Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 07:41 PM EDT

PDB ID	:	6CSD
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:

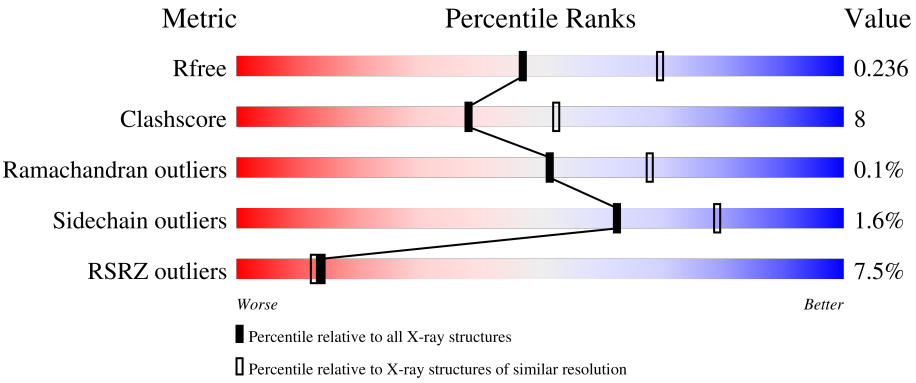
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	7% 82% 14%
1	B	479	8% 78% 15% 5%

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
1	A	462	Total	C	N	O	S	0	3	0
			3570	2276	637	643	14			
1	B	454	Total	C	N	O	S	0	3	0
			3548	2270	627	637	14			

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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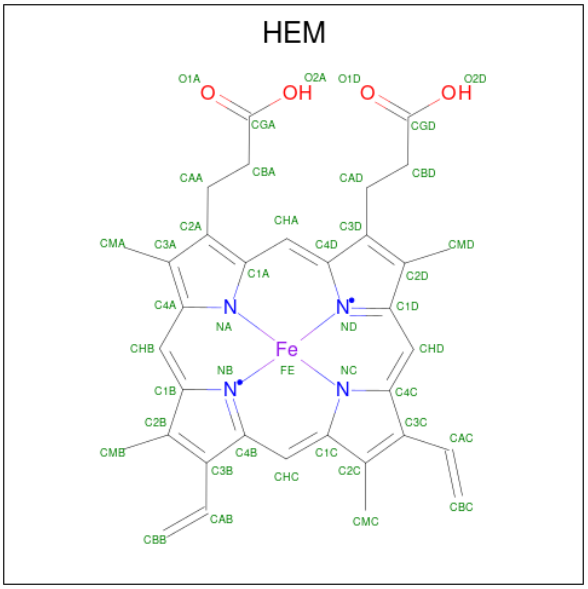
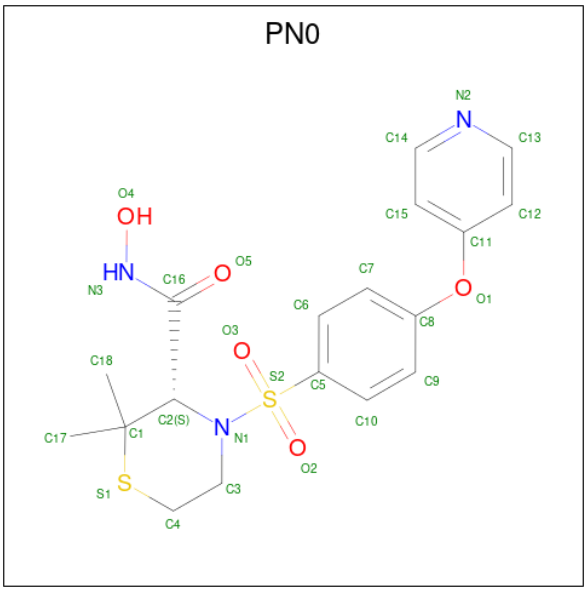
Chain	Residue	Modelled	Actual	Comment	Reference
B	32	LYS	-	expression tag	UNP P10635
B	33	LEU	-	expression tag	UNP P10635
B	308	GLU	VAL	engineered mutation	UNP P10635
B	498	HIS	-	expression tag	UNP P10635
B	499	HIS	-	expression tag	UNP P10635
B	500	HIS	-	expression tag	UNP P10635
B	501	HIS	-	expression tag	UNP P10635

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



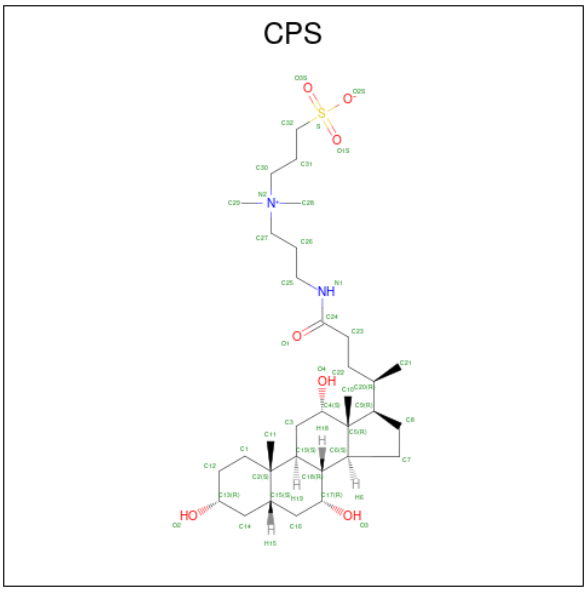
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is Prinomastat (three-letter code: PN0) (formula: $C_{18}H_{21}N_3O_5S_2$).



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

- Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).



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

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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is water.

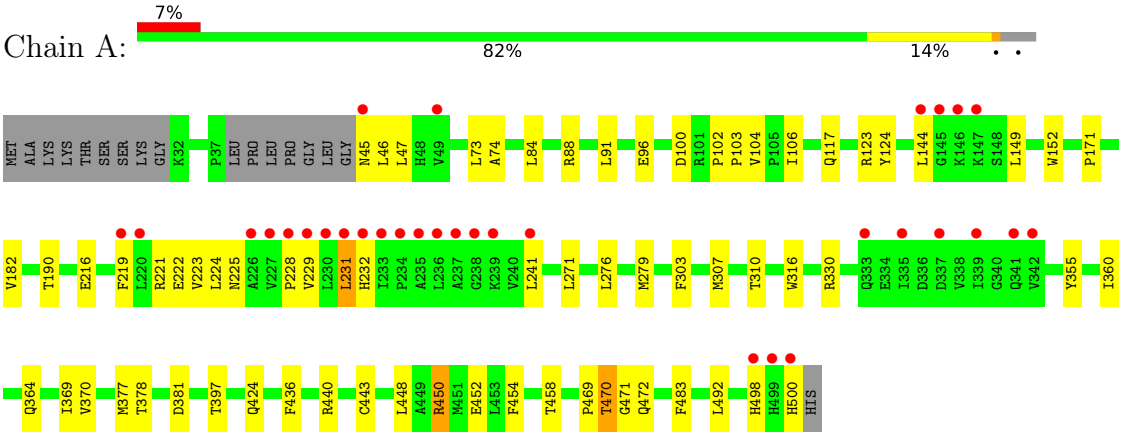
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	226	Total O 226 226	0	0
6	B	187	Total O 187 187	0	0

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.

