



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 03:41 PM UTC

PDB ID : 8RVR / pdb_00008rvr
Title : Crystal structure of Trypanosoma congolense pyruvate kinase in complex with a single-domain antibody (TcoPYK-sdAb42) in the presence of sulfate
Authors : Sterckx, Y.G.-J.
Deposited on : 2024-02-02
Resolution : 3.19 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 ⓘ 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

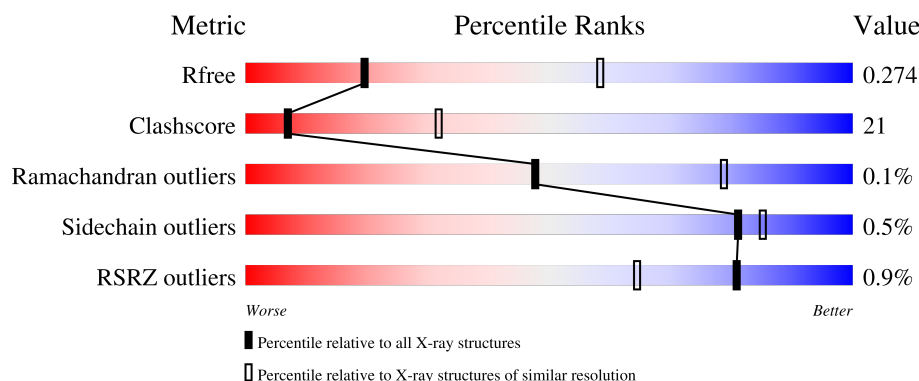
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	514	% 62% 33% ..
1	B	514	50% 28% 21%
1	C	514	2% 60% 35% ..
1	D	514	% 62% 35% .
1	E	514	48% 29% 23%

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Mol	Chain	Length	Quality of chain
1	F	514	
2	G	149	
2	H	149	
2	I	149	
2	J	149	
2	K	149	
2	L	149	

