Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:03 PM GMT

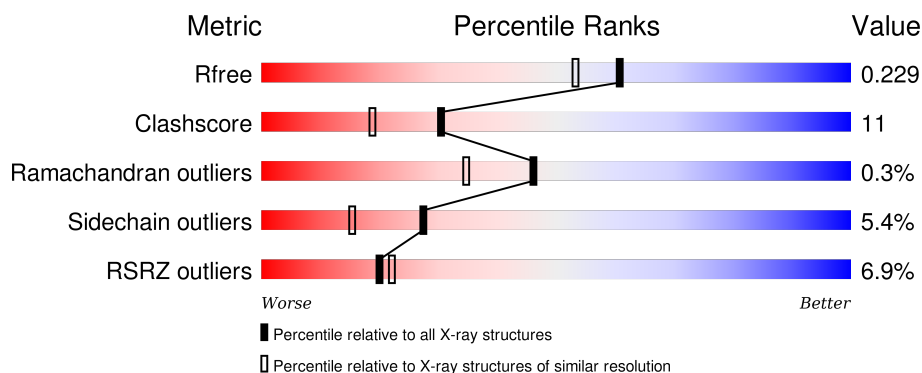|		
PDB ID	:	1DUW
Title	:	STRUCTURE OF NONAHEME CYTOCHROME C
Authors	:	Umhau, S.; Fritz, G.; Diederichs, K.; Breed, J.; Kroneck, P.M.; Welte, W.
Deposited on	:	2000-01-19
Resolution	:	1.89 Å(reported)

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 1.89 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	Percentile Ranks	Value
Rfree		0.229
Clashscore		11
Ramachandran outliers		0.3%
Sidechain outliers		5.4%
RSRZ outliers		6.9%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 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	292	7% — 75% — 21% ··

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

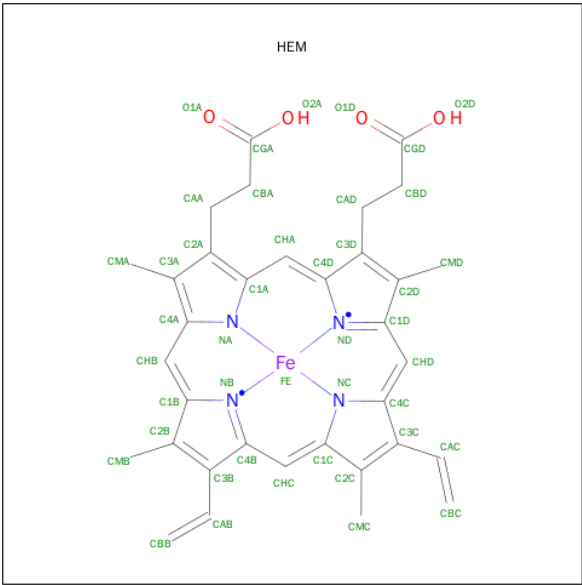| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	302	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3004 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 NONAHEME CYTOCHROME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	1	0
			2188	1334	415	411	28			

- 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		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
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	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
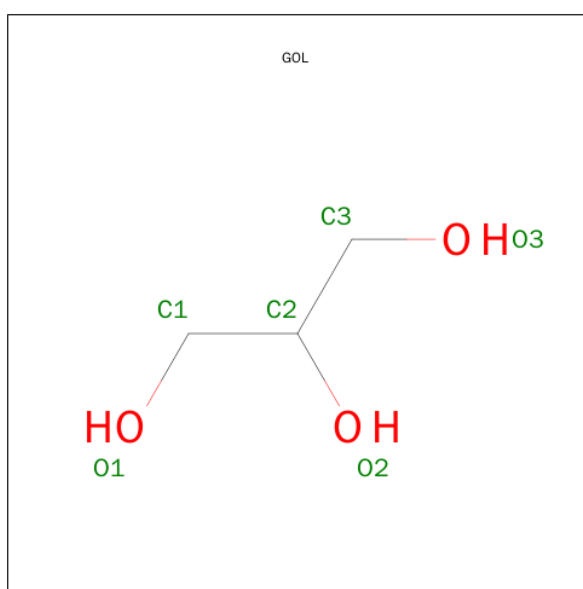
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	423	Total	O	0	0
			423	423		

