



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 05:56 AM UTC

PDB ID : 6WW0 / pdb_00006ww0
Title : Human steroidogenic cytochrome P450 17A1 with 3-keto-5alpha-abiraterone analog
Authors : Petrunak, E.M.; Bart, A.G.; Scott, E.E.
Deposited on : 2020-05-07
Resolution : 2.01 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

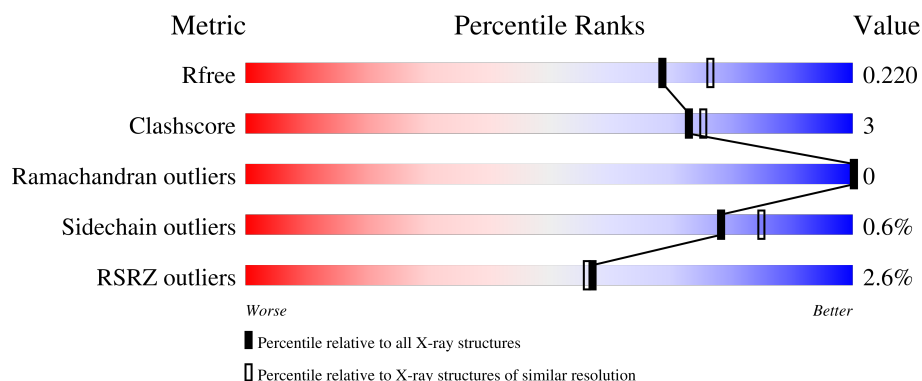
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	494	 2% 86% 8% 6%
1	B	494	 2% 88% 7% 5%
1	C	494	 3% 89% 6% 5%
1	D	494	 3% 85% 10% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31551 atoms, of which 15427 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	464	Total	C	H	N	O	S	0	0	0
			7477	2376	3777	640	669	15			
1	B	469	Total	C	H	N	O	S	0	0	0
			7561	2403	3823	647	673	15			
1	C	467	Total	C	H	N	O	S	0	0	0
			7516	2388	3794	644	675	15			
1	D	467	Total	C	H	N	O	S	0	0	0
			7508	2386	3789	643	675	15			

There are 36 discrepancies between the modelled and reference sequences:

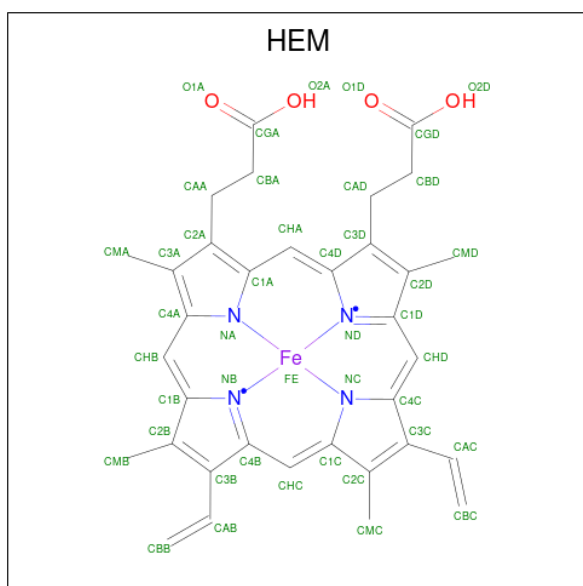
Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	initiating methionine	UNP P05093
A	20	ALA	-	expression tag	UNP P05093
A	21	LYS	-	expression tag	UNP P05093
A	22	LYS	-	expression tag	UNP P05093
A	23	THR	-	expression tag	UNP P05093
A	509	HIS	-	expression tag	UNP P05093
A	510	HIS	-	expression tag	UNP P05093
A	511	HIS	-	expression tag	UNP P05093
A	512	HIS	-	expression tag	UNP P05093
B	19	MET	-	initiating methionine	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	-	initiating methionine	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	-	initiating methionine	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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



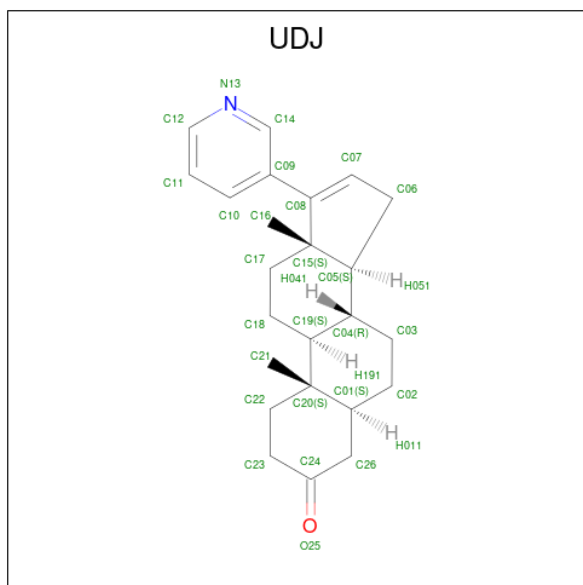
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
2	B	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
2	C	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0

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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 (5alpha,8alpha)-17-(pyridin-3-yl)androst-16-en-3-one (CCD ID: UDJ) (formula: C₂₄H₃₁NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			57	24	31	1	1		
3	B	1	Total	C	H	N	O	0	0
			57	24	31	1	1		
3	C	1	Total	C	H	N	O	0	0
			57	24	31	1	1		
3	D	1	Total	C	H	N	O	0	0
			57	24	31	1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	2	Total Cl	0	0
			2 2		

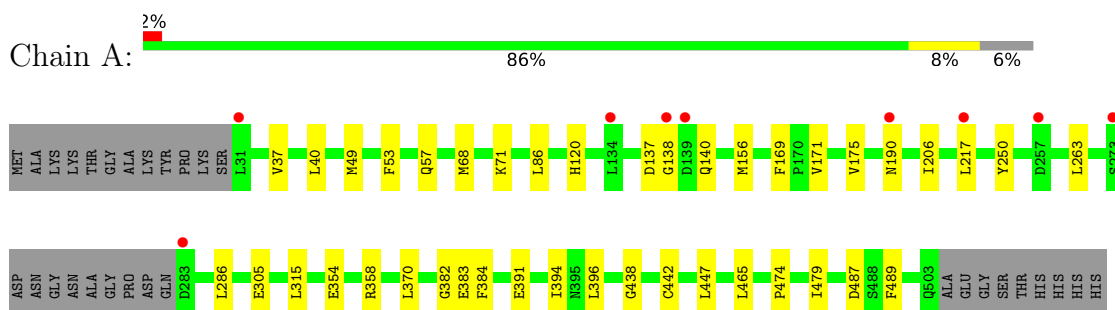
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	256	Total 256	O 256	0	0
5	B	246	Total 246	O 246	0	0
5	C	256	Total 256	O 256	0	0
5	D	209	Total 209	O 209	0	0

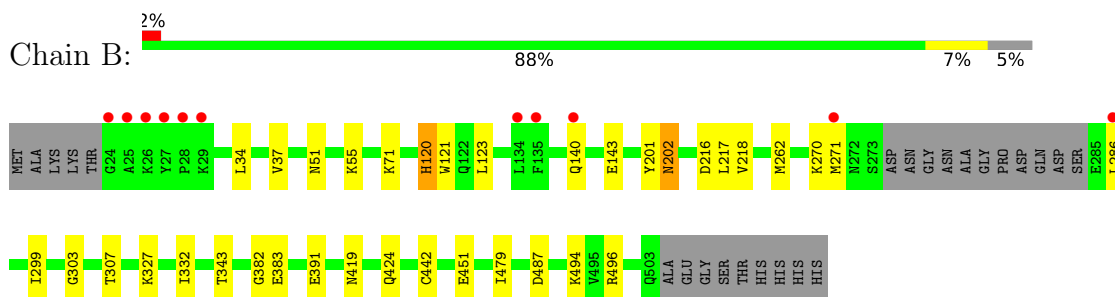
3 Residue-property plots

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.

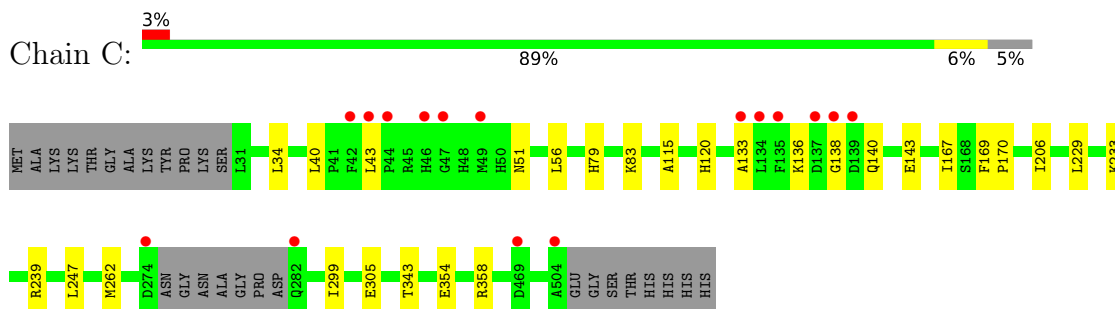
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase



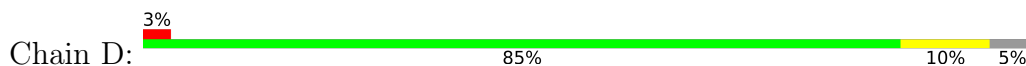
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase



- 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	85.72Å 151.18Å 169.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.68 – 2.01 38.68 – 2.01	Depositor EDS
% Data completeness (in resolution range)	98.1 (38.68-2.01) 90.4 (38.68-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.185 , 0.218 0.188 , 0.220	Depositor DCC
R_{free} test set	7240 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31551	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.45 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1683e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CL, HEM, UDJ

