



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:16 AM UTC

PDB ID : 6Y30 / pdb_00006y30
Title : NG domain of human SRP54 T115A mutant
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Deposited on : 2020-02-17
Resolution : 2.65 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

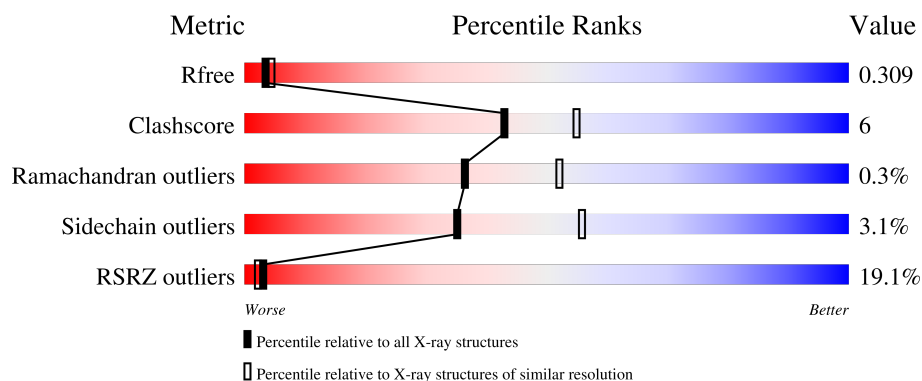
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	303	20% 82% 17% .
1	B	303	17% 78% 16% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4511 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 Signal recognition particle 54 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2300	1464	392	431	13			
1	B	284	Total	C	N	O	S	0	0	0
			2186	1389	377	407	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P61011
A	-5	GLY	-	expression tag	UNP P61011
A	-4	HIS	-	expression tag	UNP P61011
A	-3	HIS	-	expression tag	UNP P61011
A	-2	HIS	-	expression tag	UNP P61011
A	-1	HIS	-	expression tag	UNP P61011
A	0	HIS	-	expression tag	UNP P61011
A	115	ALA	THR	engineered mutation	UNP P61011
B	-6	MET	-	initiating methionine	UNP P61011
B	-5	GLY	-	expression tag	UNP P61011
B	-4	HIS	-	expression tag	UNP P61011
B	-3	HIS	-	expression tag	UNP P61011
B	-2	HIS	-	expression tag	UNP P61011
B	-1	HIS	-	expression tag	UNP P61011
B	0	HIS	-	expression tag	UNP P61011
B	115	ALA	THR	engineered mutation	UNP P61011

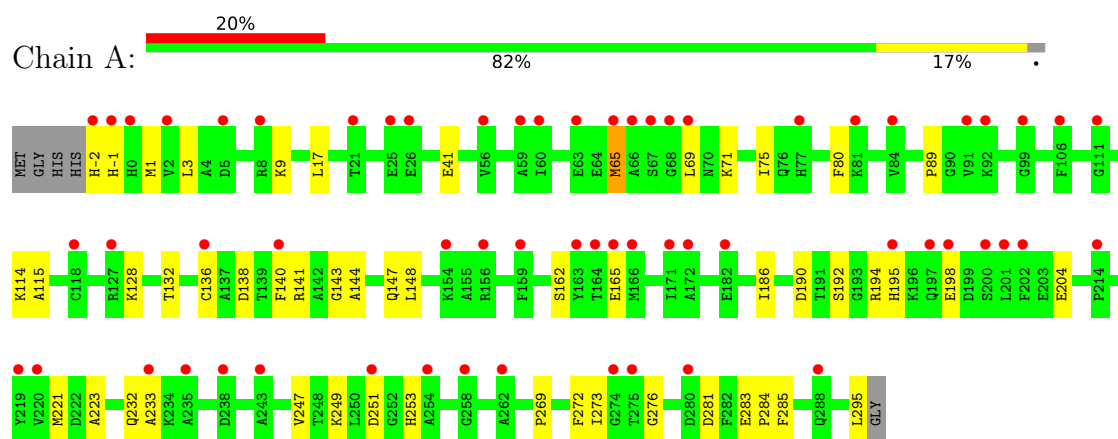
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	17	Total	O	0	0
			17	17		
2	B	8	Total	O	0	0
			8	8		

