



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:36 PM GMT

PDB ID : 3UA1
Title : Crystal structure of the cytochrome P4503A4-bromoergocryptine complex
Authors : Sevrioukova, I.F.; Poulos, T.L.
Deposited on : 2011-10-20
Resolution : 2.15 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

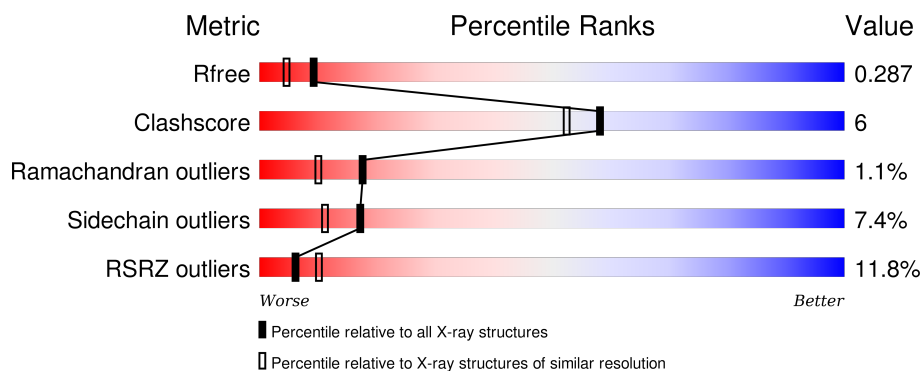
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

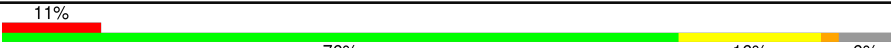
The reported resolution of this entry is 2.15 Å.

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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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 $\leq 5\%$. 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	487	

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.

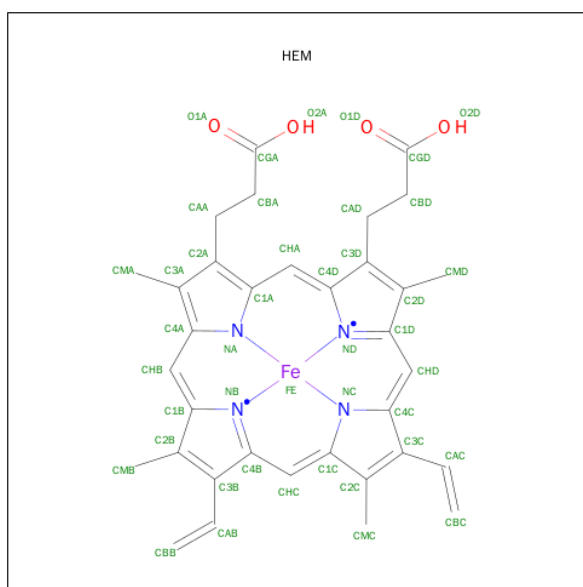
- Molecule 1 is a protein called Cytochrome P450 3A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3672	2392	601	655	24			

There are 4 discrepancies between the modelled and reference sequences:

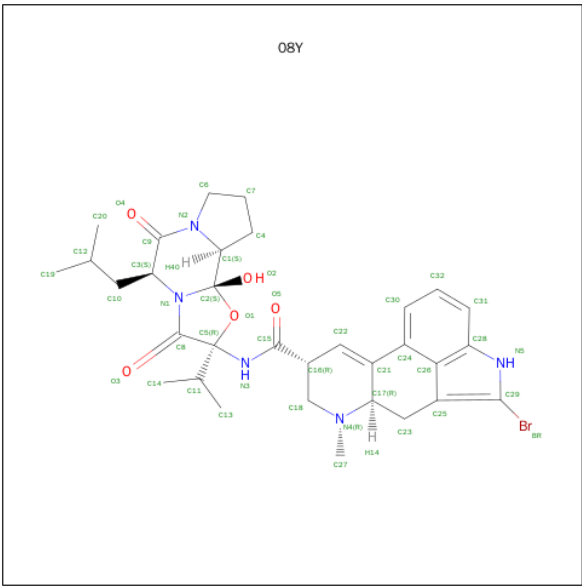
Chain	Residue	Modelled	Actual	Comment	Reference
A	504	HIS	-	EXPRESSION TAG	UNP P08684
A	505	HIS	-	EXPRESSION TAG	UNP P08684
A	506	HIS	-	EXPRESSION TAG	UNP P08684
A	507	HIS	-	EXPRESSION TAG	UNP P08684

- 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 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is BROMOERGOCRYPTINE (three-letter code: 08Y) (formula: C₃₂H₄₀BrN₅O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			43	1	32	5	5		

