



# wwPDB X-ray Structure Validation Summary Report

Sep 8, 2022 – 02:26 PM EDT

PDB ID : 7TIF  
Title : 2.85 Angstrom crystal structure of Arginyltransferase 1 (ATE1) from *Saccharomyces cerevisiae*  
Authors : Van, V.; Ejimogu, N.-E.; Smith, A.T.  
Deposited on : 2022-01-13  
Resolution : 2.85 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.29  
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) : 2.29

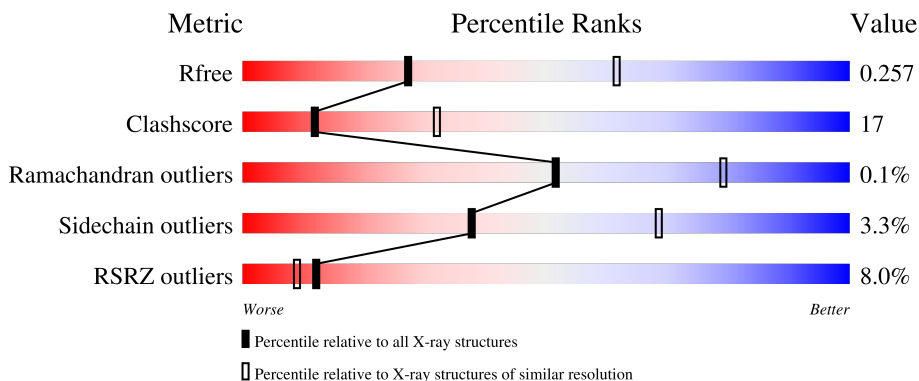
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	518	 4% 65% 24% • 10%
1	B	518	 5% 64% 24% • 10%
1	C	518	 6% 65% 22% • 10%
1	D	518	 5% 59% 27% • 12%
1	E	518	 5% 65% 23% • 10%

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Mol	Chain	Length	Quality of chain			
1	F	518	6%	59%	30%	10%
1	G	518	6%	56%	30%	12%
1	H	518	6%	59%	28%	12%
1	I	518	8%	58%	27%	13%
1	J	518	14%	48%	37%	13%
1	K	518	6%	59%	29%	11%
1	L	518	14%	46%	38%	15%

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
2	SO4	A	614	-	-	-	X
2	SO4	A	620	-	-	-	X
2	SO4	A	622	-	-	-	X
2	SO4	B	605	-	-	-	X
2	SO4	B	607	-	-	-	X
2	SO4	B	617	-	-	-	X
2	SO4	B	622	-	-	-	X
2	SO4	C	601	-	-	X	-
2	SO4	C	604	-	-	X	-
2	SO4	C	609	-	-	-	X
2	SO4	C	612	-	-	-	X
2	SO4	C	618	-	-	-	X
2	SO4	C	621	-	-	-	X
2	SO4	D	602	-	-	-	X
2	SO4	D	609	-	-	X	-
2	SO4	E	601	-	-	X	-
2	SO4	E	611	-	-	-	X
2	SO4	E	612	-	-	X	-
2	SO4	F	613	-	-	-	X
2	SO4	G	608	-	-	X	-
2	SO4	G	610	-	-	-	X
2	SO4	G	611	-	-	-	X
2	SO4	G	617	-	-	X	-
2	SO4	H	601	-	-	X	-
2	SO4	H	605	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	H	608	-	-	-	X
2	SO4	H	610	-	-	-	X
2	SO4	H	612	-	-	X	-
2	SO4	H	613	-	-	-	X
2	SO4	I	602	-	-	X	X
2	SO4	I	603	-	-	-	X
2	SO4	I	611	-	-	X	-
2	SO4	J	601	-	-	-	X
2	SO4	J	603	-	-	X	-
2	SO4	K	605	-	-	X	X
2	SO4	K	608	-	-	-	X
2	SO4	L	604	-	-	X	-
2	SO4	L	611	-	-	X	-
3	GOL	A	625	-	-	X	-
3	GOL	D	624	-	-	-	X
3	GOL	D	625	-	-	-	X
3	GOL	D	626	-	-	-	X
3	GOL	F	615	-	-	-	X
3	GOL	H	616	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 46039 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 Arginyl-tRNA--protein transferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	466	3800	2447	621	706	26	0	1	0
1	B	464	3775	2430	615	704	26	0	0	0
1	C	464	3776	2434	618	698	26	0	1	0
1	D	456	3715	2391	608	691	25	0	0	0
1	E	465	3783	2437	618	704	24	0	0	0
1	F	464	3777	2432	617	702	26	0	0	0
1	G	457	3718	2394	607	692	25	0	0	0
1	H	456	3721	2397	609	690	25	0	0	0
1	I	452	3676	2367	602	682	25	0	0	0
1	J	449	3651	2357	598	671	25	0	0	0
1	K	459	3733	2405	610	693	25	0	0	0
1	L	441	3589	2318	588	658	25	0	0	0

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	504	GLU	-	expression tag	UNP P16639
A	505	ASN	-	expression tag	UNP P16639
A	506	LEU	-	expression tag	UNP P16639
A	507	TYR	-	expression tag	UNP P16639
A	508	PHE	-	expression tag	UNP P16639

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Chain	Residue	Modelled	Actual	Comment	Reference
A	509	GLN	-	expression tag	UNP P16639
A	510	SER	-	expression tag	UNP P16639
A	511	LEU	-	expression tag	UNP P16639
A	512	GLU	-	expression tag	UNP P16639
A	513	HIS	-	expression tag	UNP P16639
A	514	HIS	-	expression tag	UNP P16639
A	515	HIS	-	expression tag	UNP P16639
A	516	HIS	-	expression tag	UNP P16639
A	517	HIS	-	expression tag	UNP P16639
A	518	HIS	-	expression tag	UNP P16639
B	504	GLU	-	expression tag	UNP P16639
B	505	ASN	-	expression tag	UNP P16639
B	506	LEU	-	expression tag	UNP P16639
B	507	TYR	-	expression tag	UNP P16639
B	508	PHE	-	expression tag	UNP P16639
B	509	GLN	-	expression tag	UNP P16639
B	510	SER	-	expression tag	UNP P16639
B	511	LEU	-	expression tag	UNP P16639
B	512	GLU	-	expression tag	UNP P16639
B	513	HIS	-	expression tag	UNP P16639
B	514	HIS	-	expression tag	UNP P16639
B	515	HIS	-	expression tag	UNP P16639
B	516	HIS	-	expression tag	UNP P16639
B	517	HIS	-	expression tag	UNP P16639
B	518	HIS	-	expression tag	UNP P16639
C	504	GLU	-	expression tag	UNP P16639
C	505	ASN	-	expression tag	UNP P16639
C	506	LEU	-	expression tag	UNP P16639
C	507	TYR	-	expression tag	UNP P16639
C	508	PHE	-	expression tag	UNP P16639
C	509	GLN	-	expression tag	UNP P16639
C	510	SER	-	expression tag	UNP P16639
C	511	LEU	-	expression tag	UNP P16639
C	512	GLU	-	expression tag	UNP P16639
C	513	HIS	-	expression tag	UNP P16639
C	514	HIS	-	expression tag	UNP P16639
C	515	HIS	-	expression tag	UNP P16639
C	516	HIS	-	expression tag	UNP P16639
C	517	HIS	-	expression tag	UNP P16639
C	518	HIS	-	expression tag	UNP P16639
D	504	GLU	-	expression tag	UNP P16639
D	505	ASN	-	expression tag	UNP P16639

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Chain	Residue	Modelled	Actual	Comment	Reference
D	506	LEU	-	expression tag	UNP P16639
D	507	TYR	-	expression tag	UNP P16639
D	508	PHE	-	expression tag	UNP P16639
D	509	GLN	-	expression tag	UNP P16639
D	510	SER	-	expression tag	UNP P16639
D	511	LEU	-	expression tag	UNP P16639
D	512	GLU	-	expression tag	UNP P16639
D	513	HIS	-	expression tag	UNP P16639
D	514	HIS	-	expression tag	UNP P16639
D	515	HIS	-	expression tag	UNP P16639
D	516	HIS	-	expression tag	UNP P16639
D	517	HIS	-	expression tag	UNP P16639
D	518	HIS	-	expression tag	UNP P16639
E	504	GLU	-	expression tag	UNP P16639
E	505	ASN	-	expression tag	UNP P16639
E	506	LEU	-	expression tag	UNP P16639
E	507	TYR	-	expression tag	UNP P16639
E	508	PHE	-	expression tag	UNP P16639
E	509	GLN	-	expression tag	UNP P16639
E	510	SER	-	expression tag	UNP P16639
E	511	LEU	-	expression tag	UNP P16639
E	512	GLU	-	expression tag	UNP P16639
E	513	HIS	-	expression tag	UNP P16639
E	514	HIS	-	expression tag	UNP P16639
E	515	HIS	-	expression tag	UNP P16639
E	516	HIS	-	expression tag	UNP P16639
E	517	HIS	-	expression tag	UNP P16639
E	518	HIS	-	expression tag	UNP P16639
F	504	GLU	-	expression tag	UNP P16639
F	505	ASN	-	expression tag	UNP P16639
F	506	LEU	-	expression tag	UNP P16639
F	507	TYR	-	expression tag	UNP P16639
F	508	PHE	-	expression tag	UNP P16639
F	509	GLN	-	expression tag	UNP P16639
F	510	SER	-	expression tag	UNP P16639
F	511	LEU	-	expression tag	UNP P16639
F	512	GLU	-	expression tag	UNP P16639
F	513	HIS	-	expression tag	UNP P16639
F	514	HIS	-	expression tag	UNP P16639
F	515	HIS	-	expression tag	UNP P16639
F	516	HIS	-	expression tag	UNP P16639
F	517	HIS	-	expression tag	UNP P16639

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Chain	Residue	Modelled	Actual	Comment	Reference
F	518	HIS	-	expression tag	UNP P16639
G	504	GLU	-	expression tag	UNP P16639
G	505	ASN	-	expression tag	UNP P16639
G	506	LEU	-	expression tag	UNP P16639
G	507	TYR	-	expression tag	UNP P16639
G	508	PHE	-	expression tag	UNP P16639
G	509	GLN	-	expression tag	UNP P16639
G	510	SER	-	expression tag	UNP P16639
G	511	LEU	-	expression tag	UNP P16639
G	512	GLU	-	expression tag	UNP P16639
G	513	HIS	-	expression tag	UNP P16639
G	514	HIS	-	expression tag	UNP P16639
G	515	HIS	-	expression tag	UNP P16639
G	516	HIS	-	expression tag	UNP P16639
G	517	HIS	-	expression tag	UNP P16639
G	518	HIS	-	expression tag	UNP P16639
H	504	GLU	-	expression tag	UNP P16639
H	505	ASN	-	expression tag	UNP P16639
H	506	LEU	-	expression tag	UNP P16639
H	507	TYR	-	expression tag	UNP P16639
H	508	PHE	-	expression tag	UNP P16639
H	509	GLN	-	expression tag	UNP P16639
H	510	SER	-	expression tag	UNP P16639
H	511	LEU	-	expression tag	UNP P16639
H	512	GLU	-	expression tag	UNP P16639
H	513	HIS	-	expression tag	UNP P16639
H	514	HIS	-	expression tag	UNP P16639
H	515	HIS	-	expression tag	UNP P16639
H	516	HIS	-	expression tag	UNP P16639
H	517	HIS	-	expression tag	UNP P16639
H	518	HIS	-	expression tag	UNP P16639
I	504	GLU	-	expression tag	UNP P16639
I	505	ASN	-	expression tag	UNP P16639
I	506	LEU	-	expression tag	UNP P16639
I	507	TYR	-	expression tag	UNP P16639
I	508	PHE	-	expression tag	UNP P16639
I	509	GLN	-	expression tag	UNP P16639
I	510	SER	-	expression tag	UNP P16639
I	511	LEU	-	expression tag	UNP P16639
I	512	GLU	-	expression tag	UNP P16639
I	513	HIS	-	expression tag	UNP P16639
I	514	HIS	-	expression tag	UNP P16639

