



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:42 AM UTC

PDB ID : 6CSD / pdb_00006csd
Title : V308E mutant of cytochrome P450 2D6 complexed with prinomastat
Authors : Yang, Y.T.; Fujita, K.; Wang, P.F.; Im, S.C.; Pearl, N.M.; Meagher, J.;
Stuckey, J.; Waskell, L.
Deposited on : 2018-03-20
Resolution : 2.39 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

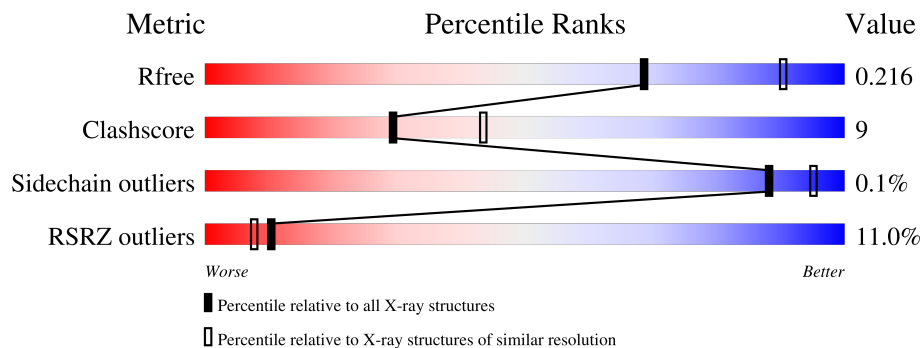
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	479	
1	B	479	

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 7727 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.

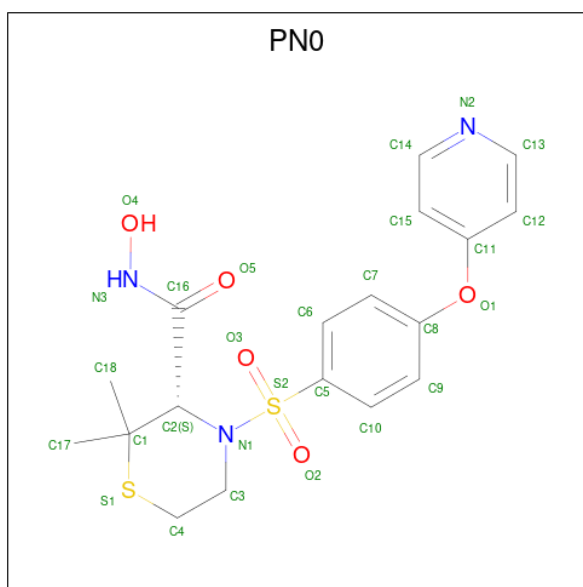
- Molecule 1 is a protein called Cytochrome P450 2D6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	462	3570	2276	637	643	14	0	3	0
1	B	454	3548	2270	627	637	14	0	3	0

There are 32 discrepancies between the modelled and reference sequences:

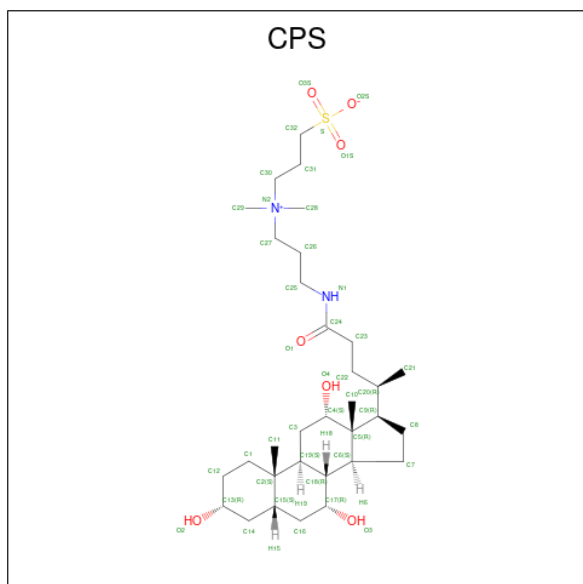
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP P10635
A	24	ALA	-	expression tag	UNP P10635
A	25	LYS	-	expression tag	UNP P10635
A	26	LYS	-	expression tag	UNP P10635
A	27	THR	-	expression tag	UNP P10635
A	28	SER	-	expression tag	UNP P10635
A	29	SER	-	expression tag	UNP P10635
A	30	LYS	-	expression tag	UNP P10635
A	31	GLY	-	expression tag	UNP P10635
A	32	LYS	-	expression tag	UNP P10635
A	33	LEU	-	expression tag	UNP P10635
A	308	GLU	VAL	engineered mutation	UNP P10635
A	498	HIS	-	expression tag	UNP P10635
A	499	HIS	-	expression tag	UNP P10635
A	500	HIS	-	expression tag	UNP P10635
A	501	HIS	-	expression tag	UNP P10635
B	23	MET	-	initiating methionine	UNP P10635
B	24	ALA	-	expression tag	UNP P10635
B	25	LYS	-	expression tag	UNP P10635
B	26	LYS	-	expression tag	UNP P10635
B	27	THR	-	expression tag	UNP P10635
B	28	SER	-	expression tag	UNP P10635
B	29	SER	-	expression tag	UNP P10635
B	30	LYS	-	expression tag	UNP P10635
B	31	GLY	-	expression tag	UNP P10635

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	28	18	3	5	2	0	0
3	B	1	28	18	3	5	2	0	0

- Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (CCD ID: CPS) (formula: C₃₂H₅₈N₂O₇S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	24	21	3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	C O	0	0
			24	21 3		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Zn	0	0
			3	3		
5	B	3	Total	Zn	0	0
			3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	226	Total	O	0	0
			226	226		
6	B	187	Total	O	0	0
			187	187		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	57.47Å 126.53Å 192.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.06 – 2.39 48.06 – 2.39	Depositor EDS
% Data completeness (in resolution range)	94.4 (48.06-2.39) 94.5 (48.06-2.39)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.198 , 0.236 (Not available) , 0.216	Depositor DCC
R_{free} test set	2628 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtrriage
Anisotropy	0.728	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7727	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.2373e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.39	0/3673	0.58	0/5005
1	B	0.36	0/3654	0.58	0/4973
All	All	0.37	0/7327	0.58	0/9978

There are no bond length outliers.

There are no bond angle outliers.

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	3570	0	3437	56	0
1	B	3548	0	3469	63	1
2	A	43	0	30	2	0
2	B	43	0	30	8	0
3	A	28	0	21	1	0
3	B	28	0	21	1	0
4	A	24	0	34	2	0
4	B	24	0	34	0	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
6	A	226	0	0	3	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	187	0	0	4	1
All	All	7727	0	7076	123	2

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 9.

