Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 02:50 PM EDT

PDB ID	:	2GNW
Title	:	Crystal structure of non-symbiotic plant hemoglobin from rice, B10 mutant F40W
Authors	:	Hoy, J.A.
Deposited on	:	2006-04-11
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

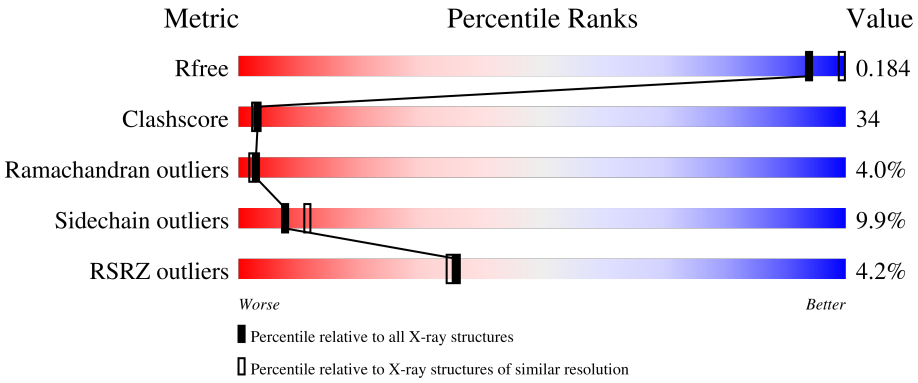
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	165	4% 32% 50% 15% ·
1	B	165	4% 35% 52% 11% ·

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2765 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.

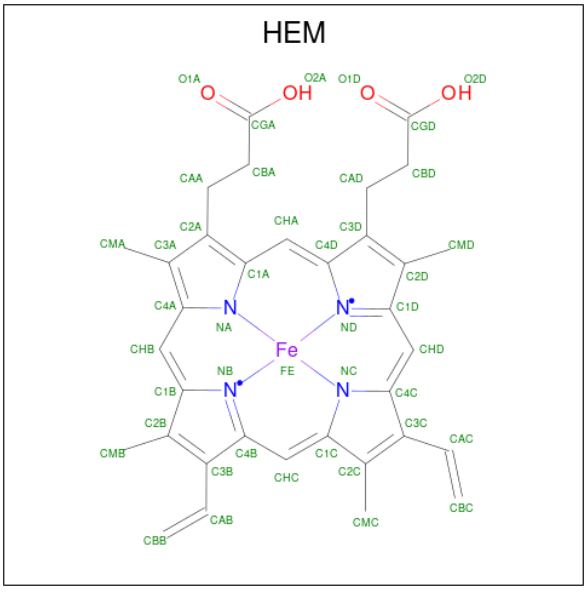
- Molecule 1 is a protein called Non-symbiotic hemoglobin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1291	829	217	238	7			
1	B	165	Total	C	N	O	S	0	0	0
			1291	829	217	238	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	TRP	PHE	engineered mutation	UNP O04986
B	40	TRP	PHE	engineered mutation	UNP O04986

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



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

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

- Molecule 3 is water.

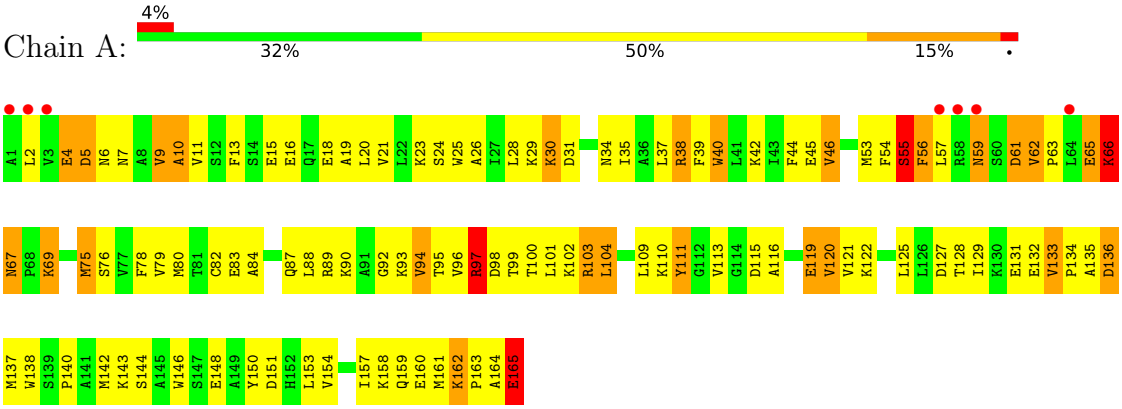
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		
3	B	47	Total	O	0	0
			47	47		

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.

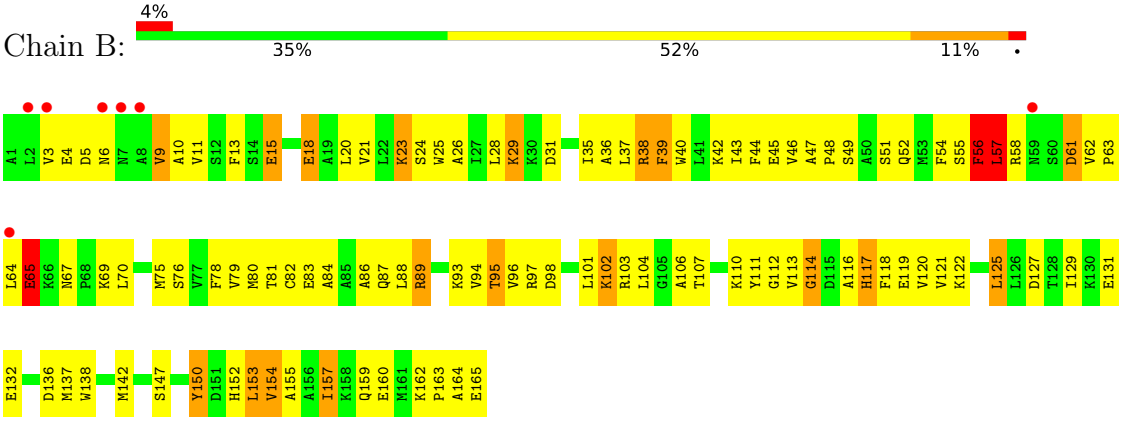
• Molecule 1: Non-symbiotic hemoglobin 1

Chain A:



• Molecule 1: Non-symbiotic hemoglobin 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	125.68Å 125.68Å 56.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40 36.28 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-2.40) 69.7 (36.28-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 1.84Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.174 , 0.204 0.175 , 0.184	Depositor DCC
R_{free} test set	1599 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	0.467 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2765	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	2.13	41/1318 (3.1%)	1.44	12/1781 (0.7%)
1	B	2.07	38/1318 (2.9%)	1.41	10/1781 (0.6%)
All	All	2.10	79/2636 (3.0%)	1.42	22/3562 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	165	GLU	CD-OE1	13.71	1.40	1.25
1	A	40	TRP	CB-CG	11.05	1.70	1.50
1	B	150	TYR	CD1-CE1	-10.15	1.24	1.39
1	A	165	GLU	CD-OE2	9.53	1.36	1.25
1	A	65	GLU	CD-OE2	9.17	1.35	1.25
1	A	165	GLU	CD-OE1	8.94	1.35	1.25
1	A	39	PHE	CE1-CZ	-8.47	1.21	1.37
1	A	53	MET	SD-CE	-8.03	1.32	1.77
1	A	39	PHE	CE2-CZ	-7.94	1.22	1.37
1	A	146	TRP	CB-CG	7.80	1.64	1.50
1	A	111	TYR	CE2-CZ	7.71	1.48	1.38
1	B	78	PHE	CD2-CE2	7.65	1.54	1.39
1	B	165	GLU	CD-OE2	7.52	1.33	1.25
1	A	21	VAL	C-O	-7.43	1.09	1.23
1	A	111	TYR	CZ-OH	7.33	1.50	1.37
1	A	69	LYS	CE-NZ	7.28	1.67	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	GLU	CG-CD	7.21	1.62	1.51
1	B	45	GLU	CG-CD	-7.18	1.41	1.51
1	A	82	CYS	CB-SG	-7.03	1.70	1.82
1	B	45	GLU	CD-OE1	-6.96	1.18	1.25
1	A	66	LYS	C-O	6.90	1.36	1.23
1	A	21	VAL	CB-CG1	-6.80	1.38	1.52
1	B	47	ALA	CA-CB	-6.75	1.38	1.52
1	A	121	VAL	CB-CG1	-6.69	1.38	1.52
1	B	138	TRP	CB-CG	6.66	1.62	1.50
1	B	165	GLU	CG-CD	6.46	1.61	1.51
1	B	147	SER	CA-C	-6.46	1.36	1.52
1	B	39	PHE	CE1-CZ	-6.43	1.25	1.37
1	A	56	PHE	CB-CG	6.27	1.62	1.51
1	B	113	VAL	CB-CG2	-6.27	1.39	1.52
1	B	82	CYS	CB-SG	-6.18	1.71	1.82
1	B	43	ILE	C-O	-6.11	1.11	1.23
1	A	13	PHE	CD1-CE1	-5.96	1.27	1.39
1	A	94	VAL	CB-CG1	5.87	1.65	1.52
1	A	13	PHE	CG-CD2	5.85	1.47	1.38
1	A	59	ASN	CB-CG	5.85	1.64	1.51
1	A	119	GLU	CG-CD	-5.78	1.43	1.51
1	B	51	SER	CB-OG	5.76	1.49	1.42
1	A	46	VAL	CB-CG1	-5.74	1.40	1.52
1	A	4	GLU	CD-OE2	5.73	1.31	1.25
1	B	38	ARG	NE-CZ	5.71	1.40	1.33
1	A	44	PHE	CE1-CZ	5.68	1.48	1.37
1	B	119	GLU	CD-OE2	-5.62	1.19	1.25
1	B	56	PHE	CB-CG	5.61	1.60	1.51
1	B	13	PHE	CG-CD1	-5.61	1.30	1.38
1	B	102	LYS	CD-CE	5.59	1.65	1.51
1	B	21	VAL	CB-CG2	-5.58	1.41	1.52
1	B	6	ASN	CB-CG	5.56	1.63	1.51
1	A	39	PHE	CD1-CE1	-5.52	1.28	1.39
1	A	4	GLU	CB-CG	5.49	1.62	1.52
1	A	5	ASP	CB-CG	5.48	1.63	1.51
1	B	18	GLU	CD-OE1	-5.46	1.19	1.25
1	A	13	PHE	CD2-CE2	-5.44	1.28	1.39
1	A	127	ASP	N-CA	5.41	1.57	1.46
1	B	117	HIS	C-O	-5.32	1.13	1.23
1	A	56	PHE	N-CA	5.32	1.56	1.46
1	B	154	VAL	CB-CG1	-5.32	1.41	1.52
1	B	153	LEU	CG-CD1	-5.27	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	PRO	C-O	5.23	1.33	1.23
1	B	111	TYR	CE1-CZ	-5.23	1.31	1.38
1	A	23	LYS	CE-NZ	-5.22	1.35	1.49
1	A	121	VAL	C-O	-5.22	1.13	1.23
1	B	65	GLU	CD-OE2	5.21	1.31	1.25
1	B	150	TYR	CG-CD1	-5.21	1.32	1.39
1	B	114	GLY	C-O	-5.17	1.15	1.23
1	B	153	LEU	C-O	-5.16	1.13	1.23
1	B	9	VAL	CB-CG2	5.15	1.63	1.52
1	B	42	LYS	CB-CG	5.15	1.66	1.52
1	B	13	PHE	C-O	-5.09	1.13	1.23
1	B	15	GLU	CG-CD	5.09	1.59	1.51
1	B	15	GLU	CD-OE2	5.08	1.31	1.25
1	A	62	VAL	CA-CB	5.07	1.65	1.54
1	A	122	LYS	C-O	-5.07	1.13	1.23
1	B	88	LEU	CG-CD2	-5.05	1.33	1.51
1	A	120	VAL	CA-CB	-5.05	1.44	1.54
1	A	61	ASP	CB-CG	5.04	1.62	1.51
1	A	19	ALA	CA-CB	5.03	1.63	1.52
1	A	26	ALA	CA-CB	5.02	1.62	1.52
1	B	55	SER	CA-CB	5.01	1.60	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	97	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	A	97	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	B	38	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	127	ASP	CB-CG-OD2	6.97	124.57	118.30
1	B	57	LEU	CA-CB-CG	6.64	130.57	115.30
1	B	136	ASP	CB-CG-OD2	6.56	124.20	118.30
1	A	5	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	136	ASP	CB-CG-OD2	6.37	124.04	118.30
1	B	160	GLU	OE1-CD-OE2	-6.36	115.67	123.30
1	B	31	ASP	CB-CG-OD2	6.25	123.93	118.30
1	B	61	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	75	MET	CG-SD-CE	5.83	109.53	100.20
1	A	30	LYS	CD-CE-NZ	-5.62	98.77	111.70
1	A	57	LEU	CA-CB-CG	5.47	127.89	115.30
1	B	18	GLU	OE1-CD-OE2	-5.39	116.83	123.30
1	A	151	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	57	LEU	CB-CG-CD1	5.34	120.08	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	104	LEU	CB-CG-CD2	5.31	120.03	111.00
1	B	136	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	A	75	MET	CG-SD-CE	-5.17	91.93	100.20
1	A	136	ASP	OD1-CG-OD2	-5.08	113.66	123.30
1	A	153	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	55	SER	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1291	0	1313	96	3
1	B	1291	0	1313	84	1
2	A	43	0	30	1	0
2	B	43	0	30	3	0
3	A	50	0	0	10	3
3	B	47	0	0	14	2
All	All	2765	0	2686	180	5

