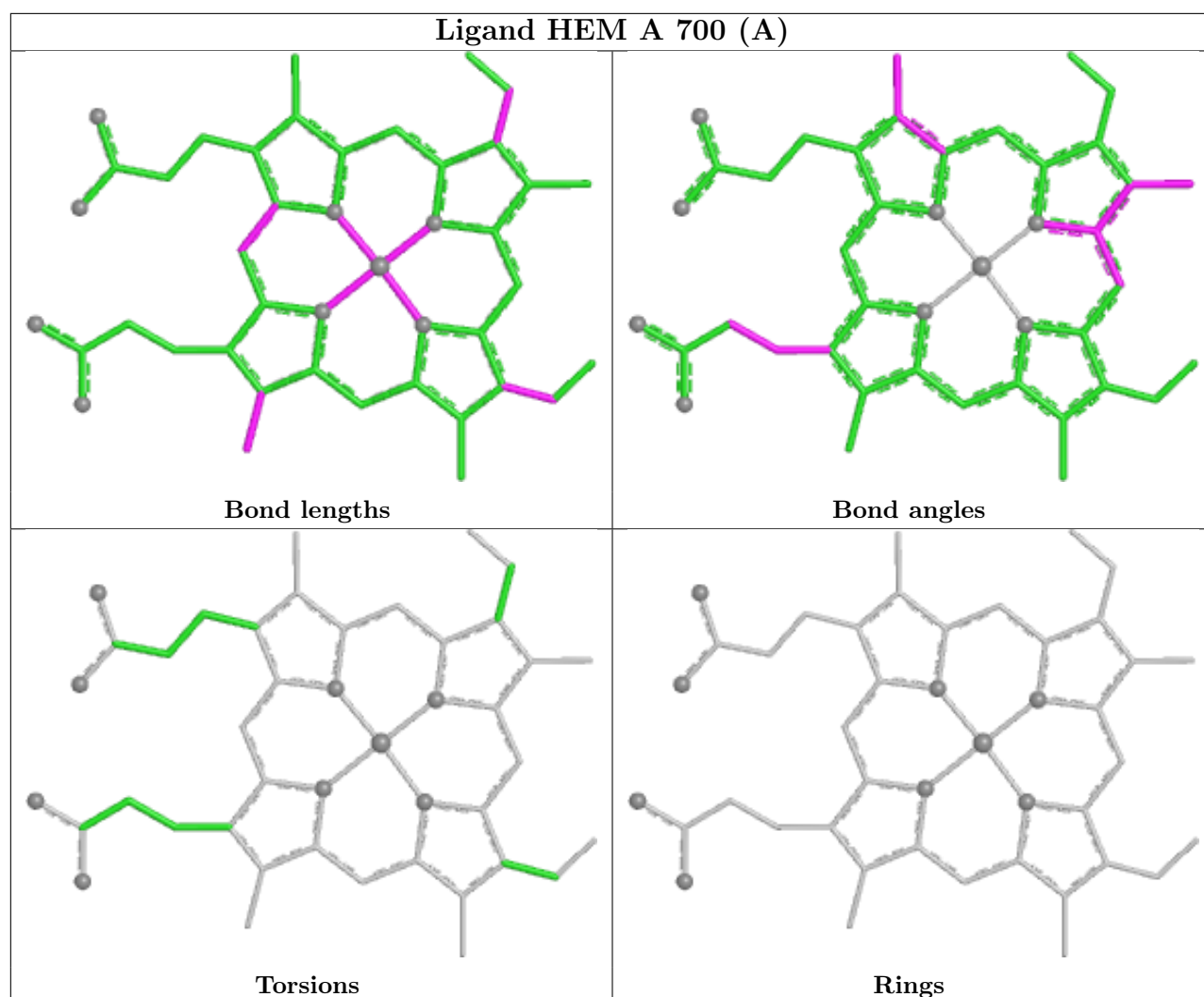
Ligand HEM B 700 (B)



Ligand HEM A 700 (B)







