



# Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2021 – 04:22 PM EDT

PDB ID : 7M8I  
Title : Human CYP11B2 and human adrenodoxin in complex with fadrozole  
Authors : Scott, E.E.; Brixius-Anderko, S.  
Deposited on : 2021-03-29  
Resolution : 2.94 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](mailto: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.

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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 : 2.18  
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) : 2.18

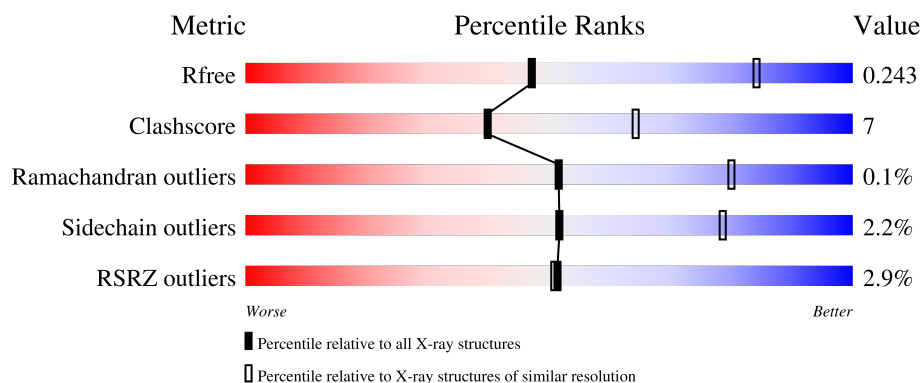
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.94 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	609	
1	B	609	
1	C	609	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27303 atoms, of which 13636 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 Adrenodoxin, Cytochrome P450 11B2, mitochondrial fusion enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	572	Total	C	H	N	O	S	0	0	0
			9221	2948	4618	808	819	28			
1	B	572	Total	C	H	N	O	S	0	0	0
			9224	2950	4618	810	818	28			
1	C	529	Total	C	H	N	O	S	0	0	0
			8536	2736	4271	752	752	25			

There are 36 discrepancies between the modelled and reference sequences:

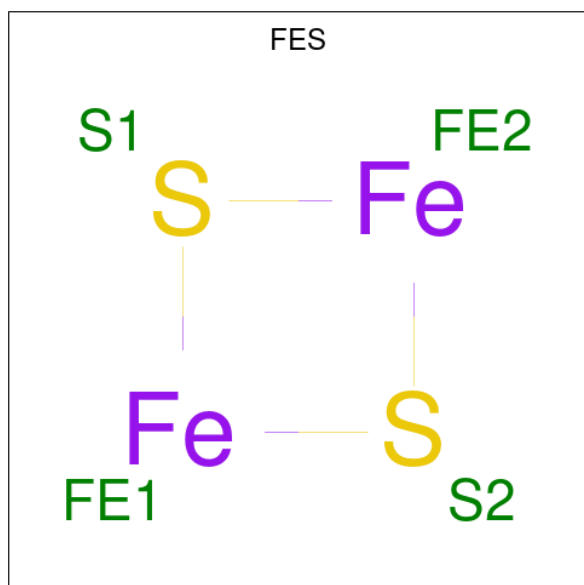
Chain	Residue	Modelled	Actual	Comment	Reference
A	60	MET	-	initiating methionine	UNP P10109
A	185	ALA	-	linker	UNP P10109
A	186	ALA	-	linker	UNP P10109
A	187	LYS	-	linker	UNP P10109
A	188	LYS	-	linker	UNP P10109
A	189	THR	-	linker	UNP P10109
A	190	SER	-	linker	UNP P10109
A	191	SER	-	linker	UNP P10109
A	1504	HIS	-	expression tag	UNP P19099
A	1505	HIS	-	expression tag	UNP P19099
A	1506	HIS	-	expression tag	UNP P19099
A	1507	HIS	-	expression tag	UNP P19099
B	60	MET	-	initiating methionine	UNP P10109
B	185	ALA	-	linker	UNP P10109
B	186	ALA	-	linker	UNP P10109
B	187	LYS	-	linker	UNP P10109
B	188	LYS	-	linker	UNP P10109
B	189	THR	-	linker	UNP P10109
B	190	SER	-	linker	UNP P10109
B	191	SER	-	linker	UNP P10109
B	1504	HIS	-	expression tag	UNP P19099
B	1505	HIS	-	expression tag	UNP P19099

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1506	HIS	-	expression tag	UNP P19099
B	1507	HIS	-	expression tag	UNP P19099
C	60	MET	-	initiating methionine	UNP P10109
C	185	ALA	-	linker	UNP P10109
C	186	ALA	-	linker	UNP P10109
C	187	LYS	-	linker	UNP P10109
C	188	LYS	-	linker	UNP P10109
C	189	THR	-	linker	UNP P10109
C	190	SER	-	linker	UNP P10109
C	191	SER	-	linker	UNP P10109
C	1504	HIS	-	expression tag	UNP P19099
C	1505	HIS	-	expression tag	UNP P19099
C	1506	HIS	-	expression tag	UNP P19099
C	1507	HIS	-	expression tag	UNP P19099

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



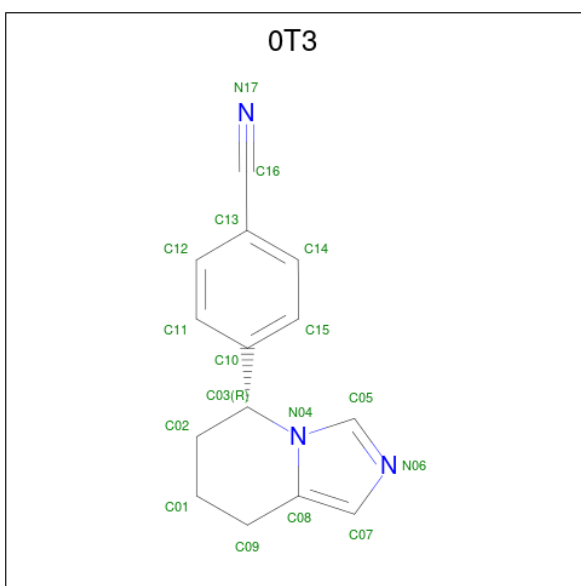
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	C	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 4 is 4-[(5R)-5,6,7,8-tetrahydroimidazo[1,5-a]pyridin-5-yl]benzonitrile (three-letter code: OT3) (formula: C<sub>14</sub>H<sub>13</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	N	0	0
			30	14	13	3		
4	B	1	Total	C	H	N	0	0
			30	14	13	3		
4	C	1	Total	C	H	N	0	0
			30	14	13	3		

