



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 07:54 PM EDT

PDB ID : 1M6C / pdb_00001m6c
Title : V68N MYOGLOBIN WITH CO
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Deposited on : 1998-08-12
Resolution : 1.90 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

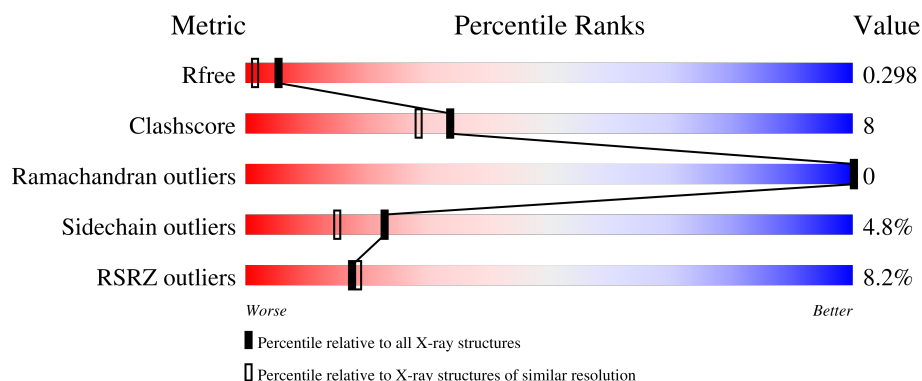
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 ≥ 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	153	
1	B	153	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3049 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.

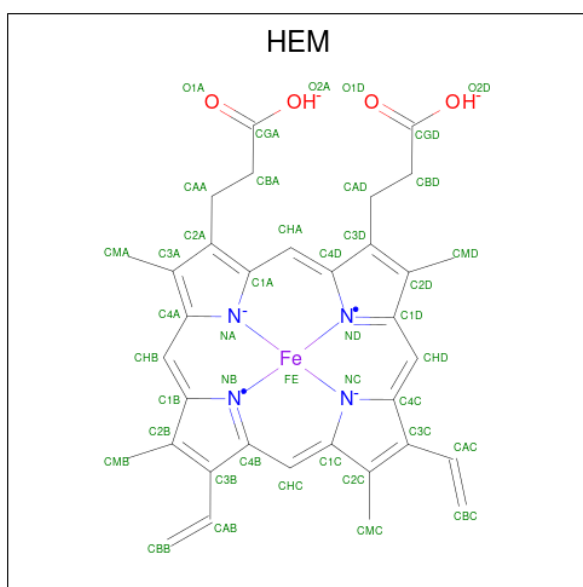
- Molecule 1 is a protein called PROTEIN (MYOGLOBIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	5	11	0
			1238	788	216	231	3			
1	B	153	Total	C	N	O	S	17	9	0
			1234	783	216	232	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	ASN	VAL	engineered mutation	UNP P02189
B	68	ASN	VAL	engineered mutation	UNP P02189

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



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

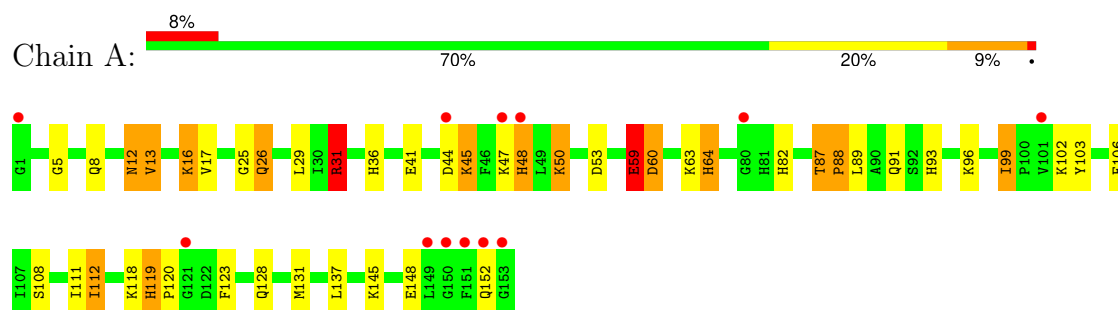
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	268	Total	O		
			268	268		
					0	0
4	B	219	Total	O		
			219	219		
					0	0

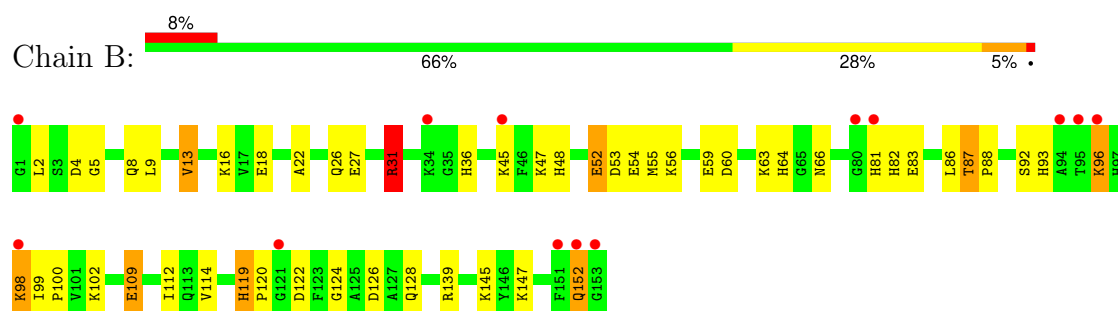
3 Residue-property plots [i](#)

