



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:53 AM UTC

PDB ID : 6DB9 / pdb_00006db9
Title : Structural basis for promiscuous binding and activation of fluorogenic dyes by DIR2s RNA aptamer
Authors : Shao, Y.; Shelke, S.A.; Laski, A.; Piccirilli, J.A.
Deposited on : 2018-05-02
Resolution : 2.02 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

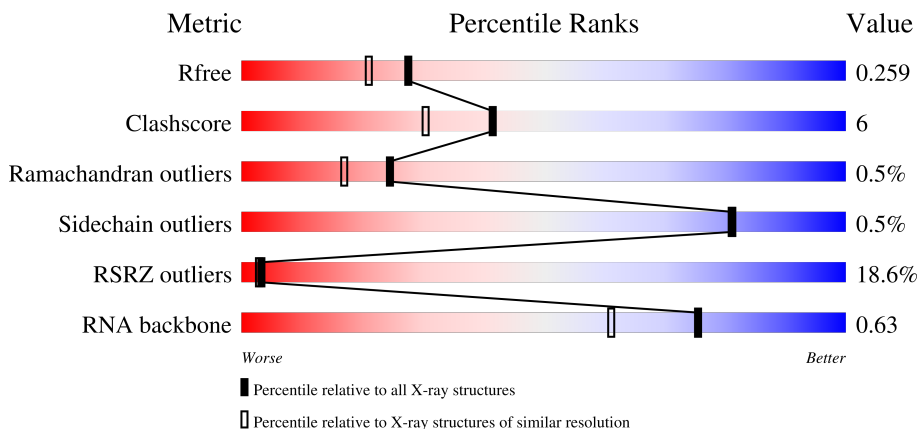
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)
RNA backbone	3983	1000 (2.38-1.66)

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	R	60	2% 80% 13% 7%
2	H	232	11% 85% 9% 6%
3	L	214	30% 81% 16% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4682 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 RNA chain called RNA (60-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	60	Total	C	N	O	P	0	0	0
			1286	574	238	414	60			

- Molecule 2 is a protein called Fab-Heavy-Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1638	1033	280	320	5			

- Molecule 3 is a protein called Fab-Light-Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	209	Total	C	N	O	S	0	0	0
			1601	999	268	329	5			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	R	2	Total	Mg	0	0
			2	2		

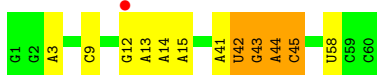
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	R	57	Total	O	0	0
			57	57		
5	H	77	Total	O	0	0
			77	77		
5	L	21	Total	O	0	0
			21	21		

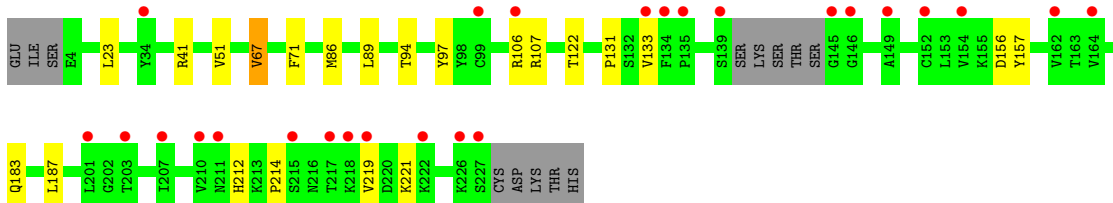
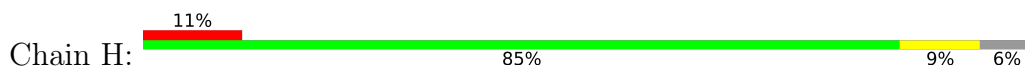
3 Residue-property plots [i](#)

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.

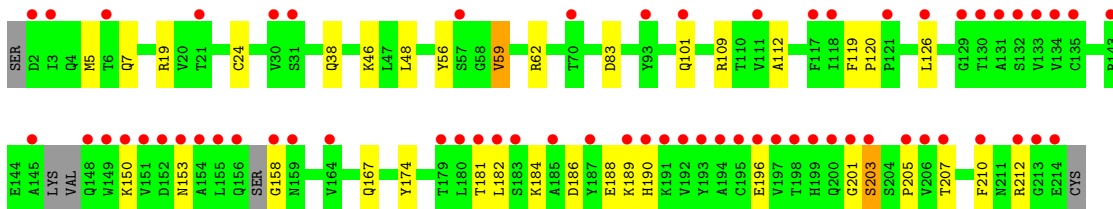
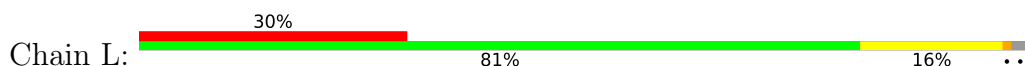
- Molecule 1: RNA (60-MER)



