



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:54 PM UTC

PDB ID : 7M8I / pdb_00007m8i
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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

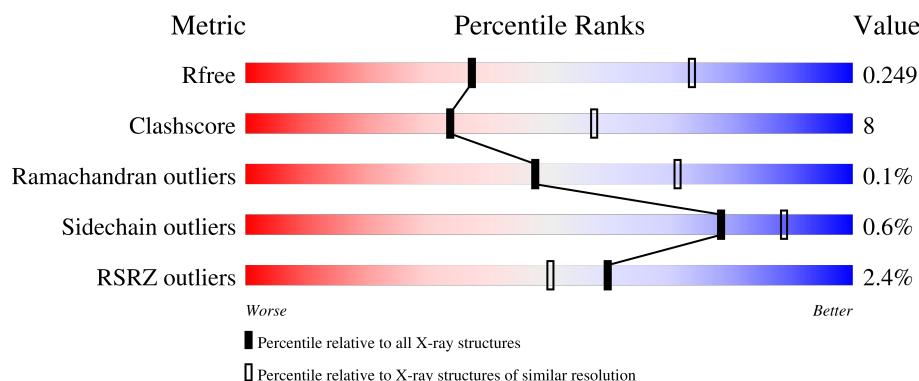
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

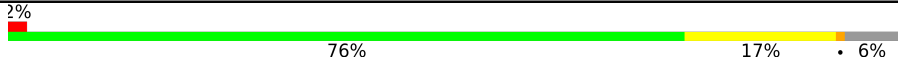
The reported resolution of this entry is 2.94 Å.

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}	180053	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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 $\leq 5\%$. 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:

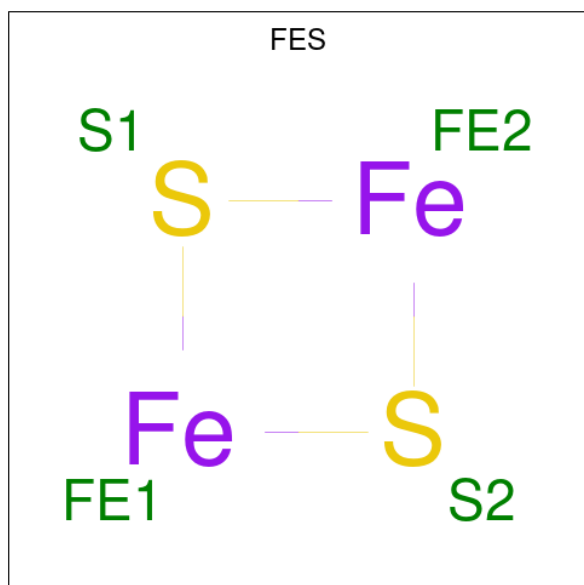
Chain	Residue	Modelled	Actual	Comment	Reference
A	60	MET	-	initiating methionine	UNP P10109
A	185	ALA	-	linker	UNP P10109
A	186	ALA	-	linker	UNP P10109
A	187	LYS	-	linker	UNP P10109
A	188	LYS	-	linker	UNP P10109
A	189	THR	-	linker	UNP P10109
A	190	SER	-	linker	UNP P10109
A	191	SER	-	linker	UNP P10109
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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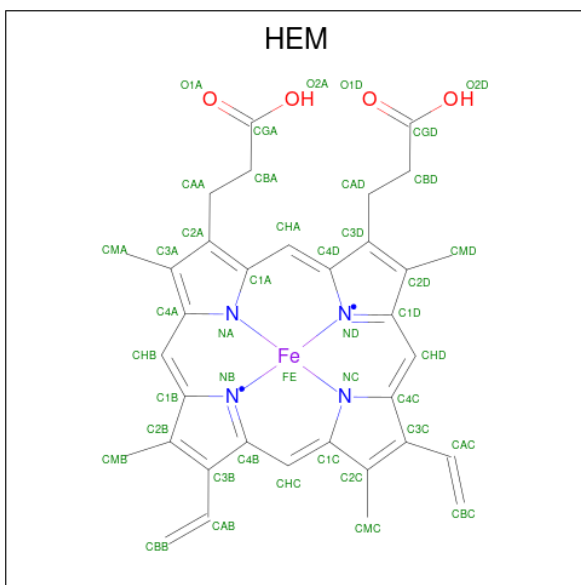
Chain	Residue	Modelled	Actual	Comment	Reference
B	1506	HIS	-	expression tag	UNP P19099
B	1507	HIS	-	expression tag	UNP P19099
C	60	MET	-	initiating methionine	UNP P10109
C	185	ALA	-	linker	UNP P10109
C	186	ALA	-	linker	UNP P10109
C	187	LYS	-	linker	UNP P10109
C	188	LYS	-	linker	UNP P10109
C	189	THR	-	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 (CCD ID: FES) (formula: Fe_2S_2).



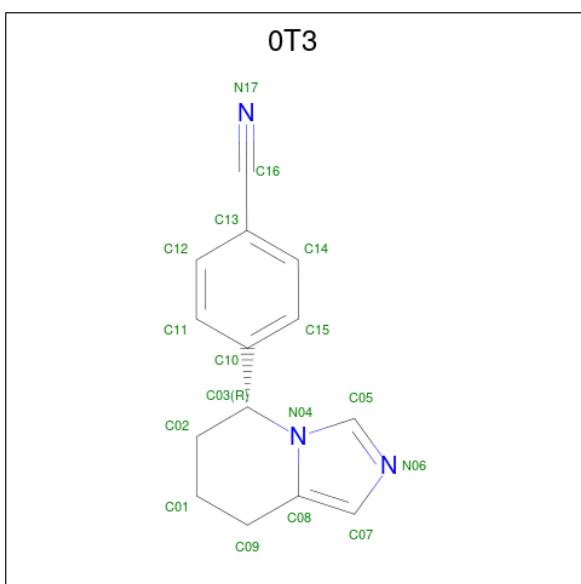
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	C	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

- Molecule 4 is 4-[(5R)-5,6,7,8-tetrahydroimidazo[1,5-a]pyridin-5-yl]benzonitrile (CCD ID: 0T3) (formula: C₁₄H₁₃N₃).



