



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 8, 2016 – 09:34 AM EDT

PDB ID : 5L6V
Title : Crystal structure of E. coli ADP-glucose pyrophosphorylase (AGPase) in complex with a negative allosteric regulator adenosine monophosphate (AMP) - AGPase*AMP
Authors : Cifuentes, J.O.; Albasa-Jove, D.; Comino, N.; Madariaga-Marcos, J.; Agirre, J.; Lopez-Fernandez, S.; Garcia-Alija, M.; Guerin, M.E.
Deposited on : 2016-05-31
Resolution : 2.67 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

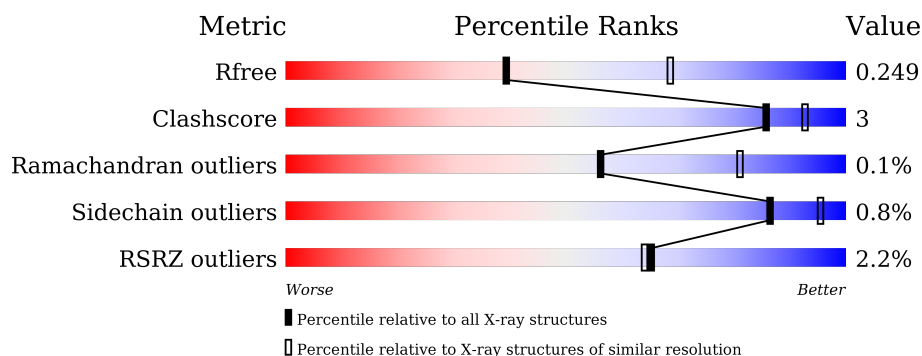
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	431	<div> <div>92%</div> <div>6%</div> <div>•</div> </div>
1	B	431	<div> <div>90%</div> <div>7%</div> <div>•</div> </div>
1	C	431	<div> <div>89%</div> <div>8%</div> <div>•</div> </div>
1	D	431	<div> <div>88%</div> <div>8%</div> <div>•</div> </div>
1	E	431	<div> <div>2%</div> <div>88%</div> <div>8%</div> <div>5%</div> </div>
1	F	431	<div> <div>88%</div> <div>7%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	431	<div><div></div><div>7%</div><div>87%</div><div>8%</div><div>5%</div></div>
1	H	431	<div><div></div><div>3%</div><div>89%</div><div>8%</div><div></div></div>
1	I	431	<div><div></div><div>7%</div><div>85%</div><div>7%</div><div>7%</div></div>
1	J	431	<div><div></div><div>3%</div><div>90%</div><div>6%</div><div></div></div>
1	K	431	<div><div></div><div>%</div><div>89%</div><div>8%</div><div></div></div>
1	L	431	<div><div></div><div>3%</div><div>87%</div><div>8%</div><div></div></div>
1	M	431	<div><div></div><div></div><div>88%</div><div>7%</div><div></div></div>
1	N	431	<div><div></div><div>%</div><div>90%</div><div>7%</div><div></div></div>
1	O	431	<div><div></div><div>2%</div><div>91%</div><div>5%</div><div></div></div>
1	P	431	<div><div></div><div></div><div>92%</div><div>6%</div><div></div></div>

2 Entry composition

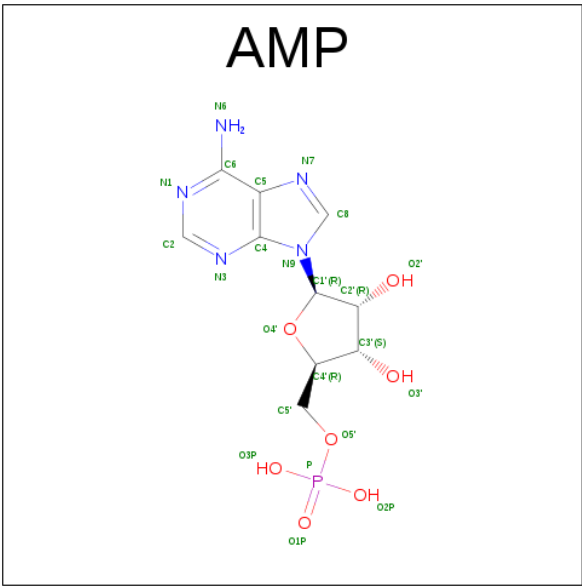
There are 5 unique types of molecules in this entry. The entry contains 53530 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	422	Total	C	N	O	S	0	3	0
			3325	2100	583	619	23			
1	B	421	Total	C	N	O	S	0	0	0
			3293	2081	579	611	22			
1	C	421	Total	C	N	O	S	0	2	0
			3325	2105	585	612	23			
1	D	413	Total	C	N	O	S	0	0	0
			3210	2028	563	599	20			
1	E	411	Total	C	N	O	S	0	1	0
			3202	2024	561	596	21			
1	F	411	Total	C	N	O	S	0	0	0
			3225	2035	567	602	21			
1	G	411	Total	C	N	O	S	0	0	0
			3127	1985	543	579	20			
1	H	416	Total	C	N	O	S	0	0	0
			3162	2008	545	589	20			
1	I	400	Total	C	N	O	S	0	0	0
			2984	1893	522	549	20			
1	J	412	Total	C	N	O	S	0	0	0
			3158	2002	555	581	20			
1	K	421	Total	C	N	O	S	0	0	0
			3292	2080	578	612	22			
1	L	412	Total	C	N	O	S	0	0	0
			3195	2022	561	591	21			
1	M	415	Total	C	N	O	S	0	0	0
			3250	2056	572	601	21			
1	N	422	Total	C	N	O	S	0	0	0
			3285	2079	575	609	22			
1	O	415	Total	C	N	O	S	0	0	0
			3237	2044	568	604	21			
1	P	423	Total	C	N	O	S	0	0	0
			3305	2090	578	615	22			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