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
4	GOL	C	603	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25987 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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			3681	2295	647	713	26			
1	B	404	Total	C	N	O	S	0	0	0
			3002	1862	540	577	23			
1	C	498	Total	C	N	O	S	0	1	0
			3667	2284	653	704	26			
1	D	498	Total	C	N	O	S	0	1	0
			3680	2294	650	710	26			
1	E	397	Total	C	N	O	S	0	0	0
			2927	1811	524	569	23			
1	F	399	Total	C	N	O	S	0	0	0
			2904	1804	515	562	23			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	500	GLU	-	expression tag	UNP G0UYF4
A	501	ASN	-	expression tag	UNP G0UYF4
A	502	LEU	-	expression tag	UNP G0UYF4
A	503	TYR	-	expression tag	UNP G0UYF4
A	504	PHE	-	expression tag	UNP G0UYF4
A	505	GLN	-	expression tag	UNP G0UYF4
A	506	SER	-	expression tag	UNP G0UYF4
A	507	GLY	-	expression tag	UNP G0UYF4
A	508	GLY	-	expression tag	UNP G0UYF4
A	509	HIS	-	expression tag	UNP G0UYF4
A	510	HIS	-	expression tag	UNP G0UYF4
A	511	HIS	-	expression tag	UNP G0UYF4
A	512	HIS	-	expression tag	UNP G0UYF4
A	513	HIS	-	expression tag	UNP G0UYF4
A	514	HIS	-	expression tag	UNP G0UYF4
B	500	GLU	-	expression tag	UNP G0UYF4
B	501	ASN	-	expression tag	UNP G0UYF4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	502	LEU	-	expression tag	UNP G0UYF4
B	503	TYR	-	expression tag	UNP G0UYF4
B	504	PHE	-	expression tag	UNP G0UYF4
B	505	GLN	-	expression tag	UNP G0UYF4
B	506	SER	-	expression tag	UNP G0UYF4
B	507	GLY	-	expression tag	UNP G0UYF4
B	508	GLY	-	expression tag	UNP G0UYF4
B	509	HIS	-	expression tag	UNP G0UYF4
B	510	HIS	-	expression tag	UNP G0UYF4
B	511	HIS	-	expression tag	UNP G0UYF4
B	512	HIS	-	expression tag	UNP G0UYF4
B	513	HIS	-	expression tag	UNP G0UYF4
B	514	HIS	-	expression tag	UNP G0UYF4
C	500	GLU	-	expression tag	UNP G0UYF4
C	501	ASN	-	expression tag	UNP G0UYF4
C	502	LEU	-	expression tag	UNP G0UYF4
C	503	TYR	-	expression tag	UNP G0UYF4
C	504	PHE	-	expression tag	UNP G0UYF4
C	505	GLN	-	expression tag	UNP G0UYF4
C	506	SER	-	expression tag	UNP G0UYF4
C	507	GLY	-	expression tag	UNP G0UYF4
C	508	GLY	-	expression tag	UNP G0UYF4
C	509	HIS	-	expression tag	UNP G0UYF4
C	510	HIS	-	expression tag	UNP G0UYF4
C	511	HIS	-	expression tag	UNP G0UYF4
C	512	HIS	-	expression tag	UNP G0UYF4
C	513	HIS	-	expression tag	UNP G0UYF4
C	514	HIS	-	expression tag	UNP G0UYF4
D	500	GLU	-	expression tag	UNP G0UYF4
D	501	ASN	-	expression tag	UNP G0UYF4
D	502	LEU	-	expression tag	UNP G0UYF4
D	503	TYR	-	expression tag	UNP G0UYF4
D	504	PHE	-	expression tag	UNP G0UYF4
D	505	GLN	-	expression tag	UNP G0UYF4
D	506	SER	-	expression tag	UNP G0UYF4
D	507	GLY	-	expression tag	UNP G0UYF4
D	508	GLY	-	expression tag	UNP G0UYF4
D	509	HIS	-	expression tag	UNP G0UYF4
D	510	HIS	-	expression tag	UNP G0UYF4
D	511	HIS	-	expression tag	UNP G0UYF4
D	512	HIS	-	expression tag	UNP G0UYF4
D	513	HIS	-	expression tag	UNP G0UYF4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	514	HIS	-	expression tag	UNP G0UYF4
E	500	GLU	-	expression tag	UNP G0UYF4
E	501	ASN	-	expression tag	UNP G0UYF4
E	502	LEU	-	expression tag	UNP G0UYF4
E	503	TYR	-	expression tag	UNP G0UYF4
E	504	PHE	-	expression tag	UNP G0UYF4
E	505	GLN	-	expression tag	UNP G0UYF4
E	506	SER	-	expression tag	UNP G0UYF4
E	507	GLY	-	expression tag	UNP G0UYF4
E	508	GLY	-	expression tag	UNP G0UYF4
E	509	HIS	-	expression tag	UNP G0UYF4
E	510	HIS	-	expression tag	UNP G0UYF4
E	511	HIS	-	expression tag	UNP G0UYF4
E	512	HIS	-	expression tag	UNP G0UYF4
E	513	HIS	-	expression tag	UNP G0UYF4
E	514	HIS	-	expression tag	UNP G0UYF4
F	500	GLU	-	expression tag	UNP G0UYF4
F	501	ASN	-	expression tag	UNP G0UYF4
F	502	LEU	-	expression tag	UNP G0UYF4
F	503	TYR	-	expression tag	UNP G0UYF4
F	504	PHE	-	expression tag	UNP G0UYF4
F	505	GLN	-	expression tag	UNP G0UYF4
F	506	SER	-	expression tag	UNP G0UYF4
F	507	GLY	-	expression tag	UNP G0UYF4
F	508	GLY	-	expression tag	UNP G0UYF4
F	509	HIS	-	expression tag	UNP G0UYF4
F	510	HIS	-	expression tag	UNP G0UYF4
F	511	HIS	-	expression tag	UNP G0UYF4
F	512	HIS	-	expression tag	UNP G0UYF4
F	513	HIS	-	expression tag	UNP G0UYF4
F	514	HIS	-	expression tag	UNP G0UYF4

- Molecule 2 is a protein called Camelid single-domain antibody 42 (sdAb42).

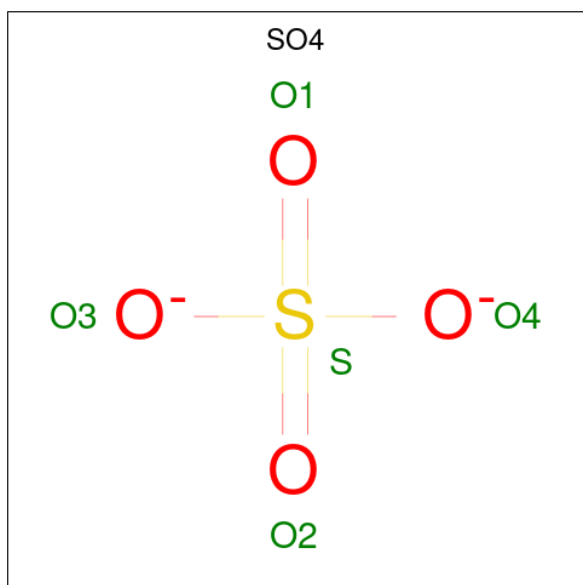
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	130	Total	C	N	O	S	0	0	0
			995	622	173	197	3			
2	H	130	Total	C	N	O	S	0	0	0
			998	623	173	199	3			
2	I	130	Total	C	N	O	S	0	0	0
			976	610	167	196	3			
2	J	131	Total	C	N	O	S	0	0	0
			1007	628	175	201	3			