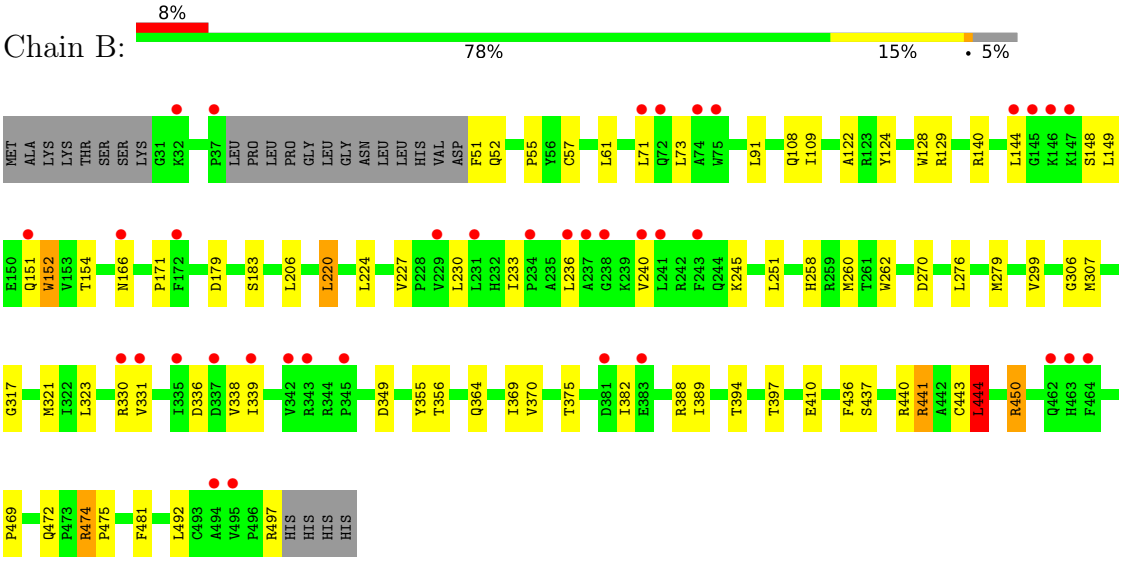
• Molecule 1: Cytochrome P450 2D6

Chain A:



• Molecule 1: Cytochrome P450 2D6

Chain B:



4 Data and refinement statistics (i)

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) 94.6 (48.06-2.39)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.198 , 0.236 0.200 , 0.236	Depositor DCC
R_{free} test set	2628 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.728	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PN0, ZN, CPS, 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	0.42	0/3673	0.60	1/5005 (0.0%)
1	B	0.40	0/3654	0.58	2/4973 (0.0%)
All	All	0.41	0/7327	0.59	3/9978 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	231	LEU	CB-CG-CD2	7.46	123.69	111.00
1	B	441	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	444	LEU	CA-CB-CG	5.51	127.97	115.30

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	51	0
1	B	3548	0	3469	55	1
2	A	43	0	30	2	0
2	B	43	0	30	7	0
3	A	28	0	21	1	0
3	B	28	0	21	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
6	B	187	0	0	4	1
All	All	7727	0	7076	110	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 8.

All (110) 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:A:276:LEU:HD23	1:A:279:MET:HE3	1.67	0.75
1:B:474:ARG:NH1	6:B:703:HOH:O	2.20	0.75
1:A:117:GLN:HE22	1:A:123:ARG:HG2	1.52	0.74
1:B:276:LEU:HD23	1:B:279:MET:HE3	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:228:PRO:C	1:A:231:LEU:HD23	2.10	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PRO:HA	1:A:377:MET:HE3	1.85	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
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:B:224:LEU:HD23	1:B:230:LEU:HD12	1.88	0.55
2:B:601:HEM:HBB2	2:B:601:HEM:HMB2	1.89	0.55
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:306:GLY:HA2	2:B:601:HEM:CMC	2.40	0.51
1:B:330[B]:ARG:HG2	1:B:355:TYR:CE2	2.45	0.51
1:A:103:PRO:HD2	1:A:377:MET:HE1	1.92	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: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:227:VAL:HG23	1:B:230:LEU:HG	1.95	0.47
1:B:339:ILE:HD11	1:B:349:ASP:CB	2.44	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
1:A:47:LEU:HD23	1:A:47:LEU:HA	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:PRO:HA	1:A:492:LEU:O	2.17	0.45
1:A:303:PHE:CE1	1:A:307:MET:HE2	2.52	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
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: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: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: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
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	2.01	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
2:B:601:HEM:C4A	3:B:602:PN0:H13	2.55	0.41
1:B:179:ASP:HB3	1:B:307:MET:HE2	2.03	0.41
1:A:84:LEU:O	1:A:88[B]:ARG:HB2	2.20	0.40
1:A:229:VAL:C	1:A:231:LEU:H	2.24	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:B:336:ASP:CG	1:B:497:ARG:HH22	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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)

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	461/479 (96%)	443 (96%)	17 (4%)	1 (0%)	47 62
1	B	454/479 (95%)	447 (98%)	7 (2%)	0	100 100
All	All	915/958 (96%)	890 (97%)	24 (3%)	1 (0%)	51 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	470	THR

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%)	365 (99%)	4 (1%)	73 87
1	B	374/409 (91%)	366 (98%)	8 (2%)	53 72
All	All	743/818 (91%)	731 (98%)	12 (2%)	62 79

