



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4YCZ / pdb_00004ycz
Title : Y-COMPLEX HUB (NUP85-NUP120-NUP145C-SEC13 COMPLEX) FROM
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Deposited on : 2015-02-20
Resolution : 4.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

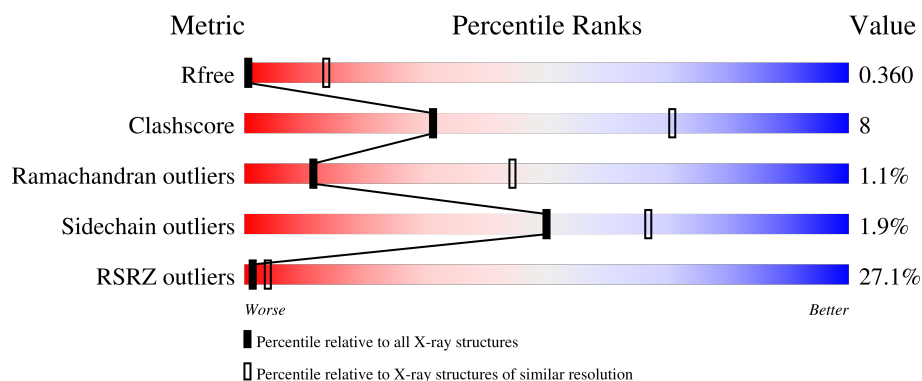
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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	876	20% 66% 14% 19%
2	B	933	20% 53% 10% 37%
3	C	313	15% 48% 14% 38%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10051 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 Fusion Protein of Sec13 and Nup145C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	0	0
			4777	3049	843	874	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP G2QES5
A	2	PRO	-	expression tag	UNP G2QES5
A	3	GLY	-	expression tag	UNP G2QES5
A	4	SER	-	expression tag	UNP G2QES5

- Molecule 2 is a protein called Nup85.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	590	Total	C	N	O	S	Se	0	0	0
			3962	2596	644	705	5	12			

There are 8 discrepancies between the modelled and reference sequences:

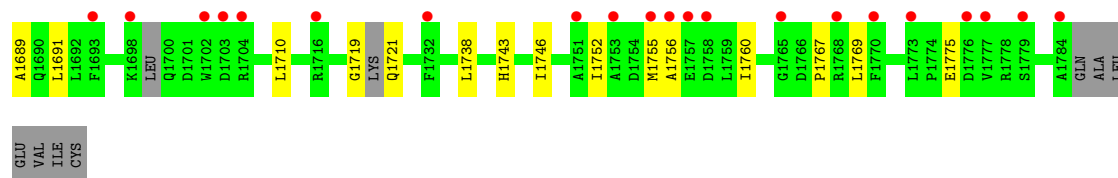
Chain	Residue	Modelled	Actual	Comment	Reference
B	249	GLY	-	expression tag	UNP G2Q7J4
B	250	PRO	-	expression tag	UNP G2Q7J4
B	251	GLY	-	expression tag	UNP G2Q7J4
B	252	SER	-	expression tag	UNP G2Q7J4
B	253	GLU	-	expression tag	UNP G2Q7J4
B	254	PHE	-	expression tag	UNP G2Q7J4
B	255	GLU	-	expression tag	UNP G2Q7J4
B	256	LEU	-	expression tag	UNP G2Q7J4

- Molecule 3 is a protein called Nup120.