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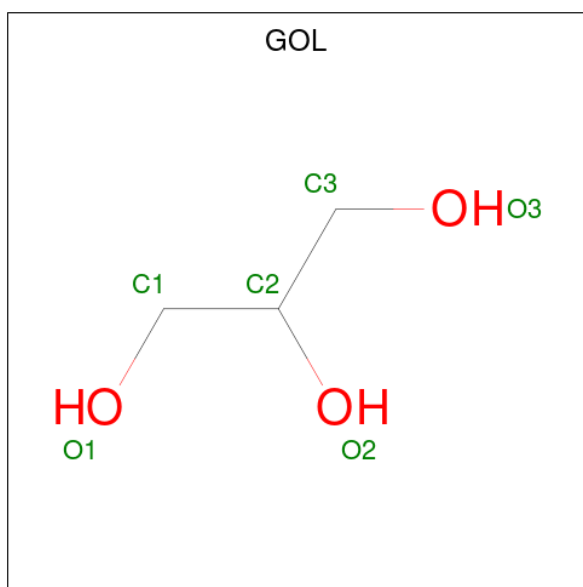
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	130	Total	C	N	O	S	0	0	0
			967	603	165	196	3			
2	L	130	Total	C	N	O	S	0	0	0
			942	585	160	194	3			

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



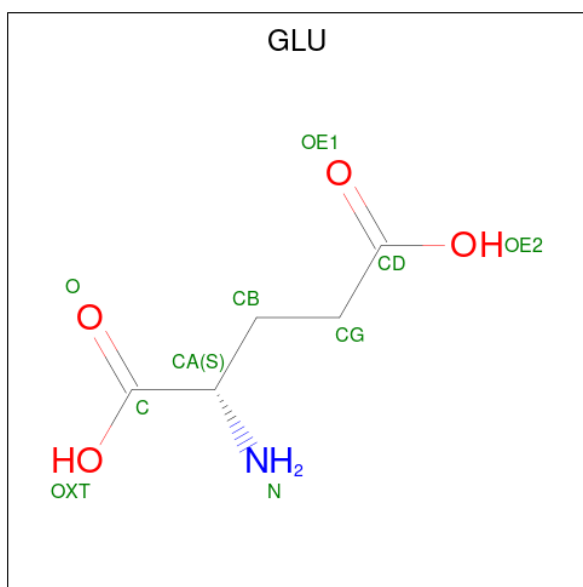
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	D	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	28	Total	O	0	0
			28	28		
6	B	14	Total	O	0	0
			14	14		
6	C	32	Total	O	0	0
			32	32		
6	D	17	Total	O	0	0
			17	17		
6	E	8	Total	O	0	0
			8	8		
6	F	8	Total	O	0	0
			8	8		
6	G	1	Total	O	0	0
			1	1		
6	H	3	Total	O	0	0
			3	3		
6	I	1	Total	O	0	0
			1	1		
6	J	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	K	1	Total	O	0	0
			1	1		
6	L	2	Total	O	0	0
			2	2		

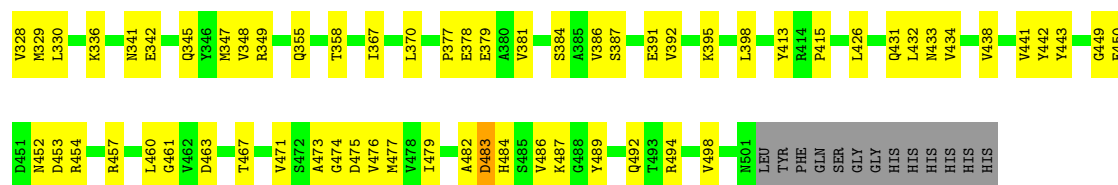
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

