wwPDB X-ray Structure Validation Summary Report (i)

Sep 12, 2023 – 07:39 AM EDT

PDB ID	:	4NKX
Title	:	Human steroidogenic cytochrome P450 17A1 mutant A105L with substrate progesterone
Authors	:	Scott, E.E.; Petrunak, E.M.
Deposited on	:	2013-11-13
Resolution	:	2.79 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

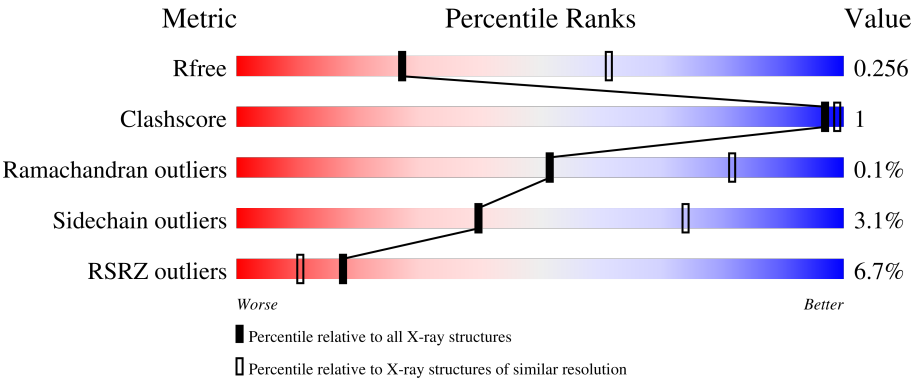
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	494	5% 90% · 6%
1	B	494	4% 91% · 5%
1	C	494	6% 90% · 5%
1	D	494	10% 90% · 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 30719 atoms, of which 15484 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 Steroid 17-alpha-hydroxylase/17,20 lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	466	Total	C	H	N	O	S	0	0	0
			7526	2387	3809	643	672	15			
1	B	468	Total	C	H	N	O	S	0	0	0
			7549	2394	3817	646	677	15			
1	C	469	Total	C	H	N	O	S	0	0	0
			7550	2398	3810	647	680	15			
1	D	468	Total	C	H	N	O	S	0	0	0
			7544	2396	3808	646	679	15			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	expression tag	UNP P05093
A	20	ALA	-	expression tag	UNP P05093
A	21	LYS	-	expression tag	UNP P05093
A	22	LYS	-	expression tag	UNP P05093
A	23	THR	-	expression tag	UNP P05093
A	105	LEU	ALA	engineered mutation	UNP P05093
A	509	HIS	-	expression tag	UNP P05093
A	510	HIS	-	expression tag	UNP P05093
A	511	HIS	-	expression tag	UNP P05093
A	512	HIS	-	expression tag	UNP P05093
B	19	MET	-	expression tag	UNP P05093
B	20	ALA	-	expression tag	UNP P05093
B	21	LYS	-	expression tag	UNP P05093
B	22	LYS	-	expression tag	UNP P05093
B	23	THR	-	expression tag	UNP P05093
B	105	LEU	ALA	engineered mutation	UNP P05093
B	509	HIS	-	expression tag	UNP P05093
B	510	HIS	-	expression tag	UNP P05093
B	511	HIS	-	expression tag	UNP P05093
B	512	HIS	-	expression tag	UNP P05093
C	19	MET	-	expression tag	UNP P05093

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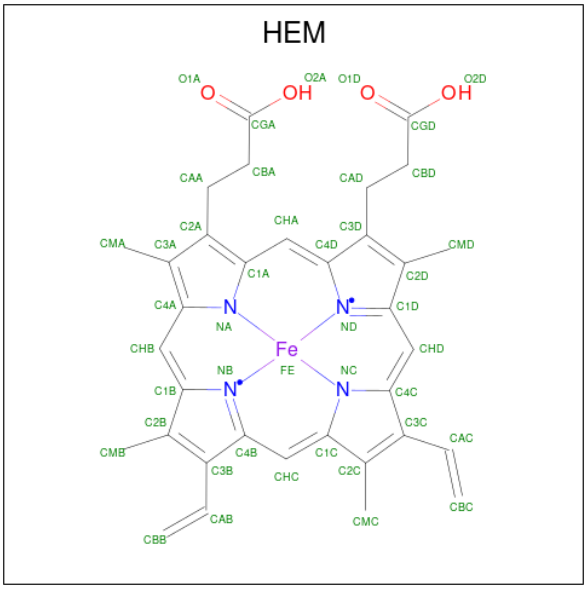
Chain	Residue	Modelled	Actual	Comment	Reference
C	20	ALA	-	expression tag	UNP P05093
C	21	LYS	-	expression tag	UNP P05093
C	22	LYS	-	expression tag	UNP P05093
C	23	THR	-	expression tag	UNP P05093
C	105	LEU	ALA	engineered mutation	UNP P05093
C	509	HIS	-	expression tag	UNP P05093
C	510	HIS	-	expression tag	UNP P05093
C	511	HIS	-	expression tag	UNP P05093
C	512	HIS	-	expression tag	UNP P05093
D	19	MET	-	expression tag	UNP P05093
D	20	ALA	-	expression tag	UNP P05093
D	21	LYS	-	expression tag	UNP P05093
D	22	LYS	-	expression tag	UNP P05093
D	23	THR	-	expression tag	UNP P05093
D	105	LEU	ALA	engineered mutation	UNP P05093
D	509	HIS	-	expression tag	UNP P05093
D	510	HIS	-	expression tag	UNP P05093
D	511	HIS	-	expression tag	UNP P05093
D	512	HIS	-	expression tag	UNP P05093

- 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	H	N	O	0	0
			73	34	1	30	4	4		

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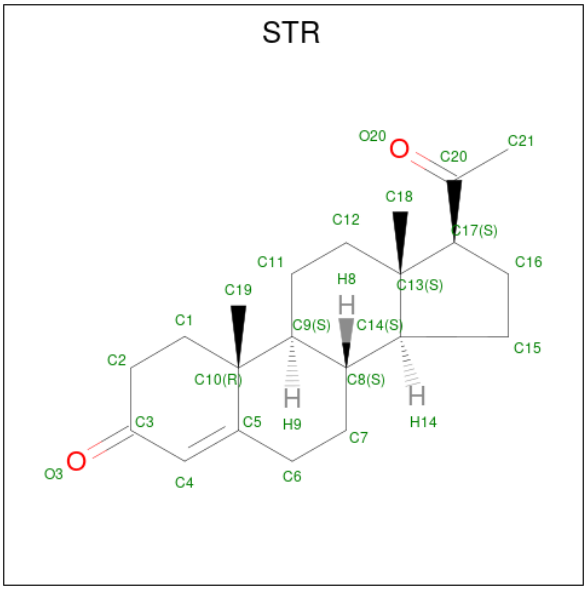
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	D	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 3 is PROGESTERONE (three-letter code: STR) (formula: $C_{21}H_{30}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			53	21	30	2		
3	B	1	Total	C	H	O	0	0
			53	21	30	2		
3	C	1	Total	C	H	O	0	0
			53	21	30	2		
3	D	1	Total	C	H	O	0	0
			53	21	30	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		
4	B	13	Total	O	0	0
			13	13		

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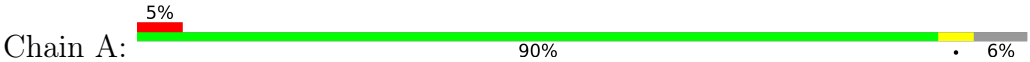
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	10	Total O 10 10	0	0
4	D	9	Total O 9 9	0	0

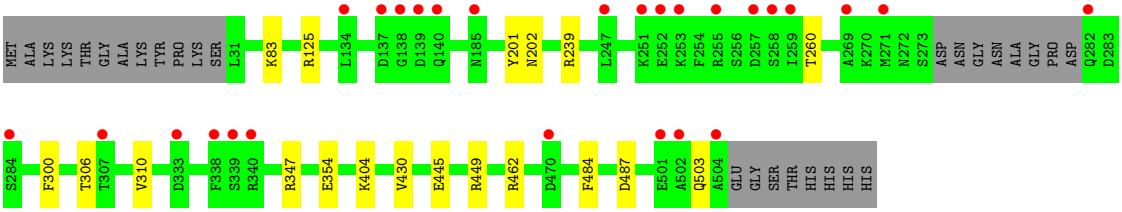
3 Residue-property plots (i)

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: Steroid 17-alpha-hydroxylase/17,20 lyase

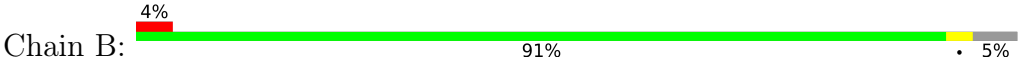
Chain A:

