Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 12:47 PM EDT

PDB ID	:	5E58
Title	:	Crystal Structure Of Cytochrome P450 2B35 from Desert Woodrat Neotoma Lepida in complex with 4-(4-chlorophenyl)imidazole
Authors	:	Shah, M.B.; Stout, C.D.; Halpert, J.R.
Deposited on	:	2015-10-08
Resolution	:	2.40 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:

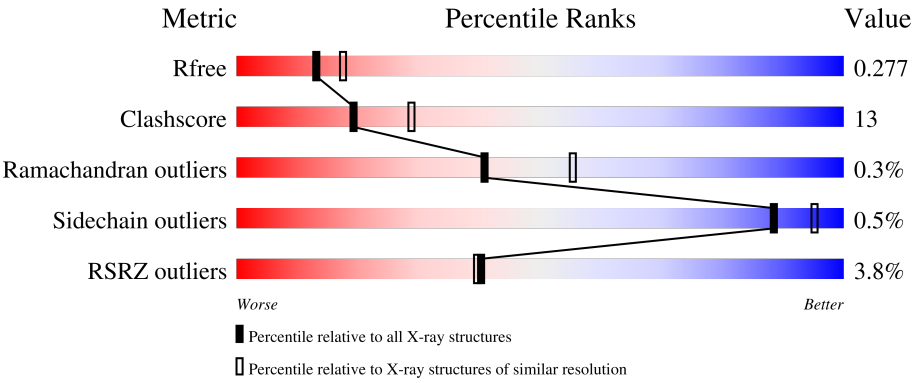
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.40 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	493	2% 83% 11% 6%
1	B	493	4% 71% 22% 7%
1	C	493	% 75% 19% 6%
1	D	493	3% 79% 15% 6%
1	E	493	3% 74% 19% 6%

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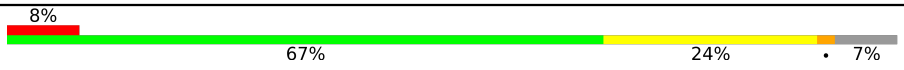
Mol	Chain	Length	Quality of chain
1	F	493	
2	G	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	G	1	-	X	-	-
2	FRU	G	2	-	-	X	-
4	CPZ	A	502	-	-	X	-
4	CPZ	B	502	-	-	X	-
4	CPZ	B	503	-	-	X	-
4	CPZ	C	502	-	-	X	-
4	CPZ	D	502	-	-	X	-
4	CPZ	E	502	-	-	X	-
4	CPZ	F	502	-	-	X	-
4	CPZ	F	503	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 23024 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.

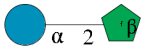
- Molecule 1 is a protein called Cytochrome P450 family 2 subfamily B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3727	2396	638	677	16			
1	B	458	Total	C	N	O	S	0	0	0
			3602	2321	607	659	15			
1	C	465	Total	C	N	O	S	0	0	0
			3685	2371	631	667	16			
1	D	463	Total	C	N	O	S	0	0	0
			3665	2360	623	666	16			
1	E	462	Total	C	N	O	S	0	0	0
			3661	2352	626	667	16			
1	F	458	Total	C	N	O	S	0	1	0
			3558	2284	608	651	15			

There are 12 discrepancies between the modelled and reference sequences:

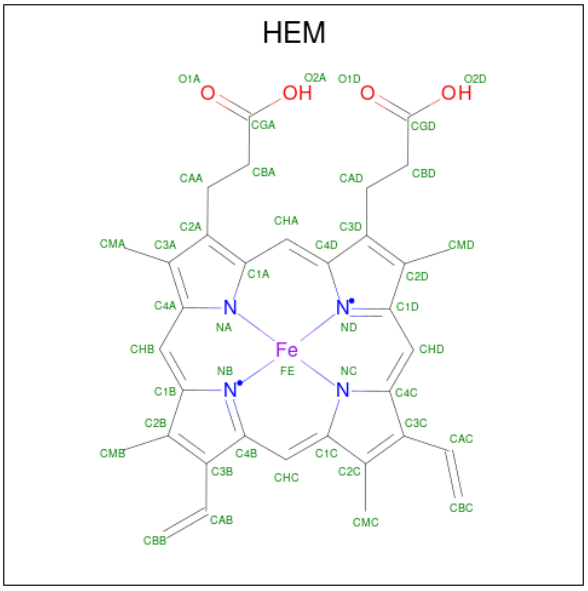
Chain	Residue	Modelled	Actual	Comment	Reference
A	492	HIS	-	expression tag	UNP J9JD66
A	493	HIS	-	expression tag	UNP J9JD66
B	492	HIS	-	expression tag	UNP J9JD66
B	493	HIS	-	expression tag	UNP J9JD66
C	492	HIS	-	expression tag	UNP J9JD66
C	493	HIS	-	expression tag	UNP J9JD66
D	492	HIS	-	expression tag	UNP J9JD66
D	493	HIS	-	expression tag	UNP J9JD66
E	492	HIS	-	expression tag	UNP J9JD66
E	493	HIS	-	expression tag	UNP J9JD66
F	492	HIS	-	expression tag	UNP J9JD66
F	493	HIS	-	expression tag	UNP J9JD66

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



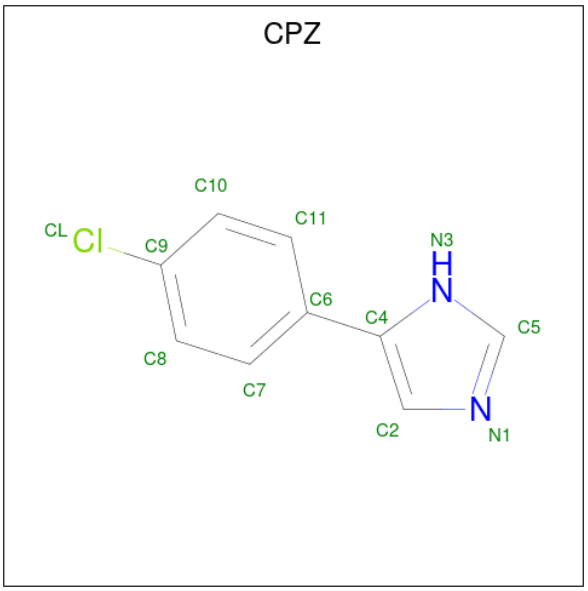
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	G	2	Total C O 23 12 11	0	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



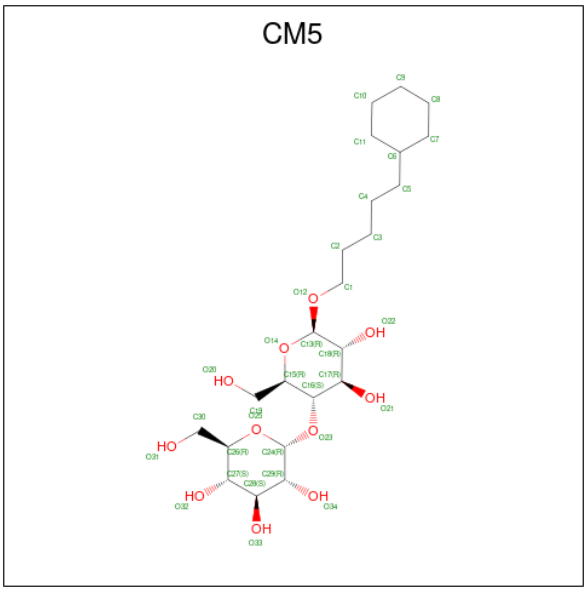
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Fe N O 43 34 1 4 4	0	0
3	B	1	Total C Fe N O 43 34 1 4 4	0	0
3	C	1	Total C Fe N O 43 34 1 4 4	0	0
3	D	1	Total C Fe N O 43 34 1 4 4	0	0
3	E	1	Total C Fe N O 43 34 1 4 4	0	0
3	F	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 4 is 4-(4-CHLOROPHENYL)IMIDAZOLE (three-letter code: CPZ) (formula: $C_9H_7ClN_2$).



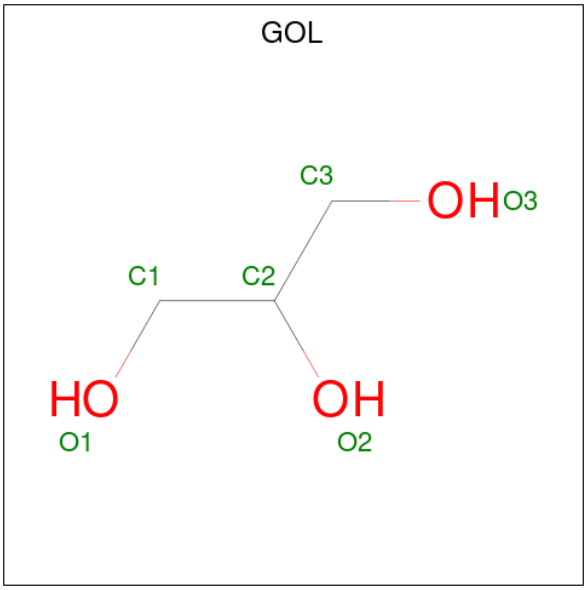
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	A	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	B	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	B	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	C	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	C	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	D	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	D	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	E	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	E	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	F	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	F	1	Total	C	Cl	N	0	0
			12	9	1	2		

- Molecule 5 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSIDE (three-letter code: CM5) (formula: $C_{23}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 6 6	0	0
5	E	1	Total C O 12 11 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 7 is water.

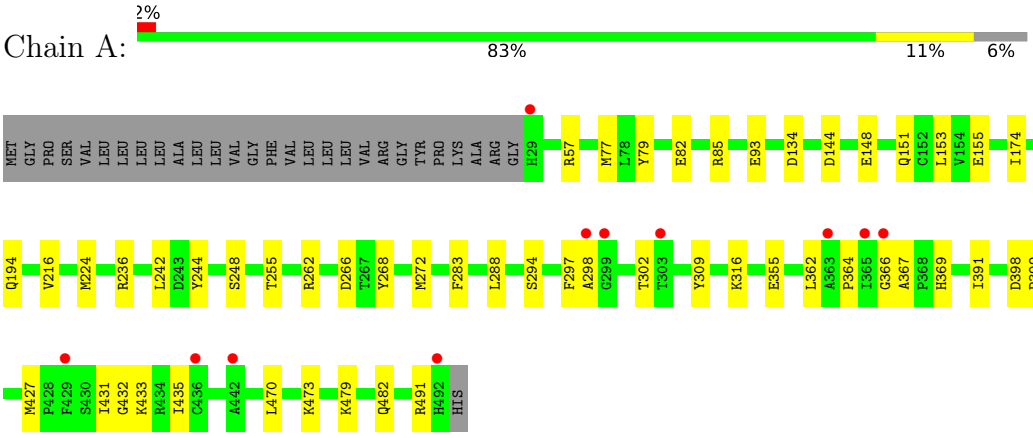
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	211	Total O 211 211	0	0
7	B	59	Total O 59 59	0	0
7	C	124	Total O 124 124	0	0
7	D	106	Total O 106 106	0	0
7	E	99	Total O 99 99	0	0
7	F	60	Total O 60 60	0	0

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.

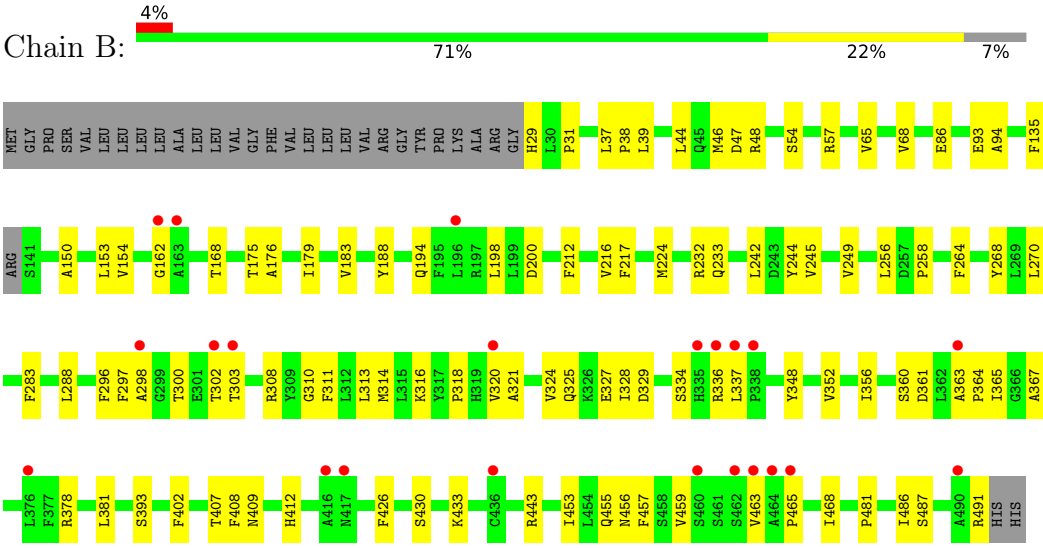
• Molecule 1: Cytochrome P450 family 2 subfamily B

Chain A:



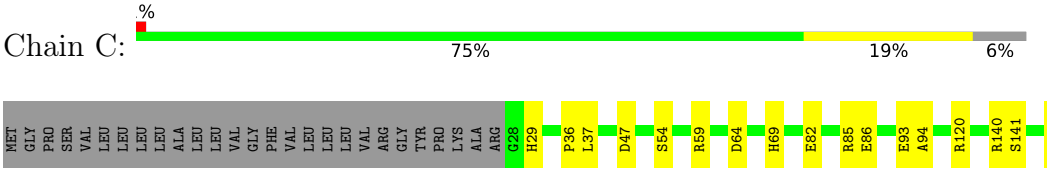
• Molecule 1: Cytochrome P450 family 2 subfamily B

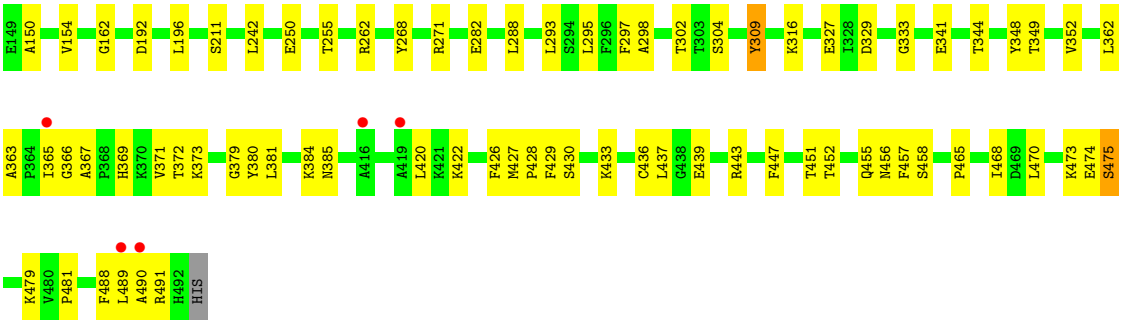
Chain B:



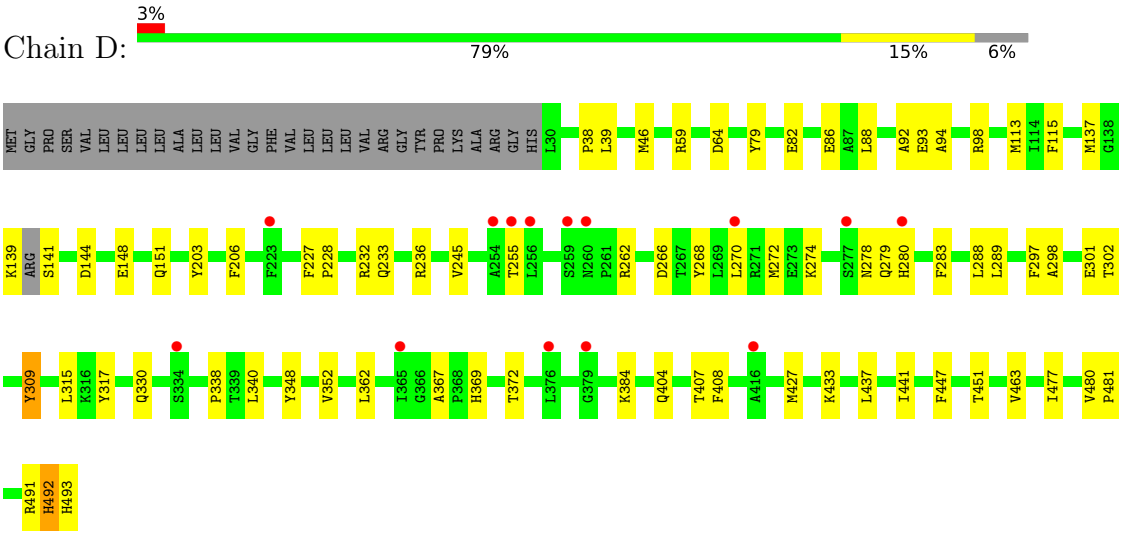
• Molecule 1: Cytochrome P450 family 2 subfamily B

Chain C:

