



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:32 AM UTC

PDB ID : 3KW4 / pdb_00003kw4
Title : Crystal structure of cytochrome 2B4 in complex with the anti-platelet drug ticlopidine
Authors : Gay, S.C.; Maekawa, K.; Roberts, A.G.; Hong, W.-X.; Zhang, Q.; Stout, C.D.; Halpert, J.R.
Deposited on : 2009-11-30
Resolution : 2.67 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

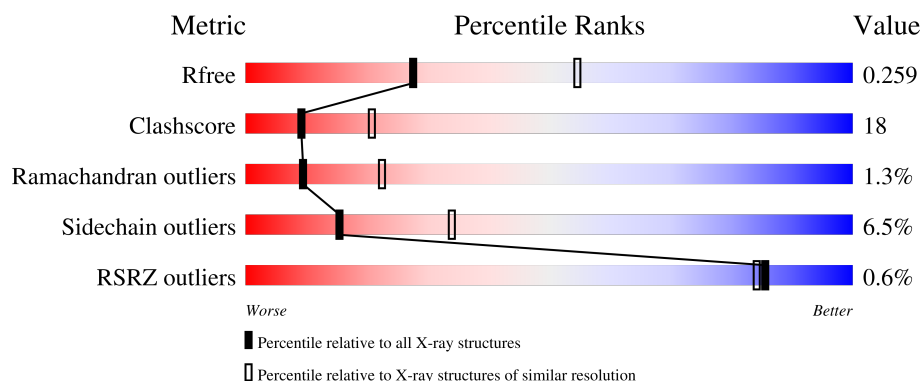
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	476	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3949 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 2B4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	0	0
			3693	2383	635	665	10			

There are 33 discrepancies between the modelled and reference sequences:

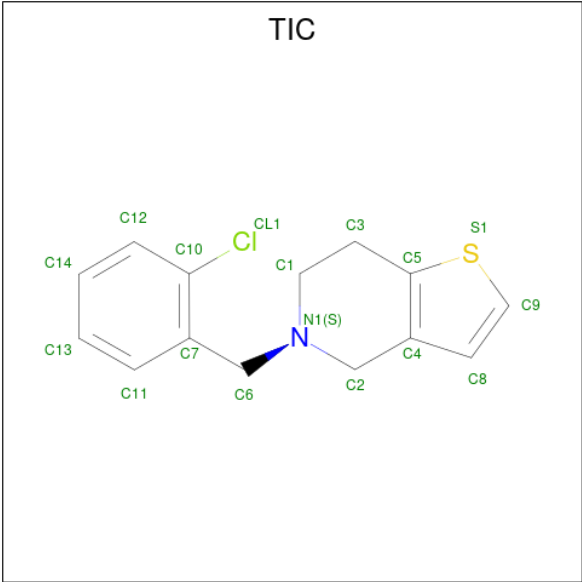
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ALA	GLU	engineered mutation	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	SER	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	ALA	deletion	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	ALA	deletion	UNP P00178
A	?	-	GLY	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	ARG	deletion	UNP P00178
A	22	LYS	GLY	engineered mutation	UNP P00178
A	23	LYS	HIS	engineered mutation	UNP P00178
A	24	THR	PRO	engineered mutation	UNP P00178
A	25	SER	LYS	engineered mutation	UNP P00178
A	26	SER	ALA	engineered mutation	UNP P00178
A	27	LYS	HIS	engineered mutation	UNP P00178
A	29	LYS	ARG	engineered mutation	UNP P00178

Continued on next page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	SER	PRO	SEE REMARK 999	UNP P00178
A	226	TYR	HIS	engineered mutation	UNP P00178
A	492	HIS	-	expression tag	UNP P00178
A	493	HIS	-	expression tag	UNP P00178
A	494	HIS	-	expression tag	UNP P00178
A	495	HIS	-	expression tag	UNP P00178

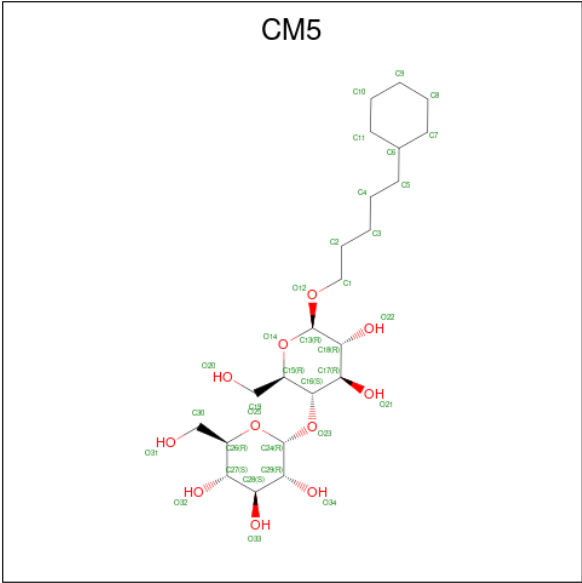
- # HEM

- Molecule 3 is ticlopidine (CCD ID: TIC) (formula: $C_{14}H_{14}ClNS$).



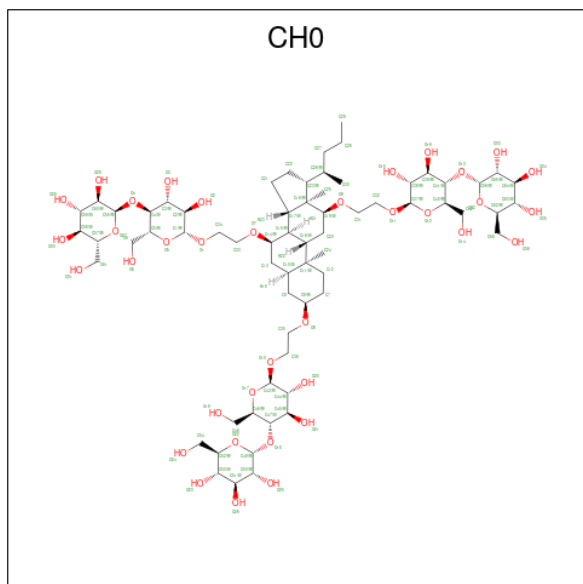
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	S	0	1
			34	28	2	2	2		

- Molecule 4 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSIDE (CCD ID: CM5) (formula: C₂₃H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			34	23	11		
4	A	1	Total	C	O	0	0
			34	23	11		

- Molecule 5 is 2-[[[(3alpha,5alpha,7alpha,8alpha,10alpha,12alpha,17alpha)-3,12-bis{2-[(4-O-alpha-D-glucopyranosyl-beta-D-glucopyranosyl)oxy]ethoxy}cholan-7-yl]oxy}ethyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (CCD ID: CH0) (formula: C₆₆H₁₁₄O₃₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	1	0
			80	54	26		

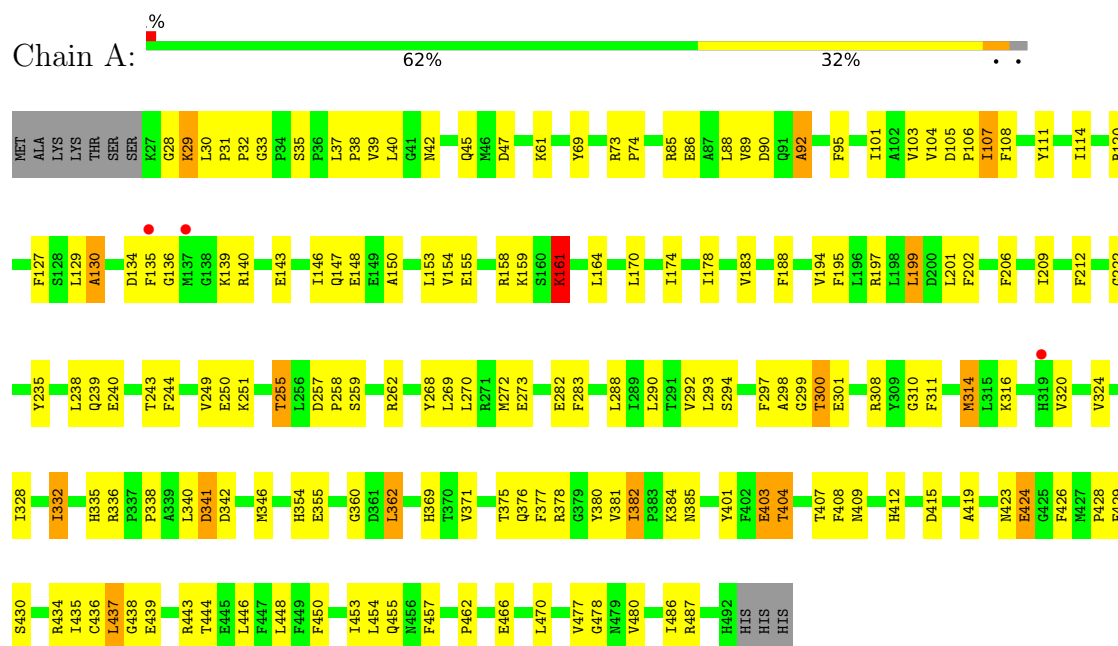
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	31	Total	O	0	0
			31	31		

