



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:44 PM UTC

PDB ID : 6UDL / pdb_00006udl
Title : Structure of Human Cytochrome P450 1A1 with Duocarmycin Prodrug (S)
ICT-2700
Authors : Bart, A.G.; Scott, E.E.
Deposited on : 2019-09-19
Resolution : 2.85 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

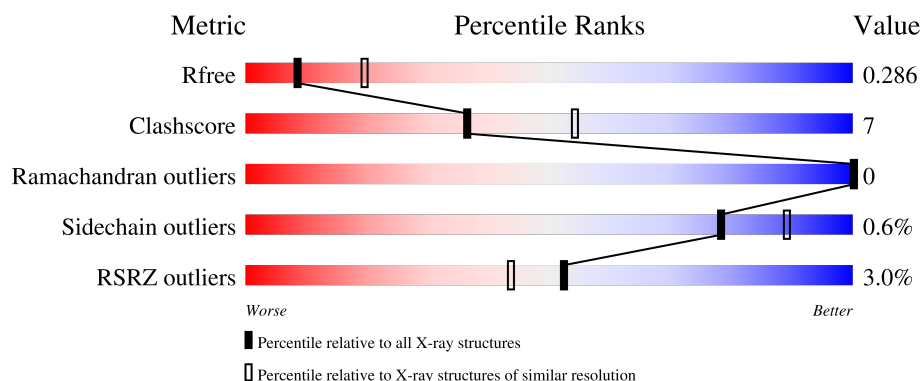
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	491	0% 82% 13% •
1	B	491	0% 86% 11% •
1	C	491	4% 78% 17% 5%
1	D	491	7% 78% 16% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30414 atoms, of which 15172 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 Cytochrome P450 1A1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	469	Total	C	H	N	O	S	0	0	0
			7510	2406	3756	653	674	21			
1	B	477	Total	C	H	N	O	S	0	0	0
			7627	2442	3811	664	689	21			
1	C	466	Total	C	H	N	O	S	0	0	0
			7456	2390	3729	648	668	21			
1	D	465	Total	C	H	N	O	S	0	0	0
			7438	2385	3720	646	666	21			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	expression tag	UNP P04798
A	29	ALA	-	expression tag	UNP P04798
A	30	LYS	-	expression tag	UNP P04798
A	31	LYS	-	expression tag	UNP P04798
A	32	THR	-	expression tag	UNP P04798
A	33	SER	-	expression tag	UNP P04798
A	34	SER	-	expression tag	UNP P04798
A	513	HIS	-	expression tag	UNP P04798
A	514	HIS	-	expression tag	UNP P04798
A	515	HIS	-	expression tag	UNP P04798
A	516	HIS	-	expression tag	UNP P04798
A	517	HIS	-	expression tag	UNP P04798
A	518	HIS	-	expression tag	UNP P04798
B	28	MET	-	expression tag	UNP P04798
B	29	ALA	-	expression tag	UNP P04798
B	30	LYS	-	expression tag	UNP P04798
B	31	LYS	-	expression tag	UNP P04798
B	32	THR	-	expression tag	UNP P04798
B	33	SER	-	expression tag	UNP P04798
B	34	SER	-	expression tag	UNP P04798
B	513	HIS	-	expression tag	UNP P04798

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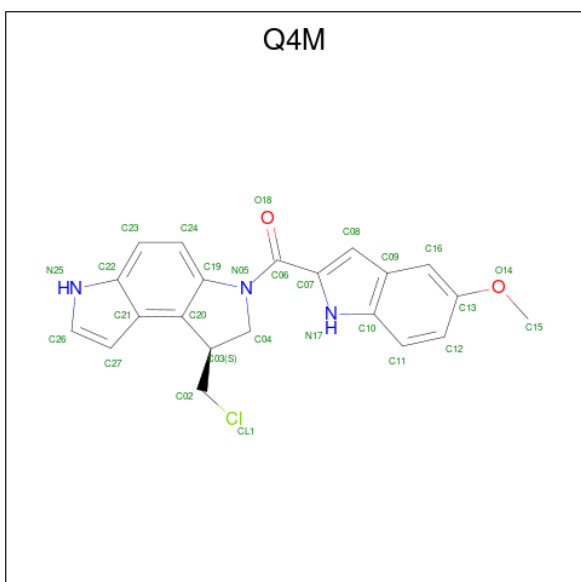
Chain	Residue	Modelled	Actual	Comment	Reference
B	514	HIS	-	expression tag	UNP P04798
B	515	HIS	-	expression tag	UNP P04798
B	516	HIS	-	expression tag	UNP P04798
B	517	HIS	-	expression tag	UNP P04798
B	518	HIS	-	expression tag	UNP P04798
C	28	MET	-	expression tag	UNP P04798
C	29	ALA	-	expression tag	UNP P04798
C	30	LYS	-	expression tag	UNP P04798
C	31	LYS	-	expression tag	UNP P04798
C	32	THR	-	expression tag	UNP P04798
C	33	SER	-	expression tag	UNP P04798
C	34	SER	-	expression tag	UNP P04798
C	513	HIS	-	expression tag	UNP P04798
C	514	HIS	-	expression tag	UNP P04798
C	515	HIS	-	expression tag	UNP P04798
C	516	HIS	-	expression tag	UNP P04798
C	517	HIS	-	expression tag	UNP P04798
C	518	HIS	-	expression tag	UNP P04798
D	28	MET	-	expression tag	UNP P04798
D	29	ALA	-	expression tag	UNP P04798
D	30	LYS	-	expression tag	UNP P04798
D	31	LYS	-	expression tag	UNP P04798
D	32	THR	-	expression tag	UNP P04798
D	33	SER	-	expression tag	UNP P04798
D	34	SER	-	expression tag	UNP P04798
D	513	HIS	-	expression tag	UNP P04798
D	514	HIS	-	expression tag	UNP P04798
D	515	HIS	-	expression tag	UNP P04798
D	516	HIS	-	expression tag	UNP P04798
D	517	HIS	-	expression tag	UNP P04798
D	518	HIS	-	expression tag	UNP P04798

- 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
2	D	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0

- Molecule 3 is [(1S)-1-(chloromethyl)-1,6-dihydropyrrolo[3,2-e]indol-3(2H)-yl](5-methoxy-1H-indol-2-yl)methanone (CCD ID: Q4M) (formula: C₂₁H₁₈ClN₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	H	N	O	0	0
			45	21	1	18	3	2		
3	B	1	Total	C	Cl	H	N	O	0	0
			45	21	1	18	3	2		

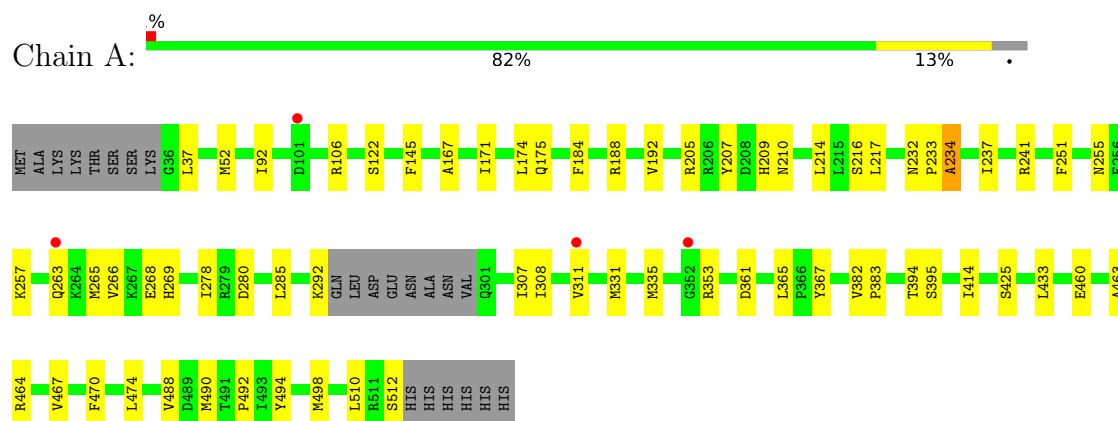
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O	0	0
			1	1		

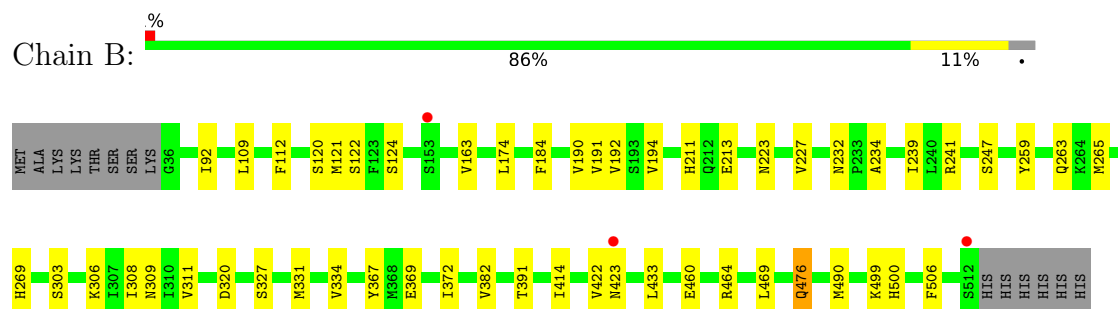
3 Residue-property plots

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.