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	0.71	2/3780 (0.1%)	0.77	2/5117 (0.0%)
1	B	0.77	4/3820 (0.1%)	0.79	3/5170 (0.1%)
1	C	0.68	2/3802 (0.1%)	0.79	3/5147 (0.1%)
1	D	0.73	5/3799 (0.1%)	0.81	7/5143 (0.1%)
All	All	0.72	13/15201 (0.1%)	0.79	15/20577 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	218	VAL	CA-C	-10.76	1.43	1.52
1	A	57	GLN	C-O	-6.09	1.16	1.24
1	D	143	GLU	C-O	-5.94	1.17	1.24
1	A	156	MET	C-O	-5.85	1.17	1.24
1	C	51	ASN	C-O	-5.79	1.17	1.24
1	B	120	HIS	C-O	-5.74	1.17	1.24
1	B	201	TYR	C-O	-5.57	1.17	1.24
1	D	40	LEU	CA-C	5.52	1.58	1.52
1	B	121	TRP	C-O	-5.52	1.17	1.24
1	D	40	LEU	C-O	-5.51	1.18	1.24
1	D	122	GLN	C-O	-5.47	1.17	1.24
1	D	47	GLY	C-O	-5.26	1.19	1.23
1	C	239	ARG	C-O	-5.07	1.18	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	46	HIS	N-CA-C	6.98	123.26	113.56
1	D	218	VAL	CA-C-O	-6.72	115.19	119.15
1	D	44	PRO	N-CA-C	6.22	122.36	113.47
1	C	43	LEU	CA-C-N	-5.97	114.61	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	LEU	C-N-CA	-5.97	114.61	120.52
1	C	138	GLY	N-CA-C	5.91	123.02	112.02
1	A	138	GLY	N-CA-C	-5.35	106.16	111.56
1	B	202	ASN	N-CA-C	-5.31	105.41	111.14
1	B	496	ARG	CA-C-N	5.26	128.10	120.79
1	B	496	ARG	C-N-CA	5.26	128.10	120.79
1	D	202	ASN	N-CA-C	-5.17	105.55	111.14
1	D	137	ASP	N-CA-C	5.10	116.94	109.24
1	D	343	THR	CA-C-N	5.10	128.66	120.30
1	D	343	THR	C-N-CA	5.10	128.66	120.30
1	A	169	PHE	O-C-N	-5.06	116.38	120.38

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	3700	3777	3775	27	0
1	B	3738	3823	3821	21	0
1	C	3722	3794	3792	16	0
1	D	3719	3789	3789	29	0
2	A	43	30	30	5	0
2	B	43	30	30	6	0
2	C	43	30	30	2	0
2	D	43	30	30	4	0
3	A	26	31	0	0	0
3	B	26	31	0	0	0
3	C	26	31	0	0	0
3	D	26	31	0	0	0
4	D	2	0	0	0	0
5	A	256	0	0	1	0
5	B	246	0	0	1	0
5	C	256	0	0	0	0
5	D	209	0	0	1	0
All	All	16124	15427	15297	97	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 (97) 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:A:600:HEM:HMC1	2:A:600:HEM:HBC2	1.72	0.71
2:C:600:HEM:HMC1	2:C:600:HEM:HBC2	1.70	0.70
1:A:68:MET:CE	1:C:40:LEU:HD12	2.22	0.69
1:A:479:ILE:HD11	1:A:487:ASP:OD1	1.92	0.69
1:C:229:LEU:HD11	1:C:233:LYS:HE3	1.75	0.69
1:B:479:ILE:HD11	1:B:487:ASP:OD1	1.94	0.68
2:D:601:HEM:HBB2	2:D:601:HEM:HHC	1.76	0.67
1:A:370:LEU:HD22	1:A:394:ILE:HB	1.75	0.67
1:A:40:LEU:HD21	1:A:68:MET:HE1	1.78	0.66
1:D:120:HIS:CE1	1:D:286:LEU:HD23	2.34	0.63
2:A:600:HEM:HBB2	2:A:600:HEM:HMB2	1.82	0.61
1:D:369:MET:HE2	1:D:393:ILE:HG21	1.82	0.60
2:C:600:HEM:HHC	2:C:600:HEM:HBB2	1.83	0.60
2:B:600:HEM:HBB2	2:B:600:HEM:HHC	1.84	0.59
1:D:315:LEU:HD21	1:D:465:LEU:HD13	1.85	0.59
1:C:206:ILE:HD11	1:C:305:GLU:HG3	1.86	0.57
1:A:71:LYS:HE2	1:A:391:GLU:OE1	2.04	0.57
1:A:447:LEU:HD23	2:A:600:HEM:HBC2	1.87	0.56
1:D:167:ILE:C	1:D:167:ILE:HD12	2.32	0.55
1:A:68:MET:HG3	1:A:217:LEU:O	2.07	0.55
1:D:231:LYS:NZ	5:D:709:HOH:O	2.39	0.54
1:B:143:GLU:OE2	1:B:343:THR:HB	2.08	0.54
1:D:53:PHE:CD2	1:D:369:MET:HE1	2.43	0.54
1:D:369:MET:HE2	1:D:393:ILE:CG2	2.39	0.53
1:B:442:CYS:HB2	2:B:600:HEM:NA	2.24	0.52
1:D:349:ARG:HH11	1:D:349:ARG:HG2	1.73	0.52
1:D:247:LEU:HD12	1:D:247:LEU:O	2.10	0.51
1:D:206:ILE:HD11	1:D:305:GLU:HG3	1.93	0.50
2:A:600:HEM:HBB2	2:A:600:HEM:CMB	2.40	0.50
1:D:363:LEU:HD11	1:D:412:PHE:HA	1.93	0.50
1:D:442:CYS:HB2	2:D:601:HEM:NA	2.27	0.50
1:C:354:GLU:O	1:C:358:ARG:HG3	2.11	0.49
2:B:600:HEM:HBC2	2:B:600:HEM:CMC	2.43	0.49
1:A:71:LYS:CE	1:A:391:GLU:OE1	2.61	0.49
1:A:442:CYS:HB2	2:A:600:HEM:NA	2.28	0.48
1:D:167:ILE:C	1:D:167:ILE:CD1	2.86	0.48
1:A:315:LEU:HD22	1:A:465:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:MET:HE3	1:C:40:LEU:HB2	1.96	0.47
1:A:384:PHE:HB3	1:C:34:LEU:HG	1.97	0.47
1:A:382:GLY:O	1:A:383:GLU:HB2	2.15	0.47
1:D:330:GLU:O	1:D:334:GLN:HG3	2.15	0.47
1:A:206:ILE:HD11	1:A:305:GLU:HG3	1.97	0.47
1:B:262:MET:SD	1:B:299:ILE:HG13	2.55	0.47
1:A:120:HIS:HB2	5:A:891:HOH:O	2.14	0.46
2:B:600:HEM:HBC2	2:B:600:HEM:HMC2	1.98	0.46
1:B:37:VAL:O	1:B:37:VAL:HG12	2.15	0.46
1:A:120:HIS:CE1	1:A:286:LEU:HD23	2.51	0.46
2:D:601:HEM:HMC2	2:D:601:HEM:HBC2	1.97	0.46
1:B:307:THR:HG21	1:B:451:GLU:OE1	2.15	0.46
1:C:133:ALA:O	1:C:136:LYS:HG2	2.15	0.45
1:A:49:MET:HE3	1:A:53:PHE:CE2	2.51	0.45
1:D:303:GLY:HA2	2:D:601:HEM:HMC2	1.98	0.45
1:D:76:VAL:HB	1:D:394:ILE:HD13	1.98	0.45
1:B:442:CYS:HB2	2:B:600:HEM:C4A	2.53	0.44
1:A:86:LEU:O	1:A:438:GLY:HA3	2.18	0.44
1:B:51:ASN:O	1:B:55:LYS:HG3	2.18	0.44
1:C:262:MET:SD	1:C:299:ILE:HG13	2.58	0.44
1:A:49:MET:CE	1:A:53:PHE:CZ	3.01	0.44
1:D:499:TRP:O	1:D:503:GLN:HG2	2.18	0.44
1:B:120:HIS:CE1	1:B:286:LEU:HA	2.53	0.43
1:C:115:ALA:HB1	1:C:120:HIS:NE2	2.32	0.43
1:D:270:LYS:HD3	1:D:287:LEU:O	2.18	0.43
1:D:344:ILE:HD13	1:D:344:ILE:HA	1.88	0.43
1:D:251:LYS:NZ	1:D:289:ASP:OD2	2.52	0.43
1:D:349:ARG:HG2	1:D:349:ARG:NH1	2.33	0.43
1:B:271:MET:HE2	1:B:271:MET:HB3	1.85	0.43
1:A:250:TYR:CG	1:A:263:LEU:HD23	2.54	0.43
1:D:229:LEU:C	1:D:229:LEU:HD23	2.43	0.43
1:A:37:VAL:HG11	1:C:56:LEU:HD21	2.01	0.42
1:C:169:PHE:HB3	1:C:170:PRO:HD3	2.01	0.42
1:A:354:GLU:O	1:A:358:ARG:HG3	2.20	0.42
1:B:270:LYS:O	1:B:270:LYS:HG2	2.19	0.42
1:D:217:LEU:HD23	1:D:217:LEU:HA	1.88	0.42
1:B:303:GLY:HA2	2:B:600:HEM:HMC2	2.01	0.41
1:D:247:LEU:HG	1:D:251:LYS:HE3	2.02	0.41
1:B:123:LEU:HD22	1:B:286:LEU:HD13	2.02	0.41
1:A:68:MET:HE2	1:C:40:LEU:HD12	2.00	0.41
1:C:143:GLU:OE2	1:C:343:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:LYS:NZ	5:B:724:HOH:O	2.54	0.41
1:C:262:MET:HE3	1:C:262:MET:HB2	1.81	0.41
1:D:55:LYS:O	1:D:58:LYS:HE2	2.19	0.41
1:D:120:HIS:CE1	1:D:286:LEU:CD2	3.02	0.41
1:D:75:ILE:HD13	1:D:393:ILE:HB	2.03	0.41
1:A:171:VAL:O	1:A:175:VAL:HG22	2.21	0.41
1:B:71:LYS:HE2	1:B:391:GLU:OE1	2.21	0.41
1:A:370:LEU:HD13	1:A:396:LEU:HB2	2.03	0.41
1:B:382:GLY:O	1:B:383:GLU:HB2	2.21	0.41
1:B:419:ASN:ND2	1:B:424:GLN:HB2	2.35	0.41
1:C:167:ILE:C	1:C:167:ILE:HD12	2.45	0.41
1:A:140:GLN:O	1:A:140:GLN:HG3	2.21	0.41
1:A:474:PRO:HB3	1:A:489:PHE:CG	2.56	0.41
1:C:79:HIS:O	1:C:83:LYS:HD2	2.20	0.41
1:B:217:LEU:HD23	1:B:217:LEU:HA	1.81	0.40
1:B:140:GLN:HG2	1:B:140:GLN:O	2.21	0.40
1:B:34:LEU:HD13	1:D:74:VAL:HG22	2.03	0.40
1:B:327:LYS:HE3	1:B:327:LYS:HB3	1.91	0.40
1:D:455:ILE:O	1:D:459:LEU:HG	2.22	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	460/494 (93%)	452 (98%)	8 (2%)	0	100	100
1	B	465/494 (94%)	458 (98%)	7 (2%)	0	100	100
1	C	463/494 (94%)	453 (98%)	10 (2%)	0	100	100
1	D	463/494 (94%)	452 (98%)	11 (2%)	0	100	100
All	All	1851/1976 (94%)	1815 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	414/436 (95%)	412 (100%)	2 (0%)	81	87
1	B	417/436 (96%)	414 (99%)	3 (1%)	76	82
1	C	416/436 (95%)	414 (100%)	2 (0%)	81	87
1	D	416/436 (95%)	413 (99%)	3 (1%)	76	82
All	All	1663/1744 (95%)	1653 (99%)	10 (1%)	78	85

