Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:44 AM GMT

PDB ID	:	3C2C
Title	:	REFINEMENT OF THE CRYSTAL STRUCTURE OF OXIDIZED RHODOSPIRILLUM 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

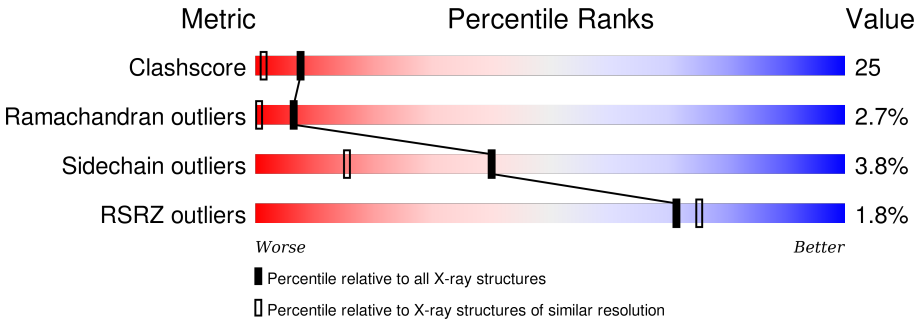
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	5317 (1.70-1.66)
Ramachandran outliers	100387	5225 (1.70-1.66)
Sidechain outliers	100360	5224 (1.70-1.66)
RSRZ outliers	91569	4813 (1.70-1.66)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	112	2% 20% 49% 26% 5%

2 Entry composition

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.

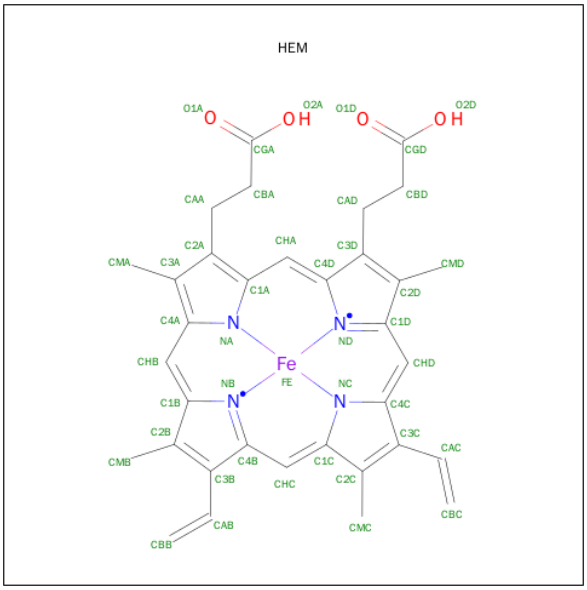
- Molecule 1 is a protein called CYTOCHROME C2.

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

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 (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		

- Molecule 3 is water.

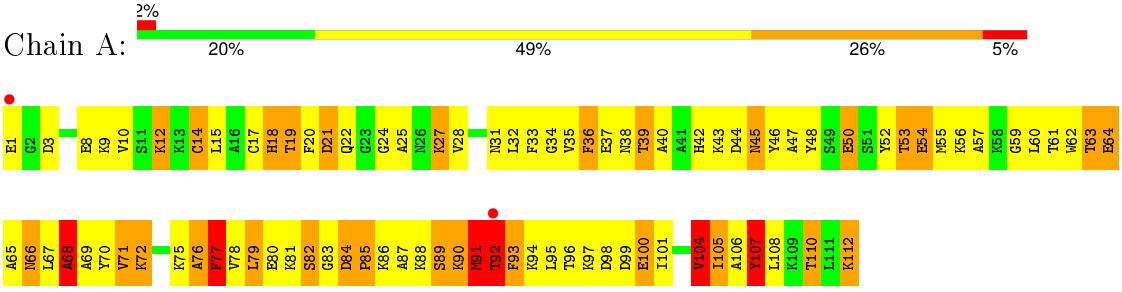
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	87	Total O 87 87	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 (i)

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 34.18 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.68) 61.4 (34.18-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	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.	DCC
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 , 62.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[1]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	3 of 7287 reflections (0.041%)	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.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	2.55	46/848 (5.4%)	3.77	135/1144 (11.8%)

