wwPDB X-ray Structure Validation Summary Report (i)

Mar 2, 2024 – 10:48 PM EST

PDB ID	:	5W6J
Title	:	Agrobacterium tumefaciens ADP-glucose pyrophosphorylase
Authors	:	Mascarenhas, R.N.; Hill, B.L.; Wu, R.; Ballicora, M.A.; Liu, D.
Deposited on	:	2017-06-16
Resolution	:	1.78 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:

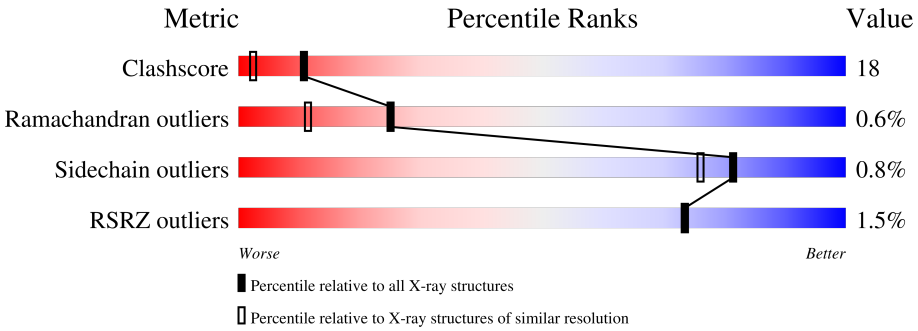
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.78 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.



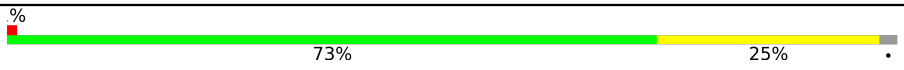
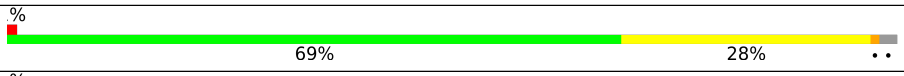
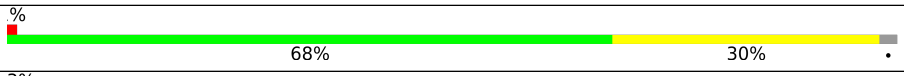
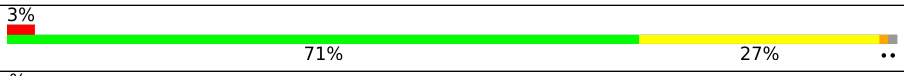
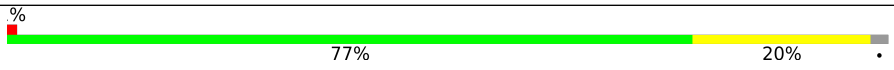
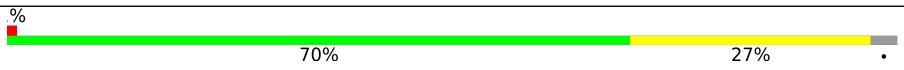
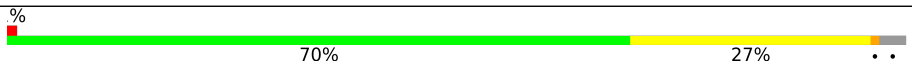
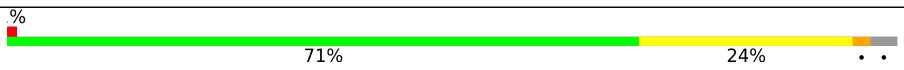
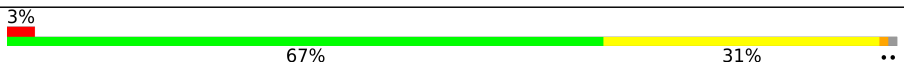
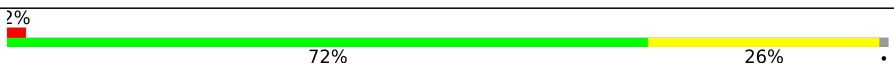
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	420	70% 28%
1	B	420	66% 30%
1	C	420	72% 26%
1	D	420	70% 27%
1	E	420	72% 24%
1	F	420	70% 27%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	420	
1	H	420	
1	I	420	
1	J	420	
1	K	420	
1	L	420	
1	M	420	
1	N	420	
1	O	420	
1	P	420	
1	Q	420	
1	R	420	
1	T	420	
1	U	420	

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	502	-	-	X	-
2	SO4	C	502	-	-	X	-
2	SO4	D	502	-	-	X	-
2	SO4	L	502	-	-	X	-
2	SO4	O	502	-	-	X	-
2	SO4	T	501	-	-	X	-
2	SO4	T	502	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 75925 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
			3252	2062	564	613	13			
1	B	415	Total	C	N	O	S	0	3	0
			3262	2068	567	614	13			
1	C	413	Total	C	N	O	S	0	1	0
			3240	2055	562	610	13			
1	D	412	Total	C	N	O	S	0	0	0
			3226	2047	558	608	13			
1	E	409	Total	C	N	O	S	0	1	0
			3202	2035	549	605	13			
1	H	409	Total	C	N	O	S	0	0	0
			3202	2034	549	606	13			
1	I	409	Total	C	N	O	S	0	1	0
			3212	2040	552	607	13			
1	J	415	Total	C	N	O	S	3	2	0
			3250	2062	561	614	13			
1	K	410	Total	C	N	O	S	0	0	0
			3213	2040	553	607	13			
1	L	410	Total	C	N	O	S	0	1	0
			3222	2045	554	610	13			
1	N	415	Total	C	N	O	S	0	0	0
			3253	2061	562	617	13			
1	O	411	Total	C	N	O	S	0	0	0
			3212	2040	551	608	13			
1	P	409	Total	C	N	O	S	0	1	0
			3212	2040	552	607	13			
1	Q	409	Total	C	N	O	S	0	1	0
			3212	2040	552	607	13			
1	R	409	Total	C	N	O	S	0	0	0
			3202	2034	549	606	13			
1	F	408	Total	C	N	O	S	5	1	0
			3214	2042	554	605	13			

Continued on next page...

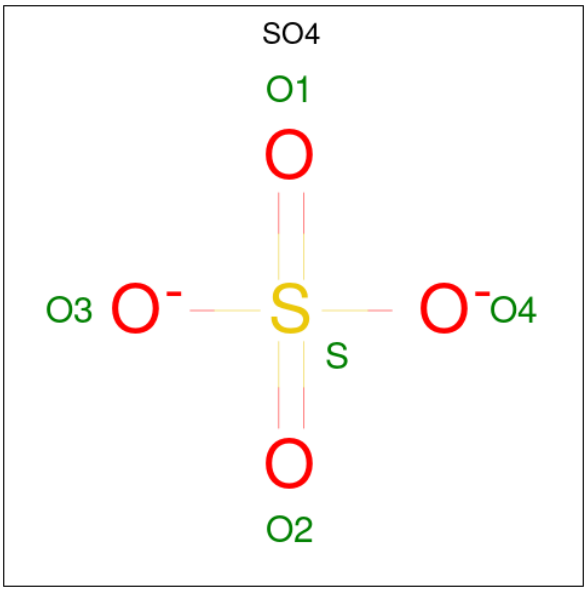
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	410	Total	C	N	O	S	0	1	0
			3227	2048	559	607	13			
1	M	410	Total	C	N	O	S	4	1	0
			3210	2037	553	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	0	1	0
			3244	2058	559	614	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	LEU	VAL	conflict	UNP P39669
B	221	LEU	VAL	conflict	UNP P39669
C	221	LEU	VAL	conflict	UNP P39669
D	221	LEU	VAL	conflict	UNP P39669
E	221	LEU	VAL	conflict	UNP P39669
H	221	LEU	VAL	conflict	UNP P39669
I	221	LEU	VAL	conflict	UNP P39669
J	221	LEU	VAL	conflict	UNP P39669
K	221	LEU	VAL	conflict	UNP P39669
L	221	LEU	VAL	conflict	UNP P39669
N	221	LEU	VAL	conflict	UNP P39669
O	221	LEU	VAL	conflict	UNP P39669
P	221	LEU	VAL	conflict	UNP P39669
Q	221	LEU	VAL	conflict	UNP P39669
R	221	LEU	VAL	conflict	UNP P39669
F	221	LEU	VAL	conflict	UNP P39669
G	221	LEU	VAL	conflict	UNP P39669
M	221	LEU	VAL	conflict	UNP P39669
T	221	LEU	VAL	conflict	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	514	Total O 514 514	0	0
3	B	531	Total O 531 531	0	0
3	C	619	Total O 619 619	0	0
3	D	573	Total O 573 573	0	0
3	E	587	Total O 587 587	0	0
3	H	544	Total O 544 544	0	0
3	I	623	Total O 623 623	0	0
3	J	654	Total O 654 654	0	0
3	K	545	Total O 545 545	0	0
3	L	514	Total O 514 514	0	0
3	N	503	Total O 503 503	0	0
3	O	603	Total O 603 603	0	0

Continued on next page...

