wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2023 – 07:30 PM EDT

PDB ID	:	2IA5
Title	:	T4 polynucleotide kinase/phosphatase with bound sulfate and magnesium.
Authors	:	Zhu, H.; Smith, P.C.; Wang, L.K.; Lima, C.D.; Shuman, S.
Deposited on	:	2006-09-07
Resolution	:	2.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

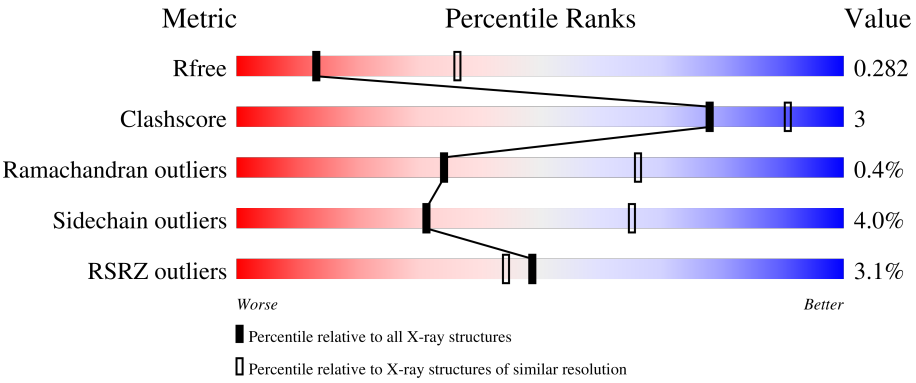
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	301	2% 86% 12%
1	B	301	% 92% 7%
1	C	301	% 89% 10%
1	D	301	3% 87% 10%
1	E	301	4% 90% 7%

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Mol	Chain	Length	Quality of chain
1	F	301	2% 89% 9%
1	G	301	2% 88% 9%
1	H	301	5% 89% 9%
1	I	301	5% 84% 11%
1	J	301	3% 89% 8%
1	K	301	4% 87% 8%
1	L	301	4% 87% 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 29589 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 Polynucleotide kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2383	1519	412	436	16			
1	B	300	Total	C	N	O	S	0	0	0
			2403	1529	415	443	16			
1	C	299	Total	C	N	O	S	0	0	0
			2399	1528	414	441	16			
1	D	296	Total	C	N	O	S	0	0	0
			2373	1513	411	433	16			
1	E	294	Total	C	N	O	S	0	0	1
			2351	1497	406	432	16			
1	F	298	Total	C	N	O	S	0	0	0
			2402	1531	413	442	16			
1	G	294	Total	C	N	O	S	0	0	0
			2353	1499	405	434	15			
1	H	301	Total	C	N	O	S	0	0	0
			2416	1538	418	444	16			
1	I	289	Total	C	N	O	S	0	0	0
			2304	1471	398	419	16			
1	J	296	Total	C	N	O	S	0	0	0
			2364	1508	409	431	16			
1	K	288	Total	C	N	O	S	0	0	0
			2318	1479	401	422	16			
1	L	291	Total	C	N	O	S	0	0	0
			2349	1499	405	429	16			

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

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

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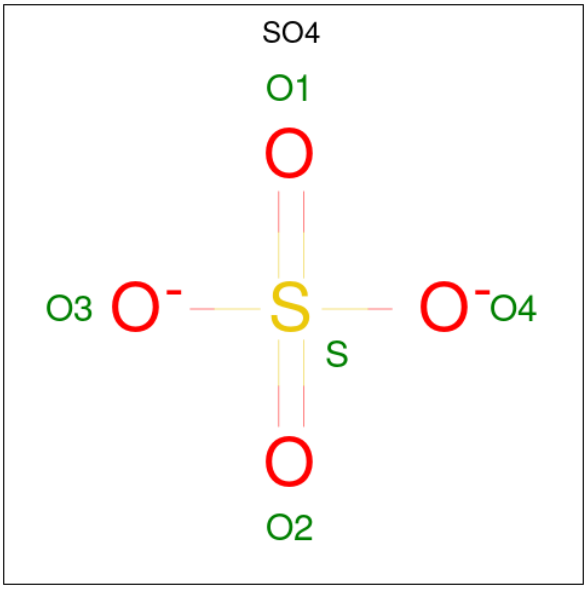
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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	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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0

- Molecule 4 is ARSENIC (three-letter code: ARS) (formula: As).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total As 1 1	0	0
4	B	1	Total As 1 1	0	0
4	C	1	Total As 1 1	0	0
4	D	1	Total As 1 1	0	0
4	E	1	Total As 1 1	0	0
4	F	1	Total As 1 1	0	0
4	G	1	Total As 1 1	0	0
4	H	1	Total As 1 1	0	0
4	I	1	Total As 1 1	0	0
4	J	1	Total As 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	1	Total As 1 1	0	0

- Molecule 5 is water.

