



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:16 AM UTC

PDB ID : 2FXK / pdb_00002fxk
Title : Crystal structure of the macro-domain of human core histone variant macroH2A1.1 (form A)
Authors : Kustatscher, G.; Hothorn, M.; Pugieux, C.; Scheffzek, K.; Ladurner, A.G.
Deposited on : 2006-02-06
Resolution : 2.54 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

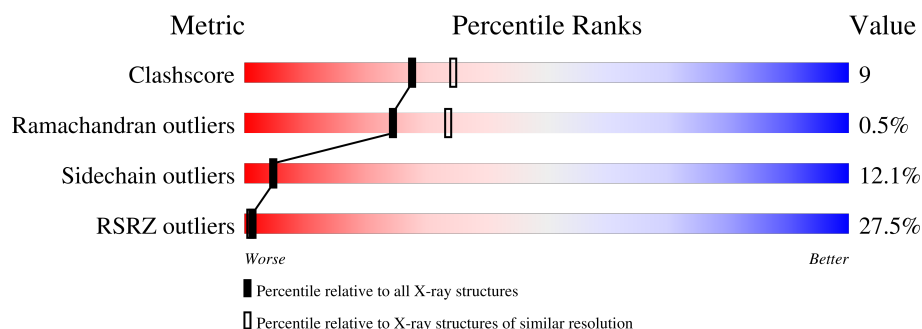
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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))
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	211	19% 65% 21% • 11%
1	B	211	30% 67% 18% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2853 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 H2A histone family, member Y isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	S	0	0	0
			1405	901	230	269	5			
1	B	187	Total	C	N	O	S	0	0	0
			1405	901	230	269	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	GLY	-	cloning artifact	GB 20336746
A	160	ALA	-	cloning artifact	GB 20336746
A	161	MET	-	cloning artifact	GB 20336746
B	159	GLY	-	cloning artifact	GB 20336746
B	160	ALA	-	cloning artifact	GB 20336746
B	161	MET	-	cloning artifact	GB 20336746

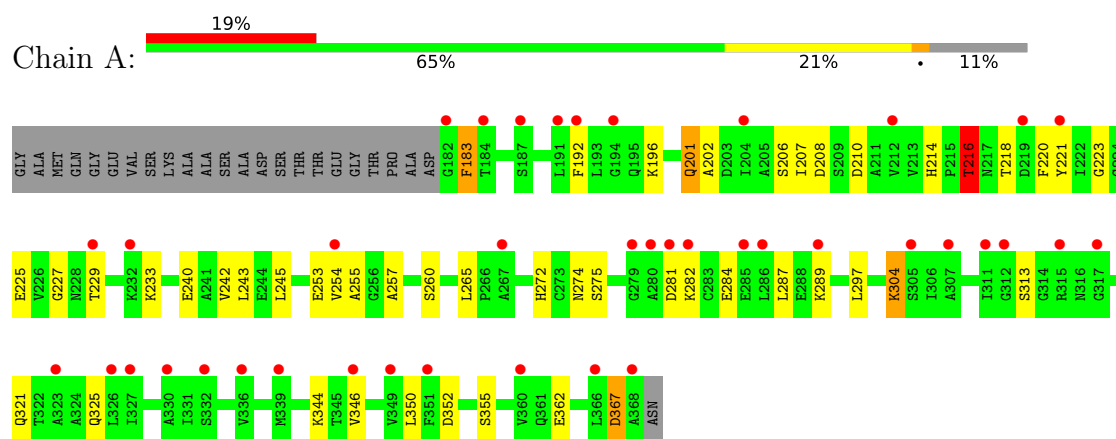
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		
2	B	22	Total	O	0	0
			22	22		