3 Residue-property plots ⓘ

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: NONAHEME CYTOCHROME C
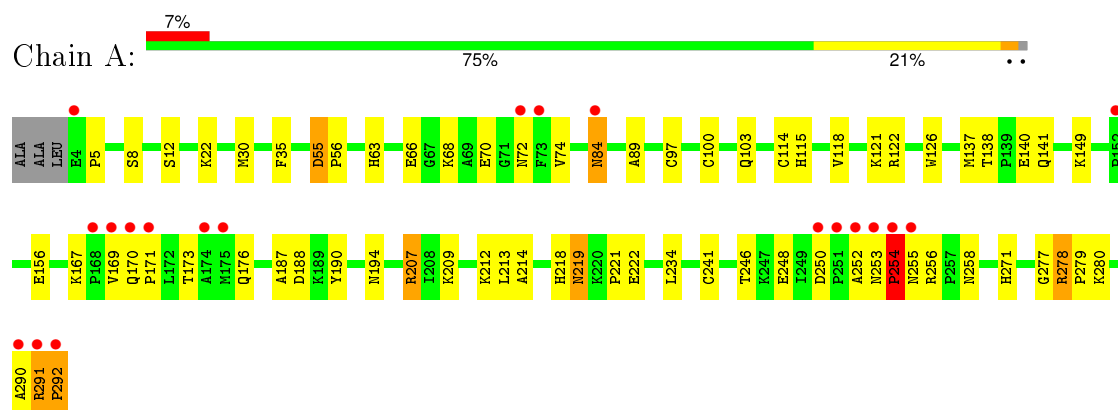
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	55.40Å　　55.40Å　　236.80Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	30.00　–　1.89 29.60　–　1.88	Depositor EDS
% Data completeness (in resolution range)	7.5 (30.00-1.89) 97.9 (29.60-1.88)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 1.88Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.183　,　0.235 0.182　,　0.229	Depositor DCC
R_{free} test set	2129 reflections (7.55%)	DCC
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 100.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 30779 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3004	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	1.84	1/2246 (0.0%)	1.13	6/3044 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	PRO	C-OXT	85.46	2.85	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	207	ARG	NE-CZ-NH1	-9.93	115.33	120.30
1	A	207	ARG	NE-CZ-NH2	7.95	124.28	120.30
1	A	254	PRO	CA-N-CD	-6.84	101.92	111.50
1	A	115	HIS	CA-CB-CG	-5.71	103.90	113.60
1	A	207	ARG	CD-NE-CZ	5.56	131.39	123.60
1	A	250	ASP	CA-CB-CG	5.24	124.94	113.40

There are no chirality outliers.

There are no planarity outliers.

