



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 09:01 am BST

PDB ID : 5YNZ
Title : Crystal structure of the dihydroorotase domain (K1556A) of human CAD
Authors : Huang, Y.H.; Chen, K.L.; Cheng, J.H.; Huang, C.Y.
Deposited on : 2017-10-26
Resolution : 2.77 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

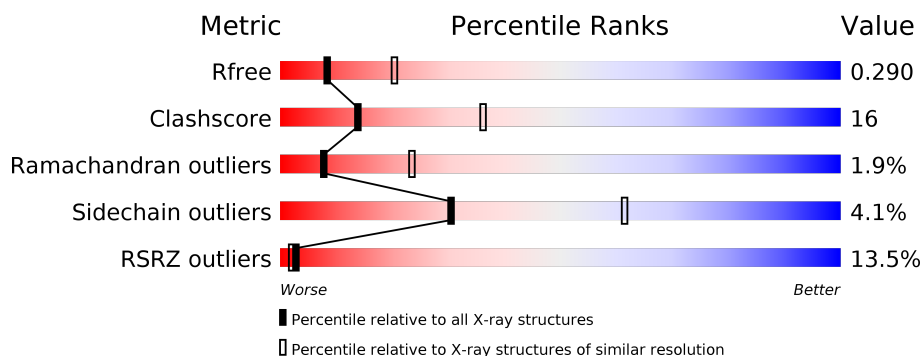
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 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	391	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2803 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 CAD protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2788	1772	497	506	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1556	ALA	LYS	engineered mutation	UNP P27708

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

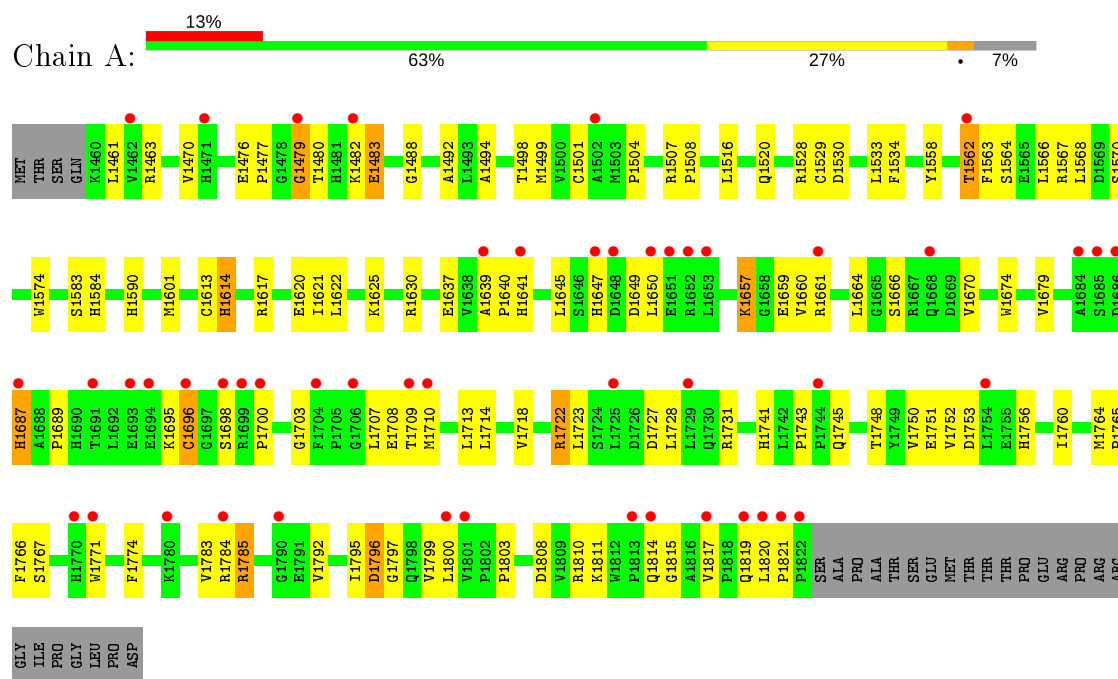
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		