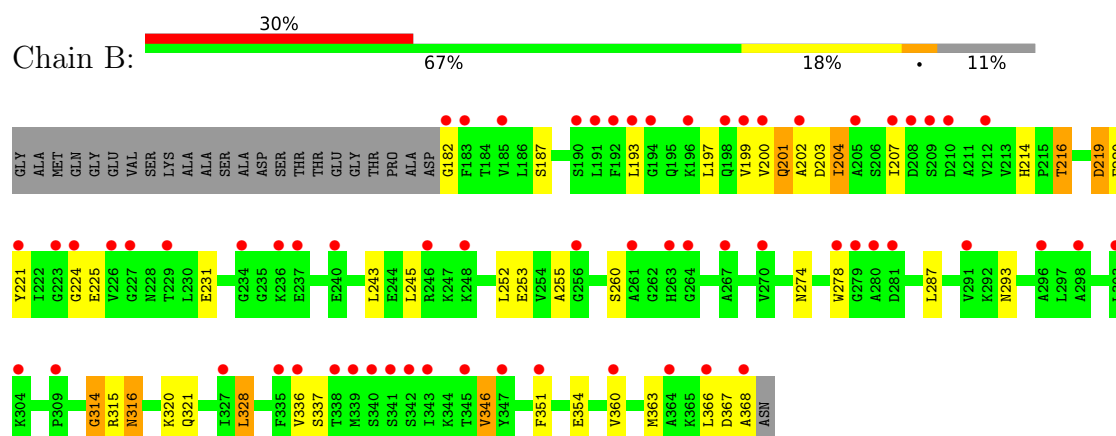
3 Residue-property plots [i](#)

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: H2A histone family, member Y isoform 1



- Molecule 1: H2A histone family, member Y isoform 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	90.77Å 98.27Å 42.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.91 – 2.54 66.68 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.0 (90.91-2.54) 98.9 (66.68-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.207 , 0.270 (Not available) , (Not available)	Depositor DCC
R_{free} test set	37 reflections (0.29%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2853	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% 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	0.91	0/1429	1.04	4/1929 (0.2%)
1	B	0.76	0/1429	0.98	1/1929 (0.1%)
All	All	0.84	0/2858	1.01	5/3858 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	ASP	N-CA-C	-7.02	103.56	111.14
1	A	265	LEU	CA-C-N	5.38	124.83	119.24
1	A	265	LEU	C-N-CA	5.38	124.83	119.24
1	A	367	ASP	N-CA-C	-5.30	106.75	113.43
1	A	216	THR	CB-CA-C	-5.12	100.36	111.11

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	1405	0	1435	25	0
1	B	1405	0	1435	26	0
2	A	21	0	0	0	0
2	B	22	0	0	6	0
All	All	2853	0	2870	51	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 9.