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ASP
1	A	190	ASN
1	B	202	ASN
1	B	216	ASP
1	B	332	ILE
1	C	140	GLN
1	C	247	LEU
1	D	45	ARG
1	D	326	LYS
1	D	470	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	348	ASN
1	B	120	HIS
1	B	196	ASN
1	C	57	GLN
1	C	140	GLN
1	C	163	GLN

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Mol	Chain	Res	Type
1	C	407	HIS
1	D	78	HIS
1	D	79	HIS
1	D	163	GLN
1	D	407	HIS
1	D	408	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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z > 2$
3	UDJ	A	601	2	30,30,30	2.66	16 (53%)	47,47,47	2.82	14 (29%)
3	UDJ	C	601	2	30,30,30	3.06	16 (53%)	47,47,47	2.67	14 (29%)
3	UDJ	B	601	2	30,30,30	3.18	18 (60%)	47,47,47	2.97	18 (38%)
2	HEM	C	600	3,1	50,50,50	1.37	6 (12%)	67,82,82	1.39	12 (17%)
2	HEM	D	601	3,1	50,50,50	1.45	12 (24%)	67,82,82	1.30	9 (13%)
3	UDJ	D	602	2	30,30,30	3.20	17 (56%)	47,47,47	2.91	14 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	B	600	3,1	50,50,50	1.42	7 (14%)	67,82,82	1.28	6 (8%)
2	HEM	A	600	3,1	50,50,50	1.44	5 (10%)	67,82,82	1.15	6 (8%)

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	UDJ	A	601	2	-	0/4/62/62	0/5/5/5
3	UDJ	C	601	2	-	0/4/62/62	0/5/5/5
3	UDJ	B	601	2	-	0/4/62/62	0/5/5/5
2	HEM	C	600	3,1	-	1/14/54/54	-
2	HEM	D	601	3,1	-	0/14/54/54	-
3	UDJ	D	602	2	-	0/4/62/62	0/5/5/5
2	HEM	B	600	3,1	-	0/14/54/54	-
2	HEM	A	600	3,1	-	1/14/54/54	-

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	UDJ	C15-C08	-8.67	1.46	1.53
3	D	602	UDJ	C16-C15	-8.42	1.40	1.54
3	D	602	UDJ	C15-C08	-7.09	1.47	1.53
3	B	601	UDJ	C15-C08	-6.65	1.47	1.53
3	C	601	UDJ	C06-C07	-5.83	1.41	1.50
3	B	601	UDJ	C17-C15	-5.82	1.43	1.54
3	B	601	UDJ	C06-C05	-5.68	1.46	1.54
3	B	601	UDJ	C06-C07	-5.44	1.42	1.50
3	D	602	UDJ	C06-C07	-4.91	1.43	1.50
3	A	601	UDJ	C15-C08	-4.68	1.49	1.53
3	B	601	UDJ	O25-C24	-4.65	1.13	1.21
3	A	601	UDJ	O25-C24	-4.49	1.13	1.21
3	C	601	UDJ	C22-C20	-4.37	1.46	1.54
3	B	601	UDJ	C22-C20	-4.30	1.46	1.54
3	D	602	UDJ	C17-C15	-4.27	1.46	1.54
3	A	601	UDJ	C26-C24	-4.26	1.43	1.50
3	A	601	UDJ	C06-C05	-4.26	1.48	1.54
3	D	602	UDJ	O25-C24	-4.23	1.14	1.21
3	C	601	UDJ	O25-C24	-4.17	1.14	1.21
3	C	601	UDJ	C20-C01	-4.14	1.49	1.55
3	A	601	UDJ	C16-C15	-4.10	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	UDJ	C21-C20	-4.10	1.47	1.54
3	A	601	UDJ	C17-C15	-4.09	1.46	1.54
2	A	600	HEM	FE-NA	4.01	2.08	1.95
3	B	601	UDJ	C20-C01	-4.00	1.49	1.55
3	D	602	UDJ	C21-C20	-3.97	1.47	1.54
3	C	601	UDJ	C16-C15	-3.95	1.48	1.54
3	D	602	UDJ	C14-N13	-3.80	1.26	1.34
3	D	602	UDJ	C20-C01	-3.73	1.49	1.55
2	B	600	HEM	FE-NC	3.73	2.07	1.95
3	A	601	UDJ	C20-C01	-3.66	1.49	1.55
3	B	601	UDJ	C14-N13	-3.59	1.26	1.34
3	A	601	UDJ	C22-C23	-3.57	1.45	1.53
3	C	601	UDJ	C14-N13	-3.45	1.26	1.34
3	B	601	UDJ	C14-C09	-3.35	1.33	1.39
2	A	600	HEM	CAB-C3B	3.34	1.56	1.47
3	B	601	UDJ	C04-C05	-3.28	1.47	1.53
3	D	602	UDJ	C06-C05	-3.23	1.49	1.54
3	B	601	UDJ	C18-C19	-3.20	1.48	1.53
3	B	601	UDJ	C16-C15	-3.19	1.49	1.54
3	C	601	UDJ	C03-C04	-3.17	1.47	1.53
2	C	600	HEM	FE-NC	3.16	2.05	1.95
3	D	602	UDJ	C14-C09	-3.16	1.34	1.39
3	A	601	UDJ	C04-C19	-3.14	1.47	1.53
3	D	602	UDJ	C22-C20	-3.13	1.48	1.54
3	A	601	UDJ	C14-N13	-3.11	1.27	1.34
2	A	600	HEM	FE-NC	3.09	2.05	1.95
2	C	600	HEM	FE-NB	3.05	2.04	1.94
2	C	600	HEM	CAC-C3C	3.05	1.55	1.47
2	C	600	HEM	CAB-C3B	3.04	1.55	1.47
2	B	600	HEM	FE-NA	2.96	2.04	1.95
3	A	601	UDJ	C14-C09	-2.87	1.34	1.39
3	C	601	UDJ	C06-C05	-2.87	1.50	1.54
3	D	602	UDJ	C26-C24	-2.83	1.46	1.50
2	B	600	HEM	CAB-C3B	2.80	1.54	1.47
2	A	600	HEM	CAC-C3C	2.78	1.54	1.47
3	B	601	UDJ	C22-C23	-2.74	1.47	1.53
2	B	600	HEM	CMB-C2B	2.73	1.56	1.50
3	B	601	UDJ	C23-C24	-2.72	1.44	1.50
2	D	601	HEM	CAB-C3B	2.71	1.54	1.47
3	D	602	UDJ	C15-C05	-2.68	1.49	1.54
3	D	602	UDJ	C03-C04	-2.65	1.48	1.53
3	B	601	UDJ	C26-C24	-2.64	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	HEM	C3B-C2B	-2.63	1.31	1.37
3	D	602	UDJ	C23-C24	-2.60	1.44	1.50
2	D	601	HEM	C1C-NC	-2.59	1.34	1.39
2	D	601	HEM	CAC-C3C	2.55	1.54	1.47
3	A	601	UDJ	C06-C07	-2.55	1.46	1.50
3	C	601	UDJ	C22-C23	-2.43	1.48	1.53
3	C	601	UDJ	C23-C24	-2.39	1.44	1.50
3	C	601	UDJ	C14-C09	-2.38	1.35	1.39
2	C	600	HEM	CMA-C3A	2.35	1.55	1.50
2	B	600	HEM	CAC-C3C	2.34	1.53	1.47
3	A	601	UDJ	C22-C20	-2.32	1.50	1.54
2	D	601	HEM	FE-NC	2.30	2.02	1.95
2	D	601	HEM	FE-ND	2.27	2.01	1.94
2	B	600	HEM	CMC-C2C	2.26	1.55	1.50
2	D	601	HEM	C2A-C3A	-2.21	1.33	1.38
3	C	601	UDJ	C07-C08	-2.19	1.30	1.33
3	A	601	UDJ	C04-C05	-2.19	1.49	1.53
2	B	600	HEM	CMA-C3A	2.18	1.55	1.50
2	C	600	HEM	CMC-C2C	2.17	1.55	1.50
2	D	601	HEM	C3C-C2C	-2.17	1.32	1.37
3	B	601	UDJ	C07-C08	-2.17	1.30	1.33
2	D	601	HEM	CMD-C2D	2.17	1.55	1.50
3	C	601	UDJ	C17-C15	-2.16	1.50	1.54
2	A	600	HEM	FE-ND	2.16	2.01	1.94
3	B	601	UDJ	C26-C01	-2.13	1.49	1.53
3	C	601	UDJ	C04-C05	-2.12	1.49	1.53
2	D	601	HEM	CMA-C3A	2.09	1.55	1.50
2	D	601	HEM	CMC-C2C	2.09	1.55	1.50
2	D	601	HEM	FE-NA	2.08	2.02	1.95
3	D	602	UDJ	C07-C08	-2.06	1.30	1.33
3	A	601	UDJ	C11-C10	-2.03	1.35	1.38
3	D	602	UDJ	C04-C05	-2.02	1.49	1.53
3	B	601	UDJ	C04-C19	-2.02	1.49	1.53
3	A	601	UDJ	C03-C04	-2.01	1.49	1.53