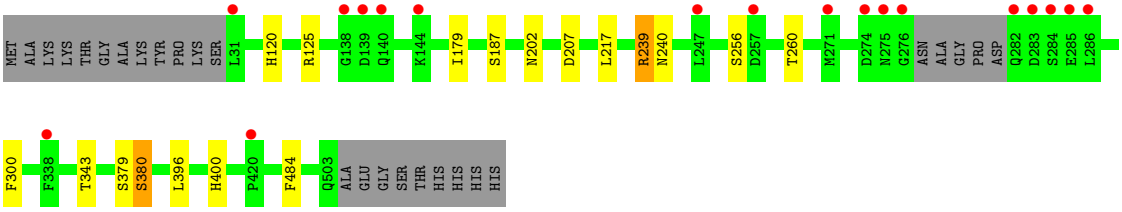




• Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

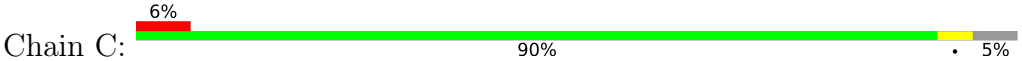
Chain B:

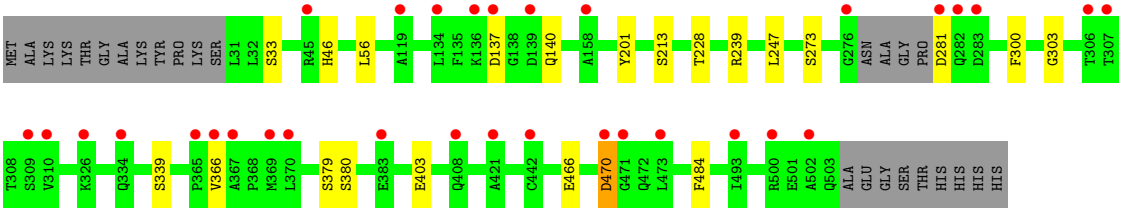




• Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

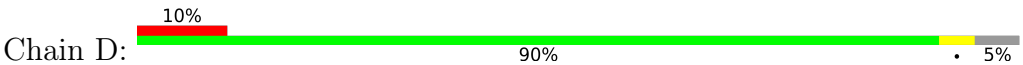
Chain C:

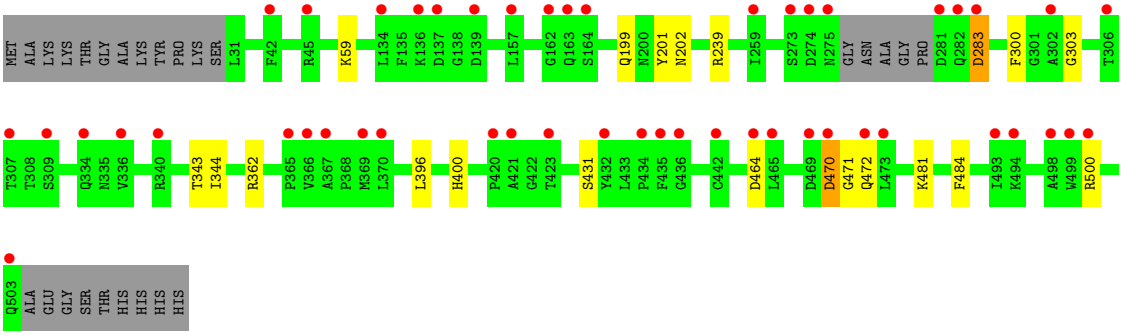




• Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

Chain D:




MET ALA LYS LYS THR GLY ALA LYS TYR PRO LYS SER L31 F42 R45 K59 L134 F135 K136 D137 G138 D139 L157 G162 Q163 S164 Q199 N200 Y201 N202 R239 I259 S273 D274 N275 GLY ASN ALA GLY PRO D281 Q282 D283 F300 G301 A302 G303 T306
T307 T308 S309 Q334 N335 V336 R340 T343 I344 R362 P365 V366 A367 P368 M369 L370 L396 H400 P420 A421 G422 T423 S431 Y432 L433 P434 F435 G436 C442 D464 L465 D469 D470 G471 Q472 L473 K481 F484 I493 K494 A498 W499 R500
Q503 ALA GLU GLY SER THR HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.93Å 153.04Å 173.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.13 – 2.79 39.13 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.13-2.79) 99.1 (39.13-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.184 , 0.257 0.187 , 0.256	Depositor DCC
R_{free} test set	2886 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	58.1	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 49.1	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	0.95	EDS
Total number of atoms	30719	wwPDB-VP
Average B, all atoms (Å^2)	59.0	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 39.90 % 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 2.9624e-04. 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: HEM, STR

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	0/3797	0.52	0/5140
1	B	0.40	0/3812	0.52	0/5160
1	C	0.39	0/3820	0.52	0/5171
1	D	0.38	0/3816	0.53	0/5166
All	All	0.39	0/15245	0.52	0/20637

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	3717	3809	3794	5	0
1	B	3732	3817	3802	5	0
1	C	3740	3810	3806	4	0
1	D	3736	3808	3803	8	0
2	A	43	30	30	2	0
2	B	43	30	30	1	0
2	C	43	30	30	4	0
2	D	43	30	30	3	0
3	A	23	30	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	23	30	30	1	0
3	C	23	30	30	0	0
3	D	23	30	30	1	0
4	A	14	0	0	0	0
4	B	13	0	0	0	0
4	C	10	0	0	0	0
4	D	9	0	0	0	0
All	All	15235	15484	15445	27	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 1.

The worst 5 of 27 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:B:239:ARG:NH1	1:B:240:ASN:OD1	2.26	0.69
2:C:600:HEM:HBC2	2:C:600:HEM:HHD	1.79	0.65
1:D:470:ASP:O	1:D:472:GLN:N	2.31	0.64
2:D:600:HEM:HBC2	2:D:600:HEM:HHD	1.81	0.63
2:C:600:HEM:HHC	2:C:600:HEM:HBB2	1.84	0.60

There are no symmetry-related clashes.

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	462/494 (94%)	438 (95%)	24 (5%)	0	100 100
1	B	464/494 (94%)	440 (95%)	23 (5%)	1 (0%)	47 78
1	C	465/494 (94%)	446 (96%)	19 (4%)	0	100 100
1	D	464/494 (94%)	450 (97%)	13 (3%)	1 (0%)	47 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1855/1976 (94%)	1774 (96%)	79 (4%)	2 (0%)	51 81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	471	GLY
1	B	217	LEU

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	416/437 (95%)	406 (98%)	10 (2%)	49 81
1	B	418/437 (96%)	407 (97%)	11 (3%)	46 79
1	C	419/437 (96%)	401 (96%)	18 (4%)	29 62
1	D	419/437 (96%)	407 (97%)	12 (3%)	42 76
All	All	1672/1748 (96%)	1621 (97%)	51 (3%)	40 74

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	228	THR
1	C	403	GLU
1	D	484	PHE
1	C	239	ARG
1	C	281	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	120	HIS
1	D	202	ASN
1	D	408	GLN

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Mol	Chain	Res	Type
1	D	407	HIS
1	B	202	ASN

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)

8 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	$\#\|Z\| > 2$
2	HEM	A	600	1	41,50,50	2.04	8 (19%)	45,82,82	1.71	5 (11%)
3	STR	D	601	-	26,26,26	4.41	17 (65%)	42,42,42	2.59	17 (40%)
3	STR	B	601	-	26,26,26	4.42	17 (65%)	42,42,42	2.51	15 (35%)
2	HEM	C	600	1	41,50,50	1.92	7 (17%)	45,82,82	1.75	10 (22%)
2	HEM	D	600	1	41,50,50	1.91	6 (14%)	45,82,82	1.67	9 (20%)
2	HEM	B	600	1	41,50,50	1.94	7 (17%)	45,82,82	1.57	7 (15%)
3	STR	A	601	-	26,26,26	4.42	17 (65%)	42,42,42	2.41	12 (28%)
3	STR	C	601	-	26,26,26	4.39	18 (69%)	42,42,42	2.52	16 (38%)

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
2	HEM	A	600	1	-	2/12/54/54	-
3	STR	D	601	-	-	0/4/62/62	0/4/4/4
3	STR	B	601	-	-	0/4/62/62	0/4/4/4
2	HEM	C	600	1	-	4/12/54/54	-
2	HEM	D	600	1	-	2/12/54/54	-
2	HEM	B	600	1	-	2/12/54/54	-
3	STR	A	601	-	-	0/4/62/62	0/4/4/4
3	STR	C	601	-	-	0/4/62/62	0/4/4/4

The worst 5 of 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	STR	C11-C9	11.66	1.73	1.53
3	D	601	STR	C11-C9	11.57	1.73	1.53
3	C	601	STR	C11-C9	11.48	1.73	1.53
3	A	601	STR	C11-C9	11.21	1.72	1.53
3	A	601	STR	C12-C11	8.87	1.72	1.53

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	HEM	C4D-ND-C1D	6.85	112.14	105.07
3	A	601	STR	C12-C13-C17	-5.85	108.95	116.10
3	B	601	STR	C16-C17-C13	-5.79	99.05	104.21
3	A	601	STR	C17-C13-C14	5.68	105.78	99.72
3	B	601	STR	C1-C2-C3	-5.65	99.51	111.62

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	600	HEM	C1A-C2A-CAA-CBA
2	C	600	HEM	C3A-C2A-CAA-CBA
2	C	600	HEM	C4B-C3B-CAB-CBB
2	B	600	HEM	C1A-C2A-CAA-CBA
2	A	600	HEM	CAA-CBA-CGA-O2A

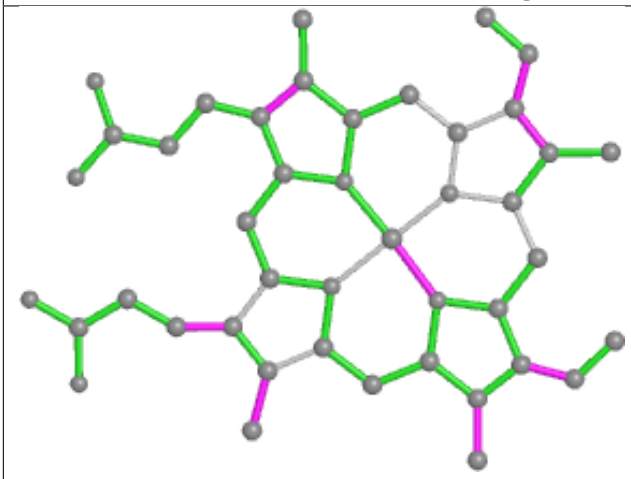
There are no ring outliers.

