



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:04 AM GMT

PDB ID : 3NZP
Title : Crystal Structure of the Biosynthetic Arginine decarboxylase SpeA from *Campylobacter jejuni*, Northeast Structural Genomics Consortium Target BR53
Authors : Forouhar, F.; Lew, S.; Seetharaman, J.; Sahdev, S.; Xiao, R.; Ciccocanti, C.; Belote, R.L.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2010-07-16
Resolution : 3.00 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

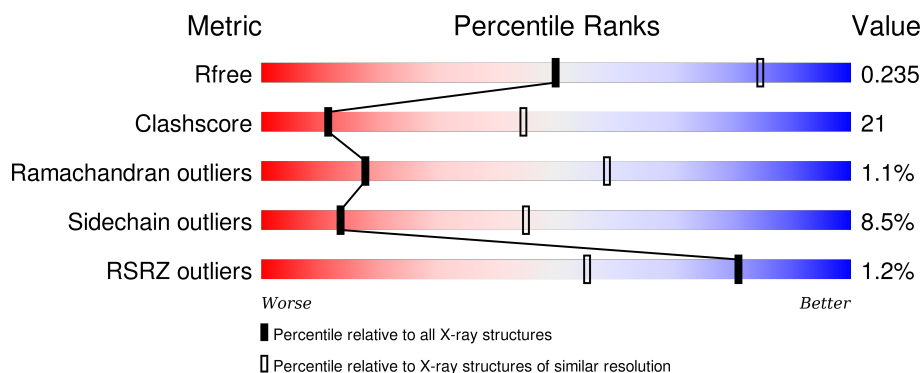
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	619	
1	B	619	

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
3	SO4	A	702	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9685 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 Arginine decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	Se	0	0	0
			4701	3035	773	881	2	10			
1	B	591	Total	C	N	O	S	Se	0	0	0
			4775	3081	793	889	2	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	612	LEU	-	expression tag	UNP Q0PAC6
A	613	GLU	-	expression tag	UNP Q0PAC6
A	614	HIS	-	expression tag	UNP Q0PAC6
A	615	HIS	-	expression tag	UNP Q0PAC6
A	616	HIS	-	expression tag	UNP Q0PAC6
A	617	HIS	-	expression tag	UNP Q0PAC6
A	618	HIS	-	expression tag	UNP Q0PAC6
A	619	HIS	-	expression tag	UNP Q0PAC6
B	612	LEU	-	expression tag	UNP Q0PAC6
B	613	GLU	-	expression tag	UNP Q0PAC6
B	614	HIS	-	expression tag	UNP Q0PAC6
B	615	HIS	-	expression tag	UNP Q0PAC6
B	616	HIS	-	expression tag	UNP Q0PAC6
B	617	HIS	-	expression tag	UNP Q0PAC6
B	618	HIS	-	expression tag	UNP Q0PAC6
B	619	HIS	-	expression tag	UNP Q0PAC6

