



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:31 AM GMT

PDB ID : 3EZ9
Title : Partition Protein
Authors : Schumacher, M.A.
Deposited on : 2008-10-22
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

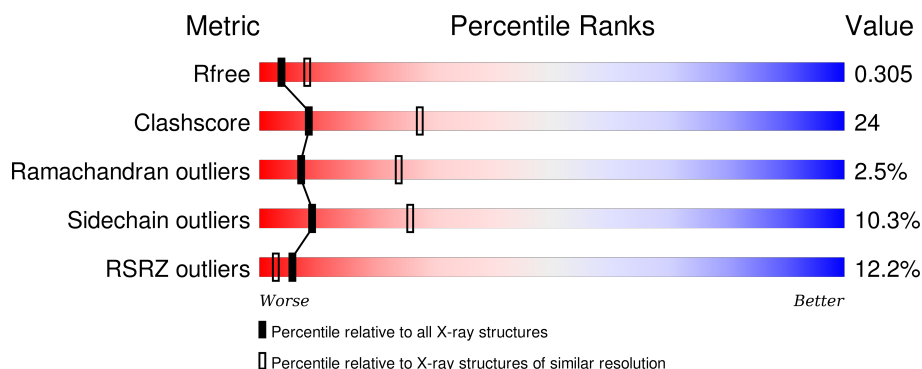
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	403	<div> <div>5%</div> <div>46%</div> <div>35%</div> <div>• •</div> <div>13%</div> </div>
1	B	403	<div> <div>16%</div> <div>45%</div> <div>35%</div> <div>6% •</div> <div>13%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	402	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5670 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 ParA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2802	1772	491	532	7			
1	B	350	Total	C	N	O	S	0	0	0
			2792	1763	491	531	7			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP B4ABW6
A	0	MET	-	EXPRESSION TAG	UNP B4ABW6
A	21	ALA	SER	CONFLICT	UNP B4ABW6
A	28	ASP	GLU	CONFLICT	UNP B4ABW6
A	35	GLN	LEU	CONFLICT	UNP B4ABW6
A	59	ASP	GLU	CONFLICT	UNP B4ABW6
A	67	GLU	ASP	CONFLICT	UNP B4ABW6
A	68	ASP	GLY	CONFLICT	UNP B4ABW6
A	71	GLN	GLU	CONFLICT	UNP B4ABW6
A	182	ASN	ASP	CONFLICT	UNP B4ABW6
A	198	VAL	ILE	CONFLICT	UNP B4ABW6
A	218	ARG	GLU	CONFLICT	UNP B4ABW6
A	219	GLU	ASP	CONFLICT	UNP B4ABW6
A	222	GLU	LYS	CONFLICT	UNP B4ABW6
A	228	GLN	MET	CONFLICT	UNP B4ABW6
A	229	ASN	LYS	CONFLICT	UNP B4ABW6
A	230	GLN	PRO	CONFLICT	UNP B4ABW6
A	231	TYR	SER	CONFLICT	UNP B4ABW6
A	233	ILE	VAL	CONFLICT	UNP B4ABW6
A	236	ARG	LYS	CONFLICT	UNP B4ABW6
A	237	ASN	LYS	CONFLICT	UNP B4ABW6
A	240	ASP	GLU	CONFLICT	UNP B4ABW6
A	360	VAL	ILE	CONFLICT	UNP B4ABW6
A	380	THR	ASN	CONFLICT	UNP B4ABW6
B	-1	MET	-	EXPRESSION TAG	UNP B4ABW6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	EXPRESSION TAG	UNP B4ABW6
B	21	ALA	SER	CONFLICT	UNP B4ABW6
B	28	ASP	GLU	CONFLICT	UNP B4ABW6
B	35	GLN	LEU	CONFLICT	UNP B4ABW6
B	59	ASP	GLU	CONFLICT	UNP B4ABW6
B	67	GLU	ASP	CONFLICT	UNP B4ABW6
B	68	ASP	GLY	CONFLICT	UNP B4ABW6
B	71	GLN	GLU	CONFLICT	UNP B4ABW6
B	182	ASN	ASP	CONFLICT	UNP B4ABW6
B	198	VAL	ILE	CONFLICT	UNP B4ABW6
B	218	ARG	GLU	CONFLICT	UNP B4ABW6
B	219	GLU	ASP	CONFLICT	UNP B4ABW6
B	222	GLU	LYS	CONFLICT	UNP B4ABW6
B	228	GLN	MET	CONFLICT	UNP B4ABW6
B	229	ASN	LYS	CONFLICT	UNP B4ABW6
B	230	GLN	PRO	CONFLICT	UNP B4ABW6
B	231	TYR	SER	CONFLICT	UNP B4ABW6
B	233	ILE	VAL	CONFLICT	UNP B4ABW6
B	236	ARG	LYS	CONFLICT	UNP B4ABW6
B	237	ASN	LYS	CONFLICT	UNP B4ABW6
B	240	ASP	GLU	CONFLICT	UNP B4ABW6
B	360	VAL	ILE	CONFLICT	UNP B4ABW6
B	380	THR	ASN	CONFLICT	UNP B4ABW6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0

