wwPDB X-ray Structure Validation Summary Report (i)

Nov 7, 2023 – 06:20 AM EST

PDB ID	:	5W5R
Title	:	Agrobacterium tumefaciens ADP-glucose pyrophosphorylase P96A mutant bound to activator pyruvate
Authors	:	Mascarenhas, R.N.; Hill, B.L.; Ballicora, M.A.; Liu, D.
Deposited on	:	2017-06-15
Resolution	:	1.75 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

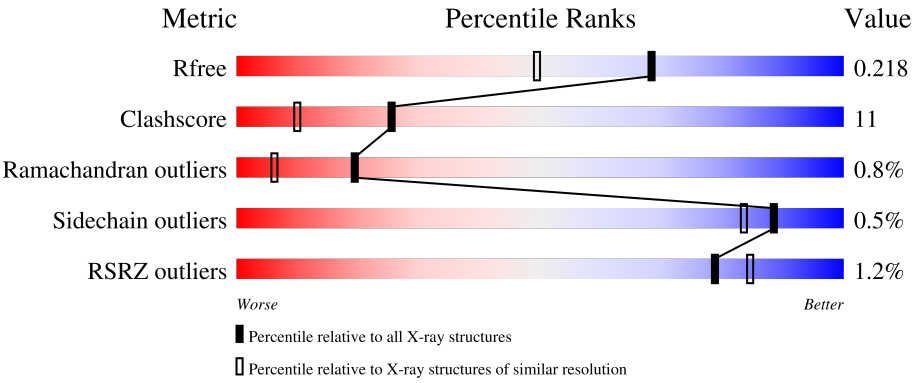
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	418	77% 22%
1	B	418	77% 21%
1	C	418	78% 20%
1	D	418	79% 19%
1	E	418	80% 17%

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Mol	Chain	Length	Quality of chain
1	F	418	81% 16%
1	G	418	78% 20%
1	H	418	77% 20%
1	I	418	78% 19%
1	J	418	80% 19%
1	K	418	80% 18%
1	L	418	78% 20%
1	M	418	78% 19%
1	N	418	3% 75% 23%
1	O	418	84% 14%
1	P	418	77% 20%
1	Q	418	80% 17%
1	R	418	82% 15%
1	T	418	78% 21%
1	U	418	80% 18%

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	B	501	-	-	X	-
2	SO4	K	502	-	-	X	-
2	SO4	P	502	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 72534 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 Glucose-1-phosphate adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	1	0
			3250	2060	564	613	13			
1	B	415	Total	C	N	O	S	8	3	0
			3262	2068	567	614	13			
1	C	415	Total	C	N	O	S	4	1	0
			3248	2059	564	612	13			
1	D	412	Total	C	N	O	S	0	2	0
			3236	2054	561	608	13			
1	E	409	Total	C	N	O	S	0	1	0
			3206	2036	552	605	13			
1	H	409	Total	C	N	O	S	0	0	0
			3206	2035	552	606	13			
1	I	409	Total	C	N	O	S	0	1	0
			3210	2038	552	607	13			
1	J	415	Total	C	N	O	S	0	3	0
			3251	2062	561	615	13			
1	K	410	Total	C	N	O	S	0	0	0
			3211	2038	553	607	13			
1	L	410	Total	C	N	O	S	0	1	0
			3220	2043	554	610	13			
1	N	415	Total	C	N	O	S	0	0	0
			3247	2056	561	617	13			
1	O	411	Total	C	N	O	S	0	0	0
			3216	2041	554	608	13			
1	P	409	Total	C	N	O	S	0	1	0
			3210	2038	552	607	13			
1	Q	409	Total	C	N	O	S	0	1	0
			3210	2038	552	607	13			
1	R	409	Total	C	N	O	S	5	2	0
			3214	2042	552	607	13			
1	F	408	Total	C	N	O	S	5	2	0
			3216	2044	554	605	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	410	Total	C	N	O	S	0	1	0
			3225	2046	559	607	13			
1	M	409	Total	C	N	O	S	0	1	0
			3216	2041	555	607	13			
1	T	415	Total	C	N	O	S	0	1	0
			3252	2062	562	615	13			
1	U	415	Total	C	N	O	S	4	1	0
			3248	2059	562	614	13			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	ALA	-	expression tag	UNP P39669
A	5	ALA	-	expression tag	UNP P39669
A	6	ALA	-	expression tag	UNP P39669
A	97	ALA	PRO	engineered mutation	UNP P39669
A	221	LEU	VAL	conflict	UNP P39669
B	4	ALA	-	expression tag	UNP P39669
B	5	ALA	-	expression tag	UNP P39669
B	6	ALA	-	expression tag	UNP P39669
B	97	ALA	PRO	engineered mutation	UNP P39669
B	221	LEU	VAL	conflict	UNP P39669
C	4	ALA	-	expression tag	UNP P39669
C	5	ALA	-	expression tag	UNP P39669
C	6	ALA	-	expression tag	UNP P39669
C	97	ALA	PRO	engineered mutation	UNP P39669
C	221	LEU	VAL	conflict	UNP P39669
D	4	ALA	-	expression tag	UNP P39669
D	5	ALA	-	expression tag	UNP P39669
D	6	ALA	-	expression tag	UNP P39669
D	97	ALA	PRO	engineered mutation	UNP P39669
D	221	LEU	VAL	conflict	UNP P39669
E	4	ALA	-	expression tag	UNP P39669
E	5	ALA	-	expression tag	UNP P39669
E	6	ALA	-	expression tag	UNP P39669
E	97	ALA	PRO	engineered mutation	UNP P39669
E	221	LEU	VAL	conflict	UNP P39669
H	4	ALA	-	expression tag	UNP P39669
H	5	ALA	-	expression tag	UNP P39669
H	6	ALA	-	expression tag	UNP P39669
H	97	ALA	PRO	engineered mutation	UNP P39669
H	221	LEU	VAL	conflict	UNP P39669
I	4	ALA	-	expression tag	UNP P39669

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Chain	Residue	Modelled	Actual	Comment	Reference
I	5	ALA	-	expression tag	UNP P39669
I	6	ALA	-	expression tag	UNP P39669
I	97	ALA	PRO	engineered mutation	UNP P39669
I	221	LEU	VAL	conflict	UNP P39669
J	4	ALA	-	expression tag	UNP P39669
J	5	ALA	-	expression tag	UNP P39669
J	6	ALA	-	expression tag	UNP P39669
J	97	ALA	PRO	engineered mutation	UNP P39669
J	221	LEU	VAL	conflict	UNP P39669
K	4	ALA	-	expression tag	UNP P39669
K	5	ALA	-	expression tag	UNP P39669
K	6	ALA	-	expression tag	UNP P39669
K	97	ALA	PRO	engineered mutation	UNP P39669
K	221	LEU	VAL	conflict	UNP P39669
L	4	ALA	-	expression tag	UNP P39669
L	5	ALA	-	expression tag	UNP P39669
L	6	ALA	-	expression tag	UNP P39669
L	97	ALA	PRO	engineered mutation	UNP P39669
L	221	LEU	VAL	conflict	UNP P39669
N	4	ALA	-	expression tag	UNP P39669
N	5	ALA	-	expression tag	UNP P39669
N	6	ALA	-	expression tag	UNP P39669
N	97	ALA	PRO	engineered mutation	UNP P39669
N	221	LEU	VAL	conflict	UNP P39669
O	4	ALA	-	expression tag	UNP P39669
O	5	ALA	-	expression tag	UNP P39669
O	6	ALA	-	expression tag	UNP P39669
O	97	ALA	PRO	engineered mutation	UNP P39669
O	221	LEU	VAL	conflict	UNP P39669
P	4	ALA	-	expression tag	UNP P39669
P	5	ALA	-	expression tag	UNP P39669
P	6	ALA	-	expression tag	UNP P39669
P	97	ALA	PRO	engineered mutation	UNP P39669
P	221	LEU	VAL	conflict	UNP P39669
Q	4	ALA	-	expression tag	UNP P39669
Q	5	ALA	-	expression tag	UNP P39669
Q	6	ALA	-	expression tag	UNP P39669
Q	97	ALA	PRO	engineered mutation	UNP P39669
Q	221	LEU	VAL	conflict	UNP P39669
R	4	ALA	-	expression tag	UNP P39669
R	5	ALA	-	expression tag	UNP P39669
R	6	ALA	-	expression tag	UNP P39669