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	152	TRP
1	A	381	ASP
1	A	450	ARG
1	B	108	GLN
1	B	152	TRP
1	B	166	ASN
1	B	220	LEU
1	B	388	ARG
1	B	444	LEU
1	B	450	ARG
1	B	474	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	472	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 monosaccharides 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	$\#\|Z\| > 2$
3	PN0	B	602	2	28,30,30	0.29	0	36,44,44	0.48	0
4	CPS	A	603	-	26,27,45	0.41	0	41,44,70	0.82	1 (2%)
4	CPS	B	603	-	26,27,45	0.21	0	41,44,70	0.47	0
2	HEM	A	601	3,1	41,50,50	1.59	8 (19%)	45,82,82	1.57	10 (22%)
3	PN0	A	602	2	28,30,30	0.22	0	36,44,44	0.44	0
2	HEM	B	601	3,1	41,50,50	1.54	6 (14%)	45,82,82	1.39	6 (13%)

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	PN0	B	602	2	-	5/21/39/39	0/3/3/3
4	CPS	A	603	-	-	2/2/67/90	0/4/4/4
4	CPS	B	603	-	-	0/2/67/90	0/4/4/4
2	HEM	A	601	3,1	-	4/12/54/54	-
3	PN0	A	602	2	-	3/21/39/39	0/3/3/3
2	HEM	B	601	3,1	-	2/12/54/54	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	C3C-C2C	-4.19	1.34	1.40
2	A	601	HEM	C3C-CAC	3.63	1.55	1.47
2	B	601	HEM	C3C-CAC	3.45	1.54	1.47
2	A	601	HEM	C3C-C2C	-3.42	1.35	1.40
2	A	601	HEM	CAB-C3B	3.04	1.55	1.47
2	B	601	HEM	CAB-C3B	2.96	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	CMB-C2B	2.81	1.56	1.50
2	B	601	HEM	CAA-C2A	2.61	1.55	1.52
2	A	601	HEM	FE-ND	2.56	2.09	1.96
2	A	601	HEM	CMA-C3A	2.40	1.56	1.51
2	A	601	HEM	FE-NB	2.15	2.07	1.96
2	A	601	HEM	CMD-C2D	2.15	1.55	1.50
2	B	601	HEM	CMD-C2D	2.10	1.55	1.50
2	B	601	HEM	C1B-NB	-2.00	1.36	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	HEM	C4B-CHC-C1C	3.95	127.77	122.56
2	A	601	HEM	C1B-NB-C4B	3.89	109.09	105.07
2	A	601	HEM	C4D-ND-C1D	3.31	108.49	105.07
2	A	601	HEM	C4C-CHD-C1D	3.05	126.58	122.56
2	A	601	HEM	CHC-C4B-NB	2.77	127.44	124.43
2	A	601	HEM	CAA-CBA-CGA	-2.63	106.39	113.76
2	A	601	HEM	CMC-C2C-C3C	2.57	129.48	124.68
4	A	603	CPS	C3-C19-C18	2.56	114.63	110.88
2	A	601	HEM	C4B-CHC-C1C	2.55	125.93	122.56
2	A	601	HEM	C3D-C4D-ND	-2.54	107.33	110.17
2	B	601	HEM	C1B-NB-C4B	2.47	107.63	105.07
2	B	601	HEM	CHC-C4B-NB	2.36	127.00	124.43
2	B	601	HEM	C3B-C2B-C1B	2.22	108.13	106.49
2	B	601	HEM	C4D-ND-C1D	2.19	107.33	105.07
2	B	601	HEM	CMC-C2C-C3C	2.16	128.71	124.68
2	A	601	HEM	CBD-CAD-C3D	-2.07	106.88	112.63
2	A	601	HEM	C2B-C1B-NB	-2.06	107.40	109.84

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-O1A

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Mol	Chain	Res	Type	Atoms
2	A	601	HEM	CAA-CBA-CGA-O2A
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	B	602	PN0	C10-C5-S2-N1
2	A	601	HEM	CAD-CBD-CGD-O1D
3	A	602	PN0	C10-C5-S2-O2

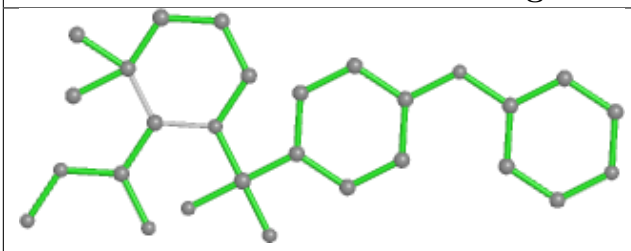
There are no ring outliers.

5 monomers are involved in 12 short contacts:

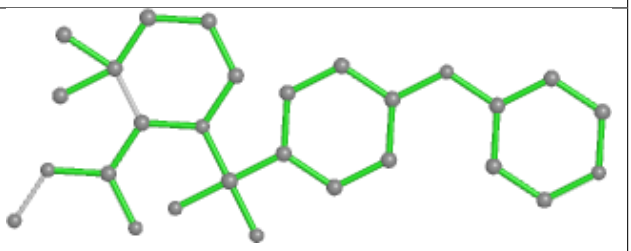
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	PN0	1	0
4	A	603	CPS	2	0
2	A	601	HEM	2	0
3	A	602	PN0	1	0
2	B	601	HEM	7	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