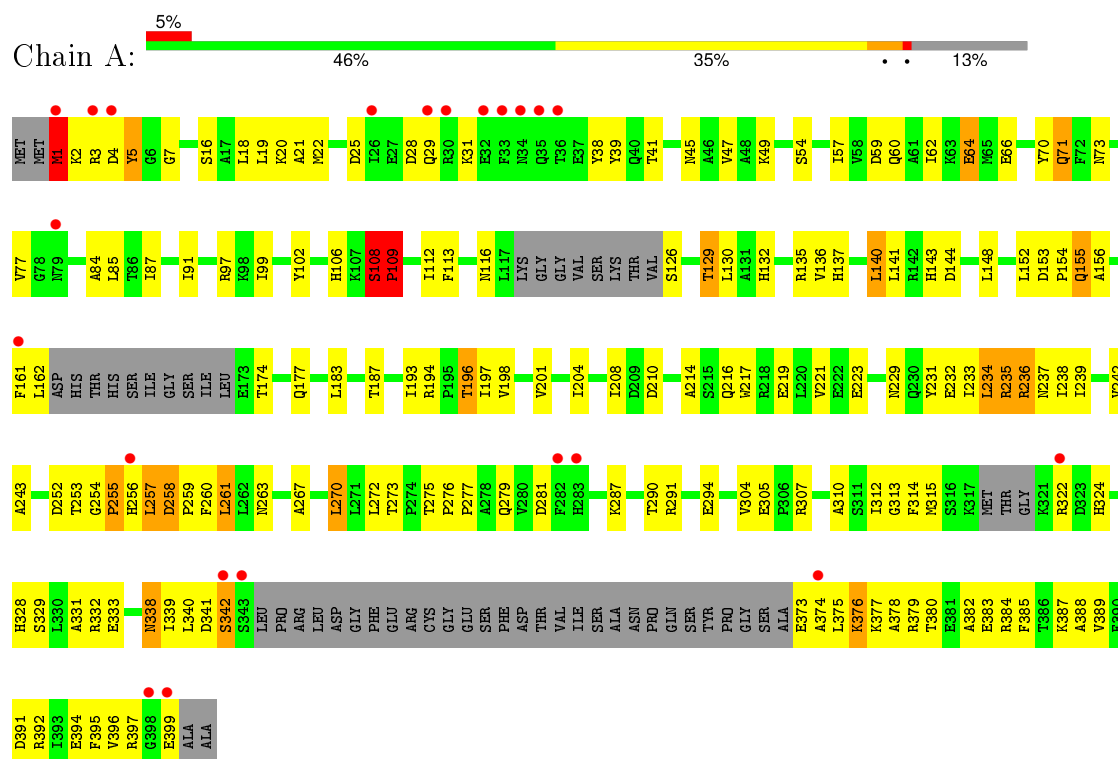
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	44	Total O 44 44	0	0
3	B	31	Total O 31 31	0	0

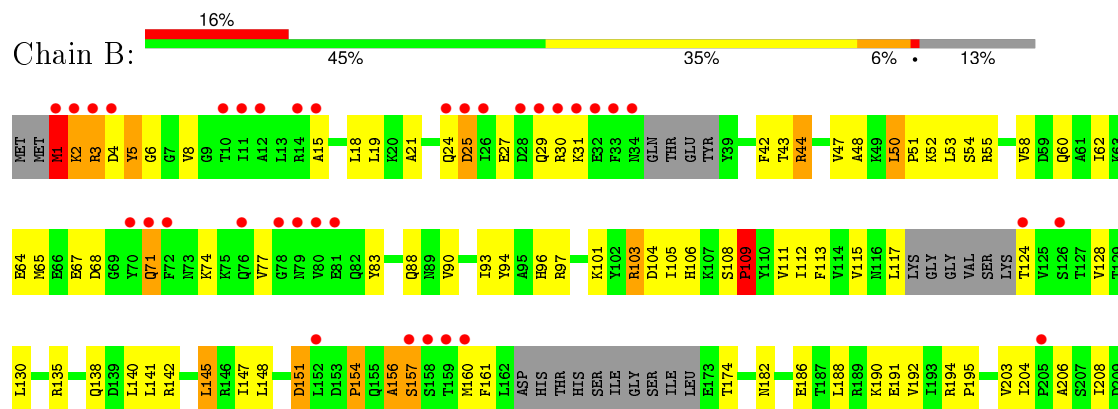
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: ParA



