



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:23 AM GMT

PDB ID : 4J14
Title : Crystal Structure of Human Cytochrome P450 CYP46A1 with Posaconazole Bound
Authors : Stout, C.D.; Mast, N.; Pikuleva, I.A.
Deposited on : 2013-01-31
Resolution : 2.50 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>

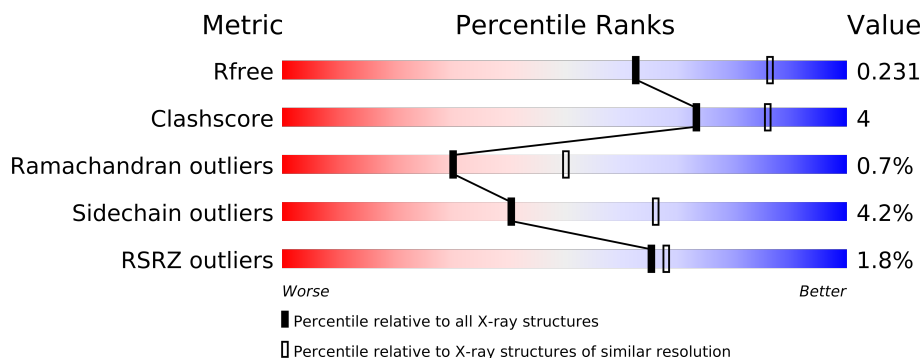
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	456	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	A	603	-	X

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 3689 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.

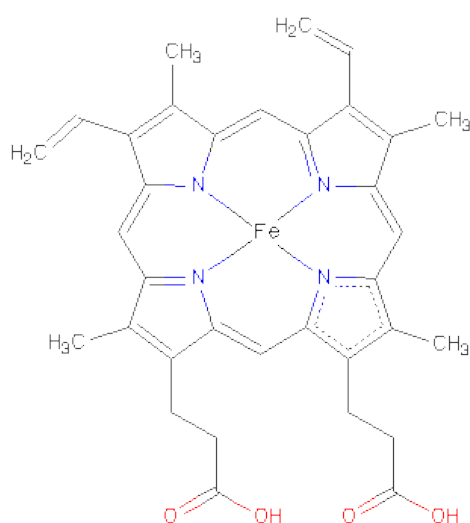
- Molecule 1 is a protein called Cholesterol 24-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	436	3507	2241	615	634	17	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

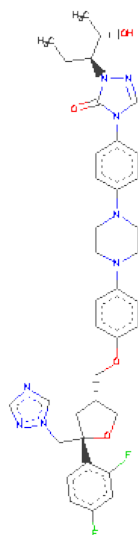
Chain	Residue	Modelled	Actual	Comment	Reference
A	49	MET	-	EXPRESSION TAG	UNP Q9Y6A2
A	50	ALA	-	EXPRESSION TAG	UNP Q9Y6A2
A	501	HIS	-	EXPRESSION TAG	UNP Q9Y6A2
A	502	HIS	-	EXPRESSION TAG	UNP Q9Y6A2
A	503	HIS	-	EXPRESSION TAG	UNP Q9Y6A2
A	504	HIS	-	EXPRESSION TAG	UNP Q9Y6A2

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



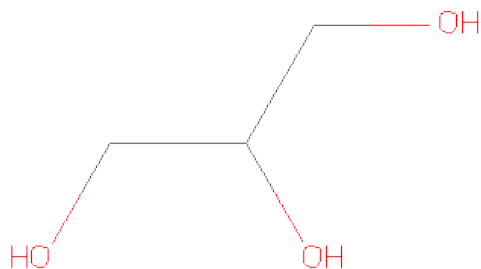
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is POSACONAZOLE (three-letter code: X2N) (formula: $C_{37}H_{42}F_2N_8O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			51	37	2	8	4		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

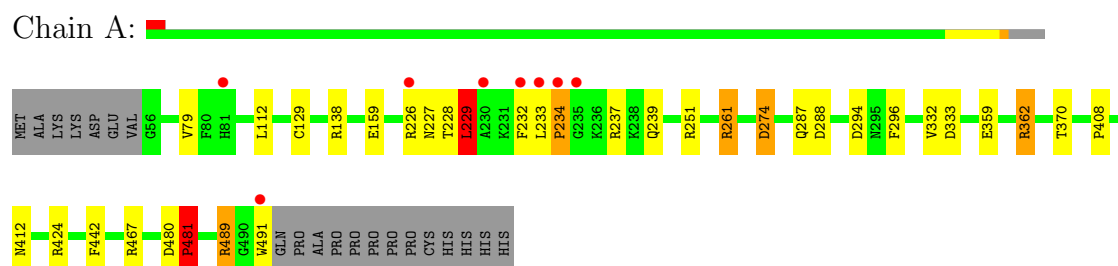
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	82	Total	O	0	0
			82	82		

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: Cholesterol 24-hydroxylase



