



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:17 PM UTC

PDB ID : 6UNJ / pdb_00006unj
Title : Human CYP3A4 bound to an inhibitor
Authors : Sevrioukova, I.
Deposited on : 2019-10-12
Resolution : 2.60 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

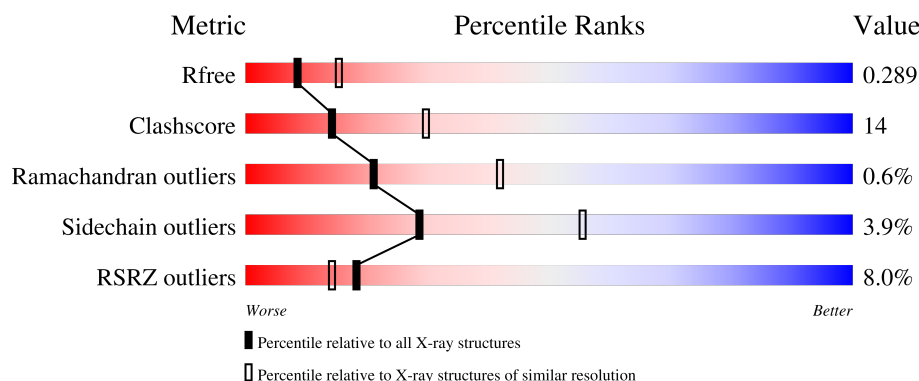
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	487	 6% 62% 27% 9%
1	B	487	 8% 64% 23% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7222 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome P450 3A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	2	0
			3566	2327	581	633	25			
1	B	433	Total	C	N	O	S	5	2	0
			3488	2280	569	614	25			

There are 12 discrepancies between the modelled and reference sequences:

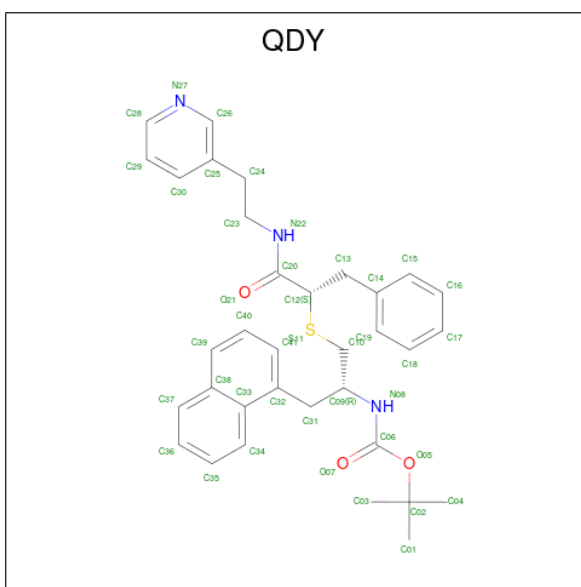
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	initiating methionine	UNP P08684
A	22	ALA	-	expression tag	UNP P08684
A	504	HIS	-	expression tag	UNP P08684
A	505	HIS	-	expression tag	UNP P08684
A	506	HIS	-	expression tag	UNP P08684
A	507	HIS	-	expression tag	UNP P08684
B	21	MET	-	initiating methionine	UNP P08684
B	22	ALA	-	expression tag	UNP P08684
B	504	HIS	-	expression tag	UNP P08684
B	505	HIS	-	expression tag	UNP P08684
B	506	HIS	-	expression tag	UNP P08684
B	507	HIS	-	expression tag	UNP P08684

- 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 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is tert-butyl [(2R)-1-(naphthalen-1-yl)-3-[(2S)-1-oxo-3-phenyl-1-{2-(pyridin-3-yl)ethyl}amino}propan-2-yl]sulfanyl}propan-2-yl]carbamate (CCD ID: QDY) (formula: C₃₄H₃₉N₃O₃S) (labeled as "Ligand of Interest" by depositor).

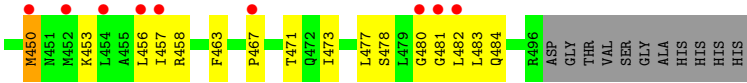


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			41	34	3	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			41	34	3	3	1		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.99Å 98.08Å 93.43Å 90.00° 124.04° 90.00°	Depositor
Resolution (Å)	47.29 – 2.60 47.29 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.2 (47.29-2.60) 92.1 (47.29-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.253 , 0.288 0.262 , 0.289	Depositor DCC
R_{free} test set	1636 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	92.2	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 92.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7222	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, QDY

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	0.20	1/3656 (0.0%)	0.48	4/4941 (0.1%)
1	B	0.21	1/3576 (0.0%)	0.43	2/4829 (0.0%)
All	All	0.21	2/7232 (0.0%)	0.46	6/9770 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	477	LEU	C-N	-7.14	1.23	1.33
1	A	477	LEU	C-N	-5.39	1.25	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	SER	N-CA-C	8.93	124.12	113.23
1	A	69	GLY	N-CA-C	6.83	118.31	111.21
1	B	69	GLY	N-CA-C	6.82	118.31	111.21
1	A	194	ASP	N-CA-C	6.36	118.14	109.11
1	A	193	ILE	N-CA-CB	5.77	120.75	111.23
1	B	193	ILE	N-CA-CB	5.75	120.71	111.23

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	3566	0	3667	114	0
1	B	3488	0	3600	90	0
2	A	43	0	30	6	0
2	B	43	0	30	4	0
3	A	41	0	0	2	0
3	B	41	0	0	2	0
All	All	7222	0	7327	207	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 14.