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	UDJ	C09-C08-C07	9.73	137.63	125.08
3	D	602	UDJ	C15-C08-C09	-9.51	115.32	125.39
3	A	601	UDJ	C09-C08-C07	8.84	136.48	125.08
3	B	601	UDJ	C15-C08-C09	-8.01	116.91	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	UDJ	C15-C08-C09	-7.90	117.02	125.39
3	B	601	UDJ	C09-C08-C07	7.89	135.26	125.08
3	A	601	UDJ	C15-C08-C09	-7.86	117.06	125.39
3	C	601	UDJ	C09-C08-C07	7.64	134.94	125.08
3	B	601	UDJ	C06-C05-C15	-7.53	98.77	104.05
3	B	601	UDJ	C06-C05-C04	-6.00	115.27	121.63
3	C	601	UDJ	C06-C05-C15	-5.85	99.95	104.05
3	B	601	UDJ	C16-C15-C17	-5.77	104.51	111.10
3	C	601	UDJ	C10-C09-C08	5.66	130.40	121.04
3	A	601	UDJ	C16-C15-C17	-5.46	104.87	111.10
3	D	602	UDJ	C06-C05-C04	-5.41	115.90	121.63
3	D	602	UDJ	C16-C15-C17	-5.33	105.01	111.10
3	D	602	UDJ	C10-C09-C08	5.25	129.72	121.04
3	A	601	UDJ	C06-C05-C04	-5.21	116.10	121.63
3	C	601	UDJ	C06-C05-C04	-5.20	116.12	121.63
3	A	601	UDJ	C10-C09-C08	4.85	129.06	121.04
3	C	601	UDJ	C10-C09-C14	-4.82	112.24	117.61
3	A	601	UDJ	C06-C05-C15	-4.75	100.72	104.05
3	D	602	UDJ	C06-C05-C15	-4.64	100.80	104.05
3	B	601	UDJ	C10-C09-C08	4.64	128.70	121.04
3	A	601	UDJ	C10-C09-C14	-4.49	112.61	117.61
3	B	601	UDJ	C10-C09-C14	-4.46	112.64	117.61
3	B	601	UDJ	C15-C08-C07	-4.43	105.72	109.66
3	D	602	UDJ	C10-C09-C14	-4.39	112.72	117.61
3	A	601	UDJ	C17-C15-C08	3.92	123.83	119.30
3	A	601	UDJ	C15-C08-C07	-3.90	106.19	109.66
2	C	600	HEM	C3B-C2B-C1B	3.85	109.30	106.41
3	D	602	UDJ	C17-C15-C08	3.63	123.50	119.30
3	C	601	UDJ	C16-C15-C17	-3.51	107.09	111.10
3	C	601	UDJ	C17-C15-C08	3.42	123.25	119.30
3	C	601	UDJ	C15-C08-C07	-3.40	106.63	109.66
2	B	600	HEM	CAA-CBA-CGA	-3.40	104.64	113.67
3	B	601	UDJ	C05-C15-C08	-3.38	96.64	99.50
2	D	601	HEM	C3B-C2B-C1B	3.31	108.89	106.41
2	B	600	HEM	O2A-CGA-CBA	3.24	124.25	114.00
3	B	601	UDJ	C05-C06-C07	-3.24	96.28	101.25
3	B	601	UDJ	C17-C15-C08	3.24	123.04	119.30
2	D	601	HEM	CHD-C4C-NC	3.23	127.97	124.45
3	A	601	UDJ	C11-C10-C09	3.21	123.52	120.36
3	A	601	UDJ	C05-C06-C07	-3.17	96.38	101.25
2	C	600	HEM	O2A-CGA-CBA	3.15	123.97	114.00
3	D	602	UDJ	C15-C08-C07	-3.15	106.86	109.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	HEM	O1A-CGA-CBA	-3.02	113.51	123.09
3	A	601	UDJ	C19-C04-C05	-2.81	105.41	109.09
2	C	600	HEM	C3B-C4B-NB	-2.76	107.48	109.47
2	D	601	HEM	CMD-C2D-C1D	2.75	129.33	125.03
3	B	601	UDJ	C19-C04-C05	-2.74	105.50	109.09
2	A	600	HEM	O1A-CGA-CBA	-2.74	114.42	123.09
2	C	600	HEM	CHA-C1A-NA	2.73	128.81	123.86
3	D	602	UDJ	C19-C04-C05	-2.72	105.53	109.09
2	C	600	HEM	C1B-NB-C4B	2.69	108.39	105.21
3	D	602	UDJ	C12-N13-C14	2.66	121.52	116.85
2	A	600	HEM	CHC-C4B-NB	2.66	127.29	124.42
2	A	600	HEM	O2A-CGA-CBA	2.62	122.29	114.00
3	B	601	UDJ	C18-C19-C04	-2.62	108.13	111.78
2	C	600	HEM	C2A-C1A-NA	-2.60	107.27	110.15
3	C	601	UDJ	C05-C06-C07	-2.55	97.34	101.25
3	D	602	UDJ	C05-C06-C07	-2.54	97.35	101.25
2	A	600	HEM	C2A-C1A-NA	-2.54	107.34	110.15
2	C	600	HEM	CAA-CBA-CGA	-2.52	106.99	113.67
3	B	601	UDJ	C11-C10-C09	2.50	122.82	120.36
3	C	601	UDJ	C12-N13-C14	2.46	121.16	116.85
2	D	601	HEM	CAC-C3C-C4C	-2.44	118.99	124.82
3	D	602	UDJ	C11-C10-C09	2.39	122.72	120.36
3	C	601	UDJ	C11-C10-C09	2.39	122.71	120.36
3	A	601	UDJ	C20-C19-C04	-2.38	110.02	112.43
2	D	601	HEM	O2A-CGA-CBA	2.36	121.45	114.00
2	C	600	HEM	O2D-CGD-CBD	2.32	121.33	114.00
3	B	601	UDJ	C16-C15-C08	2.30	111.41	107.81
2	B	600	HEM	O1A-CGA-CBA	-2.29	115.83	123.09
3	D	602	UDJ	C20-C19-C04	-2.28	110.11	112.43
3	C	601	UDJ	C19-C04-C05	-2.28	106.11	109.09
2	D	601	HEM	O1A-CGA-CBA	-2.26	115.91	123.09
2	D	601	HEM	O2D-CGD-CBD	2.24	121.08	114.00
2	D	601	HEM	CMB-C2B-C3B	-2.18	123.15	128.43
3	A	601	UDJ	C19-C20-C01	2.17	111.53	108.51
2	C	600	HEM	CAB-C3B-C2B	-2.16	121.40	128.43
2	C	600	HEM	C1A-C2A-C3A	2.12	110.15	106.87
2	A	600	HEM	C1D-C2D-C3D	2.11	109.20	106.98
2	B	600	HEM	O1D-CGD-CBD	-2.11	116.40	123.09
3	B	601	UDJ	C22-C20-C19	-2.10	108.07	111.34
3	B	601	UDJ	C12-N13-C14	2.10	120.53	116.85
3	B	601	UDJ	C09-C14-N13	2.09	126.61	123.50
2	B	600	HEM	CBA-CAA-C2A	2.08	118.28	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	HEM	C4A-NA-C1A	2.07	109.20	105.82
2	D	601	HEM	CAA-CBA-CGA	-2.07	108.17	113.67
2	C	600	HEM	C2B-C1B-NB	-2.07	107.46	109.84
2	B	600	HEM	CHB-C1B-NB	2.07	126.92	124.37
3	C	601	UDJ	C20-C19-C04	-2.04	110.36	112.43

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	600	HEM	C4B-C3B-CAB-CBB
2	A	600	HEM	CAD-CBD-CGD-O1D

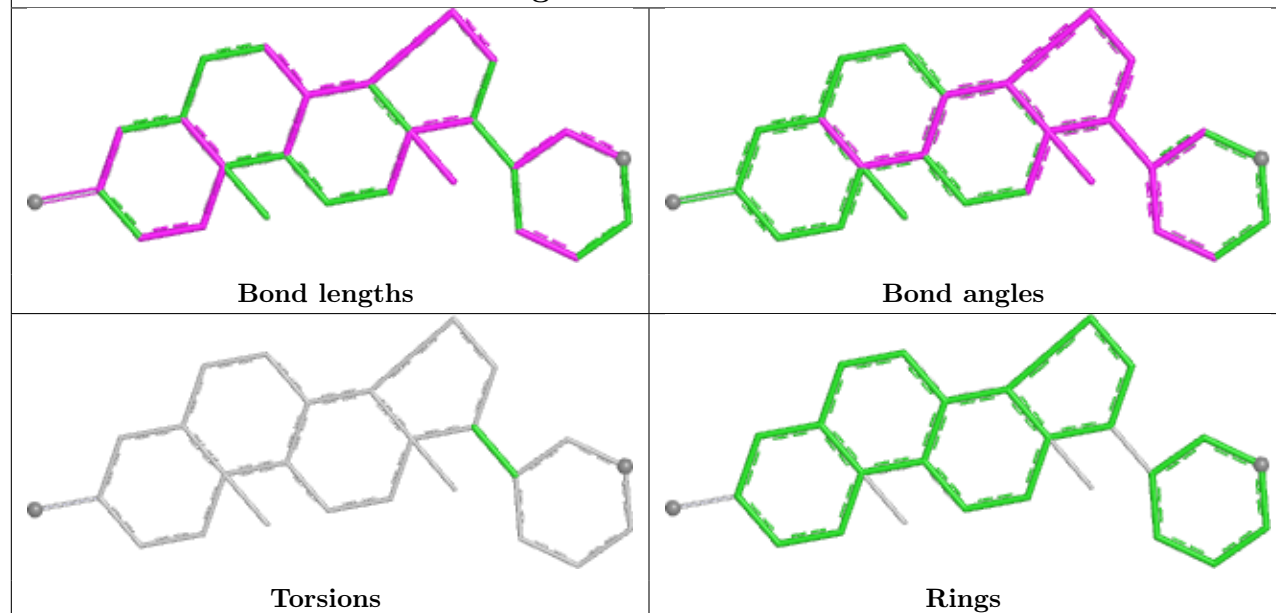
There are no ring outliers.