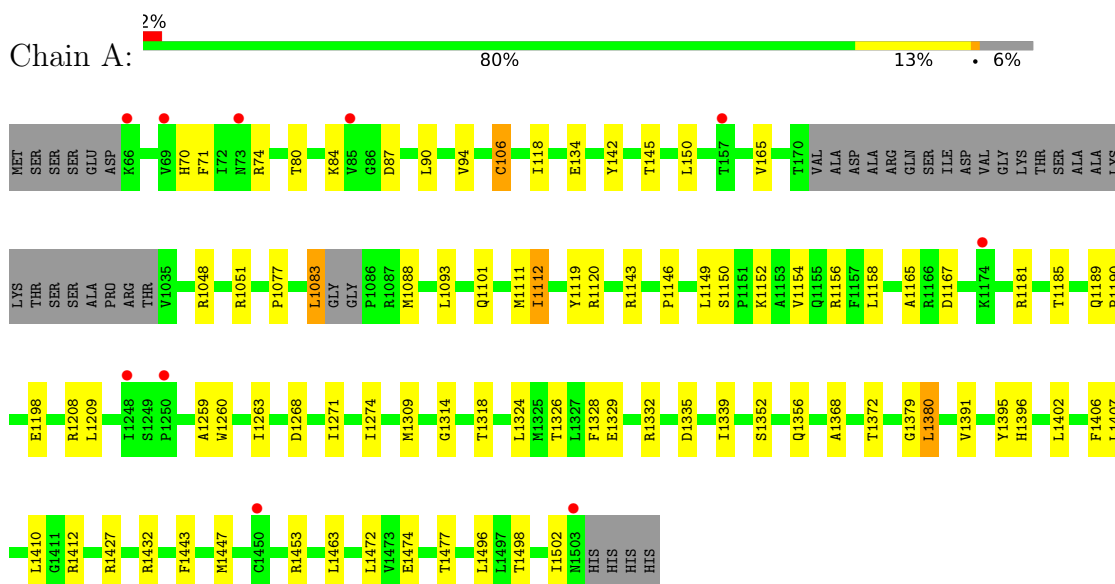
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		

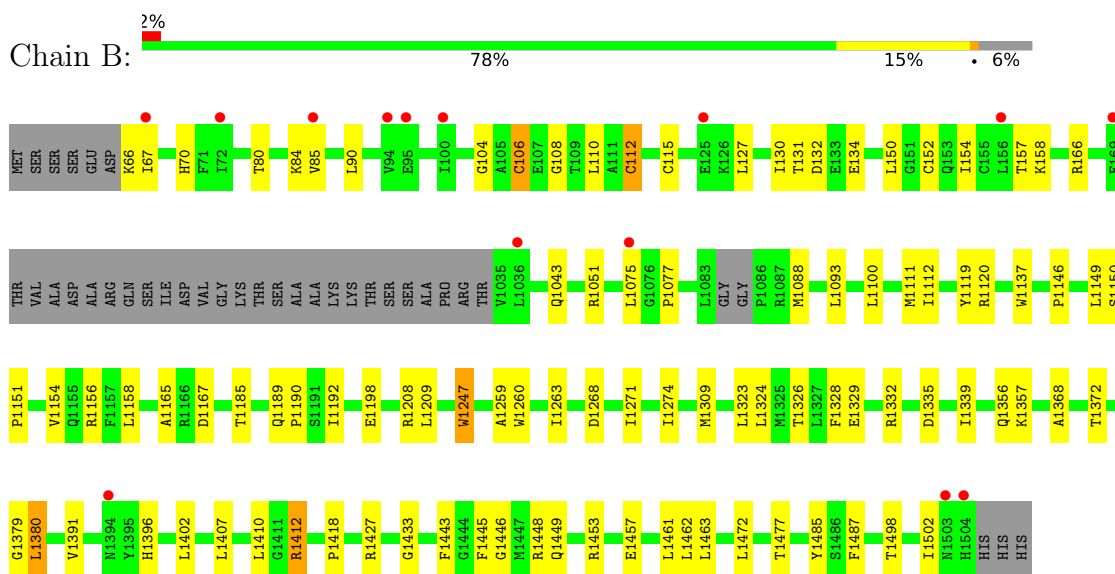
### 3 Residue-property plots

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.

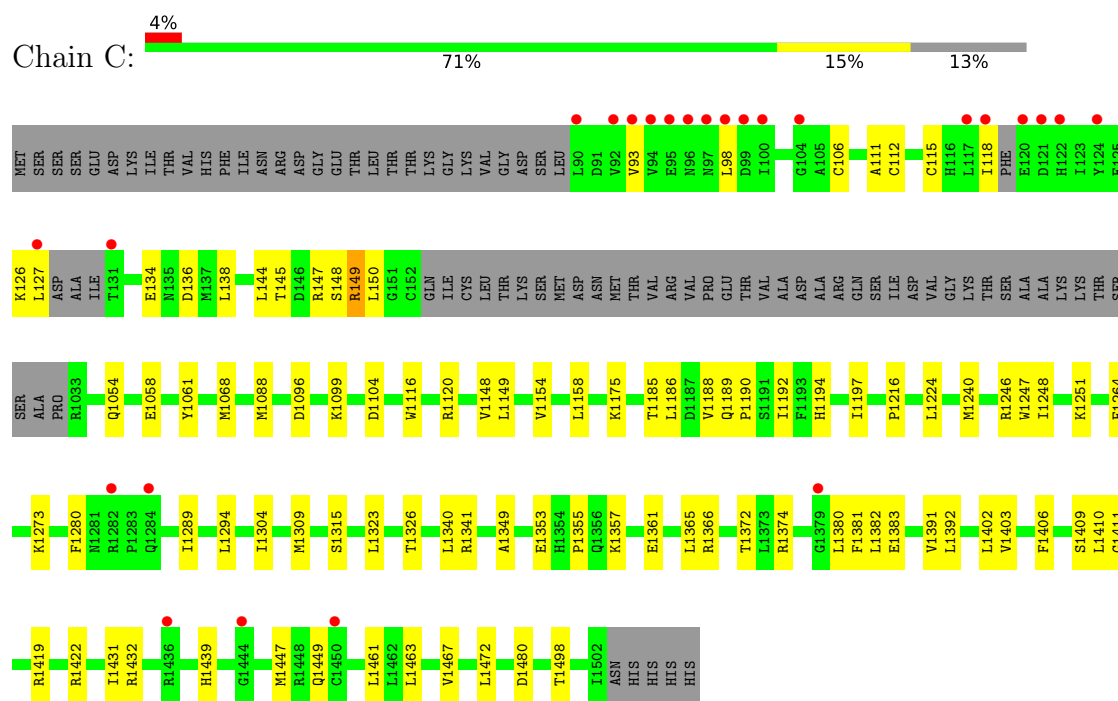
- Molecule 1: Adrenodoxin, Cytochrome P450 11B2, mitochondrial fusion enzyme



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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.58Å 208.70Å 124.92Å 90.00° 114.07° 90.00°	Depositor
Resolution (Å)	48.16 – 2.94 48.84 – 2.93	Depositor EDS
% Data completeness (in resolution range)	90.9 (48.16-2.94) 85.4 (48.84-2.93)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.210 , 0.244 0.209 , 0.243	Depositor DCC
$R_{free}$ test set	2000 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	27303	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, OT3, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.68	0/4711	0.64	0/6385
1	B	0.58	0/4715	0.62	0/6390
1	C	0.54	0/4368	0.61	0/5920
All	All	0.60	0/13794	0.62	0/18695

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 [i](#)

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	4603	4618	4618	60	0
1	B	4606	4618	4619	73	0
1	C	4265	4271	4268	56	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
3	A	43	30	30	4	0
3	B	43	30	30	4	0
3	C	43	30	30	5	0
4	A	17	13	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	17	13	13	0	0
4	C	17	13	13	0	0
5	A	1	0	0	0	0
All	All	13667	13636	13634	199	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 7.

