



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:12 am BST

PDB ID : 5IRV
Title : Human cytochrome P450 17A1 bound to inhibitor VT-464
Authors : Scott, E.E.; Petrunak, E.M.
Deposited on : 2016-03-14
Resolution : 3.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

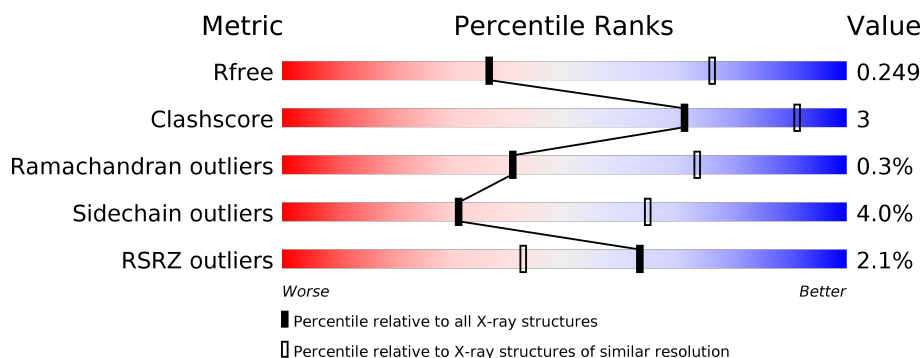
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	494	<div> <div>0%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
1	B	494	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
1	C	494	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>.</div> <div>.</div> </div> </div>
1	D	494	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>.</div> <div>.</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30314 atoms, of which 15005 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 Steroid 17-alpha-hydroxylase/17,20 lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	471	Total	C	H	N	O	S	0	0	0
			7576	2403	3827	649	682	15			
1	B	471	Total	C	H	N	O	S	0	0	0
			7576	2403	3827	649	682	15			
1	C	475	Total	C	H	N	O	S	0	0	0
			7336	2415	3564	654	688	15			
1	D	472	Total	C	H	N	O	S	0	0	0
			7354	2406	3599	650	684	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	expression tag	UNP P05093
A	20	ALA	-	expression tag	UNP P05093
A	21	LYS	-	expression tag	UNP P05093
A	22	LYS	-	expression tag	UNP P05093
A	23	THR	-	expression tag	UNP P05093
A	509	HIS	-	expression tag	UNP P05093
A	510	HIS	-	expression tag	UNP P05093
A	511	HIS	-	expression tag	UNP P05093
A	512	HIS	-	expression tag	UNP P05093
B	19	MET	-	expression tag	UNP P05093
B	20	ALA	-	expression tag	UNP P05093
B	21	LYS	-	expression tag	UNP P05093
B	22	LYS	-	expression tag	UNP P05093
B	23	THR	-	expression tag	UNP P05093
B	509	HIS	-	expression tag	UNP P05093
B	510	HIS	-	expression tag	UNP P05093
B	511	HIS	-	expression tag	UNP P05093
B	512	HIS	-	expression tag	UNP P05093
C	19	MET	-	expression tag	UNP P05093
C	20	ALA	-	expression tag	UNP P05093
C	21	LYS	-	expression tag	UNP P05093

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Chain	Residue	Modelled	Actual	Comment	Reference
C	22	LYS	-	expression tag	UNP P05093
C	23	THR	-	expression tag	UNP P05093
C	509	HIS	-	expression tag	UNP P05093
C	510	HIS	-	expression tag	UNP P05093
C	511	HIS	-	expression tag	UNP P05093
C	512	HIS	-	expression tag	UNP P05093
D	19	MET	-	expression tag	UNP P05093
D	20	ALA	-	expression tag	UNP P05093
D	21	LYS	-	expression tag	UNP P05093
D	22	LYS	-	expression tag	UNP P05093
D	23	THR	-	expression tag	UNP P05093
D	509	HIS	-	expression tag	UNP P05093
D	510	HIS	-	expression tag	UNP P05093
D	511	HIS	-	expression tag	UNP P05093
D	512	HIS	-	expression tag	UNP P05093

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



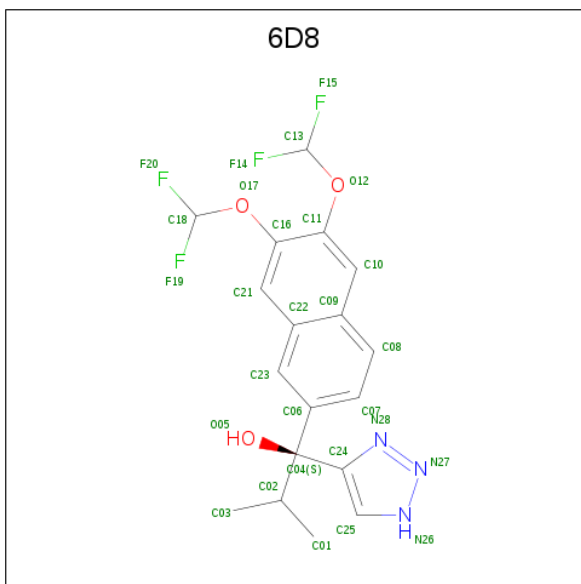
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	D	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 3 is VT-464 (three-letter code: 6D8) (formula: $C_{18}H_{17}F_4N_3O_3$).

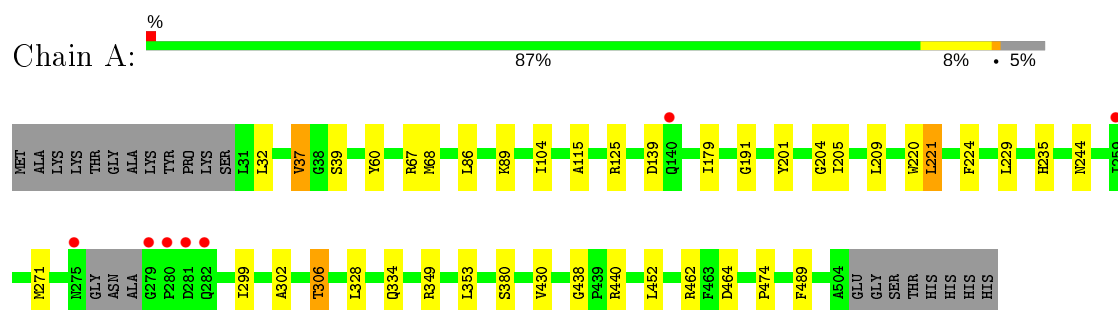


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	H	N	O	0	0
			45	18	4	17	3	3		
3	B	1	Total	C	F	H	N	O	0	0
			45	18	4	17	3	3		
3	C	1	Total	C	F	H	N	O	0	0
			45	18	4	17	3	3		
3	D	1	Total	C	F	H	N	O	0	0
			45	18	4	17	3	3		

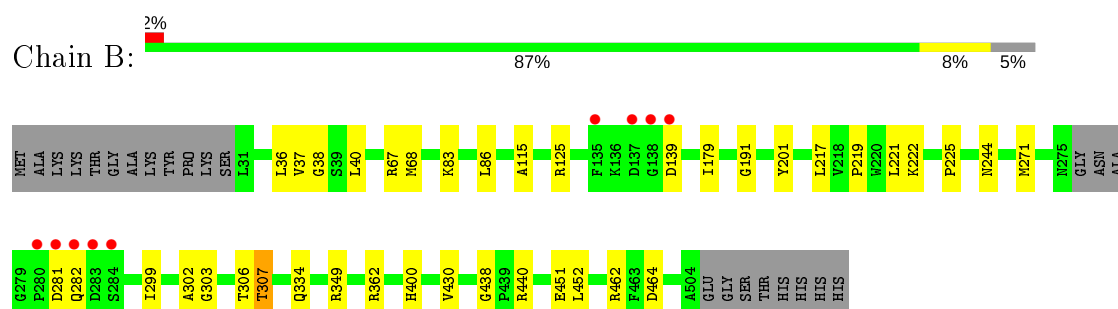
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

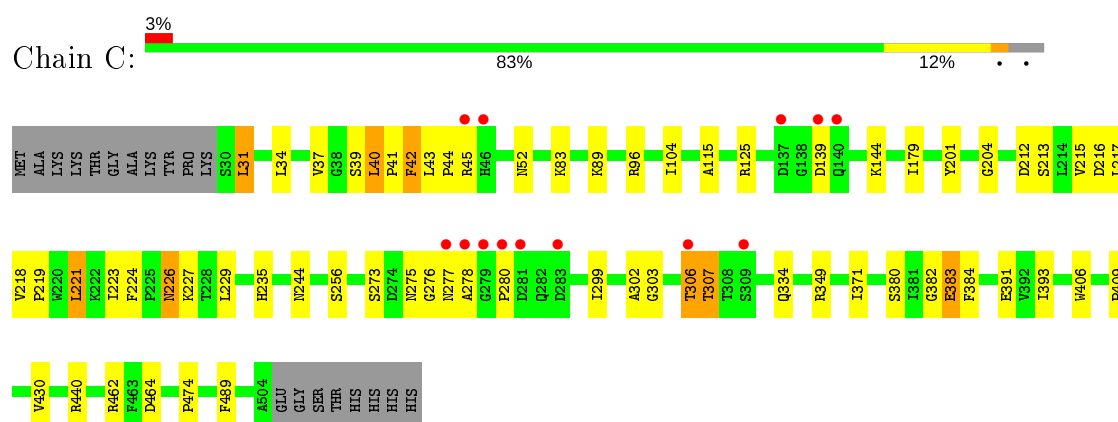
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase