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 34.

All (180) 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:29:LYS:HA	1:B:29:LYS:NZ	1.57	1.19
1:A:78:PHE:CE1	1:A:129:ILE:HD11	1.91	1.04
1:A:78:PHE:HE1	1:A:129:ILE:HD11	1.16	1.03
1:A:9:VAL:O	1:A:11:VAL:HG23	1.56	1.03
1:A:10:ALA:HB2	3:A:192:HOH:O	1.62	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:LEU:O	1:B:157:ILE:HD13	1.65	0.95
1:B:29:LYS:HA	1:B:29:LYS:HZ2	1.18	0.92
1:A:28:LEU:HD22	1:A:35:ILE:CD1	2.00	0.91
1:A:25:TRP:O	1:A:29:LYS:HG3	1.70	0.91
1:A:11:VAL:HG11	1:A:88:LEU:HD22	1.55	0.87
1:B:29:LYS:HZ2	1:B:29:LYS:CA	1.90	0.84
1:A:5:ASP:OD2	1:A:9:VAL:HG13	1.77	0.84
1:B:103:ARG:O	1:B:103:ARG:NH1	2.11	0.83
1:A:28:LEU:HD11	1:A:129:ILE:HD12	1.61	0.82
1:B:29:LYS:NZ	1:B:29:LYS:CA	2.43	0.82
1:A:10:ALA:CB	3:A:192:HOH:O	2.22	0.81
1:A:144:SER:O	1:A:148:GLU:HG2	1.80	0.80
1:B:96:VAL:HB	1:B:101:LEU:HG	1.63	0.80
1:A:35:ILE:HD12	1:A:132:GLU:HG3	1.64	0.78
1:B:29:LYS:HA	1:B:29:LYS:HZ1	1.47	0.78
1:A:11:VAL:HG11	1:A:88:LEU:CD2	2.15	0.77
1:B:38:ARG:NE	1:B:132:GLU:OE1	2.18	0.76
1:A:2:LEU:HD22	3:A:199:HOH:O	1.85	0.76
1:B:76:SER:O	1:B:80:MET:HB2	1.85	0.76
1:A:103:ARG:HH11	1:A:103:ARG:HB3	1.51	0.76
1:B:127:ASP:OD1	3:B:186:HOH:O	2.05	0.74
1:A:11:VAL:CG1	1:A:88:LEU:HD22	2.17	0.73
1:A:31:ASP:O	1:A:35:ILE:HG22	1.88	0.72
1:A:76:SER:O	1:A:80:MET:HB2	1.90	0.72
1:B:103:ARG:O	1:B:103:ARG:CZ	2.39	0.71
1:A:18:GLU:OE2	1:A:89:ARG:HG2	1.91	0.70
1:B:103:ARG:NH2	1:B:106:ALA:HB3	2.07	0.69
1:A:28:LEU:HD22	1:A:35:ILE:HD11	1.74	0.69
1:A:28:LEU:HD22	1:A:35:ILE:HD12	1.74	0.69
1:B:54:PHE:HB3	1:B:69:LYS:HZ3	1.58	0.69
1:A:59:ASN:HA	3:A:190:HOH:O	1.94	0.68
1:B:37:LEU:HD11	1:B:64:LEU:HD11	1.76	0.67
1:A:29:LYS:NZ	1:A:29:LYS:HB3	2.10	0.66
1:B:110:LYS:HE3	3:B:175:HOH:O	1.95	0.66
1:B:23:LYS:HB3	3:B:213:HOH:O	1.94	0.66
1:A:93:LYS:HE3	1:A:95:THR:HG22	1.75	0.66
1:A:83:GLU:O	1:A:87:GLN:HG3	1.96	0.66
1:A:67:ASN:N	1:A:67:ASN:HD22	1.94	0.65
1:B:96:VAL:HG22	3:B:184:HOH:O	1.97	0.65
1:A:116:ALA:O	1:A:120:VAL:HG23	1.97	0.63
1:B:120:VAL:HG12	1:B:120:VAL:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ASP:HB2	1:B:155:ALA:HB1	1.80	0.62
1:A:35:ILE:CD1	1:A:132:GLU:HG3	2.30	0.62
1:A:28:LEU:HD11	1:A:129:ILE:CD1	2.30	0.61
1:A:2:LEU:HD12	1:A:5:ASP:H	1.65	0.61
1:A:42:LYS:O	1:A:46:VAL:HG23	2.01	0.61
1:B:103:ARG:HH22	1:B:106:ALA:HB3	1.65	0.60
1:A:164:ALA:O	1:A:165:GLU:C	2.40	0.60
1:A:29:LYS:HE2	3:A:185:HOH:O	2.02	0.59
1:B:94:VAL:HG23	1:B:152:HIS:HB3	1.84	0.59
1:A:2:LEU:HD13	1:A:5:ASP:HB2	1.84	0.59
1:B:96:VAL:HB	1:B:101:LEU:CG	2.32	0.59
1:A:133:VAL:HB	1:A:137:MET:HE2	1.85	0.59
1:A:101:LEU:CD2	1:A:157:ILE:HD13	2.33	0.59
1:B:131:GLU:HG3	3:B:171:HOH:O	2.03	0.58
1:A:5:ASP:OD2	1:A:9:VAL:HG22	2.03	0.58
1:B:157:ILE:N	1:B:157:ILE:CD1	2.67	0.57
1:B:15:GLU:HG3	1:B:89:ARG:CZ	2.36	0.56
1:B:103:ARG:NH1	1:B:107:THR:OG1	2.38	0.56
1:B:35:ILE:HD12	1:B:36:ALA:N	2.22	0.55
1:B:137:MET:O	3:B:194:HOH:O	2.18	0.55
1:B:57:LEU:HB3	1:B:65:GLU:HB2	1.89	0.55
1:A:29:LYS:HB3	1:A:29:LYS:HZ2	1.70	0.55
1:B:121:VAL:HG21	2:B:166:HEM:CMC	2.37	0.55
1:A:104:LEU:HD12	1:A:157:ILE:CD1	2.37	0.55
1:A:110:LYS:NZ	1:A:111:TYR:HE1	2.05	0.55
1:B:44:PHE:O	1:B:48:PRO:HG3	2.08	0.54
1:B:94:VAL:CG2	1:B:152:HIS:HB3	2.37	0.54
1:A:101:LEU:HD23	1:A:157:ILE:HD13	1.90	0.54
1:A:110:LYS:NZ	1:A:111:TYR:CE1	2.76	0.53
1:B:157:ILE:N	1:B:157:ILE:HD12	2.24	0.53
1:B:54:PHE:HB3	1:B:69:LYS:NZ	2.22	0.53
1:A:61:ASP:HB3	1:A:66:LYS:HB3	1.89	0.53
1:B:3:VAL:HG12	1:B:4:GLU:N	2.24	0.53
1:B:103:ARG:NE	1:B:103:ARG:HA	2.24	0.53
1:A:24:SER:HB3	1:A:142:MET:HE1	1.90	0.53
1:B:125:LEU:O	1:B:129:ILE:HG13	2.09	0.53
1:A:30:LYS:NZ	3:A:189:HOH:O	2.41	0.52
1:A:67:ASN:HD22	1:A:67:ASN:H	1.57	0.52
1:A:84:ALA:O	1:A:88:LEU:HG	2.10	0.52
1:A:134:PRO:HB2	1:A:136:ASP:OD2	2.09	0.51
1:A:154:VAL:O	1:A:158:LYS:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:PHE:CZ	1:A:62:VAL:HG13	2.46	0.51