All (199) 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:1192:ILE:HG23	1:B:1323:LEU:HD23	1.49	0.94
1:B:90:LEU:HD11	1:B:104:GLY:HA3	1.56	0.87
1:C:145:THR:HG22	1:C:147:ARG:H	1.49	0.77
1:B:1192:ILE:CG2	1:B:1323:LEU:HD23	2.13	0.77
3:C:1602:HEM:HBB2	3:C:1602:HEM:HMB2	1.67	0.76
1:C:127:LEU:HD13	1:C:149:ARG:HD3	1.67	0.76
1:A:1119:TYR:CZ	1:A:1260:TRP:HB3	2.22	0.75
1:A:118:ILE:HD13	1:A:145:THR:HG21	1.71	0.71
1:A:1391:VAL:HG23	1:A:1396:HIS:HA	1.73	0.70
1:B:1472:LEU:HD13	1:B:1502:ILE:HG12	1.74	0.70
1:B:1391:VAL:HG23	1:B:1396:HIS:HA	1.73	0.69
1:A:1472:LEU:HD13	1:A:1502:ILE:HG12	1.74	0.67
1:A:1263:ILE:HG22	1:A:1309:MET:HE1	1.78	0.66
1:C:1197:ILE:HD11	1:C:1224:LEU:HD21	1.77	0.65
1:B:110:LEU:HD12	1:B:1151:PRO:HG2	1.79	0.65
1:B:1263:ILE:HG22	1:B:1309:MET:HE1	1.78	0.64
1:C:1294:LEU:HD23	1:C:1304:ILE:HD13	1.79	0.64
1:C:1326:THR:OG1	1:C:1372:THR:HG21	1.98	0.64
1:B:134:GLU:HG3	1:B:150:LEU:HD12	1.79	0.64
1:B:130:ILE:HG22	1:B:131:THR:O	2.00	0.61
1:B:1119:TYR:CZ	1:B:1260:TRP:HB3	2.36	0.61
3:A:1602:HEM:HMB2	3:A:1602:HEM:HBB2	1.83	0.60
3:C:1602:HEM:HMC2	3:C:1602:HEM:HBC2	1.84	0.60
1:C:1402:LEU:HD23	1:C:1403:VAL:N	2.16	0.59
1:C:115:CYS:SG	1:C:150:LEU:HD22	2.42	0.59
1:B:108:GLY:HA2	1:B:152:CYS:SG	2.43	0.59
3:B:1602:HEM:HBB2	3:B:1602:HEM:HMB2	1.83	0.58
1:B:66:LYS:N	1:B:84:LYS:HZ3	2.01	0.58
1:B:115:CYS:SG	1:B:150:LEU:HB3	2.43	0.58
1:A:1152:LYS:O	1:A:1156:ARG:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1477:THR:O	1:B:1477:THR:OG1	2.22	0.58
1:A:1271:ILE:HA	1:A:1274:ILE:HG22	1.86	0.57
1:A:134:GLU:HG3	1:A:150:LEU:HD12	1.85	0.57
1:B:1111:MET:SD	1:B:1402:LEU:HD13	2.45	0.57
1:B:1271:ILE:HA	1:B:1274:ILE:HG22	1.86	0.57
1:C:1381:PHE:O	1:C:1382:LEU:HD23	2.05	0.56
1:C:111:ALA:HB2	1:C:1149:LEU:HD23	1.88	0.56
1:A:1158:LEU:HD23	1:A:1356:GLN:HA	1.87	0.56
1:B:1043:GLN:O	1:B:1075:LEU:HD21	2.05	0.56
1:C:1096:ASP:HB3	1:C:1392:LEU:HD22	1.89	0.55
1:B:1158:LEU:HD23	1:B:1356:GLN:HA	1.87	0.54
1:B:90:LEU:HD11	1:B:104:GLY:CA	2.34	0.54
1:B:1380:LEU:HD12	1:B:1485:TYR:CD1	2.42	0.54
1:C:138:LEU:HG	1:C:144:LEU:HD11	1.90	0.54
1:B:1410:LEU:O	1:B:1410:LEU:HD23	2.09	0.53
1:A:1119:TYR:CE2	1:A:1260:TRP:HB3	2.43	0.53
1:A:1185:THR:HG22	1:A:1496:LEU:HG	1.91	0.53
1:C:1185:THR:HG22	1:C:1498:THR:HG23	1.91	0.53
1:C:118:ILE:HG12	1:C:148:SER:HB3	1.90	0.52
1:A:1410:LEU:HD23	1:A:1410:LEU:O	2.09	0.52
1:A:1111:MET:SD	1:A:1402:LEU:HD13	2.48	0.52
1:A:1185:THR:OG1	1:A:1498:THR:OG1	2.24	0.52
1:C:1186:LEU:HD11	1:C:1188:VAL:HG12	1.91	0.52
1:A:90:LEU:O	1:A:94:VAL:HG22	2.10	0.52
1:A:1391:VAL:HG23	1:A:1396:HIS:CA	2.40	0.52
1:B:1112:ILE:H	1:B:1112:ILE:HD12	1.74	0.52
1:A:1328:PHE:CZ	1:A:1332:ARG:HD2	2.45	0.52
1:C:1383:GLU:HG2	1:C:1402:LEU:HD21	1.91	0.52
1:C:1449:GLN:O	1:C:1449:GLN:HG3	2.09	0.51
1:B:1167:ASP:OD2	1:B:1208:ARG:NH2	2.44	0.51
3:B:1602:HEM:HBB2	3:B:1602:HEM:CMB	2.41	0.51
1:B:1192:ILE:HG23	1:B:1323:LEU:CD2	2.32	0.51
3:A:1602:HEM:HBB2	3:A:1602:HEM:CMB	2.41	0.51
1:B:1391:VAL:HG23	1:B:1396:HIS:CA	2.40	0.51
1:A:1167:ASP:OD2	1:A:1208:ARG:NH2	2.44	0.51
1:B:1328:PHE:CZ	1:B:1332:ARG:HD2	2.45	0.51
1:A:1443:PHE:CG	1:A:1453:ARG:HG3	2.46	0.50
1:C:1463:LEU:O	1:C:1467:VAL:HG23	2.12	0.50
1:A:1119:TYR:CE1	1:A:1260:TRP:HB3	2.46	0.50
1:A:1474:GLU:HB3	1:C:1280:PHE:CE2	2.46	0.50
1:A:70:HIS:ND1	1:A:80:THR:HG23	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1192:ILE:HD12	1:B:1323:LEU:CD2	2.43	0.49
1:A:1048:ARG:HD3	1:A:1083:LEU:HD23	1.95	0.49
3:C:1602:HEM:HBC2	3:C:1602:HEM:CMC	2.43	0.49
1:B:110:LEU:HD12	1:B:1151:PRO:CG	2.43	0.49
1:B:1449:GLN:O	1:B:1449:GLN:HG3	2.12	0.48
1:A:74:ARG:NH1	1:A:142:TYR:OH	2.46	0.48
1:B:70:HIS:ND1	1:B:80:THR:HG23	2.29	0.48
1:A:1185:THR:CG2	1:A:1496:LEU:HG	2.44	0.48
1:B:1198:GLU:OE2	1:B:1209:LEU:HB2	2.14	0.48
1:C:1419:ARG:HH11	1:C:1419:ARG:HG2	1.79	0.48
1:A:1260:TRP:CE3	1:A:1263:ILE:HD12	2.49	0.47
1:A:1185:THR:O	1:C:1273:LYS:HD3	2.13	0.47
3:A:1602:HEM:CMC	3:A:1602:HEM:HBC2	2.45	0.47
1:C:1154:VAL:O	1:C:1158:LEU:HB2	2.15	0.47
3:C:1602:HEM:HBB2	3:C:1602:HEM:CMB	2.40	0.47
1:B:1380:LEU:HD12	1:B:1485:TYR:HD1	1.79	0.47
1:C:134:GLU:HG3	1:C:150:LEU:HD12	1.97	0.47
1:B:1192:ILE:HD12	1:B:1323:LEU:HD21	1.97	0.47
3:B:1602:HEM:HBC2	3:B:1602:HEM:CMC	2.45	0.47
1:C:1357:LYS:HB3	1:C:1361:GLU:HG3	1.97	0.47
1:B:127:LEU:HD13	1:B:154:ILE:HD12	1.97	0.47
1:C:127:LEU:HD23	1:C:127:LEU:HA	1.74	0.47
1:C:1099:LYS:HE2	1:C:1391:VAL:O	2.15	0.47
1:A:1198:GLU:OE2	1:A:1209:LEU:HB2	2.14	0.47
1:C:1185:THR:HG22	1:C:1498:THR:OG1	2.15	0.46
1:B:1368:ALA:O	1:B:1372:THR:HG23	2.16	0.46
1:C:1186:LEU:HD21	1:C:1188:VAL:CG1	2.45	0.46
1:A:1368:ALA:O	1:A:1372:THR:HG23	2.16	0.46
1:C:1247:TRP:CE3	1:C:1248:ILE:HG23	2.51	0.46
1:C:1365:LEU:HD23	1:C:1461:LEU:HD23	1.97	0.46
1:B:1189:GLN:HG3	1:B:1324:LEU:HD21	1.98	0.46