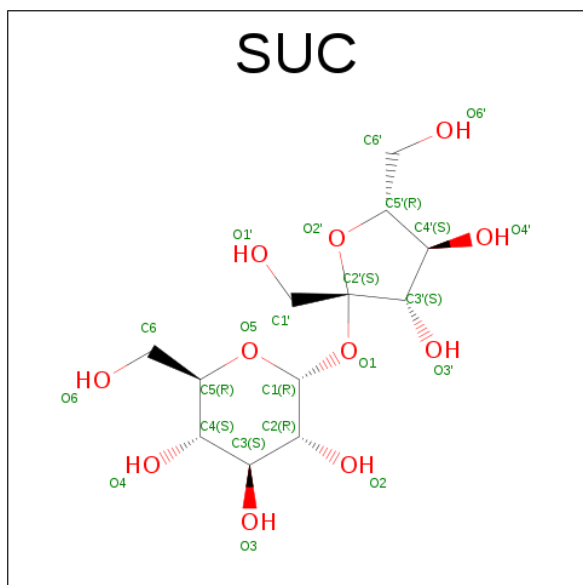
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	G	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	H	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	I	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	J	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	K	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	L	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	M	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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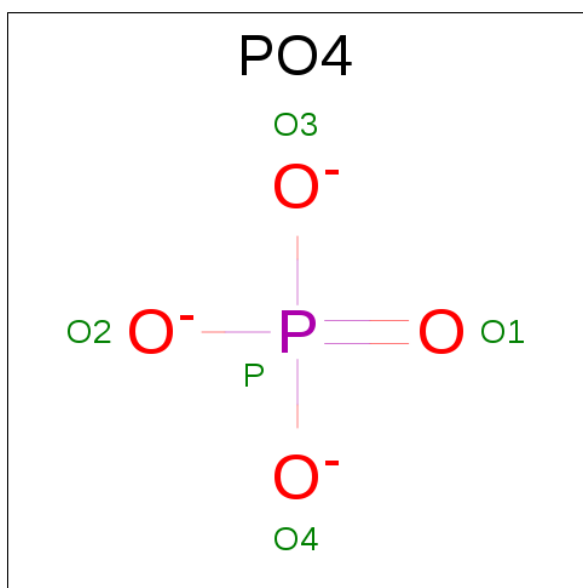
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	N	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	O	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	P	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is SUCROSE (three-letter code: SUC) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	12	11		
3	E	1	Total	C	O	0	0
			23	12	11		
3	G	1	Total	C	O	0	0
			23	12	11		
3	H	1	Total	C	O	0	0
			23	12	11		
3	I	1	Total	C	O	0	0
			23	12	11		
3	J	1	Total	C	O	0	0
			23	12	11		
3	K	1	Total	C	O	0	0
			23	12	11		
3	N	1	Total	C	O	0	0
			23	12	11		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	104	Total	O	0	0
			104	104		
5	B	85	Total	O	0	0
			85	85		
5	C	148	Total	O	0	0
			148	148		
5	D	97	Total	O	0	0
			97	97		
5	E	92	Total	O	0	0
			92	92		
5	F	101	Total	O	0	0
			101	101		
5	G	62	Total	O	0	0
			62	62		
5	H	42	Total	O	0	0
			42	42		
5	I	57	Total	O	0	0
			57	57		
5	J	74	Total	O	0	0
			74	74		

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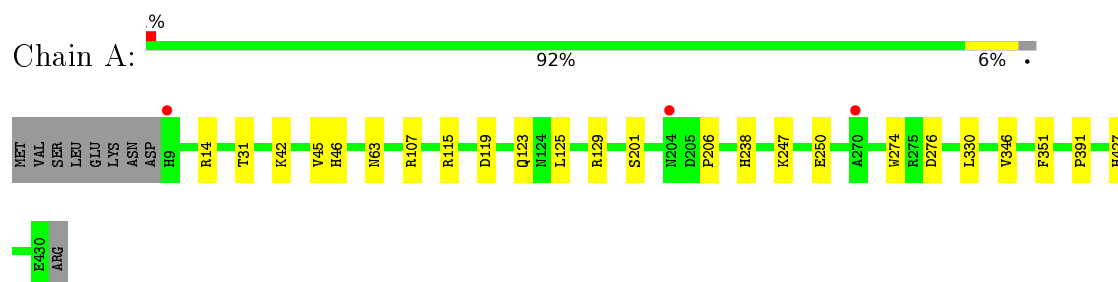
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	K	75	Total 75	O 75	0	0
5	L	81	Total 81	O 81	0	0
5	M	111	Total 111	O 111	0	0
5	N	142	Total 142	O 142	0	0
5	O	67	Total 67	O 67	0	0
5	P	60	Total 60	O 60	0	0