Chain A: %

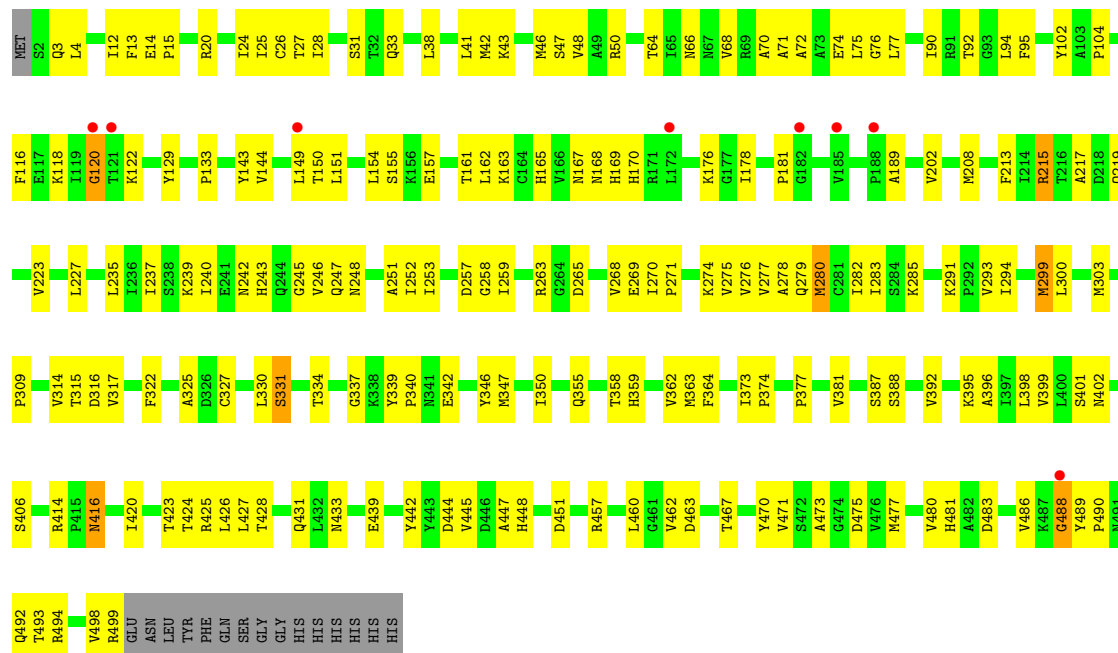
62% 33%

Sequence logo for Chain A showing amino acid conservation across 277 positions. The y-axis lists amino acids, and the x-axis shows positions 1 to 277. A color scale at the top indicates conservation from 0% (grey) to 62% (green) to 33% (yellow). The logo shows high conservation in the N-terminal region (positions 1-100) and lower conservation in the C-terminal region (positions 200-277).

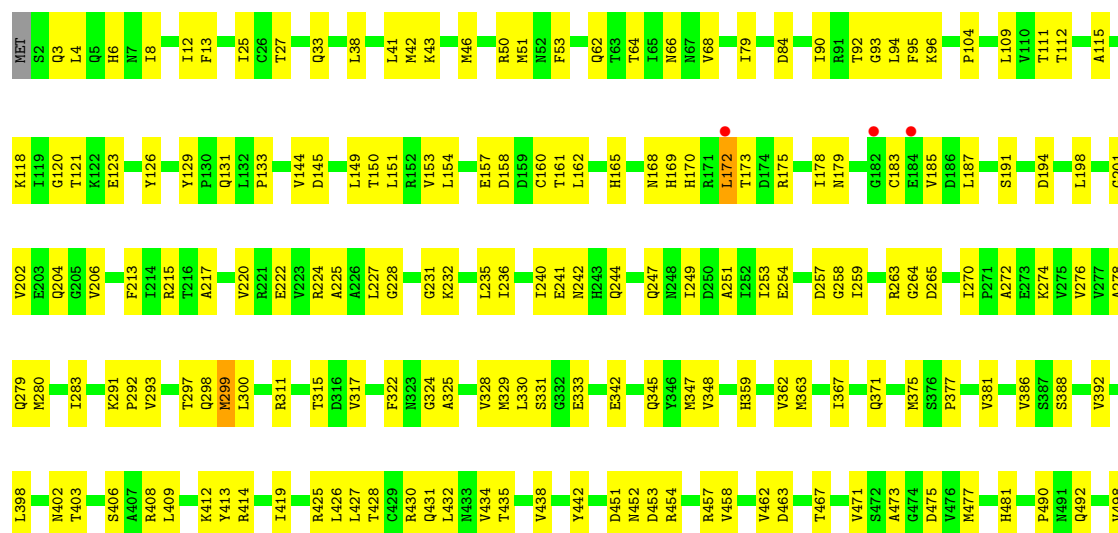
[illegible]