4 monomers are involved in 17 short contacts:

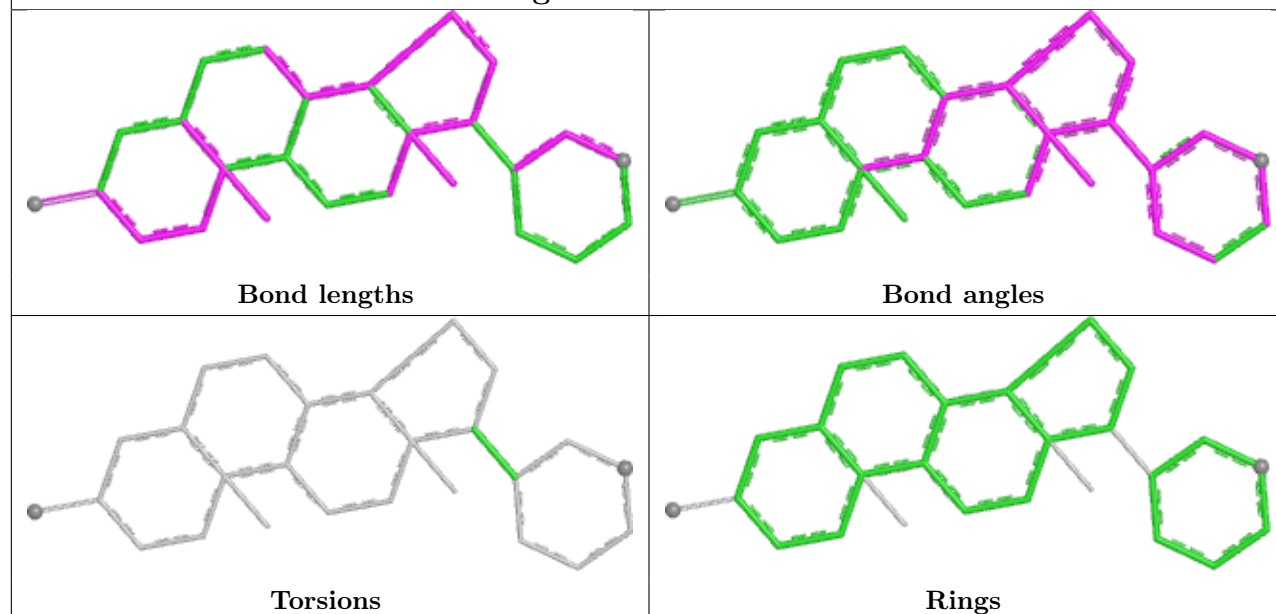
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	600	HEM	2	0
2	D	601	HEM	4	0
2	B	600	HEM	6	0
2	A	600	HEM	5	0

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.