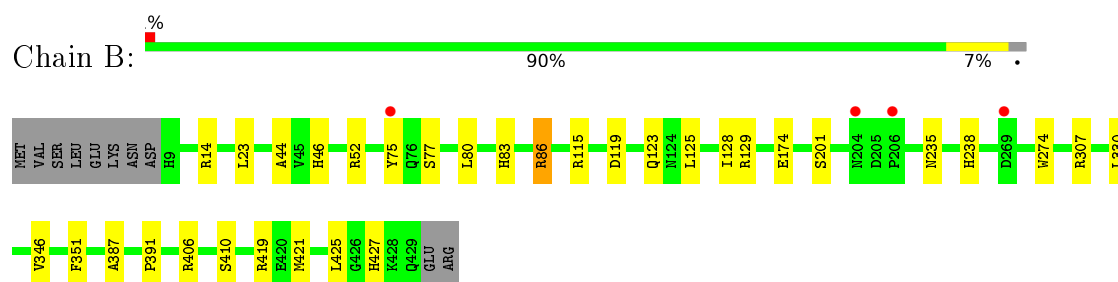
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

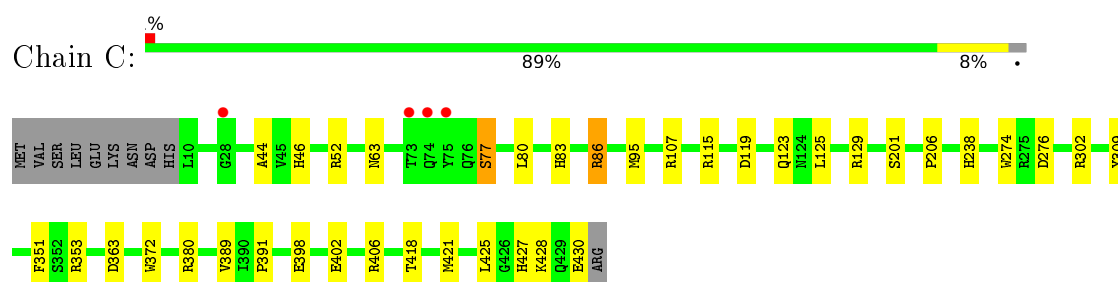
- Molecule 1: Glucose-1-phosphate adenylyltransferase



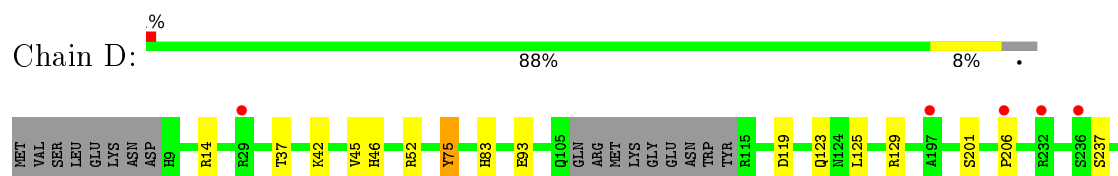
- Molecule 1: Glucose-1-phosphate adenylyltransferase



- Molecule 1: Glucose-1-phosphate adenylyltransferase

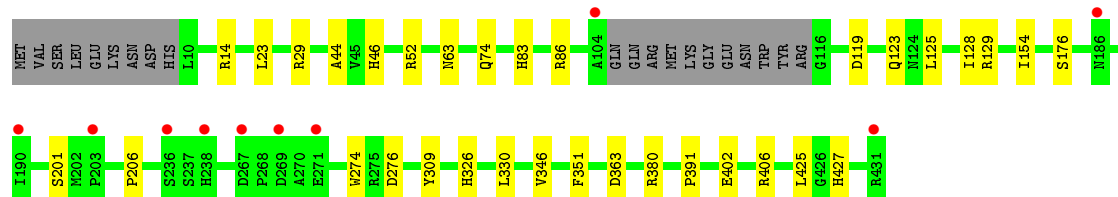
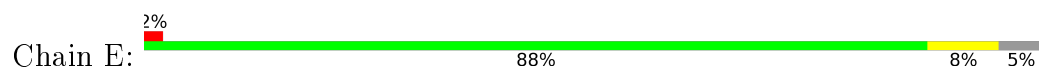


- Molecule 1: Glucose-1-phosphate adenylyltransferase

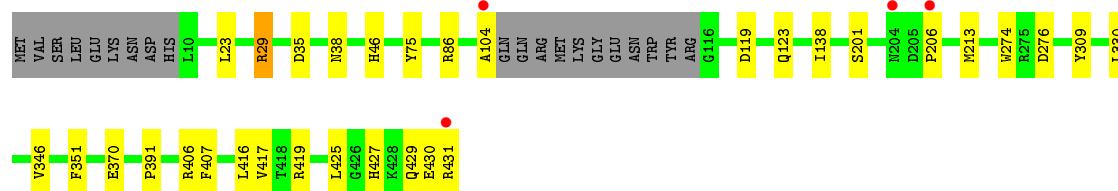
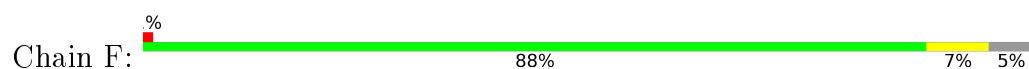