Continued from previous page...

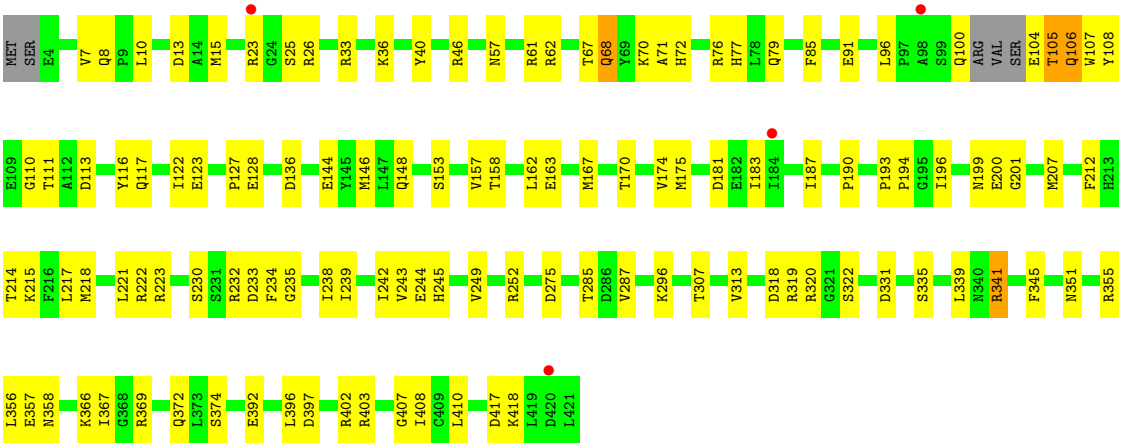
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	511	Total O 511 511	0	0
3	Q	557	Total O 557 557	0	0
3	R	597	Total O 597 597	0	0
3	F	545	Total O 545 545	0	0
3	G	489	Total O 489 489	0	0
3	M	559	Total O 559 559	0	0
3	T	589	Total O 589 589	0	0
3	U	539	Total O 539 539	0	0

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.

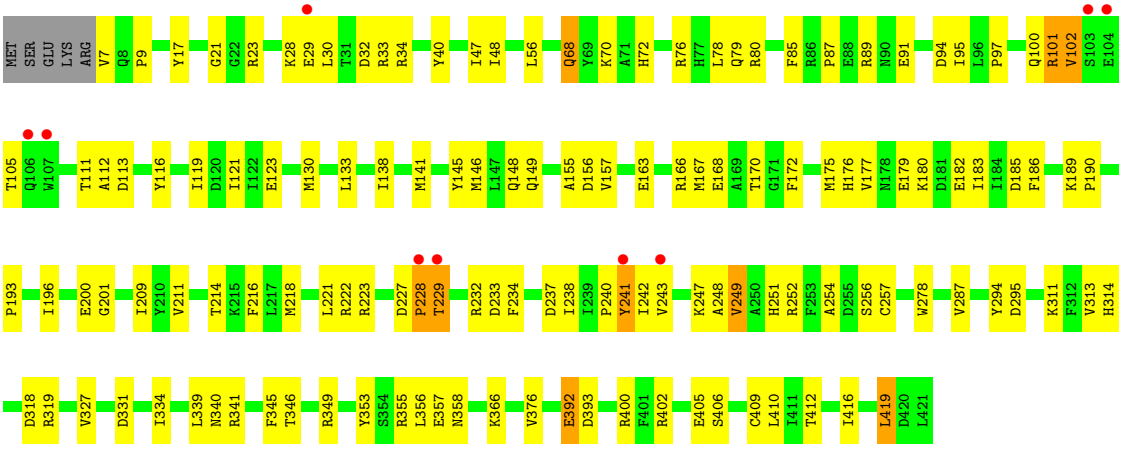
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain A:



• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain B:

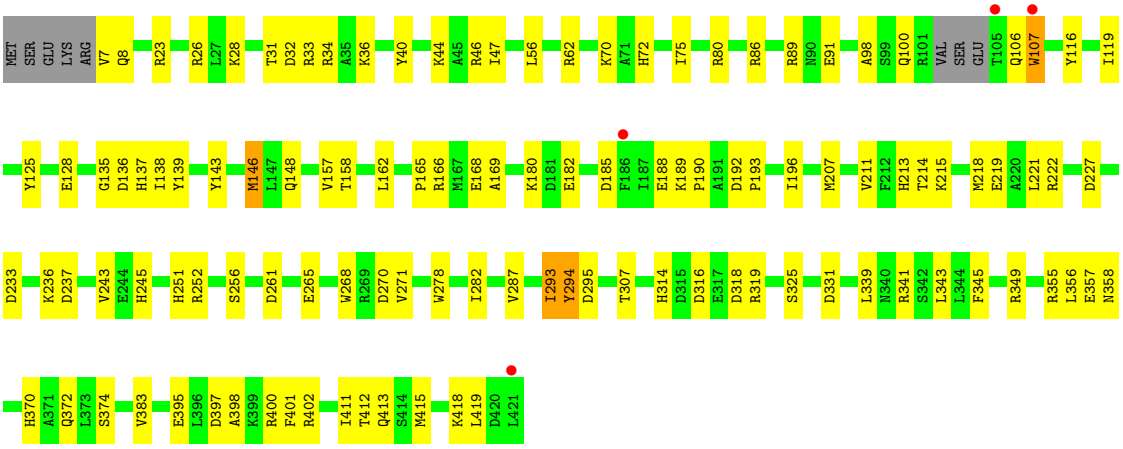


• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain C:

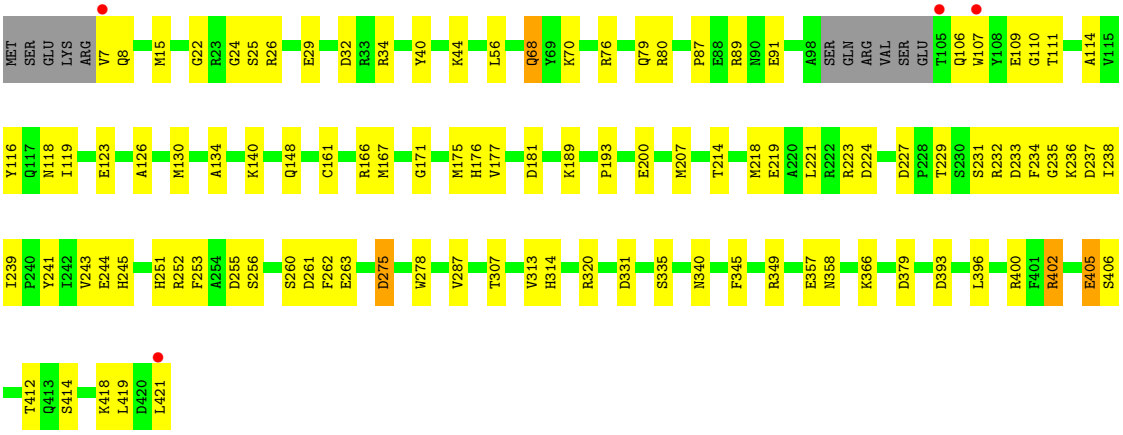
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain D:



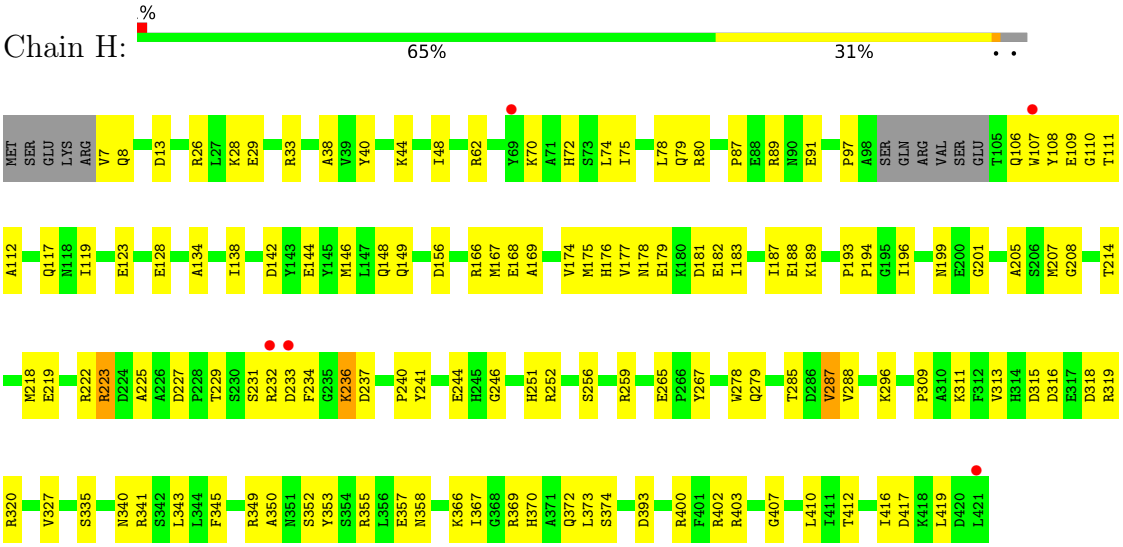
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain E:



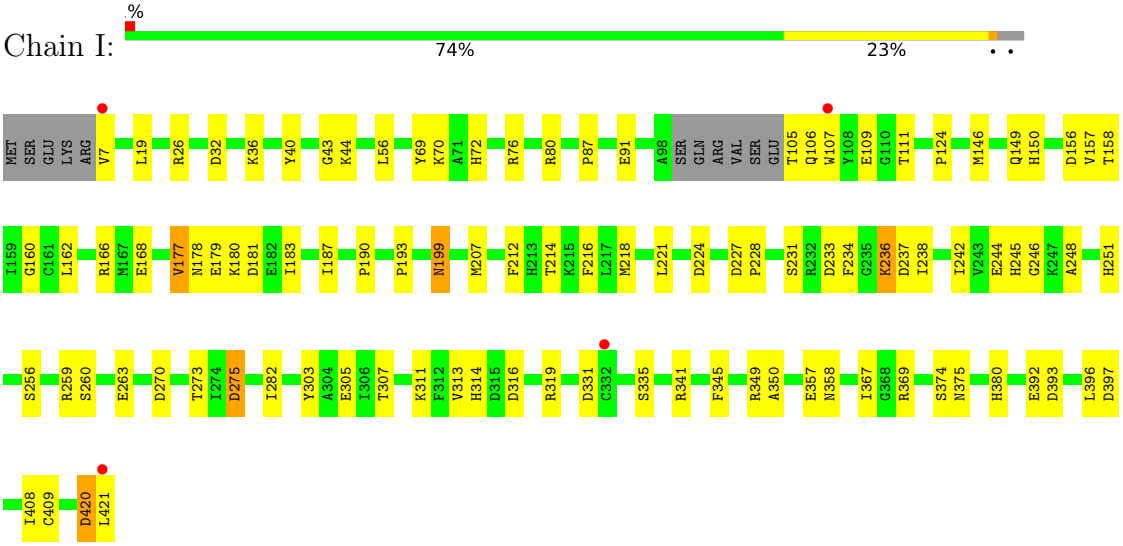
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain H:



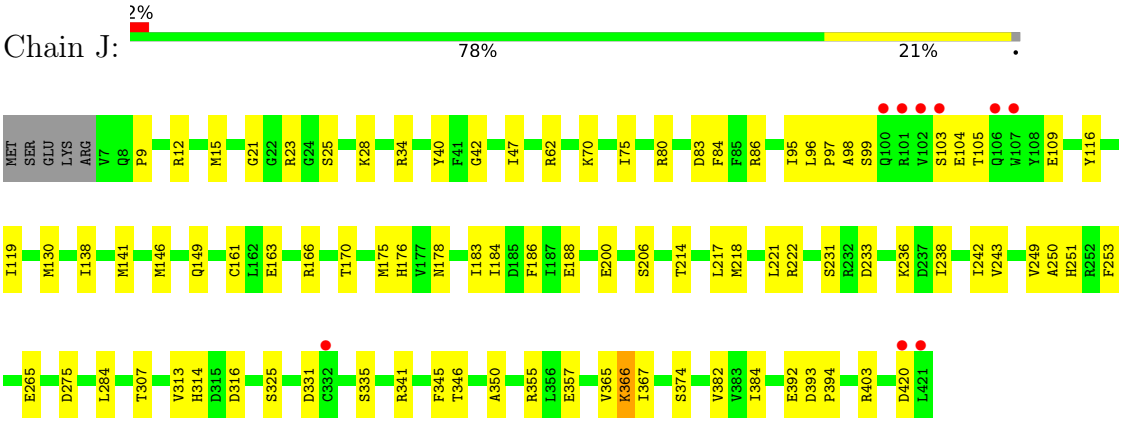
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain I:



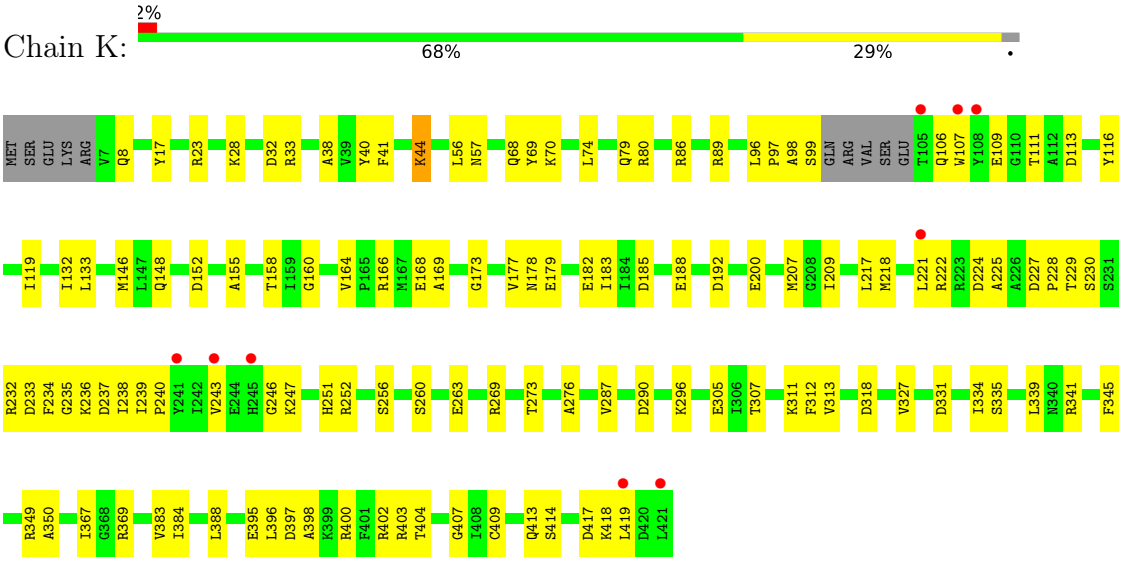
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain J:



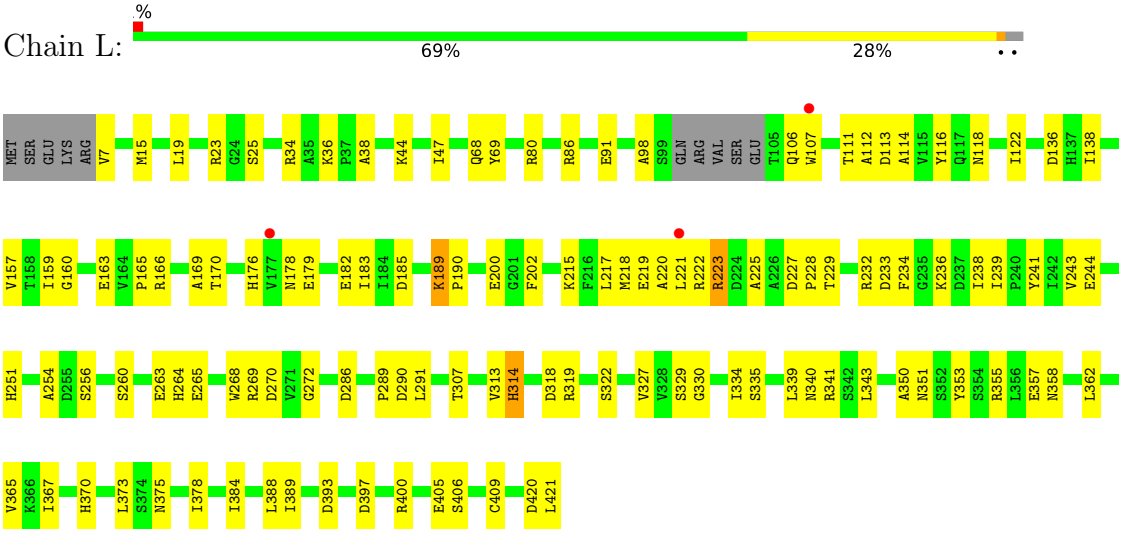
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain K:



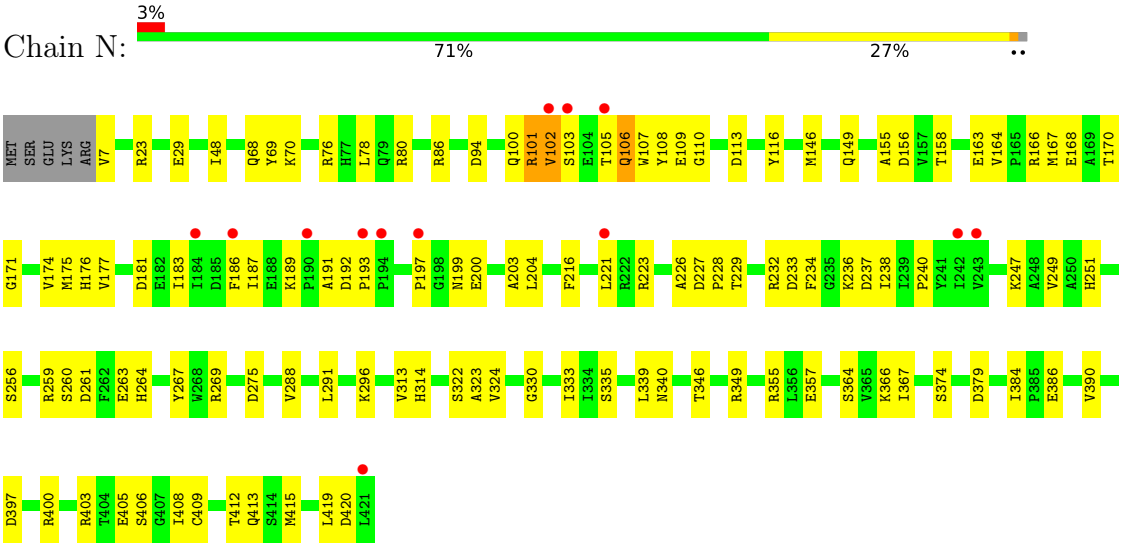
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain L:



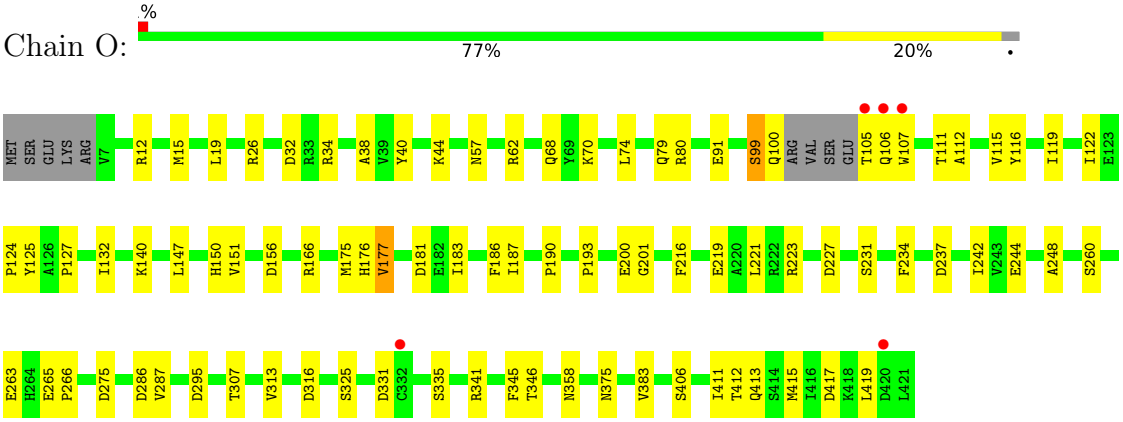
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain N:



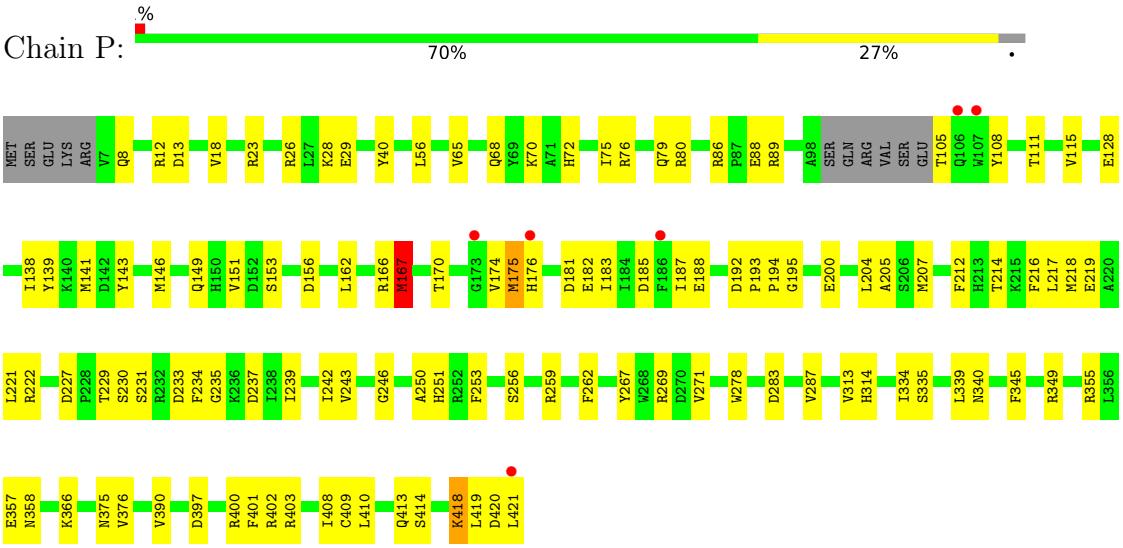
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain O:



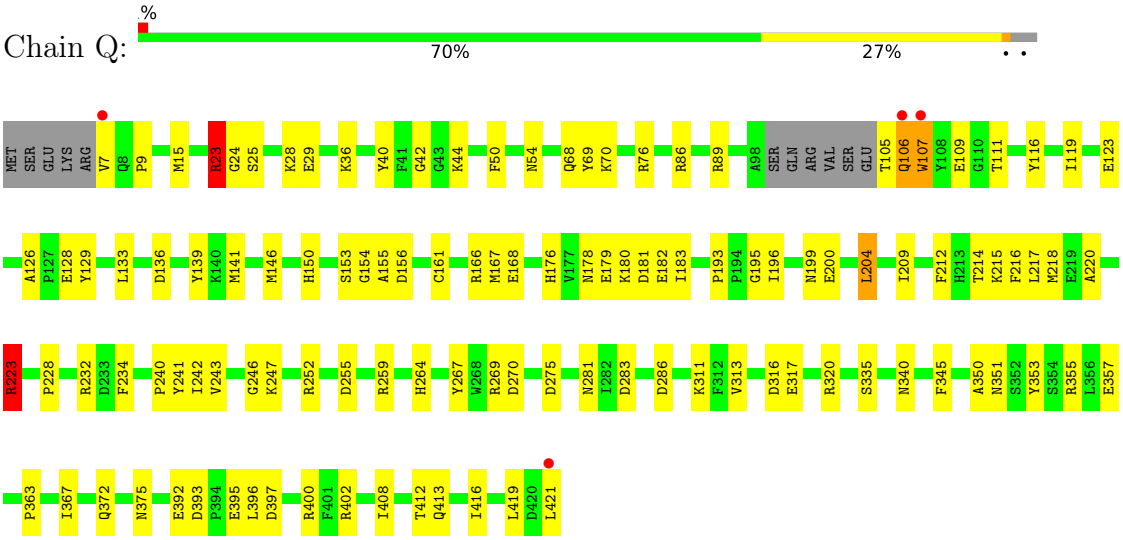
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain P:



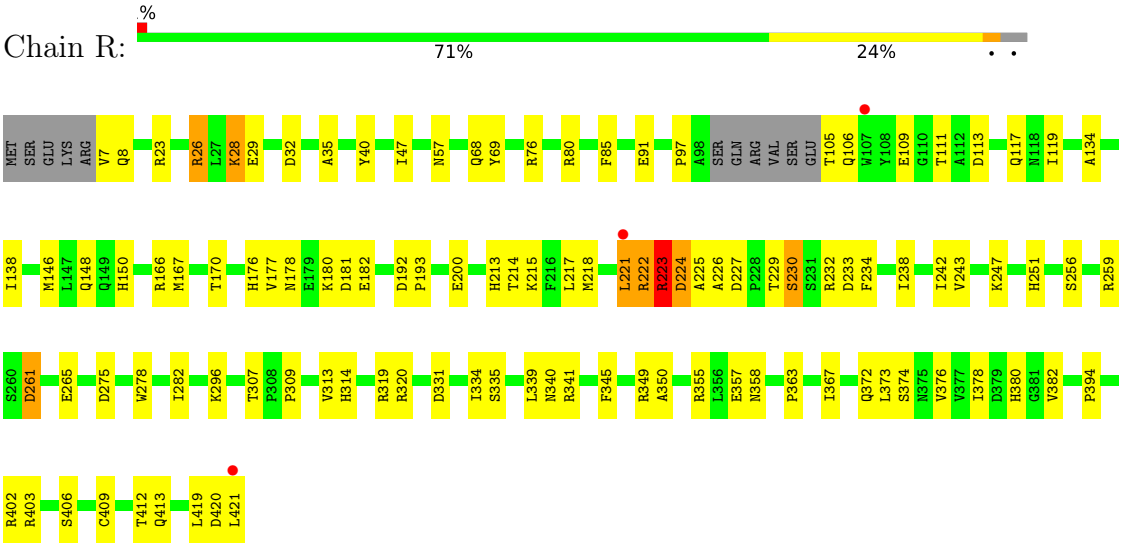
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain Q:



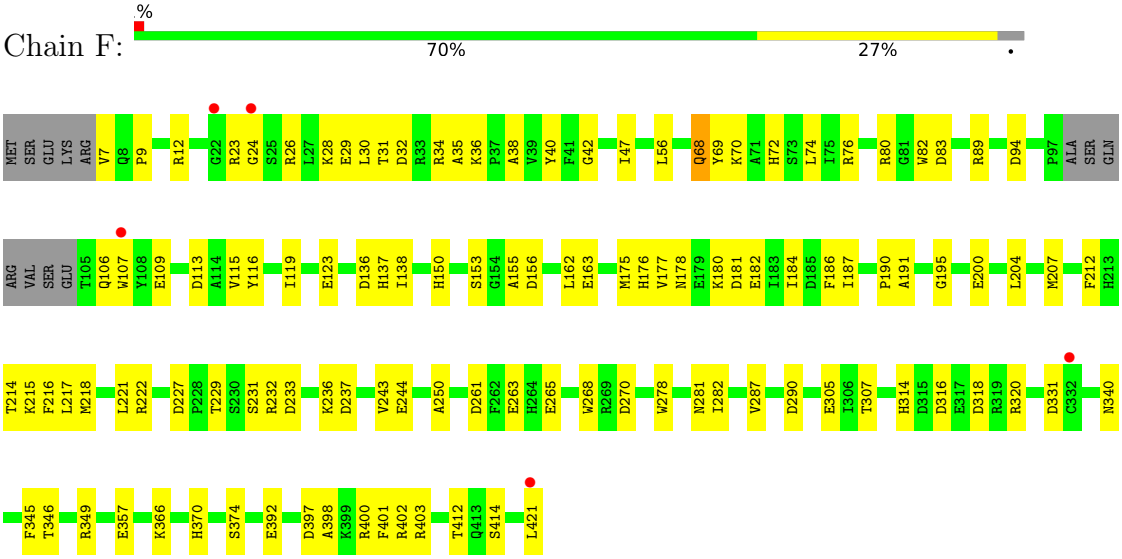
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain R:



• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain F:

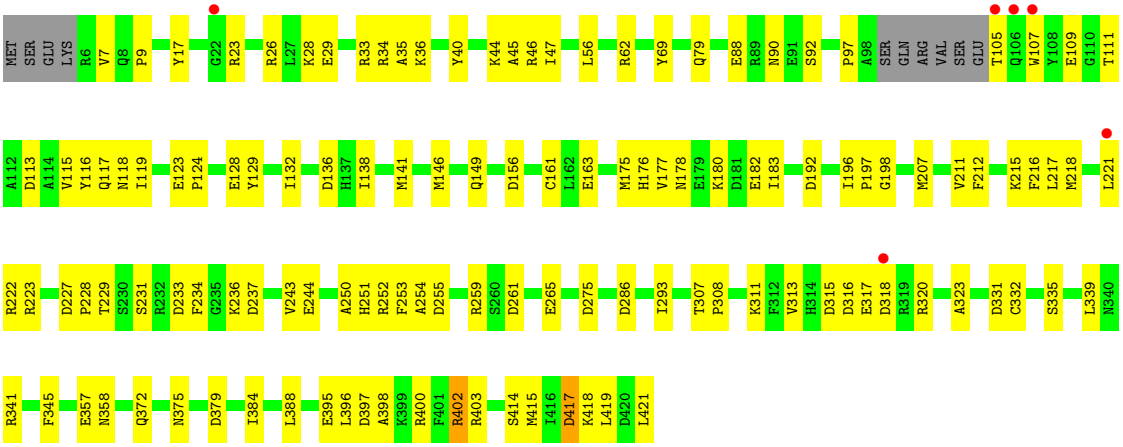


• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain G:

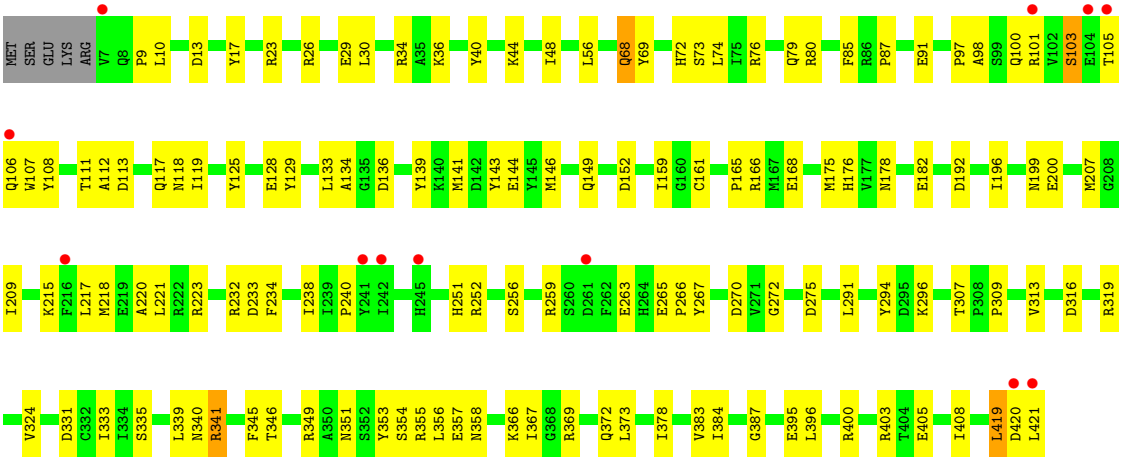
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain M:



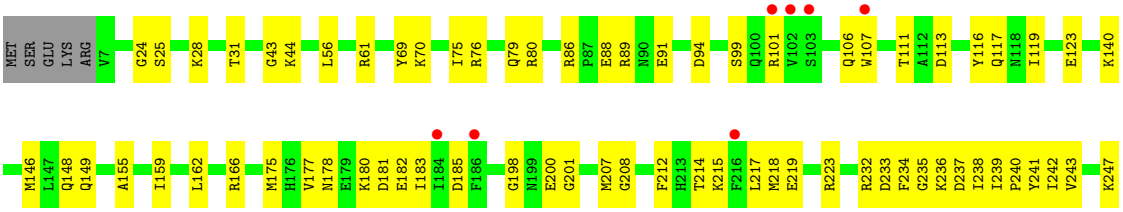
• Molecule 1: Glucose-1-phosphate adenylyltransferase

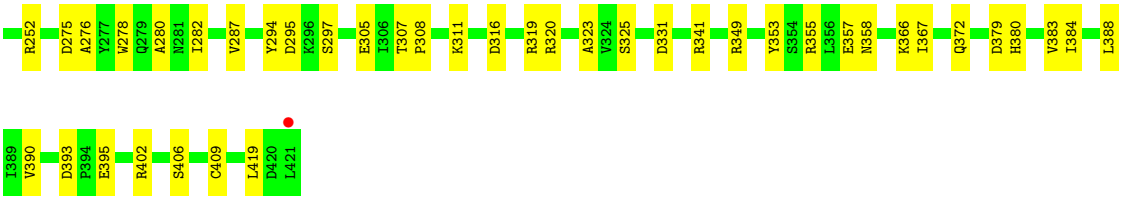
Chain T:



• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain U:




R252
D275
A276
Y277
W278
Q279
A280
N281
I282
V287
Y294
D295
K296
S297
E305
I306
T307
P308
K311
D316
R319
R320
A323
V324
S325
D331
R341
R349
Y353
S354
R355
L356
E357
N358
K366
I367
Q372
D379
H380
V383
I384
L388
I389
V390
D393
P394
E395
R402
S406
C409
L419
D420
L421

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	93.44Å 140.69Å 228.49Å 72.04° 78.19° 89.98°	Depositor
Resolution (Å)	36.55 – 1.78 36.55 – 1.78	Depositor EDS
% Data completeness (in resolution range)	97.0 (36.55-1.78) 89.6 (36.55-1.78)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.200 , 0.229 0.174 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.467 for h,-k,h-l 0.468 for -h,k,k-l 0.467 for -h,-k,-h-k+l	Xtriage
Reported twinning fraction	0.450 for h,-k,h-l	Depositor
Outliers	0 of 1003130 reflections	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	75925	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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 61.29 % 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 1.3393e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.32	0/3331	0.50	0/4523
1	B	0.40	3/3348 (0.1%)	0.54	0/4548
1	C	0.33	0/3319	0.49	0/4507
1	D	0.70	7/3302 (0.2%)	0.89	7/4485 (0.2%)
1	E	0.34	0/3281	0.50	0/4460
1	F	0.34	0/3293	0.49	0/4473
1	G	0.33	0/3306	0.49	0/4490
1	H	0.40	2/3278 (0.1%)	0.51	1/4455 (0.0%)
1	I	0.34	0/3291	0.50	0/4472
1	J	0.36	1/3333 (0.0%)	0.51	1/4530 (0.0%)
1	K	0.32	0/3289	0.49	0/4469
1	L	0.33	0/3298	0.50	0/4481
1	M	0.35	0/3288	0.51	1/4468 (0.0%)
1	N	0.37	0/3330	0.53	2/4525 (0.0%)
1	O	0.33	0/3288	0.49	0/4469
1	P	0.37	1/3291 (0.0%)	0.53	2/4472 (0.0%)
1	Q	0.41	1/3291 (0.0%)	0.64	7/4472 (0.2%)
1	R	0.48	3/3278 (0.1%)	0.61	5/4455 (0.1%)
1	T	0.34	0/3332	0.50	0/4528
1	U	0.32	0/3324	0.49	0/4518
All	All	0.38	18/66091 (0.0%)	0.54	26/89800 (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	B	0	1
1	N	0	1
1	O	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Q	0	1
1	R	0	2
1	T	0	1
All	All	0	7

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	294	TYR	CE1-CZ	-24.51	1.06	1.38
1	D	294	TYR	CG-CD2	-17.56	1.16	1.39
1	R	223	ARG	CZ-NH1	16.09	1.53	1.33
1	D	294	TYR	CD1-CE1	-12.35	1.20	1.39
1	H	236	LYS	CB-CG	8.52	1.75	1.52