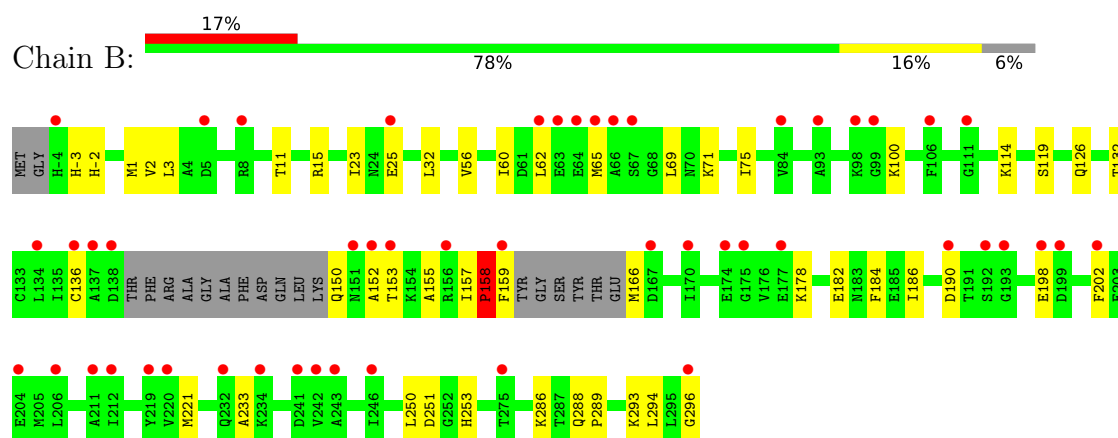
3 Residue-property plots [i](#)

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: Signal recognition particle 54 kDa protein



- Molecule 1: Signal recognition particle 54 kDa protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.80Å 53.90Å 91.37Å 90.00° 105.97° 90.00°	Depositor
Resolution (Å)	53.26 – 2.65 53.26 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.9 (53.26-2.65) 95.9 (53.26-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.276 , 0.309 0.278 , 0.309	Depositor DCC
R_{free} test set	1118 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.9	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	4511	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.76% 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	0.11	0/2337	0.30	0/3150
1	B	0.11	0/2219	0.27	0/2988
All	All	0.11	0/4556	0.29	0/6138

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

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	2300	0	2358	28	0
1	B	2186	0	2247	28	0
2	A	17	0	0	1	0
2	B	8	0	0	1	0
All	All	4511	0	4605	56	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 6.

