



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:50 AM UTC

PDB ID : 1WNW / pdb_00001wnw
Title : D136N mutant of Heme Oxygenase from *Corynebacterium diphtheriae* (HmuO)
Authors : Unno, M.; Matsui, T.; Ikeda-Saito, M.
Deposited on : 2004-08-10
Resolution : 1.70 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

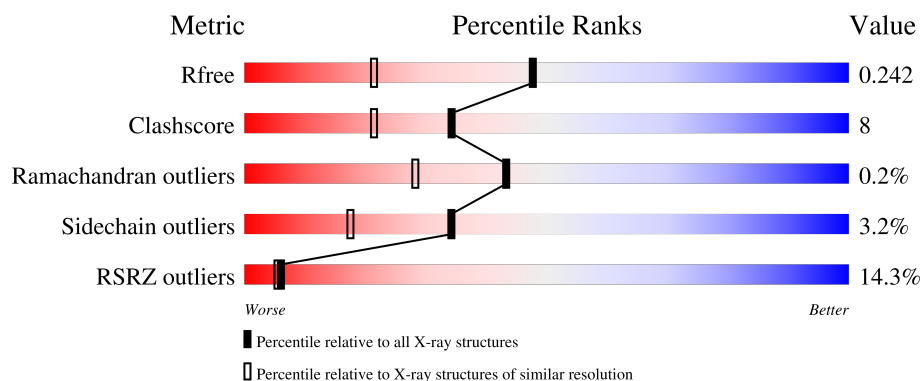
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	215	4% 88% 9% .
1	B	215	3% 88% 9% .
1	C	215	35% 71% 20% 5% .

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	IOD	A	1006	-	-	X	-
2	IOD	A	1007	-	-	X	-
2	IOD	B	1002	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5538 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 Heme oxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	1	0
			1653	1042	298	310	3			
1	B	210	Total	C	N	O	S	0	1	0
			1668	1050	300	315	3			
1	C	206	Total	C	N	O	S	0	0	0
			1635	1031	291	310	3			

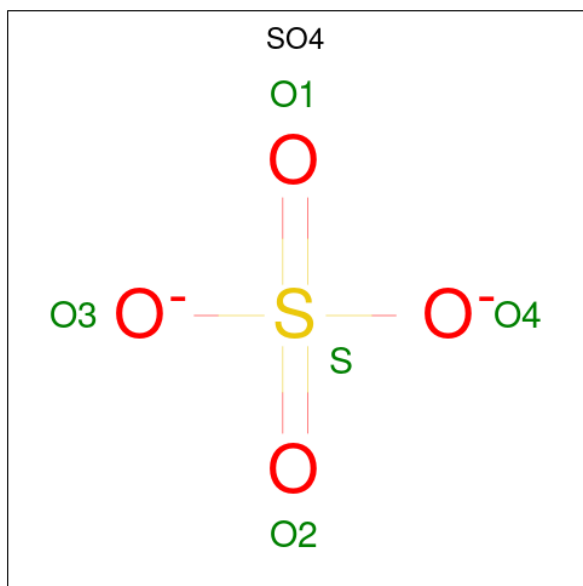
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	LYS	GLU	SEE REMARK 999	UNP P71119
A	60	VAL	ALA	SEE REMARK 999	UNP P71119
A	92	GLY	ASP	SEE REMARK 999	UNP P71119
A	93	SER	GLY	SEE REMARK 999	UNP P71119
A	136	ASN	ASP	engineered mutation	UNP P71119
A	192	HIS	ASN	SEE REMARK 999	UNP P71119
B	34	LYS	GLU	SEE REMARK 999	UNP P71119
B	60	VAL	ALA	SEE REMARK 999	UNP P71119
B	92	GLY	ASP	SEE REMARK 999	UNP P71119
B	93	SER	GLY	SEE REMARK 999	UNP P71119
B	136	ASN	ASP	engineered mutation	UNP P71119
B	192	HIS	ASN	SEE REMARK 999	UNP P71119
C	34	LYS	GLU	SEE REMARK 999	UNP P71119
C	60	VAL	ALA	SEE REMARK 999	UNP P71119
C	92	GLY	ASP	SEE REMARK 999	UNP P71119
C	93	SER	GLY	SEE REMARK 999	UNP P71119
C	136	ASN	ASP	engineered mutation	UNP P71119
C	192	HIS	ASN	SEE REMARK 999	UNP P71119

- Molecule 2 is IODIDE ION (CCD ID: IOD) (formula: I).

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

Continued on next page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- # HEM

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Na 2 2	0	0

- WORLDWIDE
PDB
PROTEIN DATA BANK

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	128	Total 128	O 128	0	0
6	B	157	Total 157	O 157	0	0
6	C	97	Total 97	O 97	0	0

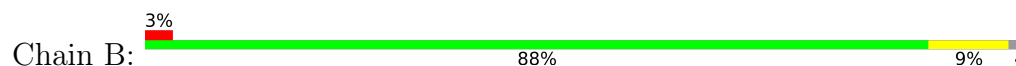
3 Residue-property plots [i](#)

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.