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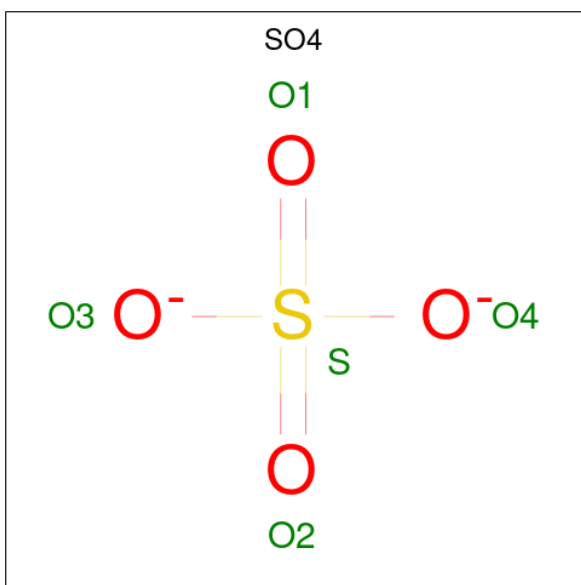
Chain	Residue	Modelled	Actual	Comment	Reference
I	515	HIS	-	expression tag	UNP P16639
I	516	HIS	-	expression tag	UNP P16639
I	517	HIS	-	expression tag	UNP P16639
I	518	HIS	-	expression tag	UNP P16639
J	504	GLU	-	expression tag	UNP P16639
J	505	ASN	-	expression tag	UNP P16639
J	506	LEU	-	expression tag	UNP P16639
J	507	TYR	-	expression tag	UNP P16639
J	508	PHE	-	expression tag	UNP P16639
J	509	GLN	-	expression tag	UNP P16639
J	510	SER	-	expression tag	UNP P16639
J	511	LEU	-	expression tag	UNP P16639
J	512	GLU	-	expression tag	UNP P16639
J	513	HIS	-	expression tag	UNP P16639
J	514	HIS	-	expression tag	UNP P16639
J	515	HIS	-	expression tag	UNP P16639
J	516	HIS	-	expression tag	UNP P16639
J	517	HIS	-	expression tag	UNP P16639
J	518	HIS	-	expression tag	UNP P16639
K	504	GLU	-	expression tag	UNP P16639
K	505	ASN	-	expression tag	UNP P16639
K	506	LEU	-	expression tag	UNP P16639
K	507	TYR	-	expression tag	UNP P16639
K	508	PHE	-	expression tag	UNP P16639
K	509	GLN	-	expression tag	UNP P16639
K	510	SER	-	expression tag	UNP P16639
K	511	LEU	-	expression tag	UNP P16639
K	512	GLU	-	expression tag	UNP P16639
K	513	HIS	-	expression tag	UNP P16639
K	514	HIS	-	expression tag	UNP P16639
K	515	HIS	-	expression tag	UNP P16639
K	516	HIS	-	expression tag	UNP P16639
K	517	HIS	-	expression tag	UNP P16639
K	518	HIS	-	expression tag	UNP P16639
L	504	GLU	-	expression tag	UNP P16639
L	505	ASN	-	expression tag	UNP P16639
L	506	LEU	-	expression tag	UNP P16639
L	507	TYR	-	expression tag	UNP P16639
L	508	PHE	-	expression tag	UNP P16639
L	509	GLN	-	expression tag	UNP P16639
L	510	SER	-	expression tag	UNP P16639
L	511	LEU	-	expression tag	UNP P16639

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Chain	Residue	Modelled	Actual	Comment	Reference
L	512	GLU	-	expression tag	UNP P16639
L	513	HIS	-	expression tag	UNP P16639
L	514	HIS	-	expression tag	UNP P16639
L	515	HIS	-	expression tag	UNP P16639
L	516	HIS	-	expression tag	UNP P16639
L	517	HIS	-	expression tag	UNP P16639
L	518	HIS	-	expression tag	UNP P16639

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		

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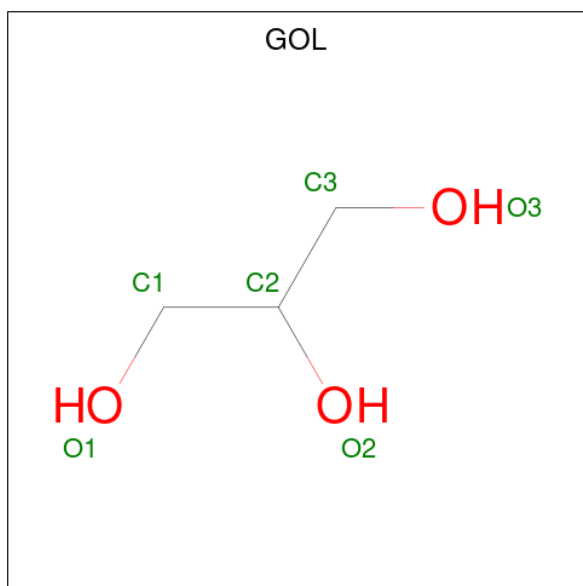
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	I	1	Total C O 6 3 3	0	0
3	J	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	L	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total O 5 5	0	0
4	B	12	Total O 12 12	0	0
4	C	5	Total O 5 5	0	0
4	D	7	Total O 7 7	0	0

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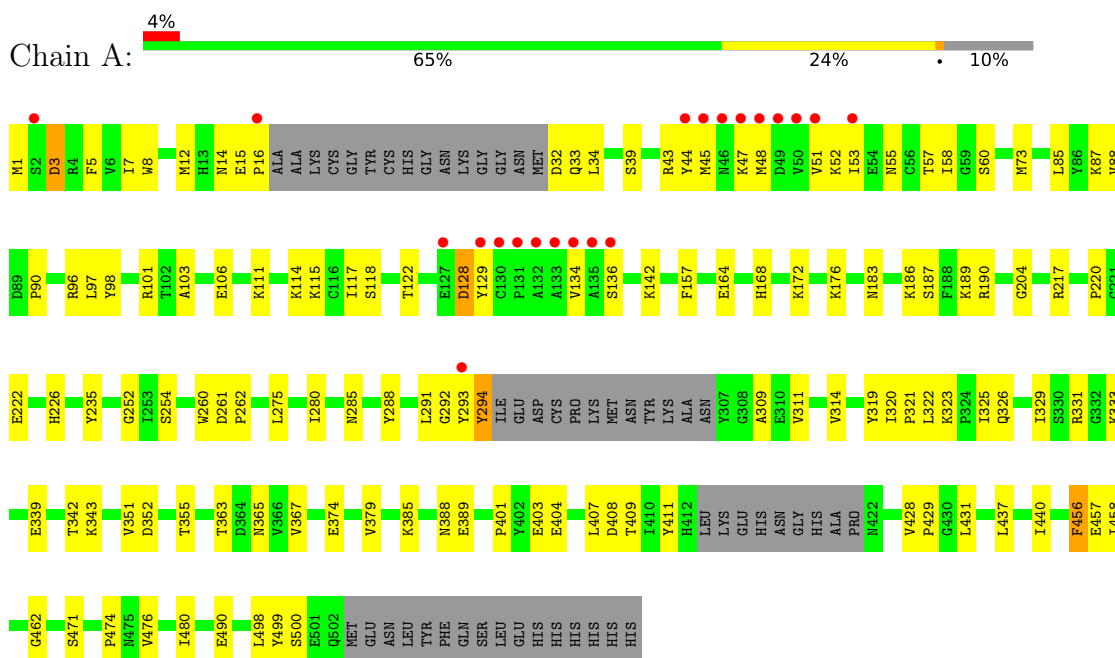
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	E	9	Total O 9 9	0	0
4	F	5	Total O 5 5	0	0
4	G	7	Total O 7 7	0	0
4	H	3	Total O 3 3	0	0
4	I	2	Total O 2 2	0	0
4	J	2	Total O 2 2	0	0
4	K	5	Total O 5 5	0	0
4	L	2	Total O 2 2	0	0

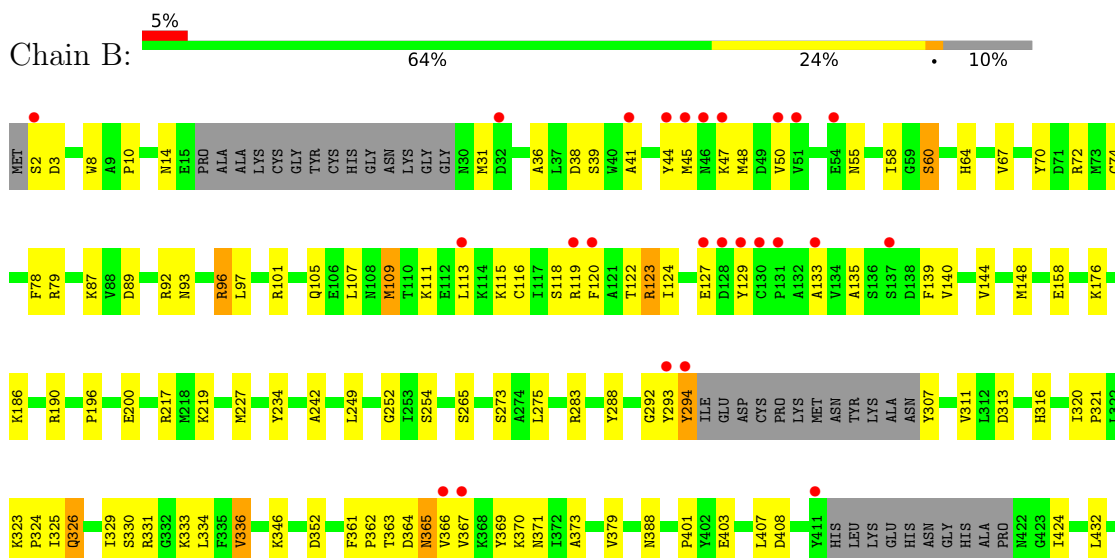
### 3 Residue-property plots [i](#)

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.

