



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 08:41 AM EST

PDB ID : 4J00
Title : Crystal Structure of CmlA, a diiron beta-hydroxylase from *Streptomyces venezuelae*
Authors : Knoot, C.J.; Makris, T.M.; Wilmot, C.M.; Lipscomb, J.D.
Deposited on : 2013-03-16
Resolution : 2.17 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

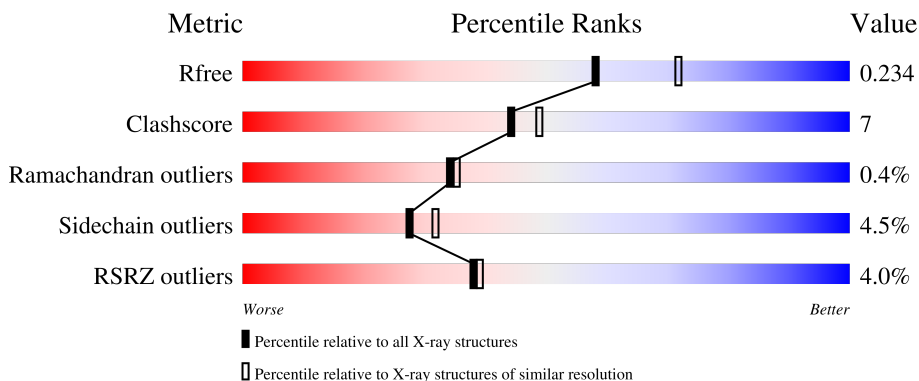
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.17 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}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	534	

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
6	GOL	A	608	-	-	X	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4440 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 CmlA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	522	4266	2701	762	789	14	0	8	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP F2RB80
A	-1	HIS	-	expression tag	UNP F2RB80
A	189	ASN	ASP	conflict	UNP F2RB80

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		

- Molecule 3 is OXYGEN ATOM (three-letter code: O) (formula: O).

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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total K 2 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

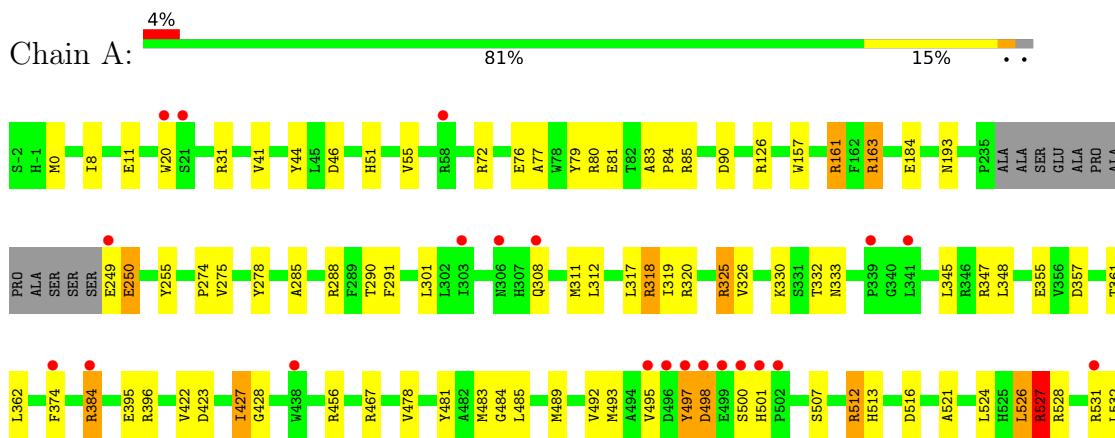
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	152	Total	O	0	1
			153	153		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: CmlA



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	153.16Å 153.16Å 93.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.66 – 2.17 38.66 – 2.17	Depositor EDS
% Data completeness (in resolution range)	96.4 (38.66-2.17) 96.4 (38.66-2.17)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.73 (at 2.18Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.233 0.208 , 0.234	Depositor DCC
R_{free} test set	2875 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtrriage
Anisotropy	0.369	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4440	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: FE, K, O, ACT, GOL

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	0.78	0/4380	0.96	14/5957 (0.2%)

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 (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	318	ARG	NE-CZ-NH1	11.23	125.92	120.30
1	A	456	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	A	318	ARG	NE-CZ-NH2	-8.41	116.10	120.30
1	A	456	ARG	CG-CD-NE	-7.22	96.64	111.80
1	A	31	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	A	347	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	A	325	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	163	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	126	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	325	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	161	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	126	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	31	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	347	ARG	NE-CZ-NH2	-5.19	117.70	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	250	GLU	Peptide

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	4266	0	4117	56	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	4	0	3	1	0
5	A	2	0	0	0	0
6	A	12	0	16	5	0
7	A	153	0	0	8	0
All	All	4440	0	4136	56	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 7.