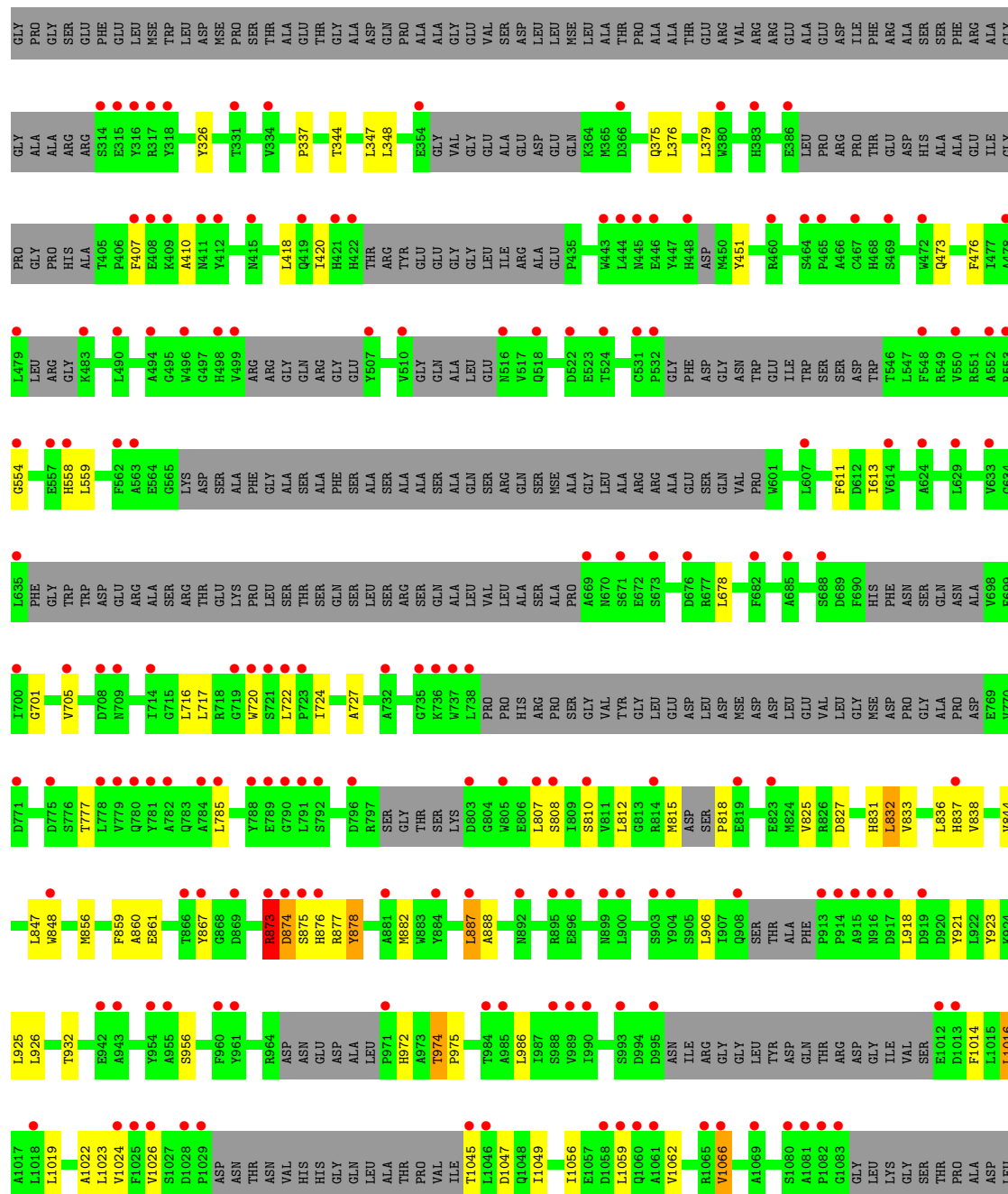
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	195	Total	C	N	O	S	0	0	0
			1312	846	220	241	5			