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

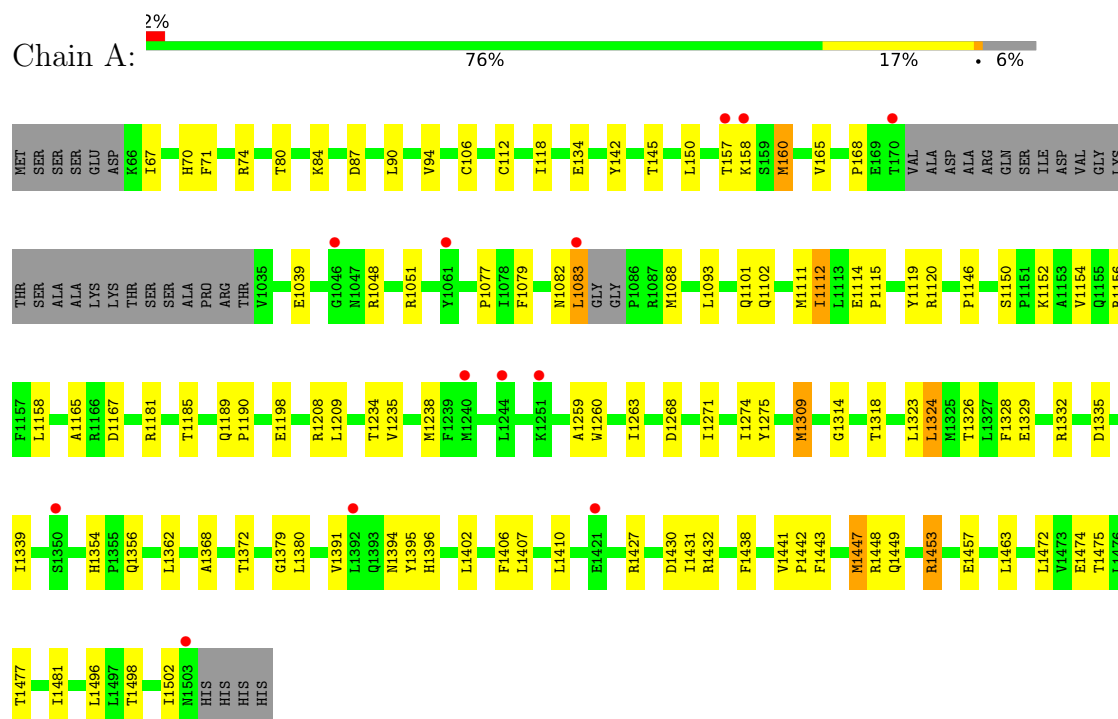
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	O 1	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: 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, α , β , γ	140.58Å 208.70Å 124.92Å 90.00° 114.07° 90.00°	Depositor
Resolution (Å)	48.16 – 2.94 48.16 – 2.94	Depositor EDS
% Data completeness (in resolution range)	90.9 (48.16-2.94) 85.8 (48.16-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.210 , 0.244 0.211 , 0.249	Depositor DCC
R_{free} test set	2000 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.86	26/4711 (0.6%)	0.75	12/6385 (0.2%)
1	B	0.72	13/4715 (0.3%)	0.72	11/6390 (0.2%)
1	C	0.67	12/4368 (0.3%)	0.68	17/5920 (0.3%)
All	All	0.76	51/13794 (0.4%)	0.72	40/18695 (0.2%)