1:A:110:LYS:HZ2	1:A:110:LYS:HB3	1.76	0.50
1:B:9:VAL:O	1:B:11:VAL:HG23	2.11	0.50
1:A:101:LEU:HD23	1:A:157:ILE:CD1	2.41	0.50
1:B:23:LYS:O	1:B:26:ALA:HB3	2.12	0.50
1:B:40:TRP:CH2	1:B:65:GLU:HB3	2.47	0.50
1:B:112:GLY:HA2	3:B:211:HOH:O	2.11	0.50
1:B:116:ALA:O	1:B:120:VAL:HG23	2.12	0.50
1:B:132:GLU:OE2	1:B:132:GLU:HA	2.12	0.49
1:B:89:ARG:HD2	3:B:181:HOH:O	2.11	0.49
1:A:15:GLU:O	1:A:15:GLU:HG2	2.11	0.49
1:A:150:TYR:CE2	1:A:154:VAL:HG21	2.48	0.49
1:A:104:LEU:HD12	1:A:157:ILE:HD11	1.94	0.48
1:B:24:SER:O	1:B:28:LEU:HD13	2.14	0.48
1:A:38:ARG:HD3	1:A:128:THR:HG23	1.94	0.48
1:A:103:ARG:HB3	1:A:103:ARG:NH1	2.26	0.48
1:A:140:PRO:O	1:A:143:LYS:HB3	2.14	0.48
1:B:26:ALA:HA	1:B:29:LYS:HG3	1.95	0.48
1:B:39:PHE:HE1	1:B:125:LEU:HA	1.79	0.47
1:A:94:VAL:HG13	1:A:96:VAL:HG23	1.95	0.47
1:A:38:ARG:CD	1:A:132:GLU:OE1	2.62	0.47
1:B:18:GLU:OE1	1:B:89:ARG:NE	2.47	0.47
1:A:15:GLU:HA	1:A:89:ARG:HD3	1.96	0.47
1:A:38:ARG:NH2	1:A:131:GLU:HG2	2.31	0.46
1:A:125:LEU:O	1:A:129:ILE:HG12	2.14	0.46
1:B:155:ALA:O	1:B:159:GLN:HG3	2.14	0.46
1:A:11:VAL:HB	1:A:92:GLY:O	2.15	0.46
1:B:11:VAL:HG13	3:B:206:HOH:O	2.13	0.46
1:B:20:LEU:HB3	1:B:142:MET:HG3	1.98	0.46
1:B:162:LYS:HE2	3:B:204:HOH:O	2.14	0.46
1:A:134:PRO:O	1:A:136:ASP:N	2.49	0.46
1:B:64:LEU:O	1:B:65:GLU:HB3	2.14	0.46
1:A:5:ASP:OD2	1:A:9:VAL:CG1	2.57	0.46
1:A:115:ASP:O	1:A:119:GLU:HG3	2.15	0.46
1:B:38:ARG:HH21	1:B:132:GLU:CD	2.18	0.46
1:A:103:ARG:HH11	1:A:103:ARG:CB	2.25	0.46
1:B:106:ALA:O	1:B:110:LYS:HB2	2.16	0.46
1:A:2:LEU:CD1	1:A:5:ASP:HB2	2.46	0.45
1:A:28:LEU:CD1	1:A:129:ILE:HD12	2.41	0.45
1:A:67:ASN:N	1:A:67:ASN:ND2	2.61	0.45
1:B:54:PHE:CD2	1:B:70:LEU:HD23	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LYS:HB2	1:B:150:TYR:CE2	2.52	0.45
1:A:67:ASN:H	1:A:67:ASN:ND2	2.15	0.45
1:B:49:SER:HA	1:B:52:GLN:HG3	1.98	0.45
1:B:83:GLU:O	1:B:87:GLN:HG3	2.17	0.45
1:B:157:ILE:CD1	1:B:157:ILE:H	2.28	0.45
1:B:29:LYS:CA	1:B:29:LYS:CE	2.94	0.45
1:A:134:PRO:O	1:A:137:MET:N	2.50	0.45
1:A:96:VAL:O	1:A:97:ARG:C	2.52	0.45
1:B:15:GLU:HG3	1:B:89:ARG:NH1	2.32	0.45
1:A:38:ARG:HD2	1:A:132:GLU:OE1	2.17	0.44
1:A:100:THR:O	1:A:104:LEU:HG	2.17	0.44
1:A:113:VAL:HG13	2:A:166:HEM:HAC	1.99	0.44
1:A:101:LEU:HD22	1:A:157:ILE:HD13	1.98	0.44
1:A:90:LYS:HB2	3:A:186:HOH:O	2.18	0.44
1:B:114:GLY:N	1:B:117:HIS:ND1	2.62	0.44
1:A:54:PHE:HA	1:A:69:LYS:NZ	2.33	0.44
1:B:96:VAL:HB	1:B:101:LEU:CD1	2.48	0.44
1:A:79:VAL:O	1:A:83:GLU:HG3	2.17	0.44
1:B:121:VAL:HG21	2:B:166:HEM:HMC2	2.00	0.43
1:B:79:VAL:O	1:B:83:GLU:HG3	2.18	0.43
1:B:154:VAL:HG22	2:B:166:HEM:HBB1	2.00	0.43
1:B:118:PHE:HB2	3:B:172:HOH:O	2.19	0.43
1:B:46:VAL:HG11	1:B:120:VAL:HG13	2.01	0.43
1:B:131:GLU:OE2	3:B:171:HOH:O	2.21	0.43
1:A:104:LEU:CD1	1:A:157:ILE:CD1	2.96	0.43
1:A:104:LEU:CD1	1:A:157:ILE:HD12	2.48	0.43
1:B:20:LEU:HD22	3:B:194:HOH:O	2.18	0.43
1:A:104:LEU:CB	1:A:157:ILE:HD12	2.49	0.42
1:B:35:ILE:HD12	1:B:35:ILE:C	2.40	0.42
1:B:3:VAL:HG12	1:B:4:GLU:H	1.84	0.42
1:B:101:LEU:HD23	1:B:104:LEU:HD12	2.00	0.42
1:A:110:LYS:NZ	1:A:110:LYS:HB3	2.34	0.42
1:A:138:TRP:CZ2	1:A:143:LYS:HB2	2.55	0.42
1:B:81:THR:O	1:B:84:ALA:HB3	2.19	0.42
1:B:93:LYS:HE3	1:B:95:THR:CG2	2.49	0.42
1:B:101:LEU:HD22	1:B:157:ILE:HD12	2.01	0.42
1:A:115:ASP:OD1	3:A:177:HOH:O	2.22	0.41
1:B:150:TYR:O	1:B:154:VAL:HG23	2.20	0.41
1:A:15:GLU:O	1:A:15:GLU:CG	2.68	0.41
1:B:98:ASP:O	1:B:102:LYS:HB2	2.19	0.41
1:A:98:ASP:OD2	1:A:98:ASP:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:O	1:A:142:MET:HE1	2.20	0.41
1:A:131:GLU:OE1	3:A:206:HOH:O	2.22	0.41
1:A:159:GLN:O	1:A:162:LYS:NZ	2.48	0.41
1:A:102:LYS:HG2	1:A:160:GLU:OE2	2.20	0.41
1:B:67:ASN:HD21	1:B:69:LYS:HG3	1.85	0.41
1:A:6:ASN:HD22	1:A:7:ASN:H	1.69	0.40
1:A:65:GLU:HA	3:A:178:HOH:O	2.20	0.40
1:B:38:ARG:NH2	1:B:132:GLU:OE1	2.53	0.40
1:B:97:ARG:NH1	3:B:182:HOH:O	2.54	0.40
1:A:109:LEU:N	1:A:161:MET:HE3	2.36	0.40
1:B:18:GLU:OE2	1:B:86:ALA:HA	2.21	0.40

