



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:36 AM UTC

PDB ID : 1I9Y / pdb_00001i9y
Title : CRYSTAL STRUCTURE OF INOSITOL POLYPHOSPHATE 5-PHOSPHATASE DOMAIN (IPP5C) OF SPSYNAPTOJANIN
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Deposited on : 2001-03-21
Resolution : 2.00 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

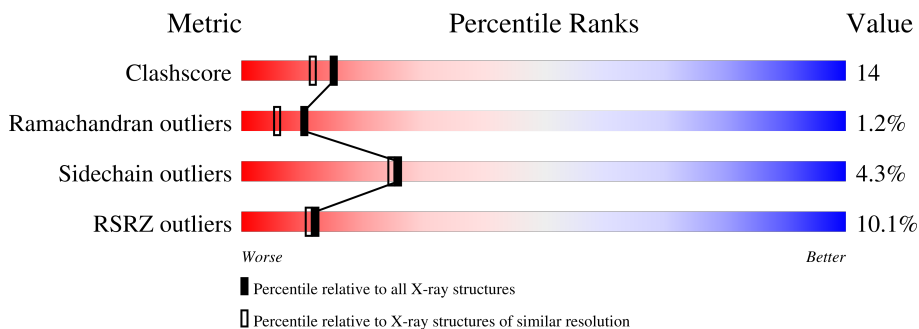
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	347	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2952 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 PHOSPHATIDYLINOSITOL PHOSPHATE PHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	1	0
			2766	1771	473	513	9			

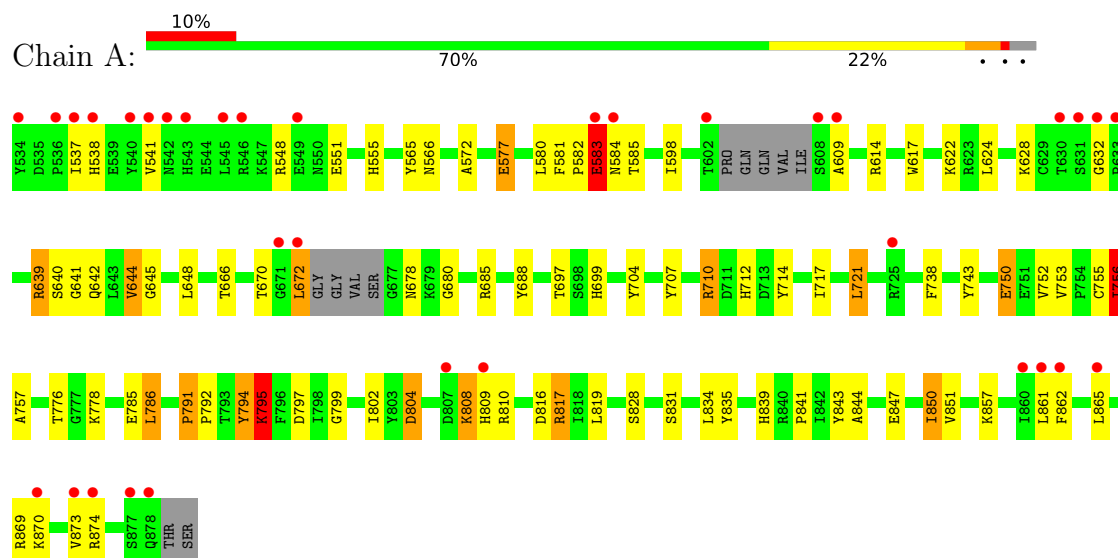
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	186	Total	O	0	0
			186	186		

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: PHOSPHATIDYLINOSITOL PHOSPHATE PHOSPHATASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.97Å 67.41Å 51.44Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 96.0 (30.00-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.97 (at 1.99Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.195 , 0.225 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.996	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2952	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.33% 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	0.98	2/2835 (0.1%)	1.23	32/3834 (0.8%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	795	LYS	N-CA	-6.73	1.37	1.46
1	A	817	ARG	CG-CD	-5.05	1.37	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	584	ASN	N-CA-C	-11.50	96.64	110.44
1	A	794	TYR	CA-C-N	8.10	137.00	121.54
1	A	794	TYR	C-N-CA	8.10	137.00	121.54
1	A	817	ARG	CA-CB-CG	-7.54	99.01	114.10
1	A	794	TYR	O-C-N	7.47	132.43	123.24
1	A	847	GLU	N-CA-C	-7.44	96.77	108.90
1	A	817	ARG	N-CA-C	7.04	119.78	109.07
1	A	639	ARG	NE-CZ-NH2	-6.87	113.02	119.20
1	A	598	ILE	N-CA-C	-6.71	102.66	111.05
1	A	797	ASP	N-CA-C	-6.68	100.54	110.23
1	A	753	VAL	CA-C-N	-6.46	112.34	119.19
1	A	753	VAL	C-N-CA	-6.46	112.34	119.19
1	A	786	LEU	CA-C-N	-6.29	113.30	119.78
1	A	786	LEU	C-N-CA	-6.29	113.30	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	632	GLY	CA-C-N	6.25	126.22	119.78
1	A	632	GLY	C-N-CA	6.25	126.22	119.78
1	A	639	ARG	CB-CG-CD	6.24	125.64	111.30
1	A	755	CYS	CA-C-N	-6.04	111.84	120.42
1	A	755	CYS	C-N-CA	-6.04	111.84	120.42
1	A	831	SER	N-CA-C	-5.96	101.18	110.42
1	A	566	ASN	N-CA-C	-5.82	99.04	108.41
1	A	704	TYR	N-CA-C	5.78	117.44	111.03
1	A	639	ARG	NE-CZ-NH1	5.73	127.23	121.50
1	A	752	VAL	N-CA-C	5.62	115.81	110.53
1	A	641	GLY	N-CA-C	-5.44	102.85	110.96
1	A	834	LEU	N-CA-C	-5.41	101.35	109.95
1	A	756	ILE	CB-CG1-CD1	-5.19	102.90	113.80
1	A	688	TYR	N-CA-C	-5.18	98.82	107.99
1	A	791	PRO	CA-C-N	5.12	125.41	119.93
1	A	791	PRO	C-N-CA	5.12	125.41	119.93
1	A	802	ILE	N-CA-C	5.04	115.57	108.36
1	A	577	GLU	N-CA-C	5.03	117.41	111.33