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1309	MET	C-N	-8.35	1.23	1.33
1	A	1309	MET	C-N	-8.28	1.23	1.33
1	C	1229	VAL	C-N	-7.68	1.23	1.33
1	A	1457	GLU	C-O	-7.29	1.15	1.24
1	C	1232	LYS	C-O	-7.27	1.15	1.24
1	A	1354	HIS	C-O	-6.98	1.17	1.24
1	A	1431	ILE	C-O	-6.83	1.16	1.24
1	A	1362	LEU	C-O	-6.68	1.16	1.24
1	A	112	CYS	C-O	-6.59	1.17	1.24
1	A	1453	ARG	C-O	-6.42	1.16	1.24
1	B	1128	GLY	C-O	-6.38	1.18	1.24
1	A	1449	GLN	C-O	-6.29	1.15	1.23
1	B	166	ARG	C-O	-6.20	1.16	1.23
1	B	1449	GLN	C-O	-6.15	1.16	1.23
1	C	1431	ILE	C-N	6.12	1.42	1.33
1	B	123	ILE	C-O	-6.04	1.17	1.23
1	C	1255	GLU	C-O	-5.94	1.16	1.24
1	A	67	ILE	C-O	-5.87	1.18	1.24
1	A	160	MET	C-O	-5.79	1.16	1.24
1	A	1447	MET	N-CA	-5.74	1.38	1.46
1	B	1488	ILE	C-O	-5.71	1.17	1.24
1	A	1481	ILE	C-O	-5.68	1.18	1.24
1	A	1448	ARG	C-O	-5.67	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1481	ILE	C-O	-5.67	1.18	1.24
1	A	1323	LEU	C-O	-5.65	1.17	1.24
1	A	1442	PRO	C-O	-5.60	1.17	1.24
1	B	1323	LEU	C-O	-5.44	1.17	1.24
1	A	1115	PRO	C-O	-5.38	1.17	1.24
1	C	136	ASP	C-O	-5.36	1.17	1.24
1	B	1432	ARG	N-CA	-5.34	1.39	1.46
1	C	1249	SER	C-O	-5.30	1.17	1.24
1	A	1457	GLU	N-CA	-5.28	1.40	1.46
1	A	1275	TYR	C-O	-5.27	1.17	1.24
1	C	1370	LYS	C-O	-5.27	1.17	1.24
1	C	1271	ILE	C-O	-5.25	1.17	1.24
1	A	1102	GLN	C-O	-5.21	1.17	1.24
1	A	1447	MET	C-O	-5.18	1.17	1.24
1	C	1139	PHE	C-O	-5.18	1.18	1.24
1	B	1362	LEU	C-O	-5.13	1.18	1.24
1	B	1438	PHE	C-O	-5.11	1.17	1.23
1	C	1363	PRO	C-O	-5.10	1.17	1.24
1	A	1438	PHE	C-O	-5.09	1.17	1.23
1	C	1275	TYR	C-O	-5.09	1.17	1.24
1	C	1438	PHE	C-O	-5.09	1.17	1.23
1	A	1039	GLU	C-O	-5.08	1.17	1.24
1	B	68	THR	C-O	-5.06	1.17	1.24
1	B	1181	ARG	C-O	-5.06	1.16	1.24
1	A	1082	ASN	C-O	-5.03	1.18	1.24
1	A	1441	VAL	C-O	-5.03	1.18	1.24
1	A	1114	GLU	C-O	-5.03	1.17	1.24
1	A	1354	HIS	CA-CB	-5.00	1.47	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1430	ASP	N-CA-C	-7.70	102.82	111.14
1	C	122	HIS	CA-C-N	6.74	130.38	120.74
1	C	122	HIS	C-N-CA	6.74	130.38	120.74
1	A	1324	LEU	CA-C-N	-6.70	110.63	120.28
1	A	1324	LEU	C-N-CA	-6.70	110.63	120.28
1	B	1324	LEU	CA-C-N	-6.68	110.66	120.28
1	B	1324	LEU	C-N-CA	-6.68	110.66	120.28
1	C	1091	VAL	O-C-N	6.59	129.84	122.92
1	C	1209	LEU	N-CA-C	6.40	121.23	113.17
1	A	1431	ILE	CB-CA-C	-6.32	103.76	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1486	SER	CA-C-N	6.29	133.55	121.54
1	C	1486	SER	C-N-CA	6.29	133.55	121.54
1	C	1450	CYS	N-CA-C	6.15	119.40	110.42
1	A	1324	LEU	O-C-N	6.15	128.73	122.09
1	B	1324	LEU	O-C-N	6.11	128.69	122.09
1	A	1475	THR	O-C-N	-5.83	117.38	123.56
1	B	1112	ILE	CB-CA-C	-5.77	103.64	111.15
1	B	1418	PRO	CA-C-O	-5.62	115.19	121.32
1	B	1486	SER	CA-C-N	5.59	132.22	121.54
1	B	1486	SER	C-N-CA	5.59	132.22	121.54
1	C	121	ASP	N-CA-C	5.55	118.09	111.71
1	C	1430	ASP	N-CA-C	-5.51	99.07	110.80
1	B	1441	VAL	CA-C-N	-5.47	114.14	120.04
1	B	1441	VAL	C-N-CA	-5.47	114.14	120.04
1	C	1431	ILE	O-C-N	5.43	128.25	122.06
1	C	1486	SER	CA-C-O	-5.34	115.31	122.31
1	A	168	PRO	N-CA-C	5.31	119.38	111.41
1	A	158	LYS	N-CA-C	5.25	117.68	111.33
1	C	1431	ILE	CA-C-N	-5.24	110.80	121.18
1	C	1431	ILE	C-N-CA	-5.24	110.80	121.18
1	A	1449	GLN	CA-C-N	5.23	128.53	121.05
1	A	1449	GLN	C-N-CA	5.23	128.53	121.05
1	C	1477	THR	N-CA-C	-5.20	102.50	110.30
1	A	1453	ARG	N-CA-C	5.17	117.59	111.33
1	B	1449	GLN	CA-C-N	5.17	128.45	121.05
1	B	1449	GLN	C-N-CA	5.17	128.45	121.05
1	C	1209	LEU	CB-CA-C	-5.10	101.57	110.09
1	A	1394	ASN	N-CA-C	5.09	118.76	112.24
1	C	1091	VAL	CA-C-N	-5.09	112.33	120.17
1	C	1091	VAL	C-N-CA	-5.09	112.33	120.17

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	4603	4618	4618	65	0
1	B	4606	4618	4619	78	0
1	C	4265	4271	4268	58	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
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	211	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 8.

