Full wwPDB X-ray Structure Validation Report (i)

Apr 8, 2025 – 12:11 PM EDT

PDB ID	:	9DFG / pdb_00009dfg
Title	:	Crystal structure of PrnB in complex with 7-Cl-Trp
Authors	:	Li, B.; Wang, Y.
Deposited on	:	2024-08-30
Resolution	:	2.42 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 (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:

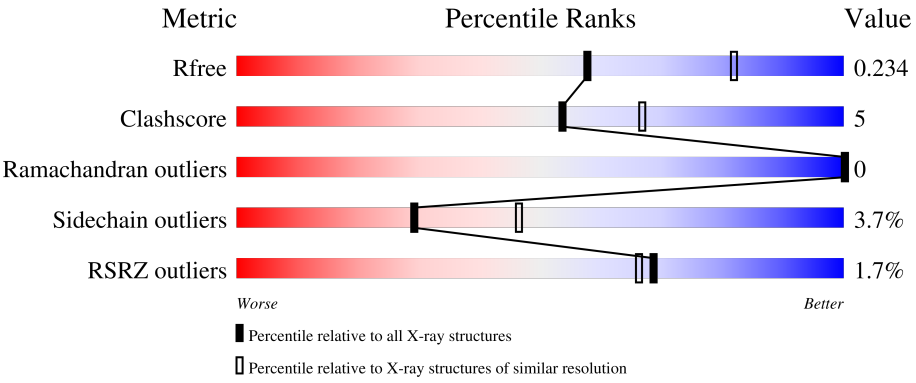
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

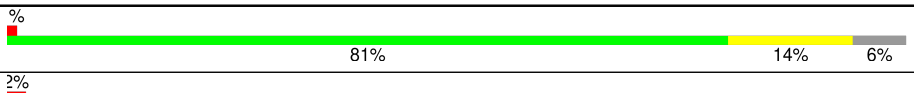
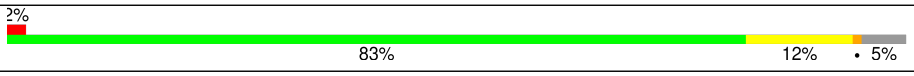
The reported resolution of this entry is 2.42 Å.

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}	164625	5670 (2.44-2.40)
Clashscore	180529	6299 (2.44-2.40)
Ramachandran outliers	177936	6232 (2.44-2.40)
Sidechain outliers	177891	6233 (2.44-2.40)
RSRZ outliers	164620	5670 (2.44-2.40)

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	370	
1	B	370	

2 Entry composition

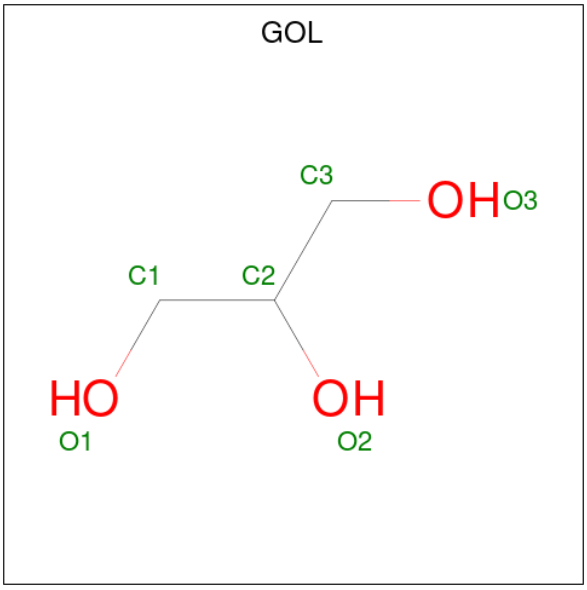
There are 5 unique types of molecules in this entry. The entry contains 5972 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PrnB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	1	0
			2764	1775	463	519	7			
1	B	352	Total	C	N	O	S	0	1	0
			2796	1798	467	524	7			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

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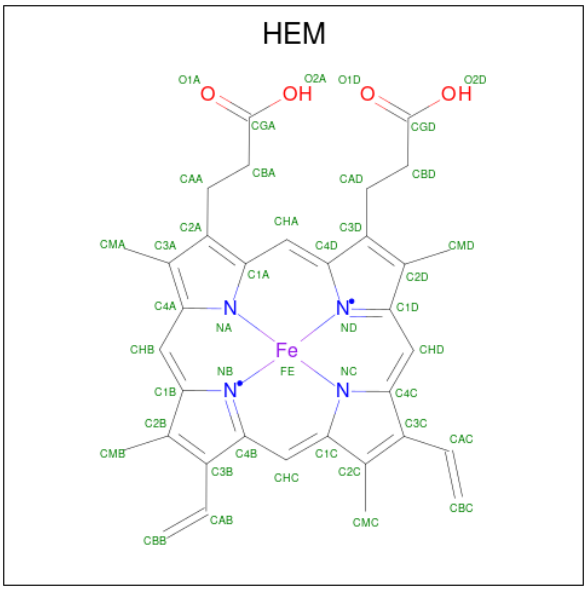
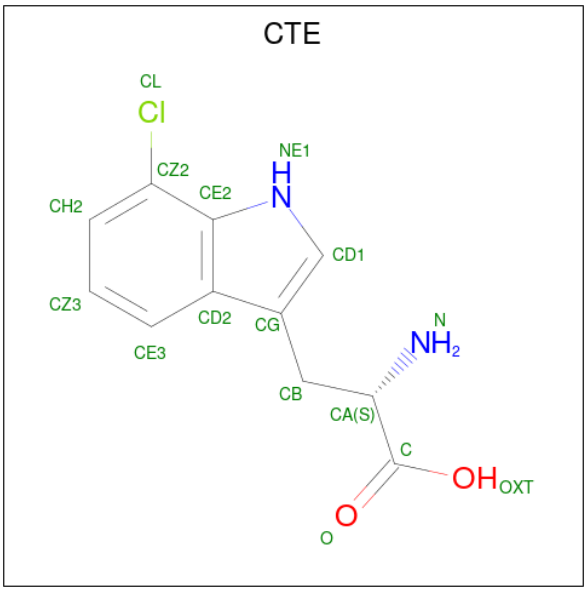
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 6 3 3	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is 7-CHLOROTRYPTOPHAN (CCD ID: CTE) (formula: $C_{11}H_{11}ClN_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			16	11	1	2	2		
4	B	1	Total	C	Cl	N	O	0	0
			16	11	1	2	2		

- Molecule 5 is water.

