



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:48 PM UTC

PDB ID : 5I9D / pdb_00005i9d
Title : Crystal structure of designed pentatricopeptide repeat protein dPPR-U8A2 in complex with its target RNA U8A2
Authors : Shen, C.; Zhang, D.; Guan, Z.; Zou, T.; Yin, P.
Deposited on : 2016-02-20
Resolution : 2.60 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

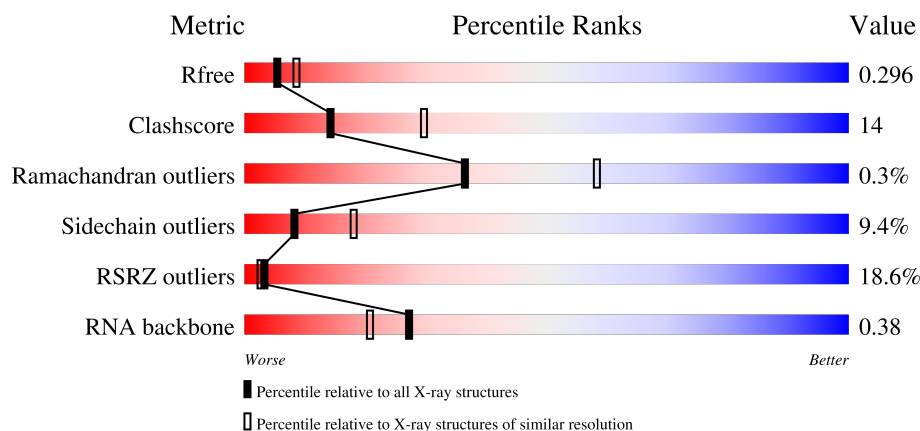
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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	460	
2	B	18	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3017 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 pentatricopeptide repeat protein dPPR-U8A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	0	0
			2778	1793	425	540	20			

- Molecule 2 is a RNA chain called RNA (5'-R(*GP*GP*GP*G*UP*UP*UP*UP*AP*AP*UP*UP*UP*CP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	P	0	0	1
			198	89	24	75	10			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		
3	B	6	Total	O	0	0
			6	6		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.55Å 84.90Å 95.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.08 – 2.60 46.08 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.08-2.60) 96.1 (46.08-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.69 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.267 , 0.293 0.271 , 0.296	Depositor DCC
R_{free} test set	704 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 61.4	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	3017	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.34% 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	0.99	3/2804 (0.1%)	1.23	15/3762 (0.4%)
2	B	0.99	3/218 (1.4%)	1.11	2/336 (0.6%)
All	All	0.99	6/3022 (0.2%)	1.22	17/4098 (0.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	ASP	N-CA	7.15	1.54	1.45
2	B	3	U	O3'-P	-5.71	1.52	1.61
2	B	4	U	O3'-P	-5.36	1.53	1.61
2	B	2	U	O3'-P	-5.21	1.53	1.61
1	A	231	THR	CA-CB	5.12	1.61	1.53
1	A	227	VAL	C-O	-5.03	1.18	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	GLU	N-CA-C	10.47	122.45	111.14
1	A	155	ASP	N-CA-C	6.51	120.09	110.46
1	A	231	THR	N-CA-CB	6.17	119.26	110.13
1	A	157	VAL	CB-CA-C	-6.17	103.82	112.14
1	A	231	THR	N-CA-C	-5.90	104.21	111.40
1	A	286	GLU	CB-CA-C	-5.71	99.26	110.10
1	A	285	GLU	CA-C-O	-5.69	114.84	120.70
2	B	2	U	C1'-C2'-O2'	5.59	116.79	108.40
1	A	328	LYS	N-CA-C	5.57	117.69	109.50
1	A	197	LEU	CA-C-N	5.40	127.57	120.60
1	A	197	LEU	C-N-CA	5.40	127.57	120.60
2	B	4	U	C4'-C3'-O3'	-5.33	105.00	113.00
1	A	286	GLU	N-CA-CB	-5.33	101.44	110.50
1	A	155	ASP	CB-CA-C	-5.30	101.28	110.45
1	A	366	VAL	N-CA-C	-5.29	105.55	110.53
1	A	112	MET	CB-CA-C	-5.10	102.87	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	VAL	N-CA-C	5.00	115.72	110.62