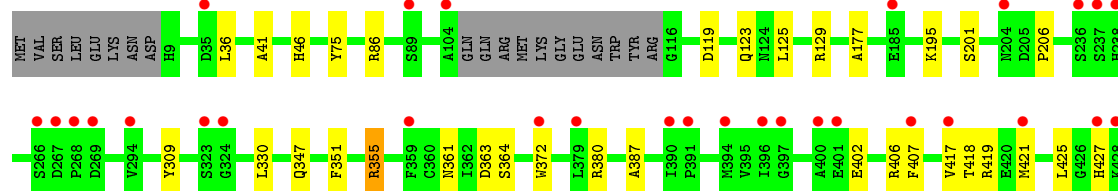
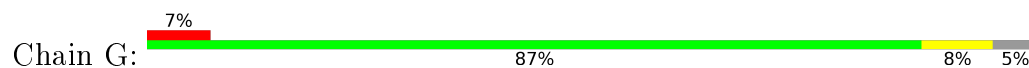
- Molecule 1: Glucose-1-phosphate adenylyltransferase



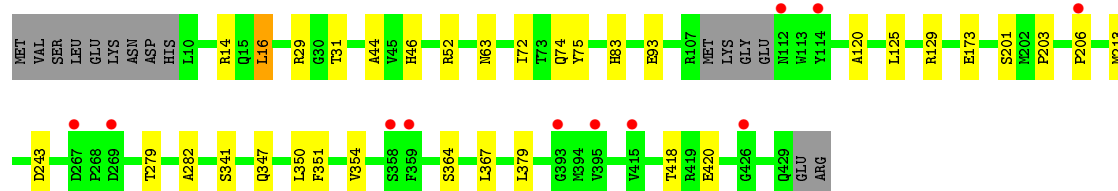
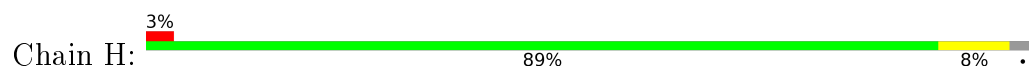
- Molecule 1: Glucose-1-phosphate adenylyltransferase



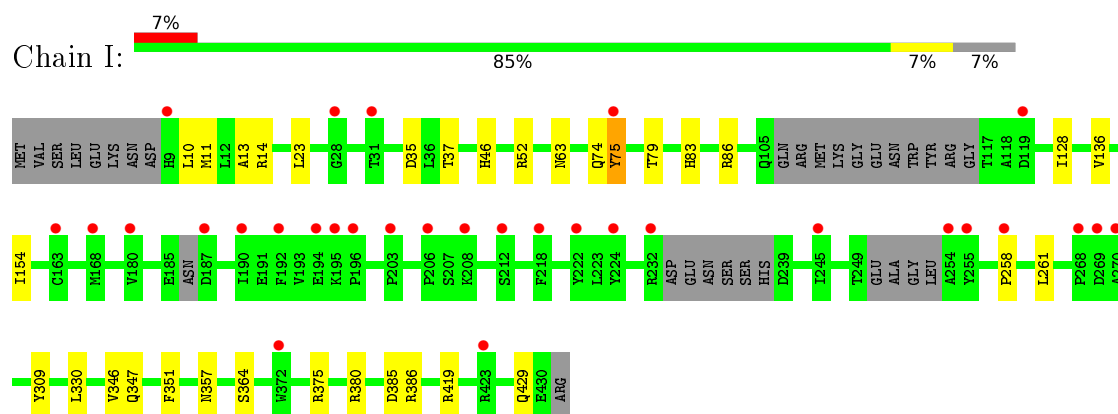
- Molecule 1: Glucose-1-phosphate adenylyltransferase



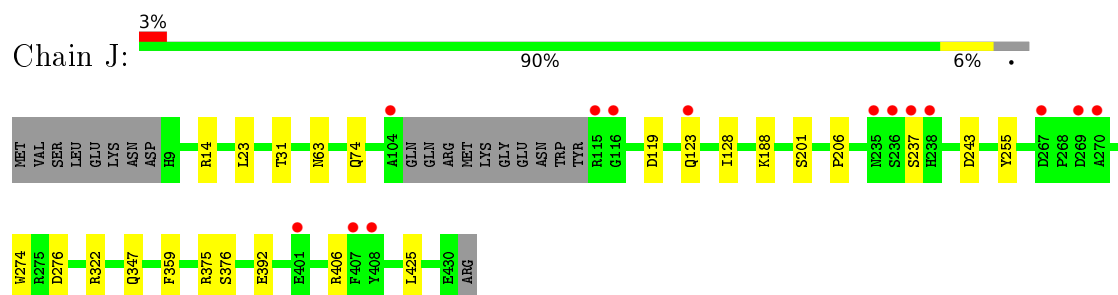
- Molecule 1: Glucose-1-phosphate adenylyltransferase



