



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 02:23 am GMT

PDB ID : 3SS4
Title : Crystal structure of mouse Glutaminase C, phosphate-bound form
Authors : Ambrosio, A.L.B.; Dias, S.M.G.; Cerione, R.A.
Deposited on : 2011-07-07
Resolution : 2.85 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

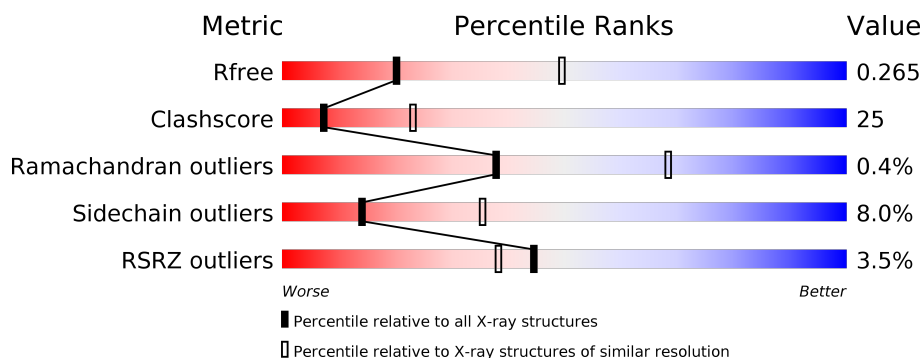
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	100719	2469 (2.90-2.82)
Clashscore	112137	2749 (2.90-2.82)
Ramachandran outliers	110173	2687 (2.90-2.82)
Sidechain outliers	110143	2690 (2.90-2.82)
RSRZ outliers	101464	2487 (2.90-2.82)

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	479	<div> <div>4%</div> <div> <div>51%</div> <div>28%</div> <div>•</div> <div>19%</div> </div> </div>
1	B	479	<div> <div>3%</div> <div> <div>50%</div> <div>27%</div> <div>•</div> <div>19%</div> </div> </div>
1	C	479	<div> <div>3%</div> <div> <div>45%</div> <div>33%</div> <div>•</div> <div>18%</div> </div> </div>
1	D	479	<div> <div>%</div> <div> <div>44%</div> <div>33%</div> <div>•</div> <div>19%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12470 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 Glutaminase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	4	0	0
			3051	1952	513	558	28			
1	B	388	Total	C	N	O	S	4	0	0
			3036	1941	511	556	28			
1	C	394	Total	C	N	O	S	5	0	0
			3083	1970	519	566	28			
1	D	387	Total	C	N	O	S	4	0	0
			3025	1930	510	557	28			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	GLY	-	EXPRESSION TAG	UNP Q69ZX9
A	126	SER	-	EXPRESSION TAG	UNP Q69ZX9
A	127	HIS	-	EXPRESSION TAG	UNP Q69ZX9
B	125	GLY	-	EXPRESSION TAG	UNP Q69ZX9
B	126	SER	-	EXPRESSION TAG	UNP Q69ZX9
B	127	HIS	-	EXPRESSION TAG	UNP Q69ZX9
C	125	GLY	-	EXPRESSION TAG	UNP Q69ZX9
C	126	SER	-	EXPRESSION TAG	UNP Q69ZX9
C	127	HIS	-	EXPRESSION TAG	UNP Q69ZX9
D	125	GLY	-	EXPRESSION TAG	UNP Q69ZX9
D	126	SER	-	EXPRESSION TAG	UNP Q69ZX9
D	127	HIS	-	EXPRESSION TAG	UNP Q69ZX9