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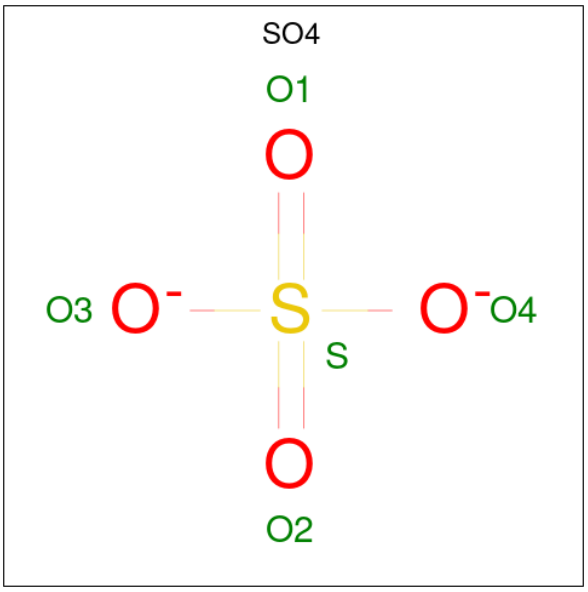
Chain	Residue	Modelled	Actual	Comment	Reference
R	97	ALA	PRO	engineered mutation	UNP P39669
R	221	LEU	VAL	conflict	UNP P39669
F	4	ALA	-	expression tag	UNP P39669
F	5	ALA	-	expression tag	UNP P39669
F	6	ALA	-	expression tag	UNP P39669
F	97	ALA	PRO	engineered mutation	UNP P39669
F	221	LEU	VAL	conflict	UNP P39669
G	4	ALA	-	expression tag	UNP P39669
G	5	ALA	-	expression tag	UNP P39669
G	6	ALA	-	expression tag	UNP P39669
G	97	ALA	PRO	engineered mutation	UNP P39669
G	221	LEU	VAL	conflict	UNP P39669
M	4	ALA	-	expression tag	UNP P39669
M	5	ALA	-	expression tag	UNP P39669
M	6	ALA	-	expression tag	UNP P39669
M	97	ALA	PRO	engineered mutation	UNP P39669
M	221	LEU	VAL	conflict	UNP P39669
T	4	ALA	-	expression tag	UNP P39669
T	5	ALA	-	expression tag	UNP P39669
T	6	ALA	-	expression tag	UNP P39669
T	97	ALA	PRO	engineered mutation	UNP P39669
T	221	LEU	VAL	conflict	UNP P39669
U	4	ALA	-	expression tag	UNP P39669
U	5	ALA	-	expression tag	UNP P39669
U	6	ALA	-	expression tag	UNP P39669
U	97	ALA	PRO	engineered mutation	UNP P39669
U	221	LEU	VAL	conflict	UNP P39669

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	N	1	Total O S 5 4 1	0	0
2	N	1	Total O S 5 4 1	0	0
2	O	1	Total O S 5 4 1	0	0
2	O	1	Total O S 5 4 1	0	0
2	P	1	Total O S 5 4 1	0	0
2	P	1	Total O S 5 4 1	0	0
2	Q	1	Total O S 5 4 1	0	0
2	Q	1	Total O S 5 4 1	0	0
2	R	1	Total O S 5 4 1	0	0
2	R	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0

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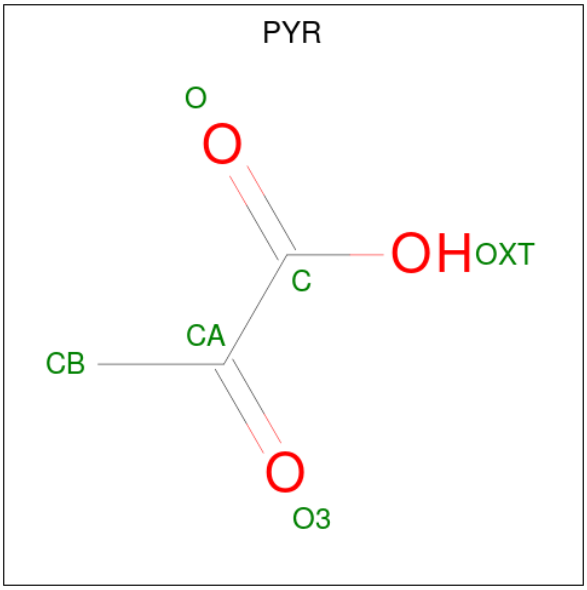
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	M	1	Total O S 5 4 1	0	0
2	M	1	Total O S 5 4 1	0	0
2	T	1	Total O S 5 4 1	0	0
2	T	1	Total O S 5 4 1	0	0
2	T	1	Total O S 5 4 1	0	0
2	U	1	Total O S 5 4 1	0	0
2	U	1	Total O S 5 4 1	0	0

- Molecule 3 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	387	Total O 387 387	0	0
4	B	372	Total O 372 372	0	0
4	C	435	Total O 435 435	0	0
4	D	407	Total O 407 407	0	0
4	E	409	Total O 409 409	0	0
4	H	365	Total O 365 365	0	0
4	I	420	Total O 420 420	0	0
4	J	451	Total O 451 451	0	0
4	K	395	Total O 395 395	0	0
4	L	312	Total O 312 312	0	0
4	N	297	Total O 297 297	0	0
4	O	436	Total O 436 436	0	0
4	P	347	Total O 347 347	0	0
4	Q	371	Total O 371 371	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	R	438	Total O 438 438	0	0
4	F	406	Total O 406 406	0	0
4	G	367	Total O 367 367	0	0
4	M	360	Total O 360 360	0	0
4	T	365	Total O 365 365	0	0
4	U	376	Total O 376 376	0	0

3 Residue-property plots (i)

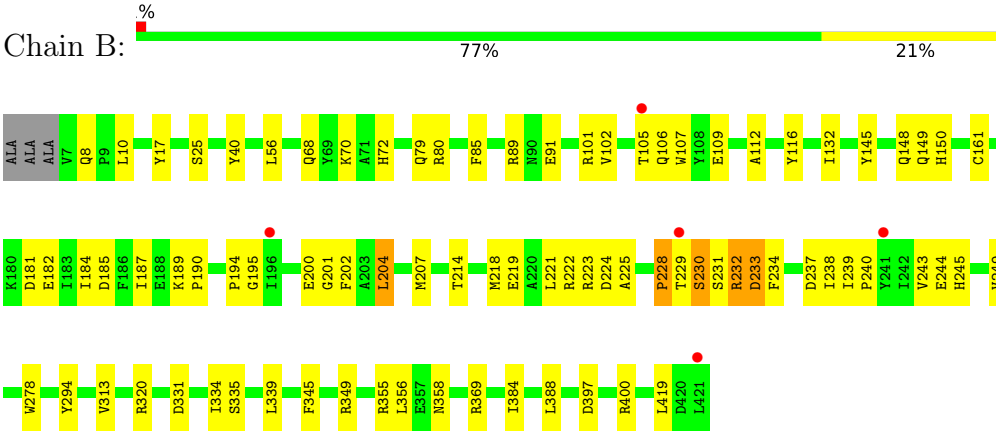
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glucose-1-phosphate adenylyltransferase

Chain A:

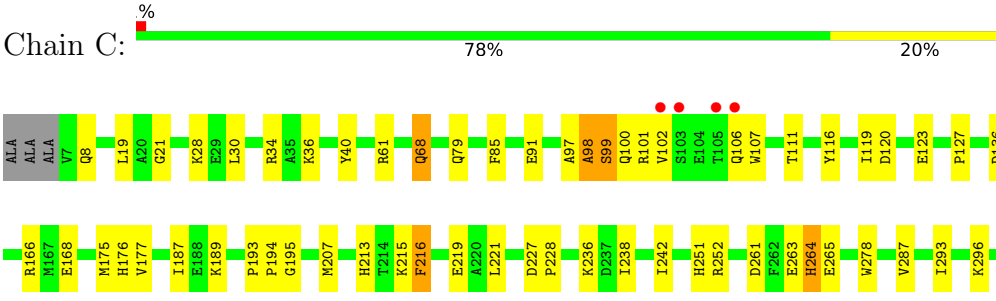
• Molecule 1: Glucose-1-phosphate adenylyltransferase

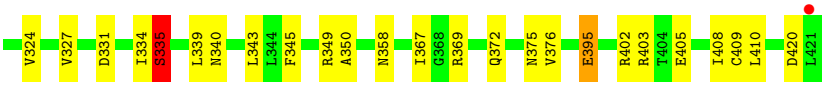
Chain B:



• Molecule 1: Glucose-1-phosphate adenylyltransferase

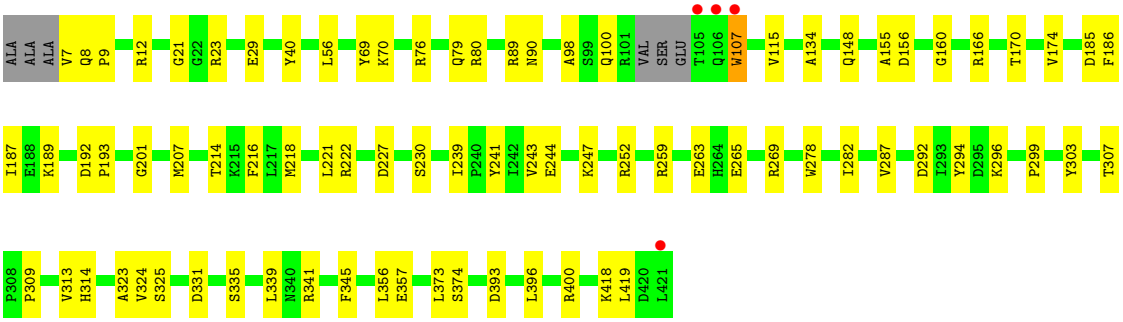
Chain C:





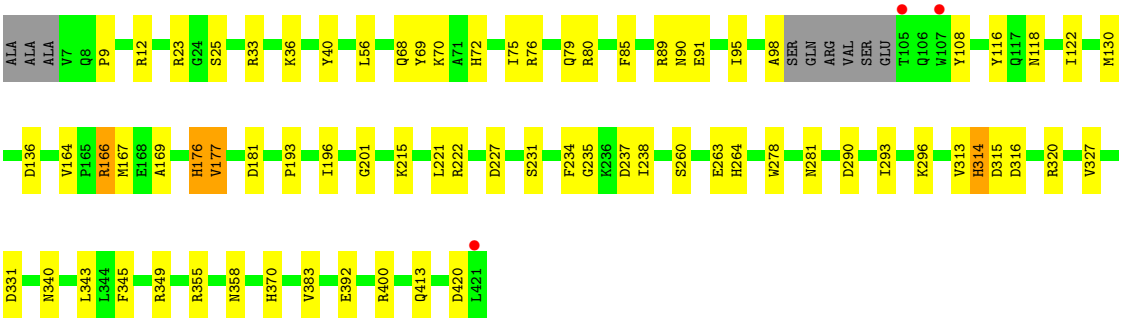
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain D:



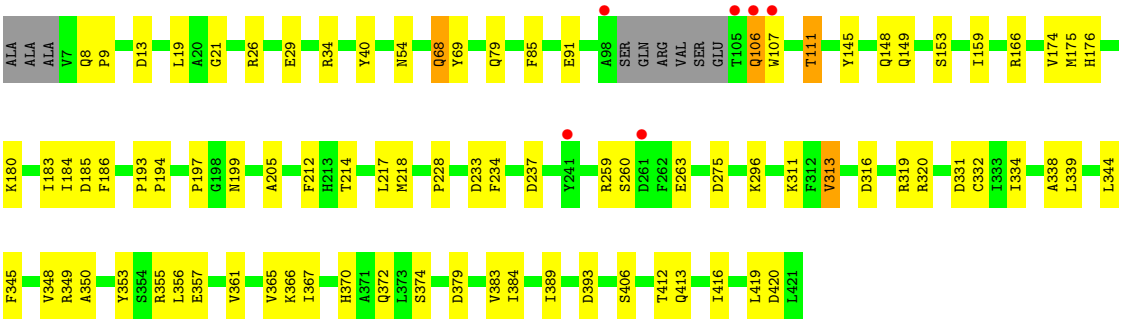
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain E:



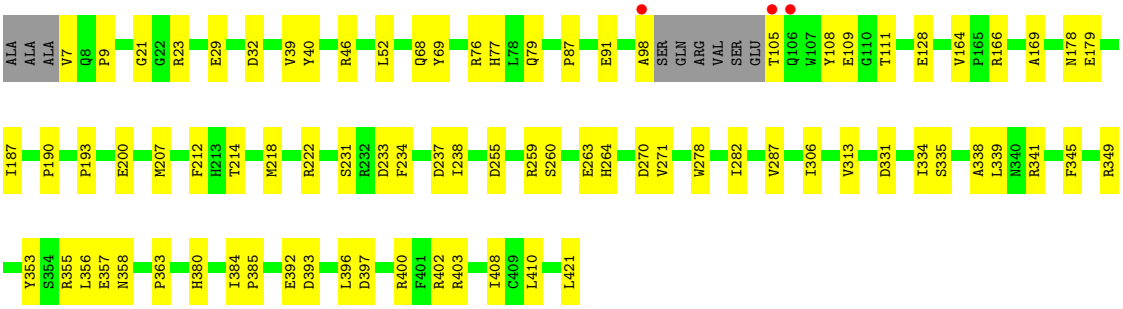
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain H:

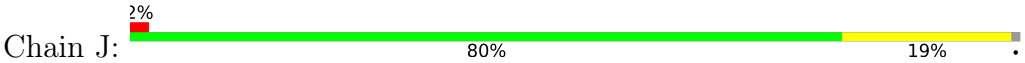


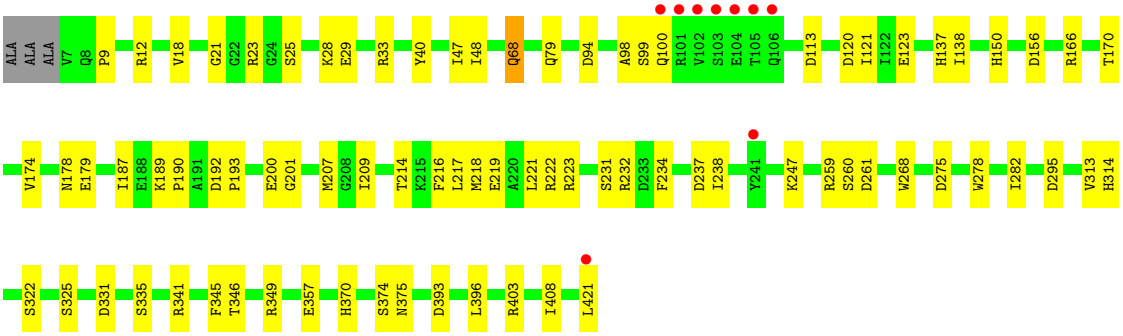
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain I:

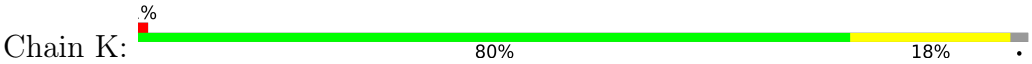


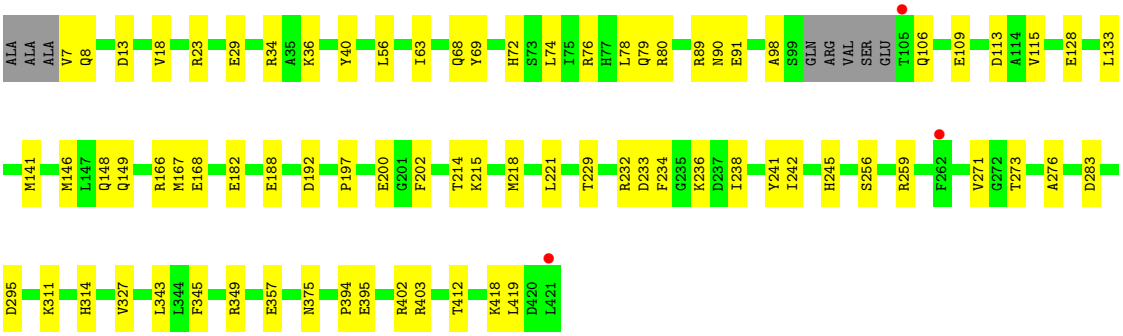
• Molecule 1: Glucose-1-phosphate adenylyltransferase



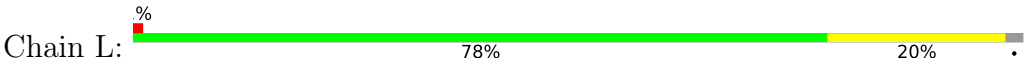


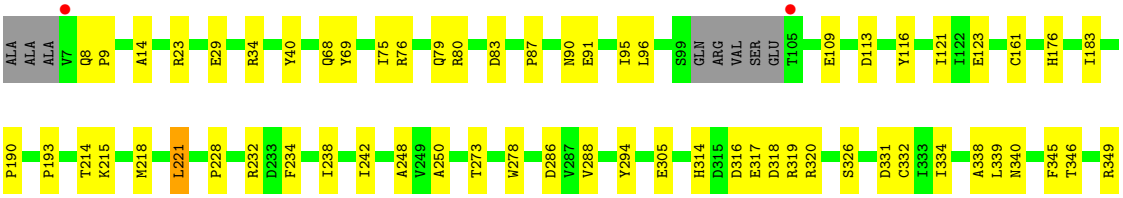
• Molecule 1: Glucose-1-phosphate adenylyltransferase

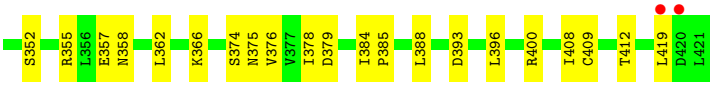




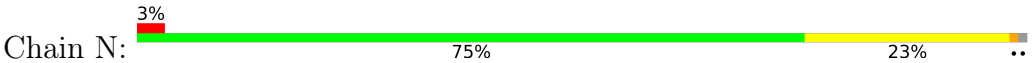
• Molecule 1: Glucose-1-phosphate adenylyltransferase

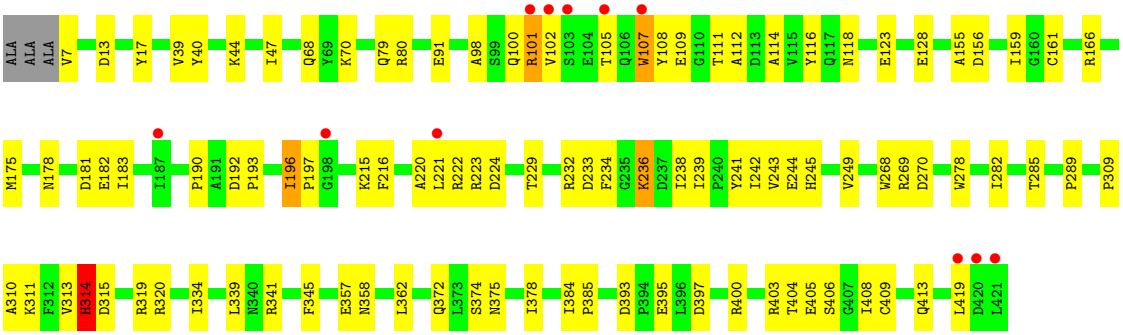




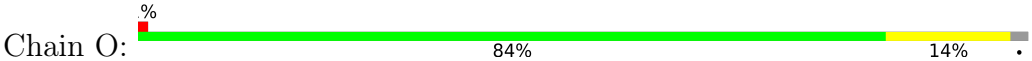


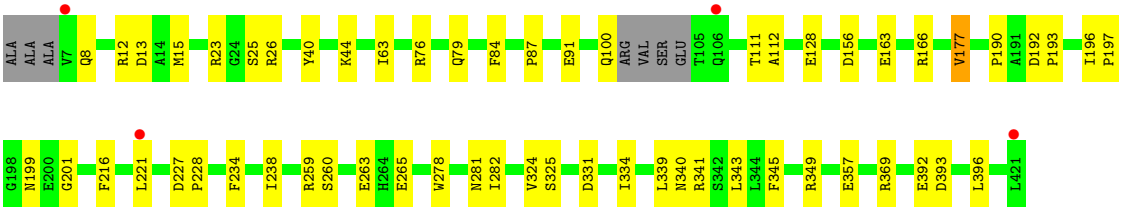
• Molecule 1: Glucose-1-phosphate adenylyltransferase



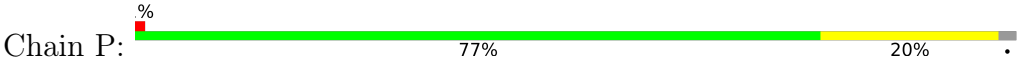


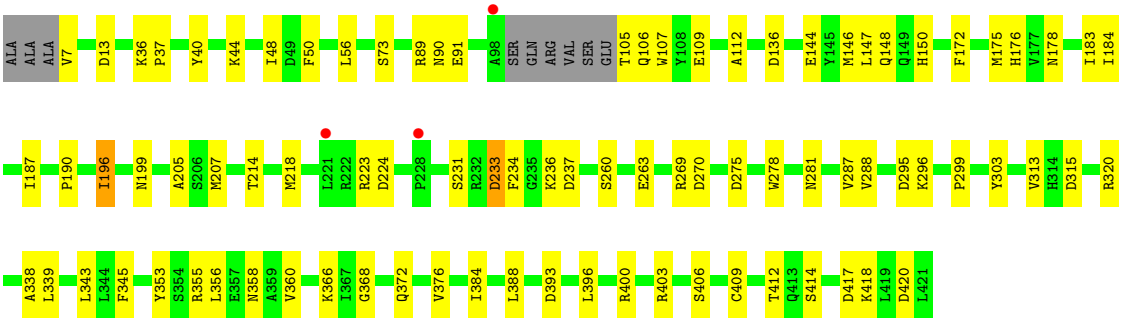
• Molecule 1: Glucose-1-phosphate adenylyltransferase