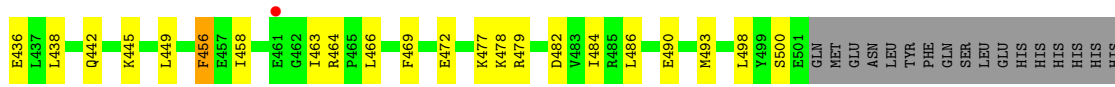
#### • Molecule 1: Arginyl-tRNA--protein transferase 1



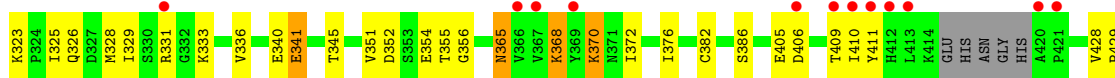
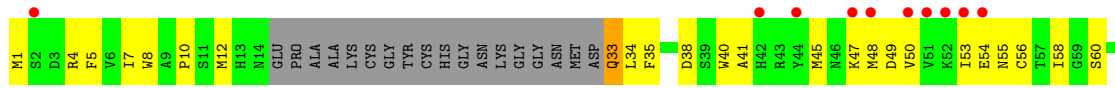
#### • Molecule 1: Arginyl-tRNA--protein transferase 1



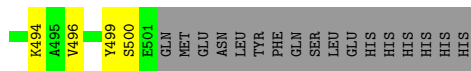
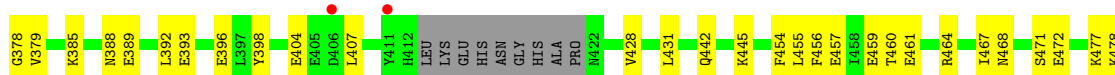
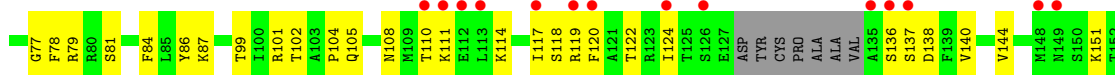




• Molecule 1: Arginyl-tRNA--protein transferase 1

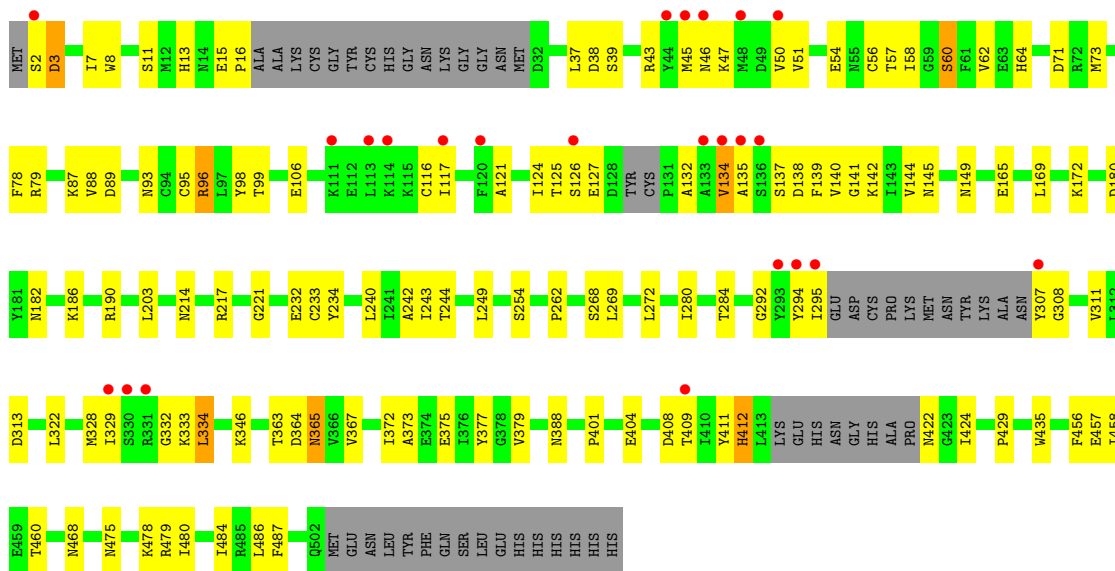


• Molecule 1: Arginyl-tRNA--protein transferase 1



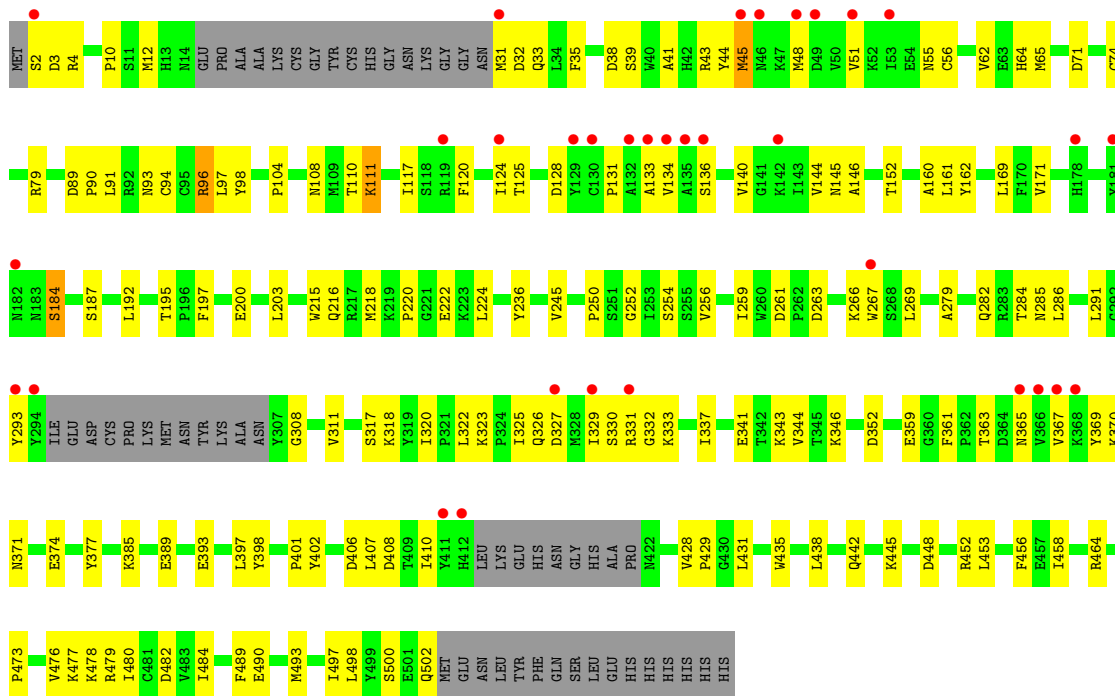
• Molecule 1: Arginyl-tRNA--protein transferase 1

Chain E: 5% 65% 23% 10%



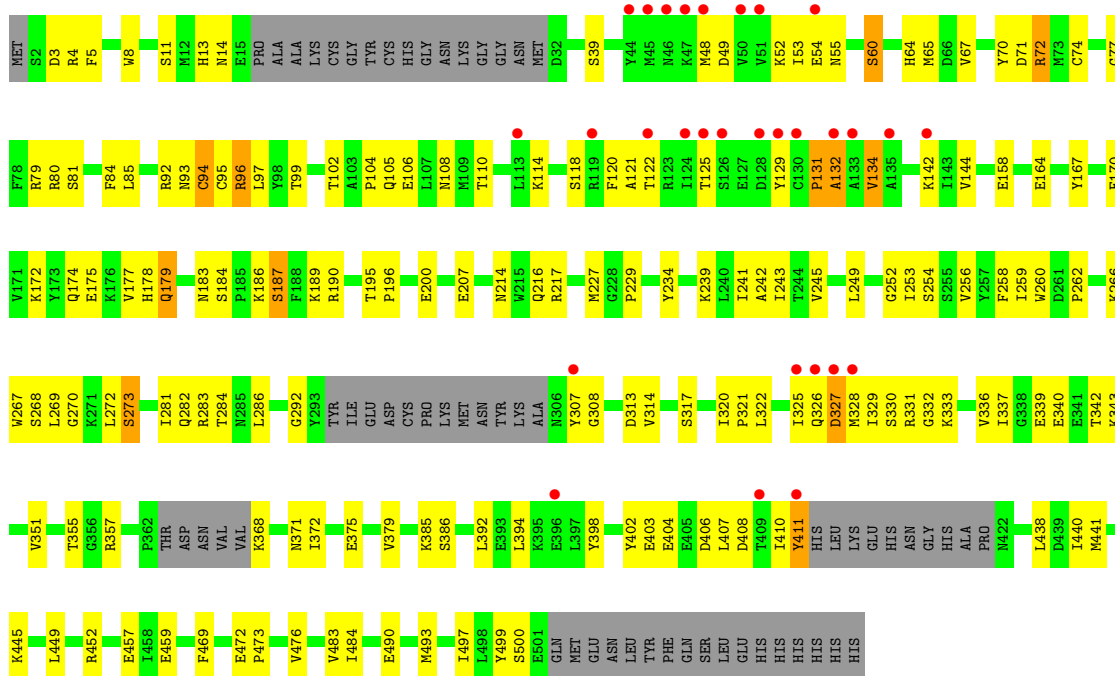
• Molecule 1: Arginyl-tRNA--protein transferase 1