All (207) 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:207:THR:O	1:A:208:LYS:HG2	1.45	1.17
1:A:482:LEU:HD11	1:A:484:GLN:OE1	1.51	1.10
1:B:482:LEU:HD11	1:B:484:GLN:OE1	1.55	1.03
1:A:217:ASP:HB3	1:A:218:PRO:HD2	1.41	1.02
1:A:482:LEU:CD1	1:A:484:GLN:CD	2.36	0.98
1:B:482:LEU:CD1	1:B:484:GLN:CD	2.39	0.96
1:A:482:LEU:HD11	1:A:484:GLN:CD	1.92	0.95
1:B:242:PRO:O	1:B:246:THR:HG23	1.71	0.91
1:B:482:LEU:HD12	1:B:484:GLN:CD	1.96	0.91
1:A:482:LEU:HD12	1:A:484:GLN:CD	2.03	0.83
1:A:184:ILE:HG13	1:A:306:GLY:HA3	1.60	0.82
1:A:209:LYS:HG3	1:A:245:VAL:HG12	1.61	0.81
1:B:482:LEU:HD11	1:B:484:GLN:CD	2.03	0.80
1:A:207:THR:O	1:A:208:LYS:CG	2.30	0.78
1:B:482:LEU:CD1	1:B:484:GLN:OE1	2.30	0.77
1:B:184:ILE:HG13	1:B:306:GLY:HA3	1.67	0.77
1:B:209:LYS:HG3	1:B:245:VAL:HG12	1.67	0.75
1:A:270:ASP:H	1:A:273:GLN:HB3	1.51	0.75
1:B:368:PRO:O	1:B:483:LEU:HD22	1.88	0.74
1:A:217:ASP:HB3	1:A:218:PRO:CD	2.17	0.73
2:B:601:HEM:HBC2	2:B:601:HEM:HHD	1.70	0.73
1:A:192:ASN:O	1:A:193:ILE:HD13	1.88	0.73
1:B:50:ILE:HD13	1:B:225:VAL:HG21	1.71	0.72
1:A:206:ASN:N	1:A:248:PHE:CZ	2.59	0.71
1:B:270:ASP:H	1:B:273:GLN:HB3	1.56	0.69
1:B:421:LYS:HA	1:B:424:LYS:HG2	1.74	0.68
1:B:246:THR:O	1:B:250:ARG:N	2.26	0.68
1:B:189:PHE:HB3	1:B:256:MET:HE2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:VAL:CG2	1:B:256:MET:SD	2.83	0.67
1:A:215:PHE:O	1:A:216:LEU:HB2	1.95	0.67
2:A:601:HEM:HHD	2:A:601:HEM:HBC2	1.77	0.66
1:A:57:PHE:HE2	1:A:481:GLY:HA2	1.61	0.65
1:A:216:LEU:HG	1:A:217:ASP:H	1.62	0.65
1:B:57:PHE:HE2	1:B:481:GLY:HA2	1.62	0.65
1:A:410:GLU:O	1:A:418:ARG:NH2	2.30	0.64
1:A:246:THR:O	1:A:250:ARG:N	2.29	0.64
1:B:410:GLU:O	1:B:418:ARG:NH2	2.31	0.64
1:A:368:PRO:O	1:A:483:LEU:HD22	1.98	0.64
1:A:212:ARG:HD3	1:A:245:VAL:HG21	1.80	0.63
1:A:50:ILE:HD13	1:A:225:VAL:HG21	1.81	0.63
1:A:421:LYS:HA	1:A:424:LYS:HG2	1.80	0.62
1:A:482:LEU:CD1	1:A:484:GLN:OE1	2.33	0.60
1:B:275:MET:HE2	1:B:290:LEU:HD21	1.83	0.59
1:B:370:ALA:O	1:B:372:ARG:N	2.33	0.59
1:A:189:PHE:HB3	1:A:256:MET:HE2	1.84	0.59
1:A:236:LEU:HB2	1:A:238:ILE:HG13	1.85	0.59
1:A:275:MET:HE2	1:A:290:LEU:HD21	1.87	0.57
1:A:191:VAL:CG2	1:A:256:MET:SD	2.93	0.57
1:A:482:LEU:CD1	1:A:484:GLN:NE2	2.68	0.56
1:B:471:THR:O	1:B:471:THR:CG2	2.54	0.56
1:B:210:LEU:HD11	1:B:303:ILE:HG22	1.87	0.56
1:B:189:PHE:HZ	1:B:299:SER:HB3	1.69	0.56
1:B:101:VAL:HG21	1:B:381:VAL:HG11	1.87	0.56
1:A:71:VAL:HG13	1:A:82:LEU:HD11	1.88	0.55
1:A:101:VAL:HG21	1:A:381:VAL:HG11	1.89	0.55
1:A:421:LYS:HG3	1:A:424:LYS:HE3	1.88	0.55
1:B:473:ILE:HG23	1:B:473:ILE:O	2.06	0.55
1:B:212:ARG:HB3	1:B:245:VAL:HG21	1.89	0.54
1:B:471:THR:O	1:B:471:THR:HG23	2.06	0.54
1:A:92:THR:HA	1:A:96:LYS:HB2	1.90	0.54
1:A:357:ASP:OD1	1:A:453:LYS:NZ	2.34	0.54
1:B:213:PHE:CD2	1:B:213:PHE:O	2.61	0.54
2:B:601:HEM:HBB2	2:B:601:HEM:HMB2	1.89	0.54
1:B:482:LEU:CD1	1:B:484:GLN:NE2	2.71	0.53
1:A:317:ILE:HG13	1:A:363:THR:HG21	1.90	0.53
1:A:347:TYR:CD1	1:A:450:MET:HE1	2.43	0.53
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.91	0.53
1:A:331:LEU:HD22	1:A:359:VAL:HG21	1.91	0.52
1:B:210:LEU:HD13	1:B:304:PHE:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:SER:C	1:A:480:GLY:H	2.17	0.52
1:A:54:HIS:CD2	1:A:55:LYS:HG3	2.45	0.52
1:A:370:ALA:HA	3:A:602:QDY:C17	2.39	0.52
1:B:478:SER:C	1:B:480:GLY:H	2.16	0.52
1:A:210:LEU:HD11	1:A:303:ILE:HG22	1.91	0.52
1:B:421:LYS:HG3	1:B:424:LYS:HE3	1.93	0.51
1:A:163:GLU:HB3	1:A:170:VAL:HG22	1.92	0.51
1:A:208:LYS:O	1:A:208:LYS:HG3	2.09	0.51
1:B:347:TYR:CD1	1:B:450:MET:HE1	2.46	0.51
1:B:357:ASP:OD1	1:B:453:LYS:NZ	2.31	0.51
1:B:146:VAL:HG21	1:B:347:TYR:HB2	1.91	0.51
1:B:223:ILE:HG23	1:B:230:ILE:HD11	1.93	0.51
1:A:172:LEU:HD11	1:A:491:LEU:HD12	1.93	0.50
1:B:420:SER:O	1:B:424:LYS:N	2.39	0.50
1:A:471:THR:OG1	1:A:490:VAL:O	2.29	0.50
1:A:210:LEU:HD13	1:A:304:PHE:HA	1.93	0.50
1:A:420:SER:O	1:A:424:LYS:N	2.41	0.50
1:B:291:SER:HB3	1:B:294:GLU:HG3	1.94	0.50
1:A:482:LEU:H	1:A:482:LEU:HD23	1.77	0.50
1:A:208:LYS:C	1:A:210:LEU:H	2.19	0.49
1:B:370:ALA:HA	3:B:602:QDY:C17	2.42	0.49
1:A:133:LEU:HD22	1:A:271:PHE:HE1	1.77	0.49
1:B:482:LEU:H	1:B:482:LEU:HD23	1.78	0.49
1:B:208:LYS:C	1:B:210:LEU:H	2.20	0.49
1:B:294:GLU:O	1:B:298:GLN:HG2	2.13	0.49
1:B:368:PRO:C	1:B:483:LEU:HD22	2.38	0.48
1:A:276:ILE:HA	1:A:279:GLN:HB3	1.95	0.48
1:B:213:PHE:O	1:B:213:PHE:CG	2.66	0.48
1:A:86:ASP:HB3	1:A:89:MET:HB2	1.95	0.48
1:A:105:ARG:HH22	2:A:601:HEM:HBD1	1.78	0.48
1:A:120:ILE:HD11	3:A:602:QDY:C35	2.44	0.48
1:A:217:ASP:O	1:A:218:PRO:C	2.55	0.48
1:A:223:ILE:HG23	1:A:230:ILE:HD11	1.95	0.48
1:B:92:THR:HA	1:B:96:LYS:HB2	1.95	0.48
1:B:331:LEU:HD22	1:B:359:VAL:HG21	1.96	0.48
1:B:467:PRO:HB3	1:B:471:THR:HG21	1.95	0.48
1:B:191:VAL:HG23	1:B:256:MET:SD	2.53	0.48
