



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:46 am BST

PDB ID : 2YBA
Title : Crystal structure of Nurf55 in complex with histone H3
Authors : Schmitges, F.W.; Prusty, A.B.; Faty, M.; Stutzer, A.; Lingaraju, G.M.; Aiwazian, J.; Sack, R.; Hess, D.; Li, L.; Zhou, S.; Bunker, R.D.; Wirth, U.; Bouwmeester, T.; Bauer, A.; Ly-Hartig, N.; Zhao, K.; Chan, H.; Gu, J.; Gut, H.; Fischle, W.; Muller, J.; Thoma, N.H.
Deposited on : 2011-03-02
Resolution : 2.55 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

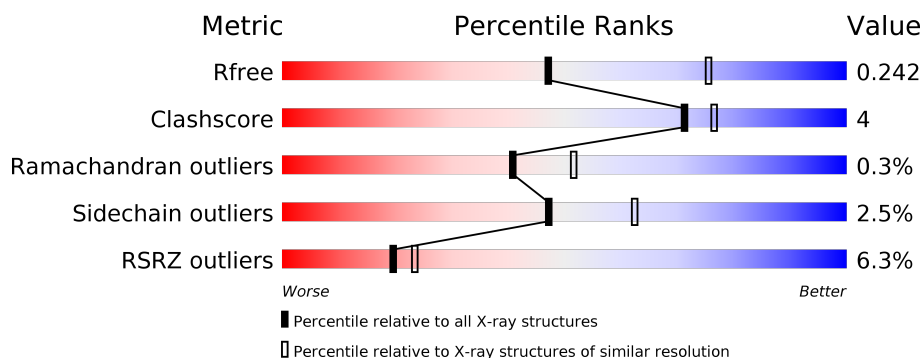
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 ≥ 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	422	<div> <div>7%</div> <div>83%</div> <div>9%</div> <div>8%</div> </div>
1	B	422	<div> <div>4%</div> <div>81%</div> <div>9%</div> <div>9%</div> </div>
2	C	19	<div> <div>11%</div> <div>47%</div> <div>11%</div> <div>42%</div> </div>
2	D	19	<div> <div>11%</div> <div>79%</div> <div>21%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6457 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 PROBABLE HISTONE-BINDING PROTEIN CAF1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3097	1952	531	603	11			
1	B	382	Total	C	N	O	S	0	0	0
			3038	1915	520	593	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q24572
A	-2	GLY	-	expression tag	UNP Q24572
A	-1	GLY	-	expression tag	UNP Q24572
A	0	ARG	-	expression tag	UNP Q24572
B	-3	GLY	-	expression tag	UNP Q24572
B	-2	GLY	-	expression tag	UNP Q24572
B	-1	GLY	-	expression tag	UNP Q24572
B	0	ARG	-	expression tag	UNP Q24572

- Molecule 2 is a protein called HISTONE H3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	0	0	0
			76	45	16	15			
2	D	15	Total	C	N	O	0	0	0
			102	60	22	20			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	B	106	Total	O	0	0
			106	106		

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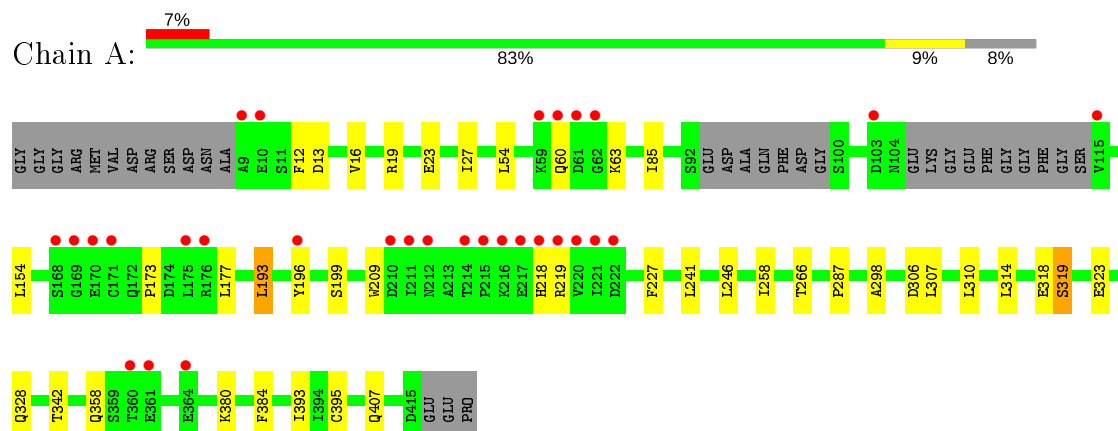
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	O	0	0
			1	1		
3	D	1	Total	O	0	0
			1	1		