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

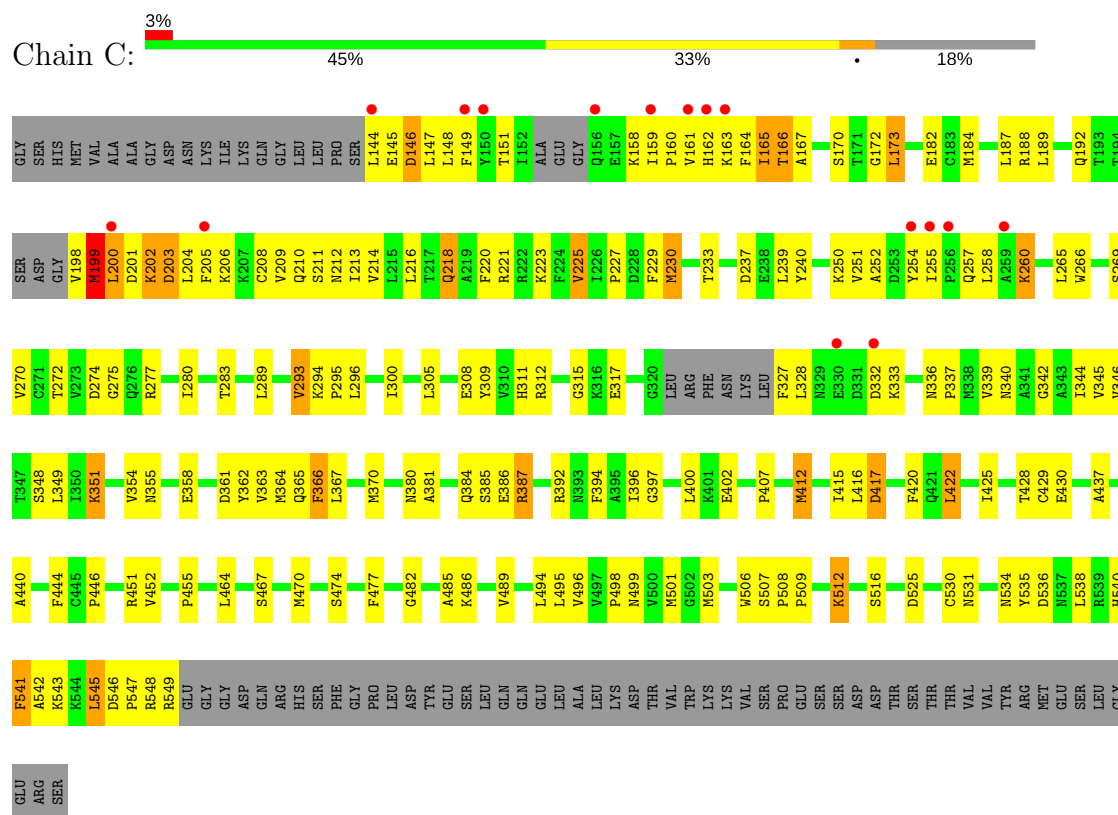


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

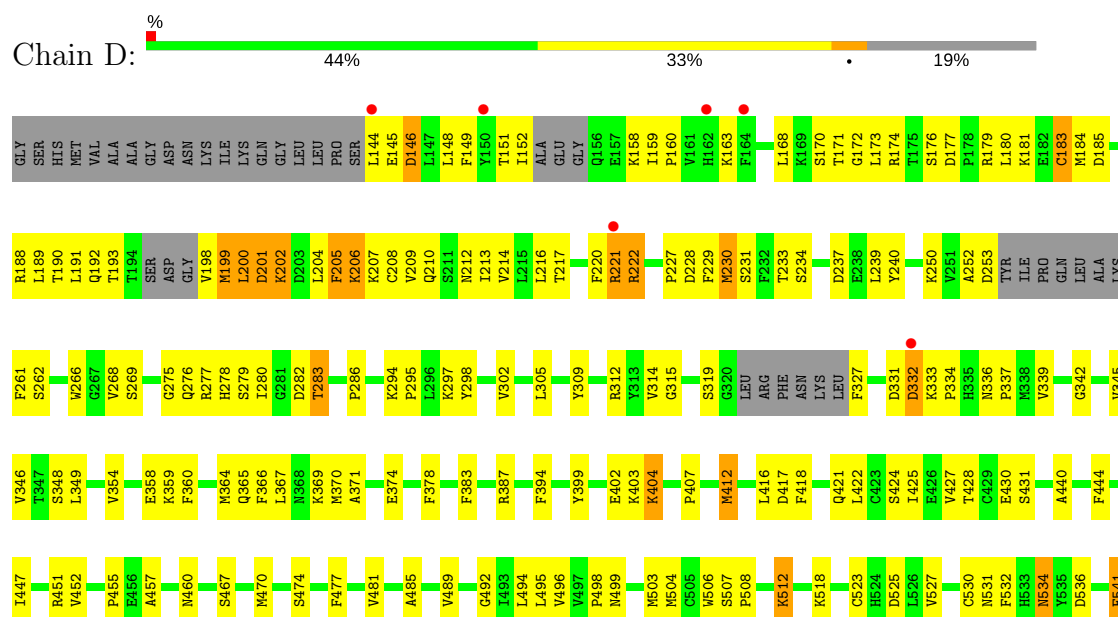
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	63	Total	O	0	0
			63	63		
3	B	71	Total	O	0	0
			71	71		
3	C	53	Total	O	0	0
			53	53		
3	D	68	Total	O	0	0
			68	68		

- Molecule 1: Glutaminase C



- Molecule 1: Glutaminase C



A542	R543	K544	L545	D546	P547	R548	R549	GLU	GLY	GLY	ASP	GLN	ARG	HIS	SER	PHE	GLY	PRO	LEU	ASP	TYR	GLU	SER	LEU	GLN	GLN	GLU	LEU	ALA	LEU	LYS	ASP	THR	VAL	TRP	LYS	LYS	VAL	SER	PRO	GLU	SER	SER	ASP	ASP	THR	SER	THR	THR	VAL	VAL	TYR	ARG	MET	GLU	SER	LEU	GLY	GLU
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ARG

SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.72Å 136.28Å 176.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.85 37.55 – 2.85	Depositor EDS
% Data completeness (in resolution range)	93.3 (19.91-2.85) 93.0 (37.55-2.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.227 , 0.270 0.222 , 0.265	Depositor DCC
R_{free} test set	2631 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12470	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.35 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.9224e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PO4

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	0.65	3/3118 (0.1%)	0.53	0/4205
1	B	0.57	2/3101 (0.1%)	0.53	0/4179
1	C	0.62	3/3150 (0.1%)	0.55	1/4249 (0.0%)
1	D	0.59	0/3089	0.53	1/4164 (0.0%)
All	All	0.61	8/12458 (0.1%)	0.54	2/16797 (0.0%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	VAL	CB-CG2	-5.57	1.41	1.52
1	B	489	VAL	CB-CG1	-5.54	1.41	1.52
1	C	362	TYR	CE2-CZ	-5.38	1.31	1.38
1	C	362	TYR	CD2-CE2	-5.32	1.31	1.39
1	A	225	VAL	CB-CG1	-5.22	1.41	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	LEU	CA-CB-CG	5.10	127.03	115.30
1	D	200	LEU	CA-CB-CG	5.07	126.97	115.30

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	3051	0	3036	147	0
1	B	3036	0	3017	131	0
1	C	3083	0	3066	176	0
1	D	3025	0	3001	159	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	63	0	0	0	0
3	B	71	0	0	0	0
3	C	53	0	0	2	0
3	D	68	0	0	0	0
All	All	12470	0	12120	603	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 25.

The worst 5 of 603 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:200:LEU:HD12	1:A:204:LEU:CD2	1.62	1.28
1:C:148:LEU:HD13	1:C:148:LEU:O	1.41	1.18
1:C:387:ARG:HH11	1:C:387:ARG:HG2	1.01	1.15
1:A:200:LEU:HD12	1:A:204:LEU:HD21	1.19	1.14
1:A:548:ARG:HG3	1:A:548:ARG:HH11	1.08	1.13

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	382/479 (80%)	366 (96%)	16 (4%)	0	100	100
1	B	378/479 (79%)	366 (97%)	10 (3%)	2 (0%)	32	64
1	C	386/479 (81%)	378 (98%)	6 (2%)	2 (0%)	32	64
1	D	377/479 (79%)	362 (96%)	13 (3%)	2 (0%)	32	64
All	All	1523/1916 (80%)	1472 (97%)	45 (3%)	6 (0%)	38	68

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	202	LYS
1	C	202	LYS
1	D	205	PHE
1	D	206	LYS
1	B	211	SER

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	339/415 (82%)	314 (93%)	25 (7%)	16	39
1	B	337/415 (81%)	308 (91%)	29 (9%)	12	32
1	C	343/415 (83%)	316 (92%)	27 (8%)	14	36
1	D	337/415 (81%)	309 (92%)	28 (8%)	13	34
All	All	1356/1660 (82%)	1247 (92%)	109 (8%)	14	35

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	422	LEU
1	C	211	SER
1	D	332	ASP
1	B	512	LYS
1	C	146	ASP

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

Mol	Chain	Res	Type
1	A	335	HIS
1	B	156	GLN
1	C	540	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	PO4	A	1	-	4,4,4	0.74	0	6,6,6	0.43	0
2	PO4	B	2	-	4,4,4	0.74	0	6,6,6	0.37	0
2	PO4	C	3	-	4,4,4	0.74	0	6,6,6	0.35	0
2	PO4	D	4	-	4,4,4	0.73	0	6,6,6	0.43	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	PO4	A	1	-	-	0/0/0/0	0/0/0/0
2	PO4	B	2	-	-	0/0/0/0	0/0/0/0
2	PO4	C	3	-	-	0/0/0/0	0/0/0/0
2	PO4	D	4	-	-	0/0/0/0	0/0/0/0

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 [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	390/479 (81%)	0.02	19 (4%) 30 26	26, 40, 75, 88	4 (1%)
1	B	388/479 (81%)	0.01	13 (3%) 46 39	26, 40, 78, 94	4 (1%)
1	C	394/479 (82%)	0.05	16 (4%) 38 32	24, 43, 82, 105	4 (1%)
1	D	387/479 (80%)	0.03	6 (1%) 72 70	24, 41, 77, 95	4 (1%)
All	All	1559/1916 (81%)	0.03	54 (3%) 44 38	24, 41, 78, 105	16 (1%)

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	150	TYR	6.8
1	A	150	TYR	5.9
1	C	149	PHE	5.7
1	A	200	LEU	4.7
1	A	257	GLN	4.6

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	PO4	A	1	5/5	0.96	0.13	-1.47	40,49,56,71	0
2	PO4	C	3	5/5	0.97	0.11	-1.61	45,49,58,74	0
2	PO4	D	4	5/5	0.94	0.12	-2.06	43,52,68,84	0
2	PO4	B	2	5/5	0.98	0.08	-2.78	49,50,67,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.