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: PROTEIN (MYOGLOBIN)



• Molecule 1: PROTEIN (MYOGLOBIN)



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.14Å 42.30Å 91.55Å 90.00° 92.49° 90.00°	Depositor
Resolution (Å)	24.00 – 1.90 24.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.0 (24.00-1.90) 95.0 (24.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.261 (Not available) , 0.298	Depositor DCC
R_{free} test set	1807 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.178 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3049	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 100.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 0.0000e+00. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CMO, 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	1.23	1/1308 (0.1%)	2.07	51/1749 (2.9%)
1	B	1.30	5/1295 (0.4%)	2.13	57/1734 (3.3%)
All	All	1.26	6/2603 (0.2%)	2.10	108/3483 (3.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	98	LYS	CD-CE	9.45	1.80	1.52
1	B	5	GLY	CA-C	6.67	1.59	1.52
1	B	93	HIS	ND1-CE1	6.05	1.38	1.32
1	B	119	HIS	C-N	-6.03	1.25	1.33
1	B	55	MET	N-CA	5.80	1.53	1.46
1	A	111	ILE	N-CA	5.04	1.52	1.46

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	HIS	CA-CB-CG	-12.44	101.36	113.80
1	B	16	LYS	CG-CD-CE	11.28	137.23	111.30
1	B	109	GLU	CB-CG-CD	9.11	128.09	112.60
1	A	53	ASP	CA-CB-CG	-8.94	103.66	112.60
1	B	93	HIS	CE1-NE2-CD2	8.91	117.91	109.00
1	B	47	LYS	CB-CA-C	8.39	126.14	110.63
1	B	112	ILE	O-C-N	8.28	129.90	121.87
1	B	82	HIS	CA-C-O	8.13	129.21	119.78
1	B	152	GLN	N-CA-CB	7.97	121.98	109.71
1	A	108	SER	CA-C-O	7.88	128.91	120.55
1	B	66	ASN	OD1-CG-ND2	7.66	130.26	122.60
1	B	2	LEU	CA-C-O	-7.53	112.64	121.46
1	B	26	GLN	OE1-CD-NE2	-7.52	115.08	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	ASP	CA-CB-CG	7.29	119.89	112.60
1	A	112[A]	ILE	O-C-N	7.27	129.03	121.91
1	A	112[B]	ILE	O-C-N	7.27	129.03	121.91
1	A	96	LYS	N-CA-C	7.14	119.14	111.36
1	B	36	HIS	CA-C-O	7.10	129.45	121.22
1	A	64	HIS	CA-C-O	-7.07	112.93	120.42
1	B	2	LEU	O-C-N	7.07	132.58	123.11
1	A	36	HIS	CA-C-O	6.94	129.27	121.22
1	B	128[A]	GLN	CB-CA-C	-6.85	100.13	110.88
1	B	128[B]	GLN	CB-CA-C	-6.85	100.13	110.88
1	A	128[A]	GLN	CB-CA-C	-6.83	100.17	110.88
1	A	128[B]	GLN	CB-CA-C	-6.83	100.17	110.88
1	B	93	HIS	ND1-CE1-NE2	-6.78	101.62	108.40
1	B	112	ILE	CA-C-N	-6.78	111.20	120.28
1	B	112	ILE	C-N-CA	-6.78	111.20	120.28
1	A	36	HIS	O-C-N	-6.76	115.42	121.17
1	A	103	TYR	CA-C-O	-6.60	112.38	119.97
1	B	36	HIS	O-C-N	-6.49	115.65	121.17
1	B	22	ALA	CA-C-N	-6.49	112.86	120.00
1	B	22	ALA	C-N-CA	-6.49	112.86	120.00
1	A	50	LYS	CB-CG-CD	6.49	126.22	111.30
1	B	122	ASP	CA-CB-CG	-6.32	106.28	112.60
1	A	112[A]	ILE	CA-C-N	-6.25	111.91	120.28
1	A	112[A]	ILE	C-N-CA	-6.25	111.91	120.28
1	A	112[B]	ILE	CA-C-N	-6.25	111.91	120.28
1	A	112[B]	ILE	C-N-CA	-6.25	111.91	120.28
1	B	145	LYS	N-CA-CB	6.24	119.91	110.30
1	A	64	HIS	O-C-N	6.08	129.08	122.15