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 (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	ASP	CG-OD1	12.19	1.53	1.25
1	A	112	LYS	C-O	11.95	1.46	1.23
1	A	37	GLU	CD-OE1	11.87	1.38	1.25
1	A	92	THR	C-O	11.84	1.45	1.23
1	A	63	THR	CB-OG1	10.04	1.63	1.43
1	A	50	GLU	CD-OE1	8.75	1.35	1.25
1	A	63	THR	CA-CB	8.54	1.75	1.53
1	A	20	PHE	N-CA	-8.51	1.29	1.46
1	A	1	GLU	CA-CB	8.15	1.71	1.53
1	A	1	GLU	C-O	8.00	1.38	1.23
1	A	34	GLY	CA-C	7.96	1.64	1.51
1	A	8	GLU	CG-CD	7.54	1.63	1.51
1	A	98	ASP	CB-CG	7.15	1.66	1.51
1	A	46	TYR	CE1-CZ	7.12	1.47	1.38
1	A	67	LEU	N-CA	7.08	1.60	1.46
1	A	93	PHE	CE2-CZ	7.05	1.50	1.37
1	A	105	ILE	CA-CB	6.92	1.70	1.54
1	A	81	LYS	CE-NZ	6.75	1.66	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	LYS	CE-NZ	6.60	1.65	1.49
1	A	9	LYS	CD-CE	6.56	1.67	1.51
1	A	52	TYR	CB-CG	6.24	1.61	1.51
1	A	90	LYS	CE-NZ	6.22	1.64	1.49
1	A	1	GLU	N-CA	6.13	1.58	1.46
1	A	94	LYS	CA-CB	6.12	1.67	1.53
1	A	19	THR	CB-OG1	6.07	1.55	1.43
1	A	92	THR	CA-CB	5.95	1.68	1.53
1	A	107	TYR	CE2-CZ	5.87	1.46	1.38
1	A	107	TYR	N-CA	5.80	1.57	1.46
1	A	92	THR	N-CA	5.74	1.57	1.46
1	A	83	GLY	CA-C	-5.66	1.42	1.51
1	A	64	GLU	CD-OE1	5.62	1.31	1.25
1	A	18	HIS	CG-CD2	5.61	1.45	1.35
1	A	28	VAL	CB-CG2	5.61	1.64	1.52
1	A	24	GLY	N-CA	-5.51	1.37	1.46
1	A	47	ALA	C-O	5.48	1.33	1.23
1	A	85	PRO	N-CA	5.46	1.56	1.47
1	A	10	VAL	CB-CG1	5.43	1.64	1.52
1	A	78	VAL	C-N	-5.41	1.21	1.34
1	A	8	GLU	CD-OE2	-5.33	1.19	1.25
1	A	62	TRP	CG-CD1	5.33	1.44	1.36
1	A	27	LYS	C-O	5.24	1.33	1.23
1	A	82	SER	CA-C	5.21	1.66	1.52
1	A	35	VAL	C-O	-5.15	1.13	1.23
1	A	71	VAL	N-CA	5.13	1.56	1.46
1	A	1	GLU	C-N	-5.11	1.23	1.33
1	A	62	TRP	CE2-CZ2	5.05	1.48	1.39