• Molecule 1: Pyruvate kinase



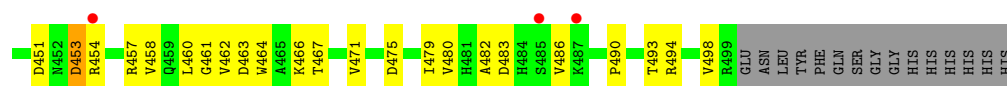
• Molecule 1: Pyruvate kinase



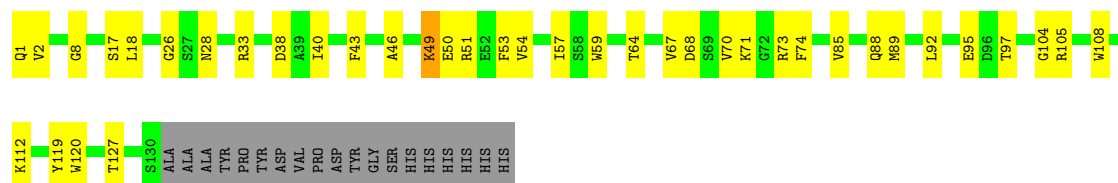
- Molecule 1: Pyruvate kinase

- Molecule 1: Pyruvate kinase

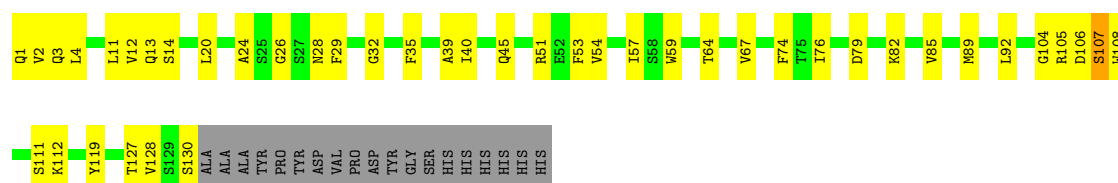
V362	V363	V364	V365	V366	V367	V368	V370	V373	V374	V375	V376	V377	V378	V381	V386	V387	V388	V389	V390	V391	V392	V393	V394	V395	V396	V397	V398	V399	V400	A407	A410	A411	A412	A413	A414	A415	A416	A417	A431	A432	A433	A434	A435	A436	A437	A438	V441	D444	A447
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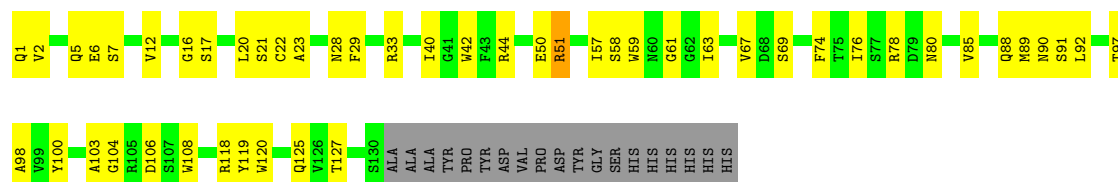
• Molecule 2: Camelid single-domain antibody 42 (sdAb42)



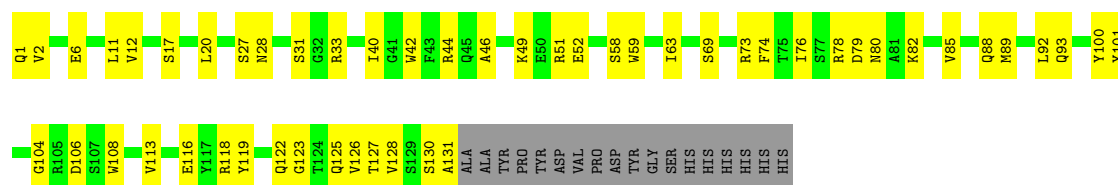
• Molecule 2: Camelid single-domain antibody 42 (sdAb42)



• Molecule 2: Camelid single-domain antibody 42 (sdAb42)



• Molecule 2: Camelid single-domain antibody 42 (sdAb42)