1:A:270:ASP:O	1:A:274:LEU:N	2.47	0.47
1:B:57:PHE:CE2	1:B:481:GLY:HA2	2.46	0.47
1:A:209:LYS:O	1:A:211:LEU:N	2.46	0.47
1:A:229:LEU:HA	1:A:232:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLU:HB3	1:B:170:VAL:HG22	1.96	0.47
1:B:219:PHE:HZ	1:B:240:VAL:HG12	1.80	0.47
1:B:482:LEU:HD12	1:B:484:GLN:NE2	2.29	0.47
1:A:368:PRO:C	1:A:370:ALA:H	2.21	0.47
1:B:450:MET:HE3	1:B:450:MET:HB2	1.79	0.46
1:A:216:LEU:HG	1:A:217:ASP:N	2.27	0.46
1:B:276:ILE:HA	1:B:279:GLN:HB3	1.96	0.46
1:B:86:ASP:HB3	1:B:89:MET:HB2	1.95	0.46
1:B:54:HIS:CD2	1:B:55:LYS:HG3	2.51	0.46
1:A:375:ARG:HH22	2:A:601:HEM:CGA	2.29	0.46
1:A:299:SER:O	1:A:303:ILE:HG13	2.16	0.45
1:B:105:ARG:HH22	2:B:601:HEM:HBD1	1.80	0.45
1:A:212:ARG:HG2	1:A:245:VAL:HG21	1.98	0.45
1:B:435:PHE:HB3	1:B:442:CYS:HB3	1.98	0.45
1:A:216:LEU:CG	1:A:217:ASP:H	2.24	0.45
1:A:368:PRO:C	1:A:483:LEU:HD22	2.42	0.45
1:A:356:LEU:O	1:A:360:VAL:HG23	2.17	0.45
1:B:232:ILE:O	1:B:235:VAL:HG12	2.17	0.45
1:B:246:THR:OG1	1:B:247:ASN:N	2.50	0.45
1:B:317:ILE:HG13	1:B:363:THR:HG21	1.99	0.45
1:A:57:PHE:CE2	1:A:481:GLY:HA2	2.47	0.45
1:B:254:LYS:HE3	1:B:254:LYS:HB2	1.70	0.45
1:A:368:PRO:C	1:A:370:ALA:N	2.75	0.45
1:B:142:LEU:HD11	1:B:447:PHE:HB2	1.99	0.45
1:A:450:MET:HE3	1:A:450:MET:HB2	1.85	0.45
1:A:275:MET:SD	1:A:295:LEU:HG	2.57	0.45
1:A:326:ASP:N	1:A:326:ASP:OD1	2.50	0.45
1:A:442:CYS:HB2	2:A:601:HEM:C4A	2.52	0.45
1:A:413:LYS:HE2	1:A:413:LYS:HB3	1.87	0.44
1:B:275:MET:SD	1:B:295:LEU:HG	2.57	0.44
1:B:395[A]:MET:HE3	1:B:395[A]:MET:HB3	1.92	0.44
1:A:291:SER:HB3	1:A:294:GLU:HG3	1.98	0.44
1:A:347:TYR:CE1	1:A:450:MET:HE1	2.52	0.44
1:A:442:CYS:HB2	2:A:601:HEM:NA	2.32	0.44
1:B:335:ILE:HD13	1:B:457:ILE:HA	1.99	0.44
1:B:228:PHE:O	1:B:231:PRO:HD2	2.17	0.44
1:B:209:LYS:O	1:B:211:LEU:N	2.44	0.43
1:B:50:ILE:HD12	1:B:221:LEU:HD11	2.00	0.43
1:B:120:ILE:HD11	3:B:602:QDY:C35	2.48	0.43
1:B:185:THR:O	1:B:189:PHE:HB2	2.18	0.43
1:A:458:ARG:HD2	1:A:458:ARG:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HD12	1:A:221:LEU:HD11	1.99	0.43
1:B:71:VAL:HG21	1:B:386:MET:HE1	2.01	0.43
1:A:101:VAL:HA	1:A:378:LYS:HG2	2.00	0.43
1:A:206:ASN:N	1:A:248:PHE:HZ	2.14	0.43
1:A:50:ILE:HG21	1:A:225:VAL:HG22	2.00	0.43
1:B:58:CYS:HB3	1:B:399:TYR:CD2	2.54	0.43
1:A:212:ARG:HG2	1:A:245:VAL:HG11	2.00	0.43
1:A:228:PHE:O	1:A:231:PRO:HD2	2.19	0.43
1:A:110:PRO:HG3	1:A:233:LEU:HB2	2.01	0.43
1:A:206:ASN:OD1	1:A:252:SER:OG	2.28	0.43
1:A:221:LEU:HD22	1:A:221:LEU:HA	1.84	0.43
1:A:335:ILE:HD13	1:A:457:ILE:HA	2.00	0.43
1:A:143:LYS:HD3	1:A:347:TYR:CG	2.54	0.43
1:B:212:ARG:NH2	1:B:304:PHE:HB2	2.34	0.43
1:A:206:ASN:C	1:A:208:LYS:H	2.27	0.43
1:A:219:PHE:HZ	1:A:240:VAL:HG12	1.84	0.43
1:A:294:GLU:O	1:A:298:GLN:HG2	2.19	0.42
1:B:375:ARG:HH22	2:B:601:HEM:CGA	2.32	0.42
1:B:458:ARG:HD2	1:B:458:ARG:HA	1.85	0.42
1:A:93:VAL:HG13	1:A:102:PHE:CG	2.55	0.42
1:A:478:SER:C	1:A:480:GLY:N	2.77	0.42
1:A:146:VAL:HG21	1:A:347:TYR:HB2	2.00	0.42
1:A:157:VAL:HG13	1:A:463:PHE:CE2	2.55	0.42
1:A:189:PHE:HZ	1:A:299:SER:HB3	1.85	0.42
1:A:232:ILE:O	1:A:235:VAL:HG12	2.20	0.42
1:B:317:ILE:HD13	1:B:456:LEU:HD11	2.00	0.42
1:A:211:LEU:O	1:A:211:LEU:HG	2.19	0.42
1:A:442:CYS:SG	1:A:445:MET:N	2.92	0.42
1:A:482:LEU:HD12	1:A:484:GLN:CG	2.50	0.42
1:A:314:LEU:O	1:A:318:MET:HG2	2.20	0.42
1:B:270:ASP:O	1:B:274:LEU:N	2.51	0.42
1:B:192:ASN:C	1:B:193:ILE:HG12	2.43	0.42
1:A:58:CYS:HB3	1:A:399:TYR:CD2	2.55	0.42
1:A:380:ASP:OD1	1:A:390:LYS:N	2.50	0.41
1:A:415:LEU:O	1:A:418:ARG:HG3	2.20	0.41
1:B:338:VAL:HB	1:B:353:MET:HE2	2.01	0.41
1:A:143:LYS:HB2	1:A:143:LYS:HE2	1.82	0.41
1:B:478:SER:C	1:B:480:GLY:N	2.77	0.41
1:A:192:ASN:C	1:A:193:ILE:HG12	2.44	0.41
1:A:446:ARG:HE	1:B:425:ASP:HB3	1.85	0.41
1:A:212:ARG:HD2	1:A:242:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:SER:O	1:B:303:ILE:HG13	2.20	0.41
1:B:413:LYS:HB3	1:B:413:LYS:HE2	1.79	0.41
1:A:208:LYS:C	1:A:210:LEU:N	2.79	0.41
1:A:254:LYS:HB2	1:A:254:LYS:HE3	1.75	0.41
1:B:93:VAL:HG21	1:B:394:VAL:HG11	2.03	0.41
1:B:370:ALA:C	1:B:372:ARG:N	2.78	0.41
1:B:230:ILE:HB	1:B:231:PRO:HD3	2.03	0.41
1:B:371:MET:O	1:B:398:SER:HB2	2.21	0.41
1:A:145:MET:O	1:A:149:ILE:HG13	2.20	0.40
1:A:47:LEU:HD22	1:A:50:ILE:HD11	2.03	0.40
1:B:87:PRO:HG3	1:B:431:ILE:HD11	2.02	0.40
1:A:321:LEU:HD21	1:A:359:VAL:HG11	2.04	0.40
1:B:157:VAL:HG13	1:B:463:PHE:CE2	2.56	0.40
1:B:368:PRO:C	1:B:370:ALA:H	2.28	0.40
1:A:477:LEU:O	1:A:479:LEU:HD12	2.22	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	437/487 (90%)	399 (91%)	34 (8%)	4 (1%)	14	30
1	B	425/487 (87%)	394 (93%)	30 (7%)	1 (0%)	43	66
All	All	862/974 (88%)	793 (92%)	64 (7%)	5 (1%)	21	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	LEU
1	A	217	ASP
1	A	218	PRO