3 Residue-property plots [i](#)

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 2B4



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.50Å 93.50Å 137.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	68.54 – 2.67 68.54 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.6 (68.54-2.67) 99.6 (68.54-2.67)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.253 0.197 , 0.259	Depositor DCC
R_{free} test set	1033 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	70.8	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3949	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: CH0, CM5, TIC, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	1/3785 (0.0%)	0.97	7/5130 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	GLY	C-N	5.86	1.41	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	GLU	N-CA-C	-9.56	96.37	110.23
1	A	136	GLY	N-CA-C	6.01	119.39	111.52
1	A	382	ILE	CA-C-N	5.37	125.31	119.78
1	A	382	ILE	C-N-CA	5.37	125.31	119.78
1	A	33	GLY	O-C-N	5.30	127.07	121.77
1	A	107	ILE	CB-CA-C	-5.12	105.26	111.87
1	A	197	ARG	N-CA-C	-5.08	105.82	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3693	0	3673	127	0
2	A	43	0	30	7	0
3	A	34	0	28	6	0
4	A	68	0	84	11	0
5	A	80	0	92	8	0
6	A	31	0	0	1	0
All	All	3949	0	3907	142	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 18.

All (142) 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:308:ARG:HD2	6:A:1023:HOH:O	1.53	1.06
1:A:255:THR:HG23	1:A:262:ARG:HH22	1.18	1.03
1:A:404:THR:HG23	1:A:407:THR:HB	1.41	1.03
1:A:342:ASP:O	1:A:346:MET:HG3	1.61	1.00
3:A:600[B]:TIC:H3	3:A:600[B]:TIC:CL1	2.04	0.94
1:A:404:THR:O	1:A:404:THR:HG22	1.72	0.88
1:A:255:THR:HG23	1:A:262:ARG:NH2	1.99	0.76
1:A:324:VAL:O	1:A:328:ILE:HG13	1.87	0.75
2:A:500:HEM:HBC2	2:A:500:HEM:HMC1	1.69	0.73
1:A:188:PHE:HE2	4:A:602:CM5:H18	1.53	0.72
1:A:354:HIS:HD2	1:A:426:PHE:CE2	2.07	0.71
1:A:404:THR:O	1:A:404:THR:CG2	2.39	0.71
1:A:404:THR:CG2	1:A:407:THR:HB	2.19	0.70
1:A:212:PHE:HB2	5:A:603:CH0:H82	1.74	0.70
1:A:28:GLY:O	1:A:29:LYS:HG2	1.94	0.68
1:A:403:GLU:O	1:A:412:HIS:NE2	2.26	0.68
1:A:316:LYS:HD3	1:A:470:LEU:HD11	1.76	0.67
1:A:251:LYS:O	1:A:255:THR:HG22	1.94	0.67
5:A:603:CH0:H64	5:A:603:CH0:H17	1.78	0.65
1:A:429:PHE:HB3	1:A:436:CYS:HB3	1.77	0.65
1:A:154:VAL:HG13	1:A:457:PHE:CE2	2.32	0.64
1:A:310:GLY:O	1:A:314:MET:HG2	1.99	0.63
1:A:206:PHE:CD2	1:A:301:GLU:HG3	2.32	0.63
1:A:42:ASN:HD22	1:A:45:GLN:NE2	1.97	0.62
1:A:244:PHE:CE1	4:A:602:CM5:H52	2.35	0.61
1:A:332:ILE:HG23	1:A:336:ARG:NH1	2.15	0.61
1:A:268:TYR:CE1	1:A:272:MET:HE2	2.38	0.59
1:A:69:TYR:CE2	1:A:74:PRO:HB3	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LEU:O	1:A:92:ALA:HA	2.03	0.59
1:A:244:PHE:CZ	4:A:602:CM5:H41	2.37	0.59
4:A:601:CM5:H11	4:A:601:CM5:O22	2.01	0.59
1:A:354:HIS:HD2	1:A:426:PHE:CZ	2.20	0.59
1:A:85:ARG:NE	1:A:424:GLU:HG3	2.18	0.59
1:A:444:THR:HG22	1:A:448:LEU:HD12	1.84	0.58
1:A:111:TYR:HB2	1:A:290:LEU:HD12	1.86	0.58
1:A:201:LEU:HD21	1:A:240:GLU:CD	2.28	0.58
1:A:316:LYS:CD	1:A:470:LEU:HD11	2.34	0.58
1:A:159:LYS:O	1:A:161:LYS:HD2	2.03	0.58
1:A:209:ILE:HG21	3:A:600[B]:TIC:H12	1.85	0.58
1:A:188:PHE:CE2	4:A:602:CM5:H18	2.38	0.57
1:A:209:ILE:CG2	3:A:600[B]:TIC:H12	2.35	0.56
1:A:195:PHE:HD1	4:A:602:CM5:H31A	1.70	0.56
1:A:183:VAL:HG11	1:A:292:VAL:HG13	1.87	0.56
1:A:38:PRO:O	1:A:39:VAL:HB	2.04	0.56
2:A:500:HEM:HMB1	2:A:500:HEM:HBB2	1.87	0.55
4:A:601:CM5:O22	4:A:601:CM5:C1	2.54	0.55
2:A:500:HEM:HBB2	2:A:500:HEM:CMB	2.37	0.55
1:A:69:TYR:CZ	1:A:74:PRO:HB3	2.43	0.54
1:A:127:PHE:CD1	1:A:127:PHE:C	2.86	0.54
1:A:206:PHE:CG	1:A:301:GLU:HG3	2.42	0.54
1:A:340:LEU:HD13	1:A:444:THR:HG23	1.90	0.54
1:A:42:ASN:HD22	1:A:45:GLN:HE21	1.54	0.54
1:A:415:ASP:OD2	1:A:419:ALA:HB3	2.08	0.54
1:A:153:LEU:HD21	1:A:453:ILE:HD11	1.90	0.53
1:A:135:PHE:O	1:A:139:LYS:HD3	2.08	0.53
1:A:129:LEU:O	1:A:130:ALA:C	2.52	0.53
1:A:143:GLU:O	1:A:147:GLN:HG3	2.09	0.53
1:A:314:MET:HE2	1:A:450:PHE:CE1	2.43	0.53
1:A:154:VAL:HG13	1:A:457:PHE:HE2	1.71	0.52
4:A:602:CM5:O20	4:A:602:CM5:H26	2.09	0.52
1:A:269:LEU:HD23	1:A:272:MET:HE3	1.92	0.52
1:A:108:PHE:CZ	1:A:293:LEU:HD23	2.45	0.51
1:A:95:PHE:O	1:A:369:HIS:HD2	1.93	0.51
1:A:311:PHE:HA	1:A:314:MET:HG3	1.92	0.51
1:A:298:ALA:HB1	3:A:600[B]:TIC:H8	1.93	0.51
1:A:268:TYR:CE1	1:A:288:LEU:HB2	2.46	0.51
1:A:300:THR:CG2	1:A:301:GLU:N	2.74	0.50
1:A:338:PRO:HD3	1:A:455:GLN:OE1	2.10	0.50
1:A:375:THR:O	1:A:381:VAL:HA	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LEU:HD23	1:A:437:LEU:O	2.12	0.50
1:A:426:PHE:CZ	1:A:428:PRO:HG3	2.46	0.49
5:A:603:CH0:H18	5:A:603:CH0:H11	1.94	0.49
1:A:478:GLY:HA3	3:A:600[B]:TIC:C13	2.43	0.49
1:A:105:ASP:N	1:A:106:PRO:CD	2.76	0.49
1:A:134:ASP:O	1:A:135:PHE:HB2	2.13	0.48
1:A:202:PHE:HE1	1:A:300:THR:HG21	1.78	0.48
1:A:47:ASP:O	4:A:601:CM5:H112	2.12	0.48
1:A:154:VAL:O	1:A:158:ARG:HG3	2.14	0.48
1:A:360:GLY:C	1:A:362:LEU:HD13	2.38	0.48
1:A:429:PHE:O	1:A:430:SER:HB3	2.13	0.48
1:A:371:VAL:HG21	1:A:382:ILE:HG22	1.97	0.47
5:A:603:CH0:H81	5:A:603:CH0:H74	1.47	0.46
1:A:31:PRO:HB3	1:A:32:PRO:HD2	1.98	0.46
1:A:401:TYR:HB3	1:A:423:ASN:OD1	2.15	0.46
1:A:439:GLU:O	1:A:443:ARG:HG3	2.16	0.46
1:A:384:LYS:O	1:A:385:ASN:HB2	2.16	0.46
1:A:114:ILE:HD11	1:A:298:ALA:HB2	1.98	0.46
1:A:268:TYR:CD1	1:A:272:MET:HE2	2.50	0.46
1:A:268:TYR:HE1	1:A:272:MET:HE2	1.80	0.46
1:A:299:GLY:HA2	2:A:500:HEM:C2C	2.50	0.46
2:A:500:HEM:HBC2	2:A:500:HEM:CMC	2.42	0.45
5:A:603:CH0:H10	5:A:603:CH0:H58	1.47	0.45
1:A:188:PHE:CE2	4:A:602:CM5:H11	2.50	0.45
1:A:199:LEU:HA	1:A:199:LEU:HD22	1.62	0.45
1:A:258:PRO:HA	1:A:270:LEU:HD21	1.98	0.45
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.56	0.45
1:A:438:GLY:HA3	2:A:500:HEM:C3C	2.52	0.45
1:A:250:GLU:O	1:A:251:LYS:C	2.59	0.45
1:A:355:GLU:OE2	1:A:409:ASN:N	2.49	0.45
1:A:297:PHE:CZ	3:A:600[B]:TIC:CL1	3.07	0.44
1:A:146:ILE:HG12	1:A:178:ILE:HD12	1.99	0.44
1:A:270:LEU:O	1:A:273:GLU:HB2	2.16	0.44
1:A:354:HIS:CD2	1:A:426:PHE:CE2	2.96	0.44
1:A:257:ASP:C	1:A:259:SER:H	2.25	0.44
5:A:603:CH0:H41	5:A:603:CH0:H46	1.74	0.44
1:A:235:TYR:CE2	1:A:239:GLN:NE2	2.85	0.44
1:A:477:VAL:O	1:A:477:VAL:HG22	2.18	0.43
1:A:150:ALA:O	1:A:154:VAL:HG23	2.18	0.43
1:A:257:ASP:O	1:A:259:SER:N	2.52	0.43
1:A:107:ILE:HG13	1:A:238:LEU:HD12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:PRO:HD3	1:A:380:TYR:CZ	2.54	0.42
1:A:251:LYS:HZ1	4:A:602:CM5:H16	1.84	0.42
1:A:272:MET:HG3	1:A:283:PHE:O	2.19	0.42
1:A:235:TYR:CZ	1:A:239:GLN:NE2	2.88	0.42
1:A:268:TYR:O	1:A:272:MET:N	2.53	0.42
1:A:320:VAL:O	1:A:324:VAL:HG23	2.20	0.42
1:A:434:ARG:O	1:A:435:ILE:C	2.61	0.42
1:A:377:PHE:O	1:A:378:ARG:C	2.61	0.42
1:A:403:GLU:O	1:A:404:THR:HB	2.19	0.42
1:A:446:LEU:O	1:A:450:PHE:HB2	2.20	0.42
1:A:148:GLU:HA	1:A:148:GLU:OE1	2.20	0.41
1:A:320:VAL:HG21	1:A:408:PHE:HE2	1.85	0.41
1:A:341:ASP:OD1	1:A:341:ASP:N	2.48	0.41
1:A:120:ARG:HA	1:A:282:GLU:HG3	2.01	0.41
1:A:369:HIS:HE1	2:A:500:HEM:O2A	2.03	0.41
5:A:603:CH0:H72	5:A:603:CH0:H60	1.66	0.41
1:A:101:ILE:HB	1:A:104:VAL:HG22	2.01	0.41
1:A:103:VAL:HG23	1:A:104:VAL:HG13	2.03	0.41
1:A:480:VAL:HG23	1:A:480:VAL:O	2.20	0.41
5:A:603:CH0:H47	5:A:603:CH0:H24	2.01	0.41
1:A:376:GLN:HA	1:A:380:TYR:O	2.21	0.41
1:A:86:GLU:O	1:A:90:ASP:HB2	2.21	0.41
1:A:164:LEU:HD21	1:A:462:PRO:HD3	2.03	0.41
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.91	0.41
1:A:466:GLU:H	1:A:466:GLU:CD	2.28	0.41
1:A:114:ILE:HG13	1:A:294:SER:HB3	2.03	0.41
1:A:300:THR:HG23	1:A:301:GLU:N	2.36	0.40
1:A:429:PHE:HB3	1:A:436:CYS:CB	2.47	0.40
1:A:314:MET:HE2	1:A:450:PHE:HE1	1.86	0.40
1:A:362:LEU:HA	1:A:362:LEU:HD12	1.77	0.40
1:A:435:ILE:O	1:A:436:CYS:C	2.64	0.40
1:A:250:GLU:HA	1:A:250:GLU:OE2	2.20	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	464/476 (98%)	426 (92%)	32 (7%)	6 (1%)	9	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	HIS
1	A	92	ALA
1	A	130	ALA
1	A	29	LYS
1	A	161	LYS
1	A	222	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	401/421 (95%)	375 (94%)	26 (6%)	15	34