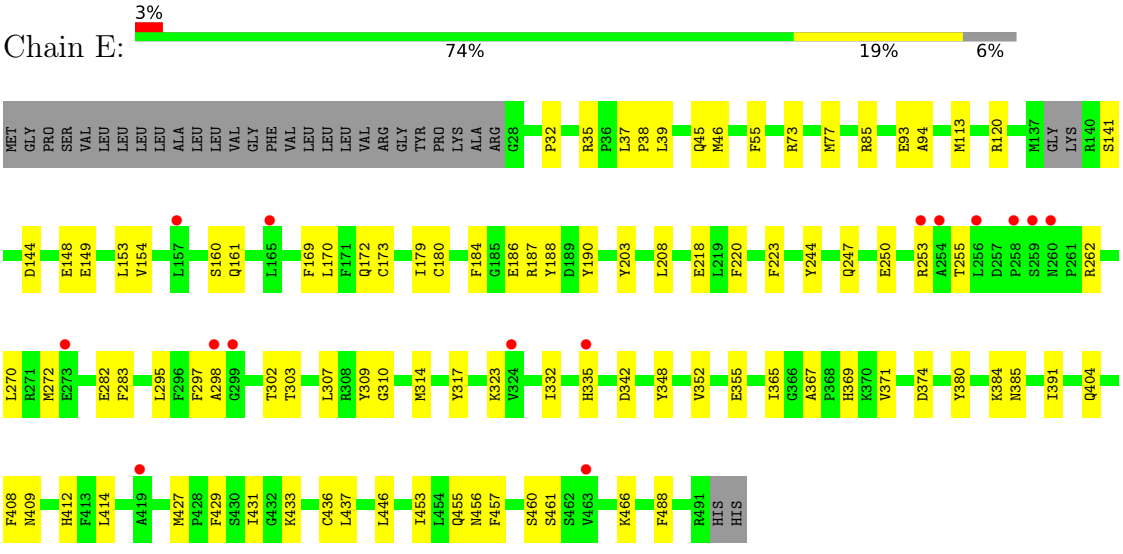




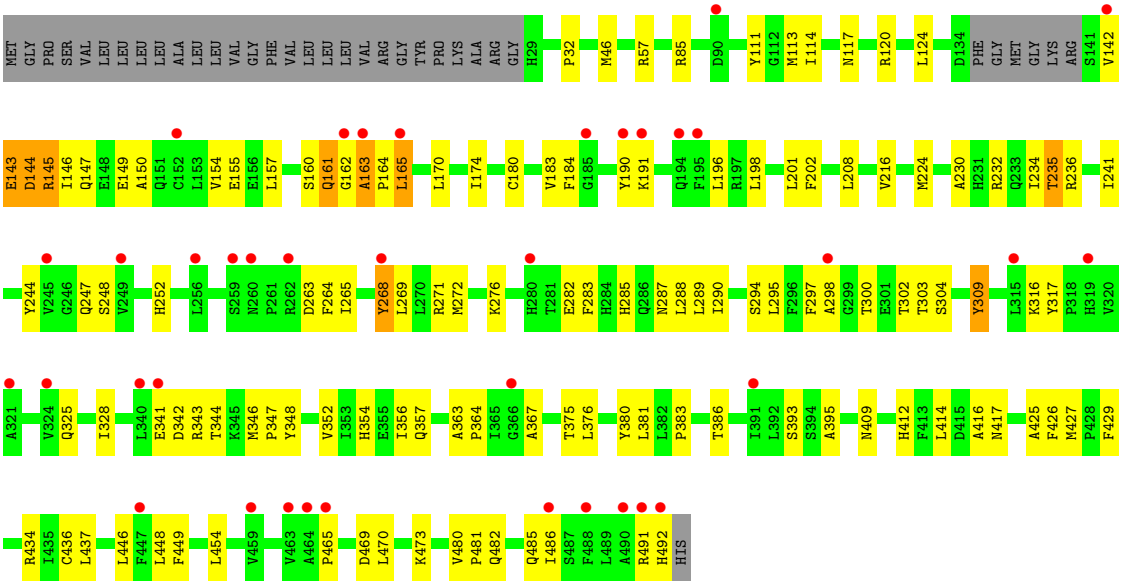
• Molecule 1: Cytochrome P450 family 2 subfamily B



• Molecule 1: Cytochrome P450 family 2 subfamily B



• Molecule 1: Cytochrome P450 family 2 subfamily B



• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	98.08Å 106.07Å 106.20Å 64.61° 82.53° 69.93°	Depositor
Resolution (Å)	40.00 – 2.40 39.72 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.9 (40.00-2.40) 94.9 (39.72-2.40)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.216 , 0.283 0.229 , 0.277	Depositor DCC
R_{free} test set	6567 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	43.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 63.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23024	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: GOL, CM5, CPZ, HEM, FRU, GLC

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	0.57	0/3819	0.67	0/5163
1	B	0.61	0/3692	0.67	0/5008
1	C	0.57	0/3778	0.67	0/5114
1	D	0.56	0/3757	0.64	0/5090
1	E	0.51	0/3752	0.64	0/5080
1	F	0.60	0/3637	0.72	0/4936
All	All	0.57	0/22435	0.67	0/30391

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	3727	0	3708	49	0
1	B	3602	0	3500	96	1
1	C	3685	0	3625	94	0
1	D	3665	0	3594	77	0
1	E	3661	0	3581	91	1
1	F	3558	0	3406	134	0
2	G	23	0	18	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	43	0	30	9	0
3	B	43	0	30	9	0
3	C	43	0	30	7	0
3	D	43	0	30	2	0
3	E	43	0	30	8	0
3	F	43	0	30	7	0
4	A	24	0	14	4	0
4	B	24	0	14	9	0
4	C	24	0	14	6	0
4	D	24	0	14	5	0
4	E	24	0	14	8	0
4	F	24	0	14	10	0
5	A	6	0	10	0	0
5	E	12	0	21	2	0
6	A	6	0	8	0	0
6	B	6	0	8	1	0
6	C	6	0	8	0	0
6	E	6	0	8	0	0
7	A	211	0	0	12	0
7	B	59	0	0	8	0
7	C	124	0	0	13	0
7	D	106	0	0	13	0
7	E	99	0	0	14	0
7	F	60	0	0	16	0
All	All	23024	0	21759	571	1

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 13.