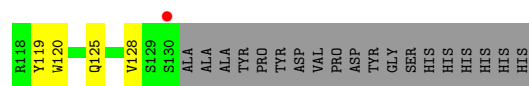


• Molecule 2: Camelid single-domain antibody 42 (sdAb42)





Chain L: 58% 30% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	167.52Å 168.42Å 177.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 3.19 49.32 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.32-3.19) 99.8 (49.32-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.221 , 0.275 0.223 , 0.274	Depositor DCC
R_{free} test set	4176 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	88.2	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 92.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.038 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25987	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.24% 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, GOL

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	0.56	0/3738	1.04	23/5091 (0.5%)
1	B	0.53	0/3043	0.82	8/4131 (0.2%)
1	C	0.54	0/3728	0.94	10/5077 (0.2%)
1	D	0.50	0/3740	0.84	8/5093 (0.2%)
1	E	0.47	0/2965	0.78	1/4026 (0.0%)
1	F	0.47	0/2943	0.90	10/4005 (0.2%)
2	G	0.54	0/1018	0.86	3/1377 (0.2%)
2	H	0.49	0/1021	0.78	2/1381 (0.1%)
2	I	0.40	0/999	0.81	3/1356 (0.2%)
2	J	0.50	0/1030	0.75	0/1393
2	K	0.35	0/989	0.78	3/1343 (0.2%)
2	L	0.34	0/964	0.73	0/1314
All	All	0.50	0/26178	0.87	71/35587 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	F	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	120	GLY	N-CA-C	22.38	146.16	113.48
1	A	296	ALA	N-CA-C	18.80	139.60	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	17	ALA	N-CA-C	12.51	128.31	111.30
1	A	336	LYS	CA-C-N	-12.20	111.61	122.47
1	A	336	LYS	C-N-CA	-12.20	111.61	122.47

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	168	ASN	Peptide
1	C	373	ILE	Peptide
1	F	233	ASP	Peptide
1	F	373	ILE	Peptide

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	3681	0	3587	147	0
1	B	3002	0	2966	132	0
1	C	3667	0	3560	169	0
1	D	3680	0	3597	158	0
1	E	2927	0	2854	122	0
1	F	2904	0	2824	162	0
2	G	995	0	932	31	0
2	H	998	0	934	42	0
2	I	976	0	891	52	0
2	J	1007	0	945	42	0
2	K	967	0	879	40	0
2	L	942	0	818	37	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	B	18	0	24	0	0
4	C	18	0	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	12	0	16	1	0
4	E	6	0	8	0	0
4	G	6	0	6	0	0
4	H	6	0	7	0	0
4	I	6	0	8	1	0
4	J	6	0	7	0	0
5	C	5	0	1	1	0
5	D	5	0	1	0	0
6	A	28	0	0	2	0
6	B	14	0	0	0	0
6	C	32	0	0	1	0
6	D	17	0	0	2	0
6	E	8	0	0	0	0
6	F	8	0	0	0	0
6	G	1	0	0	1	0
6	H	3	0	0	0	0
6	I	1	0	0	1	0
6	J	8	0	0	0	0
6	K	1	0	0	1	0
6	L	2	0	0	0	0
All	All	25987	0	24888	1072	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 1072 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)
2:H:1:GLN:HG3	2:H:2:VAL:H	1.09	1.10
1:A:93:GLY:HA3	1:A:175:ARG:H	1.14	1.09
1:D:158:ASP:HB2	1:D:161:THR:HG22	1.46	0.96
1:F:432:LEU:HD13	1:F:438:VAL:HG11	1.44	0.95
2:H:1:GLN:HG3	2:H:2:VAL:N	1.82	0.95

There are no symmetry-related clashes.

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	497/514 (97%)	454 (91%)	43 (9%)	0	100	100
1	B	400/514 (78%)	385 (96%)	15 (4%)	0	100	100
1	C	497/514 (97%)	464 (93%)	33 (7%)	0	100	100
1	D	497/514 (97%)	470 (95%)	27 (5%)	0	100	100
1	E	391/514 (76%)	369 (94%)	21 (5%)	1 (0%)	36	68
1	F	395/514 (77%)	365 (92%)	29 (7%)	1 (0%)	36	68
2	G	128/149 (86%)	125 (98%)	3 (2%)	0	100	100
2	H	128/149 (86%)	126 (98%)	2 (2%)	0	100	100
2	I	128/149 (86%)	125 (98%)	3 (2%)	0	100	100
2	J	129/149 (87%)	126 (98%)	3 (2%)	0	100	100
2	K	128/149 (86%)	123 (96%)	5 (4%)	0	100	100
2	L	128/149 (86%)	124 (97%)	4 (3%)	0	100	100
All	All	3446/3978 (87%)	3256 (94%)	188 (6%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	374	PRO
1	E	374	PRO

