



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:06 PM GMT

PDB ID : 4GL5
Title : Structure of human placental aromatase complexed with designed inhibitor HDDG029 (compound 4)
Authors : Ghosh, D.
Deposited on : 2012-08-13
Resolution : 3.48 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

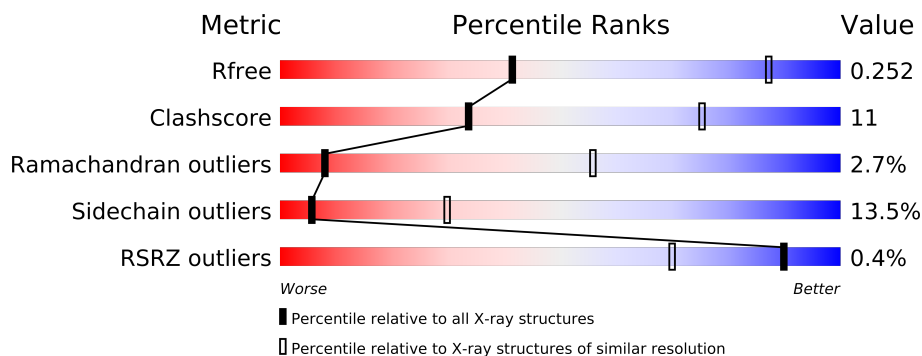
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance


The reported resolution of this entry is 3.48 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}	66092	1175 (3.66-3.30)
Clashscore	79885	1001 (3.62-3.34)
Ramachandran outliers	78287	1001 (3.64-3.32)
Sidechain outliers	78261	1002 (3.64-3.32)
RSRZ outliers	66119	1175 (3.66-3.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	503	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 3727 atoms, of which 0 are hydrogen and 0 are deuterium.

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 19A1.

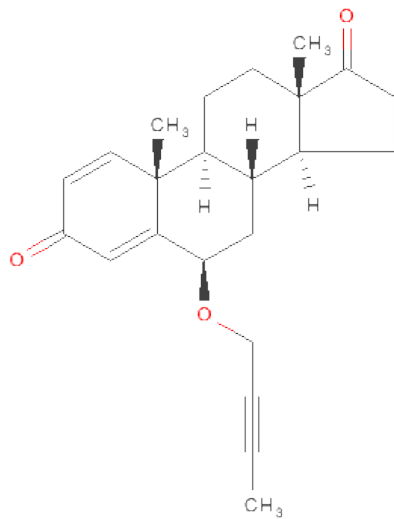
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	452	3658	2361	617	650	30	0	0	0

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

- Molecule 3 is (6ALPHA,8ALPHA)-6-(BUT-2-YN-1-YLOXY)ANDROSTA-1,4-DIENE-3,17-DIONE (three-letter code: G29) (formula: $C_{23}H_{28}O_3$).