All (211) 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
3:A:1602:HEM:HMB1	3:A:1602:HEM:HBB2	1.64	0.78
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
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
3:C:1602:HEM:HMB1	3:C:1602:HEM:HBB2	1.77	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: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:A:1263:ILE:HG22	1:A:1309:MET:HE1	1.80	0.62
1:B:1263:ILE:HG22	1:B:1309:MET:HE1	1.80	0.62
1:B:130:ILE:HG22	1:B:131:THR:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1119:TYR:CZ	1:B:1260:TRP:HB3	2.36	0.61
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:HMB2	3:B:1602:HEM:HBB2	1.83	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
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:B:66:LYS:N	1:B:84:LYS:HZ3	2.07	0.52
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:A:157:THR:OG1	1:A:160:MET:HE3	2.09	0.52
1:B:1112:ILE:HD12	1:B:1112:ILE:H	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:HG3	1:C:1449:GLN:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:1602:HEM:HBB2	3:C:1602:HEM:CMB	2.40	0.50
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
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
1:B:1410:LEU:HD23	1:B:1410:LEU:C	2.38	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:A:1410:LEU:HD23	1:A:1410:LEU:C	2.38	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:HG2	1:C:1419:ARG:HH11	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:HBC2	3:A:1602:HEM:CMC	2.45	0.47
1:C:1154:VAL:O	1:C:1158:LEU:HB2	2.15	0.47
1:B:1247:TRP:CD1	1:B:1247:TRP:C	2.91	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:A:1391:VAL:HG23	1:A:1395:TYR:C	2.40	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:C:1410:LEU:HD23	1:C:1410:LEU:C	2.40	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:1234:THR:HG22	1:A:1238:MET:HE2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1234:THR:HG22	1:B:1238:MET:HE2	1.97	0.45
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
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:HG3	1:C:1432:ARG:O	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:C:1376:TYR:HD2	1:C:1483:MET:HE2	1.83	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:B:1146:PRO:HA	1:B:1150:SER:OG	2.17	0.43
1:C:1479:GLU:CD	1:C:1479:GLU:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1230:MET:HE3	1:B:1230:MET:HB3	1.84	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: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:A:1235:VAL:HA	1:A:1238:MET:HE3	2.02	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
1:A:1120:ARG:HG2	1:A:1120:ARG:HH21	1.85	0.42
1:B:1235:VAL:HA	1:B:1238:MET:HE3	2.02	0.42
1:C:1366:ARG:HG2	1:C:1461:LEU:HD11	2.00	0.42
1:B:106:CYS:HB3	1:B:112:CYS:HB3	2.02	0.42
1:B:1120:ARG:HG2	1:B:1120:ARG:HH21	1.85	0.42
1:A:1410:LEU:C	1:A:1410:LEU:CD2	2.93	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:B:1395:TYR:O	1:B:1396:HIS:C	2.63	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:B:1410:LEU:C	1:B:1410:LEU:CD2	2.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:1447:MET:HE3	1:C:1447:MET:HB3	1.83	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:A:1079:PHE:CD2	1:A:1079:PHE:C	2.98	0.41
1:B:67:ILE:HD11	1:B:158:LYS:HA	2.03	0.41
1:B:1079:PHE:C	1:B:1079:PHE:CD2	2.98	0.41
1:B:1412:ARG:HH11	1:B:1412:ARG:HG2	1.86	0.41
1:C:1349:ALA:O	1:C:1353:GLU:HG3	2.21	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
3:A:1602:HEM:HBB2	3:A:1602:HEM:CMB	2.41	0.40
1:B:84:LYS:HD2	1:B:84:LYS:HA	2.01	0.40
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:1325:MET:HE1	1:B:1481:ILE:HD12	2.03	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
1:C:1413:ASN:CG	1:C:1416:LEU:HD12	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	30	54
1	C	521/609 (86%)	495 (95%)	26 (5%)	0	100	100
All	All	1653/1827 (90%)	1590 (96%)	61 (4%)	2 (0%)	48	71

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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%)	499 (99%)	6 (1%)	63	78
1	B	505/534 (95%)	504 (100%)	1 (0%)	87	95
1	C	464/534 (87%)	462 (100%)	2 (0%)	84	92
All	All	1474/1602 (92%)	1465 (99%)	9 (1%)	78	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1051	ARG
1	A	1083	LEU
1	A	1101	GLN
1	A	1112	ILE
1	A	1181	ARG
1	A	1427	ARG
1	B	166	ARG
1	C	136	ASP
1	C	149	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1101	GLN
1	A	1201	ASN
1	A	1342	GLN
1	A	1393	GLN
1	A	1449	GLN
1	B	1342	GLN
1	B	1393	GLN
1	B	1426	GLN
1	B	1439	HIS
1	C	135	ASN
1	C	1178	GLN
1	C	1189	GLN
1	C	1201	ASN
1	C	1393	GLN
1	C	1396	HIS
1	C	1470	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	A	1602	4,1	50,50,50	1.23	4 (8%)	67,82,82	0.93	0
2	FES	B	1601	1	0,4,4	-	-	-		
2	FES	C	1601	1	0,4,4	-	-	-		
4	OT3	C	1603	3	18,19,19	1.73	5 (27%)	18,26,26	1.18	3 (16%)
2	FES	A	1601	1	0,4,4	-	-	-		
4	OT3	B	1603	3	18,19,19	1.86	6 (33%)	18,26,26	1.44	2 (11%)
4	OT3	A	1603	3	18,19,19	1.87	6 (33%)	18,26,26	1.44	2 (11%)
3	HEM	B	1602	4,1	50,50,50	1.23	4 (8%)	67,82,82	0.93	0
3	HEM	C	1602	4,1	50,50,50	1.40	7 (14%)	67,82,82	1.01	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	1602	4,1	-	0/14/54/54	-
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	0/3/3/3
2	FES	A	1601	1	-	-	0/1/1/1
4	OT3	B	1603	3	-	0/6/16/16	0/3/3/3
4	OT3	A	1603	3	-	0/6/16/16	0/3/3/3
3	HEM	B	1602	4,1	-	0/14/54/54	-
3	HEM	C	1602	4,1	-	2/14/54/54	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1602	HEM	FE-NA	4.65	2.10	1.95
4	A	1603	OT3	C07-C08	3.66	1.41	1.36
4	B	1603	OT3	C07-C08	3.64	1.41	1.36
4	A	1603	OT3	C09-C08	3.51	1.57	1.49
4	B	1603	OT3	C09-C08	3.50	1.57	1.49
4	C	1603	OT3	C07-C08	3.22	1.41	1.36
4	C	1603	OT3	C09-C08	3.15	1.56	1.49
3	C	1602	HEM	CAC-C3C	3.00	1.55	1.47
3	C	1602	HEM	CAB-C3B	2.92	1.55	1.47
4	C	1603	OT3	C01-C09	-2.90	1.42	1.52
3	C	1602	HEM	FE-NB	2.88	2.03	1.94
3	B	1602	HEM	CAB-C3B	2.74	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1602	HEM	CAB-C3B	2.73	1.54	1.47
3	B	1602	HEM	CAC-C3C	2.65	1.54	1.47
3	A	1602	HEM	CAC-C3C	2.63	1.54	1.47
4	A	1603	OT3	C01-C09	-2.57	1.43	1.52
4	B	1603	OT3	C01-C09	-2.56	1.43	1.52
4	C	1603	OT3	C16-N17	2.55	1.20	1.14
3	C	1602	HEM	FE-ND	2.52	2.02	1.94
4	B	1603	OT3	C16-N17	2.52	1.20	1.14
4	A	1603	OT3	C16-N17	2.50	1.20	1.14
4	B	1603	OT3	C13-C16	-2.42	1.39	1.44
4	A	1603	OT3	C13-C16	-2.41	1.39	1.44
4	C	1603	OT3	C13-C16	-2.39	1.39	1.44
3	A	1602	HEM	C2A-C3A	-2.17	1.33	1.38
3	B	1602	HEM	C2A-C3A	-2.16	1.33	1.38
3	B	1602	HEM	FE-NB	2.11	2.01	1.94
4	B	1603	OT3	C10-C03	2.10	1.55	1.51
3	C	1602	HEM	CMA-C3A	2.10	1.55	1.50
4	A	1603	OT3	C10-C03	2.10	1.55	1.51
3	A	1602	HEM	FE-NB	2.10	2.01	1.94
3	C	1602	HEM	CMC-C2C	2.04	1.54	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1603	OT3	C02-C03-C10	-2.99	104.58	112.83
4	B	1603	OT3	C02-C03-C10	-2.97	104.64	112.83
4	A	1603	OT3	C15-C10-C11	-2.53	115.16	118.30
4	B	1603	OT3	C15-C10-C11	-2.53	115.17	118.30
4	C	1603	OT3	C07-N06-C05	2.32	108.28	105.24
3	C	1602	HEM	C4D-ND-C1D	2.30	107.92	105.21
4	C	1603	OT3	C12-C11-C10	2.08	123.26	121.18
4	C	1603	OT3	C15-C10-C11	-2.02	115.80	118.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1602	HEM	CAD-CBD-CGD-O1D
3	C	1602	HEM	CAD-CBD-CGD-O2D

