



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:06 PM GMT

PDB ID : 3W6W
Title : Crystal structure of melB holo-protyrosinase from *Asperugillus oryzae*
Authors : Fujieda, N.; Yabuta, S.; Ikeda, T.; Oyama, T.; Muraki, N.; Kurisu, G.; Itoh, S.
Deposited on : 2013-02-22
Resolution : 1.39 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

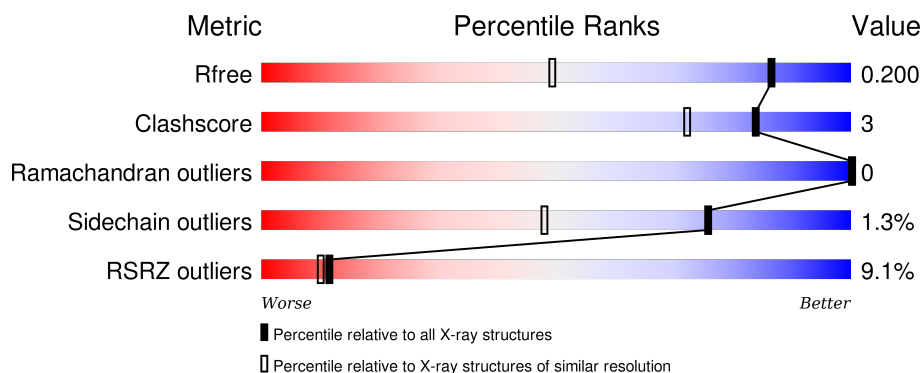
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.39 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	1199 (1.40-1.40)
Clashscore	102246	1295 (1.40-1.40)
Ramachandran outliers	100387	1259 (1.40-1.40)
Sidechain outliers	100360	1258 (1.40-1.40)
RSRZ outliers	91569	1198 (1.40-1.40)

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	620	
1	B	620	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11010 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 Tyrosinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	65	0
			5121	3305	876	923	17			
1	B	555	Total	C	N	O	S	0	43	0
			4790	3098	827	850	15			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Cu	0	0
			2	2		
2	A	2	Total	Cu	0	0
			2	2		

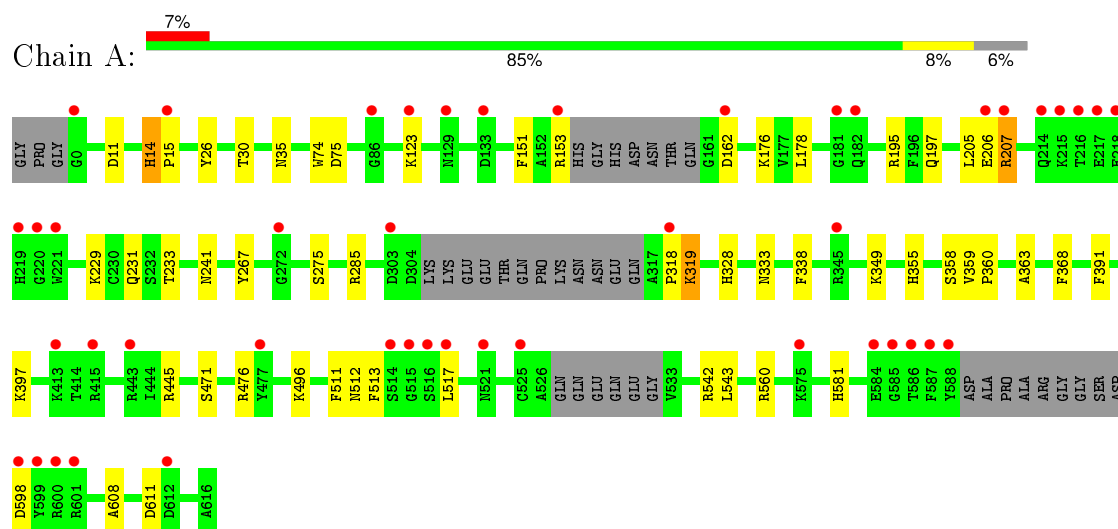
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	587	Total	O	0	0
			587	587		
3	B	508	Total	O	0	0
			508	508		