All (51) 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:B:199:VAL:HG23	1:B:363:MET:HE2	1.72	0.71
1:A:183:PHE:HD2	1:A:183:PHE:C	2.05	0.65
1:A:183:PHE:C	1:A:183:PHE:CD2	2.75	0.64
1:B:216:THR:HG22	1:B:221:TYR:O	1.99	0.63
1:A:325:GLN:CG	1:A:362:GLU:OE1	2.48	0.62
1:B:368:ALA:HB1	2:B:42:HOH:O	1.99	0.61
1:A:210:ASP:OD2	1:A:304:LYS:HG2	2.02	0.59
1:B:214:HIS:CE1	1:B:216:THR:HG23	2.38	0.59
1:A:214:HIS:CE1	1:A:216:THR:HG23	2.37	0.58
1:A:216:THR:CG2	1:A:221:TYR:O	2.51	0.58
1:A:216:THR:HG22	1:A:221:TYR:O	2.02	0.58
1:B:202:ALA:HB3	1:B:207:ILE:HD11	1.84	0.58
1:B:314:GLY:HA3	2:B:43:HOH:O	2.04	0.57
1:A:202:ALA:CB	1:A:207:ILE:HD11	2.35	0.57
1:A:321:GLN:OE1	1:A:325:GLN:NE2	2.37	0.56
1:B:202:ALA:CB	1:B:207:ILE:HD11	2.36	0.56
1:A:325:GLN:HG3	1:A:362:GLU:OE1	2.06	0.56
1:B:351:PHE:CE2	2:B:3:HOH:O	2.59	0.55
1:A:223:GLY:O	1:A:227:GLY:HA3	2.07	0.55
1:A:206:SER:HB3	1:A:233:LYS:HZ1	1.72	0.55
1:A:216:THR:HG21	1:A:220:PHE:HA	1.89	0.53
1:A:352:ASP:OD1	1:A:355:SER:OG	2.22	0.52
1:B:197:LEU:HD12	1:B:346:VAL:HG13	1.91	0.52
1:B:216:THR:CG2	1:B:221:TYR:O	2.59	0.50
1:A:281:ASP:O	1:A:282:LYS:C	2.54	0.49
1:A:202:ALA:HB3	1:A:207:ILE:HD11	1.94	0.49
1:B:182:GLY:N	2:B:16:HOH:O	2.44	0.49
1:A:254:VAL:O	1:A:255:ALA:HB3	2.13	0.47
1:B:328:LEU:HG	1:B:366:LEU:HD11	1.97	0.47
1:B:320:LYS:NZ	1:B:354:GLU:OE1	2.35	0.47
1:A:218:THR:HG22	1:A:274:ASN:ND2	2.31	0.46
1:B:216:THR:HG21	1:B:220:PHE:HA	1.98	0.46
1:A:245:LEU:HD22	1:A:260:SER:HB3	1.97	0.45
1:A:257:ALA:HA	1:A:272:HIS:O	2.16	0.45
1:B:316:ASN:N	1:B:316:ASN:HD22	2.13	0.45
1:B:219:ASP:O	1:B:220:PHE:C	2.58	0.45
1:B:255:ALA:O	1:B:293:ASN:ND2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:VAL:HG22	1:A:272:HIS:CE1	2.52	0.43
1:B:252:LEU:HD23	1:B:274:ASN:HB2	2.01	0.43
1:B:201:GLN:O	1:B:202:ALA:HB2	2.19	0.43
1:A:201:GLN:HG2	1:A:350:LEU:O	2.18	0.42
1:A:206:SER:HB3	1:A:233:LYS:NZ	2.35	0.42
1:B:245:LEU:HD22	1:B:260:SER:HB3	2.02	0.42
1:A:223:GLY:O	1:A:227:GLY:CA	2.68	0.41
1:B:224:GLY:O	1:B:225:GLU:C	2.63	0.41
1:A:192:PHE:CZ	1:A:367:ASP:HB3	2.55	0.41
1:B:351:PHE:CZ	2:B:3:HOH:O	2.57	0.41
1:B:203:ASP:O	1:B:204:ILE:C	2.64	0.41
1:B:316:ASN:ND2	2:B:23:HOH:O	2.53	0.41
1:B:200:VAL:HG12	1:B:201:GLN:N	2.35	0.40
1:B:199:VAL:CG2	1:B:363:MET:HE2	2.47	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	185/211 (88%)	175 (95%)	9 (5%)	1 (0%)	24	34
1	B	185/211 (88%)	172 (93%)	12 (6%)	1 (0%)	24	34
All	All	370/422 (88%)	347 (94%)	21 (6%)	2 (0%)	24	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	ASP
1	B	314	GLY

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	153/169 (90%)	135 (88%)	18 (12%)	5	5
1	B	153/169 (90%)	134 (88%)	19 (12%)	4	4
All	All	306/338 (90%)	269 (88%)	37 (12%)	5	5

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	PHE
1	A	196	LYS
1	A	201	GLN
1	A	216	THR
1	A	225	GLU
1	A	229	THR
1	A	240	GLU
1	A	243	LEU
1	A	253	GLU
1	A	275	SER
1	A	284	GLU
1	A	287	LEU
1	A	289	LYS
1	A	297	LEU
1	A	304	LYS
1	A	313	SER
1	A	344	LYS
1	A	346	VAL
1	B	187	SER
1	B	193	LEU
1	B	201	GLN
1	B	204	ILE
1	B	216	THR
1	B	219	ASP
1	B	231	GLU
1	B	243	LEU
1	B	253	GLU