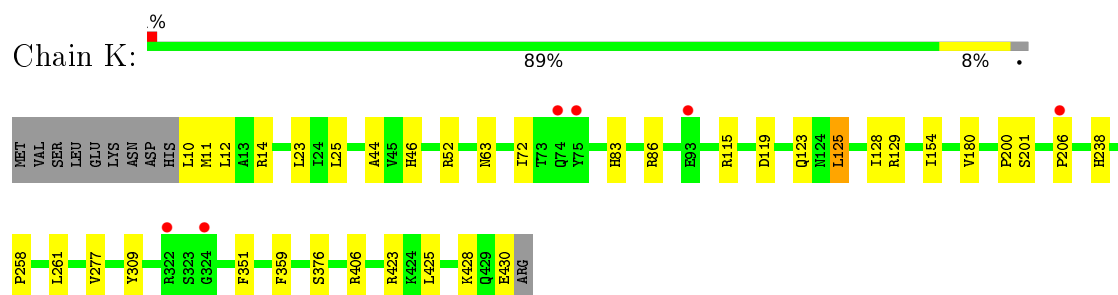
- Molecule 1: Glucose-1-phosphate adenylyltransferase



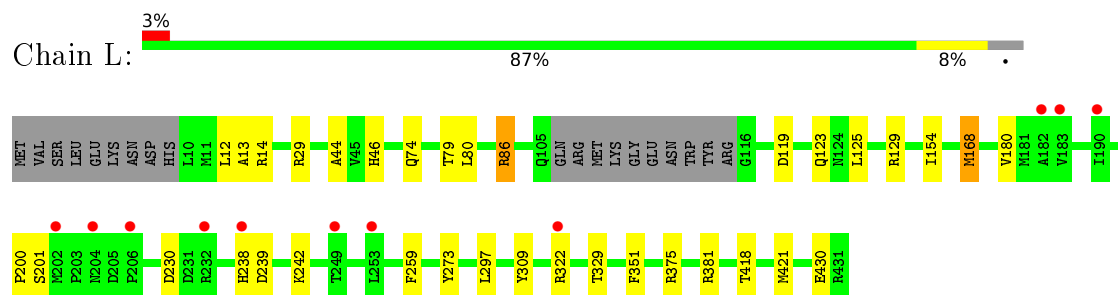
- Molecule 1: Glucose-1-phosphate adenylyltransferase



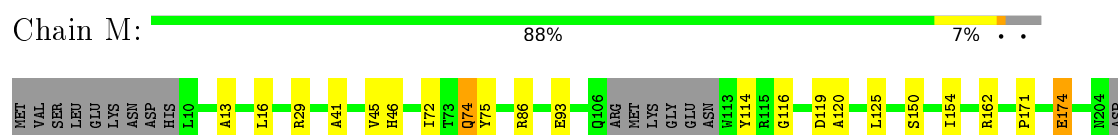
- Molecule 1: Glucose-1-phosphate adenylyltransferase



- Molecule 1: Glucose-1-phosphate adenylyltransferase

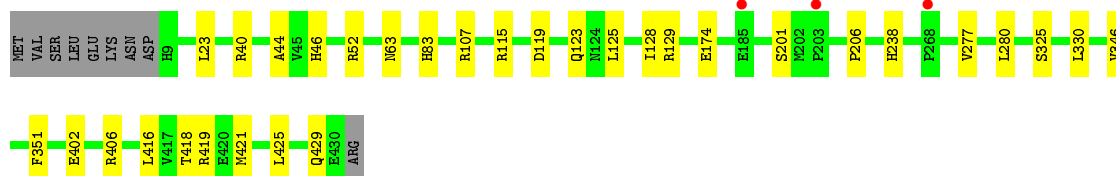
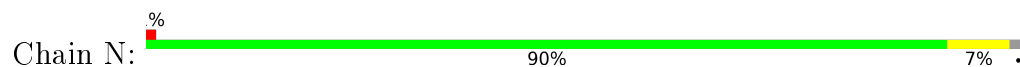


- Molecule 1: Glucose-1-phosphate adenylyltransferase

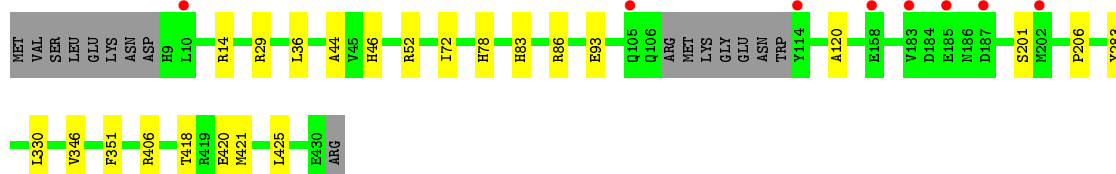




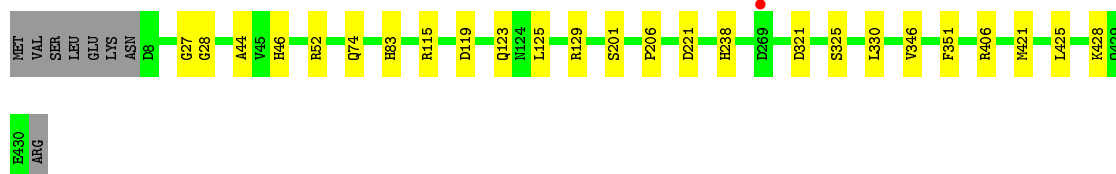
- Molecule 1: Glucose-1-phosphate adenylyltransferase