All (56) 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:311:MET:HA	7:A:849:HOH:O	1.63	0.98
1:A:384[A]:ARG:O	1:A:384[A]:ARG:HD2	1.72	0.88
1:A:161:ARG:HD2	7:A:921:HOH:O	1.74	0.87
1:A:11:GLU:OE1	1:A:163:ARG:HD3	1.74	0.86
1:A:357:ASP:OD1	1:A:384[A]:ARG:NH2	2.16	0.78
1:A:483:MET:HG2	6:A:608:GOL:H31	1.66	0.77
1:A:278:TYR:O	1:A:288:ARG:NH2	2.21	0.72
1:A:163:ARG:HG2	7:A:921:HOH:O	1.91	0.69
1:A:41:VAL:HG11	1:A:79:TYR:CD1	2.28	0.69
1:A:483:MET:CG	6:A:608:GOL:H31	2.27	0.64
1:A:72:ARG:NH2	1:A:76:GLU:OE1	2.32	0.62
1:A:184:GLU:N	1:A:184:GLU:OE1	2.31	0.62
1:A:531:ARG:O	1:A:532:LEU:CB	2.48	0.61
1:A:312:LEU:HD22	7:A:848:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:TYR:OH	6:A:608:GOL:H2	2.05	0.57
1:A:330:LYS:HA	1:A:355:GLU:OE2	2.06	0.55
1:A:8:ILE:O	1:A:318:ARG:NH2	2.39	0.55
1:A:531:ARG:O	1:A:532:LEU:HB3	2.07	0.54
1:A:384[B]:ARG:NH2	7:A:918:HOH:O	2.41	0.53
1:A:484:GLY:O	1:A:495:VAL:HG22	2.10	0.51
1:A:274:PRO:HG3	1:A:301:LEU:HD11	1.92	0.51
1:A:85:ARG:HG2	1:A:157:TRP:CE2	2.46	0.51
1:A:493:MET:HE1	4:A:604:ACT:H3	1.94	0.50
1:A:428:GLY:O	7:A:951:HOH:O	2.19	0.50
1:A:478:VAL:O	1:A:521:ALA:HA	2.11	0.50
1:A:44:TYR:HA	1:A:51:HIS:CD2	2.47	0.49
1:A:326:VAL:HG11	1:A:345:LEU:HD13	1.93	0.49
1:A:51:HIS:O	1:A:55:VAL:HG23	2.13	0.48
1:A:20:TRP:HB3	1:A:308[B]:GLN:NE2	2.29	0.47
1:A:308[B]:GLN:NE2	7:A:932:HOH:O	2.39	0.47
1:A:291:PHE:CD1	1:A:318:ARG:HD2	2.49	0.46
1:A:77:ALA:O	1:A:81:GLU:HG3	2.15	0.46
1:A:332:THR:O	1:A:333:ASN:C	2.52	0.46
1:A:483:MET:CG	6:A:608:GOL:C3	2.94	0.46
1:A:500:SER:O	1:A:501:HIS:C	2.54	0.45
1:A:526:LEU:O	1:A:527:ARG:C	2.53	0.45
1:A:317:LEU:HD21	1:A:348:LEU:HD22	1.97	0.45
1:A:526:LEU:O	1:A:527:ARG:O	2.33	0.45
1:A:427:ILE:HG13	1:A:428:GLY:N	2.31	0.45
1:A:274:PRO:HG2	7:A:849:HOH:O	2.16	0.44
1:A:498:ASP:OD2	1:A:500:SER:HB2	2.18	0.43
1:A:512:ARG:NH2	1:A:516:ASP:OD1	2.51	0.43
1:A:285:ALA:O	1:A:288:ARG:HD3	2.19	0.42
1:A:319:ILE:O	1:A:320:ARG:C	2.57	0.42
1:A:524:LEU:HD22	1:A:528:ARG:HG3	2.02	0.42
1:A:396:ARG:HE	1:A:532:LEU:C	2.22	0.42
1:A:467:ARG:HG3	1:A:513:HIS:CE1	2.54	0.42
1:A:275:VAL:HG21	1:A:489:MET:SD	2.61	0.41
1:A:291:PHE:CG	1:A:318:ARG:HD2	2.56	0.41
1:A:485:LEU:HD12	6:A:608:GOL:H11	2.03	0.41
1:A:396:ARG:HA	1:A:423:ASP:OD2	2.21	0.41
1:A:83:ALA:N	1:A:84:PRO:CD	2.84	0.41
1:A:85:ARG:HG2	1:A:157:TRP:NE1	2.36	0.41
1:A:193:ASN:HA	1:A:320:ARG:NH1	2.36	0.40
1:A:361:THR:HG22	1:A:362:LEU:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:TYR:O	1:A:498:ASP:HB3	2.22	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	526/534 (98%)	499 (95%)	25 (5%)	2 (0%)	34 35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	ARG
1	A	498	ASP