All (571) 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:E:455:GLN:NE2	7:E:601:HOH:O	1.79	1.15
2:G:1:GLC:O2	2:G:2:FRU:O3	1.70	1.06
1:A:297:PHE:O	1:A:298:ALA:HB3	1.60	1.02
1:B:297:PHE:O	1:B:298:ALA:HB3	1.60	1.01
1:F:157:LEU:O	1:F:160:SER:HB3	1.62	1.00
1:E:297:PHE:O	1:E:298:ALA:HB3	1.60	0.99
1:C:297:PHE:O	1:C:298:ALA:HB3	1.60	0.98
1:D:297:PHE:O	1:D:298:ALA:HB3	1.60	0.98
7:A:603:HOH:O	2:G:2:FRU:C6	2.12	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:LEU:HD12	1:F:165:LEU:N	1.74	0.98
1:F:297:PHE:O	1:F:298:ALA:HB3	1.60	0.97
1:A:431:ILE:CD1	2:G:2:FRU:H3	1.97	0.94
1:F:165:LEU:N	1:F:165:LEU:CD1	2.30	0.94
1:B:465:PRO:HA	1:B:468:ILE:HD12	1.50	0.93
1:B:135:PHE:HB3	7:B:602:HOH:O	1.68	0.93
1:F:234:ILE:O	1:F:234:ILE:HG22	1.67	0.92
1:D:151:GLN:HG3	7:D:675:HOH:O	1.69	0.92
1:A:255:THR:OG1	1:A:262:ARG:NH2	2.04	0.90
1:B:365:ILE:O	1:B:365:ILE:HG22	1.68	0.90
2:G:1:GLC:C2	2:G:2:FRU:O3	2.20	0.90
3:A:501:HEM:HBB2	3:A:501:HEM:HMB2	1.52	0.89
1:F:282:GLU:OE2	1:F:287:ASN:ND2	2.07	0.88
1:A:431:ILE:HD11	2:G:2:FRU:H3	1.56	0.88
1:C:365:ILE:HG22	1:C:366:GLY:H	1.39	0.87
1:F:375:THR:HG22	1:F:376:LEU:N	1.88	0.87
1:C:365:ILE:HG22	1:C:366:GLY:N	1.89	0.86
1:B:297:PHE:O	1:B:298:ALA:CB	2.23	0.85
1:D:255:THR:OG1	1:D:262:ARG:NH2	2.09	0.85
3:D:501:HEM:HBB2	3:D:501:HEM:HMB2	1.59	0.84
1:B:57:ARG:HH12	1:E:35:ARG:HE	1.25	0.84
1:D:139:LYS:O	1:D:141:SER:HB2	1.77	0.84
1:C:474:GLU:N	7:C:601:HOH:O	2.09	0.84
1:F:297:PHE:O	1:F:298:ALA:CB	2.23	0.83
1:B:93:GLU:OE1	1:B:433:LYS:NZ	2.10	0.83
1:D:298:ALA:HA	1:D:302:THR:HG23	1.60	0.83
1:F:165:LEU:CD1	1:F:165:LEU:H	1.90	0.83
1:F:248:SER:HB2	7:F:624:HOH:O	1.77	0.83
1:F:234:ILE:O	1:F:235:THR:HB	1.79	0.83
1:B:212:PHE:HZ	1:E:38:PRO:HB3	1.43	0.83
1:F:208:LEU:HB3	1:F:234:ILE:HD11	1.60	0.82
1:D:297:PHE:O	1:D:298:ALA:CB	2.23	0.81
1:C:309:TYR:CZ	1:C:481:PRO:HB3	2.16	0.81
1:E:297:PHE:O	1:E:298:ALA:CB	2.23	0.81
1:A:297:PHE:O	1:A:298:ALA:CB	2.23	0.81
1:E:298:ALA:HA	1:E:302:THR:HG23	1.62	0.81
1:C:309:TYR:CE1	1:C:481:PRO:HB3	2.16	0.81
3:B:501:HEM:HMB1	3:B:501:HEM:HBB2	1.63	0.81
1:B:463:VAL:HG12	1:B:463:VAL:O	1.81	0.80
4:C:502:CPZ:HN3	4:C:503:CPZ:HN3	1.26	0.80
3:A:501:HEM:HBB2	3:A:501:HEM:CMB	2.09	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:GLN:HB3	7:D:654:HOH:O	1.81	0.79
1:C:297:PHE:O	1:C:298:ALA:CB	2.23	0.78
1:E:255:THR:OG1	1:E:262:ARG:NH2	2.17	0.77
1:F:124:LEU:HD13	7:F:622:HOH:O	1.85	0.77
1:F:165:LEU:O	1:F:485:GLN:HA	1.86	0.76
1:F:357:GLN:HE21	1:F:426:PHE:HZ	1.34	0.75
1:E:169:PHE:CE2	1:E:173:CYS:SG	2.79	0.75
1:A:404:GLN:HE21	1:B:407:THR:HG22	1.52	0.74
1:E:369:HIS:NE2	3:E:501:HEM:O2A	2.17	0.74
1:D:233:GLN:OE1	1:D:236:ARG:NH1	2.19	0.74
1:F:375:THR:CG2	1:F:376:LEU:N	2.51	0.74
1:F:367:ALA:HB1	4:F:503:CPZ:CL	2.24	0.73
7:A:603:HOH:O	2:G:2:FRU:H61	1.82	0.73
1:C:93:GLU:OE2	1:C:433:LYS:NZ	2.21	0.72
4:E:502:CPZ:HN3	4:E:503:CPZ:HN3	1.38	0.72
1:F:247:GLN:NE2	7:F:603:HOH:O	2.20	0.72
1:E:141:SER:HA	7:E:622:HOH:O	1.88	0.72
1:C:474:GLU:O	1:C:475:SER:O	2.07	0.72
1:A:404:GLN:NE2	1:B:407:THR:HG22	2.05	0.72
1:B:308:ARG:HH21	1:B:481:PRO:HD2	1.53	0.72
1:B:200:ASP:OD1	6:B:504:GOL:H31	1.89	0.72
1:D:309:TYR:CE2	1:D:481:PRO:HB3	2.26	0.71
1:F:354:HIS:NE2	7:F:604:HOH:O	2.24	0.71
1:F:269:LEU:HD23	1:F:272:MET:SD	2.30	0.71
1:D:492:HIS:O	1:D:493:HIS:HB2	1.91	0.70
1:F:114:ILE:HD13	4:F:502:CPZ:H11	1.72	0.70
1:F:386:THR:HA	7:F:653:HOH:O	1.92	0.70
1:C:473:LYS:HG2	7:C:601:HOH:O	1.92	0.69
1:F:309:TYR:OH	1:F:470:LEU:O	2.09	0.69
1:C:140:ARG:NH2	1:C:144:ASP:OD1	2.24	0.69
1:F:375:THR:O	1:F:381:LEU:HD12	1.93	0.69
1:B:308:ARG:HH21	1:B:481:PRO:CD	2.06	0.69
1:C:298:ALA:HB2	4:C:502:CPZ:C11	2.22	0.69
1:F:469:ASP:OD2	1:F:482:GLN:NE2	2.25	0.69
1:F:201:LEU:HD23	1:F:241:ILE:HG13	1.75	0.68
1:A:236:ARG:NH1	7:A:605:HOH:O	2.26	0.68
4:A:502:CPZ:HN3	4:A:503:CPZ:HN3	1.41	0.68
1:D:384:LYS:NZ	7:D:604:HOH:O	2.26	0.68
1:A:479:LYS:HD2	7:A:735:HOH:O	1.94	0.68
1:C:439:GLU:OE2	1:C:443:ARG:NH1	2.27	0.68
1:E:46:MET:CE	7:E:650:HOH:O	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:234:ILE:O	1:F:235:THR:CB	2.40	0.67
1:B:426:PHE:HE2	1:B:443:ARG:HH21	1.41	0.67
1:C:309:TYR:CE1	1:C:481:PRO:CB	2.77	0.67
1:A:298:ALA:HA	1:A:302:THR:HG23	1.77	0.67
1:B:327:GLU:OE2	1:B:348:TYR:HB3	1.94	0.67
1:F:357:GLN:OE1	1:F:446:LEU:HD12	1.95	0.66
1:B:179:ILE:HD13	3:B:501:HEM:HBC1	1.77	0.66
1:D:278:ASN:OD1	1:D:279:GLN:N	2.29	0.66
1:F:268:TYR:O	1:F:269:LEU:C	2.34	0.66
1:C:379:GLY:O	7:C:602:HOH:O	2.12	0.66
1:F:342:ASP:O	1:F:346:MET:HG3	1.95	0.66
1:F:363:ALA:O	7:F:601:HOH:O	2.12	0.66
1:B:365:ILE:O	1:B:365:ILE:CG2	2.42	0.65
1:D:298:ALA:HB2	4:D:503:CPZ:C11	2.26	0.65
1:E:365:ILE:O	7:E:602:HOH:O	2.15	0.65
1:E:169:PHE:C	1:E:169:PHE:CD2	2.69	0.65
1:E:250:GLU:O	1:E:253:ARG:HG2	1.96	0.65
1:B:168:THR:HG23	1:B:308:ARG:HH11	1.61	0.65
1:E:46:MET:HE2	7:E:650:HOH:O	1.96	0.65
1:B:298:ALA:HB2	4:B:502:CPZ:C11	2.26	0.65
1:B:57:ARG:HH12	1:E:35:ARG:NE	1.94	0.65
1:B:402:PHE:HB3	1:B:412:HIS:HD2	1.61	0.65
1:F:165:LEU:HD12	1:F:165:LEU:H	1.50	0.64
2:G:1:GLC:C3	2:G:2:FRU:O3	2.45	0.64
1:B:336:ARG:CG	1:B:337:LEU:N	2.57	0.64
1:F:46:MET:CE	7:F:628:HOH:O	2.44	0.64
1:F:268:TYR:CD1	1:F:272:MET:HG2	2.33	0.64
1:D:309:TYR:CZ	1:D:481:PRO:HA	2.32	0.64
1:B:298:ALA:HA	1:B:302:THR:HG23	1.79	0.64
1:E:113:MET:SD	1:E:295:LEU:HD21	2.37	0.64
1:D:144:ASP:OD1	7:D:601:HOH:O	2.15	0.64
1:F:298:ALA:HA	1:F:302:THR:HG23	1.79	0.64
1:C:373:LYS:NZ	7:C:608:HOH:O	2.28	0.64
1:C:456:ASN:O	1:C:457:PHE:HD1	1.81	0.64
1:B:308:ARG:NH2	1:B:481:PRO:HD2	2.13	0.63
1:D:309:TYR:CZ	1:D:481:PRO:HB3	2.34	0.63
1:F:271:ARG:HG2	1:F:271:ARG:O	1.97	0.63
3:B:501:HEM:HBB2	3:B:501:HEM:CMB	2.28	0.63
4:D:502:CPZ:HN3	4:D:503:CPZ:HN3	1.44	0.63
1:F:191:LYS:HA	1:F:196:LEU:HD11	1.81	0.63
1:F:157:LEU:O	1:F:160:SER:CB	2.44	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:PHE:CD1	5:E:504:CM5:H111	2.34	0.62
1:B:327:GLU:CD	1:B:348:TYR:HB3	2.19	0.62
1:D:491:ARG:O	1:D:492:HIS:HB2	1.99	0.62
3:A:501:HEM:HMB2	3:A:501:HEM:CBB	2.28	0.62
1:E:144:ASP:O	1:E:148:GLU:HG3	1.98	0.62
1:F:57:ARG:NH1	7:F:606:HOH:O	2.28	0.62
1:D:362:LEU:HG	4:D:502:CPZ:H5	1.82	0.62
1:D:384:LYS:HE3	7:D:604:HOH:O	1.99	0.62
1:F:143:GLU:O	1:F:146:ILE:N	2.30	0.62
1:D:384:LYS:CE	7:D:604:HOH:O	2.48	0.62
1:E:186:GLU:HG3	1:E:188:TYR:HE1	1.63	0.62
1:B:37:LEU:HD13	7:B:639:HOH:O	1.99	0.62
1:E:250:GLU:HA	1:E:253:ARG:HE	1.64	0.62
1:A:272:MET:HG3	1:A:283:PHE:O	1.99	0.61
1:D:309:TYR:OH	1:D:481:PRO:HA	2.00	0.61
1:C:309:TYR:CD1	1:C:481:PRO:HB3	2.35	0.61
1:F:417:ASN:ND2	7:F:610:HOH:O	2.33	0.61
1:B:316:LYS:HB2	1:B:468:ILE:HG21	1.83	0.61
1:C:309:TYR:CE2	1:C:481:PRO:HB3	2.35	0.61
1:F:271:ARG:O	1:F:271:ARG:CG	2.49	0.61
1:B:233:GLN:CG	7:B:619:HOH:O	2.48	0.60
1:A:134:ASP:OD2	7:A:602:HOH:O	2.16	0.60
1:F:269:LEU:HA	1:F:272:MET:HG3	1.83	0.60
1:C:211:SER:HA	1:C:474:GLU:OE2	2.01	0.60
1:F:429:PHE:HB3	1:F:436:CYS:HB3	1.83	0.60
2:G:1:GLC:H3	2:G:2:FRU:O3	2.02	0.60
1:B:324:VAL:O	1:B:327:GLU:N	2.34	0.60
1:C:162:GLY:HA2	1:C:489:LEU:HG	1.83	0.60
1:E:85:ARG:NE	1:E:427:MET:HE3	2.17	0.60
1:B:298:ALA:HB2	4:B:502:CPZ:H11	1.82	0.60
1:C:457:PHE:CD2	1:C:488:PHE:HB3	2.36	0.60
1:F:165:LEU:H	1:F:165:LEU:HD13	1.63	0.60
1:F:348:TYR:HD1	1:F:414:LEU:HD11	1.66	0.60
3:F:501:HEM:HBA2	3:F:501:HEM:HHA	1.82	0.60
1:D:309:TYR:CE2	1:D:481:PRO:CB	2.84	0.59
1:F:232:ARG:O	1:F:235:THR:HG22	2.02	0.59
1:F:146:ILE:O	1:F:150:ALA:N	2.29	0.59
1:D:268:TYR:CE1	1:D:288:LEU:HB2	2.36	0.59
1:E:154:VAL:HG13	1:E:457:PHE:HE2	1.67	0.59
1:F:114:ILE:CD1	4:F:502:CPZ:H11	2.33	0.59
3:E:501:HEM:NB	4:E:502:CPZ:C5	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:ASN:O	1:C:457:PHE:CD1	2.56	0.59
1:F:416:ALA:HA	7:F:647:HOH:O	2.03	0.59
1:A:427:MET:HE2	1:A:431:ILE:HD13	1.85	0.58
1:D:309:TYR:CE2	1:D:481:PRO:CA	2.85	0.58
4:F:502:CPZ:HN3	4:F:503:CPZ:HN3	1.49	0.58
1:B:402:PHE:HB3	1:B:412:HIS:CD2	2.39	0.58
1:D:309:TYR:CE2	1:D:481:PRO:N	2.72	0.58
1:E:323:LYS:HB3	1:E:348:TYR:CE2	2.39	0.57
1:B:302:THR:HG21	4:B:502:CPZ:C5	2.34	0.57
1:C:479:LYS:HD2	7:C:716:HOH:O	2.03	0.57
1:D:46:MET:CE	7:D:676:HOH:O	2.52	0.57
1:F:309:TYR:CD1	1:F:481:PRO:HB3	2.39	0.57
3:D:501:HEM:HBB2	3:D:501:HEM:CMB	2.32	0.57
1:F:357:GLN:OE1	1:F:446:LEU:CD1	2.53	0.57
1:C:429:PHE:HB3	1:C:436:CYS:HB3	1.87	0.57
1:B:364:PRO:HA	1:B:393:SER:HB2	1.86	0.57
1:C:426:PHE:HE2	1:C:443:ARG:HH21	1.52	0.57
3:E:501:HEM:NB	4:E:502:CPZ:H5	2.20	0.57
3:E:501:HEM:HBB2	3:E:501:HEM:HMB2	1.86	0.57
1:C:59:ARG:NH2	1:C:64:ASP:OD1	2.25	0.57
1:B:29:HIS:HB3	1:B:381:LEU:HB3	1.86	0.57
1:F:208:LEU:CB	1:F:234:ILE:HD11	2.33	0.57
1:A:367:ALA:O	1:A:369:HIS:HD2	1.88	0.56
1:C:316:LYS:HD3	1:C:470:LEU:HD11	1.86	0.56
3:C:501:HEM:HBB2	3:C:501:HEM:HMB2	1.87	0.56
1:A:194:GLN:NE2	7:A:611:HOH:O	2.38	0.56
1:D:137:MET:HE2	1:D:441:ILE:HB	1.88	0.56
1:E:179:ILE:HD13	3:E:501:HEM:HBC1	1.86	0.56
1:F:46:MET:HE2	7:F:628:HOH:O	2.05	0.56
1:B:217:PHE:HD1	1:B:224:MET:HE2	1.71	0.55
1:F:285:HIS:NE2	1:F:289:LEU:HD11	2.22	0.55
3:F:501:HEM:C1B	4:F:502:CPZ:H5	2.41	0.55
1:A:435:ILE:HD11	2:G:2:FRU:O1	2.06	0.55
1:F:120:ARG:NE	1:F:282:GLU:OE2	2.39	0.55
1:A:179:ILE:HD13	3:A:501:HEM:HBC1	1.89	0.55
1:F:230:ALA:O	1:F:234:ILE:HD12	2.07	0.55
1:D:309:TYR:CZ	1:D:481:PRO:CA	2.89	0.55
1:D:492:HIS:O	1:D:493:HIS:CB	2.54	0.55
1:B:29:HIS:O	1:B:381:LEU:N	2.38	0.55
1:F:268:TYR:HD1	1:F:272:MET:HG2	1.69	0.55
1:E:466:LYS:HD3	1:E:466:LYS:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:375:THR:CG2	1:F:376:LEU:H	2.21	0.54
1:D:227:PHE:C	1:D:232:ARG:NH2	2.61	0.54
1:E:73:ARG:NH2	1:E:218:GLU:OE1	2.38	0.54
1:B:194:GLN:OE1	1:B:198:LEU:HG	2.07	0.54
1:D:309:TYR:CD2	1:D:481:PRO:HB3	2.42	0.54
1:B:150:ALA:O	1:B:154:VAL:HG23	2.08	0.54
1:E:37:LEU:CD1	7:E:664:HOH:O	2.55	0.54
1:E:303:THR:HG22	1:E:307:LEU:HD23	1.89	0.54
1:C:309:TYR:CZ	1:C:481:PRO:CB	2.90	0.54
1:F:248:SER:CB	7:F:624:HOH:O	2.43	0.54
1:B:296:PHE:O	1:B:300:THR:OG1	2.23	0.54
1:D:139:LYS:C	1:D:141:SER:HB2	2.27	0.54
1:A:298:ALA:HB2	4:A:502:CPZ:C11	2.38	0.54
1:C:82:GLU:O	1:C:86:GLU:HB2	2.08	0.54
1:E:365:ILE:HD13	7:E:695:HOH:O	2.06	0.54
1:C:309:TYR:CE1	1:C:481:PRO:CA	2.91	0.54
1:C:298:ALA:HA	1:C:302:THR:HG23	1.89	0.53
1:B:321:ALA:O	1:B:324:VAL:HB	2.09	0.53
1:F:46:MET:HE3	7:F:628:HOH:O	2.05	0.53
1:E:427:MET:HE1	1:E:431:ILE:HG21	1.91	0.53
1:D:427:MET:HA	7:D:663:HOH:O	2.07	0.53
1:E:208:LEU:HG	7:E:618:HOH:O	2.07	0.53
1:C:85:ARG:NE	1:C:427:MET:HE3	2.24	0.53
1:F:232:ARG:O	1:F:235:THR:CG2	2.57	0.52
1:C:489:LEU:O	1:C:490:ALA:C	2.47	0.52
1:A:85:ARG:NH2	2:G:2:FRU:O4	2.42	0.52
1:A:184:PHE:HD1	1:A:248:SER:HG	1.56	0.52
1:B:256:LEU:O	1:B:258:PRO:HD3	2.09	0.52
1:C:192:ASP:O	1:C:196:LEU:HD12	2.09	0.52
1:D:463:VAL:HA	7:D:685:HOH:O	2.07	0.52
1:E:93:GLU:HG2	1:E:433:LYS:NZ	2.24	0.52
1:F:180:CYS:O	1:F:184:PHE:N	2.35	0.52
1:F:302:THR:OG1	1:F:303:THR:N	2.43	0.52
1:B:268:TYR:CE1	1:B:288:LEU:HB2	2.45	0.52
1:E:247:GLN:HB2	7:E:660:HOH:O	2.10	0.52
1:E:37:LEU:HD11	7:E:664:HOH:O	2.10	0.52
1:F:367:ALA:HB2	4:F:503:CPZ:C9	2.40	0.52
1:F:434:ARG:NH2	7:F:617:HOH:O	2.42	0.52
1:D:330:GLN:CB	7:D:654:HOH:O	2.51	0.51
1:E:272:MET:HG2	1:E:283:PHE:O	2.10	0.51
1:D:94:ALA:HA	1:D:372:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:TYR:O	1:F:272:MET:HG3	2.10	0.51
1:D:144:ASP:O	1:D:148:GLU:HG3	2.10	0.51
1:B:409:ASN:O	1:B:412:HIS:ND1	2.32	0.51
1:A:431:ILE:HD11	2:G:2:FRU:C3	2.34	0.51
1:B:168:THR:HG23	1:B:308:ARG:NH1	2.25	0.51
1:C:250:GLU:HG2	7:C:609:HOH:O	2.11	0.51
1:C:341:GLU:O	1:C:344:THR:HG22	2.10	0.51
1:F:348:TYR:CD1	1:F:414:LEU:HD11	2.46	0.51
1:F:367:ALA:CB	4:F:503:CPZ:C9	2.89	0.51
1:A:85:ARG:NE	1:A:427:MET:HE3	2.26	0.50
1:C:211:SER:CA	1:C:474:GLU:OE2	2.59	0.50
1:D:278:ASN:OD1	1:D:280:HIS:N	2.30	0.50
1:B:320:VAL:O	1:B:324:VAL:HG23	2.11	0.50
1:C:473:LYS:HE2	7:C:664:HOH:O	2.10	0.50
1:F:325:GLN:HE21	1:F:454:LEU:HD22	1.76	0.50
1:F:269:LEU:O	1:F:272:MET:N	2.45	0.50
3:F:501:HEM:HMB2	3:F:501:HEM:HBB2	1.93	0.50
1:A:364:PRO:C	1:A:366:GLY:H	2.14	0.50
1:C:365:ILE:CG2	1:C:366:GLY:N	2.64	0.50
1:F:202:PHE:CE1	1:F:241:ILE:HD13	2.47	0.50
1:C:367:ALA:HB1	4:C:503:CPZ:CL	2.48	0.50
1:A:57:ARG:NH1	7:A:616:HOH:O	2.44	0.50
1:D:367:ALA:HB2	4:D:502:CPZ:C9	2.41	0.50
1:A:144:ASP:O	1:A:148:GLU:HG3	2.12	0.49
1:C:150:ALA:O	1:C:154:VAL:HG23	2.11	0.49
1:D:317:TYR:HE2	1:D:408:PHE:HB3	1.77	0.49
1:E:298:ALA:HB2	4:E:502:CPZ:C11	2.42	0.49
1:A:93:GLU:OE2	1:A:433:LYS:NZ	2.44	0.49
1:F:285:HIS:CD2	1:F:289:LEU:HD11	2.48	0.49
1:B:47:ASP:OD2	1:B:57:ARG:NH1	2.44	0.49