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	2188	0	2124	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	387	0	270	9	0
3	A	6	0	8	0	0
4	A	423	0	0	13	0
All	All	3004	0	2402	55	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (55) 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:254:PRO:HD2	1:A:256:ARG:H	1.39	0.87
1:A:173:THR:H	1:A:176:GLN:HE21	1.25	0.83
1:A:138:THR:H	1:A:141:GLN:HE21	1.29	0.77
1:A:56:PRO:HG3	4:A:1279:HOH:O	1.85	0.76
1:A:169:VAL:HG21	1:A:219:ASN:O	1.86	0.75
1:A:173:THR:H	1:A:176:GLN:NE2	1.86	0.74
1:A:254:PRO:HD3	4:A:1407:HOH:O	1.87	0.73
1:A:277:GLY:O	1:A:280:LYS:HE3	1.89	0.73
1:A:255:ASN:HA	4:A:1336:HOH:O	1.91	0.69
1:A:291:ARG:HD2	4:A:1045:HOH:O	1.93	0.68
1:A:22:LYS:HG3	1:A:66:GLU:OE2	1.93	0.67
1:A:68:LYS:HG3	1:A:70:GLU:OE1	1.99	0.62
1:A:89:ALA:HB2	4:A:1232:HOH:O	2.01	0.61
1:A:140:GLU:HB2	4:A:1355:HOH:O	2.05	0.56
1:A:8:SER:HB2	2:A:296:HEM:C2B	2.41	0.55
1:A:246:THR:O	1:A:258:ASN:HB2	2.10	0.52
1:A:30:MET:HG3	2:A:294:HEM:C4A	2.45	0.52
1:A:209:LYS:HB3	1:A:209:LYS:NZ	2.25	0.52
1:A:171:PRO:HA	1:A:221:PRO:HA	1.92	0.51
1:A:188:ASP:O	1:A:291:ARG:HD3	2.11	0.51
1:A:140:GLU:OE1	1:A:140:GLU:HA	2.10	0.51
1:A:138:THR:H	1:A:141:GLN:NE2	2.05	0.50
1:A:291:ARG:O	1:A:292:PRO:O	2.30	0.49
1:A:254:PRO:HD2	1:A:256:ARG:HB2	1.94	0.49
1:A:213:LEU:HD13	2:A:297:HEM:CHA	2.43	0.49
1:A:207:ARG:HG3	4:A:1322:HOH:O	2.12	0.48
2:A:300:HEM:HBC1	2:A:301:HEM:HMC3	1.95	0.48
1:A:190:TYR:CD2	1:A:290:ALA:HA	2.49	0.47
1:A:271:HIS:CE1	2:A:299:HEM:HBC1	2.50	0.47
1:A:278:ARG:HG2	1:A:279:PRO:N	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ALA:HB3	4:A:1176:HOH:O	2.15	0.47
1:A:207:ARG:NH2	4:A:1322:HOH:O	2.48	0.46
1:A:63:HIS:CE1	1:A:74:VAL:HB	2.50	0.46
1:A:241:CYS:HA	2:A:298:HEM:HHC	1.97	0.46
1:A:122:ARG:HD3	1:A:126:TRP:CH2	2.51	0.46
1:A:254:PRO:CD	1:A:256:ARG:HB2	2.46	0.45
1:A:5:PRO:HA	4:A:1301:HOH:O	2.16	0.45
1:A:114:CYS:O	1:A:118:VAL:HG23	2.17	0.45
1:A:138:THR:OG1	1:A:141:GLN:HG3	2.16	0.45
1:A:84:ASN:O	1:A:84:ASN:ND2	2.50	0.45
1:A:188:ASP:O	1:A:291:ARG:NH1	2.49	0.44
1:A:35:PHE:CZ	2:A:296:HEM:HHD	2.52	0.44
1:A:214:ALA:HB1	1:A:218:HIS:CE1	2.53	0.44
1:A:212:LYS:HD3	4:A:1058:HOH:O	2.17	0.44
1:A:241:CYS:HA	2:A:298:HEM:CHC	2.47	0.44
1:A:100:CYS:O	1:A:103:GLN:HB2	2.18	0.43
1:A:252:ALA:O	1:A:254:PRO:HA	2.18	0.43
1:A:156:GLU:HA	4:A:1152:HOH:O	2.18	0.43
1:A:248:GLU:OE1	1:A:248:GLU:HA	2.19	0.43
1:A:55:ASP:HA	1:A:56:PRO:HD3	1.90	0.42
1:A:137:MET:HA	1:A:141:GLN:NE2	2.35	0.41
1:A:222:GLU:HB2	1:A:234:LEU:HD13	2.03	0.41
1:A:97:CYS:HA	2:A:297:HEM:CHC	2.51	0.41
1:A:280:LYS:HA	1:A:280:LYS:HD3	1.91	0.40
1:A:248:GLU:HB2	4:A:1142:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	288/292 (99%)	279 (97%)	8 (3%)	1 (0%)	46	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	PRO