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 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: CAD protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	88.84Å 108.63Å 99.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.80 – 2.77 29.81 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.80-2.77) 99.5 (29.81-2.77)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.76Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.226 , 0.289 0.227 , 0.290	Depositor DCC
R_{free} test set	600 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.777	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2803	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% 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: ZN

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	0.49	0/2863	0.68	1/3907 (0.0%)

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	1785	ARG	NE-CZ-NH2	-6.73	116.94	120.30

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	2788	0	2769	88	1
2	A	1	0	0	0	0
3	A	14	0	0	0	0
All	All	2803	0	2769	88	1

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 16.

All (88) 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:1785:ARG:HG3	1:A:1795:ILE:CD1	1.74	1.16
1:A:1785:ARG:HG3	1:A:1795:ILE:HD13	1.06	1.01
1:A:1785:ARG:CG	1:A:1795:ILE:HD13	2.00	0.85
1:A:1785:ARG:CG	1:A:1795:ILE:CD1	2.58	0.81
1:A:1752:VAL:HG12	1:A:1783:VAL:HA	1.62	0.79
1:A:1709:THR:O	1:A:1713:LEU:HD12	1.88	0.73
1:A:1477:PRO:HG2	1:A:1508:PRO:HD2	1.73	0.69
1:A:1647:HIS:HA	1:A:1650:LEU:HD12	1.75	0.68
1:A:1687:HIS:CD2	1:A:1707:LEU:HD12	2.30	0.67
1:A:1820:LEU:HD22	1:A:1821:PRO:HD2	1.76	0.66
1:A:1723:LEU:HD12	1:A:1727:ASP:HB3	1.77	0.66
1:A:1808:ASP:HB3	1:A:1811:LYS:HG3	1.78	0.65
1:A:1698:SER:O	1:A:1700:PRO:HD3	1.99	0.63
1:A:1743:PRO:HB2	1:A:1814:GLN:HG2	1.81	0.63
1:A:1483:GLU:HG3	1:A:1689:PRO:CG	2.28	0.63
1:A:1792:VAL:HG12	1:A:1800:LEU:HD12	1.81	0.62
1:A:1751:GLU:OE1	1:A:1785:ARG:NH2	2.29	0.62
1:A:1785:ARG:CZ	1:A:1785:ARG:HB2	2.30	0.61
1:A:1765:PRO:HB2	1:A:1766:PHE:CD2	2.38	0.58
1:A:1617:ARG:HB2	1:A:1620:GLU:HG3	1.86	0.57
1:A:1741:HIS:HB2	1:A:1817:VAL:HG22	1.87	0.57
1:A:1479:GLY:CA	1:A:1482:LYS:NZ	2.68	0.56
1:A:1528:ARG:NH1	1:A:1803:PRO:HD3	2.21	0.56
1:A:1492:ALA:HB2	1:A:1707:LEU:HD13	1.88	0.56
1:A:1613:CYS:O	1:A:1614:HIS:ND1	2.42	0.53
1:A:1695:LYS:HZ3	1:A:1771:TRP:HZ2	1.56	0.52
1:A:1483:GLU:HG3	1:A:1689:PRO:HG3	1.92	0.52
1:A:1796:ASP:OD1	1:A:1796:ASP:O	2.28	0.51
1:A:1461:LEU:HD22	1:A:1753:ASP:HA	1.92	0.51
1:A:1479:GLY:HA2	1:A:1482:LYS:NZ	2.27	0.50
1:A:1657:LYS:HA	1:A:1695:LYS:HD3	1.93	0.50
1:A:1743:PRO:CB	1:A:1814:GLN:HG2	2.41	0.50
