



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:40 AM UTC

PDB ID : 3EXW / pdb_00003exw
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

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

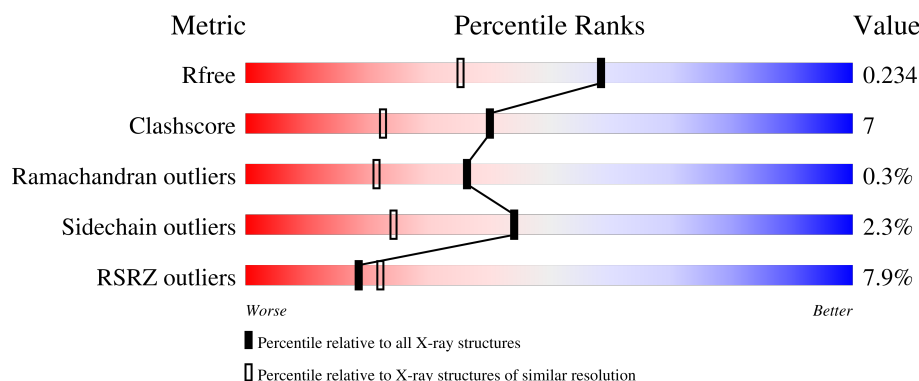
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 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	213	9% 77% 13% • 7%
1	B	213	10% 78% 13% • 7%
1	C	213	3% 83% 8% • 7%

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

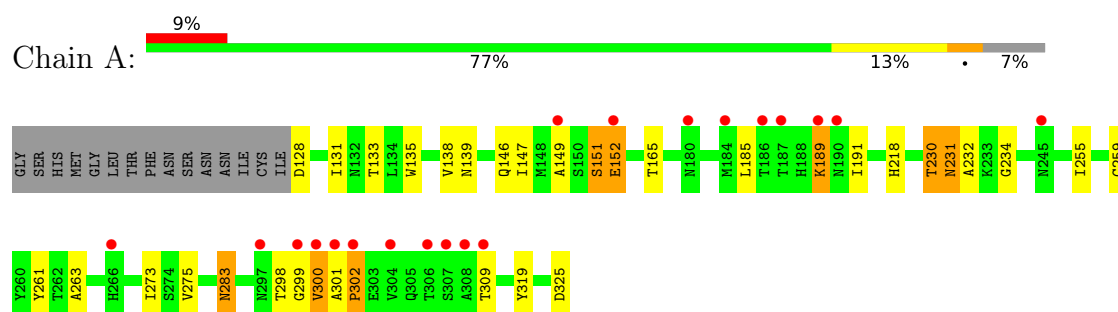
- Molecule 2 is water.

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		

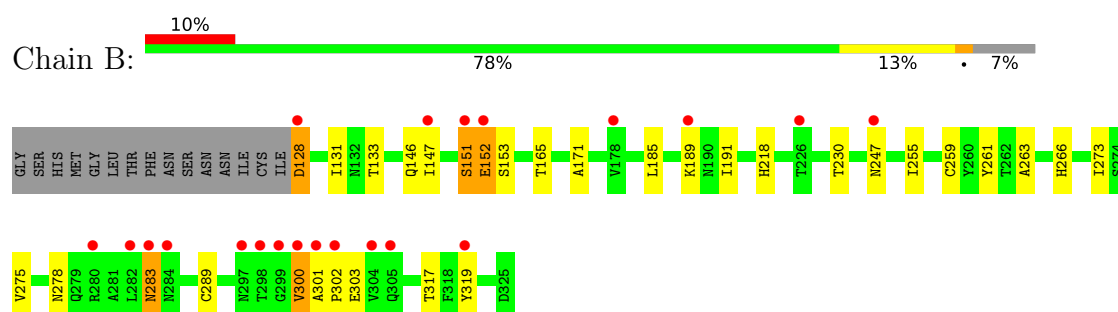
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

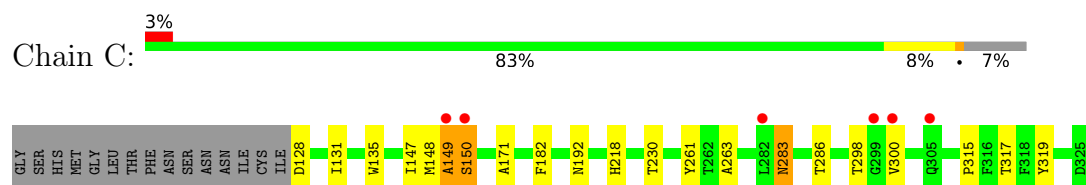
• Molecule 1: L5 fiber protein



• 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, α , β , γ	83.31Å 88.05Å 79.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.11 – 1.75 36.11 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.1 (36.11-1.75) 99.1 (36.11-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5128	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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	0.43	0/1594	0.64	3/2179 (0.1%)
1	B	0.45	0/1587	0.57	0/2169
1	C	0.44	0/1572	0.60	1/2148 (0.0%)
All	All	0.44	0/4753	0.60	4/6496 (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	5
1	B	0	3
1	C	0	2
All	All	0	10

