



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:02 AM UTC

PDB ID : 9C5F / pdb_00009c5f
Title : Crystal Structure Analysis of human PRKCB
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Deposited on : 2024-06-06
Resolution : 2.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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<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
Mogul	:	2022.3.0, CSD as543be (2022)
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

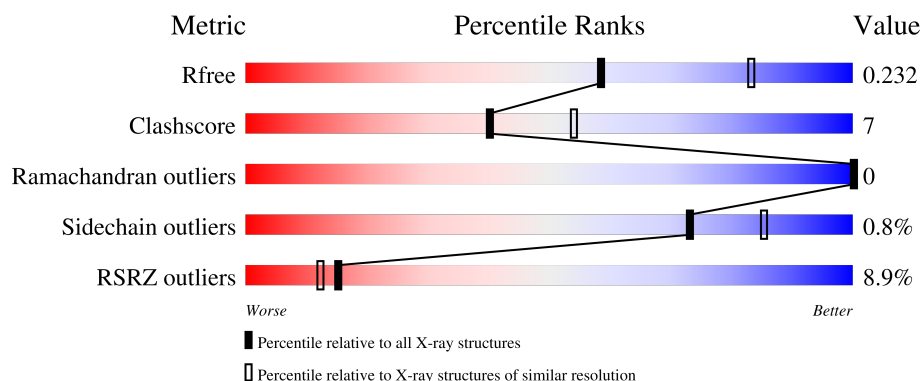
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	190	
1	B	190	

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	1010	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2362 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 Protein kinase C beta type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	0	0
			1133	721	195	213	4			
1	B	142	Total	C	N	O	S	0	0	0
			1126	714	190	218	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	MET	-	initiating methionine	UNP P05771
A	126	GLY	-	expression tag	UNP P05771
A	297	GLU	-	expression tag	UNP P05771
A	298	GLN	-	expression tag	UNP P05771
A	299	LYS	-	expression tag	UNP P05771
A	300	LEU	-	expression tag	UNP P05771
A	301	ILE	-	expression tag	UNP P05771
A	302	SER	-	expression tag	UNP P05771
A	303	GLU	-	expression tag	UNP P05771
A	304	GLU	-	expression tag	UNP P05771
A	305	ASP	-	expression tag	UNP P05771
A	306	LEU	-	expression tag	UNP P05771
A	307	LEU	-	expression tag	UNP P05771
A	308	GLU	-	expression tag	UNP P05771
A	309	HIS	-	expression tag	UNP P05771
A	310	HIS	-	expression tag	UNP P05771
A	311	HIS	-	expression tag	UNP P05771
A	312	HIS	-	expression tag	UNP P05771
A	313	HIS	-	expression tag	UNP P05771
A	314	HIS	-	expression tag	UNP P05771
B	125	MET	-	initiating methionine	UNP P05771
B	126	GLY	-	expression tag	UNP P05771
B	297	GLU	-	expression tag	UNP P05771
B	298	GLN	-	expression tag	UNP P05771
B	299	LYS	-	expression tag	UNP P05771

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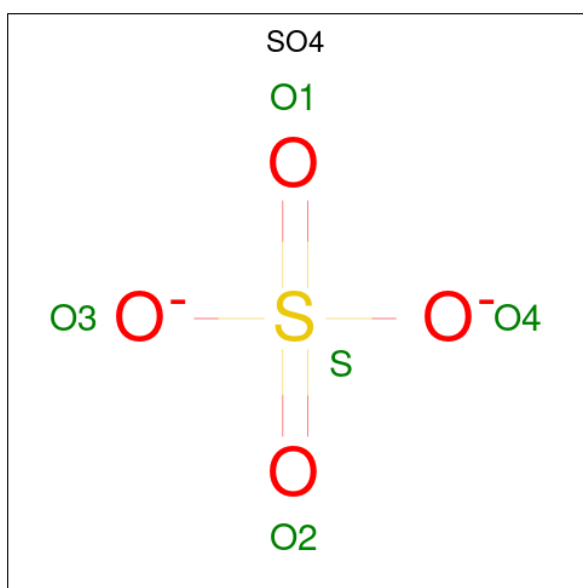
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Chain	Residue	Modelled	Actual	Comment	Reference
B	300	LEU	-	expression tag	UNP P05771
B	301	ILE	-	expression tag	UNP P05771
B	302	SER	-	expression tag	UNP P05771
B	303	GLU	-	expression tag	UNP P05771
B	304	GLU	-	expression tag	UNP P05771
B	305	ASP	-	expression tag	UNP P05771
B	306	LEU	-	expression tag	UNP P05771
B	307	LEU	-	expression tag	UNP P05771
B	308	GLU	-	expression tag	UNP P05771
B	309	HIS	-	expression tag	UNP P05771
B	310	HIS	-	expression tag	UNP P05771
B	311	HIS	-	expression tag	UNP P05771
B	312	HIS	-	expression tag	UNP P05771
B	313	HIS	-	expression tag	UNP P05771
B	314	HIS	-	expression tag	UNP P05771

