

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	4Q9H
Title	:	P-glycoprotein at 3.4 A resolution
Authors	:	McGrath, A.P.; Szewczyk, P.; Chang, G.
Deposited on	:	2014-05-01
Resolution	:	3.40 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 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)	:	1.13
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 (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.40 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}	130704	1026 (3.48-3.32)		
Clashscore	141614	1055 (3.48-3.32)		
Ramachandran outliers	138981	1038 (3.48-3.32)		
Sidechain outliers	138945	1038 (3.48-3.32)		
RSRZ outliers	127900	2173 (3.50-3.30)		

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					
			10%					
1	А	1284	78%	14%	8%			



4Q9H

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9164 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 Multidrug resistance protein 1A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	1182	Total 9164	C 5893	N 1553	O 1680	S 38	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	83	GLN	ASN	conflict	UNP P21447
А	87	GLN	ASN	conflict	UNP P21447
А	90	GLN	ASN	conflict	UNP P21447
А	1277	LEU	-	expression tag	UNP P21447
А	1278	GLU	-	expression tag	UNP P21447
А	1279	HIS	-	expression tag	UNP P21447
А	1280	HIS	-	expression tag	UNP P21447
А	1281	HIS	-	expression tag	UNP P21447
А	1282	HIS	-	expression tag	UNP P21447
А	1283	HIS	-	expression tag	UNP P21447
А	1284	HIS	-	expression tag	UNP P21447



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.

- 10% Chain A: 78% 14% 8%
- Molecule 1: Multidrug resistance protein 1A







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	87.95Å 139.18Å 186.03Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	77.33 - 3.40	Depositor
Resolution (A)	77.33 - 3.40	EDS
% Data completeness	99.2 (77.33-3.40)	Depositor
(in resolution range)	99.2 (77.33-3.40)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) > 1$	$1.95 (at 3.41 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R R.	0.260 , 0.291	Depositor
n, n_{free}	0.265 , 0.291	DCC
R_{free} test set	1615 reflections (5.06%)	wwPDB-VP
Wilson B-factor $(Å^2)$	134.3	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.25 , 24.5	EDS
L-test for twinning ²	$ L > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9164	wwPDB-VP
Average B, all atoms $(Å^2)$	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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).

Mal	Chain	Bond	lengths	Bond angles		
IVIOI	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.35	0/9333	0.53	2/12615~(0.0%)	

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	А	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	1054	LEU	CA-CB-CG	5.35	127.60	115.30
1	А	1223	CYS	CA-CB-SG	5.03	123.06	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	398	PRO	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	А	9164	0	9350	120	0
All	All	9164	0	9350	120	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 6.