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	99	ASP	CB-CG-OD2	37.38	151.94	118.30
1	A	44	ASP	CB-CG-OD1	28.03	143.53	118.30
1	A	98	ASP	CB-CG-OD2	-18.55	101.60	118.30
1	A	98	ASP	CB-CG-OD1	18.53	134.97	118.30
1	A	70	TYR	CB-CG-CD1	17.14	131.29	121.00
1	A	44	ASP	CB-CG-OD2	-17.05	102.95	118.30
1	A	99	ASP	CB-CG-OD1	-15.69	104.18	118.30
1	A	37	GLU	OE1-CD-OE2	15.05	141.36	123.30
1	A	93	PHE	CB-CG-CD2	-14.91	110.36	120.80
1	A	86	LYS	CA-CB-CG	14.89	146.16	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	50	GLU	OE1-CD-OE2	14.49	140.68	123.30
1	A	79	LEU	CB-CG-CD2	12.91	132.95	111.00
1	A	3	ASP	CB-CG-OD2	-11.79	107.69	118.30
1	A	93	PHE	CB-CG-CD1	11.59	128.91	120.80
1	A	70	TYR	CG-CD1-CE1	10.97	130.08	121.30
1	A	1	GLU	O-C-N	10.85	141.65	123.20
1	A	1	GLU	C-N-CA	-10.79	99.64	122.30
1	A	12	LYS	CB-CG-CD	10.76	139.57	111.60
1	A	48	TYR	CB-CG-CD2	-10.55	114.67	121.00
1	A	92	THR	CA-C-O	-10.36	98.33	120.10
1	A	99	ASP	OD1-CG-OD2	-10.26	103.81	123.30
1	A	63	THR	OG1-CB-CG2	-9.94	87.14	110.00
1	A	63	THR	CA-CB-CG2	-9.84	98.62	112.40
1	A	48	TYR	CG-CD1-CE1	-9.55	113.66	121.30
1	A	92	THR	O-C-N	9.53	137.95	122.70
1	A	38	ASN	CB-CG-OD1	9.13	139.87	121.60
1	A	112	LYS	CB-CA-C	9.11	128.62	110.40
1	A	9	LYS	CD-CE-NZ	-9.05	90.89	111.70
1	A	80	GLU	O-C-N	-9.03	108.26	122.70
1	A	46	TYR	CZ-CE2-CD2	8.64	127.57	119.80
1	A	19	THR	C-N-CA	8.54	143.04	121.70
1	A	25	ALA	CB-CA-C	-8.52	97.32	110.10
1	A	65	ALA	N-CA-CB	-8.52	98.17	110.10
1	A	18	HIS	CG-CD2-NE2	-8.46	93.12	109.20
1	A	54	GLU	CA-C-O	-8.26	102.76	120.10
1	A	19	THR	O-C-N	-8.06	109.80	122.70
1	A	54	GLU	CA-C-N	7.96	134.71	117.20
1	A	27	LYS	CB-CG-CD	-7.93	90.97	111.60
1	A	55	MET	CA-CB-CG	-7.87	99.92	113.30
1	A	36	PHE	CB-CG-CD1	-7.87	115.29	120.80
1	A	75	LYS	N-CA-CB	7.81	124.66	110.60
1	A	76	ALA	CB-CA-C	7.79	121.78	110.10
1	A	67	LEU	N-CA-CB	-7.79	94.82	110.40
1	A	108	LEU	CB-CG-CD1	7.75	124.18	111.00
1	A	91	MET	CA-C-O	7.47	135.78	120.10
1	A	54	GLU	OE1-CD-OE2	-7.41	114.41	123.30
1	A	68	ALA	CB-CA-C	7.37	121.15	110.10
1	A	1	GLU	CB-CA-C	-7.32	95.77	110.40
1	A	91	MET	C-N-CA	-7.31	103.43	121.70
1	A	15	LEU	CB-CG-CD2	7.29	123.40	111.00
1	A	70	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	A	81	LYS	CD-CE-NZ	-7.18	95.18	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	8	GLU	CA-CB-CG	-7.18	97.61	113.40
1	A	69	ALA	N-CA-CB	-7.17	100.06	110.10
1	A	96	THR	O-C-N	-7.09	111.35	122.70
1	A	63	THR	CA-CB-OG1	-7.05	94.18	109.00
1	A	96	THR	CA-C-N	7.05	132.72	117.20
1	A	57	ALA	O-C-N	-6.99	111.51	122.70
1	A	46	TYR	CB-CG-CD2	6.99	125.19	121.00
1	A	86	LYS	CB-CA-C	6.98	124.36	110.40
1	A	77	PHE	CB-CG-CD1	6.93	125.65	120.80
1	A	97	LYS	CB-CG-CD	6.90	129.55	111.60
1	A	19	THR	CA-C-N	6.85	132.27	117.20
1	A	20	PHE	CZ-CE2-CD2	6.82	128.28	120.10
1	A	78	VAL	CA-CB-CG1	-6.79	100.71	110.90
1	A	62	TRP	CH2-CZ2-CE2	-6.75	110.64	117.40
