



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 7, 2025 – 05:40 pm BST

PDB ID : 8RTF / pdb_00008rtf
Title : Crystal structure of Trypanosoma congolense pyruvate kinase in complex with a single-domain antibody (TcoPYK-sdAb42)
Authors : Sterckx, Y.G.-J.
Deposited on : 2024-01-26
Resolution : 2.80 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

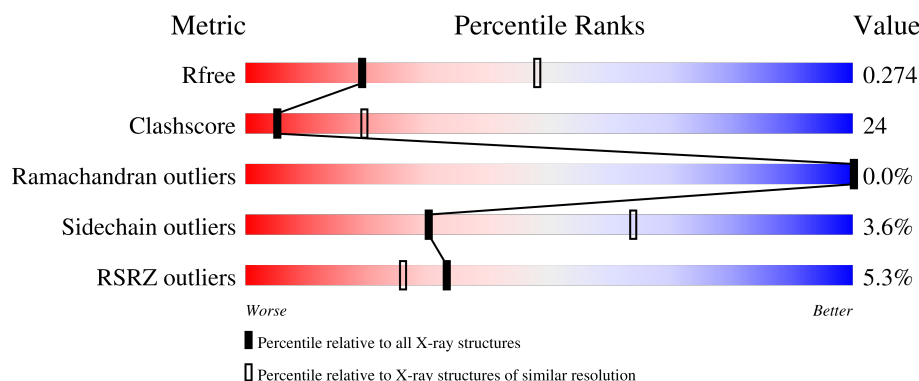
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>30%</div> <div>• •</div> </div> </div>
1	B	514	<div> <div>0%</div> <div> <div></div> <div>50%</div> <div>27%</div> <div>•</div> <div>21%</div> </div> </div>
1	C	514	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>34%</div> <div>• •</div> </div> </div>
1	D	514	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>33%</div> <div>• •</div> </div> </div>
1	E	514	<div> <div>5%</div> <div> <div></div> <div>46%</div> <div>28%</div> <div>•</div> <div>23%</div> </div> </div>

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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
3	GOL	A	601	-	X	-	-
3	GOL	B	701	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 25898 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
			3687	2298	650	713	26			
1	B	404	Total	C	N	O	S	0	0	0
			2996	1859	537	577	23			
1	C	499	Total	C	N	O	S	0	1	0
			3672	2287	654	705	26			
1	D	499	Total	C	N	O	S	0	1	0
			3691	2300	654	711	26			
1	E	395	Total	C	N	O	S	0	0	0
			2920	1807	525	565	23			
1	F	399	Total	C	N	O	S	0	0	0
			2901	1802	515	562	22			

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	515	GLU	-	expression tag	UNP G0UYF4
C	516	ASN	-	expression tag	UNP G0UYF4
C	517	LEU	-	expression tag	UNP G0UYF4
C	518	TYR	-	expression tag	UNP G0UYF4
C	519	PHE	-	expression tag	UNP G0UYF4
C	520	GLN	-	expression tag	UNP G0UYF4
C	521	SER	-	expression tag	UNP G0UYF4
C	522	GLY	-	expression tag	UNP G0UYF4
C	523	GLY	-	expression tag	UNP G0UYF4
C	524	HIS	-	expression tag	UNP G0UYF4
C	525	HIS	-	expression tag	UNP G0UYF4
C	526	HIS	-	expression tag	UNP G0UYF4
C	527	HIS	-	expression tag	UNP G0UYF4
C	528	HIS	-	expression tag	UNP G0UYF4
C	529	HIS	-	expression tag	UNP G0UYF4
D	515	GLU	-	expression tag	UNP G0UYF4
D	516	ASN	-	expression tag	UNP G0UYF4
D	517	LEU	-	expression tag	UNP G0UYF4
D	518	TYR	-	expression tag	UNP G0UYF4
D	519	PHE	-	expression tag	UNP G0UYF4
D	520	GLN	-	expression tag	UNP G0UYF4
D	521	SER	-	expression tag	UNP G0UYF4
D	522	GLY	-	expression tag	UNP G0UYF4
D	523	GLY	-	expression tag	UNP G0UYF4
D	524	HIS	-	expression tag	UNP G0UYF4
D	525	HIS	-	expression tag	UNP G0UYF4
D	526	HIS	-	expression tag	UNP G0UYF4
D	527	HIS	-	expression tag	UNP G0UYF4
D	528	HIS	-	expression tag	UNP G0UYF4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	529	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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		