All (120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:235:PHE:O	1:A:287:LYS:NZ	2.25	0.69
1:A:1172:LEU:HD13	1:A:1176:GLN:HB2	1.79	0.65
1:A:76:ASP:OD2	1:A:323:SER:OG	2.17	0.62
1:A:700:ASN:ND2	1:A:703:GLU:OE1	2.32	0.61
1:A:733:GLY:O	1:A:737:ASN:N	2.34	0.60
1:A:893:ALA:HB2	1:A:916:TYR:HE1	1.67	0.60
1:A:1154:ILE:HA	1:A:1157:LEU:CD1	2.31	0.60
1:A:1153:PHE:CE2	1:A:1176:GLN:HG2	2.37	0.59
1:A:1070:CYS:O	1:A:1074:THR:N	2.34	0.56
1:A:40:ARG:HD2	1:A:41:TYR:CZ	2.40	0.56
1:A:1154:ILE:HG21	1:A:1161:TYR:CE2	2.41	0.55
1:A:922:ILE:HB	1:A:923:PRO:HD3	1.89	0.55
1:A:1090:VAL:HG13	1:A:1097:ILE:HG12	1.87	0.55
1:A:1193:LEU:HB2	1:A:1223:CYS:HB2	1.87	0.54
1:A:1207:GLU:OE1	1:A:1229:ARG:NH2	2.41	0.54
1:A:1001:ALA:O	1:A:1005:ILE:HD12	2.08	0.54
1:A:802:ASP:OD1	1:A:804:LYS:N	2.41	0.54
1:A:729:SER:O	1:A:733:GLY:N	2.41	0.54
1:A:1030:ASN:ND2	1:A:1055:GLU:OE1	2.41	0.54
1:A:694:TRP:O	1:A:697:LEU:N	2.41	0.53
1:A:257:ILE:HG23	1:A:258:ARG:N	2.23	0.52
1:A:453:ASP:OD1	1:A:454:ILE:N	2.43	0.52
1:A:495:GLU:N	1:A:495:GLU:OE1	2.41	0.52
1:A:156:ILE:HD11	1:A:904:VAL:HG11	1.90	0.52
1:A:239:GLU:HB2	1:A:287:LYS:HZ2	1.76	0.51
1:A:518:THR:HG22	1:A:519:LEU:H	1.76	0.51
1:A:1012:PRO:HG2	1:A:1015:ASP:HB3	1.93	0.51
1:A:801:ASP:OD2	1:A:1083:TYR:OH	2.25	0.51
1:A:731:VAL:HG22	1:A:751:PHE:HB3	1.93	0.50
1:A:1136:VAL:HG12	1:A:1140:GLU:HB3	1.93	0.50
1:A:40:ARG:NH1	1:A:366:ASP:OD1	2.43	0.50
1:A:33:VAL:HG12	1:A:37:THR:OG1	2.12	0.50
1:A:707:PHE:O	1:A:711:ILE:HG12	2.12	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:572:ALA:O	1:A:576:ARG:NH1	2.45	0.50
1:A:762:SER:HA	1:A:765:THR:HG22	1.93	0.50
1:A:711:ILE:HD12	1:A:833:PHE:CD2	2.47	0.49
1:A:843:ILE:HD11	1:A:858:LEU:HD21	1.95	0.49
1:A:257:ILE:HG21	1:A:800:PHE:HD1	1.76	0.49
1:A:824:ALA:HA	1:A:828:ARG:HD3	1.95	0.49
1:A:853:LEU:HD12	1:A:973:VAL:HG11	1.94	0.49
1:A:93:GLU:OE1	1:A:93:GLU:N	2.45	0.48
1:A:544:ASN:O	1:A:544:ASN:ND2	2.46	0.48
1:A:477:ALA:O	1:A:478:THR:HG23	2.12	0.48
1:A:1110:GLY:N	1:A:1192:ILE:O	2.45	0.48
1:A:1196:ASP:OD1	1:A:1226:ILE:HD11	2.13	0.48
1:A:388:LEU:HB2	1:A:413:VAL:CG1	2.44	0.48
1:A:300:LEU:HD21	1:A:763:PHE:HB2	1.95	0.48
1:A:1144:ALA:CB	1:A:1187:VAL:HG23	2.44	0.48
1:A:604:GLU:OE1	1:A:617:ILE:N	2.45	0.47
1:A:1196:ASP:HA	1:A:1226:ILE:HG12	1.95	0.47
1:A:108:THR:HG22	1:A:954:ARG:HH12	1.79	0.47
1:A:1120:ASP:OD2	1:A:1164:ARG:NH2	2.47	0.47
1:A:1050:GLN:H	1:A:1245:GLY:HA3	1.78	0.47
1:A:518:THR:HG22	1:A:519:LEU:N	2.30	0.47
1:A:758:LEU:HA	1:A:761:ILE:HG22	1.97	0.47
1:A:257:ILE:HA	1:A:260:VAL:HG12	1.96	0.47
1:A:1204:THR:OG1	1:A:1205:GLU:N	2.48	0.47
1:A:397:TYR:O	1:A:399:SER:N	2.48	0.46
1:A:189:PHE:CE1	1:A:348:ILE:HD11	2.50	0.46
1:A:388:LEU:HB2	1:A:413:VAL:HG13	1.97	0.46
1:A:916:TYR:CE2	1:A:920:LEU:HD11	2.51	0.46
1:A:479:THR:HA	1:A:518:THR:O	2.16	0.45
1:A:419:VAL:HG23	1:A:593:VAL:HG23	1.99	0.45
1:A:86:LYS:HB2	1:A:739:GLY:CA	2.47	0.45
1:A:1052:LEU:HG	1:A:1054:LEU:HD22	1.98	0.45
1:A:1173:SER:OG	1:A:1176:GLN:OE1	2.29	0.44
1:A:1157:LEU:HB3	1:A:1158:PRO:HD2	2.00	0.44
1:A:833:PHE:HA	1:A:836:ILE:HG12	1.99	0.44
1:A:734:VAL:O	1:A:738:GLY:N	2.49	0.44
1:A:794:ARG:HG2	1:A:1012:PRO:HG3	1.99	0.44
1:A:963:GLN:HG2	1:A:964:LEU:N	2.32	0.44
1:A:372:ASP:O	1:A:373:SER:CB	2.66	0.44
1:A:409:LEU:HD13	1:A:410:ASN:N	2.33	0.44
1:A:1202:LEU:HD23	1:A:1207:GLU:HA	1.99	0.44