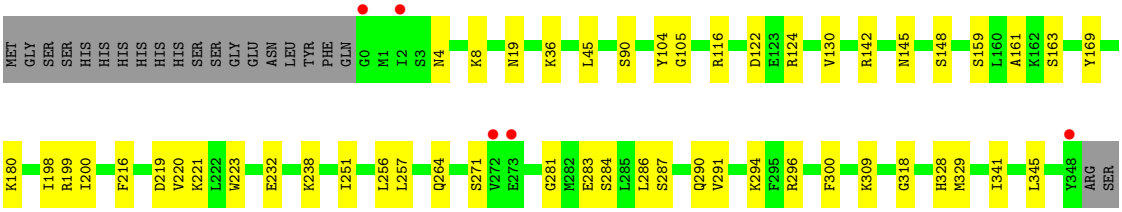
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	132	Total	O	0	0
			132	132		
5	B	132	Total	O	0	0
			132	132		

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.

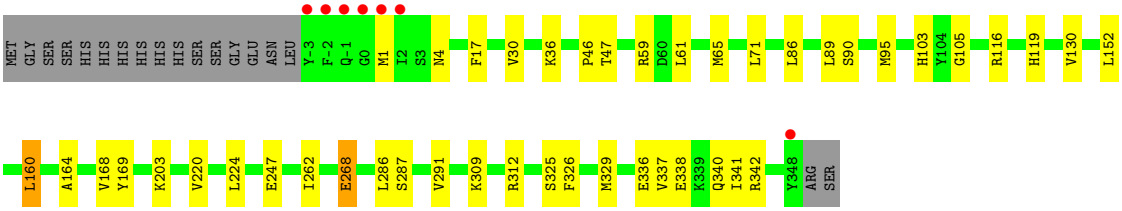
• Molecule 1: PrnB

Chain A:



• Molecule 1: PrnB

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.01Å 122.52Å 66.74Å 90.00° 94.64° 90.00°	Depositor
Resolution (Å)	46.63 – 2.42 46.63 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.63-2.42) 94.3 (46.63-2.42)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.181 , 0.234 0.181 , 0.234	Depositor DCC
R_{free} test set	40768 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å^2)	32.6	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5972	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: CTE, HEM, GOL

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	0/2828	0.61	0/3838
1	B	0.44	0/2862	0.60	0/3884
All	All	0.43	0/5690	0.60	0/7722

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	2764	0	2784	24	0
1	B	2796	0	2810	24	0
2	A	18	0	24	2	0
2	B	12	0	16	0	0
3	A	43	0	30	4	0
3	B	43	0	30	1	0
4	A	16	0	11	2	0
4	B	16	0	11	0	0
5	A	132	0	0	3	0
5	B	132	0	0	2	0
All	All	5972	0	5716	55	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 5.

All (55) 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:1:MET:HG3	1:B:247:GLU:OE2	1.87	0.74
1:A:251:ILE:HD12	1:A:251:ILE:H	1.54	0.72
1:B:116:ARG:NH1	5:B:803:HOH:O	2.31	0.63
1:A:124:ARG:HG2	5:A:716:HOH:O	2.01	0.59
1:A:286:LEU:HB2	1:A:341:ILE:HG21	1.83	0.59
1:B:309:LYS:HE2	1:B:312:ARG:NH2	2.17	0.59
3:A:604:HEM:HBB2	3:A:604:HEM:HMB1	1.88	0.55
1:B:336:GLU:O	1:B:340:GLN:HG3	2.06	0.55
1:A:116:ARG:HH12	1:A:124:ARG:CZ	2.20	0.55
1:A:19:ASN:OD1	5:A:701:HOH:O	2.18	0.54
1:B:105:GLY:HA3	1:B:130:VAL:HG23	1.89	0.54
1:A:232:GLU:HB3	1:A:329:MET:CE	2.39	0.53
3:B:703:HEM:HMB2	3:B:703:HEM:HBB2	1.93	0.50
1:B:152:LEU:HD12	1:B:268:GLU:HG2	1.94	0.50
1:B:220:VAL:HA	1:B:224:LEU:HB3	1.94	0.49
1:A:283:GLU:OE1	1:A:345:LEU:HD13	2.13	0.49
3:A:604:HEM:HHA	3:A:604:HEM:HBA2	1.94	0.48
1:B:338:GLU:HG2	1:B:342:ARG:HD2	1.95	0.48
2:A:602:GOL:O3	2:A:602:GOL:O1	2.31	0.48
1:B:90:SER:HB2	1:B:95:MET:O	2.13	0.48
1:B:262:ILE:HD13	1:B:341:ILE:HD11	1.96	0.48
1:B:164:ALA:O	1:B:168:VAL:HG23	2.15	0.47
1:A:4:ASN:O	1:A:8:LYS:HG2	2.15	0.46
1:A:220:VAL:HG11	1:A:256:LEU:HG	1.97	0.46
1:B:59:ARG:HB2	1:B:103:HIS:HB3	1.98	0.46
1:B:286:LEU:HB2	1:B:341:ILE:HG21	1.97	0.46
1:A:281:GLY:O	1:A:284:SER:OG	2.30	0.46
1:A:198:ILE:HG22	1:A:200:ILE:HG13	1.99	0.45
1:B:326:PHE:O	1:B:329:MET:HG3	2.17	0.45
1:A:145:ASN:HA	1:A:221:LYS:HE3	1.99	0.44
1:A:104:TYR:CD2	4:A:605:CTE:CL	3.08	0.44
1:B:287:SER:O	1:B:291:VAL:HG23	2.17	0.44
1:A:300:PHE:HE1	1:A:328:HIS:HB2	1.83	0.44
3:A:604:HEM:C1C	4:A:605:CTE:HE3	2.53	0.44
1:A:290:GLN:O	1:A:294:LYS:HG3	2.18	0.43
3:A:604:HEM:HBC2	3:A:604:HEM:HMC2	1.98	0.43
1:B:36:LYS:HD3	1:B:36:LYS:HA	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LYS:HD3	1:A:36:LYS:HA	1.76	0.43
1:A:105:GLY:HA3	1:A:130:VAL:HG23	2.01	0.43
1:B:65:MET:SD	1:B:86:LEU:HD11	2.59	0.43
2:A:603:GOL:H12	5:B:853:HOH:O	2.20	0.42
1:A:116:ARG:HH12	1:A:124:ARG:NH1	2.17	0.42
1:B:247:GLU:H	1:B:247:GLU:CD	2.23	0.42
1:A:216:PHE:O	1:A:220:VAL:HG23	2.19	0.42
1:A:219:ASP:OD1	1:A:223:TRP:NE1	2.50	0.41
1:A:219:ASP:OD2	1:A:296:ARG:NH2	2.52	0.41
1:B:17:PHE:CD1	1:B:36:LYS:HE3	2.56	0.41
1:B:337:VAL:O	1:B:341:ILE:HG13	2.20	0.41
1:A:287:SER:O	1:A:291:VAL:HG23	2.20	0.41
1:B:61:LEU:O	1:B:65:MET:HG3	2.20	0.41
1:A:161:ALA:HB3	1:A:284:SER:HB2	2.02	0.41
1:B:30:VAL:HB	1:B:71:LEU:HD13	2.03	0.40
1:B:160:LEU:HD12	1:B:160:LEU:HA	1.85	0.40
1:A:318:GLY:HA2	5:A:810:HOH:O	2.21	0.40
1:B:46:PRO:HB3	1:B:89:LEU:HD13	2.04	0.40