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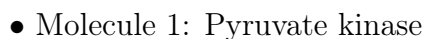
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			6	3	3		

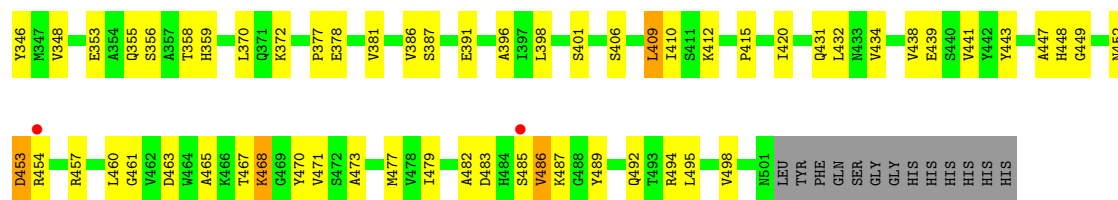
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	7	Total	O	0	0
			7	7		
4	C	25	Total	O	0	0
			25	25		
4	D	13	Total	O	0	0
			13	13		
4	E	5	Total	O	0	0
			5	5		
4	F	5	Total	O	0	0
			5	5		
4	G	2	Total	O	0	0
			2	2		
4	H	5	Total	O	0	0
			5	5		
4	I	1	Total	O	0	0
			1	1		
4	J	4	Total	O	0	0
			4	4		
4	L	1	Total	O	0	0
			1	1		

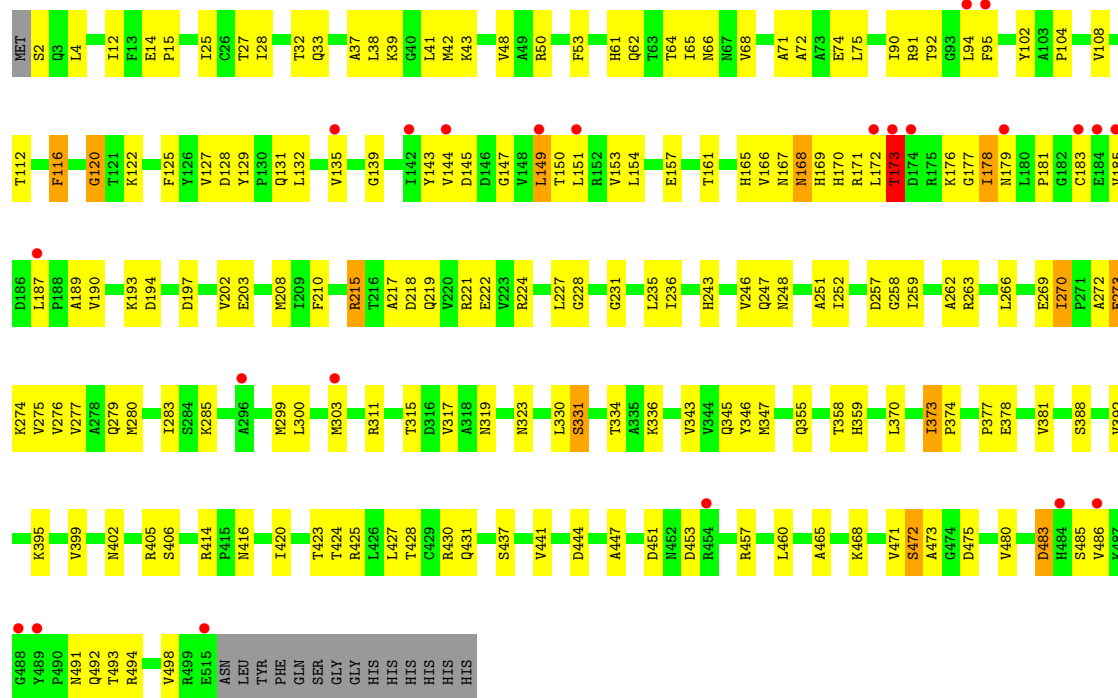
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- Molecule 1: Pyruvate kinase