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	35	SER
1	A	37	LEU
1	A	40	LEU
1	A	61	LYS
1	A	73	ARG
1	A	89	VAL
1	A	140	ARG
1	A	155	GLU
1	A	161	LYS
1	A	174	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	194	VAL
1	A	199	LEU
1	A	243	THR
1	A	249	VAL
1	A	255	THR
1	A	300	THR
1	A	314	MET
1	A	332	ILE
1	A	341	ASP
1	A	362	LEU
1	A	404	THR
1	A	424	GLU
1	A	437	LEU
1	A	486	ILE
1	A	487	ARG

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

Mol	Chain	Res	Type
1	A	45	GLN
1	A	91	GLN
1	A	109	GLN
1	A	284	HIS
1	A	354	HIS
1	A	357	GLN
1	A	369	HIS
1	A	456	ASN
1	A	485	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

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	TIC	A	600[B]	-	19,19,19	1.31	2 (10%)	25,26,26	2.00	6 (24%)
3	TIC	A	600[A]	-	19,19,19	1.18	1 (5%)	25,26,26	1.28	1 (4%)
4	CM5	A	601	-	36,36,36	0.43	0	49,49,49	1.44	10 (20%)
2	HEM	A	500	1	50,50,50	1.59	6 (12%)	67,82,82	1.37	9 (13%)
4	CM5	A	602	-	36,36,36	0.51	0	49,49,49	0.93	2 (4%)
5	CH0	A	603	-	87,87,111	0.79	4 (4%)	125,129,165	1.68	30 (24%)

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	TIC	A	600[B]	-	-	2/4/13/13	0/3/3/3
3	TIC	A	600[A]	-	-	0/4/13/13	0/3/3/3
4	CM5	A	601	-	-	9/17/65/65	0/3/3/3
2	HEM	A	500	1	-	4/14/54/54	-
4	CM5	A	602	-	-	12/17/65/65	0/3/3/3
5	CH0	A	603	-	-	25/40/185/237	1/8/8/10