1:A:1477:THR:O	1:A:1477:THR:OG1	2.26	0.46
1:C:1088:MET:HG3	1:C:1402:LEU:HB3	1.97	0.45
1:A:1432:ARG:O	1:A:1432:ARG:HG3	2.16	0.45
3:B:1602:HEM:HBC2	3:B:1602:HEM:HMC2	1.97	0.45
3:A:1602:HEM:HBC2	3:A:1602:HEM:HMC2	1.97	0.45
1:C:1431:ILE:HD13	1:C:1439:HIS:CD2	2.51	0.45
1:B:1410:LEU:HD23	1:B:1410:LEU:C	2.38	0.44
1:A:1077:PRO:HB2	1:A:1093:LEU:HD12	1.99	0.44
1:A:1146:PRO:HA	1:A:1150:SER:OG	2.17	0.44
1:C:1148:VAL:HG22	1:C:1289:ILE:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1189:GLN:HG3	1:A:1324:LEU:HD21	1.98	0.44
1:B:1165:ALA:HB1	1:B:1463:LEU:HA	2.00	0.44
1:C:1315:SER:HA	3:C:1602:HEM:HMC2	2.00	0.44
1:A:1314:GLY:HA2	4:A:1603:OT3:C15	2.47	0.44
1:B:1137:TRP:CZ2	1:B:1448:ARG:HG2	2.53	0.44
1:B:1326:THR:OG1	1:B:1372:THR:HG21	2.17	0.44
1:C:1432:ARG:O	1:C:1432:ARG:HG3	2.16	0.44
1:B:1185:THR:HG22	1:B:1498:THR:HG23	2.00	0.44
1:A:1112:ILE:HD13	1:A:1112:ILE:HG21	1.74	0.44
1:B:85:VAL:HG13	1:B:157:THR:HA	2.00	0.44
1:C:1158:LEU:HD22	1:C:1355:PRO:O	2.18	0.44
1:A:1165:ALA:HB1	1:A:1463:LEU:HA	2.00	0.44
1:A:1259:ALA:O	1:A:1263:ILE:HG13	2.17	0.44
1:B:1185:THR:HG22	1:B:1498:THR:OG1	2.18	0.44
1:C:1068:MET:HE1	1:C:1381:PHE:HE1	1.83	0.44
1:A:1410:LEU:HD23	1:A:1410:LEU:C	2.38	0.43
1:B:1146:PRO:HA	1:B:1150:SER:OG	2.17	0.43
1:A:1379:GLY:O	1:A:1407:LEU:HD12	2.18	0.43
1:B:1323:LEU:HD11	1:B:1463:LEU:HD22	2.00	0.43
1:B:1357:LYS:HE2	1:B:1357:LYS:HB3	1.82	0.43
1:A:134:GLU:CG	1:A:150:LEU:HD12	2.49	0.43
1:A:1326:THR:OG1	1:A:1372:THR:HG21	2.17	0.43
1:A:1391:VAL:HG23	1:A:1395:TYR:O	2.18	0.43
1:B:1154:VAL:O	1:B:1158:LEU:HB2	2.19	0.43
1:B:1259:ALA:O	1:B:1263:ILE:HG13	2.17	0.43
1:C:1264:PHE:HA	1:C:1309:MET:SD	2.58	0.43
1:B:1077:PRO:HB2	1:B:1093:LEU:HD12	1.99	0.43
1:B:1379:GLY:O	1:B:1407:LEU:HD12	2.18	0.43
1:C:1054:GLN:O	1:C:1058:GLU:HB2	2.18	0.43
1:C:1116:TRP:O	1:C:1120:ARG:HG2	2.18	0.43
1:A:1154:VAL:O	1:A:1158:LEU:HB2	2.19	0.43
1:C:1410:LEU:HD23	1:C:1410:LEU:O	2.17	0.43
1:B:1100:LEU:HD23	1:B:1445:PHE:HZ	1.84	0.43
1:C:1374:ARG:NH2	1:C:1411:GLY:O	2.52	0.43
1:A:1189:GLN:HB3	1:A:1190:PRO:HD3	2.01	0.42
1:B:1247:TRP:C	1:B:1247:TRP:CD1	2.91	0.42
1:C:1194:HIS:CE1	1:C:1216:PRO:HG3	2.53	0.42
1:A:1146:PRO:HA	1:A:1150:SER:HG	1.84	0.42
1:B:70:HIS:CE1	1:B:80:THR:HG23	2.55	0.42
1:C:1341:ARG:CZ	1:C:1472:LEU:HD23	2.49	0.42
1:C:1419:ARG:HG2	1:C:1419:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1120:ARG:HH21	1:A:1120:ARG:HG2	1.85	0.42
1:A:1391:VAL:HG23	1:A:1395:TYR:C	2.40	0.42
1:B:1146:PRO:HA	1:B:1150:SER:HG	1.84	0.42
1:C:1366:ARG:HG2	1:C:1461:LEU:HD11	2.00	0.42
1:C:1410:LEU:HD23	1:C:1410:LEU:C	2.40	0.42
1:B:106:CYS:HB3	1:B:112:CYS:HB3	2.02	0.42
1:B:1120:ARG:HH21	1:B:1120:ARG:HG2	1.85	0.42
1:B:1189:GLN:HB3	1:B:1190:PRO:HD3	2.01	0.42
1:B:1443:PHE:CG	1:B:1453:ARG:HG3	2.55	0.42
1:C:93:VAL:HG13	1:C:98:LEU:HB2	2.01	0.42
1:A:1088:MET:SD	1:A:1402:LEU:HD23	2.59	0.42
1:C:126:LYS:HD2	1:C:126:LYS:HA	1.71	0.42
1:C:112:CYS:HB3	1:C:1447:MET:HG2	2.01	0.41
1:C:1189:GLN:HB3	1:C:1190:PRO:HD3	2.01	0.41
1:C:1340:LEU:HD22	1:C:1365:LEU:HA	2.02	0.41
1:A:1260:TRP:CE3	1:A:1260:TRP:HA	2.54	0.41
1:B:1268:ASP:O	1:B:1271:ILE:HG22	2.20	0.41
1:A:1119:TYR:CE2	1:A:1260:TRP:CB	3.03	0.41
1:A:84:LYS:O	1:A:87:ASP:HB2	2.20	0.41
1:B:1198:GLU:OE1	1:B:1208:ARG:NH1	2.54	0.41
1:A:1329:GLU:OE2	1:A:1332:ARG:NH2	2.54	0.41
1:B:1088:MET:SD	1:B:1402:LEU:HD23	2.59	0.41
1:A:71:PHE:CE1	1:A:165:VAL:HG21	2.56	0.41
1:A:1198:GLU:OE1	1:A:1208:ARG:NH1	2.54	0.41
1:A:1268:ASP:O	1:A:1271:ILE:HG22	2.20	0.41
1:A:1335:ASP:O	1:A:1339:ILE:HG13	2.21	0.41
1:B:1418:PRO:O	1:B:1427:ARG:NH2	2.54	0.41
1:C:1186:LEU:HG	1:C:1188:VAL:HG13	2.02	0.41
1:A:1318:THR:HG21	4:A:1603:OT3:N04	2.35	0.41
1:B:1077:PRO:HB2	1:B:1093:LEU:CD1	2.51	0.41
1:B:1335:ASP:O	1:B:1339:ILE:HG13	2.21	0.41
1:B:67:ILE:HD11	1:B:158:LYS:HA	2.03	0.41
1:B:1412:ARG:HG2	1:B:1412:ARG:HH11	1.86	0.41
1:C:1349:ALA:O	1:C:1353:GLU:HG3	2.21	0.41
1:C:1406:PHE:HD2	1:C:1409:SER:HG	1.63	0.41
1:B:1329:GLU:OE2	1:B:1332:ARG:NH2	2.54	0.41
1:A:106:CYS:HB3	1:A:1447:MET:SD	2.61	0.40
1:A:1380:LEU:HD22	1:A:1406:PHE:CE1	2.56	0.40
1:B:1158:LEU:HD11	1:B:1462:LEU:HD11	2.03	0.40
1:C:1192:ILE:HG23	1:C:1323:LEU:HD23	2.02	0.40
1:B:84:LYS:HD2	1:B:84:LYS:HA	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1446:GLY:O	1:B:1449:GLN:HG2	2.22	0.40
1:B:1100:LEU:HD23	1:B:1445:PHE:CZ	2.56	0.40
1:B:1119:TYR:CE1	1:B:1260:TRP:HB3	2.56	0.40
1:B:1457:GLU:O	1:B:1461:LEU:HB2	2.22	0.40
1:C:1240:MET:SD	1:C:1248:ILE:HD11	2.61	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	566/609 (93%)	549 (97%)	17 (3%)	0	100	100
1	B	566/609 (93%)	546 (96%)	18 (3%)	2 (0%)	34	64
1	C	521/609 (86%)	495 (95%)	26 (5%)	0	100	100
All	All	1653/1827 (90%)	1590 (96%)	61 (4%)	2 (0%)	51	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1487	PHE
1	B	1433	GLY