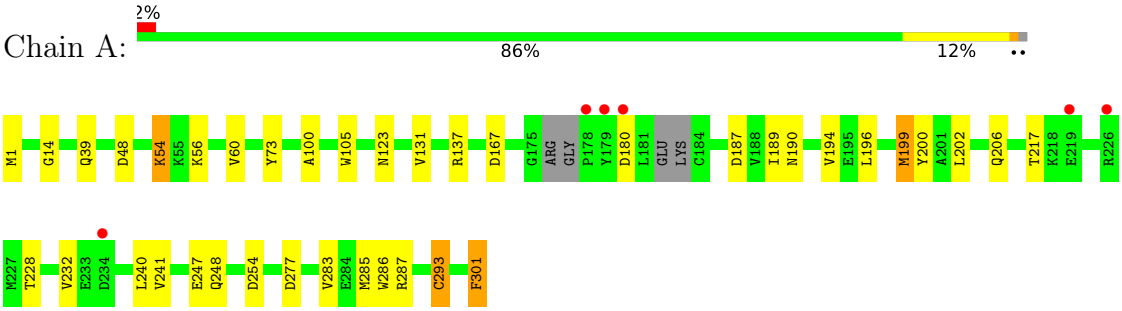
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	142	Total O 142 142	0	0
5	B	116	Total O 116 116	0	0
5	C	88	Total O 88 88	0	0
5	D	136	Total O 136 136	0	0
5	E	56	Total O 56 56	0	0
5	F	81	Total O 81 81	0	0
5	G	65	Total O 65 65	0	0
5	H	58	Total O 58 58	0	0
5	I	70	Total O 70 70	0	0
5	J	48	Total O 48 48	0	0
5	K	74	Total O 74 74	0	0
5	L	42	Total O 42 42	0	0

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.

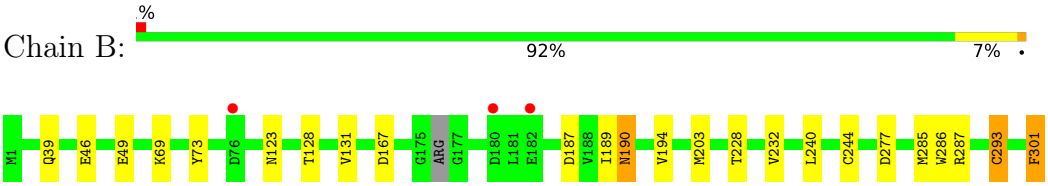
• Molecule 1: Polynucleotide kinase

Chain A:



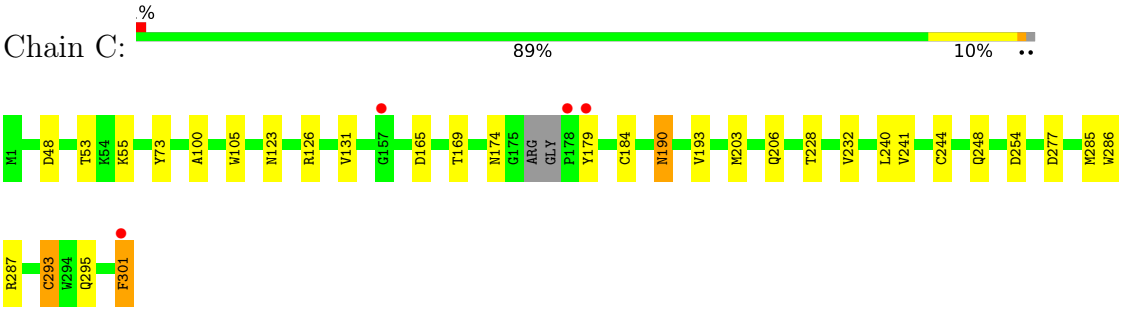
• Molecule 1: Polynucleotide kinase

Chain B:



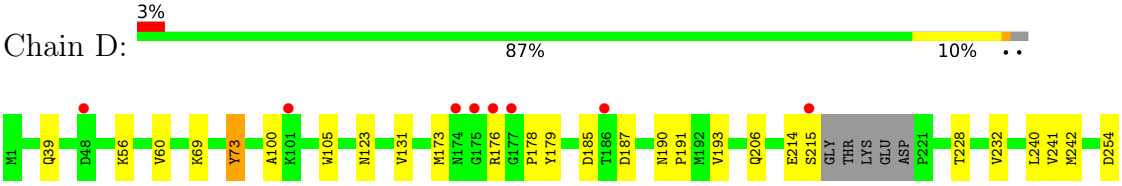
• Molecule 1: Polynucleotide kinase

Chain C:



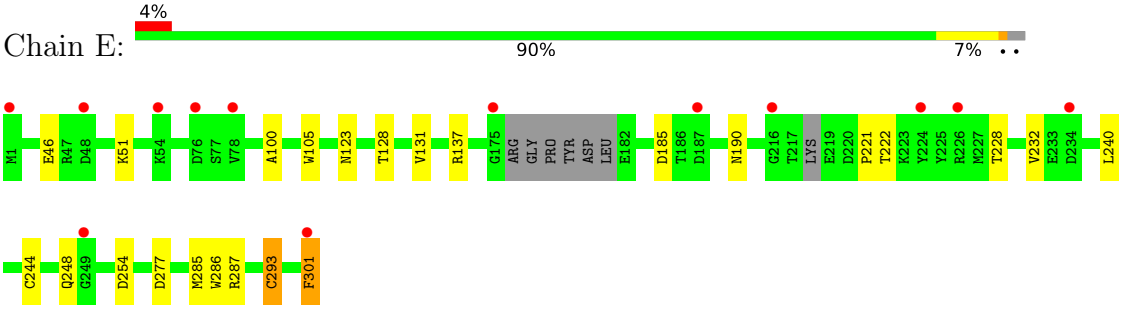
• Molecule 1: Polynucleotide kinase

Chain D:



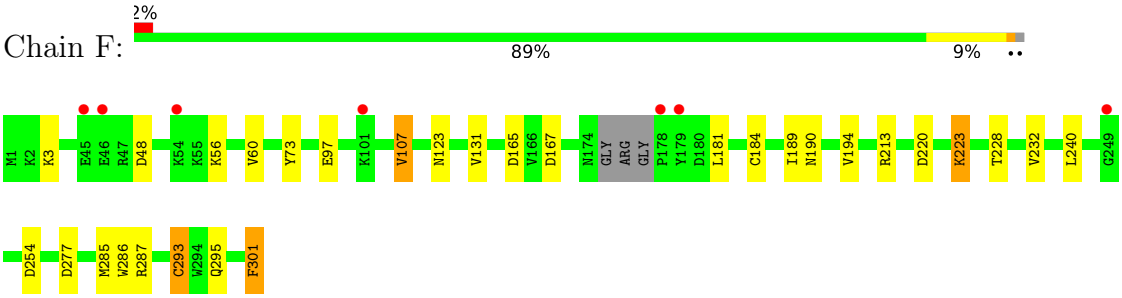
• Molecule 1: Polynucleotide kinase

Chain E:



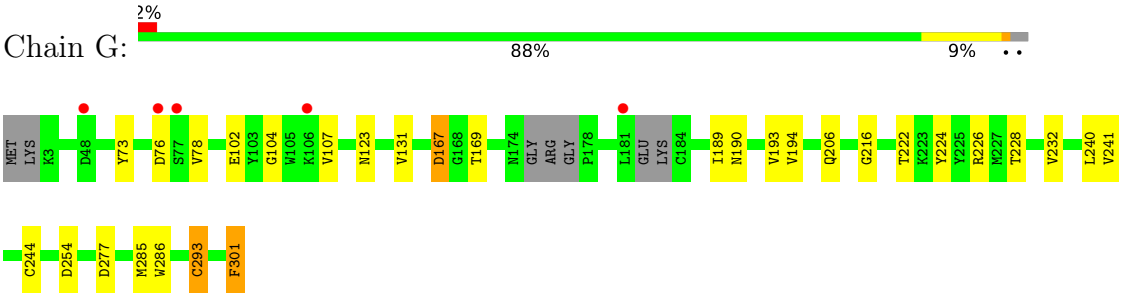
• Molecule 1: Polynucleotide kinase

Chain F:



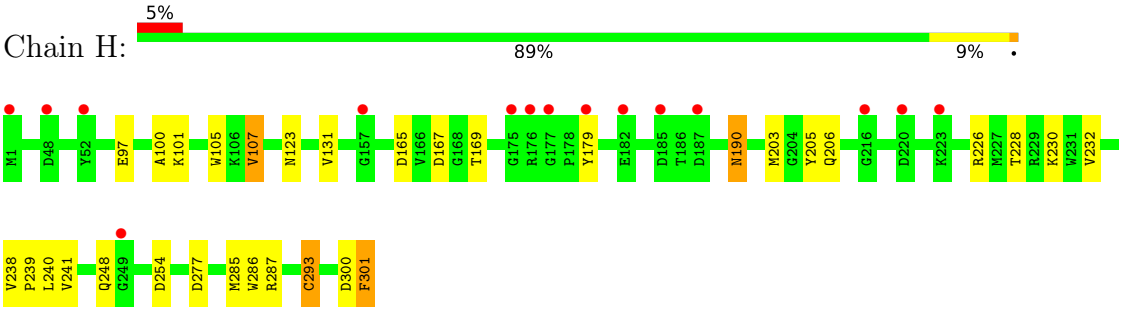
• Molecule 1: Polynucleotide kinase

Chain G:



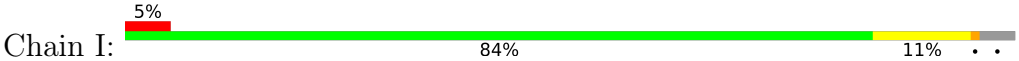
• Molecule 1: Polynucleotide kinase

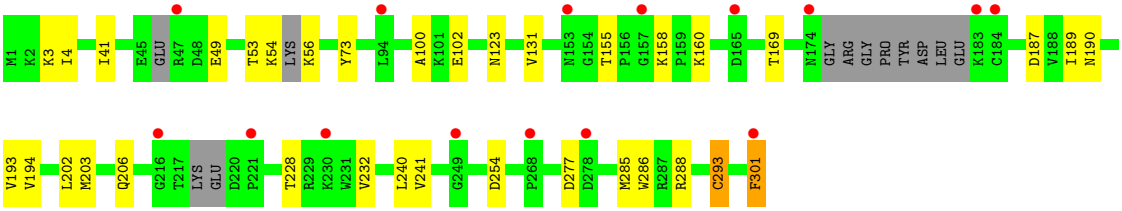
Chain H:



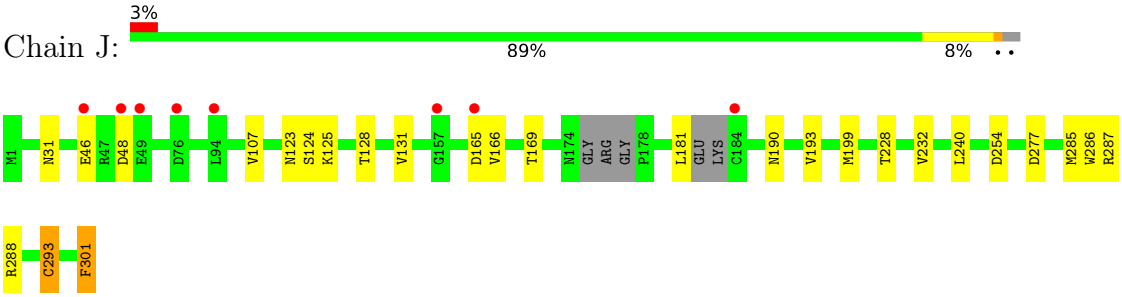
• Molecule 1: Polynucleotide kinase

Chain I:

