



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 8, 2021 – 10:07 AM JST

PDB ID : 7CVO
Title : crystal structure of Arabidopsis CO CCT domain in complex with NF-YB3/YC4 and FT CORE2 DNA
Authors : Lv, X.; Du, J.
Deposited on : 2020-08-26
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 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	:	2.20
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)	:	2.20

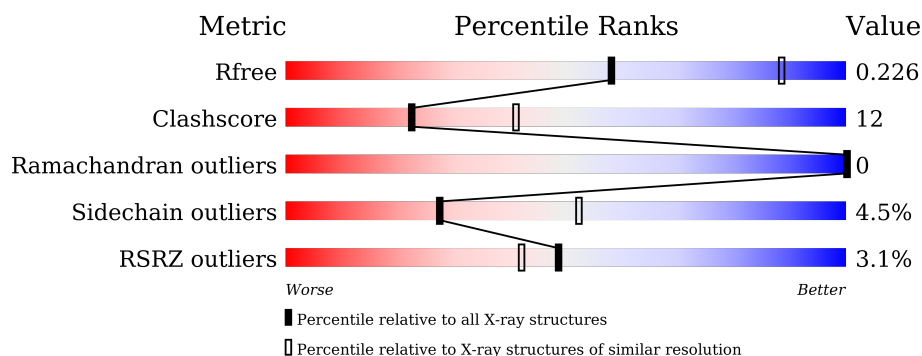
1 Overall quality at a glance

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	165	<div> <div>3%</div> <div>61%</div> <div>15%</div> <div>21%</div> </div>
1	F	165	<div> <div>2%</div> <div>41%</div> <div>16%</div> <div>41%</div> </div>
2	B	103	<div> <div>72%</div> <div>14%</div> <div>15%</div> </div>
2	G	103	<div> <div>5%</div> <div>63%</div> <div>21%</div> <div>15%</div> </div>
3	D	25	<div> <div>64%</div> <div>36%</div> </div>
4	E	25	<div> <div>68%</div> <div>32%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4376 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 Chimera of Nuclear transcription factor Y subunit C-4 and Zinc finger protein CONSTANS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	0	0
			1082	687	207	184	4			
1	F	98	Total	C	N	O	S	0	0	0
			806	513	147	142	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	278	GLY	-	linker	UNP Q9FMV5
A	279	SER	-	linker	UNP Q9FMV5
A	280	GLY	-	linker	UNP Q9FMV5
A	281	SER	-	linker	UNP Q9FMV5
A	282	GLY	-	linker	UNP Q9FMV5
A	283	SER	-	linker	UNP Q9FMV5
A	284	GLY	-	linker	UNP Q9FMV5
A	285	SER	-	linker	UNP Q9FMV5
A	286	GLY	-	linker	UNP Q9FMV5
A	287	SER	-	linker	UNP Q9FMV5
A	288	GLY	-	linker	UNP Q9FMV5
A	289	SER	-	linker	UNP Q9FMV5
F	278	GLY	-	linker	UNP Q9FMV5
F	279	SER	-	linker	UNP Q9FMV5
F	280	GLY	-	linker	UNP Q9FMV5
F	281	SER	-	linker	UNP Q9FMV5
F	282	GLY	-	linker	UNP Q9FMV5
F	283	SER	-	linker	UNP Q9FMV5
F	284	GLY	-	linker	UNP Q9FMV5
F	285	SER	-	linker	UNP Q9FMV5
F	286	GLY	-	linker	UNP Q9FMV5
F	287	SER	-	linker	UNP Q9FMV5
F	288	GLY	-	linker	UNP Q9FMV5
F	289	SER	-	linker	UNP Q9FMV5

- Molecule 2 is a protein called Nuclear transcription factor Y subunit B-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	88	Total	C	N	O	S	0	0	0
			710	451	120	135	4			
2	G	88	Total	C	N	O	S	0	0	0
			710	451	120	135	4			

- Molecule 3 is a DNA chain called FT CORE2 DNA forward strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	25	Total	C	N	O	P	0	0	0
			515	248	94	149	24			

- Molecule 4 is a DNA chain called FT CORE2 DNA reverse strand.