• Molecule 1: ParA



PHE	ASP	THR	VAL	ILE	SER	ALA	ASN	PRO	GLN	SER	TYR	PRO	GLY	SER	A372	L375	K376	K377	A378	R379	T380	E381	R384	F385	R392	I393	E394	R397	G398	E399	ALA	ALA																											
D281	F282	H283	S284	T285		L289	T290	R291	L292	P293	E294	W295		E302	R307		I312	G313	F314	N315	S316	K317	MET	THR	GLY	K321	R322	D323		S327		L330	A331	R332	F333	V334	Y335	A336	S337	N338	I339	L340	D341	S342	S343	L344	P345	ARG	LEU	ASP	GLY	PHE	GLU	ARG	CYS	GLY	GLU	SER	
D210		A214	S215	Q216	W217	R218	E219	L220	V221	E222		L225		Q228	N229	Q230	Y231	E232	I233	L234	R235	R236	N237	L238	I239	D240	R241	V242	A243		Y246		I251	D252	T253	G254	P255	H256	L257	D258	P259		L262	N263		A267	S268	D269	L270	L271	L272	T273	P274	T275	T276	P277	A278	Q279	V280

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	55.95Å 267.41Å 154.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.85 – 2.80 66.85 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.3 (66.85-2.80) 99.3 (66.85-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.65Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.254 , 0.294 0.267 , 0.305	Depositor DCC
R_{free} test set	2015 reflections (6.95%)	DCC
Wilson B-factor (Å ²)	72.3	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 33374 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5670	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	A	0.62	2/2850 (0.1%)	0.94	11/3853 (0.3%)
1	B	0.47	1/2838 (0.0%)	0.82	4/3837 (0.1%)
All	All	0.55	3/5688 (0.1%)	0.88	15/7690 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	GLN	CB-CG	-12.98	1.17	1.52
1	B	1	MET	N-CA	6.89	1.60	1.46
1	A	109	PRO	N-CA	6.31	1.57	1.47

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	PRO	CA-N-CD	-24.64	77.00	111.50
1	A	109	PRO	CA-N-CD	-23.71	78.30	111.50
1	A	108	SER	C-N-CD	-8.96	100.89	120.60
1	A	109	PRO	N-CA-CB	8.45	113.44	103.30
1	A	1	MET	N-CA-C	8.09	132.84	111.00

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	2802	0	2798	131	1
1	B	2792	0	2791	139	0
2	A	1	0	0	0	0
3	A	44	0	0	1	0
3	B	31	0	0	3	0
All	All	5670	0	5589	270	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 24.

The worst 5 of 270 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:B:279:GLN:HA	1:B:282:PHE:HB3	1.46	0.97
1:B:182:ASN:OD1	1:B:241:ARG:NH2	1.99	0.95
1:B:335:TYR:HB2	1:B:339:ILE:HG12	1.52	0.92
1:A:47:VAL:HG21	1:A:85:LEU:HD12	1.53	0.90
1:A:236:ARG:HE	1:A:237:ASN:HD21	1.19	0.89

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:60:GLN:CG	1:A:399:GLU:OE2[8_565]	1.69	0.51

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	339/403 (84%)	303 (89%)	30 (9%)	6 (2%)	11	34
1	B	338/403 (84%)	293 (87%)	34 (10%)	11 (3%)	5	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	677/806 (84%)	596 (88%)	64 (10%)	17 (2%)	7	24

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	PRO
1	B	109	PRO
1	B	161	PHE
1	A	342	SER
1	A	376	LYS

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	305/350 (87%)	272 (89%)	33 (11%)	8	23
1	B	304/350 (87%)	274 (90%)	30 (10%)	10	28
All	All	609/700 (87%)	546 (90%)	63 (10%)	9	26

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	GLU
1	B	25	ASP
1	B	375	LEU
1	A	333	GLU
1	A	376	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	GLN
1	A	298	GLN
1	B	228	GLN

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Mol	Chain	Res	Type
1	A	230	GLN
1	A	237	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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 ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	349/403 (86%)	0.30	22 (6%) 23 14	33, 65, 148, 167	0
1	B	350/403 (86%)	0.86	63 (18%) 2 1	45, 89, 163, 179	0
All	All	699/806 (86%)	0.58	85 (12%) 5 3	33, 76, 159, 179	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	343	SER	9.7
1	B	342	SER	9.5
1	B	3	ARG	9.2
1	B	334	VAL	8.9
1	B	315	MET	8.8

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	A	402	1/1	0.71	0.53	14.06	33,33,33,33	1

6.5 Other polymers ⓘ

There are no such residues in this entry.