All (5) 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)
3:A:202:HOH:O	3:A:203:HOH:O[3_564]	1.92	0.28
1:A:61:ASP:OD1	3:B:177:HOH:O[2_665]	2.03	0.17
1:A:89:ARG:NH1	3:B:176:HOH:O[2_664]	2.05	0.15
1:A:111:TYR:OH	3:A:171:HOH:O[4_555]	2.14	0.06
1:B:64:LEU:CD1	3:A:185:HOH:O[3_564]	2.18	0.02

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	163/165 (99%)	145 (89%)	12 (7%)	6 (4%)	3	2
1	B	163/165 (99%)	145 (89%)	11 (7%)	7 (4%)	2	2
All	All	326/330 (99%)	290 (89%)	23 (7%)	13 (4%)	3	2

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ALA
1	B	56	PHE
1	B	61	ASP
1	B	164	ALA
1	A	4	GLU
1	A	135	ALA
1	B	163	PRO
1	B	65	GLU
1	A	55	SER
1	A	163	PRO
1	B	10	ALA
1	B	63	PRO
1	A	9	VAL

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	137/137 (100%)	121 (88%)	16 (12%)	5 7
1	B	137/137 (100%)	126 (92%)	11 (8%)	12 18
All	All	274/274 (100%)	247 (90%)	27 (10%)	8 11

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	34	ASN
1	A	37	LEU
1	A	38	ARG
1	A	40	TRP
1	A	45	GLU
1	A	55	SER
1	A	66	LYS
1	A	67	ASN
1	A	75	MET
1	A	97	ARG

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Mol	Chain	Res	Type
1	A	99	THR
1	A	103	ARG
1	A	133	VAL
1	A	162	LYS
1	A	165	GLU
1	B	23	LYS
1	B	25	TRP
1	B	29	LYS
1	B	56	PHE
1	B	57	LEU
1	B	58	ARG
1	B	62	VAL
1	B	89	ARG
1	B	95	THR
1	B	125	LEU
1	B	157	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	34	ASN
1	A	52	GLN
1	A	67	ASN
1	B	7	ASN
1	B	159	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	166	1	27,50,50	1.49	5 (18%)	17,82,82	2.87	10 (58%)
2	HEM	B	166	1	27,50,50	1.65	6 (22%)	17,82,82	2.42	6 (35%)