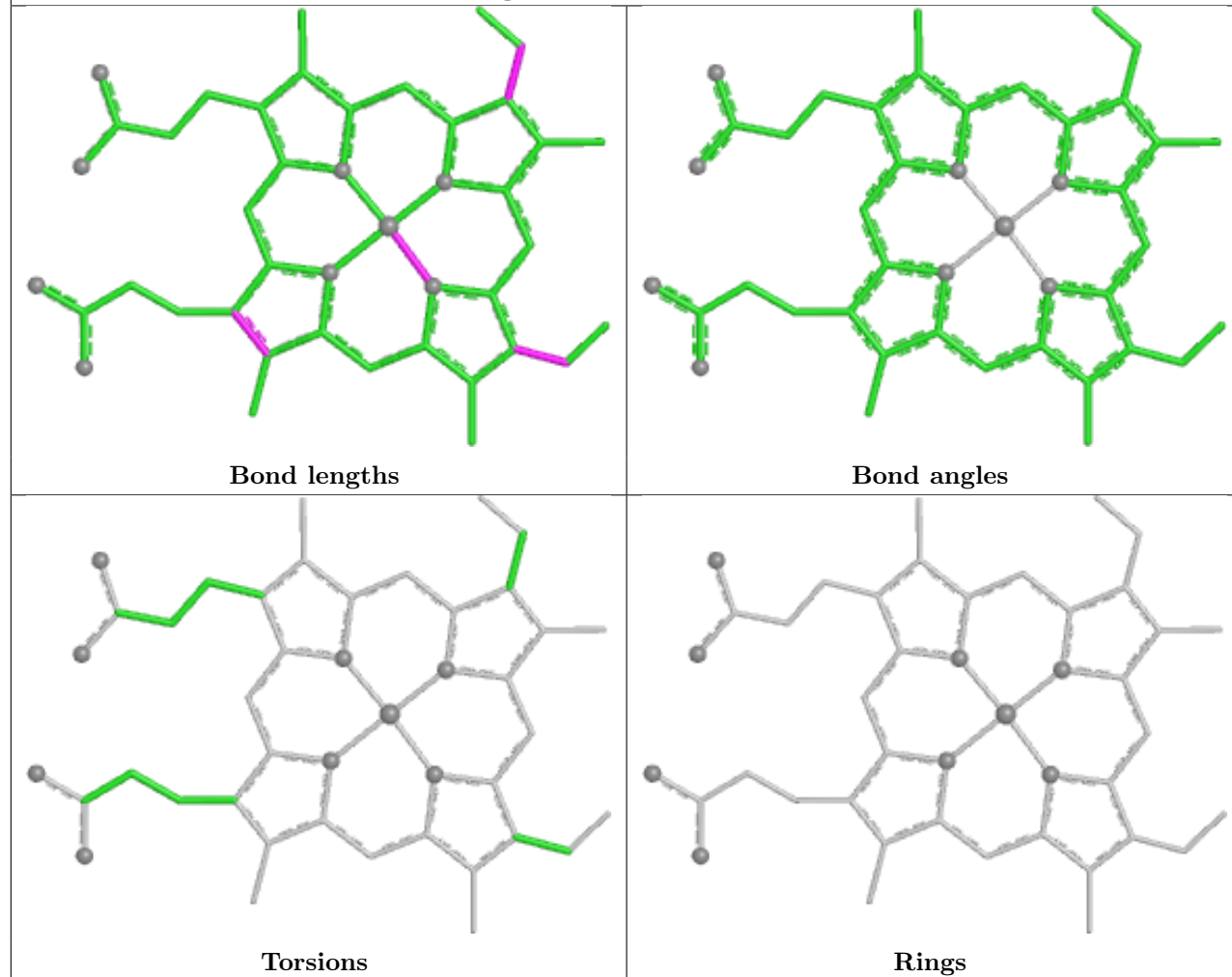
There are no ring outliers.