1	B	98	LYS	CG-CD-CE	-6.07	97.34	111.30
1	A	112[A]	ILE	CA-C-O	-6.04	114.77	121.17
1	A	112[B]	ILE	CA-C-O	-6.04	114.77	121.17
1	B	26	GLN	CG-CD-NE2	6.04	125.46	116.40
1	B	99	ILE	CA-C-N	6.03	126.00	120.03
1	B	99	ILE	C-N-CA	6.03	126.00	120.03
1	B	52	GLU	O-C-N	-6.02	115.74	122.12
1	A	5	GLY	O-C-N	6.02	128.09	122.13
1	B	22	ALA	O-C-N	5.97	128.45	122.12
1	B	4	ASP	CA-CB-CG	-5.96	106.64	112.60
1	B	112	ILE	CA-C-O	-5.87	114.84	120.95
1	A	123	PHE	CA-C-N	5.85	129.91	121.54
1	A	123	PHE	C-N-CA	5.85	129.91	121.54
1	A	29	LEU	O-C-N	5.82	128.29	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	SER	O-C-N	-5.75	116.02	122.12
1	B	31	ARG	CA-C-N	5.74	128.23	120.65
1	B	31	ARG	C-N-CA	5.74	128.23	120.65
1	A	13[A]	VAL	CA-C-O	-5.71	114.31	120.47
1	A	13[B]	VAL	CA-C-O	-5.71	114.31	120.47
1	B	93	HIS	CG-CD2-NE2	-5.70	101.50	107.20
1	A	26	GLN	N-CA-C	-5.68	105.09	111.28
1	B	139	ARG	N-CA-CB	5.64	118.19	110.01
1	B	98	LYS	CA-C-N	-5.63	118.77	122.60
1	B	98	LYS	C-N-CA	-5.63	118.77	122.60
1	A	45	LYS	CA-C-O	-5.62	111.75	119.05
1	A	87	THR	CA-C-N	5.58	125.42	119.28
1	A	87	THR	C-N-CA	5.58	125.42	119.28
1	B	82	HIS	N-CA-CB	-5.56	102.26	111.49
1	A	118	LYS	O-C-N	-5.56	114.47	122.36
1	B	124	GLY	O-C-N	-5.56	118.38	122.71
1	A	31	ARG	CG-CD-NE	5.54	124.20	112.00
1	B	126	ASP	CA-C-O	-5.54	114.55	120.42
1	A	29	LEU	CA-C-O	-5.52	114.70	120.55
1	B	82	HIS	CB-CG-CD2	5.52	138.37	131.20
1	A	106	PHE	O-C-N	5.50	127.94	122.12
1	A	59	GLU	CA-C-O	-5.47	113.68	119.97
1	A	82	HIS	CA-CB-CG	5.46	119.26	113.80
1	A	88	PRO	N-CA-CB	5.46	109.29	103.39
1	B	83[A]	GLU	CB-CA-C	5.46	120.72	110.63
1	B	83[B]	GLU	CB-CA-C	5.46	120.72	110.63
1	B	31	ARG	CA-CB-CG	5.43	124.97	114.10
1	A	25	GLY	O-C-N	5.43	127.46	122.19
1	A	50	LYS	CG-CD-CE	5.43	123.79	111.30
1	A	13[A]	VAL	N-CA-CB	5.42	120.58	110.77
1	A	13[B]	VAL	N-CA-CB	5.42	120.58	110.77
1	B	31	ARG	CG-CD-NE	5.39	123.87	112.00
1	B	48[A]	HIS	CA-C-O	-5.39	112.06	119.12
1	B	48[B]	HIS	CA-C-O	-5.39	112.06	119.12
1	B	100	PRO	N-CA-CB	5.37	109.02	103.38
1	A	17	VAL	N-CA-C	-5.29	105.35	110.42
1	B	128[A]	GLN	OE1-CD-NE2	5.27	127.87	122.60
1	B	128[B]	GLN	OE1-CD-NE2	5.27	127.87	122.60
1	A	103	TYR	O-C-N	5.27	128.75	122.27
1	A	99	ILE	N-CA-C	5.26	112.76	107.55
1	B	147	LYS	O-C-N	-5.22	116.67	122.09
1	B	93	HIS	CA-CB-CG	-5.21	108.59	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	LYS	CA-CB-CG	-5.20	103.69	114.10
1	A	12	ASN	CA-CB-CG	-5.19	107.41	112.60
1	A	119	HIS	O-C-N	5.18	127.28	121.32
1	B	86	LEU	N-CA-C	5.13	116.95	111.36
1	B	82	HIS	ND1-CG-CD2	-5.13	100.97	106.10
1	B	81	HIS	CA-C-N	5.07	130.61	122.14
1	B	81	HIS	C-N-CA	5.07	130.61	122.14
1	B	54	GLU	O-C-N	5.03	127.25	122.07
1	A	137	LEU	N-CA-CB	5.02	117.28	110.01
1	A	93	HIS	CA-CB-CG	-5.02	108.78	113.80
1	B	87	THR	O-C-N	-5.00	115.57	121.32

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	1238	0	1259	20	1
1	B	1234	0	1236	17	2
2	A	43	0	30	2	0
2	B	43	0	30	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	268	0	0	6	1
4	B	219	0	0	5	3
All	All	3049	0	2555	39	4