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	348/370 (94%)	341 (98%)	7 (2%)	0	100	100
1	B	351/370 (95%)	343 (98%)	8 (2%)	0	100	100
All	All	699/740 (94%)	684 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	310/328 (94%)	295 (95%)	15 (5%)	21 35
1	B	313/328 (95%)	305 (97%)	8 (3%)	41 60
All	All	623/656 (95%)	600 (96%)	23 (4%)	29 46

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	90	SER
1	A	122	ASP
1	A	142	ARG
1	A	148	SER
1	A	159	SER
1	A	163	SER
1	A	169	TYR
1	A	180	LYS
1	A	199	ARG
1	A	238	LYS
1	A	257	LEU
1	A	264	GLN
1	A	271	SER
1	A	309	LYS
1	B	4	ASN
1	B	47	THR
1	B	119	HIS
1	B	160	LEU
1	B	169	TYR
1	B	203	LYS
1	B	268	GLU
1	B	325	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

9 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	GOL	A	603	-	5,5,5	1.25	1 (20%)	5,5,5	0.93	0
2	GOL	A	602	-	5,5,5	0.84	0	5,5,5	1.33	1 (20%)
2	GOL	B	702	-	5,5,5	1.03	0	5,5,5	0.97	0
3	HEM	A	604	4,1	42,50,50	1.52	5 (11%)	46,82,82	1.47	8 (17%)
4	CTE	A	605	3	14,17,17	1.27	1 (7%)	11,24,24	2.01	3 (27%)
2	GOL	B	701	-	5,5,5	1.07	0	5,5,5	1.09	0
4	CTE	B	704	3	14,17,17	1.20	1 (7%)	11,24,24	2.23	3 (27%)
3	HEM	B	703	4,1	42,50,50	1.52	5 (11%)	46,82,82	1.35	7 (15%)
2	GOL	A	601	-	5,5,5	0.96	0	5,5,5	1.05	0

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	GOL	A	603	-	-	2/4/4/4	-
2	GOL	A	602	-	-	1/4/4/4	-
2	GOL	B	702	-	-	2/4/4/4	-
3	HEM	A	604	4,1	-	6/12/54/54	-
4	CTE	A	605	3	-	2/7/8/8	0/2/2/2
2	GOL	B	701	-	-	2/4/4/4	-
4	CTE	B	704	3	-	2/7/8/8	0/2/2/2
3	HEM	B	703	4,1	-	4/12/54/54	-
2	GOL	A	601	-	-	4/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	604	HEM	C3C-C2C	-4.39	1.34	1.40
3	B	703	HEM	C3C-C2C	-3.93	1.35	1.40
3	B	703	HEM	C3C-CAC	3.61	1.55	1.47
3	A	604	HEM	C3C-CAC	3.26	1.55	1.47
3	B	703	HEM	CAB-C3B	3.05	1.55	1.47
3	A	604	HEM	CAB-C3B	2.85	1.55	1.47
3	A	604	HEM	C3C-C4C	2.79	1.45	1.41
3	B	703	HEM	C3C-C4C	2.50	1.45	1.41
4	A	605	CTE	OXT-C	2.41	1.38	1.30
3	B	703	HEM	FE-NB	2.36	2.11	1.98
3	A	604	HEM	CMB-C2B	2.18	1.55	1.50
4	B	704	CTE	OXT-C	2.14	1.37	1.30
2	A	603	GOL	C1-C2	2.14	1.59	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	704	CTE	CH2-CZ2-CE2	-5.33	117.23	121.08
4	A	605	CTE	CH2-CZ2-CE2	-4.02	118.17	121.08
3	A	604	HEM	C4C-CHD-C1D	3.72	127.47	122.56
4	A	605	CTE	OXT-C-O	-3.68	115.73	124.08
3	B	703	HEM	C4C-CHD-C1D	3.20	126.78	122.56
4	B	704	CTE	CE2-CZ2-CL	3.16	121.79	118.97
4	B	704	CTE	OXT-C-O	-2.90	117.51	124.08
3	A	604	HEM	C3B-C2B-C1B	2.71	108.45	106.41
3	B	703	HEM	C3B-C2B-C1B	2.71	108.45	106.41
3	B	703	HEM	C4A-C3A-C2A	2.59	108.80	107.00
4	A	605	CTE	CB-CG-CD1	-2.57	124.79	127.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	703	HEM	CMC-C2C-C3C	2.56	129.79	124.68
3	A	604	HEM	CMA-C3A-C4A	-2.55	124.72	128.46
3	B	703	HEM	C1B-NB-C4B	2.55	108.22	105.21
3	A	604	HEM	C4D-ND-C1D	2.54	108.21	105.21
3	A	604	HEM	C1B-NB-C4B	2.51	108.17	105.21
3	B	703	HEM	C2B-C1B-NB	-2.41	107.08	109.84
2	A	602	GOL	C3-C2-C1	-2.34	103.22	111.80
3	B	703	HEM	CMA-C3A-C4A	-2.19	125.24	128.46
3	A	604	HEM	O2D-CGD-CBD	2.18	120.87	114.00
3	A	604	HEM	C4A-C3A-C2A	2.08	108.44	107.00
3	A	604	HEM	C2B-C1B-NB	-2.06	107.47	109.84