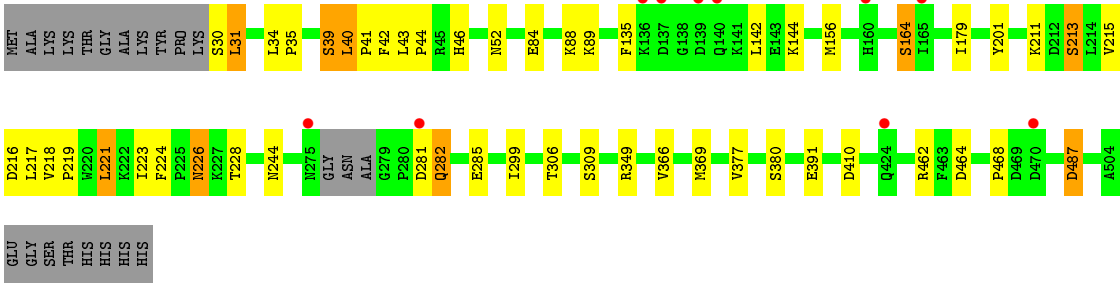
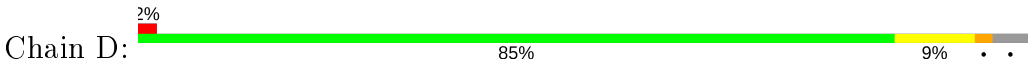
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase



- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase



- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.95Å 153.50Å 169.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.44 – 3.10 39.44 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (39.44-3.10) 88.1 (39.44-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.195 , 0.248 0.197 , 0.249	Depositor DCC
R_{free} test set	2163 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	57.7	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	30314	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: 6D8, HEM

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	0.27	0/3830	0.49	1/5186 (0.0%)
1	B	0.27	0/3830	0.49	0/5186
1	C	0.27	0/3854	0.50	0/5220
1	D	0.27	0/3836	0.50	0/5194
All	All	0.27	0/15350	0.50	1/20786 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	LEU	CA-CB-CG	5.46	127.85	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3749	3827	3812	22	0
1	B	3749	3827	3812	24	0
1	C	3772	3564	3832	42	0
1	D	3755	3599	3817	34	0
2	A	43	30	30	4	0
2	B	43	30	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	30	30	3	0
2	D	43	30	30	1	0
3	A	28	17	0	2	0
3	B	28	17	0	1	0
3	C	28	17	0	0	0
3	D	28	17	0	0	0
All	All	15309	15005	15393	107	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (107) 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:302:ALA:O	1:A:306:THR:OG1	1.95	0.84
1:B:303:GLY:O	1:B:307:THR:OG1	1.99	0.80
1:C:221:LEU:H	1:C:221:LEU:HD12	1.50	0.75
1:A:37:VAL:O	1:C:41:PRO:HD3	1.90	0.72
1:C:303:GLY:O	1:C:307:THR:OG1	2.08	0.70
1:D:223:ILE:HG13	1:D:224:PHE:CD1	2.28	0.69
1:C:302:ALA:O	1:C:306:THR:OG1	2.10	0.69
1:C:43:LEU:H	1:C:43:LEU:HD12	1.58	0.67
1:C:223:ILE:HG13	1:C:224:PHE:CD2	2.30	0.67
1:D:34:LEU:HB2	1:D:35:PRO:HD2	1.81	0.63
1:B:38:GLY:HA3	1:D:40:LEU:HD12	1.82	0.62
1:C:273:SER:O	1:C:280:PRO:HA	2.00	0.61
1:C:42:PHE:CZ	1:C:45:ARG:HG3	2.35	0.61
1:D:44:PRO:HB3	1:D:52:ASN:ND2	2.16	0.61
1:D:89:LYS:NZ	1:D:380:SER:OG	2.35	0.60
1:C:275:ASN:OD1	1:C:276:GLY:N	2.35	0.59
1:C:42:PHE:HZ	1:C:45:ARG:HG3	1.68	0.59
1:B:302:ALA:O	1:B:306:THR:OG1	2.19	0.59
1:B:281:ASP:OD1	1:B:282:GLN:N	2.35	0.58
1:A:60:TYR:CG	1:C:37:VAL:HG11	2.38	0.58
1:C:226:ASN:HD22	1:C:226:ASN:C	2.07	0.57
1:D:221:LEU:H	1:D:221:LEU:HD12	1.69	0.57
1:B:115:ALA:O	1:B:440:ARG:NH2	2.33	0.57
1:C:382:GLY:O	1:C:383:GLU:HB2	2.06	0.55
1:C:44:PRO:HB2	1:C:52:ASN:ND2	2.21	0.55
1:D:299:ILE:HG23	2:D:600:HEM:HBC1	1.89	0.54
1:C:219:PRO:O	1:C:223:ILE:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ARG:NH1	2:C:600:HEM:O1D	2.41	0.54
1:D:219:PRO:O	1:D:221:LEU:HD12	2.08	0.53
1:B:219:PRO:HD2	1:D:43:LEU:HD13	1.91	0.53
1:D:306:THR:HG23	1:D:366:VAL:HG11	1.91	0.53
2:A:600:HEM:HHD	2:A:600:HEM:HBC2	1.92	0.52
1:D:216:ASP:N	1:D:391:GLU:OE2	2.34	0.52
1:B:37:VAL:HG23	1:D:41:PRO:HG3	1.93	0.51
1:A:299:ILE:HG23	2:A:600:HEM:HBC1	1.92	0.51
1:C:41:PRO:O	1:C:42:PHE:C	2.47	0.51
1:D:215:VAL:CG2	1:D:218:VAL:HG23	2.42	0.50
1:A:224:PHE:HE2	1:C:218:VAL:HG11	1.76	0.49
1:B:37:VAL:O	1:D:41:PRO:HD3	2.14	0.48
1:C:31:LEU:HD12	1:C:31:LEU:N	2.29	0.48
1:D:213:SER:HB3	1:D:369:MET:HE3	1.95	0.48
1:A:89:LYS:NZ	1:A:380:SER:OG	2.47	0.47
1:C:115:ALA:O	1:C:440:ARG:NH2	2.30	0.47
1:A:115:ALA:O	1:A:440:ARG:NH2	2.38	0.47
1:B:299:ILE:HG23	2:B:600:HEM:HBC1	1.97	0.47
1:D:217:LEU:HD12	1:D:218:VAL:HG23	1.97	0.47
1:C:216:ASP:HB3	1:C:391:GLU:OE1	2.15	0.47
1:C:299:ILE:HG23	2:C:600:HEM:HBC1	1.96	0.47
2:C:600:HEM:HBC2	2:C:600:HEM:HHD	1.97	0.47
1:A:205:ILE:O	1:A:209:LEU:HB2	2.15	0.47
1:D:226:ASN:O	1:D:228:THR:N	2.48	0.47
1:A:86:LEU:O	1:A:438:GLY:HA3	2.14	0.46
1:A:452:LEU:HD11	2:A:600:HEM:HBB1	1.96	0.46
1:D:164:SER:HB3	1:D:468:PRO:HB3	1.97	0.46
1:C:382:GLY:O	1:C:383:GLU:CB	2.63	0.46
1:C:474:PRO:HB3	1:C:489:PHE:CG	2.50	0.46
1:C:83:LYS:NZ	1:C:430:VAL:HB	2.31	0.46
1:D:135:PHE:O	1:D:142:LEU:HB2	2.15	0.46
2:B:600:HEM:HBC2	2:B:600:HEM:HHD	1.98	0.45
1:C:280:PRO:HD2	1:D:377:VAL:HG12	1.98	0.45
1:A:474:PRO:HB3	1:A:489:PHE:CG	2.52	0.45
1:B:306:THR:HG21	3:B:601:6D8:C25	2.45	0.45
1:D:39:SER:O	1:D:40:LEU:HD13	2.17	0.45
1:D:84:GLU:HA	1:D:88:LYS:HB3	1.98	0.45
1:B:67:ARG:O	1:D:39:SER:HA	2.16	0.45
1:B:125:ARG:NH1	2:B:600:HEM:O1D	2.48	0.45
1:B:362:ARG:NH1	1:B:400:HIS:O	2.49	0.44
1:C:406:TRP:HB2	1:C:409:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:PHE:CE2	1:C:218:VAL:HG11	2.53	0.44
1:B:219:PRO:CD	1:D:43:LEU:HD13	2.47	0.44
1:B:452:LEU:HD11	2:B:600:HEM:HBB1	2.00	0.44
1:B:221:LEU:HD12	1:B:222:LYS:HG3	2.00	0.43
1:B:225:PRO:O	1:D:211:LYS:HE3	2.18	0.43
1:C:277:ASN:O	1:C:278:ALA:HB3	2.18	0.43
1:D:41:PRO:O	1:D:43:LEU:N	2.51	0.43
1:A:67:ARG:O	1:C:39:SER:HA	2.19	0.43
1:D:215:VAL:HG23	1:D:218:VAL:HG23	2.00	0.43
1:D:282:GLN:O	1:D:285:GLU:HG2	2.19	0.42
1:D:487:ASP:OD1	1:D:487:ASP:N	2.52	0.42
1:A:125:ARG:NH1	2:A:600:HEM:O1D	2.51	0.42
1:D:216:ASP:HB3	1:D:391:GLU:OE1	2.18	0.42
1:A:68:MET:CE	1:C:40:LEU:HD22	2.49	0.42
1:C:41:PRO:O	1:C:43:LEU:N	2.53	0.42
1:C:96:ARG:NH1	1:C:371:ILE:HB	2.34	0.42
1:B:86:LEU:O	1:B:438:GLY:HA3	2.19	0.42
1:B:68:MET:HE2	1:D:40:LEU:HD22	2.02	0.42
1:C:42:PHE:HZ	1:C:45:ARG:CG	2.32	0.42
1:B:83:LYS:NZ	1:B:430:VAL:HB	2.35	0.42
1:A:302:ALA:HB2	3:A:601:6D8:C08	2.50	0.41
1:B:307:THR:HG21	1:B:451:GLU:OE1	2.19	0.41
1:C:384:PHE:N	1:C:384:PHE:CD1	2.88	0.41
1:A:306:THR:HG21	3:A:601:6D8:C25	2.50	0.41
1:A:104:ILE:HD12	1:A:229:LEU:HD22	2.02	0.41
1:A:191:GLY:HA3	1:B:191:GLY:HA3	2.01	0.41
1:B:40:LEU:HD21	1:B:68:MET:HE1	2.02	0.41
1:A:328:LEU:HD21	1:A:353:LEU:HA	2.03	0.41
1:B:68:MET:CE	1:D:40:LEU:HD22	2.51	0.41
1:C:204:GLY:HA3	1:C:235:HIS:CD2	2.56	0.41
1:C:215:VAL:HG12	1:C:393:ILE:HD13	2.03	0.41
1:D:34:LEU:HB2	1:D:35:PRO:CD	2.49	0.41
1:C:42:PHE:HZ	1:C:45:ARG:CD	2.33	0.40
1:C:31:LEU:H	1:C:31:LEU:HD12	1.86	0.40
1:C:89:LYS:NZ	1:C:380:SER:OG	2.54	0.40
1:D:30:SER:O	1:D:31:LEU:CB	2.68	0.40
1:A:204:GLY:HA3	1:A:235:HIS:CD2	2.56	0.40
1:A:220:TRP:CZ3	1:C:218:VAL:HG13	2.56	0.40
1:C:104:ILE:HD11	1:C:229:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	467/494 (94%)	441 (94%)	25 (5%)	1 (0%)	47	79
1	B	467/494 (94%)	441 (94%)	26 (6%)	0	100	100
1	C	473/494 (96%)	450 (95%)	21 (4%)	2 (0%)	34	69
1	D	468/494 (95%)	443 (95%)	23 (5%)	2 (0%)	34	69
All	All	1875/1976 (95%)	1775 (95%)	95 (5%)	5 (0%)	41	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	42	PHE
1	C	383	GLU
1	C	42	PHE
1	D	226	ASN
1	A	32	LEU

