



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:07 am GMT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

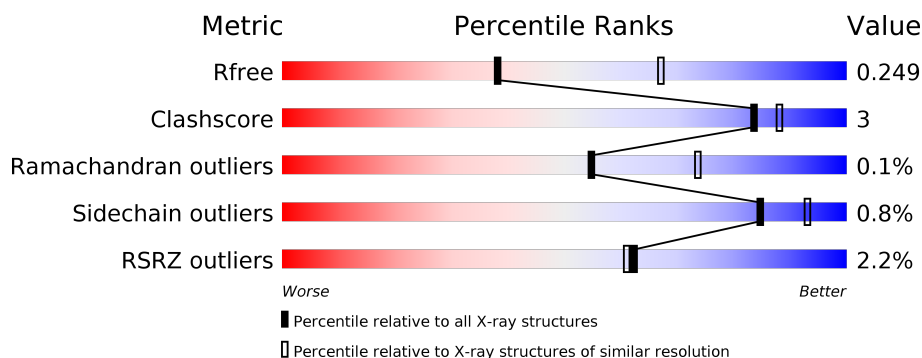
# 1 Overall quality at a glance

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))
$R_{free}$	100719	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (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  $\geq 3$ , 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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>92%</span> <span>6% •</span> </div> </div>
1	B	431	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 97%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>90%</span> <span>7% •</span> </div> </div>
1	C	431	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 97%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>89%</span> <span>8% •</span> </div> </div>
1	D	431	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 97%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>88%</span> <span>8% •</span> </div> </div>
1	E	431	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 96%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>2%</span> <span>88%</span> <span>8% 5%</span> </div> </div>
1	F	431	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 97%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>88%</span> <span>7% 5%</span> </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>2%</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 [i](#)

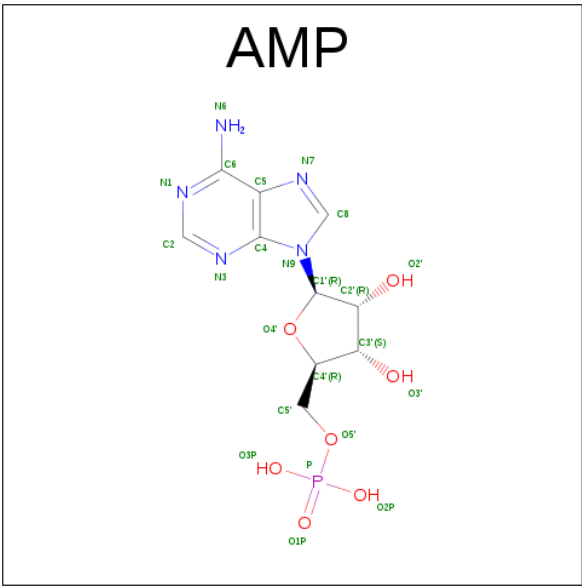
There are 5 unique types of molecules in this entry. The entry contains 53530 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



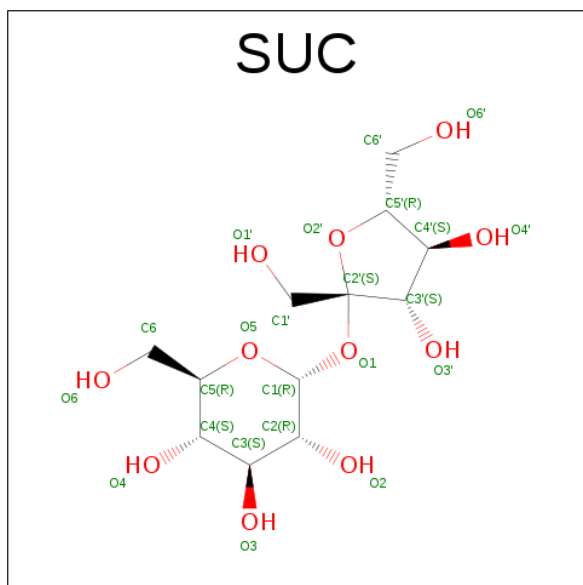
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	G	1	Total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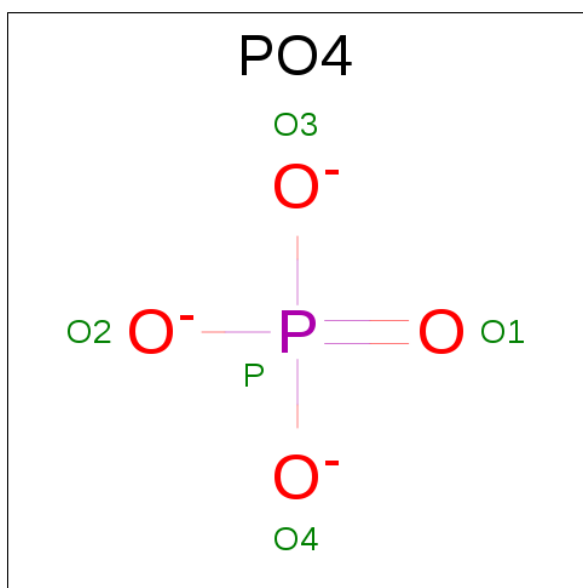
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	N	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	O	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	P	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- 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: O<sub>4</sub>P).



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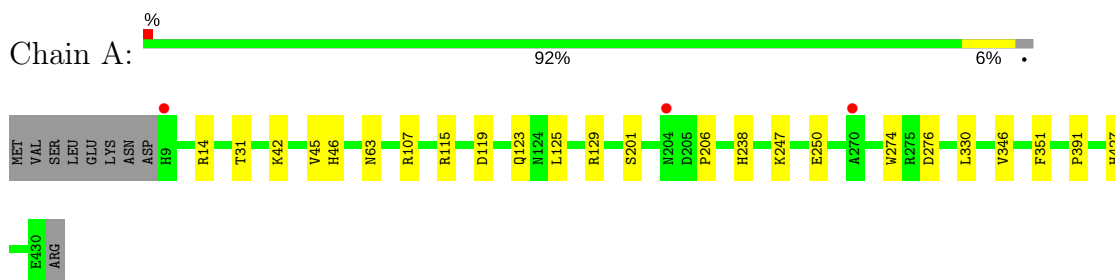
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	K	75	Total 75	O 75	0	0
5	L	81	Total 81	O 81	0	0
5	M	111	Total 111	O 111	0	0
5	N	142	Total 142	O 142	0	0
5	O	67	Total 67	O 67	0	0
5	P	60	Total 60	O 60	0	0



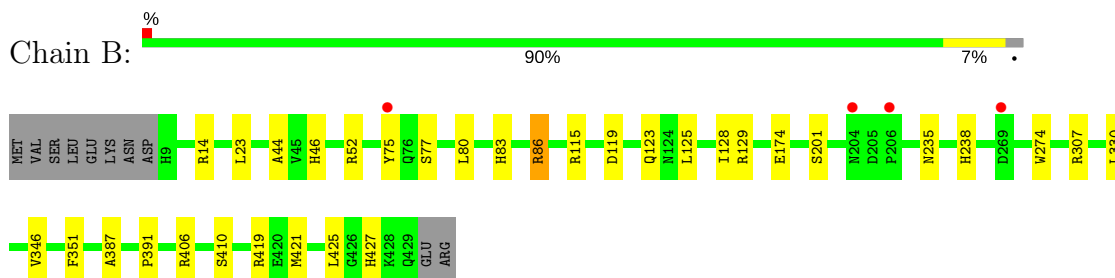
### 3 Residue-property plots [i](#)