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	2778	0	2909	85	1
2	B	198	0	99	3	0
3	A	35	0	0	27	0
3	B	6	0	0	0	0
All	All	3017	0	3008	85	1

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 (85) 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:209:GLU:CA	3:A:502:HOH:O	1.93	1.17
1:A:209:GLU:C	3:A:502:HOH:O	1.93	1.10
1:A:286:GLU:N	1:A:286:GLU:OE1	1.90	1.04
1:A:42:LEU:HD13	1:A:43:ARG:H	1.22	1.00
1:A:286:GLU:HG3	3:A:524:HOH:O	1.63	0.97
1:A:407:VAL:CB	3:A:501:HOH:O	2.13	0.96
1:A:208:ASP:O	3:A:502:HOH:O	1.85	0.92
1:A:255:LYS:HG2	1:A:256:GLY:H	1.35	0.90
1:A:285:GLU:O	1:A:286:GLU:OE1	1.92	0.88
1:A:285:GLU:C	1:A:286:GLU:OE1	2.15	0.87
1:A:407:VAL:O	3:A:504:HOH:O	1.95	0.84
1:A:114:GLU:OE2	3:A:503:HOH:O	1.95	0.83
1:A:405:ARG:NH2	3:A:506:HOH:O	2.10	0.83
1:A:286:GLU:CG	3:A:524:HOH:O	2.20	0.83
1:A:208:ASP:C	3:A:502:HOH:O	2.20	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:VAL:HG23	3:A:501:HOH:O	1.78	0.82
1:A:407:VAL:CG2	3:A:501:HOH:O	2.29	0.80
1:A:238:LYS:NZ	3:A:508:HOH:O	2.14	0.80
1:A:407:VAL:N	3:A:501:HOH:O	1.84	0.79
1:A:42:LEU:CD1	1:A:43:ARG:H	1.96	0.79
1:A:209:GLU:HA	3:A:502:HOH:O	1.69	0.78
1:A:42:LEU:HD13	1:A:43:ARG:N	1.99	0.78
1:A:407:VAL:HB	3:A:501:HOH:O	1.80	0.77
1:A:252:MET:O	3:A:505:HOH:O	2.04	0.74
1:A:286:GLU:CB	3:A:524:HOH:O	2.36	0.73
1:A:42:LEU:HD12	1:A:42:LEU:N	2.04	0.73
1:A:290:LYS:HG3	1:A:291:GLY:N	2.04	0.72
1:A:411:TYR:N	3:A:504:HOH:O	2.21	0.72
1:A:403:THR:O	3:A:501:HOH:O	2.08	0.71
1:A:286:GLU:OE2	1:A:290:LYS:NZ	2.25	0.68
1:A:286:GLU:CD	1:A:290:LYS:HD2	2.18	0.68
1:A:369:TYR:OH	3:A:507:HOH:O	2.12	0.67
1:A:61:LEU:HD13	1:A:69:GLU:HG3	1.79	0.65
1:A:242:LEU:HD11	1:A:274:ALA:CB	2.27	0.65
1:A:212:LYS:HB2	3:A:502:HOH:O	1.96	0.64
1:A:59:ASP:OD1	1:A:63:LYS:HE3	1.98	0.63
1:A:269:ASP:OD2	3:A:509:HOH:O	2.15	0.63
1:A:255:LYS:HG2	1:A:256:GLY:N	2.12	0.61
1:A:242:LEU:HD11	1:A:274:ALA:HB2	1.83	0.60
1:A:286:GLU:HB3	3:A:524:HOH:O	2.00	0.60
1:A:172:LEU:HD21	1:A:201:LEU:HD23	1.84	0.59