All (123) 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:228:PRO:O	1:A:231:LEU:HD23	1.44	1.13
1:B:129:ARG:NH1	6:B:701:HOH:O	2.03	0.91
1:B:122:ALA:O	1:B:441:ARG:NH2	2.15	0.77
1:A:450:ARG:NH1	6:A:702:HOH:O	2.17	0.77
1:A:104:VAL:HA	1:A:225:ASN:HD21	1.50	0.76
1:A:46:LEU:HD21	1:A:74:ALA:H	1.49	0.75
1:B:474:ARG:NH1	6:B:703:HOH:O	2.20	0.75
1:A:228:PRO:C	1:A:231:LEU:HD23	2.10	0.75
1:A:117:GLN:HE22	1:A:123:ARG:HG2	1.52	0.74
1:B:150:GLU:HG2	1:B:451:MET:HE2	1.69	0.73
1:A:228:PRO:O	1:A:231:LEU:CD2	2.33	0.73
1:B:469:PRO:HB2	1:B:472:GLN:HG3	1.71	0.72
1:B:306:GLY:HA2	2:B:601:HEM:HMC2	1.73	0.71
1:B:339:ILE:HD11	1:B:349:ASP:HB3	1.72	0.70
1:A:469:PRO:HB2	1:A:472:GLN:HG3	1.75	0.68
1:A:223:VAL:HG23	1:A:224:LEU:HD12	1.74	0.68
1:B:179:ASP:CG	1:B:307:MET:HE1	2.19	0.68
1:A:424:GLN:NE2	6:A:701:HOH:O	2.02	0.66
1:B:375[A]:THR:CG2	1:B:394:THR:HG23	2.26	0.64
1:B:148:SER:OG	6:B:702:HOH:O	2.15	0.63
1:A:316:TRP:CD1	1:A:369:ILE:HD11	2.35	0.62
1:B:140:ARG:HA	1:B:144:LEU:HB3	1.83	0.60
1:B:55:PRO:HG3	1:B:481:PHE:CE1	2.37	0.60
1:B:276:LEU:HA	1:B:279:MET:HE3	1.83	0.60
1:A:46:LEU:CD2	1:A:74:ALA:H	2.15	0.59
1:B:233:ILE:HD12	1:B:236:LEU:HD22	1.83	0.59
1:A:102:PRO:HA	1:A:377:MET:HE3	1.84	0.59
1:B:51:PHE:CD1	1:B:52:GLN:HG2	2.38	0.59
1:A:96:GLU:HA	1:A:440:ARG:HH22	1.68	0.58
1:B:128:TRP:CZ3	1:B:129:ARG:HG3	2.39	0.57
1:B:436:PHE:HB3	1:B:443:CYS:HB3	1.86	0.57
1:A:96:GLU:HA	1:A:440:ARG:NH2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:GLN:O	1:B:154:THR:HG22	2.04	0.57
1:A:364:GLN:OE1	1:A:450:ARG:NH2	2.22	0.57
1:B:375[A]:THR:HG21	1:B:394:THR:HG23	1.86	0.56
1:B:151:GLN:HA	1:B:154:THR:HG22	1.88	0.56
1:B:410:GLU:HG3	6:B:853:HOH:O	2.06	0.56
1:A:303:PHE:CE1	1:A:307:MET:HE2	2.41	0.55
1:B:224:LEU:HD23	1:B:230:LEU:HD12	1.88	0.55
1:A:275:PHE:CD1	1:A:279:MET:HE2	2.42	0.55
1:A:275:PHE:HD1	1:A:279:MET:HE2	1.72	0.54
4:A:603:CPS:H21A	6:A:840:HOH:O	2.07	0.54
1:B:338:VAL:HG12	1:B:339:ILE:HD12	1.89	0.54
1:B:91:LEU:HD11	1:B:397:THR:HG21	1.90	0.53
1:A:330[B]:ARG:HB3	1:A:355:TYR:CE2	2.43	0.53
1:A:144:LEU:HA	1:A:149:LEU:HD23	1.91	0.52
1:B:369:ILE:HG13	1:B:370:VAL:HG23	1.91	0.52
1:A:224:LEU:HD12	1:A:224:LEU:N	2.24	0.52
1:B:109:ILE:CG2	1:B:245:LYS:HD2	2.40	0.52
1:A:106:ILE:HG12	1:A:241:LEU:HD11	1.91	0.51
1:B:275:PHE:HD1	1:B:279:MET:HE2	1.74	0.51
1:B:306:GLY:HA2	2:B:601:HEM:CMC	2.40	0.51
1:B:179:ASP:CB	1:B:307:MET:HE1	2.40	0.51
1:B:330[B]:ARG:HG2	1:B:355:TYR:CE2	2.45	0.51
1:A:73:LEU:HD12	4:A:603:CPS:H10B	1.93	0.51
1:B:109:ILE:HG21	1:B:245:LYS:HD2	1.93	0.50
1:A:103:PRO:HD2	1:A:377:MET:HE1	1.93	0.50
1:A:498:HIS:CE1	1:A:500:HIS:H	2.30	0.50
1:A:360:ILE:HG22	1:A:450:ARG:HH22	1.77	0.49
1:A:104:VAL:HG23	1:A:225:ASN:ND2	2.27	0.49
1:A:91:LEU:HD11	1:A:397:THR:HG21	1.94	0.49
1:A:369:ILE:HG22	1:A:370:VAL:HG23	1.95	0.49
1:A:219:PHE:O	1:A:223:VAL:HG13	2.12	0.49
1:A:443:CYS:HB2	2:A:601:HEM:NA	2.28	0.49
1:B:443:CYS:HB2	2:B:601:HEM:NA	2.27	0.49
1:B:258:HIS:HE1	1:B:270:ASP:OD1	1.96	0.48
1:B:275:PHE:CD1	1:B:279:MET:HE2	2.48	0.47
1:B:227:VAL:HG23	1:B:230:LEU:HG	1.95	0.47
1:A:276:LEU:HA	1:A:279:MET:HE3	1.96	0.47
1:B:339:ILE:HD11	1:B:349:ASP:CB	2.44	0.47
1:A:279:MET:HE1	1:A:295:LEU:HD22	1.96	0.47
1:B:227:VAL:HG23	1:B:227:VAL:O	2.15	0.46
1:A:104:VAL:HG21	1:A:221:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:HD23	1:A:47:LEU:HA	1.78	0.46
1:A:303:PHE:HE1	1:A:307:MET:HE2	1.80	0.46
1:B:364:GLN:OE1	1:B:450:ARG:NH2	2.47	0.46
1:B:437:SER:HB3	2:B:601:HEM:HBA1	1.97	0.45
1:A:229:VAL:C	1:A:231:LEU:H	2.24	0.45
1:A:171:PRO:HA	1:A:492:LEU:O	2.17	0.45
1:B:336:ASP:CG	1:B:497:ARG:HH22	2.25	0.45
1:A:221:ARG:NH1	1:A:222:GLU:OE2	2.49	0.45
1:B:71:LEU:HB3	1:B:73:LEU:HD21	1.98	0.45
1:B:251:LEU:HD21	1:B:299:VAL:HG12	1.99	0.45
1:A:470:THR:HG23	1:A:471:GLY:N	2.32	0.44
1:B:317:GLY:O	1:B:321:MET:HG2	2.17	0.44
1:B:51:PHE:CG	1:B:52:GLN:N	2.86	0.44
1:B:151:GLN:HA	1:B:154:THR:CG2	2.47	0.44
1:B:444:LEU:HD22	2:B:601:HEM:HMD3	1.98	0.44
1:A:436:PHE:HB3	1:A:443:CYS:HB3	2.00	0.44
1:A:454:PHE:O	1:A:458:THR:HG23	2.18	0.44
2:A:601:HEM:HMB1	2:A:601:HEM:HBB2	1.99	0.44
2:B:601:HEM:HMB1	2:B:601:HEM:HBB2	2.00	0.44
1:B:220:LEU:CD2	1:B:240:VAL:HA	2.48	0.43
1:A:377:MET:HG2	1:A:378:THR:N	2.33	0.43
1:B:52:GLN:OE1	1:B:481:PHE:HB3	2.18	0.43
1:B:307:MET:SD	1:B:307:MET:C	3.02	0.43
1:B:57:CYS:O	1:B:61:LEU:HG	2.18	0.43
1:A:190:THR:HA	1:A:271:LEU:HB3	2.01	0.42
1:B:72:GLN:C	1:B:73:LEU:HD23	2.45	0.42
1:B:171:PRO:HA	1:B:492:LEU:O	2.19	0.42
1:A:231:LEU:HD11	1:A:232:HIS:CE1	2.54	0.42
1:A:223:VAL:CG2	1:A:224:LEU:HD12	2.48	0.42
1:A:182:VAL:HG11	1:A:310:THR:HB	2.02	0.42
1:B:124:TYR:OH	1:B:440:ARG:NH2	2.52	0.42
1:B:369:ILE:HD11	2:B:601:HEM:HMB3	2.02	0.41
1:A:448:LEU:O	1:A:452:GLU:HG3	2.20	0.41
1:A:100:ASP:HA	1:A:124:TYR:HB2	2.03	0.41
1:B:382:ILE:HG13	1:B:389:ILE:HB	2.02	0.41
1:B:220:LEU:HD23	1:B:240:VAL:HG23	2.02	0.41
1:A:216:GLU:HA	1:A:221:ARG:HD3	2.03	0.41
1:A:483:PHE:HE2	3:A:602:PN0:O1	2.04	0.41
1:B:262:TRP:CE3	1:B:276:LEU:HD13	2.56	0.41
1:A:104:VAL:HG13	1:A:104:VAL:O	2.20	0.41
1:B:331:VAL:HG13	1:B:356:THR:OG1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:HEM:C4A	3:B:602:PN0:H13	2.55	0.41
1:B:116:SER:HA	1:B:294:ASN:CG	2.46	0.41
1:A:84:LEU:O	1:A:88[B]:ARG:HB2	2.20	0.40
1:B:51:PHE:CD1	1:B:52:GLN:CG	3.04	0.40
1:B:183:SER:OG	1:B:206:LEU:HD21	2.20	0.40
1:A:72:GLN:C	1:A:73:LEU:HD23	2.45	0.40
1:B:149:LEU:HD12	1:B:152:TRP:HB3	2.02	0.40
1:B:323:LEU:HD21	1:B:475:PRO:HD2	2.04	0.40
1:A:470:THR:CG2	1:A:471:GLY:N	2.84	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:753:HOH:O	6:A:881:HOH:O[2_885]	1.96	0.24
1:B:260:MET:O	6:B:701:HOH:O[4_475]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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	369/409 (90%)	369 (100%)	0	100	100
1	B	374/409 (91%)	373 (100%)	1 (0%)	86	93
All	All	743/818 (91%)	742 (100%)	1 (0%)	88	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	444	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	167	HIS
1	A	472	GLN
1	B	60	GLN
1	B	166	ASN
1	B	210	GLN
1	B	250	GLN
1	B	350	GLN