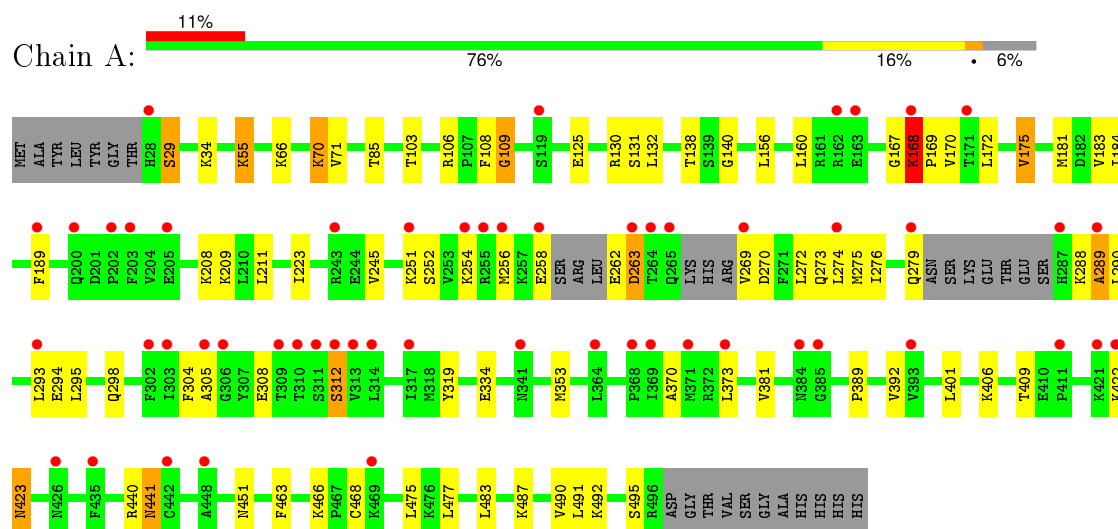
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	65	Total	O	0	0
			65	65		

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 ($\text{RSRZ} > 2$). 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 P450 3A4



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	77.67Å 99.39Å 131.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 2.15 38.26 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.8 (39.90-2.15) 96.9 (38.26-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.221 , 0.278 0.225 , 0.287	Depositor DCC
R_{free} test set	1383 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 27255 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3823	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: HEM, 08Y

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	0.65	0/3761	0.74	3/5086 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	289	ALA	CB-CA-C	9.57	124.46	110.10
1	A	440	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	A	168	LYS	CB-CA-C	5.23	120.87	110.40

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	3672	0	3750	43	0
2	A	43	0	30	2	0
3	A	43	0	40	3	0
4	A	65	0	0	0	0
All	All	3823	0	3820	45	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 6.