### 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	505/534 (95%)	493 (98%)	12 (2%)	49	77
1	B	505/534 (95%)	495 (98%)	10 (2%)	55	80
1	C	464/534 (87%)	453 (98%)	11 (2%)	49	77
All	All	1474/1602 (92%)	1441 (98%)	33 (2%)	52	78

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	CYS
1	A	1051	ARG
1	A	1083	LEU
1	A	1101	GLN
1	A	1112	ILE
1	A	1143	ARG
1	A	1149	LEU
1	A	1181	ARG
1	A	1352	SER
1	A	1380	LEU
1	A	1412	ARG
1	A	1427	ARG
1	B	106	CYS
1	B	112	CYS
1	B	132	ASP
1	B	166	ARG
1	B	1051	ARG
1	B	1149	LEU
1	B	1156	ARG
1	B	1247	TRP
1	B	1380	LEU
1	B	1412	ARG
1	C	106	CYS
1	C	136	ASP
1	C	149	ARG
1	C	1061	TYR
1	C	1104	ASP
1	C	1175	LYS
1	C	1246	ARG
1	C	1251	LYS
1	C	1380	LEU
1	C	1422	ARG
1	C	1480	ASP

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

Mol	Chain	Res	Type
1	A	1101	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	FES	A	1601	1	0,4,4	0.00	-	-		
2	FES	B	1601	1	0,4,4	0.00	-	-		
2	FES	C	1601	1	0,4,4	0.00	-	-		
4	OT3	C	1603	3	15,19,19	1.46	4 (26%)	18,26,26	1.09	1 (5%)
3	HEM	C	1602	1,4	27,50,50	1.85	5 (18%)	17,82,82	1.58	4 (23%)
4	OT3	B	1603	3	15,19,19	1.54	4 (26%)	18,26,26	1.34	2 (11%)
3	HEM	A	1602	1,4	27,50,50	1.84	4 (14%)	17,82,82	1.39	3 (17%)
4	OT3	A	1603	3	15,19,19	1.54	4 (26%)	18,26,26	1.34	2 (11%)
3	HEM	B	1602	1,4	27,50,50	1.84	4 (14%)	17,82,82	1.39	3 (17%)

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	FES	A	1601	1	-	-	0/1/1/1
2	FES	B	1601	1	-	-	0/1/1/1
2	FES	C	1601	1	-	-	0/1/1/1
4	OT3	C	1603	3	-	0/6/16/16	0/2/3/3
3	HEM	C	1602	1,4	-	0/6/54/54	-
4	OT3	B	1603	3	-	0/6/16/16	0/2/3/3
3	HEM	A	1602	1,4	-	0/6/54/54	-
4	OT3	A	1603	3	-	0/6/16/16	0/2/3/3
3	HEM	B	1602	1,4	-	0/6/54/54	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1602	HEM	C3C-C2C	-4.53	1.34	1.40
3	B	1602	HEM	C3C-C2C	-4.52	1.34	1.40
3	C	1602	HEM	C3B-C2B	-4.28	1.34	1.40
3	A	1602	HEM	C3B-C2B	-4.25	1.34	1.40
3	B	1602	HEM	C3B-C2B	-4.22	1.34	1.40
3	C	1602	HEM	C3C-CAC	3.70	1.55	1.47
3	C	1602	HEM	C3C-C2C	-3.69	1.35	1.40
3	C	1602	HEM	C3B-CAB	3.56	1.55	1.47
3	B	1602	HEM	C3B-CAB	3.32	1.54	1.47
3	A	1602	HEM	C3B-CAB	3.31	1.54	1.47
4	A	1603	OT3	C09-C08	3.25	1.57	1.50
3	B	1602	HEM	C3C-CAC	3.25	1.54	1.47
4	B	1603	OT3	C09-C08	3.24	1.57	1.50
3	A	1602	HEM	C3C-CAC	3.23	1.54	1.47
4	C	1603	OT3	C09-C08	2.89	1.56	1.50
4	C	1603	OT3	C16-N17	2.44	1.20	1.14
4	B	1603	OT3	C16-N17	2.40	1.20	1.14
4	C	1603	OT3	C01-C09	-2.39	1.42	1.51
4	A	1603	OT3	C16-N17	2.39	1.20	1.14
4	B	1603	OT3	C13-C16	-2.30	1.39	1.44
4	A	1603	OT3	C13-C16	-2.29	1.39	1.44
4	C	1603	OT3	C13-C16	-2.27	1.39	1.44
4	A	1603	OT3	C01-C09	-2.10	1.43	1.51
4	B	1603	OT3	C01-C09	-2.08	1.43	1.51
3	C	1602	HEM	CAA-C2A	2.04	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1603	OT3	C02-C03-C10	-2.86	104.58	112.77
4	B	1603	OT3	C02-C03-C10	-2.84	104.64	112.77
4	A	1603	OT3	C15-C10-C11	-2.51	115.16	118.29
3	C	1602	HEM	CMC-C2C-C3C	2.51	129.37	124.68
4	B	1603	OT3	C15-C10-C11	-2.50	115.17	118.29
3	C	1602	HEM	CMD-C2D-C1D	-2.50	124.62	128.46
3	A	1602	HEM	CAA-CBA-CGA	-2.31	108.80	112.67
3	B	1602	HEM	CAA-CBA-CGA	-2.30	108.81	112.67
3	C	1602	HEM	CMA-C3A-C4A	-2.27	124.98	128.46
3	B	1602	HEM	CMD-C2D-C1D	-2.09	125.25	128.46
3	A	1602	HEM	CMD-C2D-C1D	-2.09	125.26	128.46
4	C	1603	OT3	C12-C11-C10	2.05	123.26	121.20
3	C	1602	HEM	C1D-C2D-C3D	2.04	108.42	107.00
3	B	1602	HEM	CMC-C2C-C3C	2.03	128.47	124.68
3	A	1602	HEM	CMC-C2C-C3C	2.02	128.45	124.68

