



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1US7 / pdb_00001us7
Title : Complex of Hsp90 and P50
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Deposited on : 2003-11-20
Resolution : 2.30 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

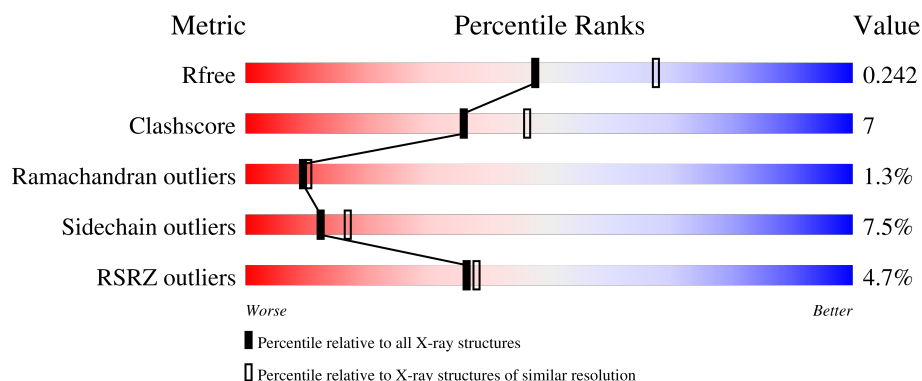
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	214	% 81% 14% • •
2	B	265	6% 48% 19% 5% • 27%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3414 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 HEAT SHOCK PROTEIN HSP82.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	1
			1639	1043	271	321	4			

- Molecule 2 is a protein called HSP90 CO-CHAPERONE CDC37.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	194	Total	C	N	O	S	0	0	1
			1599	1012	276	297	14			

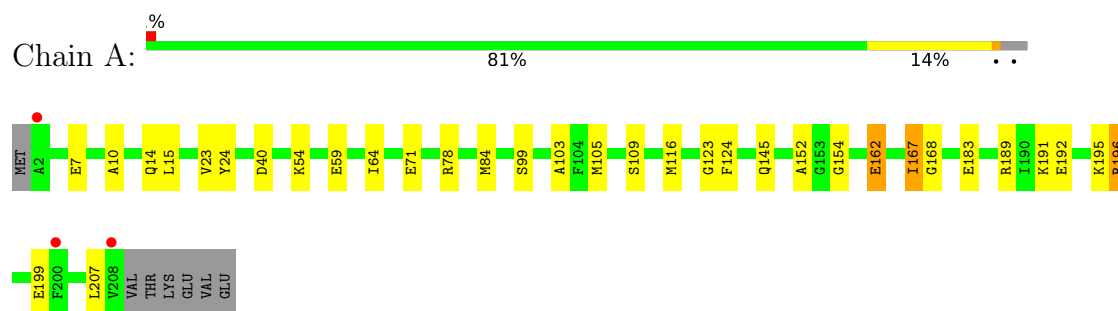
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total	O	0	0
			115	115		
3	B	61	Total	O	0	0
			61	61		

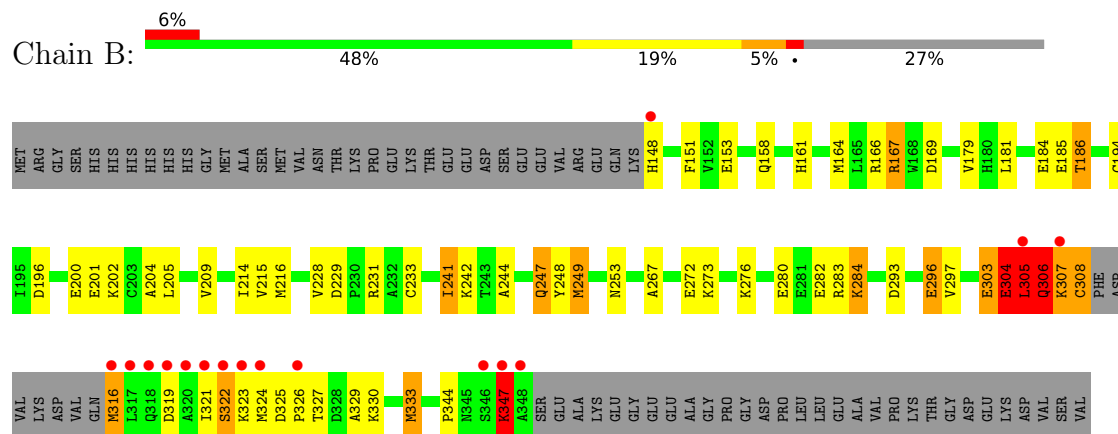
3 Residue-property plots

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: HEAT SHOCK PROTEIN HSP82



• Molecule 2: HSP90 CO-CHAPERONE CDC37



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.76Å 83.76Å 148.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	72.55 – 2.30 72.54 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.3 (72.55-2.30) 96.4 (72.54-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.185 , 0.241 (Not available) , 0.242	Depositor DCC
R_{free} test set	1334 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3414	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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	1.62	16/1663 (1.0%)	1.32	5/2241 (0.2%)
2	B	1.58	12/1629 (0.7%)	1.37	9/2184 (0.4%)
All	All	1.60	28/3292 (0.9%)	1.34	14/4425 (0.3%)