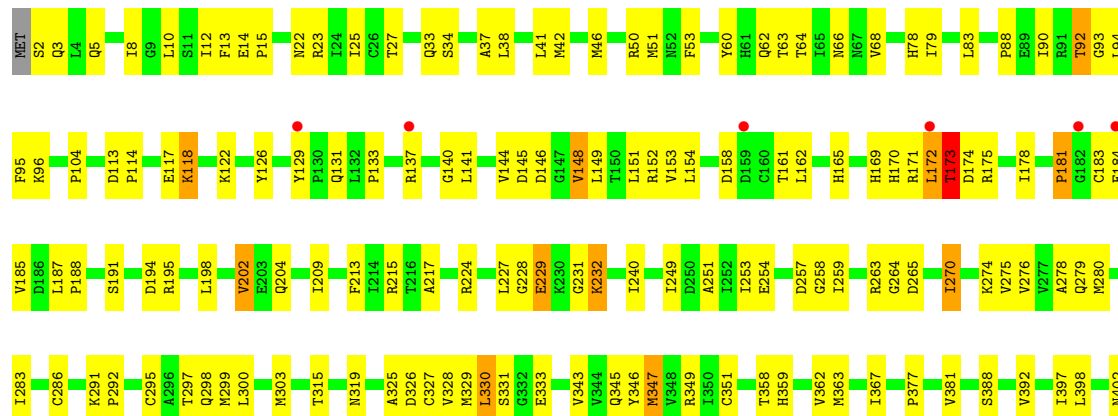


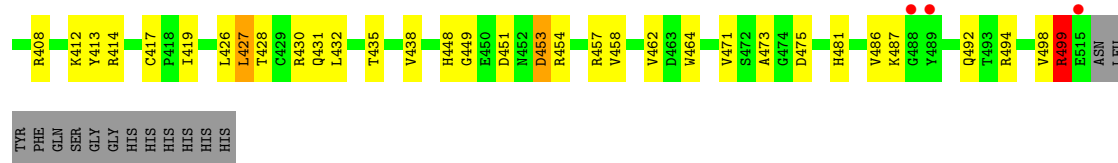


• Molecule 1: Pyruvate kinase

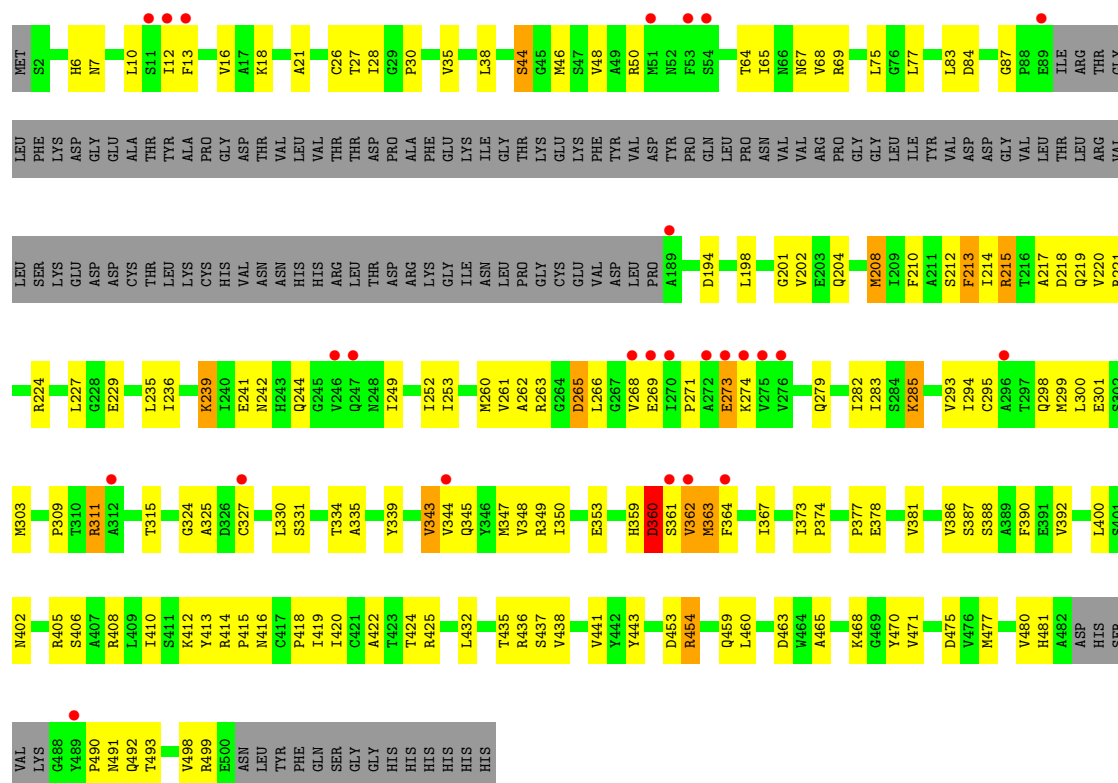


• Molecule 1: Pyruvate kinase

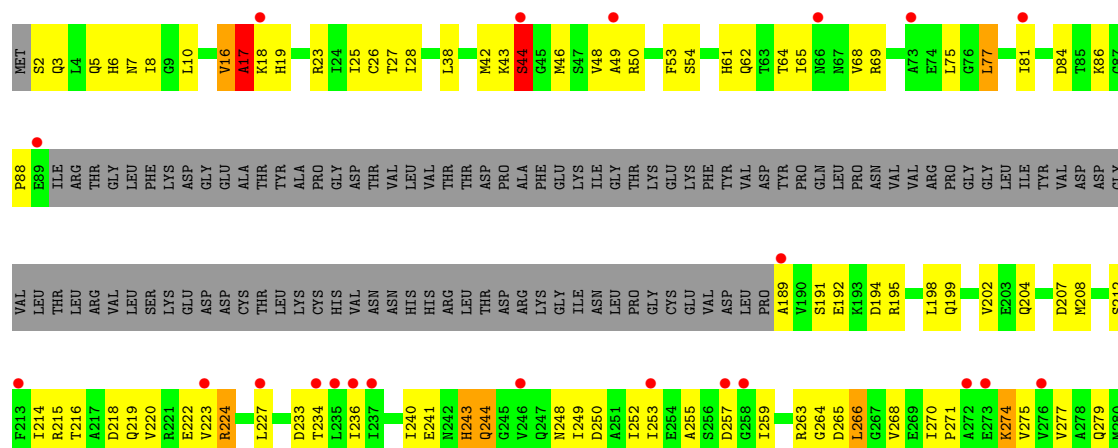




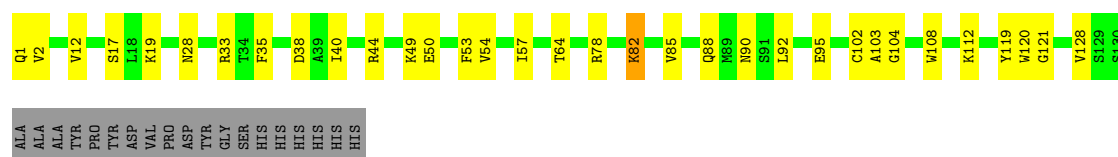