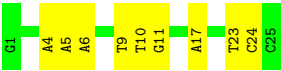
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	25	Total	C	N	O	P	0	0	0
			504	244	89	147	24			

- Molecule 5 is water.

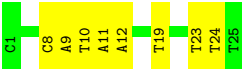
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total	O	0	0
			16	16		
5	B	3	Total	O	0	0
			3	3		
5	D	9	Total	O	0	0
			9	9		
5	E	5	Total	O	0	0
			5	5		
5	F	13	Total	O	0	0
			13	13		
5	G	3	Total	O	0	0
			3	3		

THR
THR
ALA
GLY

- Molecule 3: FT CORE2 DNA forward strand



- Molecule 4: FT CORE2 DNA reverse strand



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.74Å 139.94Å 65.57Å 90.00° 108.38° 90.00°	Depositor
Resolution (Å)	48.02 – 2.60 48.70 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.02-2.60) 99.1 (48.70-2.59)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.196 , 0.221 0.210 , 0.226	Depositor DCC
R_{free} test set	1467 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4376	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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	0.83	0/1098	0.69	0/1470
1	F	0.61	0/816	0.73	0/1095
2	B	0.82	0/721	0.68	0/968
2	G	0.50	0/721	0.59	0/968
3	D	0.79	0/578	0.93	0/892
4	E	0.96	0/564	0.91	0/867
All	All	0.76	0/4498	0.75	0/6260

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 [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	1082	0	1144	33	0
1	F	806	0	851	30	0
2	B	710	0	722	14	0
2	G	710	0	722	28	0
3	D	515	0	286	9	0
4	E	504	0	285	6	0
5	A	16	0	0	2	0
5	B	3	0	0	3	0
5	D	9	0	0	0	0
5	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	13	0	0	1	0
5	G	3	0	0	0	0
All	All	4376	0	4010	96	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 12.