1:A:63:LYS:HA	1:A:64:ALA:HB2	1.85	0.57
1:A:64:ALA:HB1	1:A:65:GLY:CA	2.35	0.57
1:A:102:LEU:HD21	1:A:131:LEU:HD23	1.86	0.57
1:A:283:LEU:O	1:A:286:GLU:CB	2.54	0.56
1:A:283:LEU:O	1:A:286:GLU:HB2	2.06	0.55
1:A:286:GLU:HG2	1:A:286:GLU:O	2.05	0.55
1:A:67:LEU:HD23	1:A:71:LEU:HD11	1.89	0.55
1:A:59:ASP:OD1	1:A:63:LYS:CE	2.55	0.55
1:A:176:LEU:CD2	1:A:197:LEU:HD22	2.37	0.55
1:A:290:LYS:HG3	1:A:291:GLY:H	1.69	0.54
1:A:98:LYS:HE3	3:A:510:HOH:O	2.08	0.53
1:A:402:LEU:CD2	1:A:406:ARG:CZ	2.87	0.53
1:A:279:GLU:HA	1:A:282:LYS:HD2	1.92	0.52
1:A:227:VAL:O	1:A:231:THR:HG23	2.10	0.51
1:A:53:THR:HG22	1:A:57:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:CD1	1:A:42:LEU:N	2.72	0.49
1:A:119:PRO:HB3	1:A:123:THR:HG21	1.92	0.49
1:A:367:VAL:HG13	2:B:5:U:N1	2.27	0.49
1:A:332:VAL:HG13	2:B:4:U:C2	2.48	0.48
1:A:271:LEU:HB2	1:A:280:ALA:HB2	1.96	0.47
1:A:286:GLU:OE1	1:A:290:LYS:HD2	2.15	0.47
1:A:286:GLU:CD	1:A:290:LYS:NZ	2.73	0.46
1:A:75:GLU:O	1:A:78:VAL:HG22	2.15	0.46
1:A:374:ASP:OD1	1:A:378:LYS:HE2	2.15	0.46
1:A:176:LEU:HD22	1:A:197:LEU:HD22	1.96	0.46
1:A:226:VAL:O	1:A:230:SER:OG	2.28	0.46
1:A:347:LEU:HD22	1:A:379:ALA:CB	2.46	0.45
1:A:347:LEU:HD21	1:A:376:LEU:HD23	1.98	0.45
1:A:299:TYR:HB2	1:A:322:MET:HE3	1.99	0.45
1:A:392:MET:HE1	1:A:403:THR:HG21	2.00	0.43
1:A:120:ASP:C	1:A:120:ASP:OD1	2.60	0.43
1:A:136:LYS:O	1:A:137:LEU:C	2.61	0.43
1:A:391:GLU:HA	1:A:394:GLU:HG2	2.00	0.43
1:A:217:MET:HE1	1:A:228:THR:HG21	2.01	0.43
1:A:67:LEU:CD2	1:A:71:LEU:HD11	2.49	0.42
1:A:67:LEU:HD23	1:A:71:LEU:CD1	2.49	0.42
1:A:214:PHE:CD2	1:A:232:LEU:HD11	2.55	0.42
1:A:82:ILE:HD12	1:A:82:ILE:N	2.35	0.41
1:A:145:GLU:HG2	1:A:146:GLU:N	2.34	0.41
1:A:67:LEU:HD21	1:A:96:LEU:CD2	2.51	0.41
1:A:74:PHE:O	1:A:78:VAL:HG13	2.20	0.41
1:A:262:VAL:HG13	2:B:2:U:C2	2.56	0.41
1:A:63:LYS:NZ	3:A:513:HOH:O	2.54	0.40
1:A:209:GLU:N	3:A:502:HOH:O	2.26	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LYS:NZ	1:A:360:LYS:O[1_655]	2.12	0.08

