



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:16 AM UTC

PDB ID : 3C2C / pdb_00003c2c
Title : REFINEMENT OF THE CRYSTAL STRUCTURE OF OXIDIZED RHO-
DOSPIRILLUM RUBRUM CYTOCHROME C2
Authors : Bhatia, G.; Finzel, B.C.; Kraut, J.
Deposited on : 1983-11-03
Resolution : 1.68 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

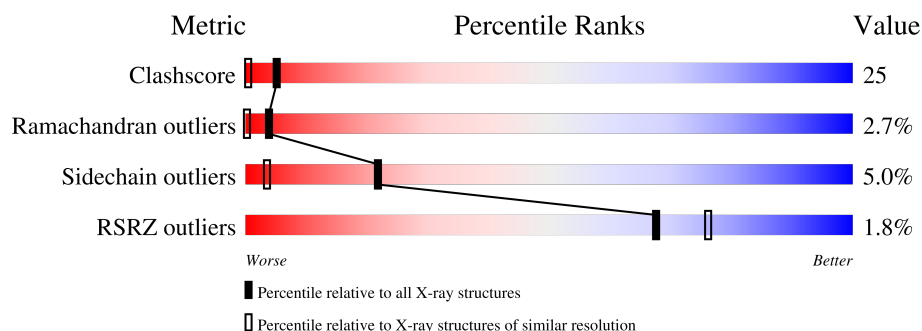
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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))
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	112	2% 7% 56% 29% 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 962 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.

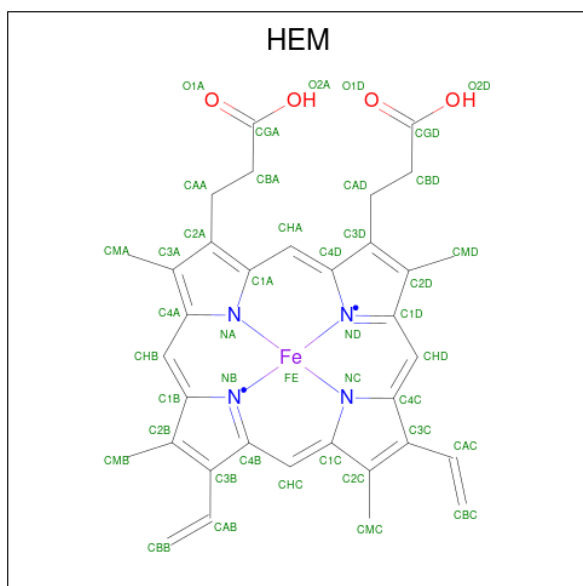
- Molecule 1 is a protein called CYTOCHROME C2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	112	832	529	137	162	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	ASN	ASP	conflict	UNP P00092
A	73	ASN	ASP	conflict	UNP P00092

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



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

- Molecule 3 is water.

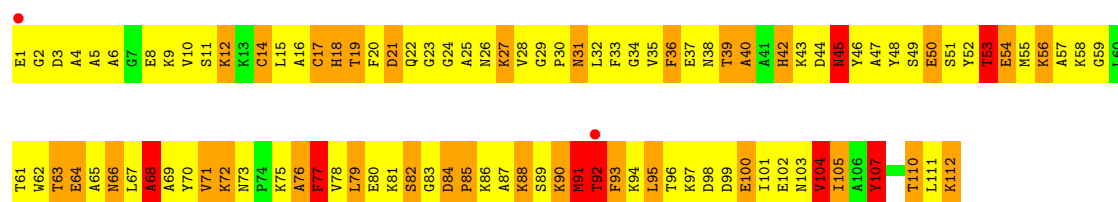
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	87	Total	O	0	0
			87	87		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: CYTOCHROME C2

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	32.22Å 37.36Å 84.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.68 42.31 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.68) 61.4 (42.31-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.175 , (Not available) 0.167 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.5	EDS
L-test for twinning ¹	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	962	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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: 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	3.34	109/848 (12.9%)	4.03	218/1144 (19.1%)

