



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:30 AM GMT

PDB ID : 3EXW  
Title : Crystal structure of the human Adenovirus type 7 fiber knob  
Authors : Persson, B.D.; Reiter, D.M.; Arnberg, N.; Stehle, T.  
Deposited on : 2008-10-17  
Resolution : 1.75 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

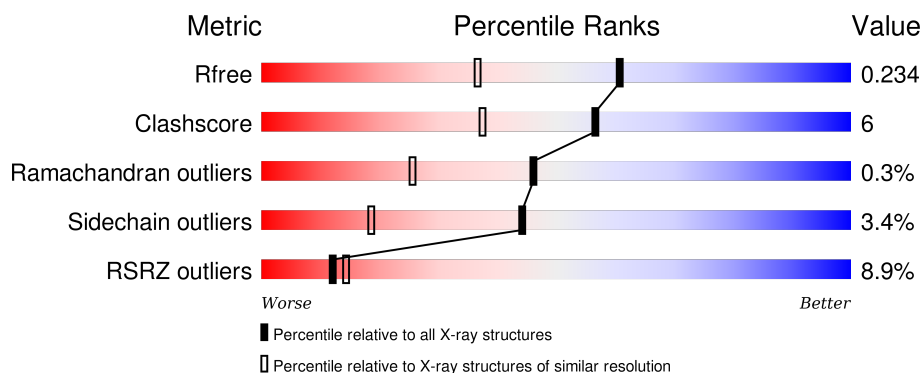
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
$R_{free}$	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	213	<div> <div>15%</div> <div>78%</div> <div>11%</div> <div>7%</div> </div>
1	B	213	<div> <div>7%</div> <div>78%</div> <div>13%</div> <div>7%</div> </div>
1	C	213	<div> <div>4%</div> <div>83%</div> <div>9%</div> <div>7%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5128 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 L5 fiber protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	3	0
			1551	981	250	311	9			
1	B	198	Total	C	N	O	S	0	2	0
			1547	978	250	310	9			
1	C	198	Total	C	N	O	S	0	0	0
			1538	970	250	309	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	GLY	-	EXPRESSION TAG	UNP Q5EY45
A	114	SER	-	EXPRESSION TAG	UNP Q5EY45
A	115	HIS	-	EXPRESSION TAG	UNP Q5EY45
A	116	MET	-	EXPRESSION TAG	UNP Q5EY45
B	113	GLY	-	EXPRESSION TAG	UNP Q5EY45
B	114	SER	-	EXPRESSION TAG	UNP Q5EY45
B	115	HIS	-	EXPRESSION TAG	UNP Q5EY45
B	116	MET	-	EXPRESSION TAG	UNP Q5EY45
C	113	GLY	-	EXPRESSION TAG	UNP Q5EY45
C	114	SER	-	EXPRESSION TAG	UNP Q5EY45
C	115	HIS	-	EXPRESSION TAG	UNP Q5EY45
C	116	MET	-	EXPRESSION TAG	UNP Q5EY45

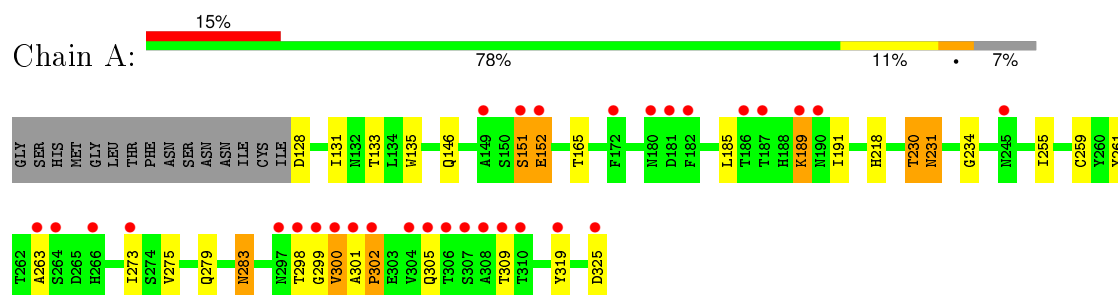
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	149	Total	O	0	0
			149	149		
2	B	177	Total	O	0	0
			177	177		
2	C	166	Total	O	0	0
			166	166		