1:A:1482:LYS:O	1:A:1483:GLU:HG2	2.12	0.49
1:A:1476:GLU:HG3	1:A:1480:THR:HG22	1.94	0.49
1:A:1745:GLN:O	1:A:1748:THR:OG1	2.19	0.49
1:A:1601:MET:HE2	1:A:1601:MET:O	2.13	0.49
1:A:1714:LEU:O	1:A:1718:VAL:HG23	2.13	0.49
1:A:1751:GLU:O	1:A:1784:ARG:HB2	2.13	0.49
1:A:1785:ARG:CG	1:A:1795:ILE:HD11	2.41	0.48
1:A:1494:ALA:O	1:A:1783:VAL:HG21	2.14	0.48
1:A:1660:VAL:O	1:A:1661:ARG:HD3	2.14	0.48
1:A:1695:LYS:NZ	1:A:1703:GLY:O	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1741:HIS:CD2	1:A:1817:VAL:HG13	2.50	0.47
1:A:1470:VAL:HA	1:A:1501:CYS:HB2	1.96	0.47
1:A:1625:LYS:HB2	1:A:1679:VAL:HG21	1.97	0.46
1:A:1820:LEU:HD13	1:A:1821:PRO:N	2.31	0.46
1:A:1463:ARG:CG	1:A:1751:GLU:HG2	2.45	0.46
1:A:1774:PHE:CD1	1:A:1774:PHE:N	2.83	0.46
1:A:1639:ALA:HB1	1:A:1641:HIS:CE1	2.51	0.45
1:A:1567:ARG:HG3	1:A:1567:ARG:HH11	1.82	0.45
1:A:1463:ARG:HG3	1:A:1751:GLU:HG2	1.98	0.45
1:A:1810:ARG:NH1	1:A:1815:GLY:O	2.50	0.45
1:A:1674:TRP:HZ3	1:A:1723:LEU:HD22	1.81	0.45
1:A:1645:LEU:HD12	1:A:1645:LEU:N	2.32	0.44
1:A:1708:GLU:HB2	1:A:1764:MET:HG3	1.98	0.44
1:A:1743:PRO:HB3	1:A:1814:GLN:C	2.37	0.44
1:A:1621:ILE:HD11	1:A:1679:VAL:HB	2.00	0.44
1:A:1640:PRO:HG3	1:A:1710:MET:HG3	1.99	0.44
1:A:1563:PHE:HB2	1:A:1566:LEU:HB2	1.99	0.44
1:A:1584:HIS:CD2	1:A:1819:GLN:HB2	2.53	0.44
1:A:1479:GLY:CA	1:A:1482:LYS:HZ3	2.31	0.44
1:A:1558:TYR:CD1	1:A:1566:LEU:HD13	2.53	0.44
1:A:1674:TRP:CE3	1:A:1722:ARG:HD2	2.52	0.44
1:A:1483:GLU:OE1	1:A:1488:GLY:N	2.51	0.43
1:A:1564:SER:O	1:A:1567:ARG:HG2	2.19	0.43
1:A:1666:SER:O	1:A:1670:VAL:HG23	2.18	0.43
1:A:1622:LEU:HA	1:A:1622:LEU:HD23	1.74	0.43
1:A:1566:LEU:HD23	1:A:1566:LEU:HA	1.71	0.43
1:A:1520:GLN:HG3	1:A:1533:LEU:HD12	1.99	0.43
1:A:1574:TRP:CD1	1:A:1574:TRP:N	2.87	0.43
1:A:1709:THR:O	1:A:1713:LEU:CD1	2.62	0.43
1:A:1641:HIS:O	1:A:1664:LEU:HD11	2.19	0.43
1:A:1795:ILE:HG22	1:A:1796:ASP:H	1.84	0.43
1:A:1567:ARG:O	1:A:1568:LEU:HD23	2.19	0.42
1:A:1562:THR:OG1	1:A:1562:THR:O	2.38	0.42
1:A:1760:ILE:HD13	1:A:1774:PHE:HB3	2.01	0.42
1:A:1714:LEU:HA	1:A:1714:LEU:HD13	1.76	0.41
1:A:1766:PHE:CE1	1:A:1799:VAL:HG23	2.55	0.41
1:A:1499:MET:HA	1:A:1530:ASP:O	2.20	0.41
1:A:1659:GLU:OE2	1:A:1661:ARG:NH2	2.54	0.41
1:A:1750:VAL:HG12	1:A:1752:VAL:HG13	2.02	0.41
1:A:1766:PHE:CZ	1:A:1799:VAL:HG23	2.55	0.41
1:A:1614:HIS:H	1:A:1637:GLU:HG3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1728:LEU:HA	1:A:1728:LEU:HD12	1.83	0.40
1:A:1498:THR:O	1:A:1529:CYS:HB2	2.20	0.40
1:A:1504:PRO:HB3	1:A:1534:PHE:O	2.22	0.40
1:A:1558:TYR:HA	1:A:1590:HIS:HB2	2.02	0.40
1:A:1476:GLU:HA	1:A:1477:PRO:HA	1.89	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1696:CYS:SG	1:A:1696:CYS:SG[2_655]	1.75	0.45