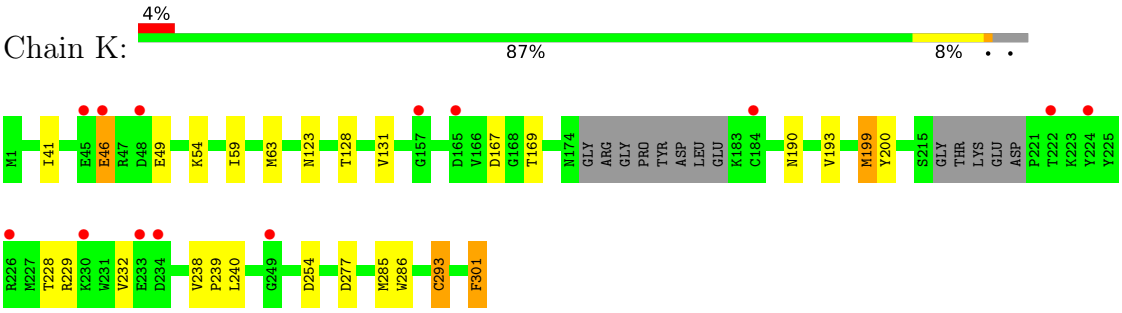




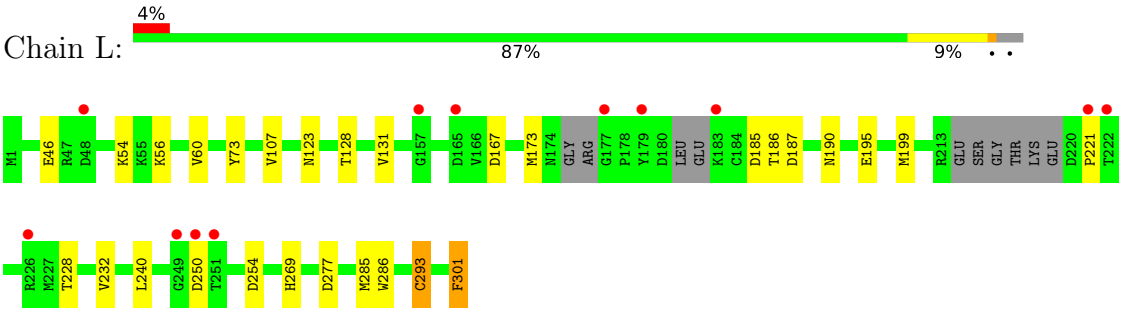
• Molecule 1: Polynucleotide kinase



• Molecule 1: Polynucleotide kinase



• Molecule 1: Polynucleotide kinase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	124.63Å 128.05Å 357.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.90 19.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	88.0 (19.99-2.90) 88.0 (19.98-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.88Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.286 0.234 , 0.282	Depositor DCC
R_{free} test set	3180 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å^2)	50.3	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 44.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	29589	wwPDB-VP
Average B, all atoms (Å^2)	60.0	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 24.36 % 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 3.8919e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, SO4, ARS

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	0.70	1/2434 (0.0%)	0.75	2/3280 (0.1%)
1	B	0.72	1/2455 (0.0%)	0.72	2/3311 (0.1%)
1	C	0.72	1/2452 (0.0%)	0.72	2/3306 (0.1%)
1	D	0.73	1/2425 (0.0%)	0.73	2/3269 (0.1%)
1	E	0.73	1/2400 (0.0%)	0.72	2/3237 (0.1%)
1	F	0.73	1/2455 (0.0%)	0.73	2/3311 (0.1%)
1	G	0.72	1/2404 (0.0%)	0.75	3/3244 (0.1%)
1	H	0.73	1/2470 (0.0%)	0.72	2/3332 (0.1%)
1	I	0.72	1/2352 (0.0%)	0.74	2/3171 (0.1%)
1	J	0.71	1/2415 (0.0%)	0.72	2/3258 (0.1%)
1	K	0.73	1/2368 (0.0%)	0.73	2/3192 (0.1%)
1	L	0.73	1/2400 (0.0%)	0.72	2/3235 (0.1%)
All	All	0.72	12/29030 (0.0%)	0.73	25/39146 (0.1%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	293	CYS	CB-SG	-9.36	1.66	1.82
1	G	293	CYS	CB-SG	-8.32	1.68	1.82
1	D	293	CYS	CB-SG	-8.26	1.68	1.82
1	E	293	CYS	CB-SG	-7.63	1.69	1.82
1	H	293	CYS	CB-SG	-7.56	1.69	1.82

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	301	PHE	CG-CD1-CE1	6.27	127.69	120.80
1	A	301	PHE	CG-CD1-CE1	6.23	127.65	120.80
1	A	301	PHE	CG-CD2-CE2	6.22	127.65	120.80
1	G	301	PHE	CG-CD1-CE1	6.20	127.62	120.80
1	J	301	PHE	CG-CD2-CE2	6.19	127.60	120.80