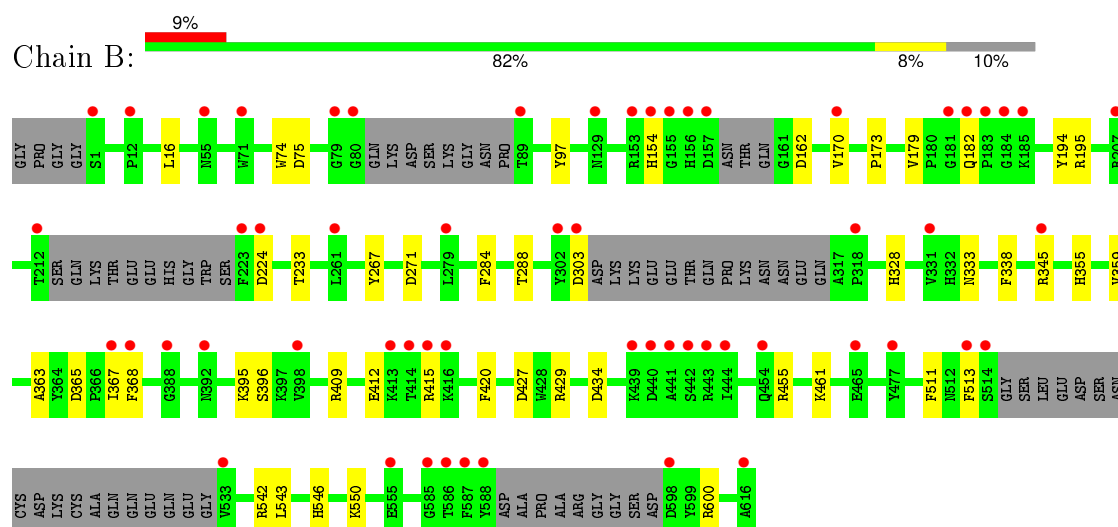
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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: Tyrosinase



• Molecule 1: Tyrosinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.31Å 118.09Å 84.21Å 90.00° 97.40° 90.00°	Depositor
Resolution (Å)	34.07 – 1.39 34.07 – 1.39	Depositor EDS
% Data completeness (in resolution range)	97.7 (34.07-1.39) 97.6 (34.07-1.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.177 , 0.199 0.177 , 0.200	Depositor DCC
R_{free} test set	9916 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	14.0	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 196365 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11010	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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: CU

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	0.34	0/5451	0.55	0/7392
1	B	0.34	0/5052	0.54	0/6857
All	All	0.34	0/10503	0.54	0/14249

There are no bond length outliers.

There are no bond angle outliers.

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	5121	0	5093	37	0
1	B	4790	0	4724	25	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	587	0	0	9	0
3	B	508	0	0	1	0
All	All	11010	0	9817	59	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 3.