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

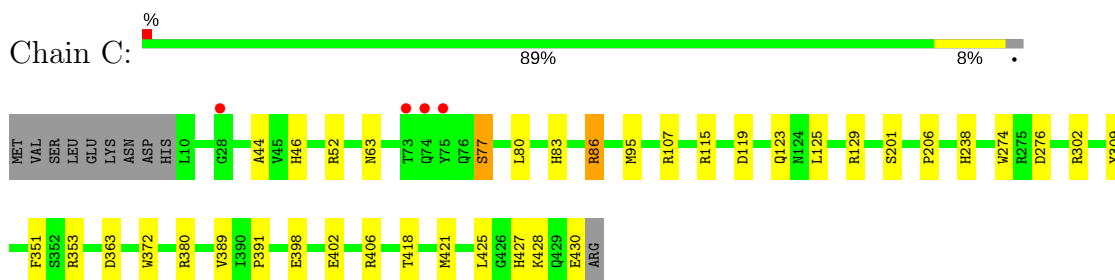
- Molecule 1: Glucose-1-phosphate adenylyltransferase



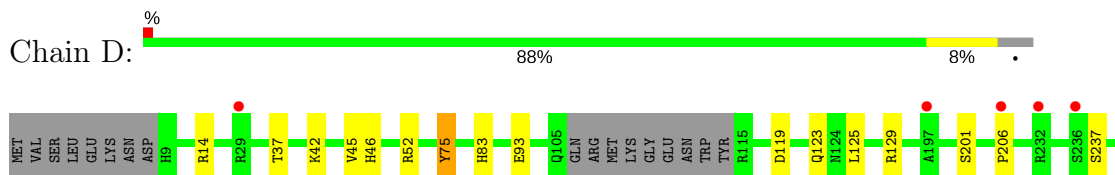
- Molecule 1: Glucose-1-phosphate adenylyltransferase



- Molecule 1: Glucose-1-phosphate adenylyltransferase

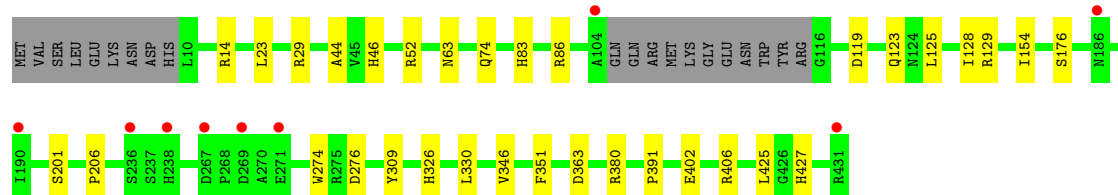
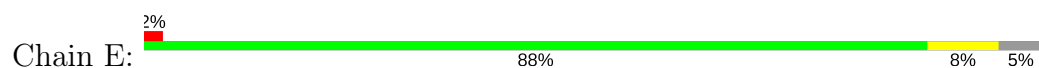


- Molecule 1: Glucose-1-phosphate adenylyltransferase

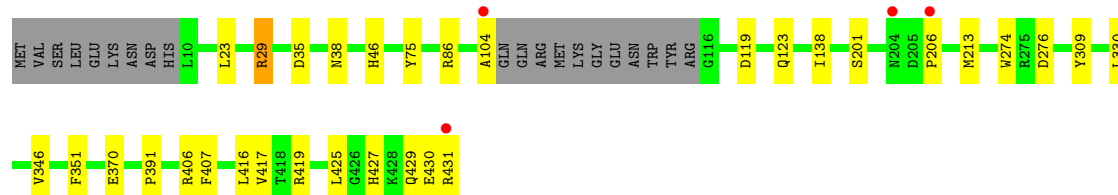
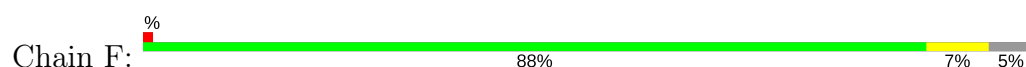




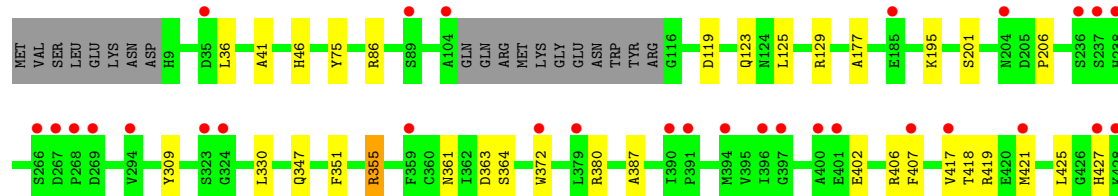
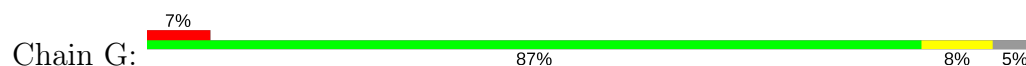
- Molecule 1: Glucose-1-phosphate adenylyltransferase



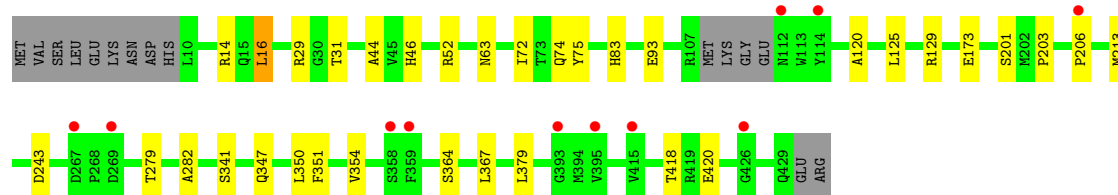
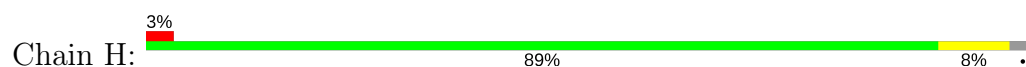
- Molecule 1: Glucose-1-phosphate adenylyltransferase



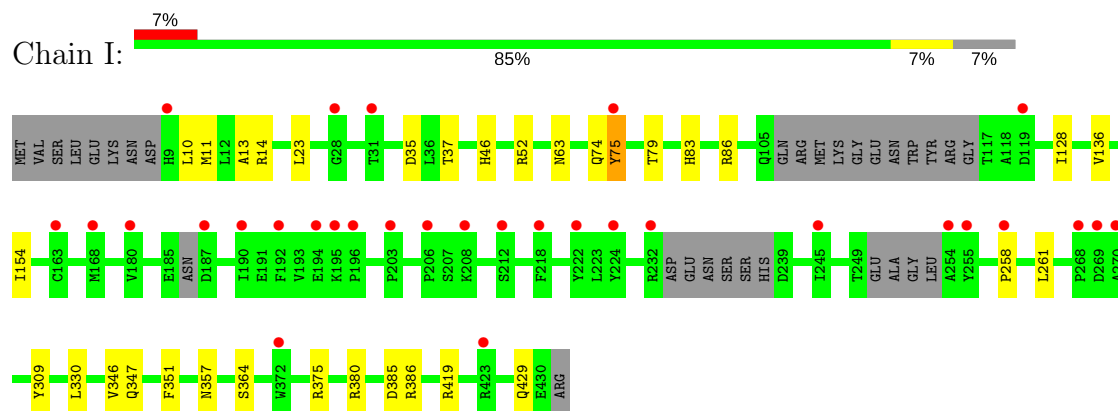
- Molecule 1: Glucose-1-phosphate adenylyltransferase