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	405/416 (97%)	0.11	7 (1%) 69 69	24, 34, 54, 77	0
1	B	402/416 (96%)	0.22	11 (2%) 56 56	25, 37, 54, 67	0
All	All	807/832 (96%)	0.17	18 (2%) 62 62	24, 36, 54, 77	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	PRO	3.6
1	A	120	PRO	3.6
1	B	259	GLN	3.1
1	B	142	ARG	2.8
1	B	239	GLY	2.7
1	A	99	ARG	2.6
1	B	323	GLU	2.5
1	B	124	GLN	2.5
1	A	239	GLY	2.4
1	B	143	SER	2.4
1	A	259	GLN	2.4
1	B	122	ALA	2.3
1	B	146	GLN	2.2
1	B	89	GLN	2.2
1	A	238	PRO	2.2
1	B	144	GLY	2.2
1	B	147	ALA	2.1
1	A	121	PRO	2.1

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

There are no oligosaccharides in this entry.

6.4 Ligands

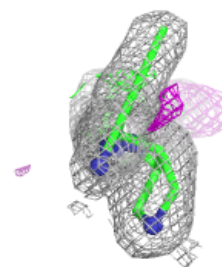
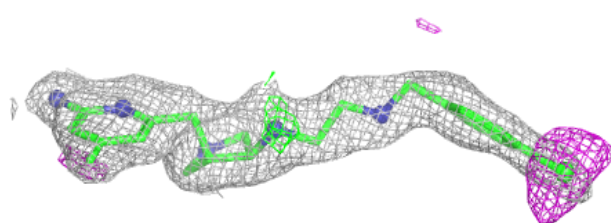
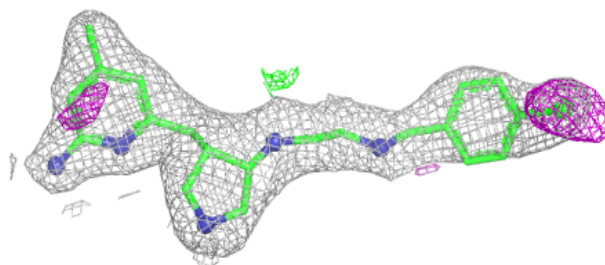
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GOL	A	880	6/6	0.85	0.17	48,50,50,51	0
7	JI3	B	800	26/26	0.87	0.13	30,36,53,56	0
8	GOL	B	880	6/6	0.87	0.17	50,52,52,53	0
7	JI3	A	800	26/26	0.88	0.11	25,34,55,59	0
3	ACT	B	860	4/4	0.95	0.10	42,42,42,43	0
6	H4B	B	760	17/17	0.95	0.07	33,34,34,34	0
3	ACT	A	860	4/4	0.95	0.08	41,41,42,42	0
6	H4B	A	760	17/17	0.97	0.06	30,31,33,33	0
2	CAC	B	850	3/5	0.97	0.14	56,56,56,56	0
5	HEM	A	700[A]	43/43	0.98	0.06	23,25,30,33	5
5	HEM	A	700[B]	43/43	0.98	0.06	23,25,29,30	5
5	HEM	B	700[A]	43/43	0.98	0.06	26,28,34,35	5
5	HEM	B	700[B]	43/43	0.98	0.06	26,28,32,34	5
2	CAC	A	850	3/5	0.98	0.09	44,44,45,48	0
4	ZN	A	900	1/1	1.00	0.01	29,29,29,29	0

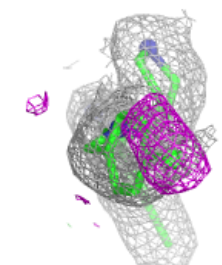
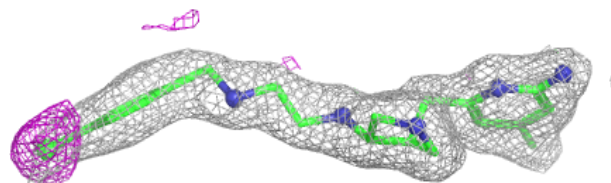
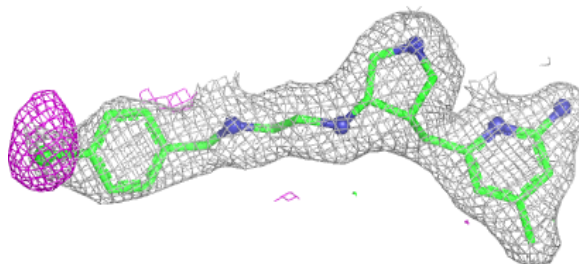
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around JI3 B 800:

