



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:05 AM UTC

PDB ID : 4KF7 / pdb_00004kf7
Title : Nup188(aa1-1160) from Myceliophthora thermophila
Authors : Schwartz, T.U.; Andersen, K.R.
Deposited on : 2013-04-26
Resolution : 2.65 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

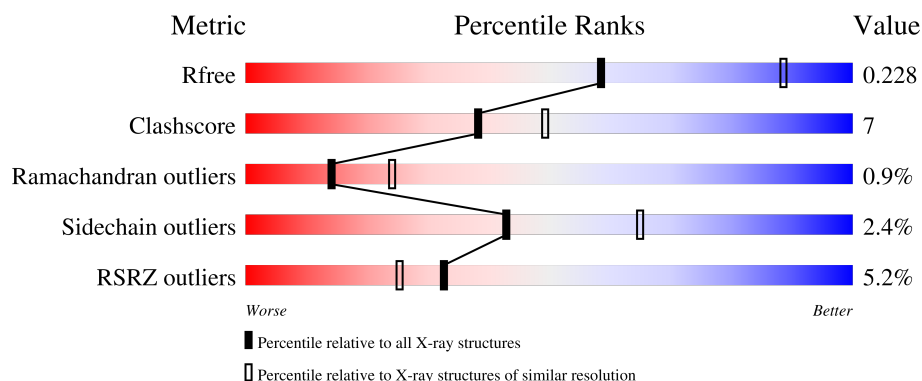
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	1160	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8644 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 Nup188.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1096	Total	C	N	O	S	0	0	0
			8516	5387	1467	1625	37			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	128	Total	O	0	0
			128	128		

WORLD WIDE
PDB
PROTEIN DATA BANK

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.03Å 94.77Å 91.64Å 90.00° 98.94° 90.00°	Depositor
Resolution (Å)	66.76 – 2.65 66.76 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (66.76-2.65) 100.0 (66.76-2.65)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.55Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.181 , 0.225 0.184 , 0.228	Depositor DCC
R_{free} test set	2120 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8644	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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 [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	0.36	0/8670	0.81	15/11781 (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 (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	277	MET	N-CA-C	-7.73	102.49	112.23
1	A	635	ASN	CA-C-N	7.58	127.46	119.05
1	A	635	ASN	C-N-CA	7.58	127.46	119.05
1	A	659	THR	N-CA-C	-7.46	103.64	112.89
1	A	658	ASN	N-CA-C	6.65	119.11	108.41
1	A	10	PHE	CA-C-N	6.63	124.50	119.66
1	A	10	PHE	C-N-CA	6.63	124.50	119.66
1	A	653	VAL	N-CA-C	-6.53	102.84	110.21
1	A	94	TYR	N-CA-C	-6.39	105.55	113.15
1	A	167	THR	N-CA-C	6.00	122.05	114.31
1	A	222	LEU	N-CA-C	-5.62	106.40	113.20
1	A	1117	LYS	N-CA-C	5.62	119.81	112.17
1	A	242	LYS	CA-C-N	5.57	125.89	119.93
1	A	242	LYS	C-N-CA	5.57	125.89	119.93
1	A	221	GLU	N-CA-C	-5.12	104.54	111.55