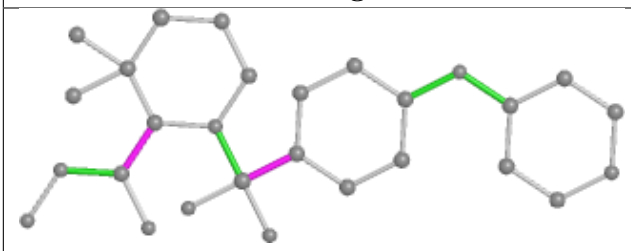
Ligand PN0 B 602



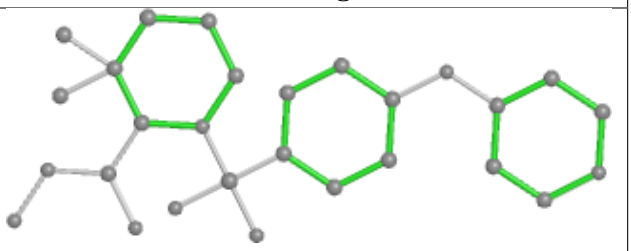
Bond lengths



Bond angles

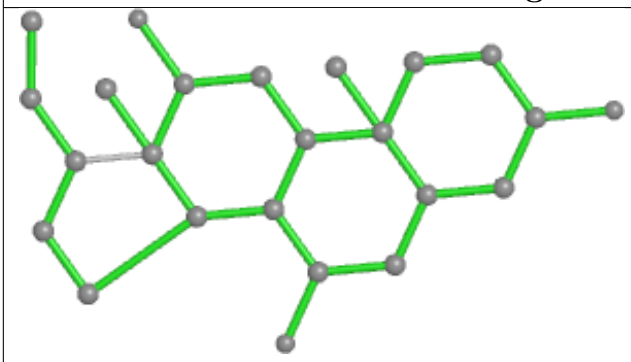


Torsions

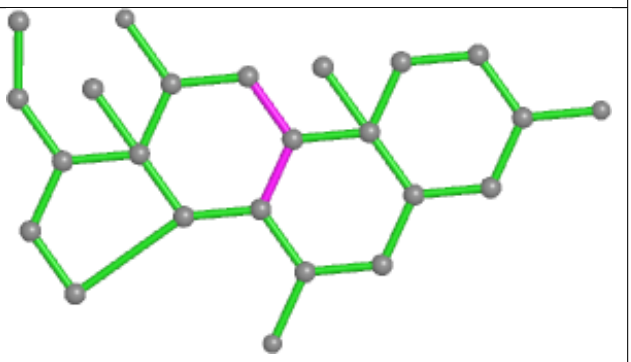


Rings

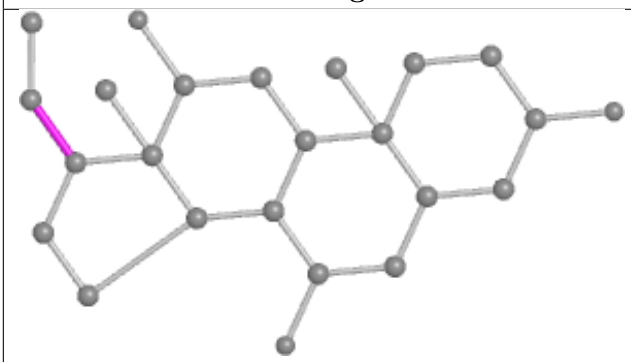
Ligand CPS A 603



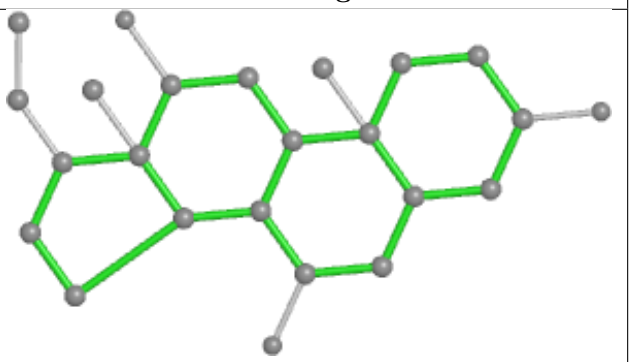
Bond lengths



Bond angles

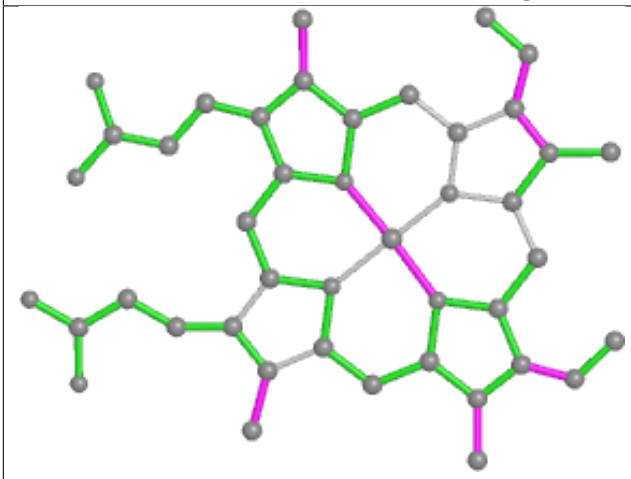


Torsions

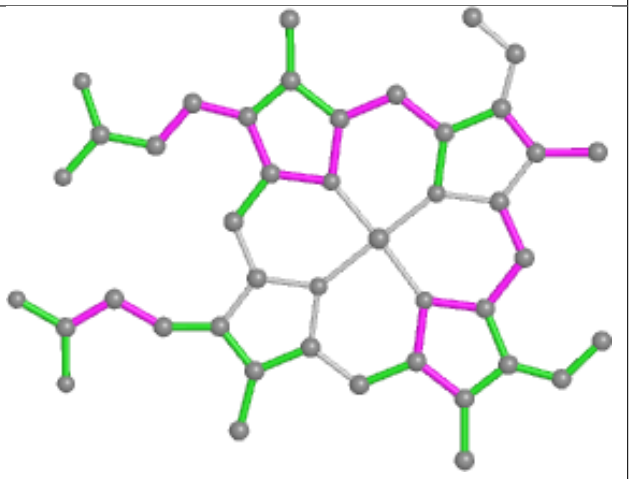


Rings

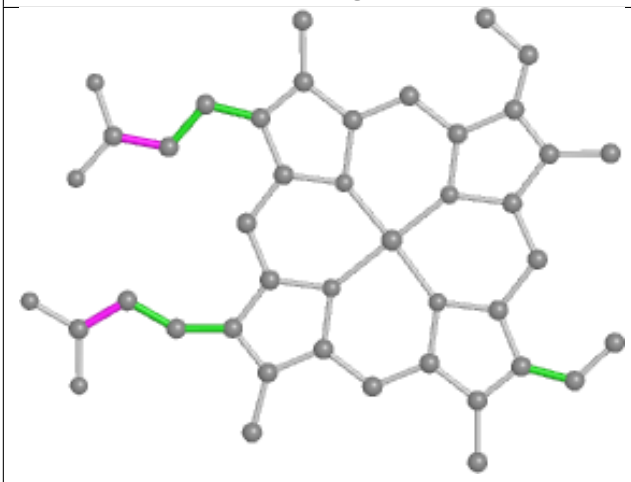
Ligand HEM A 601



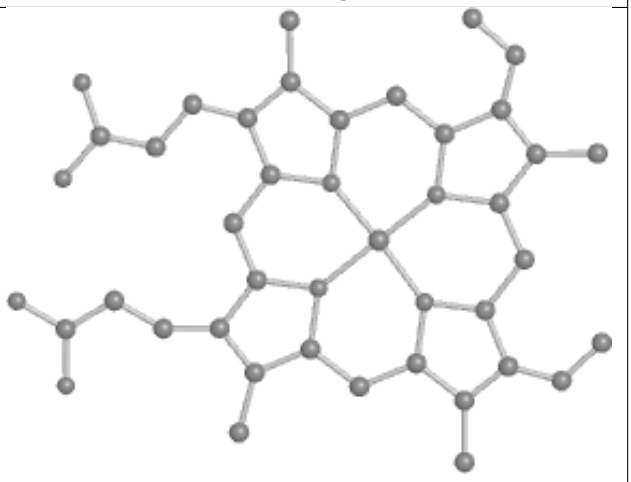
Bond lengths



Bond angles

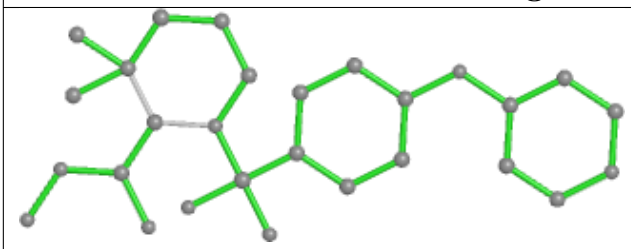


Torsions

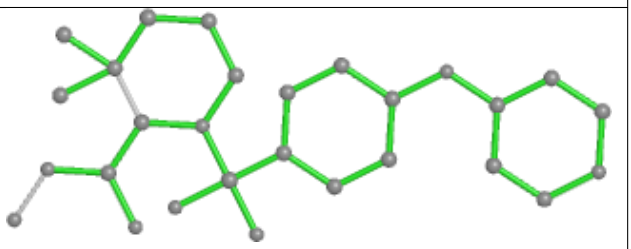


Rings

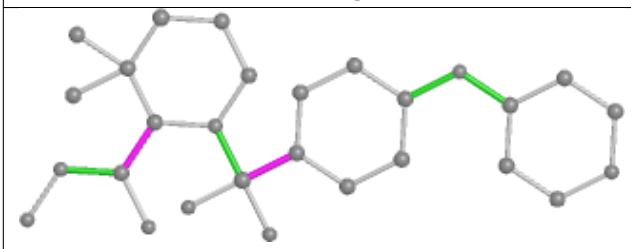
Ligand PN0 A 602



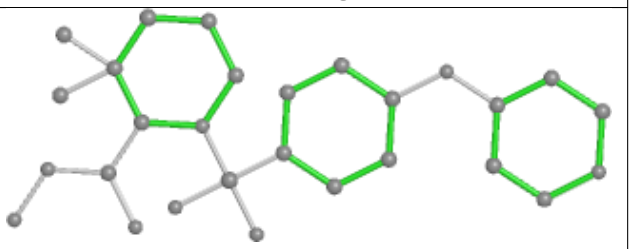
Bond lengths



Bond angles

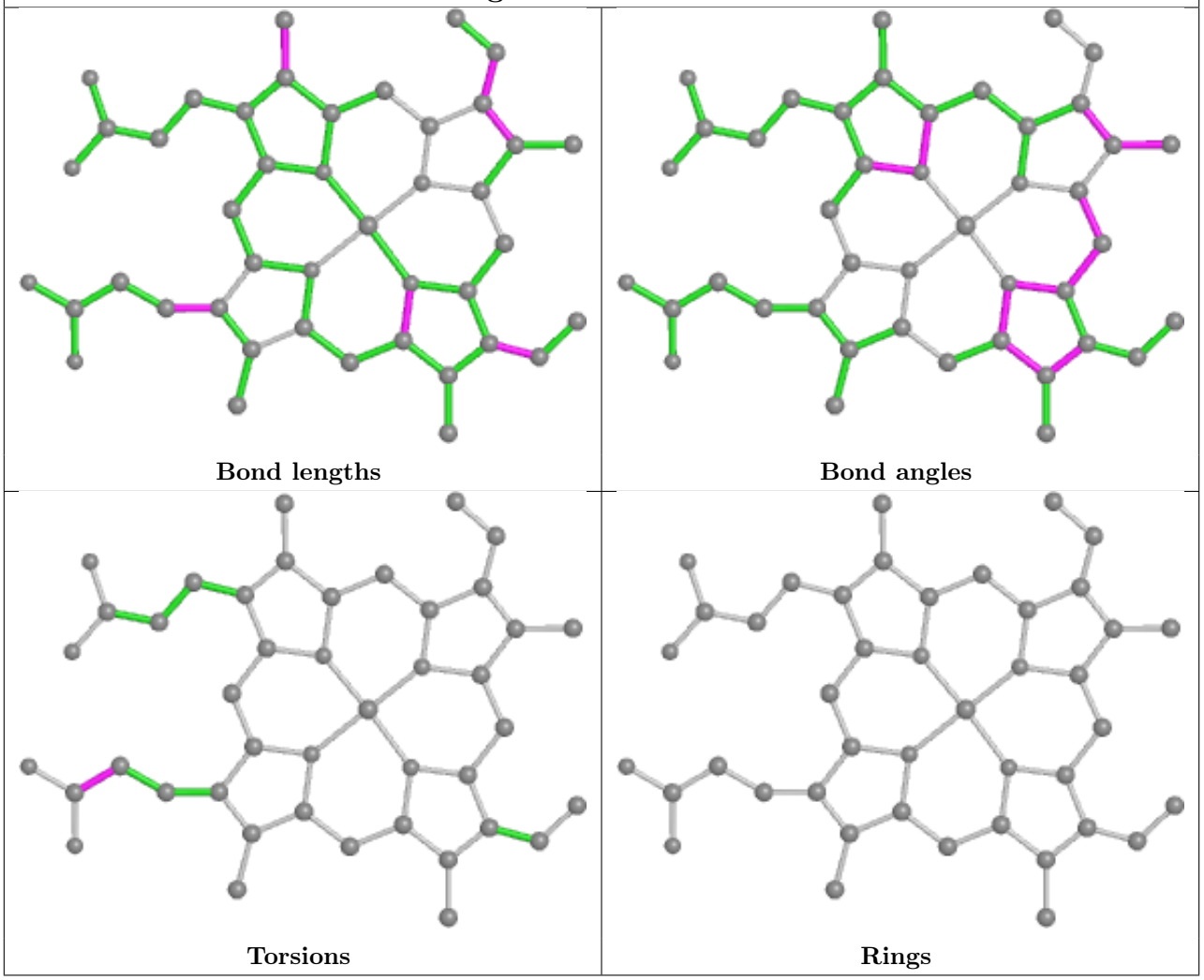


Torsions



Rings

Ligand HEM B 601



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, 95^{th} 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%)	0.18	32 (6%)	16	15	20, 40, 85, 109	0