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	419/436 (96%)	405 (97%)	14 (3%)	38	69
1	B	419/436 (96%)	407 (97%)	12 (3%)	42	72
1	C	421/436 (97%)	400 (95%)	21 (5%)	24	57
1	D	420/436 (96%)	400 (95%)	20 (5%)	25	58
All	All	1679/1744 (96%)	1612 (96%)	67 (4%)	31	65

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	39	SER
1	A	139	ASP
1	A	179	ILE
1	A	201	TYR
1	A	221	LEU
1	A	244	ASN
1	A	271	MET
1	A	306	THR
1	A	334	GLN
1	A	349	ARG
1	A	430	VAL
1	A	462	ARG
1	A	464	ASP
1	B	36	LEU
1	B	139	ASP
1	B	179	ILE
1	B	201	TYR
1	B	217	LEU
1	B	244	ASN
1	B	271	MET
1	B	307	THR
1	B	334	GLN
1	B	349	ARG
1	B	462	ARG
1	B	464	ASP
1	C	31	LEU
1	C	34	LEU
1	C	40	LEU
1	C	139	ASP
1	C	144	LYS
1	C	179	ILE
1	C	201	TYR
1	C	212	ASP
1	C	213	SER
1	C	217	LEU
1	C	221	LEU
1	C	226	ASN
1	C	227	LYS
1	C	244	ASN
1	C	256	SER
1	C	306	THR

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Mol	Chain	Res	Type
1	C	307	THR
1	C	334	GLN
1	C	349	ARG
1	C	462	ARG
1	C	464	ASP
1	D	31	LEU
1	D	39	SER
1	D	40	LEU
1	D	46	HIS
1	D	144	LYS
1	D	156	MET
1	D	164	SER
1	D	179	ILE
1	D	201	TYR
1	D	213	SER
1	D	221	LEU
1	D	244	ASN
1	D	281	ASP
1	D	282	GLN
1	D	309	SER
1	D	349	ARG
1	D	410	ASP
1	D	462	ARG
1	D	464	ASP
1	D	487	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	B	50	HIS
1	B	78	HIS
1	C	46	HIS
1	C	52	ASN
1	C	78	HIS
1	C	120	HIS
1	D	52	ASN
1	D	78	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	6D8	D	601	2	28,30,30	1.68	6 (21%)	36,44,44	1.17	4 (11%)
3	6D8	B	601	2	28,30,30	1.60	5 (17%)	36,44,44	1.11	4 (11%)
3	6D8	A	601	2	28,30,30	1.68	5 (17%)	36,44,44	1.07	2 (5%)
3	6D8	C	601	2	28,30,30	1.64	6 (21%)	36,44,44	1.09	3 (8%)
2	HEM	C	600	3	27,50,50	1.88	4 (14%)	17,82,82	1.62	3 (17%)
2	HEM	D	600	3	27,50,50	1.93	5 (18%)	17,82,82	1.68	7 (41%)
2	HEM	A	600	3	27,50,50	1.95	5 (18%)	17,82,82	1.67	5 (29%)
2	HEM	B	600	3	27,50,50	1.89	4 (14%)	17,82,82	1.63	4 (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
3	6D8	D	601	2	-	1/20/26/26	0/3/3/3
3	6D8	B	601	2	-	4/20/26/26	0/3/3/3
3	6D8	A	601	2	-	3/20/26/26	0/3/3/3
3	6D8	C	601	2	-	3/20/26/26	0/3/3/3
2	HEM	C	600	3	-	0/6/54/54	-
2	HEM	D	600	3	-	0/6/54/54	-
2	HEM	A	600	3	-	0/6/54/54	-
2	HEM	B	600	3	-	0/6/54/54	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	HEM	C3C-C2C	-5.49	1.32	1.40
2	D	600	HEM	C3C-C2C	-5.17	1.33	1.40
2	C	600	HEM	C3C-C2C	-4.96	1.33	1.40
2	B	600	HEM	C3C-C2C	-4.82	1.33	1.40
3	D	601	6D8	O12-C11	4.28	1.44	1.37
2	D	600	HEM	C3B-C2B	-4.18	1.34	1.40
3	A	601	6D8	O12-C11	4.14	1.44	1.37
3	B	601	6D8	O12-C11	4.11	1.44	1.37
3	C	601	6D8	O12-C11	4.11	1.44	1.37
2	B	600	HEM	C3B-C2B	-4.02	1.34	1.40
2	C	600	HEM	C3B-C2B	-3.94	1.34	1.40
3	A	601	6D8	O05-C04	-3.92	1.38	1.43
2	A	600	HEM	C3B-C2B	-3.90	1.35	1.40
2	C	600	HEM	C3B-CAB	3.64	1.55	1.47
3	B	601	6D8	O05-C04	-3.59	1.39	1.43
3	C	601	6D8	O05-C04	-3.55	1.39	1.43
2	D	600	HEM	C3B-CAB	3.53	1.55	1.47
2	B	600	HEM	C3C-CAC	3.52	1.55	1.47
2	A	600	HEM	C3B-CAB	3.50	1.55	1.47
2	B	600	HEM	C3B-CAB	3.43	1.54	1.47
2	C	600	HEM	C3C-CAC	3.41	1.54	1.47
2	A	600	HEM	C3C-CAC	3.41	1.54	1.47
2	D	600	HEM	C3C-CAC	3.32	1.54	1.47
3	D	601	6D8	O05-C04	-3.27	1.39	1.43
3	A	601	6D8	O17-C16	3.05	1.42	1.37
3	D	601	6D8	C04-C06	2.97	1.57	1.53
3	D	601	6D8	O17-C16	2.59	1.42	1.37
3	B	601	6D8	O17-C16	2.53	1.41	1.37
3	C	601	6D8	C04-C06	2.46	1.57	1.53
3	C	601	6D8	O17-C16	2.45	1.41	1.37
3	D	601	6D8	C07-C06	2.25	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	HEM	CAA-C2A	2.24	1.55	1.52
3	A	601	6D8	C21-C16	2.23	1.40	1.36
2	D	600	HEM	CAA-C2A	2.17	1.55	1.52
3	D	601	6D8	C10-C11	2.16	1.40	1.36
3	C	601	6D8	C07-C06	2.15	1.42	1.39
3	C	601	6D8	C10-C11	2.08	1.40	1.36
3	B	601	6D8	C07-C06	2.05	1.42	1.39
3	A	601	6D8	C04-C06	2.01	1.56	1.53
3	B	601	6D8	C10-C11	2.01	1.40	1.36