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3D-C2D	7.14	1.52	1.36
3	A	600[B]	TIC	C2-N1	4.52	1.50	1.46
3	A	600[A]	TIC	C2-N1	3.55	1.49	1.46
2	A	500	HEM	CAC-C3C	2.59	1.54	1.47
5	A	603	CH0	C18-C17	-2.49	1.51	1.55
5	A	603	CH0	O11-C37	2.39	1.44	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C2A-C3A	-2.28	1.33	1.38
2	A	500	HEM	C3C-C2C	-2.15	1.32	1.37
5	A	603	CH0	C18-C23	-2.11	1.52	1.55
2	A	500	HEM	CMB-C2B	2.08	1.55	1.50
2	A	500	HEM	CAB-C3B	2.05	1.52	1.47
5	A	603	CH0	C11-C16	-2.04	1.52	1.56
3	A	600[B]	TIC	C3-C5	-2.01	1.46	1.50

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600[B]	TIC	C6-N1-C2	5.74	117.79	110.51
5	A	603	CH0	C18-C23-C26	-5.39	112.95	119.48
5	A	603	CH0	C51-C53-C52	4.85	119.03	110.23
5	A	603	CH0	C20-C19-C18	-4.71	105.63	113.29
2	A	500	HEM	CHD-C1D-ND	4.36	129.12	124.42
3	A	600[A]	TIC	C6-N1-C2	4.25	115.90	110.51
5	A	603	CH0	C18-C17-C15	-4.07	109.56	114.72
3	A	600[B]	TIC	C3-C1-N1	3.97	114.73	111.19
5	A	603	CH0	C12-C11-C16	-3.81	105.42	111.34
5	A	603	CH0	O22-C52-C53	3.70	116.37	109.70
5	A	603	CH0	C49-O22-C52	3.54	120.63	113.72
2	A	500	HEM	CBD-CAD-C3D	-3.52	102.81	112.53
4	A	601	CM5	C24-O23-C16	-3.50	109.68	117.98
5	A	603	CH0	C45-C47-C46	3.49	118.68	110.93
5	A	603	CH0	C53-C51-C50	3.35	116.71	110.83
2	A	500	HEM	C4D-ND-C1D	3.27	109.08	105.21
4	A	601	CM5	C29-C28-C27	-3.25	105.12	110.83
5	A	603	CH0	C12-C11-C10	3.23	112.38	107.75
3	A	600[B]	TIC	C3-C5-C4	-3.19	122.42	124.66
4	A	601	CM5	C18-C17-C16	-3.16	102.51	109.68
5	A	603	CH0	O12-C37-C38	3.15	116.84	110.37
2	A	500	HEM	CHB-C1B-NB	3.04	128.12	124.37
2	A	500	HEM	CHD-C1D-C2D	-2.99	120.30	125.03
5	A	603	CH0	C23-C18-C17	2.98	103.10	100.11
5	A	603	CH0	C9-C8-C7	-2.97	107.83	111.53
5	A	603	CH0	C20-C16-C11	-2.90	110.76	113.70
5	A	603	CH0	C37-O12-C40	2.90	119.39	113.72
5	A	603	CH0	C17-C15-C14	-2.82	109.30	112.47
4	A	602	CM5	C24-O23-C16	-2.82	111.30	117.98
5	A	603	CH0	O17-C46-C47	2.77	115.44	109.72
5	A	603	CH0	C49-O18-C47	-2.74	111.49	117.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600[B]	TIC	C4-C2-N1	2.72	115.04	110.96
5	A	603	CH0	O10-C43-C44	2.65	112.29	108.27
5	A	603	CH0	C44-C45-C47	2.64	115.68	109.68
4	A	601	CM5	C24-O25-C26	2.64	118.88	113.72
3	A	600[B]	TIC	C12-C10-CL1	-2.59	113.33	118.42
4	A	601	CM5	C1-O12-C13	-2.52	109.37	113.68
5	A	603	CH0	C24-C11-C12	2.49	112.26	108.31
5	A	603	CH0	C37-C38-C39	2.48	115.22	110.01
4	A	601	CM5	O21-C17-C16	2.43	116.17	109.94
3	A	600[B]	TIC	C4-C5-S1	2.42	113.62	111.37
5	A	603	CH0	O18-C49-C50	2.41	114.02	108.09
5	A	603	CH0	C9-C10-C11	2.39	115.20	112.66
5	A	603	CH0	C34-O1-C1	-2.39	109.60	113.68
4	A	601	CM5	O12-C13-C18	-2.38	104.66	108.27
4	A	601	CM5	C13-C18-C17	-2.36	105.04	110.01
5	A	603	CH0	C21-C17-C18	2.32	105.79	103.54
4	A	601	CM5	O25-C26-C27	2.30	113.84	109.70
5	A	603	CH0	C13-C10-C9	-2.26	108.65	111.23
2	A	500	HEM	C1C-CHC-C4B	-2.22	121.30	126.02
2	A	500	HEM	CAA-CBA-CGA	-2.18	107.88	113.67
5	A	603	CH0	C49-C50-C51	2.18	114.59	110.01
2	A	500	HEM	CAD-C3D-C4D	2.14	128.43	124.70
4	A	601	CM5	C17-C16-C15	-2.09	106.30	110.93
4	A	602	CM5	C24-C29-C28	-2.04	105.71	110.01
5	A	603	CH0	C35-O8-C8	-2.04	109.91	115.53
2	A	500	HEM	C1A-CHA-C4D	-2.02	121.49	126.25
5	A	603	CH0	C25-C18-C23	-2.00	108.06	111.20

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	CM5	O14-C13-O12-C1
4	A	602	CM5	C18-C13-O12-C1
4	A	602	CM5	O14-C13-O12-C1
5	A	603	CH0	C7-C8-O8-C35
5	A	603	CH0	O5-C5-C6-O6
5	A	603	CH0	O17-C46-C48-O19
5	A	603	CH0	C47-C46-C48-O19
5	A	603	CH0	C4-C5-C6-O6
5	A	603	CH0	C53-C52-C54-O24
5	A	603	CH0	C46-C47-O18-C49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	603	CH0	O12-C40-C42-O14
5	A	603	CH0	C30-C26-C27-C28
4	A	601	CM5	C27-C26-C30-O31
3	A	600[B]	TIC	C7-C6-N1-C1
5	A	603	CH0	O22-C52-C54-O24
4	A	601	CM5	C18-C13-O12-C1
5	A	603	CH0	C44-C43-O10-C36
4	A	602	CM5	O14-C15-C19-O20
4	A	601	CM5	O25-C26-C30-O31
5	A	603	CH0	C18-C23-C26-C27
4	A	602	CM5	O12-C1-C2-C3
4	A	602	CM5	C3-C4-C5-C6
4	A	601	CM5	O14-C15-C19-O20
5	A	603	CH0	C41-C40-C42-O14
4	A	602	CM5	C16-C15-C19-O20
4	A	602	CM5	C2-C3-C4-C5
5	A	603	CH0	C18-C23-C26-C30
4	A	602	CM5	C1-C2-C3-C4
4	A	601	CM5	C2-C3-C4-C5
3	A	600[B]	TIC	N1-C6-C7-C10
5	A	603	CH0	C26-C27-C28-C29
4	A	601	CM5	C2-C1-O12-C13
5	A	603	CH0	C2-C1-O1-C34
5	A	603	CH0	C18-C19-O9-C31
5	A	603	CH0	O8-C35-C36-O10
4	A	602	CM5	C4-C5-C6-C7
5	A	603	CH0	C22-C23-C26-C27
5	A	603	CH0	C22-C23-C26-C30
5	A	603	CH0	C45-C47-O18-C49
5	A	603	CH0	O12-C37-O11-C32
5	A	603	CH0	O7-C33-C34-O1
5	A	603	CH0	C36-C35-O8-C8
4	A	602	CM5	C15-C16-O23-C24
4	A	602	CM5	C17-C16-O23-C24
2	A	500	HEM	CAA-CBA-CGA-O2A
2	A	500	HEM	CAA-CBA-CGA-O1A
4	A	601	CM5	C1-C2-C3-C4
4	A	601	CM5	C16-C15-C19-O20
4	A	602	CM5	C4-C5-C6-C11
2	A	500	HEM	CAD-CBD-CGD-O1D
2	A	500	HEM	CAD-CBD-CGD-O2D
5	A	603	CH0	C20-C19-O9-C31

