



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:35 PM UTC

PDB ID : 4Q9H / pdb_00004q9h
Title : P-glycoprotein at 3.4 Å 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

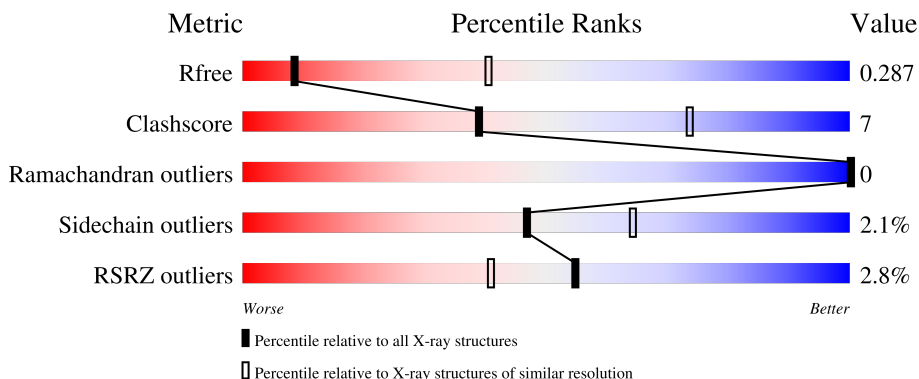
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 $\leq 5\%$. 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	1284	

2 Entry composition

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	A	1182	Total	C	N	O	S	0	0	0
			9164	5893	1553	1680	38			

There are 11 discrepancies between the modelled and reference sequences:

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

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.95Å 139.18Å 186.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.33 – 3.40 77.33 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (77.33-3.40) 99.1 (77.33-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.260 , 0.291 0.267 , 0.287	Depositor DCC
R_{free} test set	1616 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	134.3	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 77.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

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	0.47	0/9333	0.84	10/12615 (0.1%)

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	A	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	399	SER	N-CA-C	-6.17	105.75	113.28
1	A	1111	ILE	N-CA-C	6.17	117.39	109.30
1	A	1240	VAL	N-CA-C	6.07	117.43	107.24
1	A	738	GLY	N-CA-C	5.67	119.50	112.64
1	A	1168	LYS	N-CA-C	-5.62	104.43	112.13
1	A	1204	THR	CB-CA-C	-5.56	110.14	116.54
1	A	1069	GLY	N-CA-C	5.18	120.49	112.45
1	A	966	THR	N-CA-C	5.12	117.94	109.85
1	A	1053	SER	N-CA-C	5.12	116.75	108.26
1	A	1240	VAL	CB-CA-C	-5.02	104.76	110.73

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	PRO	Peptide

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	9164	0	9350	125	0
All	All	9164	0	9350	125	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 7.

All (125) 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:235:PHE:O	1:A:287:LYS:NZ	2.25	0.70
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:801:ASP:OD2	1:A:1083:TYR:OH	2.25	0.51
1:A:518:THR:HG22	1:A:519:LEU:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1012:PRO:HG2	1:A:1015:ASP:HB3	1.93	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
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:1196:ASP:CG	1:A:1226:ILE:HD11	2.41	0.46
1:A:270:LEU:C	1:A:270:LEU:HD23	2.42	0.45
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:1157:LEU:HB3	1:A:1158:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1172:LEU:HD12	1:A:1172:LEU:C	2.42	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
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:446:MET:HE2	1:A:448:SER:HB2	2.01	0.43
1:A:1269:VAL:HG13	1:A:1270:GLN:N	2.33	0.43
1:A:1132:ASN:C	1:A:1134:ARG:H	2.26	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:874:MET:HE2	1:A:937:THR:HG21	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:167:LEU:C	1:A:167:LEU:HD23	2.44	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:38:MET:HE2	1:A:182:ILE:HG22	2.02	0.41
1:A:121:VAL:HA	1:A:124:VAL:HG22	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1035:GLY:O	1:A:1088:GLY:HA3	2.20	0.41
1:A:64:LEU:HD13	1:A:64:LEU:C	2.45	0.40
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
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 ⓘ

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	1178/1284 (92%)	1130 (96%)	48 (4%)	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	973/1065 (91%)	953 (98%)	20 (2%)	47 64

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LYS
1	A	134	LEU
1	A	144	ARG
1	A	253	VAL
1	A	260	VAL
1	A	310	PHE
1	A	317	VAL
1	A	508	PHE
1	A	753	LEU
1	A	768	LEU
1	A	793	LEU
1	A	795	GLN
1	A	1014	ILE
1	A	1030	ASN
1	A	1031	VAL
1	A	1062	LEU
1	A	1151	HIS
1	A	1187	VAL
1	A	1223	CYS
1	A	1225	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	154	GLN
1	A	276	ASN
1	A	417	GLN
1	A	424	ASN
1	A	437	GLN
1	A	483	ASN
1	A	504	ASN
1	A	544	ASN
1	A	744	GLN

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Mol	Chain	Res	Type
1	A	747	ASN
1	A	838	ASN
1	A	932	HIS
1	A	1030	ASN
1	A	1114	GLN
1	A	1151	HIS
1	A	1243	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	1182/1284 (92%)	0.04	33 (2%) 55 41	40, 91, 179, 277	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	ILE	4.9
1	A	312	TYR	4.3
1	A	778	GLU	4.0
1	A	83	GLN	4.0
1	A	306	TYR	3.6
1	A	605	GLN	3.2
1	A	1083	TYR	3.0
1	A	736	THR	2.8
1	A	617	ILE	2.8
1	A	232	LEU	2.8
1	A	974	PHE	2.7
1	A	403	VAL	2.6
1	A	1260	LYS	2.5
1	A	109	THR	2.4
1	A	958	TYR	2.4
1	A	1201	ALA	2.4
1	A	934	PHE	2.4
1	A	49	TYR	2.3
1	A	227	ILE	2.3
1	A	1093	ASP	2.3
1	A	223	LEU	2.3
1	A	445	GLY	2.3
1	A	303	TYR	2.3
1	A	74	MET	2.2
1	A	228	TRP	2.2
1	A	514	HIS	2.2
1	A	952	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	446	MET	2.2
1	A	243	TYR	2.1
1	A	995	ALA	2.1
1	A	447	VAL	2.1
1	A	226	GLY	2.0
1	A	1092	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 oligosaccharides 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.