1	B	454/479 (94%)	0.30	37 (8%)	12	11	24, 44, 79, 94	0
All	All	916/958 (95%)	0.24	69 (7%)	14	13	20, 42, 80, 109	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	ALA	6.5
1	B	145	GLY	6.2
1	A	236	LEU	6.0
1	B	75	TRP	4.9
1	A	45	ASN	4.9
1	A	498	HIS	4.8
1	A	234	PRO	4.5
1	A	231	LEU	4.4
1	B	335	ILE	4.2
1	B	144	LEU	4.2
1	B	147	LYS	4.2
1	B	339	ILE	4.1
1	A	500	HIS	4.1
1	A	230	LEU	3.9
1	A	237	ALA	3.7
1	B	37	PRO	3.6
1	A	232	HIS	3.6
1	B	495	VAL	3.6
1	A	499	HIS	3.5
1	A	238	GLY	3.5
1	A	220	LEU	3.5
1	B	234	PRO	3.4
1	B	32	LYS	3.3
1	A	145	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	151	GLN	3.2
1	A	219	PHE	3.2
1	B	240	VAL	3.0
1	B	464	PHE	3.0
1	B	238	GLY	3.0
1	B	383	GLU	3.0
1	B	72	GLN	2.9
1	B	494	ALA	2.9
1	A	229	VAL	2.9
1	B	237	ALA	2.8
1	B	342	VAL	2.8
1	A	227	VAL	2.8
1	B	166	ASN	2.8
1	A	335	ILE	2.6
1	A	239	LYS	2.6
1	B	146	LYS	2.5
1	A	337	ASP	2.5
1	A	339	ILE	2.5
1	B	71	LEU	2.4
1	A	144	LEU	2.4
1	A	241	LEU	2.4
1	A	342	VAL	2.4
1	A	147	LYS	2.3
1	B	345	PRO	2.3
1	A	146	LYS	2.3
1	A	333	GLN	2.3