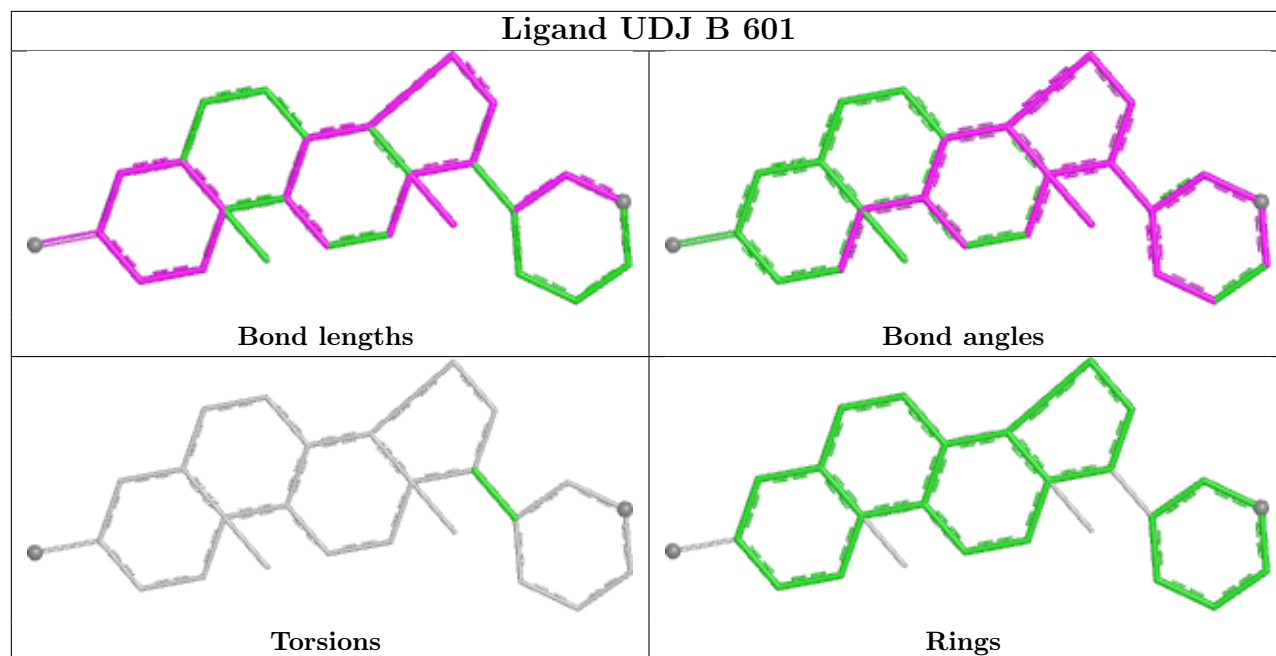
Ligand UDJ A 601



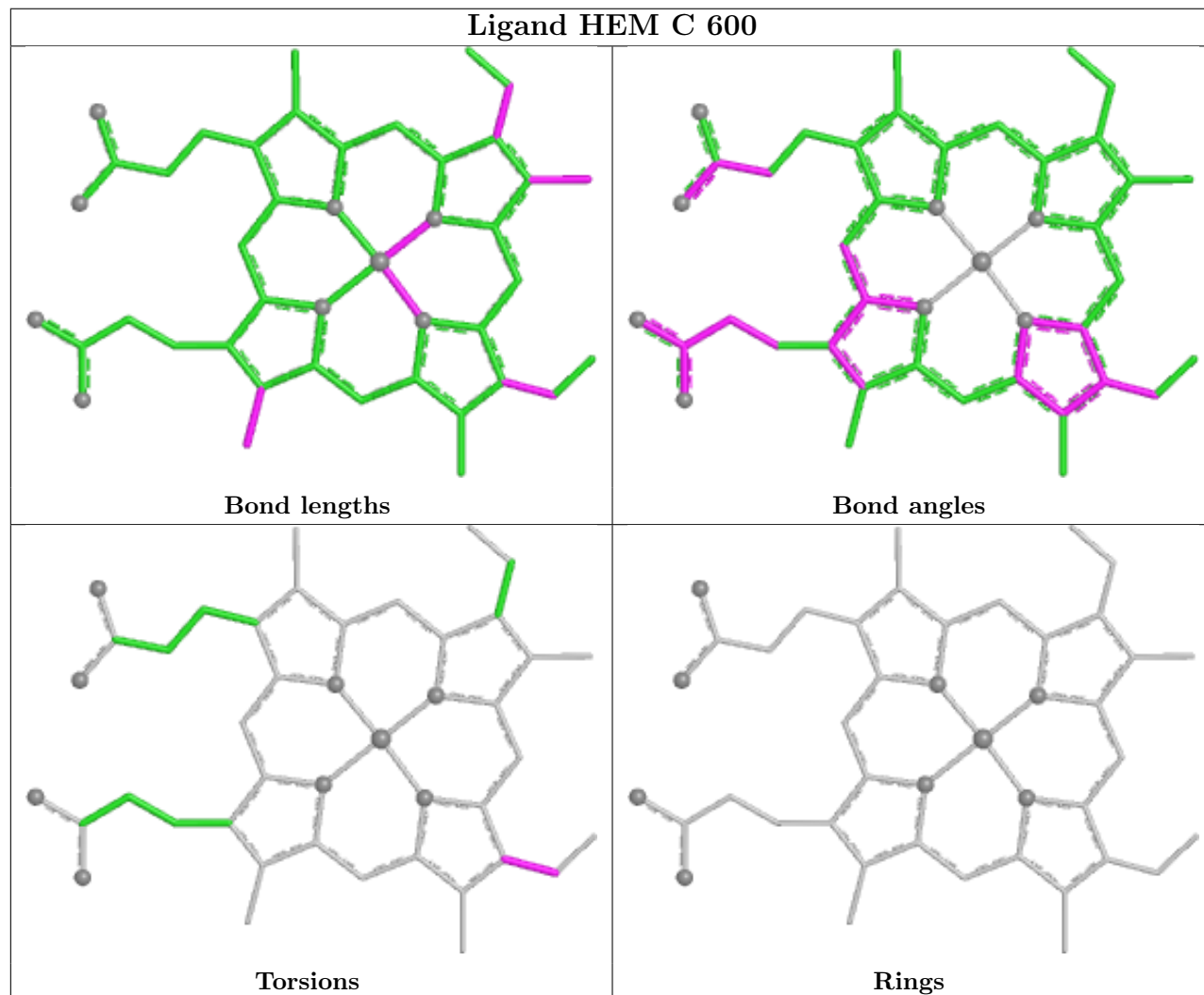
Ligand UDJ C 601

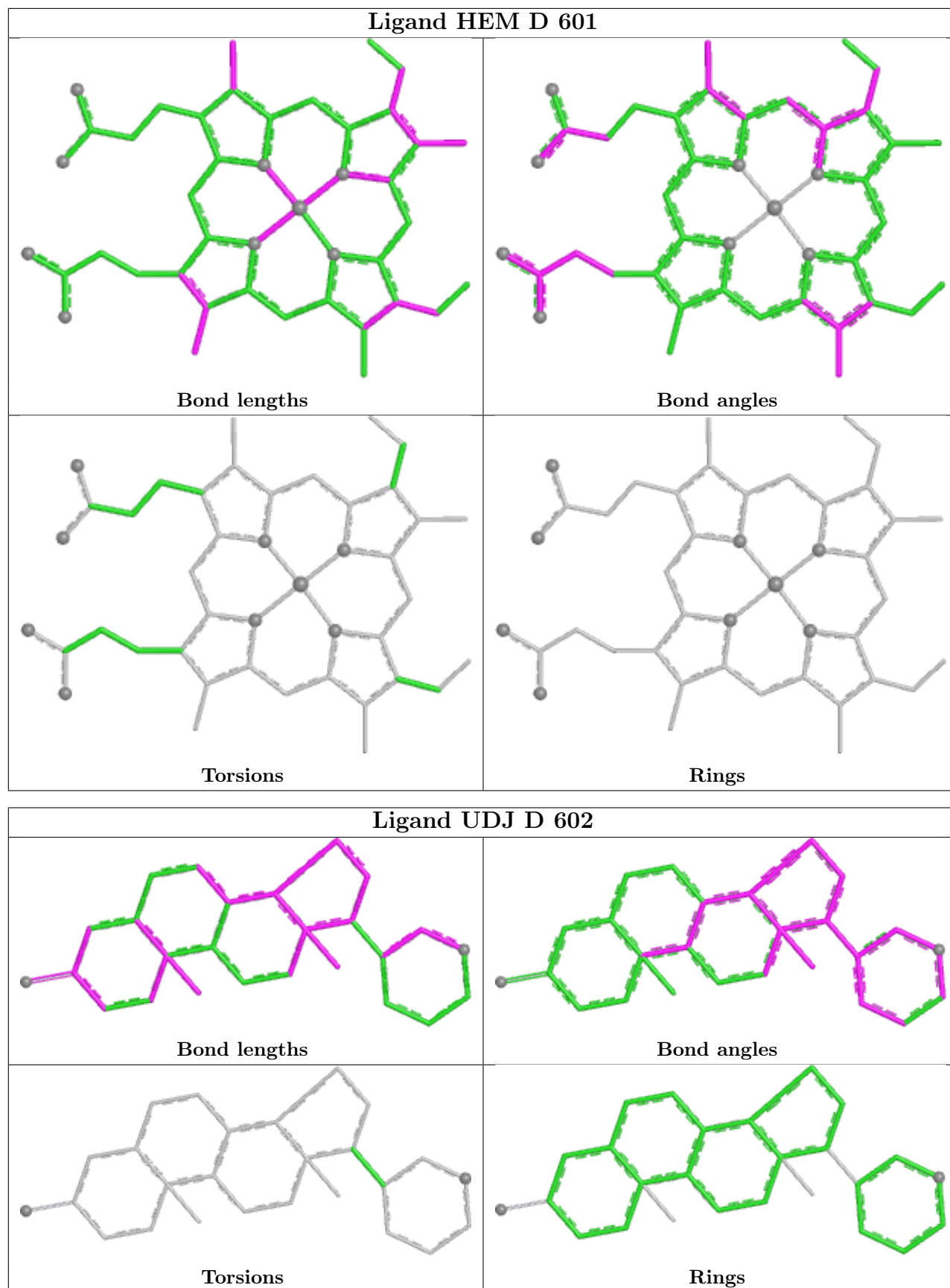


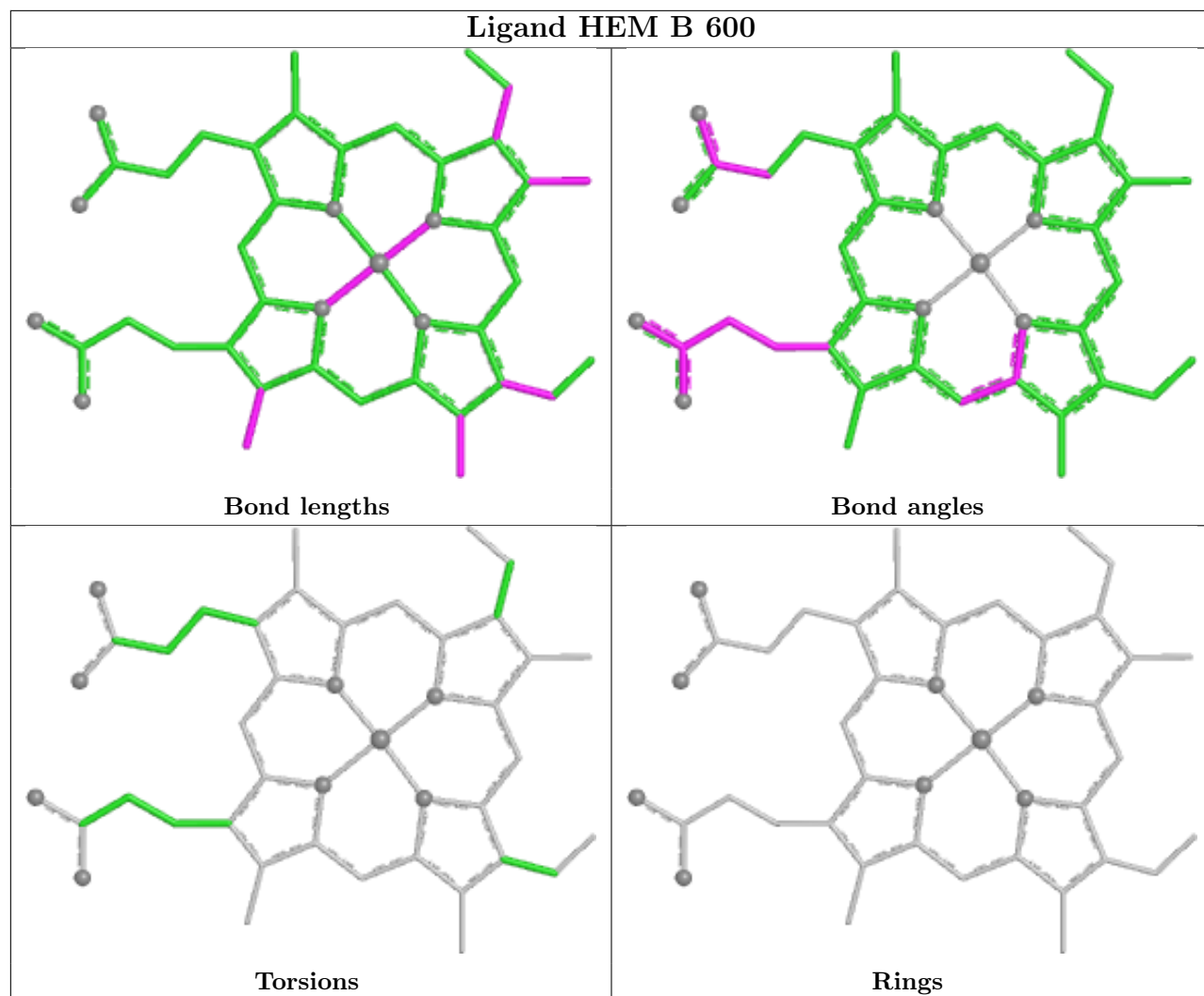
Ligand UDJ B 601

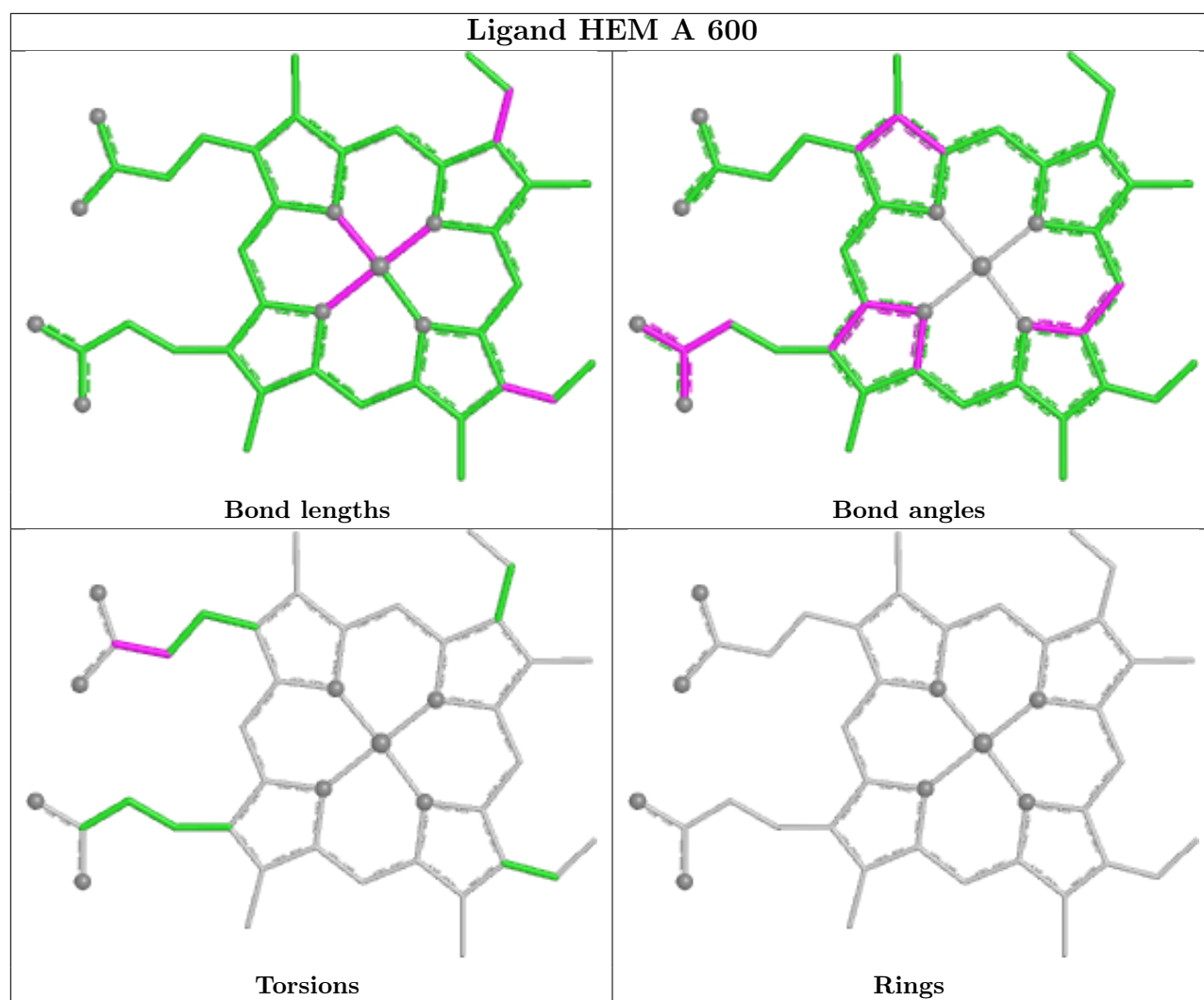


Ligand HEM C 600









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	464/494 (93%)	-0.14	9 (1%) 66 66	22, 34, 58, 93	0
1	B	469/494 (94%)	0.00	11 (2%) 61 60	23, 35, 66, 98	0
1	C	467/494 (94%)	-0.10	16 (3%) 48 47	23, 34, 61, 106	0
1	D	467/494 (94%)	0.03	13 (2%) 55 54	23, 36, 64, 97	0
All	All	1867/1976 (94%)	-0.05	49 (2%) 57 56	22, 35, 63, 106	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	504	ALA	4.5
1	C	139	ASP	4.4
1	C	46	HIS	3.8
1	B	28	PRO	3.8
1	C	42	PHE	3.8
1	D	504	ALA	3.7
1	B	27	TYR	3.6
1	B	29	LYS	3.5
1	B	25	ALA	3.4
1	D	42	PHE	3.2
1	A	31	LEU	3.1
1	D	46	HIS	3.0
1	A	139	ASP	2.8
1	D	273	SER	2.7
1	A	217	LEU	2.6
1	B	271	MET	2.5
1	C	133	ALA	2.5
1	D	47	GLY	2.5
1	B	24	GLY	2.4
1	C	138	GLY	2.4
1	C	43	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	137	ASP	2.4
1	C	47	GLY	2.4
1	C	469	ASP	2.4
1	B	135	PHE	2.4
1	C	135	PHE	2.4
1	D	139	ASP	2.3
1	B	26	LYS	2.3
1	C	49	MET	2.3
1	D	421	ALA	2.3
1	A	134	LEU	2.3
1	A	138	GLY	2.3
1	C	274	ASP	2.3
1	A	273	SER	2.3
1	D	136	LYS	2.3
1	D	274	ASP	2.2
1	C	44	PRO	2.2
1	A	283	ASP	2.2
1	C	282	GLN	2.1
1	D	471	GLY	2.1
1	A	190	ASN	2.1
1	B	134	LEU	2.1
1	B	140	GLN	2.1
1	C	134	LEU	2.1
1	A	257	ASP	2.1