- Molecule 2: Fab-Heavy-Chain



- Molecule 3: Fab-Light-Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.78Å 83.81Å 109.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.64 – 2.02 66.64 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.0 (66.64-2.02) 91.6 (66.64-2.03)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.82 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.230 , 0.257 0.233 , 0.259	Depositor DCC
R_{free} test set	2002 reflections (3.96%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4682	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	R	0.15	0/1439	0.38	0/2242
2	H	0.17	0/1678	0.43	0/2283
3	L	0.17	0/1634	0.46	0/2215
All	All	0.16	0/4751	0.42	0/6740

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	R	1286	0	651	8	0
2	H	1638	0	1597	17	0
3	L	1601	0	1542	30	0
4	R	2	0	0	0	0
5	H	77	0	0	1	0
5	L	21	0	0	1	0
5	R	57	0	0	0	0
All	All	4682	0	3790	53	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 (53) 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)
3:L:7:GLN:H	3:L:101:GLN:NE2	1.72	0.86
3:L:101:GLN:H	3:L:101:GLN:CD	1.88	0.81
3:L:181:THR:O	3:L:182:LEU:HD13	1.89	0.72
3:L:7:GLN:H	3:L:101:GLN:HE22	1.39	0.71
3:L:7:GLN:HB3	3:L:101:GLN:HE21	1.58	0.69
3:L:150:LYS:HE2	3:L:153:ASN:HA	1.75	0.69
3:L:196:GLU:HG3	3:L:207:THR:HG22	1.79	0.63
3:L:7:GLN:N	3:L:101:GLN:NE2	2.47	0.62
1:R:3:A:H61	1:R:58:U:H3	1.47	0.61
1:R:9:C:O2'	2:H:106:ARG:NH2	2.34	0.60
2:H:107:ARG:NH2	3:L:56:TYR:OH	2.35	0.59
3:L:101:GLN:CD	3:L:101:GLN:N	2.60	0.58
2:H:86:MET:HB3	2:H:89:LEU:HD21	1.86	0.58
2:H:41:ARG:HG3	2:H:51:VAL:HG21	1.86	0.58
2:H:131:PRO:HB3	2:H:157:TYR:HB3	1.87	0.57
3:L:7:GLN:HB3	3:L:101:GLN:NE2	2.19	0.57
3:L:186:ASP:HA	3:L:189:LYS:HD3	1.87	0.56
3:L:7:GLN:N	3:L:101:GLN:HE22	2.01	0.55
2:H:67:VAL:HG13	2:H:71:PHE:HB2	1.89	0.54
3:L:46:LYS:NZ	5:L:301:HOH:O	2.39	0.53
2:H:183:GLN:HG2	2:H:187:LEU:O	2.09	0.53
1:R:12:G:H2'	1:R:13:A:H2'	1.92	0.51
3:L:101:GLN:NE2	3:L:101:GLN:H	2.10	0.50
2:H:133:VAL:HG11	2:H:219:VAL:HG11	1.93	0.50
3:L:126:LEU:O	3:L:184:LYS:HD3	2.11	0.49
1:R:42:U:O2'	1:R:43:G:OP1	2.29	0.49
3:L:201:GLY:O	3:L:203:SER:HB2	2.12	0.49
3:L:189:LYS:C	3:L:190:HIS:HD2	2.22	0.48
1:R:13:A:H62	1:R:42:U:H2'	1.78	0.47
1:R:13:A:N6	1:R:42:U:H2'	2.29	0.47
3:L:158:GLY:N	3:L:182:LEU:HD11	2.29	0.47
2:H:106:ARG:HG2	2:H:106:ARG:HH11	1.80	0.47
3:L:56:TYR:O	3:L:59:VAL:HG13	2.15	0.47
2:H:156:ASP:OD2	2:H:183:GLN:NE2	2.48	0.47
2:H:23:LEU:HG	2:H:86:MET:HE2	1.97	0.47
3:L:5:MET:HE3	3:L:24:CYS:SG	2.55	0.47
2:H:221:LYS:HB2	2:H:221:LYS:HE2	1.78	0.45
2:H:94:THR:HG23	2:H:122:THR:HA	1.98	0.45
2:H:212:HIS:CE1	2:H:214:PRO:HB2	2.52	0.45
1:R:43:G:O3'	1:R:44:A:H3'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:19:ARG:HE	3:L:19:ARG:HB2	1.54	0.44
2:H:106:ARG:HG2	2:H:106:ARG:NH1	2.34	0.43
3:L:184:LYS:O	3:L:188:GLU:HG3	2.19	0.43
3:L:38:GLN:HB2	3:L:48:LEU:HD11	2.01	0.42
3:L:120:PRO:HB3	3:L:210:PHE:CE1	2.53	0.42
3:L:62:ARG:HH21	3:L:83:ASP:CG	2.28	0.42
3:L:167:GLN:HG3	3:L:174:TYR:CZ	2.54	0.42
2:H:41:ARG:HD3	2:H:97:TYR:CZ	2.56	0.41
1:R:44:A:H4'	1:R:45:C:H5'	2.02	0.41
3:L:119:PHE:HA	3:L:120:PRO:HD3	1.96	0.41
3:L:212:ARG:O	3:L:212:ARG:HG2	2.21	0.41
3:L:109:ARG:HH12	3:L:112:ALA:HB2	1.86	0.41
2:H:122:THR:HG21	5:H:355:HOH:O	2.20	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	
2	H	215/232 (93%)	207 (96%)	8 (4%)	0	100	100
3	L	203/214 (95%)	186 (92%)	15 (7%)	2 (1%)	12	5
All	All	418/446 (94%)	393 (94%)	23 (6%)	2 (0%)	24	17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	203	SER
3	L	205	PRO