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	707	TYR	Sidechain
1	A	714	TYR	Sidechain

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	2766	0	2687	74	0
2	A	186	0	0	7	0
All	All	2952	0	2687	74	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 14.

All (74) 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:583:GLU:HB2	1:A:585:THR:HG23	1.51	0.93
1:A:795:LYS:HG3	1:A:804:ASP:HB2	1.53	0.88
1:A:816:ASP:O	1:A:817:ARG:HG3	1.75	0.87
1:A:809[A]:HIS:C	1:A:810:ARG:N	2.34	0.86
1:A:808:LYS:C	1:A:809[B]:HIS:N	2.33	0.85
1:A:808:LYS:HA	1:A:808:LYS:HE2	1.63	0.81
1:A:583:GLU:HG2	1:A:585:THR:OG1	1.81	0.79
1:A:639:ARG:HD3	2:A:161:HOH:O	1.89	0.73
1:A:795:LYS:HB3	2:A:13:HOH:O	1.87	0.72
1:A:582:PRO:HG2	1:A:583:GLU:H	1.52	0.72
1:A:717:ILE:HG23	1:A:721:LEU:HD22	1.73	0.69
1:A:577:GLU:H	1:A:577:GLU:CD	2.01	0.69
1:A:808:LYS:O	1:A:809[A]:HIS:C	2.36	0.68
1:A:555:HIS:CD2	1:A:851:VAL:HG22	2.28	0.68
1:A:581:PHE:HE1	1:A:624:LEU:HG	1.59	0.68
1:A:816:ASP:OD2	1:A:839:HIS:HD2	1.78	0.67
1:A:548:ARG:HH22	1:A:861:LEU:HD22	1.60	0.67
1:A:776:THR:OG1	1:A:778:LYS:HG3	1.94	0.66
1:A:795:LYS:HG2	1:A:810:ARG:HB2	1.78	0.65
1:A:717:ILE:CG2	1:A:721:LEU:HD22	2.26	0.65
1:A:537:ILE:O	1:A:541:VAL:HG23	1.98	0.63
1:A:699:HIS:HD2	2:A:163:HOH:O	1.80	0.63
1:A:750:GLU:CD	1:A:750:GLU:H	2.05	0.62
1:A:582:PRO:HG2	1:A:583:GLU:N	2.16	0.60
1:A:670:THR:HG23	1:A:680:GLY:HA2	1.83	0.59
1:A:809[A]:HIS:O	1:A:810:ARG:N	2.36	0.57
1:A:869:ARG:O	1:A:873:VAL:HG23	2.06	0.56
1:A:678:ASN:HB2	2:A:24:HOH:O	2.07	0.55
1:A:808:LYS:C	1:A:809[B]:HIS:CB	2.80	0.55
1:A:861:LEU:O	1:A:865:LEU:HD23	2.07	0.54
1:A:548:ARG:NH2	1:A:861:LEU:HD22	2.23	0.54
1:A:869:ARG:O	1:A:869:ARG:HD3	2.08	0.54
1:A:548:ARG:NH2	1:A:861:LEU:HD13	2.23	0.53
1:A:839:HIS:HE1	2:A:177:HOH:O	1.92	0.52
1:A:756:ILE:HG13	1:A:757:ALA:N	2.24	0.52
1:A:572:ALA:HA	1:A:617:TRP:CZ2	2.45	0.51
1:A:816:ASP:C	1:A:817:ARG:HG3	2.33	0.51
1:A:644:VAL:HG12	1:A:645:GLY:N	2.25	0.51
1:A:537:ILE:HG23	1:A:869:ARG:CG	2.41	0.50
1:A:799:GLY:HA2	1:A:835:TYR:HB3	1.93	0.50
1:A:794:TYR:CG	1:A:795:LYS:N	2.78	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809[A]:HIS:CA	1:A:810:ARG:N	2.74	0.50
1:A:785:GLU:OE2	1:A:817:ARG:HG2	2.12	0.49
1:A:565:TYR:CG	1:A:841:PRO:HB3	2.48	0.49
1:A:710:ARG:HB3	1:A:743:TYR:CZ	2.48	0.49
1:A:808:LYS:C	1:A:809[B]:HIS:HB3	2.37	0.49
1:A:750:GLU:CD	1:A:750:GLU:N	2.69	0.49
1:A:537:ILE:HG23	1:A:869:ARG:HG3	1.95	0.47
1:A:666:THR:HG23	1:A:721:LEU:HD12	1.95	0.47
1:A:581:PHE:CE1	1:A:624:LEU:HG	2.43	0.47
1:A:697:THR:HA	1:A:738:PHE:O	2.16	0.46
1:A:582:PRO:CG	1:A:583:GLU:H	2.23	0.46
1:A:870:LYS:O	1:A:874:ARG:HG3	2.15	0.46
1:A:582:PRO:CG	1:A:583:GLU:N	2.78	0.45
1:A:640:SER:HA	1:A:648:LEU:O	2.16	0.45
1:A:785:GLU:HB2	1:A:819:LEU:CD2	2.46	0.45
1:A:756:ILE:HD13	1:A:791:PRO:HB3	1.99	0.45
1:A:644:VAL:HG12	1:A:645:GLY:H	1.82	0.44
1:A:614:ARG:HD3	1:A:642:GLN:OE1	2.18	0.44
1:A:645:GLY:HA3	2:A:90:HOH:O	2.18	0.44
1:A:672:LEU:HA	1:A:672:LEU:HD22	1.68	0.43
1:A:583:GLU:HB3	2:A:56:HOH:O	2.18	0.43
1:A:551:GLU:O	1:A:857:LYS:HD2	2.18	0.43
1:A:548:ARG:HB3	1:A:551:GLU:OE2	2.19	0.43
1:A:672:LEU:HB2	1:A:712:HIS:ND1	2.33	0.43
1:A:581:PHE:HA	1:A:583:GLU:OE2	2.19	0.42
1:A:828:SER:O	1:A:844:ALA:HA	2.19	0.42
1:A:808:LYS:C	1:A:809[B]:HIS:CA	2.88	0.41
1:A:538:HIS:CD2	1:A:862:PHE:HZ	2.39	0.41
1:A:581:PHE:CZ	1:A:628:LYS:HG3	2.56	0.41
1:A:582:PRO:HG3	1:A:843:TYR:CZ	2.55	0.41
1:A:685:ARG:C	1:A:685:ARG:HD3	2.46	0.41
1:A:808:LYS:HE2	1:A:808:LYS:CA	2.39	0.41
1:A:850:ILE:HA	1:A:850:ILE:HD12	1.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	329/347 (95%)	315 (96%)	10 (3%)	4 (1%)	10 6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	804	ASP
1	A	583	GLU
1	A	609	ALA
1	A	644	VAL