All (45) 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:70:LYS:HD3	1:A:71:VAL:HG23	1.68	0.75
1:A:189:PHE:CD1	1:A:272:LEU:HD23	2.23	0.72
1:A:181:MET:CE	1:A:208:LYS:HG3	2.19	0.72
1:A:181:MET:HE1	1:A:208:LYS:HG3	1.72	0.70
1:A:132:LEU:HD11	1:A:289:ALA:O	1.92	0.69
1:A:138:THR:HG22	1:A:140:GLY:H	1.57	0.68
1:A:305:ALA:HA	3:A:600:08Y:H34	1.76	0.68
2:A:508:HEM:HBC2	2:A:508:HEM:HHD	1.77	0.67
1:A:108:PHE:O	1:A:109:GLY:O	2.14	0.65
1:A:269:VAL:HG13	1:A:269:VAL:O	1.97	0.65
1:A:167:GLY:O	1:A:168:LYS:HB2	1.96	0.64
2:A:508:HEM:HBB2	2:A:508:HEM:HHC	1.80	0.63
1:A:169:PRO:HB3	1:A:468:CYS:SG	2.40	0.61
1:A:308:GLU:O	1:A:312:SER:HB2	2.02	0.59
1:A:130:ARG:HH22	1:A:441:ASN:ND2	1.99	0.59
1:A:252:SER:O	1:A:256:MET:HG2	2.05	0.57
1:A:262:GLU:HA	1:A:262:GLU:OE1	2.04	0.56
1:A:189:PHE:CG	1:A:272:LEU:HD23	2.41	0.54
1:A:275:MET:HE1	1:A:295:LEU:HA	1.92	0.52
1:A:370:ALA:HB1	3:A:600:08Y:C13	2.41	0.51
1:A:209:LYS:HB2	1:A:245:VAL:HG21	1.94	0.50
1:A:170:VAL:O	1:A:490:VAL:HA	2.12	0.49
1:A:270:ASP:O	1:A:274:LEU:HG	2.13	0.49
1:A:183:VAL:HG21	1:A:451:ASN:HD21	1.78	0.49
1:A:55:LYS:HB3	1:A:55:LYS:HE2	1.66	0.49
1:A:294:GLU:O	1:A:298:GLN:HG2	2.13	0.48
1:A:172:LEU:HD11	1:A:491:LEU:HD12	1.95	0.48
1:A:304:PHE:HE2	3:A:600:08Y:H25	1.79	0.48
1:A:156:LEU:O	1:A:160:LEU:HB2	2.13	0.47
1:A:181:MET:HE3	1:A:208:LYS:HG3	1.94	0.46
1:A:184:ILE:HA	1:A:184:ILE:HD13	1.74	0.46
1:A:156:LEU:CD1	1:A:175:VAL:HG13	2.46	0.46
1:A:275:MET:HE2	1:A:295:LEU:HG	1.98	0.46
1:A:334:GLU:OE2	1:A:353:MET:HB3	2.17	0.45
1:A:85:THR:HB	1:A:401:LEU:HD21	1.99	0.44
1:A:276:ILE:HA	1:A:279:GLN:HE21	1.83	0.43
1:A:275:MET:HE2	1:A:275:MET:HB3	1.86	0.43
1:A:269:VAL:O	1:A:269:VAL:CG1	2.68	0.42
1:A:275:MET:CE	1:A:295:LEU:HA	2.49	0.42
1:A:270:ASP:OD1	1:A:273:GLN:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:LEU:HD22	1:A:483:LEU:CD1	2.50	0.42
1:A:319:TYR:CZ	1:A:475:LEU:HB2	2.55	0.42
1:A:389:PRO:HD2	1:A:392:VAL:HG21	2.01	0.41
1:A:172:LEU:HD11	1:A:491:LEU:CD1	2.51	0.41
1:A:160:LEU:HB3	1:A:463:PHE:CE2	2.57	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	448/487 (92%)	421 (94%)	22 (5%)	5 (1%)	17 10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	GLY
1	A	423	ASN
1	A	29	SER
1	A	263	ASP
1	A	168	LYS

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	417/443 (94%)	386 (93%)	31 (7%)	17	11

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	34	LYS
1	A	55	LYS
1	A	66	LYS
1	A	70	LYS
1	A	103	THR
1	A	106	ARG
1	A	125	GLU
1	A	131	SER
1	A	175	VAL
1	A	211	LEU
1	A	223	ILE
1	A	251	LYS
1	A	254	LYS
1	A	258	GLU
1	A	263	ASP
1	A	288	LYS
1	A	290	LEU
1	A	293	LEU
1	A	312	SER
1	A	373	LEU
1	A	381	VAL
1	A	406	LYS
1	A	409	THR
1	A	422	LYS
1	A	423	ASN
1	A	441	ASN
1	A	466	LYS
1	A	487	LYS
1	A	492	LYS
1	A	495	SER

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	65	HIS
1	A	151	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	279	GLN
1	A	352	GLN
1	A	441	ASN
1	A	451	ASN
1	A	484	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 carbohydrates 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	508	1	30,50,50	1.96	8 (26%)	24,82,82	2.51	12 (50%)
3	08Y	A	600	-	44,49,49	1.61	6 (13%)	47,79,79	2.46	16 (34%)

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	508	1	-	0/10/54/54	0/0/8/8
3	08Y	A	600	-	-	0/19/93/93	0/6/7/7

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	508	HEM	C3D-C4D	-4.82	1.45	1.51
2	A	508	HEM	C3B-C4B	-4.38	1.48	1.51
2	A	508	HEM	C2C-C1C	-4.04	1.44	1.52
3	A	600	08Y	C24-C26	2.05	1.46	1.41
2	A	508	HEM	CMA-C3A	2.08	1.55	1.51
3	A	600	08Y	C25-C26	2.12	1.45	1.41
2	A	508	HEM	C3C-CAC	2.23	1.55	1.51
2	A	508	HEM	C1C-NC	2.33	1.38	1.36
3	A	600	08Y	C32-C31	2.33	1.42	1.36
2	A	508	HEM	CAA-C2A	2.68	1.56	1.52
2	A	508	HEM	C4C-NC	2.78	1.39	1.36
3	A	600	08Y	C24-C21	3.66	1.51	1.45
3	A	600	08Y	O2-C2	4.43	1.44	1.38
3	A	600	08Y	BR-C29	6.83	2.00	1.90