- Molecule 1: Glucose-1-phosphate adenylyltransferase



- Molecule 1: Glucose-1-phosphate adenylyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	166.88Å 148.19Å 180.16Å 90.00° 115.48° 90.00°	Depositor
Resolution (Å)	45.27 – 2.67 45.27 – 2.67	Depositor EDS
% Data completeness (in resolution range)	95.1 (45.27-2.67) 99.8 (45.27-2.67)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.65Å)	Xtriage
Refinement program	PHENIX (dev_2219: ???)	Depositor
R, R_{free}	0.239 , 0.263 0.221 , 0.249	Depositor DCC
R_{free} test set	11269 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.006 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	53530	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, PO4, SUC

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	0.26	0/3396	0.45	0/4605
1	B	0.26	0/3363	0.45	0/4560
1	C	0.25	0/3404	0.44	0/4613
1	D	0.25	0/3277	0.45	0/4445
1	E	0.25	0/3269	0.44	0/4432
1	F	0.25	0/3292	0.46	0/4459
1	G	0.25	0/3194	0.44	0/4341
1	H	0.25	0/3232	0.44	0/4398
1	I	0.25	0/3047	0.43	0/4148
1	J	0.26	0/3225	0.46	0/4379
1	K	0.25	0/3362	0.44	0/4556
1	L	0.25	0/3262	0.45	0/4422
1	M	0.25	0/3319	0.45	0/4497
1	N	0.25	0/3356	0.45	0/4552
1	O	0.25	0/3304	0.45	0/4480
1	P	0.25	0/3376	0.44	0/4577
All	All	0.25	0/52678	0.45	0/71464

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3325	0	3262	15	0
1	B	3293	0	3234	21	0
1	C	3325	0	3282	32	0
1	D	3210	0	3141	29	0
1	E	3202	0	3141	17	0
1	F	3225	0	3180	19	0
1	G	3127	0	3027	19	0
1	H	3162	0	3030	19	0
1	I	2984	0	2800	19	0
1	J	3158	0	3078	12	0
1	K	3292	0	3233	22	0
1	L	3195	0	3141	19	0
1	M	3250	0	3187	20	0
1	N	3285	0	3215	19	0
1	O	3237	0	3177	14	0
1	P	3305	0	3240	15	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
2	C	23	0	12	0	0
2	D	23	0	12	0	0
2	E	23	0	12	0	0
2	F	23	0	12	0	0
2	G	23	0	12	0	0
2	H	23	0	12	0	0
2	I	23	0	12	1	0
2	J	23	0	12	0	0
2	K	23	0	12	0	0
2	L	23	0	12	0	0
2	M	23	0	12	0	0
2	N	23	0	12	0	0
2	O	23	0	12	0	0
2	P	23	0	12	0	0
3	A	23	0	22	0	0
3	E	23	0	22	0	0
3	G	23	0	22	0	0
3	H	23	0	22	0	0
3	I	23	0	22	0	0
3	J	23	0	22	0	0
3	K	23	0	22	0	0
3	N	23	0	22	0	0
4	D	5	0	0	0	0
5	A	104	0	0	1	0
5	B	85	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	148	0	0	0	0
5	D	97	0	0	0	0
5	E	92	0	0	0	0
5	F	101	0	0	0	0
5	G	62	0	0	3	0
5	H	42	0	0	1	0
5	I	57	0	0	2	0
5	J	74	0	0	0	0
5	K	75	0	0	0	0
5	L	81	0	0	1	0
5	M	111	0	0	3	0
5	N	142	0	0	0	0
5	O	67	0	0	0	0
5	P	60	0	0	1	0
All	All	53530	0	50736	284	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 284 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:I:37:THR:O	1:I:75:TYR:OH	2.00	0.79
1:M:13:ALA:HA	1:M:154:ILE:HD11	1.63	0.78
1:B:235:ASN:OD1	1:K:423:ARG:NH1	2.20	0.73
1:B:274:TRP:CZ2	1:B:274:TRP:CZ3	2.76	0.70
1:J:63:ASN:O	1:K:14:ARG:NH2	2.29	0.66

There are no symmetry-related clashes.

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	423/431 (98%)	414 (98%)	9 (2%)	0	100	100
1	B	419/431 (97%)	409 (98%)	9 (2%)	1 (0%)	52	77
1	C	421/431 (98%)	409 (97%)	12 (3%)	0	100	100
1	D	409/431 (95%)	401 (98%)	8 (2%)	0	100	100
1	E	408/431 (95%)	398 (98%)	9 (2%)	1 (0%)	52	77
1	F	407/431 (94%)	397 (98%)	10 (2%)	0	100	100
1	G	407/431 (94%)	397 (98%)	10 (2%)	0	100	100
1	H	412/431 (96%)	400 (97%)	11 (3%)	1 (0%)	52	77
1	I	390/431 (90%)	377 (97%)	12 (3%)	1 (0%)	46	72
1	J	408/431 (95%)	397 (97%)	10 (2%)	1 (0%)	52	77
1	K	419/431 (97%)	410 (98%)	9 (2%)	0	100	100
1	L	408/431 (95%)	396 (97%)	11 (3%)	1 (0%)	52	77
1	M	409/431 (95%)	396 (97%)	12 (3%)	1 (0%)	52	77
1	N	420/431 (97%)	410 (98%)	10 (2%)	0	100	100
1	O	411/431 (95%)	398 (97%)	13 (3%)	0	100	100
1	P	421/431 (98%)	411 (98%)	10 (2%)	0	100	100
All	All	6592/6896 (96%)	6420 (97%)	165 (2%)	7 (0%)	56	81