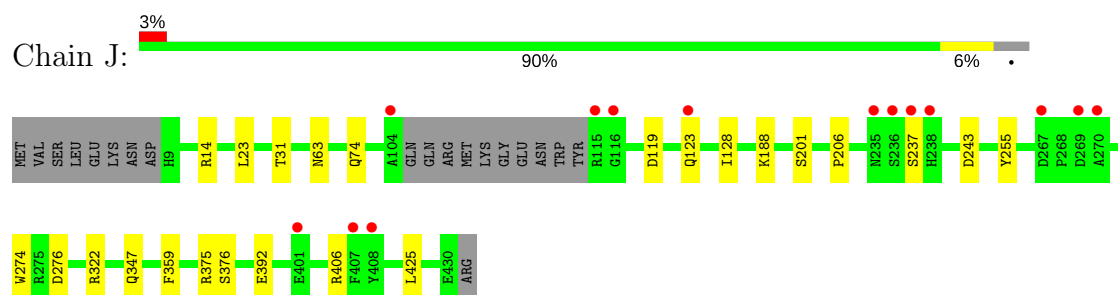
- Molecule 1: Glucose-1-phosphate adenylyltransferase



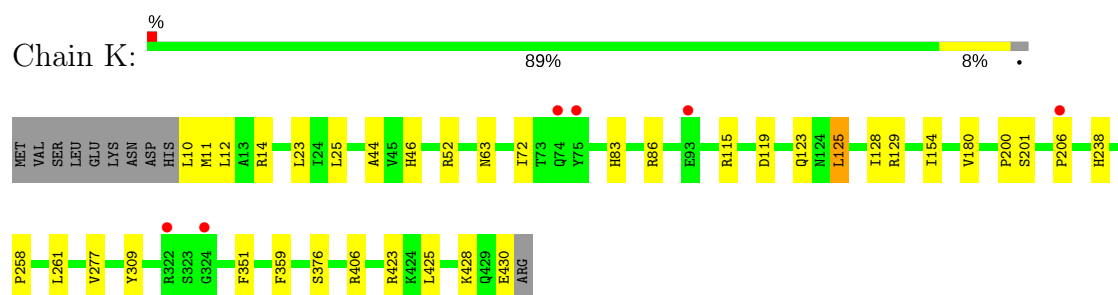
- Molecule 1: Glucose-1-phosphate adenylyltransferase



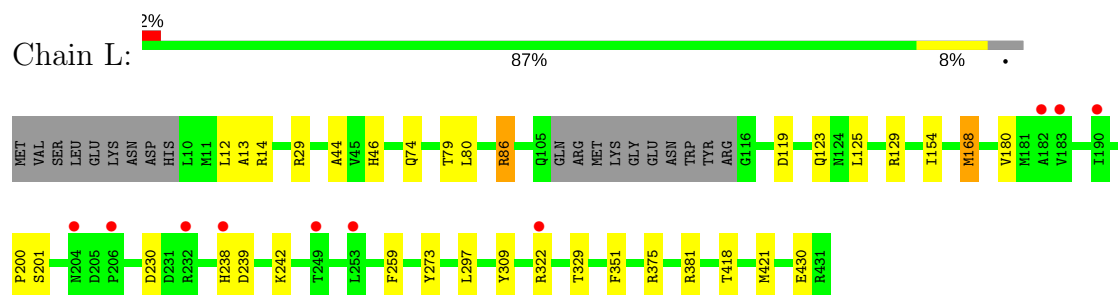
- Molecule 1: Glucose-1-phosphate adenylyltransferase



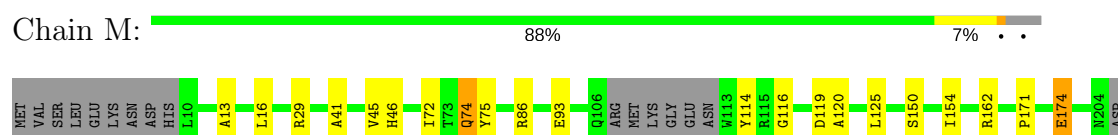
- Molecule 1: Glucose-1-phosphate adenylyltransferase



- Molecule 1: Glucose-1-phosphate adenylyltransferase

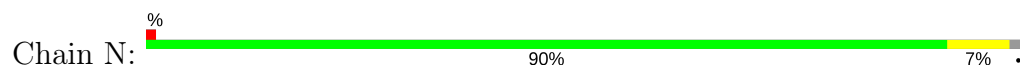


- Molecule 1: Glucose-1-phosphate adenylyltransferase

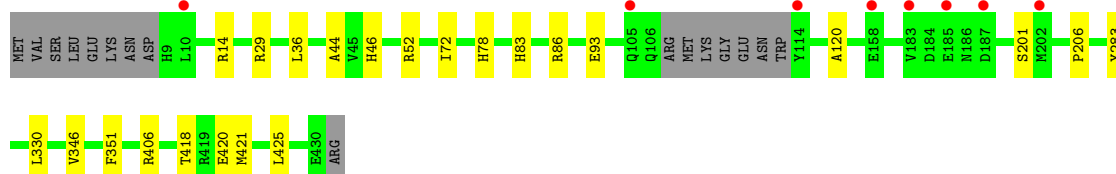




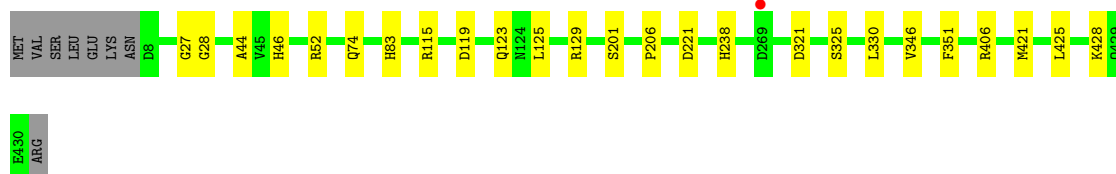
- Molecule 1: Glucose-1-phosphate adenylyltransferase