Chain F: 6% 59% 30% 10%

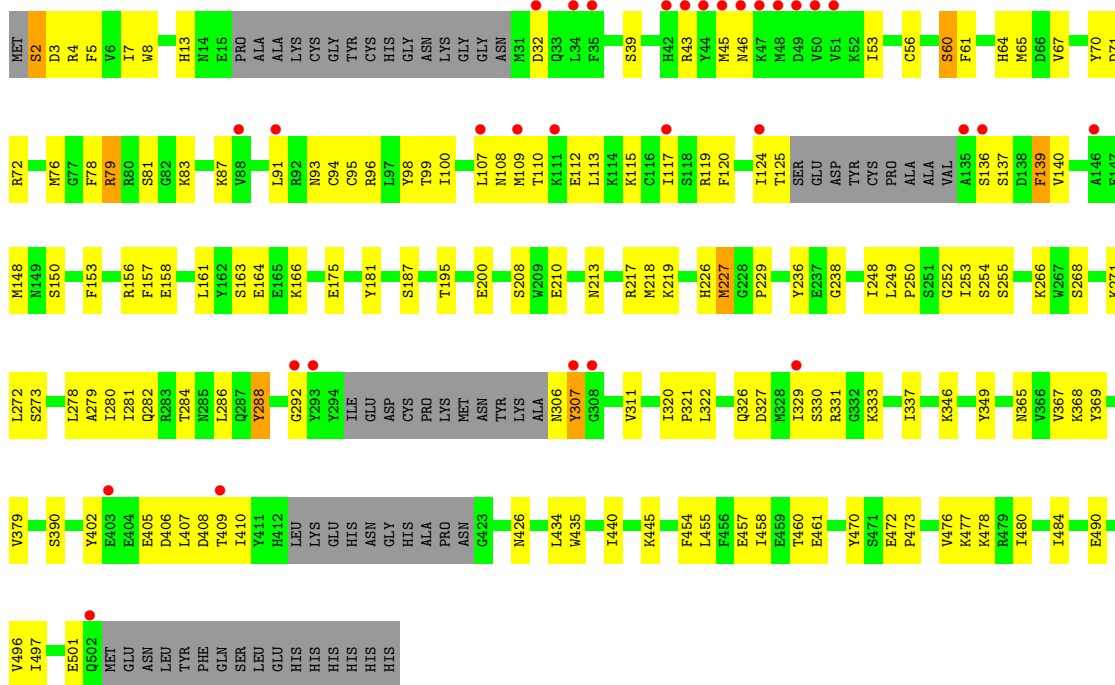


• Molecule 1: Arginyl-tRNA--protein transferase 1

Chain G: 6% 56% 30% 12%

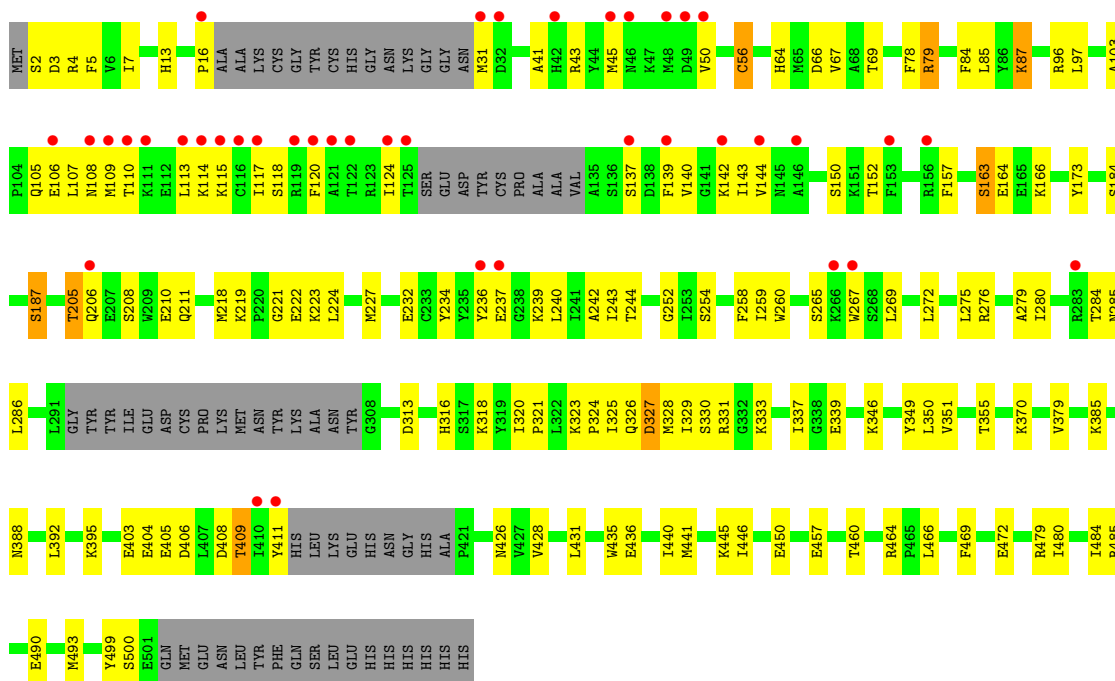


• Molecule 1: Arginyl-tRNA--protein transferase 1

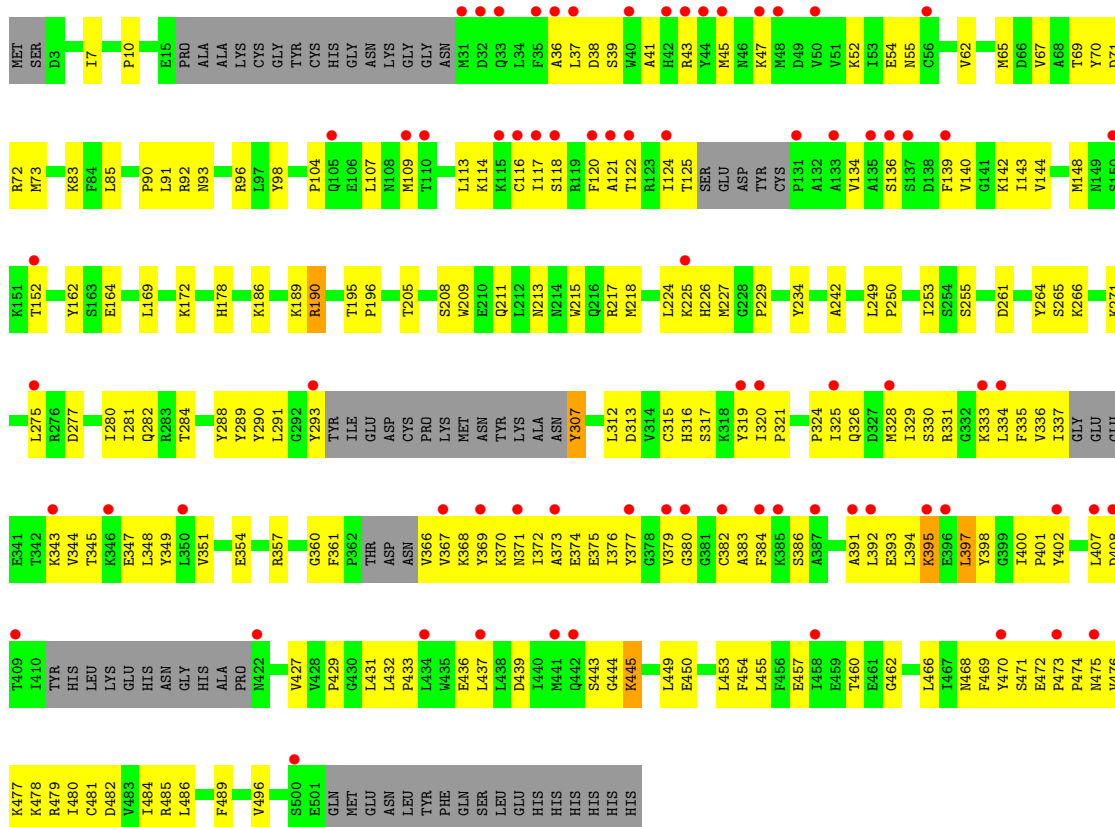


• Molecule 1: Arginyl-tRNA--protein transferase 1





- Molecule 1: Arginyl-tRNA--protein transferase 1



- Molecule 1: Arginyl-tRNA--protein transferase 1



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	235.27Å 235.27Å 171.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.25 – 2.85 65.25 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.25-2.85) 100.0 (65.25-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.86Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.200 , 0.257 0.200 , 0.257	Depositor DCC
$R_{free}$ test set	10891 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.4	Xtrriage
Anisotropy	0.111	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 84.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	46039	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	0.53	0/3898	0.68	0/5269
1	B	0.53	1/3867 (0.0%)	0.71	0/5226
1	C	0.55	0/3871	0.70	0/5229
1	D	0.50	0/3804	0.66	1/5136 (0.0%)
1	E	0.51	0/3875	0.67	1/5236 (0.0%)
1	F	0.52	1/3870 (0.0%)	0.66	0/5230
1	G	0.49	0/3808	0.65	2/5143 (0.0%)
1	H	0.48	0/3811	0.66	2/5146 (0.0%)
1	I	0.50	0/3764	0.67	1/5083 (0.0%)
1	J	0.48	0/3737	0.69	2/5043 (0.0%)
1	K	0.51	0/3823	0.70	3/5165 (0.1%)
1	L	0.49	0/3675	0.70	1/4956 (0.0%)
All	All	0.51	2/45803 (0.0%)	0.68	13/61862 (0.0%)

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	L	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	336	VAL	CB-CG1	-5.58	1.41	1.52
1	F	74	CYS	CB-SG	-5.09	1.73	1.81

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	220	PRO	N-CA-C	6.72	129.57	112.10
1	H	288	TYR	CB-CA-C	-6.17	98.06	110.40
1	G	132	ALA	N-CA-C	5.83	126.73	111.00
1	K	220	PRO	CB-CA-C	-5.74	97.65	112.00
1	G	102	THR	C-N-CA	5.57	135.63	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	104	PRO	Mainchain

## 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	3800	0	3733	103	2
1	B	3775	0	3707	102	0
1	C	3776	0	3727	110	0
1	D	3715	0	3654	116	0
1	E	3783	0	3722	122	0
1	F	3777	0	3710	129	0
1	G	3718	0	3653	164	0
1	H	3721	0	3660	123	0
1	I	3676	0	3629	132	2
1	J	3651	0	3615	183	0
1	K	3733	0	3675	140	0
1	L	3589	0	3546	206	3
2	A	115	0	0	2	1
2	B	125	0	0	3	0
2	C	115	0	0	6	0
2	D	110	0	0	2	0
2	E	125	0	0	6	0
2	F	65	0	0	1	0
2	G	85	0	0	7	0
2	H	65	0	0	6	0
2	I	65	0	0	5	0
2	J	40	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	50	0	0	5	0
2	L	55	0	0	10	0
3	A	48	0	64	9	0
3	B	30	0	39	2	0
3	C	18	0	24	0	0
3	D	24	0	32	4	0
3	E	18	0	24	3	0
3	F	12	0	16	2	0
3	G	36	0	48	5	0
3	H	24	0	32	4	0
3	I	6	0	8	0	0
3	J	6	0	8	0	0
3	K	18	0	24	1	0
3	L	6	0	8	0	0
4	A	5	0	0	0	0
4	B	12	0	0	2	0
4	C	5	0	0	0	0
4	D	7	0	0	0	0
4	E	9	0	0	3	0
4	F	5	0	0	0	0
4	G	7	0	0	0	0
4	H	3	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	5	0	0	0	0
4	L	2	0	0	0	0
All	All	46039	0	44358	1563	4

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 17.

The worst 5 of 1563 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:L:79:ARG:NH1	1:L:292:GLY:HA3	1.21	1.45
1:H:266:LYS:HD2	2:H:601:SO4:O1	1.25	1.35
1:C:189:LYS:NZ	2:C:601:SO4:O1	1.56	1.34
1:L:79:ARG:NH1	1:L:292:GLY:CA	1.93	1.30
1:D:282:GLN:NE2	2:D:609:SO4:O2	1.65	1.29

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:217:ARG:NH1	2:A:612:SO4:O3[4_555]	1.42	0.78
1:A:363:THR:CG2	1:L:210:GLU:OE2[3_554]	2.02	0.18
1:I:219:LYS:NZ	1:L:285:ASN:ND2[1_554]	2.14	0.06
1:A:217:ARG:CG	1:I:106:GLU:OE2[3_555]	2.15	0.05

## 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	459/518 (89%)	435 (95%)	24 (5%)	0	100	100
1	B	456/518 (88%)	436 (96%)	20 (4%)	0	100	100
1	C	455/518 (88%)	425 (93%)	30 (7%)	0	100	100
1	D	446/518 (86%)	420 (94%)	26 (6%)	0	100	100
1	E	455/518 (88%)	428 (94%)	26 (6%)	1 (0%)	47	75
1	F	456/518 (88%)	423 (93%)	33 (7%)	0	100	100
1	G	447/518 (86%)	417 (93%)	28 (6%)	2 (0%)	34	62
1	H	446/518 (86%)	424 (95%)	22 (5%)	0	100	100
1	I	442/518 (85%)	395 (89%)	47 (11%)	0	100	100
1	J	435/518 (84%)	394 (91%)	41 (9%)	0	100	100
1	K	449/518 (87%)	415 (92%)	32 (7%)	2 (0%)	34	62
1	L	425/518 (82%)	385 (91%)	39 (9%)	1 (0%)	47	75
All	All	5371/6216 (86%)	4997 (93%)	368 (7%)	6 (0%)	51	79

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	130	CYS
1	K	131	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	139	PHE
1	G	131	PRO
1	G	134	VAL

### 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	418/460 (91%)	409 (98%)	9 (2%)	52	79
1	B	415/460 (90%)	397 (96%)	18 (4%)	29	59
1	C	416/460 (90%)	401 (96%)	15 (4%)	35	66
1	D	409/460 (89%)	394 (96%)	15 (4%)	34	65
1	E	416/460 (90%)	399 (96%)	17 (4%)	30	61
1	F	415/460 (90%)	408 (98%)	7 (2%)	60	83
1	G	408/460 (89%)	392 (96%)	16 (4%)	32	63
1	H	409/460 (89%)	395 (97%)	14 (3%)	37	67
1	I	406/460 (88%)	394 (97%)	12 (3%)	41	72
1	J	401/460 (87%)	392 (98%)	9 (2%)	52	79
1	K	410/460 (89%)	399 (97%)	11 (3%)	44	74
1	L	394/460 (86%)	375 (95%)	19 (5%)	25	55
All	All	4917/5520 (89%)	4755 (97%)	162 (3%)	38	68

