



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:24 pm GMT

PDB ID : 2BMX
Title : MYCOBACTERIUM TUBERCULOSIS AHPC
Authors : Guimaraes, B.G.; Alzari, P.M.
Deposited on : 2005-03-16
Resolution : 2.40 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

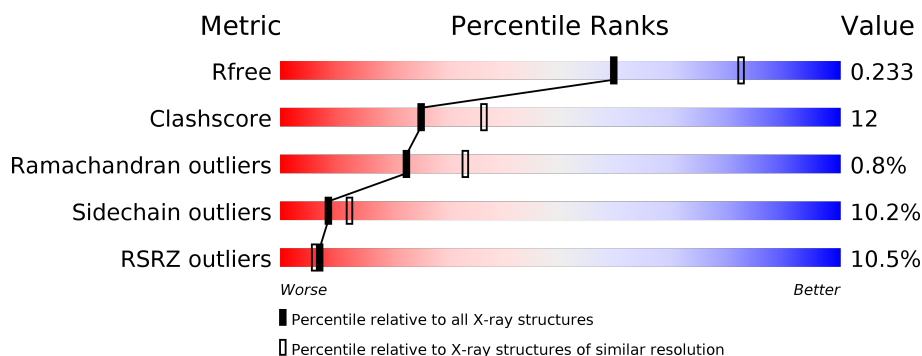
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	195	<div> <div>5%</div> <div> <div>72%</div> <div>11%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	195	<div> <div>8%</div> <div> <div>71%</div> <div>16%</div> <div>• •</div> <div>9%</div> </div> </div>
1	C	195	<div> <div>15%</div> <div> <div>56%</div> <div>24%</div> <div>5%</div> <div>•</div> <div>13%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4247 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 ALKYL HYDROPEROXIDASE C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	Se	0	0	0
			1292	829	214	247	1	1			
1	B	178	Total	C	N	O	S	Se	0	0	0
			1373	875	229	266	2	1			
1	C	169	Total	C	N	O	S	Se	0	0	0
			1298	830	215	251	1	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	176	SER	CYS	ENGINEERED MUTATION	UNP Q7BHK8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	86	Total	O	0	0
			86	86		
2	B	95	Total	O	0	0
			95	95		
2	C	103	Total	O	0	0
			103	103		

4 Data and refinement statistics

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, α , β , γ	139.26Å 139.26Å 148.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	141.42 – 2.40 29.71 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (141.42-2.40) 100.0 (29.71-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.31 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195 , 0.236 0.193 , 0.233	Depositor DCC
R_{free} test set	1712 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4247	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.94% 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

5.1 Standard geometry

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	0.85	0/1323	0.91	6/1805 (0.3%)
1	B	0.88	0/1406	1.02	7/1919 (0.4%)
1	C	0.97	2/1329 (0.2%)	0.99	6/1814 (0.3%)
All	All	0.90	2/4058 (0.0%)	0.98	19/5538 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	13	TYR	CD1-CE1	5.39	1.47	1.39
1	C	68	PHE	N-CA	5.25	1.56	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	ARG	NE-CZ-NH2	-11.95	114.32	120.30
1	B	116	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	B	116	ARG	NE-CZ-NH2	-9.87	115.36	120.30
1	C	163	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	B	97	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	B	163	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	C	163	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	A	163	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	A	83	LEU	CA-CB-CG	6.71	130.73	115.30
1	A	163	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	C	83	LEU	CB-CG-CD1	6.47	122.00	111.00
1	B	4	LEU	CB-CG-CD1	6.39	121.86	111.00
1	A	147	VAL	CB-CA-C	-6.34	99.35	111.40
1	C	4	LEU	CB-CG-CD1	6.17	121.50	111.00
1	B	106	LEU	CA-CB-CG	5.78	128.59	115.30
1	C	139	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	3	LEU	CB-CG-CD2	-5.43	101.77	111.00
1	C	5	THR	CB-CA-C	-5.22	97.51	111.60
1	A	83	LEU	CB-CG-CD1	5.01	119.52	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	1292	0	1214	24	0
1	B	1373	0	1280	21	0
1	C	1298	0	1216	48	1
2	A	86	0	0	6	0
2	B	95	0	0	3	0
2	C	103	0	0	7	0
All	All	4247	0	3710	93	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 12.