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	HEM	CMB-C2B-C3B	3.06	130.40	124.68
2	A	600	HEM	CMD-C2D-C1D	-3.00	123.85	128.46
3	B	601	6D8	C25-C24-N28	-2.95	106.92	111.33
2	B	600	HEM	CMB-C2B-C3B	2.95	130.19	124.68
3	C	601	6D8	C25-C24-N28	-2.83	107.10	111.33
2	D	600	HEM	CAA-CBA-CGA	-2.80	107.97	112.67
3	A	601	6D8	C25-C24-N28	-2.74	107.24	111.33
3	D	601	6D8	C25-C24-N28	-2.70	107.29	111.33
2	A	600	HEM	CAA-CBA-CGA	-2.66	108.21	112.67
2	B	600	HEM	CAA-CBA-CGA	-2.65	108.23	112.67
3	D	601	6D8	O05-C04-C06	2.59	114.27	108.21
2	D	600	HEM	C1D-C2D-C3D	2.52	108.75	107.00
2	B	600	HEM	CMA-C3A-C4A	-2.50	124.62	128.46
2	A	600	HEM	CMB-C2B-C3B	2.46	129.28	124.68
2	A	600	HEM	CMA-C3A-C4A	-2.44	124.71	128.46
2	D	600	HEM	CMB-C2B-C3B	2.44	129.24	124.68
3	C	601	6D8	N26-N27-N28	-2.40	108.25	111.24
3	D	601	6D8	O17-C16-C21	-2.38	119.42	124.27
3	B	601	6D8	N26-N27-N28	-2.37	108.30	111.24
3	D	601	6D8	N26-N27-N28	-2.35	108.31	111.24
2	C	600	HEM	CBA-CAA-C2A	-2.35	108.15	112.49
2	C	600	HEM	CMA-C3A-C4A	-2.33	124.88	128.46
2	D	600	HEM	C4C-C3C-C2C	2.33	108.53	106.90
3	A	601	6D8	N26-N27-N28	-2.29	108.39	111.24
2	D	600	HEM	CMD-C2D-C1D	-2.27	124.97	128.46
2	D	600	HEM	CMA-C3A-C4A	-2.24	125.02	128.46
2	A	600	HEM	C1D-C2D-C3D	2.15	108.50	107.00
3	C	601	6D8	O17-C16-C21	-2.15	119.90	124.27
2	B	600	HEM	CMD-C2D-C1D	-2.15	125.17	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	6D8	C23-C22-C21	-2.06	118.11	122.16
3	B	601	6D8	O17-C16-C21	-2.04	120.11	124.27
2	D	600	HEM	C3C-C4C-NC	-2.04	107.09	110.94

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	6D8	F20-C18-O17-C16
3	D	601	6D8	F14-C13-O12-C11
3	B	601	6D8	F20-C18-O17-C16
3	A	601	6D8	F19-C18-O17-C16
3	C	601	6D8	F14-C13-O12-C11
3	C	601	6D8	F20-C18-O17-C16
3	A	601	6D8	C16-C11-O12-C13
3	B	601	6D8	F15-C13-O12-C11
3	B	601	6D8	C16-C11-O12-C13
3	B	601	6D8	F19-C18-O17-C16
3	C	601	6D8	F19-C18-O17-C16

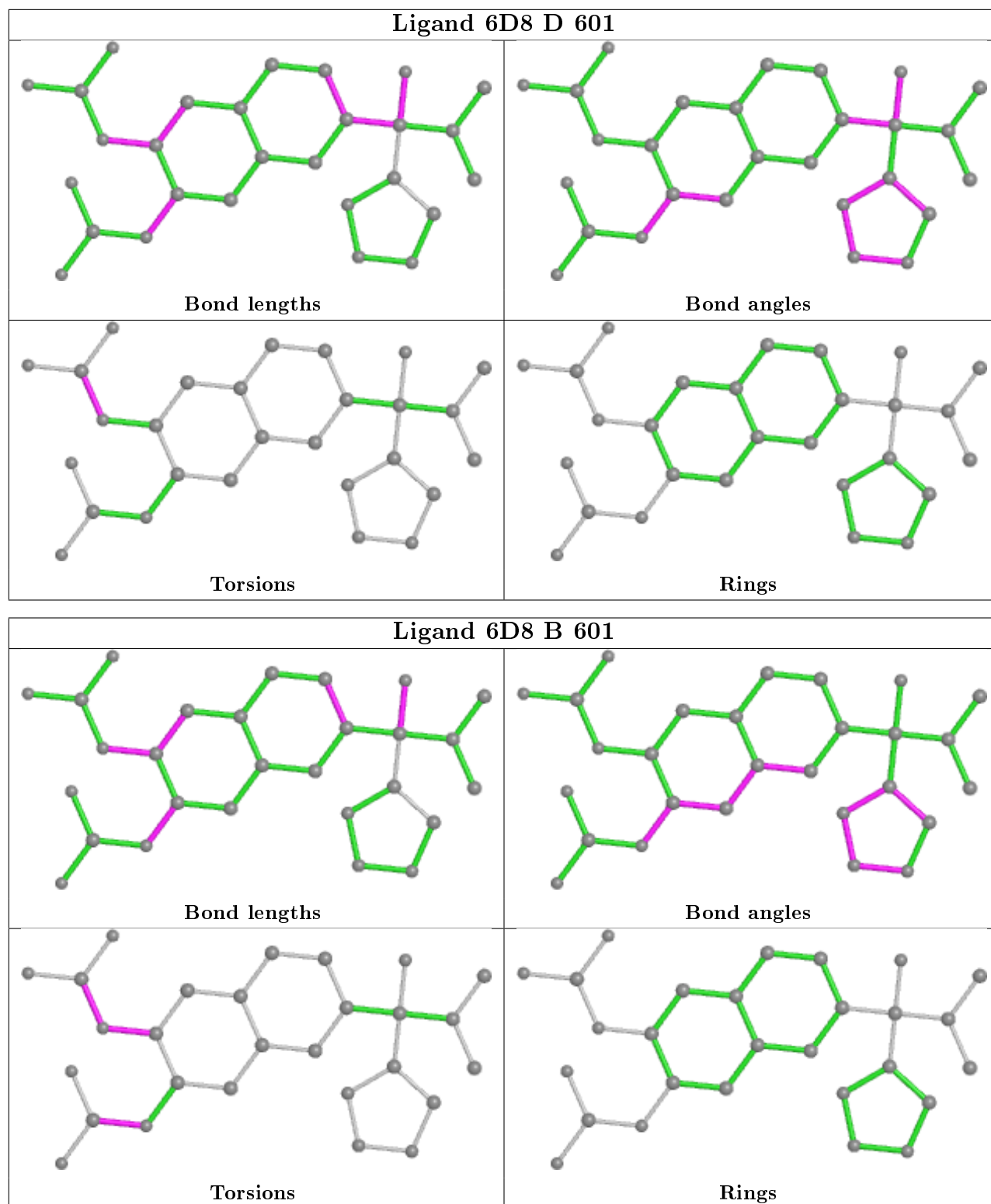
There are no ring outliers.

6 monomers are involved in 15 short contacts:

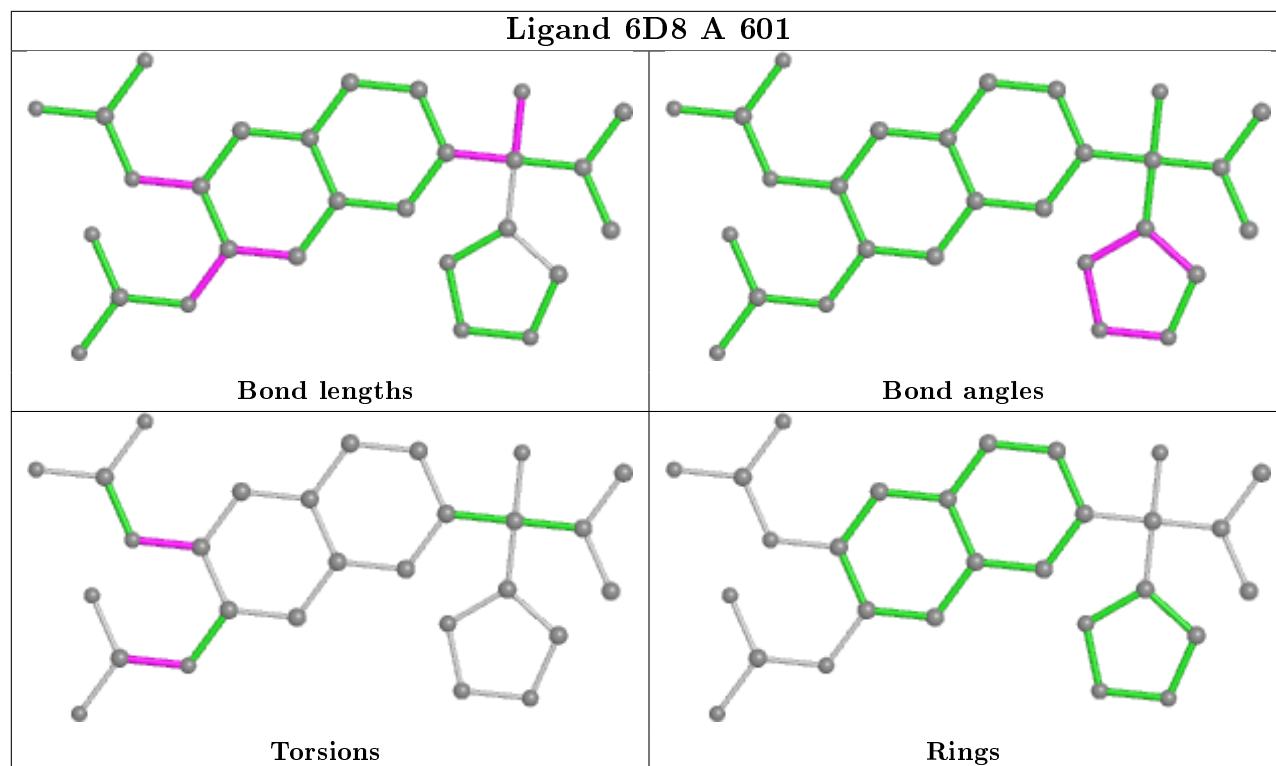
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	6D8	1	0
3	A	601	6D8	2	0
2	C	600	HEM	3	0
2	D	600	HEM	1	0
2	A	600	HEM	4	0
2	B	600	HEM	4	0