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	GOL	O1-C1-C2-C3
3	A	604	HEM	C1A-C2A-CAA-CBA
3	A	604	HEM	C3A-C2A-CAA-CBA
2	A	601	GOL	O1-C1-C2-C3
2	A	601	GOL	C1-C2-C3-O3
2	A	603	GOL	C1-C2-C3-O3
2	B	702	GOL	C1-C2-C3-O3
2	A	601	GOL	O1-C1-C2-O2
2	B	701	GOL	O1-C1-C2-O2
2	A	603	GOL	O2-C2-C3-O3
2	B	702	GOL	O2-C2-C3-O3
2	A	601	GOL	O2-C2-C3-O3
4	B	704	CTE	O-C-CA-CB
4	A	605	CTE	O-C-CA-CB
4	A	605	CTE	OXT-C-CA-CB
3	B	703	HEM	C3A-C2A-CAA-CBA
3	B	703	HEM	C1A-C2A-CAA-CBA
4	B	704	CTE	OXT-C-CA-CB
2	A	602	GOL	C1-C2-C3-O3
3	A	604	HEM	CAA-CBA-CGA-O2A
3	B	703	HEM	CAA-CBA-CGA-O2A
3	A	604	HEM	CAA-CBA-CGA-O1A
3	B	703	HEM	CAA-CBA-CGA-O1A
3	A	604	HEM	CAD-CBD-CGD-O1D
3	A	604	HEM	CAD-CBD-CGD-O2D

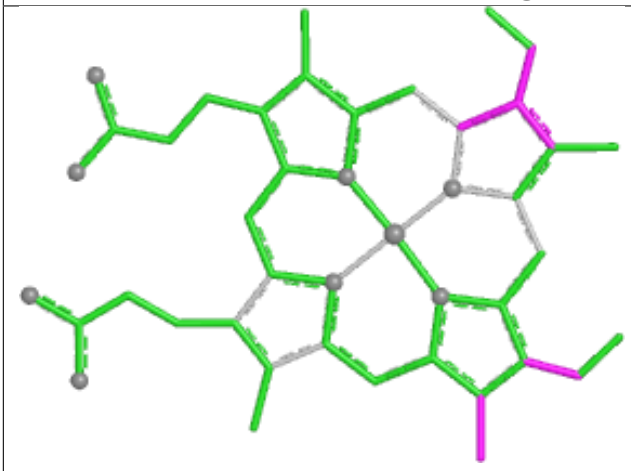
There are no ring outliers.

5 monomers are involved in 8 short contacts:

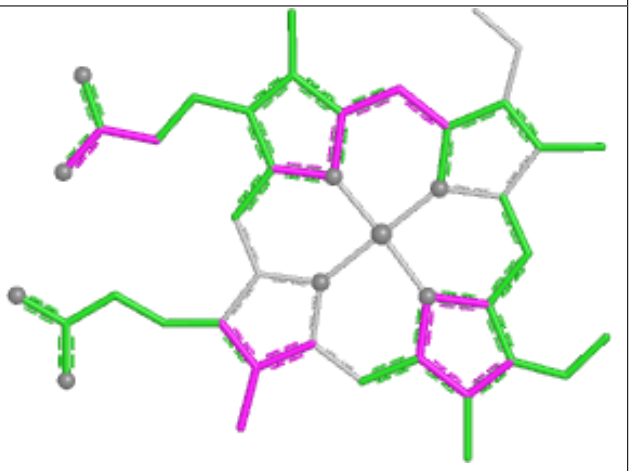
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	GOL	1	0
2	A	602	GOL	1	0
3	A	604	HEM	4	0
4	A	605	CTE	2	0
3	B	703	HEM	1	0

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.