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
2	B	0	2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	249	MET	SD-CE	-18.07	1.34	1.79
1	A	167	ILE	CA-CB	9.02	1.65	1.54
1	A	116	MET	SD-CE	8.51	2.00	1.79
2	B	164	MET	SD-CE	8.49	2.00	1.79
1	A	105	MET	SD-CE	7.06	1.97	1.79
2	B	216	MET	SD-CE	7.01	1.97	1.79
2	B	297	VAL	CA-CB	6.66	1.62	1.54
1	A	207	LEU	C-N	-6.48	1.24	1.33
2	B	205	LEU	C-O	6.47	1.31	1.24
1	A	154	GLY	C-O	-6.28	1.17	1.24
1	A	64	ILE	C-O	-6.19	1.17	1.24
2	B	347	LYS	C-N	-6.16	1.24	1.33
1	A	99	SER	C-O	-6.04	1.17	1.24
1	A	84	MET	CA-C	5.99	1.59	1.52
2	B	209	VAL	N-CA	5.91	1.53	1.46
2	B	194	CYS	N-CA	5.91	1.53	1.46
2	B	272	GLU	C-O	-5.88	1.17	1.24
1	A	7	GLU	C-O	5.71	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	215	VAL	CA-C	5.67	1.59	1.52
1	A	15	LEU	CA-C	5.65	1.60	1.52
2	B	267	ALA	CA-CB	5.64	1.62	1.53
1	A	116	MET	CB-CG	5.61	1.69	1.52
2	B	161	HIS	C-O	-5.53	1.17	1.24
1	A	14	GLN	CA-C	5.33	1.59	1.52
1	A	59	GLU	CA-C	5.32	1.59	1.52
1	A	191	LYS	CA-C	-5.15	1.46	1.52
1	A	152	ALA	CA-CB	5.14	1.60	1.53
1	A	10	ALA	CA-CB	5.03	1.61	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	LEU	O-C-N	-12.30	103.31	123.00
2	B	166	ARG	NE-CZ-NH2	-7.82	112.16	119.20
2	B	253	ASN	N-CA-C	7.41	119.36	111.28
2	B	306	GLN	N-CA-C	6.89	120.91	108.17
2	B	186	THR	OG1-CB-CG2	-6.49	96.33	109.30
2	B	276	LYS	N-CA-C	-5.91	104.42	111.69
1	A	168	GLY	N-CA-C	-5.84	105.73	112.50
2	B	327	THR	N-CA-C	-5.59	106.35	114.12
2	B	305	LEU	CB-CA-C	5.44	119.56	109.54
2	B	267	ALA	N-CA-C	-5.41	105.46	111.36
1	A	207	LEU	CA-C-N	5.39	126.97	116.20
2	B	167	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	A	207	LEU	CA-C-O	5.18	129.61	120.80
1	A	40	ASP	N-CA-C	5.11	116.85	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	304	GLU	Peptide
2	B	305	LEU	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	1639	0	1653	12	0
2	B	1599	0	1584	37	0
3	A	115	0	0	4	1
3	B	61	0	0	5	0
All	All	3414	0	3237	47	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 7.