1	A	112	LYS	CA-C-O	6.74	134.24	120.10
1	A	53	THR	N-CA-CB	-6.65	97.66	110.30
1	A	28	VAL	CA-CB-CG1	6.65	120.87	110.90
1	A	87	ALA	N-CA-CB	6.56	119.29	110.10
1	A	70	TYR	CD1-CE1-CZ	-6.54	113.92	119.80
1	A	104	VAL	CA-CB-CG2	-6.51	101.13	110.90
1	A	61	THR	CA-CB-CG2	6.47	121.46	112.40
1	A	107	TYR	CZ-CE2-CD2	-6.47	113.98	119.80
1	A	84	ASP	C-N-CD	6.44	141.93	128.40
1	A	22	GLN	CA-C-N	6.41	129.02	116.20
1	A	97	LYS	CD-CE-NZ	-6.37	97.06	111.70
1	A	3	ASP	N-CA-CB	-6.31	99.24	110.60
1	A	22	GLN	O-C-N	-6.30	112.49	123.20
1	A	36	PHE	CZ-CE2-CD2	-6.29	112.56	120.10
1	A	90	LYS	CG-CD-CE	6.21	130.53	111.90
1	A	78	VAL	CA-CB-CG2	6.20	120.20	110.90
1	A	72	LYS	CD-CE-NZ	6.17	125.89	111.70
1	A	85	PRO	O-C-N	6.17	132.56	122.70
1	A	59	GLY	CA-C-O	-6.15	109.53	120.60
1	A	62	TRP	NE1-CE2-CZ2	-6.13	123.65	130.40
1	A	38	ASN	OD1-CG-ND2	-6.12	107.83	121.90
1	A	104	VAL	CA-CB-CG1	-6.06	101.80	110.90
1	A	100	GLU	CG-CD-OE1	6.06	130.43	118.30
1	A	48	TYR	CD1-CG-CD2	6.06	124.56	117.90
1	A	85	PRO	C-N-CA	-6.02	106.66	121.70
1	A	110	THR	OG1-CB-CG2	6.01	123.82	110.00
1	A	64	GLU	CA-CB-CG	6.00	126.59	113.40
1	A	44	ASP	OD1-CG-OD2	-5.99	111.93	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	62	TRP	CB-CG-CD1	-5.94	119.28	127.00
1	A	66	ASN	C-N-CA	-5.89	106.96	121.70
1	A	70	TYR	CD1-CG-CD2	-5.88	111.44	117.90
1	A	22	GLN	CA-CB-CG	-5.85	100.53	113.40
1	A	33	PHE	CB-CG-CD2	-5.84	116.71	120.80
1	A	77	PHE	N-CA-CB	5.79	121.02	110.60
1	A	34	GLY	CA-C-O	-5.77	110.21	120.60
1	A	64	GLU	CG-CD-OE1	5.76	129.81	118.30
1	A	79	LEU	CA-CB-CG	5.67	128.33	115.30
1	A	101	ILE	N-CA-CB	-5.64	97.83	110.80
1	A	62	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	A	43	LYS	O-C-N	-5.55	113.82	122.70
1	A	80	GLU	N-CA-CB	5.53	120.56	110.60
1	A	33	PHE	CD1-CG-CD2	5.53	125.49	118.30
1	A	97	LYS	N-CA-CB	5.53	120.56	110.60
1	A	80	GLU	CA-CB-CG	5.50	125.49	113.40
1	A	82	SER	CA-C-O	-5.50	108.56	120.10
1	A	96	THR	CA-CB-CG2	5.49	120.08	112.40
1	A	22	GLN	OE1-CD-NE2	-5.48	109.29	121.90
1	A	46	TYR	N-CA-CB	-5.46	100.77	110.60
1	A	62	TRP	CD2-CE3-CZ3	-5.37	111.82	118.80
1	A	72	LYS	N-CA-CB	5.33	120.19	110.60
1	A	12	LYS	CA-CB-CG	5.32	125.11	113.40
1	A	32	LEU	C-N-CA	-5.30	108.44	121.70
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	68	ALA	N-CA-CB	5.28	117.49	110.10
1	A	107	TYR	CA-C-O	-5.28	109.02	120.10
1	A	39	THR	CA-CB-CG2	5.26	119.77	112.40
1	A	72	LYS	CB-CG-CD	5.24	125.23	111.60
1	A	106	ALA	N-CA-CB	-5.20	102.83	110.10
1	A	62	TRP	CD1-CG-CD2	5.13	110.40	106.30
1	A	78	VAL	CA-C-O	-5.13	109.33	120.10
1	A	60	LEU	CB-CG-CD2	-5.11	102.31	111.00
1	A	36	PHE	N-CA-CB	5.09	119.76	110.60
1	A	100	GLU	OE1-CD-OE2	-5.07	117.21	123.30
1	A	33	PHE	CG-CD2-CE2	-5.07	115.22	120.80
1	A	18	HIS	CE1-NE2-CD2	5.07	119.27	106.60
1	A	94	LYS	CB-CA-C	-5.05	100.29	110.40
1	A	110	THR	O-C-N	-5.02	114.67	122.70
1	A	89	SER	N-CA-CB	5.01	118.01	110.50