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	3	16

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	THR	C-O	17.35	1.45	1.24
1	A	21	ASP	CG-OD1	14.76	1.53	1.25
1	A	63	THR	CA-CB	14.46	1.75	1.53
1	A	105	ILE	CA-CB	12.69	1.70	1.54
1	A	63	THR	CB-OG1	12.24	1.63	1.43
1	A	20	PHE	N-CA	-12.02	1.29	1.46
1	A	67	LEU	N-CA	11.35	1.60	1.46
1	A	112	LYS	C-O	11.25	1.46	1.23
1	A	82	SER	CA-C	10.55	1.66	1.52
1	A	78	VAL	C-N	-10.21	1.21	1.33
1	A	71	VAL	N-CA	9.38	1.56	1.46
1	A	34	GLY	CA-C	9.23	1.64	1.51
1	A	1	GLU	CA-CB	9.22	1.71	1.53
1	A	107	TYR	N-CA	9.15	1.57	1.46
1	A	92	THR	CA-CB	9.08	1.68	1.53
1	A	92	THR	N-CA	9.03	1.57	1.46
1	A	18	HIS	CG-CD2	8.58	1.45	1.35
1	A	35	VAL	C-O	-8.22	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	GLU	C-N	8.21	1.44	1.33
1	A	42	HIS	ND1-CE1	8.20	1.40	1.32
1	A	49	SER	CA-C	8.06	1.62	1.52
1	A	61	THR	C-N	8.04	1.44	1.33
1	A	19	THR	CA-CB	7.77	1.65	1.53
1	A	99	ASP	C-O	-7.72	1.15	1.24
1	A	104	VAL	C-N	7.63	1.43	1.33
1	A	1	GLU	C-O	7.50	1.38	1.23
1	A	27	LYS	C-O	7.40	1.33	1.24
1	A	47	ALA	C-O	7.38	1.33	1.23
1	A	1	GLU	C-N	-7.35	1.23	1.32
1	A	20	PHE	C-N	7.30	1.43	1.33
1	A	19	THR	CB-OG1	7.27	1.55	1.43
1	A	98	ASP	CA-CB	7.25	1.64	1.53
1	A	78	VAL	CA-C	7.25	1.61	1.52
1	A	94	LYS	CA-C	7.22	1.61	1.52
1	A	42	HIS	CG-ND1	7.16	1.46	1.38
1	A	92	THR	C-N	-7.10	1.23	1.33
1	A	52	TYR	CA-CB	7.07	1.65	1.53
1	A	37	GLU	CD-OE1	7.03	1.38	1.25
1	A	35	VAL	CA-C	6.91	1.62	1.52
1	A	101	ILE	C-N	6.90	1.42	1.33
1	A	28	VAL	CA-C	6.88	1.61	1.52
1	A	9	LYS	C-N	6.80	1.42	1.33
1	A	52	TYR	C-N	-6.62	1.25	1.34
1	A	85	PRO	N-CA	6.59	1.56	1.47
1	A	30	PRO	CA-CB	6.57	1.62	1.53
1	A	1	GLU	N-CA	6.50	1.58	1.46
1	A	18	HIS	CA-C	6.50	1.60	1.52
1	A	111	LEU	CA-C	6.45	1.59	1.53
1	A	97	LYS	CA-C	-6.44	1.45	1.52
1	A	83	GLY	CA-C	-6.39	1.42	1.51
1	A	91	MET	C-N	6.37	1.42	1.33
1	A	73	ASN	C-O	6.34	1.32	1.24
1	A	82	SER	C-N	-6.22	1.24	1.33
1	A	31	ASN	CA-C	6.21	1.60	1.52
1	A	38	ASN	C-N	-6.13	1.25	1.33
1	A	22	GLN	C-O	6.13	1.31	1.23
1	A	46	TYR	N-CA	6.13	1.53	1.46
1	A	103	ASN	N-CA	6.12	1.53	1.46
1	A	58	LYS	N-CA	-6.12	1.38	1.46
1	A	80	GLU	C-O	6.08	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	GLU	CA-C	-6.08	1.43	1.52
1	A	73	ASN	N-CA	6.05	1.54	1.46
1	A	17	CYS	N-CA	6.04	1.53	1.45
1	A	59	GLY	N-CA	6.02	1.53	1.45
1	A	66	ASN	N-CA	5.96	1.53	1.46
1	A	44	ASP	C-N	5.90	1.42	1.33
1	A	98	ASP	CB-CG	5.89	1.66	1.52
1	A	87	ALA	C-N	5.76	1.41	1.33
1	A	56	LYS	CA-C	5.75	1.60	1.52
1	A	10	VAL	CA-CB	5.74	1.61	1.54
1	A	33	PHE	N-CA	5.74	1.53	1.45
1	A	59	GLY	C-O	5.69	1.31	1.24
1	A	71	VAL	CA-C	5.69	1.58	1.52
1	A	21	ASP	CA-CB	5.66	1.62	1.53
1	A	55	MET	C-O	5.65	1.30	1.24
1	A	24	GLY	N-CA	-5.65	1.37	1.45
1	A	4	ALA	CA-C	5.64	1.60	1.52
1	A	85	PRO	CA-C	5.63	1.61	1.52
1	A	23	GLY	C-O	-5.62	1.16	1.24
1	A	77	PHE	N-CA	-5.60	1.39	1.46
1	A	111	LEU	CA-CB	5.59	1.61	1.53
1	A	57	ALA	N-CA	5.54	1.53	1.46
1	A	81	LYS	CE-NZ	5.53	1.66	1.49
1	A	49	SER	N-CA	5.48	1.52	1.46
1	A	79	LEU	N-CA	5.46	1.52	1.46
1	A	83	GLY	N-CA	5.45	1.53	1.45
1	A	40	ALA	C-N	-5.45	1.26	1.33
1	A	22	GLN	CA-C	-5.45	1.45	1.52
1	A	97	LYS	CE-NZ	5.40	1.65	1.49
1	A	99	ASP	CG-OD1	5.40	1.35	1.25
1	A	64	GLU	CA-C	-5.38	1.45	1.52
1	A	53	THR	CA-CB	5.38	1.62	1.53
1	A	28	VAL	CA-CB	-5.35	1.47	1.54
1	A	34	GLY	C-N	-5.34	1.27	1.33
1	A	94	LYS	CA-CB	5.29	1.67	1.54
1	A	80	GLU	CA-C	-5.28	1.46	1.52
1	A	50	GLU	CD-OE1	5.23	1.35	1.25
1	A	29	GLY	C-N	5.15	1.40	1.33
1	A	23	GLY	CA-C	-5.14	1.44	1.51
1	A	38	ASN	CA-C	5.11	1.58	1.52
1	A	63	THR	C-N	-5.09	1.27	1.33
1	A	85	PRO	CA-CB	5.09	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	LYS	CE-NZ	5.08	1.64	1.49
1	A	9	LYS	CD-CE	5.07	1.67	1.52
1	A	42	HIS	CD2-NE2	-5.06	1.32	1.37
1	A	90	LYS	N-CA	5.04	1.52	1.46
1	A	46	TYR	CA-C	-5.04	1.46	1.52
1	A	61	THR	CA-C	5.02	1.58	1.52
1	A	95	LEU	CA-C	5.01	1.59	1.52