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.64Å 121.64Å 143.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.78 – 2.50 60.82 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (92.78-2.50) 99.9 (60.82-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.08 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.213 , 0.263 0.187 , 0.231	Depositor DCC
R_{free} test set	977 reflections (5.44%)	DCC
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 21.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 18945 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3689	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: GOL, X2N, 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	0.74	0/3579	0.74	4/4828 (0.1%)

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	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	PRO	N-CA-C	-6.26	95.81	112.10
1	A	362	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	A	362	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	A	138	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	ASN	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	3507	0	0	14	0
2	A	43	0	0	2	0
3	A	51	0	0	1	0
4	A	6	0	8	0	0
5	A	82	0	0	1	0
All	All	3689	0	8	15	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 4.

All (15) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:251:ARG:NH1	1:A:294:ASP:OD1	2.17	0.77
1:A:480:ASP:C	1:A:481:PRO:O	2.24	0.72
1:A:228:THR:CA	1:A:229:LEU:CB	2.71	0.68
1:A:362:ARG:NH1	1:A:408:PRO:O	2.27	0.68
1:A:370:THR:OG1	2:A:601:HEM:O2A	2.24	0.54
1:A:261:ARG:NH2	1:A:274:ASP:OD2	2.45	0.49
1:A:233:LEU:N	1:A:234:PRO:CD	2.78	0.47
1:A:480:ASP:O	1:A:481:PRO:O	2.32	0.47
1:A:296:PHE:CD1	1:A:296:PHE:C	2.89	0.47
1:A:467:ARG:N	1:A:480:ASP:OD2	2.48	0.46
1:A:333:ASP:OD2	1:A:489:ARG:NH1	2.48	0.46
1:A:129:CYS:N	5:A:711:HOH:O	2.48	0.46
1:A:491:TRP:CD1	1:A:491:TRP:C	2.90	0.45
2:A:601:HEM:C1A	3:A:602:X2N:CAS	2.99	0.42
1:A:359:GLU:OE2	1:A:412:ASN:N	2.52	0.41

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	434/456 (95%)	413 (95%)	18 (4%)	3 (1%)	30 50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	LEU
1	A	234	PRO
1	A	481	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	379/397 (96%)	363 (96%)	16 (4%)	40 66

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	VAL
1	A	112	LEU
1	A	159	GLU
1	A	226	ARG
1	A	229	LEU
1	A	232	PHE
1	A	237	ARG
1	A	239	GLN
1	A	261	ARG
1	A	274	ASP
1	A	287	GLN
1	A	288	ASP
1	A	332	VAL
1	A	424	ARG
1	A	442	PHE
1	A	489	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

3 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	601	1,3	49,50,50	7.32	25 (51%)	46,82,82	2.72	16 (34%)
3	X2N	A	602	2	57,57,57	1.67	6 (10%)	78,82,82	2.21	27 (34%)
4	GOL	A	603	-	5,5,5	0.32	0	5,5,5	0.41	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	601	1,3	-	0/14/114/114	0/0/8/8
3	X2N	A	602	2	-	0/35/59/59	0/7/7/7
4	GOL	A	603	-	-	0/4/4/4	0/0/0/0

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C2B-C1B	-37.60	1.35	1.44
2	A	601	HEM	C3D-C4D	19.08	1.49	1.44
2	A	601	HEM	C2D-C1D	17.54	1.48	1.44
2	A	601	HEM	CHB-C1B	9.97	1.50	1.35
3	A	602	X2N	CBN-NBW	-8.75	1.34	1.44
2	A	601	HEM	C4A-C3A	8.69	1.51	1.40
2	A	601	HEM	CHD-C4C	6.91	1.49	1.36
2	A	601	HEM	C3D-C2D	-6.46	1.32	1.43
2	A	601	HEM	CHC-C1C	6.23	1.48	1.36
2	A	601	HEM	FE-NB	6.09	2.19	1.97
3	A	602	X2N	OAC-CBP	5.19	1.34	1.23
2	A	601	HEM	C1A-C2A	4.90	1.51	1.43
2	A	601	HEM	CBB-CAB	3.97	1.52	1.28
2	A	601	HEM	C3C-CAC	3.75	1.52	1.40
2	A	601	HEM	C1A-CHA	3.50	1.49	1.39
2	A	601	HEM	C1A-NA	3.46	1.43	1.36
2	A	601	HEM	C3B-C4B	3.37	1.48	1.44
3	A	602	X2N	CAT-NBF	3.32	1.35	1.30
2	A	601	HEM	C3C-C2C	3.29	1.49	1.43
2	A	601	HEM	CHD-C1D	-3.22	1.31	1.39
2	A	601	HEM	C3B-C2B	3.15	1.49	1.43
2	A	601	HEM	C2C-C1C	-3.01	1.34	1.43
2	A	601	HEM	C4D-ND	-2.83	1.33	1.39
2	A	601	HEM	C1B-NB	-2.82	1.33	1.39
3	A	602	X2N	CAA-CAU	-2.56	1.32	1.50
2	A	601	HEM	CHA-C4D	-2.40	1.32	1.35
2	A	601	HEM	FE-NA	2.40	2.02	1.92
3	A	602	X2N	OBG-CBK	-2.26	1.32	1.37
2	A	601	HEM	C3B-CAB	-2.26	1.32	1.40
3	A	602	X2N	CAQ-NBE	2.10	1.35	1.31
2	A	601	HEM	CHC-C4B	-2.06	1.34	1.39