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	THR	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	8516	0	8530	117	0
2	A	128	0	0	5	0
All	All	8644	0	8530	117	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 (117) 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:325:MET:HE3	1:A:330:PHE:HA	1.59	0.83
1:A:13:LEU:HD22	1:A:81:THR:HG22	1.61	0.83
1:A:1072:ARG:HE	1:A:1115:LEU:HD12	1.45	0.82
1:A:1097:LEU:HD23	1:A:1142:TRP:HB3	1.69	0.75
1:A:366:LEU:HD22	1:A:420:GLN:HG3	1.71	0.72
1:A:842:THR:HG22	1:A:846:SER:HA	1.73	0.69
1:A:1009:LEU:HD12	1:A:1010:PRO:HD2	1.76	0.68
1:A:685:GLU:HB2	1:A:719:LYS:HZ1	1.59	0.67
1:A:124:GLU:OE2	1:A:187:ARG:NH1	2.28	0.67
1:A:1069:HIS:HA	1:A:1072:ARG:HD2	1.77	0.66
1:A:797:VAL:HA	1:A:800:GLU:HB3	1.79	0.65
1:A:1121:ARG:NH2	1:A:1124:GLU:OE2	2.29	0.65
1:A:787:ASN:OD1	1:A:829:ARG:NH2	2.30	0.64
1:A:265:ARG:NH2	2:A:1267:HOH:O	2.30	0.63
1:A:581:ARG:NH1	2:A:1257:HOH:O	2.27	0.62
1:A:840:ILE:O	1:A:842:THR:N	2.33	0.62
1:A:532:ASP:OD1	1:A:581:ARG:NH2	2.33	0.61
1:A:942:SER:HA	1:A:1025:ARG:HD2	1.83	0.61
1:A:34:GLU:HG2	1:A:37:ALA:HB2	1.83	0.60
1:A:783:ARG:HG2	1:A:787:ASN:HD22	1.67	0.59
1:A:151:VAL:H	1:A:155:GLN:HG3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ALA:HB1	1:A:591:GLN:HG2	1.84	0.58
1:A:325:MET:HE2	1:A:352:VAL:HG13	1.84	0.57
1:A:654:PHE:O	1:A:655:GLU:HB2	2.04	0.57
1:A:796:LEU:O	1:A:800:GLU:N	2.36	0.57
1:A:1111:ILE:HA	1:A:1114:GLN:HB2	1.86	0.56
1:A:215:ALA:O	1:A:220:VAL:HG21	2.06	0.56
1:A:659:THR:O	1:A:697:PHE:HB2	2.05	0.56
1:A:595:GLN:NE2	2:A:1301:HOH:O	2.38	0.56
1:A:717:PHE:CZ	1:A:745:GLY:HA3	2.41	0.55
1:A:838:PRO:HB2	1:A:849:LEU:HD22	1.88	0.55
1:A:618:LEU:HD13	1:A:624:SER:HB3	1.89	0.54
1:A:1097:LEU:HB2	1:A:1143:MET:HG2	1.88	0.54
1:A:687:CYS:SG	1:A:778:LEU:HD21	2.47	0.54
1:A:192:TYR:CZ	1:A:196:ARG:HD2	2.43	0.53
1:A:699:THR:C	1:A:701:VAL:H	2.15	0.53
1:A:792:THR:O	1:A:796:LEU:HB2	2.08	0.53
1:A:794:ASP:OD1	1:A:833:TYR:OH	2.22	0.53
1:A:685:GLU:O	1:A:719:LYS:NZ	2.36	0.53
1:A:985:SER:O	1:A:995:ARG:NH1	2.42	0.53
1:A:178:PHE:O	1:A:187:ARG:NH2	2.42	0.53
1:A:138:SER:HA	1:A:169:ALA:HB3	1.91	0.52
1:A:204:ASP:CG	1:A:519:ARG:HH22	2.17	0.52
1:A:737:LEU:HD11	1:A:742:LEU:HD13	1.92	0.52
1:A:95:ASN:HB3	1:A:98:THR:HB	1.91	0.52
1:A:719:LYS:NZ	1:A:778:LEU:O	2.43	0.51
1:A:210:LEU:HB3	1:A:230:LEU:HD21	1.93	0.51
1:A:685:GLU:HB2	1:A:719:LYS:NZ	2.26	0.51
1:A:288:ARG:HD3	1:A:340:LEU:HB3	1.92	0.51
1:A:60:ARG:HH21	1:A:233:ALA:HA	1.76	0.50
1:A:155:GLN:O	1:A:159:ILE:N	2.41	0.50
1:A:439:ARG:NH1	1:A:461:SER:OG	2.45	0.50
1:A:219:GLY:O	1:A:221:GLU:N	2.43	0.49
1:A:851:ARG:NH2	1:A:921:GLN:HB3	2.27	0.49
1:A:1030:LEU:HD22	1:A:1078:LEU:HD22	1.93	0.49
1:A:723:VAL:HG11	1:A:732:THR:HG23	1.95	0.48
1:A:598:ASN:ND2	2:A:1301:HOH:O	2.45	0.48