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](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	CPS	B	603	-	26,27,45	0.21	0	42,44,70	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	601	3,1	50,50,50	1.60	10 (20%)	67,82,82	1.31	11 (16%)
4	CPS	A	603	-	26,27,45	0.42	0	42,44,70	0.84	1 (2%)
3	PN0	A	602	2	28,30,30	0.21	0	37,44,44	0.43	0
3	PN0	B	602	2	28,30,30	0.26	0	37,44,44	0.47	0
2	HEM	B	601	3,1	50,50,50	1.40	6 (12%)	67,82,82	1.24	6 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CPS	B	603	-	-	0/2/67/90	0/4/4/4
2	HEM	A	601	3,1	-	4/14/54/54	-
4	CPS	A	603	-	-	2/2/67/90	0/4/4/4
3	PN0	A	602	2	-	3/21/39/39	0/3/3/3
3	PN0	B	602	2	-	5/21/39/39	0/3/3/3
2	HEM	B	601	3,1	-	2/14/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	FE-ND	4.75	2.09	1.94
2	A	601	HEM	FE-NB	4.10	2.07	1.94
2	B	601	HEM	FE-ND	3.52	2.05	1.94
2	A	601	HEM	CAB-C3B	3.12	1.55	1.47
2	B	601	HEM	CAB-C3B	3.03	1.55	1.47
2	A	601	HEM	CAC-C3C	2.95	1.55	1.47
2	A	601	HEM	CMB-C2B	2.91	1.56	1.50
2	A	601	HEM	CMA-C3A	2.86	1.56	1.50
2	B	601	HEM	CAC-C3C	2.81	1.54	1.47
2	A	601	HEM	FE-NA	2.77	2.04	1.95
2	B	601	HEM	FE-NB	2.71	2.03	1.94
2	A	601	HEM	CMD-C2D	2.23	1.55	1.50
2	A	601	HEM	CMC-C2C	2.22	1.55	1.50
2	B	601	HEM	CMD-C2D	2.18	1.55	1.50
2	A	601	HEM	FE-NC	2.16	2.02	1.95
2	B	601	HEM	CMA-C3A	2.12	1.55	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	C1B-NB-C4B	3.28	109.09	105.21
2	A	601	HEM	CHC-C4B-NB	2.80	127.44	124.42
2	A	601	HEM	C4D-ND-C1D	2.77	108.49	105.21
2	A	601	HEM	CAA-CBA-CGA	-2.74	106.39	113.67
2	A	601	HEM	C3D-C4D-ND	-2.59	107.33	110.17
4	A	603	CPS	C3-C19-C18	2.52	114.63	110.89
2	A	601	HEM	C2A-C1A-NA	-2.45	107.43	110.15
2	B	601	HEM	CHC-C4B-NB	2.39	127.00	124.42
2	B	601	HEM	C3B-C2B-C1B	2.29	108.13	106.41
2	A	601	HEM	C2B-C1B-NB	-2.12	107.40	109.84
2	B	601	HEM	CHC-C1C-NC	2.12	126.76	124.45
2	A	601	HEM	CHD-C4C-NC	2.10	126.75	124.45
2	B	601	HEM	CAA-C2A-C1A	2.10	129.04	124.94
2	A	601	HEM	C3B-C4B-NB	-2.08	107.97	109.47
2	A	601	HEM	C4A-NA-C1A	2.05	109.17	105.82
2	A	601	HEM	CBD-CAD-C3D	-2.05	106.88	112.53
2	B	601	HEM	C1B-NB-C4B	2.04	107.63	105.21
2	B	601	HEM	C2A-C1A-NA	-2.02	107.91	110.15