	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:330:VAL:HG23	1:A:331:PHE:N	2.32	0.44
1:A:843:ILE:CD1	1:A:858:LEU:HD11	2.48	0.43
1:A:270:LEU:HD21	1:A:786:TYR:CE1	2.53	0.43
1:A:1269:VAL:HG13	1:A:1270:GLN:N	2.33	0.43
1:A:727:ILE:HD12	1:A:758:LEU:HD23	1.99	0.43
1:A:696:ILE:HG23	1:A:697:LEU:HD12	2.01	0.43
1:A:86:LYS:HB2	1:A:739:GLY:HA2	2.00	0.43
1:A:704:TRP:N	1:A:705:PRO:HD2	2.33	0.43
1:A:81:VAL:HG21	1:A:103:LEU:CD2	2.48	0.43
1:A:151:ILE:HD12	1:A:167:LEU:HD21	2.00	0.43
1:A:474:VAL:CG1	1:A:902:THR:HG21	2.49	0.43
1:A:916:TYR:HE2	1:A:920:LEU:HD11	1.84	0.43
1:A:64:LEU:HD12	1:A:336:ILE:HG21	2.00	0.42
1:A:74:MET:SD	1:A:953:PHE:CD2	3.12	0.42
1:A:603:VAL:HG23	1:A:604:GLU:H	1.85	0.42
1:A:1165:VAL:HG12	1:A:1166:GLY:N	2.35	0.42
1:A:159:PHE:HE2	1:A:900:PHE:CG	2.38	0.42
1:A:295:MET:HG2	1:A:766:PHE:CZ	2.55	0.42
1:A:313:GLY:O	1:A:317:VAL:HG23	2.19	0.42
1:A:703:GLU:HG2	1:A:779:ILE:HD11	2.01	0.42
1:A:721:GLN:HB3	1:A:722:PRO:HD3	2.01	0.42
1:A:33:VAL:O	1:A:355:ARG:NH1	2.53	0.42
1:A:134:LEU:HD22	1:A:931:ALA:CB	2.50	0.41
1:A:802:ASP:OD1	1:A:804:LYS:HB2	2.20	0.41
1:A:121:VAL:HA	1:A:124:VAL:HG22	2.02	0.41
1:A:1196:ASP:CG	1:A:1226:ILE:HD11	2.41	0.41
1:A:1244:ASN:OD1	1:A:1244:ASN:N	2.53	0.41
1:A:408:GLY:O	1:A:409:LEU:HB2	2.20	0.41
1:A:1150:ILE:HB	1:A:1179:ARG:HB3	2.03	0.41
1:A:1152:GLN:HG3	1:A:1153:PHE:N	2.35	0.41
1:A:159:PHE:HE2	1:A:900:PHE:CD2	2.38	0.41
1:A:257:ILE:HG12	1:A:800:PHE:CE1	2.56	0.41
1:A:419:VAL:HA	1:A:593:VAL:HG23	2.02	0.41
1:A:390:PHE:HB3	1:A:409:LEU:HD12	2.01	0.41
1:A:477:ALA:HA	1:A:520:VAL:O	2.21	0.41
1:A:1154:ILE:HG21	1:A:1161:TYR:CD2	2.56	0.41
1:A:159:PHE:CE2	1:A:900:PHE:CD2	3.10	0.41
1:A:270:LEU:C	1:A:270:LEU:HD23	2.42	0.41
1:A:1035:GLY:O	1:A:1088:GLY:HA3	2.20	0.41
1:A:478:THR:HB	1:A:482:GLU:HB2	2.03	0.40
1:A:257:ILE:HA	1:A:260:VAL:CG1	2.52	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:991:ALA:N	1:A:992:PRO:HD2	2.35	0.40
1:A:1033:PHE:HD1	1:A:1036:VAL:HG21	1.87	0.40
1:A:388:LEU:HD12	1:A:388:LEU:N	2.37	0.40
1:A:711:ILE:HD12	1:A:833:PHE:HD2	1.87	0.40
1:A:1063:ALA:HB1	1:A:1233:ILE:HG12	2.02	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	Perce	entiles
1	А	1178/1284~(92%)	1130 (96%)	48 (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	А	973/1065~(91%)	963~(99%)	10 (1%)	76 88

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	310	PHE
	<i>a</i>	7	,



COntic	naea jion	i previe	as paye
Mol	Chain	\mathbf{Res}	Type
1	А	508	PHE
1	А	700	ASN
1	А	747	ASN
1	А	793	LEU
1	А	795	GLN
1	А	1030	ASN
1	А	1151	HIS
1	А	1155	ASP
1	А	1223	CYS