All (218) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	LYS	CA-CB-CG	16.03	146.16	114.10
1	A	54	GLU	CA-C-O	-15.74	102.76	120.24
1	A	92	THR	CA-C-O	-15.51	98.33	120.51
1	A	38	ASN	OD1-CG-ND2	-14.77	107.83	122.60
1	A	99	ASP	CB-CG-OD2	14.58	151.94	118.40
1	A	18	HIS	CG-CD2-NE2	-14.08	93.12	107.20
1	A	19	THR	CA-C-N	13.70	143.04	122.08
1	A	19	THR	C-N-CA	13.70	143.04	122.08
1	A	22	GLN	OE1-CD-NE2	-13.31	109.29	122.60
1	A	80	GLU	O-C-N	-12.92	108.26	122.08
1	A	12	LYS	CB-CG-CD	12.29	139.57	111.30
1	A	77	PHE	CA-CB-CG	11.81	125.61	113.80
1	A	1	GLU	O-C-N	11.65	141.65	123.00
1	A	92	THR	O-C-N	11.55	137.95	122.59
1	A	78	VAL	CA-C-O	-11.27	109.33	121.05
1	A	82	SER	CA-C-O	-11.21	108.56	120.55
1	A	63	THR	OG1-CB-CG2	-11.08	87.14	109.30
1	A	44	ASP	CB-CG-OD1	10.92	143.53	118.40
1	A	91	MET	CA-C-O	10.68	135.78	120.51
1	A	63	THR	CA-CB-OG1	-10.28	94.18	109.60
1	A	18	HIS	CE1-NE2-CD2	10.27	119.27	109.00
1	A	57	ALA	O-C-N	-10.01	111.51	122.12
1	A	67	LEU	N-CA-CB	-10.00	94.82	110.22
1	A	85	PRO	CA-C-N	-10.00	106.66	122.65
1	A	85	PRO	C-N-CA	-10.00	106.66	122.65
1	A	101	ILE	N-CA-CB	-9.96	97.83	110.57
1	A	75	LYS	N-CA-CB	9.89	124.66	110.12
1	A	112	LYS	CB-CA-C	9.74	128.62	110.10
1	A	36	PHE	CA-CB-CG	9.64	123.44	113.80
1	A	38	ASN	CB-CG-OD1	9.54	139.87	120.80
1	A	91	MET	CA-C-N	-9.48	103.43	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	MET	C-N-CA	-9.48	103.43	121.54
1	A	19	THR	O-C-N	-9.48	109.80	122.97
1	A	66	ASN	CA-C-N	-9.25	106.96	120.28
1	A	66	ASN	C-N-CA	-9.25	106.96	120.28
1	A	26	ASN	CA-CB-CG	9.07	121.67	112.60
1	A	107	TYR	CA-C-O	-9.04	109.02	119.60
1	A	96	THR	O-C-N	-8.94	111.35	122.35
1	A	27	LYS	CB-CG-CD	-8.84	90.97	111.30
1	A	40	ALA	N-CA-C	-8.70	99.04	110.53
1	A	59	GLY	CA-C-O	-8.42	109.53	119.46
1	A	90	LYS	CG-CD-CE	8.36	130.53	111.30
1	A	3	ASP	CA-CB-CG	-8.29	104.31	112.60
1	A	8	GLU	CA-CB-CG	-8.24	97.61	114.10
1	A	43	LYS	O-C-N	-8.24	113.82	123.22
1	A	80	GLU	CB-CG-CD	8.24	126.60	112.60
1	A	86	LYS	CB-CA-C	8.16	124.36	110.56
1	A	53	THR	N-CA-CB	-8.16	97.66	110.22
1	A	50	GLU	CB-CG-CD	8.06	126.31	112.60
1	A	38	ASN	CA-CB-CG	-8.03	104.57	112.60
1	A	99	ASP	OD1-CG-OD2	-7.95	103.81	122.90
1	A	34	GLY	CA-C-O	-7.93	110.21	119.02
1	A	97	LYS	CB-CG-CD	7.93	129.55	111.30
1	A	105	ILE	O-C-N	7.91	129.98	121.83
1	A	65	ALA	N-CA-CB	-7.81	98.17	110.28
1	A	32	LEU	CA-C-N	-7.80	108.44	121.39
1	A	32	LEU	C-N-CA	-7.80	108.44	121.39
1	A	96	THR	N-CA-C	-7.73	103.67	113.72
1	A	22	GLN	O-C-N	-7.72	112.49	123.07
1	A	37	GLU	OE1-CD-OE2	7.69	141.36	122.90
1	A	1	GLU	CA-C-N	-7.59	99.64	121.88
1	A	1	GLU	C-N-CA	-7.59	99.64	121.88
1	A	42	HIS	CG-CD2-NE2	7.59	114.79	107.20
1	A	4	ALA	N-CA-C	-7.56	103.94	113.01
1	A	85	PRO	O-C-N	7.55	132.56	122.30
1	A	1	GLU	CB-CA-C	-7.54	95.77	110.10
1	A	18	HIS	ND1-CG-CD2	7.53	113.63	106.10
1	A	53	THR	CA-C-N	7.51	133.42	120.58
1	A	53	THR	C-N-CA	7.51	133.42	120.58
1	A	23	GLY	CA-C-N	7.50	130.81	121.06
1	A	23	GLY	C-N-CA	7.50	130.81	121.06
1	A	57	ALA	CA-C-N	7.44	133.15	120.72