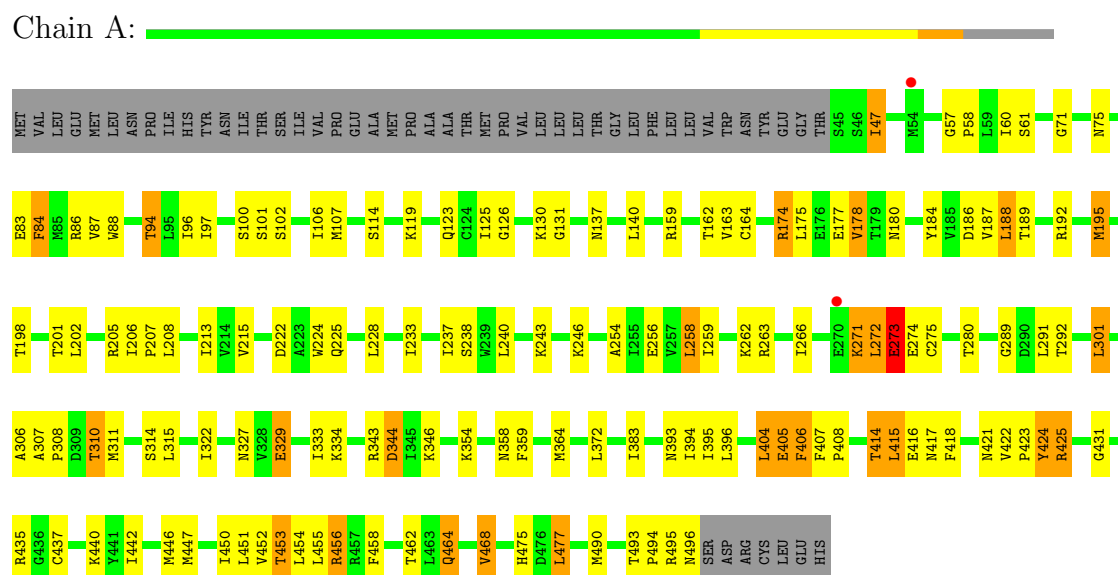


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	26	23	3	0	0

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: Cytochrome P450 19A1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.33Å 140.33Å 118.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.48 30.38 – 3.48	Depositor EDS
% Data completeness (in resolution range)	91.2 (50.00-3.48) 91.4 (30.38-3.48)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.210 , 0.260 0.206 , 0.252	Depositor DCC
R_{free} test set	832 reflections (5.44%)	DCC
Wilson B-factor (Å ²)	87.7	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 29.0	EDS
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 16132 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3727	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, G29

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	0.47	0/3737	0.62	1/5035 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	301	LEU	CA-CB-CG	6.63	130.56	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	GLY	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the

Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3658	0	3735	83	0
2	A	43	0	30	0	0
3	A	26	0	28	3	0
All	All	3727	0	3793	83	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (83) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:94:THR:HB	1:A:393:ASN:HB2	1.55	0.88
1:A:225:GLN:HG3	1:A:477:LEU:HB2	1.61	0.81
1:A:310:THR:HG22	3:A:601:G29:H13	1.66	0.77
1:A:71:GLY:HA2	1:A:372:LEU:HD21	1.68	0.75
1:A:315:LEU:HD13	1:A:450:ILE:HD11	1.71	0.73
1:A:97:ILE:HG21	1:A:102:SER:HB2	1.75	0.68
1:A:322:ILE:HD13	1:A:455:LEU:HD11	1.77	0.67
1:A:87:VAL:CG1	1:A:88:TRP:N	2.59	0.66
1:A:47:ILE:HD11	1:A:84:PHE:HE2	1.60	0.65
1:A:424:TYR:HD1	1:A:424:TYR:O	1.82	0.63
1:A:358:ASN:ND2	1:A:418:PHE:HB3	2.14	0.62
1:A:477:LEU:HD22	3:A:601:G29:H25	1.81	0.61
1:A:106:ILE:HD13	1:A:394:ILE:HG21	1.81	0.61
1:A:87:VAL:HG12	1:A:88:TRP:N	2.15	0.61
1:A:358:ASN:HD22	1:A:418:PHE:HB3	1.67	0.60
1:A:452:VAL:O	1:A:456:ARG:HB3	2.02	0.60
1:A:358:ASN:ND2	1:A:418:PHE:O	2.36	0.59
1:A:75:ASN:HD22	1:A:475:HIS:HE1	1.51	0.59
1:A:424:TYR:C	1:A:424:TYR:CD1	2.77	0.58
1:A:437:CYS:HB3	1:A:440:LYS:HB3	1.85	0.58
1:A:311:MET:CE	1:A:447:MET:HG3	2.33	0.58
1:A:83:GLU:HA	1:A:83:GLU:OE1	2.04	0.57
1:A:329:GLU:O	1:A:333:ILE:HG12	2.06	0.56
1:A:406:PHE:CE2	1:A:422:VAL:HG12	2.41	0.56
1:A:174:ARG:HG2	1:A:177:GLU:HG3	1.87	0.56
1:A:195:MET:HA	1:A:195:MET:CE	2.36	0.55
1:A:414:THR:C	1:A:416:GLU:H	2.11	0.54
1:A:464:GLN:HE21	1:A:464:GLN:N	2.05	0.54
1:A:178:VAL:HG13	1:A:186:ASP:H	1.73	0.54
1:A:187:VAL:HG21	1:A:490:MET:HG3	1.89	0.54
1:A:97:ILE:HG21	1:A:102:SER:CB	2.38	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:208:LEU:HB3	1:A:258:LEU:HD21	1.90	0.54
1:A:107:MET:CE	1:A:431:GLY:HA2	2.39	0.53
1:A:57:GLY:O	1:A:60:ILE:HG13	2.10	0.52
1:A:87:VAL:CG1	1:A:88:TRP:H	2.22	0.52
1:A:266:ILE:HD13	1:A:280:THR:HG23	1.92	0.51
1:A:343:ARG:HG2	1:A:344:ASP:H	1.76	0.51
1:A:96:ILE:HG22	1:A:395:ILE:HB	1.92	0.51
1:A:358:ASN:HD22	1:A:418:PHE:CB	2.25	0.50
1:A:311:MET:HE3	1:A:447:MET:HG3	1.93	0.49
1:A:442:ILE:O	1:A:446:MET:HG3	2.11	0.49
1:A:306:ALA:O	1:A:310:THR:HG23	2.12	0.49
1:A:61:SER:HB2	1:A:87:VAL:HG13	1.93	0.49
1:A:195:MET:HE3	1:A:195:MET:HA	1.95	0.48
1:A:310:THR:CG2	3:A:601:G29:H13	2.40	0.48
1:A:87:VAL:HG13	1:A:88:TRP:H	1.78	0.48
1:A:106:ILE:HD12	1:A:396:LEU:HD21	1.95	0.47
1:A:100:SER:HB3	1:A:405:GLU:OE1	2.14	0.47
1:A:262:LYS:O	1:A:266:ILE:HG13	2.14	0.47
1:A:424:TYR:C	1:A:424:TYR:HD1	2.17	0.47
1:A:126:GLY:O	1:A:130:LYS:HE3	2.14	0.47
1:A:159:ARG:O	1:A:163:VAL:HG23	2.15	0.46
1:A:119:LYS:O	1:A:123:GLN:HB2	2.16	0.46
1:A:458:PHE:O	1:A:495:ARG:NH1	2.49	0.46
1:A:71:GLY:HA2	1:A:372:LEU:CD2	2.42	0.45
1:A:125:ILE:HG21	1:A:224:TRP:HA	1.99	0.45
1:A:180:ASN:HB2	1:A:184:TYR:HB2	1.97	0.45
1:A:315:LEU:HD22	1:A:450:ILE:HD11	1.99	0.45
1:A:188:LEU:O	1:A:192:ARG:HG3	2.17	0.45
1:A:101:SER:HA	1:A:425:ARG:HH22	1.82	0.44
1:A:259:ILE:HD13	1:A:263:ARG:HH12	1.82	0.44
1:A:58:PRO:HA	1:A:88:TRP:HB2	1.99	0.44
1:A:315:LEU:HD13	1:A:450:ILE:CD1	2.43	0.44
1:A:452:VAL:HG12	1:A:453:THR:N	2.32	0.44
1:A:311:MET:HE1	1:A:446:MET:HB2	2.00	0.43
1:A:271:LYS:O	1:A:274:GLU:HG3	2.17	0.43
1:A:414:THR:HB	1:A:416:GLU:HB2	1.99	0.43
1:A:238:SER:C	1:A:240:LEU:H	2.22	0.43
1:A:343:ARG:HG2	1:A:344:ASP:N	2.34	0.42
1:A:307:ALA:HB3	1:A:308:PRO:HD3	2.01	0.42
1:A:107:MET:HE1	1:A:431:GLY:HA2	2.02	0.42
1:A:359:PHE:HA	1:A:415:LEU:HD21	2.02	0.42
1:A:83:GLU:CA	1:A:83:GLU:OE1	2.68	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:322:ILE:HG13	1:A:359:PHE:CZ	2.55	0.41
1:A:206:ILE:HA	1:A:207:PRO:HD2	1.88	0.41
1:A:83:GLU:OE2	1:A:404:LEU:HD21	2.21	0.41
1:A:273:GLU:CD	1:A:273:GLU:H	2.24	0.41
1:A:114:SER:HA	1:A:435:ARG:NH1	2.36	0.41
1:A:137:ASN:HB3	1:A:140:LEU:HB3	2.02	0.41
1:A:208:LEU:HD13	1:A:213:ILE:HG13	2.03	0.41
1:A:315:LEU:HD21	1:A:447:MET:HG2	2.03	0.40
1:A:254:ALA:O	1:A:258:LEU:HD12	2.22	0.40
1:A:407:PHE:CD1	1:A:417:ASN:HB3	2.57	0.40

There are no symmetry-related clashes.

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	450/503 (90%)	387 (86%)	51 (11%)	12 (3%)	8 56

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	PHE
1	A	272	LEU
1	A	421	ASN
1	A	84	PHE
1	A	494	PRO
1	A	271	LYS
1	A	273	GLU
1	A	174	ARG
1	A	289	GLY
1	A	423	PRO
1	A	468	VAL
1	A	408	PRO

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	406/452 (90%)	351 (86%)	55 (14%)	6 30

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ILE
1	A	86	ARG
1	A	94	THR
1	A	162	THR
1	A	164	CYS
1	A	175	LEU
1	A	178	VAL
1	A	188	LEU
1	A	189	THR
1	A	195	MET
1	A	198	THR
1	A	201	THR
1	A	202	LEU
1	A	205	ARG
1	A	215	VAL
1	A	222	ASP
1	A	228	LEU
1	A	233	ILE
1	A	237	ILE
1	A	243	LYS
1	A	246	LYS
1	A	256	GLU
1	A	258	LEU
1	A	272	LEU
1	A	273	GLU
1	A	275	CYS
1	A	291	LEU
1	A	292	THR
1	A	301	LEU
1	A	310	THR
1	A	314	SER