6 monomers are involved in 12 short contacts:

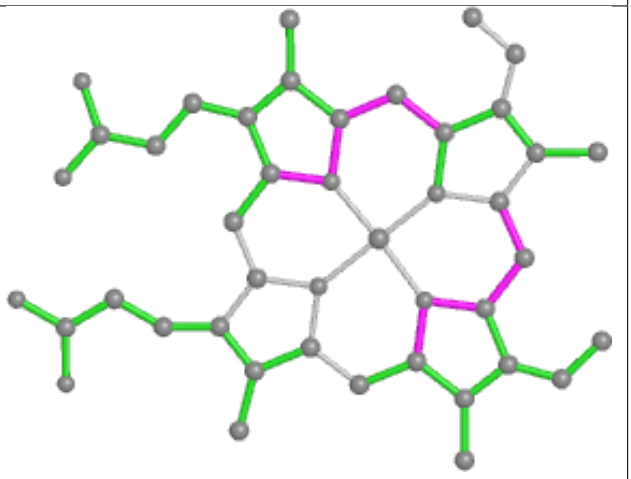
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	HEM	2	0
3	D	601	STR	1	0
3	B	601	STR	1	0
2	C	600	HEM	4	0
2	D	600	HEM	3	0
2	B	600	HEM	1	0

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.