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	A	166	1	-	0/6/54/54	-
2	HEM	B	166	1	-	3/6/54/54	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	166	HEM	C3B-C2B	-3.45	1.35	1.40
2	B	166	HEM	CBC-CAC	3.04	1.49	1.29
2	A	166	HEM	C3B-C2B	-2.92	1.36	1.40
2	B	166	HEM	C1D-ND	-2.88	1.30	1.36
2	A	166	HEM	CBB-CAB	2.75	1.47	1.29
2	A	166	HEM	CAD-C3D	2.67	1.56	1.52
2	B	166	HEM	C3B-CAB	-2.67	1.42	1.47
2	B	166	HEM	CAA-C2A	2.61	1.55	1.52
2	B	166	HEM	CBB-CAB	2.58	1.46	1.29
2	A	166	HEM	C1B-C2B	2.16	1.47	1.42
2	A	166	HEM	CMA-C3A	2.08	1.56	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	166	HEM	CBA-CAA-C2A	6.92	125.25	112.49
2	A	166	HEM	CBA-CAA-C2A	6.72	124.87	112.49
2	A	166	HEM	CMA-C3A-C4A	-4.96	120.83	128.46
2	A	166	HEM	CMC-C2C-C3C	4.15	132.44	124.68
2	A	166	HEM	C4A-C3A-C2A	3.35	109.33	107.00
2	B	166	HEM	CAA-CBA-CGA	3.04	117.76	112.67
2	A	166	HEM	CBD-CAD-C3D	2.97	117.96	112.48
2	A	166	HEM	CAD-C3D-C2D	2.83	135.37	127.25
2	B	166	HEM	CAD-CBD-CGD	2.79	117.35	112.67
2	B	166	HEM	C1D-C2D-C3D	2.73	108.89	107.00
2	B	166	HEM	CMA-C3A-C4A	-2.70	124.31	128.46
2	A	166	HEM	CMA-C3A-C2A	2.59	129.82	124.94
2	B	166	HEM	CMD-C2D-C3D	-2.47	120.29	124.94
2	A	166	HEM	C3B-C4B-NB	2.46	112.39	109.21
2	A	166	HEM	CMB-C2B-C3B	-2.07	120.80	124.68
2	A	166	HEM	C3C-C4C-NC	-2.05	107.07	110.94

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	166	HEM	C1A-C2A-CAA-CBA
2	B	166	HEM	C3A-C2A-CAA-CBA
2	B	166	HEM	C2A-CAA-CBA-CGA

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	166	HEM	1	0
2	B	166	HEM	3	0

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

equivalents in the CSD to analyse the geometry.

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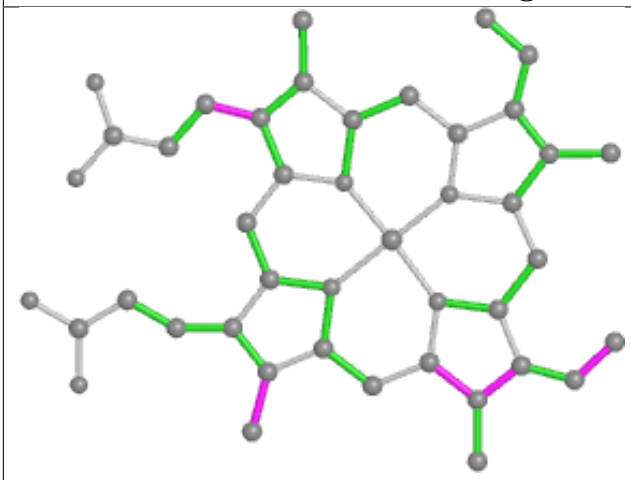
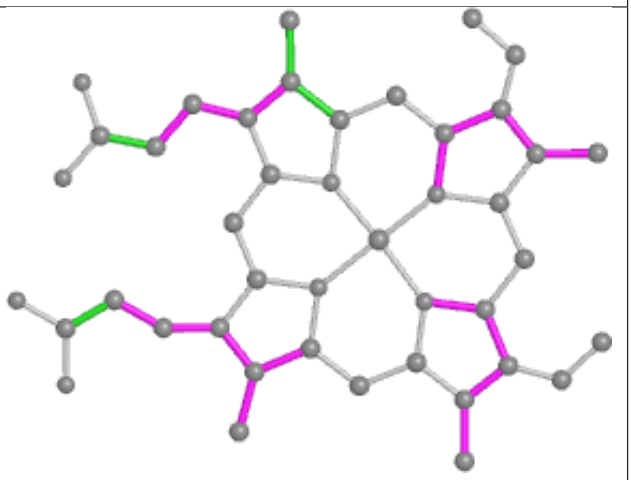
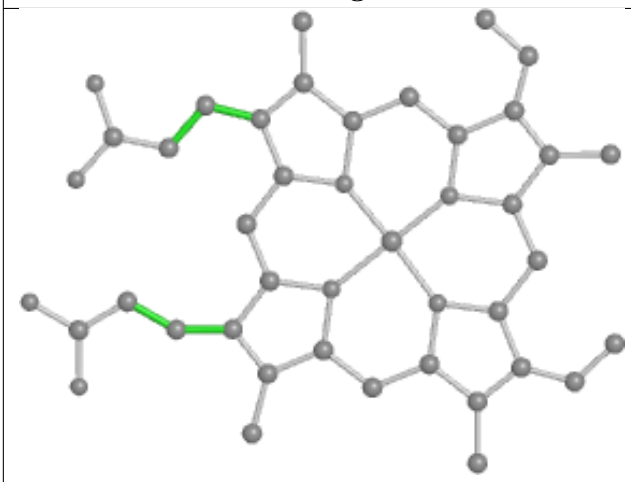