4 monomers are involved in 15 short contacts:

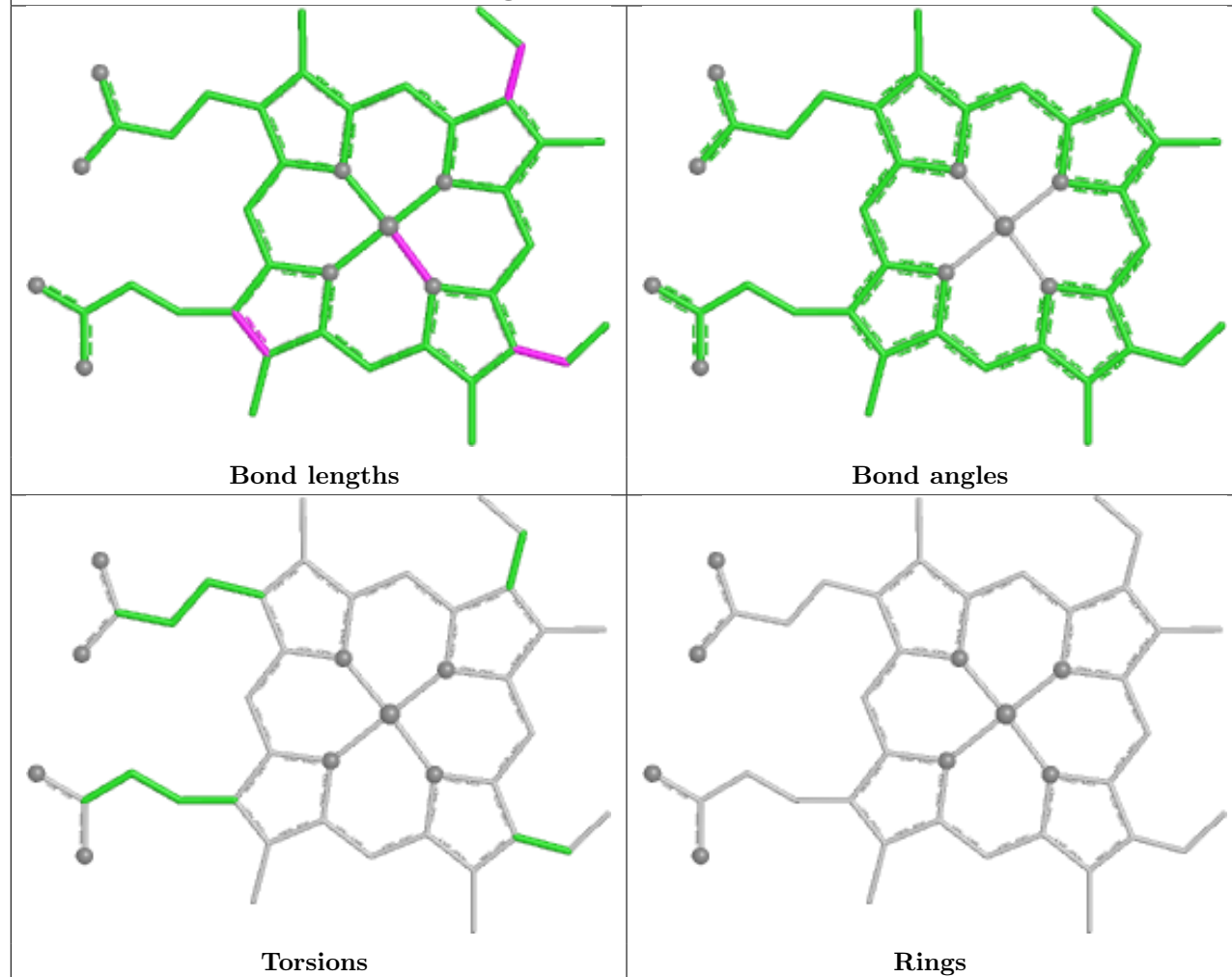
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1602	HEM	4	0
4	A	1603	OT3	2	0
3	B	1602	HEM	4	0
3	C	1602	HEM	5	0