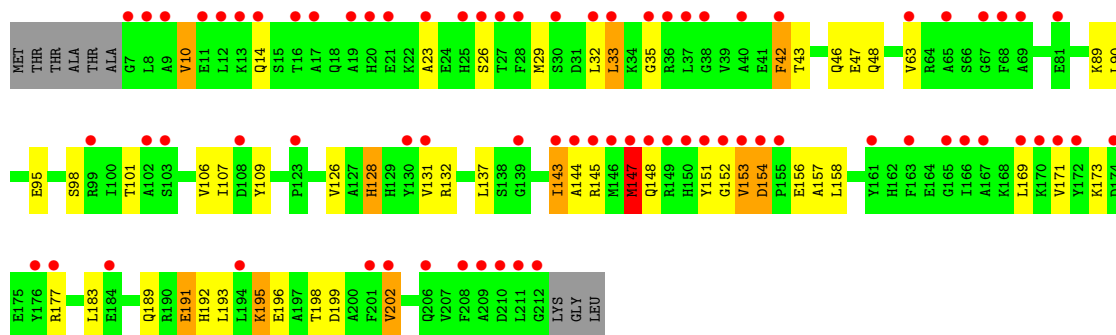
• Molecule 1: Heme oxygenase



• Molecule 1: Heme oxygenase



• Molecule 1: Heme oxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.06Å 63.10Å 107.16Å 90.00° 101.03° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 20.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-1.70) 97.1 (20.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.196 , 0.233 0.208 , 0.242	Depositor DCC
R_{free} test set	7616 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5538	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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: SO4, IOD, NA, 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	1.28	3/1692 (0.2%)	1.17	1/2285 (0.0%)
1	B	1.28	3/1707 (0.2%)	1.15	1/2303 (0.0%)
1	C	1.38	12/1667 (0.7%)	1.29	12/2254 (0.5%)
All	All	1.32	18/5066 (0.4%)	1.20	14/6842 (0.2%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	128	HIS	C-O	-10.41	1.11	1.24
1	C	145	ARG	C-O	8.36	1.34	1.24
1	A	124	ALA	CA-CB	-8.35	1.40	1.53
1	B	102	ALA	CA-CB	-8.06	1.40	1.53
1	C	148	GLN	N-CA	6.78	1.54	1.46
1	C	143	ILE	N-CA	6.67	1.54	1.46
1	C	63	VAL	CA-CB	-6.64	1.46	1.54
1	C	10	VAL	C-N	6.37	1.43	1.33
1	B	84	ALA	CA-CB	-6.07	1.43	1.53
1	C	137	LEU	C-O	5.72	1.31	1.24
1	B	62	ALA	C-O	-5.70	1.17	1.24
1	A	105	ALA	CA-CB	-5.58	1.44	1.53
1	C	154	ASP	CA-C	-5.53	1.46	1.52
1	A	151	TYR	C-O	-5.45	1.16	1.24
1	C	153	VAL	CA-CB	-5.42	1.47	1.54
1	C	46	GLN	C-O	-5.35	1.17	1.24
1	C	144	ALA	N-CA	5.10	1.52	1.46
1	C	143	ILE	CA-C	5.06	1.59	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	HIS	N-CA-C	7.72	122.70	113.28
1	C	131	VAL	N-CA-C	7.12	117.25	110.42
1	C	109	TYR	N-CA-C	-6.79	103.34	111.69
1	C	126	VAL	N-CA-C	-6.76	103.89	110.72
1	C	189	GLN	N-CA-C	-6.34	104.45	111.36
1	C	191	GLU	N-CA-C	-6.34	104.46	111.82
1	C	42	PHE	N-CA-C	-6.13	104.68	111.36
1	C	171	VAL	N-CA-C	-6.05	104.85	110.53
1	C	147	MET	N-CA-C	5.47	117.33	111.36
1	C	152	GLY	N-CA-C	-5.24	106.83	114.90
1	B	37	LEU	CA-C-O	5.23	120.98	117.94
1	C	192	HIS	N-CA-C	-5.23	105.26	111.69
1	C	98	SER	N-CA-C	5.20	119.61	113.16
1	C	131	VAL	CB-CA-C	-5.02	105.54	111.97