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

Mol	Chain	Res	Type
1	А	452	GLN
1	А	1030	ASN
1	А	1151	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 (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, 95^{th} 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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	1182/1284~(92%)	0.73	130 (10%) 5 6	40, 91, 179, 277	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	306	TYR	5.6
1	А	231	ILE	5.3
1	А	605	GLN	5.2
1	А	574	GLU	5.0
1	А	312	TYR	5.0
1	А	228	TRP	4.9
1	А	235	PHE	4.8
1	А	974	PHE	4.8
1	А	299	PHE	4.6
1	А	952	CYS	4.6
1	А	83	GLN	4.6
1	А	222	GLY	4.1
1	А	226	GLY	4.1
1	А	303	TYR	4.0
1	А	736	THR	4.0
1	А	953	PHE	4.0
1	А	324	ILE	3.9
1	А	732	VAL	3.8
1	А	959	LEU	3.8
1	А	423	GLY	3.8
1	А	955	PHE	3.7
1	А	738	GLY	3.7
1	А	269	GLU	3.6
1	А	236	THR	3.6
1	А	85	SER	3.5
1	А	224	SER	3.5
1	А	132	TRP	3.5



Mol	Chain	Res	Type	RSRZ
1	А	971	LEU	3.5
1	А	556	ALA	3.4
1	А	78	PHE	3.4
1	А	405	ILE	3.3
1	А	1250	HIS	3.3
1	А	778	GLU	3.3
1	А	554	THR	3.3
1	А	886	LEU	3.3
1	А	769	GLN	3.3
1	А	484	ILE	3.2
1	А	946	TYR	3.2
1	А	1165	VAL	3.2
1	А	773	PHE	3.2
1	A	785	ARG	3.2
1	А	223	LEU	3.2
1	А	1105	LEU	3.1
1	А	548	LEU	3.1
1	А	422	VAL	3.1
1	А	557	LEU	3.0
1	А	229	ALA	3.0
1	А	706	TYR	3.0
1	А	606	GLY	3.0
1	А	220	VAL	3.0
1	А	1054	LEU	3.0
1	А	549	LEU	3.0
1	А	1225	VAL	2.9
1	А	210	LEU	2.9
1	А	1067	SER	2.9
1	А	424	ASN	2.9
1	A	182	ILE	2.8
1	А	295	MET	2.8
1	А	103	LEU	2.8
1	A	1150	ILE	2.8
1	А	852	GLN	2.7
1	A	522	GLU	2.7
1	A	328	LEU	2.7
1	А	1033	PHE	2.7
1	A	618	TYR	2.7
1	А	720	LEU	2.7
1	A	934	PHE	2.7
1	А	970	VAL	2.7
1	А	486	TYR	2.6



Mol	Chain	Res	Type	RSRZ
1	А	233	SER	2.6
1	А	735	PHE	2.6
1	А	230	LYS	2.6
1	А	784	LEU	2.6
1	А	878	GLN	2.6
1	А	71	PHE	2.6
1	А	310	PHE	2.5
1	А	724	PHE	2.5
1	А	84	VAL	2.5
1	А	584	ARG	2.5
1	А	1195	LEU	2.5
1	А	139	GLN	2.5
1	А	1260	LYS	2.5
1	А	967	PHE	2.4
1	А	700	ASN	2.4
1	А	1219	GLU	2.4
1	А	134	LEU	2.4
1	А	1065	VAL	2.4
1	А	266	GLN	2.3
1	А	1064	LEU	2.3
1	А	1080	GLU	2.3
1	А	1079	LEU	2.3
1	А	476	PHE	2.3
1	А	1263	TYR	2.3
1	А	208	TRP	2.3
1	А	49	TYR	2.3
1	А	1031	VAL	2.3
1	А	143	ILE	2.3
1	А	1205	GLU	2.2
1	А	1100	LEU	2.2
1	А	789	PHE	2.2
1	A	480	ILE	2.2
1	A	1242	ILE	2.2
1	А	243	TYR	2.2
1	A	357	ALA	2.2
1	A	734	VAL	2.2
1	А	449	ILE	2.2
1	A	315	SER	2.2
1	A	1262	ILE	2.2
1	A	468	VAL	2.2
1	A	792	MET	2.1
1	А	569	LEU	2.1



Mol	Chain	Res	Type	RSRZ
1	А	1161	TYR	2.1
1	А	175	VAL	2.1
1	А	978	VAL	2.1
1	А	972	LEU	2.1
1	А	432	THR	2.1
1	А	1004	ILE	2.1
1	А	1193	LEU	2.1
1	А	227	ILE	2.1
1	А	395	PHE	2.1
1	А	138	ARG	2.1
1	А	131	PHE	2.1
1	А	99	MET	2.1
1	А	707	PHE	2.0
1	А	1093	ASP	2.0
1	А	217	ILE	2.0
1	А	254	LEU	2.0
1	А	331	PHE	2.0
1	А	1214	LEU	2.0
1	А	1230	LEU	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.