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

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

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

## 5 Model quality

### 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.

All (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
1:L:381:ARG:NH1	1:N:325:SER:HB2	2.12	0.65
1:D:52:ARG:HG3	1:D:83:HIS:CE1	2.32	0.64
1:A:63:ASN:O	1:D:14:ARG:NH2	2.31	0.64
1:H:279:THR:HG23	1:H:282:ALA:H	1.63	0.64
1:N:44:ALA:O	1:N:52:ARG:NH1	2.31	0.64
1:M:330:LEU:HB3	1:M:346:VAL:HG22	1.80	0.64
1:J:14:ARG:NH2	1:K:63:ASN:O	2.31	0.63
1:D:37:THR:O	1:D:75:TYR:OH	2.15	0.63
1:L:13:ALA:HA	1:L:154:ILE:HD11	1.81	0.62
1:B:387:ALA:O	1:B:419:ARG:NH1	2.33	0.62
1:O:44:ALA:O	1:O:52:ARG:NH1	2.33	0.61
1:K:180:VAL:HG21	1:K:200:PRO:HD2	1.81	0.61
1:N:115:ARG:HG2	1:N:238:HIS:HD2	1.66	0.60
1:C:302:ARG:HH22	1:D:353:ARG:HE	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:427:HIS:HE1	5:G:651:HOH:O	1.84	0.60
1:E:14:ARG:NH2	1:H:63:ASN:O	2.34	0.60
1:O:52:ARG:HD2	1:O:83:HIS:CG	2.36	0.60
1:C:115:ARG:HG2	1:C:238:HIS:HD2	1.66	0.60
1:H:52:ARG:HD2	1:H:83:HIS:CG	2.37	0.60
1:K:115:ARG:HG2	1:K:238:HIS:HD2	1.66	0.59
1:N:63:ASN:O	1:O:14:ARG:NH2	2.35	0.59
1:B:52:ARG:HD2	1:B:83:HIS:CG	2.38	0.59
1:H:29:ARG:HD3	1:H:31:THR:HG22	1.84	0.59
1:C:52:ARG:HD2	1:C:83:HIS:CG	2.38	0.58
1:C:302:ARG:NH2	1:D:353:ARG:HE	2.01	0.58
1:K:428:LYS:HG2	1:K:430:GLU:H	1.68	0.58
1:I:63:ASN:O	1:L:14:ARG:NH1	2.36	0.58
1:L:180:VAL:HG21	1:L:200:PRO:HD2	1.85	0.58
1:C:119:ASP:O	1:C:123:GLN:HG3	2.03	0.58
1:D:119:ASP:O	1:D:123:GLN:HG3	2.04	0.58
1:A:119:ASP:O	1:A:123:GLN:HG3	2.04	0.57
1:I:330:LEU:HB3	1:I:346:VAL:HG22	1.85	0.57
1:H:418:THR:HG22	1:H:420:GLU:H	1.68	0.57
1:N:119:ASP:O	1:N:123:GLN:HG3	2.05	0.57
1:F:430:GLU:HA	1:F:431:ARG:CB	2.35	0.57
1:P:44:ALA:O	1:P:52:ARG:NH1	2.37	0.56
1:P:52:ARG:HD2	1:P:83:HIS:CG	2.41	0.56
1:K:52:ARG:HD2	1:K:83:HIS:CG	2.41	0.56
1:K:44:ALA:O	1:K:52:ARG:NH1	2.38	0.56
1:N:52:ARG:HD2	1:N:83:HIS:CG	2.40	0.56
1:B:119:ASP:O	1:B:123:GLN:HG3	2.05	0.56
1:H:29:ARG:HG3	1:H:75:TYR:CZ	2.41	0.55
1:I:419:ARG:NH2	1:I:429:GLN:O	2.39	0.55
1:F:119:ASP:O	1:F:123:GLN:HG3	2.06	0.55
1:K:119:ASP:O	1:K:123:GLN:HG3	2.07	0.55
1:A:115:ARG:HG2	1:A:238:HIS:HD2	1.70	0.55
1:H:350:LEU:HD22	1:H:354:VAL:HG11	1.88	0.55
1:M:16:LEU:HD12	1:M:154:ILE:HD13	1.89	0.55
1:E:63:ASN:O	1:H:14:ARG:NH2	2.40	0.55
1:J:322:ARG:HH12	1:J:375:ARG:NH1	2.04	0.55
1:P:27:GLY:HA3	1:P:74:GLN:H	1.72	0.55
1:P:330:LEU:HB3	1:P:346:VAL:HG22	1.89	0.55
1:P:406:ARG:HB3	1:P:425:LEU:HD21	1.88	0.54
1:E:44:ALA:O	1:E:52:ARG:NH1	2.40	0.54
1:F:29:ARG:HG3	1:F:75:TYR:CZ	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:201:SER:HB2	1:K:206:PRO:HA	1.90	0.54
1:C:302:ARG:HH22	1:D:353:ARG:NE	2.04	0.54
1:B:115:ARG:HG2	1:B:238:HIS:HD2	1.73	0.54
1:I:23:LEU:HD13	1:I:136:VAL:HG13	1.90	0.54
1:A:274:TRP:CH2	1:A:276:ASP:HB3	2.43	0.53
1:B:14:ARG:NH2	1:C:63:ASN:O	2.41	0.53
1:M:86:ARG:NH2	1:O:93:GLU:OE1	2.41	0.53
1:F:274:TRP:CH2	1:F:276:ASP:HB3	2.43	0.53
1:K:115:ARG:HG2	1:K:238:HIS:CD2	2.43	0.53
1:O:418:THR:HG22	1:O:420:GLU:H	1.73	0.53
1:N:201:SER:HB2	1:N:206:PRO:HA	1.90	0.53
1:E:52:ARG:HD2	1:E:83:HIS:CG	2.44	0.53
1:A:201:SER:HB2	1:A:206:PRO:HA	1.90	0.53
1:F:86:ARG:NH2	1:H:93:GLU:OE1	2.41	0.53
1:H:44:ALA:O	1:H:52:ARG:NH1	2.41	0.53
1:B:406:ARG:HB3	1:B:425:LEU:HD21	1.91	0.53
1:E:119:ASP:O	1:E:123:GLN:HG3	2.09	0.53
1:I:380:ARG:NH1	5:I:602:HOH:O	2.41	0.53
1:J:406:ARG:HB3	1:J:425:LEU:HD21	1.92	0.52
1:F:201:SER:HB2	1:F:206:PRO:HA	1.91	0.52
1:D:406:ARG:HB3	1:D:425:LEU:HD21	1.92	0.52
1:C:302:ARG:HH22	1:D:353:ARG:HH21	1.58	0.52
1:N:280:LEU:HD13	1:N:416:LEU:HD12	1.92	0.52
1:C:302:ARG:NH2	1:D:353:ARG:NE	2.57	0.52
1:G:201:SER:HB2	1:G:206:PRO:HA	1.91	0.51
1:L:119:ASP:O	1:L:123:GLN:HG3	2.11	0.51
1:P:119:ASP:O	1:P:123:GLN:HG3	2.10	0.51
1:F:419:ARG:NH2	1:F:429:GLN:O	2.44	0.51
1:E:274:TRP:CH2	1:E:276:ASP:HB3	2.46	0.50
1:C:201:SER:HB2	1:C:206:PRO:HA	1.94	0.50
1:P:201:SER:HB2	1:P:206:PRO:HA	1.92	0.50
1:B:235:ASN:HD21	1:K:423:ARG:HD2	1.77	0.50
1:G:419:ARG:NH2	1:G:429:GLN:O	2.45	0.50
1:G:177:ALA:O	1:G:195:LYS:NZ	2.45	0.50