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

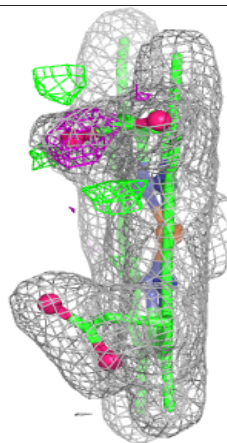
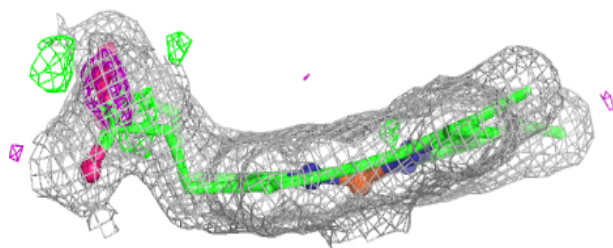
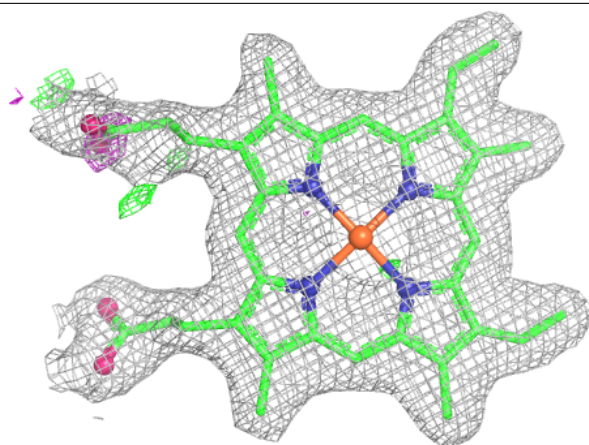
**Electron density around JI3 A 800:**

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



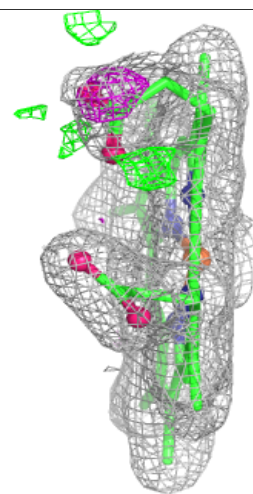
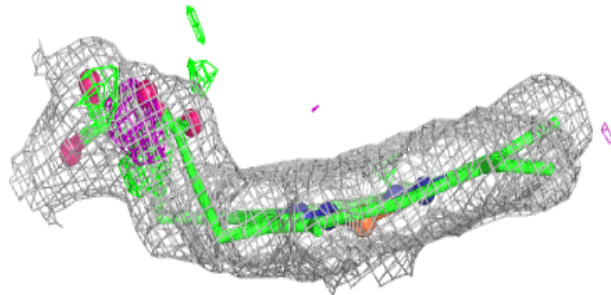
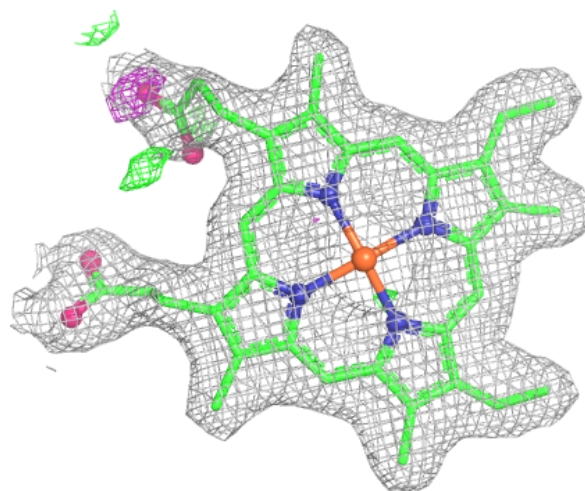
Electron density around HEM A 700 (A):