All (96) 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:304:MET:HG2	2:G:37:LYS:CG	1.74	1.18
1:A:304:MET:CG	2:G:37:LYS:HG3	1.89	1.01
1:A:304:MET:HG2	2:G:37:LYS:HG3	0.93	0.92
1:A:89:LYS:HB3	1:A:327:ARG:NH2	1.86	0.89
1:A:301:LEU:HG	1:A:305:ASP:HB3	1.58	0.86
1:F:300:GLN:HG3	1:F:301:LEU:H	1.48	0.78
1:F:104:LEU:O	1:F:104:LEU:HD13	1.86	0.76
1:A:314:ARG:NH1	2:G:96:ASP:O	2.20	0.75
1:A:78:GLN:O	1:A:78:GLN:NE2	2.21	0.72
1:A:94:VAL:O	1:A:327:ARG:NH1	2.23	0.71
2:B:105:LEU:HB3	5:B:203:HOH:O	1.90	0.71
1:A:78:GLN:HG3	2:B:34:ILE:HD11	1.73	0.70
1:A:309:ARG:HD3	2:B:67:GLU:OE2	1.92	0.70
1:A:153:ILE:HD11	2:B:59:GLU:HG3	1.74	0.69
1:A:309:ARG:NH1	2:B:67:GLU:OE2	2.25	0.68
1:A:89:LYS:HB3	1:A:327:ARG:HH21	1.59	0.68
2:G:44:LYS:HE3	2:G:45:ILE:H	1.60	0.66
3:D:9:DT:H2''	3:D:10:DT:OP2	1.95	0.65
1:F:300:GLN:HG3	1:F:301:LEU:N	2.11	0.65
1:F:153:ILE:HD11	2:G:59:GLU:HG3	1.78	0.65
4:E:10:DT:H4'	4:E:11:DA:OP1	1.94	0.64
1:A:304:MET:HG2	2:G:37:LYS:CB	2.27	0.64
1:A:341:VAL:HG23	1:A:346:ALA:HB2	1.80	0.64
1:F:316:LYS:NZ	1:F:317:ARG:HH21	1.97	0.62
1:F:301:LEU:HG	1:F:305:ASP:HB3	1.80	0.62
2:G:67:GLU:HG3	2:G:92:LEU:HD11	1.82	0.62
1:F:309:ARG:NH1	5:F:502:HOH:O	2.34	0.60
2:G:87:TRP:O	2:G:91:THR:HG23	2.02	0.59
1:F:129:ARG:NH2	1:F:136:ASP:OD2	2.36	0.59
4:E:23:DT:H2''	4:E:24:DT:OP2	2.02	0.59
2:G:53:VAL:O	2:G:57:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:5:DA:H2''	3:D:6:DA:OP2	2.04	0.57
2:B:98:VAL:HG12	2:B:102:LYS:HE2	1.87	0.57
1:F:94:VAL:O	1:F:95:ARG:HB2	2.03	0.56
2:B:106:GLN:HB3	5:B:203:HOH:O	2.05	0.56
3:D:10:DT:H2''	3:D:11:DG:C8	2.41	0.56
3:D:9:DT:H2''	3:D:10:DT:H72	1.86	0.55
2:G:85:LEU:O	2:G:89:MET:HG3	2.06	0.54
1:F:119:ARG:HD3	1:F:144:THR:HG21	1.90	0.54
1:A:340:ARG:HA	1:A:344:ARG:O	2.08	0.54
1:A:104:LEU:HD13	2:B:105:LEU:HD13	1.90	0.54
1:F:137:ILE:HD13	2:G:53:VAL:HG23	1.91	0.53
1:A:304:MET:CG	2:G:37:LYS:CB	2.87	0.53
1:F:104:LEU:HD11	2:G:101:LEU:HD13	1.89	0.53
1:F:316:LYS:HZ2	1:F:317:ARG:HH21	1.57	0.52
1:A:89:LYS:O	1:A:327:ARG:NH2	2.39	0.52
3:D:23:DT:H2''	3:D:24:DC:H5''	1.91	0.51
1:F:300:GLN:CG	1:F:301:LEU:N	2.73	0.51
3:D:4:DA:H2''	3:D:5:DA:OP2	2.11	0.50
1:F:104:LEU:HD13	1:F:104:LEU:C	2.31	0.50
1:A:328:TYR:HB2	1:A:331:ARG:HD2	1.94	0.48
1:A:301:LEU:HD21	1:A:309:ARG:NE	2.28	0.48
1:A:307:GLU:OE1	1:F:110:GLU:OE2	2.31	0.48
2:B:53:VAL:O	2:B:57:VAL:HG23	2.13	0.48
1:A:143:ARG:HD3	5:A:501:HOH:O	2.13	0.48
1:F:98:SER:HB3	2:G:81:ASN:HA	1.95	0.47
1:A:304:MET:CG	2:G:37:LYS:CG	2.66	0.47
1:F:313:TYR:OH	2:G:59:GLU:OE2	2.33	0.47
1:A:299:THR:HG22	1:A:300:GLN:N	2.29	0.47
1:F:79:LEU:HD23	2:G:30:ASN:HB3	1.97	0.47
1:F:101:ALA:HB3	1:F:102:PRO:HD3	1.97	0.47
2:G:37:LYS:HD3	2:G:37:LYS:HA	1.65	0.46
1:A:101:ALA:HB3	1:A:102:PRO:HD3	1.97	0.46
1:A:306:ARG:NH1	5:A:503:HOH:O	2.38	0.46
2:B:105:LEU:HA	2:B:105:LEU:HD12	1.81	0.46
1:A:107:LYS:HA	1:A:107:LYS:HD3	1.74	0.45
2:G:23:ASP:N	2:G:23:ASP:OD1	2.49	0.45
2:G:67:GLU:CG	2:G:92:LEU:HD11	2.47	0.45
3:D:10:DT:H2''	3:D:11:DG:N7	2.32	0.45
1:F:152:ASP:OD2	1:F:314:ARG:HD2	2.17	0.44
4:E:10:DT:O3'	4:E:11:DA:C8	2.70	0.44
1:A:328:TYR:CD2	4:E:19:DT:H5''	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:GLN:N	5:B:203:HOH:O	2.51	0.43
3:D:17:DA:C8	3:D:17:DA:OP2	2.70	0.43
1:F:300:GLN:HE21	1:F:300:GLN:HB2	1.61	0.43
3:D:17:DA:OP2	3:D:17:DA:H8	2.01	0.43
1:F:309:ARG:HD3	2:G:67:GLU:OE1	2.18	0.43
1:A:304:MET:HG3	2:G:37:LYS:HB3	2.00	0.42
1:A:304:MET:HE2	1:A:304:MET:HB2	1.95	0.42
4:E:11:DA:H2''	4:E:12:DA:OP2	2.19	0.42
1:F:120:SER:OG	1:F:137:ILE:HA	2.19	0.42
2:G:87:TRP:CZ2	2:G:91:THR:HG21	2.54	0.42
1:F:128:LYS:HE2	1:F:128:LYS:HB2	1.93	0.42
1:A:311:LEU:O	1:A:315:GLU:HG3	2.20	0.42
2:B:24:ARG:H	2:B:24:ARG:HG2	1.68	0.42
1:F:302:SER:O	1:F:303:PRO:C	2.56	0.42
2:G:47:LYS:HD3	2:G:47:LYS:HA	1.75	0.41
1:F:317:ARG:NE	1:F:317:ARG:HA	2.35	0.41
1:F:312:ARG:HH21	1:F:312:ARG:HG2	1.86	0.41
2:B:99:GLU:OE2	2:B:102:LYS:HE3	2.21	0.41
4:E:8:DC:H2''	4:E:9:DA:C8	2.56	0.41
1:F:104:LEU:C	1:F:104:LEU:CD1	2.88	0.41
2:G:44:LYS:HD2	2:G:44:LYS:HA	1.82	0.41
1:F:146:ILE:HD12	2:G:94:PHE:CE1	2.56	0.40
1:A:104:LEU:HD23	2:B:85:LEU:HD12	2.02	0.40
2:G:71:LYS:HA	2:G:74:ARG:NH2	2.37	0.40