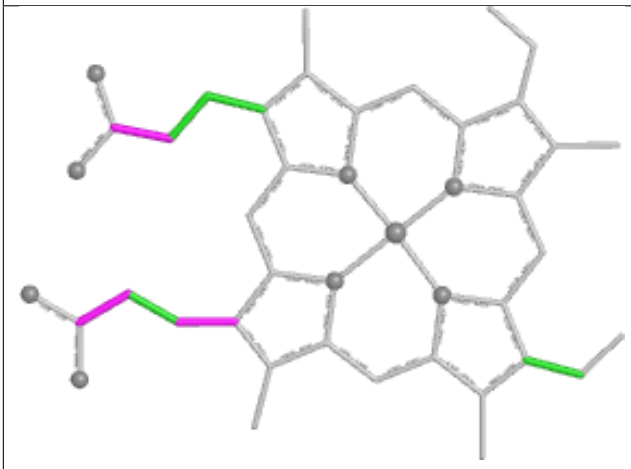
Ligand HEM A 604



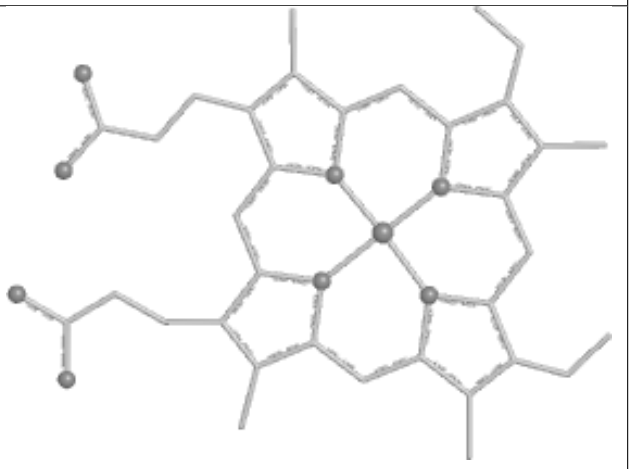
Bond lengths



Bond angles

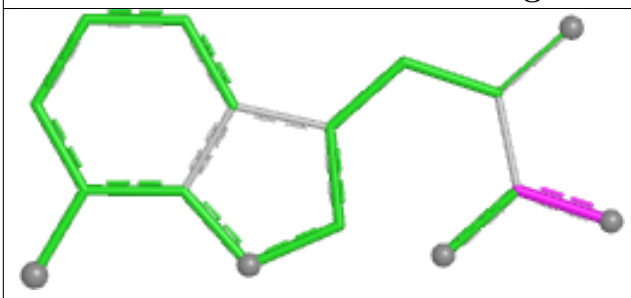


Torsions

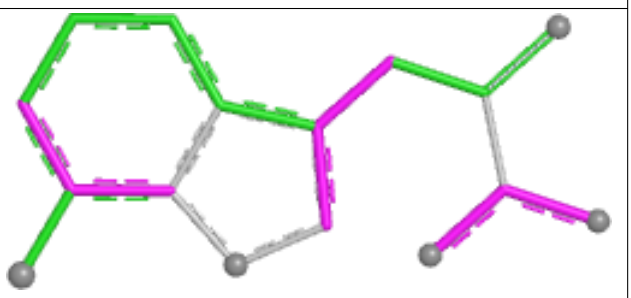


Rings

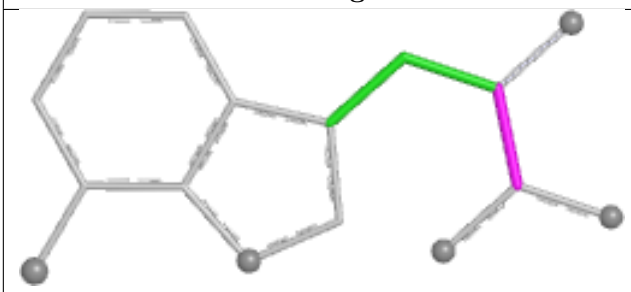
Ligand CTE A 605



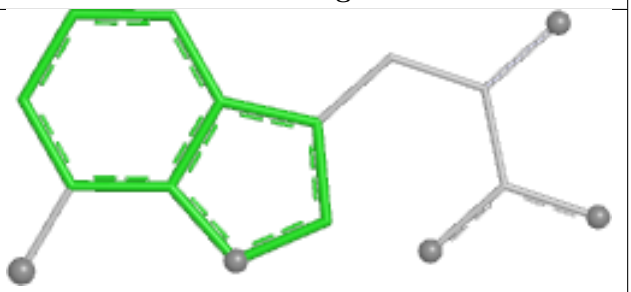
Bond lengths



Bond angles

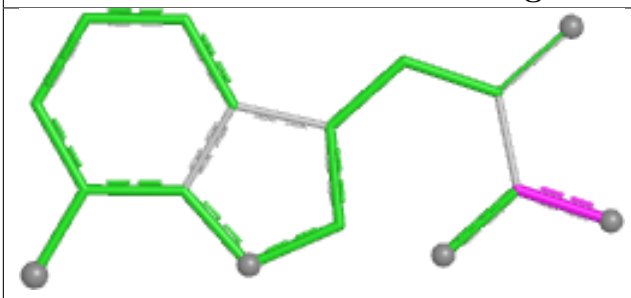


Torsions

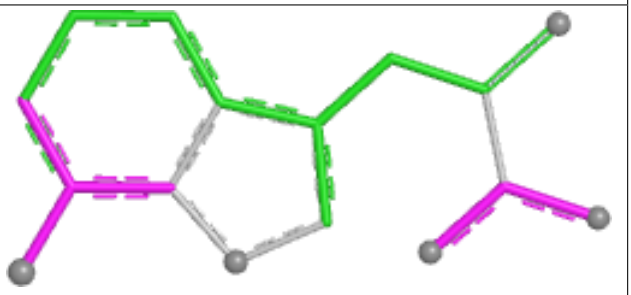


Rings

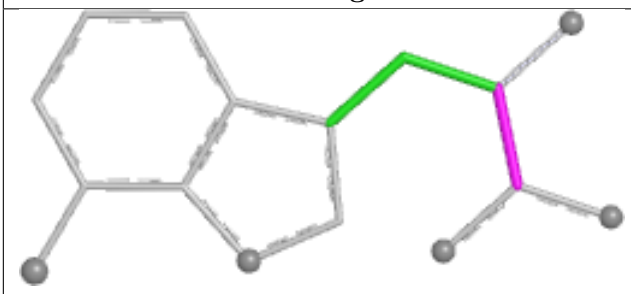
Ligand CTE B 704



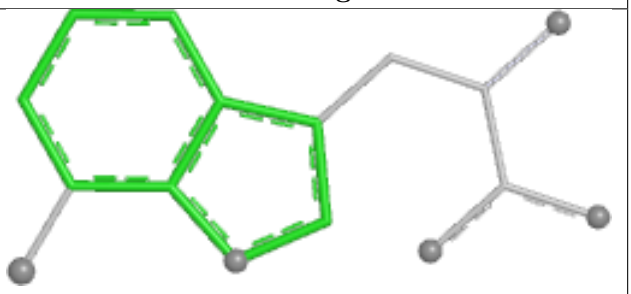
Bond lengths



Bond angles

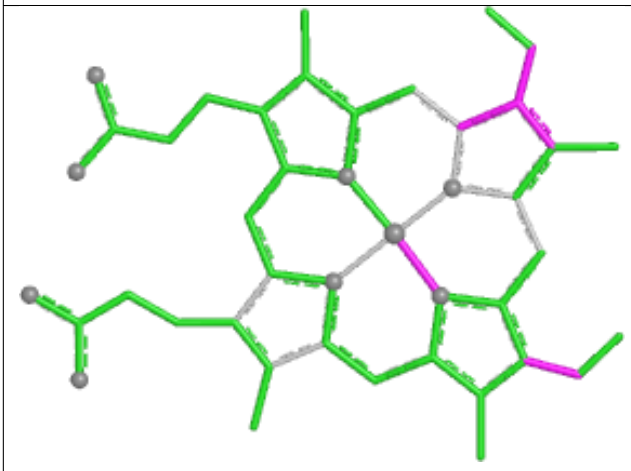


Torsions

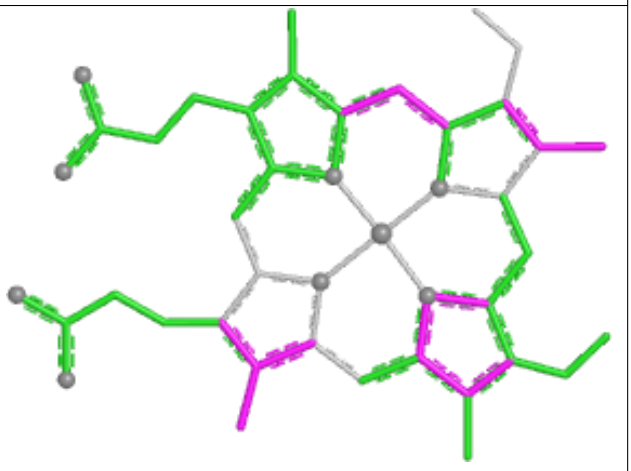