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	242/242 (100%)	229 (95%)	13 (5%)	27	15

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	55	ASP
1	A	72	ASN
1	A	84	ASN
1	A	121	LYS
1	A	149	LYS
1	A	167	LYS
1	A	170	GLN
1	A	194	ASN
1	A	219	ASN
1	A	253	ASN
1	A	278	ARG
1	A	291	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	103	GLN
1	A	141	GLN
1	A	154	GLN
1	A	176	GLN
1	A	194	ASN

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Mol	Chain	Res	Type
1	A	219	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 ⓘ

10 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	293	1	30,50,50	2.42	8 (26%)	24,82,82	3.10	13 (54%)
2	HEM	A	294	1	30,50,50	2.39	9 (30%)	24,82,82	3.29	12 (50%)
2	HEM	A	295	1	30,50,50	2.48	6 (20%)	24,82,82	3.35	11 (45%)
2	HEM	A	296	1	30,50,50	2.41	7 (23%)	24,82,82	3.34	13 (54%)
2	HEM	A	297	1	30,50,50	2.48	7 (23%)	24,82,82	3.13	16 (66%)
2	HEM	A	298	1	30,50,50	2.44	8 (26%)	24,82,82	3.42	14 (58%)
2	HEM	A	299	1	30,50,50	2.43	8 (26%)	24,82,82	3.57	13 (54%)
2	HEM	A	300	1	30,50,50	2.43	6 (20%)	24,82,82	3.33	13 (54%)
2	HEM	A	301	1	30,50,50	2.52	6 (20%)	24,82,82	3.38	14 (58%)
3	GOL	A	302	-	5,5,5	0.73	0	5,5,5	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	293	1	-	0/10/54/54	0/0/8/8
2	HEM	A	294	1	-	0/10/54/54	0/0/8/8
2	HEM	A	295	1	-	0/10/54/54	0/0/8/8
2	HEM	A	296	1	-	0/10/54/54	0/0/8/8
2	HEM	A	297	1	-	0/10/54/54	0/0/8/8
2	HEM	A	298	1	-	0/10/54/54	0/0/8/8
2	HEM	A	299	1	-	0/10/54/54	0/0/8/8
2	HEM	A	300	1	-	0/10/54/54	0/0/8/8
2	HEM	A	301	1	-	0/10/54/54	0/0/8/8
3	GOL	A	302	-	-	0/4/4/4	0/0/0/0

