



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:16 PM UTC

PDB ID : 1N7P / pdb_00001n7p
Title : Streptococcus pneumoniae Hyaluronate Lyase W292A/F343V Double Mutant
Authors : Nukui, M.; Taylor, K.B.; McPherson, D.T.; Shigenaga, M.; Jedrzejas, M.J.
Deposited on : 2002-11-16
Resolution : 1.55 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

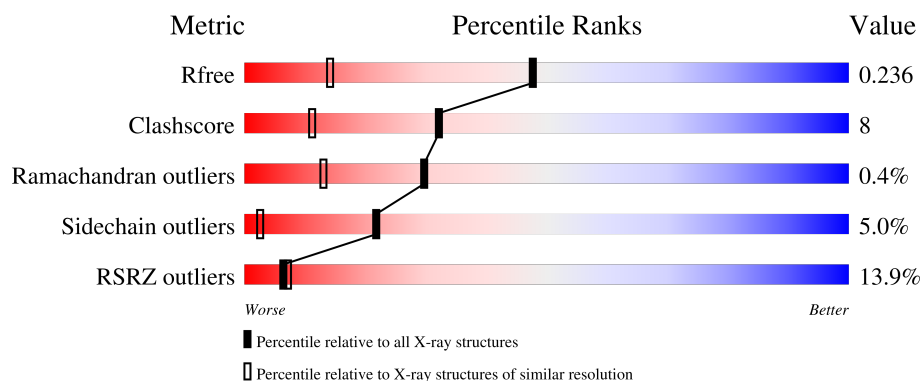
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	721	14% 85% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6441 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 HYALURONIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	721	Total	C	N	O	S	0	0	0
			5771	3626	967	1156	22			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	292	ALA	TRP	engineered mutation	UNP Q54873
A	343	VAL	PHE	engineered mutation	UNP Q54873
A	731	VAL	GLY	SEE REMARK 999	UNP Q54873

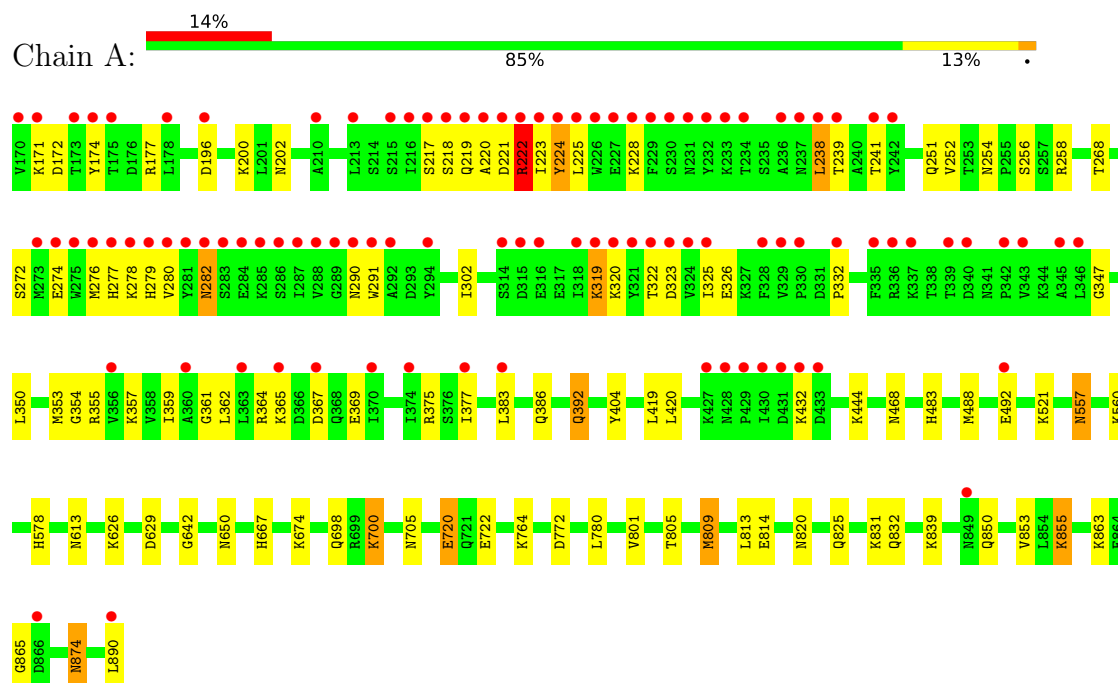
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	670	Total	O	0	0
			670	670		

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: HYALURONIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.98Å 103.72Å 100.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.55 20.00 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-1.55) 99.4 (20.00-1.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.55Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.190 , 0.234 (Not available) , 0.236	Depositor DCC
R_{free} test set	1281 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6441	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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	0.79	1/5887 (0.0%)	0.88	1/7951 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	809	MET	SD-CE	-12.16	1.49	1.79

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ASP	N-CA-C	5.20	115.00	108.45

There are no chirality outliers.