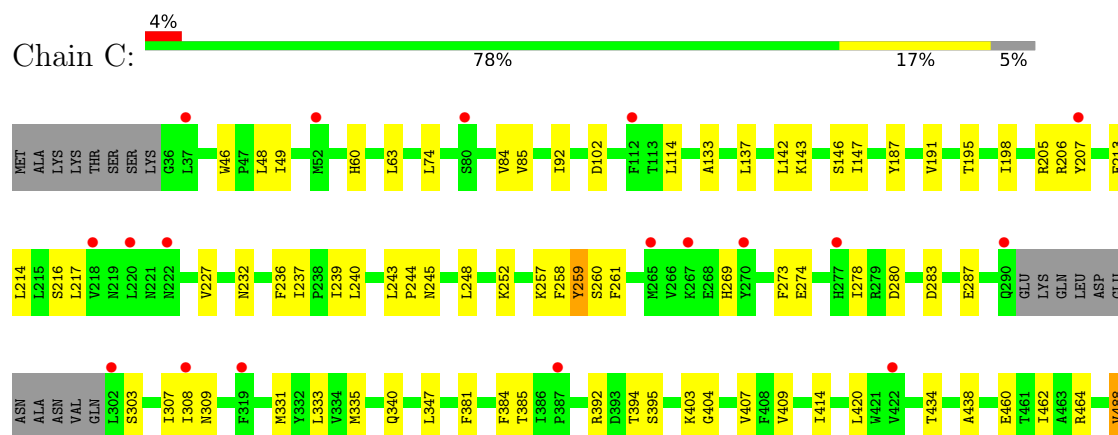
• Molecule 1: Cytochrome P450 1A1

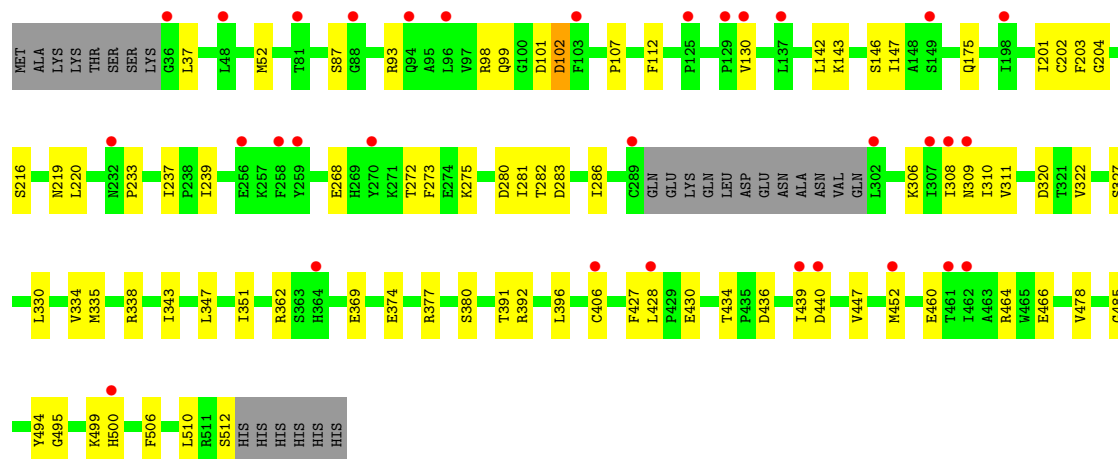


• Molecule 1: Cytochrome P450 1A1



• Molecule 1: Cytochrome P450 1A1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.37Å 196.15Å 237.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.85 48.80 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.80-2.85) 88.2 (48.80-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.68 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.238 , 0.287 0.239 , 0.286	Depositor DCC
R_{free} test set	1990 reflections (2.75%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 20.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	30414	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: HEM, Q4M

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	0.38	4/3848 (0.1%)	0.39	2/5212 (0.0%)
1	B	0.42	8/3911 (0.2%)	0.39	2/5300 (0.0%)
1	C	0.39	3/3821 (0.1%)	0.49	4/5177 (0.1%)
1	D	0.50	3/3812 (0.1%)	0.52	2/5165 (0.0%)
All	All	0.43	18/15392 (0.1%)	0.45	10/20854 (0.0%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227	VAL	C-N	-10.08	1.23	1.33
1	A	234	ALA	C-O	-8.23	1.13	1.24
1	B	122	SER	CA-C	-7.00	1.43	1.52
1	B	122	SER	C-O	-6.77	1.15	1.24
1	B	122	SER	CA-CB	-6.67	1.43	1.53
1	B	227	VAL	C-O	-6.65	1.15	1.24
1	D	101	ASP	C-O	-6.55	1.16	1.24
1	B	121	MET	C-O	-6.21	1.16	1.24
1	A	232	ASN	C-O	-6.04	1.16	1.24
1	C	245	ASN	N-CA	-6.03	1.41	1.46
1	C	488	VAL	C-O	-5.97	1.17	1.24
1	B	232	ASN	C-O	-5.72	1.17	1.24
1	D	101	ASP	N-CA	-5.69	1.39	1.46
1	B	476	GLN	C-O	-5.50	1.17	1.24
1	A	233	PRO	C-O	-5.37	1.17	1.24
1	C	245	ASN	C-O	-5.24	1.19	1.24
1	A	37	LEU	C-O	-5.20	1.17	1.23
1	D	99	GLN	CA-C	-5.16	1.45	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	102	ASP	N-CA-C	8.85	121.01	111.36
1	C	309	ASN	CB-CA-C	-8.00	93.58	110.31
1	C	259	TYR	N-CA-C	-7.51	103.11	111.82
1	A	232	ASN	CA-C-N	5.34	124.97	119.05
1	A	232	ASN	C-N-CA	5.34	124.97	119.05
1	D	440	ASP	N-CA-C	-5.24	102.11	109.96
1	B	122	SER	CB-CA-C	-5.22	100.11	109.24
1	C	245	ASN	CA-C-N	-5.10	113.39	119.05
1	C	245	ASN	C-N-CA	-5.10	113.39	119.05
1	B	227	VAL	N-CA-C	5.10	116.56	111.00

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	3754	3756	3753	44	0
1	B	3816	3811	3809	31	0
1	C	3727	3729	3727	73	0
1	D	3718	3720	3719	56	0
2	A	43	30	30	6	0
2	B	43	30	30	6	0
2	C	43	30	30	4	0
2	D	43	30	30	5	0
3	A	27	18	0	0	0
3	B	27	18	0	0	0
4	B	1	0	0	0	0
All	All	15242	15172	15128	218	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 7.