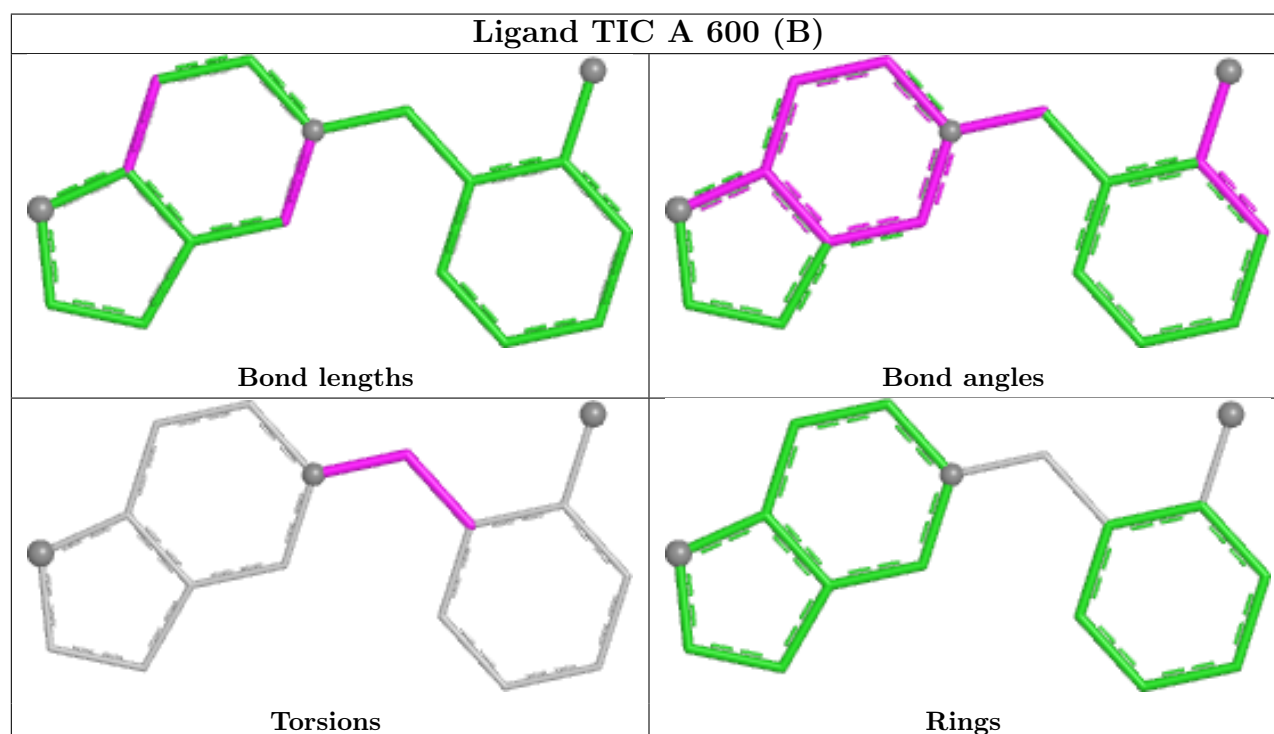
All (1) ring outliers are listed below:

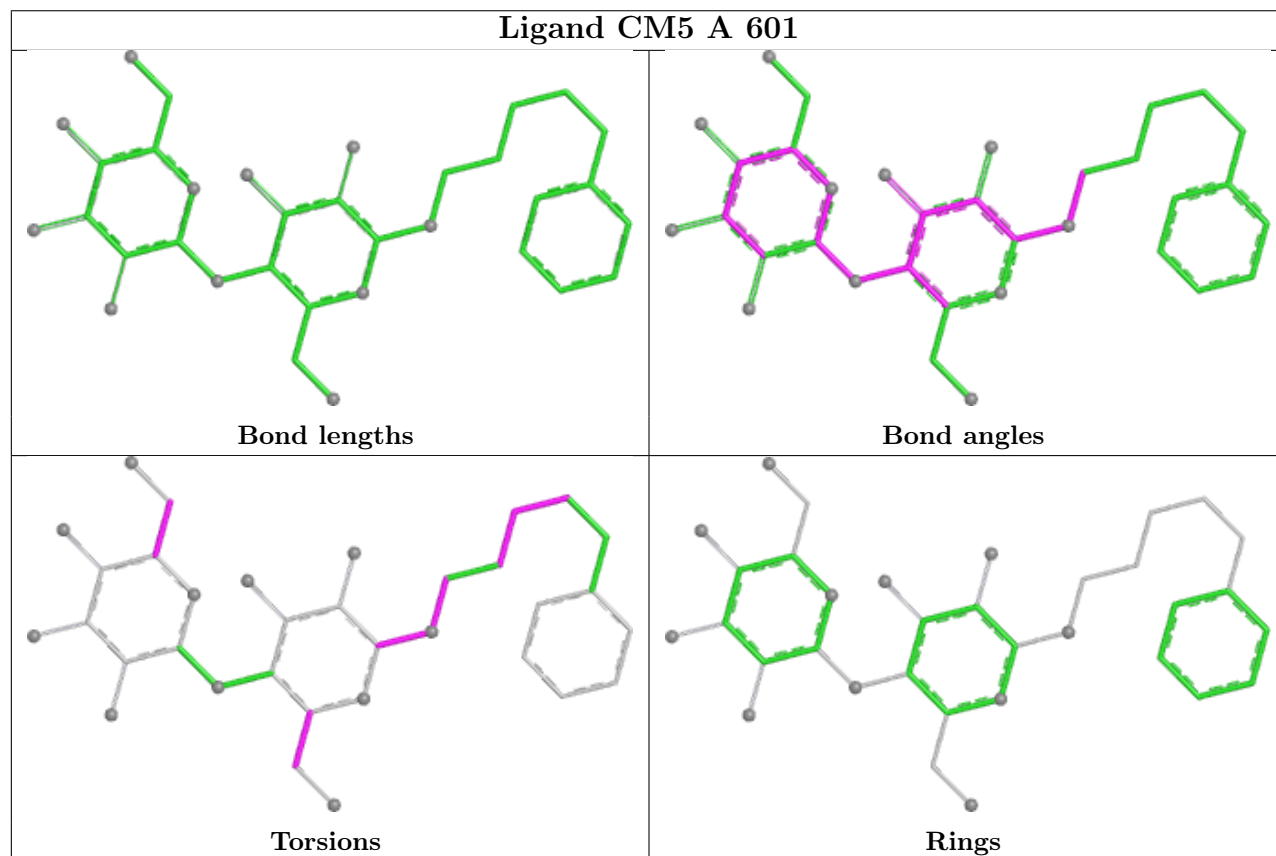
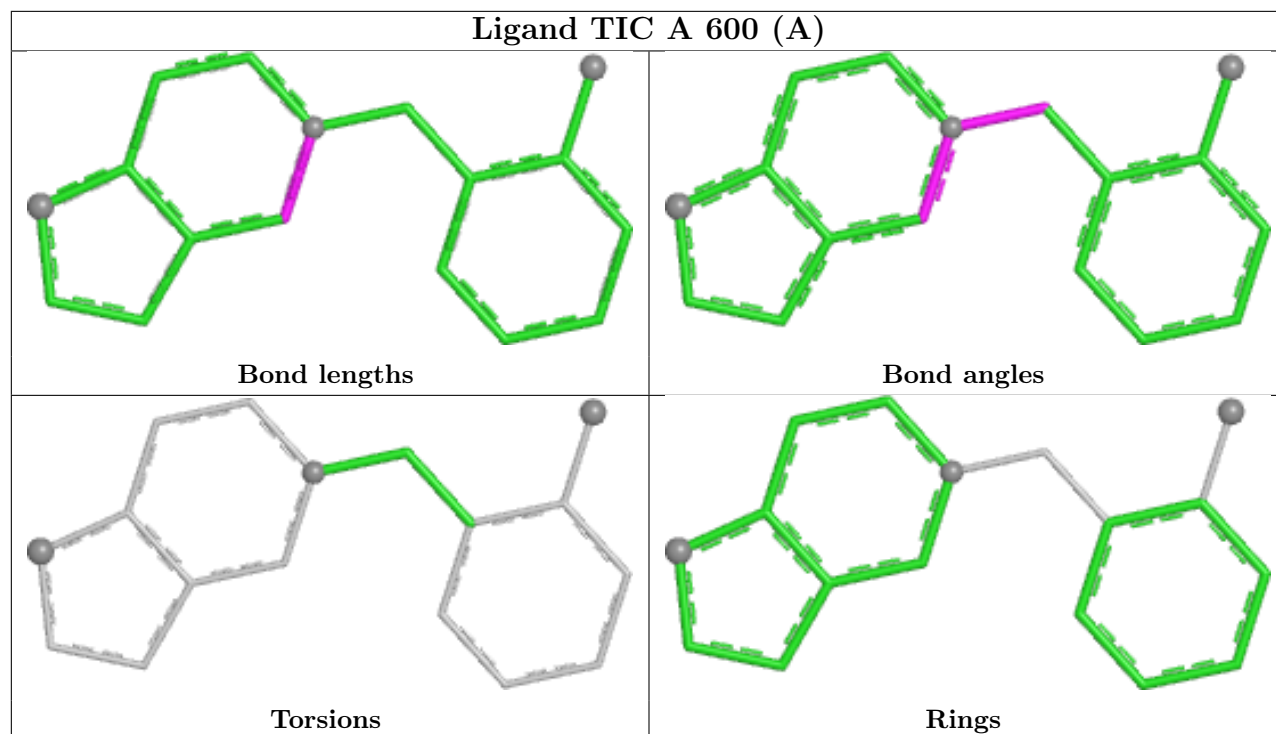
Mol	Chain	Res	Type	Atoms
5	A	603	CH0	C10-C11-C13-C14-C15-C16