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	297	HEM	C3B-C4B	-8.00	1.44	1.51
2	A	301	HEM	C3B-C4B	-7.53	1.45	1.51
2	A	295	HEM	C3B-C4B	-7.30	1.45	1.51
2	A	298	HEM	C3B-C4B	-7.14	1.45	1.51
2	A	293	HEM	C3B-C4B	-6.92	1.45	1.51
2	A	300	HEM	C3B-C4B	-6.65	1.45	1.51
2	A	299	HEM	C3B-C4B	-6.45	1.46	1.51
2	A	296	HEM	C3B-C4B	-6.41	1.46	1.51
2	A	294	HEM	C3B-C4B	-6.30	1.46	1.51
2	A	296	HEM	C2D-C3D	-6.02	1.36	1.54
2	A	298	HEM	C2D-C3D	-5.95	1.36	1.54
2	A	295	HEM	C2D-C3D	-5.85	1.37	1.54
2	A	293	HEM	C2D-C3D	-5.82	1.37	1.54
2	A	300	HEM	C2D-C3D	-5.79	1.37	1.54
2	A	299	HEM	C2D-C3D	-5.79	1.37	1.54
2	A	294	HEM	C2D-C3D	-5.77	1.37	1.54
2	A	297	HEM	C2D-C3D	-5.71	1.37	1.54
2	A	301	HEM	C2D-C3D	-5.71	1.37	1.54
2	A	300	HEM	C3D-C4D	-5.57	1.44	1.51
2	A	301	HEM	C3D-C4D	-5.47	1.44	1.51
2	A	294	HEM	C3D-C4D	-5.39	1.44	1.51
2	A	299	HEM	C3D-C4D	-5.31	1.44	1.51
2	A	295	HEM	C3D-C4D	-5.20	1.44	1.51
2	A	293	HEM	C3D-C4D	-4.98	1.45	1.51
2	A	296	HEM	C3D-C4D	-4.49	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	297	HEM	C3D-C4D	-4.43	1.45	1.51
2	A	298	HEM	C3D-C4D	-4.27	1.46	1.51
2	A	298	HEM	C2C-C1C	-4.24	1.44	1.52
2	A	296	HEM	C2C-C1C	-4.10	1.44	1.52
2	A	297	HEM	C2C-C1C	-3.96	1.45	1.52
2	A	301	HEM	C2C-C1C	-3.90	1.45	1.52
2	A	295	HEM	C2C-C1C	-3.76	1.45	1.52
2	A	300	HEM	C2C-C1C	-3.73	1.45	1.52
2	A	293	HEM	C2C-C1C	-3.71	1.45	1.52
2	A	299	HEM	C2C-C1C	-3.67	1.45	1.52
2	A	294	HEM	C2C-C1C	-3.49	1.46	1.52
2	A	293	HEM	C2B-C1B	-2.20	1.44	1.51
2	A	299	HEM	C2D-C1D	-2.16	1.44	1.51
2	A	293	HEM	C2D-C1D	-2.14	1.44	1.51
2	A	294	HEM	C2B-C1B	-2.06	1.45	1.51
2	A	297	HEM	C2B-C1B	-2.04	1.45	1.51
2	A	294	HEM	C2D-C1D	-2.03	1.45	1.51
2	A	299	HEM	C2B-C1B	-2.03	1.45	1.51
2	A	298	HEM	C2D-C1D	-2.02	1.45	1.51
2	A	298	HEM	C2B-C1B	-2.01	1.45	1.51
2	A	294	HEM	C4C-NC	2.21	1.38	1.36
2	A	296	HEM	C4C-NC	2.34	1.38	1.36
2	A	297	HEM	CBC-CAC	3.85	1.51	1.29
2	A	294	HEM	CBC-CAC	3.91	1.51	1.29
2	A	300	HEM	CBB-CAB	4.01	1.52	1.29
2	A	293	HEM	CBC-CAC	4.01	1.52	1.29
2	A	297	HEM	CBB-CAB	4.03	1.52	1.29
2	A	299	HEM	CBC-CAC	4.08	1.52	1.29
2	A	301	HEM	CBB-CAB	4.08	1.52	1.29
2	A	293	HEM	CBB-CAB	4.09	1.52	1.29
2	A	298	HEM	CBC-CAC	4.09	1.52	1.29
2	A	298	HEM	CBB-CAB	4.09	1.52	1.29
2	A	296	HEM	CBC-CAC	4.10	1.53	1.29
2	A	295	HEM	CBB-CAB	4.10	1.53	1.29
2	A	295	HEM	CBC-CAC	4.11	1.53	1.29
2	A	296	HEM	CBB-CAB	4.17	1.53	1.29
2	A	301	HEM	CBC-CAC	4.19	1.53	1.29
2	A	294	HEM	CBB-CAB	4.19	1.53	1.29
2	A	299	HEM	CBB-CAB	4.19	1.53	1.29
2	A	300	HEM	CBC-CAC	4.30	1.54	1.29