All (218) 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:D:216:SER:HA	1:D:220:LEU:HD22	1.66	0.77
1:D:362:ARG:NH2	1:D:369:GLU:HG3	2.04	0.71
1:D:362:ARG:HH21	1:D:369:GLU:HG3	1.56	0.69
1:A:335:MET:CE	1:A:488:VAL:HG21	2.23	0.69
1:D:219:ASN:O	1:D:220:LEU:HD12	1.92	0.68
2:B:601:HEM:HMC2	2:B:601:HEM:HBC2	1.76	0.67
1:C:257:LYS:HA	1:C:260:SER:HB3	1.76	0.67
1:C:335:MET:SD	1:C:488:VAL:HG21	2.34	0.67
1:D:343:ILE:O	1:D:347:LEU:HD12	1.94	0.66
1:D:320:ASP:OD1	1:D:499:LYS:NZ	2.28	0.66
1:D:175:GLN:HE21	1:D:510:LEU:HD11	1.61	0.64
1:A:488:VAL:HG22	1:D:485:GLY:CA	2.28	0.64
1:B:476:GLN:HG2	1:B:476:GLN:O	1.98	0.64
1:D:146:SER:OG	1:D:147:ILE:N	2.28	0.64
1:D:204:GLY:N	1:D:280:ASP:OD2	2.32	0.63
1:C:205:ARG:HE	1:C:205:ARG:HA	1.64	0.63
1:C:488:VAL:HG23	1:C:488:VAL:O	1.98	0.62
1:C:143:LYS:HA	1:C:146:SER:OG	1.99	0.62
1:C:239:ILE:HD12	1:C:239:ILE:H	1.64	0.62
1:C:48:LEU:H	1:C:48:LEU:HD23	1.64	0.61
1:C:74:LEU:HD11	1:C:85:VAL:HB	1.81	0.61
1:A:106:ARG:NH2	2:A:601:HEM:O2A	2.33	0.61
2:C:601:HEM:HBB2	2:C:601:HEM:HMB2	1.83	0.60
1:B:239:ILE:H	1:B:239:ILE:HD12	1.68	0.59
1:C:46:TRP:HD1	1:C:49:ILE:HD11	1.66	0.59
1:A:265:MET:O	1:A:269:HIS:ND1	2.35	0.59
1:C:60:HIS:CE1	1:C:498:MET:HE1	2.38	0.59
1:A:106:ARG:NH1	1:A:122:SER:O	2.35	0.59
1:D:391:THR:HG23	1:D:392:ARG:HD3	1.84	0.59
1:D:439:ILE:O	1:D:439:ILE:HG13	2.02	0.59
1:C:260:SER:OG	1:C:261:PHE:N	2.35	0.59
1:B:382:VAL:HG21	2:B:601:HEM:HMB1	1.85	0.58
1:C:331:MET:CB	1:C:490:MET:HE1	2.34	0.58
1:A:488:VAL:HG22	1:D:485:GLY:HA2	1.86	0.58
1:C:460:GLU:OE1	1:C:464:ARG:NH1	2.37	0.57
1:D:327:SER:OG	1:D:500:HIS:NE2	2.36	0.57
1:C:207:TYR:HB2	1:C:214:LEU:HD22	1.87	0.57
1:C:494:TYR:HA	1:C:498:MET:HE3	1.85	0.57
1:C:102:ASP:OD1	1:C:392:ARG:NH1	2.37	0.57
1:D:447:VAL:HG23	1:D:447:VAL:O	2.04	0.57
1:D:52:MET:HE2	1:D:233:PRO:HB3	1.87	0.57
1:C:331:MET:HB3	1:C:490:MET:HE1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ALA:O	1:B:241:ARG:NH1	2.39	0.56
1:C:133:ALA:O	1:C:137:LEU:HD12	2.05	0.56
1:A:269:HIS:NE2	1:A:280:ASP:OD2	2.38	0.56
2:B:601:HEM:HMB2	2:B:601:HEM:HBB2	1.88	0.56
2:D:601:HEM:HBB2	2:D:601:HEM:HMB2	1.87	0.56
1:C:46:TRP:CD1	1:C:49:ILE:HD11	2.40	0.56
1:C:333:LEU:HD22	1:C:340:GLN:HG3	1.87	0.56
2:A:601:HEM:HMB2	2:A:601:HEM:HBB2	1.88	0.55
1:D:330:LEU:O	1:D:334:VAL:HG13	2.06	0.54
1:A:488:VAL:HG23	1:A:488:VAL:O	2.08	0.54
1:A:188:ARG:NH1	1:A:209:HIS:O	2.40	0.54
1:A:205:ARG:NH2	1:A:268:GLU:OE1	2.40	0.54
1:B:331:MET:HE3	1:B:490:MET:SD	2.49	0.53
1:C:213:GLU:HA	1:C:216:SER:HB2	1.89	0.53
1:C:331:MET:HE3	1:C:490:MET:SD	2.48	0.53
1:C:227:VAL:O	1:C:232:ASN:ND2	2.41	0.53
1:C:92:ILE:HD12	1:C:414:ILE:HD11	1.91	0.53
1:C:195:THR:HA	1:C:198:ILE:HG22	1.91	0.53
1:A:331:MET:HB3	1:A:490:MET:HE1	1.92	0.52
1:C:74:LEU:HD11	1:C:85:VAL:CG2	2.40	0.52
1:C:146:SER:OG	1:C:147:ILE:N	2.42	0.52
1:A:460:GLU:OE2	1:A:464:ARG:NH1	2.42	0.52
1:C:462:ILE:HD12	1:C:462:ILE:H	1.74	0.52
1:C:278:ILE:HG23	1:C:283:ASP:HB3	1.92	0.52
2:A:601:HEM:HBC2	2:A:601:HEM:HMC2	1.90	0.52
1:B:308:ILE:O	1:B:311:VAL:HG22	2.09	0.52
1:B:303:SER:HB2	1:B:306:LYS:H	1.75	0.52
2:B:601:HEM:HBC2	2:B:601:HEM:CMC	2.39	0.51
1:D:93:ARG:HG2	1:D:452:MET:HE1	1.91	0.51
1:A:175:GLN:OE1	1:A:510:LEU:HD11	2.10	0.51
2:A:601:HEM:HBB2	2:A:601:HEM:CMB	2.41	0.51
1:D:239:ILE:HD12	1:D:239:ILE:H	1.76	0.51
1:C:142:LEU:O	1:C:146:SER:N	2.44	0.51
1:C:205:ARG:HE	1:C:206:ARG:H	1.58	0.51
2:D:601:HEM:HBC2	2:D:601:HEM:HMC2	1.92	0.51
1:B:223:ASN:ND2	1:B:247:SER:O	2.44	0.51
1:A:188:ARG:NH2	1:A:210:ASN:OD1	2.38	0.51
1:A:214:LEU:O	1:A:217:LEU:N	2.41	0.50
1:B:92:ILE:HD12	1:B:414:ILE:HD11	1.93	0.50
1:D:268:GLU:O	1:D:272:THR:HG22	2.11	0.50
1:A:174:LEU:HD22	1:A:184:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:HEM:HBB2	2:B:601:HEM:CMB	2.41	0.50
1:C:434:THR:HG23	1:C:438:ALA:O	2.12	0.50
1:C:512:SER:O	1:C:512:SER:OG	2.23	0.50
1:A:361:ASP:O	1:A:365:LEU:HD12	2.12	0.50
1:B:320:ASP:OD1	1:B:499:LYS:NZ	2.44	0.50
1:D:362:ARG:HH21	1:D:369:GLU:CG	2.25	0.50
1:A:492:PRO:CB	1:A:498:MET:HE3	2.42	0.50
1:C:392:ARG:O	1:C:394:THR:OG1	2.30	0.50
1:A:463:ALA:O	1:A:467:VAL:HG23	2.12	0.49
1:B:120:SER:O	1:B:124:SER:HB3	2.11	0.49
1:C:273:PHE:HD1	1:C:274:GLU:N	2.10	0.49
1:D:52:MET:HE1	1:D:237:ILE:HG13	1.94	0.49
2:C:601:HEM:HMC2	2:C:601:HEM:HBC2	1.93	0.49
1:D:478:VAL:HG12	1:D:510:LEU:HA	1.95	0.48
2:D:601:HEM:HHA	2:D:601:HEM:HBD1	1.95	0.48
1:B:460:GLU:OE1	1:B:464:ARG:NH1	2.47	0.48
1:D:201:ILE:HG22	1:D:281:ILE:HD12	1.96	0.48
1:B:331:MET:HA	1:B:334:VAL:HG22	1.96	0.48
2:D:601:HEM:HBB2	2:D:601:HEM:CMB	2.43	0.48
1:C:217:LEU:HD23	1:C:258:PHE:CE2	2.49	0.48
1:A:192:VAL:HG11	1:A:209:HIS:HA	1.96	0.48
1:B:422:VAL:HG23	1:B:423:ASN:N	2.29	0.47
2:C:601:HEM:HBB2	2:C:601:HEM:CMB	2.43	0.47
1:D:202:CYS:O	1:D:282:THR:HG23	2.14	0.47
1:D:434:THR:OG1	1:D:436:ASP:OD1	2.31	0.47
1:A:335:MET:HE3	1:A:488:VAL:HG21	1.94	0.47
1:C:492:PRO:HB2	1:C:498:MET:HE2	1.96	0.47
1:A:335:MET:HE1	1:A:488:VAL:HG21	1.95	0.47
1:C:84:VAL:O	1:C:407:VAL:HA	2.15	0.47
1:C:278:ILE:HD11	1:C:287:GLU:OE1	2.15	0.47
1:D:219:ASN:O	1:D:220:LEU:CD1	2.59	0.47
1:B:369:GLU:HA	1:B:372:ILE:HG12	1.97	0.47
2:D:601:HEM:HBC2	2:D:601:HEM:CMC	2.44	0.47
1:D:427:PHE:O	1:D:428:LEU:HD23	2.16	0.46
1:A:488:VAL:HG22	1:D:485:GLY:HA3	1.95	0.46
1:A:492:PRO:HB2	1:A:498:MET:HE3	1.98	0.46
1:D:143:LYS:HA	1:D:146:SER:OG	2.15	0.46
1:A:394:THR:OG1	1:A:395:SER:N	2.48	0.46
1:C:216:SER:HB3	1:C:217:LEU:HD12	1.97	0.46
1:A:269:HIS:CD2	1:A:280:ASP:OD2	2.69	0.46
1:A:367:TYR:HD1	1:A:433:LEU:HD11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:LEU:HD23	1:D:281:ILE:CD1	2.45	0.46
1:D:107:PRO:HB3	1:D:406:CYS:HB2	1.97	0.46
1:A:494:TYR:HA	1:A:498:MET:SD	2.55	0.46
1:C:248:LEU:HD23	1:C:252:LYS:HD2	1.98	0.46
1:D:308:ILE:O	1:D:311:VAL:HG12	2.16	0.46
1:C:205:ARG:HE	1:C:205:ARG:CA	2.29	0.45
1:C:143:LYS:HD2	1:C:147:ILE:HD12	1.99	0.45
1:D:273:PHE:CE1	1:D:275:LYS:HA	2.51	0.45
1:B:334:VAL:HG11	1:B:506:PHE:CE2	2.52	0.45
1:D:273:PHE:CE2	1:D:286:ILE:HG23	2.52	0.45
1:D:374:GLU:OE1	1:D:377:ARG:NE	2.44	0.45
1:B:163:VAL:HG11	1:B:469:LEU:HB3	1.99	0.45
1:B:190:VAL:O	1:B:194:VAL:HG23	2.17	0.45
1:D:102:ASP:OD1	1:D:102:ASP:N	2.49	0.45
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.46	0.45
1:D:362:ARG:NH2	1:D:369:GLU:CG	2.76	0.45
1:B:422:VAL:HG23	1:B:423:ASN:OD1	2.17	0.44
1:C:331:MET:HB2	1:C:490:MET:HE1	1.99	0.44
1:D:203:PHE:CD1	1:D:282:THR:HG21	2.52	0.44
1:A:145:PHE:HZ	1:A:278:ILE:HG22	1.82	0.44
1:A:308:ILE:O	1:A:311:VAL:HG12	2.18	0.44
2:C:601:HEM:HBC2	2:C:601:HEM:CMC	2.47	0.44
1:C:187:TYR:O	1:C:191:VAL:HB	2.17	0.44
1:C:385:THR:HG23	1:C:409:VAL:HB	1.99	0.44
1:C:394:THR:HG22	1:C:395:SER:N	2.32	0.44
1:D:37:LEU:HD23	1:D:37:LEU:HA	1.76	0.44
1:B:327:SER:OG	1:B:500:HIS:NE2	2.44	0.44
1:C:278:ILE:HG23	1:C:283:ASP:CB	2.48	0.44
1:D:239:ILE:HD12	1:D:239:ILE:N	2.33	0.44
1:D:494:TYR:CG	1:D:495:GLY:N	2.85	0.44
1:B:331:MET:HG2	1:B:506:PHE:CZ	2.53	0.43
1:C:74:LEU:CD1	1:C:85:VAL:HB	2.46	0.43
1:D:322:VAL:HG11	1:D:466:GLU:CD	2.43	0.43
1:B:191:VAL:HG13	1:B:192:VAL:HG13	2.01	0.43
1:D:334:VAL:HG11	1:D:506:PHE:CE2	2.53	0.43
1:C:257:LYS:O	1:C:257:LYS:HG2	2.18	0.43
1:A:353:ARG:NH1	1:A:512:SER:HB3	2.34	0.43
1:B:382:VAL:HG11	2:B:601:HEM:HMA2	1.99	0.43
1:C:347:LEU:HD12	1:C:347:LEU:N	2.34	0.43
1:C:74:LEU:HD11	1:C:85:VAL:CB	2.46	0.43
1:D:309:ASN:OD1	1:D:310:ILE:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:LEU:HG	1:C:85:VAL:O	2.19	0.43
1:A:251:PHE:O	1:A:255:ASN:ND2	2.49	0.42
1:B:109:LEU:HD12	1:B:112:PHE:CZ	2.54	0.42
1:B:391:THR:O	1:B:391:THR:HG22	2.17	0.42
1:C:63:LEU:HD12	1:C:384:PHE:HZ	1.84	0.42
1:C:248:LEU:CD2	1:C:252:LYS:HD2	2.49	0.42
1:D:334:VAL:HG23	1:D:335:MET:CG	2.50	0.42
1:A:92:ILE:HD12	1:A:414:ILE:HD11	2.01	0.42
1:C:303:SER:O	1:C:307:ILE:HG12	2.20	0.42
1:C:213:GLU:O	1:C:213:GLU:CG	2.67	0.42
1:D:112:PHE:N	1:D:112:PHE:CD1	2.82	0.42
1:D:201:ILE:HG22	1:D:281:ILE:CD1	2.50	0.42
1:C:213:GLU:O	1:C:216:SER:HB3	2.20	0.42
1:C:237:ILE:HD11	1:C:240:LEU:HD11	2.02	0.42
1:C:236:PHE:CD1	1:C:236:PHE:N	2.88	0.42
1:C:403:LYS:HG2	1:C:404:GLY:N	2.35	0.42
1:A:470:PHE:O	1:A:474:LEU:HD13	2.20	0.42
1:C:213:GLU:O	1:C:213:GLU:HG2	2.19	0.42
1:C:243:LEU:HD23	1:C:243:LEU:N	2.34	0.42
1:C:48:LEU:HD23	1:C:48:LEU:N	2.30	0.41
1:D:334:VAL:HG11	1:D:506:PHE:CZ	2.55	0.41
1:A:52:MET:HE1	1:A:237:ILE:HG13	2.02	0.41
1:A:234:ALA:O	1:A:241:ARG:NH1	2.53	0.41
1:C:385:THR:CG2	1:C:409:VAL:HB	2.50	0.41
1:B:309:ASN:OD1	1:B:309:ASN:C	2.63	0.41
1:D:478:VAL:HG12	1:D:510:LEU:HG	2.03	0.41
1:A:216:SER:OG	1:A:257:LYS:HE2	2.20	0.41
1:B:174:LEU:HD22	1:B:184:PHE:CZ	2.55	0.41
1:D:283:ASP:HA	1:D:286:ILE:HG22	2.02	0.41
1:C:239:ILE:HD12	1:C:239:ILE:N	2.34	0.41
1:A:382:VAL:HG11	2:A:601:HEM:HMA2	2.02	0.41
1:B:211:HIS:NE2	1:B:213:GLU:HB3	2.36	0.41
1:C:420:LEU:N	1:C:420:LEU:HD23	2.36	0.41
1:C:205:ARG:HA	1:C:205:ARG:NE	2.33	0.41
1:C:494:TYR:CG	1:C:495:GLY:N	2.88	0.41
1:A:167:ALA:O	1:A:171:ILE:HG13	2.21	0.41
1:B:259:TYR:O	1:B:263:GLN:HG3	2.21	0.41
1:D:306:LYS:HA	1:D:309:ASN:ND2	2.36	0.41
1:D:338:ARG:NH1	1:D:430:GLU:OE2	2.54	0.41
1:D:351:ILE:O	1:D:351:ILE:HG22	2.21	0.41
1:C:195:THR:HA	1:C:198:ILE:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:PHE:HA	1:C:498:MET:HG2	2.01	0.41
1:D:460:GLU:OE2	1:D:464:ARG:NH1	2.54	0.41
1:A:367:TYR:CD1	1:A:433:LEU:HD11	2.55	0.40
1:C:269:HIS:CD2	1:C:280:ASP:OD2	2.75	0.40
1:A:263:GLN:HA	1:A:266:VAL:HG12	2.02	0.40
1:B:367:TYR:HD1	1:B:433:LEU:HD11	1.86	0.40
1:D:377:ARG:O	1:D:380:SER:OG	2.40	0.40
1:C:114:LEU:HD13	1:C:252:LYS:HG2	2.02	0.40
1:A:207:TYR:HB2	1:A:214:LEU:HD22	2.03	0.40
1:A:285:LEU:HD22	1:A:307:ILE:O	2.21	0.40
1:A:383:PRO:HD3	1:A:498:MET:HG3	2.03	0.40
1:B:265:MET:O	1:B:269:HIS:ND1	2.53	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	465/491 (95%)	452 (97%)	13 (3%)	0	100	100
1	B	475/491 (97%)	457 (96%)	18 (4%)	0	100	100
1	C	462/491 (94%)	442 (96%)	20 (4%)	0	100	100
1	D	461/491 (94%)	441 (96%)	20 (4%)	0	100	100
All	All	1863/1964 (95%)	1792 (96%)	71 (4%)	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	419/439 (95%)	417 (100%)	2 (0%)	81	90
1	B	426/439 (97%)	426 (100%)	0	100	100
1	C	416/439 (95%)	413 (99%)	3 (1%)	76	87
1	D	415/439 (94%)	410 (99%)	5 (1%)	63	80
All	All	1676/1756 (95%)	1666 (99%)	10 (1%)	78	89