Rings

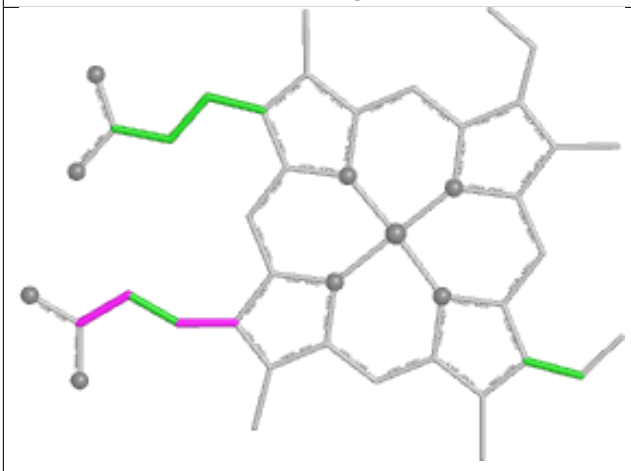
Ligand HEM B 703



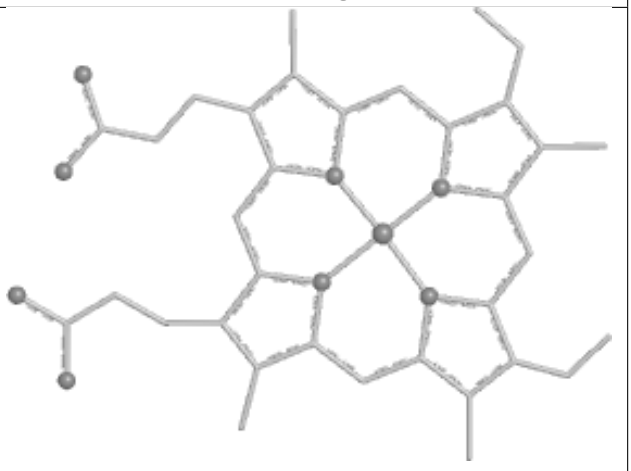
Bond lengths



Bond angles



Torsions



Rings

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	349/370 (94%)	-0.08	5 (1%)	73	71	22, 39, 61, 75	1 (0%)
1	B	352/370 (95%)	-0.09	7 (1%)	64	62	20, 38, 59, 81	1 (0%)
All	All	701/740 (94%)	-0.08	12 (1%)	69	66	20, 39, 61, 81	2 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ILE	4.6
1	B	-2	PHE	4.6
1	B	-1	GLN	4.1
1	B	0	GLY	3.3
1	B	1	MET	3.1
1	B	348	TYR	2.9
1	A	0	GLY	2.7
1	A	273	GLU	2.7
1	B	2	ILE	2.5
1	B	-3	TYR	2.3
1	A	272	VAL	2.2
1	A	348	TYR	2.1

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 (i)