All (93) 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:C:133:ARG:NH1	1:C:152:GLY:O	1.93	1.01
1:C:87:ILE:HD12	1:C:116:ARG:HH22	1.36	0.90
1:C:39:THR:HG22	1:C:41:ASP:H	1.35	0.89
1:C:60:VAL:HB	2:C:2051:HOH:O	1.74	0.87
1:C:61:CYS:HB2	2:C:2052:HOH:O	1.77	0.83
1:C:87:ILE:HD12	1:C:116:ARG:NH2	1.97	0.79
1:C:87:ILE:CD1	1:C:116:ARG:NH2	2.46	0.78
1:C:56:ASP:OD2	1:C:93:HIS:HD2	1.73	0.71
1:A:4:LEU:HD22	1:A:122:ALA:HA	1.71	0.70
1:A:96:TRP:CD1	1:A:100:HIS:HD2	2.09	0.70
1:C:69:SER:HB2	1:C:107:PRO:HD3	1.72	0.70
1:A:133:ARG:HG3	1:A:133:ARG:NH1	2.07	0.69
1:C:87:ILE:CD1	1:C:116:ARG:HH22	2.03	0.68
1:C:59:PHE:HD2	2:C:2050:HOH:O	1.76	0.68
1:A:133:ARG:HG3	1:A:133:ARG:HH11	1.59	0.67
1:C:48:ARG:HH22	1:C:142:ASN:HD22	1.42	0.66
1:C:4:LEU:HD22	1:C:122:ALA:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:THR:HG21	1:B:154:VAL:HB	1.79	0.65
1:C:39:THR:CG2	1:C:41:ASP:H	2.10	0.64
1:C:59:PHE:CD2	2:C:2050:HOH:O	2.50	0.64
1:B:60:VAL:HG11	1:B:65:ILE:HD11	1.80	0.63
1:A:136:PHE:CE2	1:A:147:VAL:HG13	2.33	0.63
1:C:87:ILE:HD13	1:C:116:ARG:NH2	2.14	0.62
1:C:69:SER:HB3	1:C:106:LEU:HD23	1.80	0.62
1:B:4:LEU:HD22	1:B:122:ALA:HA	1.82	0.62
1:C:96:TRP:CD1	1:C:100:HIS:HD2	2.19	0.60
1:C:69:SER:HB3	1:C:106:LEU:CD2	2.32	0.60
1:A:53:TRP:CZ2	1:A:110:MSE:HE3	2.37	0.60
1:B:58:THR:HG21	2:B:2045:HOH:O	2.02	0.59
1:A:95:GLN:HG3	2:A:2050:HOH:O	2.03	0.58
1:A:96:TRP:HD1	1:A:100:HIS:HD2	1.51	0.58
1:B:163:ARG:HG3	1:B:178:TRP:CG	2.39	0.57
1:A:43:HIS:HB3	1:A:46:LYS:CG	2.35	0.56
1:C:58:THR:HG21	2:C:2046:HOH:O	2.04	0.56
1:C:48:ARG:HH22	1:C:142:ASN:ND2	2.02	0.56
1:B:14:GLN:HG3	1:B:39:THR:HG22	1.86	0.55
1:C:53:TRP:CZ2	1:C:110:MSE:HE3	2.42	0.55
1:B:87:ILE:HG12	1:B:116:ARG:HG3	1.89	0.55
1:A:43:HIS:HB3	1:A:46:LYS:HG3	1.90	0.54
1:C:66:ALA:O	1:C:70:LYS:CB	2.56	0.54
1:C:69:SER:CB	1:C:106:LEU:HD23	2.38	0.54
1:C:69:SER:CB	1:C:106:LEU:CD2	2.86	0.53
1:B:137:ILE:HB	1:B:146:PHE:HB3	1.90	0.53
1:B:87:ILE:HG12	1:B:116:ARG:CG	2.39	0.52
1:C:61:CYS:SG	1:C:64:GLU:HG2	2.49	0.52
1:C:39:THR:HG22	1:C:41:ASP:N	2.16	0.52
1:C:96:TRP:CD1	1:C:100:HIS:CD2	2.97	0.52