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

Mol	Chain	Res	Type
1	A	292	LYS
1	A	425	SER
1	C	244	PRO
1	C	259	TYR
1	C	308	ILE
1	D	87	SER
1	D	98	ARG
1	D	130	VAL
1	D	396	LEU
1	D	512	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	139	GLN
1	A	221	ASN
1	A	288	HIS
1	A	416	HIS
1	C	58	ASN
1	C	185	ASN
1	C	249	ASN
1	C	290	GLN
1	D	75	GLN
1	D	139	GLN
1	D	175	GLN
1	D	269	HIS

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Mol	Chain	Res	Type
1	D	364	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	Q4M	A	602	-	31,31,31	2.41	12 (38%)	37,46,46	2.50	15 (40%)
3	Q4M	B	602	-	31,31,31	2.52	12 (38%)	37,46,46	2.52	12 (32%)
2	HEM	C	601	-	50,50,50	1.38	7 (14%)	67,82,82	1.05	4 (5%)
2	HEM	A	601	-	50,50,50	1.39	7 (14%)	67,82,82	1.08	4 (5%)
2	HEM	B	601	1	50,50,50	1.40	9 (18%)	67,82,82	1.08	3 (4%)
2	HEM	D	601	-	50,50,50	1.37	9 (18%)	67,82,82	1.06	3 (4%)

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	Q4M	A	602	-	-	3/12/24/24	0/5/5/5
3	Q4M	B	602	-	-	5/12/24/24	0/5/5/5
2	HEM	C	601	-	-	2/14/54/54	-
2	HEM	A	601	-	-	5/14/54/54	-
2	HEM	B	601	1	-	6/14/54/54	-
2	HEM	D	601	-	-	1/14/54/54	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	Q4M	C09-C10	-6.48	1.30	1.41
3	A	602	Q4M	C21-C22	-5.41	1.36	1.41
3	A	602	Q4M	C09-C10	-4.95	1.33	1.41
3	B	602	Q4M	C22-N25	-4.70	1.30	1.37
3	B	602	Q4M	C07-N17	-4.43	1.32	1.38
3	B	602	Q4M	C12-C13	-4.04	1.31	1.38
3	A	602	Q4M	C02-C03	-3.99	1.43	1.52
2	B	601	HEM	FE-ND	3.95	2.07	1.94
3	B	602	Q4M	O14-C13	-3.69	1.30	1.37
2	A	601	HEM	FE-ND	3.60	2.06	1.94
3	A	602	Q4M	C10-N17	-3.60	1.32	1.38
3	B	602	Q4M	C02-CL1	3.55	1.96	1.78
3	A	602	Q4M	O14-C13	-3.43	1.30	1.37
2	C	601	HEM	FE-NB	3.36	2.05	1.94
3	A	602	Q4M	C12-C13	-3.34	1.32	1.38
2	D	601	HEM	FE-NC	3.31	2.06	1.95
2	A	601	HEM	FE-NC	3.21	2.05	1.95
3	A	602	Q4M	C19-N05	3.08	1.45	1.39
2	D	601	HEM	FE-NB	3.02	2.04	1.94
2	C	601	HEM	CAC-C3C	3.01	1.55	1.47
2	C	601	HEM	FE-NC	3.00	2.05	1.95
2	D	601	HEM	CAB-C3B	3.00	1.55	1.47
2	C	601	HEM	CAB-C3B	3.00	1.55	1.47
2	D	601	HEM	CAC-C3C	2.99	1.55	1.47
2	B	601	HEM	CAC-C3C	2.98	1.55	1.47
2	A	601	HEM	CAC-C3C	2.98	1.55	1.47
2	A	601	HEM	CAB-C3B	2.93	1.55	1.47
2	B	601	HEM	CAB-C3B	2.91	1.55	1.47
3	A	602	Q4M	C16-C09	-2.88	1.35	1.40
2	D	601	HEM	FE-ND	2.84	2.03	1.94
2	C	601	HEM	FE-NA	2.84	2.04	1.95
2	A	601	HEM	FE-NA	2.79	2.04	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	FE-NA	2.75	2.04	1.95
2	C	601	HEM	FE-ND	2.67	2.03	1.94
2	B	601	HEM	FE-NB	2.66	2.03	1.94
3	B	602	Q4M	O14-C15	-2.66	1.35	1.42
2	B	601	HEM	FE-NC	2.59	2.03	1.95
2	D	601	HEM	FE-NA	2.55	2.03	1.95
3	B	602	Q4M	C23-C22	-2.54	1.35	1.39
2	A	601	HEM	FE-NB	2.45	2.02	1.94
3	B	602	Q4M	C10-N17	-2.44	1.34	1.38
3	A	602	Q4M	C26-C27	2.35	1.40	1.36
3	B	602	Q4M	C09-C08	-2.35	1.36	1.44
3	B	602	Q4M	C26-C27	2.31	1.40	1.36
3	A	602	Q4M	C16-C13	-2.28	1.35	1.39
3	A	602	Q4M	C07-N17	-2.19	1.35	1.38
3	A	602	Q4M	C20-C03	-2.15	1.46	1.51
3	B	602	Q4M	C26-N25	-2.12	1.34	1.38
2	D	601	HEM	CMB-C2B	2.06	1.55	1.50
2	B	601	HEM	CMD-C2D	2.05	1.55	1.50
2	A	601	HEM	CMC-C2C	2.03	1.54	1.50
2	D	601	HEM	CMC-C2C	2.03	1.54	1.50
2	B	601	HEM	CMB-C2B	2.02	1.54	1.50
2	B	601	HEM	CMC-C2C	2.01	1.54	1.50
2	C	601	HEM	CMB-C2B	2.01	1.54	1.50
2	D	601	HEM	CMD-C2D	2.01	1.54	1.50

