Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 03:47 AM EDT

PDB ID	:	3LO7
Title	:	Crystal structure of PBPA from Mycobacterium tuberculosis
Authors	:	Fedarovich, A.; Davies, C.
Deposited on	:	2010-02-03
Resolution	:	2.05 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 (i) 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 (1)) were used in the production of this report:

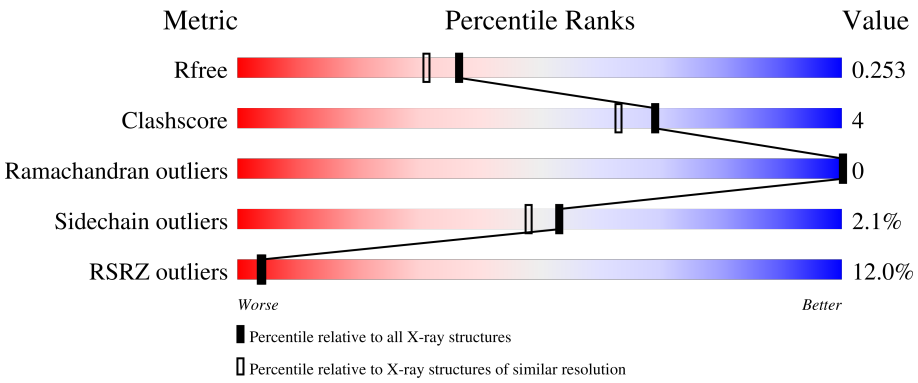
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 <=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	483	10% 79% 8% 13%
1	B	483	10% 70% 9% 21%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5984 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 Penicillin-binding protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	420	3093	1936	550	598	9	0	0	0
			Total	C	N	O	S			
1	B	383	2815	1761	501	544	9	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	EXPRESSION TAG	UNP P71586
A	10	SER	-	EXPRESSION TAG	UNP P71586
A	11	TYR	-	EXPRESSION TAG	UNP P71586
A	12	TYR	-	EXPRESSION TAG	UNP P71586
A	13	HIS	-	EXPRESSION TAG	UNP P71586
A	14	HIS	-	EXPRESSION TAG	UNP P71586
A	15	HIS	-	EXPRESSION TAG	UNP P71586
A	16	HIS	-	EXPRESSION TAG	UNP P71586
A	17	HIS	-	EXPRESSION TAG	UNP P71586
A	18	HIS	-	EXPRESSION TAG	UNP P71586
A	19	ASP	-	EXPRESSION TAG	UNP P71586
A	20	TYR	-	EXPRESSION TAG	UNP P71586
A	21	ASP	-	EXPRESSION TAG	UNP P71586
A	22	ILE	-	EXPRESSION TAG	UNP P71586
A	23	PRO	-	EXPRESSION TAG	UNP P71586
A	24	THR	-	EXPRESSION TAG	UNP P71586
A	25	GLU	-	EXPRESSION TAG	UNP P71586
A	26	ASN	-	EXPRESSION TAG	UNP P71586
A	27	LEU	-	EXPRESSION TAG	UNP P71586
A	28	TYR	-	EXPRESSION TAG	UNP P71586
A	29	PHE	-	EXPRESSION TAG	UNP P71586
A	30	GLN	-	EXPRESSION TAG	UNP P71586
A	31	GLY	-	EXPRESSION TAG	UNP P71586
A	32	ALA	-	EXPRESSION TAG	UNP P71586
A	33	MET	-	EXPRESSION TAG	UNP P71586

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	EXPRESSION TAG	UNP P71586
B	9	MET	-	EXPRESSION TAG	UNP P71586
B	10	SER	-	EXPRESSION TAG	UNP P71586
B	11	TYR	-	EXPRESSION TAG	UNP P71586
B	12	TYR	-	EXPRESSION TAG	UNP P71586
B	13	HIS	-	EXPRESSION TAG	UNP P71586
B	14	HIS	-	EXPRESSION TAG	UNP P71586
B	15	HIS	-	EXPRESSION TAG	UNP P71586
B	16	HIS	-	EXPRESSION TAG	UNP P71586
B	17	HIS	-	EXPRESSION TAG	UNP P71586
B	18	HIS	-	EXPRESSION TAG	UNP P71586
B	19	ASP	-	EXPRESSION TAG	UNP P71586
B	20	TYR	-	EXPRESSION TAG	UNP P71586
B	21	ASP	-	EXPRESSION TAG	UNP P71586
B	22	ILE	-	EXPRESSION TAG	UNP P71586
B	23	PRO	-	EXPRESSION TAG	UNP P71586
B	24	THR	-	EXPRESSION TAG	UNP P71586
B	25	GLU	-	EXPRESSION TAG	UNP P71586
B	26	ASN	-	EXPRESSION TAG	UNP P71586
B	27	LEU	-	EXPRESSION TAG	UNP P71586
B	28	TYR	-	EXPRESSION TAG	UNP P71586
B	29	PHE	-	EXPRESSION TAG	UNP P71586
B	30	GLN	-	EXPRESSION TAG	UNP P71586
B	31	GLY	-	EXPRESSION TAG	UNP P71586
B	32	ALA	-	EXPRESSION TAG	UNP P71586
B	33	MET	-	EXPRESSION TAG	UNP P71586
B	34	GLY	-	EXPRESSION TAG	UNP P71586