1:C:68:PHE:HA	1:C:158:VAL:HG11	1.91	0.52
1:C:43:HIS:HD2	2:C:2028:HOH:O	1.94	0.51
1:C:97:ARG:HD2	1:C:103:LEU:O	2.11	0.50
1:C:67:ALA:O	1:C:71:LEU:N	2.31	0.50
1:A:133:ARG:CG	1:A:133:ARG:NH1	2.74	0.50
1:C:96:TRP:NE1	1:C:100:HIS:HD2	2.10	0.49
1:A:67:ALA:O	1:A:71:LEU:HB2	2.13	0.49
1:A:60:VAL:HG11	1:A:65:ILE:HD11	1.95	0.48
1:C:64:GLU:O	1:C:68:PHE:N	2.46	0.47
1:A:136:PHE:CD2	1:A:147:VAL:HG13	2.49	0.46
1:B:146:PHE:CZ	1:B:148:SER:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLU:HG2	2:A:2026:HOH:O	2.14	0.46
1:A:150:THR:HG21	2:A:2075:HOH:O	2.17	0.45
1:B:124:VAL:HG22	1:B:134:VAL:HG11	1.99	0.45
1:C:93:HIS:HE1	1:C:111:LEU:O	2.00	0.45
1:B:53:TRP:CZ2	1:B:110:MSE:HE3	2.52	0.45
1:C:96:TRP:NE1	1:C:100:HIS:CD2	2.85	0.44
1:A:150:THR:HG23	2:A:2073:HOH:O	2.16	0.44
1:C:160:GLU:OE2	1:C:163:ARG:NH1	2.51	0.44
1:B:87:ILE:CG1	1:B:116:ARG:HG3	2.47	0.44
1:C:135:THR:OG1	1:C:156:ARG:HD3	2.18	0.44
1:A:139:ASP:HB2	1:A:140:PRO:CD	2.48	0.43
1:A:139:ASP:HB2	1:A:140:PRO:HD2	1.99	0.43
1:B:67:ALA:O	1:B:71:LEU:HB2	2.19	0.43
1:A:150:THR:CG2	2:A:2073:HOH:O	2.66	0.42
1:C:48:ARG:NH2	1:C:142:ASN:HD22	2.14	0.42
1:B:95:GLN:NE2	2:B:2057:HOH:O	2.53	0.42
1:C:69:SER:HB2	1:C:107:PRO:CD	2.47	0.42
1:C:93:HIS:CD2	1:C:110:MSE:HE2	2.54	0.42
1:C:53:TRP:HZ2	1:C:110:MSE:HE3	1.84	0.42
1:A:43:HIS:HB3	1:A:46:LYS:HG2	2.02	0.41
1:B:116:ARG:NH2	2:B:2065:HOH:O	2.51	0.41
1:C:67:ALA:O	1:C:68:PHE:C	2.58	0.41
1:A:116:ARG:NH2	2:A:2056:HOH:O	2.51	0.41
1:A:96:TRP:HD1	1:A:100:HIS:CD2	2.33	0.41
1:B:18:LEU:HD23	1:B:97:ARG:HD3	2.03	0.41
1:C:137:ILE:HB	1:C:146:PHE:HB3	2.02	0.41
1:C:43:HIS:CD2	2:C:2028:HOH:O	2.72	0.41
1:B:108:PHE:HB2	1:B:109:PRO:CD	2.50	0.41
1:B:100:HIS:CD2	1:B:103:LEU:HD12	2.56	0.41
1:B:51:PHE:CE1	1:B:68:PHE:HE1	2.38	0.41
1:C:52:PHE:HA	1:C:85:VAL:O	2.21	0.41
1:B:139:ASP:HB2	1:B:140:PRO:CD	2.51	0.40
1:A:96:TRP:HE3	1:A:110:MSE:HE1	1.86	0.40
1:C:27:ASP:O	1:C:29:LYS:N	2.50	0.40
1:C:87:ILE:HD11	1:C:130:VAL:HG12	2.03	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:C:116:ARG:NH1	1:C:116:ARG:NH2[12_556]	1.95	0.25

