



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2020 – 02:13 PM JST

PDB ID : 6LU0  
Title : Crystal structure of Cas12i2 ternary complex with 12 nt spacer  
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Deposited on : 2020-01-24  
Resolution : 3.22 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](mailto: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.

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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	:	2.14.6
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)	:	2.14.6

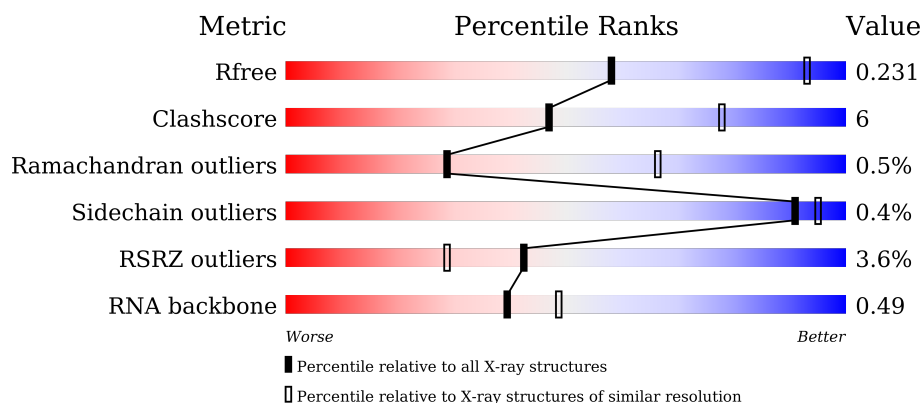
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.22 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)
RNA backbone	3102	1023 (3.54-2.90)

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  $\geq 3$ , 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	1055	<div> <div>3%</div> <div>75%</div> <div>13%</div> <div>11%</div> </div>
2	B	58	<div> <div>2%</div> <div>33%</div> <div>19%</div> <div>5%</div> <div>43%</div> </div>
3	D	11	<div> <div>55%</div> <div>27%</div> <div>9%</div> <div>9%</div> </div>
4	C	21	<div> <div>10%</div> <div>43%</div> <div>38%</div> <div>19%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8719 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 Cas12i2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	937	Total	C	N	O	S	0	0	0
			7448	4732	1320	1373	23			

- Molecule 2 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	33	Total	C	N	O	P	0	0	0
			702	316	130	224	32			

- Molecule 3 is a DNA chain called DNA (5'-D(\*GP\*CP\*CP\*GP\*CP\*TP\*TP\*TP\*CP\*TP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	10	Total	C	N	O	P	0	0	0
			197	96	30	62	9			

- Molecule 4 is a DNA chain called DNA (5'-D(\*GP\*CP\*TP\*TP\*GP\*CP\*TP\*CP\*TP\*GP\*TP\*TP\*GP\*AP\*AP\*AP\*GP\*CP\*GP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	17	Total	C	N	O	P	0	0	0
			351	166	65	103	17			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	3	Total	O	0	0
			3	3		
5	D	3	Total	O	0	0
			3	3		

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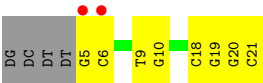
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	4	Total	O	0	0
			4	4		





● Molecule 4: DNA (5'-D(\*GP\*CP\*TP\*TP\*GP\*CP\*TP\*CP\*TP\*GP\*TP\*TP\*GP\*AP\*AP\*AP\*GP\*CP\*GP\*GP\*C)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.55Å 122.67Å 284.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.56 – 3.22 29.56 – 3.22	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.56-3.22) 97.6 (29.56-3.22)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.33 (at 3.24Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.207 , 0.231 0.207 , 0.231	Depositor DCC
$R_{free}$ test set	1339 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.6	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 30.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8719	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.29	0/7592	0.50	0/10251
2	B	0.27	0/786	0.84	1/1223 (0.1%)
3	D	0.58	0/218	1.02	1/334 (0.3%)
4	C	0.57	0/393	0.92	0/605
All	All	0.32	0/8989	0.59	2/12413 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	31	C	N1-C1'-C2'	-7.26	104.02	112.00
3	D	5	DC	O4'-C4'-C3'	-5.37	102.35	104.50