1:G:427:HIS:CE1	5:G:651:HOH:O	2.61	0.50
1:J:201:SER:HB2	1:J:206:PRO:HA	1.93	0.50
1:A:330:LEU:HB3	1:A:346:VAL:HG22	1.92	0.49
1:D:311:GLU:OE2	1:D:353:ARG:NH1	2.45	0.49
1:H:125:LEU:O	1:H:129:ARG:HG3	2.12	0.49
1:C:302:ARG:HH22	1:D:353:ARG:NH2	2.10	0.49
1:G:119:ASP:O	1:G:123:GLN:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:HIS:HB3	1:F:351:PHE:CE2	2.48	0.49
1:O:406:ARG:HB3	1:O:425:LEU:HD21	1.94	0.49
1:E:125:LEU:O	1:E:129:ARG:HG3	2.13	0.49
1:N:330:LEU:HB3	1:N:346:VAL:HG22	1.95	0.49
1:K:23:LEU:HD21	1:K:128:ILE:HD13	1.94	0.49
1:O:72:ILE:HG21	1:O:120:ALA:HB1	1.95	0.49
1:B:23:LEU:HD21	1:B:128:ILE:HD13	1.94	0.48
1:C:380:ARG:HH21	1:C:398:GLU:HG2	1.77	0.48
1:I:11:MET:SD	1:L:154:ILE:HD12	2.53	0.48
1:C:46:HIS:HB3	1:C:351:PHE:CE2	2.48	0.48
1:C:274:TRP:CH2	1:C:276:ASP:HB3	2.48	0.48
1:H:46:HIS:HB3	1:H:351:PHE:CE2	2.49	0.48
1:C:115:ARG:HG2	1:C:238:HIS:CD2	2.47	0.48
1:E:201:SER:HB2	1:E:206:PRO:HA	1.94	0.48
1:I:46:HIS:HB3	1:I:351:PHE:CE2	2.49	0.48
1:J:274:TRP:CH2	1:J:276:ASP:HB3	2.48	0.48
1:J:119:ASP:O	1:J:123:GLN:HG3	2.13	0.48
1:P:28:GLY:H	1:P:74:GLN:HB2	1.78	0.48
1:H:213:MET:HE2	1:H:213:MET:HB2	1.71	0.48
1:K:46:HIS:HB3	1:K:351:PHE:CE2	2.49	0.47
1:G:46:HIS:HB3	1:G:351:PHE:CE2	2.49	0.47
1:M:93:GLU:OE1	1:O:86:ARG:NH2	2.47	0.47
1:N:107:ARG:HD3	1:N:123:GLN:HE21	1.79	0.47
1:C:86:ARG:HB3	1:C:309:TYR:CD1	2.50	0.47
1:K:125:LEU:O	1:K:129:ARG:HG3	2.14	0.47
1:F:370:GLU:HB3	1:F:431:ARG:NH2	2.30	0.47
1:N:115:ARG:HG2	1:N:238:HIS:CD2	2.46	0.47
1:N:277:VAL:O	1:N:277:VAL:HG12	2.15	0.47
1:A:125:LEU:O	1:A:129:ARG:HG3	2.15	0.47
1:C:125:LEU:O	1:C:129:ARG:HG3	2.15	0.47
1:I:357:ASN:HB3	1:I:375:ARG:HG2	1.96	0.47
1:F:406:ARG:HB3	1:F:425:LEU:HD11	1.97	0.47
1:E:23:LEU:HD21	1:E:128:ILE:HD13	1.98	0.46
1:N:125:LEU:O	1:N:129:ARG:HG3	2.15	0.46
1:I:375:ARG:NH2	5:I:601:HOH:O	2.38	0.46
1:B:330:LEU:HB3	1:B:346:VAL:HG22	1.96	0.46
1:P:46:HIS:HB3	1:P:351:PHE:CE2	2.50	0.46
1:L:168:MET:HG3	1:L:259:PHE:HB3	1.98	0.46
1:O:46:HIS:HB3	1:O:351:PHE:CE2	2.50	0.46
1:A:46:HIS:HB3	1:A:351:PHE:CE2	2.50	0.46
1:B:44:ALA:O	1:B:52:ARG:NH1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:10:LEU:HD13	1:K:12:LEU:H	1.81	0.46
1:K:25:LEU:HD23	1:K:72:ILE:HD12	1.96	0.46
1:B:125:LEU:O	1:B:129:ARG:HG3	2.15	0.46
1:D:421:MET:O	1:D:425:LEU:HD13	2.17	0.45
1:F:35:ASP:HB2	1:F:416:LEU:HD11	1.99	0.45
1:I:13:ALA:HA	1:I:154:ILE:HD11	1.98	0.45
1:C:353:ARG:HH22	1:D:302:ARG:NH2	2.13	0.45
1:I:258:PRO:HD2	1:I:261:LEU:HD12	1.99	0.45
1:I:23:LEU:HD21	1:I:128:ILE:HD13	1.98	0.45
1:A:115:ARG:HG2	1:A:238:HIS:CD2	2.50	0.45
1:L:125:LEU:O	1:L:129:ARG:HG3	2.16	0.45
1:L:418:THR:OG1	1:L:421:MET:HG3	2.17	0.45
1:P:221:ASP:HB2	5:P:644:HOH:O	2.17	0.45
1:O:201:SER:HB3	1:O:206:PRO:HA	1.98	0.45
1:P:125:LEU:O	1:P:129:ARG:HG3	2.17	0.45
1:A:14:ARG:NH1	5:A:603:HOH:O	2.41	0.44
1:B:46:HIS:HB3	1:B:351:PHE:CE2	2.52	0.44
1:C:428:LYS:NZ	1:C:430:GLU:HB2	2.33	0.44
1:H:72:ILE:HG21	1:H:120:ALA:HB1	2.00	0.44
1:J:23:LEU:HD21	1:J:128:ILE:HD13	1.98	0.44
1:N:23:LEU:HD21	1:N:128:ILE:HD13	1.99	0.44
1:O:421:MET:O	1:O:425:LEU:HD13	2.17	0.44
1:B:86:ARG:NH2	1:D:93:GLU:HG2	2.32	0.44
1:M:72:ILE:HG21	1:M:120:ALA:HB1	1.99	0.44
1:N:418:THR:OG1	1:N:421:MET:HG3	2.17	0.44
1:P:115:ARG:HG2	1:P:238:HIS:HD2	1.81	0.44
1:P:28:GLY:N	1:P:74:GLN:HB2	2.32	0.44
1:G:363:ASP:O	1:G:380:ARG:HA	2.18	0.44
1:A:247:LYS:HB2	1:A:247:LYS:HE3	1.74	0.44
1:I:52:ARG:HD2	1:I:83:HIS:CG	2.53	0.44
1:A:42:LYS:HA	1:A:45:VAL:HG23	2.00	0.44
1:B:86:ARG:NE	1:D:93:GLU:OE2	2.51	0.44
1:G:86:ARG:HB3	1:G:309:TYR:CD1	2.52	0.44
1:D:274:TRP:CH2	1:D:276:ASP:HB3	2.53	0.44
1:E:86:ARG:HB3	1:E:309:TYR:CD1	2.53	0.44
1:K:406:ARG:HB3	1:K:425:LEU:HD11	1.99	0.44
1:M:46:HIS:HB3	1:M:351:PHE:CE2	2.53	0.44
1:E:125:LEU:HA	1:E:125:LEU:HD12	1.85	0.44
1:C:107:ARG:HD3	1:C:123:GLN:HE21	1.83	0.43
1:E:46:HIS:HB3	1:E:351:PHE:CE2	2.53	0.43
1:M:74:GLN:HE22	1:M:114:TYR:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:419:ARG:NH2	1:N:429:GLN:O	2.52	0.43
1:A:125:LEU:HD12	1:A:125:LEU:HA	1.87	0.43
1:J:375:ARG:NH1	1:J:392:GLU:OE1	2.50	0.43
1:P:321:ASP:OD2	1:P:325:SER:HB3	2.18	0.43
1:G:387:ALA:HB3	1:G:419:ARG:HD2	1.99	0.43