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	Q4M	C21-C22-N25	6.05	110.54	107.09
3	B	602	Q4M	C08-C07-N17	-5.87	103.33	109.15
3	A	602	Q4M	C03-C02-CL1	-5.72	101.39	111.53
3	B	602	Q4M	O18-C06-N05	-5.62	111.44	122.02
3	A	602	Q4M	C24-C19-C20	-5.08	115.91	122.16
3	A	602	Q4M	C04-C03-C20	4.81	106.94	102.43
3	B	602	Q4M	C23-C24-C19	4.26	127.66	119.10
3	A	602	Q4M	O18-C06-N05	-4.18	114.17	122.02
3	A	602	Q4M	C19-N05-C06	4.15	132.11	124.92
3	B	602	Q4M	C24-C19-C20	-4.08	117.14	122.16
3	A	602	Q4M	C08-C07-N17	-3.86	105.33	109.15
3	B	602	Q4M	C03-C02-CL1	3.71	118.09	111.53
3	A	602	Q4M	C27-C26-N25	-3.63	106.05	110.25
3	A	602	Q4M	C23-C22-C21	-3.39	119.97	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	Q4M	C19-C20-C03	-3.28	107.11	110.72
3	B	602	Q4M	C24-C23-C22	-3.26	113.28	119.57
3	B	602	Q4M	C09-C08-C07	3.24	110.31	107.41
3	A	602	Q4M	C21-C22-N25	2.99	108.80	107.09
3	A	602	Q4M	C22-N25-C26	2.69	110.88	108.91
3	A	602	Q4M	C15-O14-C13	-2.67	111.77	117.50
3	B	602	Q4M	C09-C16-C13	-2.57	117.54	120.46
3	B	602	Q4M	O18-C06-C07	-2.54	114.52	119.25
3	A	602	Q4M	O18-C06-C07	-2.52	114.56	119.25
3	A	602	Q4M	C23-C24-C19	2.51	124.13	119.10
2	B	601	HEM	C1B-NB-C4B	2.47	108.13	105.21
3	B	602	Q4M	C22-C21-C27	-2.43	105.25	107.02
2	A	601	HEM	C1B-NB-C4B	2.36	108.00	105.21
3	B	602	Q4M	C21-C20-C03	2.36	135.18	131.79
2	A	601	HEM	CAA-CBA-CGA	-2.33	107.49	113.67
3	A	602	Q4M	C04-N05-C19	-2.30	106.77	109.33
2	D	601	HEM	C4D-ND-C1D	2.29	107.91	105.21
2	C	601	HEM	C1B-NB-C4B	2.27	107.90	105.21
2	A	601	HEM	C3B-C2B-C1B	2.27	108.11	106.41
2	B	601	HEM	C3B-C2B-C1B	2.26	108.11	106.41
2	D	601	HEM	C1B-NB-C4B	2.25	107.88	105.21
2	C	601	HEM	C4D-ND-C1D	2.22	107.84	105.21
2	C	601	HEM	C3B-C2B-C1B	2.21	108.07	106.41
2	D	601	HEM	C3B-C2B-C1B	2.12	108.01	106.41
2	B	601	HEM	C4D-ND-C1D	2.08	107.67	105.21
2	A	601	HEM	C4D-ND-C1D	2.04	107.63	105.21
2	C	601	HEM	CAA-CBA-CGA	-2.03	108.28	113.67

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	Q4M	O18-C06-N05-C19
3	B	602	Q4M	CL1-C02-C03-C04
3	B	602	Q4M	O18-C06-N05-C19
3	A	602	Q4M	C12-C13-O14-C15
3	A	602	Q4M	C16-C13-O14-C15
3	B	602	Q4M	C12-C13-O14-C15
3	B	602	Q4M	C16-C13-O14-C15
2	B	601	HEM	C3A-C2A-CAA-CBA
2	B	601	HEM	C1A-C2A-CAA-CBA
3	B	602	Q4M	CL1-C02-C03-C20

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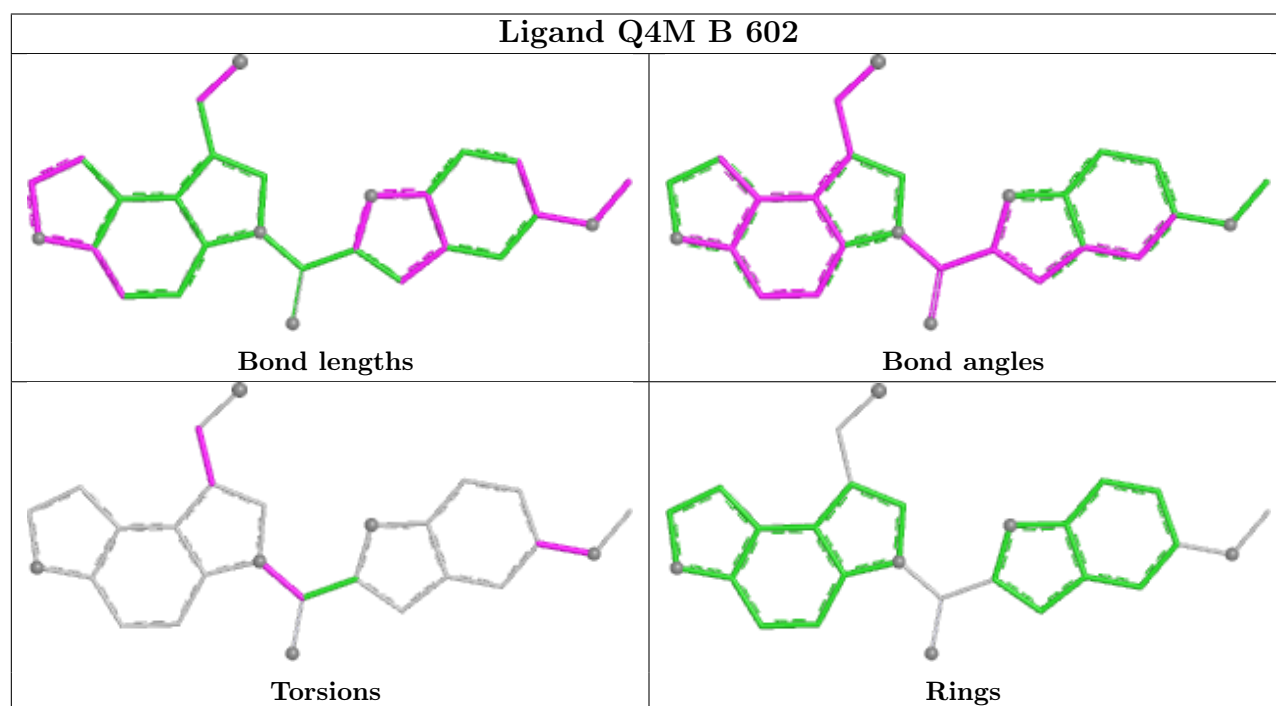
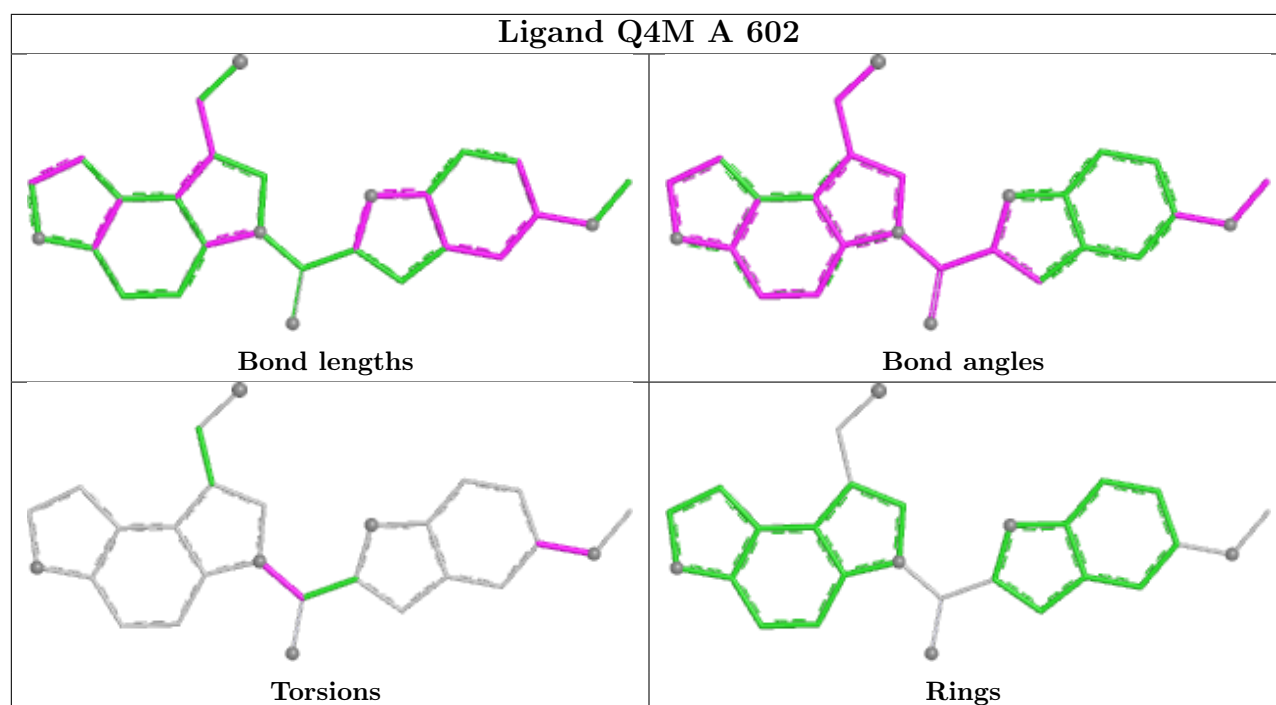
Mol	Chain	Res	Type	Atoms
2	A	601	HEM	C3A-C2A-CAA-CBA
2	A	601	HEM	C1A-C2A-CAA-CBA
2	C	601	HEM	CAA-CBA-CGA-O2A
2	C	601	HEM	CAA-CBA-CGA-O1A
2	A	601	HEM	CAA-CBA-CGA-O2A
2	A	601	HEM	CAD-CBD-CGD-O1D
2	B	601	HEM	CAD-CBD-CGD-O2D
2	D	601	HEM	C4D-C3D-CAD-CBD
2	A	601	HEM	CAA-CBA-CGA-O1A
2	B	601	HEM	CAA-CBA-CGA-O2A
2	B	601	HEM	CAD-CBD-CGD-O1D
2	B	601	HEM	CAA-CBA-CGA-O1A