1:C:327:GLU:OE2	1:C:349:THR:OG1	2.27	0.49
1:E:409:ASN:HB3	1:E:412:HIS:CE1	2.47	0.49
1:B:46:MET:HE3	7:B:642:HOH:O	2.12	0.49
1:B:409:ASN:HB3	1:B:412:HIS:CE1	2.47	0.49
1:F:269:LEU:CA	1:F:272:MET:HG3	2.42	0.49
3:A:501:HEM:C1B	4:A:502:CPZ:H5	2.48	0.49
1:C:430:SER:HB2	3:C:501:HEM:HBA1	1.95	0.49
1:C:430:SER:CB	3:C:501:HEM:HBA1	2.42	0.49
1:E:94:ALA:O	1:E:371:VAL:HA	2.12	0.49
1:F:409:ASN:O	1:F:412:HIS:ND1	2.44	0.49
1:E:172:GLN:OE1	7:E:603:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:LEU:O	1:F:485:GLN:CA	2.57	0.49
1:B:44:LEU:HA	1:E:37:LEU:HD23	1.95	0.49
1:B:360:SER:O	1:B:361:ASP:C	2.51	0.49
1:C:309:TYR:CZ	1:C:481:PRO:HA	2.48	0.49
1:D:274:LYS:O	1:D:274:LYS:HG3	2.13	0.49
1:A:355:GLU:HG3	1:A:408:PHE:CD1	2.48	0.48
1:B:188:TYR:OH	1:B:244:TYR:OH	2.28	0.48
1:C:474:GLU:O	1:C:475:SER:C	2.51	0.48
1:D:206:PHE:HB2	1:D:301:GLU:HG2	1.95	0.48
1:F:352:VAL:O	1:F:356:ILE:HG13	2.13	0.48
1:D:46:MET:HE2	7:D:676:HOH:O	2.11	0.48
1:C:255:THR:OG1	1:C:262:ARG:NH2	2.42	0.48
1:A:482:GLN:HG2	7:A:797:HOH:O	2.13	0.48
1:B:325:GLN:O	1:B:328:ILE:N	2.46	0.48
1:C:268:TYR:CG	1:C:288:LEU:HD13	2.48	0.48
1:C:316:LYS:HB2	1:C:468:ILE:HG21	1.96	0.48
1:F:147:GLN:O	1:F:150:ALA:HB3	2.13	0.48
1:F:367:ALA:CB	4:F:503:CPZ:CL	2.96	0.48
1:F:473:LYS:N	1:F:480:VAL:O	2.43	0.48
1:F:357:GLN:NE2	1:F:426:PHE:HZ	2.08	0.48
1:B:188:TYR:HH	1:B:244:TYR:HH	1.57	0.48
1:B:367:ALA:HB1	4:B:503:CPZ:CL	2.50	0.48
1:C:94:ALA:O	1:C:371:VAL:HA	2.14	0.48
1:C:309:TYR:CD1	1:C:481:PRO:HD3	2.49	0.48
1:D:262:ARG:HG2	1:D:266:ASP:OD2	2.13	0.48
1:E:160:SER:O	1:E:161:GLN:CG	2.61	0.48
1:F:357:GLN:NE2	7:F:619:HOH:O	2.46	0.48
1:B:367:ALA:HB2	4:B:503:CPZ:C9	2.44	0.48
1:F:170:LEU:O	1:F:174:ILE:HG23	2.14	0.48
1:C:473:LYS:O	1:C:474:GLU:HB2	2.13	0.47
1:D:491:ARG:O	1:D:492:HIS:CB	2.60	0.47
1:B:363:ALA:HB2	4:B:503:CPZ:C2	2.44	0.47
1:E:32:PRO:HD3	1:E:380:TYR:CE1	2.49	0.47
1:E:355:GLU:HG3	1:E:408:PHE:CE1	2.48	0.47
1:F:146:ILE:HD12	1:F:448:LEU:HD12	1.96	0.47
3:F:501:HEM:HBB2	3:F:501:HEM:CMB	2.43	0.47
1:D:59:ARG:HD2	1:D:79:TYR:CD2	2.49	0.47
1:E:46:MET:HE3	7:E:650:HOH:O	2.10	0.47
1:F:183:VAL:HA	1:F:264:PHE:HB3	1.96	0.47
1:D:338:PRO:HG2	1:D:451:THR:HG23	1.96	0.47
1:E:153:LEU:HD21	1:E:453:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ALA:HB2	1:B:300:THR:HG23	1.96	0.47
1:F:114:ILE:HD12	1:F:294:SER:HB3	1.96	0.47
3:A:501:HEM:HBC2	3:A:501:HEM:CMC	2.45	0.47
1:B:216:VAL:HG11	1:E:39:LEU:HD13	1.96	0.47
1:C:29:HIS:HB3	1:C:381:LEU:HB3	1.97	0.47
1:C:36:PRO:HG3	1:C:69:HIS:CE1	2.50	0.47
1:C:369:HIS:NE2	3:C:501:HEM:O2A	2.38	0.47
1:E:37:LEU:N	1:E:37:LEU:HD12	2.30	0.47
1:F:165:LEU:CD1	1:F:486:ILE:O	2.63	0.47
3:F:501:HEM:NB	4:F:502:CPZ:H5	2.30	0.47
1:B:232:ARG:HB2	7:B:656:HOH:O	2.14	0.47
1:B:369:HIS:NE2	3:B:501:HEM:O2A	2.41	0.47
1:C:37:LEU:CD1	7:C:619:HOH:O	2.63	0.47
1:F:143:GLU:O	1:F:145:ARG:N	2.48	0.47
1:F:303:THR:HG23	1:F:446:LEU:HG	1.96	0.47
1:C:465:PRO:HA	1:C:468:ILE:HG13	1.96	0.46
1:F:201:LEU:HD23	1:F:241:ILE:CG1	2.44	0.46
1:F:346:MET:O	1:F:348:TYR:N	2.48	0.46
1:C:363:ALA:O	1:C:365:ILE:O	2.33	0.46
1:B:272:MET:HG3	1:B:283:PHE:O	2.15	0.46
1:D:480:VAL:HG13	1:D:481:PRO:HD2	1.96	0.46
1:E:367:ALA:HB2	4:E:503:CPZ:C9	2.45	0.46
1:F:85:ARG:NE	1:F:427:MET:HE3	2.30	0.46
1:F:142:VAL:O	1:F:145:ARG:HG3	2.15	0.46
1:A:431:ILE:HD12	2:G:2:FRU:H3	1.94	0.46
1:D:477:ILE:O	4:D:502:CPZ:H2	2.14	0.46
1:F:165:LEU:N	1:F:165:LEU:HD13	2.22	0.46
1:E:172:GLN:HE22	1:E:203:TYR:HB2	1.80	0.46
1:F:300:THR:O	1:F:304:SER:OG	2.30	0.46
3:B:501:HEM:NB	4:B:502:CPZ:H5	2.29	0.46
1:D:203:TYR:HA	1:D:301:GLU:OE2	2.14	0.46
1:D:309:TYR:CZ	1:D:481:PRO:CB	2.99	0.46
1:D:317:TYR:CE2	1:D:408:PHE:HB3	2.51	0.46
1:F:341:GLU:O	1:F:344:THR:HG22	2.16	0.46
1:F:364:PRO:HA	1:F:393:SER:HB2	1.98	0.46
1:B:38:PRO:O	1:B:39:LEU:HB2	2.14	0.46
1:C:304:SER:OG	7:C:603:HOH:O	2.21	0.46
1:C:309:TYR:CZ	1:C:481:PRO:CA	2.99	0.46
1:D:245:VAL:HG12	1:D:289:LEU:HD23	1.97	0.46
1:E:298:ALA:HA	1:E:302:THR:CG2	2.40	0.46
1:F:395:ALA:O	1:F:425:ALA:HB1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:491:ARG:O	1:F:492:HIS:CG	2.69	0.46
1:F:113:MET:SD	1:F:295:LEU:HD21	2.56	0.46
1:B:47:ASP:N	1:B:54:SER:OG	2.46	0.45
1:B:430:SER:CB	3:B:501:HEM:HBA1	2.46	0.45
1:A:491:ARG:NH1	7:A:627:HOH:O	2.50	0.45
1:B:459:VAL:HB	1:B:486:ILE:HD11	1.98	0.45
1:E:85:ARG:CZ	1:E:427:MET:HE3	2.46	0.45
1:F:268:TYR:CE1	1:F:272:MET:HG2	2.51	0.45
1:B:233:GLN:HG3	7:B:619:HOH:O	2.14	0.45
1:C:447:PHE:O	1:C:451:THR:HG23	2.16	0.45
1:E:187:ARG:C	1:E:188:TYR:HD1	2.19	0.45
1:F:269:LEU:HA	1:F:272:MET:SD	2.55	0.45
1:B:363:ALA:HB2	4:B:503:CPZ:H2	1.99	0.45
3:E:501:HEM:C1B	4:E:502:CPZ:H5	2.51	0.45
1:B:311:PHE:HA	1:B:314:MET:HB2	1.97	0.45
1:E:348:TYR:O	1:E:352:VAL:HG23	2.17	0.45
1:A:153:LEU:HD22	1:A:174:ILE:HD13	1.98	0.45
1:C:141:SER:HB2	1:C:145:ARG:HH12	1.82	0.45
1:D:297:PHE:CD2	1:D:298:ALA:N	2.85	0.45
1:A:82:GLU:H	1:A:82:GLU:CD	2.19	0.45
1:E:369:HIS:HE2	3:E:501:HEM:CGA	2.22	0.45
1:C:309:TYR:CE1	1:C:481:PRO:N	2.85	0.45
1:A:262:ARG:NH1	1:A:266:ASP:OD2	2.50	0.45
1:A:297:PHE:CD2	1:A:298:ALA:N	2.85	0.45
1:B:94:ALA:O	1:B:371:VAL:HA	2.16	0.44
1:E:180:CYS:O	1:E:184:PHE:N	2.45	0.44
1:C:47:ASP:HB3	1:C:54:SER:OG	2.16	0.44
3:C:501:HEM:C1B	4:C:502:CPZ:H5	2.52	0.44
1:E:297:PHE:CD2	1:E:298:ALA:N	2.85	0.44
1:F:160:SER:O	1:F:161:GLN:CB	2.65	0.44
1:C:144:ASP:O	1:C:148:GLU:HG3	2.16	0.44
1:C:297:PHE:CD2	1:C:298:ALA:N	2.85	0.44
1:C:426:PHE:CZ	1:C:428:PRO:HG3	2.52	0.44
1:E:310:GLY:O	1:E:314:MET:HG2	2.16	0.44
1:C:295:LEU:HD22	3:C:501:HEM:HBC1	2.00	0.44
1:C:298:ALA:HB2	4:C:502:CPZ:H11	1.97	0.44
1:D:268:TYR:CG	1:D:288:LEU:HD13	2.53	0.44
1:D:272:MET:HG2	1:D:283:PHE:O	2.18	0.44
1:E:77:MET:HB3	1:E:391:ILE:HD11	1.99	0.44
1:B:153:LEU:HD21	1:B:453:ILE:HD11	1.99	0.44
1:C:309:TYR:CE1	1:C:481:PRO:CD	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:GLY:O	1:C:455:GLN:NE2	2.47	0.44
1:E:93:GLU:HG2	1:E:433:LYS:HZ1	1.83	0.44
1:E:437:LEU:HA	1:E:437:LEU:HD12	1.79	0.44
1:E:460:SER:OG	1:E:461:SER:N	2.51	0.44
1:F:174:ILE:HD12	1:F:449:PHE:CD1	2.53	0.44
1:A:362:LEU:HB2	7:A:720:HOH:O	2.17	0.44
1:E:172:GLN:NE2	1:E:203:TYR:HB2	2.32	0.44
1:F:198:LEU:HD11	1:F:244:TYR:CD2	2.53	0.44
1:F:216:VAL:HG12	1:F:224:MET:SD	2.58	0.44
1:F:297:PHE:CD2	1:F:298:ALA:N	2.85	0.44
1:B:455:GLN:HG2	1:B:456:ASN:ND2	2.33	0.44
1:C:316:LYS:HG3	1:C:465:PRO:O	2.18	0.44
1:F:162:GLY:O	1:F:163:ALA:O	2.35	0.44
1:F:268:TYR:OH	1:F:283:PHE:HA	2.18	0.44
1:B:179:ILE:CD1	3:B:501:HEM:HBC1	2.46	0.44
1:B:297:PHE:CD2	1:B:298:ALA:N	2.85	0.44
1:D:93:GLU:OE2	1:D:433:LYS:HE3	2.18	0.44
1:F:367:ALA:HB2	4:F:503:CPZ:C8	2.48	0.44
1:F:111:TYR:HB2	1:F:290:ILE:HG13	1.99	0.43
1:F:316:LYS:HG3	1:F:465:PRO:O	2.19	0.43
1:C:37:LEU:HD13	7:C:661:HOH:O	2.18	0.43
1:D:404:GLN:O	1:D:407:THR:HG22	2.18	0.43
1:E:149:GLU:OE1	1:E:190:TYR:OH	2.24	0.43
1:E:188:TYR:OH	1:E:244:TYR:OH	2.29	0.43
1:F:328:ILE:HA	1:F:346:MET:HE1	2.00	0.43
1:A:194:GLN:HE21	1:A:244:TYR:HD1	1.65	0.43
1:A:216:VAL:HG12	1:A:224:MET:SD	2.58	0.43
1:A:355:GLU:HG3	1:A:408:PHE:CE1	2.54	0.43
1:A:473:LYS:HB2	1:A:482:GLN:HA	2.00	0.43
1:B:179:ILE:HD13	3:B:501:HEM:CBC	2.48	0.43
1:C:309:TYR:CD2	1:C:481:PRO:HB3	2.54	0.43
1:E:169:PHE:HD2	1:E:170:LEU:N	2.16	0.43
1:E:404:GLN:HG3	7:E:685:HOH:O	2.19	0.43
3:A:501:HEM:HBC2	3:A:501:HEM:HMC1	1.99	0.43
1:D:59:ARG:NH2	1:D:64:ASP:OD1	2.42	0.43
1:E:332:ILE:HG12	1:E:342:ASP:OD2	2.19	0.43
1:B:329:ASP:OD1	1:B:491:ARG:NH2	2.51	0.43
1:C:37:LEU:HD11	7:C:619:HOH:O	2.17	0.43
1:A:432:GLY:HA2	1:D:493:HIS:C	2.39	0.43
1:B:245:VAL:O	1:B:249:VAL:HG23	2.18	0.43
3:C:501:HEM:HBB2	3:C:501:HEM:CMB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:302:THR:OG1	1:E:303:THR:N	2.51	0.43
1:F:117:ASN:HA	7:F:617:HOH:O	2.18	0.43
1:F:437:LEU:HB2	3:F:501:HEM:CMD	2.49	0.43
1:E:120:ARG:HA	1:E:282:GLU:HG3	2.00	0.43
1:F:235:THR:HG23	1:F:236:ARG:N	2.32	0.43
7:A:603:HOH:O	2:G:2:FRU:O6	2.20	0.43
1:C:29:HIS:O	1:C:380:TYR:HB3	2.18	0.43
1:C:348:TYR:O	1:C:352:VAL:HG23	2.18	0.43
1:C:372:THR:HA	7:C:679:HOH:O	2.19	0.43
1:F:114:ILE:CD1	1:F:294:SER:HB3	2.49	0.43
1:B:31:PRO:HB3	1:B:65:VAL:HG12	2.01	0.43
1:B:183:VAL:HA	1:B:264:PHE:HB3	2.00	0.43
1:F:316:LYS:HG2	1:F:317:TYR:CE1	2.53	0.43
1:F:346:MET:O	1:F:347:PRO:C	2.57	0.43
1:B:46:MET:HE1	1:B:68:VAL:HG11	2.00	0.42
1:D:315:LEU:HA	1:D:315:LEU:HD23	1.75	0.42
1:B:46:MET:CE	7:B:642:HOH:O	2.67	0.42
1:B:336:ARG:CG	1:B:337:LEU:H	2.32	0.42
1:E:179:ILE:CD1	3:E:501:HEM:HBC1	2.49	0.42
1:F:252:HIS:CD2	1:F:265:ILE:HB	2.54	0.42
1:B:86:GLU:OE2	1:B:378:ARG:NH2	2.32	0.42
1:C:271:ARG:NH2	7:C:627:HOH:O	2.51	0.42
1:D:92:ALA:HA	7:D:637:HOH:O	2.18	0.42
1:E:270:LEU:HD23	1:E:270:LEU:HA	1.85	0.42
1:E:348:TYR:HD1	1:E:414:LEU:HD11	1.85	0.42
1:E:374:ASP:OD1	1:E:384:LYS:N	2.46	0.42
3:B:501:HEM:HMB1	3:B:501:HEM:CBB	2.43	0.42
1:A:179:ILE:HD13	3:A:501:HEM:CBC	2.50	0.42
1:B:270:LEU:HA	1:B:270:LEU:HD23	1.77	0.42
1:B:308:ARG:HE	1:B:481:PRO:HG3	1.85	0.42
1:E:154:VAL:HG11	1:E:456:ASN:ND2	2.35	0.42
1:F:309:TYR:CE1	1:F:481:PRO:HB3	2.55	0.42
1:A:79:TYR:HE2	7:A:730:HOH:O	2.03	0.42
1:F:276:LYS:O	1:F:276:LYS:HG3	2.19	0.42
1:B:154:VAL:HG13	1:B:457:PHE:HE2	1.84	0.42
1:B:242:LEU:HD12	1:B:242:LEU:HA	1.76	0.42
1:B:310:GLY:O	1:B:314:MET:HG2	2.20	0.42
1:D:262:ARG:HG2	1:D:262:ARG:H	1.60	0.42
1:E:113:MET:SD	1:E:295:LEU:CD2	3.08	0.42
1:E:250:GLU:HA	1:E:253:ARG:NE	2.33	0.42
1:F:165:LEU:HD13	1:F:486:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:LEU:HD12	1:D:437:LEU:HA	1.93	0.42
3:A:501:HEM:NB	4:A:502:CPZ:H5	2.34	0.41
1:C:329:ASP:OD2	1:C:491:ARG:NH2	2.48	0.41
1:C:420:LEU:CD2	1:C:422:LYS:HE3	2.50	0.41
1:D:228:PRO:HA	1:D:232:ARG:CZ	2.50	0.41
1:E:355:GLU:HG3	1:E:408:PHE:CD1	2.55	0.41
1:A:77:MET:HB3	1:A:391:ILE:CD1	2.50	0.41
1:C:362:LEU:HG	4:C:503:CPZ:H5	2.02	0.41
1:D:447:PHE:O	1:D:451:THR:HG22	2.20	0.41
1:A:268:TYR:CE1	1:A:288:LEU:HB2	2.55	0.41
1:E:113:MET:H	1:E:113:MET:HG2	1.64	0.41
1:B:154:VAL:HG13	1:B:457:PHE:CE2	2.55	0.41
1:C:94:ALA:HB2	1:C:373:LYS:HE2	2.03	0.41
1:D:98:ARG:HG2	1:D:115:PHE:HA	2.02	0.41
1:F:32:PRO:HD3	1:F:380:TYR:CE1	2.55	0.41
1:F:434:ARG:HD3	3:F:501:HEM:O1D	2.20	0.41
1:B:352:VAL:O	1:B:356:ILE:HG13	2.20	0.41
1:C:120:ARG:HA	1:C:282:GLU:HG3	2.02	0.41
1:C:242:LEU:HD13	1:C:293:LEU:HD22	2.02	0.41
1:C:437:LEU:HD12	1:C:437:LEU:HA	1.87	0.41
1:F:163:ALA:HA	1:F:164:PRO:HD2	1.75	0.41
1:B:162:GLY:O	1:B:487:SER:HB3	2.20	0.41
1:B:316:LYS:C	1:B:318:PRO:HD3	2.40	0.41
1:F:269:LEU:HA	1:F:272:MET:CG	2.48	0.41
1:A:316:LYS:HD3	1:A:470:LEU:HD11	2.03	0.41
1:C:384:LYS:O	1:C:385:ASN:HB2	2.20	0.41
1:D:348:TYR:O	1:D:352:VAL:HG23	2.21	0.41
1:E:384:LYS:O	1:E:385:ASN:HB2	2.21	0.41
1:F:143:GLU:O	1:F:144:ASP:C	2.59	0.41
1:F:252:HIS:NE2	1:F:263:ASP:OD2	2.30	0.41
1:A:151:GLN:O	1:A:155:GLU:HG3	2.21	0.41
1:B:313:LEU:HD22	1:B:408:PHE:CD1	2.56	0.41
4:B:502:CPZ:H7	4:B:503:CPZ:C6	2.50	0.41
1:C:150:ALA:HB1	1:C:452:THR:HG21	2.03	0.41
1:C:309:TYR:CG	1:C:481:PRO:HB3	2.55	0.41
1:E:307:LEU:HD22	1:E:446:LEU:HD23	2.03	0.41
1:E:409:ASN:O	1:E:412:HIS:ND1	2.51	0.41
1:E:457:PHE:CD1	1:E:488:PHE:HB3	2.55	0.41
1:F:154:VAL:O	1:F:155:GLU:C	2.56	0.41
1:F:268:TYR:CG	1:F:288:LEU:HD13	2.56	0.41
1:C:268:TYR:CE1	1:C:288:LEU:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:TYR:OH	1:C:481:PRO:HA	2.21	0.41
1:D:82:GLU:O	1:D:86:GLU:HB2	2.20	0.41
1:D:367:ALA:O	1:D:369:HIS:HD2	2.03	0.41
1:A:242:LEU:HD12	1:A:242:LEU:HA	1.91	0.40
1:C:82:GLU:OE1	1:C:82:GLU:N	2.54	0.40
1:D:38:PRO:O	1:D:39:LEU:HB2	2.21	0.40
1:D:46:MET:HE3	7:D:676:HOH:O	2.16	0.40
1:E:223:PHE:HB2	5:E:504:CM5:H51	2.03	0.40
1:E:302:THR:HG21	4:E:502:CPZ:C5	2.51	0.40
1:F:348:TYR:HA	1:F:414:LEU:HD21	2.03	0.40
1:F:381:LEU:O	1:F:383:PRO:HD3	2.21	0.40
1:A:294:SER:O	1:A:297:PHE:O	2.39	0.40
1:B:48:ARG:HE	1:B:48:ARG:HB2	1.34	0.40
1:B:232:ARG:CB	7:B:656:HOH:O	2.70	0.40
1:C:211:SER:CB	1:C:474:GLU:OE2	2.68	0.40
1:D:268:TYR:CD1	1:D:288:LEU:HD13	2.56	0.40
1:D:340:LEU:HD23	1:D:340:LEU:HA	1.87	0.40
1:E:45:GLN:HG3	7:E:621:HOH:O	2.21	0.40
1:D:88:LEU:HA	1:D:88:LEU:HD23	1.82	0.40
1:D:228:PRO:N	1:D:232:ARG:CZ	2.85	0.40
1:E:317:TYR:CE2	1:E:408:PHE:HB3	2.55	0.40
1:F:149:GLU:OE1	1:F:190:TYR:OH	2.33	0.40
1:A:398:ASP:HA	1:A:399:PRO:HD3	1.95	0.40
1:D:266:ASP:O	1:D:270:LEU:HG	2.21	0.40
1:E:367:ALA:O	1:E:369:HIS:HD2	2.04	0.40
1:E:429:PHE:HB3	1:E:436:CYS:HB3	2.02	0.40
1:B:175:THR:HG21	1:B:303:THR:HB	2.04	0.40
1:E:46:MET:HE1	1:E:55:PHE:HE1	1.86	0.40
1:E:367:ALA:HB1	4:E:503:CPZ:CL	2.59	0.40