There are no chirality outliers.

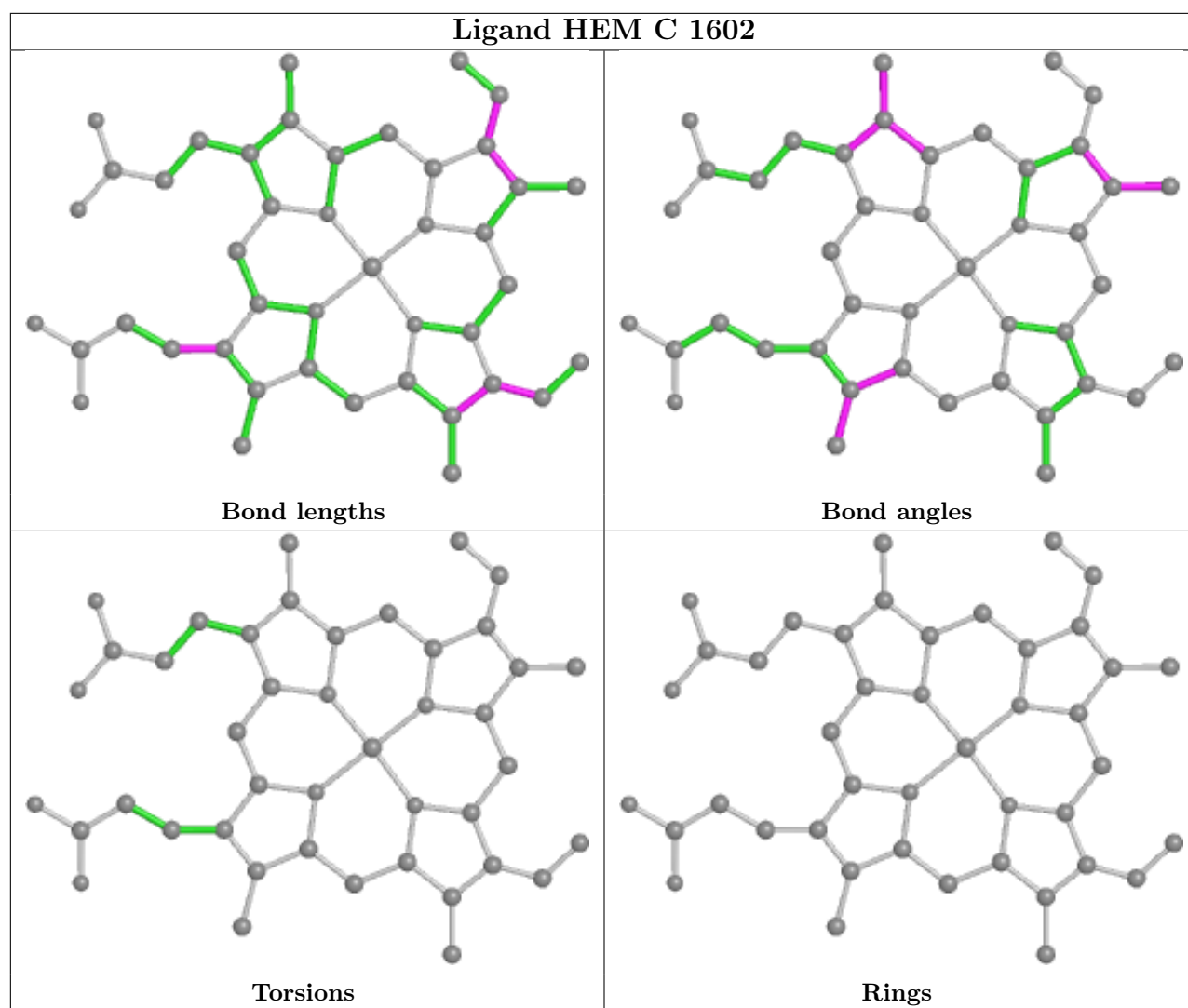
There are no torsion outliers.

There are no ring outliers.