• Molecule 1: Pyruvate kinase



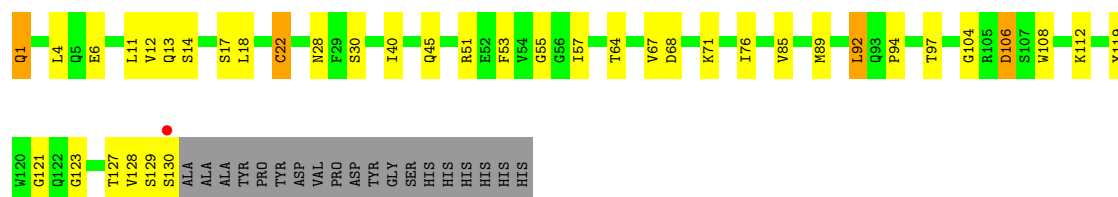
• Molecule 1: Pyruvate kinase



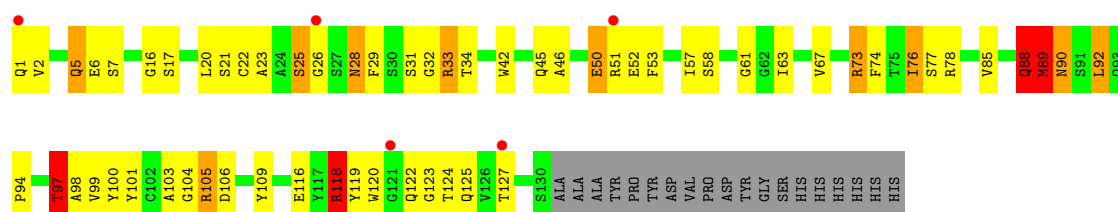
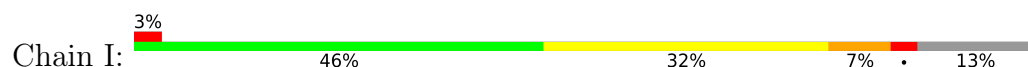
- Molecule 2: Camelid single-domain antibody 42 (sdAb42)