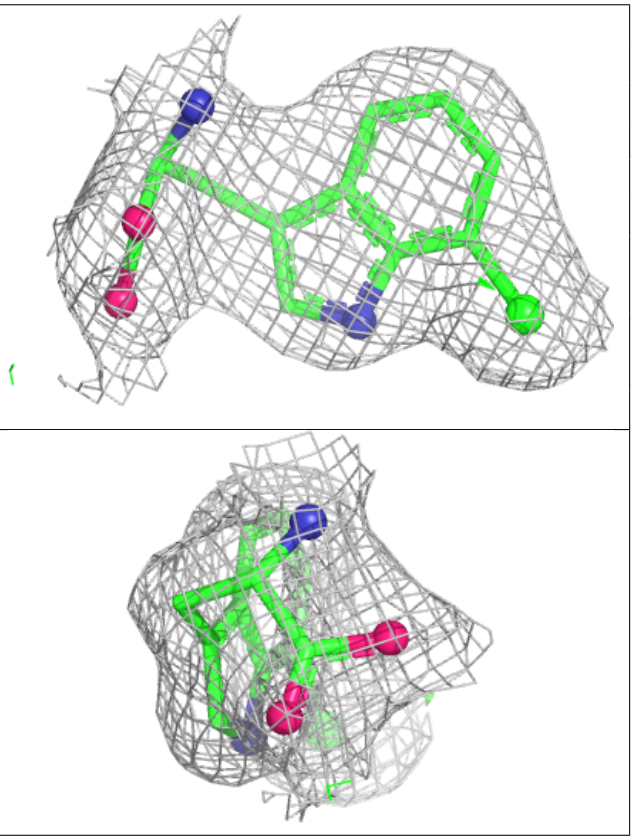
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	GOL	B	701	6/6	0.52	0.25	59,63,74,76	0
2	GOL	A	603	6/6	0.73	0.22	47,54,64,65	0
2	GOL	A	601	6/6	0.83	0.17	56,57,59,60	0
2	GOL	B	702	6/6	0.84	0.15	54,57,67,69	0
2	GOL	A	602	6/6	0.87	0.15	53,64,66,70	0
4	CTE	A	605	16/16	0.96	0.08	31,35,44,53	0
4	CTE	B	704	16/16	0.96	0.08	30,33,42,47	0
3	HEM	A	604	43/43	0.98	0.08	27,33,40,45	0
3	HEM	B	703	43/43	0.98	0.07	26,33,40,41	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.

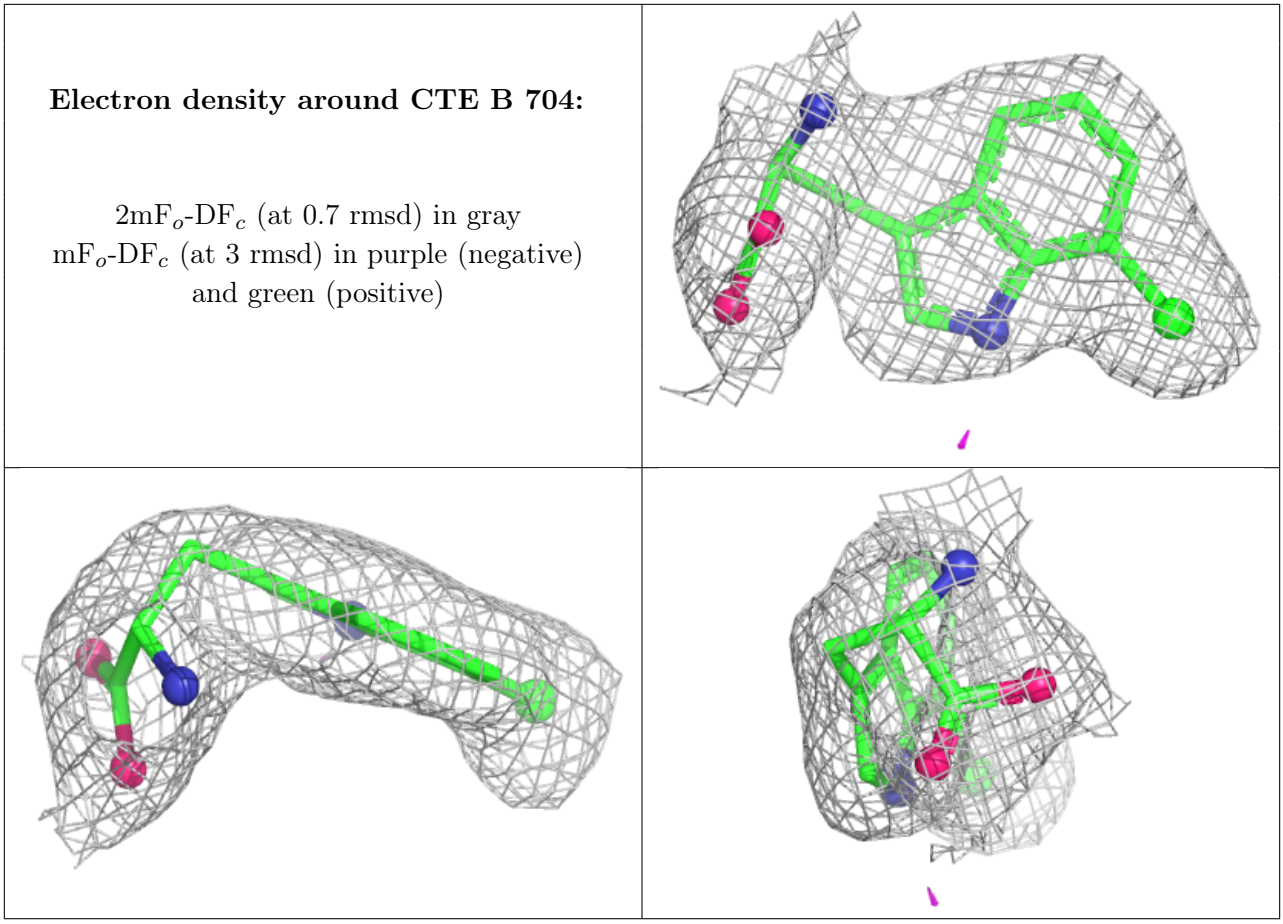
Electron density around CTE A 605:

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



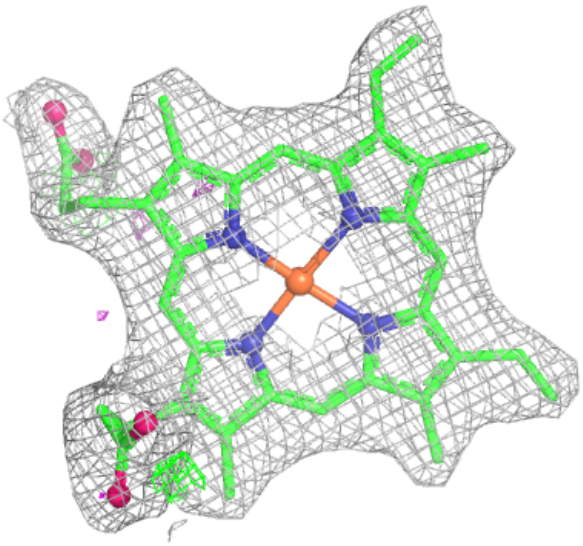
Electron density around CTE B 704:

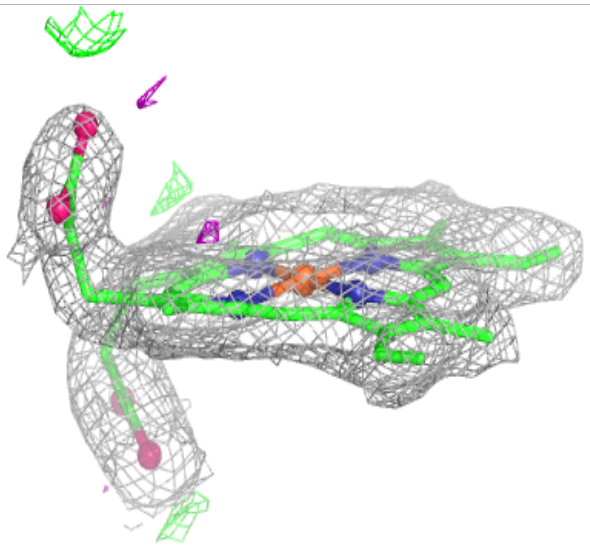
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

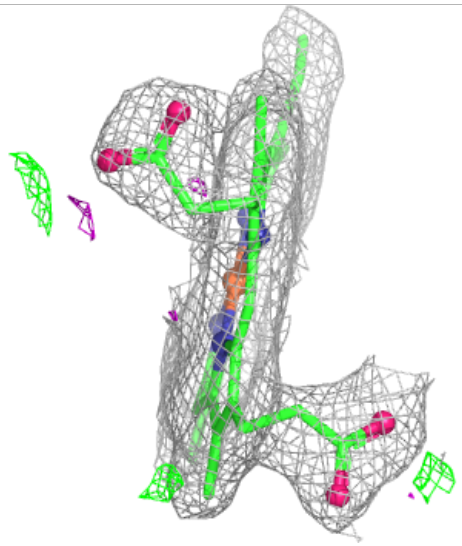


Electron density around HEM A 604:

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

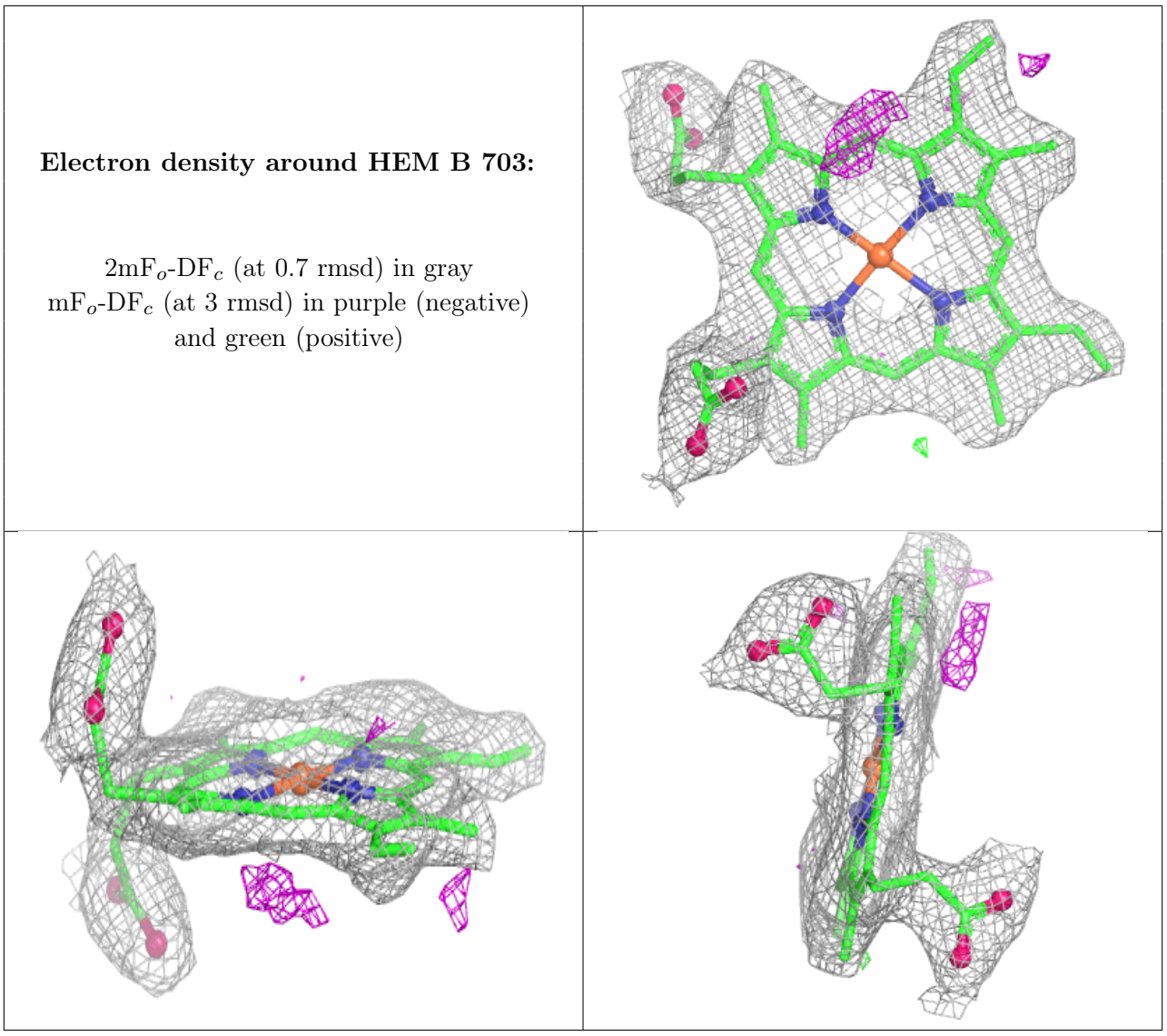






Electron density around HEM B 703:

$2mF_o$-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.