All (59) 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:205:LEU:O	1:A:207[B]:ARG:NH1	2.26	0.69
1:B:412:GLU:OE1	1:B:415[A]:ARG:NH2	2.27	0.67
1:B:16[B]:LEU:HG	1:B:434:ASP:HB2	1.78	0.65
1:A:241[B]:ASN:HD21	1:B:154:HIS:CE1	2.15	0.64
1:B:16[B]:LEU:HD21	1:B:429[B]:ARG:HG2	1.79	0.64
1:A:11[A]:ASP:HB3	1:A:14[A]:HIS:HD2	1.68	0.59
1:A:15:PRO:HA	3:A:1561:HOH:O	2.02	0.59
1:A:318:PRO:HB3	1:A:471:SER:HB3	1.84	0.59
1:A:476[B]:ARG:HH11	1:A:517:LEU:HA	1.68	0.58
1:A:11[A]:ASP:HB3	1:A:14[A]:HIS:CD2	2.40	0.56
1:B:303:ASP:HB3	1:B:395:LYS:HE3	1.88	0.55
1:B:546:HIS:CE1	1:B:550:LYS:HE2	2.41	0.55
1:B:170[A]:VAL:HG21	1:B:367[A]:ILE:HD13	1.90	0.53
1:A:391:PHE:O	1:A:397:LYS:HE3	2.11	0.51
1:A:319:LYS:H	1:A:319:LYS:NZ	2.09	0.50
1:A:151:PHE:CG	1:A:162:ASP:HB3	2.46	0.50
1:A:496:LYS:NZ	1:A:611:ASP:OD2	2.45	0.49
1:A:206:GLU:HG3	3:A:1269:HOH:O	2.12	0.49
1:B:74:TRP:CE3	1:B:75:ASP:HB2	2.48	0.49
1:B:233:THR:HA	1:B:355:HIS:CE1	2.48	0.48
1:B:365:ASP:OD1	1:B:367[A]:ILE:HG22	2.12	0.48
1:A:123[B]:LYS:NZ	3:A:1376:HOH:O	2.29	0.48
1:A:349[A]:LYS:NZ	3:A:1270:HOH:O	2.47	0.47
1:A:598:ASP:OD1	1:A:598:ASP:N	2.48	0.46
1:A:318:PRO:HG2	1:A:581:HIS:CE1	2.50	0.46
1:A:233:THR:HA	1:A:355:HIS:CE1	2.51	0.46
1:B:267:TYR:OH	1:B:543:LEU:HB3	2.15	0.46
1:A:275:SER:OG	1:B:345:ARG:NH2	2.49	0.46
1:A:285:ARG:NH2	3:A:1399:HOH:O	2.49	0.46
1:B:179[A]:VAL:HG23	1:B:182:GLN:HB2	1.98	0.45
1:B:173:PRO:HG3	1:B:194:TYR:CZ	2.51	0.45
1:B:162:ASP:HB2	1:B:455[B]:ARG:NH2	2.32	0.45
1:B:363:ALA:HA	1:B:368:PHE:CG	2.53	0.44
1:B:600[B]:ARG:NH1	3:B:1271:HOH:O	2.51	0.44
1:A:363:ALA:HA	1:A:368:PHE:CG	2.52	0.44
1:A:476[A]:ARG:HG3	1:A:512:ASN:OD1	2.18	0.43
1:A:197:GLN:HG3	1:A:231:GLN:HG2	2.01	0.43
1:B:427:ASP:OD1	1:B:429[B]:ARG:NE	2.47	0.43
1:B:97:TYR:CD2	1:B:396:SER:HA	2.54	0.43
1:A:267:TYR:OH	1:A:543:LEU:HB3	2.19	0.42
1:A:359[A]:VAL:HG22	1:A:513:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:ASP:CG	1:B:367[A]:ILE:HG22	2.41	0.42
1:A:319:LYS:O	3:A:1577:HOH:O	2.21	0.41
1:A:153[B]:ARG:NH2	3:A:1563:HOH:O	2.52	0.41
1:A:560[B]:ARG:NH2	1:A:608:ALA:HA	2.36	0.41
1:A:35:ASN:O	1:A:178:LEU:HD11	2.20	0.41
1:A:496:LYS:HE3	1:B:271:ASP:OD1	2.20	0.41
1:B:284:PHE:CE1	1:B:288:THR:HG21	2.55	0.41
1:B:333:ASN:HB2	1:B:511:PHE:CD2	2.56	0.41
1:A:229:LYS:HE2	3:A:1351:HOH:O	2.19	0.41
1:A:445[B]:ARG:HD2	1:A:445[B]:ARG:HA	1.93	0.41
1:A:358:SER:OG	1:A:360:PRO:HD2	2.20	0.41
1:A:26:TYR:CZ	1:A:30:THR:HG21	2.56	0.41
1:A:74:TRP:CE3	1:A:75:ASP:HB2	2.55	0.41
1:A:176:LYS:HE2	3:A:1427:HOH:O	2.21	0.41
1:B:359[A]:VAL:HG22	1:B:513:PHE:CE2	2.56	0.41
1:A:333:ASN:HB2	1:A:511:PHE:CD2	2.56	0.40
1:B:409:ARG:HB3	1:B:420:PHE:CE1	2.55	0.40
1:A:319:LYS:H	1:A:319:LYS:HZ1	1.70	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	637/620 (103%)	627 (98%)	10 (2%)	0	100	100
1	B	584/620 (94%)	575 (98%)	9 (2%)	0	100	100
All	All	1221/1240 (98%)	1202 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	568/537 (106%)	559 (98%)	9 (2%)	70	38
1	B	520/537 (97%)	514 (99%)	6 (1%)	78	52
All	All	1088/1074 (101%)	1073 (99%)	15 (1%)	76	45