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	294	TYR	CB-CG-CD1	33.54	141.12	121.00
1	D	294	TYR	CB-CG-CD2	-28.05	104.17	121.00
1	R	223	ARG	NE-CZ-NH1	-17.47	111.56	120.30
1	Q	23	ARG	NE-CZ-NH2	-15.28	112.66	120.30
1	Q	23	ARG	NE-CZ-NH1	14.61	127.61	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	419	LEU	Peptide
1	N	419	LEU	Peptide
1	O	419	LEU	Peptide
1	Q	23	ARG	Sidechain
1	R	222	ARG	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	3252	0	3146	121	0
1	B	3262	0	3165	153	0
1	C	3240	0	3143	109	0
1	D	3226	0	3124	135	0
1	E	3202	0	3105	112	0
1	F	3214	0	3130	140	0
1	G	3227	0	3139	105	0
1	H	3202	0	3102	145	0
1	I	3212	0	3120	94	0
1	J	3250	0	3147	86	0
1	K	3213	0	3115	112	1
1	L	3222	0	3120	120	0
1	M	3210	0	3115	134	0
1	N	3253	0	3151	137	0
1	O	3212	0	3106	89	0
1	P	3212	0	3120	116	0
1	Q	3212	0	3120	116	0
1	R	3202	0	3102	118	0
1	T	3252	0	3152	133	0
1	U	3244	0	3136	108	0
2	A	10	0	0	1	0
2	B	10	0	0	3	0
2	C	10	0	0	3	0
2	D	10	0	0	3	0
2	E	15	0	0	1	0
2	F	10	0	0	0	0
2	G	10	0	0	0	0
2	H	10	0	0	0	0
2	I	10	0	0	2	0
2	J	10	0	0	1	0
2	K	10	0	0	2	0
2	L	10	0	0	3	0
2	M	10	0	0	1	0
2	N	10	0	0	0	0
2	O	10	0	0	3	0
2	P	10	0	0	0	0
2	Q	10	0	0	1	0
2	R	10	0	0	0	0
2	T	15	0	0	5	0
2	U	10	0	0	0	0
3	A	514	0	0	77	5
3	B	531	0	0	63	2
3	C	619	0	0	66	2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	573	0	0	72	3
3	E	587	0	0	66	8
3	F	545	0	0	76	1
3	G	489	0	0	66	1
3	H	544	0	0	80	9
3	I	623	0	0	44	2
3	J	654	0	0	56	23
3	K	545	0	0	61	0
3	L	514	0	0	61	16
3	M	559	0	0	60	5
3	N	503	0	0	62	26
3	O	603	0	0	54	20
3	P	511	0	0	69	11
3	Q	557	0	0	54	1
3	R	597	0	0	58	17
3	T	589	0	0	71	8
3	U	539	0	0	61	5
All	All	75925	0	62558	2326	83

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 18.

The worst 5 of 2326 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:H:236:LYS:CB	1:H:236:LYS:CG	1.75	1.63
1:C:259:ARG:NH2	3:C:601:HOH:O	1.81	1.11
1:N:113:ASP:OD1	1:N:232:ARG:NH1	1.82	1.11
1:A:223:ARG:NH2	3:A:601:HOH:O	1.81	1.11
1:N:113:ASP:OD2	1:N:232:ARG:NH2	1.85	1.08

The worst 5 of 83 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)
3:M:1066:HOH:O	3:U:1036:HOH:O[1_565]	1.68	0.52
3:J:1187:HOH:O	3:L:1071:HOH:O[1_546]	1.69	0.51
3:J:831:HOH:O	3:N:787:HOH:O[1_655]	1.71	0.49
3:I:648:HOH:O	3:J:742:HOH:O[1_455]	1.74	0.46
3:J:1031:HOH:O	3:N:1056:HOH:O[1_655]	1.79	0.41

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	412/420 (98%)	384 (93%)	25 (6%)	3 (1%)	22 9
1	B	416/420 (99%)	384 (92%)	25 (6%)	7 (2%)	9 2
1	C	410/420 (98%)	391 (95%)	16 (4%)	3 (1%)	22 9
1	D	408/420 (97%)	387 (95%)	17 (4%)	4 (1%)	15 4
1	E	406/420 (97%)	387 (95%)	17 (4%)	2 (0%)	29 14
1	F	405/420 (96%)	380 (94%)	24 (6%)	1 (0%)	47 32
1	G	407/420 (97%)	388 (95%)	19 (5%)	0	100 100
1	H	405/420 (96%)	378 (93%)	26 (6%)	1 (0%)	47 32
1	I	406/420 (97%)	385 (95%)	19 (5%)	2 (0%)	29 14
1	J	415/420 (99%)	395 (95%)	19 (5%)	1 (0%)	47 32
1	K	406/420 (97%)	384 (95%)	19 (5%)	3 (1%)	22 9
1	L	407/420 (97%)	383 (94%)	21 (5%)	3 (1%)	22 9
1	M	407/420 (97%)	384 (94%)	22 (5%)	1 (0%)	47 32
1	N	413/420 (98%)	377 (91%)	28 (7%)	8 (2%)	8 1
1	O	407/420 (97%)	392 (96%)	14 (3%)	1 (0%)	47 32
1	P	406/420 (97%)	383 (94%)	21 (5%)	2 (0%)	29 14
1	Q	406/420 (97%)	378 (93%)	24 (6%)	4 (1%)	15 4
1	R	405/420 (96%)	385 (95%)	18 (4%)	2 (0%)	29 14
1	T	414/420 (99%)	390 (94%)	22 (5%)	2 (0%)	29 14
1	U	414/420 (99%)	396 (96%)	18 (4%)	0	100 100
All	All	8175/8400 (97%)	7711 (94%)	414 (5%)	50 (1%)	25 11

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	102	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	105	THR
1	C	98	ALA
1	L	244	GLU
1	N	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	340/352 (97%)	338 (99%)	2 (1%)	86	82
1	B	342/352 (97%)	341 (100%)	1 (0%)	92	90
1	C	340/352 (97%)	335 (98%)	5 (2%)	65	53
1	D	338/352 (96%)	337 (100%)	1 (0%)	92	90
1	E	337/352 (96%)	331 (98%)	6 (2%)	59	45
1	F	340/352 (97%)	338 (99%)	2 (1%)	86	82
1	G	340/352 (97%)	340 (100%)	0	100	100
1	H	337/352 (96%)	335 (99%)	2 (1%)	86	82
1	I	339/352 (96%)	334 (98%)	5 (2%)	65	53
1	J	341/352 (97%)	340 (100%)	1 (0%)	92	90
1	K	338/352 (96%)	336 (99%)	2 (1%)	86	82
1	L	339/352 (96%)	338 (100%)	1 (0%)	92	90
1	M	338/352 (96%)	335 (99%)	3 (1%)	78	72
1	N	343/352 (97%)	343 (100%)	0	100	100
1	O	337/352 (96%)	335 (99%)	2 (1%)	86	82
1	P	339/352 (96%)	333 (98%)	6 (2%)	59	45
1	Q	339/352 (96%)	336 (99%)	3 (1%)	78	72
1	R	337/352 (96%)	332 (98%)	5 (2%)	65	53
1	T	342/352 (97%)	340 (99%)	2 (1%)	86	82
1	U	340/352 (97%)	336 (99%)	4 (1%)	71	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6786/7040 (96%)	6733 (99%)	53 (1%)	81 76

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	153	SER
1	Q	176	HIS
1	U	28	LYS
1	P	167	MET
1	P	219	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	90	ASN
1	M	176	HIS
1	T	340	ASN
1	K	57	ASN
1	J	351	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)