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Mol	Chain	Res	Type
1	B	278	TRP
1	B	287	LEU
1	B	315	ARG
1	B	316	ASN
1	B	321	GLN
1	B	328	LEU
1	B	336	VAL
1	B	337	SER
1	B	346	VAL
1	B	360	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	ASN
1	A	325	GLN
1	B	228	ASN
1	B	249	ASN
1	B	316	ASN
1	B	361	GLN

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	187/211 (88%)	1.42	40 (21%) 2 2	53, 60, 69, 78	0
1	B	187/211 (88%)	1.78	63 (33%) 1 0	50, 58, 65, 68	0
All	All	374/422 (88%)	1.60	103 (27%) 1 1	50, 59, 67, 78	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	ALA	5.0
1	B	368	ALA	4.9
1	A	279	GLY	4.7
1	B	192	PHE	4.3
1	B	279	GLY	4.0
1	B	280	ALA	4.0
1	B	351	PHE	3.9
1	B	261	ALA	3.9
1	B	193	LEU	3.8
1	B	240	GLU	3.7
1	B	303	LEU	3.6
1	A	182	GLY	3.5
1	B	298	ALA	3.5
1	B	343	ILE	3.4
1	B	208	ASP	3.3
1	B	264	GLY	3.3
1	B	267	ALA	3.3
1	B	234	GLY	3.2
1	B	281	ASP	3.1
1	B	205	ALA	3.1
1	A	192	PHE	3.1
1	B	338	THR	3.0
1	B	194	GLY	3.0
1	A	232	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	351	PHE	3.0
1	B	191	LEU	2.9
1	B	183	PHE	2.9
1	B	226	VAL	2.9
1	B	263	HIS	2.9
1	B	207	ILE	2.8
1	B	199	VAL	2.8
1	B	339	MET	2.8
1	B	304	LYS	2.8
1	A	312	GLY	2.8
1	A	281	ASP	2.8
1	A	317	GLY	2.7
1	B	278	TRP	2.7
1	A	289	LYS	2.7
1	A	336	VAL	2.7
1	A	285	GLU	2.6
1	A	332	SER	2.6
1	B	229	THR	2.6
1	A	311	ILE	2.5
1	B	270	VAL	2.5
1	B	340	SER	2.5
1	A	327	ILE	2.5
1	B	366	LEU	2.5
1	B	182	GLY	2.5
1	B	335	PHE	2.5
1	A	360	VAL	2.5
1	B	360	VAL	2.5
1	B	296	ALA	2.5
1	B	342	SER	2.5
1	A	282	LYS	2.4
1	A	212	VAL	2.4
1	B	224	GLY	2.4
1	A	221	TYR	2.4
1	A	339	MET	2.4
1	B	345	THR	2.4
1	A	267	ALA	2.4
1	A	184	THR	2.3
1	A	204	ILE	2.3
1	A	346	VAL	2.3
1	B	200	VAL	2.3
1	B	347	TYR	2.3
1	A	330	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	256	GLY	2.3
1	B	198	GLN	2.3
1	A	323	ALA	2.2
1	B	227	GLY	2.2
1	B	190	SER	2.2
1	A	280	ALA	2.2
1	B	196	LYS	2.2
1	A	229	THR	2.2
1	A	326	LEU	2.2
1	B	209	SER	2.2
1	A	219	ASP	2.2
1	B	185	VAL	2.2
1	B	291	VAL	2.1
1	A	191	LEU	2.1
1	A	315	ARG	2.1
1	B	364	ALA	2.1
1	B	327	ILE	2.1
1	B	248	LYS	2.1
1	B	309	PRO	2.1
1	A	307	ALA	2.1
1	B	202	ALA	2.1
1	A	286	LEU	2.1
1	A	366	LEU	2.1
1	A	187	SER	2.1
1	A	254	VAL	2.1
1	B	212	VAL	2.1
1	B	237	GLU	2.1
1	B	236	LYS	2.1
1	A	349	VAL	2.0
1	A	194	GLY	2.0
1	B	223	GLY	2.0
1	B	221	TYR	2.0
1	A	305	SER	2.0
1	B	341	SER	2.0
1	B	246	ARG	2.0
1	B	336	VAL	2.0
1	B	210	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 [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.