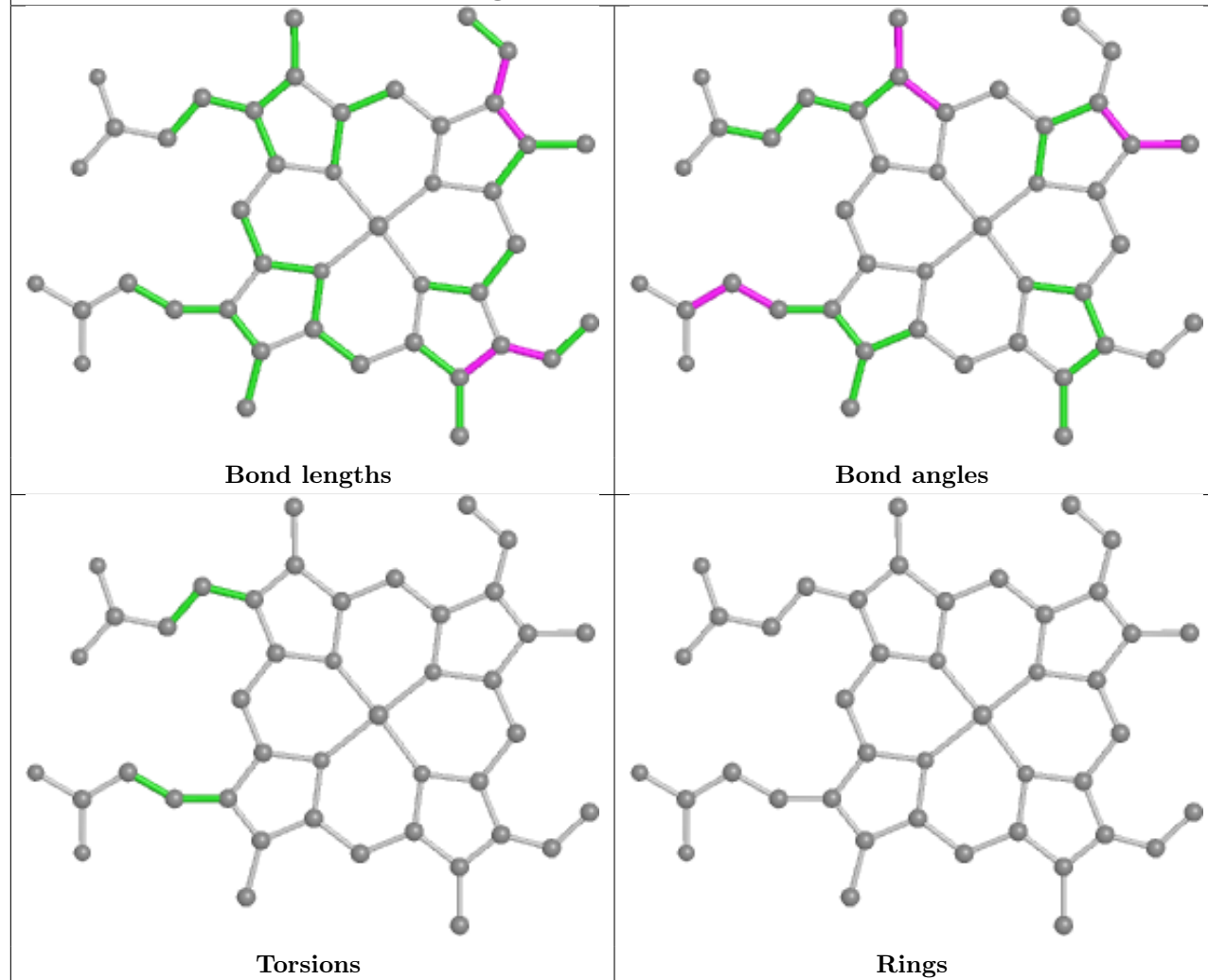
4 monomers are involved in 15 short contacts:

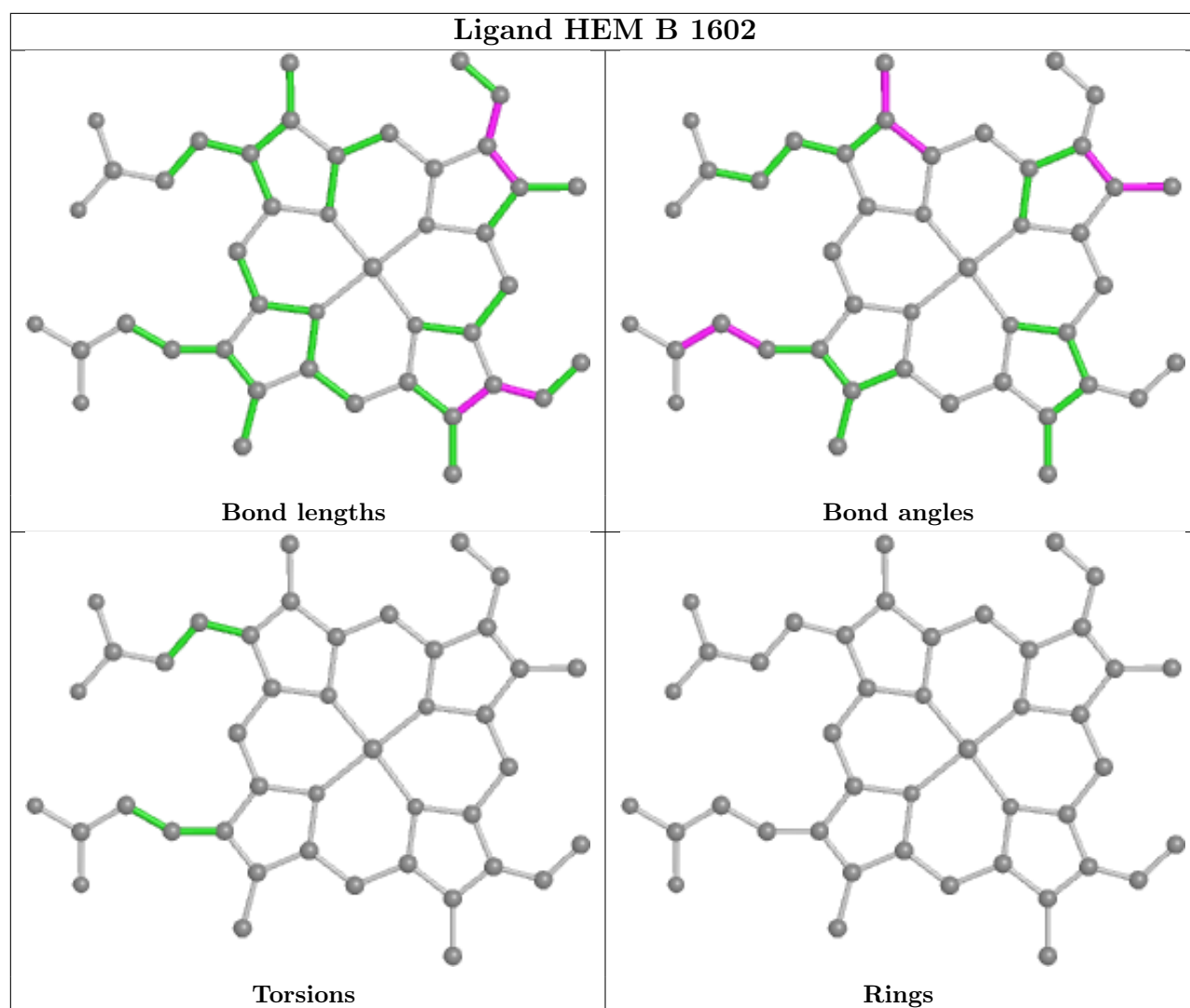
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1602	HEM	5	0
3	A	1602	HEM	4	0
4	A	1603	OT3	2	0
3	B	1602	HEM	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## Ligand HEM A 1602





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	572/609 (93%)	0.34	10 (1%) 70 71	25, 45, 71, 92	0
1	B	572/609 (93%)	0.27	14 (2%) 59 59	31, 55, 78, 99	0
1	C	529/609 (86%)	0.30	25 (4%) 31 31	31, 52, 91, 115	0
All	All	1673/1827 (91%)	0.30	49 (2%) 51 51	25, 51, 79, 115	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	94	VAL	4.9
1	C	98	LEU	4.9
1	C	118	ILE	4.6
1	C	96	ASN	4.5
1	A	157	THR	4.1
1	B	1504	HIS	4.1
1	C	100	ILE	4.0
1	C	92	VAL	4.0
1	C	120	GLU	3.9
1	C	122	HIS	3.5
1	B	94	VAL	3.3
1	C	93	VAL	3.1
1	C	97	ASN	3.1
1	C	95	GLU	3.1
1	C	117	LEU	3.0
1	B	1394	ASN	3.0
1	B	1036	LEU	2.9
1	C	124	TYR	2.8
1	C	1450	CYS	2.7
1	A	1503	ASN	2.7
1	A	1174	LYS	2.6
1	B	67	ILE	2.6
1	C	90	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	127	LEU	2.5
1	B	169	GLU	2.4
1	B	1075	LEU	2.4
1	B	1503	ASN	2.4
1	C	99	ASP	2.3
1	A	1250	PRO	2.3
1	C	1282	ARG	2.3
1	A	1248	ILE	2.2
1	C	1436	ARG	2.2
1	B	125	GLU	2.2
1	B	100	ILE	2.2
1	A	85	VAL	2.1
1	B	85	VAL	2.1
1	C	104	GLY	2.1
1	C	1379	GLY	2.1
1	B	72	ILE	2.1
1	C	131	THR	2.1
1	C	1444	GLY	2.1
1	A	73	ASN	2.1
1	C	1284	GLN	2.1
1	A	1450	CYS	2.1
1	B	156	LEU	2.1
1	C	121	ASP	2.0
1	A	69	VAL	2.0
1	A	66	LYS	2.0
1	B	95	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