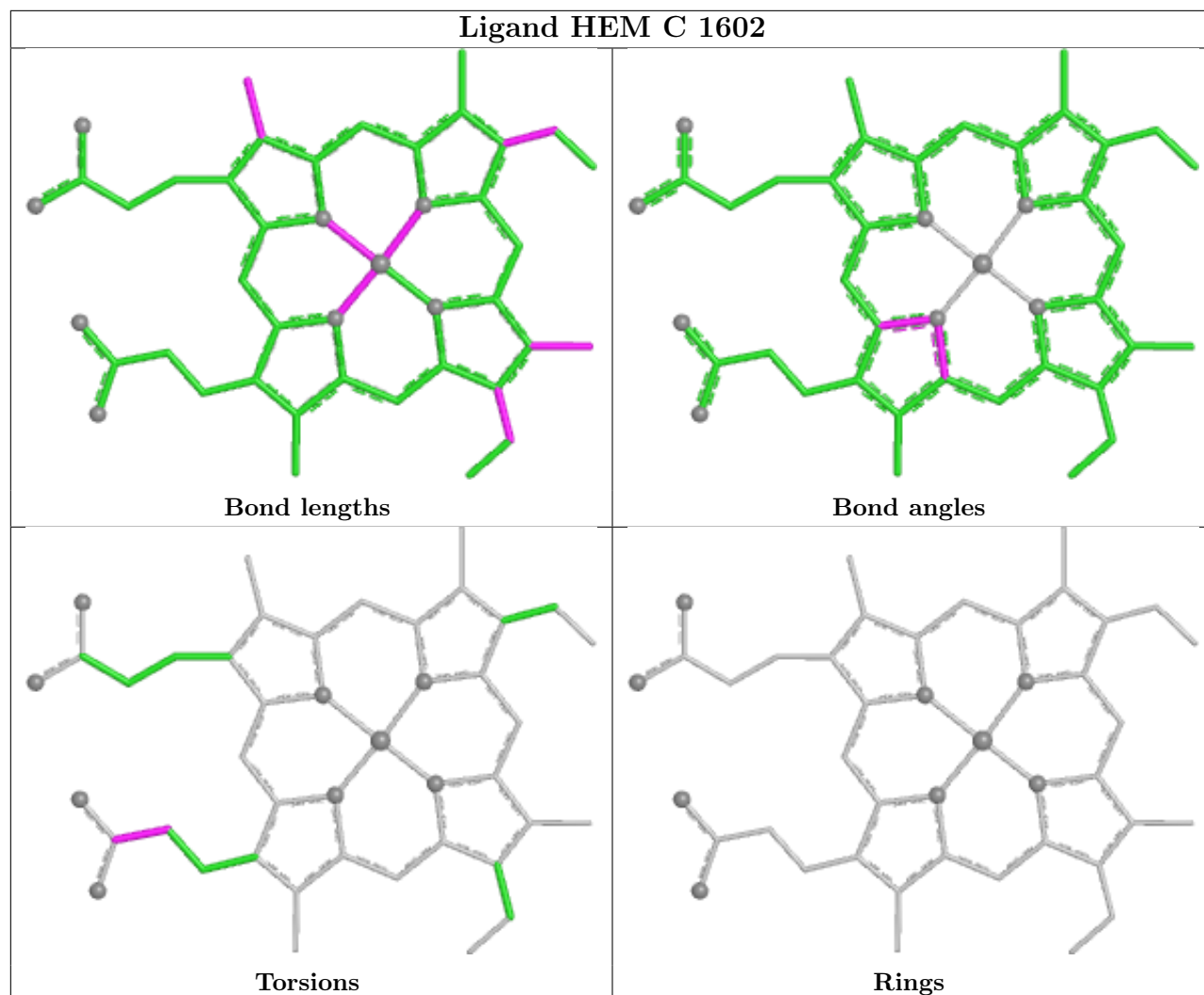
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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



Ligand HEM B 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, 95th 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	572/609 (93%)	0.15	13 (2%) 61 52	27, 50, 79, 112	0
1	B	572/609 (93%)	0.09	10 (1%) 69 61	34, 61, 86, 108	0
1	C	529/609 (86%)	0.08	17 (3%) 50 42	34, 57, 101, 124	0
All	All	1673/1827 (91%)	0.11	40 (2%) 59 50	27, 56, 88, 124	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1083	LEU	3.8
1	C	151	GLY	3.8
1	B	1061	TYR	3.4
1	C	118	ILE	3.3
1	B	1504	HIS	3.3
1	B	1387	SER	3.2
1	C	127	LEU	3.2
1	C	1477	THR	3.1
1	C	90	LEU	3.1
1	C	149	ARG	3.0
1	C	131	THR	3.0
1	A	1240	MET	2.9
1	A	158	LYS	2.9
1	B	1435	GLY	2.8
1	A	1061	TYR	2.8
1	B	1056	TRP	2.7
1	C	1081	TYR	2.6
1	C	152	CYS	2.6
1	A	1503	ASN	2.6
1	B	1493	THR	2.5
1	C	133	GLU	2.5
1	A	1421	GLU	2.5
1	B	169	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1046	GLY	2.4
1	C	1063	HIS	2.4
1	C	123	ILE	2.4
1	B	1083	LEU	2.4
1	C	1436	ARG	2.3
1	A	1244	LEU	2.3
1	C	1111	MET	2.3
1	A	1251	LYS	2.3
1	A	157	THR	2.3
1	C	1493	THR	2.3
1	B	1086	PRO	2.2
1	C	1056	TRP	2.1
1	C	1431	ILE	2.1
1	A	1350	SER	2.0
1	B	1354	HIS	2.0
1	A	170	THR	2.0
1	A	1392	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](#)

There are no oligosaccharides 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, 95th 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	A	1603	17/17	0.96	0.10	26,41,54,59	0
4	OT3	B	1603	17/17	0.96	0.12	32,48,69,79	0
4	OT3	C	1603	17/17	0.96	0.10	25,44,57,63	0
2	FES	B	1601	4/4	0.97	0.07	43,49,55,63	0
3	HEM	C	1602	43/43	0.98	0.08	25,40,63,65	0
2	FES	C	1601	4/4	0.98	0.05	53,70,82,83	0