All (56) 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:276:GLY:N	1:A:281:ASP:OD2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ARG:NH1	1:A:147:GLN:OE1	2.24	0.70
1:A:1:MET:HG2	1:A:3:LEU:H	1.55	0.69
1:B:1:MET:HG2	1:B:294:LEU:HD13	1.73	0.69
1:A:192:SER:OG	1:A:195:HIS:NE2	2.27	0.68
1:A:249:LYS:O	1:A:253:HIS:NE2	2.20	0.67
1:A:136:CYS:HB2	1:A:148:LEU:HD22	1.80	0.63
1:B:286:LYS:HE2	1:B:289:PRO:HG2	1.80	0.61
1:B:152:ALA:HB3	1:B:159:PHE:HB2	1.81	0.61
1:B:114:LYS:NZ	1:B:190:ASP:OD1	2.32	0.59
1:B:60:ILE:HD13	1:B:75:ILE:HG12	1.85	0.59
1:B:-2:HIS:ND1	1:B:296:GLY:O	2.36	0.57
1:A:273:ILE:HD11	1:A:285:PHE:HD1	1.68	0.56
1:A:221:MET:HE1	1:A:233:ALA:HB2	1.87	0.56
1:B:253:HIS:O	2:B:301:HOH:O	2.17	0.56
1:A:71:LYS:O	1:A:75:ILE:HG12	2.05	0.56
1:A:115:ALA:HB2	1:A:141:ARG:HH22	1.70	0.56
1:A:9:LYS:NZ	1:A:41:GLU:OE2	2.31	0.55
1:A:132:THR:HG22	1:A:186:ILE:HB	1.88	0.55
1:B:132:THR:HG22	1:B:186:ILE:HB	1.87	0.55
1:B:1:MET:HE2	1:B:294:LEU:HB2	1.89	0.55
1:A:-1:HIS:O	1:A:-1:HIS:ND1	2.41	0.53
1:A:80:PHE:HD1	1:A:295:LEU:HD12	1.74	0.53
1:B:126:GLN:NE2	1:B:155:ALA:O	2.41	0.53
1:B:11:THR:O	1:B:15:ARG:N	2.34	0.51
1:A:128:LYS:NZ	2:A:302:HOH:O	2.43	0.51
1:A:138:ASP:OD2	1:A:192:SER:HA	2.11	0.51
1:A:141:ARG:HB3	1:A:144:ALA:HB2	1.94	0.50
1:A:223:ALA:HB2	1:A:247:VAL:HG13	1.94	0.50
1:A:192:SER:OG	1:A:204:GLU:OE1	2.29	0.50
1:B:1:MET:HG3	1:B:3:LEU:H	1.75	0.49
1:B:1:MET:HG3	1:B:2:VAL:N	2.27	0.49
1:B:158:PRO:HG2	1:B:184:PHE:CE1	2.47	0.49
1:B:221:MET:HE1	1:B:233:ALA:HB2	1.94	0.48
1:B:65:MET:HE2	1:B:69:LEU:HD12	1.95	0.47
1:B:32:LEU:HD21	1:B:56:VAL:HG11	1.97	0.47
1:B:150:GLN:N	1:B:153:THR:HG1	2.13	0.47
1:A:141:ARG:HA	1:A:194:ARG:NH1	2.30	0.46
1:B:251:ASP:OD1	1:B:251:ASP:N	2.46	0.46
1:A:251:ASP:OD1	1:A:251:ASP:N	2.49	0.45
1:B:62:LEU:O	1:B:71:LYS:NZ	2.50	0.45
1:A:114:LYS:NZ	1:A:190:ASP:OD1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:PRO:HG3	1:A:269:PRO:HA	1.98	0.44
1:B:158:PRO:HG2	1:B:184:PHE:HE1	1.81	0.44
1:A:71:LYS:H	1:A:71:LYS:HG2	1.44	0.44
1:A:162:SER:OG	1:A:165:GLU:HG2	2.17	0.43
1:B:157:ILE:O	1:B:159:PHE:N	2.51	0.43
1:B:293:LYS:HA	1:B:293:LYS:HD3	1.84	0.43
1:B:136:CYS:HA	1:B:190:ASP:HB3	2.00	0.42
1:A:272:PHE:HA	1:A:284:PRO:HA	2.02	0.42
1:B:198:GLU:HG3	1:B:202:PHE:CE2	2.55	0.42
1:B:2:VAL:HG21	1:B:250:LEU:HB3	2.02	0.41
1:B:178:LYS:O	1:B:182:GLU:HG2	2.21	0.41
1:A:65:MET:HG2	1:A:71:LYS:HD3	2.02	0.41
1:B:288:GLN:HB3	1:B:289:PRO:HD3	2.03	0.41
1:A:114:LYS:HE3	1:A:114:LYS:HB3	1.94	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	296/303 (98%)	292 (99%)	3 (1%)	1 (0%)	36	52
1	B	278/303 (92%)	273 (98%)	4 (1%)	1 (0%)	30	45
All	All	574/606 (95%)	565 (98%)	7 (1%)	2 (0%)	36	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	158	PRO
1	A	143	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	248/251 (99%)	240 (97%)	8 (3%)	34	55
1	B	237/251 (94%)	230 (97%)	7 (3%)	36	57
All	All	485/502 (97%)	470 (97%)	15 (3%)	35	56

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS
1	A	17	LEU
1	A	65	MET
1	A	69	LEU
1	A	140	PHE
1	A	198	GLU
1	A	232	GLN
1	A	283	GLU
1	B	-3	HIS
1	B	23	ILE
1	B	25	GLU
1	B	100	LYS
1	B	119	SER
1	B	158	PRO
1	B	166	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	51	GLN
1	A	278	HIS
1	B	45	ASN
1	B	51	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