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 (39) 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:27[A]:GLU:HG2	1:B:114:VAL:HG22	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:THR:HG23	1:A:145[A]:LYS:HE2	1.65	0.78
1:B:27[A]:GLU:HG3	4:B:180:HOH:O	1.88	0.74
1:B:27[A]:GLU:HG2	1:B:114:VAL:CG2	2.19	0.72
1:B:18:GLU:OE1	4:B:188:HOH:O	2.09	0.71
1:A:44:ASP:HA	1:A:47:LYS:HD3	1.76	0.67
1:A:44:ASP:O	1:A:47:LYS:HG2	1.96	0.65
1:A:99:ILE:HD12	2:A:154:HEM:HAC	1.81	0.63
1:B:53:ASP:HB3	4:B:280:HOH:O	1.97	0.63
2:B:154:HEM:HMC1	2:B:154:HEM:HBC2	1.79	0.62
1:B:9:LEU:O	1:B:13[A]:VAL:HG12	2.00	0.61
1:B:87:THR:HB	1:B:88:PRO:HD3	1.82	0.61
1:B:45:LYS:HD3	1:B:60:ASP:OD2	2.02	0.59
1:B:63:LYS:HD2	4:B:355:HOH:O	2.04	0.58
1:A:59:GLU:O	1:A:63:LYS:HG3	2.05	0.57
1:B:52:GLU:HG2	1:B:56:LYS:HE2	1.89	0.55
1:B:8:GLN:NE2	4:B:238:HOH:O	2.40	0.53
1:A:88:PRO:HA	1:A:91:GLN:HE21	1.73	0.52
1:A:148:GLU:HG2	4:A:379:HOH:O	2.10	0.51
1:B:59:GLU:O	1:B:63:LYS:HG3	2.12	0.50
1:A:145[A]:LYS:NZ	4:A:226:HOH:O	2.45	0.50
2:B:154:HEM:HBC2	2:B:154:HEM:CMC	2.42	0.50
1:A:8[B]:GLN:NE2	1:A:12:ASN:OD1	2.42	0.49
1:A:31:ARG:NH1	4:A:219:HOH:O	2.46	0.48
1:B:119:HIS:N	1:B:120:PRO:CD	2.77	0.47
1:A:45:LYS:O	1:A:48:HIS:CE1	2.67	0.47
1:B:87:THR:HB	1:B:88:PRO:CD	2.45	0.47
1:A:60:ASP:O	1:A:64:HIS:HD2	1.97	0.47
1:B:92:SER:O	1:B:96:LYS:HB2	2.15	0.47
1:A:89:LEU:HD11	2:A:154:HEM:CHB	2.45	0.46
1:A:63:LYS:HG2	4:A:386:HOH:O	2.16	0.45
1:A:26:GLN:NE2	4:A:271:HOH:O	2.49	0.45
1:A:87:THR:HG23	1:A:145[A]:LYS:CE	2.41	0.43
1:A:112[B]:ILE:HD11	1:A:131:MET:HG3	2.01	0.42
1:A:63:LYS:HD2	4:A:394:HOH:O	2.20	0.42
1:B:64:HIS:HE1	2:B:154:HEM:CGD	2.33	0.42
1:A:41:GLU:HA	1:A:47:LYS:HE3	2.02	0.41
1:A:119:HIS:N	1:A:120:PRO:CD	2.84	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLU:OE1	4:B:240:HOH:O[2_645]	1.83	0.37
1:B:109:GLU:CD	4:B:240:HOH:O[2_645]	2.02	0.18
1:A:16:LYS:NZ	4:A:335:HOH:O[2_646]	2.19	0.01
4:B:205:HOH:O	4:B:350:HOH:O[2_645]	2.19	0.01

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	162/153 (106%)	157 (97%)	5 (3%)	0	100	100
1	B	160/153 (105%)	155 (97%)	5 (3%)	0	100	100
All	All	322/306 (105%)	312 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	134/124 (108%)	127 (95%)	7 (5%)	21	13
1	B	132/124 (106%)	125 (95%)	7 (5%)	20	12
All	All	266/248 (107%)	252 (95%)	14 (5%)	23	12

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13[A]	VAL
1	A	13[B]	VAL
1	A	31	ARG
1	A	50	LYS
1	A	59	GLU
1	A	102	LYS
1	A	152	GLN
1	B	13[A]	VAL
1	B	13[B]	VAL
1	B	31	ARG
1	B	96	LYS
1	B	98	LYS
1	B	102	LYS
1	B	152	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	64	HIS
1	A	91	GLN
1	A	116	GLN
1	B	8	GLN
1	B	64	HIS
1	B	91	GLN
1	B	140	ASN

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

4 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	CMO	B	155	-	0,1,1	-	-	-		
2	HEM	B	154	1	50,50,50	2.04	23 (46%)	67,82,82	2.08	20 (29%)
2	HEM	A	154	1	50,50,50	1.53	12 (24%)	67,82,82	1.37	10 (14%)
3	CMO	A	155	-	0,1,1	-	-	-		