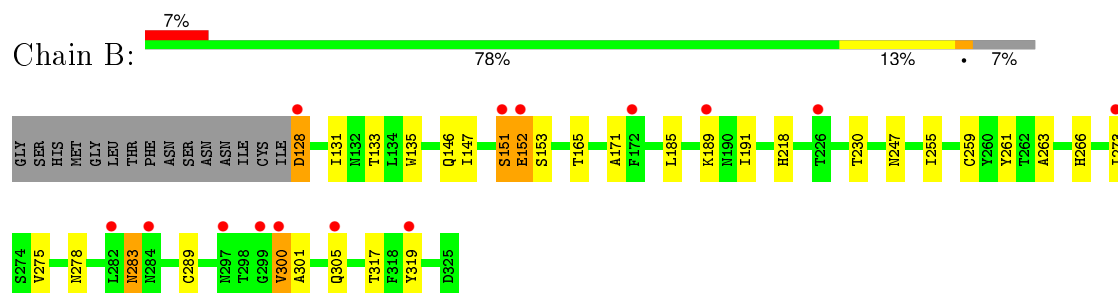
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

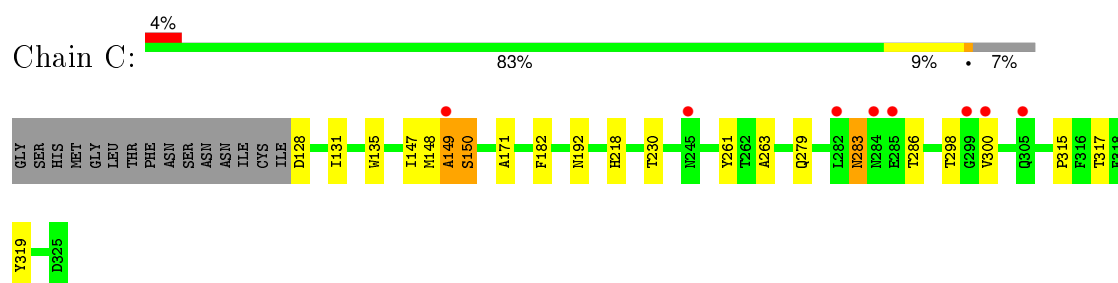
#### • Molecule 1: L5 fiber protein



#### • Molecule 1: L5 fiber protein



#### • Molecule 1: L5 fiber protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.31Å 88.05Å 79.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.11 – 1.75 36.10 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.1 (36.11-1.75) 99.1 (36.10-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, $R_{free}$	0.192 , 0.230 0.198 , 0.234	Depositor DCC
$R_{free}$ test set	5916 reflections (11.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.3	EDS
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 58883 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5128	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.35	0/1594	0.46	0/2179
1	B	0.36	0/1587	0.43	0/2169
1	C	0.35	0/1572	0.43	0/2148
All	All	0.35	0/4753	0.44	0/6496

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	5
1	B	0	3
1	C	0	2
All	All	0	10