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	298/303 (98%)	1.40	61 (20%) 2 1	37, 65, 92, 119	0
1	B	284/303 (93%)	1.32	50 (17%) 4 3	35, 61, 99, 119	0
All	All	582/606 (96%)	1.36	111 (19%) 3 2	35, 63, 95, 119	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	296	GLY	6.8
1	A	67	SER	6.0
1	A	66	ALA	4.5
1	B	153	THR	4.5
1	A	118	CYS	4.4
1	B	243	ALA	4.4
1	A	140	PHE	4.0
1	A	238	ASP	3.9
1	A	59	ALA	3.8
1	B	5	ASP	3.8
1	A	68	GLY	3.7
1	A	5	ASP	3.7
1	A	254	ALA	3.6
1	B	8	ARG	3.5
1	B	167	ASP	3.5
1	B	152	ALA	3.4
1	B	159	PHE	3.4
1	A	195	HIS	3.3
1	B	63	GLU	3.3
1	B	65	MET	3.1
1	A	274	GLY	3.0
1	B	198	GLU	3.0
1	A	92	LYS	2.9
1	B	206	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	138	ASP	2.9
1	A	65	MET	2.9
1	A	258	GLY	2.9
1	B	111	GLY	2.9
1	B	242	VAL	2.9
1	A	220	VAL	2.8
1	B	174	GLU	2.8
1	A	111	GLY	2.8
1	A	-1	HIS	2.8
1	B	-4	HIS	2.8
1	B	25	GLU	2.8
1	A	166	MET	2.7
1	B	93	ALA	2.7
1	A	163	TYR	2.7
1	B	193	GLY	2.6
1	B	204	GLU	2.6
1	A	164	THR	2.6
1	A	69	LEU	2.6
1	A	219	TYR	2.6
1	B	136	CYS	2.6
1	A	200	SER	2.5
1	A	81	LYS	2.5
1	B	156	ARG	2.5
1	A	63	GLU	2.5
1	A	165	GLU	2.5
1	B	275	THR	2.5
1	A	60	ILE	2.5
1	A	172	ALA	2.5
1	B	137	ALA	2.5
1	A	156	ARG	2.5
1	A	-2	HIS	2.5
1	A	182	GLU	2.5
1	A	56	VAL	2.5
1	B	98	LYS	2.4
1	B	246	ILE	2.4
1	B	177	GLU	2.4
1	A	159	PHE	2.4
1	A	202	PHE	2.4
1	B	66	ALA	2.4
1	B	192	SER	2.4
1	A	25	GLU	2.4
1	B	202	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	201	LEU	2.4
1	B	62	LEU	2.4
1	B	134	LEU	2.4
1	B	232	GLN	2.4
1	A	8	ARG	2.4
1	A	243	ALA	2.4
1	A	198	GLU	2.3
1	B	219	TYR	2.3
1	A	0	HIS	2.3
1	A	26	GLU	2.3
1	B	199	ASP	2.3
1	A	171	ILE	2.2
1	A	154	LYS	2.2
1	A	197	GLN	2.2
1	B	64	GLU	2.2
1	A	99	GLY	2.2
1	A	251	ASP	2.2
1	B	212	ILE	2.2
1	B	211	ALA	2.2
1	A	275	THR	2.2
1	B	151	ASN	2.2
1	A	2	VAL	2.2
1	A	21	THR	2.2
1	A	136	CYS	2.2
1	A	77	HIS	2.1
1	B	241	ASP	2.1
1	A	127	ARG	2.1
1	A	214	PRO	2.1
1	A	288	GLN	2.1
1	B	84	VAL	2.1
1	B	106	PHE	2.1
1	B	67	SER	2.1
1	B	234	LYS	2.1
1	B	99	GLY	2.1
1	A	91	VAL	2.1
1	B	220	VAL	2.1
1	A	106	PHE	2.1
1	B	190	ASP	2.0
1	A	233	ALA	2.0
1	A	235	ALA	2.0
1	B	175	GLY	2.0
1	A	262	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	280	ASP	2.0
1	B	170	ILE	2.0
1	A	84	VAL	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.