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	301/309 (97%)	288 (96%)	13 (4%)	26 25

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

Mol	Chain	Res	Type
1	A	580	LEU
1	A	583	GLU
1	A	622	LYS
1	A	672	LEU
1	A	710	ARG
1	A	721	LEU
1	A	750	GLU

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Mol	Chain	Res	Type
1	A	756	ILE
1	A	786	LEU
1	A	792	PRO
1	A	795	LYS
1	A	808	LYS
1	A	850	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	542	ASN
1	A	555	HIS
1	A	557	ASN
1	A	578	ASN
1	A	600	GLN
1	A	678	ASN
1	A	699	HIS
1	A	827	HIS
1	A	839	HIS
1	A	849	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	809[A]:HIS	C	810:ARG	N	2.34
1	A	808:LYS	C	809[B]:HIS	N	2.33

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	336/347 (96%)	0.23	34 (10%) 12 11	15, 26, 71, 77	1 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	583	GLU	5.1
1	A	809[A]	HIS	4.5
1	A	534	TYR	4.2
1	A	672	LEU	3.9
1	A	608	SER	3.9
1	A	878	GLN	3.9
1	A	633	PRO	3.9
1	A	861	LEU	3.8
1	A	609	ALA	3.3
1	A	537	ILE	3.2
1	A	602	THR	3.2
1	A	862	PHE	3.1
1	A	874	ARG	3.1
1	A	546	ARG	3.0
1	A	671	GLY	3.0
1	A	632	GLY	3.0
1	A	584	ASN	2.9
1	A	860	ILE	2.9
1	A	630	THR	2.8
1	A	873	VAL	2.7
1	A	542	ASN	2.7
1	A	536	PRO	2.7
1	A	807	ASP	2.6
1	A	543	HIS	2.6
1	A	877	SER	2.4
1	A	870	LYS	2.4
1	A	549	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	540	TYR	2.3
1	A	631	SER	2.3
1	A	545	LEU	2.3
1	A	865	LEU	2.3
1	A	538	HIS	2.2
1	A	541	VAL	2.1
1	A	725	ARG	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.