All (1) 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)
1:B:280:HIS:O	1:E:335:HIS:NE2[1_554]	2.03	0.17

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	462/493 (94%)	447 (97%)	15 (3%)	0	100 100
1	B	454/493 (92%)	432 (95%)	22 (5%)	0	100 100
1	C	463/493 (94%)	450 (97%)	12 (3%)	1 (0%)	47 62
1	D	459/493 (93%)	446 (97%)	12 (3%)	1 (0%)	47 62
1	E	458/493 (93%)	444 (97%)	14 (3%)	0	100 100
1	F	455/493 (92%)	424 (93%)	26 (6%)	5 (1%)	14 20
All	All	2751/2958 (93%)	2643 (96%)	101 (4%)	7 (0%)	41 55

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	475	SER
1	F	163	ALA
1	F	144	ASP
1	F	235	THR
1	D	492	HIS
1	F	161	GLN
1	F	143	GLU

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	408/433 (94%)	407 (100%)	1 (0%)	93 97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	384/433 (89%)	383 (100%)	1 (0%)	92 97
1	C	396/433 (92%)	394 (100%)	2 (0%)	88 95
1	D	395/433 (91%)	393 (100%)	2 (0%)	88 95
1	E	393/433 (91%)	392 (100%)	1 (0%)	92 97
1	F	370/433 (86%)	365 (99%)	5 (1%)	67 82
All	All	2346/2598 (90%)	2334 (100%)	12 (0%)	88 95

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

Mol	Chain	Res	Type
1	A	309	TYR
1	B	334	SER
1	C	309	TYR
1	C	458	SER
1	D	113	MET
1	D	309	TYR
1	E	309	TYR
1	F	145	ARG
1	F	165	LEU
1	F	268	TYR
1	F	309	TYR
1	F	343	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	325	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)

2 monosaccharides 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	GLC	G	1	2	11,11,12	3.30	8 (72%)	15,15,17	3.30	10 (66%)
2	FRU	G	2	2	11,12,12	0.58	0	10,18,18	0.54	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	GLC	G	1	2	-	2/2/19/22	0/1/1/1
2	FRU	G	2	2	-	3/5/24/24	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	GLC	O5-C1	-5.00	1.35	1.43
2	G	1	GLC	C2-C3	-4.10	1.46	1.52
2	G	1	GLC	C4-C3	-4.05	1.42	1.52
2	G	1	GLC	O2-C2	-3.92	1.35	1.43
2	G	1	GLC	O4-C4	-3.75	1.34	1.43
2	G	1	GLC	O3-C3	-3.63	1.34	1.43
2	G	1	GLC	C4-C5	-3.24	1.46	1.53
2	G	1	GLC	O5-C5	-2.27	1.38	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1	GLC	O5-C1-C2	-7.64	98.98	110.77
2	G	1	GLC	O4-C4-C3	-4.45	100.06	110.35
2	G	1	GLC	O5-C5-C6	3.85	113.23	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1	GLC	C1-C2-C3	3.83	114.38	109.67
2	G	1	GLC	O2-C2-C1	3.61	116.53	109.15
2	G	1	GLC	C3-C4-C5	-3.30	104.36	110.24
2	G	1	GLC	C2-C3-C4	-3.18	105.40	110.89
2	G	1	GLC	O3-C3-C4	-2.78	103.91	110.35
2	G	1	GLC	C1-O5-C5	-2.52	108.77	112.19
2	G	1	GLC	C6-C5-C4	-2.31	107.59	113.00

There are no chirality outliers.