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	390/435 (90%)	388 (100%)	2 (0%)	81	85
1	B	321/435 (74%)	320 (100%)	1 (0%)	86	88
1	C	385/435 (88%)	382 (99%)	3 (1%)	73	82
1	D	391/435 (90%)	387 (99%)	4 (1%)	68	80
1	E	309/435 (71%)	307 (99%)	2 (1%)	78	84
1	F	304/435 (70%)	304 (100%)	0	100	100
2	G	104/121 (86%)	104 (100%)	0	100	100
2	H	105/121 (87%)	104 (99%)	1 (1%)	68	80
2	I	100/121 (83%)	100 (100%)	0	100	100
2	J	106/121 (88%)	106 (100%)	0	100	100
2	K	99/121 (82%)	99 (100%)	0	100	100
2	L	92/121 (76%)	92 (100%)	0	100	100
All	All	2706/3336 (81%)	2693 (100%)	13 (0%)	81	85

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	185	VAL
1	D	187	LEU
2	H	107	SER
1	E	263	ARG
1	E	425	ARG

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

Mol	Chain	Res	Type
1	E	6	HIS
1	F	6	HIS
1	E	33	GLN
1	E	416	ASN
1	F	298	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

21 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	$\# Z > 2$
4	GOL	C	603	-	5,5,5	1.79	2 (40%)	5,5,5	0.77	0
4	GOL	B	604	-	5,5,5	1.54	2 (40%)	5,5,5	0.97	0
4	GOL	G	201	-	5,5,5	1.79	1 (20%)	5,5,5	1.79	3 (60%)
3	SO4	C	605	-	4,4,4	0.31	0	6,6,6	0.56	0
5	GLU	D	601	-	3,4,9	0.92	0	2,4,11	0.71	0
4	GOL	B	603	-	5,5,5	0.87	0	5,5,5	1.25	1 (20%)
4	GOL	J	201	-	5,5,5	1.38	1 (20%)	5,5,5	1.42	1 (20%)
4	GOL	I	201	-	5,5,5	0.89	0	5,5,5	1.75	2 (40%)
4	GOL	B	602	-	5,5,5	1.36	1 (20%)	5,5,5	1.12	0
4	GOL	C	604	-	5,5,5	1.36	1 (20%)	5,5,5	1.12	1 (20%)
4	GOL	E	601	-	5,5,5	0.96	0	5,5,5	1.03	0
3	SO4	E	602	-	4,4,4	0.42	0	6,6,6	0.76	0
4	GOL	D	602	-	5,5,5	1.11	0	5,5,5	1.06	0
3	SO4	F	601	-	4,4,4	0.37	0	6,6,6	0.50	0
3	SO4	D	604	-	4,4,4	0.18	0	6,6,6	0.81	0
3	SO4	A	601	-	4,4,4	0.41	0	6,6,6	0.70	0
4	GOL	C	602	-	5,5,5	1.35	1 (20%)	5,5,5	1.31	0
4	GOL	D	603	-	5,5,5	0.94	0	5,5,5	1.06	0
3	SO4	B	601	-	4,4,4	0.53	0	6,6,6	0.59	0
5	GLU	C	601	-	3,4,9	0.68	0	2,4,11	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	H	201	-	5,5,5	1.34	1 (20%)	5,5,5	1.43	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
4	GOL	C	604	-	-	1/4/4/4	-
4	GOL	C	603	-	-	4/4/4/4	-
4	GOL	B	604	-	-	2/4/4/4	-
4	GOL	G	201	-	-	0/4/4/4	-
4	GOL	D	603	-	-	2/4/4/4	-
5	GLU	D	601	-	-	0/1/2/9	-
4	GOL	B	603	-	-	4/4/4/4	-
4	GOL	J	201	-	-	3/4/4/4	-
4	GOL	C	602	-	-	3/4/4/4	-
4	GOL	E	601	-	-	1/4/4/4	-
4	GOL	I	201	-	-	0/4/4/4	-
5	GLU	C	601	-	-	0/1/2/9	-
4	GOL	H	201	-	-	2/4/4/4	-
4	GOL	D	602	-	-	2/4/4/4	-
4	GOL	B	602	-	-	4/4/4/4	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	201	GOL	O2-C2	-3.32	1.33	1.43
4	J	201	GOL	O2-C2	-2.82	1.35	1.43
4	C	603	GOL	C3-C2	2.73	1.62	1.51
4	C	603	GOL	C1-C2	2.68	1.62	1.51
4	H	201	GOL	O2-C2	-2.60	1.35	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	201	GOL	C3-C2-C1	-2.27	103.46	111.80
4	I	201	GOL	C3-C2-C1	-2.26	103.49	111.80
4	G	201	GOL	O1-C1-C2	-2.18	100.54	110.38
4	B	603	GOL	C3-C2-C1	-2.18	103.82	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	201	GOL	C3-C2-C1	-2.17	103.85	111.80