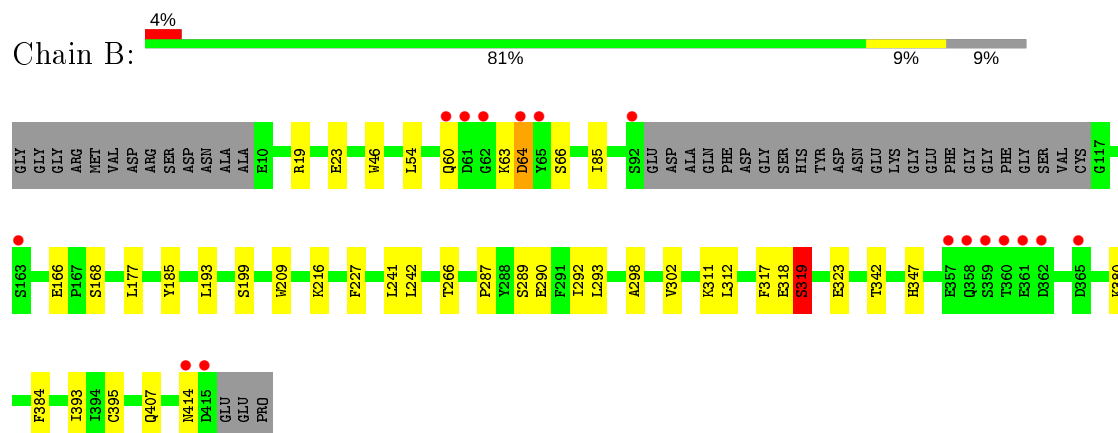
3 Residue-property plots [i](#)

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

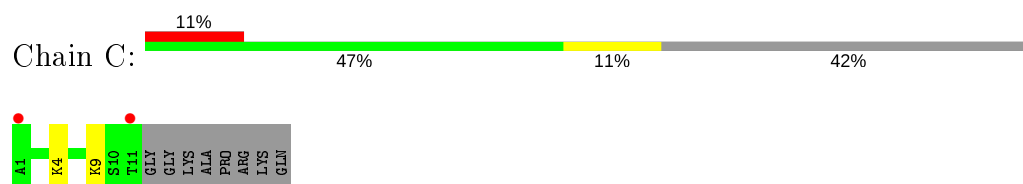
• Molecule 1: PROBABLE HISTONE-BINDING PROTEIN CAF1



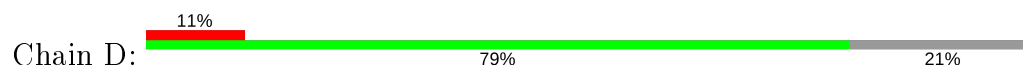
• Molecule 1: PROBABLE HISTONE-BINDING PROTEIN CAF1

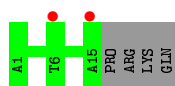


• Molecule 2: HISTONE H3



• Molecule 2: HISTONE H3





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.98 Å 88.16 Å 204.07 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.47 – 2.55 40.47 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.7 (40.47-2.55) 96.7 (40.47-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.54 Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.182 , 0.222 0.197 , 0.242	Depositor DCC
R_{free} test set	1651 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.948	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6457	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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	0.46	0/3181	0.67	0/4342
1	B	0.50	0/3121	0.69	0/4262
2	C	0.45	0/75	0.61	0/99
2	D	0.58	0/101	0.87	0/132
All	All	0.48	0/6478	0.68	0/8835

There are no bond length outliers.