There are no chirality outliers.

All (16) torsion outliers are listed below:

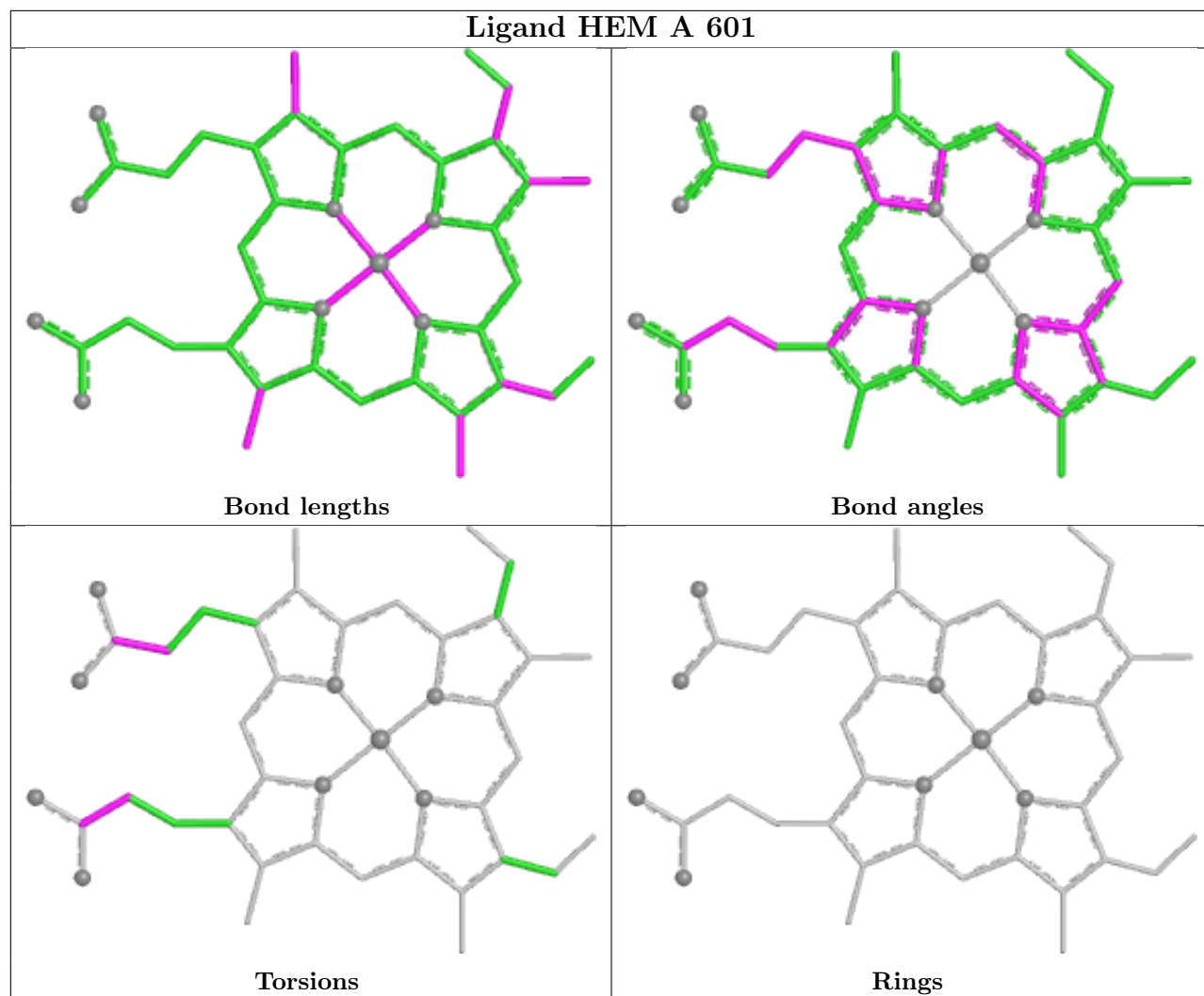
Mol	Chain	Res	Type	Atoms
4	A	603	CPS	C21-C20-C9-C8
3	A	602	PN0	N3-C16-C2-N1
3	B	602	PN0	N3-C16-C2-N1
3	A	602	PN0	O5-C16-C2-N1
3	B	602	PN0	O5-C16-C2-N1
4	A	603	CPS	C21-C20-C9-C5
3	B	602	PN0	C10-C5-S2-O2
2	A	601	HEM	CAA-CBA-CGA-O2A
2	A	601	HEM	CAA-CBA-CGA-O1A
2	B	601	HEM	CAA-CBA-CGA-O2A
2	B	601	HEM	CAA-CBA-CGA-O1A
3	B	602	PN0	C6-C5-S2-O2
2	A	601	HEM	CAD-CBD-CGD-O2D
3	A	602	PN0	C10-C5-S2-O2
2	A	601	HEM	CAD-CBD-CGD-O1D
3	B	602	PN0	C10-C5-S2-N1