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	1653	0	1611	17	0
1	B	1668	0	1622	11	0
1	C	1635	0	1585	35	0
2	A	4	0	0	6	0
2	B	4	0	0	3	0
2	C	1	0	0	0	0
3	A	15	0	0	0	0
3	B	25	0	0	0	0
3	C	20	0	0	0	0
4	A	43	0	30	14	0
4	B	43	0	30	4	0
4	C	43	0	30	2	0
5	B	2	0	0	0	0
6	A	128	0	0	6	0
6	B	157	0	0	7	0
6	C	97	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5538	0	4908	77	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 (77) 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)
2:A:1006:IOD:I	6:A:2132:HOH:O	2.23	1.23
4:B:902:HEM:HBC2	4:B:902:HEM:HHD	1.31	1.07
1:A:204:ASN:HD21	4:A:901:HEM:CBB	1.76	0.99
2:B:1002:IOD:I	6:B:4097:HOH:O	2.50	0.98
1:A:204:ASN:HD21	4:A:901:HEM:HBB1	1.26	0.97
4:A:901:HEM:HBD2	6:A:2126:HOH:O	1.66	0.94
2:A:1008:IOD:I	6:A:2127:HOH:O	2.57	0.92
1:A:204:ASN:ND2	4:A:901:HEM:CBB	2.38	0.85
1:A:204:ASN:ND2	4:A:901:HEM:HBB1	1.94	0.81
2:A:1007:IOD:I	4:A:901:HEM:HAB	2.52	0.80
4:B:902:HEM:HBC2	4:B:902:HEM:CHD	2.04	0.79
1:C:42:PHE:HB2	1:C:147:MET:HE2	1.64	0.79
1:C:191:GLU:O	1:C:195:LYS:HD3	1.87	0.73
4:B:902:HEM:HHD	4:B:902:HEM:CBC	2.16	0.72
2:A:1006:IOD:I	2:A:1007:IOD:I	3.47	0.72
1:A:23:ALA:HB1	4:A:901:HEM:HBB2	1.72	0.72
1:A:23:ALA:HB1	4:A:901:HEM:CBB	2.20	0.72
1:C:32:LEU:CD2	1:C:147:MET:HE1	2.19	0.71
1:C:32:LEU:HD21	1:C:147:MET:HE1	1.73	0.69
1:A:29:MET:HA	1:A:29:MET:HE2	1.74	0.69
2:A:1006:IOD:I	6:A:2083:HOH:O	2.81	0.69
1:C:199:ASP:O	1:C:202:VAL:HG13	1.93	0.67
1:C:128:HIS:HE1	1:C:196:GLU:OE2	1.77	0.67
2:A:1007:IOD:I	6:A:2032:HOH:O	2.84	0.65
1:B:99:ARG:O	1:B:99:ARG:HG2	1.97	0.64
1:B:190:ARG:NH1	6:B:4092:HOH:O	2.33	0.61
1:C:35:GLY:HA2	1:C:151:TYR:CZ	2.36	0.61
1:C:199:ASP:HA	1:C:202:VAL:CG1	2.32	0.60
1:C:169:LEU:HG	1:C:173:LYS:HE2	1.85	0.59
1:C:42:PHE:CB	1:C:147:MET:HE2	2.34	0.58
4:A:901:HEM:CGD	4:A:901:HEM:HHA	2.34	0.58
1:C:154:ASP:OD2	1:C:156:GLU:HG2	2.03	0.58
1:A:138:SER:HB3	4:A:901:HEM:HAD1	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:LYS:HD2	1:C:156:GLU:O	2.04	0.57
1:B:99:ARG:NH2	6:B:4140:HOH:O	2.37	0.56
1:B:42:PHE:CG	1:B:147:MET:HE2	2.41	0.56
1:C:177:ARG:NH1	6:C:2078:HOH:O	2.38	0.56
1:B:141:GLN:NE2	6:B:4119:HOH:O	2.40	0.55
1:C:42:PHE:CG	1:C:147:MET:HE2	2.42	0.55
1:C:89:LYS:NZ	6:C:2099:HOH:O	2.35	0.54
1:C:95:GLU:HG2	6:C:2030:HOH:O	2.07	0.54
1:C:95:GLU:CD	6:C:2069:HOH:O	2.52	0.53
1:B:187:ASP:O	1:B:191:GLU:HG3	2.09	0.52
1:C:89:LYS:HD3	1:C:156:GLU:HG3	1.90	0.52
1:C:153:VAL:HG11	1:C:158:LEU:HD21	1.92	0.52
1:A:34:LYS:HG3	1:A:36:ARG:HG3	1.92	0.51
1:C:32:LEU:CG	1:C:147:MET:HE1	2.41	0.51
1:A:89:LYS:NZ	6:A:2130:HOH:O	2.44	0.50
1:A:23:ALA:CB	4:A:901:HEM:HBB2	2.41	0.50
1:A:146:MET:HA	1:A:146:MET:HE2	1.94	0.50
1:C:33:LEU:HD11	1:C:143:ILE:HD13	1.95	0.49
1:C:193:LEU:C	1:C:193:LEU:HD23	2.37	0.49
2:B:1002:IOD:I	4:B:902:HEM:HAB	2.84	0.48
1:B:81:GLU:HG3	6:B:4071:HOH:O	2.14	0.47
1:B:44:ARG:NH2	6:B:4124:HOH:O	2.46	0.47
1:C:32:LEU:HG	1:C:147:MET:HE1	1.97	0.47
1:C:193:LEU:HD23	1:C:193:LEU:O	2.15	0.47
1:C:35:GLY:HA2	1:C:151:TYR:OH	2.15	0.46
1:C:23:ALA:HB1	4:C:903:HEM:CBB	2.47	0.45
1:C:33:LEU:HD11	4:C:903:HEM:HBC2	2.00	0.44
1:C:33:LEU:N	1:C:33:LEU:HD23	2.33	0.43
1:A:138:SER:OG	1:A:173:LYS:HE3	2.18	0.43
1:C:90:LEU:HG	1:C:157:ALA:HB1	1.99	0.43
1:C:199:ASP:HA	1:C:202:VAL:HG12	1.99	0.43
1:C:48:GLN:OE1	1:C:106:VAL:HG21	2.19	0.43
1:B:145:ARG:HD2	2:B:1005:IOD:I	2.89	0.43
1:A:146:MET:HE2	1:A:146:MET:CA	2.49	0.42
1:B:89:LYS:HD2	1:B:156:GLU:O	2.19	0.42
1:C:183:LEU:O	6:C:2057:HOH:O	2.21	0.42
1:C:43:THR:O	1:C:47:GLU:HG3	2.19	0.42
1:C:42:PHE:CD1	1:C:147:MET:HE2	2.55	0.41
4:A:901:HEM:HHB	4:A:901:HEM:O1D	2.20	0.41
1:A:208:PHE:CE2	4:A:901:HEM:HBB1	2.56	0.41
1:B:81:GLU:OE1	6:B:4057:HOH:O	2.22	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:VAL:O	1:C:14:GLN:HG3	2.20	0.41
1:A:134:LEU:HD12	1:A:134:LEU:HA	1.92	0.41
1:A:13:LYS:HE3	4:A:901:HEM:O2D	2.21	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	207/215 (96%)	201 (97%)	5 (2%)	1 (0%)	24	12
1	B	209/215 (97%)	205 (98%)	4 (2%)	0	100	100
1	C	204/215 (95%)	201 (98%)	3 (2%)	0	100	100
All	All	620/645 (96%)	607 (98%)	12 (2%)	1 (0%)	43	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	PHE

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	169/175 (97%)	167 (99%)	2 (1%)	63	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	170/175 (97%)	166 (98%)	4 (2%)	43	26
1	C	167/175 (95%)	157 (94%)	10 (6%)	17	5
All	All	506/525 (96%)	490 (97%)	16 (3%)	34	17

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	LYS
1	A	191	GLU
1	B	18	GLN
1	B	95	GLU
1	B	198	THR
1	B	204	ASN
1	C	26	SER
1	C	29	MET
1	C	33	LEU
1	C	101	THR
1	C	107	ILE
1	C	132	ARG
1	C	147	MET
1	C	195	LYS
1	C	198	THR
1	C	202	VAL

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	78	ASN
1	A	150	HIS
1	A	182	ASN
1	A	204	ASN
1	B	78	ASN
1	B	148	GLN
1	B	150	HIS
1	B	162	HIS
1	B	182	ASN
1	C	25	HIS
1	C	78	ASN
1	C	128	HIS
1	C	148	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	150	HIS
1	C	182	ASN
1	C	206	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 11 are monoatomic - leaving 15 for Mogul analysis.