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	C3B-C4B-NB	-9.19	107.43	114.00
3	A	602	X2N	NBE-CAQ-NBD	-7.03	109.55	116.05
3	A	602	X2N	CAQ-NBE-NBV	5.53	107.68	102.81
2	A	601	HEM	C1B-NB-C4B	5.28	110.56	105.16
2	A	601	HEM	C4A-C3A-C2A	5.07	110.52	107.00
2	A	601	HEM	CHC-C1C-NC	-4.76	120.60	124.73
3	A	602	X2N	CAS-NBD-CAQ	4.73	105.73	102.31
3	A	602	X2N	CAT-NBF-NBX	4.70	109.69	103.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	X2N	CBP-NBX-NBF	-4.55	107.36	109.58
2	A	601	HEM	CHC-C4B-NB	4.44	128.28	124.58
3	A	602	X2N	CAY-NBU-CBM	-4.13	106.82	118.05
2	A	601	HEM	CAA-C2A-C3A	-4.13	117.22	129.00
2	A	601	HEM	CHD-C4C-NC	4.01	128.22	124.73
2	A	601	HEM	C4C-NC-C1C	3.99	109.68	105.53
3	A	602	X2N	CAO-CBN-CAN	-3.89	115.34	121.29
3	A	602	X2N	CAM-CAO-CBN	3.74	123.17	119.29
2	A	601	HEM	C2D-C1D-ND	-3.56	108.72	112.93
2	A	601	HEM	C4A-CHB-C1B	-3.56	122.79	127.47
2	A	601	HEM	CBD-CAD-C3D	-3.46	106.82	114.37
2	A	601	HEM	CMA-C3A-C4A	-3.39	123.41	128.62
2	A	601	HEM	C4D-ND-C1D	3.35	108.59	105.16
3	A	602	X2N	CAL-CAN-CBN	3.35	122.77	119.29
3	A	602	X2N	CAW-CAY-NBU	-3.34	104.33	110.62
3	A	602	X2N	FAE-CBI-CAG	-3.06	112.63	118.54
3	A	602	X2N	CBS-NBX-NBF	-3.03	118.61	121.17
3	A	602	X2N	CAN-CBN-NBW	2.92	123.57	119.55
3	A	602	X2N	CBB-C7-C32	-2.91	105.14	111.11
2	A	601	HEM	CHA-C4D-ND	2.90	128.29	124.31
3	A	602	X2N	CAX-NBT-CAW	2.86	117.56	111.67
2	A	601	HEM	C1A-C2A-C3A	-2.85	103.97	106.92
3	A	602	X2N	CAM-CBM-NBU	-2.74	117.46	121.37
3	A	602	X2N	CAL-CBM-NBU	2.74	125.28	121.37
3	A	602	X2N	CAS-NBV-NBE	-2.67	107.75	110.33
3	A	602	X2N	CAA-CAU-CBS	2.63	118.05	113.60
3	A	602	X2N	CBO-CAP-CAG	-2.58	119.77	123.32
3	A	602	X2N	FAE-CBI-CAR	2.46	121.57	118.85
3	A	602	X2N	CBC-NBV-CAS	2.38	135.96	129.88
3	A	602	X2N	CBC-C2-CAR	2.28	116.61	110.62
3	A	602	X2N	CBC-NBV-NBE	-2.27	116.28	121.44
2	A	601	HEM	CAA-C2A-C1A	-2.16	118.97	125.50
3	A	602	X2N	NBF-CAT-NBW	-2.09	106.42	109.98
3	A	602	X2N	CAV-C7-CBB	2.03	117.93	110.68
3	A	602	X2N	NBD-CAS-NBV	-2.01	109.26	111.89

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	436/456 (95%)	-0.05	8 (1%) 65 68	14, 36, 71, 113	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	HIS	4.1
1	A	230	ALA	3.4
1	A	491	TRP	3.2
1	A	233	LEU	2.9
1	A	232	PHE	2.6
1	A	226	ARG	2.3
1	A	234	PRO	2.2
1	A	235	GLY	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(\AA^2)	Q<0.9
4	GOL	A	603	6/6	0.27	6.60	79,80,81,81	0
3	X2N	A	602	51/51	0.20	0.38	28,57,99,100	0
2	HEM	A	601	43/43	0.13	-0.27	11,17,25,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.