1	A	57	ALA	C-N-CA	7.44	133.15	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	LEU	CB-CG-CD2	7.42	132.95	110.70
1	A	50	GLU	OE1-CD-OE2	7.41	140.68	122.90
1	A	15	LEU	CA-C-O	-7.38	110.56	119.49
1	A	98	ASP	CB-CG-OD2	-7.30	101.60	118.40
1	A	52	TYR	CA-C-O	-7.30	111.17	119.79
1	A	110	THR	OG1-CB-CG2	7.26	123.82	109.30
1	A	98	ASP	CB-CG-OD1	7.21	134.97	118.40
1	A	25	ALA	CB-CA-C	-7.15	97.32	109.83
1	A	53	THR	CA-CB-OG1	-7.13	98.90	109.60
1	A	55	MET	CA-CB-CG	-7.09	99.92	114.10
1	A	80	GLU	N-CA-CB	7.07	120.56	109.82
1	A	70	TYR	CB-CG-CD1	6.99	131.29	120.80
1	A	63	THR	CA-CB-CG2	-6.99	98.62	110.50
1	A	104	VAL	CA-C-O	6.94	128.17	120.95
1	A	62	TRP	CA-C-N	6.94	134.10	121.06
1	A	62	TRP	C-N-CA	6.94	134.10	121.06
1	A	6	ALA	CA-C-O	6.87	127.83	119.31
1	A	78	VAL	N-CA-CB	6.87	119.06	110.47
1	A	3	ASP	N-CA-CB	-6.86	99.24	110.42
1	A	69	ALA	N-CA-CB	-6.84	100.06	110.12
1	A	22	GLN	CA-CB-CG	-6.78	100.53	114.10
1	A	82	SER	O-C-N	6.73	130.31	122.17
1	A	44	ASP	CB-CG-OD2	-6.72	102.95	118.40
1	A	84	ASP	CA-C-N	-6.71	112.78	119.56
1	A	84	ASP	C-N-CA	-6.71	112.78	119.56
1	A	4	ALA	CA-C-O	-6.69	110.36	119.05
1	A	81	LYS	CA-C-O	6.65	127.05	119.27
1	A	76	ALA	CB-CA-C	6.62	121.78	110.79
1	A	68	ALA	CB-CA-C	6.62	121.15	110.96
1	A	18	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	A	36	PHE	N-CA-CB	6.58	119.76	109.69
1	A	9	LYS	CD-CE-NZ	-6.57	90.89	111.90
1	A	54	GLU	N-CA-C	-6.57	103.61	111.69
1	A	57	ALA	N-CA-C	6.55	119.25	111.33
1	A	70	TYR	CA-C-N	-6.53	111.08	121.34
1	A	70	TYR	C-N-CA	-6.53	111.08	121.34
1	A	1	GLU	CA-C-O	-6.51	109.74	120.80
1	A	3	ASP	CA-C-O	-6.49	113.41	120.36
1	A	77	PHE	CA-C-O	-6.49	111.23	120.51
1	A	61	THR	CA-CB-CG2	6.45	121.46	110.50
1	A	72	LYS	N-CA-CB	6.42	120.19	110.30
1	A	64	GLU	N-CA-CB	6.41	119.55	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ASN	N-CA-C	-6.41	100.21	110.14
1	A	97	LYS	N-CA-CB	6.36	120.56	110.57
1	A	87	ALA	N-CA-CB	6.33	119.29	109.48
1	A	17	CYS	CA-C-N	-6.32	112.67	122.59
1	A	17	CYS	C-N-CA	-6.32	112.67	122.59
1	A	9	LYS	N-CA-C	6.30	118.71	111.02
1	A	88	LYS	CA-C-O	6.30	128.22	121.11
1	A	55	MET	N-CA-C	-6.28	104.44	111.28
1	A	64	GLU	CA-CB-CG	6.25	126.59	114.10
1	A	77	PHE	N-CA-CB	6.23	121.02	110.49
1	A	61	THR	CA-C-O	6.22	128.13	121.11
1	A	99	ASP	CB-CG-OD1	-6.18	104.18	118.40
1	A	46	TYR	N-CA-CB	-6.16	100.77	110.69
1	A	28	VAL	CA-CB-CG1	6.16	120.87	110.40
1	A	32	LEU	N-CA-C	-6.16	103.92	112.30
1	A	70	TYR	O-C-N	6.15	128.48	122.09
1	A	24	GLY	O-C-N	-6.10	115.71	122.60
1	A	93	PHE	CB-CG-CD2	-6.08	110.36	120.70
1	A	105	ILE	CB-CG1-CD1	6.07	126.54	113.80
1	A	72	LYS	CB-CG-CD	6.06	125.23	111.30
1	A	57	ALA	CA-C-O	6.04	127.16	120.63
1	A	21	ASP	CA-CB-CG	-6.03	106.57	112.60
1	A	2	GLY	O-C-N	6.03	128.72	122.75
1	A	20	PHE	CA-C-O	5.99	125.37	118.55
1	A	23	GLY	N-CA-C	-5.98	107.07	115.32
1	A	11	SER	O-C-N	5.96	130.14	122.39
1	A	19	THR	CA-CB-OG1	-5.96	100.67	109.60
1	A	52	TYR	O-C-N	5.93	130.28	122.33
1	A	103	ASN	CA-CB-CG	5.92	118.52	112.60
1	A	70	TYR	CG-CD1-CE1	5.92	130.08	121.20