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



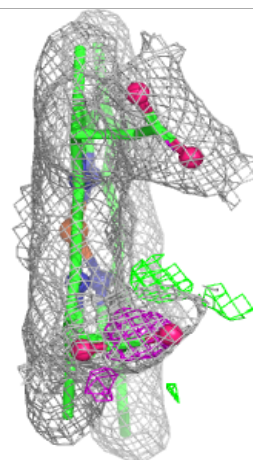
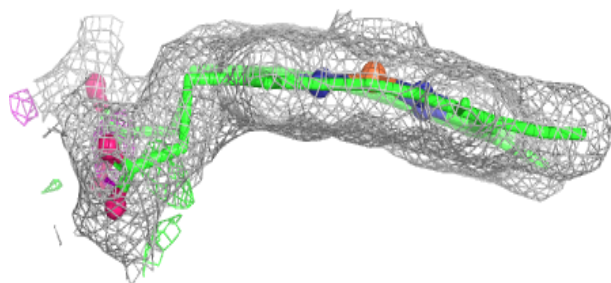
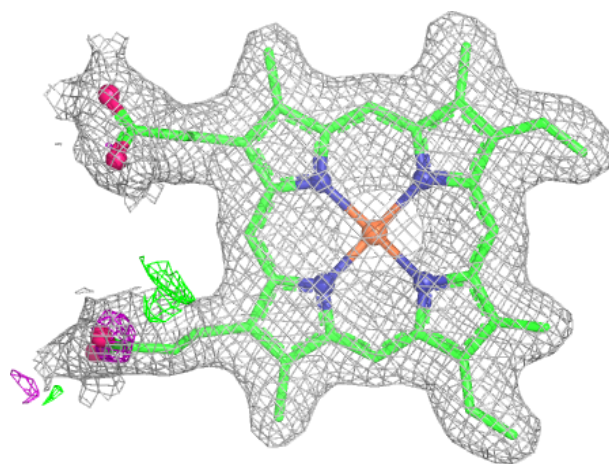
Electron density around HEM A 700 (B):

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



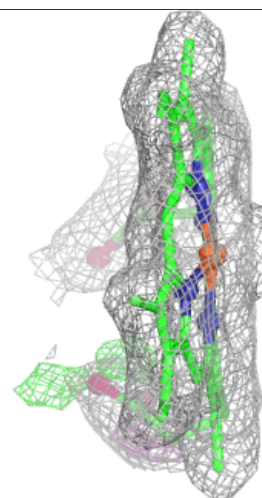
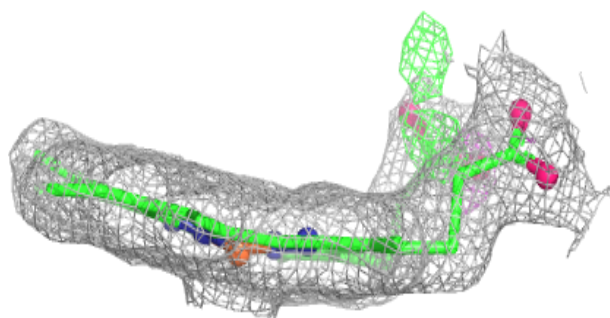
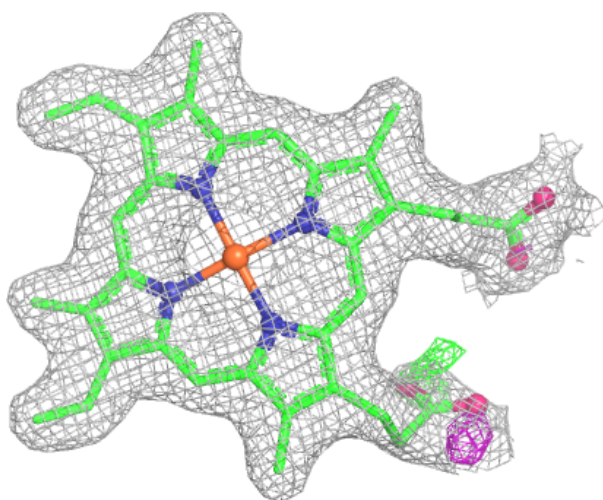
Electron density around HEM B 700 (A):

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



Electron density around HEM B 700 (B):

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



6.5 Other polymers ⓘ

There are no such residues in this entry.