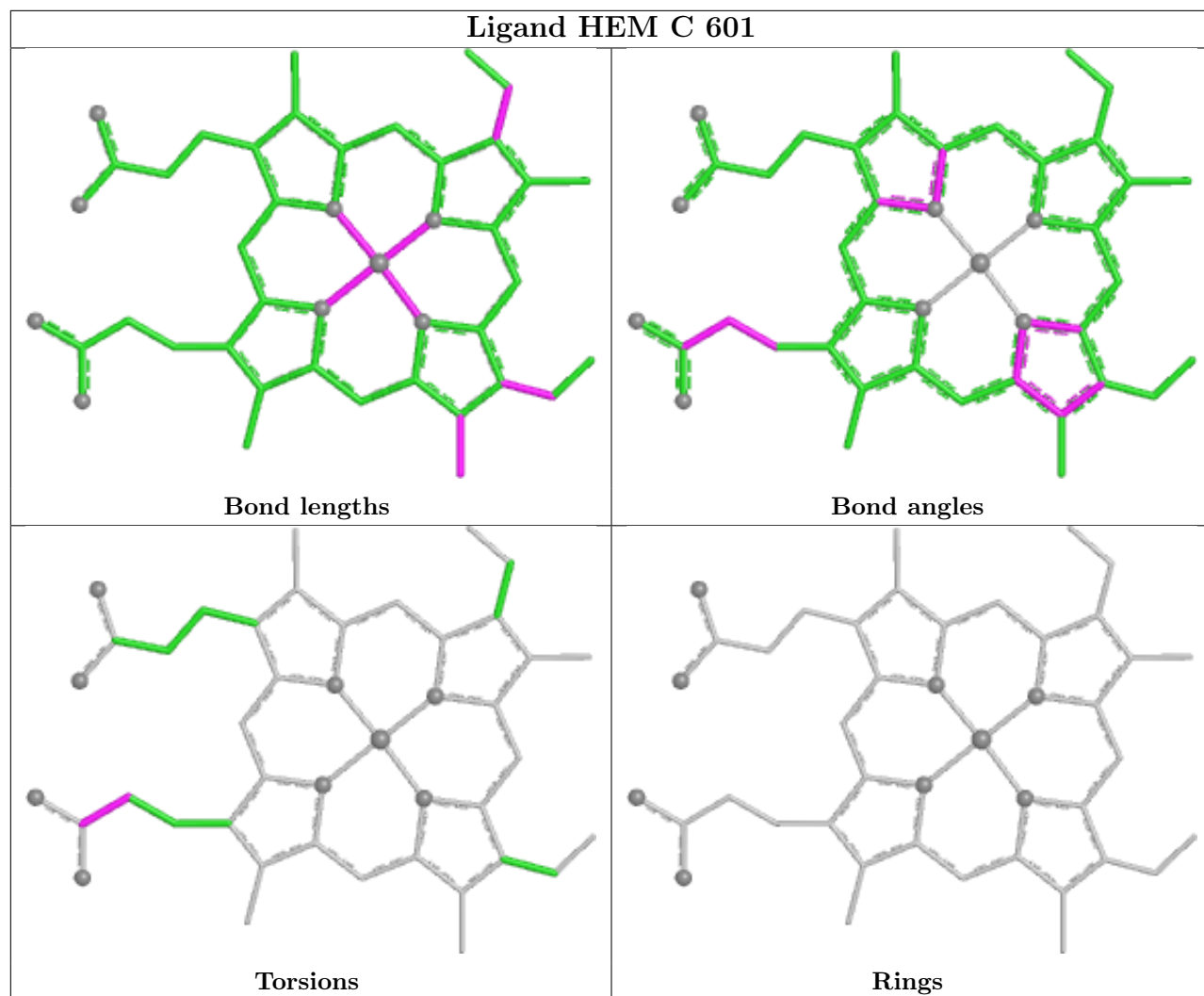
There are no ring outliers.

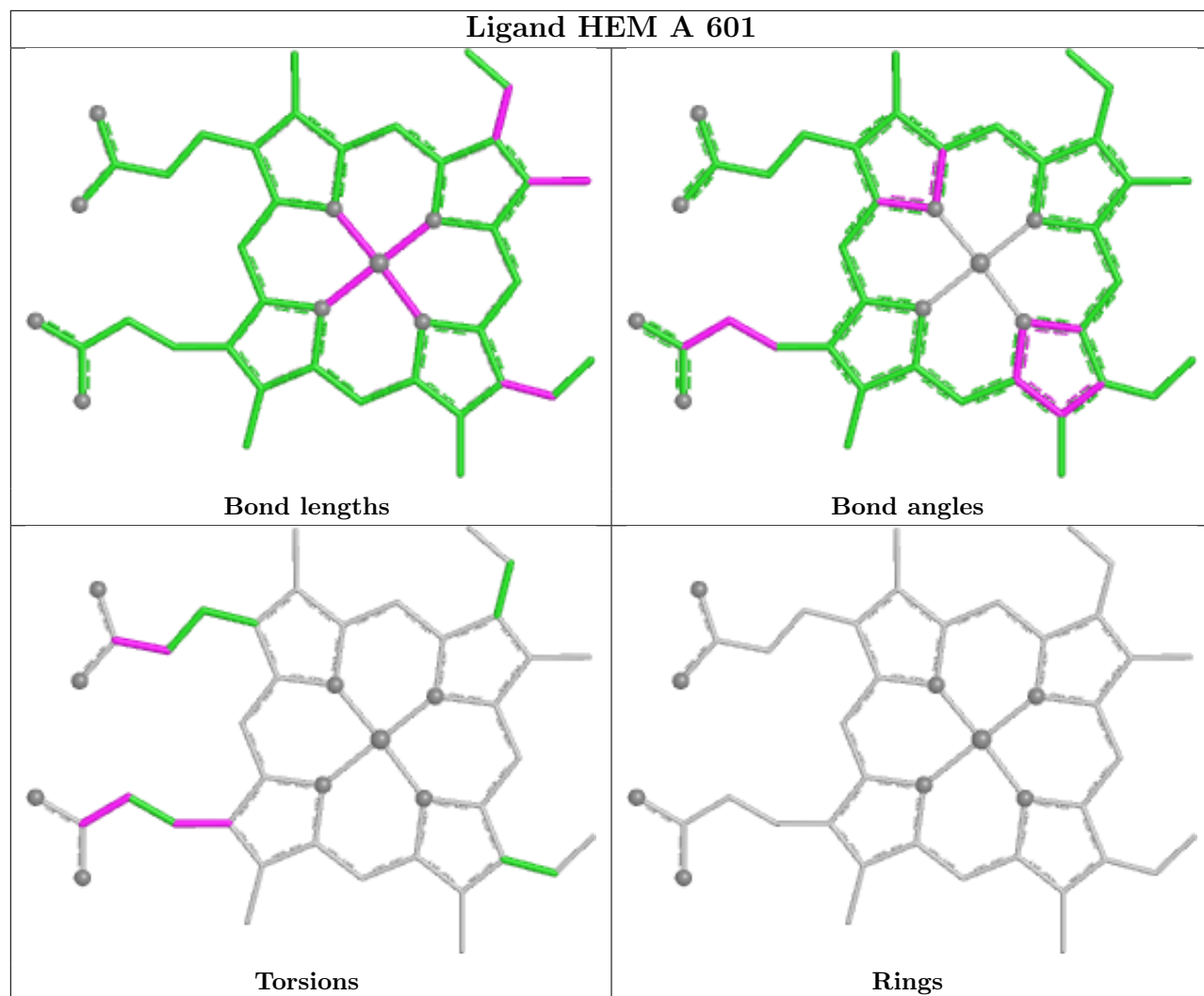
4 monomers are involved in 21 short contacts:

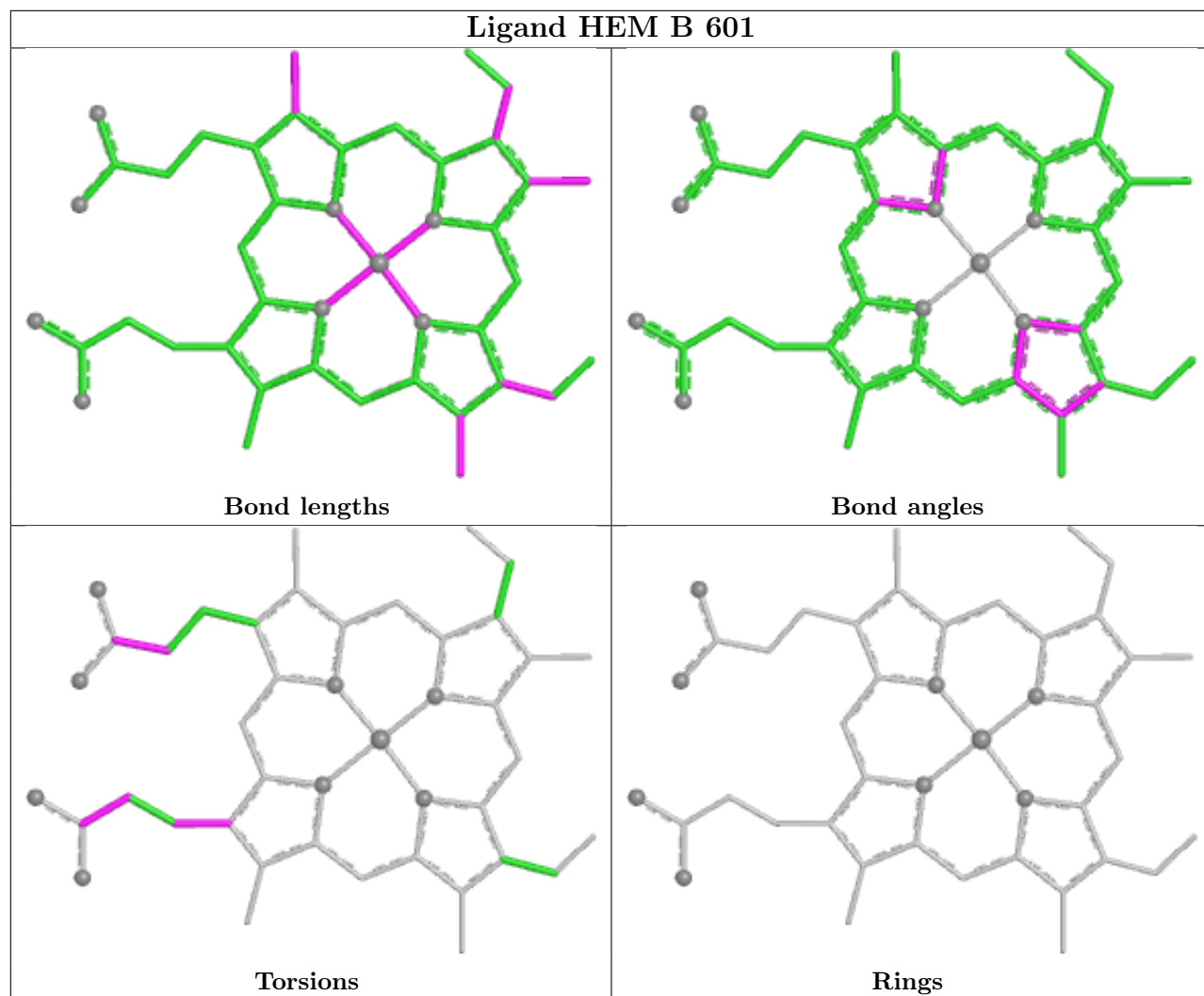
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	HEM	4	0
2	A	601	HEM	6	0
2	B	601	HEM	6	0
2	D	601	HEM	5	0

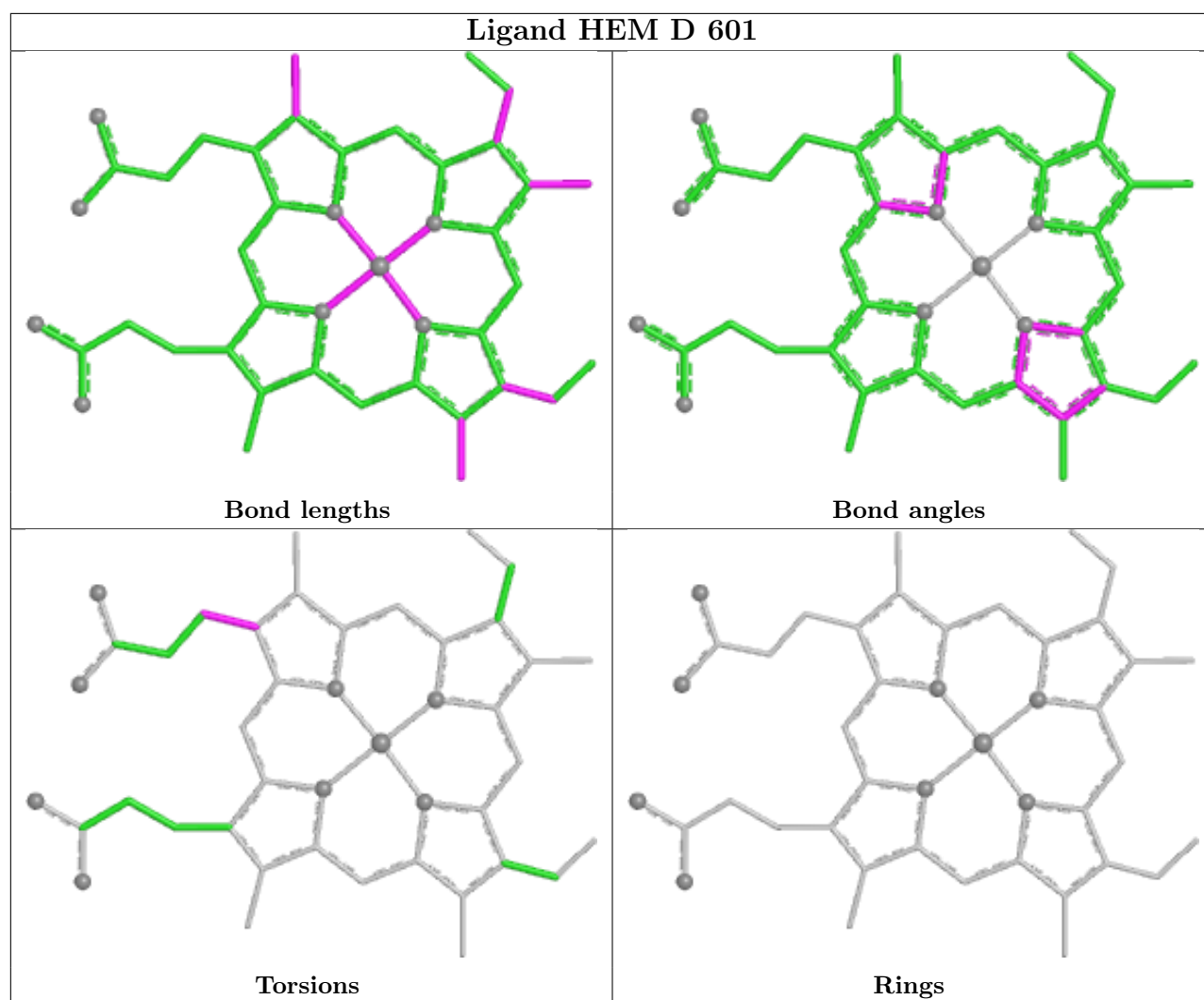
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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	469/491 (95%)	0.25	4 (0%)	81 76	43, 63, 89, 106	0
1	B	477/491 (97%)	0.16	3 (0%)	85 82	40, 57, 81, 98	0
1	C	466/491 (94%)	0.64	18 (3%)	43 34	57, 85, 105, 111	0
1	D	465/491 (94%)	0.90	32 (6%)	23 17	71, 93, 106, 116	0
All	All	1877/1964 (95%)	0.48	57 (3%)	52 44	40, 75, 103, 116	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	302	LEU	4.3
1	C	302	LEU	3.9
1	D	500	HIS	3.3
1	D	289	CYS	3.2
1	D	137	LEU	3.2
1	D	130	VAL	3.2
1	C	222	ASN	3.1
1	D	440	ASP	3.1
1	C	319	PHE	3.0
1	C	218	VAL	3.0
1	A	352	GLY	2.8
1	D	462	ILE	2.8
1	C	37	LEU	2.8
1	C	290	GLN	2.7
1	D	258	PHE	2.6
1	C	270	TYR	2.6
1	C	207	TYR	2.5
1	D	232	ASN	2.5
1	D	259	TYR	2.5
1	D	309	ASN	2.5
1	D	364	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	52	MET	2.5
1	D	48	LEU	2.5
1	C	277	HIS	2.5
1	D	96	LEU	2.4
1	D	256	GLU	2.4
1	D	81	THR	2.4
1	C	267	LYS	2.4
1	D	406	CYS	2.4
1	C	112	PHE	2.4
1	D	308	ILE	2.4
1	D	129	PRO	2.4
1	D	103	PHE	2.3
1	A	101	ASP	2.3
1	A	263	GLN	2.3
1	A	311	VAL	2.3
1	C	387	PRO	2.2
1	B	423	ASN	2.2
1	B	153	SER	2.2
1	D	36	GLY	2.2
1	C	220	LEU	2.2
1	D	94	GLN	2.2
1	C	422	VAL	2.2
1	D	198	ILE	2.2
1	D	88	GLY	2.2
1	D	149	SER	2.2
1	B	512	SER	2.1
1	D	428	LEU	2.1
1	D	270	TYR	2.1
1	D	307	ILE	2.1
1	C	80	SER	2.1
1	C	265	MET	2.1
1	D	125	PRO	2.1
1	C	308	ILE	2.1
1	D	452	MET	2.0
1	D	439	ILE	2.0
1	D	461	THR	2.0

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

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

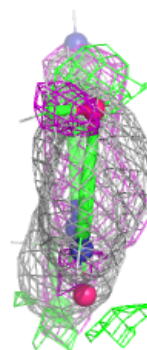
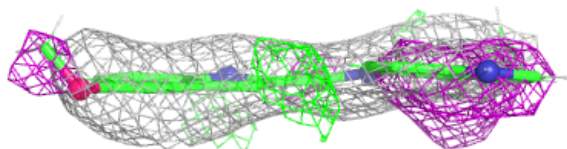
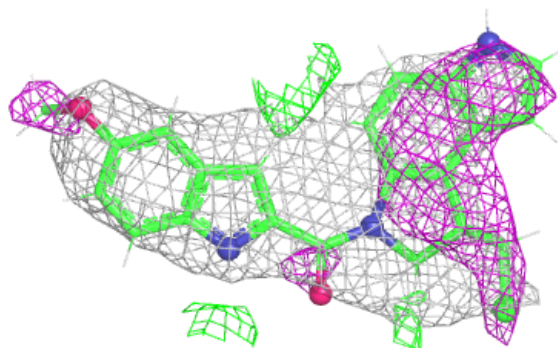
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	Q4M	A	602	27/27	0.75	0.19	52,61,68,86	0
3	Q4M	B	602	27/27	0.81	0.16	46,50,60,71	0
2	HEM	C	601	43/43	0.97	0.12	52,58,72,78	0
2	HEM	D	601	43/43	0.97	0.13	66,72,80,85	0
2	HEM	A	601	43/43	0.97	0.11	43,48,53,55	0
2	HEM	B	601	43/43	0.97	0.12	39,44,49,51	0