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	299	HEM	C3B-CAB-CBB	-9.09	110.52	124.46
2	A	298	HEM	C3C-CAC-CBC	-8.20	111.89	124.46
2	A	296	HEM	C3B-CAB-CBB	-8.07	112.07	124.46
2	A	299	HEM	C3C-CAC-CBC	-7.84	112.43	124.46
2	A	295	HEM	C3C-CAC-CBC	-7.75	112.57	124.46
2	A	300	HEM	C3C-CAC-CBC	-6.96	113.79	124.46
2	A	301	HEM	C3B-CAB-CBB	-6.91	113.86	124.46
2	A	300	HEM	CAA-C2A-C1A	-6.89	119.53	127.01
2	A	294	HEM	C3B-CAB-CBB	-6.89	113.89	124.46
2	A	297	HEM	C3B-CAB-CBB	-6.80	114.03	124.46
2	A	298	HEM	C3B-CAB-CBB	-6.63	114.29	124.46
2	A	293	HEM	C3C-CAC-CBC	-6.44	114.58	124.46
2	A	295	HEM	C3B-CAB-CBB	-6.29	114.81	124.46
2	A	300	HEM	C3B-CAB-CBB	-6.01	115.23	124.46
2	A	296	HEM	CAA-C2A-C1A	-5.92	120.58	127.01
2	A	294	HEM	C3C-CAC-CBC	-5.54	115.97	124.46
2	A	293	HEM	C3B-CAB-CBB	-5.51	116.00	124.46
2	A	296	HEM	C3C-CAC-CBC	-5.38	116.20	124.46
2	A	301	HEM	C3C-CAC-CBC	-5.27	116.36	124.46
2	A	296	HEM	C1D-CHD-C4C	-4.88	117.66	125.82
2	A	301	HEM	CAA-C2A-C1A	-4.79	121.80	127.01
2	A	294	HEM	CAA-C2A-C1A	-4.34	122.29	127.01
2	A	299	HEM	CAA-C2A-C1A	-4.24	122.40	127.01
2	A	298	HEM	C4B-CHC-C1C	-4.01	119.11	125.82
2	A	297	HEM	CAA-C2A-C1A	-3.83	122.85	127.01
2	A	295	HEM	C4B-CHC-C1C	-3.80	119.48	125.82
2	A	294	HEM	C1D-CHD-C4C	-3.73	119.59	125.82
2	A	294	HEM	C4B-CHC-C1C	-3.71	119.62	125.82
2	A	299	HEM	CMA-C3A-C4A	-3.64	122.34	128.36
2	A	297	HEM	C4B-CHC-C1C	-3.63	119.76	125.82
2	A	300	HEM	C1D-CHD-C4C	-3.56	119.87	125.82
2	A	293	HEM	CAA-C2A-C1A	-3.54	123.16	127.01
2	A	293	HEM	C1D-CHD-C4C	-3.52	119.93	125.82
2	A	301	HEM	C4B-CHC-C1C	-3.50	119.96	125.82
2	A	297	HEM	C3C-CAC-CBC	-3.47	119.13	124.46
2	A	293	HEM	CMA-C3A-C4A	-3.32	122.88	128.36
2	A	297	HEM	CMA-C3A-C4A	-3.29	122.93	128.36
2	A	295	HEM	CAA-C2A-C1A	-3.28	123.44	127.01
2	A	301	HEM	C1D-CHD-C4C	-3.04	120.75	125.82
2	A	295	HEM	CMA-C3A-C4A	-3.00	123.40	128.36
2	A	300	HEM	CMA-C3A-C4A	-2.99	123.42	128.36
2	A	298	HEM	C1D-CHD-C4C	-2.95	120.88	125.82
2	A	298	HEM	CAA-C2A-C1A	-2.74	124.03	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	296	HEM	CMA-C3A-C4A	-2.55	124.14	128.36
2	A	297	HEM	C1D-CHD-C4C	-2.49	121.66	125.82
2	A	299	HEM	C1D-CHD-C4C	-2.46	121.71	125.82
2	A	296	HEM	C4B-CHC-C1C	-2.41	121.79	125.82
2	A	300	HEM	C2C-C1C-NC	-2.36	106.24	110.21