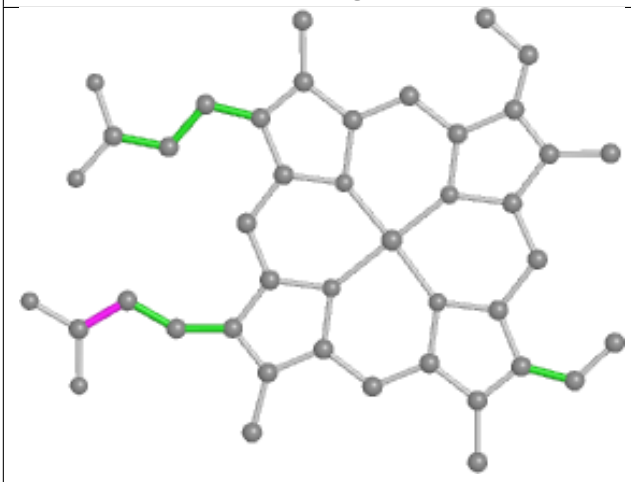
Ligand HEM A 600



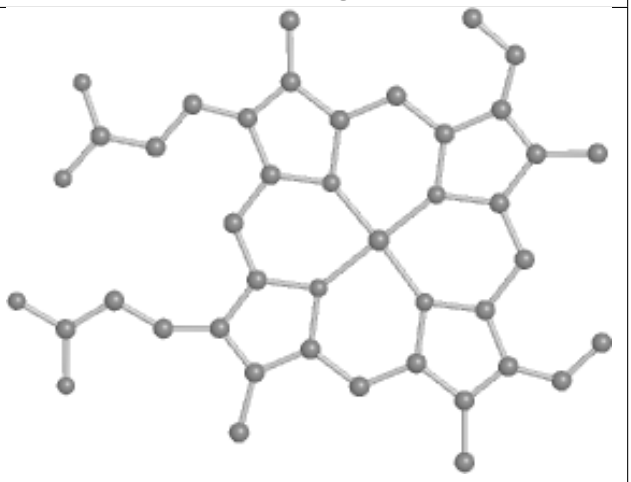
Bond lengths



Bond angles

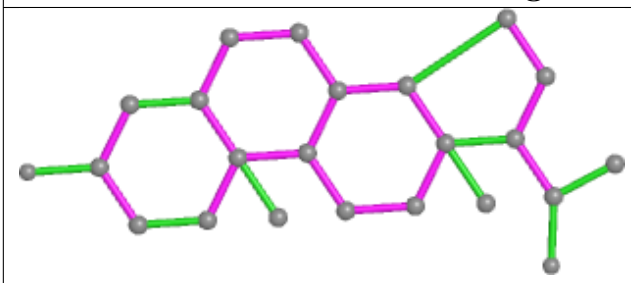


Torsions

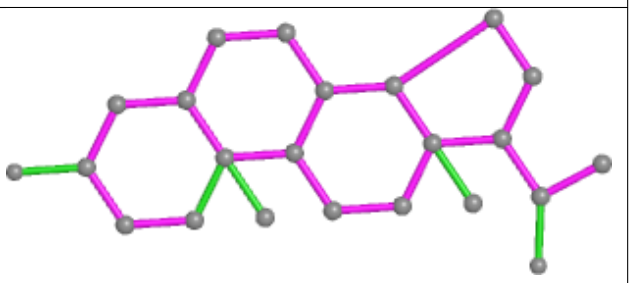


Rings

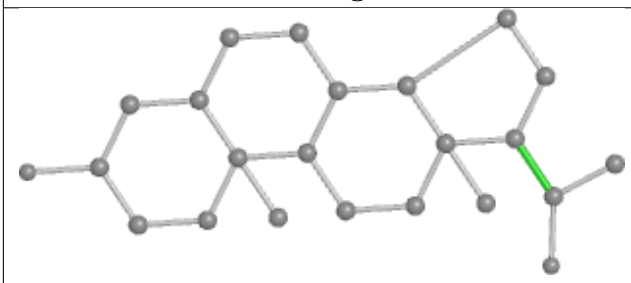
Ligand STR D 601



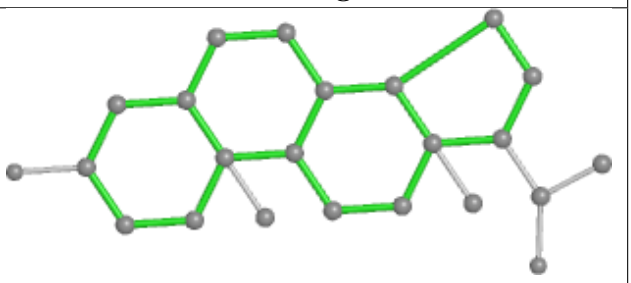
Bond lengths



Bond angles

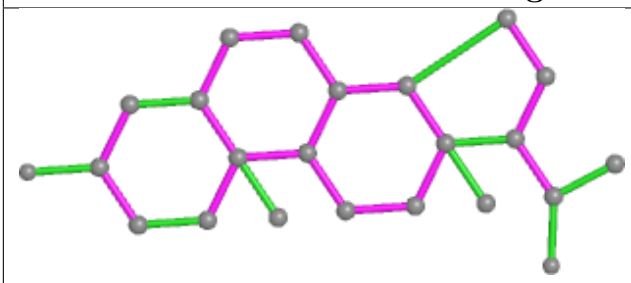


Torsions

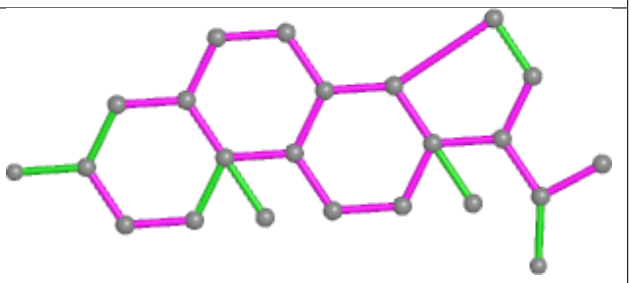


Rings

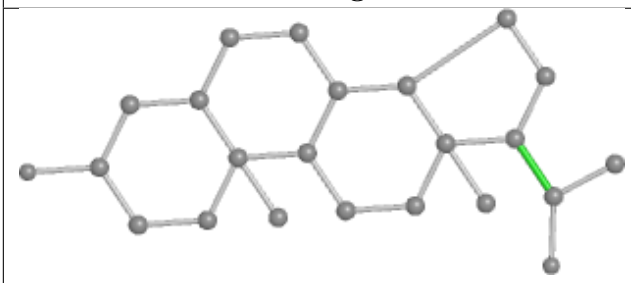
Ligand STR B 601



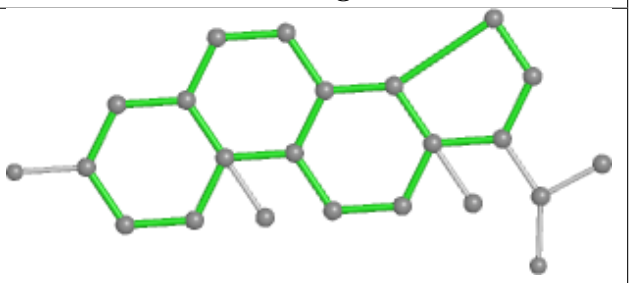
Bond lengths



Bond angles

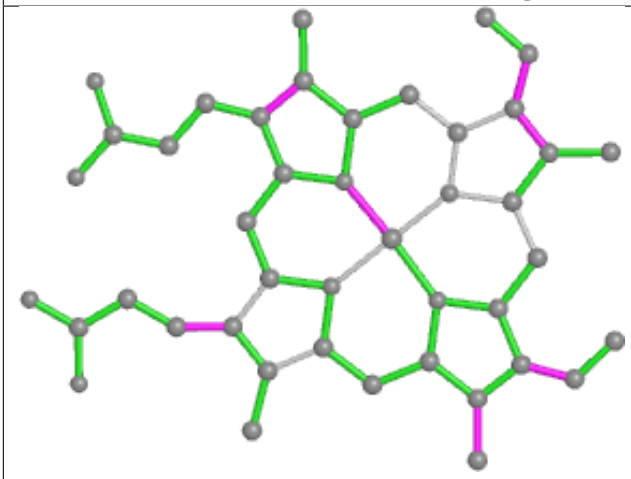


Torsions

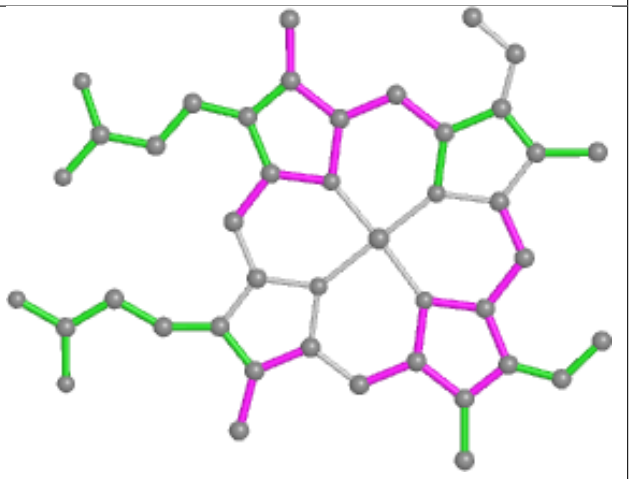


Rings

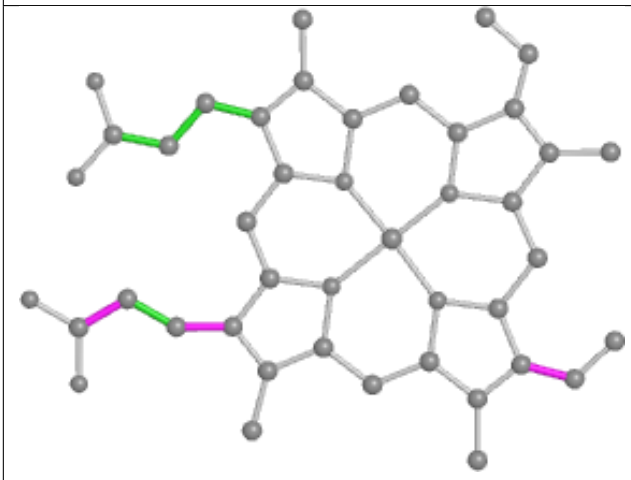
Ligand HEM C 600



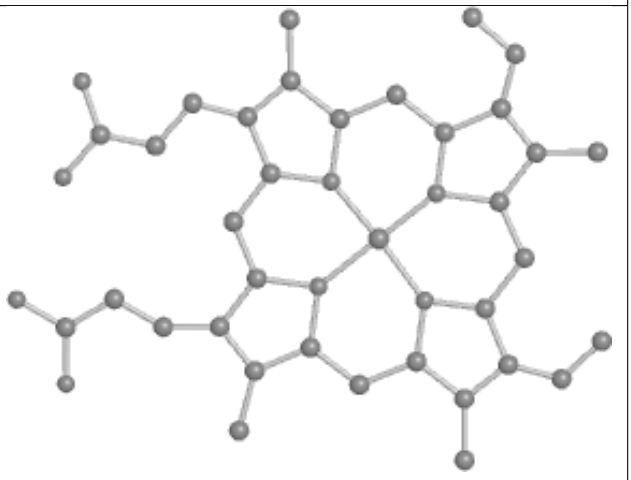
Bond lengths



Bond angles

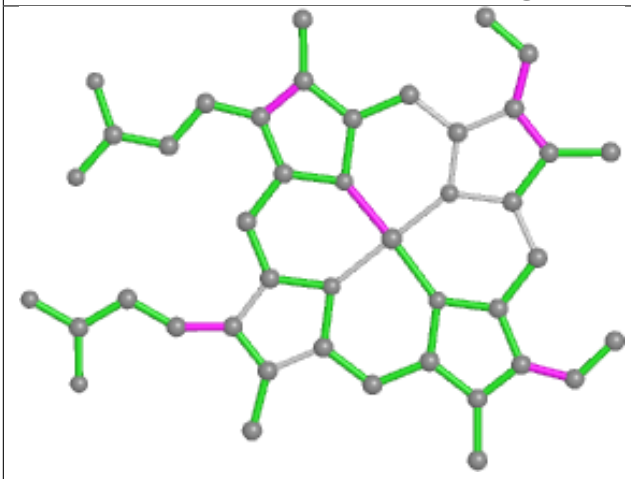


Torsions

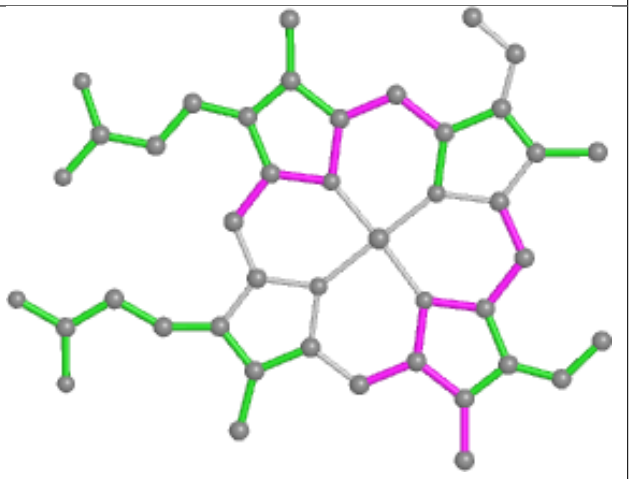


Rings

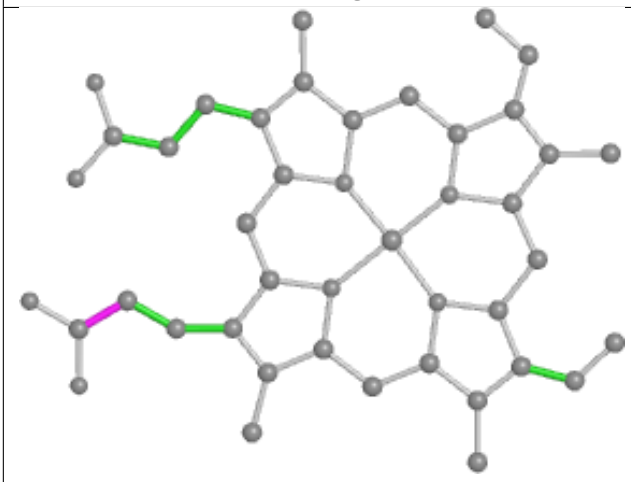
Ligand HEM D 600



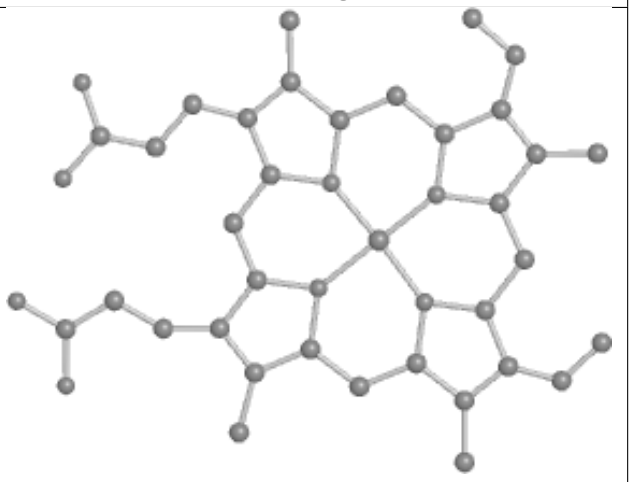