1	A	73	ASN	O-C-N	-5.90	114.53	121.32
1	A	28	VAL	O-C-N	5.89	129.94	122.57
1	A	2	GLY	CA-C-N	-5.86	114.98	122.77
1	A	2	GLY	C-N-CA	-5.86	114.98	122.77
1	A	84	ASP	CB-CA-C	5.84	116.65	110.17
1	A	80	GLU	CA-C-N	5.83	131.91	121.66
1	A	80	GLU	C-N-CA	5.83	131.91	121.66
1	A	68	ALA	N-CA-C	-5.82	104.63	110.97
1	A	68	ALA	O-C-N	-5.80	116.00	122.03
1	A	50	GLU	CA-CB-CG	-5.79	102.52	114.10
1	A	78	VAL	CA-CB-CG2	5.76	120.20	110.40
1	A	5	ALA	N-CA-C	-5.73	105.40	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	VAL	CA-CB-CG1	-5.70	100.71	110.40
1	A	80	GLU	CA-CB-CG	5.69	125.49	114.10
1	A	83	GLY	N-CA-C	-5.65	107.46	115.43
1	A	96	THR	CA-CB-CG2	5.64	120.08	110.50
1	A	73	ASN	OD1-CG-ND2	5.62	128.22	122.60
1	A	45	ASN	CA-CB-CG	5.61	118.21	112.60
1	A	16	ALA	CA-C-N	-5.58	113.47	122.24
1	A	16	ALA	C-N-CA	-5.58	113.47	122.24
1	A	86	LYS	N-CA-C	-5.58	106.05	112.92
1	A	88	LYS	O-C-N	-5.57	115.95	123.19
1	A	82	SER	CA-CB-OG	5.56	122.22	111.10
1	A	86	LYS	CA-C-O	5.55	126.06	119.56
1	A	53	THR	O-C-N	-5.55	115.73	122.22
1	A	62	TRP	O-C-N	-5.52	115.89	122.46
1	A	35	VAL	N-CA-CB	5.52	120.76	110.77
1	A	12	LYS	CA-CB-CG	5.50	125.11	114.10
1	A	110	THR	O-C-N	-5.45	114.67	122.41
1	A	39	THR	CA-CB-CG2	5.45	119.77	110.50
1	A	104	VAL	CA-CB-CG2	-5.45	101.13	110.40
1	A	110	THR	CA-C-N	5.41	129.58	122.06
1	A	110	THR	C-N-CA	5.41	129.58	122.06
1	A	44	ASP	O-C-N	5.38	128.89	122.27
1	A	20	PHE	CA-C-N	-5.38	111.27	122.07
1	A	20	PHE	C-N-CA	-5.38	111.27	122.07
1	A	6	ALA	CA-C-N	5.37	125.90	119.94
1	A	6	ALA	C-N-CA	5.37	125.90	119.94
1	A	64	GLU	CA-C-N	-5.36	112.16	120.31
1	A	64	GLU	C-N-CA	-5.36	112.16	120.31
1	A	45	ASN	CA-C-N	-5.35	115.17	122.93
1	A	45	ASN	C-N-CA	-5.35	115.17	122.93
1	A	79	LEU	CA-C-N	5.34	128.21	120.79
1	A	79	LEU	C-N-CA	5.34	128.21	120.79
1	A	77	PHE	O-C-N	-5.33	115.50	122.59
1	A	59	GLY	O-C-N	5.32	128.63	122.30
1	A	37	GLU	CA-CB-CG	-5.32	103.46	114.10
1	A	51	SER	O-C-N	-5.30	116.01	122.22
1	A	20	PHE	CE1-CZ-CE2	-5.29	110.47	120.00
1	A	36	PHE	CE1-CZ-CE2	5.29	129.51	120.00
1	A	65	ALA	N-CA-C	5.29	117.95	111.82
1	A	59	GLY	N-CA-C	-5.28	106.42	115.08
1	A	62	TRP	CH2-CZ2-CE2	-5.27	110.64	117.50
1	A	64	GLU	O-C-N	5.25	127.69	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	GLU	CG-CD-OE1	5.23	130.43	118.40
1	A	26	ASN	CA-C-O	-5.22	115.73	121.58
1	A	81	LYS	CD-CE-NZ	-5.22	95.18	111.90
1	A	62	TRP	CD2-CE3-CZ3	-5.22	111.82	118.60
1	A	68	ALA	N-CA-CB	5.19	117.49	109.91
1	A	25	ALA	N-CA-C	-5.16	102.88	110.52
1	A	53	THR	CA-C-O	5.16	125.93	120.10
1	A	102	GLU	CA-C-N	5.15	127.13	120.44
1	A	102	GLU	C-N-CA	5.15	127.13	120.44
1	A	105	ILE	CA-CB-CG1	-5.11	101.72	110.40
1	A	99	ASP	CB-CA-C	5.08	118.86	110.88
1	A	62	TRP	CB-CG-CD1	-5.08	119.28	126.90
1	A	104	VAL	CA-CB-CG1	-5.06	101.80	110.40
1	A	85	PRO	CA-N-CD	-5.04	104.95	112.00
1	A	48	TYR	CG-CD1-CE1	-5.03	113.66	121.20
1	A	56	LYS	N-CA-C	-5.02	105.72	111.14
1	A	17	CYS	CA-C-O	5.02	124.34	118.77
1	A	44	ASP	CA-C-N	-5.01	113.94	122.56
1	A	44	ASP	C-N-CA	-5.01	113.94	122.56