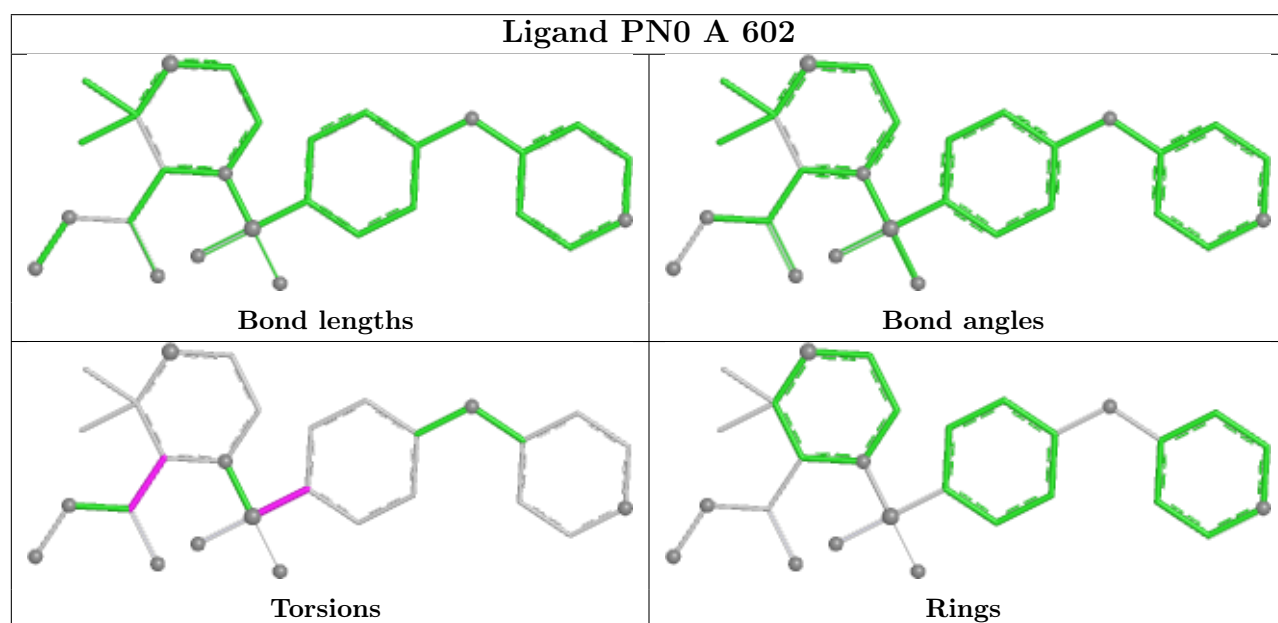
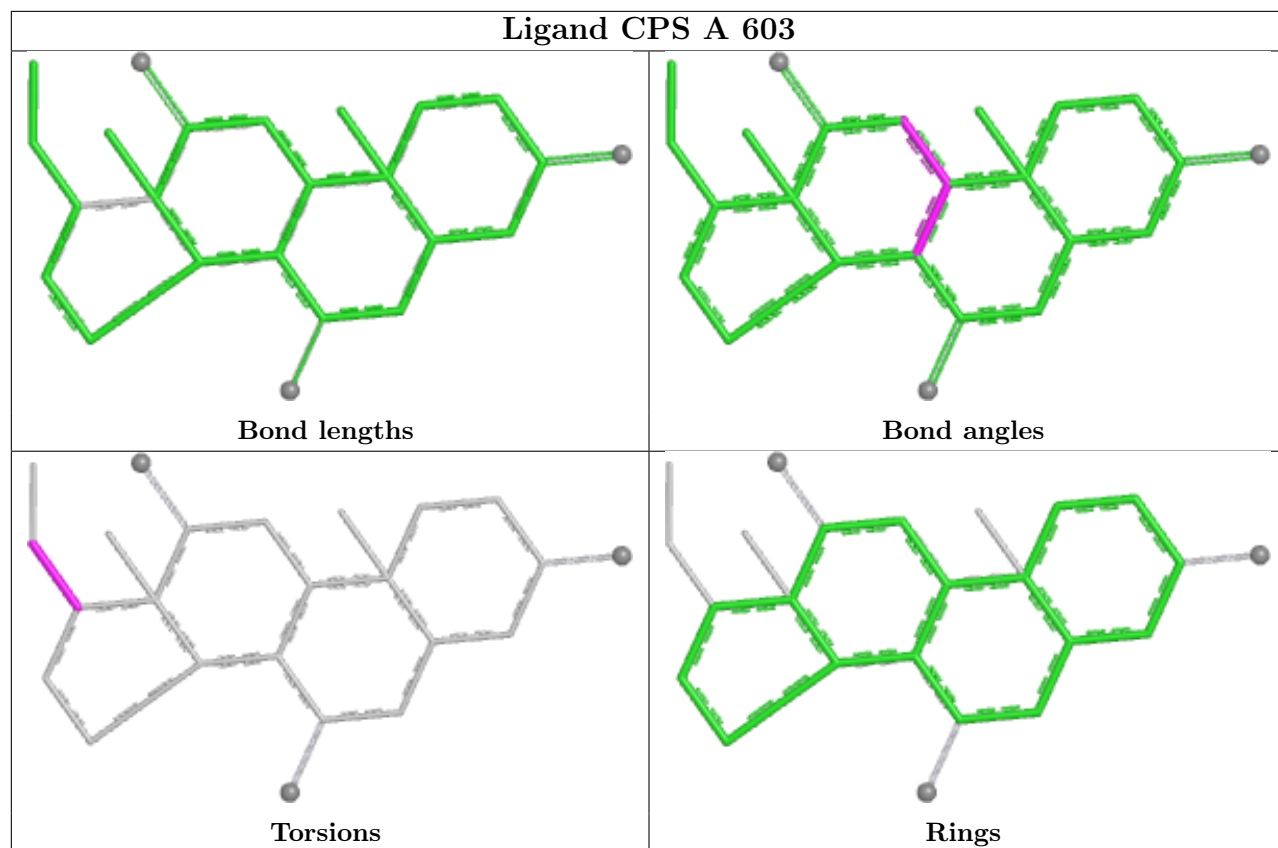
There are no ring outliers.