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	96	ARG
1	L	31	MET
1	I	187	SER
1	J	395	LYS
1	L	136	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	D	14	ASN
1	F	178	HIS
1	G	145	ASN
1	K	365	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

244 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	D	618	-	4,4,4	0.17	0	6,6,6	0.12	0
2	SO4	K	610	-	4,4,4	0.63	0	6,6,6	0.13	0
2	SO4	K	604	-	4,4,4	0.15	0	6,6,6	0.18	0
2	SO4	C	619	-	4,4,4	0.41	0	6,6,6	0.05	0
2	SO4	J	602	-	4,4,4	0.52	0	6,6,6	0.08	0
2	SO4	E	619	-	4,4,4	0.14	0	6,6,6	0.15	0
2	SO4	H	602	-	4,4,4	0.15	0	6,6,6	0.15	0
2	SO4	A	618	-	4,4,4	0.44	0	6,6,6	0.06	0
2	SO4	E	613	-	4,4,4	0.13	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	K	601	-	4,4,4	0.17	0	6,6,6	0.26	0
3	GOL	A	627	-	5,5,5	0.90	0	5,5,5	0.93	0
2	SO4	F	611	-	4,4,4	0.17	0	6,6,6	0.11	0
2	SO4	E	609	-	4,4,4	0.17	0	6,6,6	0.26	0
2	SO4	A	609	-	4,4,4	0.18	0	6,6,6	0.20	0
2	SO4	A	602	-	4,4,4	0.12	0	6,6,6	0.41	0
3	GOL	D	623	-	5,5,5	1.18	0	5,5,5	0.76	0
2	SO4	H	604	-	4,4,4	0.15	0	6,6,6	0.24	0
2	SO4	I	603	-	4,4,4	0.14	0	6,6,6	0.20	0
2	SO4	C	604	-	4,4,4	0.46	0	6,6,6	0.07	0
2	SO4	B	617	-	4,4,4	0.15	0	6,6,6	0.14	0
3	GOL	A	631	-	5,5,5	0.09	0	5,5,5	0.27	0
2	SO4	I	601	-	4,4,4	0.45	0	6,6,6	0.07	0
2	SO4	A	616	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	C	611	-	4,4,4	0.52	0	6,6,6	0.09	0
2	SO4	D	621	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	B	603	-	4,4,4	0.09	0	6,6,6	0.26	0
2	SO4	A	601	-	4,4,4	0.20	0	6,6,6	0.48	0
3	GOL	J	609	-	5,5,5	1.26	1 (20%)	5,5,5	0.78	0
2	SO4	L	602	-	4,4,4	0.11	0	6,6,6	0.15	0
3	GOL	G	621	-	5,5,5	0.94	0	5,5,5	1.15	0
2	SO4	B	616	-	4,4,4	0.47	0	6,6,6	0.06	0
2	SO4	G	607	-	4,4,4	0.43	0	6,6,6	0.06	0
2	SO4	J	601	-	4,4,4	0.15	0	6,6,6	0.25	0
2	SO4	C	617	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	G	603	-	4,4,4	0.12	0	6,6,6	0.18	0
2	SO4	B	618	-	4,4,4	0.42	0	6,6,6	0.05	0
2	SO4	D	617	-	4,4,4	0.49	0	6,6,6	0.08	0
2	SO4	E	625	-	4,4,4	0.15	0	6,6,6	0.22	0
3	GOL	H	616	-	5,5,5	0.88	0	5,5,5	1.13	0
2	SO4	A	613	-	4,4,4	0.42	0	6,6,6	0.04	0
2	SO4	G	613	-	4,4,4	0.15	0	6,6,6	0.17	0
2	SO4	F	606	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	L	608	-	4,4,4	0.49	0	6,6,6	0.08	0
2	SO4	G	616	-	4,4,4	0.17	0	6,6,6	0.12	0
2	SO4	I	612	-	4,4,4	0.45	0	6,6,6	0.05	0
2	SO4	L	601	-	4,4,4	0.48	0	6,6,6	0.08	0
2	SO4	E	608	-	4,4,4	0.13	0	6,6,6	0.45	0
2	SO4	F	602	-	4,4,4	0.14	0	6,6,6	0.15	0
3	GOL	H	617	-	5,5,5	1.67	2 (40%)	5,5,5	1.00	0
2	SO4	G	601	-	4,4,4	0.21	0	6,6,6	0.37	0
2	SO4	B	623	-	4,4,4	0.14	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	I	610	-	4,4,4	0.57	0	6,6,6	0.09	0
3	GOL	G	618	-	5,5,5	0.78	0	5,5,5	1.14	1 (20%)
2	SO4	B	609	-	4,4,4	0.17	0	6,6,6	0.37	0
2	SO4	B	615	-	4,4,4	0.14	0	6,6,6	0.08	0
3	GOL	G	620	-	5,5,5	1.09	0	5,5,5	0.90	0
2	SO4	H	609	-	4,4,4	0.13	0	6,6,6	0.26	0
2	SO4	C	612	-	4,4,4	0.15	0	6,6,6	0.25	0
2	SO4	B	610	-	4,4,4	0.51	0	6,6,6	0.05	0
3	GOL	B	626	-	5,5,5	1.09	0	5,5,5	0.91	0
2	SO4	C	622	-	4,4,4	0.14	0	6,6,6	0.12	0
3	GOL	F	614	-	5,5,5	1.09	0	5,5,5	0.97	0
2	SO4	B	620	-	4,4,4	0.19	0	6,6,6	0.15	0
2	SO4	I	613	-	4,4,4	0.45	0	6,6,6	0.06	0
2	SO4	G	615	-	4,4,4	0.47	0	6,6,6	0.08	0
2	SO4	E	605	-	4,4,4	0.19	0	6,6,6	0.14	0
2	SO4	C	614	-	4,4,4	0.17	0	6,6,6	0.16	0
2	SO4	I	604	-	4,4,4	0.14	0	6,6,6	0.22	0
2	SO4	D	610	-	4,4,4	0.13	0	6,6,6	0.18	0
2	SO4	B	613	-	4,4,4	0.13	0	6,6,6	0.11	0
3	GOL	B	628	-	5,5,5	1.26	1 (20%)	5,5,5	1.04	0
2	SO4	F	603	-	4,4,4	0.19	0	6,6,6	0.23	0
2	SO4	D	611	-	4,4,4	0.15	0	6,6,6	0.17	0
2	SO4	H	603	-	4,4,4	0.15	0	6,6,6	0.19	0
2	SO4	F	608	-	4,4,4	0.20	0	6,6,6	0.23	0
2	SO4	C	608	-	4,4,4	0.11	0	6,6,6	0.19	0
2	SO4	D	607	-	4,4,4	0.15	0	6,6,6	0.43	0
2	SO4	F	612	-	4,4,4	0.14	0	6,6,6	0.11	0
3	GOL	B	627	-	5,5,5	1.16	1 (20%)	5,5,5	1.15	0
2	SO4	B	604	-	4,4,4	0.18	0	6,6,6	0.13	0
2	SO4	E	620	-	4,4,4	0.13	0	6,6,6	0.19	0
2	SO4	G	606	-	4,4,4	0.15	0	6,6,6	0.24	0
2	SO4	E	618	-	4,4,4	0.13	0	6,6,6	0.17	0
2	SO4	J	608	-	4,4,4	0.12	0	6,6,6	0.08	0
2	SO4	B	601	-	4,4,4	0.19	0	6,6,6	0.22	0
2	SO4	J	604	-	4,4,4	0.49	0	6,6,6	0.06	0
2	SO4	I	602	-	4,4,4	0.15	0	6,6,6	0.18	0
2	SO4	E	611	-	4,4,4	0.23	0	6,6,6	0.49	0
2	SO4	D	615	-	4,4,4	0.50	0	6,6,6	0.07	0
2	SO4	H	601	-	4,4,4	0.45	0	6,6,6	0.07	0
2	SO4	A	623	-	4,4,4	0.48	0	6,6,6	0.07	0
2	SO4	I	607	-	4,4,4	0.12	0	6,6,6	0.12	0
3	GOL	E	627	-	5,5,5	0.85	0	5,5,5	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	B	624	-	4,4,4	0.12	0	6,6,6	0.10	0
2	SO4	C	618	-	4,4,4	0.52	0	6,6,6	0.09	0
3	GOL	A	629	-	5,5,5	0.79	0	5,5,5	1.09	0
2	SO4	G	605	-	4,4,4	0.15	0	6,6,6	0.24	0
2	SO4	L	607	-	4,4,4	0.18	0	6,6,6	0.14	0
2	SO4	E	617	-	4,4,4	0.17	0	6,6,6	0.16	0
2	SO4	B	607	-	4,4,4	0.12	0	6,6,6	0.24	0
2	SO4	G	614	-	4,4,4	0.16	0	6,6,6	0.09	0
2	SO4	A	612	-	4,4,4	0.49	0	6,6,6	0.06	0
3	GOL	A	626	-	5,5,5	1.17	1 (20%)	5,5,5	0.80	0
2	SO4	F	605	-	4,4,4	0.13	0	6,6,6	0.25	0
2	SO4	I	606	-	4,4,4	0.55	0	6,6,6	0.09	0
2	SO4	H	607	-	4,4,4	0.12	0	6,6,6	0.17	0
2	SO4	L	611	-	4,4,4	0.48	0	6,6,6	0.08	0
3	GOL	E	626	-	5,5,5	1.28	1 (20%)	5,5,5	0.88	0
2	SO4	A	606	-	4,4,4	0.12	0	6,6,6	0.22	0
2	SO4	D	616	-	4,4,4	0.12	0	6,6,6	0.18	0
2	SO4	C	606	-	4,4,4	0.17	0	6,6,6	0.17	0
2	SO4	C	609	-	4,4,4	0.20	0	6,6,6	0.23	0
2	SO4	B	612	-	4,4,4	0.55	0	6,6,6	0.13	0
2	SO4	G	609	-	4,4,4	0.12	0	6,6,6	0.14	0
2	SO4	D	609	-	4,4,4	0.49	0	6,6,6	0.09	0
2	SO4	A	611	-	4,4,4	0.50	0	6,6,6	0.06	0
2	SO4	B	606	-	4,4,4	0.11	0	6,6,6	0.50	0
2	SO4	G	602	-	4,4,4	0.11	0	6,6,6	0.47	0
2	SO4	A	607	-	4,4,4	0.15	0	6,6,6	0.29	0
2	SO4	B	619	-	4,4,4	0.16	0	6,6,6	0.13	0
2	SO4	K	606	-	4,4,4	0.12	0	6,6,6	0.17	0
3	GOL	B	630	-	5,5,5	1.06	0	5,5,5	0.89	0
2	SO4	C	607	-	4,4,4	0.15	0	6,6,6	0.22	0
2	SO4	C	621	-	4,4,4	0.17	0	6,6,6	0.14	0
2	SO4	H	612	-	4,4,4	0.52	0	6,6,6	0.06	0
3	GOL	E	628	-	5,5,5	0.77	0	5,5,5	0.99	0
2	SO4	H	606	-	4,4,4	0.18	0	6,6,6	0.30	0
2	SO4	I	605	-	4,4,4	0.16	0	6,6,6	0.21	0
2	SO4	E	616	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	F	613	-	4,4,4	0.13	0	6,6,6	0.14	0
2	SO4	K	607	-	4,4,4	0.16	0	6,6,6	0.19	0
2	SO4	D	606	-	4,4,4	0.17	0	6,6,6	0.09	0
2	SO4	D	622	-	4,4,4	0.46	0	6,6,6	0.06	0
2	SO4	C	613	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	H	613	-	4,4,4	0.17	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	D	626	-	5,5,5	1.04	0	5,5,5	0.86	0
2	SO4	K	605	-	4,4,4	0.42	0	6,6,6	0.05	0
2	SO4	L	610	-	4,4,4	0.44	0	6,6,6	0.05	0