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	39	THR	CB
1	A	110	THR	CB
1	A	112	LYS	CA

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	TYR	Mainchain
1	A	14	CYS	Mainchain
1	A	18	HIS	Mainchain,Sidechain
1	A	19	THR	Mainchain
1	A	27	LYS	Mainchain
1	A	31	ASN	Mainchain
1	A	36	PHE	Mainchain
1	A	54	GLU	Mainchain
1	A	66	ASN	Sidechain
1	A	68	ALA	Mainchain
1	A	77	PHE	Mainchain
1	A	82	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	A	84	ASP	Mainchain
1	A	85	PRO	Mainchain
1	A	89	SER	Mainchain

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	832	0	796	42	10
2	A	43	0	30	16	0
3	A	87	0	0	8	10
All	All	962	0	826	42	10

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 25.

All (42) 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:A:63:THR:CA	1:A:63:THR:CB	1.75	1.60
1:A:14:CYS:SG	2:A:113:HEM:CAB	2.17	1.31
1:A:88:LYS:CB	3:A:185:HOH:O	1.79	1.27
1:A:91:MET:O	1:A:92:THR:CB	1.86	1.24
1:A:17:CYS:SG	2:A:113:HEM:CAC	2.34	1.16
1:A:92:THR:CB	3:A:156:HOH:O	2.05	1.02
1:A:39:THR:HG23	1:A:40:ALA:O	1.60	1.02
1:A:100:GLU:O	1:A:104:VAL:HG23	1.62	0.99
1:A:14:CYS:SG	2:A:113:HEM:HAB	2.05	0.94
1:A:63:THR:CA	1:A:63:THR:CG2	2.53	0.86
1:A:17:CYS:HG	2:A:113:HEM:CAC	1.86	0.85
1:A:63:THR:HG22	3:A:141:HOH:O	1.77	0.83
1:A:17:CYS:SG	2:A:113:HEM:HAC	2.22	0.79
1:A:42:HIS:ND1	2:A:113:HEM:O2A	2.16	0.72
1:A:63:THR:CB	1:A:63:THR:N	2.53	0.72
1:A:63:THR:CB	1:A:63:THR:C	2.64	0.70
1:A:14:CYS:SG	2:A:113:HEM:CBB	2.79	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:CYS:SG	2:A:113:HEM:C3C	2.90	0.64
1:A:107:TYR:O	1:A:110:THR:HG22	1.97	0.64
1:A:63:THR:CA	1:A:63:THR:OG1	2.48	0.62
1:A:63:THR:CG2	3:A:141:HOH:O	2.43	0.62
1:A:68:ALA:O	1:A:72:LYS:HE2	1.99	0.62
1:A:14:CYS:SG	2:A:113:HEM:C3B	2.93	0.60
1:A:93:PHE:N	3:A:190:HOH:O	2.35	0.60
1:A:39:THR:HG21	1:A:56:LYS:HD2	1.86	0.56
1:A:64:GLU:HG3	1:A:105:ILE:HG21	1.89	0.55
1:A:91:MET:HB2	2:A:113:HEM:C1D	2.43	0.53
1:A:50:GLU:O	1:A:53:THR:HB	2.10	0.52
1:A:72:LYS:O	3:A:152:HOH:O	2.19	0.52
1:A:17:CYS:SG	2:A:113:HEM:CBC	2.96	0.51
1:A:95:LEU:HD11	1:A:104:VAL:HG21	1.93	0.51
1:A:71:VAL:HB	3:A:142:HOH:O	2.13	0.48
1:A:12:LYS:CD	3:A:205:HOH:O	2.61	0.48
1:A:76:ALA:O	1:A:77:PHE:C	2.54	0.48
1:A:17:CYS:HG	2:A:113:HEM:CBC	2.27	0.46
1:A:93:PHE:CG	2:A:113:HEM:HMC2	2.51	0.46
1:A:45:ASN:HD22	1:A:45:ASN:H	1.64	0.44
1:A:91:MET:HE3	2:A:113:HEM:C4B	2.54	0.43
1:A:104:VAL:HG23	1:A:104:VAL:H	1.70	0.41
1:A:39:THR:O	1:A:42:HIS:HB3	2.21	0.41
1:A:91:MET:HB2	2:A:113:HEM:ND	2.35	0.41
1:A:91:MET:CE	2:A:113:HEM:NB	2.83	0.41