2	A	296	HEM	CBA-CAA-C2A	-2.31	108.39	112.53
2	A	299	HEM	C4B-CHC-C1C	-2.31	121.97	125.82
2	A	293	HEM	C4B-CHC-C1C	-2.30	121.97	125.82
2	A	294	HEM	CMA-C3A-C4A	-2.18	124.75	128.36
2	A	300	HEM	C4B-CHC-C1C	-2.15	122.23	125.82
2	A	298	HEM	C3B-C4B-NB	-2.10	107.61	111.63
2	A	298	HEM	CMA-C3A-C4A	-2.07	124.93	128.36
2	A	297	HEM	C3B-C4B-NB	-2.02	107.77	111.63
2	A	297	HEM	CAA-CBA-CGA	2.04	116.48	112.75
2	A	301	HEM	CAA-CBA-CGA	2.07	116.53	112.75
2	A	297	HEM	CHD-C1D-ND	2.07	129.51	124.52
2	A	297	HEM	CHC-C4B-NB	2.07	129.51	124.52
2	A	301	HEM	CHD-C1D-ND	2.29	130.05	124.52
2	A	301	HEM	CHC-C4B-NB	2.35	130.18	124.52
2	A	298	HEM	CHC-C4B-NB	2.36	130.21	124.52
2	A	293	HEM	CHD-C1D-ND	2.38	130.26	124.52
2	A	299	HEM	CMD-C2D-C3D	2.45	125.20	114.35
2	A	293	HEM	CAD-C3D-C4D	2.48	121.20	112.47
2	A	298	HEM	CAD-C3D-C4D	2.57	121.54	112.47
2	A	299	HEM	CBA-CAA-C2A	2.83	117.60	112.53
2	A	295	HEM	CMD-C2D-C3D	2.85	126.94	114.35
2	A	296	HEM	CAD-C3D-C4D	2.89	122.67	112.47
2	A	294	HEM	CMD-C2D-C3D	2.89	127.14	114.35
2	A	300	HEM	CMD-C2D-C3D	2.96	127.45	114.35
2	A	300	HEM	CAD-C3D-C4D	3.01	123.08	112.47
2	A	296	HEM	C2D-C3D-C4D	3.13	106.81	101.50
2	A	296	HEM	CMC-C2C-C3C	3.14	124.38	116.53
2	A	301	HEM	CAD-C3D-C4D	3.25	123.94	112.47
2	A	298	HEM	CMD-C2D-C3D	3.29	128.89	114.35
2	A	297	HEM	CMD-C2D-C3D	3.40	129.38	114.35
2	A	299	HEM	CAD-C3D-C4D	3.42	124.53	112.47
2	A	301	HEM	CMD-C2D-C3D	3.49	129.80	114.35
2	A	293	HEM	CMD-C2D-C3D	3.51	129.87	114.35
2	A	300	HEM	C2D-C3D-C4D	3.57	107.54	101.50
2	A	299	HEM	C2D-C3D-C4D	3.59	107.58	101.50
2	A	297	HEM	CAD-C3D-C4D	3.60	125.16	112.47
2	A	294	HEM	CAD-C3D-C4D	3.64	125.31	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	294	HEM	C2D-C3D-C4D	3.66	107.70	101.50
2	A	296	HEM	CMB-C2B-C3B	3.68	125.72	116.53
2	A	295	HEM	C2D-C3D-C4D	3.69	107.76	101.50
2	A	298	HEM	C2D-C3D-C4D	3.70	107.78	101.50
2	A	296	HEM	CMD-C2D-C3D	3.72	130.78	114.35
2	A	300	HEM	CAD-C3D-C2D	3.73	123.93	113.22
2	A	301	HEM	C2D-C3D-C4D	3.77	107.89	101.50
2	A	293	HEM	C2D-C3D-C4D	3.82	107.98	101.50
2	A	295	HEM	CAD-C3D-C4D	3.82	125.95	112.47
2	A	297	HEM	C2D-C3D-C4D	4.19	108.60	101.50
2	A	297	HEM	CAD-C3D-C2D	4.24	125.39	113.22
2	A	299	HEM	CMB-C2B-C3B	4.43	127.58	116.53
2	A	295	HEM	CAD-C3D-C2D	4.54	126.28	113.22