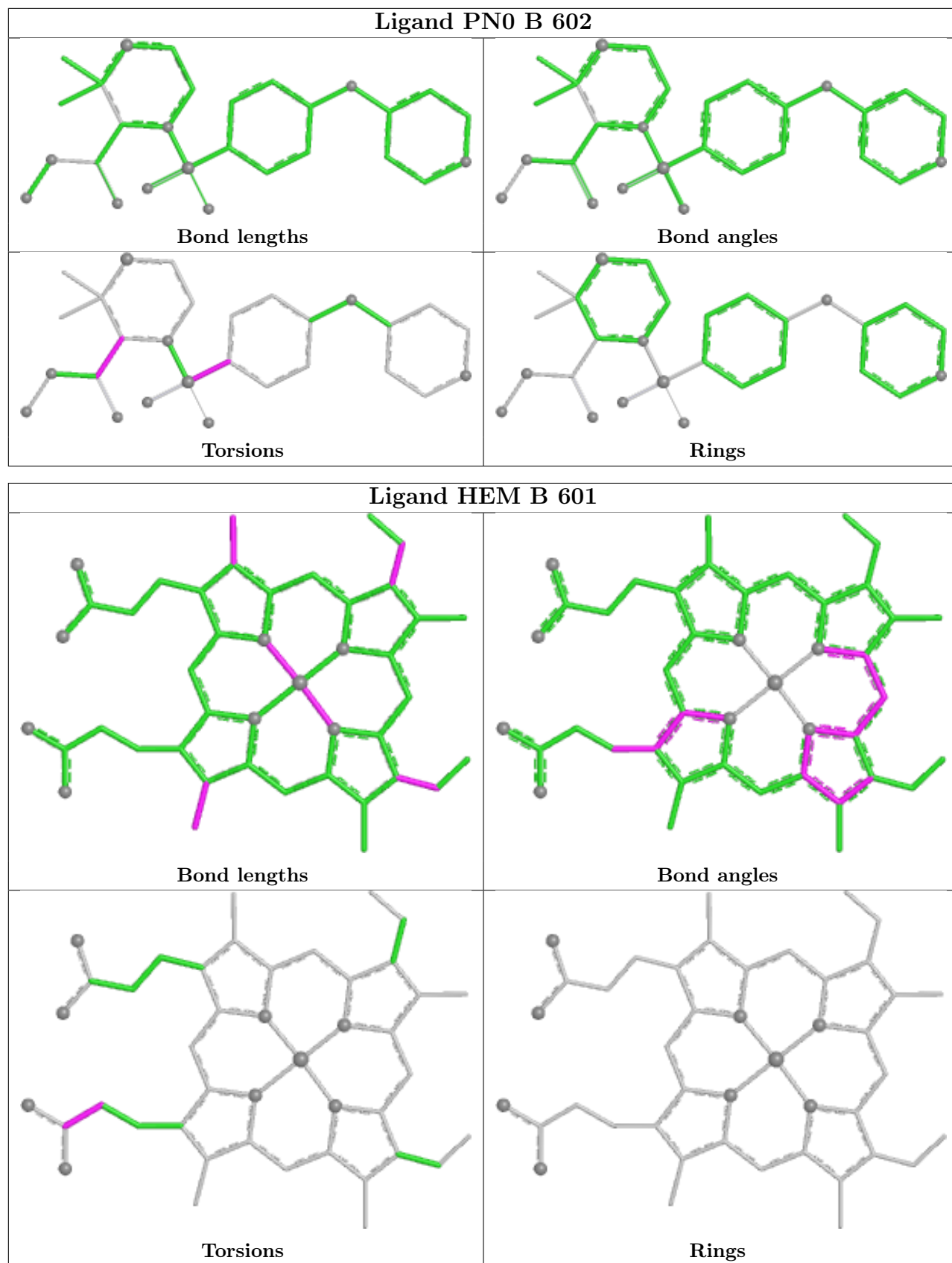
5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	2	0
4	A	603	CPS	2	0
3	A	602	PN0	1	0
3	B	602	PN0	1	0
2	B	601	HEM	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

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	462/479 (96%)	0.57	48 (10%) 11 9	20, 40, 85, 109	3 (0%)
1	B	454/479 (94%)	0.73	53 (11%) 9 7	18, 44, 79, 94	3 (0%)
All	All	916/958 (95%)	0.65	101 (11%) 10 8	18, 42, 80, 109	6 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	145	GLY	5.4
1	A	229	VAL	5.1
1	A	228	PRO	4.9
1	B	144	LEU	4.7
1	A	219	PHE	4.2
1	A	231	LEU	4.2
1	A	46	LEU	4.1
1	A	498	HIS	4.1
1	B	147	LYS	4.1
1	A	230	LEU	4.1
1	B	75	TRP	4.1
1	B	51	PHE	3.9
1	A	236	LEU	3.8
1	A	235	ALA	3.7
1	B	74	ALA	3.7
1	B	481	PHE	3.7
1	B	330[A]	ARG	3.7
1	A	330[A]	ARG	3.5
1	A	48	HIS	3.5
1	A	47	LEU	3.5
1	A	233	ILE	3.5
1	A	45	ASN	3.5
1	B	33	LEU	3.5
1	A	146	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	218	GLY	3.4
1	B	32	LYS	3.4
1	A	226	ALA	3.4
1	B	31	GLY	3.4
1	B	37	PRO	3.3
1	B	146	LYS	3.3
1	B	152	TRP	3.3
1	A	251	LEU	3.2
1	B	166	ASN	3.2
1	B	307	MET	3.2
1	B	202	PHE	3.2
1	B	240	VAL	3.1
1	B	470	THR	3.1
1	B	53	ASN	3.1
1	B	110	LEU	3.1
1	A	88[A]	ARG	3.0
1	A	74	ALA	3.0
1	A	49	VAL	3.0
1	B	477[A]	HIS	2.9
1	A	232	HIS	2.9
1	A	240	VAL	2.9
1	A	470	THR	2.9
1	B	143	GLY	2.8
1	A	481	PHE	2.8
1	A	500	HIS	2.8
1	B	56	TYR	2.8
1	A	51	PHE	2.8
1	B	482	ALA	2.8
1	B	339	ILE	2.7
1	A	224	LEU	2.7
1	A	220	LEU	2.7
1	A	482	ALA	2.6
1	A	234	PRO	2.6
1	A	144	LEU	2.6
1	A	145	GLY	2.6
1	B	71	LEU	2.6
1	B	383	GLU	2.6
1	B	464	PHE	2.6
1	B	480	VAL	2.6
1	A	307	MET	2.6
1	B	236	LEU	2.5
1	B	52	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	243	PHE	2.4
1	B	241	LEU	2.4
1	B	242	ARG	2.4
1	A	75	TRP	2.4
1	B	458	THR	2.3
1	B	129	ARG	2.3
1	A	499	HIS	2.3
1	B	106	ILE	2.3
1	B	227	VAL	2.3
1	B	150	GLU	2.3
1	A	32	LYS	2.3
1	B	63	ARG	2.2
1	A	56	TYR	2.2
1	A	84	LEU	2.2
1	B	65	PHE	2.2
1	A	337	ASP	2.2
1	A	469	PRO	2.2
1	B	337	ASP	2.2
1	A	217	SER	2.2
1	B	226	ALA	2.2
1	A	339	ILE	2.1
1	A	222	GLU	2.1
1	B	114	PRO	2.1
1	B	426	HIS	2.1
1	A	114	PRO	2.1
1	B	55	PRO	2.1
1	B	380	ARG	2.1
1	B	116	SER	2.1
1	B	148	SER	2.1
1	A	237	ALA	2.1
1	B	494	ALA	2.1
1	B	230	LEU	2.1
1	A	59	ASP	2.1
1	B	382	ILE	2.1
1	A	382	ILE	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