2	SO4	F	604	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	F	609	-	4,4,4	0.43	0	6,6,6	0.05	0
2	SO4	C	603	-	4,4,4	0.19	0	6,6,6	0.40	0
3	GOL	F	615	-	5,5,5	1.33	1 (20%)	5,5,5	1.11	0
2	SO4	E	601	-	4,4,4	0.13	0	6,6,6	0.12	0
2	SO4	A	610	-	4,4,4	0.15	0	6,6,6	0.15	0
2	SO4	A	615	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	A	622	-	4,4,4	0.10	0	6,6,6	0.29	0
2	SO4	E	607	-	4,4,4	0.13	0	6,6,6	0.17	0
2	SO4	B	605	-	4,4,4	0.49	0	6,6,6	0.07	0
2	SO4	E	614	-	4,4,4	0.13	0	6,6,6	0.17	0
2	SO4	F	601	-	4,4,4	0.20	0	6,6,6	0.44	0
2	SO4	C	615	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	K	603	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	E	606	-	4,4,4	0.13	0	6,6,6	0.22	0
3	GOL	I	614	-	5,5,5	0.89	0	5,5,5	1.08	0
2	SO4	D	605	-	4,4,4	0.15	0	6,6,6	0.09	0
3	GOL	K	612	-	5,5,5	0.99	0	5,5,5	0.88	0
2	SO4	J	605	-	4,4,4	0.43	0	6,6,6	0.06	0
2	SO4	C	616	-	4,4,4	0.15	0	6,6,6	0.15	0
2	SO4	H	605	-	4,4,4	0.59	0	6,6,6	0.10	0
2	SO4	G	611	-	4,4,4	0.13	0	6,6,6	0.14	0
2	SO4	A	620	-	4,4,4	0.51	0	6,6,6	0.09	0
2	SO4	C	601	-	4,4,4	0.47	0	6,6,6	0.08	0
2	SO4	C	620	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SO4	D	612	-	4,4,4	0.17	0	6,6,6	0.18	0
2	SO4	E	615	-	4,4,4	0.13	0	6,6,6	0.22	0
2	SO4	L	604	-	4,4,4	0.52	0	6,6,6	0.09	0
2	SO4	A	608	-	4,4,4	0.57	0	6,6,6	0.09	0
2	SO4	D	601	-	4,4,4	0.18	0	6,6,6	0.41	0
2	SO4	D	603	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	B	625	-	4,4,4	0.16	0	6,6,6	0.11	0
3	GOL	L	612	-	5,5,5	1.02	0	5,5,5	1.19	1 (20%)
3	GOL	H	614	-	5,5,5	1.41	0	5,5,5	0.66	0
3	GOL	K	611	-	5,5,5	1.41	1 (20%)	5,5,5	0.54	0
2	SO4	K	602	-	4,4,4	0.15	0	6,6,6	0.25	0
2	SO4	B	602	-	4,4,4	0.09	0	6,6,6	0.42	0
2	SO4	J	603	-	4,4,4	0.55	0	6,6,6	0.05	0
2	SO4	D	619	-	4,4,4	0.13	0	6,6,6	0.25	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	E	623	-	4,4,4	0.13	0	6,6,6	0.12	0
2	SO4	F	610	-	4,4,4	0.16	0	6,6,6	0.10	0
2	SO4	D	613	-	4,4,4	0.44	0	6,6,6	0.05	0
2	SO4	K	608	-	4,4,4	0.14	0	6,6,6	0.33	0
2	SO4	E	622	-	4,4,4	0.16	0	6,6,6	0.08	0
3	GOL	K	613	-	5,5,5	1.17	0	5,5,5	0.90	0
2	SO4	B	622	-	4,4,4	0.44	0	6,6,6	0.06	0
2	SO4	A	617	-	4,4,4	0.53	0	6,6,6	0.07	0
2	SO4	A	621	-	4,4,4	0.13	0	6,6,6	0.14	0
2	SO4	D	620	-	4,4,4	0.55	0	6,6,6	0.05	0
2	SO4	L	603	-	4,4,4	0.50	0	6,6,6	0.07	0
2	SO4	C	605	-	4,4,4	0.21	0	6,6,6	0.23	0
2	SO4	H	608	-	4,4,4	0.51	0	6,6,6	0.06	0
2	SO4	K	609	-	4,4,4	0.14	0	6,6,6	0.15	0
2	SO4	C	610	-	4,4,4	0.15	0	6,6,6	0.16	0
2	SO4	I	611	-	4,4,4	0.54	0	6,6,6	0.08	0
2	SO4	A	603	-	4,4,4	0.48	0	6,6,6	0.07	0
2	SO4	C	623	-	4,4,4	0.15	0	6,6,6	0.08	0
3	GOL	C	626	-	5,5,5	1.05	0	5,5,5	1.19	0
2	SO4	E	602	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	E	603	-	4,4,4	0.45	0	6,6,6	0.05	0
2	SO4	B	621	-	4,4,4	0.13	0	6,6,6	0.12	0
2	SO4	B	614	-	4,4,4	0.20	0	6,6,6	0.22	0
2	SO4	B	611	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	I	608	-	4,4,4	0.17	0	6,6,6	0.11	0
3	GOL	H	615	-	5,5,5	0.88	0	5,5,5	0.98	0
3	GOL	G	622	-	5,5,5	1.16	0	5,5,5	0.97	0
3	GOL	G	619	-	5,5,5	0.86	0	5,5,5	1.11	0
3	GOL	A	628	-	5,5,5	1.10	0	5,5,5	0.95	0
3	GOL	A	630	-	5,5,5	1.09	0	5,5,5	0.76	0
2	SO4	E	604	-	4,4,4	0.19	0	6,6,6	0.28	0
2	SO4	G	610	-	4,4,4	0.46	0	6,6,6	0.07	0
2	SO4	H	611	-	4,4,4	0.44	0	6,6,6	0.05	0
2	SO4	J	607	-	4,4,4	0.43	0	6,6,6	0.05	0
3	GOL	C	624	-	5,5,5	0.99	0	5,5,5	0.90	0
2	SO4	J	606	-	4,4,4	0.56	0	6,6,6	0.07	0
2	SO4	L	606	-	4,4,4	0.12	0	6,6,6	0.12	0
2	SO4	B	608	-	4,4,4	0.61	0	6,6,6	0.14	0
2	SO4	D	602	-	4,4,4	0.14	0	6,6,6	0.11	0
3	GOL	D	624	-	5,5,5	0.93	0	5,5,5	0.84	0
2	SO4	D	608	-	4,4,4	0.12	0	6,6,6	0.15	0
2	SO4	A	614	-	4,4,4	0.16	0	6,6,6	0.16	0
2	SO4	E	610	-	4,4,4	0.16	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	B	629	-	5,5,5	1.23	0	5,5,5	0.88	0
3	GOL	A	625	-	5,5,5	1.51	1 (20%)	5,5,5	0.67	0
2	SO4	L	609	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SO4	D	604	-	4,4,4	0.14	0	6,6,6	0.11	0
3	GOL	G	623	-	5,5,5	0.66	0	5,5,5	1.33	1 (20%)
2	SO4	G	608	-	4,4,4	0.47	0	6,6,6	0.06	0
2	SO4	L	605	-	4,4,4	0.16	0	6,6,6	0.45	0
2	SO4	F	607	-	4,4,4	0.19	0	6,6,6	0.32	0
2	SO4	G	604	-	4,4,4	0.13	0	6,6,6	0.20	0
2	SO4	E	624	-	4,4,4	0.46	0	6,6,6	0.07	0
2	SO4	H	610	-	4,4,4	0.15	0	6,6,6	0.17	0
3	GOL	A	624	-	5,5,5	1.16	0	5,5,5	1.02	0
2	SO4	I	609	-	4,4,4	0.44	0	6,6,6	0.06	0
2	SO4	A	605	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	E	621	-	4,4,4	0.14	0	6,6,6	0.13	0
2	SO4	G	612	-	4,4,4	0.17	0	6,6,6	0.10	0
2	SO4	G	617	-	4,4,4	0.44	0	6,6,6	0.06	0
2	SO4	D	614	-	4,4,4	0.13	0	6,6,6	0.14	0
3	GOL	C	625	-	5,5,5	1.07	0	5,5,5	0.97	0
2	SO4	A	604	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	E	612	-	4,4,4	0.52	0	6,6,6	0.09	0
3	GOL	D	625	-	5,5,5	1.16	0	5,5,5	0.86	0
2	SO4	C	602	-	4,4,4	0.13	0	6,6,6	0.22	0
2	SO4	A	619	-	4,4,4	0.16	0	6,6,6	0.14	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	G	620	-	-	3/4/4/4	-
3	GOL	E	626	-	-	3/4/4/4	-
3	GOL	A	627	-	-	0/4/4/4	-
3	GOL	B	626	-	-	1/4/4/4	-
3	GOL	C	626	-	-	2/4/4/4	-
3	GOL	F	614	-	-	1/4/4/4	-
3	GOL	D	623	-	-	2/4/4/4	-
3	GOL	B	630	-	-	1/4/4/4	-
3	GOL	E	628	-	-	2/4/4/4	-
3	GOL	H	615	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	G	622	-	-	0/4/4/4	-
3	GOL	G	619	-	-	4/4/4/4	-
3	GOL	A	628	-	-	0/4/4/4	-
3	GOL	A	631	-	-	0/4/4/4	-
3	GOL	D	626	-	-	2/4/4/4	-
3	GOL	A	630	-	-	0/4/4/4	-
3	GOL	B	628	-	-	4/4/4/4	-
3	GOL	B	627	-	-	2/4/4/4	-
3	GOL	C	624	-	-	2/4/4/4	-
3	GOL	F	615	-	-	3/4/4/4	-
3	GOL	D	624	-	-	1/4/4/4	-
3	GOL	I	614	-	-	0/4/4/4	-
3	GOL	J	609	-	-	0/4/4/4	-
3	GOL	B	629	-	-	2/4/4/4	-
3	GOL	K	612	-	-	4/4/4/4	-
3	GOL	A	625	-	-	2/4/4/4	-
3	GOL	G	621	-	-	2/4/4/4	-
3	GOL	G	623	-	-	1/4/4/4	-
3	GOL	H	616	-	-	2/4/4/4	-
3	GOL	L	612	-	-	2/4/4/4	-
3	GOL	A	624	-	-	0/4/4/4	-
3	GOL	E	627	-	-	4/4/4/4	-
3	GOL	H	614	-	-	4/4/4/4	-
3	GOL	A	629	-	-	2/4/4/4	-
3	GOL	K	611	-	-	2/4/4/4	-
3	GOL	C	625	-	-	4/4/4/4	-
3	GOL	H	617	-	-	1/4/4/4	-
3	GOL	K	613	-	-	0/4/4/4	-
3	GOL	D	625	-	-	0/4/4/4	-
3	GOL	A	626	-	-	3/4/4/4	-
3	GOL	G	618	-	-	3/4/4/4	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	617	GOL	C1-C2	2.64	1.62	1.51
3	H	617	GOL	C3-C2	2.54	1.62	1.51
3	B	628	GOL	O2-C2	-2.47	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	625	GOL	C3-C2	2.40	1.61	1.51
3	E	626	GOL	C3-C2	2.17	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	612	GOL	C3-C2-C1	-2.18	103.21	111.70
3	G	618	GOL	C3-C2-C1	-2.14	103.40	111.70
3	G	623	GOL	C3-C2-C1	-2.13	103.44	111.70

There are no chirality outliers.