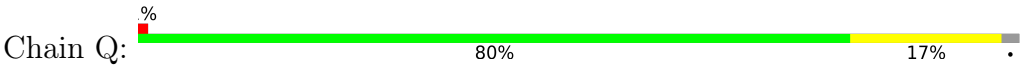


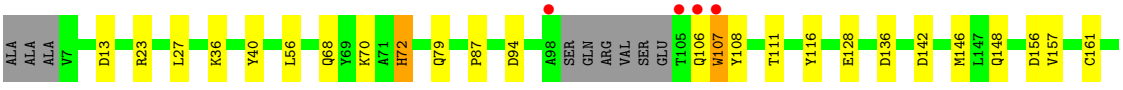
• Molecule 1: Glucose-1-phosphate adenylyltransferase

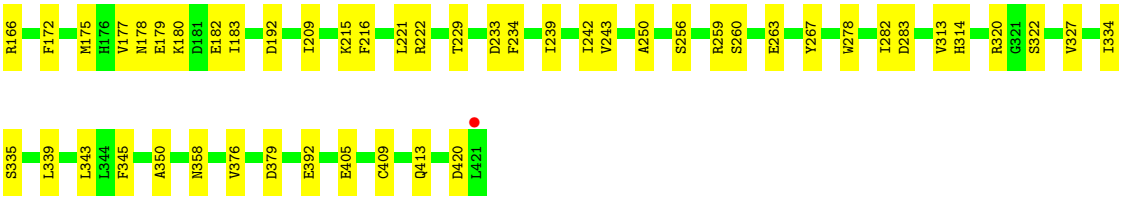




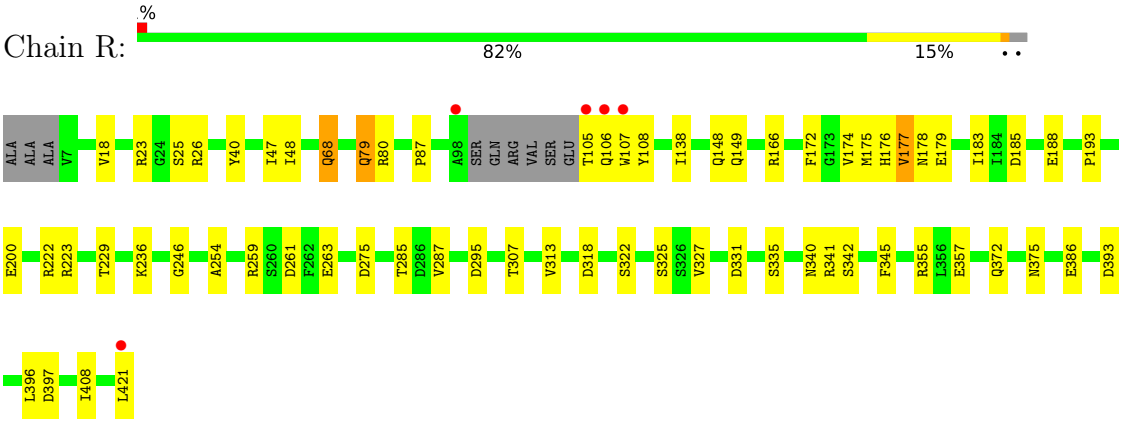
• Molecule 1: Glucose-1-phosphate adenylyltransferase



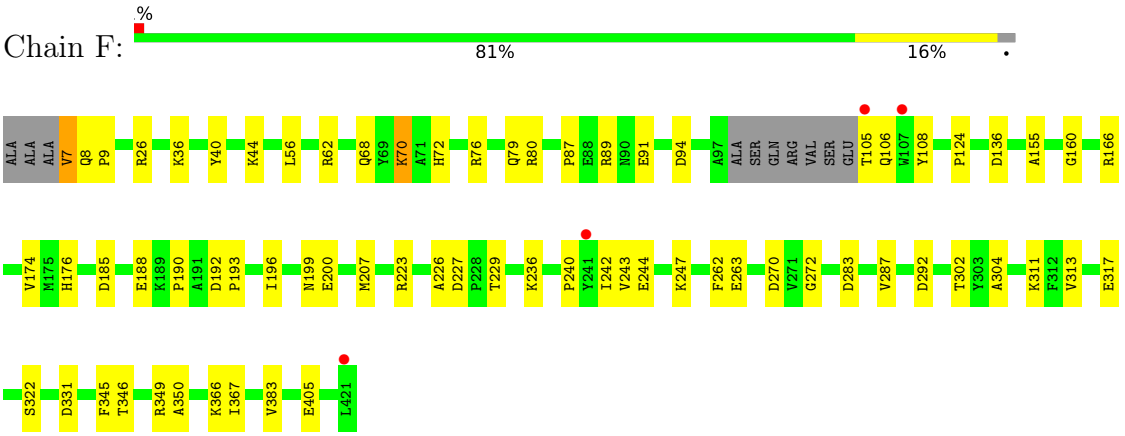




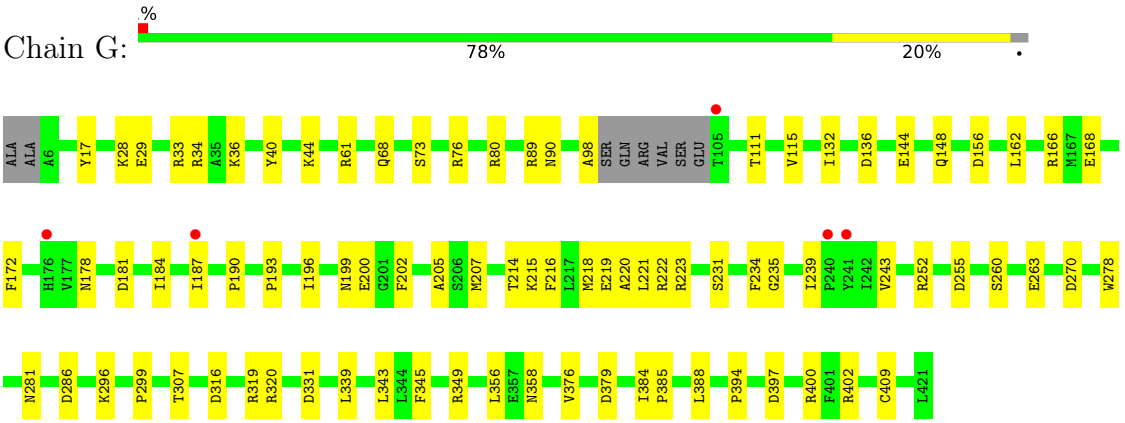
• Molecule 1: Glucose-1-phosphate adenylyltransferase