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	SO4	B	2006	-	4,4,4	0.30	0	6,6,6	0.44	0
3	SO4	B	2005	-	4,4,4	0.29	0	6,6,6	0.40	0
3	SO4	B	2008	-	4,4,4	0.27	0	6,6,6	0.20	0
3	SO4	B	2003	-	4,4,4	0.41	0	6,6,6	0.55	0
4	HEM	C	903	6,1	50,50,50	1.81	11 (22%)	67,82,82	1.39	9 (13%)
3	SO4	A	2009	-	4,4,4	0.36	0	6,6,6	0.45	0
3	SO4	C	2001	-	4,4,4	0.20	0	6,6,6	0.68	0
3	SO4	A	2007	-	4,4,4	0.18	0	6,6,6	0.30	0
3	SO4	C	2012	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	A	2011	-	4,4,4	0.18	0	6,6,6	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEM	A	901	6,1	50,50,50	1.75	9 (18%)	67,82,82	1.98	20 (29%)
4	HEM	B	902	6,1	50,50,50	1.67	8 (16%)	67,82,82	1.63	14 (20%)
3	SO4	C	2010	-	4,4,4	0.29	0	6,6,6	0.38	0
3	SO4	C	2002	-	4,4,4	0.37	0	6,6,6	0.87	0
3	SO4	B	2004	-	4,4,4	0.23	0	6,6,6	0.43	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	HEM	B	902	6,1	-	5/14/54/54	-
4	HEM	C	903	6,1	-	2/14/54/54	-
4	HEM	A	901	6,1	-	7/14/54/54	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	903	HEM	C3D-C2D	7.21	1.52	1.36
4	A	901	HEM	C3D-C2D	6.25	1.50	1.36
4	B	902	HEM	C3D-C2D	6.01	1.49	1.36
4	B	902	HEM	FE-ND	4.23	2.07	1.94
4	A	901	HEM	C1B-NB	-3.83	1.33	1.40
4	A	901	HEM	FE-NB	3.83	2.06	1.94
4	A	901	HEM	CHA-C4D	-3.68	1.31	1.38
4	C	903	HEM	CMB-C2B	3.57	1.58	1.50
4	A	901	HEM	CBD-CGD	3.22	1.58	1.50
4	C	903	HEM	CAC-C3C	3.18	1.55	1.47
4	C	903	HEM	FE-NC	3.08	2.05	1.95
4	B	902	HEM	C4B-NB	-2.74	1.33	1.38
4	B	902	HEM	CHA-C4D	-2.63	1.33	1.38
4	C	903	HEM	O1A-CGA	2.53	1.30	1.22
4	C	903	HEM	CAB-C3B	2.42	1.53	1.47
4	B	902	HEM	C3C-C2C	-2.38	1.32	1.37
4	B	902	HEM	CMA-C3A	2.37	1.55	1.50
4	B	902	HEM	C3B-C2B	-2.36	1.32	1.37
4	A	901	HEM	C2A-C3A	-2.35	1.32	1.38
4	C	903	HEM	FE-ND	2.26	2.01	1.94
4	C	903	HEM	C2A-C3A	-2.25	1.33	1.38
4	C	903	HEM	CAD-C3D	2.24	1.57	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	903	HEM	CHA-C1A	-2.23	1.34	1.39
4	B	902	HEM	CAB-C3B	2.16	1.53	1.47
4	A	901	HEM	C1D-ND	2.03	1.42	1.38
4	A	901	HEM	CAC-C3C	2.03	1.52	1.47
4	A	901	HEM	C3B-C2B	-2.02	1.33	1.37
4	C	903	HEM	O1D-CGD	2.02	1.28	1.22

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	HEM	C3B-C4B-NB	-6.35	104.90	109.47
4	A	901	HEM	C1B-NB-C4B	5.26	111.43	105.21
4	B	902	HEM	C4D-ND-C1D	4.73	110.81	105.21
4	B	902	HEM	CHD-C1D-ND	4.45	129.21	124.42
4	A	901	HEM	C4B-C3B-C2B	4.17	111.11	107.28
4	C	903	HEM	C4D-ND-C1D	4.14	110.11	105.21
4	B	902	HEM	C4C-C3C-C2C	3.73	110.05	106.81
4	A	901	HEM	CBB-CAB-C3B	-3.63	109.39	127.53
4	B	902	HEM	CBD-CAD-C3D	-3.52	102.81	112.53
4	B	902	HEM	CAA-CBA-CGA	-3.52	104.34	113.67
4	C	903	HEM	CAA-CBA-CGA	-3.43	104.56	113.67
4	C	903	HEM	C4D-C3D-C2D	-3.38	101.97	106.89
4	A	901	HEM	CHA-C4D-C3D	-3.29	119.16	125.23
4	A	901	HEM	CAA-CBA-CGA	-3.21	105.15	113.67
4	C	903	HEM	CHD-C1D-ND	3.09	127.74	124.42
4	A	901	HEM	CHD-C4C-NC	2.89	127.60	124.45
4	A	901	HEM	C4D-C3D-C2D	-2.79	102.83	106.89
4	A	901	HEM	CHA-C4D-ND	2.78	127.80	124.37
4	A	901	HEM	CMD-C2D-C1D	2.75	129.33	125.03
4	A	901	HEM	C3D-C4D-ND	2.60	113.02	110.17
4	C	903	HEM	CAB-C3B-C2B	-2.57	120.09	128.43
4	B	902	HEM	CHC-C1C-NC	2.53	127.20	124.45
4	A	901	HEM	C1A-CHA-C4D	-2.46	120.46	126.25
4	B	902	HEM	CAD-C3D-C4D	2.43	128.94	124.70
4	A	901	HEM	C2B-C1B-NB	-2.40	107.08	109.84
4	A	901	HEM	CHC-C1C-NC	2.40	127.06	124.45
4	C	903	HEM	CHA-C4D-ND	2.35	127.28	124.37
4	C	903	HEM	C3B-C2B-C1B	2.33	108.16	106.41
4	A	901	HEM	CMB-C2B-C1B	-2.33	121.40	125.03
4	C	903	HEM	CHC-C4B-NB	-2.32	121.92	124.42
4	B	902	HEM	CHA-C4D-ND	2.27	127.18	124.37
4	B	902	HEM	C1B-NB-C4B	2.26	107.89	105.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	902	HEM	C4D-C3D-C2D	-2.25	103.62	106.89
4	C	903	HEM	CHA-C4D-C3D	-2.22	121.12	125.23
4	A	901	HEM	O2A-CGA-CBA	2.22	121.02	114.00
4	B	902	HEM	O1A-CGA-CBA	-2.20	116.12	123.09
4	B	902	HEM	CHB-C1B-NB	2.17	127.05	124.37
4	A	901	HEM	CHB-C1B-NB	2.13	127.01	124.37
4	A	901	HEM	C4C-NC-C1C	2.13	109.30	105.82
4	A	901	HEM	CAA-C2A-C1A	2.10	129.05	124.94
4	A	901	HEM	CHC-C4B-C3B	2.10	129.27	125.07
4	B	902	HEM	O2D-CGD-CBD	2.03	120.42	114.00
4	B	902	HEM	CBC-CAC-C3C	-2.03	117.38	127.53

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	HEM	C2B-C3B-CAB-CBB
4	A	901	HEM	C4B-C3B-CAB-CBB
4	A	901	HEM	C2C-C3C-CAC-CBC
4	B	902	HEM	C2B-C3B-CAB-CBB
4	A	901	HEM	C4C-C3C-CAC-CBC
4	B	902	HEM	C4C-C3C-CAC-CBC
4	B	902	HEM	C4B-C3B-CAB-CBB
4	B	902	HEM	CAA-CBA-CGA-O1A
4	B	902	HEM	CAA-CBA-CGA-O2A
4	C	903	HEM	CAA-CBA-CGA-O1A
4	C	903	HEM	CAA-CBA-CGA-O2A
4	A	901	HEM	CAA-CBA-CGA-O1A
4	A	901	HEM	CAA-CBA-CGA-O2A
4	A	901	HEM	CAD-CBD-CGD-O1D