Bond lengths



Bond angles

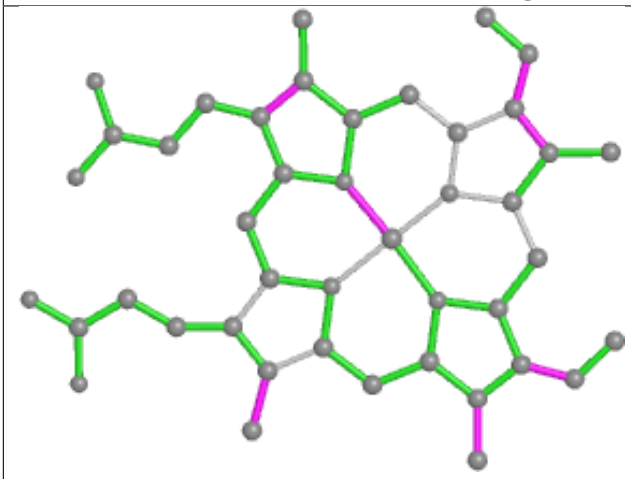


Torsions

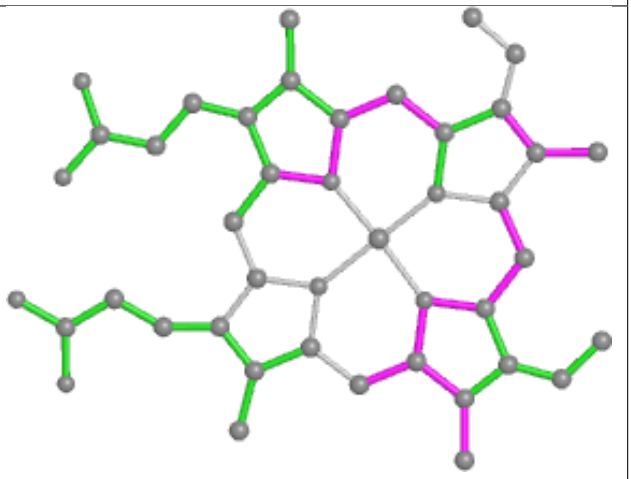


Rings

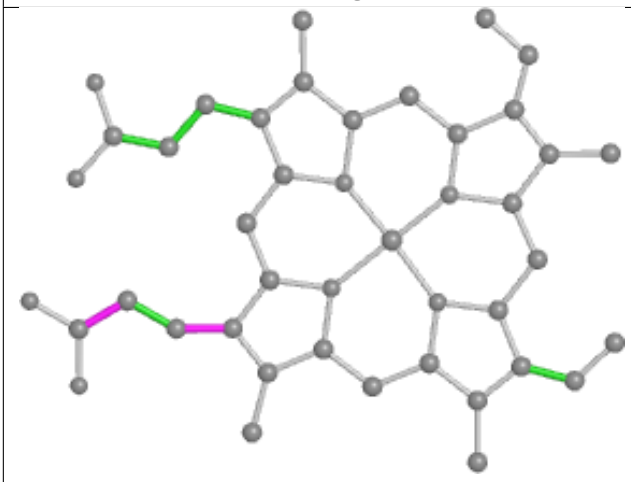
Ligand HEM B 600



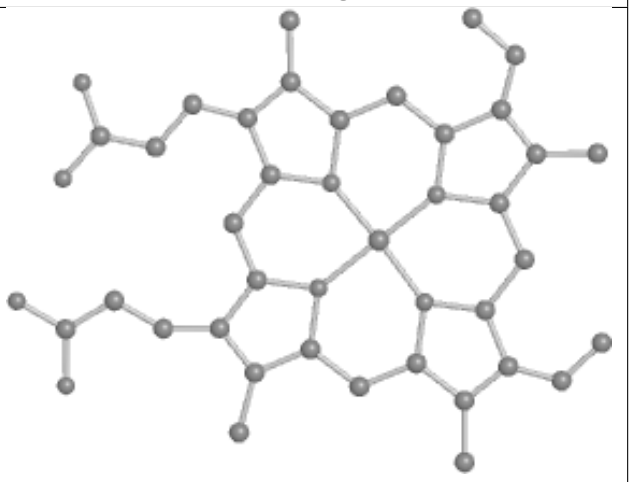
Bond lengths



Bond angles

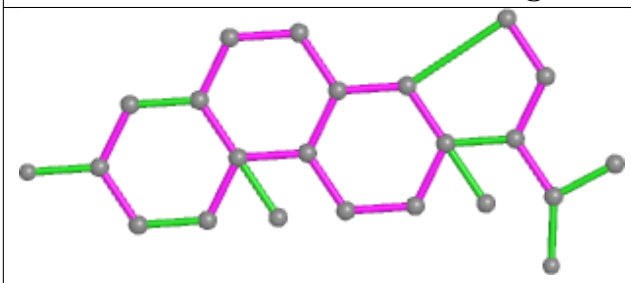


Torsions

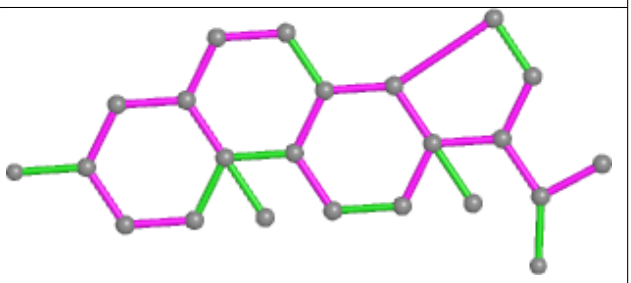


Rings

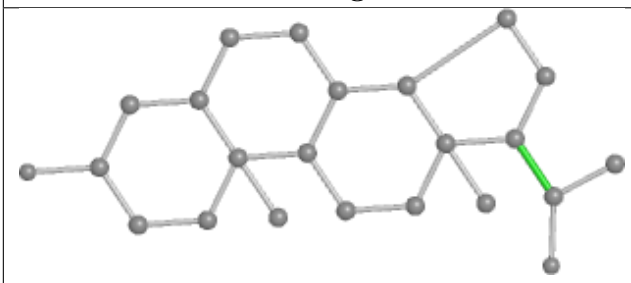
Ligand STR A 601



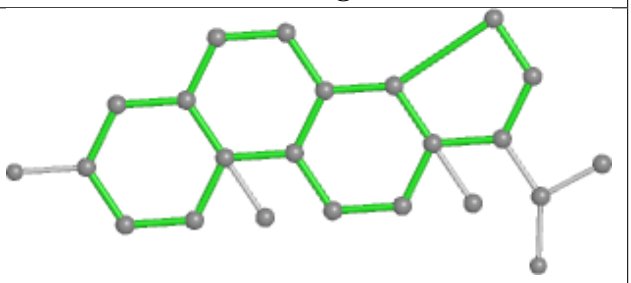
Bond lengths



Bond angles

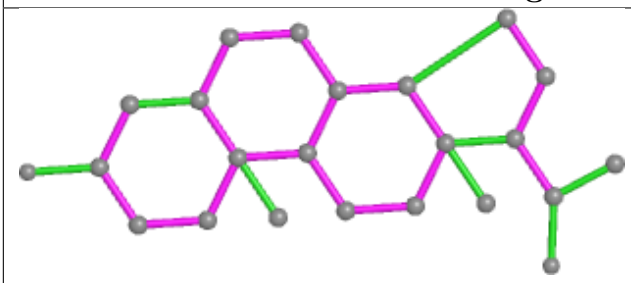


Torsions

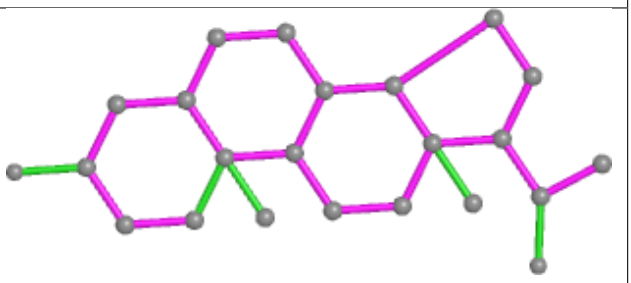


Rings

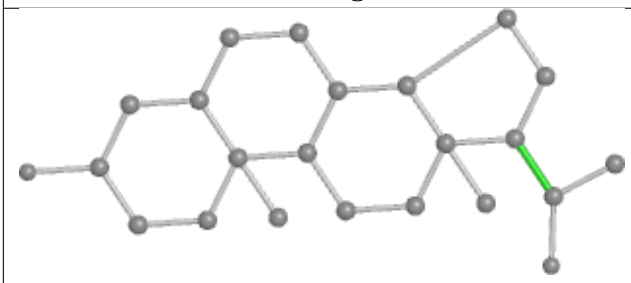
Ligand STR C 601



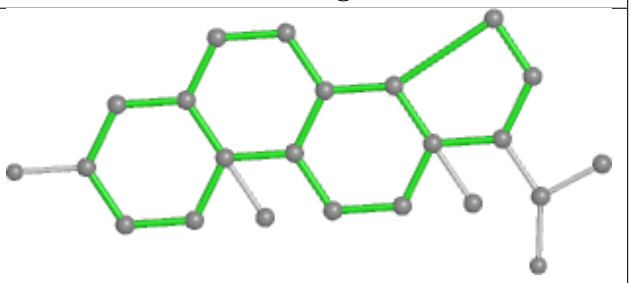
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	466/494 (94%)	0.29	27 (5%) 23 15	27, 49, 82, 109	0
1	B	468/494 (94%)	0.26	18 (3%) 40 30	28, 47, 76, 114	0
1	C	469/494 (94%)	0.46	32 (6%) 17 10	30, 51, 85, 103	0
1	D	468/494 (94%)	0.59	49 (10%) 6 3	31, 54, 92, 129	0
All	All	1871/1976 (94%)	0.40	126 (6%) 17 10	27, 50, 87, 129	0