• Molecule 1: Glucose-1-phosphate adenylyltransferase

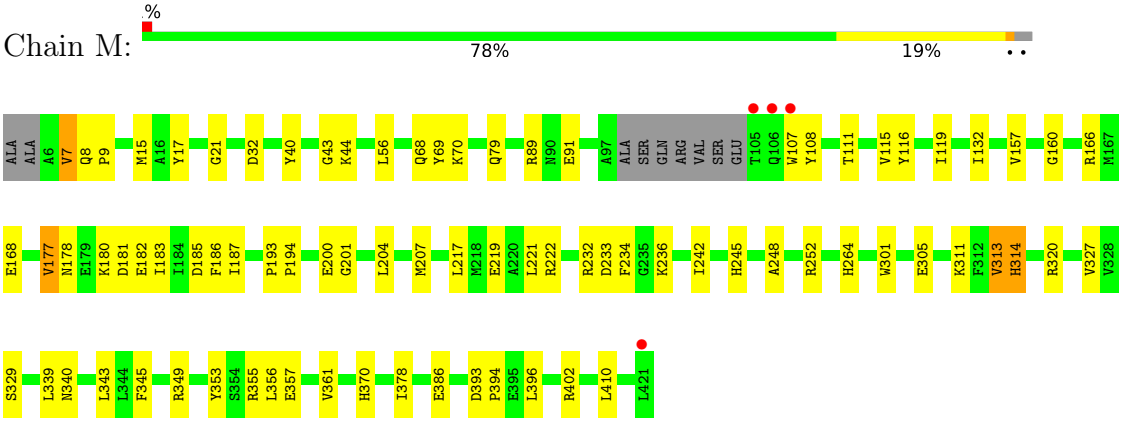


• Molecule 1: Glucose-1-phosphate adenylyltransferase



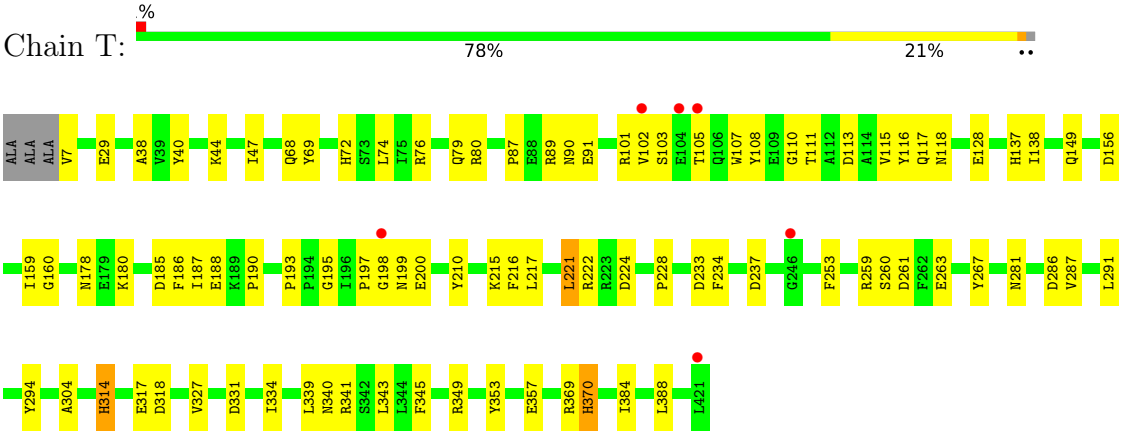
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain M:



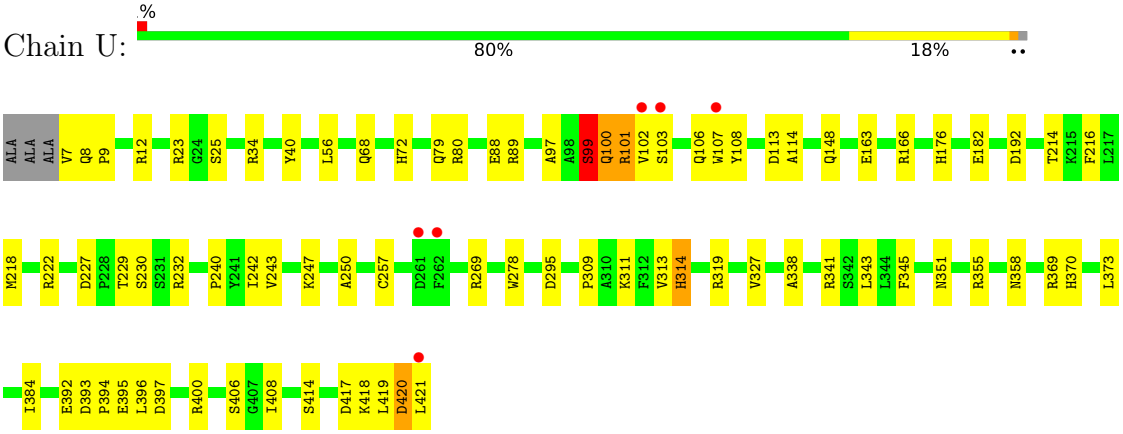
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain T:



• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain U:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	93.40Å 140.99Å 228.21Å 72.00° 78.18° 90.01°	Depositor
Resolution (Å)	46.88 – 1.75 46.88 – 1.75	Depositor EDS
% Data completeness (in resolution range)	44.0 (46.88-1.75) 47.2 (46.88-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.201 , 0.228 0.189 , 0.218	Depositor DCC
R_{free} test set	1112 reflections (0.21%)	wwPDB-VP
Wilson B-factor (Å^2)	18.6	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.457 for h,-k,h-l 0.467 for -h,k,k-l 0.467 for -h,-k,-h-k+l	Xtriage
Reported twinning fraction	0.490 for h,-k,h-l	Depositor
Outliers	0 of 535072 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	72534	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.4601e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PYR, 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	0.23	0/3328	0.44	1/4518 (0.0%)
1	B	0.25	0/3347	0.46	1/4546 (0.0%)
1	C	0.26	0/3327	0.46	0/4519
1	D	0.23	0/3317	0.42	0/4504
1	E	0.23	0/3284	0.42	0/4462
1	F	0.25	0/3297	0.42	0/4478
1	G	0.23	0/3303	0.41	0/4485
1	H	0.23	0/3281	0.42	0/4457
1	I	0.24	0/3288	0.43	0/4467
1	J	0.23	0/3336	0.42	0/4533
1	K	0.23	0/3286	0.41	0/4464
1	L	0.24	0/3295	0.43	0/4476
1	M	0.25	0/3294	0.43	1/4474 (0.0%)
1	N	0.25	0/3323	0.46	0/4516
1	O	0.24	0/3291	0.42	0/4471
1	P	0.24	0/3288	0.44	0/4467
1	Q	0.26	0/3288	0.45	0/4467
1	R	0.23	0/3295	0.42	0/4476
1	T	0.24	0/3331	0.45	0/4526
1	U	0.23	0/3327	0.43	0/4520
All	All	0.24	0/66126	0.43	3/89826 (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	A	0	1
1	C	0	1
1	F	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1
1	M	0	1
1	N	0	2
All	All	0	7

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	204	LEU	CB-CG-CD1	-7.31	98.58	111.00
1	M	313	VAL	C-N-CA	5.58	135.65	121.70
1	A	313	VAL	C-N-CA	5.33	135.01	121.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	VAL	Peptide
1	C	263	GLU	Peptide
1	I	212	PHE	Peptide
1	N	100	GLN	Peptide
1	N	244	GLU	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	3250	0	3153	79	0
1	B	3262	0	3170	75	0
1	C	3248	0	3146	67	0
1	D	3236	0	3144	71	0
1	E	3206	0	3114	65	0
1	F	3216	0	3137	71	0
1	G	3225	0	3140	80	0
1	H	3206	0	3111	76	0
1	I	3210	0	3118	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	3251	0	3150	62	1
1	K	3211	0	3113	66	0
1	L	3220	0	3118	64	0
1	M	3216	0	3129	73	0
1	N	3247	0	3138	95	0
1	O	3216	0	3115	44	0
1	P	3210	0	3118	74	0
1	Q	3210	0	3118	65	0
1	R	3214	0	3127	57	1
1	T	3252	0	3157	77	0
1	U	3248	0	3145	71	0
2	A	10	0	0	1	0
2	B	10	0	0	2	0
2	C	10	0	0	2	0
2	D	10	0	0	0	0
2	E	15	0	0	0	0
2	F	10	0	0	0	0
2	G	10	0	0	1	0
2	H	10	0	0	0	0
2	I	10	0	0	0	0
2	J	10	0	0	0	0
2	K	10	0	0	3	0
2	L	10	0	0	0	0
2	M	10	0	0	0	0
2	N	10	0	0	0	0
2	O	10	0	0	1	0
2	P	10	0	0	3	0
2	Q	10	0	0	0	0
2	R	10	0	0	0	0
2	T	15	0	0	2	0
2	U	10	0	0	1	0
3	A	6	0	0	1	0
3	D	6	0	0	1	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	H	6	0	0	2	0
3	I	6	0	0	0	0
3	J	6	0	0	1	0
3	K	6	0	0	0	0
3	U	6	0	0	0	0
4	A	387	0	0	36	4
4	B	372	0	0	31	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	435	0	0	24	0
4	D	407	0	0	33	0
4	E	409	0	0	24	0
4	F	406	0	0	37	0
4	G	367	0	0	46	1
4	H	365	0	0	33	1
4	I	420	0	0	32	0
4	J	451	0	0	30	1
4	K	395	0	0	43	1
4	L	312	0	0	32	1
4	M	360	0	0	31	2
4	N	297	0	0	50	5
4	O	436	0	0	14	5
4	P	347	0	0	39	2
4	Q	371	0	0	35	1
4	R	438	0	0	35	2
4	T	365	0	0	33	1
4	U	376	0	0	36	2
All	All	72534	0	62661	1352	16

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 11.