1	B	463	HIS	2.3
1	B	229	VAL	2.2
1	B	331	VAL	2.2
1	B	462	GLN	2.2
1	B	231	LEU	2.2
1	A	49	VAL	2.2
1	A	233	ILE	2.2
1	B	74	ALA	2.1
1	B	172	PHE	2.1
1	B	243	PHE	2.1
1	B	381	ASP	2.1
1	A	341	GLN	2.1
1	B	330[A]	ARG	2.1
1	A	228	PRO	2.1
1	A	226	ALA	2.0
1	B	241	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	236	LEU	2.0
1	B	337	ASP	2.0
1	B	343	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

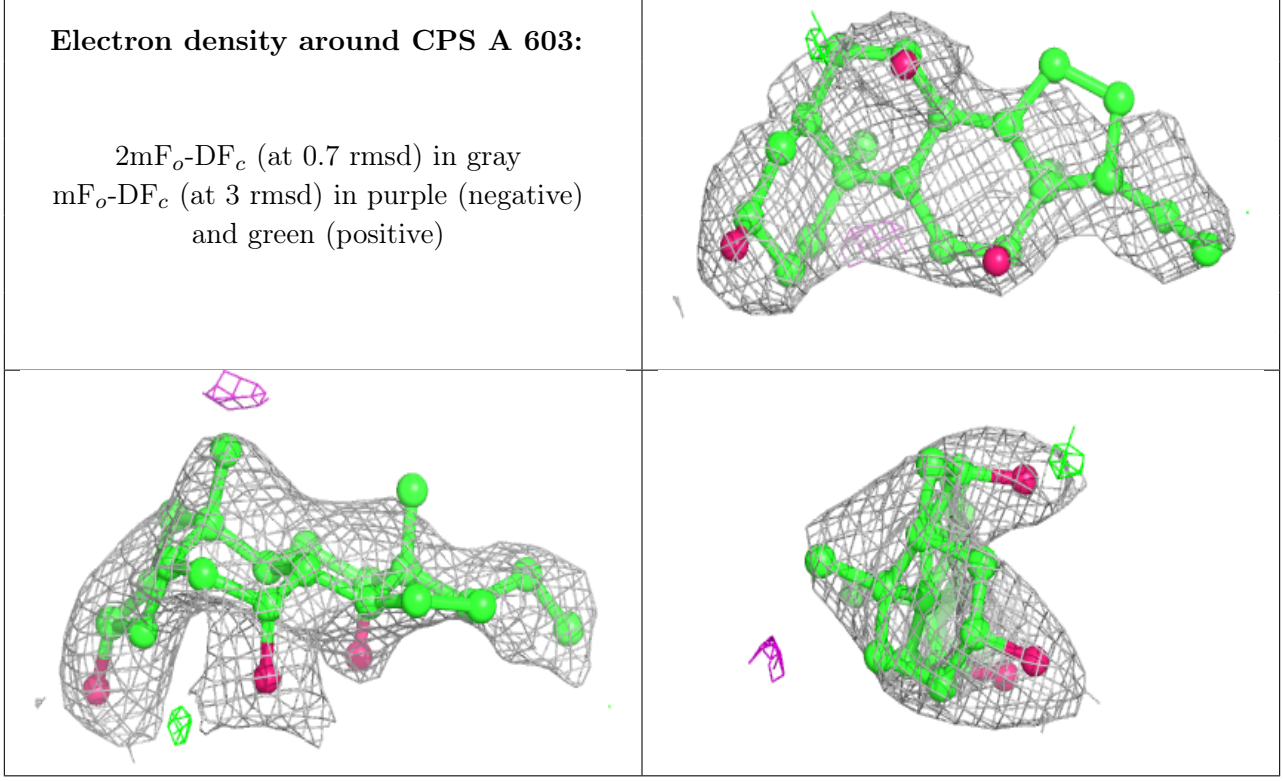
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	ZN	B	605	1/1	0.82	0.19	120,120,120,120	0
4	CPS	A	603	24/42	0.83	0.25	49,69,77,79	0
5	ZN	A	605	1/1	0.84	0.08	77,77,77,77	0
5	ZN	B	606	1/1	0.94	0.51	103,103,103,103	0
4	CPS	B	603	24/42	0.95	0.10	43,53,64,66	0
3	PN0	B	602	28/28	0.97	0.11	27,42,52,57	0
3	PN0	A	602	28/28	0.97	0.11	22,39,48,51	0
2	HEM	B	601	43/43	0.98	0.17	22,28,32,34	0
2	HEM	A	601	43/43	0.98	0.13	17,25,30,33	0
5	ZN	A	606	1/1	0.99	0.14	42,42,42,42	1
5	ZN	A	604	1/1	1.00	0.10	29,29,29,29	0
5	ZN	B	604	1/1	1.00	0.14	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.