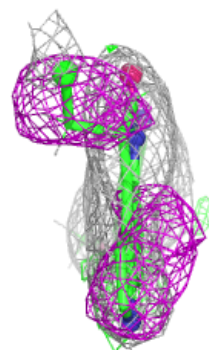
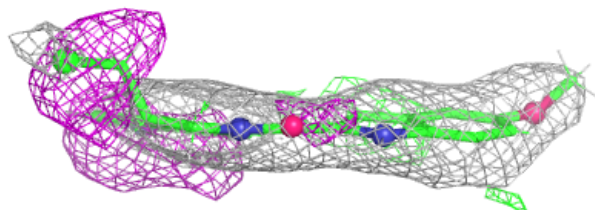
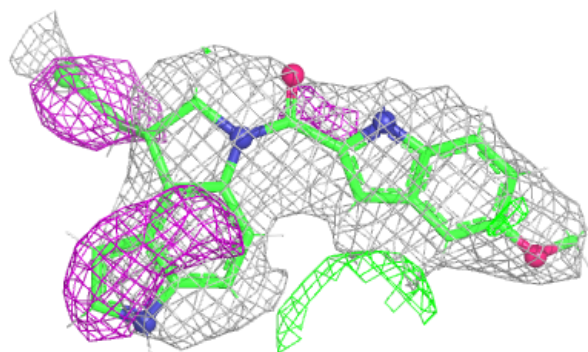
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around Q4M A 602:

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

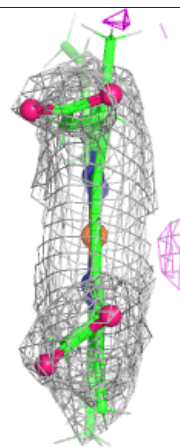
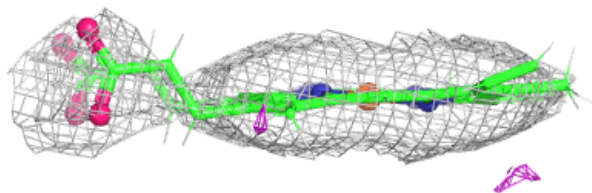
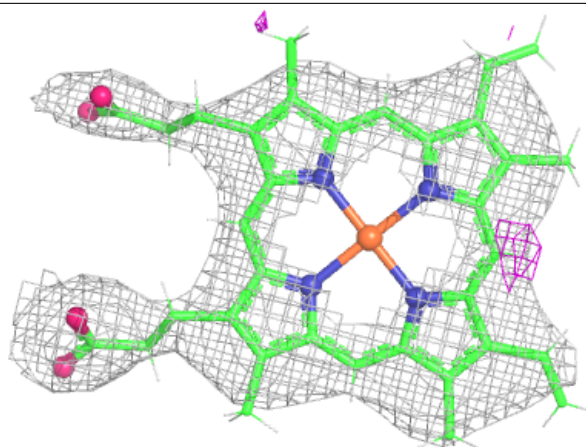
**Electron density around Q4M B 602:**

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



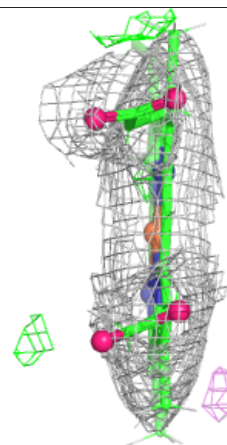
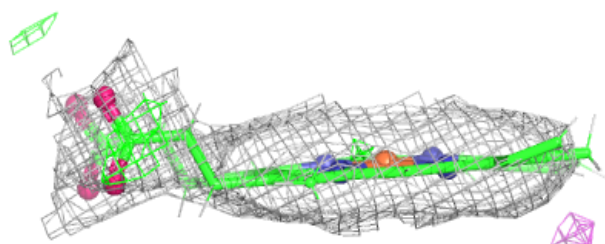
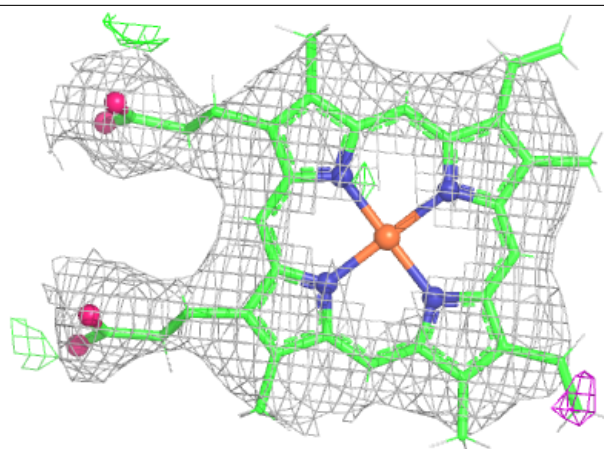
Electron density around HEM C 601:

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



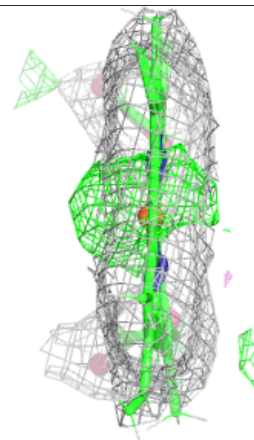
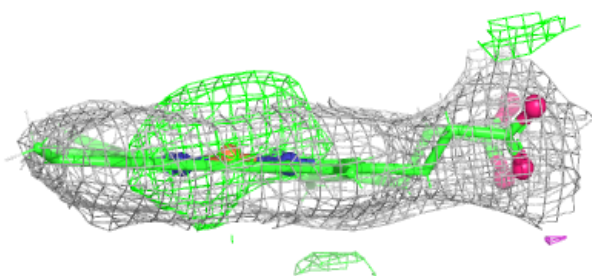
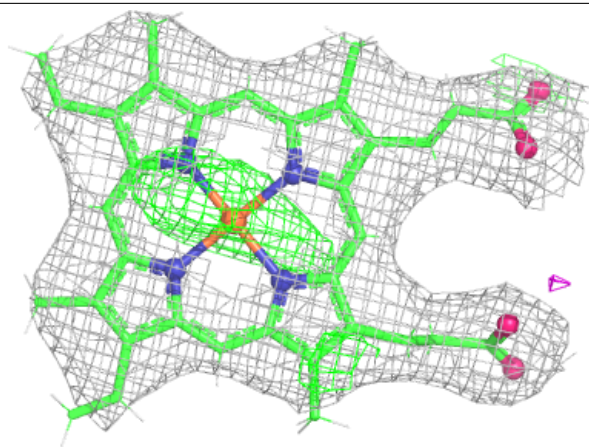
Electron density around HEM D 601:

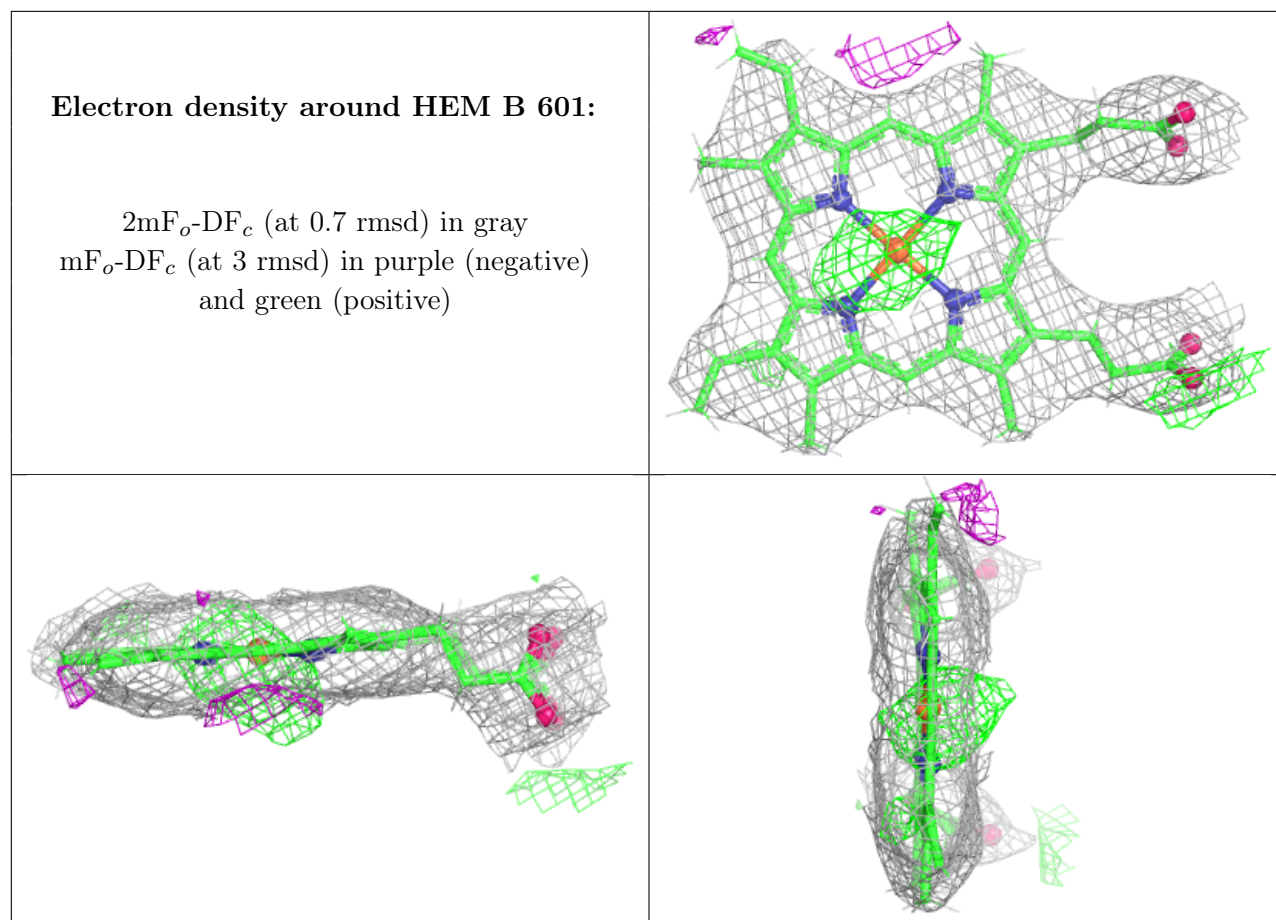
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 601:

$2mF_o-DF_c$ (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.