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

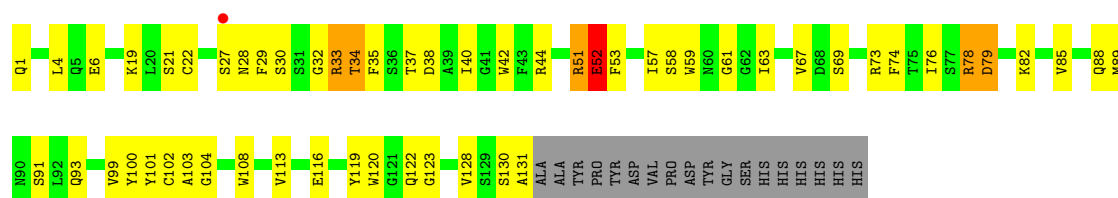


- Molecule 2: Camelid single-domain antibody 42 (sdAb42)

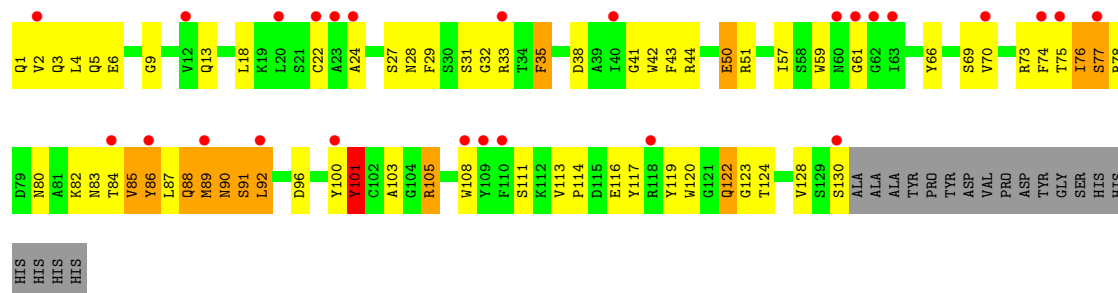
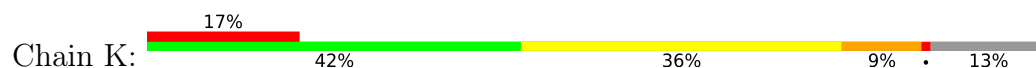


- Molecule 2: Camelid single-domain antibody 42 (sdAb42)