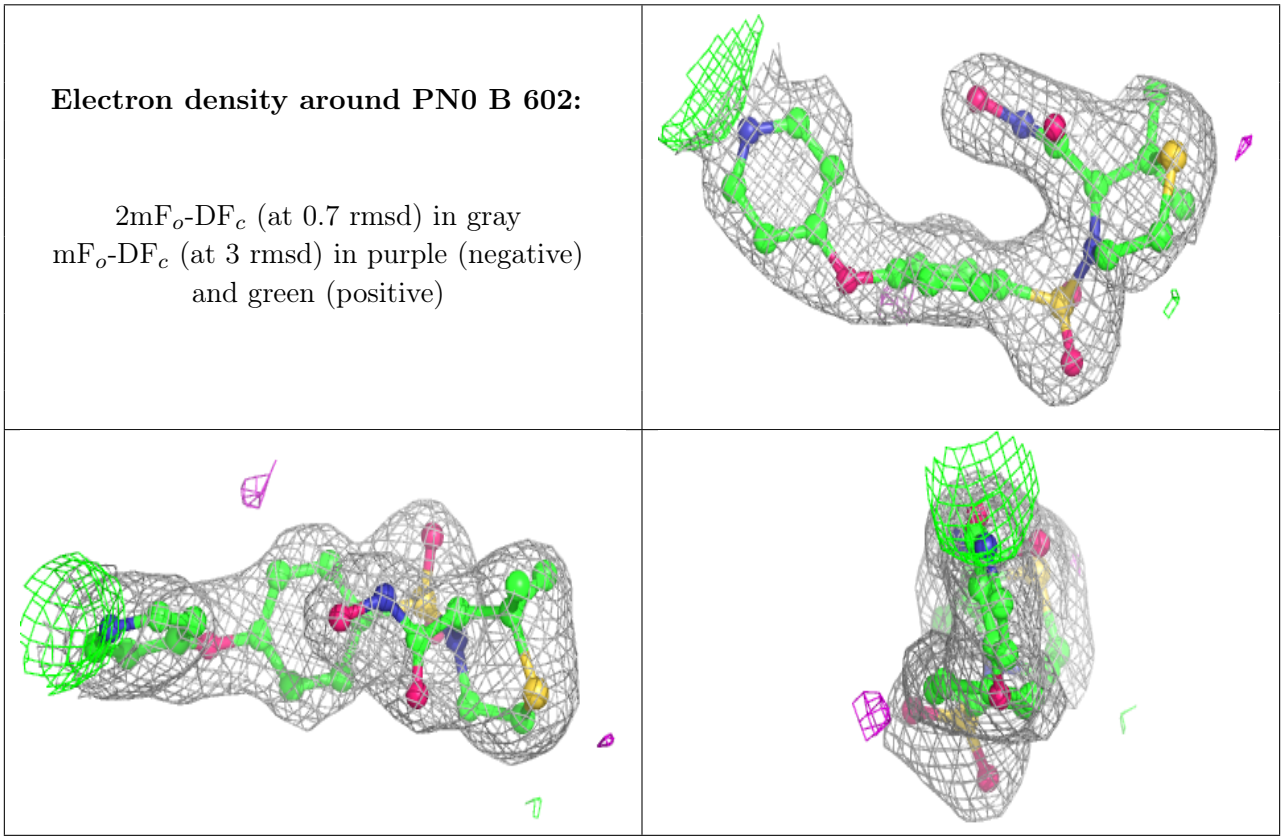
Electron density around CPS A 603:

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



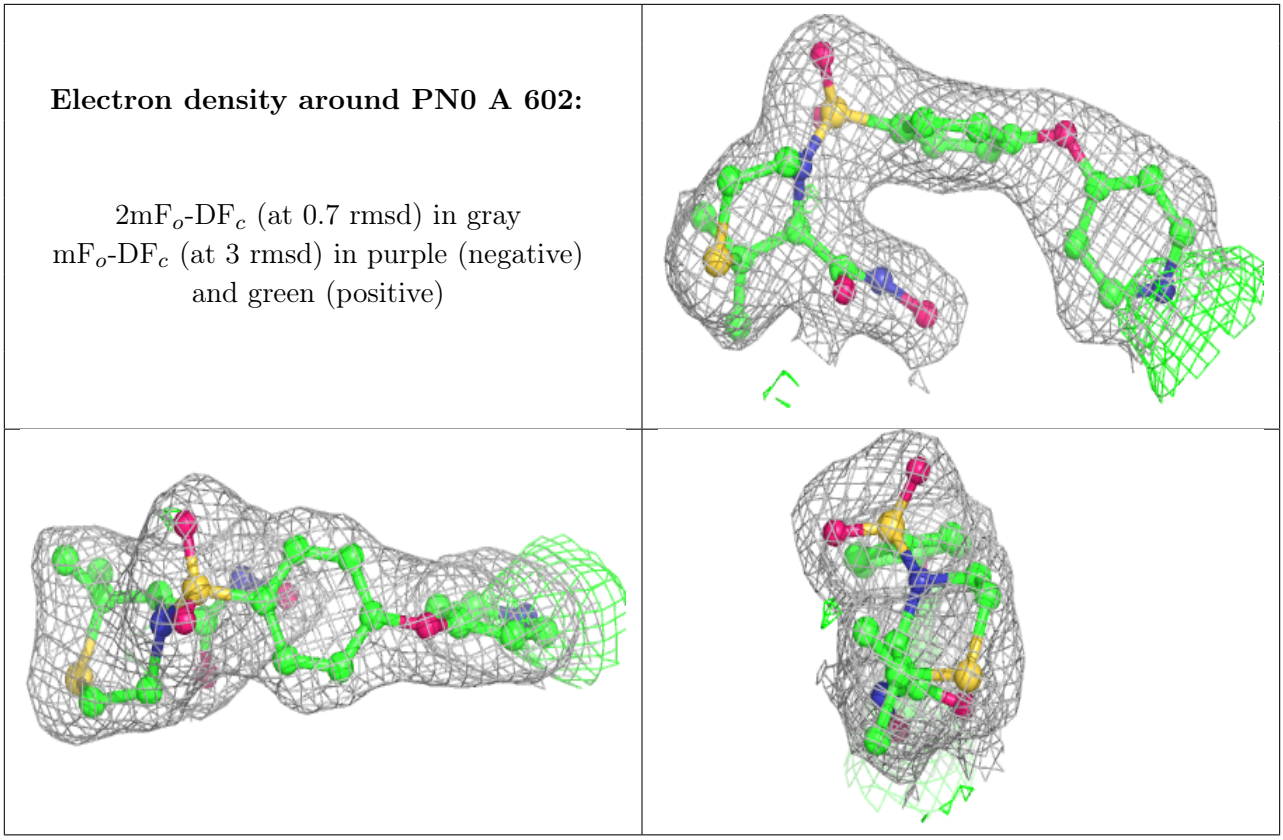
Electron density around PN0 B 602:

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



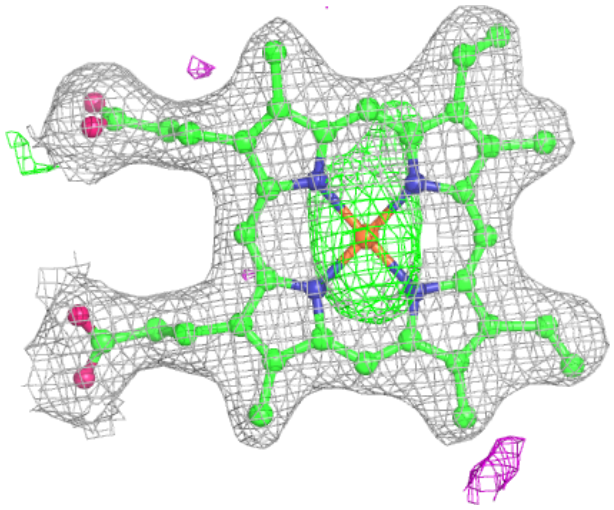
Electron density around PN0 A 602:

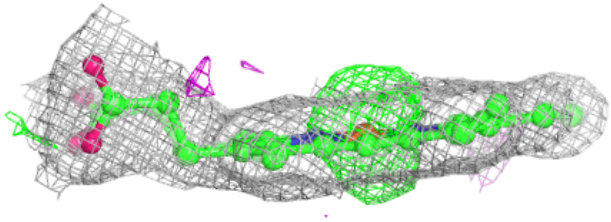
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

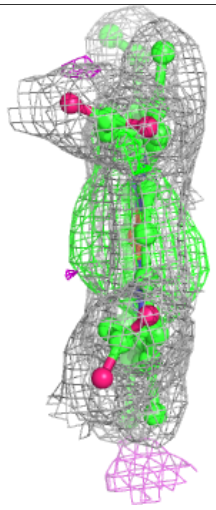


Electron density around HEM B 601:

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

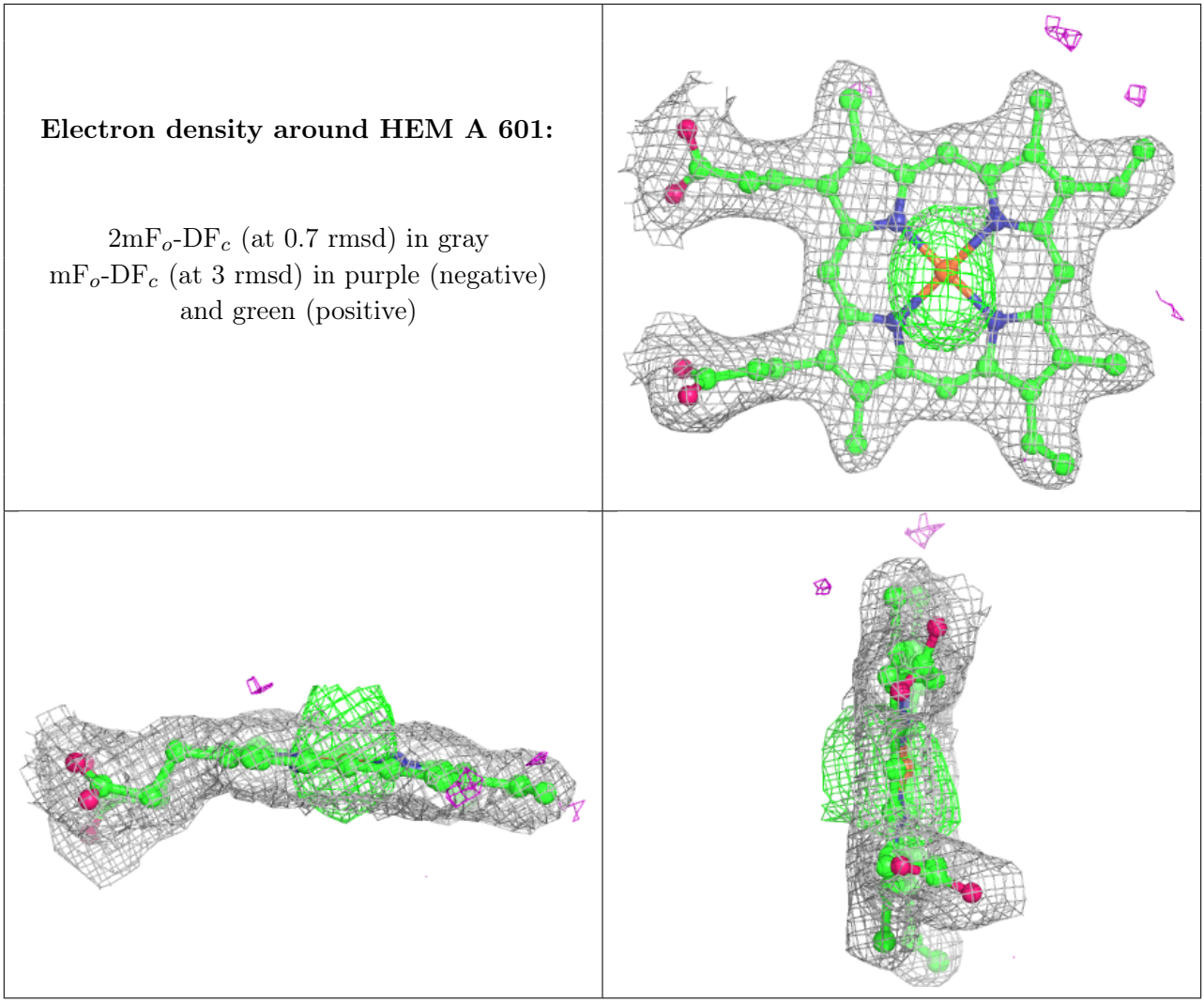






Electron density around HEM A 601:

$2mF_o$-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.