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Mol	Chain	Res	Type
1	A	327	ASN
1	A	329	GLU
1	A	334	LYS
1	A	344	ASP
1	A	346	LYS
1	A	354	LYS
1	A	364	MET
1	A	383	ILE
1	A	404	LEU
1	A	405	GLU
1	A	414	THR
1	A	415	LEU
1	A	424	TYR
1	A	425	ARG
1	A	451	LEU
1	A	453	THR
1	A	454	LEU
1	A	456	ARG
1	A	462	THR
1	A	464	GLN
1	A	468	VAL
1	A	477	LEU
1	A	493	THR
1	A	496	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	325	HIS
1	A	358	ASN
1	A	393	ASN
1	A	464	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	600	1	49,50,50	2.10	13 (26%)	46,82,82	2.11	9 (19%)
3	G29	A	601	-	29,29,29	1.69	6 (20%)	45,45,45	1.72	11 (24%)

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	600	1	-	0/14/114/114	0/0/8/8
3	G29	A	601	-	-	0/4/66/66	0/0/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	HEM	C3B-C2B	-6.13	1.33	1.43
2	A	600	HEM	C3D-C2D	5.30	1.53	1.43
2	A	600	HEM	C3C-C2C	-5.12	1.34	1.43
2	A	600	HEM	C3C-CAC	4.73	1.55	1.40
2	A	600	HEM	C3B-CAB	4.38	1.54	1.40
3	A	601	G29	C4-C5	4.04	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	G29	C10-C9	-4.01	1.53	1.57
3	A	601	G29	C2-C1	3.60	1.39	1.33
2	A	600	HEM	C4A-C3A	3.43	1.44	1.40
3	A	601	G29	C10-C1	-3.43	1.46	1.50
2	A	600	HEM	FE-ND	3.35	2.10	1.97
2	A	600	HEM	FE-NC	2.86	2.08	1.97
3	A	601	G29	C2-C3	-2.82	1.39	1.46
2	A	600	HEM	CMC-C2C	2.49	1.55	1.47
2	A	600	HEM	CMB-C2B	2.37	1.54	1.47
2	A	600	HEM	CMD-C2D	2.17	1.54	1.47
2	A	600	HEM	FE-NA	2.17	2.01	1.92
3	A	601	G29	C4-C3	-2.16	1.40	1.45
2	A	600	HEM	C2D-C1D	2.09	1.45	1.44

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	HEM	C3B-C4B-NB	-9.00	107.56	114.00
2	A	600	HEM	C4D-ND-C1D	6.13	111.44	105.16
3	A	601	G29	C10-C9-C8	-4.57	108.46	112.02
2	A	600	HEM	C2D-C1D-ND	-3.87	108.36	112.93
3	A	601	G29	C16-C17-C13	3.67	112.30	108.60
3	A	601	G29	O-C6-C5	3.64	115.89	108.24
3	A	601	G29	C15-C14-C13	3.38	106.99	104.06
2	A	600	HEM	CHC-C4B-NB	3.05	127.12	124.58
3	A	601	G29	C2-C3-C4	2.86	120.18	117.12
2	A	600	HEM	CHD-C1D-ND	2.70	126.83	124.58
2	A	600	HEM	CBD-CAD-C3D	-2.67	108.55	114.37
3	A	601	G29	O-C23-C24	2.62	118.66	111.55
2	A	600	HEM	C1B-NB-C4B	2.53	107.75	105.16
3	A	601	G29	O2-C17-C16	-2.41	122.61	125.72
3	A	601	G29	C11-C9-C8	2.31	115.06	111.73
2	A	600	HEM	CBA-CAA-C2A	-2.23	108.76	112.69
3	A	601	G29	C14-C13-C17	-2.15	97.95	100.52
3	A	601	G29	C15-C16-C17	-2.10	103.49	105.67
2	A	600	HEM	CMA-C3A-C4A	-2.06	125.45	128.62
3	A	601	G29	C23-O-C6	2.01	117.08	113.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	452/503 (89%)	-0.10	2 (0%)	90 70	68, 91, 116, 129	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	MET	2.3
1	A	270	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	HEM	A	600	43/43	0.25	0.20	57,59,62,65	0
3	G29	A	601	26/26	0.23	0.08	72,75,77,78	0

6.5 Other polymers ⓘ

There are no such residues in this entry.