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	ALA	N-CA-C	-8.39	102.48	112.89
1	A	232	ALA	N-CA-C	-6.61	103.91	112.23
1	C	135	TRP	N-CA-C	5.36	115.62	108.38
1	A	135	TRP	N-CA-C	5.36	116.14	108.74

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

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Mol	Chain	Res	Type	Group
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 [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	1551	0	1505	24	0
1	B	1547	0	1498	25	0
1	C	1538	0	1480	15	0
2	A	149	0	0	5	0
2	B	177	0	0	6	0
2	C	166	0	0	2	0
All	All	5128	0	4483	60	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 (60) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:283:ASN:C	1:A:283:ASN:HD22	2.04	0.65
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:B:283:ASN:C	1:B:283:ASN:HD22	2.06	0.63
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
1:A:298:THR:C	2:A:493:HOH:O	2.46	0.58
1:C:283:ASN:HD22	1:C:283:ASN:C	2.15	0.54
1:B:218:HIS:CE1	1:B:230:THR:H	2.17	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: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:301:ALA:O	1:A:302:PRO:C	2.57	0.47
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:B:283:ASN:C	1:B:283:ASN:ND2	2.77	0.43
1:A:300:VAL:HG22	1:A:301:ALA:H	1.83	0.42
1:B:302:PRO:C	1:B:303:GLU:HG2	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:VAL:O	1:A:139:ASN:C	2.64	0.41
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:A:234:GLY:HA3	1:A:325:ASP:OD1	2.21	0.41
1:B:278:ASN:ND2	1:B:289:CYS:H	2.19	0.41
1:B:171:ALA:O	1:B:317:THR:HA	2.21	0.40
1:B:247:ASN:CG	2:B:414:HOH:O	2.58	0.40
1:C:171:ALA:O	1:C:317:THR:HA	2.21	0.40
1:B:319:TYR:HH	1:C:319:TYR:HH	1.66	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	199/213 (93%)	188 (94%)	10 (5%)	1 (0%)	24	11
1	B	198/213 (93%)	192 (97%)	6 (3%)	0	100	100
1	C	196/213 (92%)	192 (98%)	3 (2%)	1 (0%)	24	11
All	All	593/639 (93%)	572 (96%)	19 (3%)	2 (0%)	36	21

All (2) Ramachandran outliers are listed below:

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

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	A	178/188 (95%)	172 (97%)	6 (3%)	32	13
1	B	177/188 (94%)	173 (98%)	4 (2%)	44	24
1	C	175/188 (93%)	172 (98%)	3 (2%)	53	36
All	All	530/564 (94%)	517 (98%)	13 (2%)	44	22

All (13) residues with a non-rotameric sidechain are listed below:

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	180	ASN
1	A	218	HIS
1	A	222	GLN
1	A	253	ASN
1	A	279	GLN
1	A	283	ASN
1	A	297	ASN
1	B	146	GLN
1	B	180	ASN
1	B	204	ASN
1	B	218	HIS

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Mol	Chain	Res	Type
1	B	222	GLN
1	B	247	ASN
1	B	266	HIS
1	B	278	ASN
1	B	279	GLN
1	B	283	ASN
1	B	297	ASN
1	C	204	ASN
1	C	218	HIS
1	C	222	GLN
1	C	253	ASN
1	C	283	ASN

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 [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, 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	198/213 (92%)	0.50	20 (10%)	12 14	9, 21, 33, 41	3 (1%)
1	B	198/213 (92%)	0.41	21 (10%)	11 13	9, 21, 35, 42	2 (1%)
1	C	198/213 (92%)	0.21	6 (3%)	52 59	12, 21, 32, 39	0
All	All	594/639 (92%)	0.37	47 (7%)	18 22	9, 21, 33, 42	5 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	VAL	5.3
1	C	149	ALA	5.1
1	B	282	LEU	4.5
1	B	300	VAL	4.5
1	A	304	VAL	4.3
1	A	301	ALA	4.3
1	B	152	GLU	3.9
1	C	300	VAL	3.7
1	B	189	LYS	3.5
1	A	152	GLU	3.4
1	A	180	ASN	3.4
1	A	245	ASN	3.4
1	B	128	ASP	3.3
1	A	187	THR	3.2
1	A	149	ALA	3.2
1	B	305	GLN	3.1
1	B	299	GLY	3.1
1	B	284	ASN	3.0
1	A	306	THR	3.0
1	A	266	HIS	2.9
1	A	307	SER	2.7
1	B	301	ALA	2.7
1	B	304	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	299	GLY	2.6
1	A	189	LYS	2.6
1	A	309[A]	THR	2.5
1	B	302	PRO	2.5
1	C	282	LEU	2.5
1	C	150	SER	2.5
1	A	190	ASN	2.5
1	A	302	PRO	2.5
1	A	186	THR	2.5
1	B	283	ASN	2.4
1	B	147	ILE	2.3
1	B	226	THR	2.3
1	B	178	VAL	2.2
1	B	297	ASN	2.2
1	A	297	ASN	2.2
1	B	319	TYR	2.2
1	C	305	GLN	2.1
1	A	308	ALA	2.1
1	B	151	SER	2.1
1	B	280	ARG	2.1
1	C	299	GLY	2.1
1	B	298	THR	2.1
1	B	247	ASN	2.0
1	A	184	MET	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.