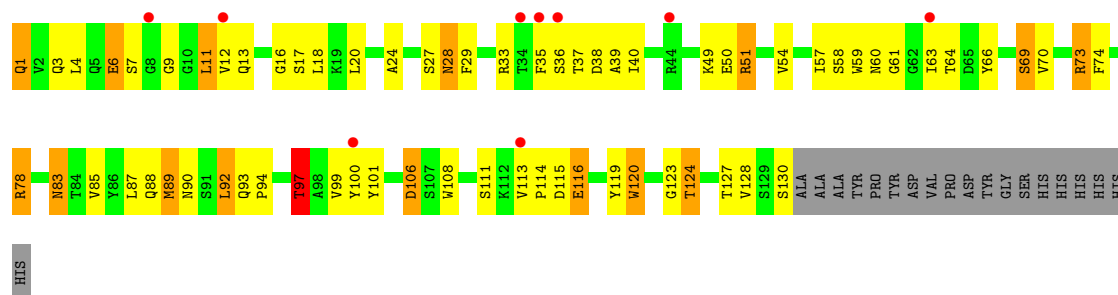
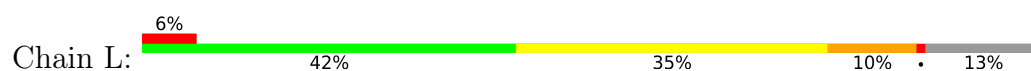




• Molecule 2: Camelid single-domain antibody 42 (sdAb42)



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



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 170.81Å 177.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.35 – 2.80 48.35 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.35-2.80) 99.8 (48.35-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.228 , 0.272 0.236 , 0.274	Depositor DCC
R_{free} test set	6274 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	84.9	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25898	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.29% 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:
 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	0.70	1/3744 (0.0%)	0.89	5/5098 (0.1%)
1	B	0.72	3/3037 (0.1%)	0.91	6/4124 (0.1%)
1	C	0.70	1/3733 (0.0%)	0.96	20/5084 (0.4%)
1	D	0.65	3/3751 (0.1%)	0.94	15/5107 (0.3%)
1	E	0.65	1/2958 (0.0%)	1.03	13/4015 (0.3%)
1	F	0.75	5/2940 (0.2%)	1.24	32/4002 (0.8%)
2	G	0.86	3/1018 (0.3%)	0.99	5/1377 (0.4%)
2	H	0.69	0/1021	0.96	3/1381 (0.2%)
2	I	0.75	2/999 (0.2%)	1.19	15/1356 (1.1%)
2	J	0.67	0/1030	1.03	7/1393 (0.5%)
2	K	0.82	3/989 (0.3%)	1.39	16/1343 (1.2%)
2	L	0.74	2/964 (0.2%)	1.30	16/1314 (1.2%)
All	All	0.71	24/26184 (0.1%)	1.03	153/35594 (0.4%)

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	A	0	1
1	B	0	1
1	C	0	4
1	D	0	3
1	E	0	1
1	F	0	8
2	G	0	1
2	I	0	5
2	J	0	2
2	K	0	5
2	L	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	35

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	91	SER	CB-OG	-14.07	1.24	1.42
1	F	374	PRO	N-CD	10.76	1.62	1.47
1	D	295	CYS	CB-SG	-9.04	1.66	1.82
1	F	391	GLU	C-O	8.36	1.39	1.23
2	I	88	GLN	CG-CD	-8.00	1.32	1.51

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	391	GLU	OE1-CD-OE2	-19.83	99.51	123.30
1	F	460	LEU	CB-CG-CD2	-17.60	81.09	111.00
2	L	51	ARG	CG-CD-NE	15.62	144.61	111.80
1	E	361	SER	N-CA-C	15.55	152.99	111.00
2	K	50	GLU	CB-CA-C	-15.33	79.74	110.40

There are no chirality outliers.

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	332	GLY	Peptide
1	B	372	LYS	Peptide
1	C	120	GLY	Peptide
1	C	168	ASN	Peptide
1	C	173	THR	Peptide

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	3687	0	3598	165	0
1	B	2996	0	2955	131	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3672	0	3562	187	0
1	D	3691	0	3610	167	0
1	E	2920	0	2857	143	1
1	F	2901	0	2817	176	7
2	G	995	0	932	30	1
2	H	998	0	934	33	0
2	I	976	0	891	72	0
2	J	1007	0	945	43	1
2	K	967	0	878	67	6
2	L	942	0	818	69	0
3	A	6	0	8	0	0
3	B	18	0	24	0	0
3	C	12	0	15	0	0
3	D	12	0	16	1	0
3	E	6	0	8	2	0
3	F	6	0	8	1	0
4	A	18	0	0	1	0
4	B	7	0	0	0	0
4	C	25	0	0	0	0
4	D	13	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	2	0	0	1	0
4	H	5	0	0	0	0
4	I	1	0	0	0	0
4	J	4	0	0	0	0
4	L	1	0	0	0	0
All	All	25898	0	24876	1216	8

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 24.