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total 3 Ca 3	0	0
2	B	3	Total 3 Ca 3	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

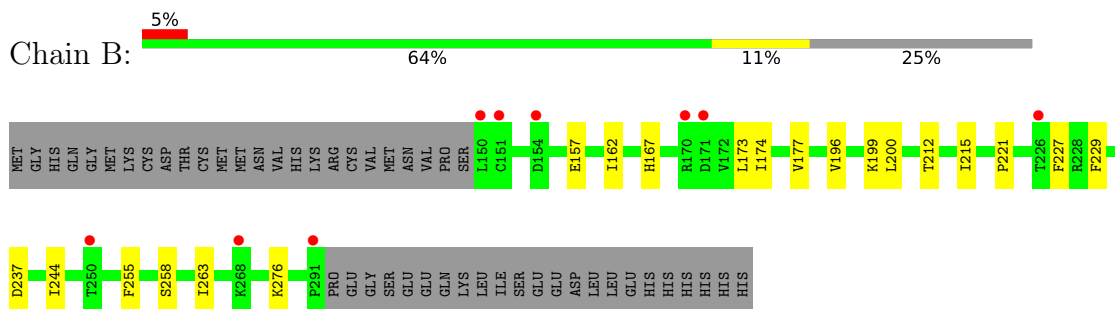


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B	8	Total O 8 8	0	0

- Molecule 1: Protein kinase C beta type



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.12Å 144.12Å 70.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.30 – 2.41 61.30 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.3 (61.30-2.41) 99.4 (61.30-2.41)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.40Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286: ???)	Depositor
R, R_{free}	0.213 , 0.232 0.214 , 0.232	Depositor DCC
R_{free} test set	1638 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	70.7	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2362	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% 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: SO4, CA

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	0.14	0/1158	0.40	0/1565
1	B	0.13	0/1152	0.35	0/1565
All	All	0.14	0/2310	0.38	0/3130

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	1133	0	1111	19	1
1	B	1126	0	1071	11	1
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	35	0	0	2	0
3	B	45	0	0	1	0
4	A	9	0	0	1	0
4	B	8	0	0	0	0
All	All	2362	0	2182	30	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 7.

All (30) 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:232:LYS:HE2	1:A:234:SER:H	1.52	0.74
1:A:209:LYS:NZ	3:A:1010:SO4:S	2.73	0.61
1:A:209:LYS:NZ	3:A:1010:SO4:O3	2.34	0.60
1:A:162:ILE:HD12	1:A:244:ILE:HD11	1.83	0.60
1:A:276:LYS:O	4:A:1101:HOH:O	2.17	0.58
1:B:162:ILE:HD12	1:B:244:ILE:HD11	1.84	0.58
1:B:200:LEU:HD22	1:B:263:ILE:HD11	1.85	0.58
1:A:165:GLN:NE2	1:A:272:ASP:OD2	2.40	0.54
1:B:173:LEU:HB3	1:B:229:PHE:HB2	1.91	0.53
1:A:202:PRO:HD2	1:A:238:ARG:HG2	1.92	0.52
1:B:199:LYS:NZ	3:B:410:SO4:O3	2.36	0.51
1:A:235:ASP:OD1	1:A:238:ARG:NH2	2.41	0.51
1:A:177:VAL:HG21	1:A:212:THR:HG21	1.91	0.51
1:B:167:HIS:HE1	1:B:174:ILE:HD12	1.74	0.50
1:A:165:GLN:HB2	1:A:176:LEU:HB3	1.93	0.50
1:B:196:VAL:HG22	1:B:244:ILE:HG12	1.96	0.47
1:A:276:LYS:HG2	1:A:290:VAL:HG22	1.97	0.47
1:B:212:THR:HG22	1:B:227:PHE:CZ	2.51	0.46
1:A:168:ILE:HD12	1:A:267:GLN:HG3	1.97	0.46
1:B:157:GLU:HB2	1:B:276:LYS:HD3	1.97	0.46
1:B:215:ILE:HD12	1:B:221:PRO:HB2	1.98	0.45
1:A:196:VAL:HG22	1:A:244:ILE:HG12	1.98	0.45
1:A:213:LYS:HA	1:A:213:LYS:HD2	1.63	0.45
1:B:177:VAL:HG21	1:B:212:THR:HG21	1.98	0.45
1:A:213:LYS:HE3	1:A:214:THR:H	1.82	0.44
1:B:255:PHE:CZ	1:B:258:SER:HB2	2.52	0.44
1:A:212:THR:HG22	1:A:227:PHE:CZ	2.53	0.44
1:A:173:LEU:HB3	1:A:229:PHE:HB2	1.99	0.43
1:A:186:MET:HE2	1:A:254:ASP:HB3	2.00	0.42
1:A:232:LYS:HE3	1:A:232:LYS:HB2	1.66	0.41

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:216:LYS:NZ	1:B:237:ASP:OD1[3_565]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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	136/190 (72%)	128 (94%)	8 (6%)	0	100	100
1	B	140/190 (74%)	132 (94%)	8 (6%)	0	100	100
All	All	276/380 (73%)	260 (94%)	16 (6%)	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	127/177 (72%)	125 (98%)	2 (2%)	55	74
1	B	124/177 (70%)	124 (100%)	0	100	100
All	All	251/354 (71%)	249 (99%)	2 (1%)	73	85

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

Mol	Chain	Res	Type
1	A	228	ARG
1	A	267	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	167	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 for Mogul analysis.