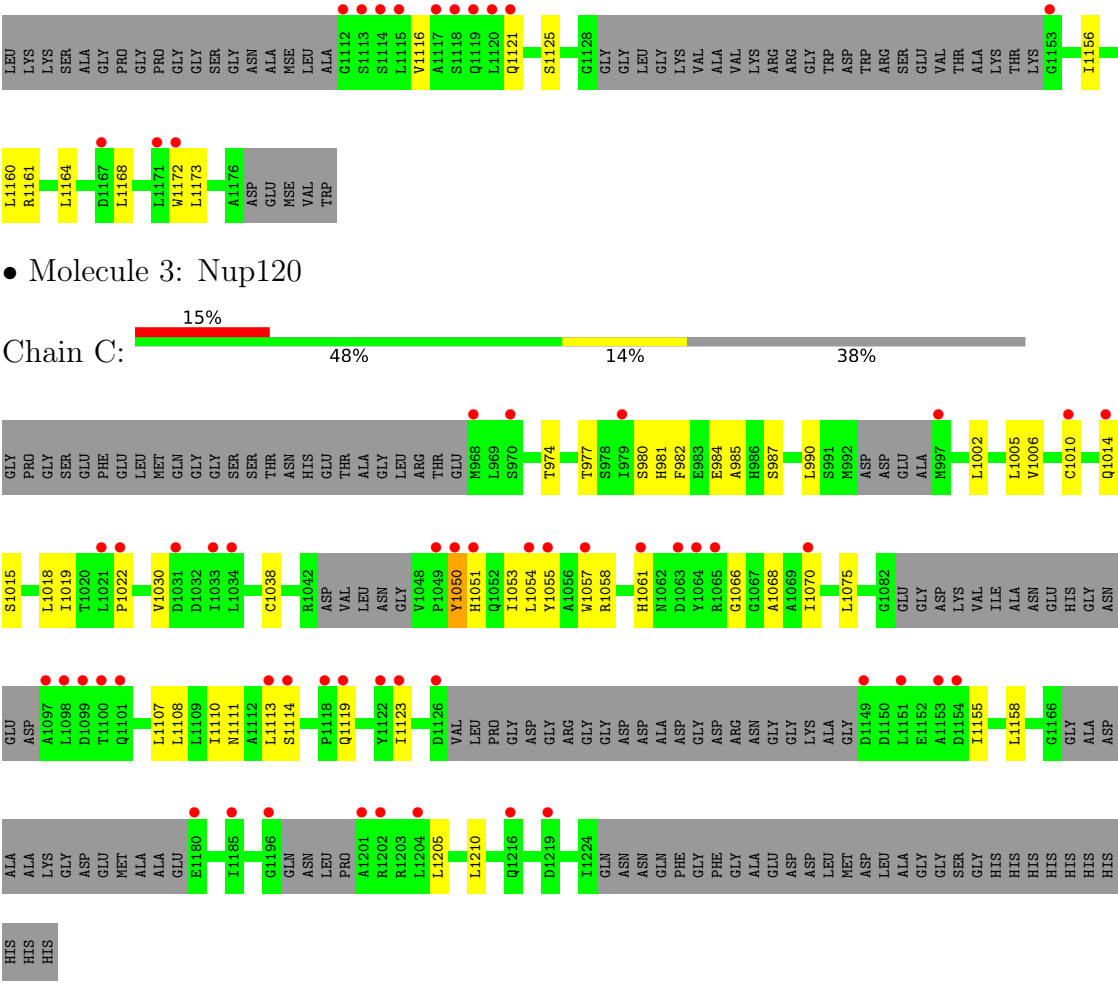
There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	943	GLY	-	expression tag	UNP G2Q2S2
C	944	PRO	-	expression tag	UNP G2Q2S2
C	945	GLY	-	expression tag	UNP G2Q2S2
C	946	SER	-	expression tag	UNP G2Q2S2
C	947	GLU	-	expression tag	UNP G2Q2S2
C	948	PHE	-	expression tag	UNP G2Q2S2
C	949	GLU	-	expression tag	UNP G2Q2S2
C	950	LEU	-	expression tag	UNP G2Q2S2
C	951	MET	-	expression tag	UNP G2Q2S2
C	1242	GLY	-	expression tag	UNP G2Q2S2
C	1243	GLY	-	expression tag	UNP G2Q2S2
C	1244	SER	-	expression tag	UNP G2Q2S2
C	1245	GLY	-	expression tag	UNP G2Q2S2
C	1246	HIS	-	expression tag	UNP G2Q2S2
C	1247	HIS	-	expression tag	UNP G2Q2S2
C	1248	HIS	-	expression tag	UNP G2Q2S2
C	1249	HIS	-	expression tag	UNP G2Q2S2
C	1250	HIS	-	expression tag	UNP G2Q2S2
C	1251	HIS	-	expression tag	UNP G2Q2S2
C	1252	HIS	-	expression tag	UNP G2Q2S2
C	1253	HIS	-	expression tag	UNP G2Q2S2
C	1254	HIS	-	expression tag	UNP G2Q2S2
C	1255	HIS	-	expression tag	UNP G2Q2S2