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

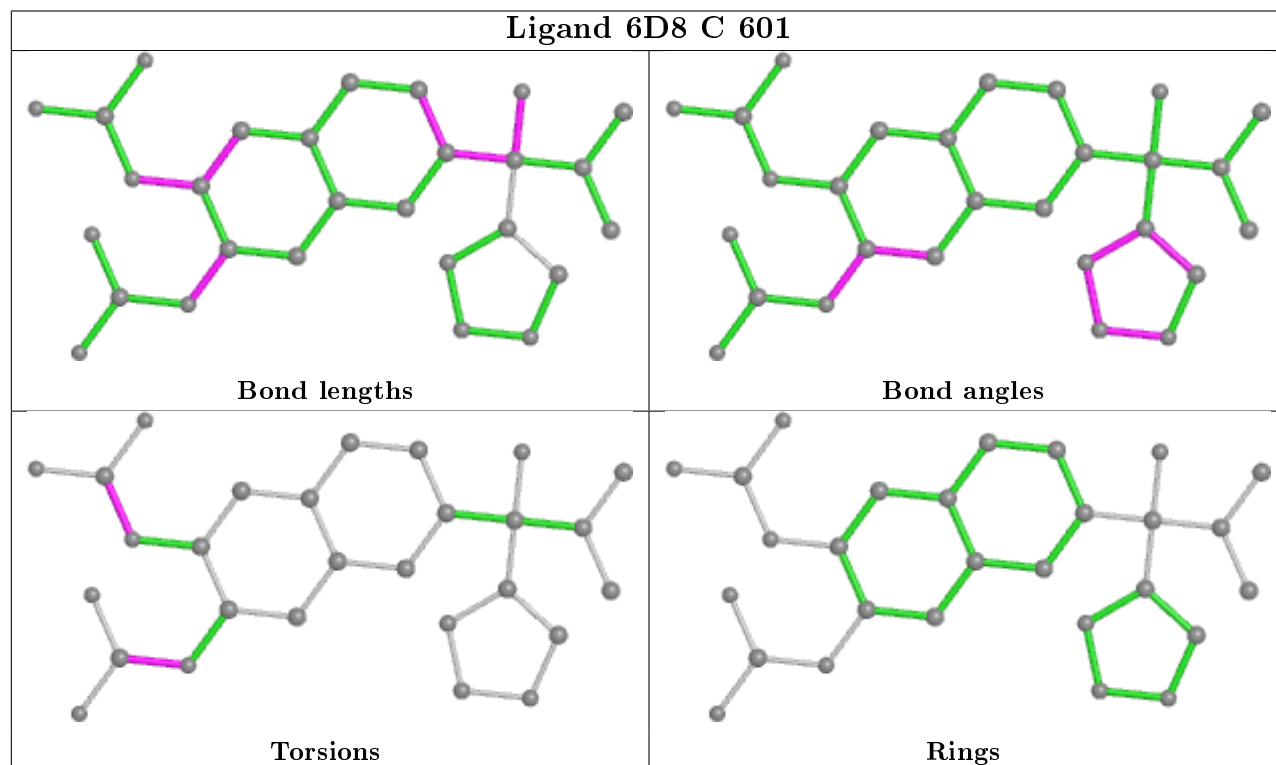
equivalents in the CSD to analyse the geometry.