- Molecule 2 is water.

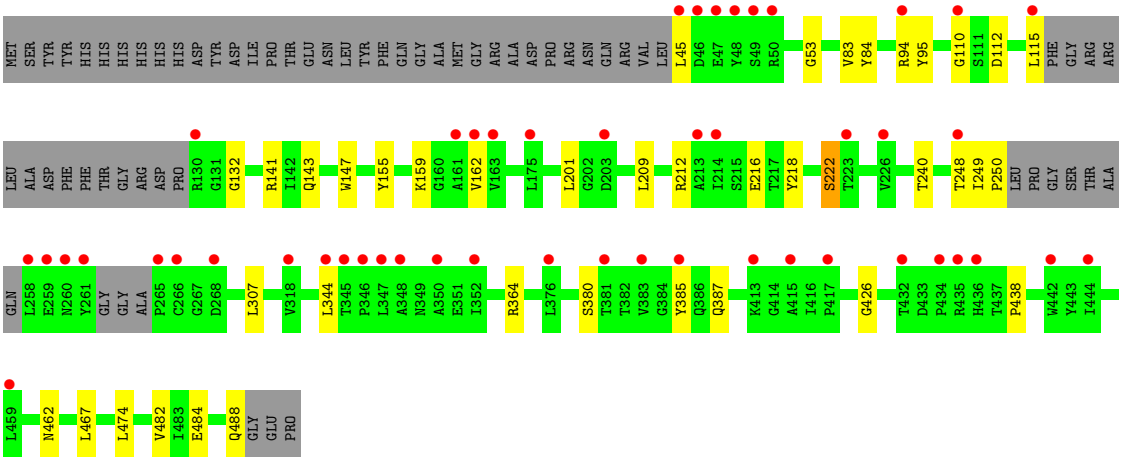
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	57	57	57	0	0
			Total	O		
2	B	19	19	19	0	0

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.

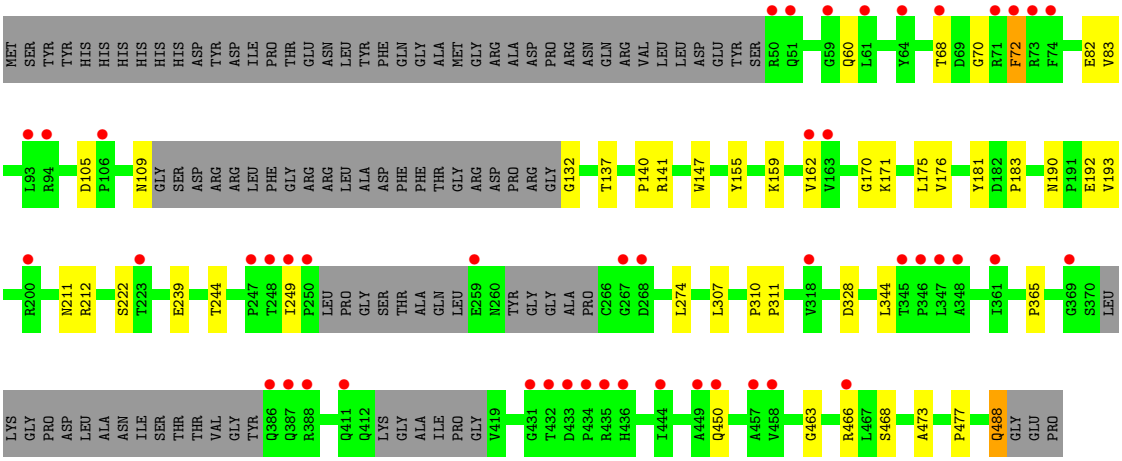
• Molecule 1: Penicillin-binding protein A