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

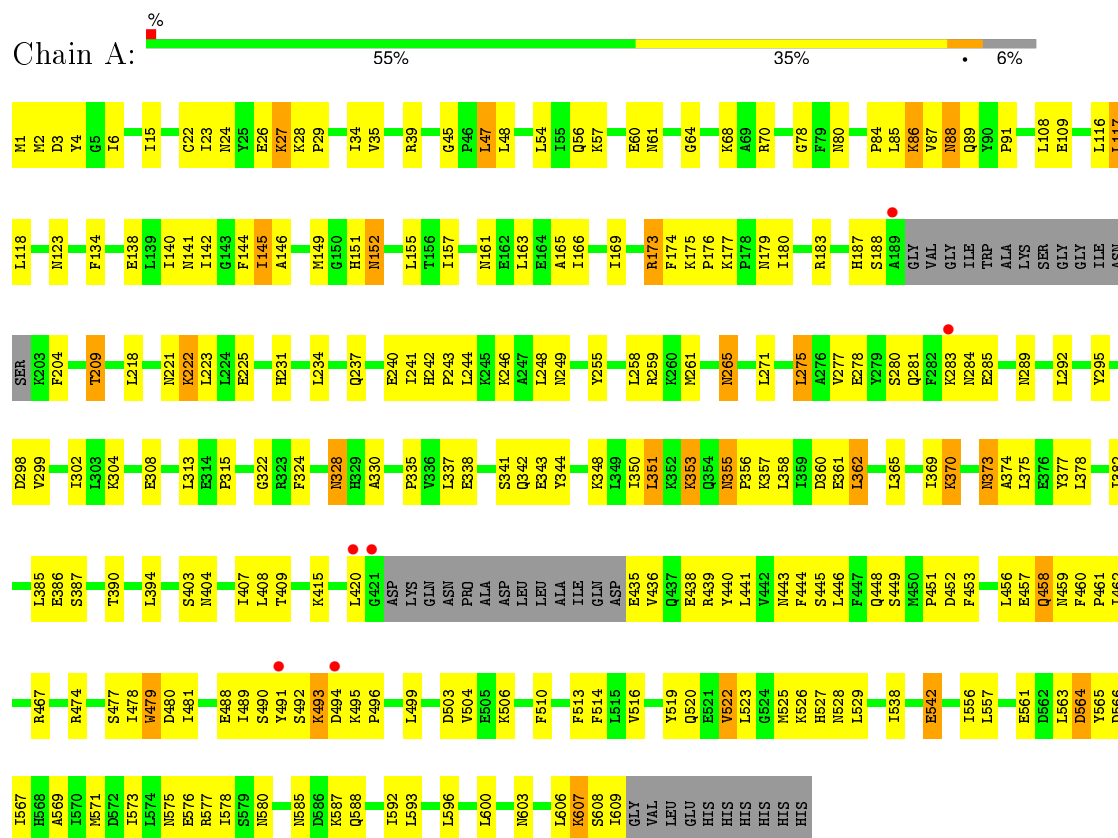
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	93	Total	O	0	0
			93	93		
4	B	71	Total	O	0	0
			71	71		

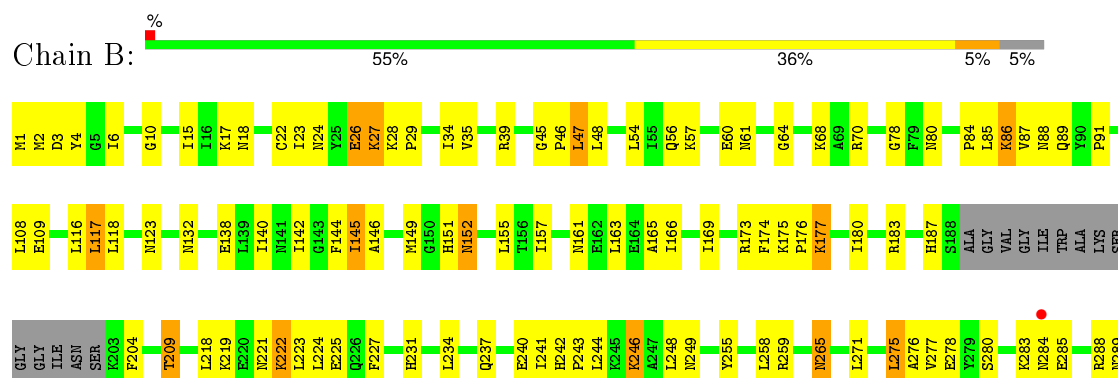
3 Residue-property plots

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: Arginine decarboxylase



• Molecule 1: Arginine decarboxylase



I556	L557	F460	I461	I462	L465	R474	S475	A476	I478	H479	D480	I481	S485	E488	I489	S490	Y491	S492	K493	D494	K495	P496	L499	D503	K506	E507	N508	Y509	F510	F513	F514	L515	V516	Y519	Q520	E521	V522	L523	G524	M525	K526	H527	N528	L529	I538	N541	E542					
L385	L389	T390	L394	L399	Q400	S403	I407	L408	T409	I412	K415	L419	L420	ASP	LYS	GLN	ASN	PRO	ALA	L339	ASP	S341	LEU	LEU	ALA	ILE	GLN	ASP	GLU	V436	Q437	E438	R439	Y440	L441	V442	M443	F444	S445	L446	F447	Q448	S449	P450	P451	D452	F453	H454	G455	L456	E457	Q458
L292	D298	V299	I302	L303	K304	E308	L313	E314	P315	F324	H328	H329	A330	I333	A334	P335	V336	L337	E338	L339	F340	S341	Q342	E343	L351	K352	K353	Q354	I355	P356	K357	L358	I359	D360	E361	L362	Y366	I369	K370	N373	A374	L375	L376	L382								