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	7448	0	7373	94	0
2	B	702	0	358	6	0
3	D	197	0	116	3	0
4	C	351	0	192	6	0
5	A	11	0	0	1	0
5	B	3	0	0	0	0
5	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	3	0	0	0	0
All	All	8719	0	8039	103	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 (103) 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:730:ARG:NH1	1:A:789:ASP:OD2	2.13	0.81
1:A:940:LEU:HD13	1:A:949:GLU:HB3	1.71	0.73
1:A:41:GLN:HE22	1:A:81:SER:HB2	1.55	0.71
1:A:323:GLU:OE1	1:A:425:GLN:NE2	2.24	0.70
4:C:5:DG:H2''	4:C:6:DC:H5''	1.74	0.69
1:A:831:ARG:HD3	1:A:875:PHE:HB2	1.77	0.67
1:A:806:LYS:NZ	2:B:11:C:OP1	2.25	0.65
1:A:82:LEU:HD22	1:A:120:TYR:HB2	1.79	0.65
1:A:945:LEU:HD11	1:A:972:LEU:HD21	1.78	0.65
1:A:831:ARG:CD	1:A:875:PHE:HB2	2.27	0.65
1:A:612:GLU:HB2	1:A:630:ILE:HD11	1.79	0.64
1:A:14:PRO:HG2	1:A:19:ASN:HB2	1.80	0.62
1:A:857:ARG:HD3	4:C:6:DC:O3'	2.00	0.61
1:A:424:GLN:O	1:A:428:ARG:HG2	2.01	0.61
1:A:994:PHE:HB3	1:A:1013:VAL:HG21	1.83	0.60
1:A:688:GLU:OE2	1:A:688:GLU:HA	2.01	0.59
1:A:831:ARG:HH12	1:A:1030:VAL:HA	1.68	0.59
1:A:56:THR:HG21	1:A:63:GLN:HB2	1.84	0.58
4:C:20:DG:H2''	4:C:21:DC:H5''	1.84	0.58
1:A:86:ILE:HD13	1:A:91:LEU:HD23	1.83	0.58
1:A:887:PRO:HG2	1:A:999:VAL:HG21	1.86	0.58
1:A:81:SER:OG	5:A:1101:HOH:O	2.17	0.58
1:A:946:GLN:O	1:A:949:GLU:HG3	2.04	0.57
1:A:666:ALA:HB1	1:A:710:TYR:CE1	2.38	0.57
1:A:458:ARG:NH2	1:A:499:TYR:O	2.36	0.57
1:A:667:SER:HA	1:A:670:VAL:HG12	1.86	0.57
1:A:472:TYR:CE2	1:A:484:LYS:HD3	2.40	0.56
1:A:68:TRP:CE2	1:A:158:ALA:HB1	2.40	0.56
1:A:924:LYS:HD3	1:A:933:HIS:ND1	2.22	0.55
1:A:70:ALA:HB2	1:A:107:ILE:HD12	1.89	0.54
1:A:639:THR:OG1	1:A:648:GLN:NE2	2.41	0.54
3:D:5:DC:H2'	3:D:6:DT:C6	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:THR:OG1	1:A:558:ASN:HB3	2.09	0.53
1:A:816:ASN:ND2	2:B:22:G:O3'	2.41	0.53
4:C:9:DT:H2''	4:C:10:DG:H5''	1.92	0.52
1:A:599:ASP:HB2	1:A:1026:ILE:HD12	1.91	0.52
1:A:816:ASN:ND2	2:B:22:G:H5''	2.23	0.52
1:A:163:GLN:HB3	1:A:166:SER:OG	2.10	0.51
1:A:165:ASN:HD21	1:A:297:ASN:HB2	1.75	0.51
1:A:853:ASP:OD1	1:A:854:TRP:N	2.43	0.51
1:A:178:GLU:HB3	3:D:8:DT:H5''	1.92	0.51
1:A:723:LEU:CD2	1:A:723:LEU:N	2.73	0.51
1:A:663:ARG:HD2	1:A:697:CYS:SG	2.51	0.51
1:A:675:ILE:HG13	1:A:689:ALA:HB2	1.93	0.51
1:A:323:GLU:CD	1:A:425:GLN:HE22	2.14	0.50
1:A:928:THR:HG1	1:A:988:ARG:HH22	1.57	0.50
1:A:900:ARG:HD3	1:A:990:GLY:O	2.12	0.50
1:A:569:ASN:ND2	1:A:573:GLN:OE1	2.37	0.50
1:A:105:ASP:O	1:A:109:GLN:HG2	2.13	0.49