Chain A:



• Molecule 1: Penicillin-binding protein A

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	120.60Å 120.60Å 92.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.30 – 2.05 36.29 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.30-2.05) 99.8 (36.29-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.252 0.213 , 0.253	Depositor DCC
R_{free} test set	2388 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5984	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 67.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9725e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.54	0/3155	0.61	0/4308
1	B	0.55	1/2869 (0.0%)	0.60	0/3918
All	All	0.54	1/6024 (0.0%)	0.61	0/8226

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	GLY	N-CA	12.77	1.65	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	72	PHE	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	3093	0	3087	21	0
1	B	2815	0	2804	26	0
2	A	57	0	0	0	0
2	B	19	0	0	0	0
All	All	5984	0	5891	44	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 4.

All (44) 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:B:190:ASN:HD22	1:B:193:VAL:HG23	1.31	0.95
1:B:141:ARG:HD3	1:B:488:GLN:HE21	1.35	0.89
1:B:170:GLY:O	1:B:365:PRO:HA	1.88	0.73
1:B:141:ARG:HD3	1:B:488:GLN:NE2	2.09	0.68
1:A:474:LEU:HD13	1:B:155:TYR:OH	2.01	0.61
1:A:112:ASP:HB3	1:A:115:LEU:HD12	1.85	0.59
1:A:94:ARG:HD2	1:A:95:TYR:CZ	2.39	0.57
1:A:307:LEU:HD21	1:A:344:LEU:HD11	1.86	0.57
1:A:467:LEU:HD11	1:B:463:GLY:HA2	1.86	0.57
1:B:60:GLN:HG3	1:B:140:PRO:HG2	1.87	0.56
1:A:364:ARG:HB2	1:A:387:GLN:HG3	1.90	0.54
1:A:141:ARG:NH2	1:A:488:GLN:HB2	2.24	0.52
1:B:473:ALA:O	1:B:477:PRO:HD3	2.10	0.51
1:A:155:TYR:HB2	1:B:468:SER:HB3	1.93	0.50
1:A:162:VAL:HG11	1:A:482:VAL:HG21	1.93	0.50
1:A:201:LEU:HD13	1:A:209:LEU:HD21	1.93	0.49
1:B:159:LYS:HE3	1:B:212:ARG:HH11	1.78	0.49
1:A:94:ARG:HD2	1:A:95:TYR:CE1	2.49	0.48
1:B:307:LEU:HD21	1:B:344:LEU:HD11	1.96	0.47
1:A:53:GLY:HA3	1:A:132:GLY:O	2.14	0.47
1:B:141:ARG:CD	1:B:488:GLN:HE21	2.18	0.47
1:A:216:GLU:HG2	1:A:218:TYR:CZ	2.50	0.46
1:A:84:TYR:CE2	1:A:143:GLN:HG2	2.52	0.45
1:B:239:GLU:HA	1:B:274:LEU:HB3	1.99	0.45
1:A:222:SER:HB2	1:A:426:GLY:HA3	1.98	0.44
1:A:438:PRO:HB2	1:A:462:ASN:HB3	1.99	0.44
1:B:70:GLY:C	1:B:72:PHE:H	2.20	0.44
1:A:159:LYS:HD2	1:A:212:ARG:NH1	2.33	0.44
1:B:159:LYS:HE3	1:B:212:ARG:NH1	2.34	0.43
1:B:175:LEU:HD21	1:B:211:ASN:HD21	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:VAL:HG22	1:A:147:TRP:CD1	2.53	0.43
1:A:249:ILE:HG13	1:A:250:PRO:HD2	2.00	0.42
1:B:83:VAL:HG22	1:B:147:TRP:CD1	2.54	0.42
1:B:70:GLY:C	1:B:72:PHE:N	2.72	0.42
1:B:310:PRO:HA	1:B:311:PRO:HD3	1.92	0.42
1:B:190:ASN:HD21	1:B:192:GLU:HB3	1.83	0.42
1:A:484:GLU:O	1:A:488:GLN:HG3	2.19	0.42
1:B:162:VAL:HB	1:B:176:VAL:HB	2.02	0.42
1:B:105:ASP:O	1:B:109:ASN:N	2.53	0.41
1:B:137:THR:HB	1:B:171:LYS:HB2	2.03	0.41
1:B:190:ASN:ND2	1:B:192:GLU:HB3	2.36	0.41
1:A:110:GLY:HA2	1:A:115:LEU:HD13	2.03	0.41
1:B:244:THR:HG21	1:B:249:ILE:HD12	2.04	0.40
1:B:181:TYR:O	1:B:183:PRO:HD3	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	412/483 (85%)	400 (97%)	12 (3%)	0	100	100
1	B	371/483 (77%)	353 (95%)	18 (5%)	0	100	100
All	All	783/966 (81%)	753 (96%)	30 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	320/370 (86%)	314 (98%)	6 (2%)	57	53
1	B	291/370 (79%)	284 (98%)	7 (2%)	49	42
All	All	611/740 (83%)	598 (98%)	13 (2%)	53	48