5 of 73 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	625	GOL	O1-C1-C2-C3
3	B	627	GOL	O1-C1-C2-C3
3	C	625	GOL	O1-C1-C2-C3
3	C	625	GOL	C1-C2-C3-O3
3	C	626	GOL	O1-C1-C2-C3

There are no ring outliers.

49 monomers are involved in 86 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	601	SO4	1	0
2	C	604	SO4	2	0
3	A	631	GOL	2	0
2	A	616	SO4	1	0
2	C	611	SO4	1	0
2	L	602	SO4	1	0
3	G	621	GOL	2	0
3	H	617	GOL	3	0
2	G	601	SO4	1	0
2	I	610	SO4	1	0
2	B	610	SO4	1	0
2	B	613	SO4	1	0
3	B	628	GOL	1	0
3	B	627	GOL	1	0
2	B	604	SO4	1	0
2	I	602	SO4	2	0
2	H	601	SO4	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	627	GOL	1	0
3	A	629	GOL	1	0
2	A	612	SO4	0	1
2	L	611	SO4	3	0
3	E	626	GOL	1	0
2	D	609	SO4	2	0
2	H	612	SO4	2	0
3	E	628	GOL	1	0
2	K	607	SO4	1	0
3	D	626	GOL	2	0
2	K	605	SO4	2	0
2	F	604	SO4	1	0
3	F	615	GOL	2	0
2	E	601	SO4	3	0
2	K	603	SO4	1	0
2	C	601	SO4	3	0
2	L	604	SO4	6	0
2	A	608	SO4	1	0
3	H	614	GOL	1	0
3	K	611	GOL	1	0
2	J	603	SO4	2	0
2	I	611	SO4	2	0
3	G	619	GOL	1	0
2	G	610	SO4	1	0
3	D	624	GOL	1	0
3	A	625	GOL	5	0
3	G	623	GOL	2	0
2	G	608	SO4	2	0
3	A	624	GOL	1	0
2	G	617	SO4	3	0
2	E	612	SO4	3	0
3	D	625	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	466/518 (89%)	0.19	21 (4%) 33 28	37, 65, 138, 195	0
1	B	464/518 (89%)	0.31	26 (5%) 24 20	42, 65, 138, 195	0
1	C	464/518 (89%)	0.29	29 (6%) 20 15	38, 67, 153, 188	0
1	D	456/518 (88%)	0.29	28 (6%) 21 17	40, 72, 143, 195	0
1	E	465/518 (89%)	0.24	24 (5%) 27 22	30, 67, 146, 216	0
1	F	464/518 (89%)	0.34	33 (7%) 16 12	30, 73, 152, 216	0
1	G	457/518 (88%)	0.39	29 (6%) 20 15	30, 74, 146, 202	0
1	H	456/518 (88%)	0.35	31 (6%) 17 13	30, 78, 146, 223	0
1	I	452/518 (87%)	0.47	40 (8%) 10 6	30, 80, 155, 186	0
1	J	449/518 (86%)	0.83	75 (16%) 1 1	55, 108, 166, 205	0
1	K	459/518 (88%)	0.36	33 (7%) 15 11	30, 79, 163, 228	0
1	L	441/518 (85%)	0.76	70 (15%) 1 1	30, 110, 171, 221	0
All	All	5493/6216 (88%)	0.40	439 (7%) 12 9	30, 77, 154, 228	0

The worst 5 of 439 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	129	TYR	10.1
1	B	46	ASN	9.2
1	I	113	LEU	8.5
1	F	133	ALA	8.4
1	H	46	ASN	8.2