All (5) torsion outliers are listed below:

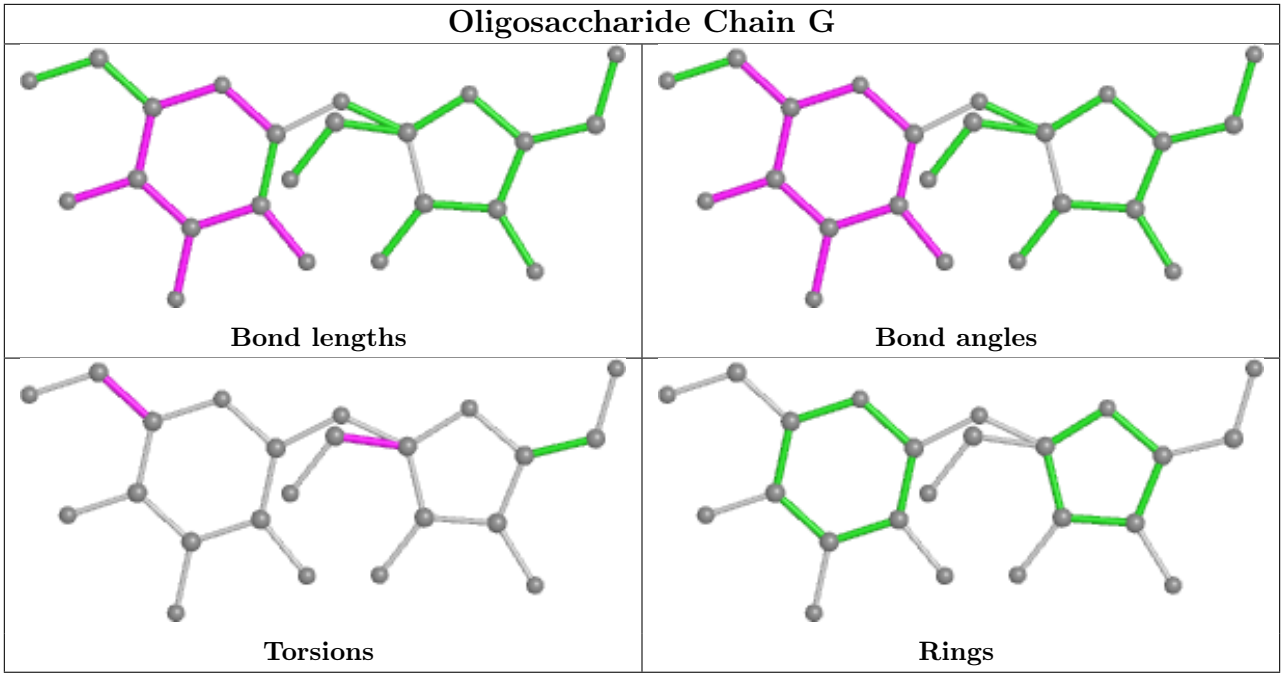
Mol	Chain	Res	Type	Atoms
2	G	2	FRU	O1-C1-C2-C3
2	G	2	FRU	O1-C1-C2-O2
2	G	1	GLC	C4-C5-C6-O6
2	G	1	GLC	O5-C5-C6-O6
2	G	2	FRU	O1-C1-C2-O5

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	GLC	4	0
2	G	2	FRU	13	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry (i)

24 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	$\#\|Z\| > 2$
4	CPZ	C	502	3	10,13,13	1.01	0	9,17,17	0.81	0
4	CPZ	E	503	-	10,13,13	1.00	0	9,17,17	0.80	0
4	CPZ	A	503	-	10,13,13	1.00	0	9,17,17	0.79	0
4	CPZ	C	503	-	10,13,13	1.00	0	9,17,17	0.79	0
6	GOL	A	506	-	5,5,5	0.57	0	5,5,5	0.96	0
3	HEM	C	501	4,1	41,50,50	2.10	9 (21%)	45,82,82	1.41	7 (15%)
4	CPZ	A	502	3	10,13,13	1.00	0	9,17,17	0.80	0
6	GOL	C	504	-	5,5,5	0.41	0	5,5,5	0.60	0
4	CPZ	E	502	3	10,13,13	1.00	0	9,17,17	0.80	0
4	CPZ	B	502	3	10,13,13	1.24	1 (10%)	9,17,17	1.04	0
3	HEM	A	501	4,1	41,50,50	2.24	13 (31%)	45,82,82	1.53	9 (20%)
6	GOL	E	505	-	5,5,5	0.47	0	5,5,5	0.57	0
4	CPZ	B	503	-	10,13,13	0.98	0	9,17,17	1.53	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEM	E	501	4,1	41,50,50	2.11	6 (14%)	45,82,82	1.68	7 (15%)
3	HEM	F	501	4	41,50,50	2.00	8 (19%)	45,82,82	1.92	8 (17%)
3	HEM	B	501	4,1	41,50,50	1.90	6 (14%)	45,82,82	1.57	9 (20%)
4	CPZ	D	502	-	10,13,13	1.00	0	9,17,17	0.80	0
4	CPZ	F	502	3	10,13,13	1.00	0	9,17,17	0.80	0
4	CPZ	D	503	3	10,13,13	0.99	0	9,17,17	0.77	0
4	CPZ	F	503	-	10,13,13	1.01	0	9,17,17	0.80	0
5	CM5	E	504	-	12,12,36	1.15	1 (8%)	13,13,49	1.16	0
3	HEM	D	501	4,1	41,50,50	1.87	6 (14%)	45,82,82	1.78	8 (17%)
6	GOL	B	504	-	5,5,5	0.49	0	5,5,5	0.78	0
5	CM5	A	505	-	6,6,36	0.38	0	6,6,49	0.62	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
4	CPZ	C	502	3	-	0/0/4/4	0/2/2/2
4	CPZ	E	503	-	-	0/0/4/4	0/2/2/2
4	CPZ	A	503	-	-	0/0/4/4	0/2/2/2
4	CPZ	C	503	-	-	0/0/4/4	0/2/2/2
6	GOL	A	506	-	-	2/4/4/4	-
3	HEM	C	501	4,1	-	2/12/54/54	-
4	CPZ	A	502	3	-	0/0/4/4	0/2/2/2
6	GOL	C	504	-	-	0/4/4/4	-
4	CPZ	E	502	3	-	0/0/4/4	0/2/2/2
4	CPZ	B	502	3	-	0/0/4/4	0/2/2/2
3	HEM	A	501	4,1	-	4/12/54/54	-
6	GOL	E	505	-	-	4/4/4/4	-
4	CPZ	B	503	-	-	0/0/4/4	0/2/2/2
3	HEM	E	501	4,1	-	4/12/54/54	-
3	HEM	F	501	4	-	8/12/54/54	-
3	HEM	B	501	4,1	-	4/12/54/54	-
4	CPZ	D	502	-	-	0/0/4/4	0/2/2/2
4	CPZ	F	502	3	-	0/0/4/4	0/2/2/2
4	CPZ	D	503	3	-	0/0/4/4	0/2/2/2
4	CPZ	F	503	-	-	0/0/4/4	0/2/2/2
5	CM5	E	504	-	-	2/6/14/65	0/1/1/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	D	501	4,1	-	4/12/54/54	-
6	GOL	B	504	-	-	4/4/4/4	-
5	CM5	A	505	-	-	-	0/1/1/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	501	HEM	C3D-C2D	8.27	1.54	1.36
3	C	501	HEM	C3D-C2D	7.98	1.53	1.36
3	B	501	HEM	C3D-C2D	7.77	1.53	1.36
3	F	501	HEM	C3D-C2D	7.50	1.52	1.36
3	D	501	HEM	C3D-C2D	7.01	1.51	1.36
3	A	501	HEM	C3C-C2C	-6.05	1.32	1.40
3	C	501	HEM	C3C-C2C	-6.04	1.32	1.40
3	A	501	HEM	C3D-C2D	5.84	1.49	1.36
3	F	501	HEM	C3C-C2C	-5.57	1.32	1.40
3	E	501	HEM	C3C-C2C	-5.36	1.32	1.40
3	D	501	HEM	C3C-C2C	-4.63	1.34	1.40
3	B	501	HEM	C3C-C2C	-4.41	1.34	1.40
3	A	501	HEM	C3B-C2B	-4.08	1.29	1.37
3	E	501	HEM	FE-ND	3.86	2.16	1.96
3	A	501	HEM	O2A-CGA	-3.86	1.17	1.30
3	F	501	HEM	C3C-CAC	3.77	1.55	1.47
3	A	501	HEM	FE-NB	-3.73	1.78	1.96
3	E	501	HEM	C3C-CAC	3.50	1.55	1.47
3	B	501	HEM	C3C-CAC	3.44	1.54	1.47
3	C	501	HEM	C3C-CAC	3.38	1.54	1.47
3	D	501	HEM	CAB-C3B	3.19	1.56	1.47
3	A	501	HEM	O2D-CGD	-3.18	1.20	1.30
3	D	501	HEM	C3C-CAC	3.13	1.54	1.47
3	A	501	HEM	C4D-C3D	-3.04	1.39	1.45
3	B	501	HEM	CMB-C2B	3.03	1.57	1.50
3	C	501	HEM	CMB-C2B	2.96	1.57	1.50
3	C	501	HEM	CAA-C2A	2.89	1.56	1.52
3	A	501	HEM	C3C-CAC	2.89	1.53	1.47
3	A	501	HEM	C2A-C3A	-2.87	1.29	1.37
3	C	501	HEM	CMA-C3A	2.81	1.57	1.51
3	C	501	HEM	CAB-C3B	2.53	1.54	1.47
3	C	501	HEM	FE-ND	2.43	2.08	1.96
3	E	501	HEM	CMB-C2B	2.42	1.55	1.50
3	A	501	HEM	CAB-C3B	2.39	1.54	1.47
3	E	501	HEM	CAB-C3B	2.39	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	501	HEM	C3B-C2B	-2.38	1.32	1.37
3	A	501	HEM	C1A-CHA	-2.38	1.34	1.41
3	F	501	HEM	CMB-C2B	2.31	1.55	1.50
3	A	501	HEM	C4A-CHB	-2.26	1.34	1.41
3	F	501	HEM	CAB-C3B	2.26	1.53	1.47
4	B	502	CPZ	C7-C8	2.18	1.41	1.36
3	D	501	HEM	CMC-C2C	2.12	1.56	1.51
3	F	501	HEM	CMD-C2D	2.09	1.55	1.50
3	C	501	HEM	O1A-CGA	2.08	1.29	1.22
3	F	501	HEM	C4A-CHB	-2.06	1.35	1.41
3	B	501	HEM	CMD-C2D	2.05	1.55	1.50
3	A	501	HEM	C4D-ND	-2.03	1.36	1.40
3	B	501	HEM	CAB-C3B	2.03	1.52	1.47
3	D	501	HEM	C3B-C2B	-2.02	1.33	1.37
5	E	504	CM5	C11-C6	-2.02	1.46	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	501	HEM	C4D-ND-C1D	6.26	111.54	105.07
3	D	501	HEM	C4D-ND-C1D	5.72	110.98	105.07
3	F	501	HEM	C4D-ND-C1D	5.34	110.59	105.07
3	F	501	HEM	CAD-CBD-CGD	-4.62	103.67	113.60
3	C	501	HEM	C4D-ND-C1D	4.51	109.73	105.07
3	D	501	HEM	CMA-C3A-C4A	-4.39	121.72	128.46
3	E	501	HEM	CMA-C3A-C4A	-4.38	121.74	128.46
3	F	501	HEM	C2C-C3C-C4C	4.18	109.81	106.90
3	F	501	HEM	C4C-CHD-C1D	4.16	128.04	122.56
4	B	503	CPZ	C11-C6-C7	3.74	121.97	118.65
3	B	501	HEM	C4D-ND-C1D	3.71	108.91	105.07
3	D	501	HEM	C4C-CHD-C1D	3.61	127.32	122.56
3	B	501	HEM	CAD-CBD-CGD	-3.54	105.98	113.60
3	F	501	HEM	CBA-CAA-C2A	-3.51	106.63	112.62
3	E	501	HEM	C4C-CHD-C1D	3.42	127.07	122.56
3	A	501	HEM	C1B-NB-C4B	-3.41	101.55	105.07
3	A	501	HEM	C4D-ND-C1D	3.37	108.56	105.07
3	F	501	HEM	CMD-C2D-C1D	3.34	130.12	125.04
3	C	501	HEM	CAD-CBD-CGD	-3.17	106.79	113.60
3	D	501	HEM	C4B-CHC-C1C	3.17	126.74	122.56
3	B	501	HEM	C4B-CHC-C1C	2.99	126.50	122.56
3	D	501	HEM	CHC-C4B-NB	2.92	127.60	124.43
3	B	501	HEM	CHA-C4D-ND	2.91	127.97	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	501	HEM	CMA-C3A-C2A	2.79	130.20	124.94
3	B	501	HEM	C1D-C2D-C3D	-2.75	104.07	106.96
3	C	501	HEM	C2C-C3C-C4C	2.74	108.81	106.90
3	F	501	HEM	C3C-C4C-NC	-2.70	105.85	110.94
3	C	501	HEM	O1D-CGD-CBD	-2.64	114.61	123.08
3	E	501	HEM	CMA-C3A-C2A	2.57	129.79	124.94
3	A	501	HEM	CMD-C2D-C1D	2.54	128.90	125.04
3	E	501	HEM	C4D-C3D-C2D	-2.54	103.20	106.90
3	A	501	HEM	O2A-CGA-CBA	2.47	121.98	114.03
3	D	501	HEM	CAA-CBA-CGA	-2.47	106.82	113.76
3	B	501	HEM	CAA-CBA-CGA	-2.43	106.95	113.76
3	F	501	HEM	CMA-C3A-C4A	-2.38	124.81	128.46
3	B	501	HEM	CMA-C3A-C4A	-2.36	124.84	128.46
3	C	501	HEM	O2D-CGD-CBD	2.35	121.58	114.03
3	A	501	HEM	CHC-C4B-NB	2.30	126.93	124.43
3	A	501	HEM	C4C-CHD-C1D	2.30	125.59	122.56
3	A	501	HEM	C1D-C2D-C3D	-2.27	104.57	106.96
3	E	501	HEM	O2A-CGA-CBA	2.26	121.30	114.03
3	A	501	HEM	O2D-CGD-CBD	2.23	121.18	114.03
3	B	501	HEM	CMD-C2D-C1D	2.22	128.42	125.04
3	A	501	HEM	C2B-C1B-NB	2.13	112.36	109.84
3	E	501	HEM	C4A-C3A-C2A	2.11	108.47	107.00
3	C	501	HEM	CMA-C3A-C4A	-2.10	125.24	128.46
3	C	501	HEM	C4C-CHD-C1D	2.04	125.25	122.56
3	B	501	HEM	O2A-CGA-CBA	2.03	120.54	114.03
3	D	501	HEM	CAD-CBD-CGD	-2.01	109.28	113.60

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	501	HEM	C1A-C2A-CAA-CBA
3	F	501	HEM	C3A-C2A-CAA-CBA
6	A	506	GOL	C1-C2-C3-O3
6	A	506	GOL	O2-C2-C3-O3
6	B	504	GOL	O1-C1-C2-C3
6	B	504	GOL	C1-C2-C3-O3
6	E	505	GOL	O1-C1-C2-C3
6	E	505	GOL	C1-C2-C3-O3
6	B	504	GOL	O2-C2-C3-O3
6	E	505	GOL	O2-C2-C3-O3
6	B	504	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	E	505	GOL	O1-C1-C2-O2
5	E	504	CM5	O12-C1-C2-C3
5	E	504	CM5	C2-C3-C4-C5
3	F	501	HEM	CAA-CBA-CGA-O2A
3	F	501	HEM	CAA-CBA-CGA-O1A
3	F	501	HEM	CAD-CBD-CGD-O2D
3	D	501	HEM	CAD-CBD-CGD-O1D
3	F	501	HEM	C2D-C3D-CAD-CBD
3	E	501	HEM	CAD-CBD-CGD-O1D
3	B	501	HEM	CAA-CBA-CGA-O2A
3	E	501	HEM	CAA-CBA-CGA-O2A
3	C	501	HEM	CAD-CBD-CGD-O1D
3	F	501	HEM	CAD-CBD-CGD-O1D
3	B	501	HEM	CAA-CBA-CGA-O1A
3	A	501	HEM	CAA-CBA-CGA-O1A
3	F	501	HEM	C4D-C3D-CAD-CBD
3	D	501	HEM	CAA-CBA-CGA-O2A
3	A	501	HEM	CAA-CBA-CGA-O2A
3	D	501	HEM	CAA-CBA-CGA-O1A
3	E	501	HEM	CAA-CBA-CGA-O1A
3	A	501	HEM	CAD-CBD-CGD-O1D
3	B	501	HEM	CAD-CBD-CGD-O1D
3	C	501	HEM	CAD-CBD-CGD-O2D
3	D	501	HEM	CAD-CBD-CGD-O2D
3	B	501	HEM	CAD-CBD-CGD-O2D
3	E	501	HEM	CAD-CBD-CGD-O2D
3	A	501	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

20 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	502	CPZ	4	0
4	E	503	CPZ	3	0
4	A	503	CPZ	1	0
4	C	503	CPZ	3	0
3	C	501	HEM	7	0
4	A	502	CPZ	4	0
4	E	502	CPZ	6	0
4	B	502	CPZ	5	0
3	A	501	HEM	9	0
4	B	503	CPZ	5	0

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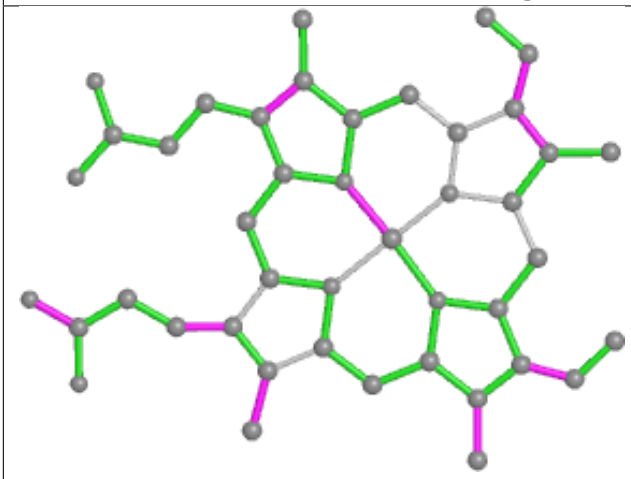
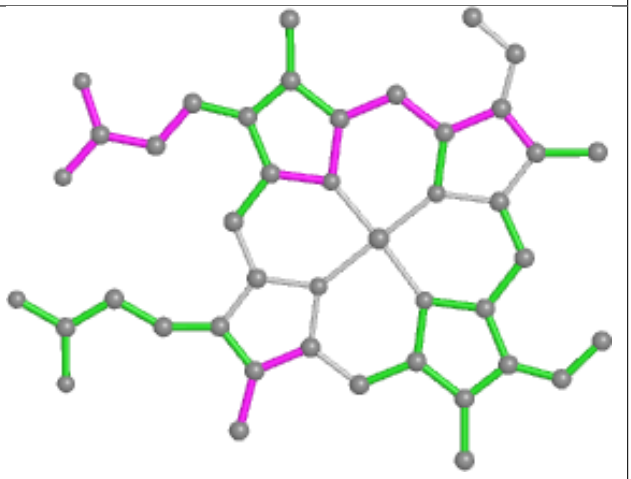
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	501	HEM	8	0
3	F	501	HEM	7	0
3	B	501	HEM	9	0
4	D	502	CPZ	4	0
4	F	502	CPZ	5	0
4	D	503	CPZ	2	0
4	F	503	CPZ	6	0
5	E	504	CM5	2	0
3	D	501	HEM	2	0
6	B	504	GOL	1	0

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.