1:M:244:LEU:O	1:M:248:ILE:HG13	2.19	0.43
1:M:406:ARG:HB3	1:M:425:LEU:HD11	1.99	0.43
1:O:330:LEU:HB3	1:O:346:VAL:HG22	2.00	0.43
1:F:104:ALA:HB1	1:F:123:GLN:OE1	2.17	0.43
1:D:419:ARG:NH2	1:D:429:GLN:O	2.49	0.43
1:G:125:LEU:O	1:G:129:ARG:HG3	2.18	0.43
1:A:391:PRO:HG3	1:A:427:HIS:CG	2.54	0.43
1:D:201:SER:HB2	1:D:206:PRO:HA	1.99	0.43
5:M:708:HOH:O	1:O:78:HIS:HA	2.18	0.43
1:J:237:SER:OG	1:J:243:ASP:OD1	2.31	0.43
1:M:45:VAL:HG13	5:M:699:HOH:O	2.18	0.43
1:A:107:ARG:HD3	1:A:123:GLN:HE21	1.83	0.43
1:F:213:MET:HE2	1:F:213:MET:HB2	1.74	0.43
1:G:355:ARG:HG3	1:G:372:TRP:CZ3	2.54	0.43
1:H:350:LEU:HD23	1:H:367:LEU:HB2	2.00	0.43
1:I:347:GLN:O	1:I:364:SER:HA	2.19	0.42
1:L:46:HIS:HB3	1:L:351:PHE:CE2	2.54	0.42
1:M:41:ALA:HB2	1:M:75:TYR:O	2.18	0.42
1:D:237:SER:OG	1:D:243:ASP:OD2	2.25	0.42
1:E:406:ARG:HB3	1:E:425:LEU:HD11	2.01	0.42
1:G:36:LEU:HD12	1:G:36:LEU:HA	1.93	0.42
1:H:16:LEU:HA	1:H:16:LEU:HD12	1.88	0.42
1:L:239:ASP:HB3	1:L:242:LYS:HB3	2.01	0.42
1:C:406:ARG:HB3	1:C:425:LEU:HD21	2.02	0.42
1:D:46:HIS:HB3	1:D:351:PHE:CE2	2.54	0.42
1:F:23:LEU:HB2	1:F:138:ILE:HD13	2.01	0.42
1:G:407:PHE:CG	1:G:417:VAL:HG22	2.55	0.42
1:K:86:ARG:HB3	1:K:309:TYR:CD1	2.54	0.42
1:L:322:ARG:HD2	1:L:375:ARG:HD3	2.00	0.42
1:N:46:HIS:HB3	1:N:351:PHE:CE2	2.55	0.42
1:C:44:ALA:O	1:C:52:ARG:NH1	2.51	0.42
1:E:402:GLU:O	1:E:406:ARG:HD3	2.19	0.42
1:L:230:ASP:OD1	1:L:238:HIS:ND1	2.39	0.42
1:B:77:SER:HB3	1:B:80:LEU:HB3	2.00	0.42
1:M:116:GLY:H	1:M:119:ASP:HB3	1.85	0.42
1:O:36:LEU:HD21	1:O:283:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:GLU:O	1:C:406:ARG:HD3	2.20	0.42
1:C:77:SER:HB2	1:C:80:LEU:HB3	2.02	0.42
1:D:125:LEU:O	1:D:129:ARG:HG3	2.19	0.42
1:D:402:GLU:O	1:D:406:ARG:HD3	2.20	0.42
1:J:188:LYS:HE2	1:J:255:TYR:CZ	2.55	0.42
1:D:418:THR:OG1	1:D:421:MET:HG3	2.20	0.41
1:E:391:PRO:HG3	1:E:427:HIS:CG	2.55	0.41
1:F:86:ARG:HB3	1:F:309:TYR:CD1	2.55	0.41
1:H:201:SER:HB2	1:H:206:PRO:HA	2.00	0.41
1:J:359:PHE:O	1:J:376:SER:HA	2.19	0.41
1:L:86:ARG:HB3	1:L:309:TYR:CD1	2.54	0.41
1:D:275:ARG:NH2	1:D:296:GLU:OE1	2.53	0.41
1:G:330:LEU:HA	5:G:630:HOH:O	2.19	0.41
1:I:86:ARG:HB3	1:I:309:TYR:CD1	2.55	0.41
1:L:273:TYR:CE2	1:L:297:LEU:HB2	2.55	0.41
1:M:375:ARG:HB3	1:M:392:GLU:HG3	2.02	0.41
1:C:391:PRO:HG3	1:C:427:HIS:CG	2.56	0.41
1:E:363:ASP:O	1:E:380:ARG:HA	2.20	0.41
1:L:13:ALA:CA	1:L:154:ILE:HD11	2.48	0.41
1:C:418:THR:OG1	1:C:421:MET:HG3	2.21	0.41
1:M:150:SER:O	1:M:154:ILE:HG12	2.21	0.41
1:M:228:GLU:HG3	5:M:618:HOH:O	2.21	0.41
1:C:302:ARG:HH22	1:D:353:ARG:CZ	2.34	0.41
1:C:406:ARG:HG2	1:C:425:LEU:HD21	2.03	0.41
1:F:407:PHE:CG	1:F:417:VAL:HG22	2.56	0.41
1:G:41:ALA:HB2	1:G:75:TYR:O	2.20	0.41
1:G:418:THR:OG1	1:G:421:MET:HG3	2.21	0.41
1:B:421:MET:O	1:B:425:LEU:HD13	2.21	0.41
1:C:372[B]:TRP:CE3	1:C:389:VAL:HG13	2.56	0.41
1:I:14:ARG:HG2	1:L:14:ARG:HA	2.02	0.41
1:K:359:PHE:O	1:K:376:SER:HA	2.21	0.41
1:F:391:PRO:HG3	1:F:427:HIS:CG	2.55	0.41
1:D:125:LEU:HA	1:D:125:LEU:HD12	1.89	0.41
1:M:171:PRO:HB2	1:M:174:GLU:HG3	2.02	0.41
1:D:42:LYS:HA	1:D:45:VAL:HG23	2.03	0.41
1:E:330:LEU:HB3	1:E:346:VAL:HG22	2.03	0.41
1:F:330:LEU:HB3	1:F:346:VAL:HG22	2.01	0.41
1:I:385:ASP:OD1	1:I:386:ARG:N	2.51	0.41
1:M:125:LEU:HA	1:M:125:LEU:HD12	1.91	0.41
1:M:402:GLU:O	1:M:406:ARG:HD3	2.21	0.41
1:B:115:ARG:HG2	1:B:238:HIS:CD2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:ARG:NH2	1:C:398:GLU:HG2	2.36	0.40
1:H:203:PRO:HD3	5:H:631:HOH:O	2.21	0.40
1:I:386:ARG:NH1	2:I:501:AMP:O2P	2.54	0.40
1:N:402:GLU:O	1:N:406:ARG:HD3	2.20	0.40
1:K:10:LEU:HD22	1:K:11:MET:H	1.86	0.40
1:M:277:VAL:HG13	1:M:283:TYR:HA	2.04	0.40
1:N:406:ARG:HB3	1:N:425:LEU:HD11	2.03	0.40
1:P:421:MET:O	1:P:425:LEU:HD13	2.22	0.40
1:C:363:ASP:O	1:C:380:ARG:HA	2.22	0.40
1:H:347:GLN:O	1:H:364:SER:HA	2.22	0.40
1:L:79:THR:HG23	5:L:657:HOH:O	2.22	0.40
1:G:347:GLN:O	1:G:364:SER:HA	2.21	0.40
1:K:258:PRO:HD2	1:K:261:LEU:HD12	2.03	0.40
1:L:44:ALA:HB2	1:L:80:LEU:HB2	2.04	0.40
1:B:391:PRO:HG3	1:B:427:HIS:CG	2.56	0.40
1:B:307:ARG:HB2	1:C:95:MET:SD	2.62	0.40
1:D:363:ASP:O	1:D:380:ARG:HA	2.22	0.40
1:F:29:ARG:NH2	1:F:38:ASN:OD1	2.54	0.40
1:G:402:GLU:O	1:G:406:ARG:HD3	2.21	0.40