There are no planarity outliers.

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	5771	0	5590	91	0
2	A	670	0	0	56	1
All	All	6441	0	5590	91	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 8.

All (91) 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:890:LEU:C	2:A:1541:HOH:O	1.85	1.15
1:A:613:ASN:H	1:A:698:GLN:HE22	1.14	0.93
1:A:863:LYS:NZ	1:A:865:GLY:O	2.04	0.91
1:A:805:THR:HG22	1:A:809:MET:HE2	1.52	0.89
1:A:355:ARG:C	2:A:1490:HOH:O	2.18	0.84
1:A:650:ASN:HD21	1:A:832:GLN:HE22	1.32	0.78
1:A:392:GLN:NE2	2:A:1480:HOH:O	2.17	0.75
1:A:357:LYS:HD3	2:A:1420:HOH:O	1.89	0.71
1:A:177:ARG:HG3	2:A:1495:HOH:O	1.90	0.71
1:A:323:ASP:HA	2:A:1500:HOH:O	1.91	0.70
1:A:874:ASN:C	1:A:874:ASN:HD22	1.99	0.70
1:A:319:LYS:HG2	2:A:1506:HOH:O	1.92	0.69
1:A:354:GLY:HA3	1:A:377:ILE:HD11	1.75	0.68
1:A:369:GLU:HG2	2:A:1516:HOH:O	1.92	0.67
1:A:801:VAL:HG11	1:A:809:MET:HE1	1.77	0.67
1:A:483:HIS:HE1	2:A:1215:HOH:O	1.77	0.67
1:A:277:HIS:NE2	2:A:1386:HOH:O	2.27	0.67
1:A:238:LEU:HD12	2:A:1436:HOH:O	1.94	0.66
1:A:357:LYS:HB3	2:A:1516:HOH:O	1.95	0.66
1:A:362:LEU:CD2	2:A:1495:HOH:O	2.44	0.66
1:A:362:LEU:HA	2:A:1481:HOH:O	1.95	0.65
1:A:557:ASN:HD22	1:A:557:ASN:C	2.04	0.65
1:A:320:LYS:HG3	2:A:1386:HOH:O	1.96	0.64
1:A:241:THR:HG21	1:A:276:MET:HE3	1.79	0.63
1:A:277:HIS:CE1	2:A:1386:HOH:O	2.55	0.60
1:A:353:MET:HG3	2:A:1420:HOH:O	2.01	0.60
1:A:705:ASN:ND2	2:A:1402:HOH:O	2.36	0.59
1:A:302:ILE:HG21	2:A:1511:HOH:O	2.03	0.58
1:A:674:LYS:NZ	2:A:1169:HOH:O	2.37	0.58
1:A:801:VAL:HG21	1:A:809:MET:HE1	1.85	0.58
1:A:350:LEU:HB3	2:A:1389:HOH:O	2.03	0.58
1:A:322:THR:HG21	2:A:1549:HOH:O	2.04	0.57
1:A:361:GLY:O	2:A:1481:HOH:O	2.17	0.57
1:A:364:ARG:CZ	2:A:1506:HOH:O	2.53	0.56
1:A:217:SER:HB3	1:A:222:ARG:HG2	1.88	0.55
1:A:362:LEU:HD22	2:A:1495:HOH:O	2.07	0.55
1:A:254:ASN:C	1:A:254:ASN:HD22	2.12	0.55
1:A:325:ILE:HA	2:A:1357:HOH:O	2.06	0.55
1:A:578:HIS:CD2	1:A:578:HIS:C	2.85	0.55
1:A:814:GLU:HG2	2:A:1364:HOH:O	2.07	0.54
1:A:805:THR:HG22	1:A:809:MET:CE	2.33	0.54
1:A:359:ILE:HG12	2:A:1490:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ASN:ND2	1:A:560:LYS:H	2.06	0.54