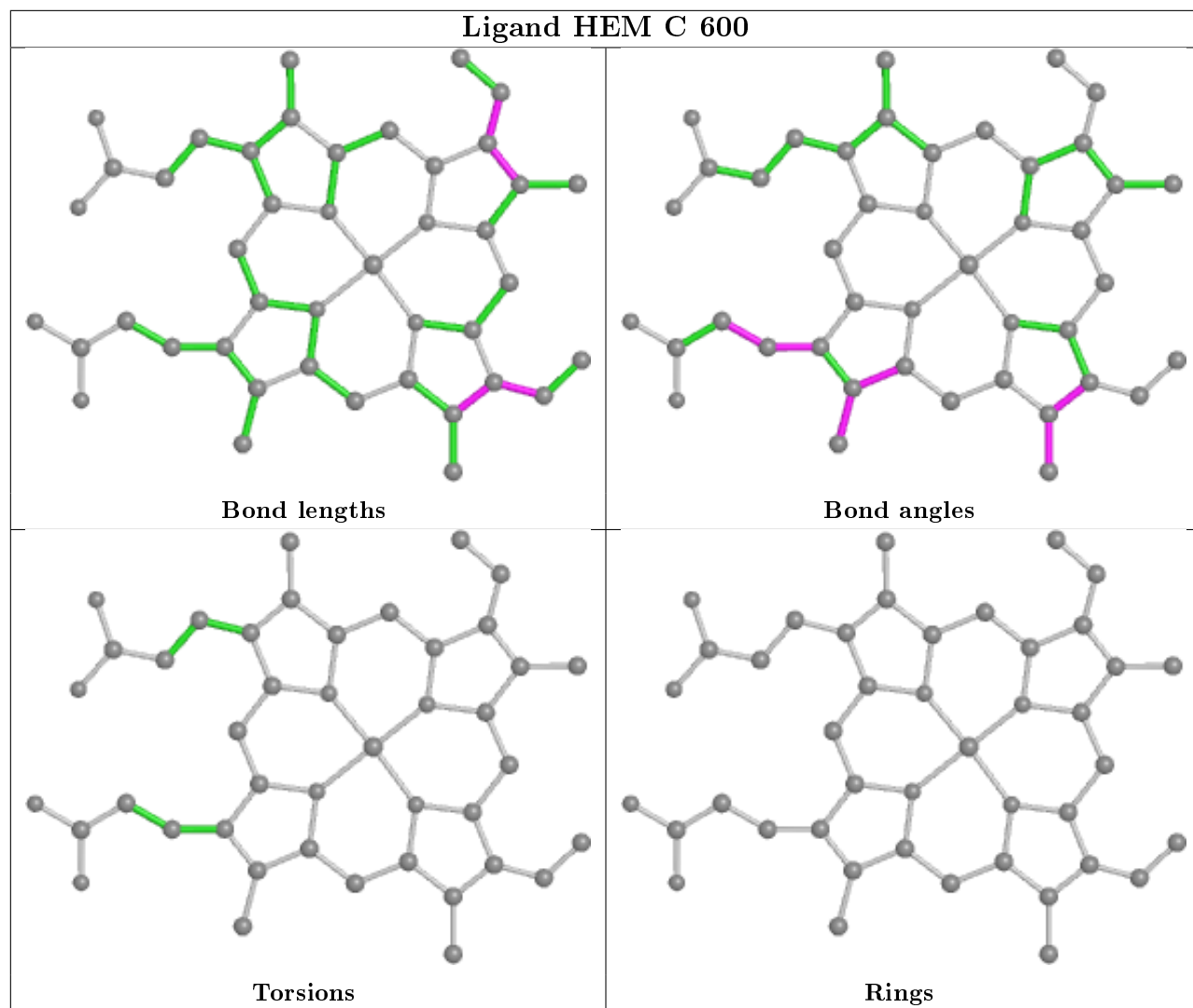


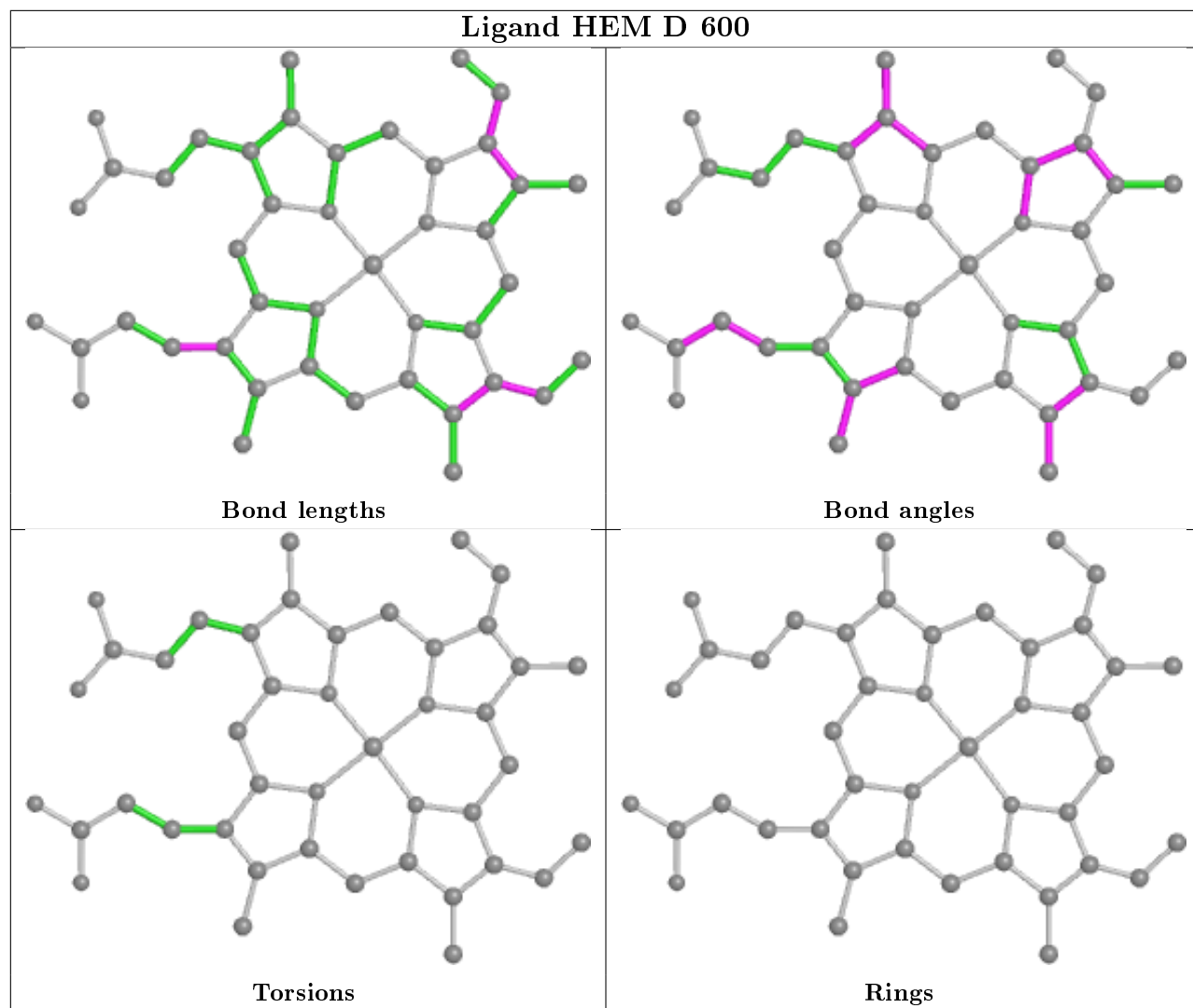
Ligand 6D8 A 601

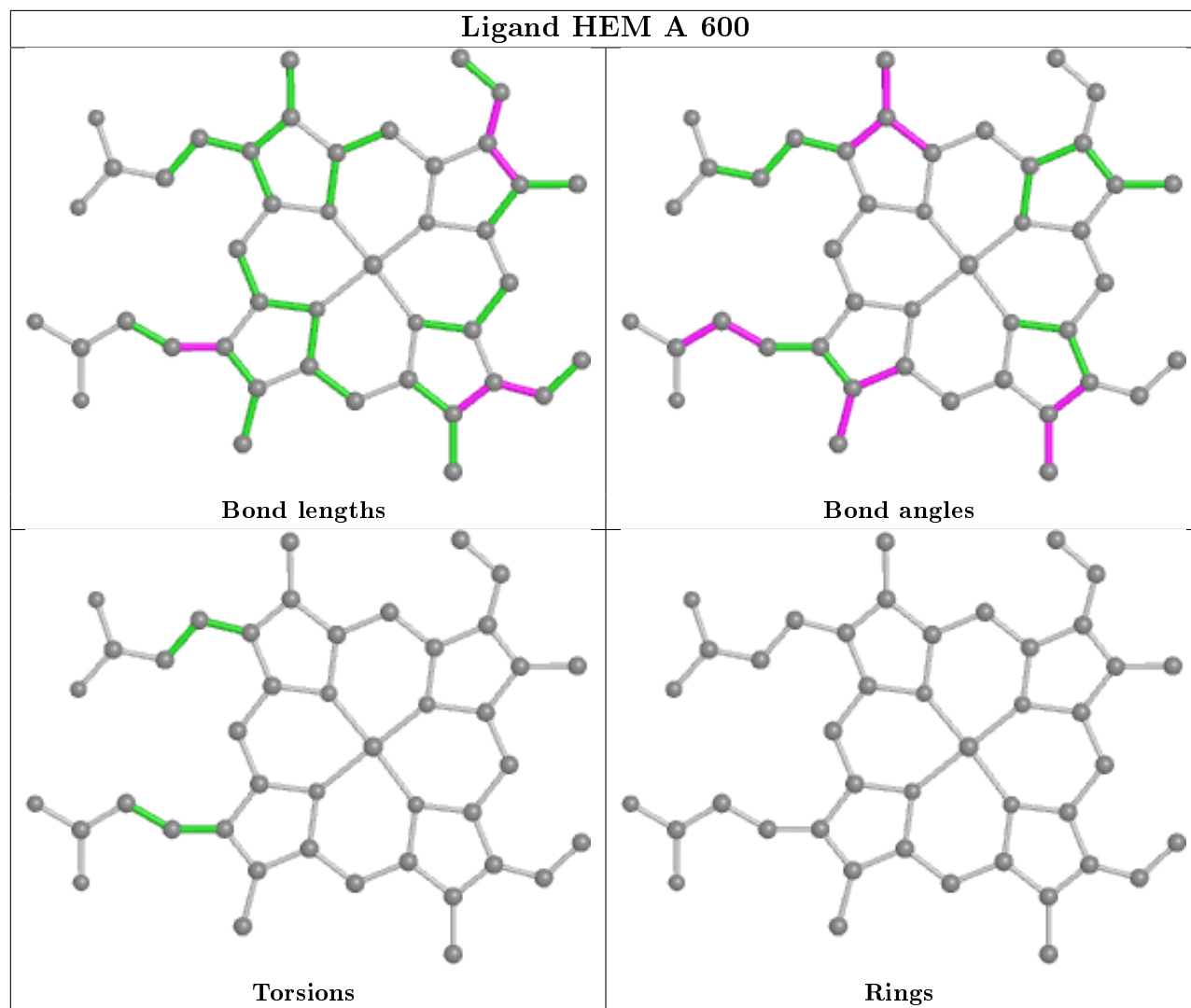


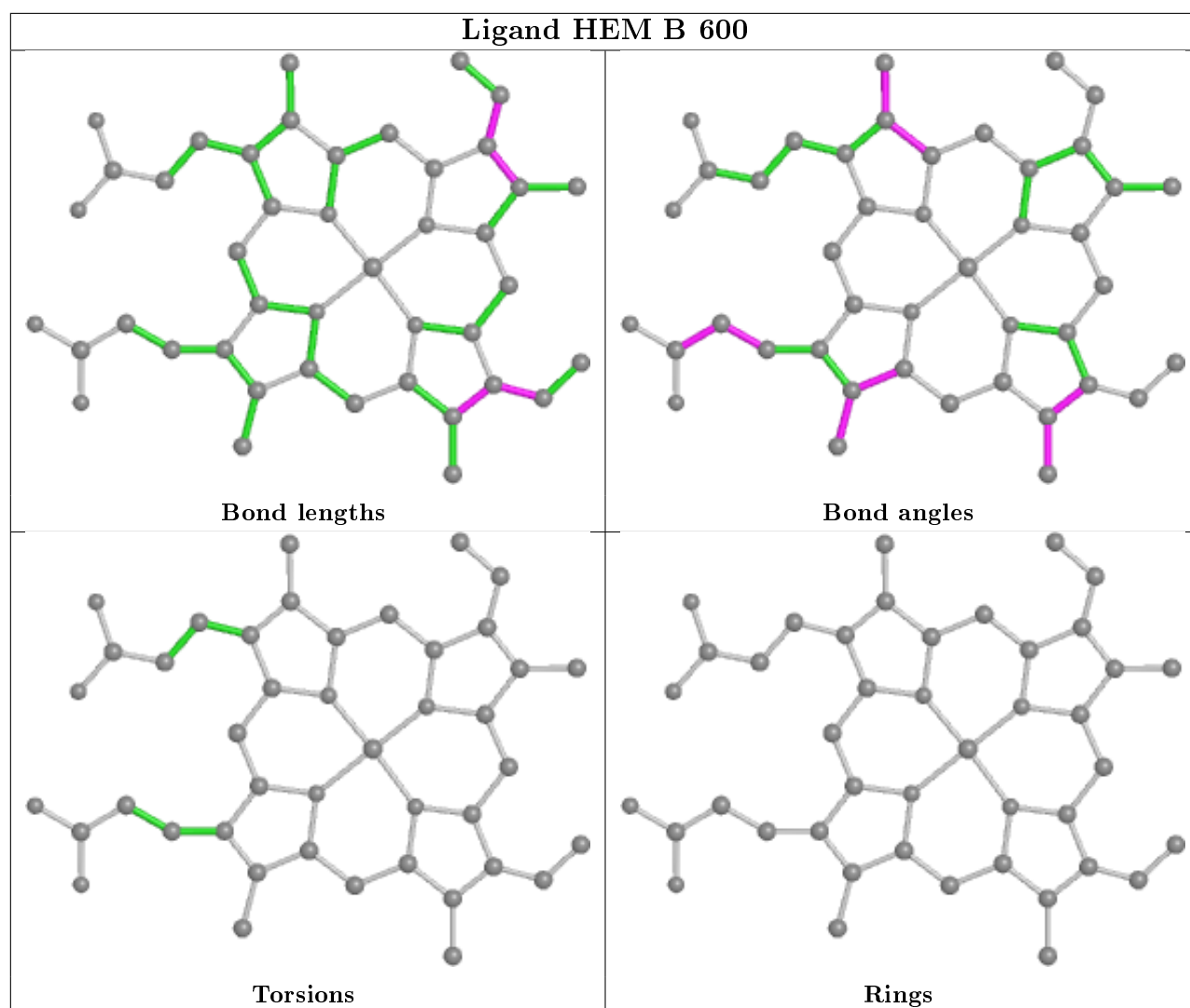
Ligand 6D8 C 601











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	471/494 (95%)	-0.02	7 (1%) 73 54	31, 58, 92, 131	0
1	B	471/494 (95%)	0.01	9 (1%) 66 46	31, 60, 93, 129	0
1	C	475/494 (96%)	0.08	13 (2%) 54 31	31, 58, 85, 126	0
1	D	472/494 (95%)	0.06	10 (2%) 63 43	36, 63, 93, 124	0
All	All	1889/1976 (95%)	0.03	39 (2%) 63 43	31, 59, 91, 131	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	139	ASP	5.4
1	C	277	ASN	5.0
1	B	139	ASP	4.5
1	A	279	GLY	4.3
1	B	280	PRO	4.1
1	A	140	GLN	4.1
1	D	139	ASP	3.4
1	C	140	GLN	3.4
1	C	280	PRO	3.3
1	C	137	ASP	3.2
1	B	284	SER	3.2
1	B	135	PHE	3.0
1	B	138	GLY	3.0
1	D	470	ASP	2.8
1	A	280	PRO	2.8
1	C	45	ARG	2.7
1	C	279	GLY	2.7
1	D	275	ASN	2.7
1	B	281	ASP	2.7
1	A	282	GLN	2.7
1	D	137	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	275	ASN	2.5
1	C	306	THR	2.5
1	D	140	GLN	2.4
1	B	282	GLN	2.4
1	C	309	SER	2.3
1	C	278	ALA	2.3
1	C	281	ASP	2.3
1	D	424	GLN	2.3
1	B	283	ASP	2.3
1	B	137	ASP	2.3
1	C	46	HIS	2.2