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	SER	Peptide
1	A	230	THR	Peptide
1	A	231	ASN	Peptide
1	A	300	VAL	Peptide
1	A	302	PRO	Peptide
1	B	128	ASP	Peptide
1	B	151	SER	Peptide
1	B	300	VAL	Peptide
1	C	148	MET	Peptide
1	C	149	ALA	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	1551	0	1505	24	0
1	B	1547	0	1498	22	0
1	C	1538	0	1480	14	0
2	A	149	0	0	5	0
2	B	177	0	0	5	0
2	C	166	0	0	2	0
All	All	5128	0	4483	56	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 (56) 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:319:TYR:OH	1:B:319:TYR:OH	1.73	1.04
1:C:150:SER:OG	2:C:333:HOH:O	1.82	0.96
1:A:189:LYS:HB2	2:A:493:HOH:O	1.74	0.86
1:C:218:HIS:HE1	1:C:230:THR:H	1.24	0.84
1:B:218:HIS:HE1	1:B:230:THR:H	1.28	0.80
1:C:298:THR:OG1	2:C:485:HOH:O	1.99	0.79
1:B:128:ASP:N	1:B:131:ILE:HG12	1.99	0.77
1:B:247:ASN:ND2	2:B:414:HOH:O	2.20	0.73
1:B:165[B]:THR:HG22	2:B:431:HOH:O	1.87	0.73
1:A:165[A]:THR:HG23	2:B:431:HOH:O	1.90	0.71
1:A:218:HIS:HE1	1:A:230:THR:H	1.37	0.71
1:B:259:CYS:SG	1:B:273[B]:ILE:HD11	2.32	0.70
1:B:146:GLN:NE2	1:B:151:SER:O	2.25	0.70
1:C:218:HIS:CE1	1:C:230:THR:H	2.07	0.69
1:A:146:GLN:NE2	1:A:151:SER:O	2.28	0.67
1:A:298:THR:O	2:A:493:HOH:O	2.13	0.66
1:B:185:LEU:HD22	1:B:191:ILE:HD12	1.79	0.64
1:A:185:LEU:HD22	1:A:191:ILE:HD12	1.79	0.64
1:A:259:CYS:SG	1:A:273[B]:ILE:HD11	2.39	0.63
1:B:319:TYR:OH	1:C:319:TYR:OH	2.17	0.61
1:B:266:HIS:HD2	2:B:356:HOH:O	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ASN:C	1:A:283:ASN:HD22	2.04	0.60
1:B:283:ASN:C	1:B:283:ASN:HD22	2.06	0.59
1:B:218:HIS:CE1	1:B:230:THR:H	2.17	0.54
1:A:298:THR:C	2:A:493:HOH:O	2.46	0.54
1:C:128:ASP:O	1:C:131:ILE:HG12	2.09	0.53
1:B:300:VAL:HG22	1:B:301:ALA:H	1.74	0.51
1:A:319:TYR:HH	1:B:319:TYR:HH	1.36	0.51
1:C:283:ASN:HD22	1:C:283:ASN:C	2.15	0.50
1:B:133:THR:O	1:B:218:HIS:HD2	1.95	0.49
1:C:298:THR:OG1	1:C:300:VAL:O	2.30	0.49
1:B:152:GLU:HB3	1:B:153:SER:H	1.37	0.48
1:B:278:ASN:HD22	1:B:289:CYS:H	1.61	0.48
1:A:133:THR:O	1:A:218:HIS:HD2	1.97	0.47
1:C:218:HIS:HE1	1:C:230:THR:N	2.03	0.47
1:C:283:ASN:ND2	1:C:286:THR:HG23	2.30	0.46
1:A:261:TYR:CE2	1:A:263:ALA:HA	2.50	0.45
1:A:319:TYR:CZ	1:B:319:TYR:OH	2.61	0.45
1:C:147:ILE:HG21	1:C:182:PHE:CE1	2.51	0.45
1:A:300:VAL:N	2:A:493:HOH:O	2.49	0.45
1:B:261:TYR:CE2	1:B:263:ALA:HA	2.52	0.45
1:A:189:LYS:NZ	1:A:299:GLY:O	2.51	0.44
1:B:255:ILE:HB	1:B:275:VAL:HB	1.99	0.44
1:A:325:ASP:HA	2:A:380:HOH:O	2.17	0.44
1:A:218:HIS:HE1	1:A:230:THR:N	2.10	0.44
2:B:411:HOH:O	1:C:315:PRO:HG2	2.18	0.43
1:A:301:ALA:O	1:A:302:PRO:C	2.57	0.43
1:A:300:VAL:HG22	1:A:301:ALA:H	1.83	0.42
1:A:151:SER:HA	1:A:152:GLU:HB2	2.00	0.42
1:A:255:ILE:HB	1:A:275:VAL:HB	2.01	0.42
1:A:128:ASP:O	1:A:131:ILE:HG12	2.21	0.41
1:C:261:TYR:CE2	1:C:263:ALA:HA	2.56	0.41
1:B:278:ASN:ND2	1:B:289:CYS:H	2.19	0.41
1:A:234:GLY:HA3	1:A:325:ASP:OD1	2.21	0.41
1:B:171:ALA:O	1:B:317:THR:HA	2.21	0.40
1:C:171:ALA:O	1:C:317:THR:HA	2.21	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	199/213 (93%)	188 (94%)	10 (5%)	1 (0%)	34	14
1	B	198/213 (93%)	192 (97%)	6 (3%)	0	100	100
1	C	196/213 (92%)	192 (98%)	3 (2%)	1 (0%)	34	14
All	All	593/639 (93%)	572 (96%)	19 (3%)	2 (0%)	46	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	149	ALA
1	A	231	ASN