The worst 5 of 1352 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:T:370:HIS:O	4:T:601:HOH:O	1.79	1.00
1:P:368:GLY:N	4:P:601:HOH:O	1.96	0.99
1:R:148:GLN:OE1	4:R:601:HOH:O	1.81	0.98
1:C:409:CYS:SG	4:C:796:HOH:O	2.22	0.97
1:J:341:ARG:NH2	4:J:602:HOH:O	1.98	0.96

The worst 5 of 16 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)
4:A:660:HOH:O	4:O:729:HOH:O[1_654]	1.86	0.34
4:N:848:HOH:O	4:G:679:HOH:O[1_545]	1.95	0.25
4:H:807:HOH:O	4:T:703:HOH:O[1_565]	1.97	0.23
4:O:1003:HOH:O	4:P:695:HOH:O[1_456]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:614:HOH:O	4:Q:633:HOH:O[1_455]	1.99	0.21

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	412/418 (99%)	388 (94%)	15 (4%)	9 (2%)	6 1
1	B	416/418 (100%)	391 (94%)	19 (5%)	6 (1%)	11 2
1	C	414/418 (99%)	395 (95%)	12 (3%)	7 (2%)	9 1
1	D	410/418 (98%)	392 (96%)	16 (4%)	2 (0%)	29 12
1	E	406/418 (97%)	389 (96%)	14 (3%)	3 (1%)	22 8
1	F	406/418 (97%)	386 (95%)	18 (4%)	2 (0%)	29 12
1	G	407/418 (97%)	392 (96%)	15 (4%)	0	100 100
1	H	405/418 (97%)	385 (95%)	14 (4%)	6 (2%)	10 2
1	I	406/418 (97%)	393 (97%)	12 (3%)	1 (0%)	47 29
1	J	416/418 (100%)	395 (95%)	19 (5%)	2 (0%)	29 12
1	K	406/418 (97%)	390 (96%)	12 (3%)	4 (1%)	15 4
1	L	407/418 (97%)	381 (94%)	25 (6%)	1 (0%)	47 29
1	M	406/418 (97%)	387 (95%)	18 (4%)	1 (0%)	47 29
1	N	413/418 (99%)	383 (93%)	24 (6%)	6 (2%)	10 2
1	O	407/418 (97%)	391 (96%)	16 (4%)	0	100 100
1	P	406/418 (97%)	390 (96%)	16 (4%)	0	100 100
1	Q	406/418 (97%)	386 (95%)	17 (4%)	3 (1%)	22 8
1	R	407/418 (97%)	392 (96%)	14 (3%)	1 (0%)	47 29
1	T	414/418 (99%)	390 (94%)	21 (5%)	3 (1%)	22 8
1	U	414/418 (99%)	387 (94%)	19 (5%)	8 (2%)	8 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	8184/8360 (98%)	7783 (95%)	336 (4%)	65 (1%)	19 6

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	THR
1	A	106	GLN
1	A	314	HIS
1	A	420	ASP
1	B	102	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	339/346 (98%)	338 (100%)	1 (0%)	92 89
1	B	342/346 (99%)	338 (99%)	4 (1%)	71 56
1	C	339/346 (98%)	335 (99%)	4 (1%)	71 56
1	D	339/346 (98%)	339 (100%)	0	100 100
1	E	337/346 (97%)	334 (99%)	3 (1%)	78 67
1	F	340/346 (98%)	339 (100%)	1 (0%)	92 89
1	G	339/346 (98%)	338 (100%)	1 (0%)	92 89
1	H	337/346 (97%)	334 (99%)	3 (1%)	78 67
1	I	338/346 (98%)	338 (100%)	0	100 100
1	J	341/346 (99%)	341 (100%)	0	100 100
1	K	337/346 (97%)	336 (100%)	1 (0%)	92 89
1	L	338/346 (98%)	336 (99%)	2 (1%)	86 79
1	M	339/346 (98%)	338 (100%)	1 (0%)	92 89
1	N	341/346 (99%)	339 (99%)	2 (1%)	86 79
1	O	337/346 (97%)	336 (100%)	1 (0%)	92 89
1	P	338/346 (98%)	335 (99%)	3 (1%)	78 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	338/346 (98%)	337 (100%)	1 (0%)	92	89
1	R	339/346 (98%)	337 (99%)	2 (1%)	86	79
1	T	342/346 (99%)	339 (99%)	3 (1%)	78	67
1	U	340/346 (98%)	339 (100%)	1 (0%)	92	89
All	All	6780/6920 (98%)	6746 (100%)	34 (0%)	88	83

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	296	LYS
1	M	177	VAL
1	T	221	LEU
1	H	13	ASP
1	E	293	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	245	HIS
1	O	8	GLN
1	T	79	GLN
1	N	118	ASN
1	Q	72	HIS

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)

51 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	PYR	H	503	-	5,5,5	1.11	0	3,6,6	1.42	0
2	SO4	A	501	-	4,4,4	0.15	0	6,6,6	0.11	0
3	PYR	A	503	-	5,5,5	1.02	0	3,6,6	1.63	1 (33%)
2	SO4	J	502	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	K	502	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	A	502	-	4,4,4	0.15	0	6,6,6	0.04	0
3	PYR	I	503	-	5,5,5	1.04	0	3,6,6	1.36	0
3	PYR	F	503	-	5,5,5	1.03	0	3,6,6	1.59	1 (33%)
2	SO4	R	501	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	L	501	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	D	502	-	4,4,4	0.15	0	6,6,6	0.08	0
2	SO4	F	501	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	T	502	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	U	501	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	L	502	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	F	502	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	G	501	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	U	502	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	E	502	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	O	501	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	G	502	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	B	501	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	Q	502	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	O	502	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	P	501	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	M	501	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	H	502	-	4,4,4	0.14	0	6,6,6	0.06	0
3	PYR	K	503	-	5,5,5	0.99	0	3,6,6	1.54	1 (33%)
3	PYR	J	503	-	5,5,5	1.03	0	3,6,6	1.62	1 (33%)
2	SO4	R	502	-	4,4,4	0.15	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	P	502	-	4,4,4	0.15	0	6,6,6	0.07	0
3	PYR	U	503	-	5,5,5	1.02	0	3,6,6	1.57	1 (33%)
2	SO4	H	501	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	I	501	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	B	502	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	T	501	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	N	501	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	M	502	-	4,4,4	0.16	0	6,6,6	0.09	0
3	PYR	E	504	-	5,5,5	0.99	0	3,6,6	1.69	1 (33%)
2	SO4	C	501	-	4,4,4	0.15	0	6,6,6	0.08	0
2	SO4	J	501	-	4,4,4	0.16	0	6,6,6	0.09	0
2	SO4	D	501	-	4,4,4	0.17	0	6,6,6	0.09	0
2	SO4	K	501	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	T	503	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	I	502	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	E	503	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	Q	501	-	4,4,4	0.16	0	6,6,6	0.05	0
3	PYR	D	503	-	5,5,5	1.11	0	3,6,6	1.40	0
2	SO4	N	502	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	E	501	-	4,4,4	0.17	0	6,6,6	0.08	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	PYR	U	503	-	-	0/4/4/4	-
3	PYR	H	503	-	-	0/4/4/4	-
3	PYR	A	503	-	-	0/4/4/4	-
3	PYR	K	503	-	-	0/4/4/4	-
3	PYR	J	503	-	-	0/4/4/4	-
3	PYR	E	504	-	-	0/4/4/4	-
3	PYR	I	503	-	-	0/4/4/4	-
3	PYR	F	503	-	-	0/4/4/4	-
3	PYR	D	503	-	-	0/4/4/4	-