1:A:720:GLU:CG	2:A:1318:HOH:O	2.56	0.54
1:A:332:PRO:HB3	2:A:1420:HOH:O	2.08	0.53
1:A:831:LYS:NZ	2:A:1383:HOH:O	2.29	0.53
1:A:839:LYS:HD2	1:A:853:VAL:HG23	1.91	0.52
1:A:831:LYS:CE	2:A:1383:HOH:O	2.57	0.52
1:A:667:HIS:HE1	2:A:1228:HOH:O	1.92	0.52
1:A:225:LEU:HG	1:A:276:MET:HE2	1.92	0.51
1:A:347:GLY:O	2:A:1389:HOH:O	2.19	0.51
1:A:764:LYS:HD2	1:A:772:ASP:HB3	1.92	0.51
1:A:386:GLN:NE2	2:A:1056:HOH:O	2.44	0.51
1:A:820:ASN:HD22	1:A:825:GLN:HG2	1.74	0.51
1:A:279:HIS:CE1	2:A:1380:HOH:O	2.66	0.49
1:A:280:VAL:HG13	2:A:1487:HOH:O	2.12	0.49
1:A:290:ASN:HD22	1:A:291:TRP:N	2.10	0.49
1:A:720:GLU:OE2	2:A:1318:HOH:O	2.20	0.49
1:A:700:LYS:HD2	2:A:961:HOH:O	2.12	0.48
1:A:217:SER:CB	1:A:222:ARG:HG2	2.43	0.48
1:A:326:GLU:HB3	2:A:1484:HOH:O	2.12	0.48
1:A:282:ASN:HB2	2:A:1292:HOH:O	2.12	0.48
1:A:274:GLU:OE2	1:A:320:LYS:NZ	2.41	0.47
1:A:420:LEU:HB3	1:A:488:MET:HE1	1.96	0.47
1:A:174:TYR:HA	2:A:1495:HOH:O	2.14	0.47
1:A:224:TYR:O	1:A:224:TYR:HD2	1.98	0.47
1:A:280:VAL:HG22	2:A:1487:HOH:O	2.14	0.47
1:A:354:GLY:CA	1:A:377:ILE:HD11	2.44	0.47
1:A:222:ARG:HD3	2:A:1423:HOH:O	2.15	0.46
1:A:578:HIS:CE1	1:A:629:ASP:O	2.69	0.45
1:A:367:ASP:N	2:A:1415:HOH:O	2.49	0.44
1:A:225:LEU:N	2:A:1423:HOH:O	2.50	0.44
1:A:254:ASN:ND2	1:A:256:SER:H	2.16	0.44
1:A:171:LYS:HB2	2:A:1542:HOH:O	2.17	0.44
1:A:224:TYR:C	2:A:1423:HOH:O	2.59	0.44
1:A:353:MET:CG	2:A:1420:HOH:O	2.64	0.44
1:A:202:ASN:ND2	1:A:251:GLN:HE22	2.15	0.44
1:A:241:THR:HG21	1:A:276:MET:CE	2.47	0.44
1:A:722:GLU:HG3	2:A:1536:HOH:O	2.17	0.44
1:A:642:GLY:HA2	2:A:1366:HOH:O	2.18	0.43
1:A:220:ALA:O	1:A:222:ARG:N	2.51	0.43
1:A:302:ILE:HD13	2:A:1511:HOH:O	2.19	0.43
1:A:357:LYS:C	2:A:1516:HOH:O	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:HD12	1:A:276:MET:HE3	2.01	0.42
1:A:254:ASN:C	1:A:254:ASN:ND2	2.78	0.42
1:A:364:ARG:HG2	2:A:1506:HOH:O	2.19	0.42
1:A:432:LYS:HD2	2:A:1534:HOH:O	2.20	0.42
1:A:855:LYS:HE3	1:A:855:LYS:HB3	1.82	0.41
1:A:365:LYS:HA	2:A:1481:HOH:O	2.18	0.41
1:A:268:THR:O	1:A:272:SER:HB2	2.21	0.41
1:A:557:ASN:C	1:A:557:ASN:ND2	2.76	0.41