• Molecule 2: Nup85





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.98Å 212.02Å 170.64Å 90.00° 107.21° 90.00°	Depositor
Resolution (Å)	163.00 – 4.10 163.00 – 4.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (163.00-4.10) 97.5 (163.00-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 4.15Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1951)	Depositor
R, R_{free}	0.319 , 0.358 0.320 , 0.360	Depositor DCC
R_{free} test set	1975 reflections (7.07%)	wwPDB-VP
Wilson B-factor (Å ²)	160.4	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 704.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	10051	wwPDB-VP
Average B, all atoms (Å ²)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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	0.28	0/4879	0.72	2/6697 (0.0%)
2	B	0.27	0/4014	0.71	3/5488 (0.1%)
3	C	0.28	0/1322	0.73	0/1805
All	All	0.28	0/10215	0.72	5/13990 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	873	ARG	CB-CA-C	-5.69	110.00	116.54
1	A	1403	ASN	CB-CA-C	-5.50	109.75	117.23
1	A	1337	GLN	CB-CA-C	-5.43	109.84	117.23
2	B	337	PRO	N-CA-C	5.26	117.12	110.70
2	B	918	LEU	CB-CA-C	-5.08	110.32	117.23

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	4777	0	4010	74	0
2	B	3962	0	3566	58	0
3	C	1312	0	1190	32	0
All	All	10051	0	8766	155	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 8.

The worst 5 of 155 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:62:ASP:HB2	1:A:85:ASP:HB3	1.75	0.69
1:A:1605:GLY:HA2	1:A:1637:ALA:HB1	1.76	0.68
2:B:722:LEU:HD13	2:B:724:ILE:HD12	1.76	0.67
2:B:1023:LEU:HG	2:B:1160:LEU:HD23	1.80	0.64
2:B:815:MSE:HB3	2:B:818:PRO:HG2	1.79	0.64

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	679/876 (78%)	611 (90%)	61 (9%)	7 (1%)	12	46
2	B	548/933 (59%)	507 (92%)	36 (7%)	5 (1%)	14	49
3	C	181/313 (58%)	164 (91%)	14 (8%)	3 (2%)	7	36
All	All	1408/2122 (66%)	1282 (91%)	111 (8%)	15 (1%)	11	44

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	TRP
2	B	878	TYR
1	A	1514	PRO
2	B	837	HIS
2	B	875	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	356/700 (51%)	352 (99%)	4 (1%)	65	74
2	B	320/725 (44%)	310 (97%)	10 (3%)	35	56
3	C	108/253 (43%)	107 (99%)	1 (1%)	70	76
All	All	784/1678 (47%)	769 (98%)	15 (2%)	50	67

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	873	ARG
2	B	1066	VAL
2	B	874	ASP
3	C	1050	TYR
2	B	974	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1718	GLN
3	C	1014	GLN
3	C	1027	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 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 [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	713/876 (81%)	1.35	175 (24%) 2 4	60, 142, 204, 287	0
2	B	578/933 (61%)	1.63	182 (31%) 1 3	82, 166, 228, 311	0
3	C	195/313 (62%)	1.30	46 (23%) 2 4	85, 178, 243, 270	0
All	All	1486/2122 (70%)	1.45	403 (27%) 1 4	60, 156, 226, 311	0

The worst 5 of 403 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	988	SER	8.7
3	C	1050	TYR	7.9
2	B	899	ASN	7.2
2	B	516	ASN	7.1
2	B	805	TRP	6.6

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.