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	348/460 (76%)	319 (92%)	28 (8%)	1 (0%)	36	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	LYS

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	308/393 (78%)	279 (91%)	29 (9%)	8	18

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	63	LYS
1	A	107	LYS
1	A	145	GLU
1	A	152	ILE
1	A	162	LEU
1	A	176	LEU
1	A	188	LYS
1	A	228	THR
1	A	230	SER

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Mol	Chain	Res	Type
1	A	231	THR
1	A	250	GLU
1	A	263	THR
1	A	287	MET
1	A	292	ILE
1	A	323	VAL
1	A	327	ILE
1	A	328	LYS
1	A	358	VAL
1	A	367	VAL
1	A	373	ILE
1	A	382	LEU
1	A	386	LEU
1	A	393	VAL
1	A	394	GLU
1	A	400	ASP
1	A	402	LEU
1	A	403	THR
1	A	411	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	9/18 (50%)	3 (33%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	U
2	B	3	U
2	B	6	C

There are no RNA pucker outliers to report.

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 [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	360/460 (78%)	1.21	68 (18%) 3 2	28, 48, 80, 107	0
2	B	11/18 (61%)	0.20	1 (9%) 15 11	36, 40, 62, 64	0
All	All	371/478 (77%)	1.18	69 (18%) 3 3	28, 48, 80, 107	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	LEU	6.2
2	B	-4	U	5.4
1	A	411	TYR	4.6
1	A	363	LYS	4.6
1	A	67	LEU	4.5
1	A	409	GLU	4.4
1	A	408	VAL	4.3
1	A	287	MET	4.1
1	A	358	VAL	4.1
1	A	382	LEU	4.0
1	A	404	TYR	4.0
1	A	379	ALA	3.9
1	A	257	ILE	3.9
1	A	66	LYS	3.7
1	A	380	GLY	3.6
1	A	69	GLU	3.6
1	A	64	ALA	3.4
1	A	407	VAL	3.2
1	A	68	ASP	3.1
1	A	209	GLU	3.1
1	A	78	VAL	3.1
1	A	377	CYS	3.0
1	A	255	LYS	3.0
1	A	401	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	361	GLY	3.0
1	A	359	GLU	3.0
1	A	107	LYS	3.0
1	A	74	PHE	2.9
1	A	49	PRO	2.9
1	A	395	LYS	2.9
1	A	362	ILE	2.9
1	A	145	GLU	2.8
1	A	285	GLU	2.7
1	A	399	PRO	2.7
1	A	393	VAL	2.7
1	A	177	LYS	2.7
1	A	299	TYR	2.7
1	A	139	GLU	2.7
1	A	63	LYS	2.6
1	A	386	LEU	2.6
1	A	79	GLU	2.6
1	A	369	TYR	2.6
1	A	290	LYS	2.6
1	A	80	LYS	2.5
1	A	400	ASP	2.5
1	A	148	VAL	2.5
1	A	183	VAL	2.5
1	A	54	TYR	2.4
1	A	397	ILE	2.4
1	A	61	LEU	2.4
1	A	76	GLU	2.4
1	A	72	LYS	2.4
1	A	231	THR	2.3
1	A	83	LYS	2.3
1	A	212	LYS	2.3
1	A	43	ARG	2.3
1	A	402	LEU	2.2
1	A	406	ARG	2.2
1	A	313	ASP	2.2
1	A	247	LYS	2.2
1	A	142	LYS	2.1
1	A	281	LEU	2.1
1	A	60	GLY	2.1
1	A	385	ALA	2.0
1	A	176	LEU	2.0
1	A	317	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	405	ARG	2.0
1	A	65	GLY	2.0
1	A	357	MET	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.