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	361/391 (92%)	328 (91%)	26 (7%)	7 (2%)	8	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1722	ARG
1	A	1797	GLY
1	A	1483	GLU
1	A	1687	HIS
1	A	1796	ASP
1	A	1583	SER
1	A	1479	GLY

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	296 / 321 (92%)	284 (96%)	12 (4%)	30 61

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1507	ARG
1	A	1516	LEU
1	A	1562	THR
1	A	1570	SER
1	A	1614	HIS
1	A	1630	ARG
1	A	1649	ASP
1	A	1657	LYS
1	A	1696	CYS
1	A	1731	ARG
1	A	1756	HIS
1	A	1767	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1741	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	363/391 (92%)	0.70	49 (13%) 3 2	37, 65, 108, 130	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1698	SER	6.8
1	A	1821	PRO	5.1
1	A	1699	ARG	5.0
1	A	1822	PRO	4.6
1	A	1653	LEU	3.8
1	A	1817	VAL	3.7
1	A	1562	THR	3.6
1	A	1647	HIS	3.4
1	A	1684	ALA	3.4
1	A	1790	GLY	3.3
1	A	1651	GLU	3.2
1	A	1820	LEU	3.2
1	A	1706	GLY	3.1
1	A	1639	ALA	3.0
1	A	1819	GLN	2.9
1	A	1693	GLU	2.9
1	A	1685	SER	2.9
1	A	1471	HIS	2.9
1	A	1686	ASP	2.9
1	A	1479	GLY	2.9
1	A	1814	GLN	2.8
1	A	1709	THR	2.7
1	A	1482	LYS	2.7
1	A	1650	LEU	2.6
1	A	1661	ARG	2.6
1	A	1800	LEU	2.6
1	A	1462	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1770	HIS	2.5
1	A	1784	ARG	2.4
1	A	1725	LEU	2.4
1	A	1780	LYS	2.4
1	A	1687	HIS	2.3
1	A	1696	CYS	2.3
1	A	1641	HIS	2.2
1	A	1801	VAL	2.2
1	A	1691	THR	2.2
1	A	1744	PRO	2.1
1	A	1729	LEU	2.1
1	A	1813	PRO	2.1
1	A	1771	TRP	2.1
1	A	1668	GLN	2.1
1	A	1754	LEU	2.1
1	A	1652	ARG	2.1
1	A	1710	MET	2.1
1	A	1648	ASP	2.1
1	A	1694	GLU	2.1
1	A	1502	ALA	2.0
1	A	1704	PHE	2.0
1	A	1700	PRO	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. 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(\AA^2)	Q<0.9
2	ZN	A	1901	1/1	0.92	0.27	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.