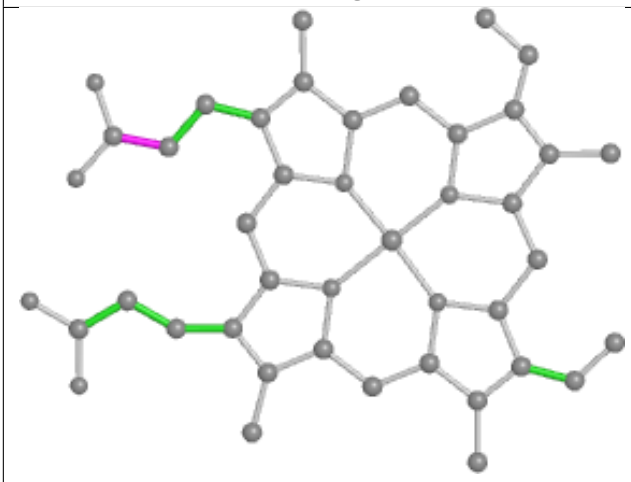
Ligand HEM C 501



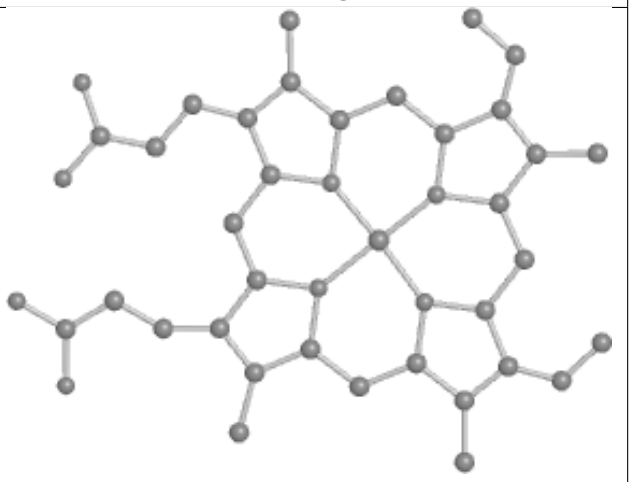
Bond lengths



Bond angles

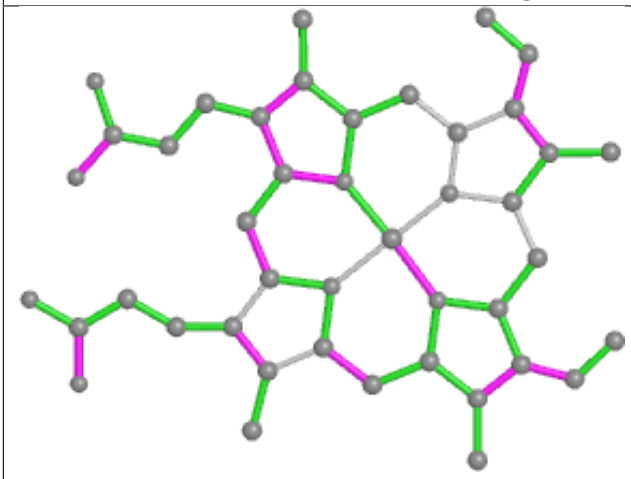


Torsions

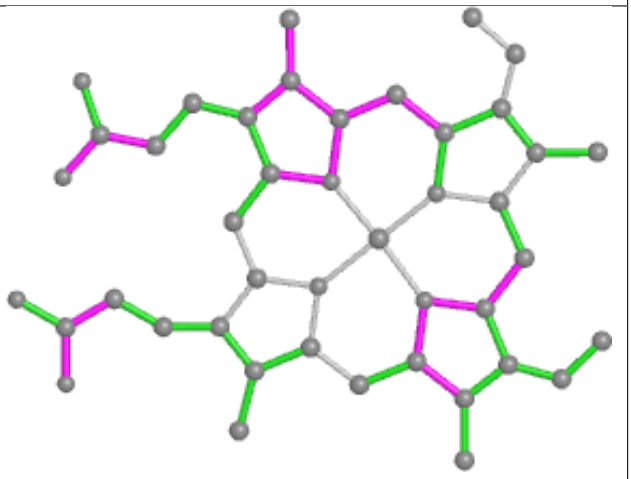


Rings

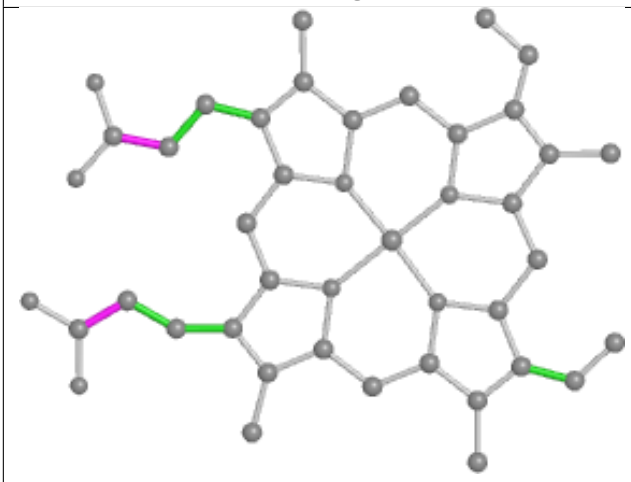
Ligand HEM A 501



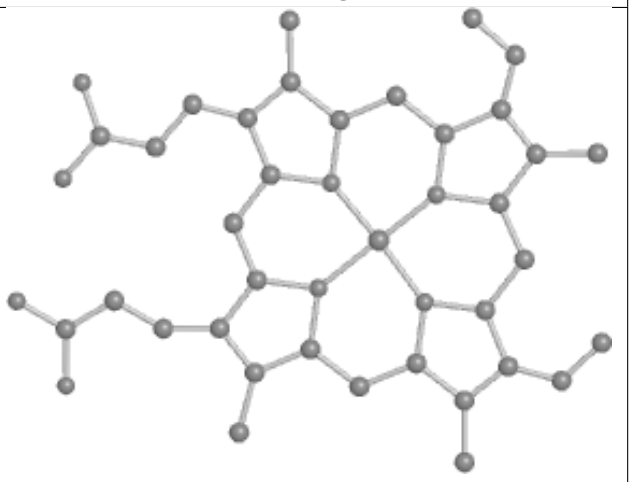
Bond lengths



Bond angles

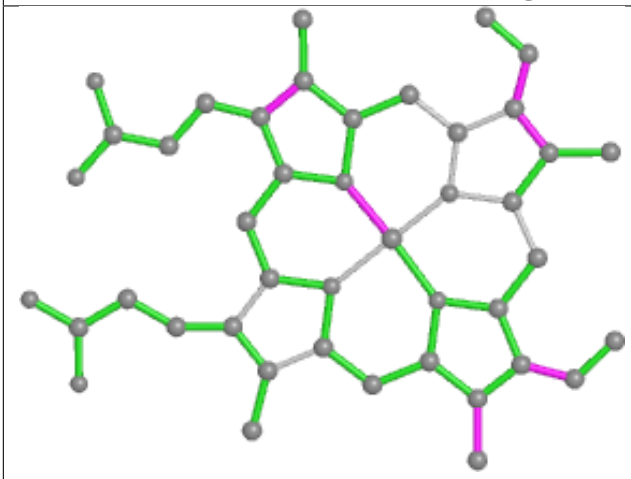


Torsions

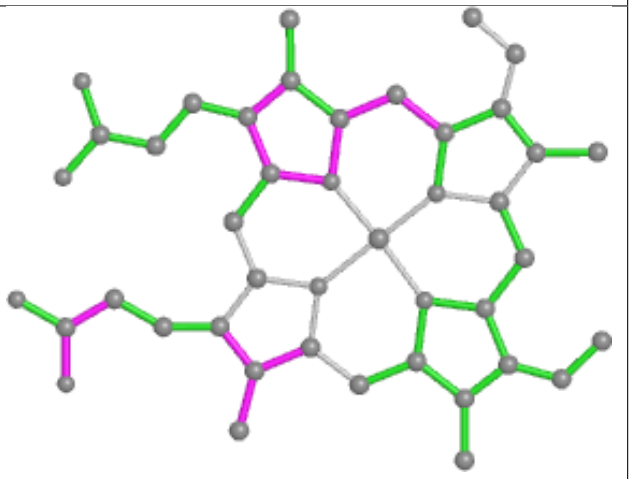


Rings

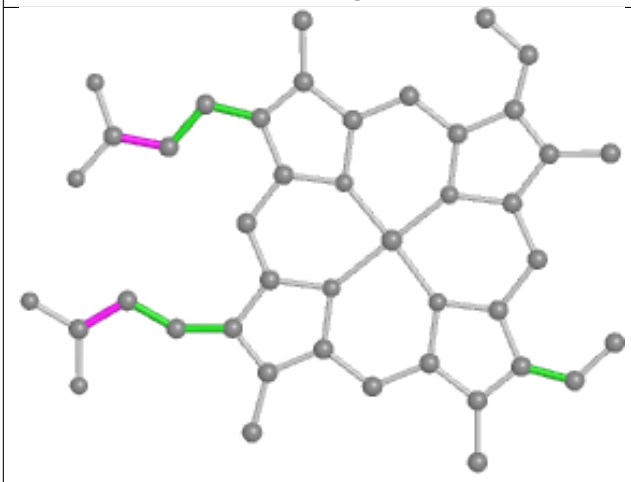
Ligand HEM E 501



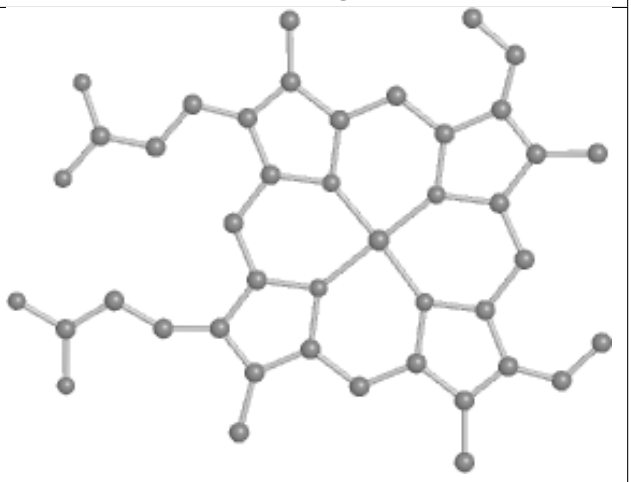
Bond lengths



Bond angles

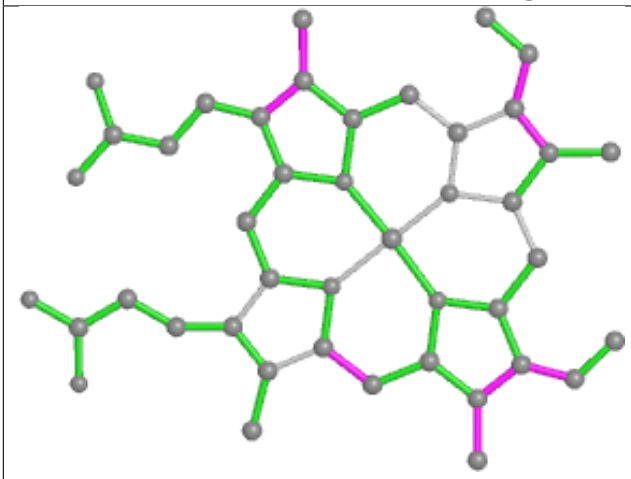


Torsions

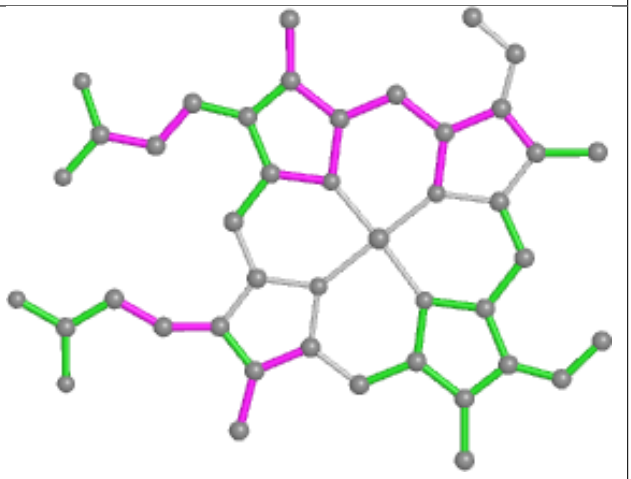


Rings

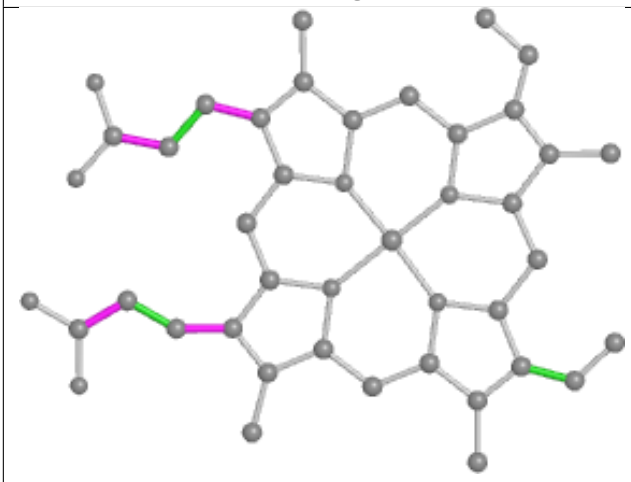
Ligand HEM F 501



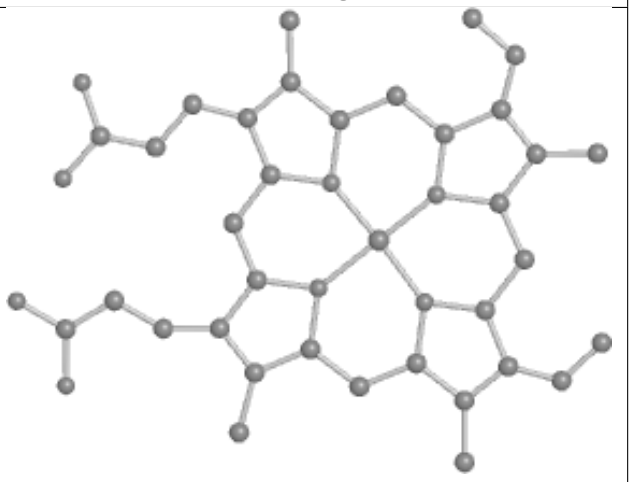
Bond lengths



Bond angles

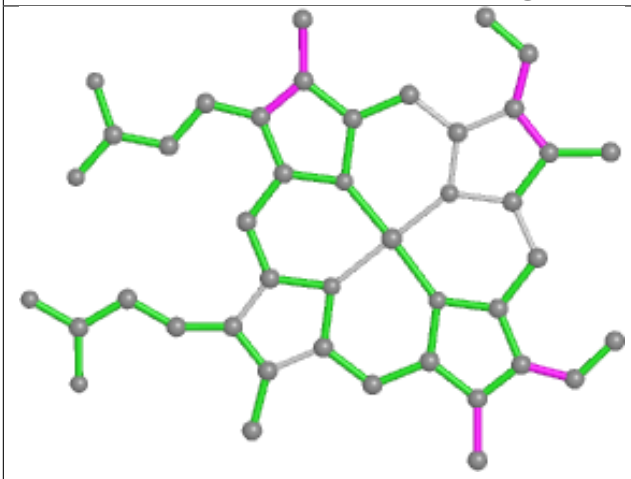


Torsions

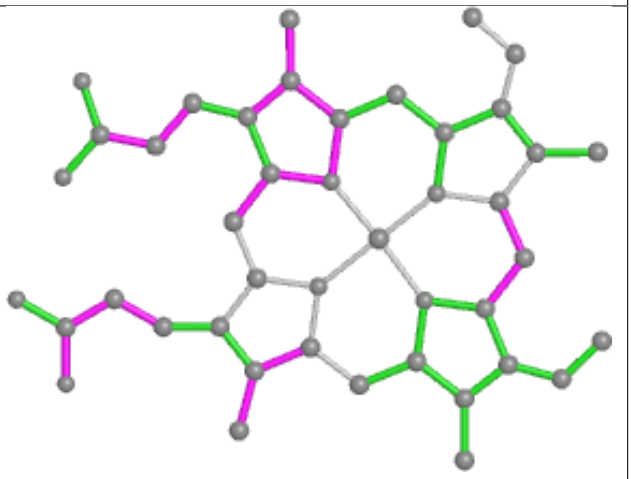


Rings

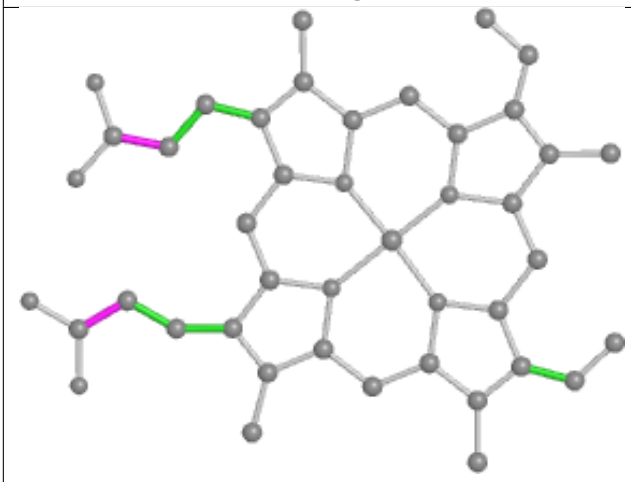
Ligand HEM B 501



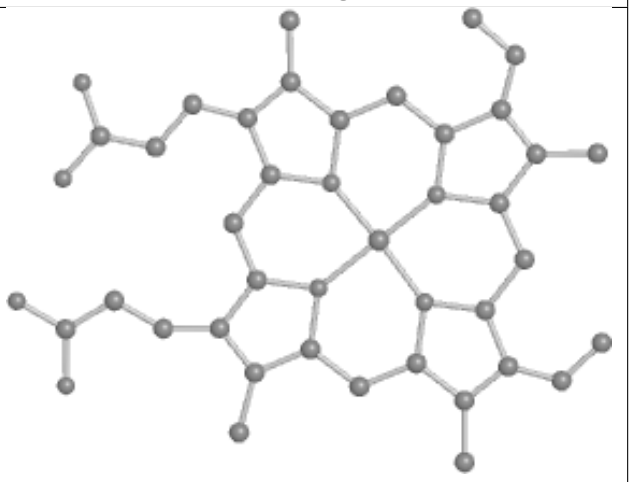
Bond lengths



Bond angles

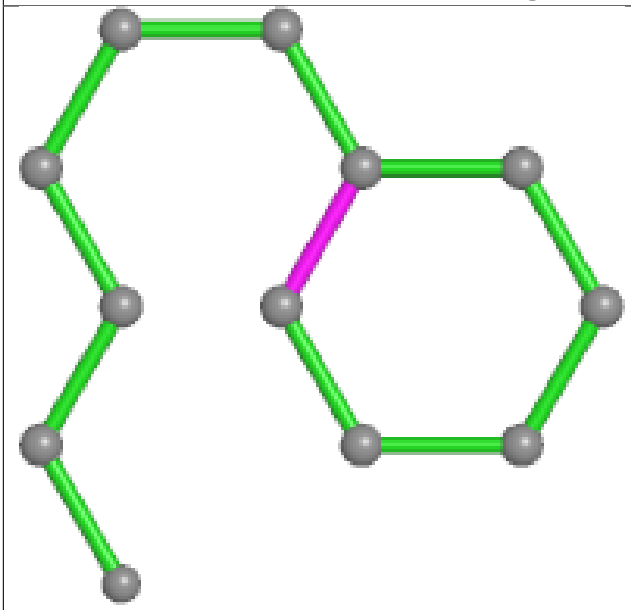


Torsions

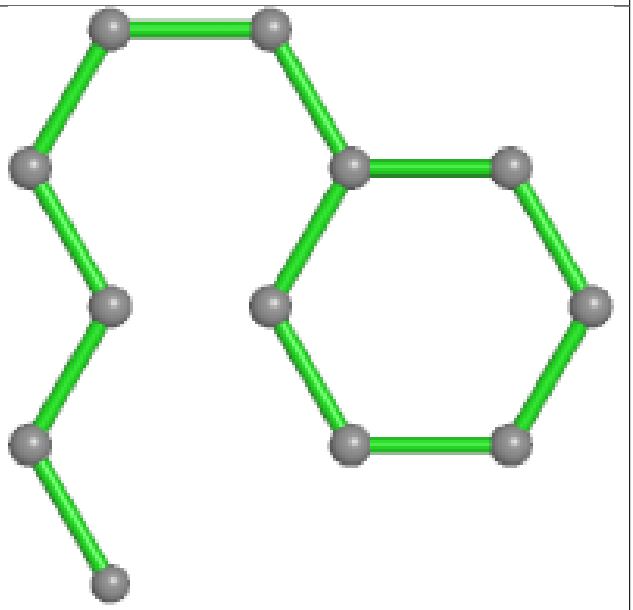


Rings

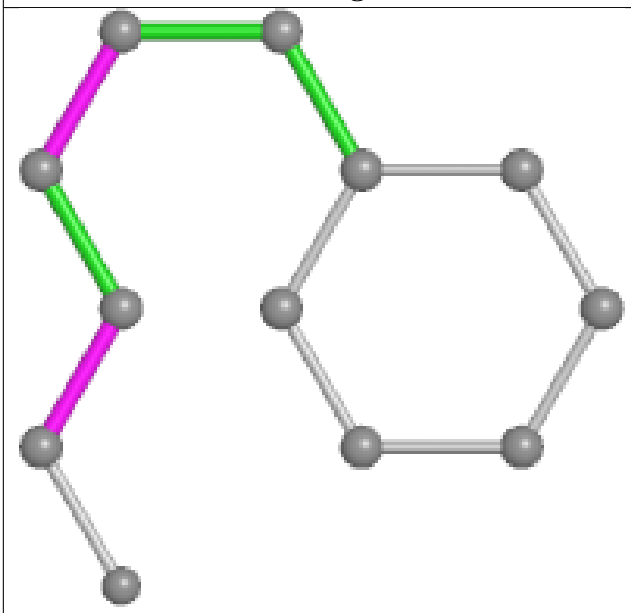
Ligand CM5 E 504



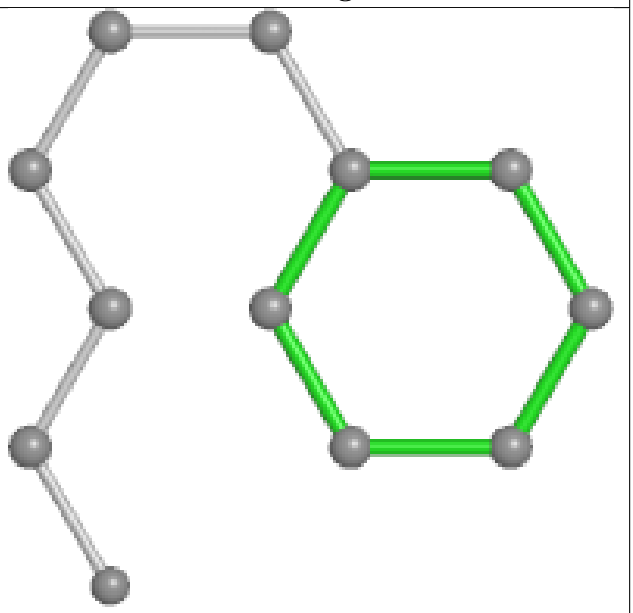
Bond lengths



Bond angles

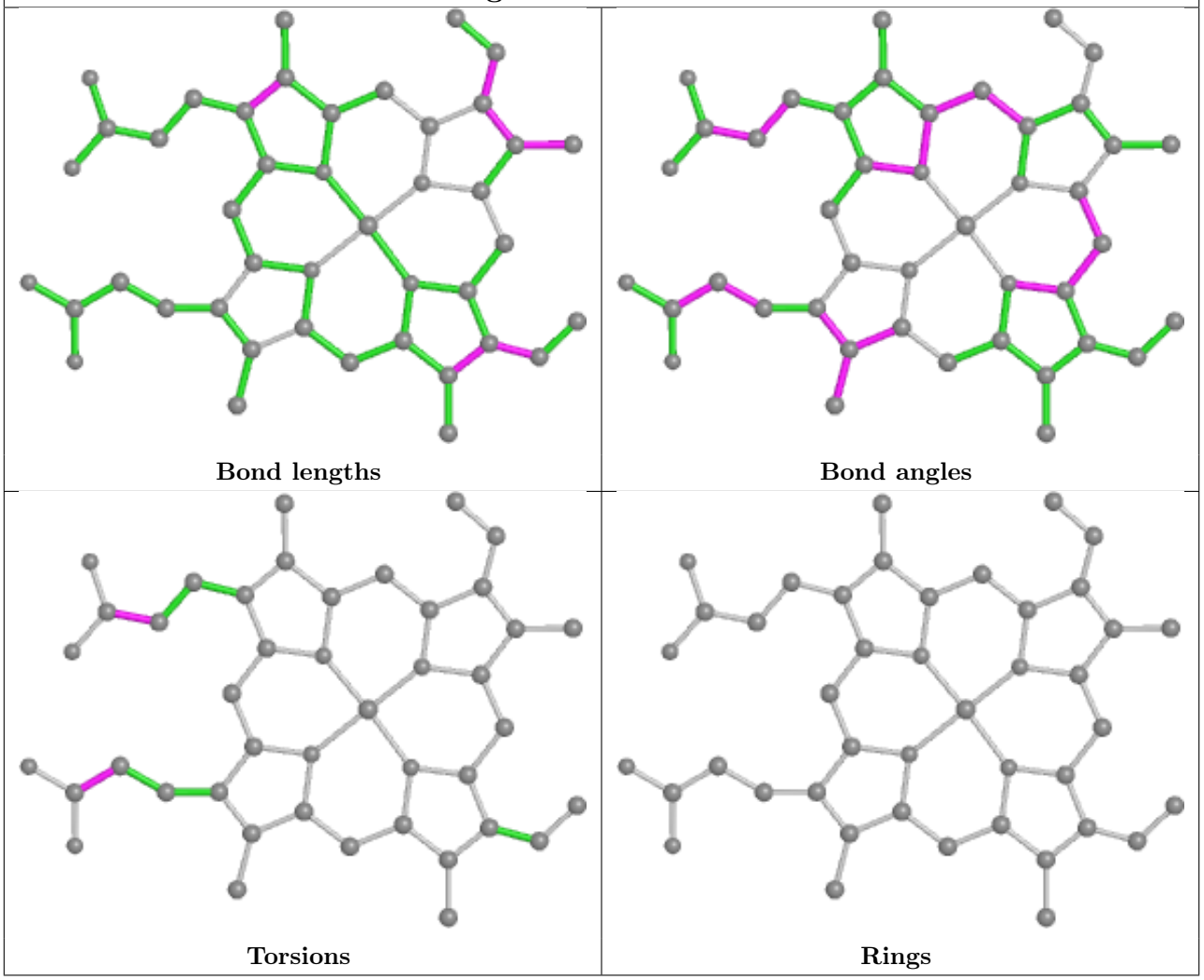


Torsions



Rings

Ligand HEM D 501



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	464/493 (94%)	-0.21	11 (2%)	59	57	19, 35, 60, 90	0
1	B	458/493 (92%)	0.13	22 (4%)	30	29	30, 50, 73, 86	0
1	C	465/493 (94%)	-0.17	5 (1%)	80	79	22, 43, 71, 90	0
1	D	463/493 (93%)	-0.10	14 (3%)	50	49	24, 45, 63, 84	0
1	E	462/493 (93%)	-0.03	15 (3%)	47	46	27, 48, 71, 79	0
1	F	458/493 (92%)	0.40	38 (8%)	11	10	27, 57, 75, 95	0
All	All	2770/2958 (93%)	0.00	105 (3%)	40	39	19, 47, 71, 95	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	492	HIS	5.1
1	F	490	ALA	5.0
1	F	259	SER	4.8
1	F	260	ASN	4.7
1	F	280	HIS	4.5
1	F	465	PRO	4.1
1	F	194	GLN	4.0
1	E	259	SER	4.0
1	F	491	ARG	3.8
1	D	254	ALA	3.7
1	C	416	ALA	3.7
1	B	162	GLY	3.6
1	D	223	PHE	3.5
1	F	315	LEU	3.4
1	C	419	ALA	3.4
1	D	256	LEU	3.4
1	E	298	ALA	3.3
1	F	190	TYR	3.3
1	F	298	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	492	HIS	3.2
1	D	334	SER	3.1
1	B	320	VAL	3.1
1	F	488	PHE	3.1
1	D	379	GLY	3.1
1	E	260	ASN	3.1
1	B	464	ALA	3.1
1	E	324	VAL	3.1
1	D	280	HIS	3.0
1	E	157	LEU	3.0
1	E	419	ALA	3.0
1	F	191	LYS	3.0
1	F	486	ILE	2.8
1	F	165	LEU	2.8
1	E	463	VAL	2.8
1	D	277	SER	2.8
1	A	365	ILE	2.7
1	D	365	ILE	2.7
1	F	340	LEU	2.7
1	F	249	VAL	2.7
1	B	303	THR	2.7
1	E	299	GLY	2.7
1	F	366	GLY	2.7
1	B	337	LEU	2.6
1	E	256	LEU	2.6
1	B	490	ALA	2.6
1	B	436	CYS	2.6
1	B	163	ALA	2.5
1	B	463	VAL	2.5
1	F	195	PHE	2.5
1	B	462	SER	2.5
1	F	268	TYR	2.5
1	B	465	PRO	2.5
1	F	163	ALA	2.5
1	B	302	THR	2.5
1	B	416	ALA	2.5
1	A	436	CYS	2.4
1	B	376	LEU	2.4
1	F	463	VAL	2.4
1	E	253	ARG	2.4
1	A	363	ALA	2.4
1	E	254	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	258	PRO	2.4
1	A	442	ALA	2.4
1	F	321	ALA	2.4
1	F	152	CYS	2.4
1	A	366	GLY	2.3
1	F	142	VAL	2.3
1	E	335	HIS	2.3
1	B	298	ALA	2.3
1	B	363	ALA	2.3
1	F	464	ALA	2.3
1	B	336	ARG	2.3
1	F	162	GLY	2.3
1	F	262	ARG	2.3
1	F	90	ASP	2.3
1	A	429	PHE	2.3
1	B	417	ASN	2.3
1	A	298	ALA	2.3
1	F	447	PHE	2.3
1	C	489	LEU	2.3
1	E	273	GLU	2.2
1	C	490	ALA	2.2
1	D	270	LEU	2.2
1	E	165	LEU	2.2
1	F	324	VAL	2.2
1	A	29	HIS	2.2
1	B	335	HIS	2.2
1	B	460	SER	2.2
1	D	416	ALA	2.2
1	A	299	GLY	2.2
1	D	376	LEU	2.2
1	F	245	VAL	2.2
1	F	459	VAL	2.2
1	B	338	PRO	2.1
1	D	260	ASN	2.1
1	F	341	GLU	2.1
1	F	391	ILE	2.1
1	F	319	HIS	2.1
1	C	365	ILE	2.1
1	A	303	THR	2.1
1	D	259	SER	2.1
1	D	255	THR	2.0
1	B	196	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	185	GLY	2.0
1	F	256	LEU	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)

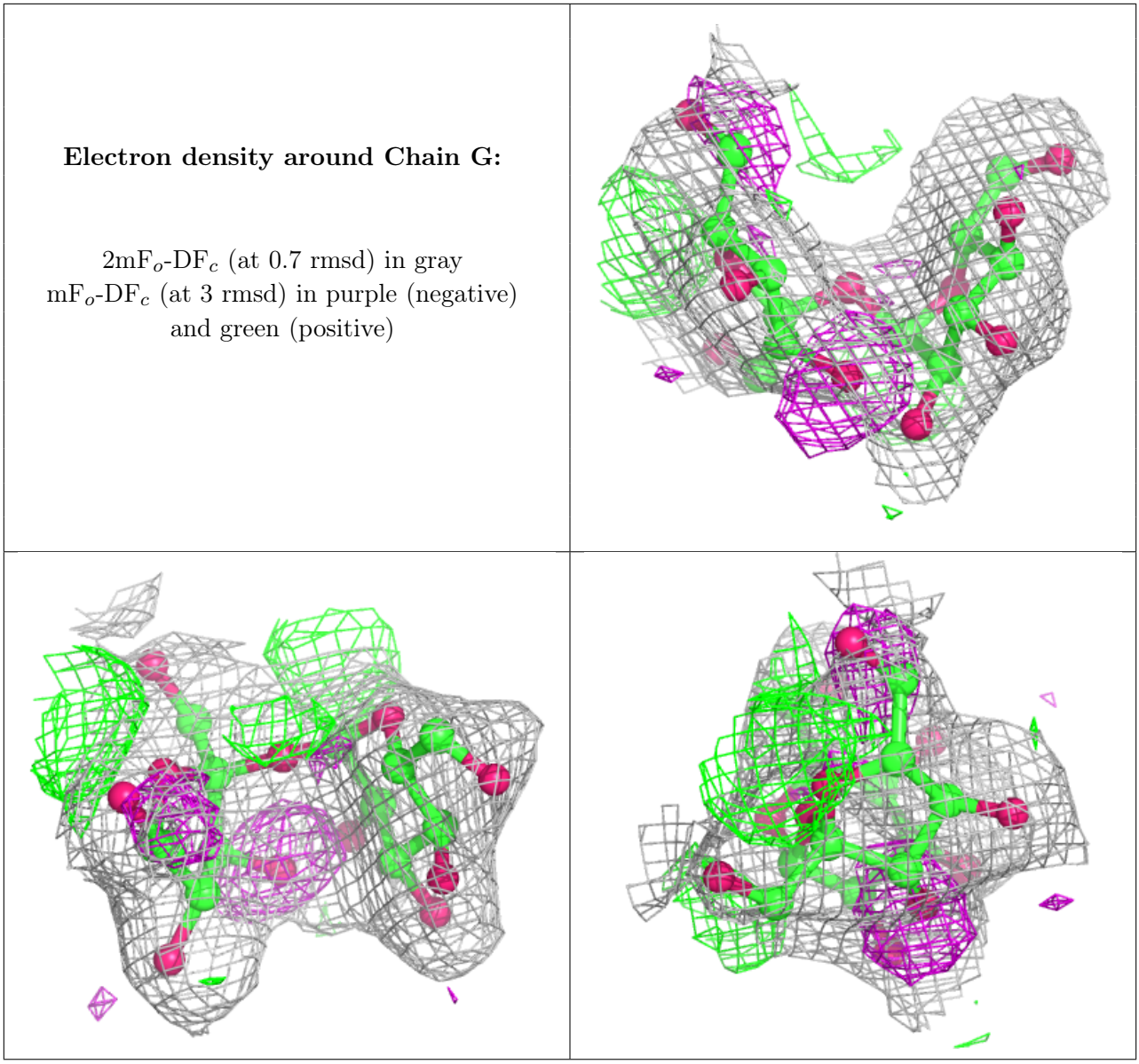
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	FRU	G	2	12/12	0.70	0.24	35,45,54,55	0
2	GLC	G	1	11/12	0.88	0.11	59,60,62,63	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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



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
6	GOL	A	506	6/6	0.74	0.09	47,52,53,54	0
6	GOL	C	504	6/6	0.74	0.14	65,69,69,71	0
6	GOL	E	505	6/6	0.83	0.13	65,67,68,69	0
4	CPZ	D	502	12/12	0.84	0.22	57,58,61,65	0
6	GOL	B	504	6/6	0.84	0.15	54,59,60,61	0

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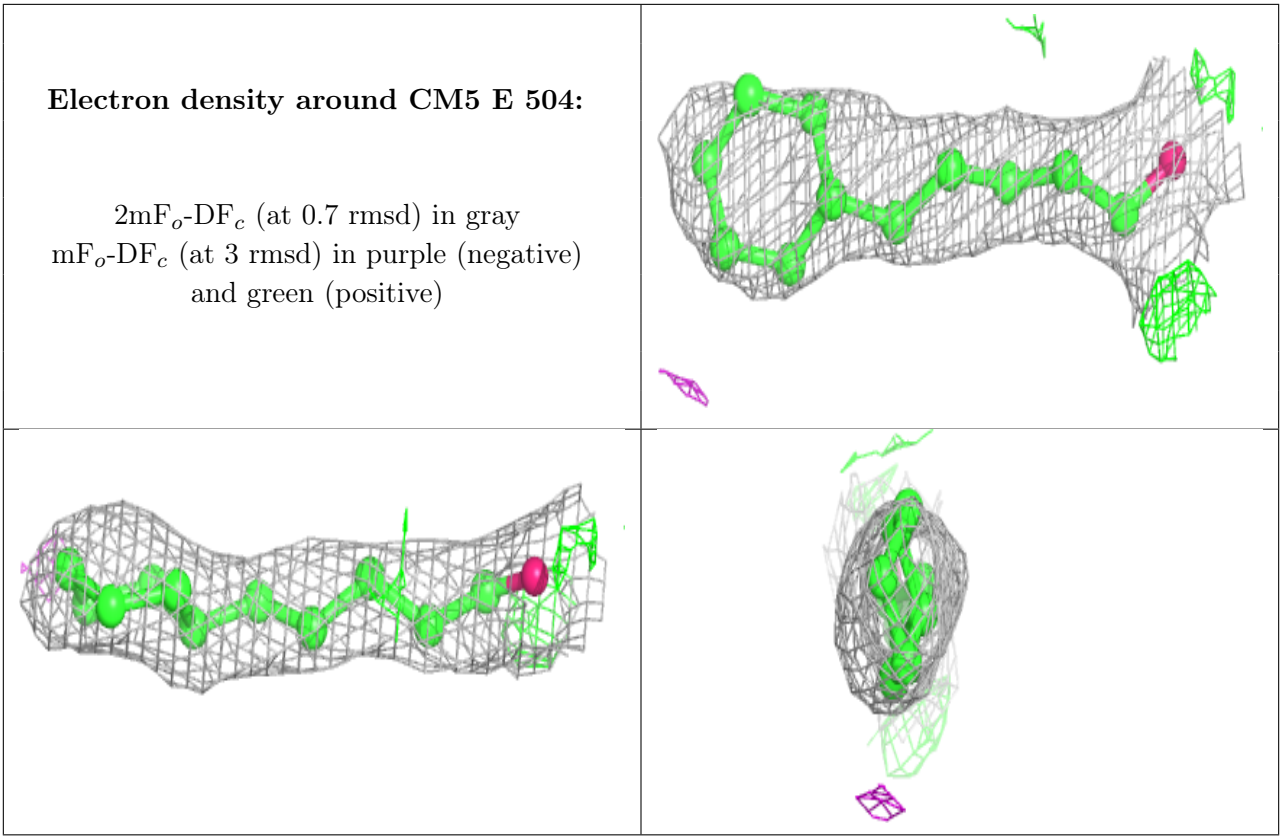
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CPZ	A	503	12/12	0.85	0.23	49,52,56,60	0
4	CPZ	B	503	12/12	0.86	0.27	68,70,74,76	0
4	CPZ	F	503	12/12	0.88	0.23	68,69,71,71	0
5	CM5	E	504	12/34	0.88	0.18	63,66,67,67	0
4	CPZ	E	503	12/12	0.90	0.23	69,71,72,76	0
4	CPZ	F	502	12/12	0.92	0.25	54,65,69,72	0
5	CM5	A	505	6/34	0.93	0.16	55,55,56,56	0
4	CPZ	C	503	12/12	0.93	0.16	49,51,53,60	0
4	CPZ	D	503	12/12	0.95	0.17	35,42,49,52	0
3	HEM	E	501	43/43	0.96	0.20	33,38,42,47	0
4	CPZ	B	502	12/12	0.96	0.20	39,41,43,44	0
4	CPZ	E	502	12/12	0.96	0.21	42,46,46,47	0
3	HEM	F	501	43/43	0.97	0.18	40,44,49,53	0
4	CPZ	A	502	12/12	0.97	0.18	31,33,35,37	0
4	CPZ	C	502	12/12	0.97	0.18	40,42,44,45	0
3	HEM	B	501	43/43	0.97	0.20	29,35,37,39	0
3	HEM	D	501	43/43	0.98	0.17	23,30,34,39	0
3	HEM	A	501	43/43	0.98	0.20	12,17,21,26	0
3	HEM	C	501	43/43	0.98	0.16	16,24,29,37	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.