All (47) 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)
2:B:293:ASP:HB3	2:B:296:GLU:HG3	1.39	1.02
2:B:307:LYS:HE3	2:B:307:LYS:H	1.53	0.73
2:B:284:LYS:HE2	3:B:2053:HOH:O	1.91	0.71
2:B:316:MET:SD	2:B:316:MET:N	2.64	0.70
1:A:145:GLN:HE22	1:A:167:ILE:H	1.42	0.67
2:B:228:VAL:HG12	2:B:229:ASP:N	2.08	0.67
1:A:196:ARG:NH1	3:A:2109:HOH:O	2.27	0.65
1:A:162:GLU:HG2	3:A:2097:HOH:O	1.96	0.64
2:B:244:ALA:HB3	2:B:249:MET:HE3	1.78	0.64
2:B:247:GLN:HE21	2:B:247:GLN:H	1.45	0.64
1:A:195:LYS:O	1:A:199:GLU:HG3	2.01	0.61
2:B:248:TYR:HD2	2:B:249:MET:HE2	1.66	0.61
2:B:179:VAL:HG21	3:B:2040:HOH:O	2.03	0.59
2:B:228:VAL:CG1	2:B:229:ASP:N	2.69	0.56
2:B:179:VAL:HG12	2:B:231:ARG:HG2	1.90	0.54
2:B:316:MET:HE2	3:B:2057:HOH:O	2.08	0.52
2:B:181:LEU:O	2:B:186:THR:HG21	2.12	0.50
1:A:23:VAL:O	1:A:24:TYR:C	2.56	0.49
2:B:229:ASP:OD1	2:B:231:ARG:HB2	2.13	0.48
2:B:167:ARG:NH2	3:B:2017:HOH:O	2.46	0.48
2:B:200:GLU:O	2:B:201:GLU:HB2	2.14	0.48
2:B:329:ALA:O	2:B:333:MET:HB2	2.15	0.47
2:B:333:MET:HE2	2:B:333:MET:CA	2.46	0.46
2:B:241:ILE:HD11	2:B:249:MET:HE1	1.98	0.46
2:B:241:ILE:CD1	2:B:249:MET:HE1	2.45	0.45
2:B:306:GLN:C	2:B:308:CYS:N	2.73	0.45
2:B:306:GLN:HB3	2:B:308:CYS:HB2	1.98	0.45
1:A:103:ALA:HB2	2:B:204:ALA:HB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:GLU:O	2:B:304:GLU:CB	2.66	0.44
1:A:78:ARG:NH2	3:A:2046:HOH:O	2.43	0.44
2:B:185:GLU:HG3	3:B:2003:HOH:O	2.17	0.43
2:B:280:GLU:O	2:B:283:ARG:HB3	2.18	0.43
1:A:145:GLN:NE2	1:A:167:ILE:H	2.10	0.43
2:B:304:GLU:HB3	2:B:305:LEU:HD23	2.00	0.43
1:A:123:GLY:O	1:A:124:PHE:C	2.60	0.43
2:B:344:PRO:HB2	2:B:347:LYS:HA	2.01	0.43
1:A:183:GLU:HG3	1:A:189:ARG:HG2	2.01	0.43
2:B:333:MET:HE2	2:B:333:MET:N	2.33	0.43
2:B:158:GLN:HB3	2:B:181:LEU:HD11	2.00	0.42
1:A:109:SER:OG	2:B:202:LYS:NZ	2.52	0.42
2:B:319:ASP:O	2:B:322:SER:HB3	2.20	0.41
2:B:169:ASP:OD1	2:B:242:LYS:HE3	2.19	0.41
1:A:145:GLN:NE2	3:A:2085:HOH:O	2.54	0.41
2:B:151:PHE:HE2	2:B:186:THR:HG22	1.85	0.41
2:B:181:LEU:O	2:B:186:THR:CG2	2.69	0.41
2:B:196:ASP:O	2:B:200:GLU:HG3	2.21	0.40
2:B:228:VAL:CG1	2:B:229:ASP:H	2.34	0.40

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)
3:A:2007:HOH:O	3:A:2007:HOH:O[4_555]	2.03	0.17

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	197/214 (92%)	192 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	181/265 (68%)	168 (93%)	8 (4%)	5 (3%)	4 2
All	All	378/479 (79%)	360 (95%)	13 (3%)	5 (1%)	9 10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	326	PRO
2	B	304	GLU
2	B	347	LYS
2	B	325	ASP
2	B	322	SER

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	174/189 (92%)	169 (97%)	5 (3%)	37 55
2	B	174/236 (74%)	153 (88%)	21 (12%)	5 5
All	All	348/425 (82%)	322 (92%)	26 (8%)	12 17

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	71	GLU
1	A	162	GLU
1	A	192	GLU
1	A	196	ARG
2	B	148	HIS
2	B	153	GLU
2	B	184	GLU
2	B	214	ILE
2	B	233	CYS
2	B	241	ILE

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Mol	Chain	Res	Type
2	B	247	GLN
2	B	273	LYS
2	B	282	GLU
2	B	284	LYS
2	B	296	GLU
2	B	303	GLU
2	B	306	GLN
2	B	307	LYS
2	B	308	CYS
2	B	316	MET
2	B	321	ILE
2	B	323	LYS
2	B	324	MET
2	B	330	LYS
2	B	333	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	141	ASN
1	A	145	GLN
1	A	181	GLN
2	B	148	HIS
2	B	158	GLN
2	B	178	ASN
2	B	247	GLN
2	B	332	HIS

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	207/214 (96%)	-0.48	3 (1%) 73 75	15, 26, 51, 63	0
2	B	194/265 (73%)	0.27	16 (8%) 17 19	17, 38, 88, 101	0
All	All	401/479 (83%)	-0.12	19 (4%) 36 38	15, 31, 76, 101	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	VAL	7.9
2	B	317	LEU	5.9
2	B	321	ILE	4.9
2	B	348	ALA	4.5
2	B	305	LEU	4.2
2	B	324	MET	3.7
2	B	326	PRO	3.4
2	B	322	SER	3.4
2	B	319	ASP	3.4
2	B	148	HIS	3.3
2	B	316	MET	3.2
2	B	347	LYS	3.1
2	B	320	ALA	3.1
1	A	200	PHE	2.5
2	B	323	LYS	2.4
2	B	346	SER	2.3
1	A	2	ALA	2.2
2	B	307	LYS	2.2
2	B	318	GLN	2.2

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.