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	$\# Z > 2$
3	SO4	A	1005	-	4,4,4	0.68	0	6,6,6	0.09	0
3	SO4	A	1009	-	4,4,4	0.67	0	6,6,6	0.06	0
3	SO4	A	1006	-	4,4,4	0.67	0	6,6,6	0.09	0
3	SO4	A	1007	-	4,4,4	0.67	0	6,6,6	0.09	0
3	SO4	B	411	-	4,4,4	0.67	0	6,6,6	0.08	0
3	SO4	B	406	-	4,4,4	0.67	0	6,6,6	0.12	0
3	SO4	B	408	-	4,4,4	0.67	0	6,6,6	0.06	0
3	SO4	B	405	2	4,4,4	0.67	0	6,6,6	0.07	0
3	SO4	B	409	-	4,4,4	0.67	0	6,6,6	0.09	0
3	SO4	A	1008	-	4,4,4	0.67	0	6,6,6	0.11	0
3	SO4	B	410	-	4,4,4	0.67	0	6,6,6	0.08	0
3	SO4	B	407	-	4,4,4	0.67	0	6,6,6	0.10	0
3	SO4	A	1004	2	4,4,4	0.66	0	6,6,6	0.08	0
3	SO4	B	404	2	4,4,4	0.67	0	6,6,6	0.11	0
3	SO4	A	1010	-	4,4,4	0.66	0	6,6,6	0.08	0
3	SO4	B	412	-	4,4,4	0.67	0	6,6,6	0.08	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	410	SO4	1	0
3	A	1010	SO4	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 ⓘ

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	140/190 (73%)	0.68	16 (11%) 10 7	56, 78, 114, 129	0
1	B	142/190 (74%)	0.62	9 (6%) 26 22	56, 86, 115, 127	0
All	All	282/380 (74%)	0.65	25 (8%) 15 12	56, 82, 115, 129	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	151	CYS	6.6
1	B	291	PRO	5.9
1	A	291	PRO	5.6
1	B	150	LEU	5.3
1	A	150	LEU	5.2
1	B	170	ARG	5.1
1	B	171	ASP	4.0
1	B	154	ASP	3.8
1	A	154	ASP	3.7
1	A	169	ASP	3.4
1	A	156	THR	3.4
1	A	170	ARG	3.2
1	B	268	LYS	3.2
1	A	213	LYS	3.0
1	A	204	PRO	3.0
1	A	233	GLU	3.0
1	A	171	ASP	2.9
1	B	151	CYS	2.6
1	B	226	THR	2.6
1	A	205	LYS	2.6
1	A	167	HIS	2.2
1	A	237	ASP	2.2
1	A	228	ARG	2.2
1	A	155	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	250	THR	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(Å ²)	Q<0.9
3	SO4	B	405	5/5	0.61	0.16	90,119,147,151	0
3	SO4	A	1010	5/5	0.66	0.14	124,136,139,167	0
3	SO4	B	410	5/5	0.70	0.12	117,126,135,166	0
3	SO4	A	1005	5/5	0.78	0.19	82,87,113,125	0
3	SO4	B	412	5/5	0.80	0.10	124,127,136,156	0
3	SO4	B	411	5/5	0.81	0.12	106,107,131,134	0
3	SO4	B	407	5/5	0.83	0.10	99,123,143,143	0
3	SO4	B	409	5/5	0.86	0.10	99,115,128,143	0
3	SO4	A	1009	5/5	0.88	0.10	109,112,119,138	0
3	SO4	B	408	5/5	0.88	0.12	108,116,127,128	0
3	SO4	A	1008	5/5	0.89	0.10	77,102,120,125	0
3	SO4	B	404	5/5	0.90	0.10	77,88,102,113	0
3	SO4	B	406	5/5	0.95	0.11	72,82,96,98	0
3	SO4	A	1004	5/5	0.96	0.07	76,77,83,87	0
3	SO4	A	1006	5/5	0.96	0.08	67,78,85,95	0
3	SO4	A	1007	5/5	0.96	0.09	78,87,101,101	0
2	CA	B	401	1/1	0.97	0.06	64,64,64,64	0
2	CA	B	403	1/1	0.98	0.04	77,77,77,77	0
2	CA	B	402	1/1	0.99	0.04	57,57,57,57	0
2	CA	A	1003	1/1	0.99	0.04	69,69,69,69	0
2	CA	A	1001	1/1	1.00	0.02	59,59,59,59	0
2	CA	A	1002	1/1	1.00	0.02	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.