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	126/165 (76%)	123 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	94/165 (57%)	89 (95%)	5 (5%)	0	100	100
2	B	86/103 (84%)	85 (99%)	1 (1%)	0	100	100
2	G	86/103 (84%)	83 (96%)	3 (4%)	0	100	100
All	All	392/536 (73%)	380 (97%)	12 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	114/140 (81%)	108 (95%)	6 (5%)	22	45
1	F	87/140 (62%)	82 (94%)	5 (6%)	20	41
2	B	78/90 (87%)	76 (97%)	2 (3%)	46	72
2	G	78/90 (87%)	75 (96%)	3 (4%)	33	59
All	All	357/460 (78%)	341 (96%)	16 (4%)	27	52

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LYS
1	A	105	PHE
1	A	107	LYS
1	A	301	LEU
1	A	304	MET
1	A	305	ASP
2	B	23	ASP
2	B	42	ASN
1	F	98	SER
1	F	104	LEU
1	F	105	PHE
1	F	301	LEU
1	F	302	SER

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Mol	Chain	Res	Type
2	G	24	ARG
2	G	42	ASN
2	G	44	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	GLN
1	F	300	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 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 [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	130/165 (78%)	0.46	5 (3%) 40 33	31, 51, 86, 109	0
1	F	98/165 (59%)	0.36	4 (4%) 37 30	34, 57, 87, 111	0
2	B	88/103 (85%)	0.19	0 100 100	32, 47, 79, 101	0
2	G	88/103 (85%)	0.36	5 (5%) 23 18	35, 56, 96, 112	0
3	D	25/25 (100%)	0.49	0 100 100	47, 56, 76, 85	0
4	E	25/25 (100%)	0.56	0 100 100	49, 60, 77, 80	0
All	All	454/586 (77%)	0.38	14 (3%) 49 42	31, 54, 87, 112	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	94	VAL	4.7
1	A	337	ILE	3.6
2	G	77	ARG	3.6
2	G	78	LYS	3.5
2	G	110	GLU	3.4
1	F	95	ARG	2.9
1	A	334	TYR	2.7
1	A	156	ARG	2.7
1	F	92	GLU	2.5
1	A	335	ALA	2.4
1	F	93	ASP	2.4
2	G	76	LYS	2.3
1	A	336	GLU	2.1
2	G	80	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.