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	Sidechain,Mainchain
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
1	A	84	ASP	Mainchain
1	A	85	PRO	Mainchain
1	A	89	SER	Mainchain

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	832	0	795	43	10
2	A	43	0	30	17	0
3	A	87	0	0	8	10
All	All	962	0	825	43	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 (43) 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:14:CYS:HG	2:A:113:HEM:CAB	1.56	1.13
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:17:CYS:HG	2:A:113:HEM:CAC	1.76	0.98
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: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:14:CYS:SG	2:A:113:HEM:CBB	2.79	0.70
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:CB	1:A:63:THR:C	2.64	0.62
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: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:14:CYS:SG	2:A:113:HEM:C3B	2.93	0.51
1:A:17:CYS:HG	2:A:113:HEM:CBC	2.21	0.51
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:14:CYS:HG	2:A:113:HEM:CBB	2.20	0.47
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:76:ALA:O	1:A:77:PHE:C	2.54	0.43
1:A:104:VAL:H	1:A:104:VAL:HG23	1.70	0.41
1:A:39:THR:O	1:A:42:HIS:HB3	2.21	0.41
1:A:91:MET:CE	2:A:113:HEM:NB	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:MET:HB2	2:A:113:HEM:ND	2.35	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%)	6 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%)	77 (96%)	3 (4%)	40 15

All (3) residues with a non-rotameric sidechain are listed below:

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	45	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 carbohydrates in this entry.

5.6 Ligand geometry

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	30,50,50	3.65	12 (40%)	24,82,82	2.99	15 (62%)

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	-	0/10/54/54	0/0/8/8

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	113	HEM	C3B-C4B	-12.98	1.40	1.51
2	A	113	HEM	C3D-C4D	-7.59	1.41	1.51
2	A	113	HEM	C2D-C3D	-6.47	1.35	1.54
2	A	113	HEM	C2D-C1D	-2.77	1.42	1.51
2	A	113	HEM	C2B-C1B	-2.70	1.43	1.51
2	A	113	HEM	C3C-CAC	2.24	1.55	1.51
2	A	113	HEM	CMD-C2D	2.29	1.58	1.53
2	A	113	HEM	C4C-NC	2.63	1.39	1.36
2	A	113	HEM	CBB-CAB	2.86	1.45	1.29
2	A	113	HEM	CMA-C3A	3.90	1.59	1.51
2	A	113	HEM	CAA-C2A	4.84	1.60	1.52
2	A	113	HEM	C3B-CAB	5.37	1.61	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	113	HEM	C3B-CAB-CBB	-3.83	118.58	124.46
2	A	113	HEM	CAA-C2A-C1A	-3.54	123.16	127.01
2	A	113	HEM	CBD-CAD-C3D	-2.87	105.19	113.55
2	A	113	HEM	C4B-CHC-C1C	-2.77	121.20	125.82
2	A	113	HEM	CMA-C3A-C4A	-2.41	124.38	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	113	HEM	C3B-C4B-NB	-2.28	107.27	111.63
2	A	113	HEM	C2C-C1C-NC	-2.18	106.53	110.21
2	A	113	HEM	CHC-C4B-NB	2.01	129.37	124.52
2	A	113	HEM	CBA-CAA-C2A	2.31	116.66	112.53
2	A	113	HEM	CAD-C3D-C4D	3.12	123.49	112.47
2	A	113	HEM	CMD-C2D-C3D	4.05	132.25	114.35
2	A	113	HEM	C2D-C3D-C4D	4.42	108.99	101.50
2	A	113	HEM	CAD-C3D-C2D	4.79	127.00	113.22
2	A	113	HEM	CMB-C2B-C3B	5.61	130.53	116.53
2	A	113	HEM	CMC-C2C-C3C	6.65	133.13	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	113	HEM	17	0

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	112/112 (100%)	-0.49	2 (1%) 71 75	4, 11, 22, 49	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	92	THR	4.4
1	A	1	GLU	2.1

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 carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	HEM	A	113	43/43	0.99	0.06	-0.82	2,3,10,13	0

6.5 Other polymers (i)

There are no such residues in this entry.