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
2	HEM	B	154	1	-	5/14/54/54	-
2	HEM	A	154	1	-	3/14/54/54	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	154	HEM	FE-ND	4.86	2.09	1.94
2	A	154	HEM	FE-ND	3.50	2.05	1.94
2	B	154	HEM	FE-NB	3.50	2.05	1.94
2	B	154	HEM	C1A-NA	3.41	1.46	1.39
2	B	154	HEM	FE-NA	-3.28	1.84	1.95
2	A	154	HEM	CAB-C3B	3.18	1.55	1.47
2	B	154	HEM	C3C-C4C	-3.03	1.40	1.46
2	B	154	HEM	CAC-C3C	3.02	1.55	1.47
2	B	154	HEM	C4D-ND	-2.98	1.35	1.40
2	B	154	HEM	CMA-C3A	2.91	1.56	1.50
2	B	154	HEM	CMB-C2B	2.79	1.56	1.50
2	B	154	HEM	C4B-NB	-2.68	1.33	1.38
2	B	154	HEM	C1B-NB	-2.67	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	154	HEM	CMB-C2B	2.66	1.56	1.50
2	B	154	HEM	CAB-C3B	2.66	1.54	1.47
2	A	154	HEM	CMC-C2C	2.64	1.56	1.50
2	B	154	HEM	CAA-C2A	2.54	1.57	1.51
2	A	154	HEM	CAC-C3C	2.49	1.54	1.47
2	B	154	HEM	C1D-ND	-2.41	1.34	1.38
2	B	154	HEM	C3B-C4B	2.40	1.49	1.44
2	A	154	HEM	CMA-C3A	2.37	1.55	1.50
2	A	154	HEM	FE-NA	2.31	2.02	1.95
2	B	154	HEM	CMD-C2D	2.30	1.55	1.50
2	B	154	HEM	C3B-C2B	-2.28	1.32	1.37
2	B	154	HEM	C2A-C3A	-2.26	1.33	1.38
2	A	154	HEM	C3B-C2B	-2.25	1.32	1.37
2	B	154	HEM	C1D-C2D	2.23	1.49	1.44
2	A	154	HEM	C4D-ND	-2.21	1.36	1.40
2	B	154	HEM	C3D-C2D	-2.18	1.32	1.36
2	B	154	HEM	C1A-C2A	-2.12	1.40	1.44
2	A	154	HEM	CMD-C2D	2.11	1.55	1.50
2	A	154	HEM	CAA-C2A	2.10	1.56	1.51
2	B	154	HEM	CAD-C3D	2.08	1.56	1.51
2	B	154	HEM	C4C-NC	2.05	1.43	1.39
2	A	154	HEM	C3C-C4C	-2.01	1.42	1.46

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	154	HEM	C1B-NB-C4B	5.27	111.45	105.21
2	B	154	HEM	CHC-C4B-NB	5.23	130.05	124.42
2	B	154	HEM	CHD-C1D-ND	5.08	129.89	124.42
2	B	154	HEM	C4D-ND-C1D	4.66	110.73	105.21
2	B	154	HEM	C3B-C4B-NB	-4.28	106.39	109.47
2	A	154	HEM	CHD-C1D-ND	4.17	128.91	124.42
2	B	154	HEM	CMA-C3A-C4A	-3.39	120.25	125.42
2	B	154	HEM	C4A-NA-C1A	-3.24	100.54	105.82
2	B	154	HEM	CMA-C3A-C2A	3.16	132.33	125.62
2	B	154	HEM	CMB-C2B-C1B	-3.12	120.15	125.03
2	B	154	HEM	CHB-C1B-NB	3.11	128.21	124.37
2	A	154	HEM	C3B-C2B-C1B	3.07	108.72	106.41
2	A	154	HEM	C4D-ND-C1D	2.89	108.63	105.21
2	A	154	HEM	CHB-C1B-NB	2.86	127.91	124.37
2	B	154	HEM	C3D-C4D-ND	-2.77	107.13	110.17
2	B	154	HEM	C4C-NC-C1C	-2.75	101.34	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	154	HEM	C2D-C1D-ND	-2.73	106.75	109.90
2	A	154	HEM	C1B-NB-C4B	2.66	108.36	105.21
2	B	154	HEM	C2B-C1B-NB	-2.59	106.86	109.84
2	A	154	HEM	C2B-C1B-NB	-2.53	106.93	109.84
2	B	154	HEM	CHA-C4D-ND	2.44	127.39	124.37
2	B	154	HEM	O1D-CGD-CBD	-2.44	115.34	123.09
2	B	154	HEM	CHA-C1A-NA	-2.32	119.66	123.86
2	B	154	HEM	C4A-CHB-C1B	-2.25	120.95	126.25
2	A	154	HEM	CHC-C4B-NB	2.25	126.84	124.42
2	A	154	HEM	C3D-C4D-ND	-2.18	107.78	110.17
2	B	154	HEM	CHB-C4A-C3A	-2.10	121.32	127.43
2	A	154	HEM	C2D-C1D-ND	-2.08	107.50	109.90
2	B	154	HEM	C4C-CHD-C1D	-2.04	121.68	126.02
2	A	154	HEM	C4C-C3C-C2C	2.04	108.58	106.81