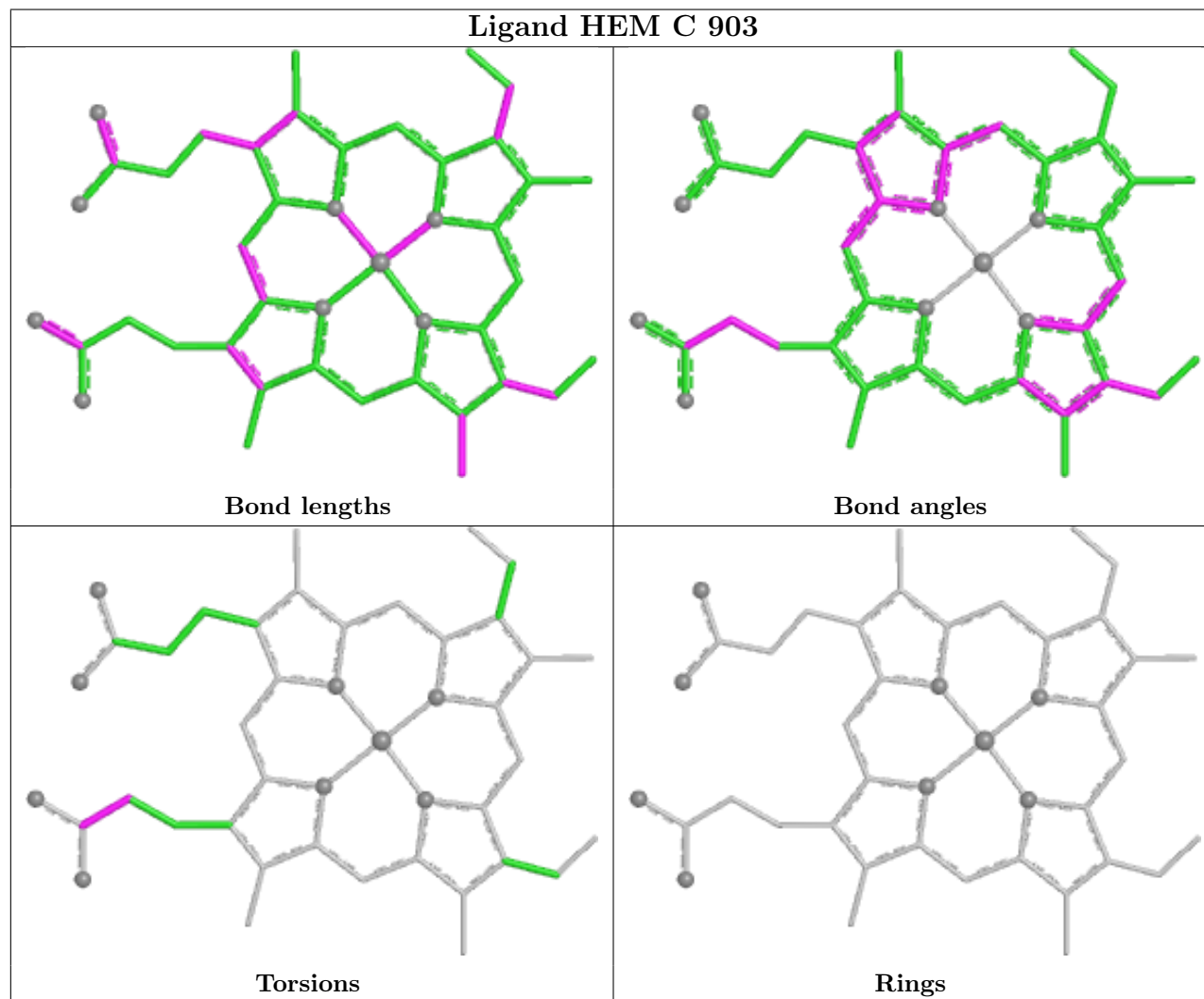
There are no ring outliers.

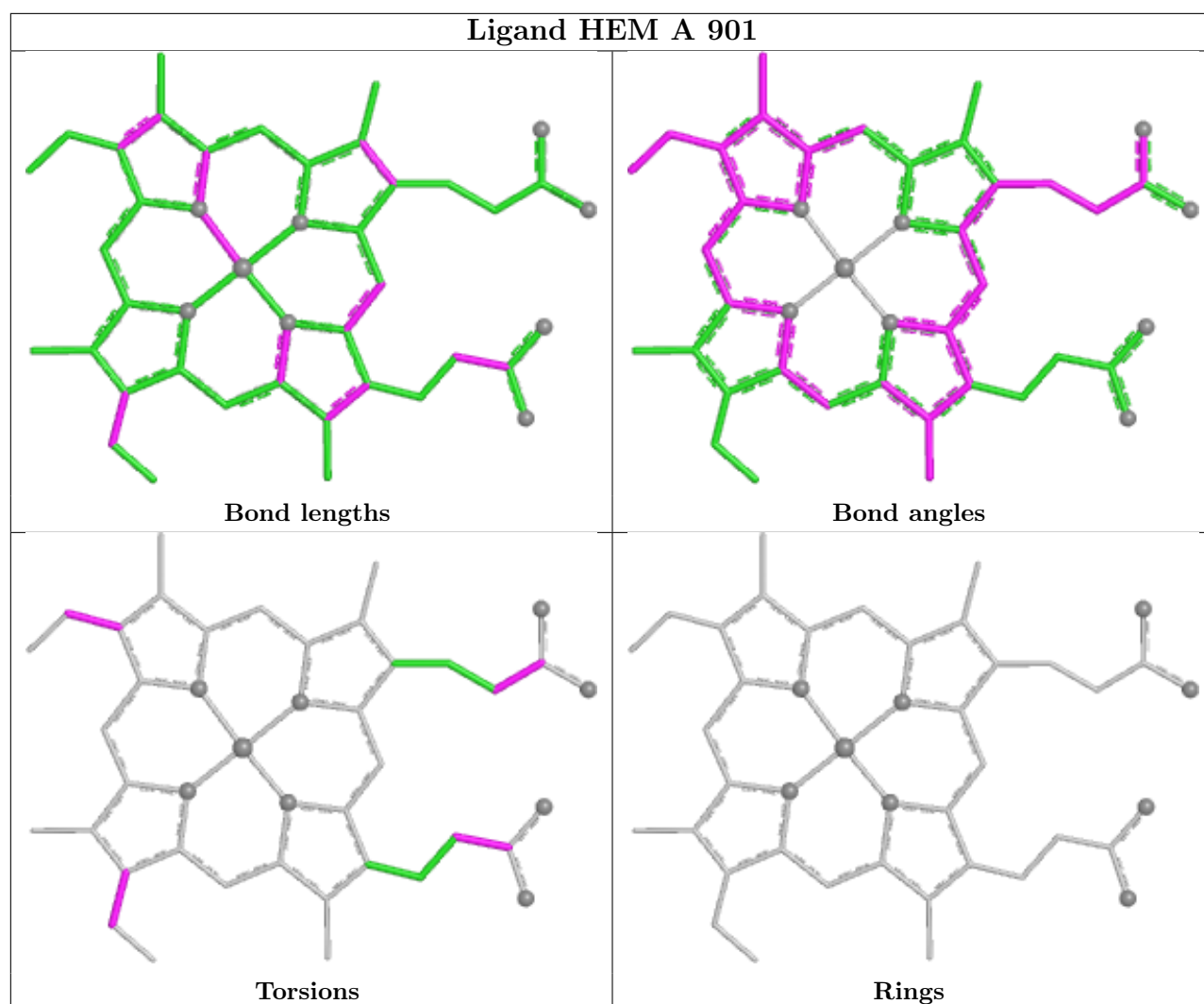
3 monomers are involved in 20 short contacts:

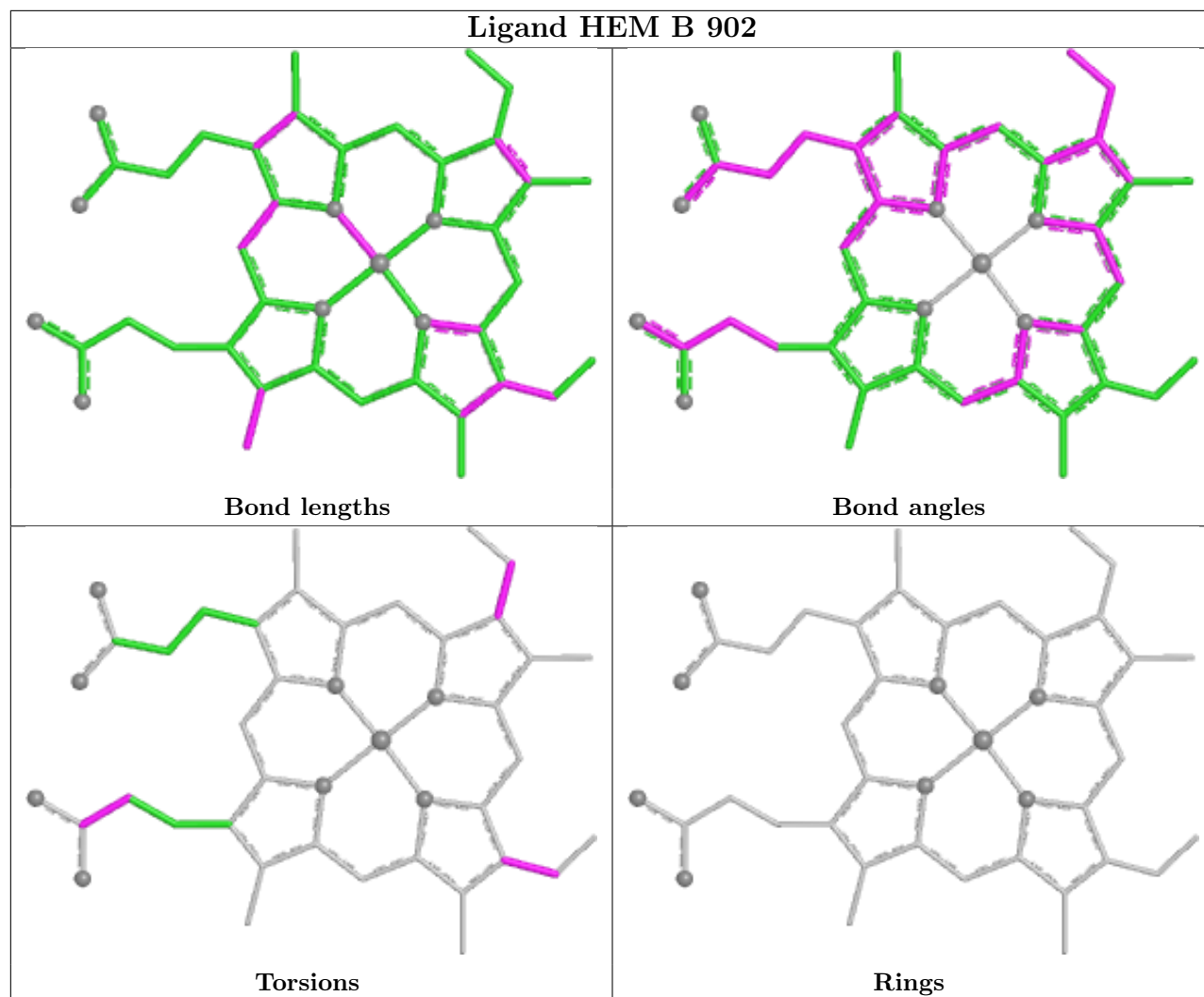
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	903	HEM	2	0
4	A	901	HEM	14	0
4	B	902	HEM	4	0

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.