1:A:67:LEU:HD21	1:A:314:ALA:HB3	1.95	0.48
1:A:761:LYS:NZ	1:A:800:GLU:OE1	2.38	0.48
2:B:33:A:H4'	2:B:33:A:OP1	2.13	0.48
1:A:471:LEU:HD13	1:A:473:LEU:HD21	1.95	0.47
1:A:217:ALA:HB2	1:A:225:VAL:HG21	1.97	0.47
1:A:831:ARG:HH12	1:A:1031:LYS:H	1.63	0.46
1:A:821:THR:O	1:A:825:ASN:ND2	2.47	0.46
1:A:143:THR:O	1:A:147:GLU:HG3	2.15	0.46
1:A:635:ILE:HG23	1:A:817:SER:HB3	1.98	0.46
1:A:735:ARG:HG2	1:A:739:GLN:HB2	1.98	0.46
3:D:7:DT:H2'	3:D:8:DT:C6	2.50	0.46
1:A:194:ILE:HD11	1:A:248:PHE:HZ	1.81	0.45
1:A:472:TYR:CD2	1:A:484:LYS:HD3	2.51	0.45
1:A:831:ARG:NH1	1:A:1031:LYS:H	2.14	0.45
1:A:780:ILE:O	1:A:780:ILE:HG13	2.17	0.45
1:A:831:ARG:HA	1:A:831:ARG:HD2	1.82	0.45
1:A:919:GLN:O	1:A:923:ALA:N	2.48	0.45
1:A:184:LEU:HG	1:A:188:LYS:HE2	1.99	0.45
1:A:12:LEU:HD23	1:A:489:PHE:HB3	1.99	0.45
1:A:718:VAL:HG22	1:A:729:ILE:HG21	1.99	0.45
1:A:502:GLY:HA2	1:A:554:LEU:HD23	2.00	0.44
1:A:730:ARG:HH12	1:A:789:ASP:CG	2.20	0.44
1:A:223:ARG:HD2	1:A:237:GLU:OE1	2.18	0.44
1:A:255:THR:HG22	1:A:259:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:CYS:HB3	1:A:157:VAL:HG21	1.98	0.44
1:A:239:PHE:O	1:A:242:LYS:HG2	2.17	0.44
1:A:761:LYS:HB3	1:A:761:LYS:HE2	1.70	0.44
1:A:496:GLN:HB2	1:A:545:ILE:HD11	1.99	0.43
1:A:757:VAL:HG11	1:A:803:ARG:HG3	2.00	0.43
1:A:656:TYR:HA	1:A:659:TYR:CE1	2.54	0.42
1:A:323:GLU:OE1	1:A:421:LYS:HD3	2.19	0.42
1:A:82:LEU:HD12	1:A:83:THR:N	2.34	0.42
1:A:833:ALA:HA	1:A:877:CYS:O	2.19	0.42
4:C:6:DC:H6	4:C:6:DC:H5''	1.85	0.42
1:A:472:TYR:HA	1:A:485:HIS:O	2.20	0.42
1:A:688:GLU:C	1:A:690:LYS:H	2.23	0.42
1:A:183:LYS:HE2	1:A:227:ALA:HA	2.00	0.41
1:A:428:ARG:HD2	2:B:32:A:OP1	2.20	0.41
1:A:32:GLY:HA2	1:A:284:THR:HG22	2.02	0.41
1:A:924:LYS:HD2	1:A:924:LYS:HA	1.90	0.41
1:A:165:ASN:ND2	1:A:297:ASN:HB2	2.36	0.41
1:A:900:ARG:HB3	1:A:932:TYR:OH	2.20	0.41
1:A:75:ARG:HD3	1:A:437:SER:OG	2.21	0.41
1:A:70:ALA:HB2	1:A:107:ILE:CD1	2.50	0.41
1:A:515:ARG:NH2	1:A:866:LEU:HD22	2.35	0.41
1:A:928:THR:OG1	1:A:988:ARG:NH2	2.34	0.41
1:A:179:ASP:OD2	1:A:182:VAL:HG23	2.20	0.41
1:A:796:LEU:HD23	1:A:796:LEU:HA	1.82	0.41
1:A:946:GLN:OE1	1:A:946:GLN:N	2.47	0.40
2:B:17:U:H4'	2:B:18:U:H5'	2.04	0.40
1:A:223:ARG:HG2	1:A:229:ASN:HA	2.03	0.40
1:A:320:GLN:O	1:A:324:ILE:HG13	2.21	0.40
4:C:18:DC:H2''	4:C:19:DG:C8	2.56	0.40
1:A:940:LEU:CD1	1:A:949:GLU:HB3	2.46	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	929/1055 (88%)	881 (95%)	43 (5%)	5 (0%)	29	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ALA
1	A	164	ASN
1	A	689	ALA
1	A	687	VAL
1	A	688	GLU