### 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 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SO4	C	612	5/5	0.44	0.51	188,189,191,191	0
2	SO4	H	601	5/5	0.49	0.27	190,193,193,194	0
3	GOL	F	614	6/6	0.49	0.29	102,116,120,121	0
3	GOL	D	625	6/6	0.50	0.47	109,115,120,122	0
2	SO4	A	620	5/5	0.53	0.66	201,202,202,203	0
2	SO4	G	611	5/5	0.55	0.49	192,193,194,195	0
2	SO4	B	622	5/5	0.55	0.53	196,196,197,197	0
2	SO4	G	607	5/5	0.56	0.33	177,178,180,180	0
2	SO4	A	623	5/5	0.59	0.22	198,199,200,201	0
2	SO4	F	613	5/5	0.60	0.44	184,185,187,188	0
2	SO4	J	607	5/5	0.61	0.28	192,192,193,194	0
2	SO4	B	618	5/5	0.61	0.32	214,215,216,216	0
2	SO4	D	617	5/5	0.61	0.18	155,159,163,166	0
2	SO4	F	609	5/5	0.62	0.28	180,185,186,188	0
2	SO4	G	610	5/5	0.63	0.54	206,206,207,208	0
2	SO4	C	601	5/5	0.63	0.21	157,159,161,161	0
2	SO4	A	618	5/5	0.63	0.29	181,182,183,184	0
2	SO4	H	611	5/5	0.64	0.22	185,187,187,188	0
2	SO4	A	621	5/5	0.66	0.29	195,196,197,197	0
2	SO4	E	623	5/5	0.66	0.21	185,185,186,187	0
2	SO4	D	609	5/5	0.67	0.31	184,186,187,188	0
3	GOL	D	626	6/6	0.67	0.44	123,126,128,130	0
2	SO4	E	624	5/5	0.67	0.19	192,197,198,199	0
2	SO4	I	602	5/5	0.68	0.44	185,188,189,190	0
2	SO4	H	613	5/5	0.68	0.44	174,178,178,182	0
2	SO4	L	603	5/5	0.68	0.21	172,173,174,177	0
2	SO4	C	604	5/5	0.69	0.25	190,191,192,192	0
2	SO4	D	616	5/5	0.69	0.37	165,169,171,171	0
2	SO4	B	617	5/5	0.69	0.52	182,184,185,186	0
2	SO4	E	612	5/5	0.69	0.28	154,154,158,160	0
2	SO4	D	602	5/5	0.69	0.41	180,181,181,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	627	6/6	0.70	0.32	107,114,120,127	0
2	SO4	C	616	5/5	0.70	0.33	164,164,166,166	0
2	SO4	G	608	5/5	0.71	0.18	175,176,177,178	0
2	SO4	H	612	5/5	0.71	0.36	161,161,164,168	0
2	SO4	F	610	5/5	0.71	0.34	173,174,175,177	0
2	SO4	A	622	5/5	0.71	0.46	156,159,161,166	0
2	SO4	C	619	5/5	0.71	0.38	167,167,169,169	0
2	SO4	C	615	5/5	0.72	0.33	182,184,184,185	0
3	GOL	A	628	6/6	0.72	0.30	98,110,112,112	0
2	SO4	K	605	5/5	0.72	0.40	203,205,206,207	0
2	SO4	K	609	5/5	0.72	0.22	184,185,185,185	0
2	SO4	H	608	5/5	0.72	0.45	174,178,178,179	0
3	GOL	H	616	6/6	0.72	0.64	125,129,134,140	0
2	SO4	L	609	5/5	0.73	0.25	185,185,186,188	0
2	SO4	I	610	5/5	0.73	0.27	175,176,177,179	0
2	SO4	J	605	5/5	0.73	0.38	171,171,173,174	0
3	GOL	A	630	6/6	0.73	0.23	99,106,111,111	0
2	SO4	C	618	5/5	0.73	0.41	164,164,166,167	0
2	SO4	A	614	5/5	0.73	0.47	166,166,169,171	0
2	SO4	A	612	5/5	0.73	0.21	190,192,193,194	0
2	SO4	D	618	5/5	0.73	0.16	167,169,169,169	0
2	SO4	C	609	5/5	0.74	0.43	149,152,157,158	0
2	SO4	A	613	5/5	0.74	0.30	159,161,162,164	0
2	SO4	I	606	5/5	0.74	0.29	154,157,159,160	0
2	SO4	C	621	5/5	0.74	0.72	183,183,185,187	0
2	SO4	J	601	5/5	0.74	0.40	156,156,159,159	0
2	SO4	G	616	5/5	0.74	0.27	185,185,187,188	0
3	GOL	H	617	6/6	0.74	0.27	80,86,94,95	0
2	SO4	C	622	5/5	0.75	0.14	181,182,184,185	0
3	GOL	A	626	6/6	0.75	0.17	84,88,90,91	0
2	SO4	E	601	5/5	0.75	0.30	173,174,175,178	0
2	SO4	J	602	5/5	0.75	0.37	168,170,173,173	0
2	SO4	B	623	5/5	0.75	0.28	164,165,167,168	0
2	SO4	C	611	5/5	0.75	0.37	146,149,154,155	0
2	SO4	K	604	5/5	0.75	0.23	163,165,166,166	0
2	SO4	B	605	5/5	0.75	0.42	183,184,184,185	0
3	GOL	F	615	6/6	0.75	0.44	78,92,107,114	0
2	SO4	F	605	5/5	0.75	0.37	150,154,156,159	0
2	SO4	A	603	5/5	0.75	0.28	170,170,171,172	0
2	SO4	K	607	5/5	0.76	0.35	157,159,163,165	0
2	SO4	H	602	5/5	0.76	0.25	145,147,149,150	0
2	SO4	D	615	5/5	0.76	0.17	166,169,170,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	I	604	5/5	0.76	0.35	145,150,151,153	0
2	SO4	D	610	5/5	0.76	0.23	175,176,178,180	0
2	SO4	I	609	5/5	0.76	0.26	162,164,166,168	0
2	SO4	E	614	5/5	0.76	0.23	154,157,158,160	0
2	SO4	L	602	5/5	0.77	0.32	146,147,149,154	0
2	SO4	E	617	5/5	0.77	0.33	155,156,158,160	0
2	SO4	H	605	5/5	0.77	0.50	171,173,176,177	0
2	SO4	I	612	5/5	0.77	0.38	171,173,177,177	0
2	SO4	E	620	5/5	0.77	0.34	161,164,167,167	0
2	SO4	B	616	5/5	0.77	0.33	180,181,184,184	0
2	SO4	E	603	5/5	0.77	0.21	187,188,189,190	0
3	GOL	D	624	6/6	0.77	0.42	116,127,129,133	0
2	SO4	E	611	5/5	0.77	0.45	151,156,159,160	0
2	SO4	J	608	5/5	0.77	0.31	178,179,179,180	0
2	SO4	G	614	5/5	0.77	0.39	171,172,174,176	0
2	SO4	B	624	5/5	0.77	0.38	177,178,182,182	0
2	SO4	B	625	5/5	0.77	0.21	168,169,172,173	0
2	SO4	I	608	5/5	0.77	0.23	166,167,167,168	0
2	SO4	D	612	5/5	0.78	0.34	162,164,165,166	0
2	SO4	A	604	5/5	0.78	0.22	153,154,155,157	0
3	GOL	B	630	6/6	0.78	0.23	93,99,100,104	0
2	SO4	K	608	5/5	0.78	0.45	137,139,141,143	0
2	SO4	A	615	5/5	0.78	0.21	166,167,168,168	0
2	SO4	A	617	5/5	0.78	0.31	186,187,191,194	0
2	SO4	H	604	5/5	0.78	0.18	171,172,172,173	0
2	SO4	E	613	5/5	0.78	0.29	173,173,174,174	0
2	SO4	C	605	5/5	0.78	0.29	134,138,142,142	0
2	SO4	H	610	5/5	0.78	0.55	172,173,174,176	0
3	GOL	K	611	6/6	0.78	0.25	93,114,118,121	0
2	SO4	D	614	5/5	0.79	0.22	168,170,171,175	0
2	SO4	I	603	5/5	0.79	0.57	159,163,166,167	0
2	SO4	E	608	5/5	0.79	0.20	122,131,133,133	0
3	GOL	G	620	6/6	0.79	0.28	78,99,104,110	0
2	SO4	E	622	5/5	0.79	0.28	163,164,165,168	0
2	SO4	C	623	5/5	0.79	0.25	194,195,196,197	0
2	SO4	J	604	5/5	0.79	0.23	154,156,158,160	0
2	SO4	G	615	5/5	0.80	0.29	180,182,183,183	0
2	SO4	D	613	5/5	0.80	0.20	165,167,170,170	0
2	SO4	B	603	5/5	0.80	0.28	135,138,140,144	0
2	SO4	B	607	5/5	0.80	0.56	186,187,188,190	0
2	SO4	E	621	5/5	0.80	0.32	154,156,160,163	0
2	SO4	B	614	5/5	0.80	0.33	152,153,157,159	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	F	612	5/5	0.80	0.26	155,156,157,159	0
2	SO4	H	609	5/5	0.80	0.29	147,147,153,156	0
3	GOL	K	613	6/6	0.80	0.27	108,110,112,115	0
3	GOL	L	612	6/6	0.80	0.41	131,134,136,137	0
2	SO4	E	616	5/5	0.81	0.30	166,170,171,172	0
3	GOL	G	621	6/6	0.81	0.22	92,102,106,111	0
3	GOL	H	614	6/6	0.81	0.23	78,90,94,99	0
3	GOL	A	625	6/6	0.81	0.42	73,87,90,92	0
2	SO4	F	602	5/5	0.81	0.14	151,157,158,159	0
2	SO4	D	620	5/5	0.81	0.27	163,164,166,166	0
2	SO4	C	607	5/5	0.81	0.26	167,169,170,172	0
2	SO4	K	606	5/5	0.81	0.36	144,146,148,153	0
2	SO4	B	613	5/5	0.82	0.30	194,196,197,199	0
2	SO4	D	608	5/5	0.82	0.24	146,148,149,152	0
2	SO4	E	605	5/5	0.82	0.30	152,155,159,159	0
2	SO4	E	615	5/5	0.82	0.27	143,145,148,154	0
3	GOL	I	614	6/6	0.82	0.33	105,111,114,115	0
2	SO4	C	613	5/5	0.82	0.27	165,166,167,169	0
2	SO4	C	608	5/5	0.82	0.15	162,162,164,164	0
2	SO4	K	602	5/5	0.82	0.20	139,139,144,149	0
2	SO4	E	619	5/5	0.83	0.25	186,187,188,188	0
2	SO4	B	606	5/5	0.83	0.26	127,134,135,140	0
2	SO4	F	608	5/5	0.83	0.31	160,161,163,163	0
2	SO4	I	607	5/5	0.83	0.21	151,152,152,153	0
2	SO4	G	613	5/5	0.83	0.68	204,205,206,207	0
3	GOL	B	626	6/6	0.83	0.19	75,101,103,104	0
2	SO4	J	606	5/5	0.83	0.32	137,141,144,145	0
3	GOL	C	625	6/6	0.83	0.30	90,98,100,101	0
2	SO4	G	605	5/5	0.83	0.34	155,159,161,163	0
2	SO4	C	617	5/5	0.83	0.22	164,164,167,168	0
2	SO4	I	611	5/5	0.83	0.58	178,178,180,180	0
2	SO4	J	603	5/5	0.84	0.18	195,195,196,198	0
2	SO4	C	620	5/5	0.84	0.25	162,163,164,165	0
2	SO4	D	603	5/5	0.84	0.18	193,194,195,198	0
2	SO4	D	604	5/5	0.84	0.38	208,209,210,211	0
3	GOL	E	627	6/6	0.84	0.30	115,115,117,121	0
2	SO4	L	608	5/5	0.84	0.17	154,158,161,163	0
2	SO4	D	605	5/5	0.84	0.24	162,162,163,167	0
2	SO4	B	609	5/5	0.84	0.26	125,130,138,140	0
2	SO4	E	610	5/5	0.84	0.21	147,149,152,154	0
2	SO4	K	603	5/5	0.84	0.30	149,152,153,154	0
3	GOL	H	615	6/6	0.84	0.27	88,97,109,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	616	5/5	0.84	0.26	193,194,196,196	0
2	SO4	B	619	5/5	0.84	0.49	167,169,169,169	0
3	GOL	A	631	6/6	0.84	0.38	20,20,20,20	0
3	GOL	J	609	6/6	0.84	0.20	95,98,100,101	0
2	SO4	G	602	5/5	0.84	0.26	119,128,137,138	0
3	GOL	K	612	6/6	0.84	0.17	91,114,115,120	0
3	GOL	B	629	6/6	0.84	0.26	99,103,107,107	0
2	SO4	D	619	5/5	0.84	0.34	158,159,160,164	0
2	SO4	A	606	5/5	0.85	0.30	127,131,134,135	0
2	SO4	I	601	5/5	0.85	0.25	174,174,176,179	0
3	GOL	G	622	6/6	0.85	0.24	85,88,94,98	0
2	SO4	D	621	5/5	0.85	0.28	176,177,178,180	0
2	SO4	L	604	5/5	0.85	0.37	184,187,189,190	0
2	SO4	L	606	5/5	0.85	0.19	155,156,158,160	0
2	SO4	L	607	5/5	0.85	0.19	141,143,150,151	0
2	SO4	B	610	5/5	0.85	0.17	162,164,165,166	0
2	SO4	E	625	5/5	0.85	0.41	158,158,160,163	0
2	SO4	D	607	5/5	0.85	0.29	115,120,123,127	0
2	SO4	D	611	5/5	0.85	0.25	148,151,159,160	0
2	SO4	G	606	5/5	0.85	0.22	138,141,143,145	0
2	SO4	E	606	5/5	0.85	0.23	136,143,144,146	0
2	SO4	E	602	5/5	0.86	0.16	176,177,178,178	0
2	SO4	F	611	5/5	0.86	0.22	165,166,167,168	0
2	SO4	C	606	5/5	0.86	0.24	128,134,135,139	0
3	GOL	A	624	6/6	0.86	0.40	74,86,91,91	0
3	GOL	G	618	6/6	0.86	0.26	98,100,101,102	0
2	SO4	B	620	5/5	0.86	0.16	159,162,163,166	0
2	SO4	F	606	5/5	0.86	0.14	162,163,165,165	0
2	SO4	B	612	5/5	0.86	0.61	180,181,184,186	0
2	SO4	E	607	5/5	0.86	0.23	137,140,144,148	0
2	SO4	H	606	5/5	0.87	0.27	128,131,132,132	0
2	SO4	H	603	5/5	0.87	0.29	134,137,137,141	0
2	SO4	B	615	5/5	0.87	0.21	154,156,158,160	0
2	SO4	G	609	5/5	0.87	0.14	158,161,162,162	0
2	SO4	L	601	5/5	0.88	0.13	177,180,180,182	0
2	SO4	D	606	5/5	0.88	0.29	166,167,167,167	0
2	SO4	A	610	5/5	0.88	0.34	157,163,165,166	0
2	SO4	A	619	5/5	0.88	0.27	167,167,170,171	0
2	SO4	L	605	5/5	0.88	0.17	87,119,127,128	0
2	SO4	G	603	5/5	0.88	0.27	139,143,144,148	0
2	SO4	F	603	5/5	0.88	0.28	139,139,141,141	0
2	SO4	B	611	5/5	0.88	0.19	169,170,171,173	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	C	626	6/6	0.89	0.50	120,120,122,123	0
2	SO4	F	604	5/5	0.89	0.25	137,138,142,146	0
3	GOL	G	619	6/6	0.89	0.24	112,114,115,117	0
2	SO4	C	610	5/5	0.89	0.27	163,165,166,167	0
2	SO4	A	611	5/5	0.89	0.35	174,174,175,175	0
3	GOL	A	629	6/6	0.89	0.34	95,99,103,103	0
3	GOL	E	628	6/6	0.89	0.39	105,107,108,108	0
2	SO4	A	605	5/5	0.89	0.14	144,144,147,149	0
2	SO4	A	607	5/5	0.90	0.28	118,123,128,129	0
3	GOL	B	627	6/6	0.90	0.45	87,98,104,105	0
2	SO4	G	612	5/5	0.90	0.14	152,154,155,156	0
2	SO4	F	607	5/5	0.90	0.38	135,139,140,141	0
3	GOL	E	626	6/6	0.90	0.32	68,72,83,84	0
2	SO4	L	611	5/5	0.90	0.54	30,30,30,30	0
2	SO4	A	608	5/5	0.91	0.28	136,144,146,148	0
2	SO4	A	609	5/5	0.91	0.23	127,131,134,138	0
2	SO4	D	601	5/5	0.91	0.38	118,121,125,134	0
2	SO4	C	614	5/5	0.91	0.34	160,161,162,165	0
2	SO4	B	608	5/5	0.91	0.33	142,147,148,148	0
3	GOL	G	623	6/6	0.91	0.57	87,93,100,111	0
2	SO4	A	601	5/5	0.91	0.34	96,102,116,116	0
2	SO4	E	609	5/5	0.91	0.34	121,135,138,139	0
2	SO4	I	605	5/5	0.92	0.22	140,143,143,143	0
2	SO4	E	618	5/5	0.92	0.28	135,139,142,143	0
2	SO4	B	621	5/5	0.92	0.33	156,157,159,159	0
2	SO4	D	622	5/5	0.92	0.50	30,30,30,30	0
2	SO4	E	604	5/5	0.92	0.36	114,124,128,134	0
2	SO4	B	604	5/5	0.92	0.18	115,120,123,129	0
2	SO4	I	613	5/5	0.93	0.49	30,30,30,30	0
3	GOL	B	628	6/6	0.93	0.31	62,78,80,82	0
2	SO4	C	603	5/5	0.93	0.17	87,91,93,97	0
2	SO4	F	601	5/5	0.93	0.21	80,104,106,106	0
2	SO4	G	604	5/5	0.93	0.37	133,135,137,137	0
2	SO4	H	607	5/5	0.94	0.20	144,146,150,151	0
2	SO4	B	602	5/5	0.94	0.30	99,102,110,113	0
2	SO4	C	602	5/5	0.94	0.27	108,117,118,122	0
2	SO4	G	601	5/5	0.94	0.23	92,93,101,111	0
2	SO4	A	602	5/5	0.94	0.19	80,94,96,98	0
2	SO4	K	610	5/5	0.95	0.58	30,30,30,30	0
2	SO4	G	617	5/5	0.95	0.48	30,30,30,30	0
3	GOL	D	623	6/6	0.95	0.34	70,80,84,90	0
2	SO4	L	610	5/5	0.96	0.54	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	K	601	5/5	0.96	0.14	87,87,101,106	0
3	GOL	C	624	6/6	0.97	0.25	66,70,75,76	0
2	SO4	B	601	5/5	0.97	0.18	120,121,125,130	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.