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	281	ASP	7.9
1	A	139	ASP	7.2
1	B	139	ASP	6.6
1	B	275	ASN	5.9
1	C	281	ASP	5.7

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

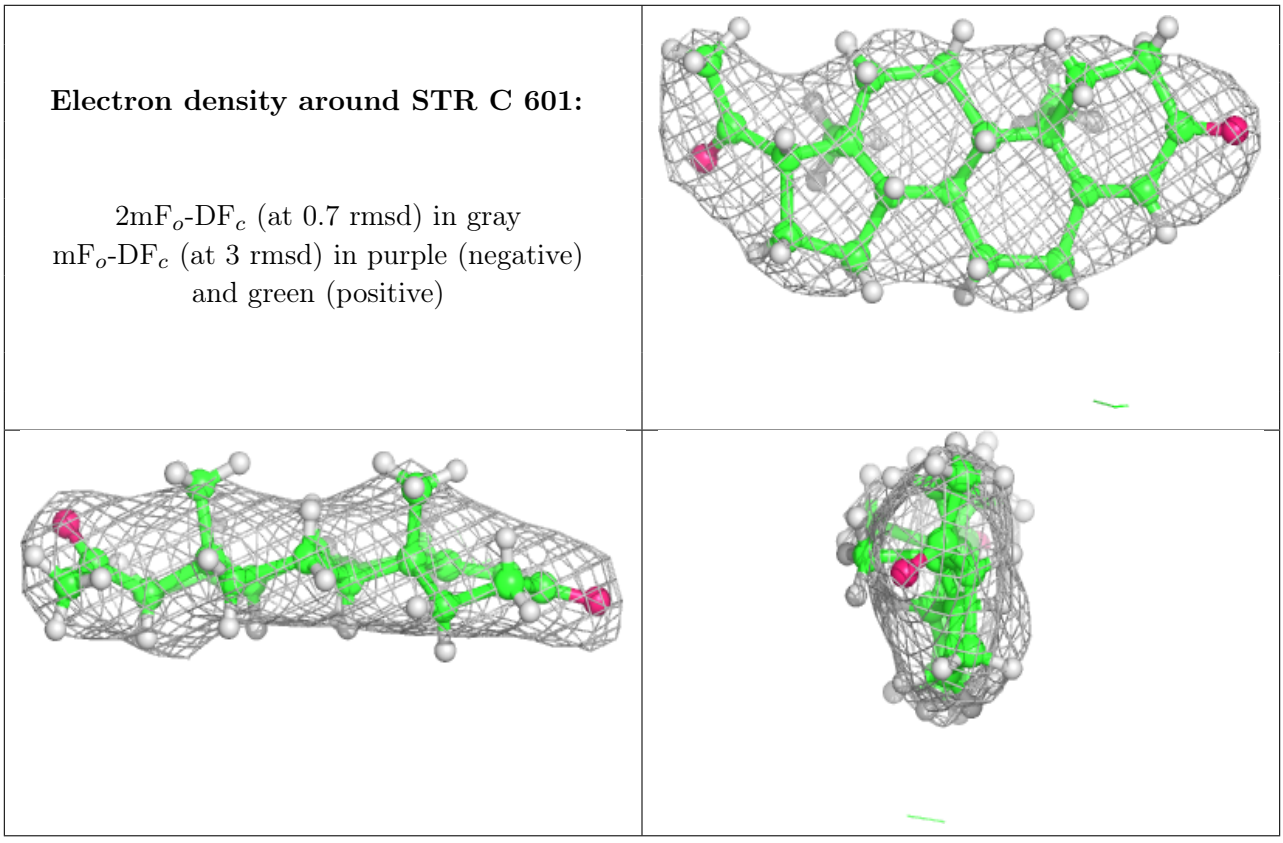
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	STR	C	601	23/23	0.95	0.30	30,42,52,57	0
3	STR	D	601	23/23	0.96	0.31	39,50,57,61	0
3	STR	A	601	23/23	0.97	0.24	35,45,55,55	0
2	HEM	C	600	43/43	0.97	0.31	27,39,53,57	0
2	HEM	D	600	43/43	0.97	0.33	29,43,55,62	0
3	STR	B	601	23/23	0.98	0.28	33,43,54,56	0
2	HEM	B	600	43/43	0.98	0.26	26,38,47,58	0
2	HEM	A	600	43/43	0.98	0.26	25,44,56,62	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.

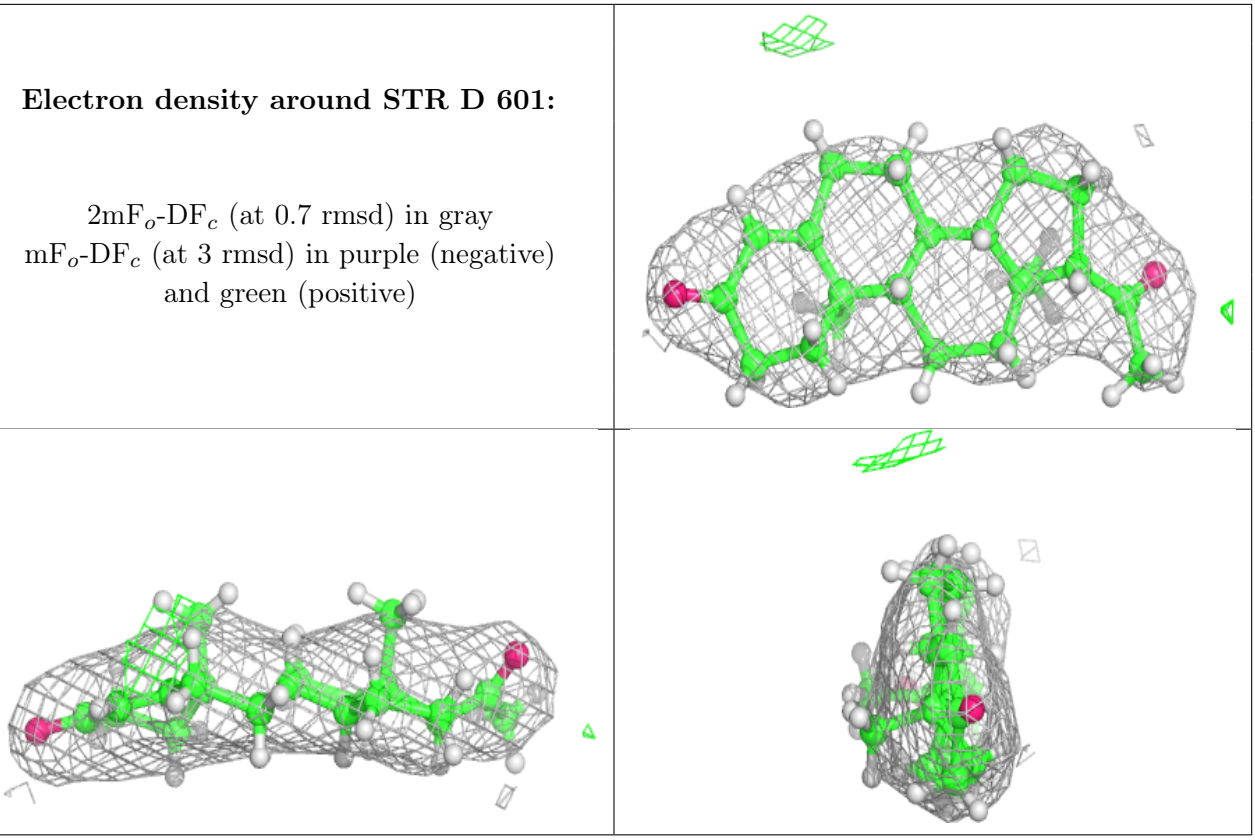
Electron density around STR C 601:

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



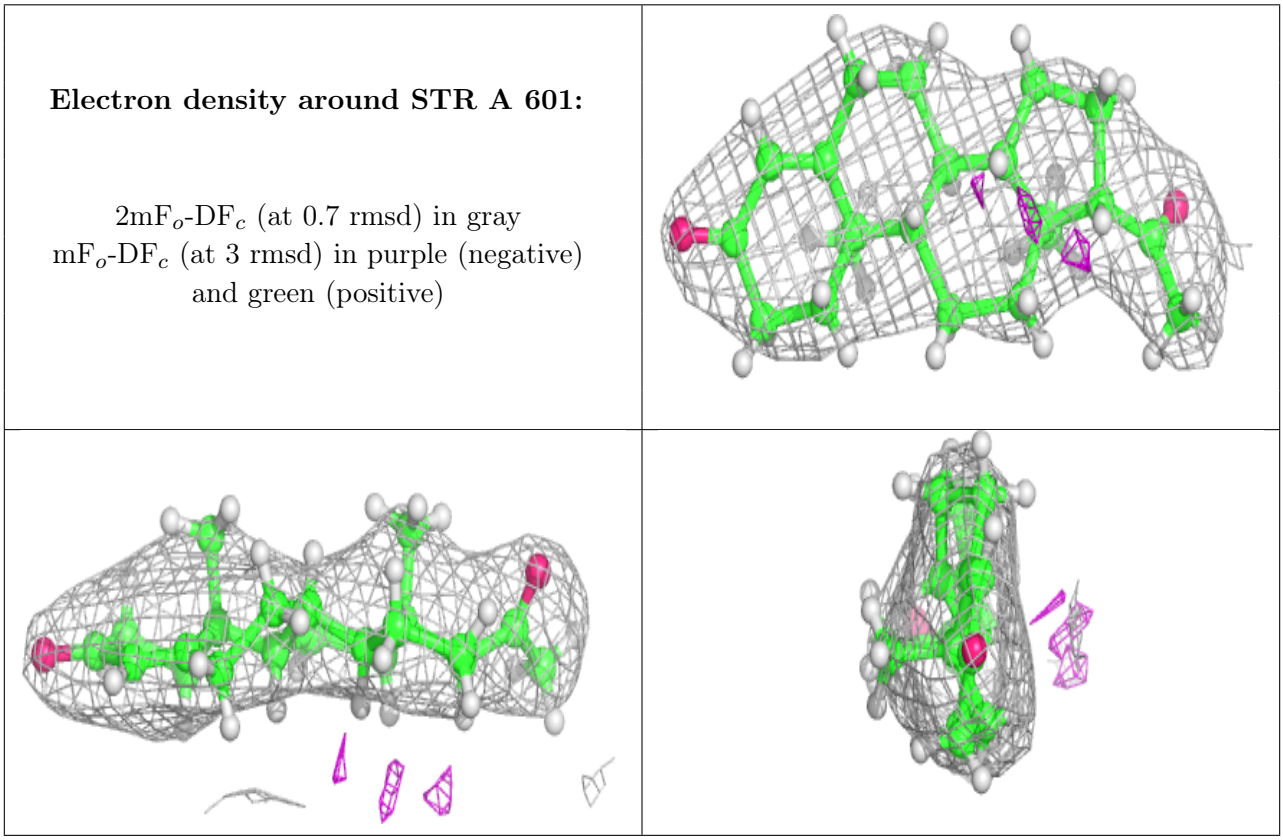
Electron density around STR D 601:

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



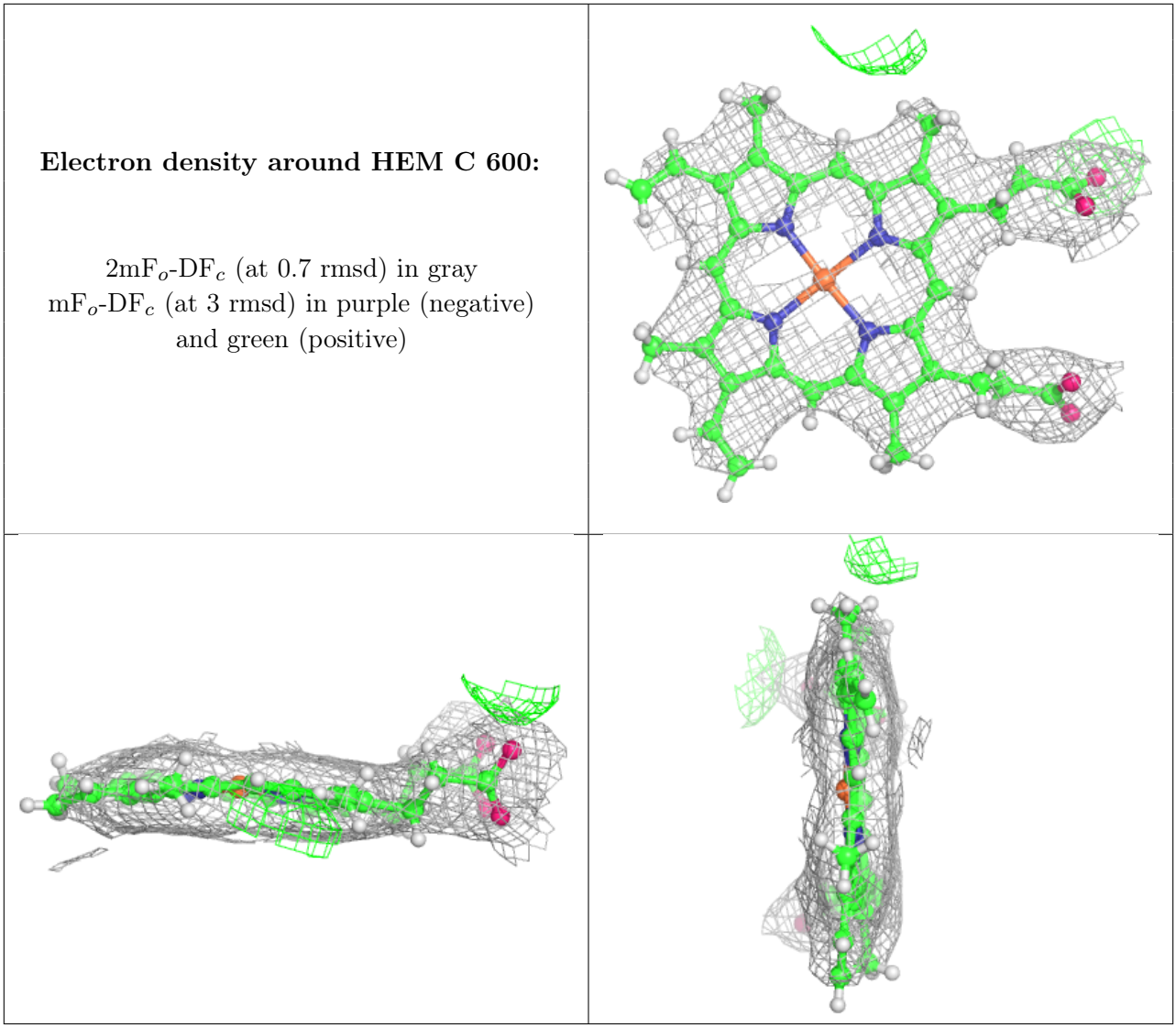
Electron density around STR A 601:

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



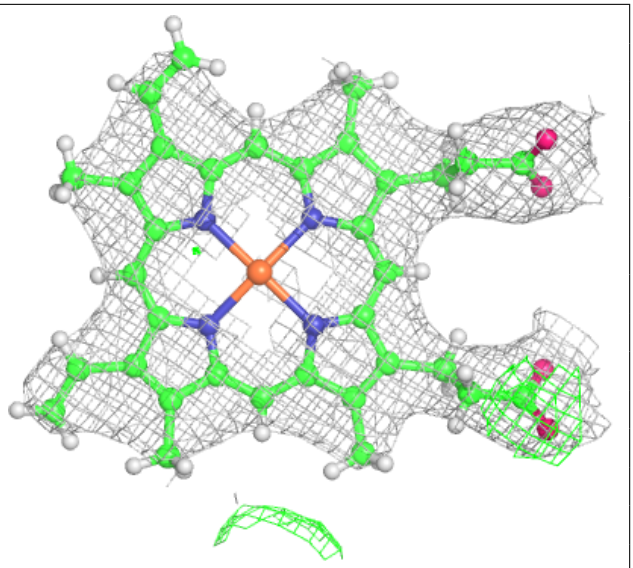
Electron density around HEM C 600:

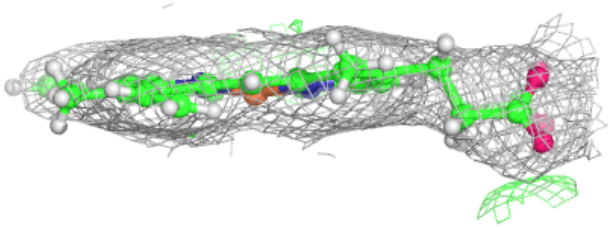
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

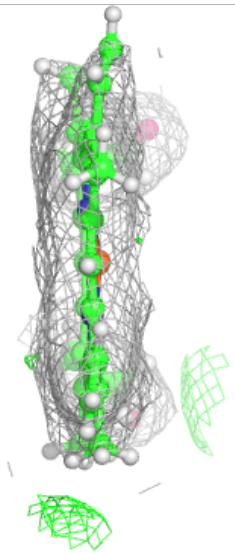


Electron density around HEM D 600:

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

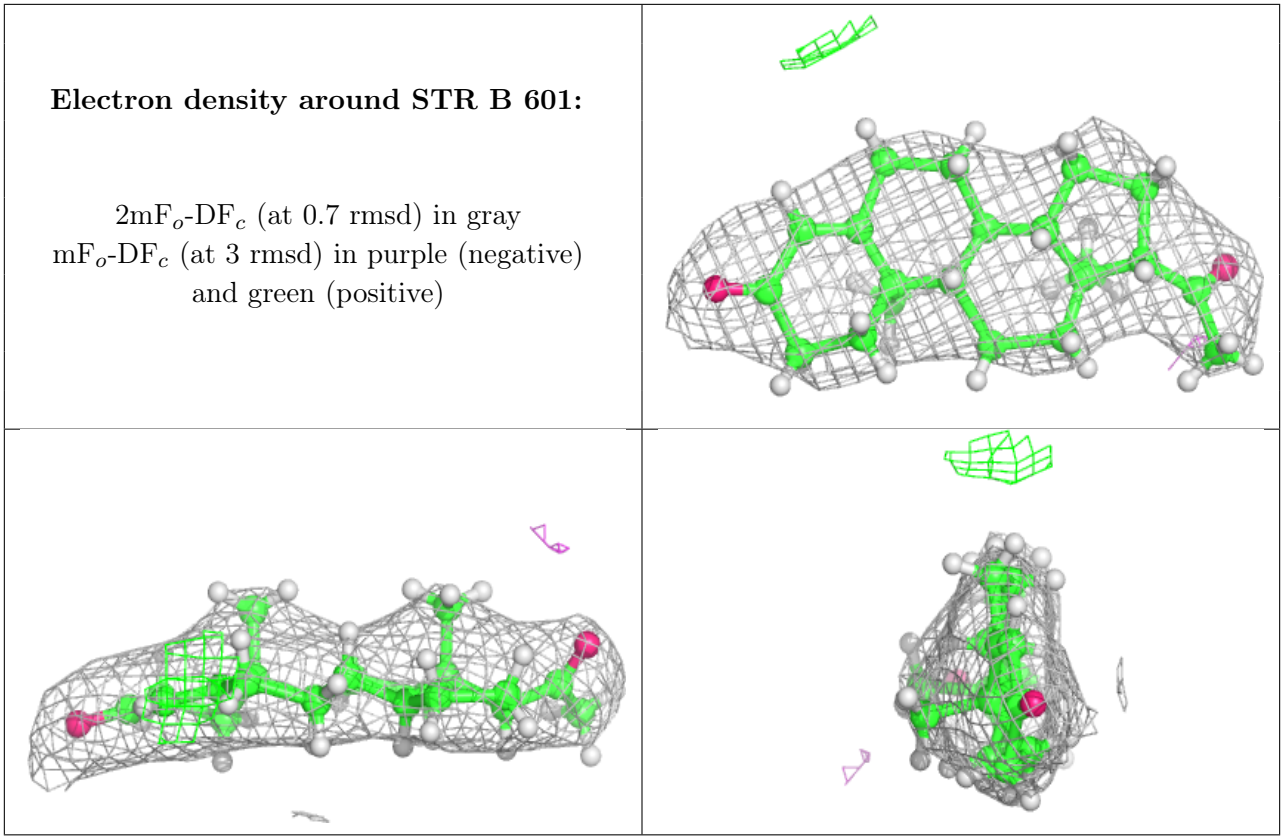






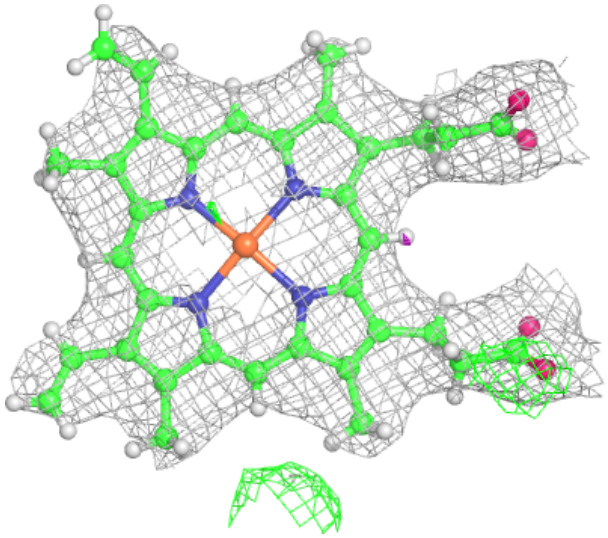
Electron density around STR B 601:

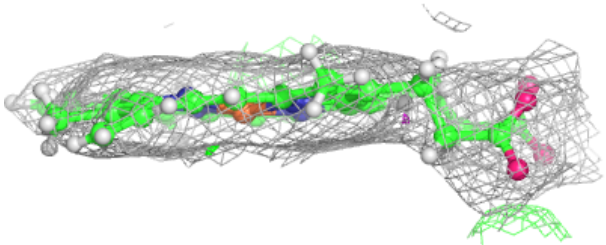
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

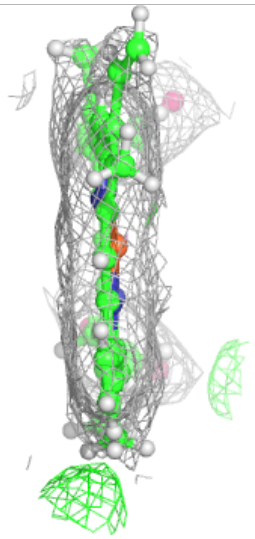


Electron density around HEM B 600:

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

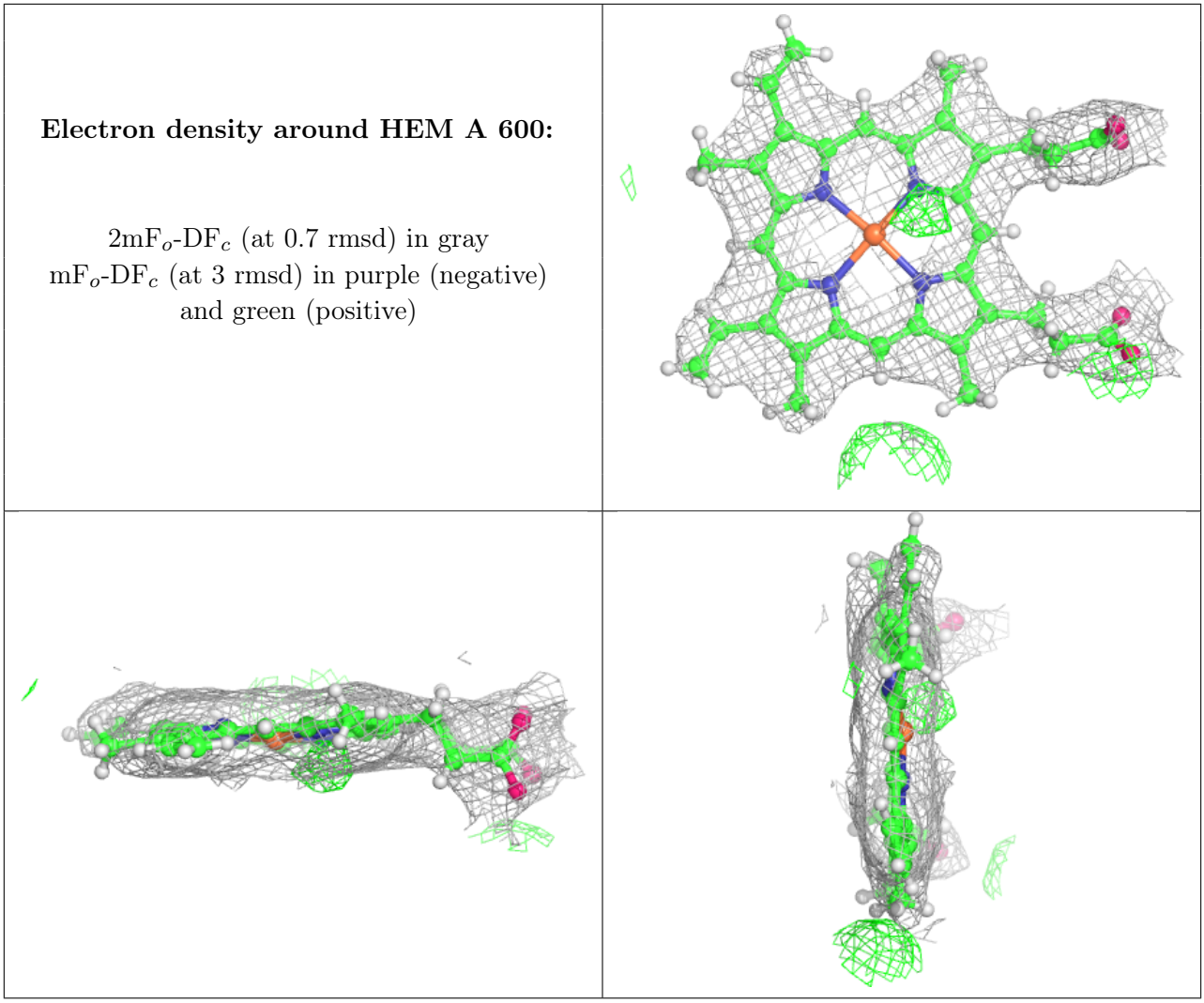






Electron density around HEM A 600:

$2mF_o$-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.