1:A:848:ARG:HD2	1:A:851:ARG:CZ	2.44	0.48
1:A:1111:ILE:O	1:A:1115:LEU:N	2.46	0.48
1:A:851:ARG:HH22	1:A:921:GLN:HB3	1.80	0.47
1:A:946:ARG:HA	1:A:1028:THR:HG21	1.96	0.47
1:A:672:ASP:HB2	1:A:731:ASP:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:ALA:HB2	1:A:911:ILE:HG23	1.97	0.46
1:A:22:ILE:HG13	1:A:1117:LYS:HG2	1.97	0.46
1:A:185:ARG:NH1	2:A:1252:HOH:O	2.26	0.46
1:A:365:THR:HG23	1:A:383:LEU:HD21	1.97	0.46
1:A:685:GLU:OE2	1:A:780:SER:HB3	2.15	0.46
1:A:221:GLU:O	1:A:224:PRO:HD2	2.16	0.46
1:A:955:LEU:O	1:A:959:THR:OG1	2.33	0.46
1:A:93:PRO:C	1:A:95:ASN:H	2.24	0.45
1:A:543:TYR:CD1	1:A:599:ARG:NH2	2.84	0.45
1:A:1030:LEU:O	1:A:1034:THR:HG23	2.17	0.45
1:A:1133:SER:HB3	1:A:1137:ARG:NH1	2.32	0.45
1:A:236:PHE:HE2	1:A:245:THR:HG22	1.82	0.45
1:A:670:LEU:HB2	1:A:687:CYS:HB2	2.00	0.44
1:A:725:LEU:HD21	1:A:792:THR:HA	1.99	0.44
1:A:914:ARG:HD2	1:A:914:ARG:HA	1.78	0.44
1:A:1143:MET:HE3	1:A:1143:MET:HB3	1.91	0.44
1:A:1072:ARG:HB3	1:A:1115:LEU:HD11	1.98	0.44
1:A:823:LEU:HB3	1:A:824:PRO:HD3	1.98	0.44
1:A:921:GLN:HG2	1:A:981:TYR:CE2	2.52	0.44
1:A:332:GLU:OE1	1:A:406:SER:OG	2.33	0.43
1:A:159:ILE:HA	1:A:162:LEU:HG	2.00	0.43
1:A:365:THR:HG23	1:A:383:LEU:HD11	1.98	0.43
1:A:503:MET:HE2	1:A:530:PHE:HB3	2.00	0.43
1:A:1093:PRO:HA	1:A:1094:PRO:HD3	1.95	0.43
1:A:654:PHE:CG	1:A:655:GLU:N	2.86	0.43
1:A:374:ASP:OD1	1:A:374:ASP:N	2.45	0.43
1:A:921:GLN:HG2	1:A:981:TYR:CZ	2.54	0.43
1:A:1114:GLN:O	1:A:1118:PRO:HD3	2.19	0.43
1:A:1061:ILE:HG21	1:A:1078:LEU:HD23	1.99	0.43
1:A:41:LEU:HD12	1:A:41:LEU:HA	1.91	0.43
1:A:362:VAL:O	1:A:366:LEU:HG	2.19	0.43
1:A:1130:ARG:O	1:A:1134:THR:HG23	2.19	0.42
1:A:39:ASP:N	1:A:39:ASP:OD1	2.52	0.42
1:A:1097:LEU:HD12	1:A:1097:LEU:O	2.19	0.42
1:A:653:VAL:H	1:A:662:PHE:HA	1.84	0.42
1:A:133:LEU:HD12	1:A:1111:ILE:HD12	2.02	0.42
1:A:162:LEU:O	1:A:165:VAL:HG12	2.19	0.42
1:A:1097:LEU:HD11	1:A:1102:PRO:HA	2.01	0.42
1:A:683:PRO:HB2	1:A:685:GLU:HG3	2.01	0.42
1:A:409:PRO:HD3	1:A:502:LEU:HD23	2.02	0.42
1:A:656:GLU:HB2	1:A:657:GLU:H	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ALA:O	1:A:253:PRO:HD2	2.20	0.41
1:A:838:PRO:HA	1:A:841:ASN:ND2	2.35	0.41
1:A:151:VAL:O	1:A:155:GLN:NE2	2.53	0.41
1:A:780:SER:HB2	1:A:781:ARG:HG3	2.03	0.41
1:A:797:VAL:CG1	1:A:849:LEU:HD21	2.50	0.41
1:A:74:LYS:O	1:A:78:GLU:HG2	2.21	0.41
1:A:334:VAL:HG21	1:A:345:LEU:HD21	2.02	0.41
1:A:148:ALA:HB2	1:A:1056:LYS:HB2	2.03	0.41
1:A:746:ILE:HB	1:A:814:SER:HB3	2.03	0.41
1:A:952:MET:HB3	1:A:982:VAL:HG11	2.03	0.41
1:A:1062:ALA:O	1:A:1065:PRO:HD2	2.21	0.41
1:A:317:LEU:HD12	1:A:317:LEU:HA	1.87	0.41
1:A:1052:THR:O	1:A:1056:LYS:HG2	2.21	0.41
1:A:850:SER:HA	1:A:853:THR:HG22	2.03	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	1084/1160 (93%)	1030 (95%)	44 (4%)	10 (1%)	14 24