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Mol	Chain	Res	Type
1	A	190	GLY
1	B	190	GLY

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	406/443 (92%)	388 (96%)	18 (4%)	25	50
1	B	396/443 (89%)	383 (97%)	13 (3%)	33	61
All	All	802/886 (90%)	771 (96%)	31 (4%)	28	55

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	118	ILE
1	A	132	LEU
1	A	142	LEU
1	A	158	ARG
1	A	163	GLU
1	A	184	ILE
1	A	193	ILE
1	A	197	ASN
1	A	207	THR
1	A	212	ARG
1	A	221	LEU
1	A	223	ILE
1	A	251	LYS
1	A	312	SER
1	A	425	ASP
1	A	426	ASN
1	A	443	ILE
1	B	47	LEU
1	B	118	ILE
1	B	132	LEU

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Mol	Chain	Res	Type
1	B	142	LEU
1	B	163	GLU
1	B	184	ILE
1	B	193	ILE
1	B	221	LEU
1	B	244	GLU
1	B	251	LYS
1	B	425	ASP
1	B	426	ASN
1	B	450	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	A	279	GLN
1	A	451	ASN
1	B	451	ASN

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 ⓘ

4 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	QDY	B	602	-	43,44,44	1.26	4 (9%)	53,59,59	1.49	6 (11%)
2	HEM	A	601	-	50,50,50	1.32	7 (14%)	67,82,82	1.29	9 (13%)
3	QDY	A	602	-	43,44,44	1.14	6 (13%)	53,59,59	1.55	4 (7%)
2	HEM	B	601	-	50,50,50	1.42	8 (16%)	67,82,82	1.25	5 (7%)

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	QDY	B	602	-	-	10/32/32/32	0/4/4/4
2	HEM	A	601	-	-	5/14/54/54	-
3	QDY	A	602	-	-	12/32/32/32	0/4/4/4
2	HEM	B	601	-	-	5/14/54/54	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	QDY	C06-N08	3.98	1.44	1.34
2	B	601	HEM	FE-NC	3.54	2.06	1.95
3	B	602	QDY	C10-S11	3.43	1.85	1.82
3	B	602	QDY	C06-N08	3.35	1.43	1.34
2	B	601	HEM	FE-NB	3.31	2.05	1.94
2	B	601	HEM	FE-NA	3.16	2.05	1.95
3	B	602	QDY	C20-N22	3.15	1.41	1.33
2	B	601	HEM	CAB-C3B	3.15	1.55	1.47
2	A	601	HEM	FE-ND	3.05	2.04	1.94
2	A	601	HEM	CAC-C3C	3.05	1.55	1.47
2	A	601	HEM	FE-NC	3.03	2.05	1.95
2	B	601	HEM	CAC-C3C	2.98	1.55	1.47
2	A	601	HEM	CAB-C3B	2.68	1.54	1.47
3	B	602	QDY	C31-C09	2.67	1.59	1.53
3	A	602	QDY	C20-N22	2.64	1.39	1.33
2	B	601	HEM	FE-ND	2.48	2.02	1.94
3	A	602	QDY	C31-C09	2.45	1.58	1.53
3	A	602	QDY	O05-C06	2.35	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	QDY	C40-C41	2.25	1.42	1.38
2	A	601	HEM	FE-NA	2.24	2.02	1.95
2	A	601	HEM	FE-NB	2.21	2.01	1.94
3	A	602	QDY	C09-N08	2.18	1.51	1.46
2	B	601	HEM	CMA-C3A	2.17	1.55	1.50
2	B	601	HEM	CMB-C2B	2.16	1.55	1.50
2	A	601	HEM	CMC-C2C	2.01	1.54	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	QDY	O05-C06-N08	5.66	119.30	110.03
3	B	602	QDY	O05-C06-N08	5.35	118.78	110.03
3	B	602	QDY	O07-C06-N08	-4.74	117.09	124.86
3	A	602	QDY	O07-C06-N08	-4.72	117.12	124.86
3	A	602	QDY	C09-N08-C06	4.39	128.99	122.23
3	B	602	QDY	C09-N08-C06	3.91	128.25	122.23
3	B	602	QDY	O21-C20-N22	-3.43	115.72	122.98
3	A	602	QDY	O21-C20-N22	-3.32	115.95	122.98
2	B	601	HEM	C3D-C4D-ND	-2.73	107.18	110.17
2	A	601	HEM	C2A-C1A-NA	-2.55	107.32	110.15
2	A	601	HEM	CBA-CAA-C2A	-2.55	105.48	112.53
2	B	601	HEM	C4D-ND-C1D	2.54	108.21	105.21
2	A	601	HEM	C3D-C4D-ND	-2.48	107.45	110.17
2	A	601	HEM	CAD-C3D-C2D	-2.41	123.35	127.87
2	B	601	HEM	CHD-C1D-ND	2.36	126.96	124.42
2	B	601	HEM	CAD-C3D-C2D	-2.35	123.46	127.87
2	B	601	HEM	C2A-C1A-NA	-2.35	107.54	110.15
2	A	601	HEM	CAC-C3C-C4C	2.33	130.40	124.82
2	A	601	HEM	CHC-C1C-NC	2.29	126.95	124.45
2	A	601	HEM	C4D-ND-C1D	2.19	107.80	105.21
2	A	601	HEM	CAD-C3D-C4D	2.11	128.37	124.70
2	A	601	HEM	O1A-CGA-CBA	-2.11	116.41	123.09
3	B	602	QDY	C32-C31-C09	2.05	116.77	113.75
3	B	602	QDY	C02-O05-C06	2.01	124.01	120.97

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	QDY	C20-C12-C13-C14
3	A	602	QDY	S11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
3	A	602	QDY	C10-C09-C31-C32
3	A	602	QDY	N08-C09-C31-C32
3	A	602	QDY	N22-C23-C24-C25
3	B	602	QDY	C20-C12-C13-C14
3	B	602	QDY	S11-C12-C13-C14
3	B	602	QDY	C10-C09-C31-C32
3	B	602	QDY	N08-C09-C31-C32
3	B	602	QDY	N22-C23-C24-C25
3	A	602	QDY	N08-C06-O05-C02
3	A	602	QDY	O07-C06-O05-C02
3	A	602	QDY	C04-C02-O05-C06
2	A	601	HEM	C4C-C3C-CAC-CBC
2	B	601	HEM	C4C-C3C-CAC-CBC
3	A	602	QDY	C03-C02-O05-C06
2	B	601	HEM	C4D-C3D-CAD-CBD
3	A	602	QDY	C09-C31-C32-C33
3	B	602	QDY	C09-C31-C32-C33
3	B	602	QDY	N08-C06-O05-C02
3	A	602	QDY	C09-C10-S11-C12
3	B	602	QDY	C09-C10-S11-C12
2	B	601	HEM	C2D-C3D-CAD-CBD
3	B	602	QDY	O07-C06-O05-C02
2	A	601	HEM	CAD-CBD-CGD-O2D
2	B	601	HEM	CAD-CBD-CGD-O1D
2	A	601	HEM	CAD-CBD-CGD-O1D
2	B	601	HEM	CAD-CBD-CGD-O2D
2	A	601	HEM	C4D-C3D-CAD-CBD
3	A	602	QDY	C09-C31-C32-C41
3	B	602	QDY	C09-C31-C32-C41
2	A	601	HEM	C2D-C3D-CAD-CBD