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	2383	0	2382	18	0
1	B	2403	0	2393	12	0
1	C	2399	0	2386	18	0
1	D	2373	0	2357	19	0
1	E	2351	0	2336	10	0
1	F	2402	0	2395	15	0
1	G	2353	0	2329	10	1
1	H	2416	0	2403	16	0
1	I	2304	0	2285	14	0
1	J	2364	0	2351	13	0
1	K	2318	0	2315	13	0
1	L	2349	0	2342	8	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	H	1	0	0	0	0
2	J	1	0	0	0	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
3	C	15	0	0	1	0
3	D	15	0	0	0	0
3	E	15	0	0	0	0
3	F	15	0	0	0	0
3	G	15	0	0	0	0
3	H	15	0	0	0	0
3	I	15	0	0	0	0
3	J	15	0	0	0	0
3	K	15	0	0	0	0
3	L	15	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	1	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	1	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
5	A	142	0	0	8	0
5	B	116	0	0	6	0
5	C	88	0	0	5	0
5	D	136	0	0	7	0
5	E	56	0	0	2	0
5	F	81	0	0	3	0
5	G	65	0	0	2	0
5	H	58	0	0	5	0
5	I	70	0	0	2	0
5	J	48	0	0	2	0
5	K	74	0	0	7	0
5	L	42	0	0	1	0
All	All	29589	0	28274	161	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 3.

The worst 5 of 161 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:D:214:GLU:C	1:D:215:SER:CA	2.46	0.84
1:D:123:ASN:HD21	1:D:131:VAL:H	1.38	0.70
1:A:123:ASN:HD21	1:A:131:VAL:H	1.37	0.70
1:K:123:ASN:HD21	1:K:131:VAL:H	1.39	0.68
1:J:123:ASN:HD21	1:J:131:VAL:H	1.42	0.68

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:G:76:ASP:OD1	1:L:269:HIS:CE1[2_665]	1.85	0.35

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	291/301 (97%)	275 (94%)	13 (4%)	3 (1%)	15	45
1	B	296/301 (98%)	285 (96%)	10 (3%)	1 (0%)	41	71
1	C	295/301 (98%)	283 (96%)	12 (4%)	0	100	100
1	D	291/301 (97%)	272 (94%)	19 (6%)	0	100	100
1	E	287/301 (95%)	277 (96%)	10 (4%)	0	100	100
1	F	294/301 (98%)	280 (95%)	13 (4%)	1 (0%)	41	71
1	G	288/301 (96%)	274 (95%)	12 (4%)	2 (1%)	22	54
1	H	299/301 (99%)	286 (96%)	11 (4%)	2 (1%)	22	54
1	I	279/301 (93%)	266 (95%)	12 (4%)	1 (0%)	34	66
1	J	290/301 (96%)	274 (94%)	15 (5%)	1 (0%)	41	71
1	K	282/301 (94%)	265 (94%)	16 (6%)	1 (0%)	34	66
1	L	283/301 (94%)	267 (94%)	13 (5%)	3 (1%)	14	42
All	All	3475/3612 (96%)	3304 (95%)	156 (4%)	15 (0%)	34	66

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	ASP
1	H	205	TYR
1	K	167	ASP
1	A	248	GLN
1	B	167	ASP

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	257/263 (98%)	241 (94%)	16 (6%)	18	47
1	B	259/263 (98%)	251 (97%)	8 (3%)	40	74
1	C	258/263 (98%)	248 (96%)	10 (4%)	32	66
1	D	253/263 (96%)	243 (96%)	10 (4%)	31	65
1	E	253/263 (96%)	245 (97%)	8 (3%)	39	73
1	F	260/263 (99%)	249 (96%)	11 (4%)	30	63
1	G	253/263 (96%)	244 (96%)	9 (4%)	35	69
1	H	259/263 (98%)	249 (96%)	10 (4%)	32	66
1	I	246/263 (94%)	235 (96%)	11 (4%)	27	61
1	J	253/263 (96%)	245 (97%)	8 (3%)	39	73
1	K	250/263 (95%)	240 (96%)	10 (4%)	31	65
1	L	254/263 (97%)	242 (95%)	12 (5%)	26	59
All	All	3055/3156 (97%)	2932 (96%)	123 (4%)	31	65