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	
2	H	180/193 (93%)	179 (99%)	1 (1%)	78	79
3	L	184/189 (97%)	183 (100%)	1 (0%)	81	81
All	All	364/382 (95%)	362 (100%)	2 (0%)	81	81

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	67	VAL
3	L	59	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	85	GLN
3	L	101	GLN
3	L	200	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	59/60 (98%)	6 (10%)	1 (1%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	14	A
1	R	15	A
1	R	41	A
1	R	43	G
1	R	44	A
1	R	45	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	42	U

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	R	60/60 (100%)	-0.13	1 (1%) 69 69	47, 63, 76, 83	0
2	H	219/232 (94%)	0.87	26 (11%) 9 8	41, 57, 77, 107	0
3	L	209/214 (97%)	1.63	64 (30%) 1 1	42, 65, 101, 111	0
All	All	488/506 (96%)	1.07	91 (18%) 3 3	41, 61, 94, 111	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	154	ALA	6.4
3	L	151	VAL	5.9
3	L	192	VAL	5.7
3	L	155	LEU	5.7
3	L	201	GLY	5.3
2	H	219	VAL	4.3
3	L	197	VAL	4.3
3	L	213	GLY	4.2
3	L	191	LYS	4.2
3	L	156	GLN	4.2
3	L	190	HIS	4.2
3	L	148	GLN	4.2
2	H	226	LYS	4.0
3	L	31	SER	4.0
2	H	145	GLY	3.9
3	L	6	THR	3.8
3	L	145	ALA	3.8
3	L	132	SER	3.7
2	H	227	SER	3.7
3	L	203	SER	3.7
3	L	126	LEU	3.7
3	L	206	VAL	3.6
3	L	182	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
3	L	212	ARG	3.6
3	L	149	TRP	3.6
3	L	207	THR	3.5
3	L	158	GLY	3.5
3	L	198	THR	3.5
3	L	210	PHE	3.4
2	H	139	SER	3.3
3	L	152	ASP	3.3
3	L	150	LYS	3.3
3	L	187	TYR	3.1
3	L	2	ASP	3.1
3	L	133	VAL	3.1
2	H	211	ASN	3.1
3	L	194	ALA	3.1
2	H	222	LYS	3.0
3	L	153	ASN	3.0
3	L	214	GLU	3.0
3	L	143	ARG	2.9
3	L	21	THR	2.9
2	H	106	ARG	2.9
3	L	193	TYR	2.9
2	H	217	THR	2.8
3	L	195	CYS	2.8
3	L	205	PRO	2.8
3	L	180	LEU	2.8
3	L	111	VAL	2.8
3	L	164	VAL	2.8
2	H	203	THR	2.8
2	H	218	LYS	2.7
3	L	129	GLY	2.7
2	H	152	CYS	2.7
3	L	130	THR	2.6
3	L	181	THR	2.6
3	L	117	PHE	2.6
3	L	101	GLN	2.6
2	H	201	LEU	2.6
3	L	135	CYS	2.5
3	L	179	THR	2.5
2	H	162	VAL	2.5
2	H	207	ILE	2.5
2	H	135	PRO	2.5
1	R	12	G	2.5

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Mol	Chain	Res	Type	RSRZ
3	L	70	THR	2.4
3	L	183	SER	2.4
2	H	133	VAL	2.4
3	L	131	ALA	2.4
3	L	189	LYS	2.4
3	L	196	GLU	2.4
3	L	30	VAL	2.4
2	H	134	PHE	2.4
3	L	57	SER	2.4
3	L	200	GLN	2.3
3	L	93	TYR	2.3
2	H	146	GLY	2.3
3	L	134	VAL	2.3
3	L	118	ILE	2.2
2	H	149	ALA	2.2
2	H	99	CYS	2.2
2	H	210	VAL	2.2
2	H	164	VAL	2.1
3	L	159	ASN	2.1
3	L	121	PRO	2.1
3	L	3	ILE	2.1
2	H	154	VAL	2.1
2	H	215	SER	2.1
3	L	185	ALA	2.1
3	L	199	HIS	2.0
2	H	34	TYR	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	R	102	1/1	0.99	0.03	53,53,53,53	0
4	MG	R	101	1/1	1.00	0.02	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.