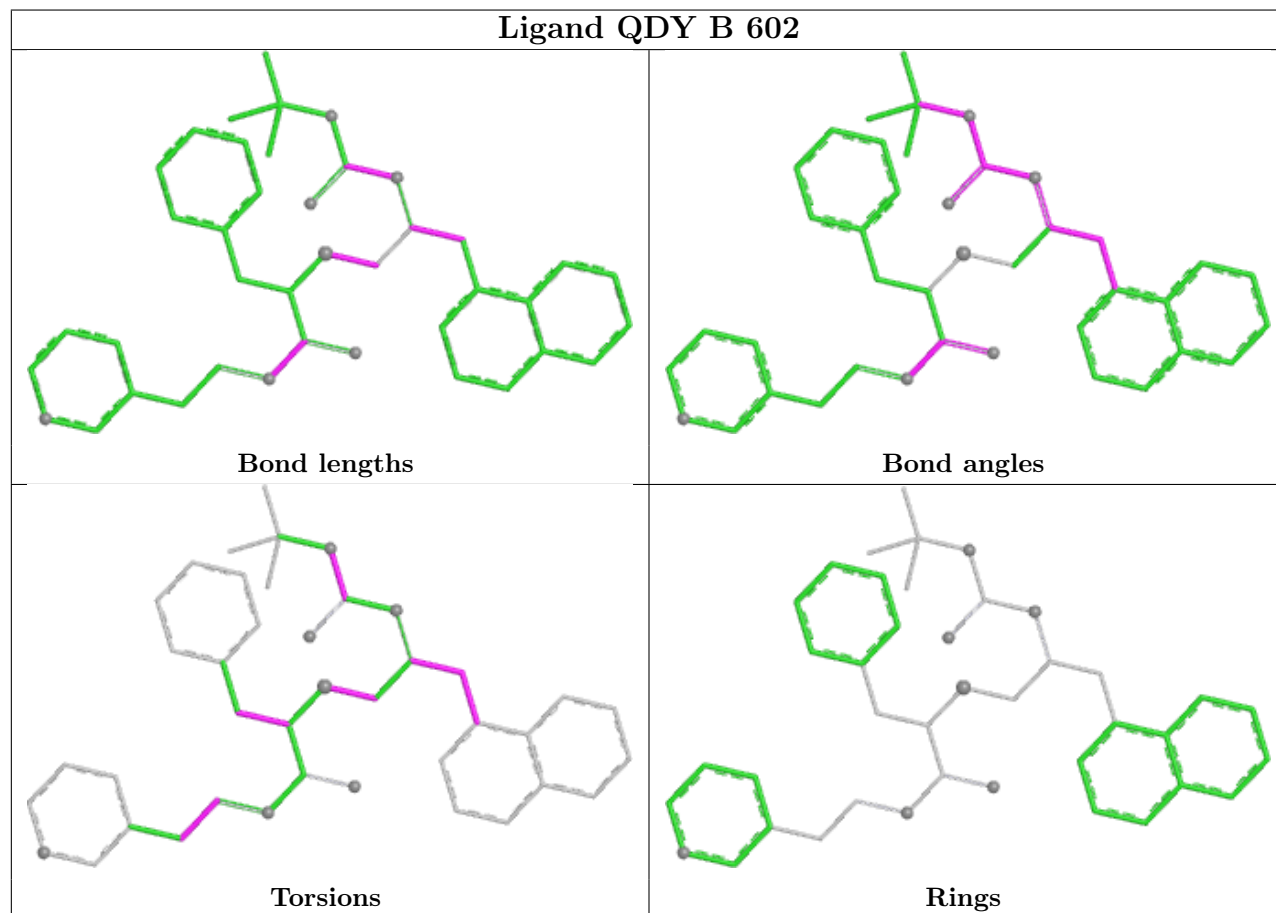
There are no ring outliers.

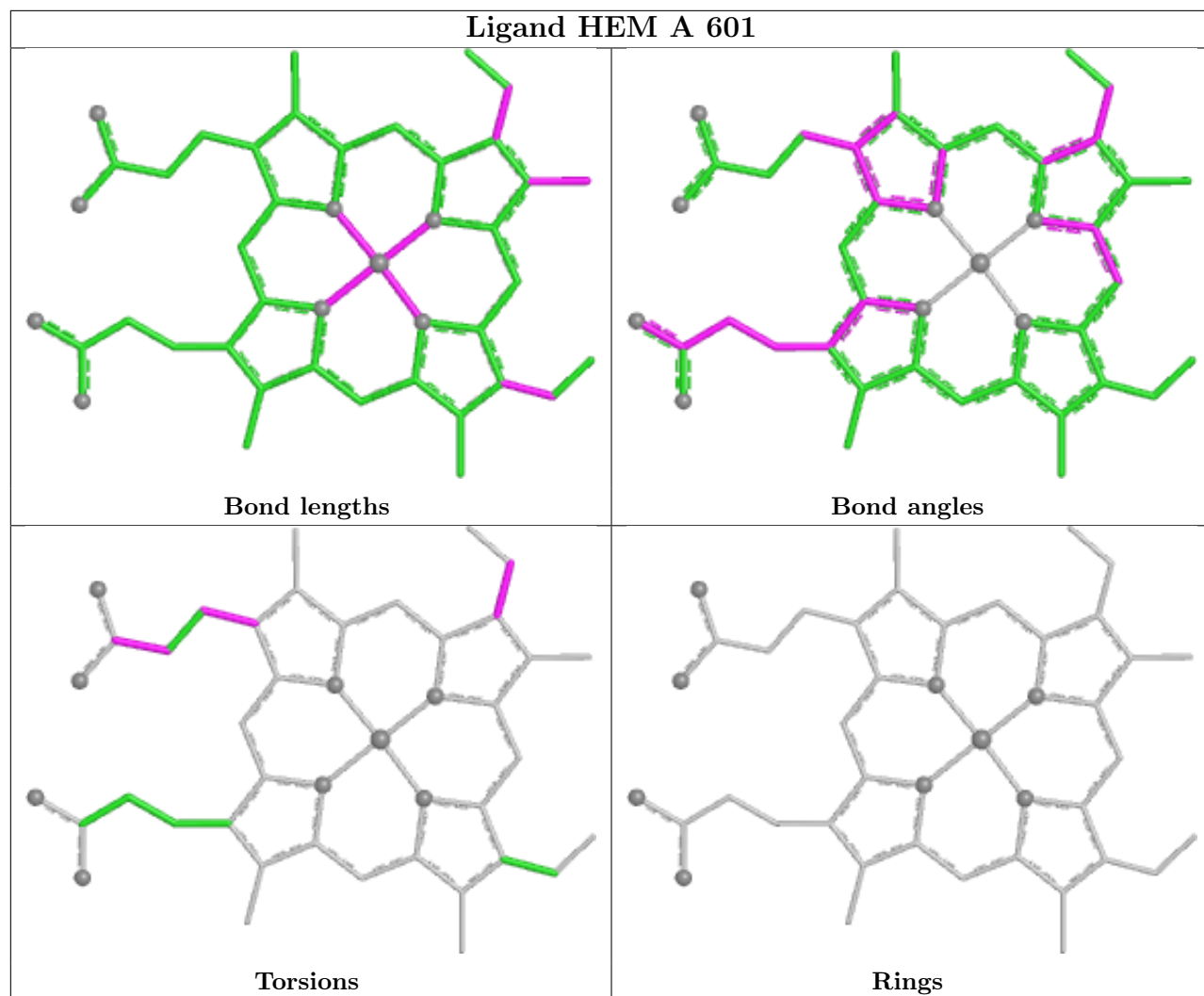
4 monomers are involved in 14 short contacts:

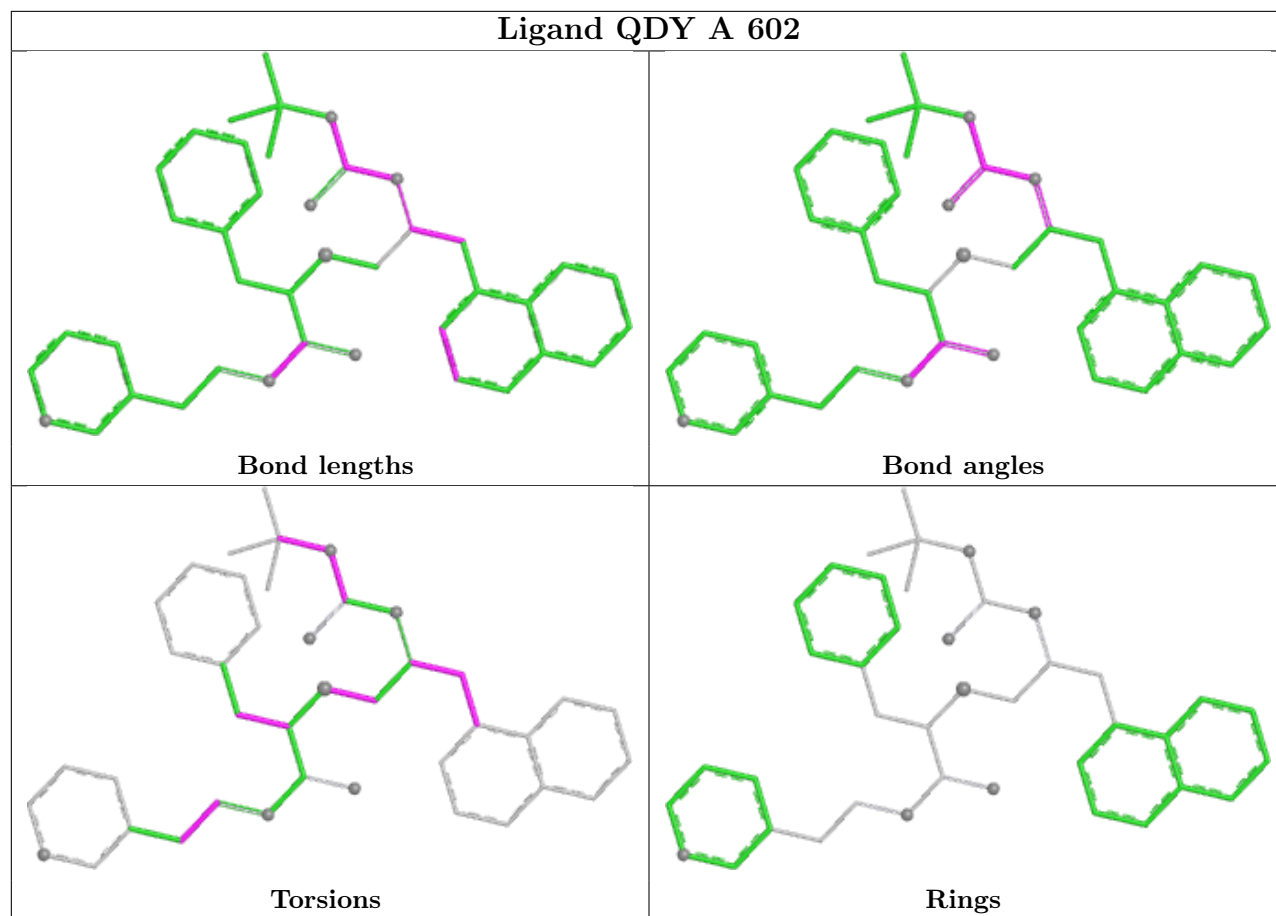
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	QDY	2	0
2	A	601	HEM	6	0
3	A	602	QDY	2	0
2	B	601	HEM	4	0

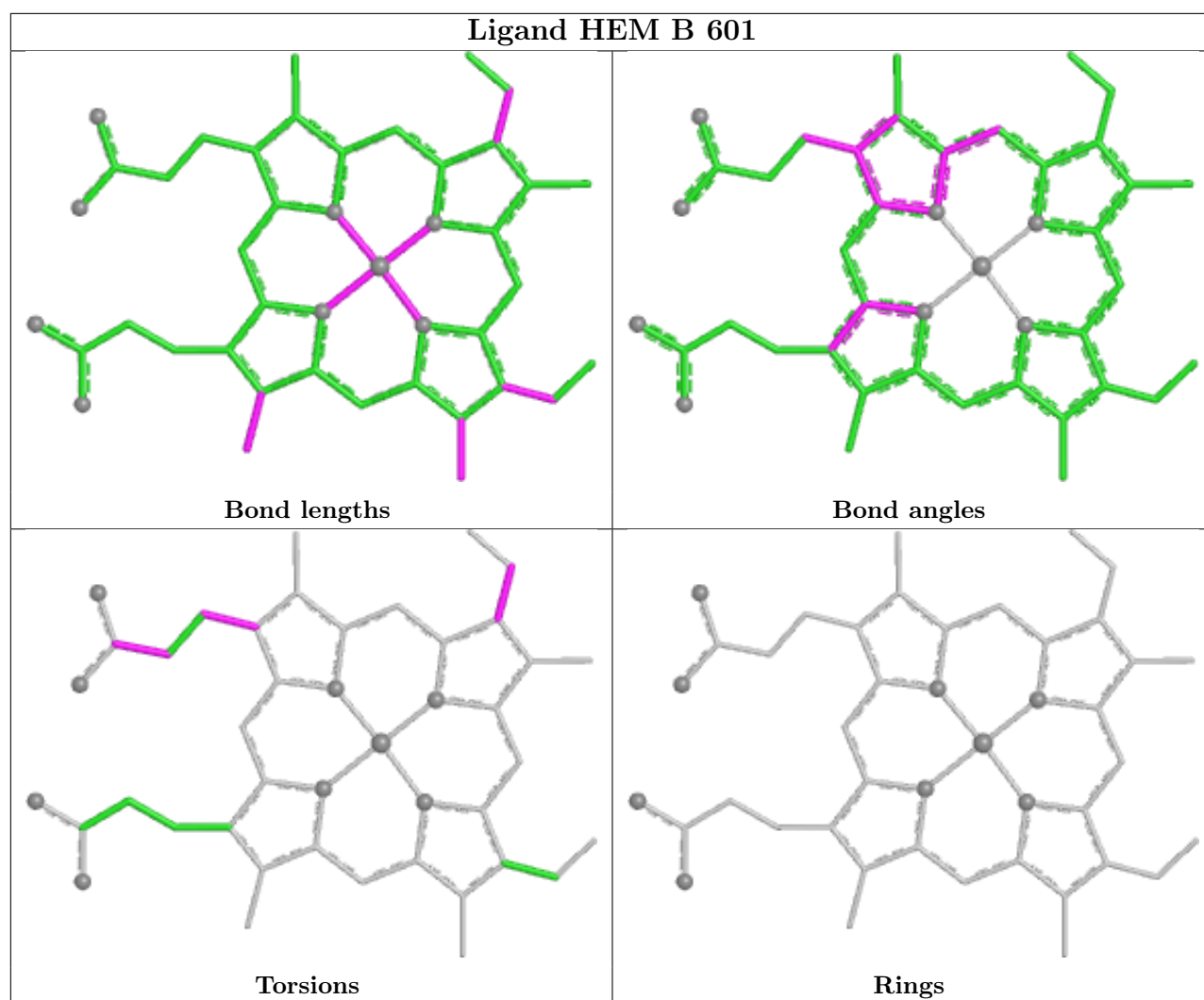
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.