2	A	293	HEM	CMB-C2B-C3B	4.58	127.96	116.53
2	A	293	HEM	CMC-C2C-C3C	4.62	128.07	116.53
2	A	298	HEM	CMC-C2C-C3C	4.74	128.36	116.53
2	A	294	HEM	CAD-C3D-C2D	4.76	126.91	113.22
2	A	299	HEM	CMC-C2C-C3C	4.82	128.56	116.53
2	A	300	HEM	CMB-C2B-C3B	4.82	128.56	116.53
2	A	300	HEM	CMC-C2C-C3C	4.85	128.63	116.53
2	A	293	HEM	CAD-C3D-C2D	4.85	127.15	113.22
2	A	296	HEM	CAD-C3D-C2D	5.03	127.67	113.22
2	A	301	HEM	CMB-C2B-C3B	5.04	129.10	116.53
2	A	297	HEM	CMB-C2B-C3B	5.07	129.17	116.53
2	A	297	HEM	CMC-C2C-C3C	5.10	129.25	116.53
2	A	299	HEM	CAD-C3D-C2D	5.10	127.88	113.22
2	A	301	HEM	CAD-C3D-C2D	5.17	128.08	113.22
2	A	295	HEM	CMB-C2B-C3B	5.29	129.72	116.53
2	A	294	HEM	CMB-C2B-C3B	5.29	129.74	116.53
2	A	298	HEM	CMB-C2B-C3B	5.37	129.93	116.53
2	A	294	HEM	CMC-C2C-C3C	5.54	130.35	116.53
2	A	295	HEM	CMC-C2C-C3C	5.57	130.43	116.53
2	A	298	HEM	CAD-C3D-C2D	5.72	129.67	113.22
2	A	301	HEM	CMC-C2C-C3C	6.30	132.26	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	294	HEM	1	0
2	A	296	HEM	2	0
2	A	297	HEM	2	0
2	A	298	HEM	2	0
2	A	299	HEM	1	0
2	A	300	HEM	1	0
2	A	301	HEM	1	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 (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(Å²)	Q<0.9
1	A	289/292 (98%)	0.26	20 (6%)	20	22	18, 27, 53, 93	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	PRO	6.2
1	A	253	ASN	5.0
1	A	254	PRO	4.4
1	A	84	ASN	4.1
1	A	291	ARG	4.0
1	A	290	ALA	3.8
1	A	169	VAL	3.6
1	A	170	GLN	3.3
1	A	168	PRO	3.3
1	A	251	PRO	2.8
1	A	250	ASP	2.7
1	A	174	ALA	2.5
1	A	171	PRO	2.4
1	A	72	ASN	2.3
1	A	252	ALA	2.2
1	A	255	ASN	2.2
1	A	175	MET	2.2
1	A	73	PHE	2.2
1	A	152	PRO	2.1
1	A	4	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	A	302	6/6	0.93	0.14	2.92	28,38,42,46	0
2	HEM	A	297	43/43	0.96	0.14	1.11	18,22,26,31	0
2	HEM	A	296	43/43	0.96	0.12	0.37	17,27,33,36	0
2	HEM	A	294	43/43	0.98	0.11	0.09	16,22,24,26	0
2	HEM	A	301	43/43	0.98	0.11	0.05	16,21,28,33	0
2	HEM	A	295	43/43	0.98	0.09	-0.19	16,21,36,45	0
2	HEM	A	298	43/43	0.96	0.11	-0.26	17,22,32,51	0
2	HEM	A	293	43/43	0.96	0.11	-0.27	18,23,37,46	0
2	HEM	A	300	43/43	0.98	0.10	-0.31	15,20,29,36	0
2	HEM	A	299	43/43	0.98	0.09	-0.53	14,25,29,30	0

6.5 Other polymers (i)

There are no such residues in this entry.