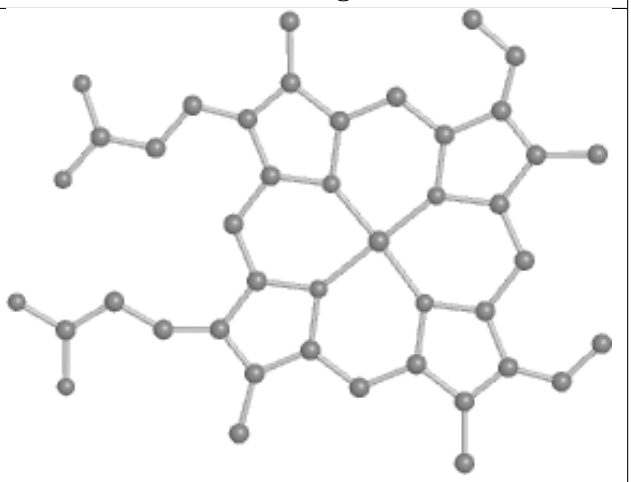
Bond lengths



Bond angles

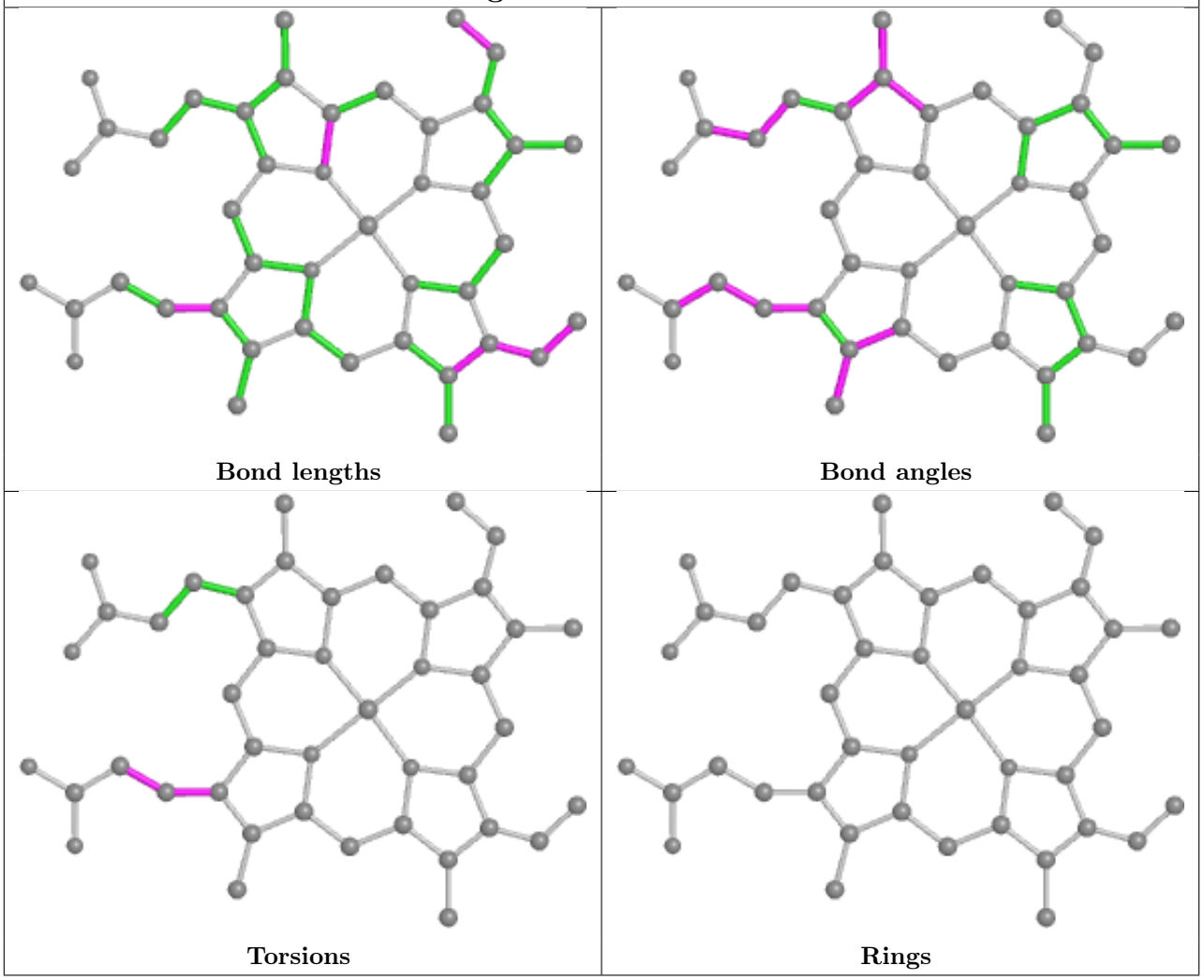


Torsions



Rings

Ligand HEM B 166



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	165/165 (100%)	-0.68	7 (4%)	36	35	28, 40, 101, 107	0
1	B	165/165 (100%)	-0.60	7 (4%)	36	35	25, 43, 105, 110	0
All	All	330/330 (100%)	-0.64	14 (4%)	36	35	25, 42, 103, 110	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	ASN	4.6
1	B	8	ALA	4.0
1	A	2	LEU	3.6
1	B	6	ASN	3.6
1	A	1	ALA	3.4
1	B	64	LEU	3.3
1	A	57	LEU	2.7
1	A	3	VAL	2.6
1	B	2	LEU	2.6
1	B	3	VAL	2.5
1	A	59	ASN	2.2
1	A	64	LEU	2.2
1	A	58	ARG	2.2
1	B	59	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