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%)	51	69
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%)	51	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	51	69
1	I	390/431 (90%)	377 (97%)	12 (3%)	1 (0%)	44	62
1	J	408/431 (95%)	397 (97%)	10 (2%)	1 (0%)	51	69
1	K	419/431 (97%)	410 (98%)	9 (2%)	0	100	100
1	L	408/431 (95%)	396 (97%)	11 (3%)	1 (0%)	51	69
1	M	409/431 (95%)	396 (97%)	12 (3%)	1 (0%)	51	69
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%)	55	73

All (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
1	E	74	GLN
1	I	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%)	89	95
1	B	354/373 (95%)	350 (99%)	4 (1%)	78	90
1	C	358/373 (96%)	356 (99%)	2 (1%)	89	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	343/373 (92%)	342 (100%)	1 (0%)	94	97
1	E	343/373 (92%)	339 (99%)	4 (1%)	75	89
1	F	349/373 (94%)	348 (100%)	1 (0%)	94	97
1	G	326/373 (87%)	323 (99%)	3 (1%)	82	91
1	H	328/373 (88%)	323 (98%)	5 (2%)	70	85
1	I	297/373 (80%)	293 (99%)	4 (1%)	73	88
1	J	331/373 (89%)	329 (99%)	2 (1%)	89	95
1	K	353/373 (95%)	350 (99%)	3 (1%)	85	93
1	L	341/373 (91%)	334 (98%)	7 (2%)	59	78
1	M	347/373 (93%)	343 (99%)	4 (1%)	75	89
1	N	350/373 (94%)	348 (99%)	2 (1%)	89	95
1	O	348/373 (93%)	347 (100%)	1 (0%)	94	97
1	P	354/373 (95%)	353 (100%)	1 (0%)	94	97
All	All	5479/5968 (92%)	5433 (99%)	46 (1%)	85	93

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	THR
1	A	250	GLU
1	B	86	ARG
1	B	174	GLU
1	B	201	SER
1	B	410	SER
1	C	77	SER
1	C	86	ARG
1	D	75	TYR
1	E	29	ARG
1	E	154	ILE
1	E	176	SER
1	E	326	HIS
1	F	29	ARG
1	G	355	ARG
1	G	361	ASN
1	G	425	LEU
1	H	16	LEU
1	H	173	GLU

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Mol	Chain	Res	Type
1	H	243	ASP
1	H	341	SER
1	H	379	LEU
1	I	10	LEU
1	I	35	ASP
1	I	75	TYR
1	I	79	THR
1	J	31	THR
1	J	347	GLN
1	K	125	LEU
1	K	154	ILE
1	K	277	VAL
1	L	12	LEU
1	L	29	ARG
1	L	86	ARG
1	L	168	MET
1	L	201	SER
1	L	329	THR
1	L	430	GLU
1	M	29	ARG
1	M	162	ARG
1	M	174	GLU
1	M	375	ARG
1	N	40	ARG
1	N	174	GLU
1	O	29	ARG
1	P	428	LYS

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	24,38,38	0.82	1 (4%)
3	SUC	A	502	-	24,24,24	0.46	0	36,36,36	0.70	0
2	AMP	B	501	-	22,25,25	0.68	0	24,38,38	0.88	1 (4%)
2	AMP	C	501	-	22,25,25	0.70	0	24,38,38	0.85	1 (4%)
2	AMP	D	501	-	22,25,25	0.65	0	24,38,38	0.83	1 (4%)
4	PO4	D	502	-	4,4,4	0.74	0	6,6,6	0.38	0
2	AMP	E	501	-	22,25,25	0.69	0	24,38,38	0.85	1 (4%)
3	SUC	E	502	-	24,24,24	0.46	0	36,36,36	0.70	0
2	AMP	F	501	-	22,25,25	0.62	0	24,38,38	0.82	1 (4%)
2	AMP	G	501	-	22,25,25	0.61	0	24,38,38	0.79	1 (4%)
3	SUC	G	502	-	24,24,24	0.47	0	36,36,36	0.69	0
2	AMP	H	501	-	22,25,25	0.60	0	24,38,38	0.82	1 (4%)
3	SUC	H	502	-	24,24,24	0.47	0	36,36,36	0.67	0
2	AMP	I	501	-	22,25,25	0.66	0	24,38,38	0.84	1 (4%)
3	SUC	I	502	-	24,24,24	0.46	0	36,36,36	0.70	0
2	AMP	J	501	-	22,25,25	0.68	0	24,38,38	0.83	1 (4%)
3	SUC	J	502	-	24,24,24	0.49	0	36,36,36	0.68	0
2	AMP	K	501	-	22,25,25	0.63	0	24,38,38	0.82	1 (4%)
3	SUC	K	502	-	24,24,24	0.45	0	36,36,36	0.68	0
2	AMP	L	501	-	22,25,25	0.70	0	24,38,38	0.84	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	AMP	M	501	-	22,25,25	0.65	0	24,38,38	0.82	1 (4%)
2	AMP	N	501	-	22,25,25	0.72	1 (4%)	24,38,38	0.89	1 (4%)
3	SUC	N	502	-	24,24,24	0.46	0	36,36,36	0.72	0
2	AMP	O	501	-	22,25,25	0.65	0	24,38,38	0.88	1 (4%)
2	AMP	P	501	-	22,25,25	0.72	1 (4%)	24,38,38	0.87	1 (4%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	501	AMP	P-O2P	-2.13	1.46	1.54
2	P	501	AMP	P-O2P	-2.12	1.46	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	501	AMP	P-O5'-C5'	2.33	124.72	118.30
2	G	501	AMP	P-O5'-C5'	2.55	125.32	118.30
2	I	501	AMP	P-O5'-C5'	2.65	125.59	118.30
2	P	501	AMP	P-O5'-C5'	2.69	125.70	118.30
2	E	501	AMP	P-O5'-C5'	2.75	125.86	118.30
2	L	501	AMP	P-O5'-C5'	2.75	125.86	118.30
2	M	501	AMP	P-O5'-C5'	2.78	125.95	118.30
2	C	501	AMP	P-O5'-C5'	2.79	125.99	118.30
2	A	501	AMP	P-O5'-C5'	2.80	126.02	118.30
2	D	501	AMP	P-O5'-C5'	2.81	126.04	118.30
2	H	501	AMP	P-O5'-C5'	2.82	126.06	118.30
2	K	501	AMP	P-O5'-C5'	2.82	126.07	118.30
2	F	501	AMP	P-O5'-C5'	2.91	126.32	118.30
2	N	501	AMP	P-O5'-C5'	2.92	126.33	118.30
2	B	501	AMP	P-O5'-C5'	2.96	126.46	118.30
2	O	501	AMP	P-O5'-C5'	3.00	126.56	118.30