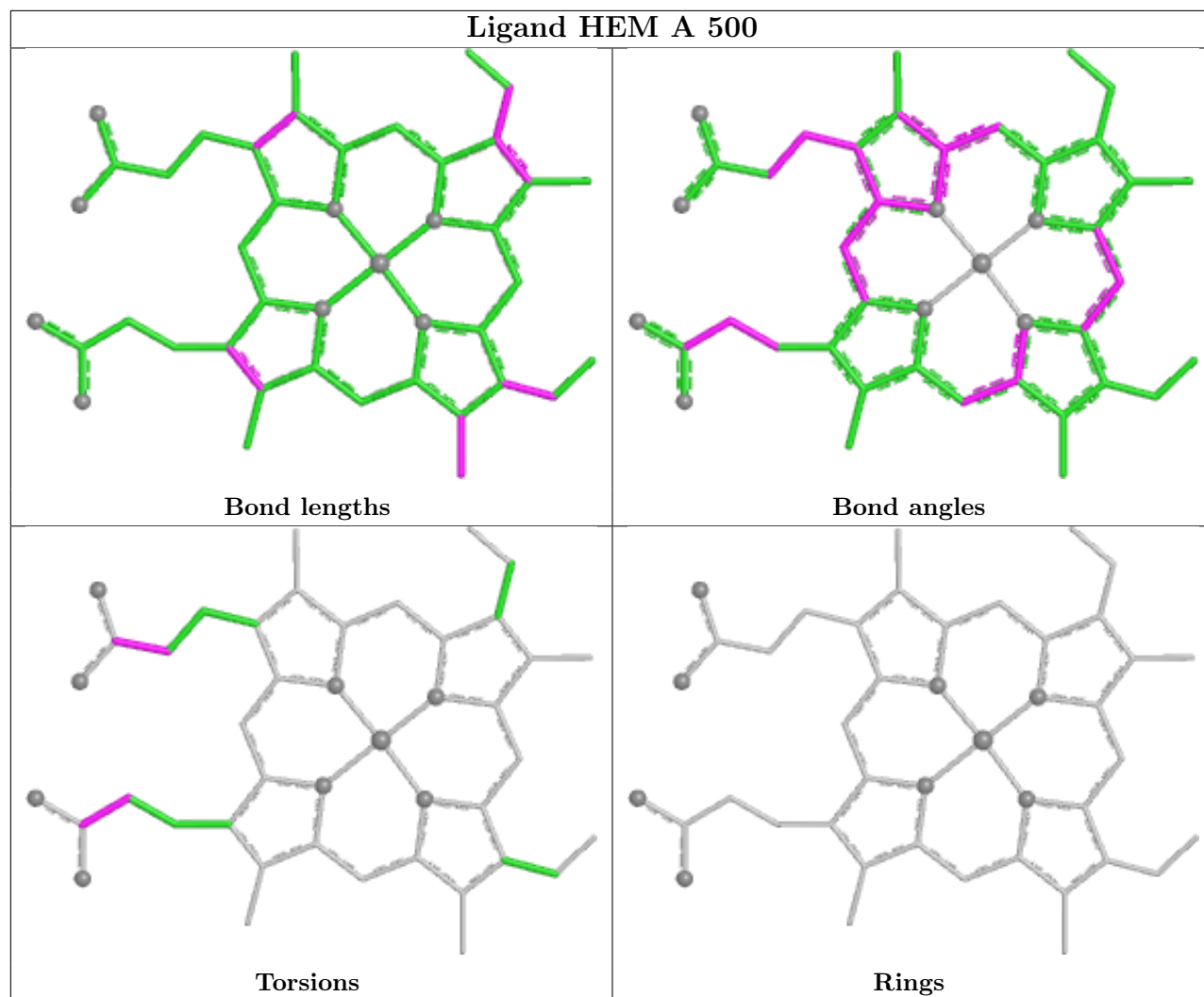
5 monomers are involved in 32 short contacts:

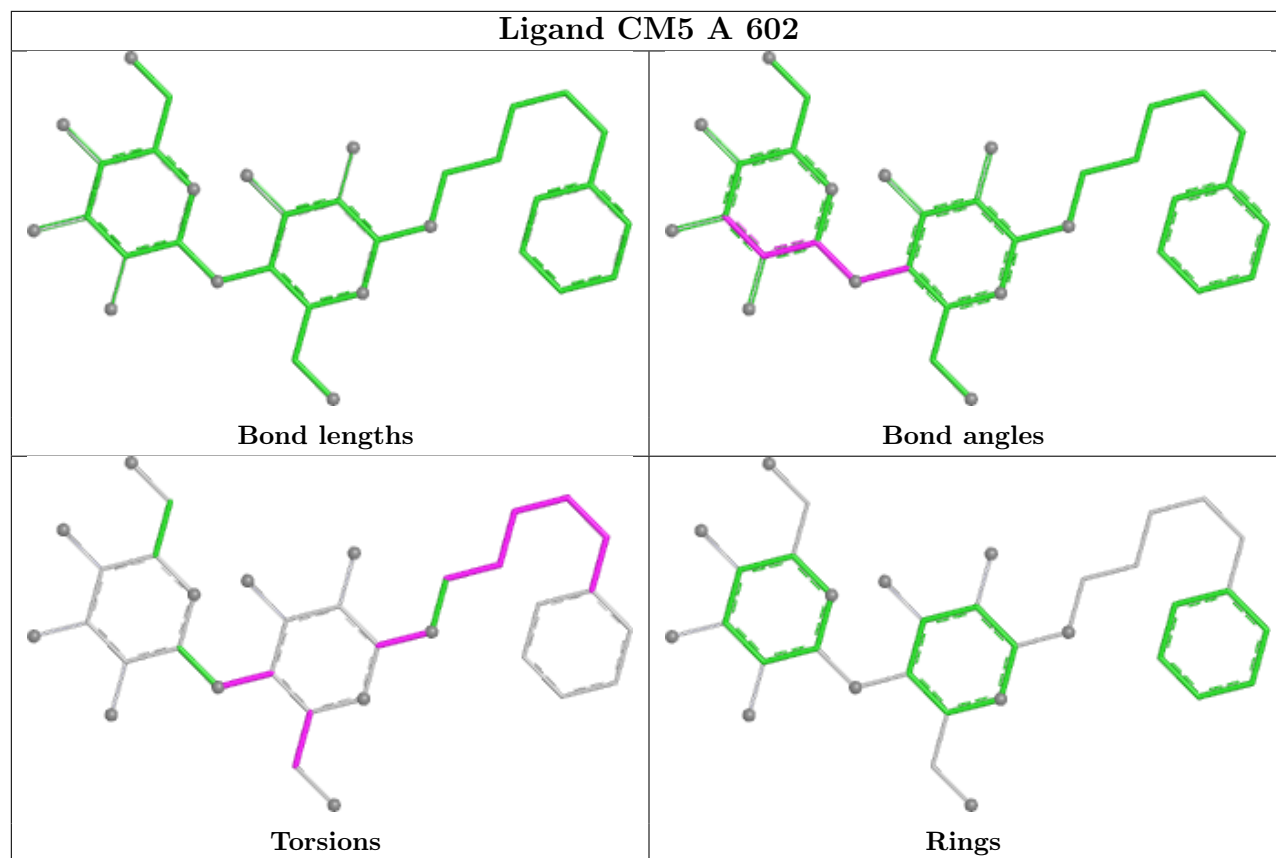
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600[B]	TIC	6	0
4	A	601	CM5	3	0
2	A	500	HEM	7	0
4	A	602	CM5	8	0
5	A	603	CH0	8	0