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	167/195 (86%)	160 (96%)	6 (4%)	1 (1%)	28	41
1	B	176/195 (90%)	166 (94%)	9 (5%)	1 (1%)	28	41
1	C	167/195 (86%)	154 (92%)	11 (7%)	2 (1%)	15	21
All	All	510/585 (87%)	480 (94%)	26 (5%)	4 (1%)	22	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	PHE
1	C	28	ALA
1	A	27	ASP
1	C	26	VAL

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	133/162 (82%)	125 (94%)	8 (6%)	22	35
1	B	143/162 (88%)	130 (91%)	13 (9%)	11	16
1	C	135/162 (83%)	114 (84%)	21 (16%)	3	3
All	All	411/486 (85%)	369 (90%)	42 (10%)	8	12

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	23	LEU
1	A	71	LEU
1	A	83	LEU
1	A	133	ARG
1	A	150	THR
1	A	159	ASP
1	A	170	SER
1	B	4	LEU
1	B	19	ILE
1	B	36	THR
1	B	58	THR
1	B	61	CYS
1	B	87	ILE
1	B	102	ASP
1	B	106	LEU
1	B	116	ARG
1	B	134	VAL
1	B	138	VAL
1	B	153	SER
1	B	163	ARG
1	C	2	PRO
1	C	4	LEU
1	C	5	THR
1	C	23	LEU
1	C	33	ASP
1	C	58	THR
1	C	59	PHE
1	C	61	CYS
1	C	64	GLU
1	C	65	ILE
1	C	68	PHE
1	C	69	SER
1	C	83	LEU
1	C	97	ARG
1	C	102	ASP
1	C	105	THR
1	C	106	LEU
1	C	116	ARG
1	C	159	ASP
1	C	163	ARG
1	C	170	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	HIS
1	B	43	HIS
1	B	100	HIS
1	C	43	HIS
1	C	93	HIS
1	C	100	HIS
1	C	142	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	168/195 (86%)	0.11	9 (5%) 26 25	28, 39, 52, 59	0
1	B	177/195 (90%)	0.30	16 (9%) 10 9	27, 38, 58, 64	0
1	C	168/195 (86%)	0.61	29 (17%) 2 1	24, 39, 60, 64	0
All	All	513/585 (87%)	0.34	54 (10%) 7 6	24, 38, 57, 64	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	28	ALA	7.5
1	C	63	THR	6.5
1	C	67	ALA	5.8
1	B	61	CYS	5.3
1	B	28	ALA	5.2
1	B	62	PRO	5.0
1	C	59	PHE	4.6
1	B	63	THR	4.6
1	C	69	SER	4.3
1	C	27	ASP	4.2
1	C	62	PRO	4.1
1	A	29	LYS	4.1
1	C	26	VAL	4.0
1	B	67	ALA	4.0
1	C	61	CYS	3.7
1	B	100	HIS	3.6
1	C	33	ASP	3.6
1	B	60	VAL	3.6
1	C	31	PRO	3.5
1	A	61	CYS	3.3
1	C	65	ILE	3.3
1	B	59	PHE	3.3
1	A	31	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	66	ALA	3.2
1	C	29	LYS	3.1
1	C	101	ASN	3.1
1	C	60	VAL	3.0
1	B	50	VAL	3.0
1	B	171	ASP	2.9
1	C	24	SER	2.9
1	B	177	ASN	2.9
1	A	22	ASP	2.7
1	C	102	ASP	2.7
1	B	66	ALA	2.5
1	A	28	ALA	2.5
1	C	135	THR	2.4
1	C	68	PHE	2.4
1	C	64	GLU	2.4
1	B	135	THR	2.3
1	B	102	ASP	2.3
1	C	85	VAL	2.3
1	C	83	LEU	2.3
1	C	50	VAL	2.2
1	C	134	VAL	2.2
1	C	100	HIS	2.2
1	C	30	GLN	2.2
1	A	100	HIS	2.1
1	A	170	SER	2.1
1	A	51	PHE	2.1
1	A	135	THR	2.1
1	B	148	SER	2.1
1	C	111	LEU	2.1
1	B	85	VAL	2.0
1	C	52	PHE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.