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	422/431 (97%)	-0.34	3 (0%) 87 88	17, 25, 40, 53	0
1	B	421/431 (97%)	-0.19	4 (0%) 82 82	20, 30, 47, 62	0
1	C	421/431 (97%)	-0.32	4 (0%) 82 82	14, 22, 37, 63	0
1	D	413/431 (95%)	-0.08	5 (1%) 79 79	15, 30, 56, 65	0
1	E	411/431 (95%)	-0.06	9 (2%) 62 61	16, 33, 56, 71	0
1	F	411/431 (95%)	-0.16	4 (0%) 82 82	16, 28, 48, 61	0
1	G	411/431 (95%)	0.32	30 (7%) 16 13	23, 42, 65, 76	0
1	H	416/431 (96%)	0.29	11 (2%) 56 55	28, 48, 67, 73	0
1	I	400/431 (92%)	0.40	31 (7%) 14 11	23, 45, 77, 85	0
1	J	412/431 (95%)	0.10	14 (3%) 46 44	25, 37, 61, 76	0
1	K	421/431 (97%)	-0.10	6 (1%) 75 74	20, 34, 48, 60	0
1	L	412/431 (95%)	0.15	10 (2%) 59 58	19, 36, 62, 76	0
1	M	415/431 (96%)	-0.24	1 (0%) 94 95	14, 26, 44, 55	0
1	N	422/431 (97%)	-0.27	3 (0%) 87 88	15, 25, 45, 64	0
1	O	415/431 (96%)	-0.18	8 (1%) 67 66	16, 29, 50, 63	0
1	P	423/431 (98%)	-0.35	1 (0%) 94 95	14, 23, 38, 59	0
All	All	6646/6896 (96%)	-0.07	144 (2%) 62 61	14, 31, 60, 85	0

All (144) RSRZ outliers are listed below:

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

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Mol	Chain	Res	Type	RSRZ
1	C	74	GLN	4.1
1	I	163	CYS	3.7
1	F	104	ALA	3.6
1	E	269	ASP	3.5
1	F	206	PRO	3.5
1	B	75	TYR	3.5
1	I	245	ILE	3.5
1	L	182	ALA	3.5
1	H	393	GLY	3.4
1	J	115	ARG	3.4
1	K	206	PRO	3.2
1	K	74	GLN	3.2
1	G	396	ILE	3.2
1	I	254	ALA	3.2
1	G	400	ALA	3.1
1	G	407	PHE	3.1
1	D	232	ARG	3.0
1	H	395	VAL	3.0
1	D	29	ARG	2.9
1	G	427	HIS	2.9
1	L	183	VAL	2.9
1	I	190	ILE	2.8
1	N	185	GLU	2.8
1	G	421	MET	2.8
1	J	236	SER	2.7
1	I	75	TYR	2.7
1	G	324	GLY	2.7
1	L	190	ILE	2.7
1	G	268	PRO	2.7
1	G	390	ILE	2.7
1	O	114	TYR	2.7
1	D	206	PRO	2.6
1	G	269	ASP	2.6
1	I	194	GLU	2.6
1	C	73	THR	2.6
1	J	270	ALA	2.6
1	K	75	TYR	2.6
1	J	238	HIS	2.6
1	I	196	PRO	2.5
1	O	10	LEU	2.5
1	O	105	GLN	2.5
1	B	206	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	204	ASN	2.5
1	L	253	LEU	2.5
1	G	89	SER	2.5
1	J	235	ASN	2.5
1	H	267	ASP	2.5
1	H	359	PHE	2.5
1	A	204	ASN	2.5
1	L	232	ARG	2.5
1	H	415	VAL	2.5
1	G	372	TRP	2.5
1	I	28	GLY	2.5
1	G	397	GLY	2.4
1	J	123	GLN	2.4
1	I	232	ARG	2.4
1	G	417	VAL	2.4
1	I	218	PHE	2.4
1	J	407	PHE	2.4
1	I	168	MET	2.4
1	N	203	PRO	2.4
1	G	359	PHE	2.4
1	I	222	TYR	2.4
1	G	35	ASP	2.4
1	H	114	TYR	2.4
1	E	104	ALA	2.4
1	E	190	ILE	2.4
1	H	426	GLY	2.4
1	J	237	SER	2.3
1	G	391	PRO	2.3
1	I	119	ASP	2.3
1	E	236	SER	2.3
1	H	358	SER	2.3
1	I	187	ASP	2.3
1	B	269	ASP	2.3
1	G	323	SER	2.3
1	H	112	ASN	2.3
1	A	270	ALA	2.3
1	O	185	GLU	2.3
1	K	322	ARG	2.3
1	I	258	PRO	2.3
1	L	204	ASN	2.3
1	G	294	VAL	2.3
1	G	204	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	266	SER	2.2
1	N	268	PRO	2.2
1	L	249	THR	2.2
1	G	267	ASP	2.2
1	J	267	ASP	2.2
1	G	236	SER	2.2
1	I	206	PRO	2.2
1	I	372	TRP	2.2
1	I	212	SER	2.2
1	L	238	HIS	2.2
1	I	224	TYR	2.2
1	G	428	LYS	2.2
1	I	192	PHE	2.2
1	D	236	SER	2.2
1	G	104	ALA	2.2
1	J	401	GLU	2.2
1	C	75	TYR	2.2
1	L	206	PRO	2.2
1	I	195	LYS	2.2
1	M	225	GLU	2.2
1	G	237	SER	2.2
1	I	269	ASP	2.2
1	I	31	THR	2.2
1	I	423	ARG	2.2
1	I	268	PRO	2.1
1	I	270	ALA	2.1
1	K	93	GLU	2.1
1	I	203	PRO	2.1
1	O	158	GLU	2.1
1	E	238	HIS	2.1
1	G	238	HIS	2.1
1	J	408	TYR	2.1
1	G	394	MET	2.1
1	C	28	GLY	2.1
1	P	269	ASP	2.1
1	G	185	GLU	2.1
1	A	9	HIS	2.1
1	O	202	MET	2.1
1	G	401	GLU	2.1
1	F	431	ARG	2.1
1	E	267	ASP	2.1
1	D	197	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	208	LYS	2.0
1	G	379	LEU	2.0
1	I	9	HIS	2.0
1	E	431	ARG	2.0
1	L	322	ARG	2.0
1	E	271	GLU	2.0
1	O	183	VAL	2.0
1	E	186	ASN	2.0
1	H	269	ASP	2.0
1	J	269	ASP	2.0
1	K	324	GLY	2.0
1	O	187	ASP	2.0
1	I	180	VAL	2.0

## 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 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SUC	I	502	23/23	0.80	0.35	1.86	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	0.41	55,56,57,58	0
2	AMP	I	501	23/23	0.95	0.19	0.31	33,38,41,43	0
3	SUC	H	502	23/23	0.84	0.19	0.30	46,57,77,85	0
3	SUC	A	502	23/23	0.94	0.14	0.18	22,27,33,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
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	-0.60	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	O	501	23/23	0.96	0.13	-0.84	22,24,26,28	0
2	AMP	J	501	23/23	0.96	0.14	-0.85	28,32,34,35	0
2	AMP	C	501	23/23	0.97	0.12	-1.32	18,20,21,21	0
2	AMP	G	501	23/23	0.95	0.14	-2.01	34,40,44,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.