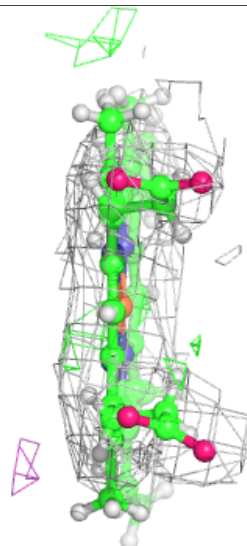
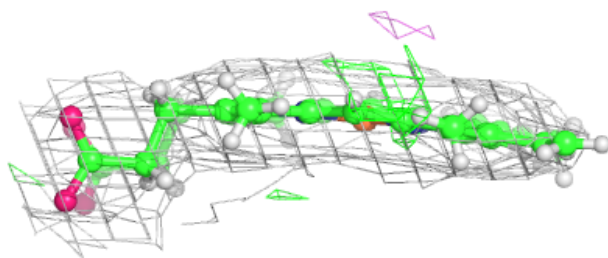
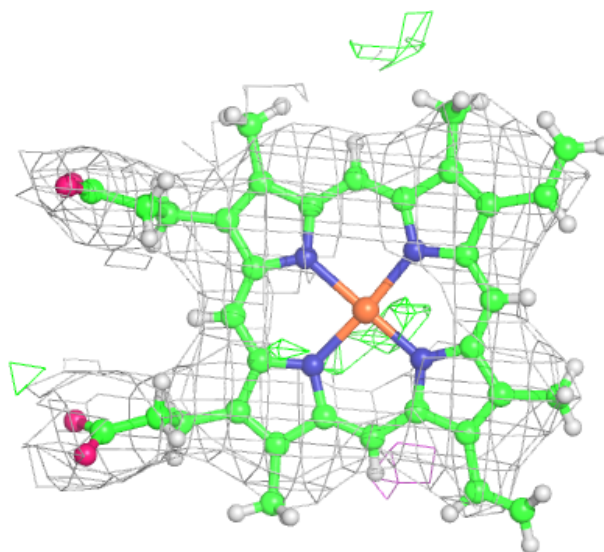
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	OT3	C	1603	17/17	0.93	0.27	25,44,57,63	0
4	OT3	B	1603	17/17	0.96	0.29	32,48,69,79	0
4	OT3	A	1603	17/17	0.96	0.27	26,41,54,59	0
3	HEM	C	1602	43/43	0.97	0.28	25,40,63,65	0
2	FES	C	1601	4/4	0.97	0.16	53,70,82,83	0
3	HEM	A	1602	43/43	0.97	0.29	20,33,47,57	0
3	HEM	B	1602	43/43	0.97	0.27	23,41,60,69	0
2	FES	B	1601	4/4	0.98	0.18	43,49,55,63	0
2	FES	A	1601	4/4	0.99	0.19	36,37,40,43	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.

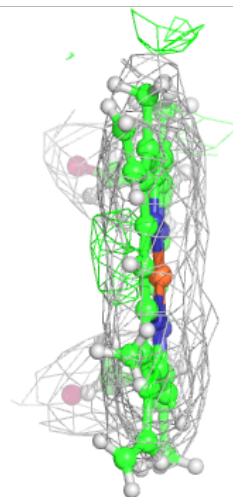
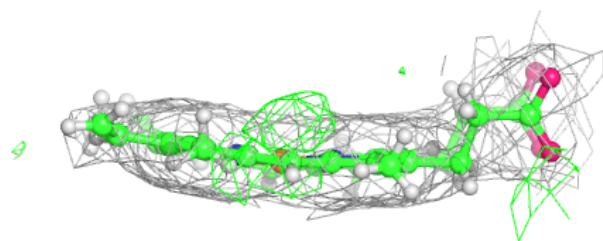
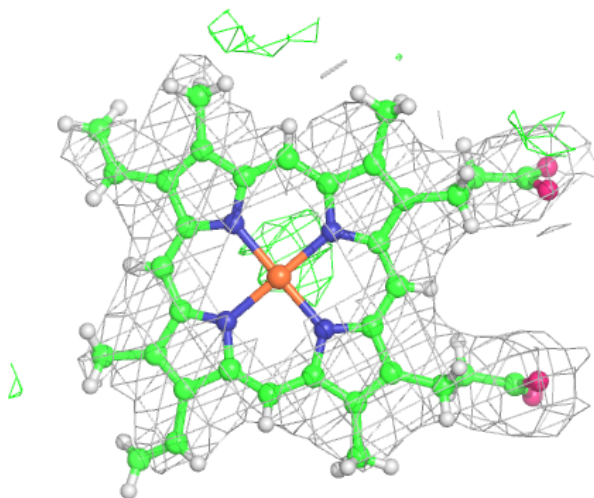
**Electron density around HEM C 1602:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



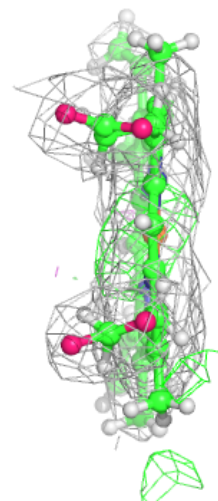
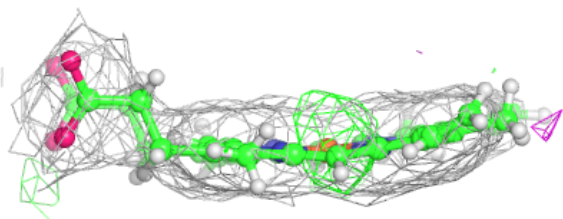
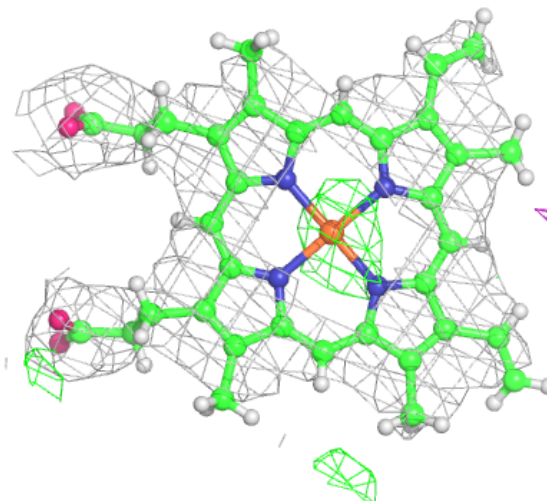
**Electron density around HEM A 1602:**

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



**Electron density around HEM B 1602:**

$2mF_o-DF_c$  (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.