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	208/215 (96%)	0.35	8 (3%) 44 48	17, 27, 45, 51	1 (0%)
1	B	210/215 (97%)	0.26	6 (2%) 53 58	16, 25, 38, 43	1 (0%)
1	C	206/215 (95%)	1.66	75 (36%) 1 1	19, 40, 61, 78	0
All	All	624/645 (96%)	0.76	89 (14%) 6 5	16, 29, 53, 78	2 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	35	GLY	7.0
1	C	152	GLY	6.4
1	C	147	MET	5.4
1	C	143	ILE	4.8
1	C	27	THR	4.7
1	B	6	ALA	4.6
1	C	209	ALA	4.5
1	C	37	LEU	4.3
1	C	169	LEU	4.3
1	C	67	GLY	4.3
1	A	94	SER	4.2
1	C	146	MET	4.2
1	C	150	HIS	4.2
1	C	212	GLY	3.9
1	C	194	LEU	3.8
1	C	9	ALA	3.8
1	C	210	ASP	3.6
1	C	40	ALA	3.6
1	C	208	PHE	3.6
1	A	6	ALA	3.6
1	C	165	GLY	3.6
1	B	164	GLU	3.5
1	C	153	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	202	VAL	3.4
1	C	16	THR	3.4
1	A	95	GLU	3.3
1	A	7	GLY	3.3
1	C	17	ALA	3.3
1	C	32	LEU	3.2
1	C	151	TYR	3.1
1	C	21	GLU	3.1
1	C	68	PHE	3.1
1	C	30	SER	3.1
1	C	12	LEU	3.0
1	C	38	GLY	3.0
1	C	171	VAL	3.0
1	C	25	HIS	3.0
1	C	19	ALA	2.9
1	C	26	SER	2.9
1	C	42	PHE	2.9
1	C	170	LYS	2.8
1	C	176	TYR	2.8
1	C	211	LEU	2.8
1	C	154	ASP	2.8
1	C	63	VAL	2.8
1	C	166	ILE	2.8
1	C	20	HIS	2.7
1	A	208	PHE	2.7
1	C	206	GLN	2.7
1	C	144	ALA	2.7
1	B	99	ARG	2.6
1	C	23	ALA	2.6
1	C	69	ALA	2.6
1	C	148	GLN	2.6
1	C	8	LEU	2.6
1	A	25	HIS	2.6
1	C	7	GLY	2.6
1	C	13	LYS	2.6
1	C	36	ARG	2.6
1	B	165	GLY	2.5
1	C	108	ASP	2.5
1	A	93	SER	2.5
1	C	201	PHE	2.5
1	C	139	GLY	2.5
1	C	33	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	11	GLU	2.4
1	C	161	TYR	2.4
1	C	81	GLU	2.4
1	C	167	ALA	2.4
1	C	103	SER	2.3
1	C	28	PHE	2.3
1	C	131	VAL	2.3
1	C	99	ARG	2.3
1	C	149	ARG	2.3
1	C	14	GLN	2.3
1	C	177	ARG	2.3
1	C	172	TYR	2.3
1	B	142	VAL	2.3
1	C	155	PRO	2.2
1	C	163	PHE	2.1
1	B	184	GLU	2.1
1	C	145	ARG	2.1
1	C	184	GLU	2.1
1	C	123	PRO	2.1
1	C	130	TYR	2.1
1	C	65	ALA	2.1
1	A	212	GLY	2.0
1	C	102	ALA	2.0
1	C	174	ASP	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](#)

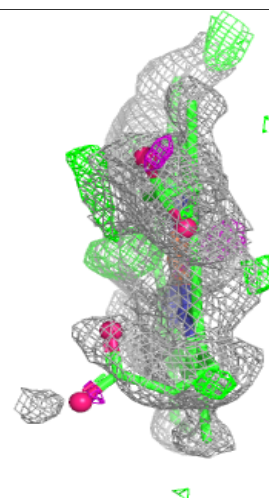
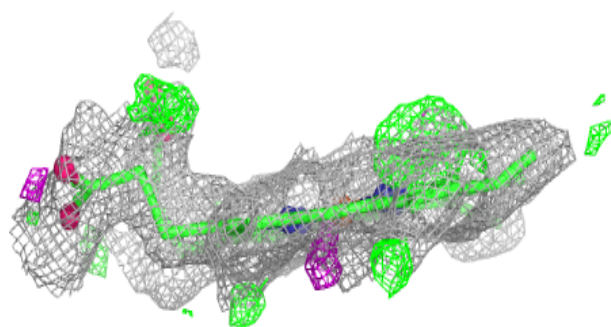
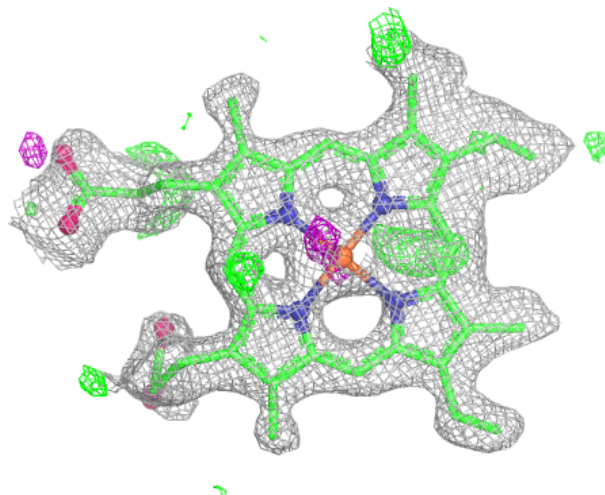
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	SO4	B	2008	5/5	0.55	0.18	95,95,96,96	0
3	SO4	B	2006	5/5	0.61	0.18	80,80,81,82	0
3	SO4	A	2009	5/5	0.65	0.18	62,64,68,69	0
3	SO4	C	2002	5/5	0.68	0.16	62,62,64,64	0
3	SO4	B	2005	5/5	0.70	0.16	62,67,68,69	0
3	SO4	C	2012	5/5	0.74	0.12	76,76,77,77	0
3	SO4	B	2003	5/5	0.78	0.17	63,64,66,67	0
3	SO4	C	2010	5/5	0.82	0.15	40,49,54,54	0
3	SO4	A	2007	5/5	0.86	0.13	79,79,80,81	0
3	SO4	A	2011	5/5	0.88	0.12	51,55,56,58	0
5	NA	B	4002	1/1	0.88	0.08	57,57,57,57	0
4	HEM	C	903	43/43	0.90	0.13	31,38,52,61	0
2	IOD	C	1001	1/1	0.90	0.10	41,41,41,41	0
3	SO4	C	2001	5/5	0.91	0.09	53,55,57,57	0
2	IOD	B	1005	1/1	0.92	0.13	44,44,44,44	0
2	IOD	A	1006	1/1	0.93	0.30	77,77,77,77	0
2	IOD	B	1004	1/1	0.93	0.16	74,74,74,74	0
3	SO4	B	2004	5/5	0.93	0.09	40,43,45,47	0
5	NA	B	4001	1/1	0.94	0.07	50,50,50,50	0
4	HEM	A	901	43/43	0.96	0.10	18,28,46,56	0
2	IOD	A	1008	1/1	0.97	0.14	56,56,56,56	0
2	IOD	A	1007	1/1	0.97	0.26	54,54,54,54	0
2	IOD	B	1002	1/1	0.98	0.23	45,45,45,45	0
2	IOD	B	1003	1/1	0.98	0.21	64,64,64,64	0
4	HEM	B	902	43/43	0.98	0.07	18,26,41,54	0
2	IOD	A	1009	1/1	0.99	0.23	49,49,49,49	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.