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	190	ASN
1	K	285	MET
1	G	285	MET
1	K	277	ASP
1	L	240	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	123	ASN
1	K	281	GLN
1	G	295	GLN
1	K	245	GLN
1	L	245	GLN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 54 ligands modelled in this entry, 18 are monoatomic - leaving 36 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	E	923	-	4,4,4	0.50	0	6,6,6	0.15	0
3	SO4	A	912	-	4,4,4	0.50	0	6,6,6	0.24	0
3	SO4	B	915	-	4,4,4	0.52	0	6,6,6	0.20	0
3	SO4	L	945	-	4,4,4	0.47	0	6,6,6	0.12	0
3	SO4	K	941	-	4,4,4	0.53	0	6,6,6	0.16	0
3	SO4	D	920	-	4,4,4	0.49	0	6,6,6	0.21	0
3	SO4	I	937	-	4,4,4	0.50	0	6,6,6	0.09	0
3	SO4	D	921	-	4,4,4	0.52	0	6,6,6	0.24	0
3	SO4	J	938	-	4,4,4	0.54	0	6,6,6	0.21	0
3	SO4	H	932	-	4,4,4	0.53	0	6,6,6	0.19	0
3	SO4	L	944	-	4,4,4	0.52	0	6,6,6	0.11	0
3	SO4	J	940	-	4,4,4	0.52	0	6,6,6	0.13	0
3	SO4	C	918	-	4,4,4	0.48	0	6,6,6	0.13	0
3	SO4	I	936	-	4,4,4	0.50	0	6,6,6	0.15	0
3	SO4	C	919	-	4,4,4	0.50	0	6,6,6	0.07	0
3	SO4	H	934	-	4,4,4	0.51	0	6,6,6	0.06	0
3	SO4	E	924	-	4,4,4	0.47	0	6,6,6	0.21	0
3	SO4	K	942	-	4,4,4	0.48	0	6,6,6	0.11	0
3	SO4	B	916	-	4,4,4	0.50	0	6,6,6	0.12	0
3	SO4	J	939	-	4,4,4	0.48	0	6,6,6	0.15	0
3	SO4	G	930	-	4,4,4	0.51	0	6,6,6	0.14	0
3	SO4	F	926	-	4,4,4	0.52	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	K	943	-	4,4,4	0.52	0	6,6,6	0.08	0
3	SO4	C	917	-	4,4,4	0.53	0	6,6,6	0.23	0
3	SO4	E	925	-	4,4,4	0.54	0	6,6,6	0.07	0
3	SO4	H	933	-	4,4,4	0.51	0	6,6,6	0.11	0
3	SO4	A	913	-	4,4,4	0.52	0	6,6,6	0.04	0
3	SO4	F	927	-	4,4,4	0.50	0	6,6,6	0.23	0
3	SO4	F	928	-	4,4,4	0.47	0	6,6,6	0.19	0
3	SO4	I	935	-	4,4,4	0.48	0	6,6,6	0.06	0
3	SO4	A	911	-	4,4,4	0.54	0	6,6,6	0.42	0
3	SO4	G	931	-	4,4,4	0.48	0	6,6,6	0.06	0
3	SO4	B	914	-	4,4,4	0.46	0	6,6,6	0.17	0
3	SO4	D	922	-	4,4,4	0.49	0	6,6,6	0.09	0
3	SO4	G	929	-	4,4,4	0.49	0	6,6,6	0.22	0
3	SO4	L	946	-	4,4,4	0.50	0	6,6,6	0.10	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	917	SO4	1	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, 95^{th} 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	297/301 (98%)	-0.28	6 (2%)	65	63	7, 40, 100, 144	0
1	B	300/301 (99%)	-0.28	3 (1%)	82	82	10, 45, 97, 165	0
1	C	299/301 (99%)	-0.19	4 (1%)	77	77	13, 50, 106, 140	0
1	D	296/301 (98%)	-0.13	8 (2%)	54	50	10, 43, 103, 149	0
1	E	294/301 (97%)	0.12	13 (4%)	34	30	24, 63, 121, 175	0
1	F	298/301 (99%)	-0.19	7 (2%)	60	58	9, 44, 103, 134	0
1	G	294/301 (97%)	-0.12	5 (1%)	70	69	7, 51, 102, 171	0
1	H	301/301 (100%)	0.21	15 (4%)	28	25	28, 65, 121, 153	0
1	I	289/301 (96%)	0.30	15 (5%)	27	23	35, 70, 109, 148	0
1	J	296/301 (98%)	0.11	8 (2%)	54	50	32, 63, 106, 140	0
1	K	288/301 (95%)	0.15	13 (4%)	33	29	33, 62, 119, 148	0
1	L	291/301 (96%)	0.26	12 (4%)	37	32	34, 73, 121, 146	0
All	All	3543/3612 (98%)	-0.00	109 (3%)	49	44	7, 57, 112, 175	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	183	LYS	5.4
1	D	175	GLY	5.2
1	J	48	ASP	5.1
1	I	230	LYS	4.8
1	E	175	GLY	4.7