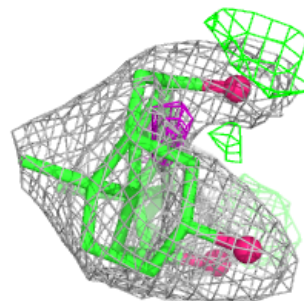
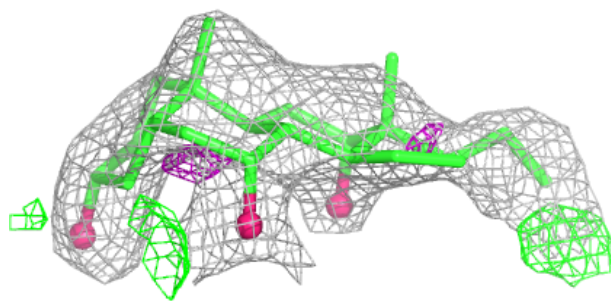
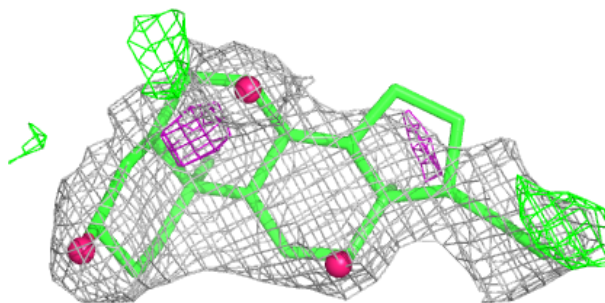
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CPS	A	603	24/42	0.74	0.20	49,69,77,79	0
5	ZN	B	605	1/1	0.85	0.17	120,120,120,120	0
4	CPS	B	603	24/42	0.89	0.12	43,53,64,66	0
5	ZN	B	606	1/1	0.91	0.52	103,103,103,103	0
5	ZN	A	605	1/1	0.92	0.09	77,77,77,77	0
3	PN0	B	602	28/28	0.96	0.08	27,42,52,57	0
3	PN0	A	602	28/28	0.96	0.07	22,39,48,51	0
2	HEM	B	601	43/43	0.98	0.07	22,28,32,34	0
2	HEM	A	601	43/43	0.98	0.07	17,25,30,33	0
5	ZN	A	606	1/1	0.99	0.08	42,42,42,42	1
5	ZN	A	604	1/1	1.00	0.01	29,29,29,29	0
5	ZN	B	604	1/1	1.00	0.05	31,31,31,31	0

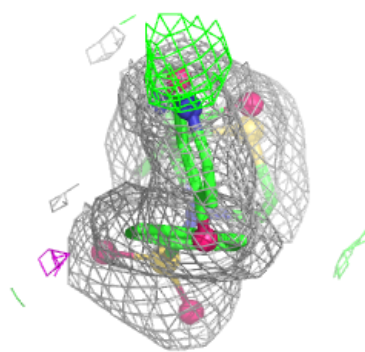
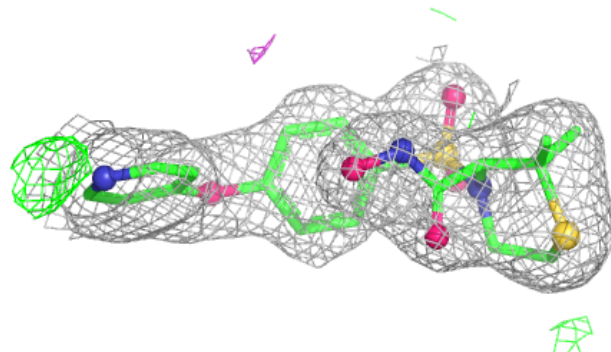
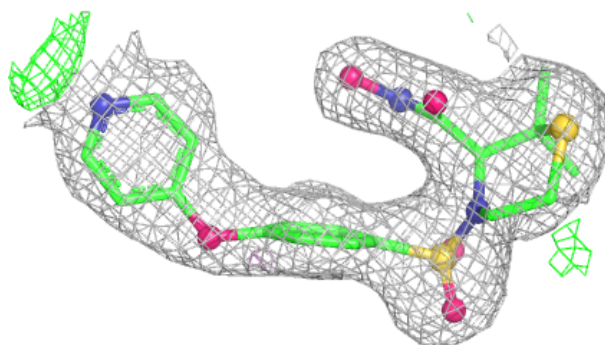
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CPS 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)

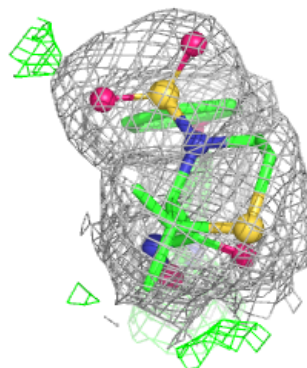
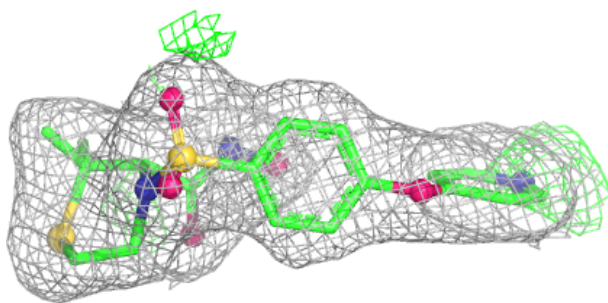
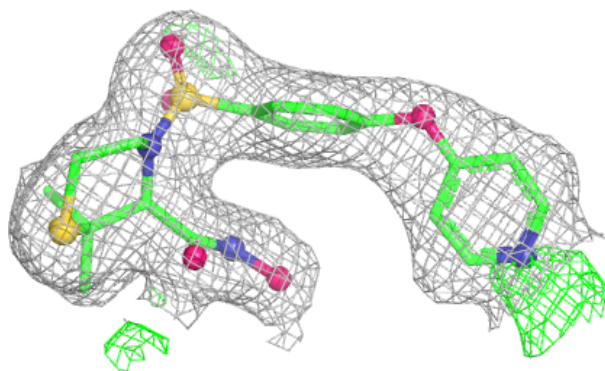
**Electron density around PN0 B 602:**