There are no bond angle outliers.

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	3097	0	2903	22	0
1	B	3038	0	2851	26	0
2	C	76	0	81	2	0
2	D	102	0	111	0	0
3	A	36	0	0	0	0
3	B	106	0	0	2	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	6457	0	5946	43	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 4.

All (43) 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:342:THR:HA	1:B:380:LYS:HG3	1.60	0.84
1:A:16:VAL:HG11	1:B:292:ILE:HD11	1.71	0.72
1:A:27:ILE:HD13	1:B:312:LEU:HD11	1.72	0.71
1:B:342:THR:HG22	1:B:380:LYS:HD3	1.75	0.68
1:A:318:GLU:O	1:A:319:SER:HB3	1.96	0.65
1:A:60:GLN:HG2	1:A:63:LYS:HG3	1.79	0.64
1:A:298:ALA:HA	1:A:323:GLU:HG3	1.79	0.64
1:B:168:SER:HB3	3:B:2038:HOH:O	2.01	0.60
1:B:318:GLU:O	1:B:319:SER:HB2	2.01	0.60
1:B:298:ALA:HA	1:B:323:GLU:HG3	1.88	0.55
1:A:306:ASP:HB2	1:A:314:LEU:HD11	1.91	0.53
1:B:242:LEU:HD22	1:B:290:GLU:HB3	1.90	0.52
1:B:177:LEU:HB3	1:B:209:TRP:CE2	2.46	0.51
1:A:241:LEU:HD12	1:A:287:PRO:HA	1.94	0.50
1:A:342:THR:HG22	1:A:380:LYS:HD3	1.94	0.50
1:A:60:GLN:CG	1:A:63:LYS:HG3	2.43	0.49
1:A:177:LEU:HB3	1:A:209:TRP:CE2	2.48	0.48
1:A:393:ILE:HG12	1:A:407:GLN:HB2	1.94	0.48
1:A:12:PHE:CD2	1:B:289:SER:HB2	2.48	0.48
1:B:393:ILE:HG12	1:B:407:GLN:HB2	1.96	0.47
1:A:13:ASP:OD1	1:B:289:SER:OG	2.28	0.47
1:B:64:ASP:N	1:B:64:ASP:OD1	2.40	0.47
1:A:54:LEU:HD11	1:A:85:ILE:HD12	1.98	0.45
1:B:46:TRP:CH2	2:C:9:LYS:HB2	2.52	0.45
1:B:60:GLN:HG3	1:B:63:LYS:HG3	1.98	0.45
1:B:241:LEU:HD12	1:B:287:PRO:HA	1.98	0.44
1:B:54:LEU:HD11	1:B:85:ILE:HD12	1.99	0.44
1:B:166:GLU:CB	3:B:2038:HOH:O	2.65	0.44
1:B:380:LYS:HE3	1:B:380:LYS:HB2	1.53	0.44
1:A:193:LEU:HD22	1:A:196:TYR:CD1	2.53	0.44
1:B:384:PHE:HA	1:B:395:CYS:O	2.18	0.43
1:A:154:LEU:HD22	1:A:173:PRO:HG3	2.00	0.43
1:B:302:VAL:HB	1:B:317:PHE:HB2	2.00	0.43
1:B:185:TYR:OH	2:C:4:LYS:HE2	2.19	0.43
1:A:199:SER:HB3	1:A:209:TRP:HZ3	1.84	0.43
1:A:246:LEU:HD11	1:A:258:ILE:CG2	2.49	0.42
1:B:193:LEU:HA	1:B:193:LEU:HD12	1.91	0.42
1:A:384:PHE:HA	1:A:395:CYS:O	2.20	0.42
1:B:199:SER:HB3	1:B:209:TRP:HZ3	1.84	0.42
1:A:307:LEU:HD23	1:A:310:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:PHE:HA	1:B:266:THR:O	2.20	0.42
1:A:12:PHE:HD2	1:B:289:SER:HB2	1.85	0.42
1:A:227:PHE:HA	1:A:266:THR:O	2.21	0.41