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	08Y	O2-C2-N1	-5.53	108.53	113.17
2	A	508	HEM	C3B-CAB-CBB	-4.95	116.87	124.46
3	A	600	08Y	C31-C28-C26	-3.29	115.47	121.11
3	A	600	08Y	C24-C21-C22	-2.82	119.72	123.08
3	A	600	08Y	O3-C8-C5	-2.73	122.67	125.59
2	A	508	HEM	CBA-CAA-C2A	-2.69	107.71	112.53
2	A	508	HEM	CBD-CAD-C3D	-2.53	106.19	113.55
3	A	600	08Y	C4-C1-C2	-2.40	115.12	117.70
2	A	508	HEM	C3B-C4B-NB	-2.06	107.69	111.63
2	A	508	HEM	C3C-CAC-CBC	-2.00	121.39	124.46
3	A	600	08Y	C24-C26-C25	2.07	126.49	122.59
3	A	600	08Y	C31-C28-N5	2.12	137.03	130.72
3	A	600	08Y	C6-N2-C9	2.13	126.51	123.02
3	A	600	08Y	C7-C6-N2	2.17	106.64	103.25
3	A	600	08Y	C9-C3-N1	2.20	113.98	111.72
2	A	508	HEM	C2D-C3D-C4D	2.38	105.54	101.50
2	A	508	HEM	CMC-C2C-C3C	2.46	122.68	116.53
3	A	600	08Y	C4-C1-N2	2.61	105.57	102.65
2	A	508	HEM	CMD-C2D-C3D	2.97	127.51	114.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	600	08Y	C23-C25-C29	3.11	137.37	131.91
3	A	600	08Y	C23-C17-C21	3.37	116.91	113.23
3	A	600	08Y	C24-C21-C17	3.37	119.91	114.86
2	A	508	HEM	C3B-C4B-CHC	3.64	128.29	123.16
3	A	600	08Y	C27-N4-C18	3.68	115.77	109.50
2	A	508	HEM	CMB-C2B-C3B	3.95	126.39	116.53
2	A	508	HEM	CAD-C3D-C4D	4.19	127.24	112.47
2	A	508	HEM	CAD-C3D-C2D	4.87	127.21	113.22
3	A	600	08Y	C27-N4-C17	10.70	123.29	111.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	508	HEM	2	0
3	A	600	08Y	3	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, 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	456/487 (93%)	0.76	54 (11%) 6 10	30, 50, 82, 118	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	THR	7.0
1	A	263	ASP	5.8
1	A	287	HIS	5.7
1	A	189	PHE	5.4
1	A	28	HIS	5.3
1	A	202	PRO	5.1
1	A	310	THR	4.4
1	A	269	VAL	4.1
1	A	162	ARG	4.0
1	A	313	VAL	4.0
1	A	168	LYS	3.9
1	A	422	LYS	3.8
1	A	258	GLU	3.7
1	A	163	GLU	3.6
1	A	200	GLN	3.6
1	A	314	LEU	3.6
1	A	469	LYS	3.5
1	A	448	ALA	3.5
1	A	306	GLY	3.5
1	A	171	THR	3.4
1	A	255	ARG	3.4
1	A	293	LEU	3.3
1	A	309	THR	3.3
1	A	426	ASN	3.2
1	A	265	GLN	3.1
1	A	251	LYS	3.1
1	A	205	GLU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	302	PHE	3.0
1	A	435	PHE	3.0
1	A	274	LEU	3.0
1	A	305	ALA	3.0
1	A	384	ASN	3.0
1	A	421	LYS	2.9
1	A	254	LYS	2.9
1	A	369	ILE	2.9
1	A	373	LEU	2.9
1	A	279	GLN	2.8
1	A	203	PHE	2.7
1	A	317	ILE	2.6
1	A	368	PRO	2.6
1	A	442	CYS	2.6
1	A	289	ALA	2.6
1	A	411	PRO	2.5
1	A	256	MET	2.4
1	A	311	SER	2.4
1	A	371	MET	2.3
1	A	341	ASN	2.3
1	A	385	GLY	2.2
1	A	119	SER	2.2
1	A	364	LEU	2.2
1	A	312	SER	2.1
1	A	393	VAL	2.1
1	A	243	ARG	2.1
1	A	303	ILE	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(\AA^2)	Q<0.9
3	08Y	A	600	43/43	0.87	0.20	0.28	52,58,71,73	0
2	HEM	A	508	43/43	0.97	0.19	-0.41	19,25,27,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.