All (10) 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:A:90:LYS:NZ	3:A:134:HOH:O[4_556]	1.28	0.92
1:A:90:LYS:CE	3:A:134:HOH:O[4_556]	1.31	0.89
1:A:112:LYS:CB	3:A:181:HOH:O[4_456]	1.32	0.88
1:A:64:GLU:OE2	3:A:200:HOH:O[3_745]	1.41	0.79
1:A:63:THR:CB	3:A:203:HOH:O[3_745]	1.47	0.73
1:A:112:LYS:CB	3:A:182:HOH:O[4_456]	1.52	0.68
1:A:64:GLU:CB	3:A:200:HOH:O[3_745]	1.93	0.27
1:A:64:GLU:CD	3:A:200:HOH:O[3_745]	2.16	0.04
1:A:21:ASP:CB	3:A:183:HOH:O[4_456]	2.17	0.03
1:A:21:ASP:CB	3:A:194:HOH:O[4_456]	2.18	0.02

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	110/112 (98%)	101 (92%)	6 (6%)	3 (3%)	4 0

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	THR
1	A	77	PHE
1	A	91	MET

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	80/89 (90%)	76 (95%)	4 (5%)	22 3

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	53	THR
1	A	79	LEU
1	A	104	VAL

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

Mol	Chain	Res	Type
1	A	45	ASN

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](#)

1 ligand is 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	113	1	50,50,50	2.22	19 (38%)	67,82,82	2.09	17 (25%)

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	113	1	-	0/14/54/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	113	HEM	C1C-C2C	5.48	1.56	1.45
2	A	113	HEM	CAB-C3B	5.25	1.61	1.47
2	A	113	HEM	CMA-C3A	4.34	1.59	1.50
2	A	113	HEM	CMD-C2D	3.76	1.58	1.50
2	A	113	HEM	CAA-C2A	3.49	1.60	1.51
2	A	113	HEM	CMB-C2B	3.34	1.57	1.50
2	A	113	HEM	CBB-CAB	3.21	1.45	1.30
2	A	113	HEM	FE-NA	3.13	2.05	1.95
2	A	113	HEM	CAC-C3C	3.05	1.55	1.47
2	A	113	HEM	O1A-CGA	2.93	1.31	1.22
2	A	113	HEM	C4D-ND	2.84	1.45	1.40
2	A	113	HEM	CHB-C1B	2.79	1.44	1.38
2	A	113	HEM	C1A-NA	-2.55	1.34	1.39
2	A	113	HEM	CHC-C1C	-2.49	1.33	1.38
2	A	113	HEM	C3B-C4B	-2.41	1.40	1.44
2	A	113	HEM	CAD-C3D	2.30	1.57	1.51
2	A	113	HEM	C2A-C3A	-2.26	1.33	1.38
2	A	113	HEM	FE-NC	2.20	2.02	1.95
2	A	113	HEM	C3C-C2C	-2.13	1.32	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	113	HEM	C4B-C3B-C2B	5.54	112.38	107.28
2	A	113	HEM	CHB-C4A-NA	4.74	132.45	123.86
2	A	113	HEM	CHC-C4B-NB	4.59	129.37	124.42
2	A	113	HEM	CMC-C2C-C1C	-4.46	116.88	124.73
2	A	113	HEM	CHC-C1C-NC	4.07	128.88	124.45
2	A	113	HEM	CHA-C1A-NA	3.86	130.85	123.86
2	A	113	HEM	CMD-C2D-C1D	-3.80	119.09	125.03
2	A	113	HEM	C2A-C1A-NA	-3.76	105.98	110.15
2	A	113	HEM	C4A-CHB-C1B	-3.74	117.46	126.25
2	A	113	HEM	C4A-NA-C1A	3.68	111.82	105.82
2	A	113	HEM	C3A-C4A-NA	-3.56	104.44	110.14
2	A	113	HEM	C3B-C2B-C1B	-3.14	104.06	106.41
2	A	113	HEM	C3B-C4B-NB	-3.07	107.27	109.47
2	A	113	HEM	CBD-CAD-C3D	-2.65	105.19	112.53
2	A	113	HEM	C1C-CHC-C4B	-2.27	121.20	126.02
2	A	113	HEM	CMD-C2D-C3D	2.26	132.25	126.15
2	A	113	HEM	C1A-CHA-C4D	-2.21	121.04	126.25

There are no chirality outliers.