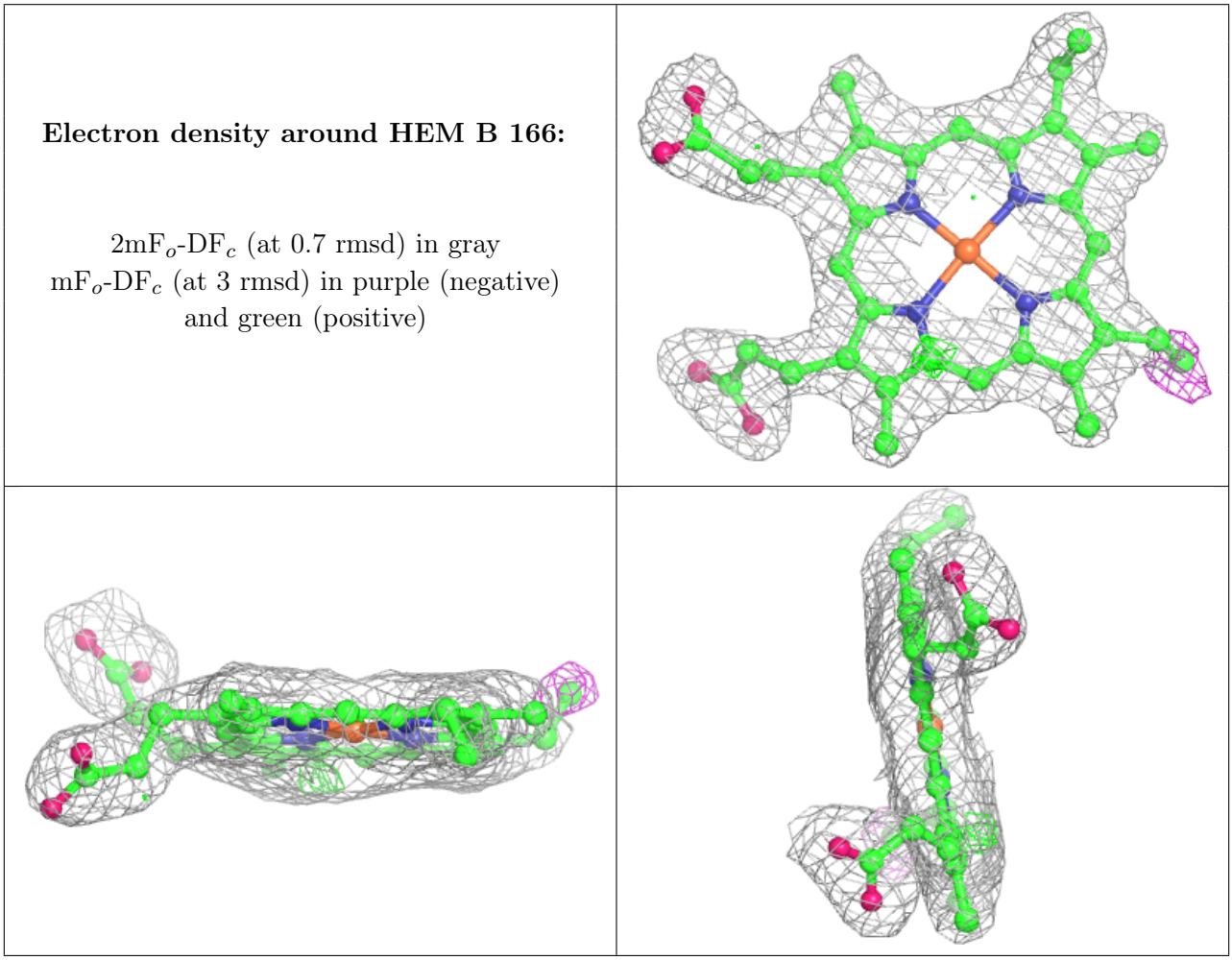
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	B	166	43/43	0.97	0.12	41,49,63,68	0
2	HEM	A	166	43/43	0.98	0.12	24,38,49,50	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.

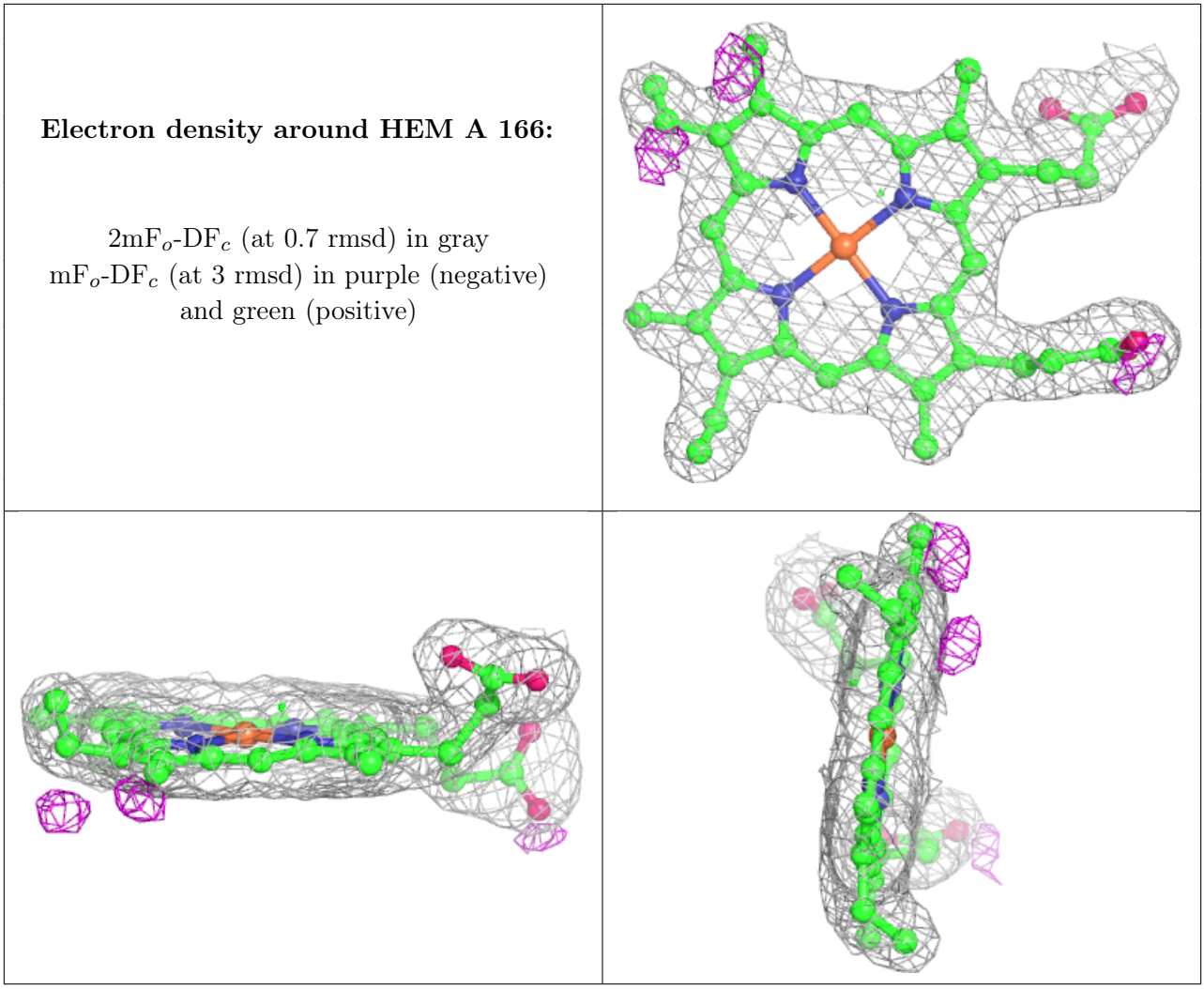
Electron density around HEM B 166:

$2mF_o$-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 166:

$2mF_o$-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.