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	384/422 (91%)	372 (97%)	11 (3%)	1 (0%)	41	51
1	B	378/422 (90%)	368 (97%)	9 (2%)	1 (0%)	41	51
2	C	9/19 (47%)	9 (100%)	0	0	100	100
2	D	13/19 (68%)	12 (92%)	1 (8%)	0	100	100
All	All	784/882 (89%)	761 (97%)	21 (3%)	2 (0%)	41	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	SER
1	B	319	SER

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	341/372 (92%)	334 (98%)	7 (2%)	53	68
1	B	335/372 (90%)	325 (97%)	10 (3%)	41	55
2	C	7/14 (50%)	7 (100%)	0	100	100
2	D	9/14 (64%)	9 (100%)	0	100	100
All	All	692/772 (90%)	675 (98%)	17 (2%)	47	62

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	23	GLU
1	A	193	LEU
1	A	218	HIS
1	A	219	ARG
1	A	328	GLN
1	A	358	GLN
1	B	19	ARG
1	B	23	GLU
1	B	64	ASP
1	B	66	SER
1	B	216	LYS
1	B	293	LEU
1	B	311	LYS
1	B	319	SER
1	B	347	HIS
1	B	414	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	HIS
1	B	204	HIS

5.3.3 RNA ⓘ

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, 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	390/422 (92%)	0.30	30 (7%) 13 17	34, 60, 96, 125	0
1	B	382/422 (90%)	-0.01	16 (4%) 36 42	19, 37, 71, 119	0
2	C	11/19 (57%)	0.77	2 (18%) 1 1	51, 64, 78, 100	0
2	D	15/19 (78%)	0.66	2 (13%) 3 4	71, 79, 87, 109	0
All	All	798/882 (90%)	0.17	50 (6%) 20 23	19, 49, 93, 125	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	ILE	6.9
1	A	9	ALA	6.2
1	B	360	THR	5.0
1	B	62	GLY	4.9
1	B	361	GLU	4.6
1	A	219	ARG	4.6
1	B	414	ASN	4.5
1	B	359	SER	4.4
1	A	62	GLY	4.2
2	D	15	ALA	4.1
1	B	415	ASP	3.9
1	B	64	ASP	3.8
1	A	170	GLU	3.6
1	A	168	SER	3.5
1	A	360	THR	3.4
1	A	214	THR	3.2
1	A	61	ASP	3.1
1	B	362	ASP	3.1
1	B	365	ASP	3.0
1	A	10	GLU	2.9
1	A	176	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	60	GLN	2.8
2	C	11	THR	2.8
2	C	1	ALA	2.7
1	A	196	TYR	2.7
1	A	171	CYS	2.7
1	A	215	PRO	2.7
1	A	169	GLY	2.6
1	B	60	GLN	2.6
1	A	218	HIS	2.6
1	A	222	ASP	2.6
1	A	221	ILE	2.5
1	A	220	VAL	2.5
1	A	361	GLU	2.4
1	B	61	ASP	2.4
1	B	92	SER	2.4
1	A	364	GLU	2.3
1	B	357	GLU	2.3
1	A	59	LYS	2.2
1	B	358	GLN	2.1
1	A	115	VAL	2.1
2	D	6	THR	2.1
1	A	175	LEU	2.1
1	A	103	ASP	2.1
1	A	210	ASP	2.1
1	B	163	SER	2.1
1	A	217	GLU	2.1
1	A	216	LYS	2.0
1	B	65	TYR	2.0
1	A	212	ASN	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.