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	443/487 (90%)	0.70	30 (6%)	23 19	55, 120, 178, 211	2 (0%)
1	B	433/487 (88%)	0.75	40 (9%)	14 11	63, 167, 246, 315	2 (0%)
All	All	876/974 (89%)	0.72	70 (7%)	18 14	55, 140, 233, 315	4 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	ARG	6.9
1	A	191	VAL	5.8
1	B	232	ILE	5.0
1	A	213	PHE	4.9
1	A	211	LEU	4.4
1	B	226	PHE	4.2
1	A	224	THR	4.0
1	A	108	PHE	4.0
1	A	206	ASN	3.7
1	B	117	ALA	3.7
1	B	189	PHE	3.7
1	B	229	LEU	3.5
1	A	226	PHE	3.5
1	B	213	PHE	3.4
1	B	46	PHE	3.4
1	B	241	PHE	3.4
1	B	212	ARG	3.3
1	B	120	ILE	3.2
1	B	156	LEU	3.2
1	B	228	PHE	3.2
1	A	207	THR	3.1
1	A	481	GLY	3.1
1	B	233	LEU	3.1
1	B	253	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	456	LEU	2.9
1	B	222	SER	2.9
1	A	215	PHE	2.9
1	B	454	LEU	2.9
1	A	210	LEU	2.9
1	B	108	PHE	2.8
1	B	110	PRO	2.7
1	A	124	GLU	2.7
1	A	289	ALA	2.7
1	B	299	SER	2.7
1	B	221	LEU	2.6
1	A	479	LEU	2.6
1	B	160	LEU	2.5
1	A	189	PHE	2.5
1	A	259	SER	2.5
1	B	452	MET	2.5
1	B	159	ASN	2.5
1	A	57	PHE	2.5
1	A	241	PHE	2.5
1	B	481	GLY	2.4
1	B	225	VAL	2.4
1	B	482	LEU	2.4
1	B	334	GLU	2.4
1	A	245	VAL	2.4
1	A	133	LEU	2.4
1	A	301	ILE	2.4
1	A	127	LYS	2.4
1	B	457	ILE	2.4
1	A	148	ILE	2.3
1	A	353	MET	2.3
1	B	480	GLY	2.3
1	B	132	LEU	2.3
1	B	133	LEU	2.3
1	B	248	PHE	2.3
1	A	298	GLN	2.2
1	B	313	VAL	2.2
1	B	359	VAL	2.2
1	B	430	TYR	2.2
1	B	467	PRO	2.2
1	A	223	ILE	2.2
1	A	335	ILE	2.1
1	B	301	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	450	MET	2.1
1	A	276	ILE	2.1
1	A	269	VAL	2.1
1	B	303	ILE	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](#)

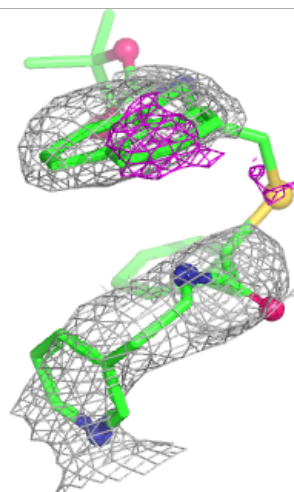
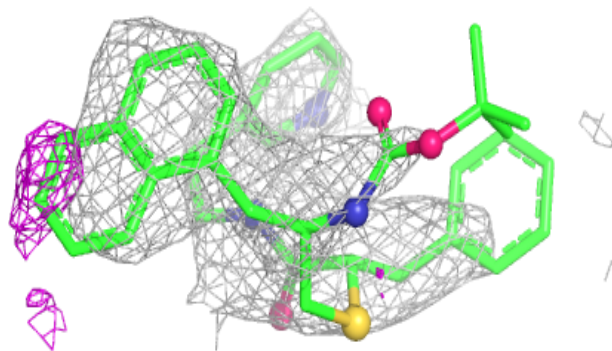
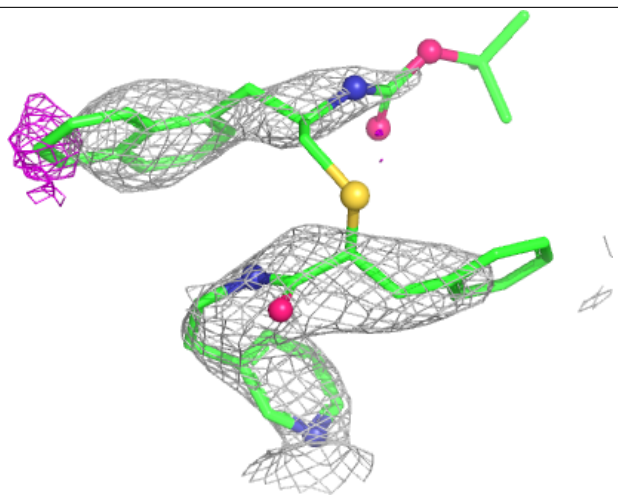
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	QDY	B	602	41/41	0.85	0.14	139,162,197,212	0
3	QDY	A	602	41/41	0.88	0.19	80,112,131,143	0
2	HEM	A	601	43/43	0.97	0.09	52,70,92,100	0
2	HEM	B	601	43/43	0.97	0.08	80,111,134,149	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.