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	602	GOL	O1-C1-C2-C3
4	B	602	GOL	C1-C2-C3-O3
4	B	604	GOL	O1-C1-C2-C3
4	C	603	GOL	O1-C1-C2-C3
4	D	603	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	605	SO4	1	0
4	I	201	GOL	1	0
4	D	603	GOL	1	0
5	C	601	GLU	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 [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	499/514 (97%)	-0.18	6 (1%) 76 58	57, 79, 214, 272	0
1	B	404/514 (78%)	-0.32	1 (0%) 91 85	61, 85, 131, 226	0
1	C	498/514 (96%)	-0.18	8 (1%) 70 51	61, 83, 194, 247	1 (0%)
1	D	498/514 (96%)	-0.24	3 (0%) 85 73	68, 97, 169, 261	1 (0%)
1	E	397/514 (77%)	-0.15	2 (0%) 87 76	85, 115, 154, 190	0
1	F	399/514 (77%)	0.14	8 (2%) 65 45	104, 135, 181, 258	0
2	G	130/149 (87%)	-0.37	0 100 100	68, 86, 108, 143	0
2	H	130/149 (87%)	-0.31	0 100 100	76, 95, 138, 171	0
2	I	130/149 (87%)	-0.06	0 100 100	85, 130, 188, 212	0
2	J	131/149 (87%)	-0.35	0 100 100	67, 91, 126, 158	0
2	K	130/149 (87%)	0.19	1 (0%) 82 67	120, 163, 220, 261	0
2	L	130/149 (87%)	0.10	1 (0%) 82 67	132, 167, 225, 264	0
All	All	3476/3978 (87%)	-0.15	30 (0%) 81 64	57, 104, 194, 272	2 (0%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	295	CYS	3.1
1	F	237	ILE	2.9
1	D	184	GLU	2.9
1	A	185	VAL	2.9
1	A	141	LEU	2.8

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 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
5	GLU	C	601	5/10	0.38	0.20	93,100,104,104	0
5	GLU	D	601	5/10	0.51	0.21	106,107,108,111	0
4	GOL	C	603	6/6	0.56	0.21	88,100,103,103	0
4	GOL	C	602	6/6	0.63	0.12	85,89,91,100	0
4	GOL	I	201	6/6	0.68	0.10	107,109,113,115	0
4	GOL	B	604	6/6	0.75	0.14	104,112,114,114	0
4	GOL	E	601	6/6	0.76	0.09	134,137,138,138	0
4	GOL	J	201	6/6	0.80	0.12	96,105,110,110	0
4	GOL	H	201	6/6	0.84	0.08	90,98,102,107	0
4	GOL	D	603	6/6	0.85	0.11	83,86,87,89	0
4	GOL	B	603	6/6	0.88	0.09	84,88,89,89	0
3	SO4	E	602	5/5	0.90	0.13	121,124,132,140	0
3	SO4	F	601	5/5	0.90	0.07	146,148,154,168	0
4	GOL	G	201	6/6	0.90	0.10	72,77,86,90	0
3	SO4	B	601	5/5	0.90	0.10	102,104,114,131	0
4	GOL	C	604	6/6	0.91	0.16	67,68,71,77	0
4	GOL	B	602	6/6	0.92	0.11	76,77,87,89	0
4	GOL	D	602	6/6	0.93	0.09	79,86,89,90	0
3	SO4	C	605	5/5	0.93	0.15	85,94,108,109	0
3	SO4	D	604	5/5	0.93	0.10	110,111,114,120	0
3	SO4	A	601	5/5	0.96	0.09	89,92,105,106	0

6.5 Other polymers [i](#)

There are no such residues in this entry.