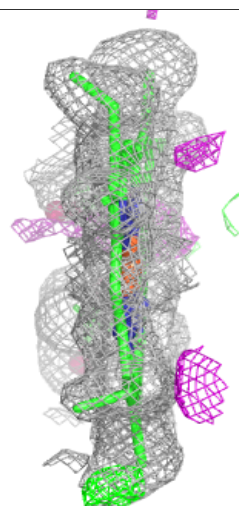
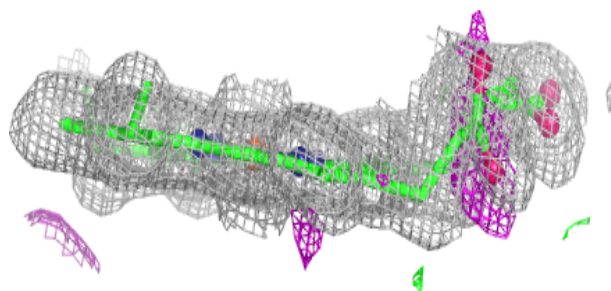
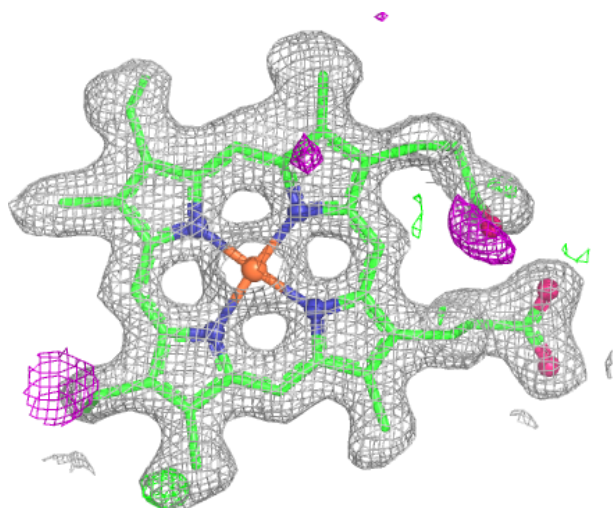
Electron density around HEM C 903:

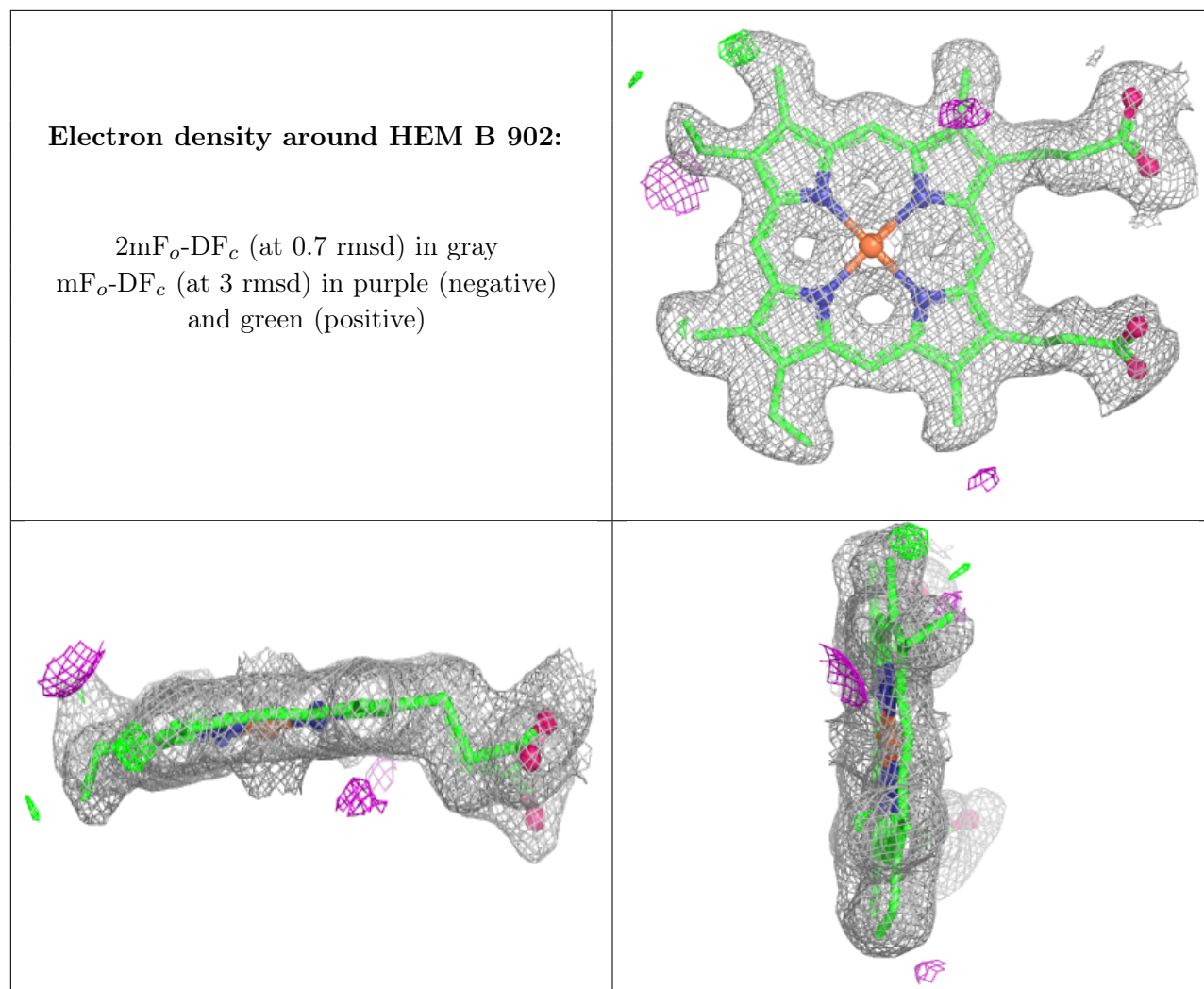
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 901:

$2mF_o-DF_c$ (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.