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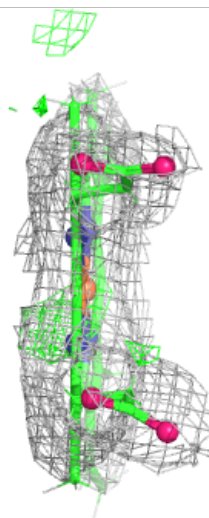
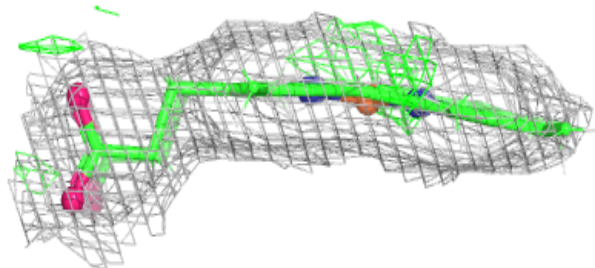
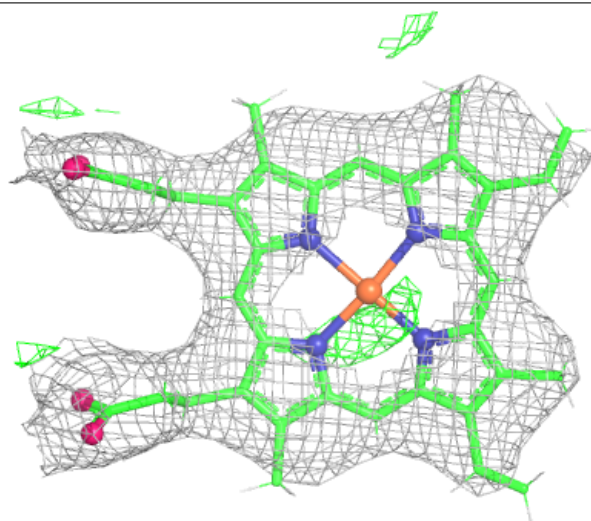
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEM	A	1602	43/43	0.98	0.08	20,33,47,57	0
3	HEM	B	1602	43/43	0.98	0.09	23,41,60,69	0
2	FES	A	1601	4/4	0.99	0.06	36,37,40,43	0

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.

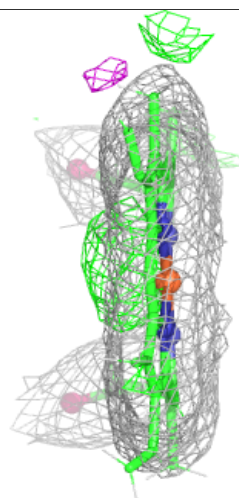
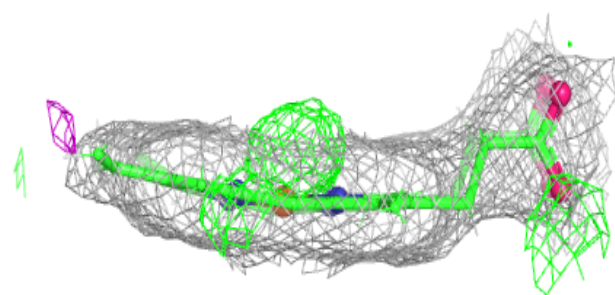
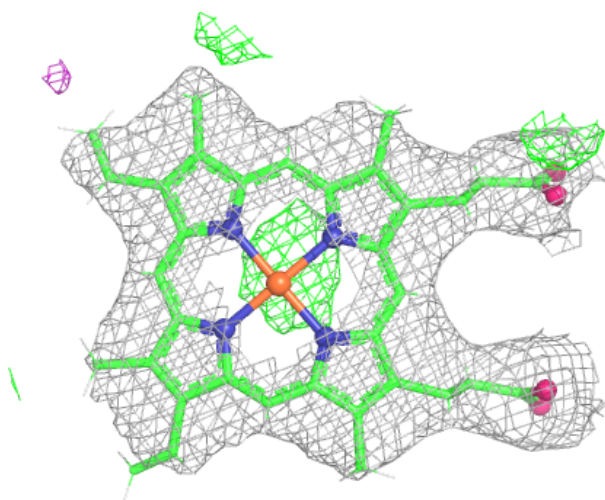
Electron density around HEM C 1602:

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



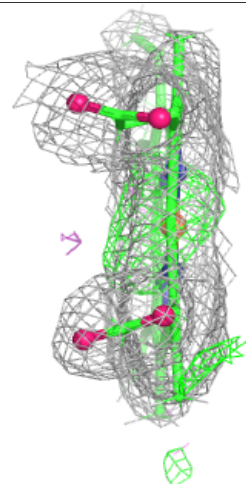
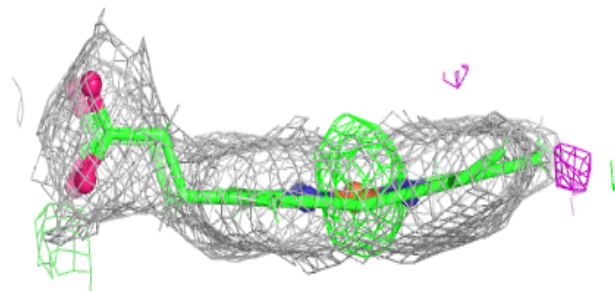
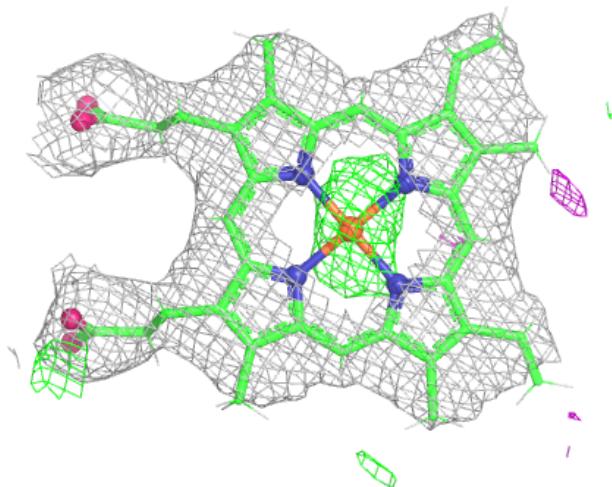
Electron density around HEM A 1602:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.