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.07Å 203.07Å 101.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 3.00 29.37 – 3.00	Depositor EDS
% Data completeness (in resolution range)	86.6 (19.96-3.00) 97.5 (29.37-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 3.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.180 , 0.219 0.196 , 0.235	Depositor DCC
R_{free} test set	4732 reflections (11.47%)	DCC
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.8	EDS
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 93938 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9685	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PLP

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	0.44	0/4784	0.58	0/6440
1	B	0.44	0/4864	0.58	0/6549
All	All	0.44	0/9648	0.58	0/12989

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	A	4701	0	4734	201	0
1	B	4775	0	4794	214	0
2	A	15	0	7	2	0
2	B	15	0	7	2	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
4	A	93	0	0	4	0
4	B	71	0	0	3	0
All	All	9685	0	9542	392	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 21.

The worst 5 of 392 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:355:ASN:HB3	1:B:359:ILE:HD11	1.26	1.10
1:B:370:LYS:H	1:B:373:ASN:HD21	1.01	1.00
1:A:353:LYS:HD3	1:A:353:LYS:H	1.30	0.95
1:A:2:MSE:HE2	1:A:4:TYR:H	1.33	0.94
1:A:1:MSE:HG2	1:A:2:MSE:H	1.33	0.94

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	577/619 (93%)	527 (91%)	43 (8%)	7 (1%)	16	56
1	B	585/619 (94%)	527 (90%)	52 (9%)	6 (1%)	19	61
All	All	1162/1238 (94%)	1054 (91%)	95 (8%)	13 (1%)	17	58

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	HIS
1	B	527	HIS
1	A	188	SER
1	B	351	LEU
1	A	88	ASN

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	511/529 (97%)	470 (92%)	41 (8%)	15	47
1	B	519/529 (98%)	472 (91%)	47 (9%)	12	41
All	All	1030/1058 (97%)	942 (92%)	88 (8%)	13	45

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	587	LYS
1	B	145	ILE
1	B	507	GLU
1	A	607	LYS
1	B	80	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	24	ASN
1	B	151	HIS
1	B	603	ASN
1	B	105	ASN
1	B	152	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

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PLP	A	701	-	15,15,16	1.78	3 (20%)	21,22,23	1.01	1 (4%)
3	SO4	A	702	-	4,4,4	0.33	0	6,6,6	0.11	0
2	PLP	B	701	-	15,15,16	1.79	3 (20%)	21,22,23	0.99	1 (4%)
3	SO4	B	702	-	4,4,4	0.33	0	6,6,6	0.17	0
3	SO4	B	703	-	4,4,4	0.27	0	6,6,6	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	701	-	-	0/6/6/8	0/1/1/1
3	SO4	A	702	-	-	0/0/0/0	0/0/0/0
2	PLP	B	701	-	-	0/6/6/8	0/1/1/1
3	SO4	B	702	-	-	0/0/0/0	0/0/0/0
3	SO4	B	703	-	-	0/0/0/0	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	PLP	C3-C4	2.19	1.45	1.40
2	B	701	PLP	C3-C4	2.60	1.46	1.40
2	B	701	PLP	C3-C2	3.42	1.43	1.40
2	A	701	PLP	C3-C2	3.44	1.43	1.40
2	B	701	PLP	C5-C4	4.08	1.45	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	PLP	C6-N1-C2	2.03	123.42	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	PLP	C6-N1-C2	2.13	123.63	119.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	PLP	2	0
2	B	701	PLP	2	0

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 [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	573/619 (92%)	-0.50	6 (1%) 84 60	22, 44, 82, 119	0
1	B	581/619 (93%)	-0.39	8 (1%) 78 51	25, 46, 87, 121	0
All	All	1154/1238 (93%)	-0.45	14 (1%) 81 55	22, 45, 86, 121	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	494	ASP	3.6
1	B	455	GLY	3.6
1	A	494	ASP	3.5
1	B	491	TYR	3.3
1	B	506	LYS	3.0

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 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
3	SO4	A	702	5/5	0.88	0.22	2.83	96,96,101,104	0
2	PLP	A	701	15/16	0.94	0.24	1.49	36,72,88,100	0
3	SO4	B	703	5/5	0.91	0.23	0.91	88,91,94,100	0
2	PLP	B	701	15/16	0.95	0.18	0.79	35,59,76,79	0
3	SO4	B	702	5/5	0.90	0.16	-1.83	77,85,91,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.