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	503	PYR	OXT-C-CA	2.42	120.60	113.97
3	E	504	PYR	OXT-C-CA	2.39	120.50	113.97
3	F	503	PYR	OXT-C-CA	2.31	120.28	113.97
3	J	503	PYR	OXT-C-CA	2.31	120.28	113.97
3	U	503	PYR	OXT-C-CA	2.28	120.20	113.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	503	PYR	2	0
2	A	501	SO4	1	0
3	A	503	PYR	1	0
2	K	502	SO4	3	0
2	T	502	SO4	1	0
2	U	501	SO4	1	0
2	O	501	SO4	1	0
2	G	502	SO4	1	0
2	C	502	SO4	1	0
2	B	501	SO4	2	0
2	P	501	SO4	1	0
3	J	503	PYR	1	0
2	P	502	SO4	2	0
2	T	501	SO4	1	0
2	C	501	SO4	1	0
3	D	503	PYR	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	415/418 (99%)	-0.15	5 (1%)	79	84	12, 25, 45, 72	0
1	B	415/418 (99%)	-0.05	5 (1%)	79	84	13, 25, 48, 67	0
1	C	415/418 (99%)	-0.20	5 (1%)	79	84	11, 22, 38, 69	0
1	D	412/418 (98%)	-0.22	4 (0%)	82	87	10, 21, 40, 74	0
1	E	409/418 (97%)	-0.29	3 (0%)	87	92	12, 22, 37, 61	0
1	F	408/418 (97%)	-0.18	4 (0%)	82	87	11, 21, 38, 61	0
1	G	410/418 (98%)	-0.07	5 (1%)	79	84	13, 26, 46, 64	0
1	H	409/418 (97%)	-0.18	6 (1%)	73	80	12, 25, 42, 64	0
1	I	409/418 (97%)	-0.26	3 (0%)	87	92	11, 21, 39, 67	0
1	J	415/418 (99%)	-0.15	9 (2%)	62	69	10, 21, 42, 74	0
1	K	410/418 (98%)	-0.21	3 (0%)	87	92	11, 24, 42, 63	0
1	L	410/418 (98%)	-0.13	4 (0%)	82	87	14, 28, 45, 66	0
1	M	409/418 (97%)	-0.15	4 (0%)	82	87	12, 23, 40, 66	0
1	N	415/418 (99%)	0.10	11 (2%)	54	60	14, 28, 50, 64	0
1	O	411/418 (98%)	-0.22	4 (0%)	82	87	11, 21, 40, 58	0
1	P	409/418 (97%)	-0.16	3 (0%)	87	92	13, 26, 45, 65	0
1	Q	409/418 (97%)	-0.17	5 (1%)	79	84	11, 22, 40, 62	0
1	R	409/418 (97%)	-0.16	5 (1%)	79	84	11, 21, 41, 64	0
1	T	415/418 (99%)	-0.13	6 (1%)	75	82	13, 25, 46, 71	0
1	U	415/418 (99%)	-0.17	6 (1%)	75	82	11, 24, 44, 73	0
All	All	8229/8360 (98%)	-0.16	100 (1%)	79	84	10, 24, 44, 74	0

The worst 5 of 100 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	421	LEU	7.7
1	Q	421	LEU	6.9
1	D	421	LEU	5.9
1	F	107	TRP	5.1
1	M	105	THR	5.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PYR	D	503	6/6	0.94	0.07	11,19,26,30	0
3	PYR	K	503	6/6	0.94	0.10	11,17,22,34	0
3	PYR	H	503	6/6	0.95	0.08	16,22,24,26	0
3	PYR	U	503	6/6	0.95	0.07	12,24,25,25	0
3	PYR	F	503	6/6	0.96	0.07	15,20,22,24	0
3	PYR	A	503	6/6	0.96	0.07	17,18,21,26	0
3	PYR	E	504	6/6	0.97	0.08	13,19,20,23	0
2	SO4	R	502	5/5	0.97	0.09	21,25,27,28	0
3	PYR	I	503	6/6	0.97	0.08	14,17,22,23	0
2	SO4	M	502	5/5	0.97	0.10	27,28,35,37	0
2	SO4	L	502	5/5	0.97	0.08	34,36,42,49	0
2	SO4	N	502	5/5	0.97	0.07	27,30,37,44	0
2	SO4	P	502	5/5	0.98	0.06	23,32,37,41	0
2	SO4	Q	502	5/5	0.98	0.08	23,24,26,28	0
2	SO4	B	502	5/5	0.98	0.09	19,22,32,37	0
2	SO4	F	502	5/5	0.98	0.07	21,24,29,42	0
2	SO4	G	501	5/5	0.98	0.07	25,27,32,36	0
2	SO4	C	502	5/5	0.98	0.07	17,25,29,31	0
2	SO4	T	501	5/5	0.98	0.08	24,26,31,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	T	502	5/5	0.98	0.06	25,25,29,30	0
2	SO4	T	503	5/5	0.98	0.07	26,28,36,41	0
2	SO4	U	501	5/5	0.98	0.07	24,24,30,30	0
2	SO4	U	502	5/5	0.98	0.07	20,20,26,32	0
2	SO4	E	502	5/5	0.98	0.09	22,26,32,32	0
2	SO4	I	502	5/5	0.98	0.09	19,22,27,31	0
2	SO4	J	502	5/5	0.98	0.07	19,19,23,28	0
2	SO4	K	502	5/5	0.98	0.09	20,23,26,33	0
2	SO4	L	501	5/5	0.98	0.08	21,29,36,40	0
3	PYR	J	503	6/6	0.98	0.07	12,17,20,25	0
2	SO4	A	502	5/5	0.98	0.07	23,28,31,31	0
2	SO4	N	501	5/5	0.98	0.08	19,25,29,31	0
2	SO4	B	501	5/5	0.98	0.06	22,24,27,27	0
2	SO4	J	501	5/5	0.99	0.07	19,20,22,24	0
2	SO4	D	501	5/5	0.99	0.08	20,21,22,27	0
2	SO4	G	502	5/5	0.99	0.06	23,27,34,36	0
2	SO4	M	501	5/5	0.99	0.08	17,17,21,28	0
2	SO4	K	501	5/5	0.99	0.08	22,23,23,41	0
2	SO4	D	502	5/5	0.99	0.07	19,25,27,39	0
2	SO4	E	501	5/5	0.99	0.08	17,18,21,23	0
2	SO4	C	501	5/5	0.99	0.07	18,19,21,21	0
2	SO4	E	503	5/5	0.99	0.06	26,33,35,37	0
2	SO4	H	501	5/5	0.99	0.06	24,27,32,35	0
2	SO4	O	501	5/5	0.99	0.07	15,16,18,20	0
2	SO4	O	502	5/5	0.99	0.08	18,22,24,27	0
2	SO4	P	501	5/5	0.99	0.05	19,21,29,36	0
2	SO4	H	502	5/5	0.99	0.07	22,25,29,31	0
2	SO4	Q	501	5/5	0.99	0.06	16,20,23,27	0
2	SO4	I	501	5/5	0.99	0.08	12,16,16,18	0
2	SO4	R	501	5/5	0.99	0.07	17,20,21,21	0
2	SO4	A	501	5/5	0.99	0.07	25,26,28,33	0
2	SO4	F	501	5/5	0.99	0.08	20,22,23,25	0

6.5 Other polymers (i)

There are no such residues in this entry.