1	A	259	ILE	2.2
1	C	283	ASP	2.2
1	D	136	LYS	2.2
1	A	281	ASP	2.1
1	D	165	ILE	2.1
1	D	281	ASP	2.0
1	D	160	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
3	6D8	D	601	28/28	0.92	0.29	33,44,58,69	0
3	6D8	B	601	28/28	0.92	0.30	32,50,59,67	0
3	6D8	C	601	28/28	0.93	0.30	28,40,58,61	0
3	6D8	A	601	28/28	0.95	0.28	34,45,57,60	0
2	HEM	C	600	43/43	0.96	0.33	28,53,68,80	0

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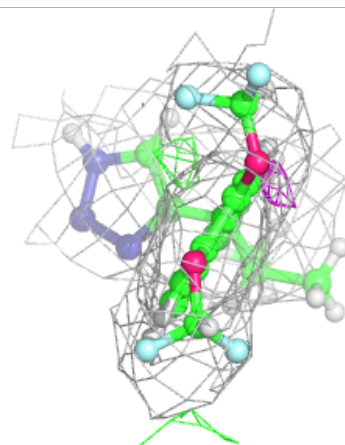
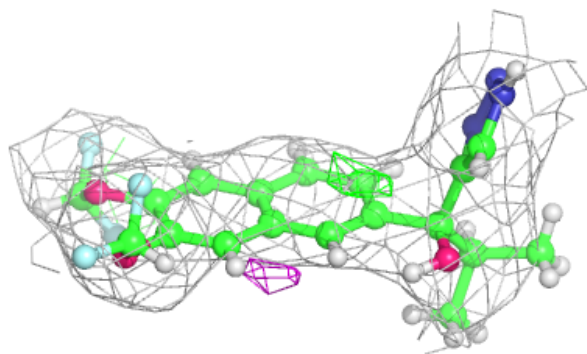
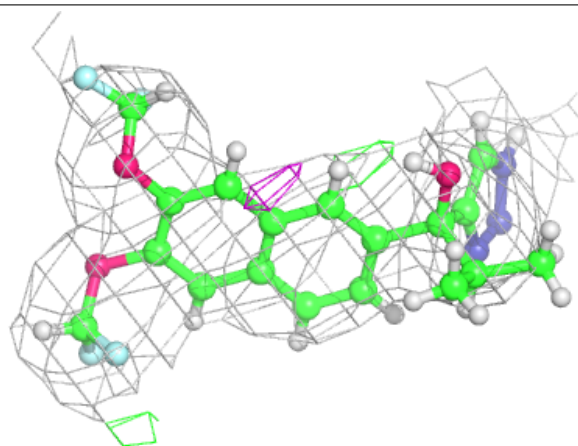
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HEM	D	600	43/43	0.96	0.34	40,58,73,76	0
2	HEM	A	600	43/43	0.97	0.30	35,49,67,72	0
2	HEM	B	600	43/43	0.97	0.33	33,51,65,68	0

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.

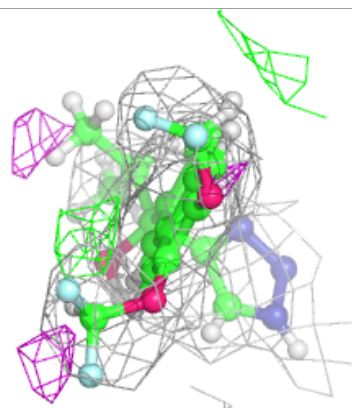
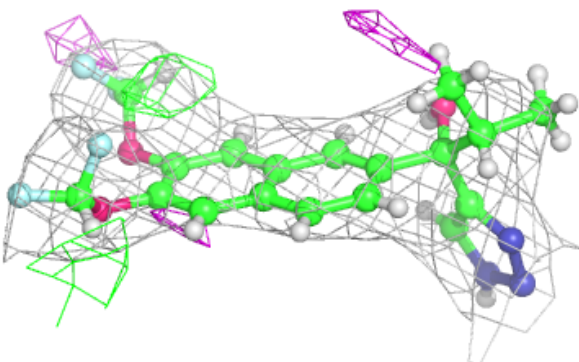
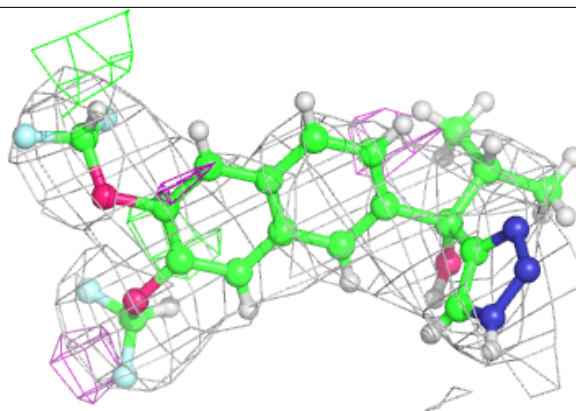
Electron density around 6D8 D 601:

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

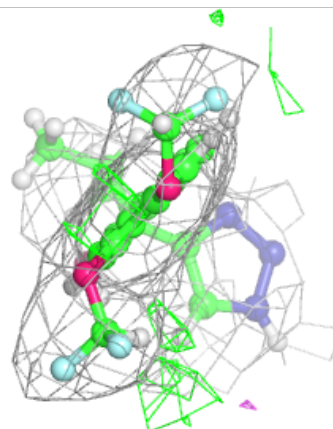
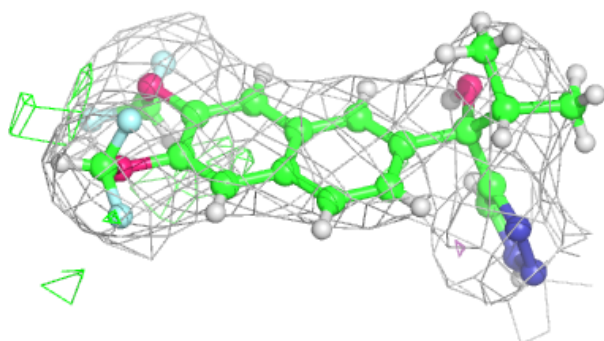
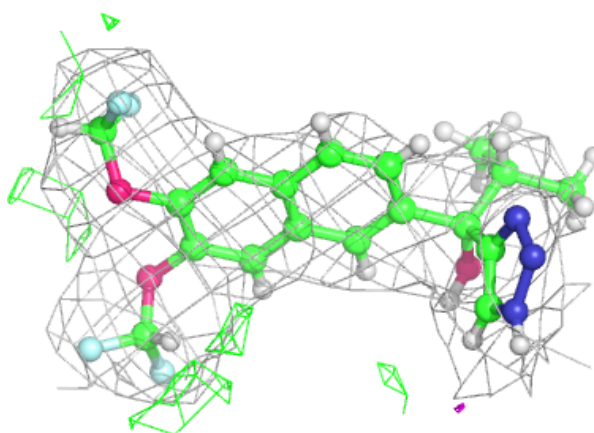


Electron density around 6D8 B 601:

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

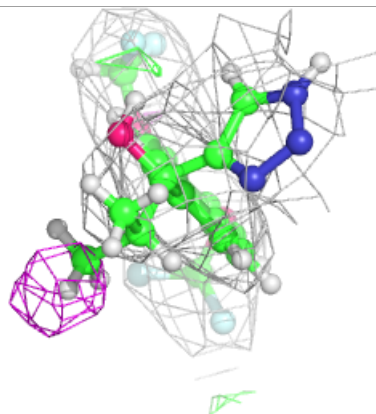
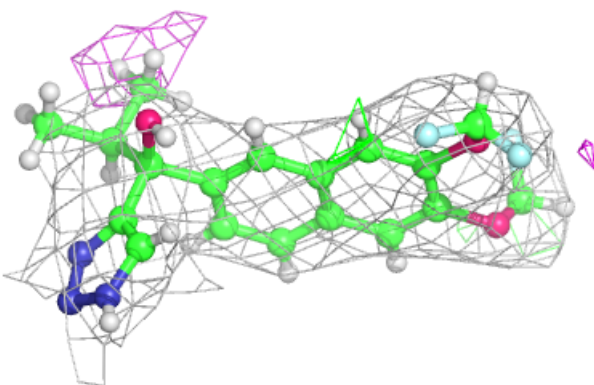
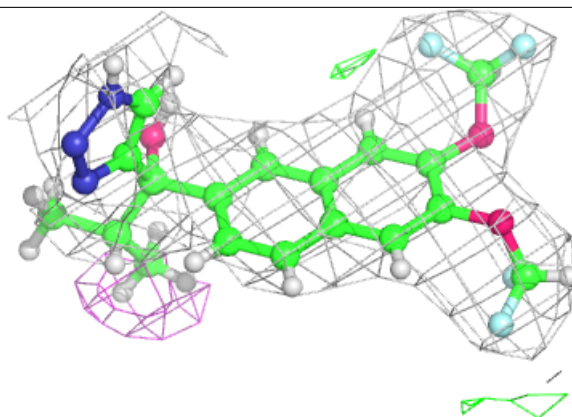
**Electron density around 6D8 C 601:**

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



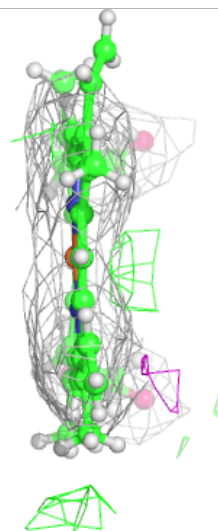
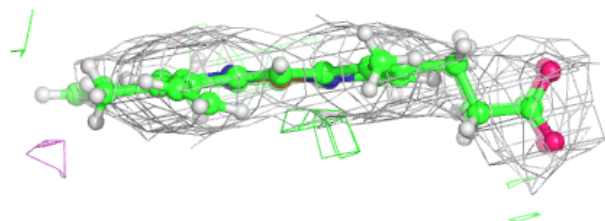
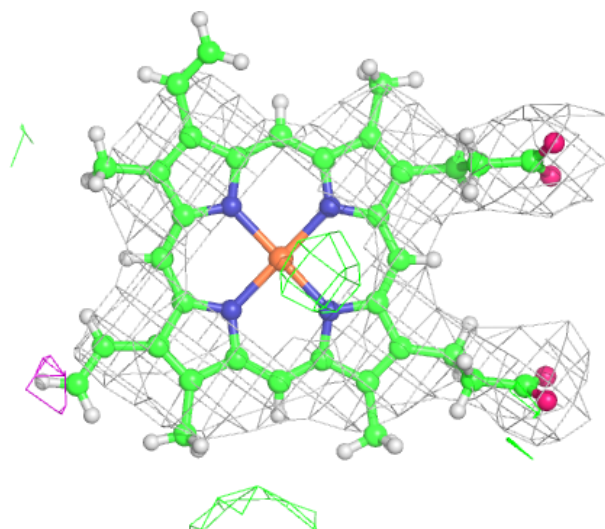
Electron density around 6D8 A 601:

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



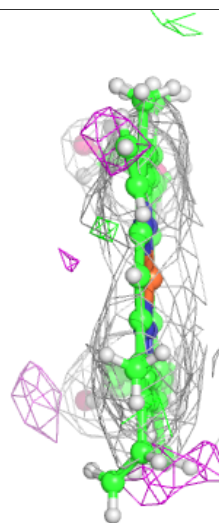
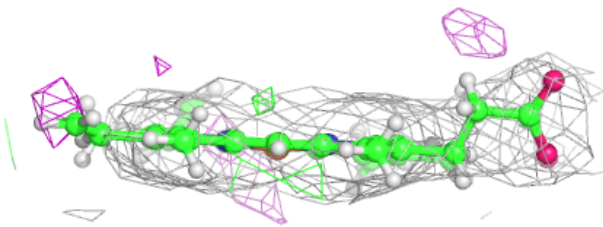
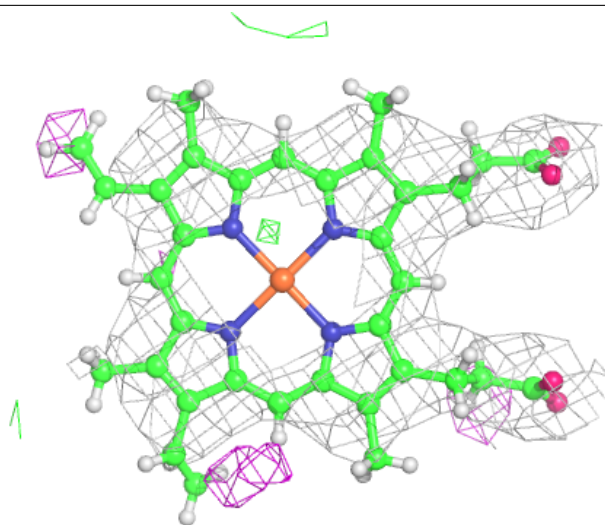
Electron density around HEM C 600:

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



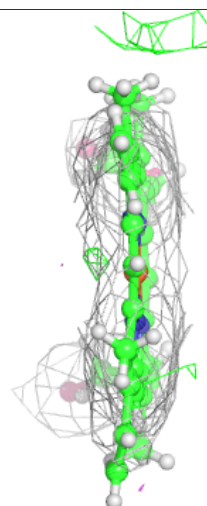
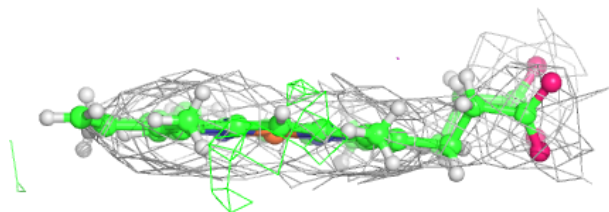
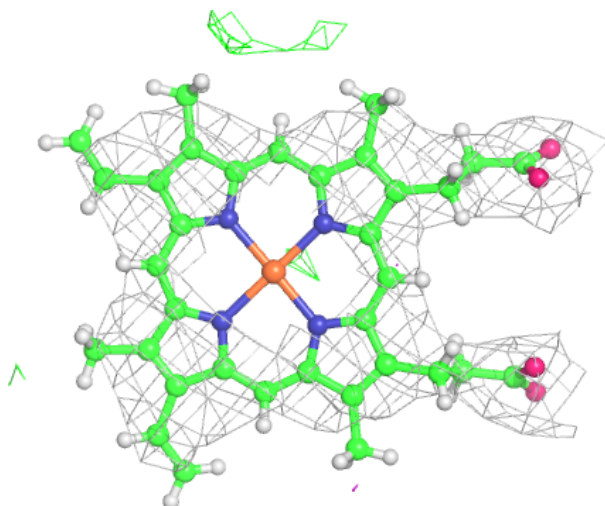
Electron density around HEM D 600:

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



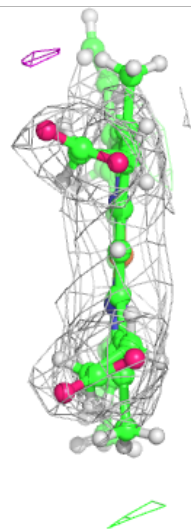
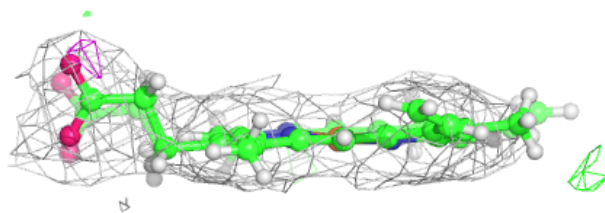
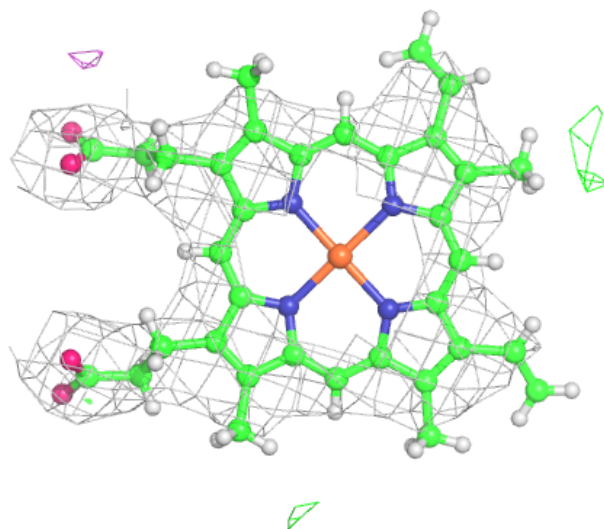
Electron density around HEM A 600:

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



Electron density around HEM B 600:

$2mF_o-DF_c$ (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.