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	154	HEM	C2A-CAA-CBA-CGA
2	A	154	HEM	CAA-CBA-CGA-O2A
2	B	154	HEM	CAA-CBA-CGA-O1A
2	B	154	HEM	CAD-CBD-CGD-O1D
2	B	154	HEM	CAD-CBD-CGD-O2D
2	B	154	HEM	CAA-CBA-CGA-O2A
2	A	154	HEM	CAA-CBA-CGA-O1A
2	A	154	HEM	CAD-CBD-CGD-O1D

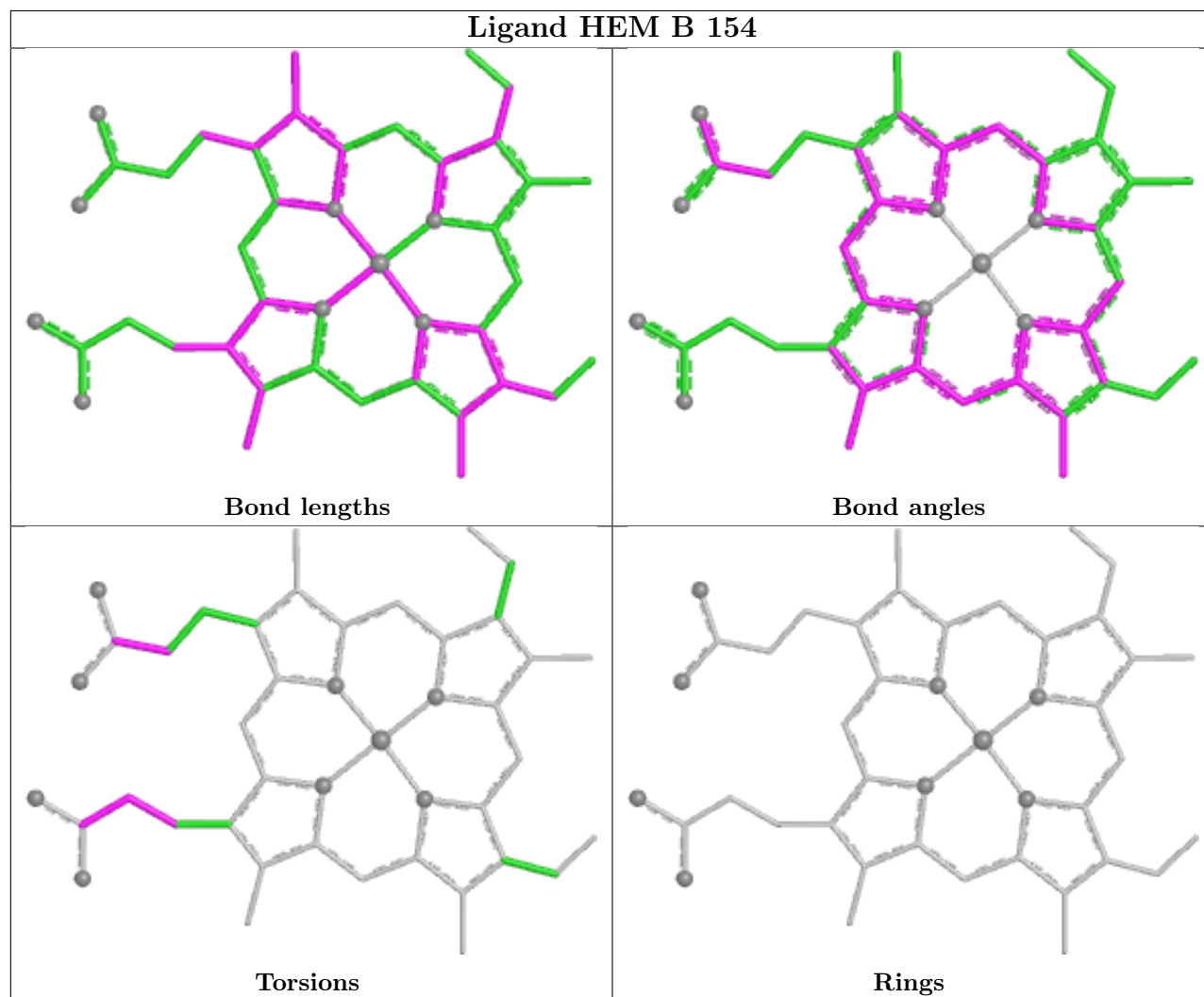
There are no ring outliers.