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	449/448 (100%)	428 (95%)	21 (5%)	26 30

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET

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Mol	Chain	Res	Type
1	A	46	ASP
1	A	80	ARG
1	A	90	ASP
1	A	249	GLU
1	A	250	GLU
1	A	290	THR
1	A	325	ARG
1	A	374	PHE
1	A	384[A]	ARG
1	A	384[B]	ARG
1	A	395	GLU
1	A	422	VAL
1	A	427	ILE
1	A	481	TYR
1	A	492	VAL
1	A	497	TYR
1	A	507	SER
1	A	512	ARG
1	A	526	LEU
1	A	527	ARG

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

Mol	Chain	Res	Type
1	A	459	ASN
1	A	525	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 for Mogul analysis.

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
6	GOL	A	607	-	5,5,5	0.54	0	5,5,5	0.74	0
6	GOL	A	608	-	5,5,5	0.35	0	5,5,5	0.60	0
4	ACT	A	604	2	3,3,3	0.82	0	3,3,3	0.70	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	607	-	-	4/4/4/4	-
6	GOL	A	608	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	607	GOL	O1-C1-C2-O2
6	A	607	GOL	O1-C1-C2-C3
6	A	607	GOL	C1-C2-C3-O3
6	A	608	GOL	O1-C1-C2-C3
6	A	608	GOL	C1-C2-C3-O3
6	A	608	GOL	O1-C1-C2-O2
6	A	608	GOL	O2-C2-C3-O3
6	A	607	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	608	GOL	5	0
4	A	604	ACT	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(Å ²)	Q<0.9
1	A	522/534 (97%)	-0.02	21 (4%) 38 39	27, 50, 78, 124	7 (1%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	497	TYR	9.2
1	A	500	SER	6.6
1	A	499	GLU	4.5
1	A	308[A]	GLN	4.4
1	A	498	ASP	3.5
1	A	58	ARG	3.3
1	A	384[A]	ARG	2.7
1	A	531	ARG	2.6
1	A	495	VAL	2.6
1	A	341	LEU	2.4
1	A	496	ASP	2.4
1	A	249	GLU	2.3
1	A	21[A]	SER	2.3
1	A	502	PRO	2.3
1	A	303	ILE	2.2
1	A	438[A]	TRP	2.2
1	A	306	ASN	2.1
1	A	339	PRO	2.1
1	A	501	HIS	2.1
1	A	374	PHE	2.1
1	A	20	TRP	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 monosaccharides 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. 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	B-factors(Å ²)	Q<0.9
6	GOL	A	608	6/6	0.73	0.50	56,60,62,63	6
6	GOL	A	607	6/6	0.90	0.10	60,65,67,71	0
4	ACT	A	604	4/4	0.93	0.34	57,57,63,67	4
5	K	A	606	1/1	0.94	0.17	81,81,81,81	0
5	K	A	605	1/1	0.99	0.04	59,59,59,59	0
3	O	A	603	1/1	1.00	0.11	44,44,44,44	0
2	FE	A	601	1/1	1.00	0.12	42,42,42,42	0
2	FE	A	602	1/1	1.00	0.16	47,47,47,47	1

6.5 Other polymers [i](#)

There are no such residues in this entry.