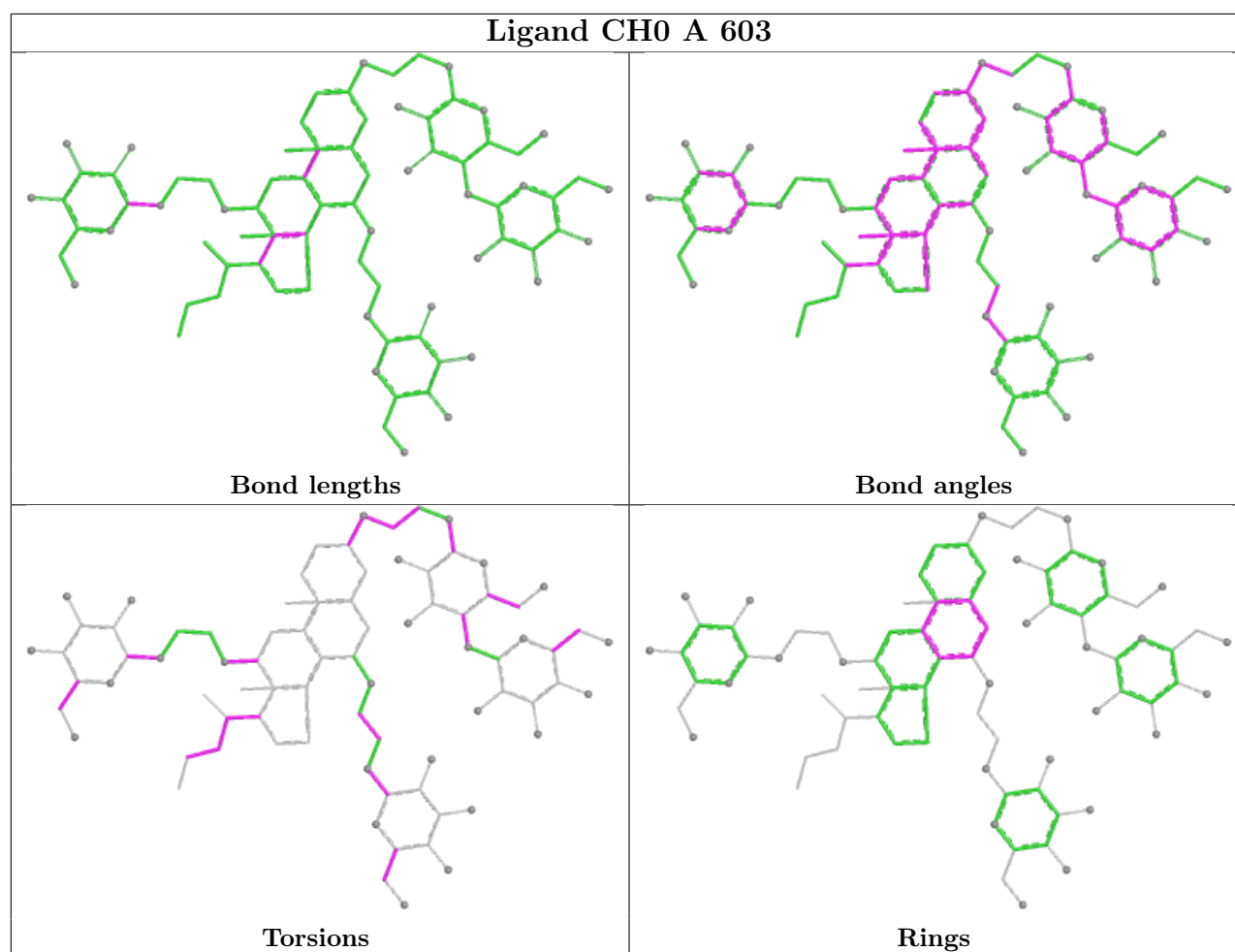
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	466/476 (97%)	0.03	3 (0%) 85 84	45, 62, 100, 133	5 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	MET	3.1
1	A	135	PHE	2.7
1	A	319	HIS	2.3

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
5	CH0	A	603	80/102	0.83	0.16	82,118,136,142	2
4	CM5	A	602	34/34	0.85	0.12	58,104,125,125	0
3	TIC	A	600[A]	17/17	0.87	0.16	65,68,70,72	17
3	TIC	A	600[B]	17/17	0.87	0.16	64,67,78,79	17

Continued on next page...

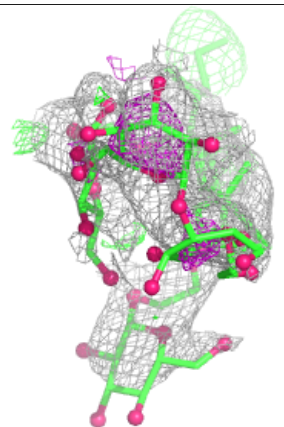
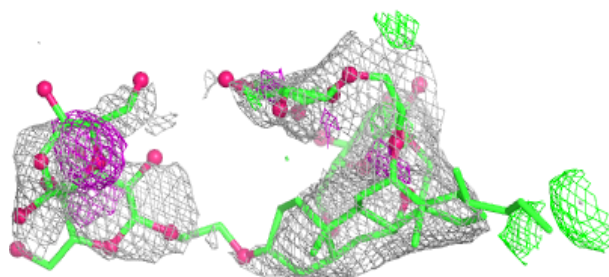
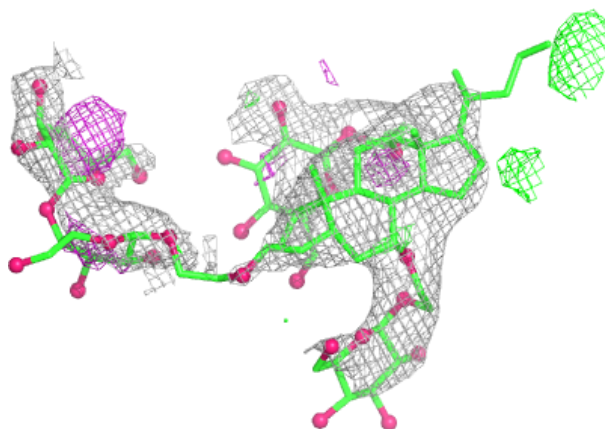
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CM5	A	601	34/34	0.90	0.12	53,92,127,127	0
2	HEM	A	500	43/43	0.98	0.09	40,48,56,66	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.

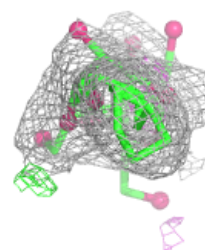
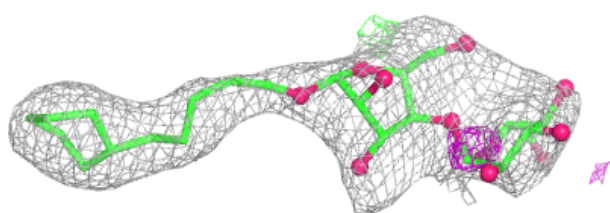
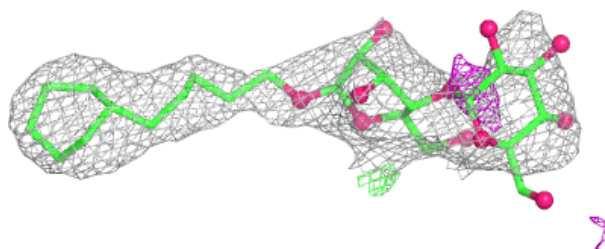
Electron density around CH0 A 603:

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

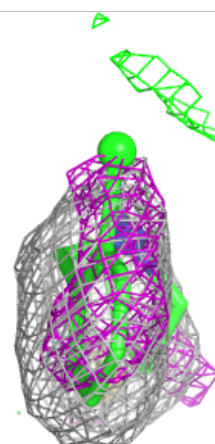
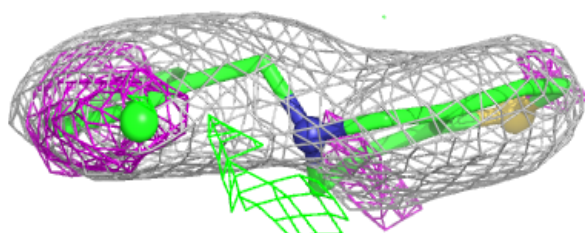
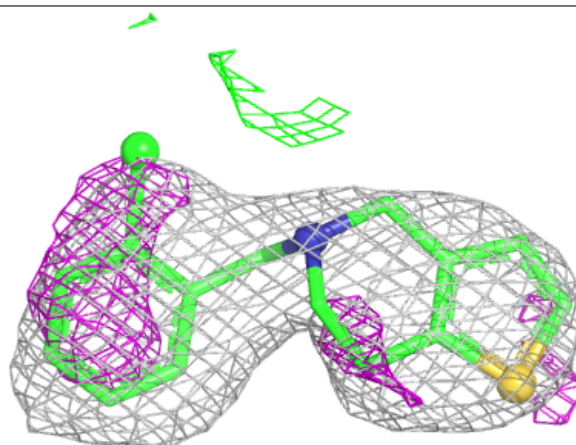


Electron density around CM5 A 602:

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

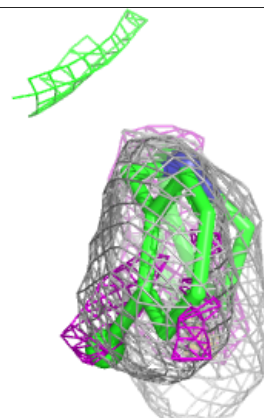
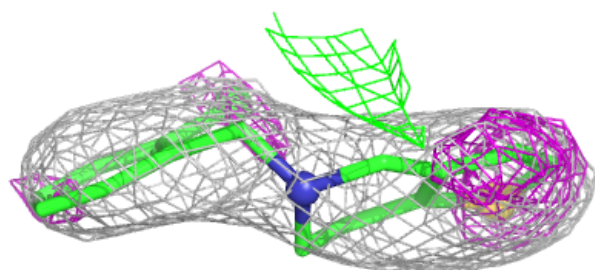
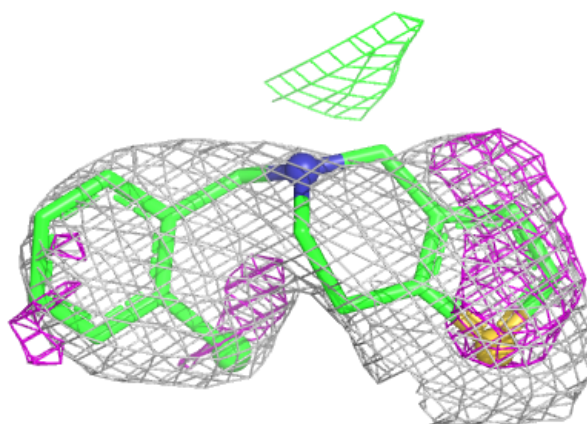
**Electron density around TIC A 600 (A):**

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

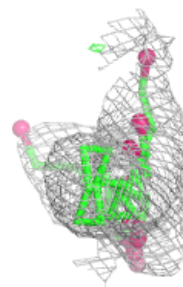
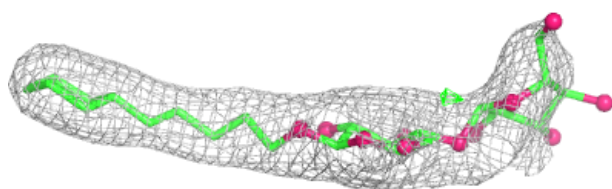
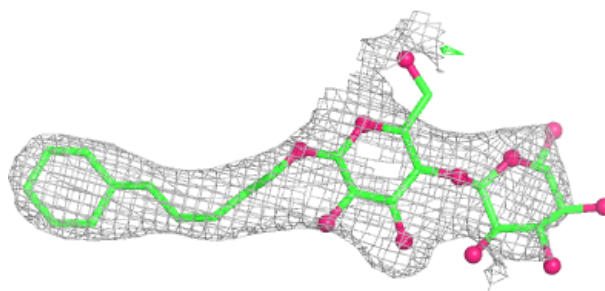


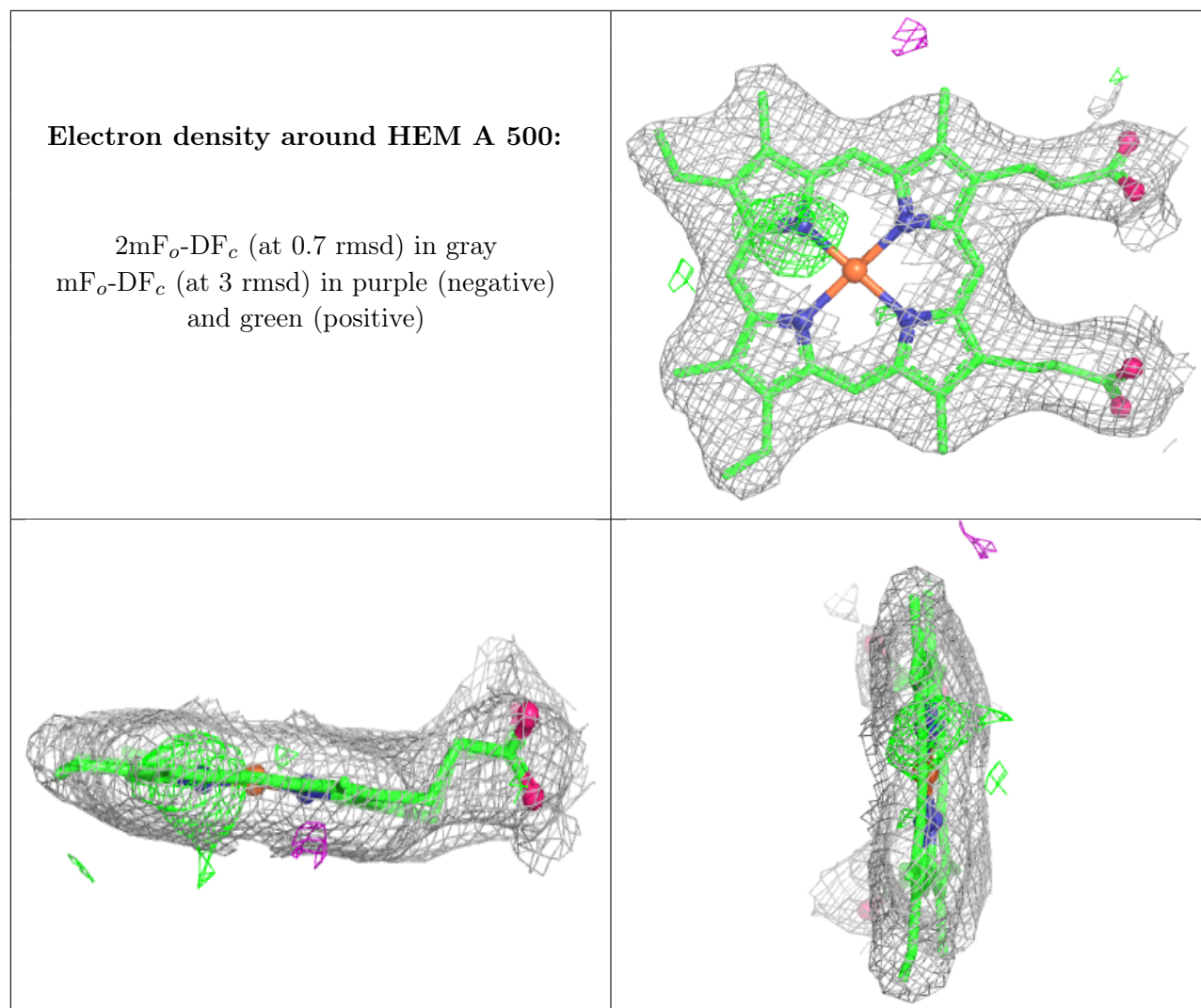
Electron density around TIC A 600 (B):

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

**Electron density around CM5 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.