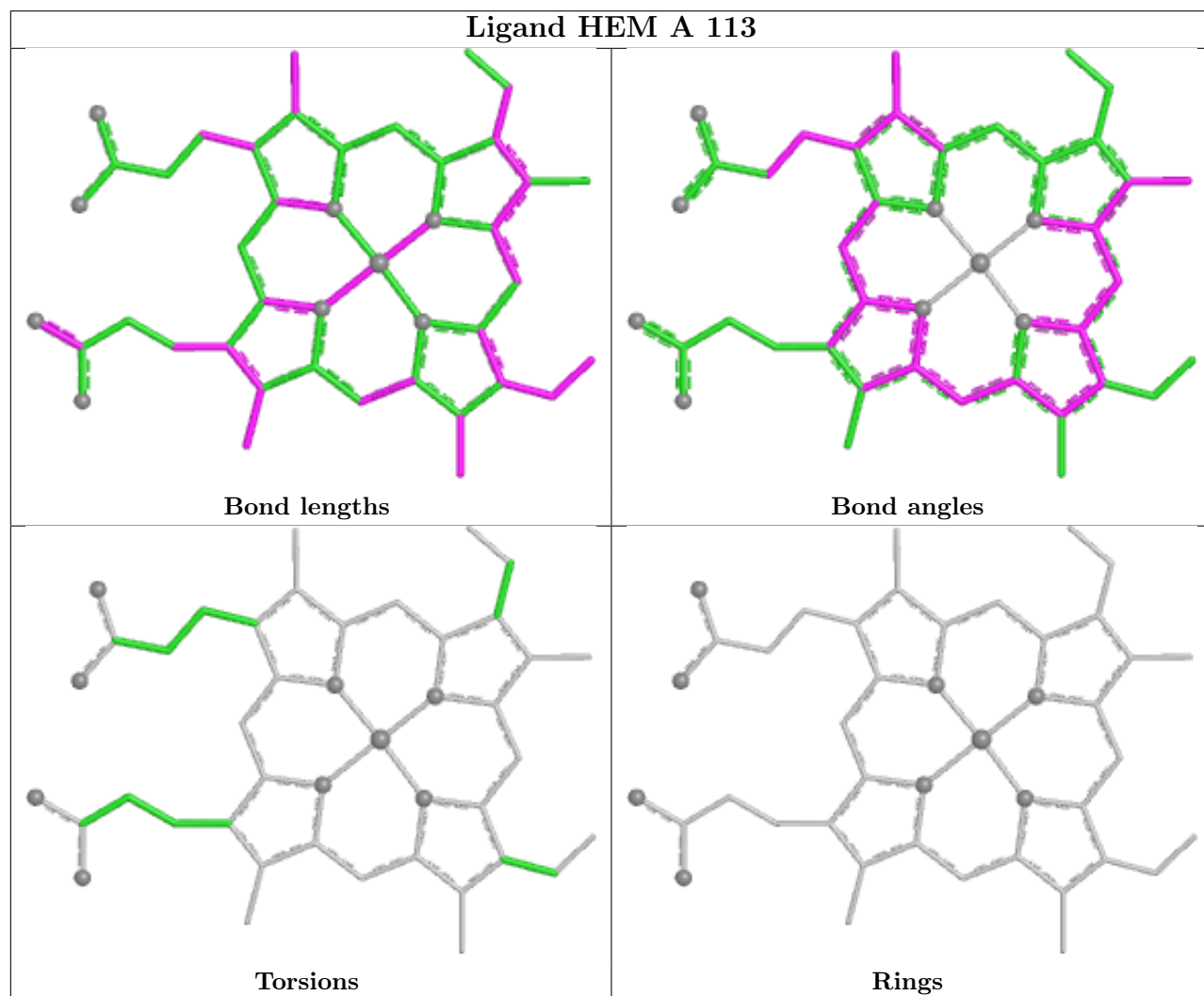
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	113	HEM	16	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	112/112 (100%)	-0.64	2 (1%) 67 76	4, 11, 22, 49	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	92	THR	4.6
1	A	1	GLU	2.8

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](#)

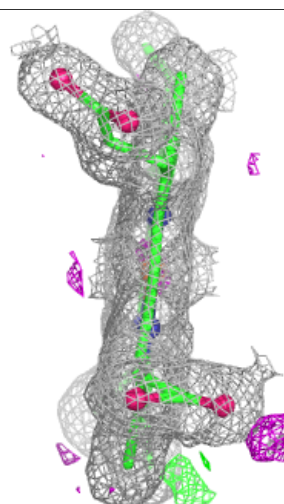
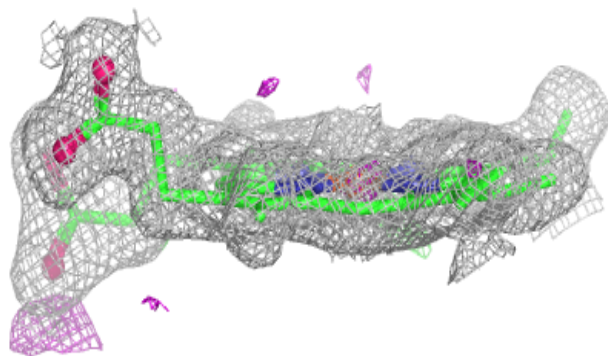
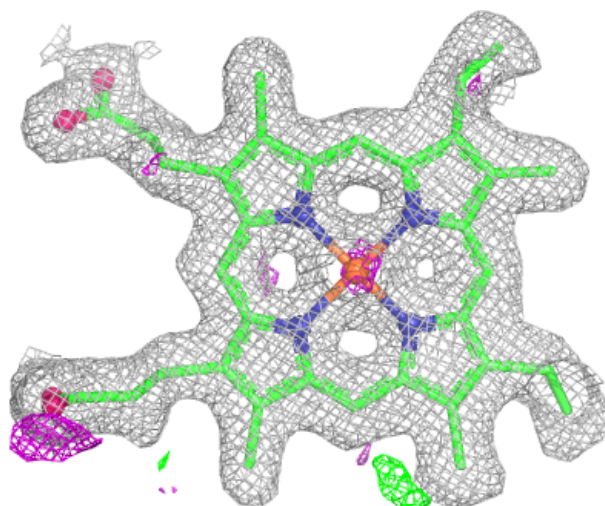
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	A	113	43/43	0.99	0.04	2,3,10,13	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 A 113:

$2mF_o-DF_c$ (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.