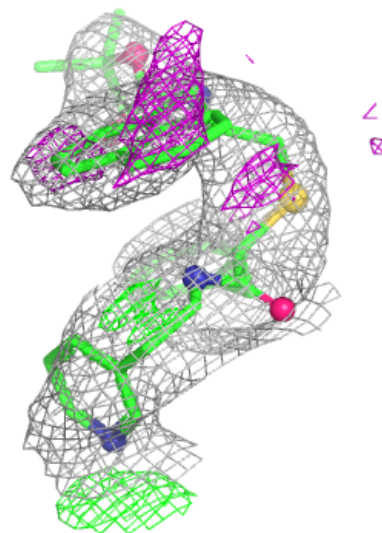
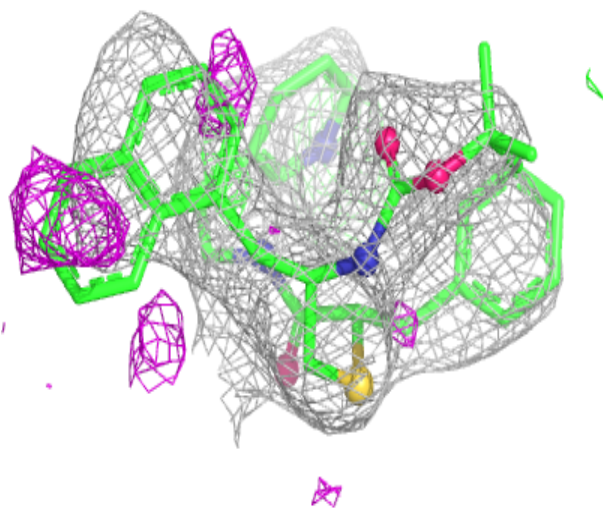
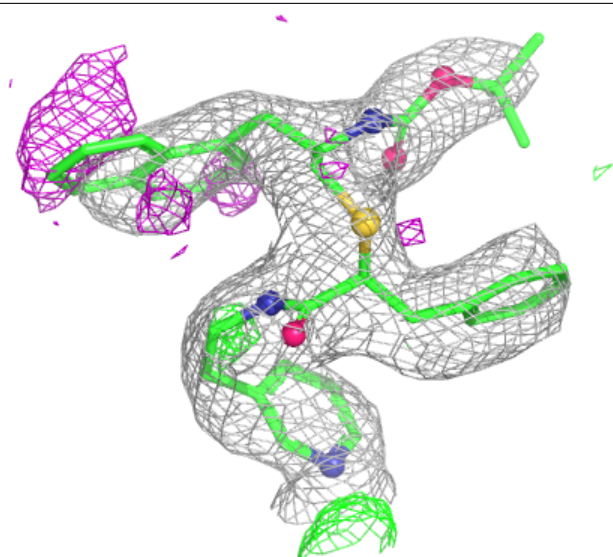
Electron density around QDY B 602:

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



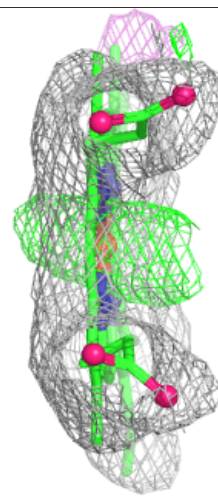
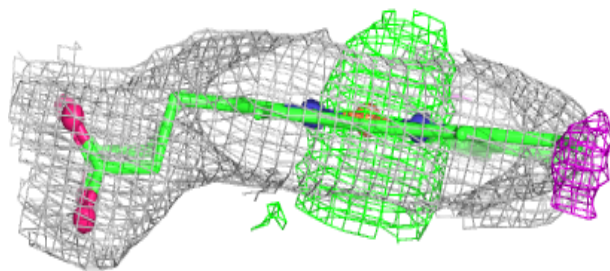
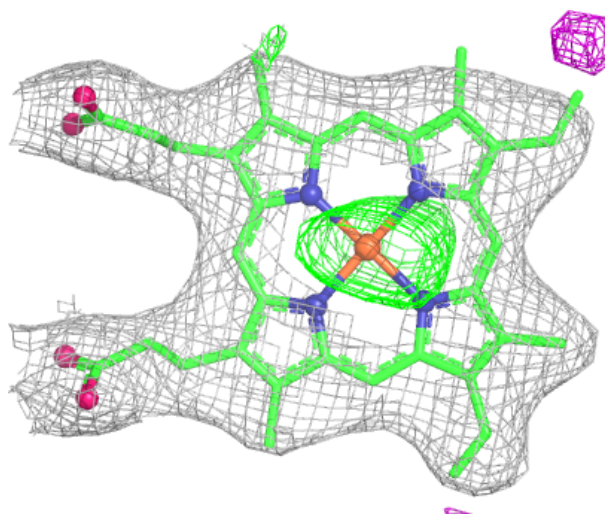
Electron density around QDY A 602:

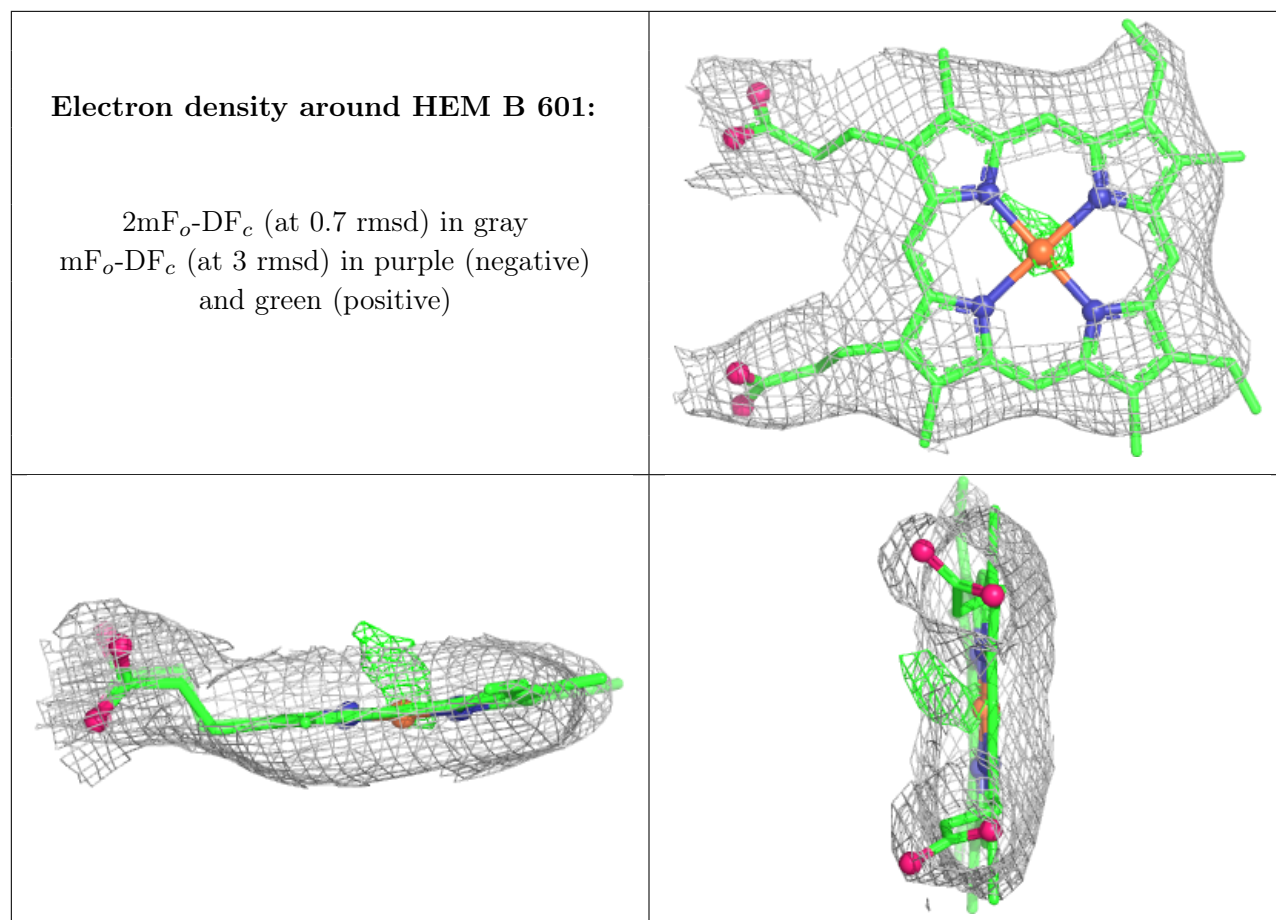
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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 [i](#)

There are no such residues in this entry.