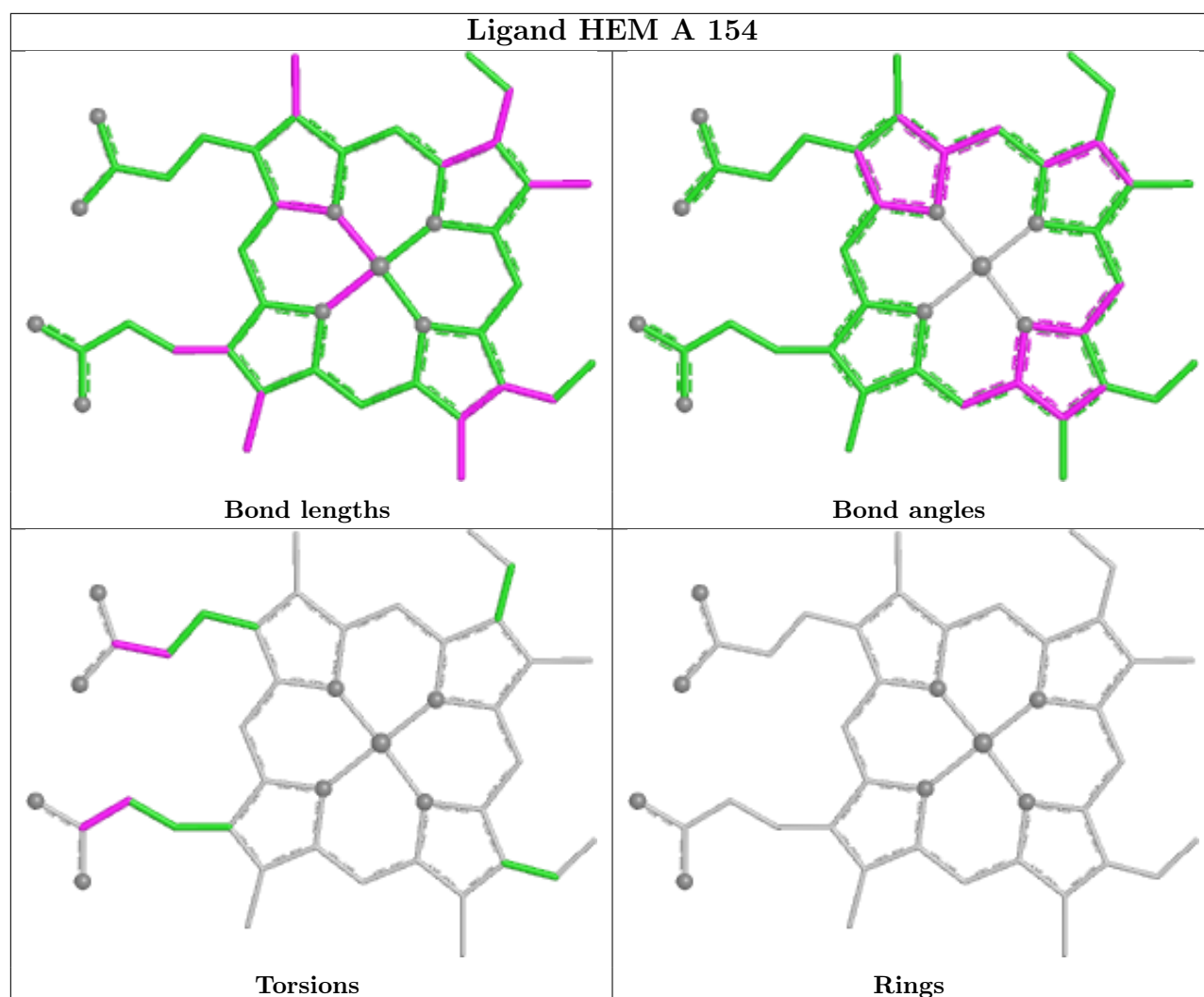
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	154	HEM	3	0
2	A	154	HEM	2	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	153/153 (100%)	0.42	12 (7%)	19 20	-1666, 26, 47, 60	13 (8%)
1	B	153/153 (100%)	0.49	13 (8%)	16 17	-4770, 24, 45, 88	14 (9%)
All	All	306/306 (100%)	0.46	25 (8%)	17 18	-4770, 25, 46, 88	27 (8%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	153	GLY	9.6
1	A	153	GLY	5.1
1	B	151	PHE	4.9
1	B	80[A]	GLY	4.3
1	A	151	PHE	4.3
1	A	152	GLN	4.3
1	A	80[A]	GLY	4.2
1	B	1	GLY	3.6
1	B	152	GLN	3.6
1	A	149	LEU	3.6
1	B	95	THR	3.5
1	B	121	GLY	3.4
1	A	48	HIS	3.2
1	B	94	ALA	3.1
1	A	44	ASP	2.9
1	A	121	GLY	2.7
1	A	47	LYS	2.7
1	A	101	VAL	2.6
1	B	96	LYS	2.6
1	A	1	GLY	2.5
1	A	150	GLY	2.4
1	B	45	LYS	2.3
1	B	98	LYS	2.2
1	B	81	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	34	LYS	2.1

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](#)