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	74	GLN
1	J	74	GLN
1	B	75	TYR
1	H	74	GLN
1	M	74	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	357/373 (96%)	355 (99%)	2 (1%)	90	97
1	B	354/373 (95%)	350 (99%)	4 (1%)	80	93
1	C	358/373 (96%)	356 (99%)	2 (1%)	90	97
1	D	343/373 (92%)	342 (100%)	1 (0%)	94	99
1	E	343/373 (92%)	339 (99%)	4 (1%)	78	92
1	F	349/373 (94%)	348 (100%)	1 (0%)	94	99
1	G	326/373 (87%)	323 (99%)	3 (1%)	84	95
1	H	328/373 (88%)	323 (98%)	5 (2%)	72	90
1	I	297/373 (80%)	293 (99%)	4 (1%)	76	91
1	J	331/373 (89%)	329 (99%)	2 (1%)	90	97
1	K	353/373 (95%)	350 (99%)	3 (1%)	86	95
1	L	341/373 (91%)	334 (98%)	7 (2%)	61	85
1	M	347/373 (93%)	343 (99%)	4 (1%)	78	92
1	N	350/373 (94%)	348 (99%)	2 (1%)	90	97
1	O	348/373 (93%)	347 (100%)	1 (0%)	94	99
1	P	354/373 (95%)	353 (100%)	1 (0%)	94	99
All	All	5479/5968 (92%)	5433 (99%)	46 (1%)	86	95

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	341	SER
1	I	79	THR
1	N	40	ARG
1	H	379	LEU
1	I	35	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	106	GLN
1	H	123	GLN
1	K	112	ASN
1	P	106	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

25 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	AMP	A	501	-	22,25,25	0.52	0	22,38,38	0.39	0
3	SUC	A	502	-	24,24,24	0.45	0	36,36,36	0.67	0
2	AMP	B	501	-	22,25,25	0.73	1 (4%)	22,38,38	0.51	0
2	AMP	C	501	-	22,25,25	0.76	1 (4%)	22,38,38	0.48	0
2	AMP	D	501	-	22,25,25	0.67	0	22,38,38	0.41	0
4	PO4	D	502	-	4,4,4	0.63	0	6,6,6	0.23	0
2	AMP	E	501	-	22,25,25	0.73	1 (4%)	22,38,38	0.50	0
3	SUC	E	502	-	24,24,24	0.45	0	36,36,36	0.66	0
2	AMP	F	501	-	22,25,25	0.64	0	22,38,38	0.35	0
2	AMP	G	501	-	22,25,25	0.62	0	22,38,38	0.39	0
3	SUC	G	502	-	24,24,24	0.46	0	36,36,36	0.66	0
2	AMP	H	501	-	22,25,25	0.62	0	22,38,38	0.38	0
3	SUC	H	502	-	24,24,24	0.46	0	36,36,36	0.64	0
2	AMP	I	501	-	22,25,25	0.70	1 (4%)	22,38,38	0.51	0
3	SUC	I	502	-	24,24,24	0.46	0	36,36,36	0.67	0
2	AMP	J	501	-	22,25,25	0.73	1 (4%)	22,38,38	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SUC	J	502	-	24,24,24	0.48	0	36,36,36	0.65	0
2	AMP	K	501	-	22,25,25	0.65	0	22,38,38	0.40	0
3	SUC	K	502	-	24,24,24	0.45	0	36,36,36	0.64	0
2	AMP	L	501	-	22,25,25	0.75	1 (4%)	22,38,38	0.50	0
2	AMP	M	501	-	22,25,25	0.68	0	22,38,38	0.38	0
2	AMP	N	501	-	22,25,25	0.78	1 (4%)	22,38,38	0.53	0
3	SUC	N	502	-	24,24,24	0.46	0	36,36,36	0.68	0
2	AMP	O	501	-	22,25,25	0.67	0	22,38,38	0.47	0
2	AMP	P	501	-	22,25,25	0.78	1 (4%)	22,38,38	0.54	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
2	AMP	A	501	-	-	0/6/26/26	0/3/3/3
3	SUC	A	502	-	-	0/12/51/51	0/2/2/2
2	AMP	B	501	-	-	0/6/26/26	0/3/3/3
2	AMP	C	501	-	-	0/6/26/26	0/3/3/3
2	AMP	D	501	-	-	0/6/26/26	0/3/3/3
4	PO4	D	502	-	-	0/0/0/0	0/0/0/0
2	AMP	E	501	-	-	0/6/26/26	0/3/3/3
3	SUC	E	502	-	-	0/12/51/51	0/2/2/2
2	AMP	F	501	-	-	0/6/26/26	0/3/3/3
2	AMP	G	501	-	-	0/6/26/26	0/3/3/3
3	SUC	G	502	-	-	0/12/51/51	0/2/2/2
2	AMP	H	501	-	-	0/6/26/26	0/3/3/3
3	SUC	H	502	-	-	0/12/51/51	0/2/2/2
2	AMP	I	501	-	-	0/6/26/26	0/3/3/3
3	SUC	I	502	-	-	0/12/51/51	0/2/2/2
2	AMP	J	501	-	-	0/6/26/26	0/3/3/3
3	SUC	J	502	-	-	0/12/51/51	0/2/2/2
2	AMP	K	501	-	-	0/6/26/26	0/3/3/3
3	SUC	K	502	-	-	0/12/51/51	0/2/2/2
2	AMP	L	501	-	-	0/6/26/26	0/3/3/3
2	AMP	M	501	-	-	0/6/26/26	0/3/3/3
2	AMP	N	501	-	-	0/6/26/26	0/3/3/3
3	SUC	N	502	-	-	0/12/51/51	0/2/2/2
2	AMP	O	501	-	-	0/6/26/26	0/3/3/3
2	AMP	P	501	-	-	0/6/26/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	501	AMP	P-O2P	-2.52	1.46	1.54
2	P	501	AMP	P-O2P	-2.50	1.46	1.54
2	L	501	AMP	P-O2P	-2.36	1.46	1.54
2	C	501	AMP	P-O2P	-2.34	1.46	1.54
2	J	501	AMP	P-O2P	-2.23	1.47	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	501	AMP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	422/431 (97%)	-0.34	3 (0%) 89 89	17, 25, 40, 53	0
1	B	421/431 (97%)	-0.19	4 (0%) 84 84	20, 30, 47, 62	0
1	C	421/431 (97%)	-0.32	4 (0%) 84 84	14, 22, 37, 63	0
1	D	413/431 (95%)	-0.08	5 (1%) 81 80	15, 30, 56, 65	0
1	E	411/431 (95%)	-0.06	10 (2%) 62 60	16, 33, 56, 71	0
1	F	411/431 (95%)	-0.16	4 (0%) 84 84	16, 28, 48, 61	0
1	G	411/431 (95%)	0.32	30 (7%) 18 15	23, 42, 65, 76	0
1	H	416/431 (96%)	0.29	11 (2%) 59 58	28, 48, 67, 73	0
1	I	400/431 (92%)	0.40	31 (7%) 16 13	23, 45, 77, 85	0
1	J	412/431 (95%)	0.10	14 (3%) 49 47	25, 37, 61, 76	0
1	K	421/431 (97%)	-0.10	6 (1%) 78 76	20, 34, 48, 60	0
1	L	412/431 (95%)	0.15	11 (2%) 58 56	19, 36, 62, 76	0
1	M	415/431 (96%)	-0.24	1 (0%) 95 96	14, 26, 44, 55	0
1	N	422/431 (97%)	-0.27	3 (0%) 89 89	15, 25, 45, 64	0
1	O	415/431 (96%)	-0.18	8 (1%) 70 69	16, 29, 50, 63	0
1	P	423/431 (98%)	-0.35	1 (0%) 95 96	14, 23, 38, 59	0
All	All	6646/6896 (96%)	-0.07	146 (2%) 65 64	14, 31, 60, 85	0