The worst 5 of 1216 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:G:82:LYS:NZ	2:G:82:LYS:CE	1.68	1.56
1:D:185:VAL:HG12	1:D:187:LEU:CD2	1.53	1.35
1:F:441:VAL:CG1	1:F:460:LEU:HD21	1.54	1.35
1:F:441:VAL:HG11	1:F:460:LEU:CD2	1.60	1.31
1:A:143:TYR:CD1	1:A:150:THR:HG22	1.66	1.29

The worst 5 of 8 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:F:274:LYS:NZ	2:K:108:TRP:CD1[3_455]	1.04	1.16
1:F:274:LYS:NZ	2:K:108:TRP:NE1[3_455]	1.49	0.71
1:F:274:LYS:NZ	2:K:108:TRP:CG[3_455]	1.59	0.61
1:E:311:ARG:NH2	1:F:316:ASP:OD1[3_445]	1.77	0.43
2:G:128:VAL:O	2:J:91:SER:OG[4_454]	2.10	0.10

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	497/514 (97%)	461 (93%)	36 (7%)	0	100	100
1	B	400/514 (78%)	386 (96%)	14 (4%)	0	100	100
1	C	498/514 (97%)	474 (95%)	23 (5%)	1 (0%)	44	73
1	D	498/514 (97%)	473 (95%)	25 (5%)	0	100	100
1	E	389/514 (76%)	370 (95%)	19 (5%)	0	100	100
1	F	395/514 (77%)	370 (94%)	25 (6%)	0	100	100
2	G	128/149 (86%)	126 (98%)	2 (2%)	0	100	100
2	H	128/149 (86%)	122 (95%)	6 (5%)	0	100	100
2	I	128/149 (86%)	121 (94%)	7 (6%)	0	100	100
2	J	129/149 (87%)	123 (95%)	6 (5%)	0	100	100
2	K	128/149 (86%)	122 (95%)	6 (5%)	0	100	100
2	L	128/149 (86%)	122 (95%)	6 (5%)	0	100	100
All	All	3446/3978 (87%)	3270 (95%)	175 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	374	PRO

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	391/435 (90%)	380 (97%)	11 (3%)	38	72
1	B	320/435 (74%)	314 (98%)	6 (2%)	52	82
1	C	385/435 (88%)	375 (97%)	10 (3%)	41	75
1	D	392/435 (90%)	377 (96%)	15 (4%)	28	62
1	E	309/435 (71%)	299 (97%)	10 (3%)	34	68
1	F	303/435 (70%)	284 (94%)	19 (6%)	15	42
2	G	104/121 (86%)	103 (99%)	1 (1%)	73	91
2	H	105/121 (87%)	103 (98%)	2 (2%)	52	82
2	I	100/121 (83%)	92 (92%)	8 (8%)	10	30
2	J	106/121 (88%)	103 (97%)	3 (3%)	38	72
2	K	99/121 (82%)	94 (95%)	5 (5%)	20	51
2	L	92/121 (76%)	84 (91%)	8 (9%)	8	26
All	All	2706/3336 (81%)	2608 (96%)	98 (4%)	30	64