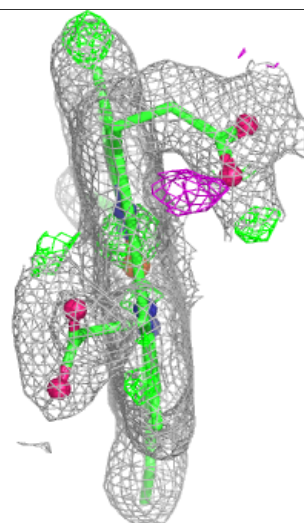
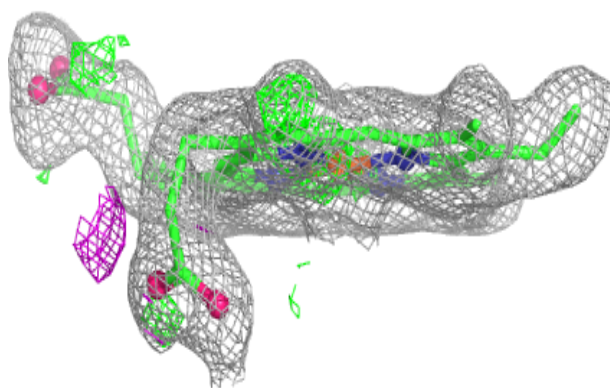
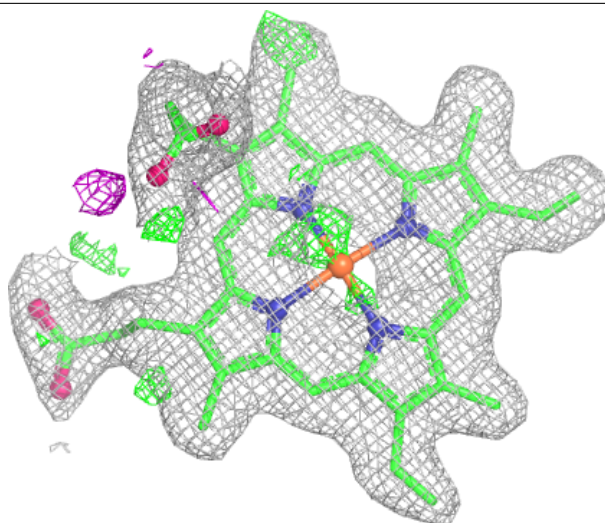
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CMO	B	155	2/2	0.94	0.10	22,22,22,24	0
3	CMO	A	155	2/2	0.95	0.09	21,21,21,25	0
2	HEM	B	154	43/43	0.97	0.08	14,22,35,38	0
2	HEM	A	154	43/43	0.98	0.07	13,23,30,38	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.

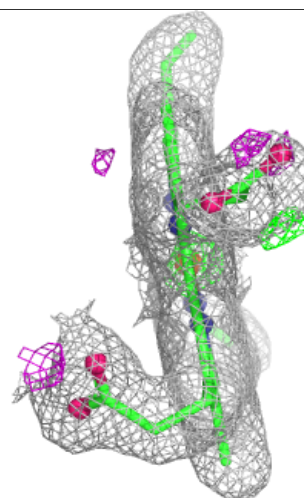
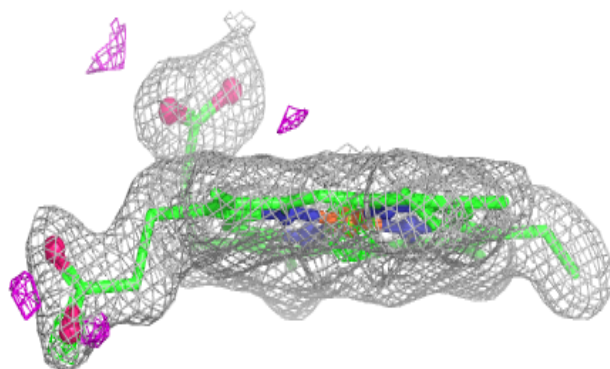
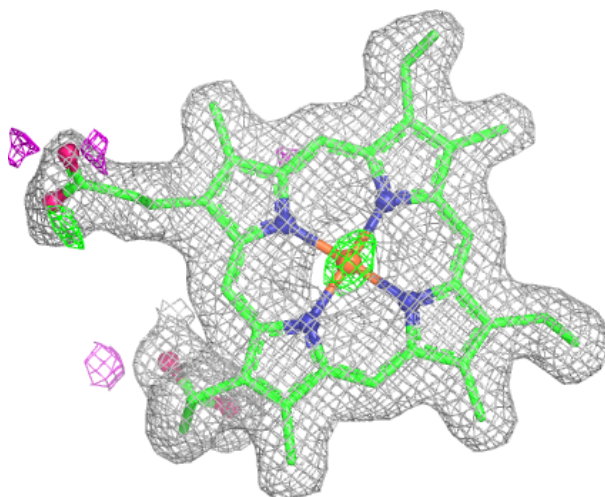
Electron density around HEM B 154:

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



Electron density around HEM A 154:

$2mF_o-DF_c$ (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.