1	D	138	GLY	2.1
1	B	286	LEU	2.0
1	D	45	ARG	2.0
1	D	271	MET	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 oligosaccharides 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,

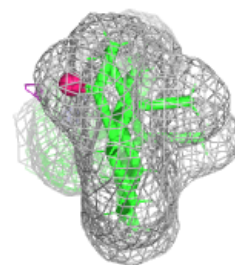
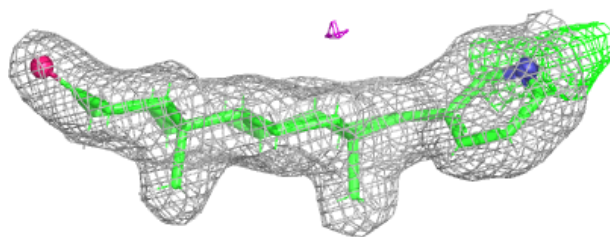
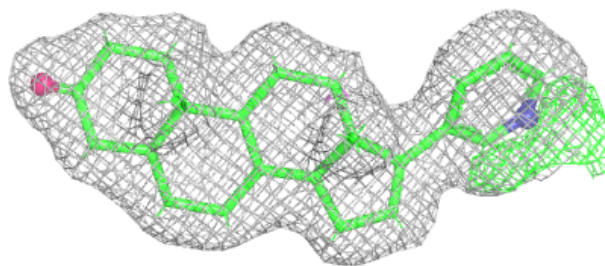
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	UDJ	C	601	26/26	0.94	0.06	19,27,34,35	0
4	CL	D	604	1/1	0.94	0.11	48,48,48,48	0
3	UDJ	A	601	26/26	0.95	0.06	19,26,33,33	0
3	UDJ	D	602	26/26	0.95	0.06	20,27,33,33	0
3	UDJ	B	601	26/26	0.95	0.06	21,27,34,35	0
2	HEM	D	601	43/43	0.98	0.06	19,24,36,44	0
2	HEM	A	600	43/43	0.98	0.06	17,24,34,41	0
2	HEM	B	600	43/43	0.98	0.06	19,27,35,43	0
4	CL	D	603	1/1	0.99	0.04	28,28,28,28	0
2	HEM	C	600	43/43	0.99	0.06	17,22,33,40	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.

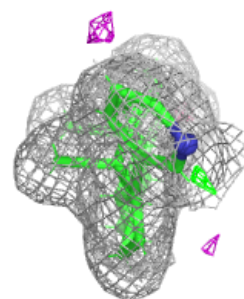
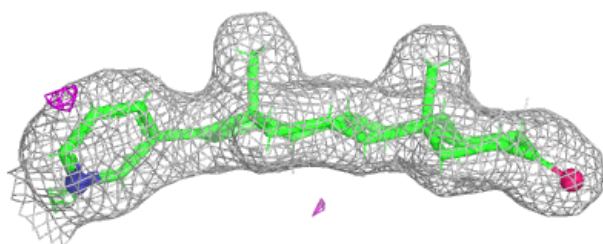
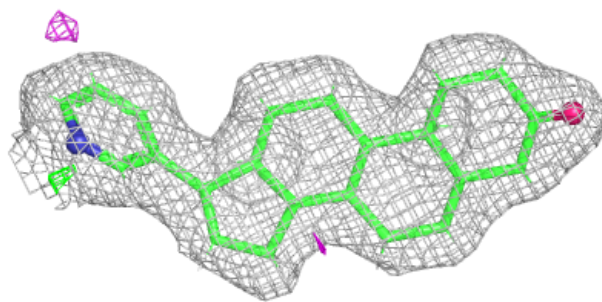
Electron density around UDJ C 601:

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

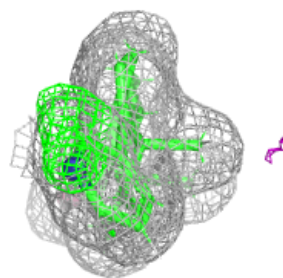
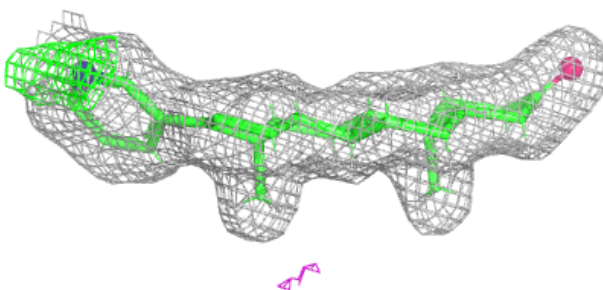
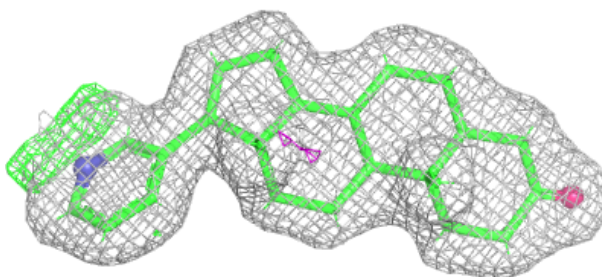


Electron density around UDJ A 601:

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

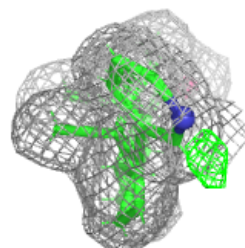
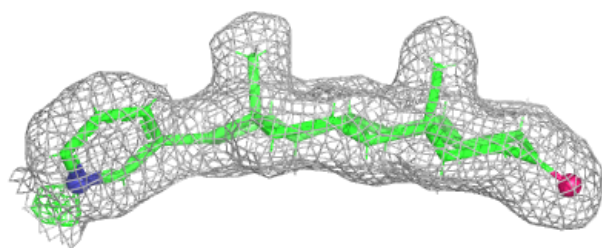
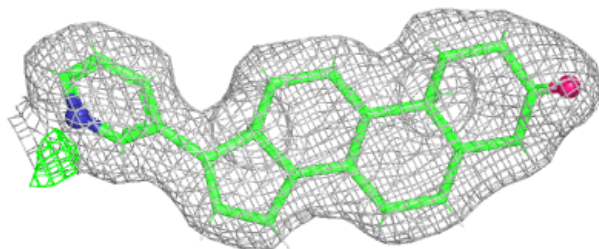
**Electron density around UDJ D 602:**