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



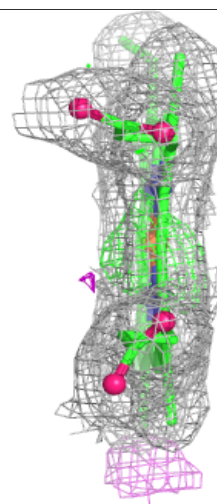
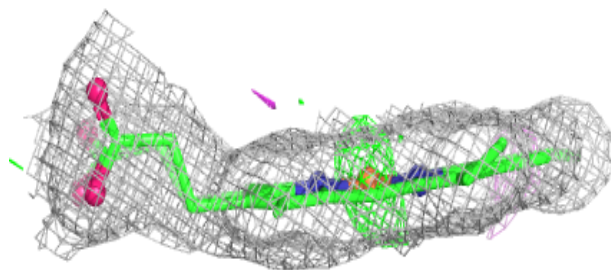
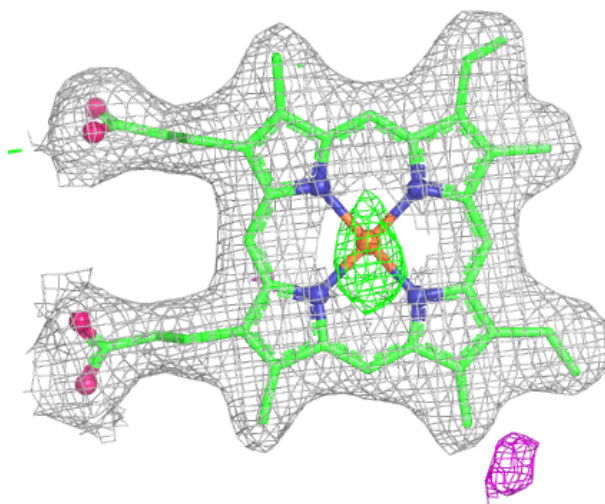
Electron density around PN0 A 602:

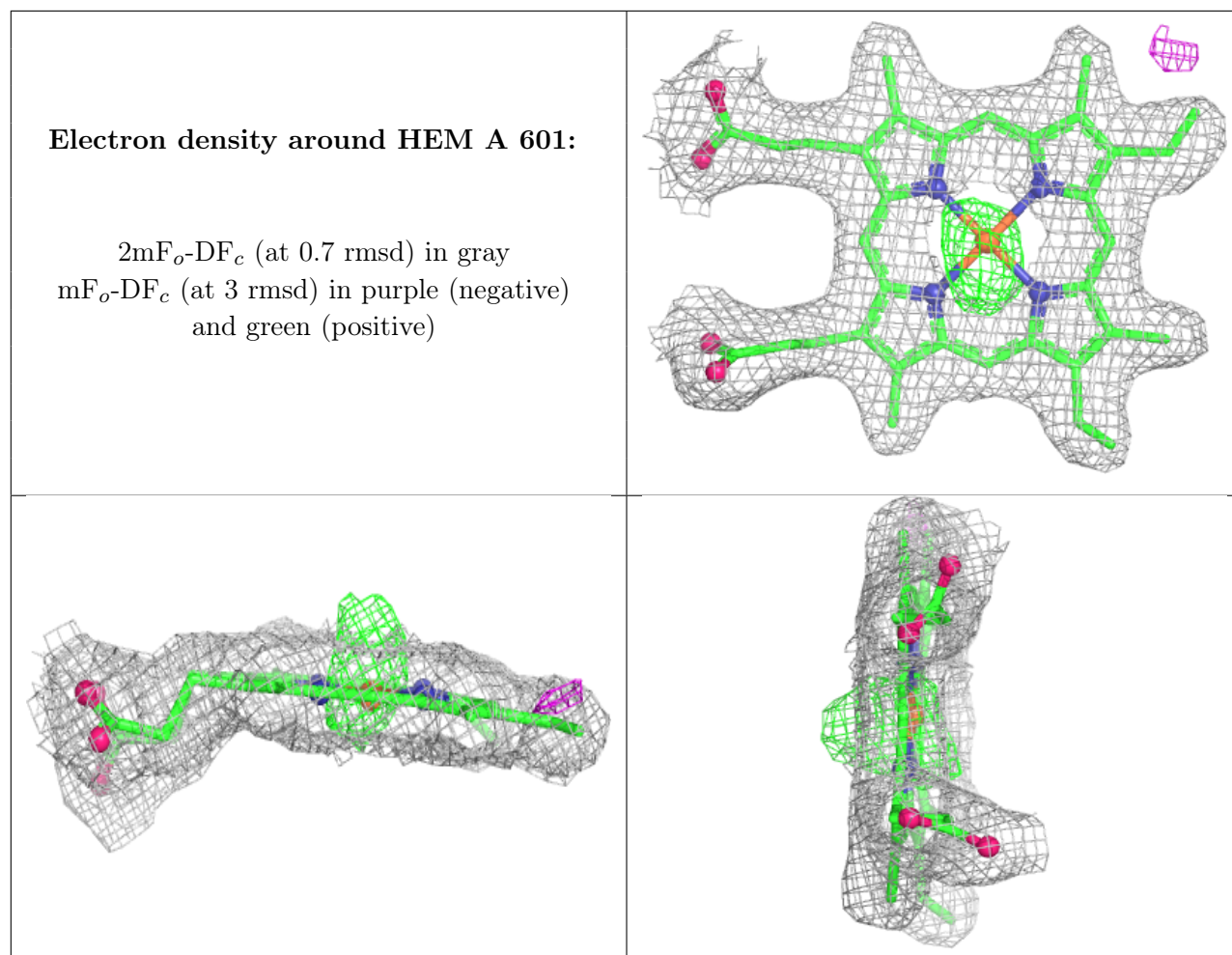
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 601:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.