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	I	937	5/5	0.79	0.26	54,57,60,62	5
2	MG	J	907	1/1	0.85	0.28	64,64,64,64	0
4	ARS	E	955	1/1	0.85	0.11	117,117,117,117	0
4	ARS	I	959	1/1	0.85	0.19	134,134,134,134	0
4	ARS	C	953	1/1	0.87	0.10	98,98,98,98	0
3	SO4	L	946	5/5	0.90	0.19	52,53,56,57	5
4	ARS	K	961	1/1	0.91	0.14	124,124,124,124	0
3	SO4	G	931	5/5	0.92	0.16	53,56,59,62	5
3	SO4	A	913	5/5	0.93	0.14	53,54,56,57	5
4	ARS	J	960	1/1	0.93	0.08	104,104,104,104	0
4	ARS	F	956	1/1	0.93	0.09	85,85,85,85	0
3	SO4	D	922	5/5	0.94	0.16	49,51,57,58	5
3	SO4	J	939	5/5	0.94	0.14	54,58,65,66	0
3	SO4	E	924	5/5	0.94	0.15	65,66,69,72	0
4	ARS	B	952	1/1	0.94	0.10	95,95,95,95	0
3	SO4	C	918	5/5	0.94	0.15	59,66,71,72	0
4	ARS	A	951	1/1	0.95	0.08	103,103,103,103	0
3	SO4	E	925	5/5	0.95	0.12	45,48,49,50	5
3	SO4	F	928	5/5	0.95	0.13	44,51,53,54	5
2	MG	B	902	1/1	0.95	0.18	43,43,43,43	0
3	SO4	C	919	5/5	0.95	0.25	62,64,67,68	5
4	ARS	G	957	1/1	0.95	0.07	83,83,83,83	0
2	MG	E	905	1/1	0.95	0.26	51,51,51,51	0
3	SO4	K	943	5/5	0.95	0.12	48,49,52,52	5
3	SO4	B	915	5/5	0.95	0.15	48,55,58,65	0
3	SO4	F	927	5/5	0.96	0.12	52,57,67,68	0
3	SO4	L	945	5/5	0.96	0.10	64,65,65,70	0
3	SO4	I	936	5/5	0.96	0.09	54,60,64,65	0
2	MG	A	901	1/1	0.96	0.48	66,66,66,66	0
3	SO4	G	930	5/5	0.96	0.12	57,63,69,70	0
3	SO4	J	940	5/5	0.96	0.16	54,58,61,63	5
3	SO4	H	932	5/5	0.97	0.12	46,48,52,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ARS	D	954	1/1	0.97	0.08	103,103,103,103	0
3	SO4	K	942	5/5	0.97	0.11	53,54,62,63	0
3	SO4	H	933	5/5	0.97	0.10	69,70,75,76	0
3	SO4	H	934	5/5	0.97	0.16	50,50,52,52	5
4	ARS	H	958	1/1	0.97	0.07	113,113,113,113	0
3	SO4	B	916	5/5	0.97	0.12	47,50,54,55	5
3	SO4	D	921	5/5	0.97	0.12	52,57,62,64	0
3	SO4	A	912	5/5	0.97	0.12	47,51,60,61	0
3	SO4	I	935	5/5	0.98	0.08	54,57,63,65	0
3	SO4	E	923	5/5	0.98	0.09	49,52,53,59	0
3	SO4	L	944	5/5	0.98	0.09	60,60,62,62	0
2	MG	H	906	1/1	0.98	0.12	81,81,81,81	0
3	SO4	J	938	5/5	0.98	0.09	45,46,52,55	0
3	SO4	G	929	5/5	0.98	0.11	39,42,51,52	0
2	MG	C	903	1/1	0.98	0.32	57,57,57,57	0
3	SO4	K	941	5/5	0.98	0.10	42,42,48,49	0
3	SO4	C	917	5/5	0.99	0.06	27,30,38,51	0
3	SO4	B	914	5/5	0.99	0.08	26,29,35,41	0
2	MG	D	904	1/1	0.99	0.25	52,52,52,52	0
3	SO4	D	920	5/5	0.99	0.09	23,31,37,44	0
3	SO4	F	926	5/5	0.99	0.08	31,31,36,39	0
3	SO4	A	911	5/5	0.99	0.08	32,32,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.