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	222	SER
1	A	240	THR
1	A	248	THR
1	A	380	SER
1	A	385	TYR
1	B	68	THR
1	B	82	GLU
1	B	222	SER
1	B	328	ASP
1	B	450	GLN
1	B	466	ARG
1	B	488	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	190	ASN
1	B	412	GLN
1	B	488	GLN

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 (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 (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	420/483 (86%)	0.50	49 (11%)	4	4	28, 42, 68, 78	0
1	B	383/483 (79%)	0.68	47 (12%)	4	3	31, 56, 88, 113	0
All	All	803/966 (83%)	0.58	96 (11%)	4	4	28, 47, 81, 113	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	LEU	8.8
1	B	436	HIS	5.4
1	A	48	TYR	5.2
1	A	436	HIS	5.1
1	B	71	ARG	5.1
1	A	258	LEU	4.7
1	A	46	ASP	4.6
1	B	268	ASP	4.3
1	B	94	ARG	4.2
1	B	435	ARG	4.2
1	B	388	ARG	4.1
1	B	250	PRO	4.0
1	B	248	THR	4.0
1	B	259	GLU	4.0
1	A	50	ARG	4.0
1	B	59	GLY	3.8
1	A	347	LEU	3.7
1	B	72	PHE	3.7
1	B	73	ARG	3.7
1	B	386	GLN	3.6
1	B	247	PRO	3.6
1	A	381	THR	3.6
1	A	47	GLU	3.6
1	B	369	GLY	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	435	ARG	3.4
1	B	387	GLN	3.4
1	A	203	ASP	3.2
1	A	49	SER	3.2
1	B	74	PHE	3.1
1	A	348	ALA	3.1
1	B	249	ILE	3.1
1	A	268	ASP	3.0
1	A	163	VAL	3.0
1	B	68	THR	3.0
1	A	417	PRO	3.0
1	B	93	LEU	3.0
1	A	383	VAL	2.9
1	A	259	GLU	2.9
1	A	385	TYR	2.9
1	A	434	PRO	2.8
1	A	432	THR	2.8
1	B	348	ALA	2.7
1	A	318	VAL	2.7
1	B	347	LEU	2.7
1	A	444	ILE	2.7
1	A	130	ARG	2.7
1	A	261	TYR	2.6
1	B	318	VAL	2.6
1	A	223	THR	2.6
1	B	434	PRO	2.6
1	A	344	LEU	2.6
1	B	162	VAL	2.5
1	A	214	ILE	2.5
1	A	415	ALA	2.5
1	A	213	ALA	2.5
1	A	94	ARG	2.4
1	B	267	GLY	2.4
1	B	432	THR	2.4
1	A	442	TRP	2.4
1	B	346	PRO	2.4
1	B	458	VAL	2.4
1	B	106	PRO	2.4
1	A	346	PRO	2.4
1	B	64	TYR	2.4
1	B	200	ARG	2.4
1	B	163	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	413	LYS	2.3
1	A	110	GLY	2.3
1	A	161	ALA	2.2
1	B	433	ASP	2.2
1	B	466	ARG	2.2
1	B	431	GLY	2.2
1	B	51	GLN	2.2
1	B	450	GLN	2.2
1	B	411	GLN	2.2
1	A	352	ILE	2.2
1	B	50	ARG	2.2
1	B	61	LEU	2.1
1	A	226	VAL	2.1
1	A	248	THR	2.1
1	A	345	THR	2.1
1	A	459	LEU	2.1
1	B	223	THR	2.1
1	A	376	LEU	2.1
1	A	260	ASN	2.1
1	B	457	ALA	2.1
1	A	115	LEU	2.1
1	A	265	PRO	2.0
1	A	266	CYS	2.0
1	A	175	LEU	2.0
1	B	449	ALA	2.0
1	A	162	VAL	2.0
1	A	350	ALA	2.0
1	B	345	THR	2.0
1	B	361	ILE	2.0
1	B	444	ILE	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.