42 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	B	501	-	4,4,4	0.17	0	6,6,6	0.32	0
2	SO4	L	502	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	R	501	-	4,4,4	0.19	0	6,6,6	0.13	0
2	SO4	R	502	-	4,4,4	0.15	0	6,6,6	0.24	0
2	SO4	U	501	-	4,4,4	0.19	0	6,6,6	0.31	0
2	SO4	A	502	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	D	501	-	4,4,4	0.23	0	6,6,6	0.22	0
2	SO4	H	501	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	K	502	-	4,4,4	0.15	0	6,6,6	0.28	0
2	SO4	J	501	-	4,4,4	0.20	0	6,6,6	0.25	0
2	SO4	C	501	-	4,4,4	0.23	0	6,6,6	0.15	0
2	SO4	Q	501	-	4,4,4	0.20	0	6,6,6	0.23	0
2	SO4	J	502	-	4,4,4	0.18	0	6,6,6	0.19	0
2	SO4	N	501	-	4,4,4	0.16	0	6,6,6	0.11	0
2	SO4	P	501	-	4,4,4	0.15	0	6,6,6	0.28	0
2	SO4	C	502	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	Q	502	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	T	503	-	4,4,4	0.17	0	6,6,6	0.21	0
2	SO4	N	502	-	4,4,4	0.18	0	6,6,6	0.23	0
2	SO4	F	501	-	4,4,4	0.19	0	6,6,6	0.14	0
2	SO4	P	502	-	4,4,4	0.17	0	6,6,6	0.14	0
2	SO4	G	502	-	4,4,4	0.19	0	6,6,6	0.11	0
2	SO4	M	501	-	4,4,4	0.17	0	6,6,6	0.14	0
2	SO4	O	501	-	4,4,4	0.21	0	6,6,6	0.15	0
2	SO4	I	501	-	4,4,4	0.24	0	6,6,6	0.22	0
2	SO4	B	502	-	4,4,4	0.15	0	6,6,6	0.26	0
2	SO4	I	502	-	4,4,4	0.20	0	6,6,6	0.13	0
2	SO4	L	501	-	4,4,4	0.19	0	6,6,6	0.07	0
2	SO4	U	502	-	4,4,4	0.15	0	6,6,6	0.16	0
2	SO4	F	502	-	4,4,4	0.17	0	6,6,6	0.19	0
2	SO4	E	501	-	4,4,4	0.21	0	6,6,6	0.14	0
2	SO4	T	502	-	4,4,4	0.19	0	6,6,6	0.19	0
2	SO4	A	501	-	4,4,4	0.17	0	6,6,6	0.18	0
2	SO4	D	502	-	4,4,4	0.21	0	6,6,6	0.13	0
2	SO4	G	501	-	4,4,4	0.15	0	6,6,6	0.15	0
2	SO4	M	502	-	4,4,4	0.17	0	6,6,6	0.13	0
2	SO4	E	502	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	H	502	-	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	$\#\|Z\| > 2$
2	SO4	O	502	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	E	503	-	4,4,4	0.18	0	6,6,6	0.15	0
2	SO4	T	501	-	4,4,4	0.21	0	6,6,6	0.30	0
2	SO4	K	501	-	4,4,4	0.21	0	6,6,6	0.18	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	SO4	1	0
2	L	502	SO4	2	0
2	K	502	SO4	1	0
2	J	502	SO4	1	0
2	C	502	SO4	3	0
2	Q	502	SO4	1	0
2	I	501	SO4	1	0
2	B	502	SO4	2	0
2	I	502	SO4	1	0
2	L	501	SO4	1	0
2	T	502	SO4	2	0
2	A	501	SO4	1	0
2	D	502	SO4	3	0
2	M	502	SO4	1	0
2	E	502	SO4	1	0
2	O	502	SO4	3	0
2	T	501	SO4	3	0
2	K	501	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	415/420 (98%)	-0.25	4 (0%)	82	82	19, 32, 52, 62	0
1	B	415/420 (98%)	-0.16	9 (2%)	62	61	19, 32, 53, 70	0
1	C	413/420 (98%)	-0.28	6 (1%)	73	73	17, 28, 44, 58	0
1	D	412/420 (98%)	-0.26	4 (0%)	82	82	16, 29, 46, 58	0
1	E	409/420 (97%)	-0.27	4 (0%)	82	82	17, 29, 44, 60	0
1	F	408/420 (97%)	-0.25	5 (1%)	79	79	16, 29, 49, 59	0
1	G	410/420 (97%)	-0.22	4 (0%)	82	82	18, 32, 51, 62	0
1	H	409/420 (97%)	-0.23	5 (1%)	79	79	19, 32, 53, 69	0
1	I	409/420 (97%)	-0.30	4 (0%)	82	82	16, 26, 44, 57	0
1	J	415/420 (98%)	-0.24	9 (2%)	62	61	15, 25, 42, 74	0
1	K	410/420 (97%)	-0.18	9 (2%)	62	61	17, 32, 52, 62	0
1	L	410/420 (97%)	-0.18	3 (0%)	87	88	19, 33, 51, 63	0
1	M	410/420 (97%)	-0.19	6 (1%)	73	73	18, 32, 50, 67	0
1	N	415/420 (98%)	-0.10	13 (3%)	49	47	17, 33, 61, 82	0
1	O	411/420 (97%)	-0.30	5 (1%)	79	79	15, 25, 42, 65	0
1	P	409/420 (97%)	-0.18	6 (1%)	73	73	19, 33, 53, 66	0
1	Q	409/420 (97%)	-0.19	4 (0%)	82	82	19, 32, 50, 68	0
1	R	409/420 (97%)	-0.25	3 (0%)	87	88	15, 25, 47, 66	0
1	T	415/420 (98%)	-0.16	12 (2%)	51	50	18, 32, 55, 73	0
1	U	415/420 (98%)	-0.16	8 (1%)	66	67	18, 32, 51, 70	0
All	All	8228/8400 (97%)	-0.22	123 (1%)	73	73	15, 30, 51, 82	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	107	TRP	8.4
1	U	102	VAL	8.2
1	U	421	LEU	7.7
1	H	421	LEU	6.9
1	J	102	VAL	6.4

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
2	SO4	A	501	5/5	0.98	0.07	38,38,39,39	0
2	SO4	G	501	5/5	0.98	0.07	38,40,41,46	0
2	SO4	T	503	5/5	0.98	0.07	28,32,34,35	0
2	SO4	B	502	5/5	0.99	0.08	21,26,29,29	0
2	SO4	C	502	5/5	0.99	0.07	21,26,26,34	0
2	SO4	D	502	5/5	0.99	0.08	20,22,23,27	0
2	SO4	E	502	5/5	0.99	0.05	30,30,34,44	0
2	SO4	E	503	5/5	0.99	0.09	32,33,33,34	0
2	SO4	H	501	5/5	0.99	0.07	24,26,28,31	0
2	SO4	H	502	5/5	0.99	0.09	43,43,44,44	0
2	SO4	I	501	5/5	0.99	0.10	20,24,25,28	0
2	SO4	I	502	5/5	0.99	0.08	39,39,41,42	0
2	SO4	J	501	5/5	0.99	0.08	19,23,25,25	0
2	SO4	K	501	5/5	0.99	0.08	27,27,27,28	0
2	SO4	K	502	5/5	0.99	0.05	28,29,31,33	0
2	SO4	L	501	5/5	0.99	0.08	28,30,32,32	0
2	SO4	L	502	5/5	0.99	0.06	31,32,32,35	0
2	SO4	N	501	5/5	0.99	0.07	22,24,29,30	0
2	SO4	N	502	5/5	0.99	0.08	30,31,31,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	O	502	5/5	0.99	0.06	26,28,29,32	0
2	SO4	P	501	5/5	0.99	0.07	21,21,25,25	0
2	SO4	P	502	5/5	0.99	0.08	39,40,41,46	0
2	SO4	Q	501	5/5	0.99	0.08	19,22,23,29	0
2	SO4	Q	502	5/5	0.99	0.09	38,39,39,44	0
2	SO4	R	502	5/5	0.99	0.07	33,34,34,39	0
2	SO4	F	501	5/5	0.99	0.09	23,23,23,28	0
2	SO4	F	502	5/5	0.99	0.06	30,31,33,34	0
2	SO4	A	502	5/5	0.99	0.05	43,44,45,45	0
2	SO4	M	501	5/5	0.99	0.06	26,26,27,29	0
2	SO4	M	502	5/5	0.99	0.08	31,31,34,41	0
2	SO4	T	501	5/5	0.99	0.09	23,24,30,39	0
2	SO4	B	501	5/5	0.99	0.07	26,27,30,31	0
2	SO4	U	501	5/5	0.99	0.09	23,24,27,28	0
2	SO4	U	502	5/5	0.99	0.07	33,34,34,35	0
2	SO4	G	502	5/5	1.00	0.06	29,30,31,31	0
2	SO4	O	501	5/5	1.00	0.10	21,21,22,24	0
2	SO4	R	501	5/5	1.00	0.08	21,21,24,26	0
2	SO4	D	501	5/5	1.00	0.08	19,22,25,25	0
2	SO4	T	502	5/5	1.00	0.07	27,28,29,30	0
2	SO4	J	502	5/5	1.00	0.06	19,21,26,27	0
2	SO4	C	501	5/5	1.00	0.09	19,25,25,28	0
2	SO4	E	501	5/5	1.00	0.07	23,25,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.