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	281	CYS
2	G	102	CYS
1	F	299	MET
1	F	373	ILE
2	I	28	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	6	HIS
2	I	88	GLN
1	F	7	ASN
2	G	88	GLN
2	J	5	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
3	GOL	E	601	-	5,5,5	0.84	0	5,5,5	0.94	0
3	GOL	B	702	-	5,5,5	0.91	0	5,5,5	1.15	1 (20%)
3	GOL	B	701	-	5,5,5	1.47	2 (40%)	5,5,5	1.00	0
3	GOL	D	601	-	5,5,5	1.27	1 (20%)	5,5,5	0.95	0
3	GOL	C	602	-	5,5,5	1.44	2 (40%)	5,5,5	1.34	0
3	GOL	B	703	-	5,5,5	0.90	0	5,5,5	0.88	0
3	GOL	C	601	-	5,5,5	1.59	1 (20%)	5,5,5	1.44	1 (20%)
3	GOL	D	602	-	5,5,5	0.91	0	5,5,5	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	601	-	5,5,5	2.42	2 (40%)	5,5,5	0.95	0
3	GOL	F	601	-	5,5,5	1.26	1 (20%)	5,5,5	0.72	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
3	GOL	E	601	-	-	4/4/4/4	-
3	GOL	B	702	-	-	4/4/4/4	-
3	GOL	B	701	-	-	4/4/4/4	-
3	GOL	D	601	-	-	0/4/4/4	-
3	GOL	C	602	-	-	2/4/4/4	-
3	GOL	B	703	-	-	1/4/4/4	-
3	GOL	C	601	-	-	1/4/4/4	-
3	GOL	D	602	-	-	2/4/4/4	-
3	GOL	A	601	-	-	4/4/4/4	-
3	GOL	F	601	-	-	2/4/4/4	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	GOL	C3-C2	4.40	1.69	1.51
3	C	601	GOL	C1-C2	3.04	1.64	1.51
3	C	602	GOL	C1-C2	2.28	1.61	1.51
3	B	701	GOL	C3-C2	2.24	1.60	1.51
3	D	601	GOL	C3-C2	2.20	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	GOL	O3-C3-C2	-2.37	98.82	110.20
3	B	702	GOL	C3-C2-C1	-2.04	103.77	111.70

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	GOL	C1-C2-C3-O3
3	B	701	GOL	O1-C1-C2-C3
3	B	701	GOL	C1-C2-C3-O3
3	B	702	GOL	O1-C1-C2-O2
3	B	702	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	601	GOL	2	0
3	D	602	GOL	1	0
3	F	601	GOL	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, 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%)	-0.05	16 (3%) 50 42	57, 71, 179, 197	0
1	B	404/514 (78%)	-0.16	4 (0%) 79 73	61, 83, 120, 173	0
1	C	499/514 (97%)	0.06	23 (4%) 38 30	51, 78, 173, 191	1 (0%)
1	D	499/514 (97%)	0.04	9 (1%) 67 60	64, 92, 140, 182	1 (0%)
1	E	395/514 (76%)	0.49	26 (6%) 26 19	73, 108, 130, 164	0
1	F	399/514 (77%)	1.13	63 (15%) 6 5	100, 124, 182, 219	0
2	G	130/149 (87%)	-0.18	0 100 100	64, 78, 100, 130	0
2	H	130/149 (87%)	-0.08	1 (0%) 82 77	75, 92, 127, 152	0
2	I	130/149 (87%)	0.60	5 (3%) 44 36	90, 131, 188, 206	0
2	J	131/149 (87%)	0.00	1 (0%) 82 77	69, 88, 112, 136	0
2	K	130/149 (87%)	1.34	26 (20%) 3 3	100, 170, 223, 236	0
2	L	130/149 (87%)	0.86	9 (6%) 24 18	115, 163, 211, 218	0
All	All	3476/3978 (87%)	0.27	183 (5%) 33 26	51, 96, 179, 236	2 (0%)

The worst 5 of 183 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	61	GLY	5.2
1	E	272	ALA	4.8
2	K	100	TYR	4.7
1	F	237	ILE	4.6
1	A	179	ASN	4.4

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, 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(\AA^2)	Q<0.9
3	GOL	C	602	6/6	0.58	0.22	89,93,95,98	0
3	GOL	C	601	6/6	0.65	0.16	84,87,94,108	0
3	GOL	A	601	6/6	0.66	0.21	78,85,85,86	0
3	GOL	F	601	6/6	0.74	0.14	104,110,112,112	0
3	GOL	B	702	6/6	0.79	0.12	92,94,95,101	0
3	GOL	E	601	6/6	0.81	0.10	112,115,116,118	0
3	GOL	D	602	6/6	0.82	0.13	90,92,94,94	0
3	GOL	B	703	6/6	0.87	0.11	95,100,100,103	0
3	GOL	B	701	6/6	0.87	0.17	82,84,85,87	0
3	GOL	D	601	6/6	0.90	0.12	85,89,92,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.