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)
2:A:1379:HOH:O	2:A:1540:HOH:O[4_446]	2.12	0.08

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	719/721 (100%)	692 (96%)	24 (3%)	3 (0%)	30	13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	GLN
1	A	221	ASP
1	A	222	ARG

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	637/639 (100%)	605 (95%)	32 (5%)	22 2

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	ASP
1	A	200	LYS
1	A	218	SER
1	A	222	ARG
1	A	223	ILE
1	A	224	TYR
1	A	228	LYS
1	A	238	LEU
1	A	239	THR
1	A	252	VAL
1	A	258	ARG
1	A	278	LYS
1	A	282	ASN
1	A	319	LYS
1	A	375	ARG
1	A	383	LEU
1	A	392	GLN
1	A	404	TYR
1	A	419	LEU
1	A	444	LYS
1	A	468	ASN
1	A	492	GLU
1	A	521	LYS
1	A	557	ASN
1	A	626	LYS
1	A	700	LYS
1	A	720	GLU
1	A	780	LEU
1	A	813	LEU
1	A	850	GLN

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Mol	Chain	Res	Type
1	A	855	LYS
1	A	874	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	231	ASN
1	A	237	ASN
1	A	254	ASN
1	A	261	GLN
1	A	282	ASN
1	A	290	ASN
1	A	349	ASN
1	A	386	GLN
1	A	436	GLN
1	A	468	ASN
1	A	483	HIS
1	A	557	ASN
1	A	578	HIS
1	A	667	HIS
1	A	683	ASN
1	A	698	GLN
1	A	759	GLN
1	A	820	ASN
1	A	825	GLN
1	A	832	GLN
1	A	874	ASN

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	721/721 (100%)	0.60	100 (13%) 6 7	12, 22, 46, 66	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	TYR	8.1
1	A	223	ILE	7.8
1	A	225	LEU	7.4
1	A	170	VAL	6.8
1	A	219	GLN	6.2
1	A	220	ALA	6.1
1	A	280	VAL	5.3
1	A	232	TYR	5.3
1	A	229	PHE	5.2
1	A	890	LEU	5.1
1	A	275	TRP	4.8
1	A	174	TYR	4.7
1	A	221	ASP	4.5
1	A	429	PRO	4.4
1	A	222	ARG	4.2
1	A	276	MET	4.2
1	A	226	TRP	4.2
1	A	433	ASP	4.0
1	A	171	LYS	3.7
1	A	318	ILE	3.7
1	A	281	TYR	3.7
1	A	319	LYS	3.7
1	A	277	HIS	3.6
1	A	278	LYS	3.6
1	A	321	TYR	3.5
1	A	288	VAL	3.5
1	A	234	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	217	SER	3.5
1	A	279	HIS	3.5
1	A	218	SER	3.5
1	A	216	ILE	3.4
1	A	377	ILE	3.4
1	A	230	SER	3.3
1	A	228	LYS	3.3
1	A	325	ILE	3.2
1	A	287	ILE	3.2
1	A	238	LEU	3.1
1	A	236	ALA	3.1
1	A	363	LEU	3.0
1	A	866	ASP	3.0
1	A	322	THR	3.0
1	A	283	SER	3.0
1	A	242	TYR	2.9
1	A	173	THR	2.9
1	A	324	VAL	2.9
1	A	316	GLU	2.8
1	A	237	ASN	2.8
1	A	292	ALA	2.8
1	A	282	ASN	2.8
1	A	340	ASP	2.8
1	A	432	LYS	2.8
1	A	289	GLY	2.7
1	A	360	ALA	2.7
1	A	227	GLU	2.7
1	A	328	PHE	2.7
1	A	233	LYS	2.6
1	A	291	TRP	2.5
1	A	374	ILE	2.5
1	A	346	LEU	2.5
1	A	329	VAL	2.5
1	A	241	THR	2.5
1	A	178	LEU	2.5
1	A	492	GLU	2.5
1	A	284	GLU	2.4
1	A	343	VAL	2.4
1	A	370	ILE	2.4
1	A	339	THR	2.4
1	A	342	PRO	2.4
1	A	285	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	196	ASP	2.3
1	A	215	SER	2.3
1	A	274	GLU	2.3
1	A	849	ASN	2.3
1	A	356	VAL	2.3
1	A	213	LEU	2.3
1	A	383	LEU	2.3
1	A	332	PRO	2.2
1	A	315	ASP	2.2
1	A	323	ASP	2.2
1	A	286	SER	2.2
1	A	273	MET	2.2
1	A	365	LYS	2.2
1	A	431	ASP	2.2
1	A	336	ARG	2.2
1	A	320	LYS	2.2
1	A	337	LYS	2.2
1	A	330	PRO	2.1
1	A	427	LYS	2.1
1	A	314	SER	2.1
1	A	210	ALA	2.1
1	A	345	ALA	2.1
1	A	290	ASN	2.1
1	A	239	THR	2.1
1	A	294	TYR	2.1
1	A	428	ASN	2.1
1	A	335	PHE	2.0
1	A	430	ILE	2.0
1	A	231	ASN	2.0
1	A	175	THR	2.0
1	A	367	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.