### 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	783/930 (84%)	780 (100%)	3 (0%)	91	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	THR
1	A	586	LYS
1	A	723	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	32/58 (55%)	9 (28%)	2 (6%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	G
2	B	4	A
2	B	6	U
2	B	7	C
2	B	13	U
2	B	18	U
2	B	24	A
2	B	32	A
2	B	33	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	3	A
2	B	32	A

## 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 monosaccharides 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	937/1055 (88%)	-0.05	33 (3%) 44 29	21, 59, 125, 152	0
2	B	33/58 (56%)	-0.18	1 (3%) 50 36	23, 40, 77, 128	0
3	D	10/11 (90%)	-0.61	0 100 100	27, 34, 41, 72	0
4	C	17/21 (80%)	0.04	2 (11%) 4 3	28, 33, 92, 101	0
All	All	997/1145 (87%)	-0.06	36 (3%) 42 29	21, 58, 124, 152	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	ASN	5.5
1	A	327	LEU	4.9
1	A	925	ASN	4.7
1	A	331	LEU	4.2
1	A	957	SER	4.1
1	A	418	ALA	3.9
1	A	958	ASP	3.9
1	A	851	SER	3.9
1	A	959	ARG	3.6
1	A	926	ILE	3.5
1	A	881	TYR	3.3
1	A	777	ASN	3.3
4	C	5	DG	3.2
1	A	338	ASP	3.2
1	A	852	MET	3.1
1	A	335	LYS	3.1
1	A	411	CYS	3.0
1	A	329	ASN	2.7
4	C	6	DC	2.7
1	A	912	TRP	2.6
2	B	33	A	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	105	ASP	2.6
1	A	835	ASP	2.5
1	A	928	THR	2.5
1	A	927	GLY	2.5
1	A	0	SER	2.3
1	A	337	ASN	2.3
1	A	687	VAL	2.3
1	A	965	CYS	2.2
1	A	416	ILE	2.2
1	A	962	ASN	2.2
1	A	878	GLY	2.1
1	A	419	ALA	2.1
1	A	911	ASP	2.0
1	A	776	LYS	2.0
1	A	915	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 monosaccharides 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.