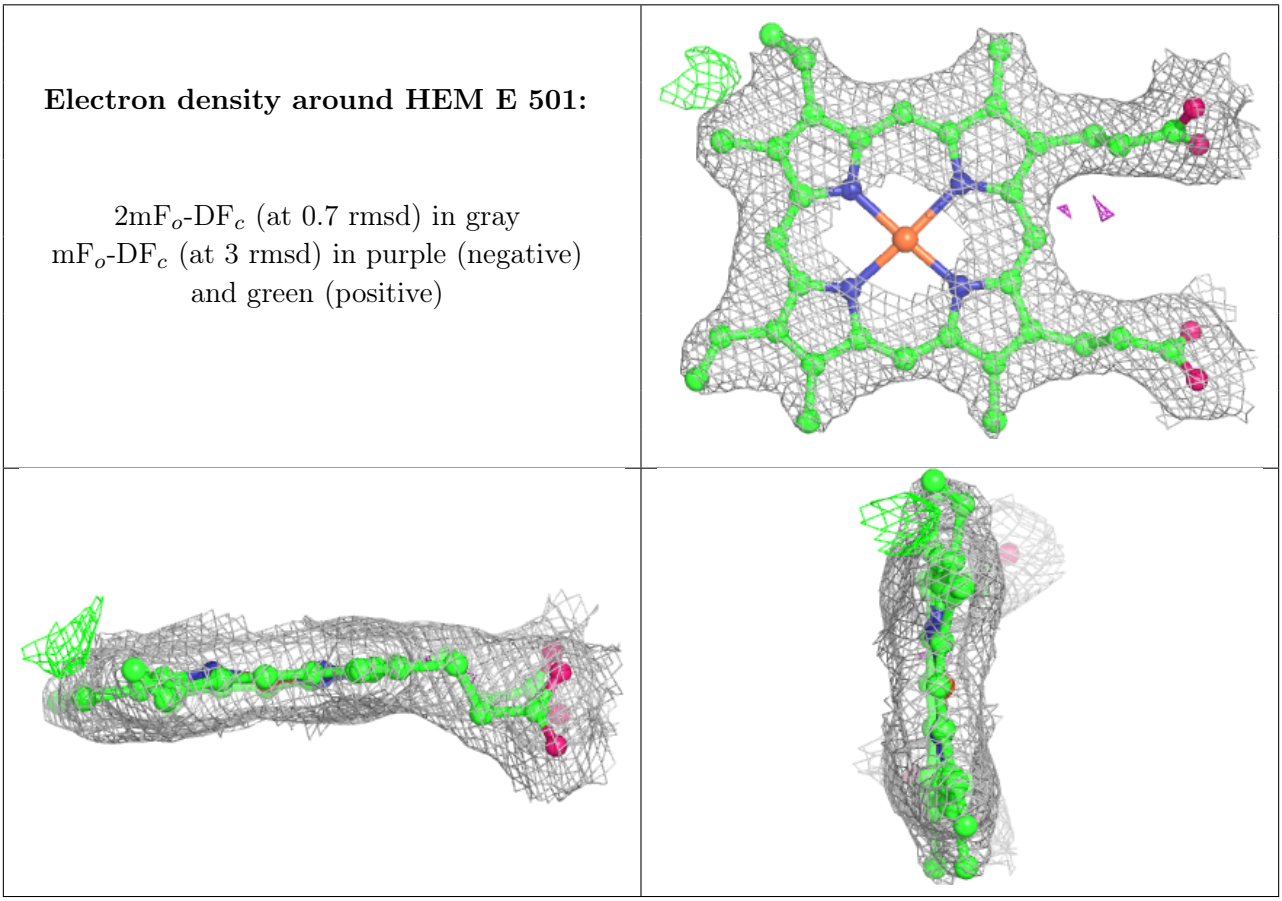
Electron density around CM5 E 504:

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



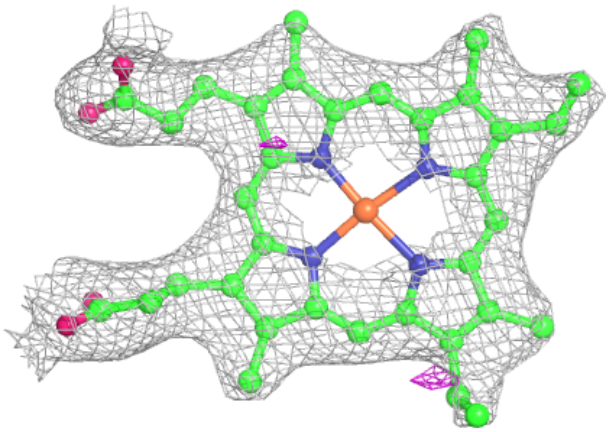
Electron density around HEM E 501:

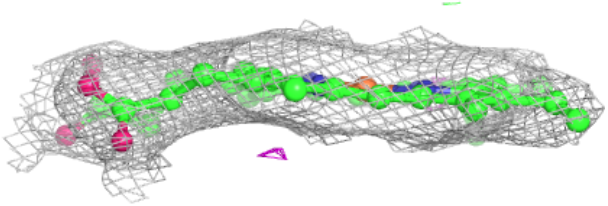
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

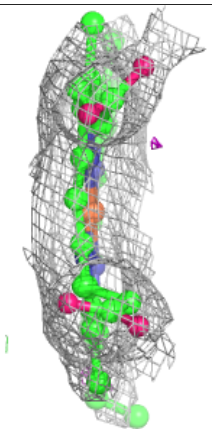


Electron density around HEM F 501:

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

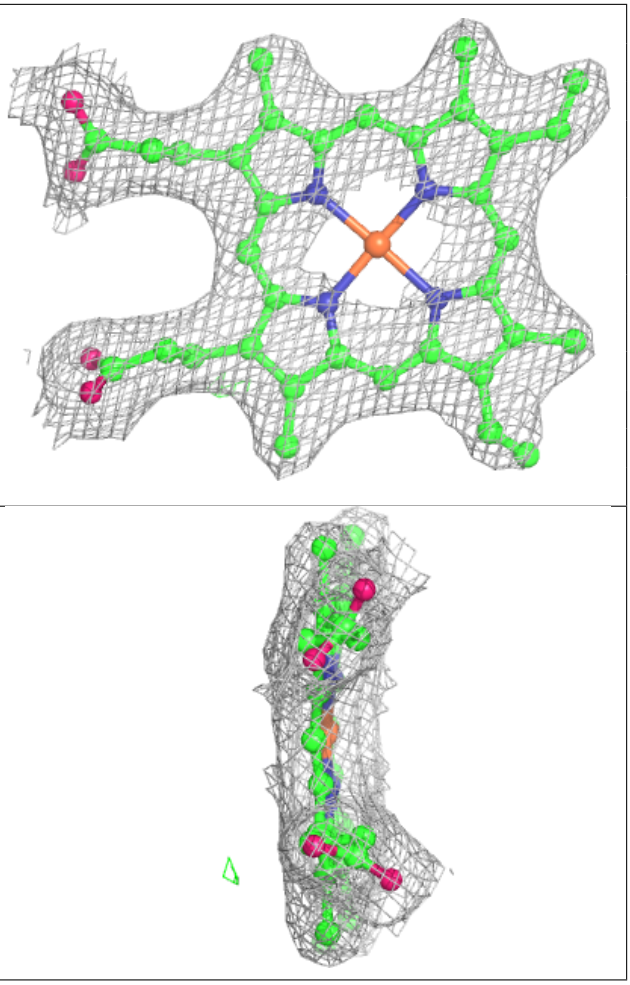






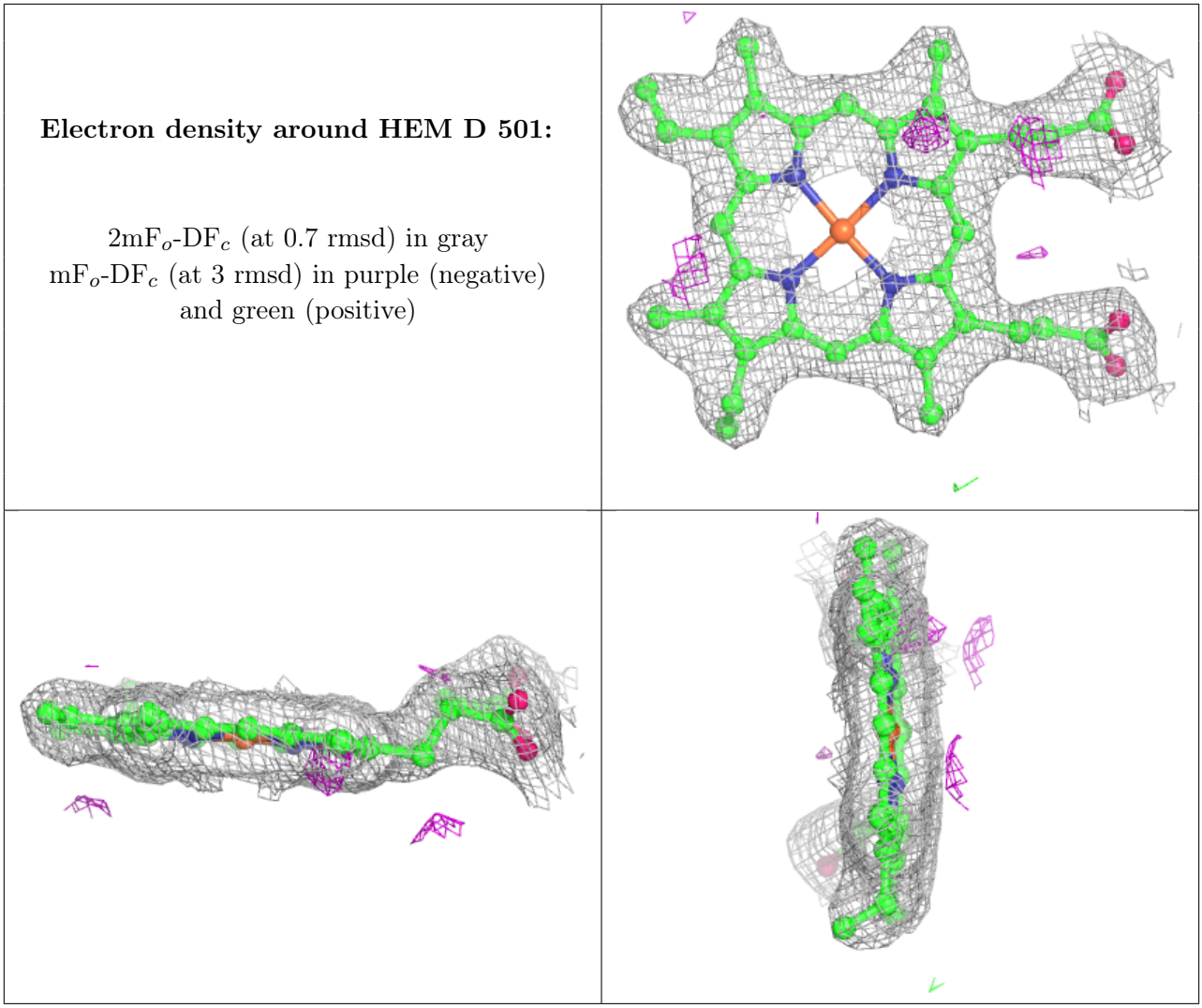
Electron density around HEM B 501:

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



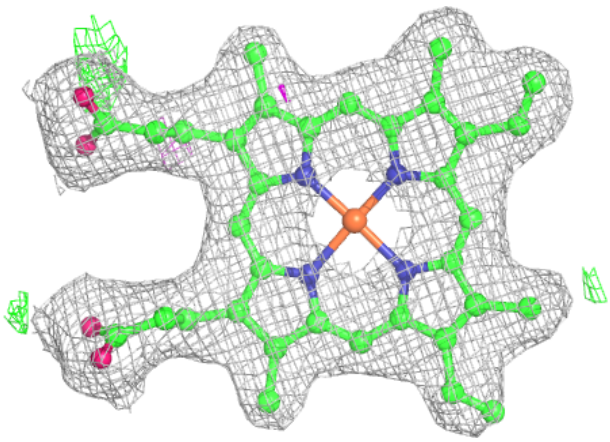
Electron density around HEM D 501:

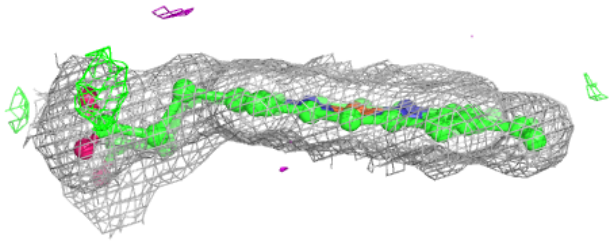
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

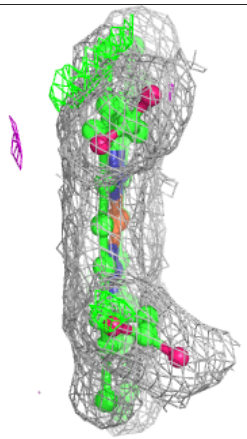


Electron density around HEM A 501:

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

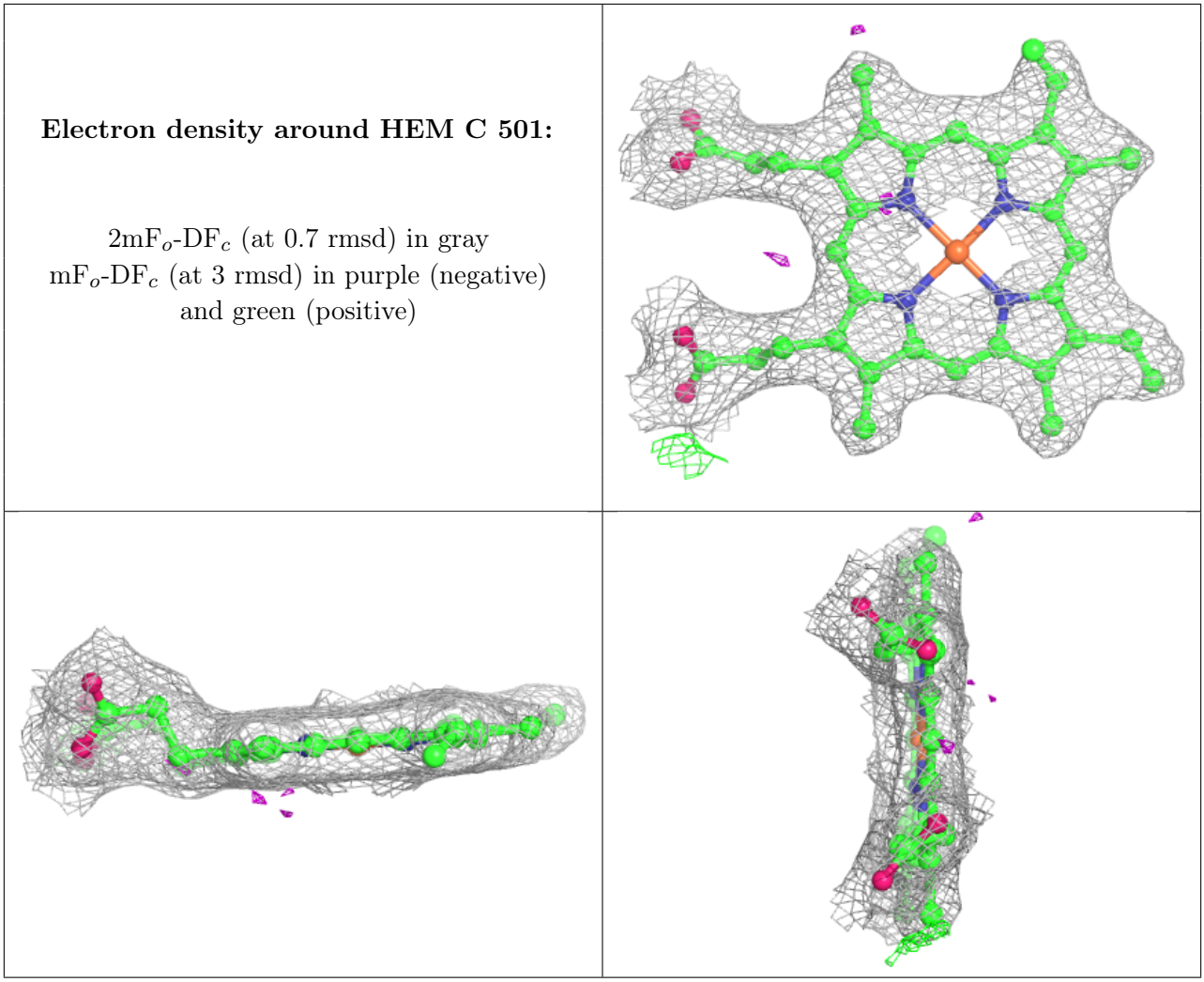






Electron density around HEM C 501:

$2mF_o$-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

There are no such residues in this entry.