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	655	GLU
1	A	657	GLU
1	A	841	ASN
1	A	220	VAL
1	A	166	THR
1	A	1044	ASN
1	A	656	GLU

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Mol	Chain	Res	Type
1	A	660	ASN
1	A	1048	ALA
1	A	765	PRO

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	924/979 (94%)	902 (98%)	22 (2%)	43	65

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	THR
1	A	107	SER
1	A	165	VAL
1	A	168	VAL
1	A	221	GLU
1	A	300	LEU
1	A	334	VAL
1	A	386	SER
1	A	463	VAL
1	A	483	ILE
1	A	641	ASN
1	A	656	GLU
1	A	685	GLU
1	A	749	LEU
1	A	796	LEU
1	A	797	VAL
1	A	842	THR
1	A	856	LEU
1	A	877	VAL
1	A	1012	THR
1	A	1044	ASN
1	A	1110	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	HIS
1	A	155	GLN
1	A	247	GLN
1	A	349	HIS
1	A	420	GLN
1	A	426	GLN
1	A	498	GLN
1	A	531	GLN
1	A	539	HIS
1	A	595	GLN
1	A	622	ASN
1	A	921	GLN
1	A	1069	HIS
1	A	1114	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 oligosaccharides 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 ⓘ

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	1096/1160 (94%)	-0.03	57 (5%)	33 25	17, 58, 132, 182	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	687	CYS	5.9
1	A	2	ALA	4.3
1	A	36	LEU	4.3
1	A	654	PHE	4.1
1	A	446	LEU	4.0
1	A	674	ALA	3.8
1	A	903	PRO	3.8
1	A	1114	GLN	3.7
1	A	852	ILE	3.6
1	A	801	LEU	3.5
1	A	971	LEU	3.5
1	A	84	ILE	3.5
1	A	853	THR	3.3
1	A	804	LEU	3.3
1	A	162	LEU	3.3
1	A	218	THR	3.3
1	A	842	THR	3.3
1	A	151	VAL	3.2
1	A	93	PRO	3.2
1	A	844	THR	3.1
1	A	215	ALA	3.0
1	A	736	TYR	3.0
1	A	962	VAL	3.0
1	A	168	VAL	3.0
1	A	849	LEU	2.9
1	A	156	ALA	2.8
1	A	462	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	220	VAL	2.8
1	A	1118	PRO	2.8
1	A	83	ALA	2.8
1	A	599	ARG	2.7
1	A	163	LEU	2.7
1	A	444	PHE	2.6
1	A	885	VAL	2.6
1	A	683	PRO	2.6
1	A	802	ALA	2.6
1	A	335	PRO	2.6
1	A	171	ALA	2.5
1	A	701	VAL	2.5
1	A	905	ILE	2.4
1	A	175	TRP	2.4
1	A	841	ASN	2.3
1	A	859	LEU	2.3
1	A	855	ASN	2.2
1	A	653	VAL	2.2
1	A	37	ALA	2.2
1	A	972	THR	2.2
1	A	803	ASP	2.2
1	A	992	SER	2.2
1	A	1113	ALA	2.1
1	A	154	ALA	2.1
1	A	1142	TRP	2.1
1	A	167	THR	2.1
1	A	1	MET	2.1
1	A	166	THR	2.1
1	A	1042	TYR	2.0
1	A	782	GLY	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.