The worst 5 of 146 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	104	ALA	6.2
1	J	116	GLY	6.2
1	H	206	PRO	4.8
1	I	255	TYR	4.6
1	B	204	ASN	4.2

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SUC	I	502	23/23	0.80	0.35	1.85	69,69,69,69	0
3	SUC	G	502	23/23	0.91	0.22	1.28	36,51,73,76	0
2	AMP	E	501	23/23	0.96	0.19	0.61	22,32,34,37	0
3	SUC	N	502	23/23	0.90	0.15	0.51	25,34,39,41	0
4	PO4	D	502	5/5	0.91	0.24	0.42	55,56,57,58	0
3	SUC	H	502	23/23	0.84	0.19	0.30	46,57,77,85	0
2	AMP	I	501	23/23	0.95	0.19	0.30	33,38,41,43	0
3	SUC	A	502	23/23	0.94	0.14	0.21	22,27,33,34	0
3	SUC	J	502	23/23	0.87	0.17	0.12	37,56,66,67	0
2	AMP	K	501	23/23	0.94	0.17	0.08	25,41,47,48	0
2	AMP	B	501	23/23	0.94	0.16	0.08	28,35,36,36	0
2	AMP	H	501	23/23	0.94	0.20	0.01	40,51,53,54	0
3	SUC	E	502	23/23	0.90	0.17	-0.06	40,51,61,70	0
2	AMP	L	501	23/23	0.96	0.15	-0.17	24,25,26,26	0
2	AMP	D	501	23/23	0.97	0.15	-0.31	26,33,34,36	0
3	SUC	K	502	23/23	0.93	0.14	-0.35	28,42,53,54	0
2	AMP	A	501	23/23	0.96	0.15	-0.40	20,26,30,33	0
2	AMP	N	501	23/23	0.97	0.14	-0.51	21,21,22,22	0
2	AMP	F	501	23/23	0.97	0.13	-0.59	24,29,30,30	0
2	AMP	M	501	23/23	0.97	0.14	-0.66	21,23,24,25	0
2	AMP	P	501	23/23	0.96	0.15	-0.71	23,24,25,25	0
2	AMP	J	501	23/23	0.96	0.14	-0.83	28,32,34,35	0
2	AMP	O	501	23/23	0.96	0.13	-0.88	22,24,26,28	0
2	AMP	C	501	23/23	0.97	0.12	-1.30	18,20,21,21	0
2	AMP	G	501	23/23	0.95	0.14	-1.98	34,40,44,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.