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14[A]	HIS
1	A	14[B]	HIS
1	A	195	ARG
1	A	207[A]	ARG
1	A	207[B]	ARG
1	A	319	LYS
1	A	328	HIS
1	A	338	PHE
1	A	542	ARG
1	B	195	ARG
1	B	224	ASP
1	B	328	HIS
1	B	338	PHE
1	B	461	LYS
1	B	542	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 molecules 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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are 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 [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	583/620 (94%)	0.39	45 (7%) 16 14	8, 15, 34, 54	0
1	B	555/620 (89%)	0.48	58 (10%) 8 7	9, 16, 36, 51	0
All	All	1138/1240 (91%)	0.44	103 (9%) 11 10	8, 16, 35, 54	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	477	TYR	7.7
1	B	443	ARG	6.8
1	B	156	HIS	6.7
1	B	440	ASP	6.6
1	B	223	PHE	6.4
1	B	155	GLY	5.9
1	A	587	PHE	5.8
1	B	441	ALA	5.8
1	B	89	THR	5.5
1	B	157	ASP	5.4
1	A	219	HIS	5.4
1	B	181	GLY	5.0
1	A	181	GLY	4.8
1	B	80	GLY	4.8
1	A	525	CYS	4.7
1	B	212	THR	4.7
1	B	442	SER	4.6
1	A	586	THR	4.1
1	B	414	THR	4.1
1	B	154	HIS	4.1
1	A	588	TYR	4.1
1	A	600	ARG	4.0
1	B	588	TYR	3.8
1	B	587	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	345	ARG	3.7
1	A	514	SER	3.5
1	A	153[A]	ARG	3.4
1	B	153[A]	ARG	3.4
1	B	533	VAL	3.4
1	A	216	THR	3.3
1	B	183	PRO	3.3
1	B	207	ARG	3.2
1	B	444	ILE	3.2
1	B	585	GLY	3.2
1	A	0	GLY	3.1
1	A	515	GLY	3.1
1	A	413	LYS	3.1
1	A	182	GLN	3.0
1	A	345	ARG	3.0
1	B	79	GLY	3.0
1	A	598	ASP	3.0
1	B	303	ASP	3.0
1	B	302	TYR	2.9
1	B	261[A]	LEU	2.9
1	B	367[A]	ILE	2.9
1	B	392	ASN	2.9
1	A	303[A]	ASP	2.9
1	B	129	ASN	2.8
1	B	224	ASP	2.8
1	B	416	LYS	2.8
1	B	12	PRO	2.8
1	B	514	SER	2.8
1	A	218[A]	GLU	2.8
1	A	221	TRP	2.8
1	B	71[A]	TRP	2.8
1	B	598	ASP	2.7
1	A	584	GLU	2.7
1	B	184	GLY	2.7
1	B	586	THR	2.7
1	B	439	LYS	2.6
1	A	443	ARG	2.6
1	B	465	GLU	2.6
1	A	220	GLY	2.5
1	B	413	LYS	2.5
1	B	415[A]	ARG	2.5
1	A	15	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	215	LYS	2.5
1	A	521	ASN	2.5
1	A	129	ASN	2.5
1	B	454[A]	GLN	2.4
1	A	162	ASP	2.4
1	A	612	ASP	2.4
1	A	415	ARG	2.4
1	A	601	ARG	2.4
1	A	599	TYR	2.4
1	A	585	GLY	2.4
1	A	517	LEU	2.4
1	B	555	GLU	2.4
1	B	398	VAL	2.4
1	B	318	PRO	2.3
1	B	513	PHE	2.3
1	B	185	LYS	2.3
1	B	331	VAL	2.3
1	A	318	PRO	2.3
1	A	206	GLU	2.2
1	A	86	GLY	2.2
1	A	214	GLN	2.2
1	B	182	GLN	2.2
1	A	207[A]	ARG	2.2
1	A	272	GLY	2.2
1	A	516	SER	2.2
1	A	123[A]	LYS	2.2
1	A	477	TYR	2.2
1	B	1	SER	2.1
1	B	368	PHE	2.1
1	B	388	GLY	2.1
1	B	279	LEU	2.1
1	B	616	ALA	2.1
1	B	170[A]	VAL	2.1
1	B	55	ASN	2.1
1	A	575	LYS	2.0
1	A	217	GLU	2.0
1	A	133	ASP	2.0

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 [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
2	CU	B	701	1/1	1.00	0.02	-2.15	17,17,17,17	0
2	CU	B	702	1/1	1.00	0.03	-2.85	17,17,17,17	0
2	CU	A	701	1/1	1.00	0.02	-4.23	15,15,15,15	0
2	CU	A	702	1/1	1.00	0.02	-6.05	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.