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



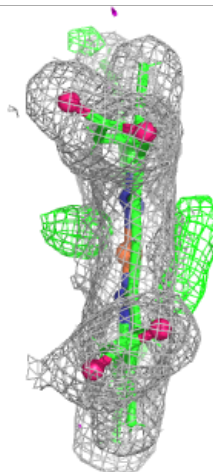
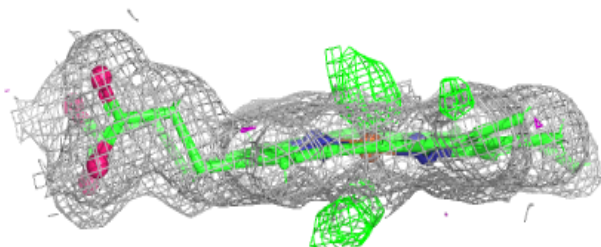
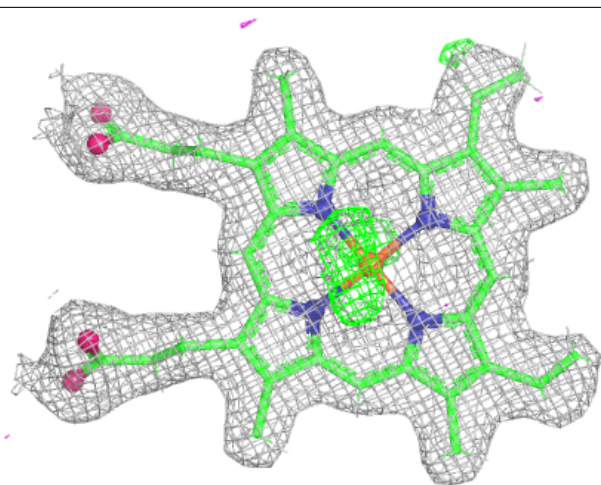
Electron density around UDJ B 601:

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



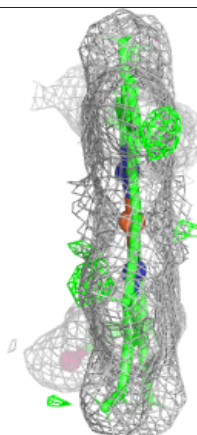
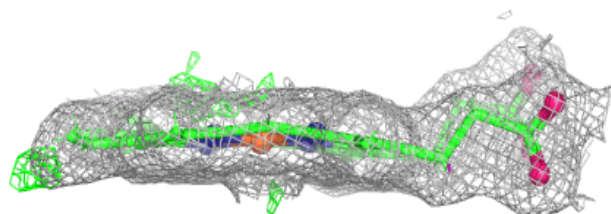
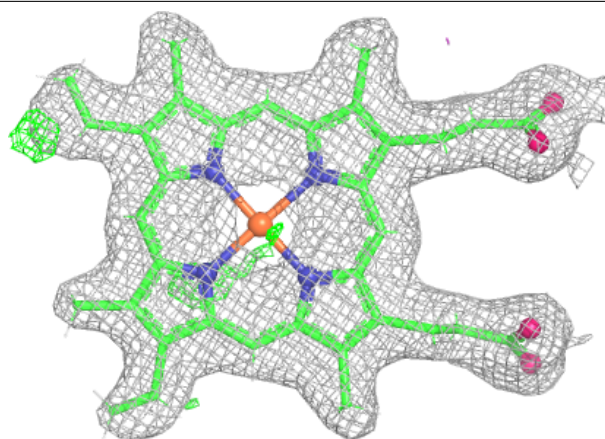
Electron density around HEM D 601:

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



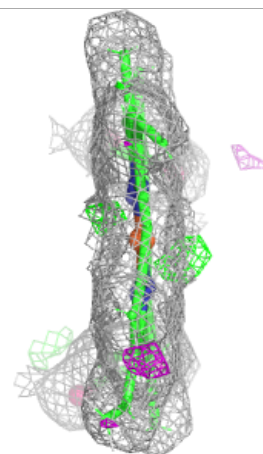
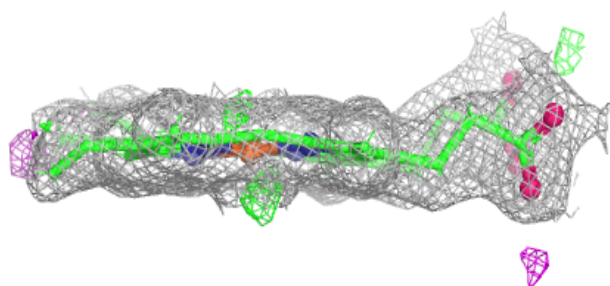
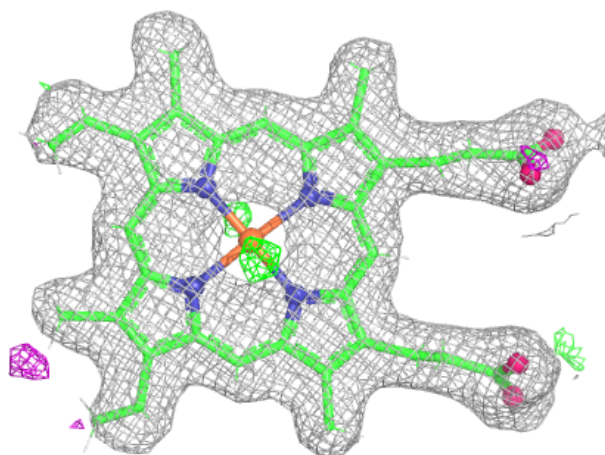
Electron density around HEM A 600:

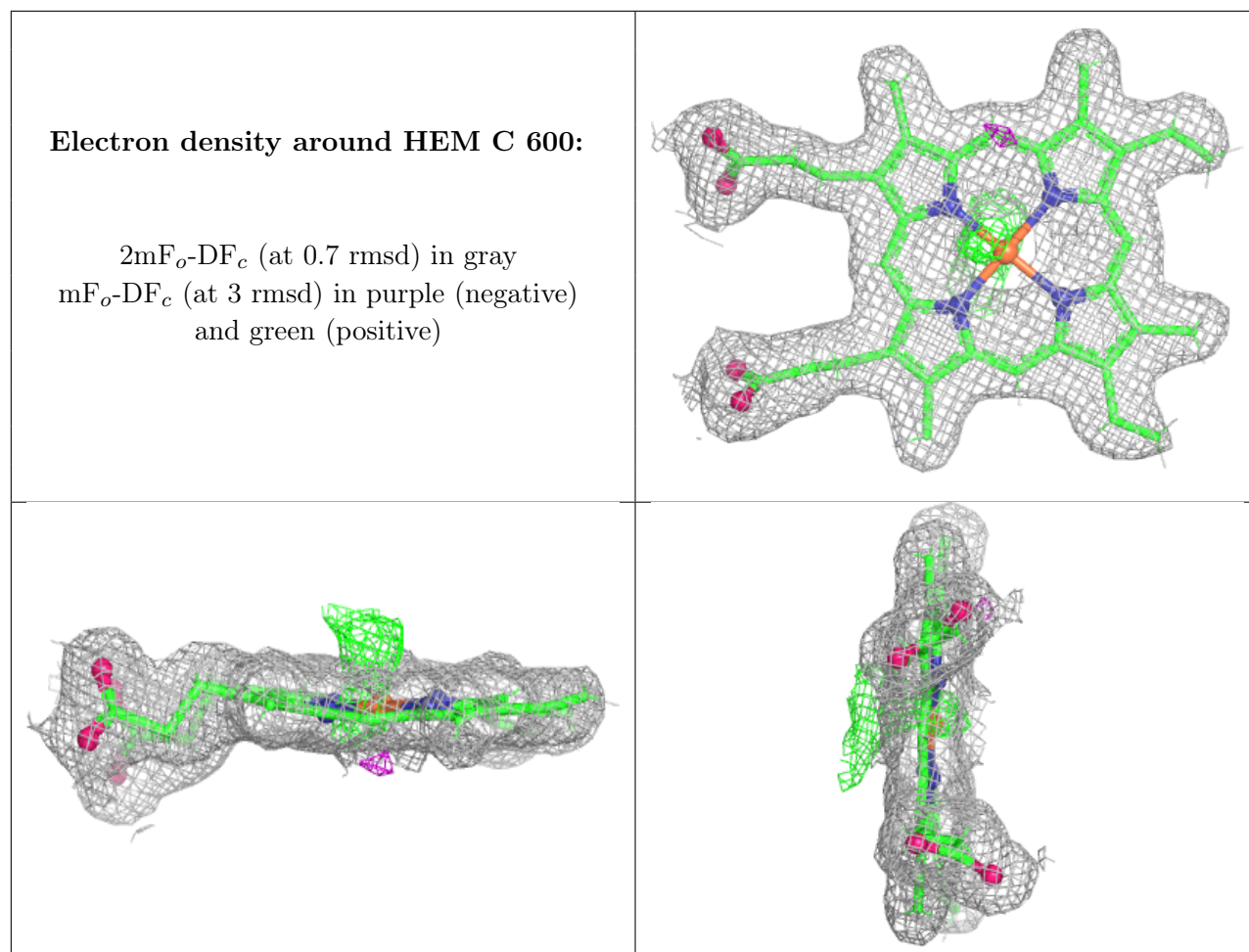
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 [i](#)

There are no such residues in this entry.