### 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	178/188 (95%)	170 (96%)	8 (4%)	34	11
1	B	177/188 (94%)	171 (97%)	6 (3%)	44	18
1	C	175/188 (93%)	170 (97%)	5 (3%)	50	24
All	All	530/564 (94%)	511 (96%)	19 (4%)	44	16

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	TRP

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Mol	Chain	Res	Type
1	A	152	GLU
1	A	189	LYS
1	A	279	GLN
1	A	283	ASN
1	A	305	GLN
1	A	309[A]	THR
1	A	309[B]	THR
1	B	135	TRP
1	B	147	ILE
1	B	152	GLU
1	B	189	LYS
1	B	283	ASN
1	B	305	GLN
1	C	135	TRP
1	C	150	SER
1	C	192	ASN
1	C	279	GLN
1	C	283	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	204	ASN
1	A	218	HIS
1	A	222	GLN
1	A	279	GLN
1	A	283	ASN
1	B	146	GLN
1	B	204	ASN
1	B	218	HIS
1	B	222	GLN
1	B	266	HIS
1	B	278	ASN
1	B	283	ASN
1	C	204	ASN
1	C	218	HIS
1	C	222	GLN
1	C	253	ASN
1	C	283	ASN
1	C	305	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 carbohydrates 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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	198/213 (92%)	0.79	31 (15%) 3 4	13, 21, 33, 41	0
1	B	198/213 (92%)	0.50	14 (7%) 19 24	13, 21, 35, 42	0
1	C	198/213 (92%)	0.28	8 (4%) 42 48	12, 21, 32, 39	0
All	All	594/639 (92%)	0.52	53 (8%) 12 14	12, 21, 33, 42	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	304	VAL	7.2
1	A	300	VAL	6.1
1	A	149	ALA	5.9
1	B	152	GLU	5.8
1	C	149	ALA	5.4
1	B	282	LEU	5.3
1	A	306	THR	5.2
1	B	300	VAL	5.0
1	A	307	SER	5.0
1	A	266	HIS	5.0
1	A	152	GLU	4.9
1	A	309[A]	THR	4.9
1	C	300	VAL	4.5
1	A	301	ALA	4.3
1	A	180	ASN	4.1
1	B	128	ASP	4.0
1	A	305	GLN	3.9
1	A	302	PRO	3.8
1	A	308	ALA	3.7
1	A	297	ASN	3.5
1	B	299	GLY	3.4
1	A	245	ASN	3.4
1	A	186	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	189	LYS	3.2
1	A	299	GLY	3.1
1	C	282	LEU	3.0
1	B	284	ASN	3.0
1	A	187	THR	2.9
1	C	299	GLY	2.8
1	A	264	SER	2.8
1	B	319	TYR	2.8
1	B	226	THR	2.7
1	C	284	ASN	2.6
1	A	189	LYS	2.6
1	A	263	ALA	2.5
1	A	273[A]	ILE	2.5
1	A	190	ASN	2.4
1	B	172	PHE	2.4
1	B	151	SER	2.4
1	A	151	SER	2.3
1	B	305	GLN	2.3
1	C	305	GLN	2.3
1	A	298	THR	2.2
1	A	181	ASP	2.2
1	B	273[A]	ILE	2.2
1	C	245	ASN	2.2
1	A	325	ASP	2.2
1	A	172	PHE	2.1
1	A	319	TYR	2.1
1	B	297	ASN	2.1
1	A	310	THR	2.0
1	C	285	GLU	2.0
1	A	182	PHE	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 carbohydrates 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.