



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:05 am GMT

PDB ID : 5L6S  
Title : Crystal structure of E. coli ADP-glucose pyrophosphorylase (AGPase) in complex with a positive allosteric regulator beta-fructose-1,6-diphosphate (FBP) - AGPase\*FBP  
Authors : Cifuentes, J.O.; Albesa-Jove, D.; Comino, N.; Madariaga-Marcos, J.; Agirre, J.; Lopez-Fernandez, S.; Garcia-Alija, M.; Guerin, M.E.  
Deposited on : 2016-05-31  
Resolution : 3.04 Å(reported)

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

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

A user guide is available at

<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

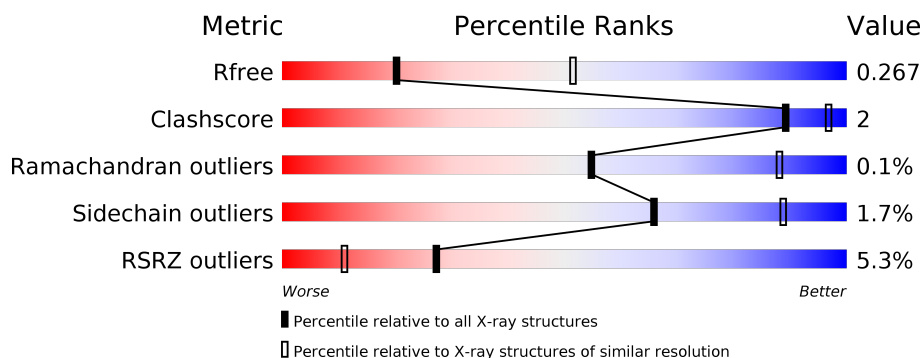
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.04 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.











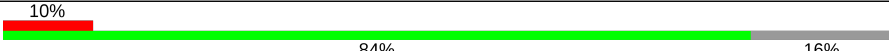
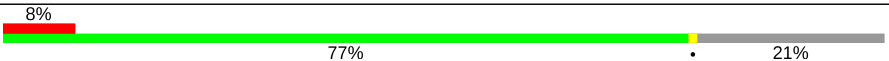
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2176 (3.08-3.00)
Clashscore	112137	2542 (3.08-3.00)
Ramachandran outliers	110173	2458 (3.08-3.00)
Sidechain outliers	110143	2461 (3.08-3.00)
RSRZ outliers	101464	2202 (3.08-3.00)

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>4%</div> <div> <div></div> <div>90%</div> <div>5%</div> </div> </div>
1	B	431	<div> <div></div> <div> <div>89%</div> <div>7%</div> <div></div> </div> </div>
1	C	431	<div> <div></div> <div> <div>88%</div> <div>8%</div> <div></div> </div> </div>
1	D	431	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>7%</div> </div> </div>
1	E	431	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>
1	F	431	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	431	
1	H	431	
1	I	431	
1	J	431	
1	K	431	
1	L	431	
1	M	431	
1	N	431	
1	O	431	
1	P	431	

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	E	501	-	-	X	-
2	SO4	F	501	-	-	X	-
2	SO4	I	501	-	-	X	-
2	SO4	J	501	-	-	X	-
2	SO4	K	503	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 45056 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	409	Total	C	N	O	S	0	0	0
			3016	1913	518	567	18			
1	B	417	Total	C	N	O	S	0	0	0
			3194	2023	563	588	20			
1	C	418	Total	C	N	O	S	0	0	0
			3283	2071	580	611	21			
1	D	402	Total	C	N	O	S	0	0	0
			2938	1849	521	550	18			
1	E	408	Total	C	N	O	S	0	0	0
			3108	1969	544	575	20			
1	F	402	Total	C	N	O	S	0	0	0
			3059	1929	541	570	19			
1	G	409	Total	C	N	O	S	0	0	0
			3144	1988	551	585	20			
1	H	408	Total	C	N	O	S	0	0	0
			3076	1955	536	565	20			
1	I	409	Total	C	N	O	S	0	0	0
			3138	1983	551	585	19			
1	J	407	Total	C	N	O	S	0	0	0
			3074	1942	536	577	19			
1	K	409	Total	C	N	O	S	0	0	0
			3115	1966	546	583	20			
1	L	415	Total	C	N	O	S	0	0	0
			3196	2020	558	598	20			
1	M	229	Total	C	N	O		0	0	0
			1185	703	242	240				
1	N	369	Total	C	N	O	S	0	0	0
			2278	1416	407	443	12			
1	O	364	Total	C	N	O	S	0	0	0
			2145	1348	385	407	5			
1	P	339	Total	C	N	O	S	0	0	0
			1832	1096	367	361	8			

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



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

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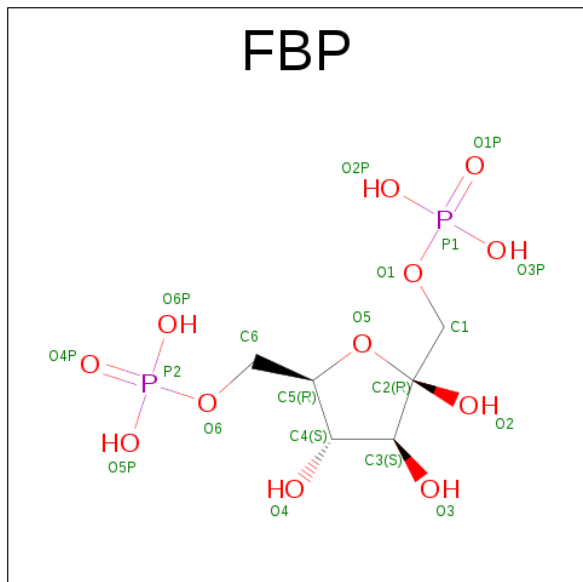
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total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

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

- Molecule 3 is BETA-FRUCTOSE-1,6-DIPHOSPHATE (three-letter code: FBP) (formula:  $C_6H_{14}O_{12}P_2$ ).

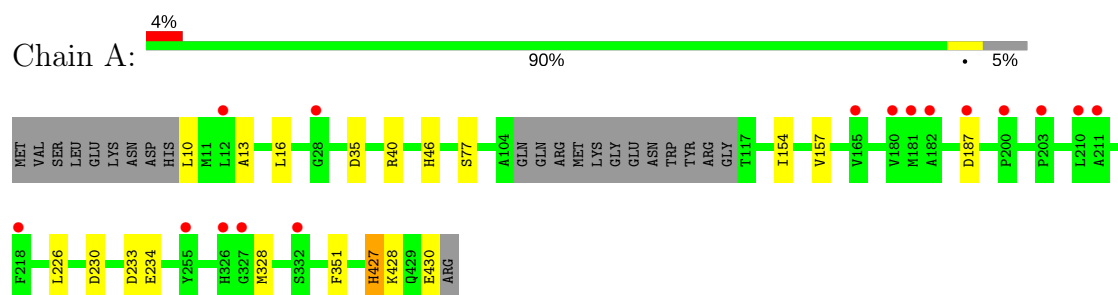


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	O	P	0	0
			20	6	12	2		
3	G	1	Total	C	O	P	0	0
			20	6	12	2		
3	I	1	Total	C	O	P	0	0
			20	6	12	2		
3	L	1	Total	C	O	P	0	0
			20	6	12	2		

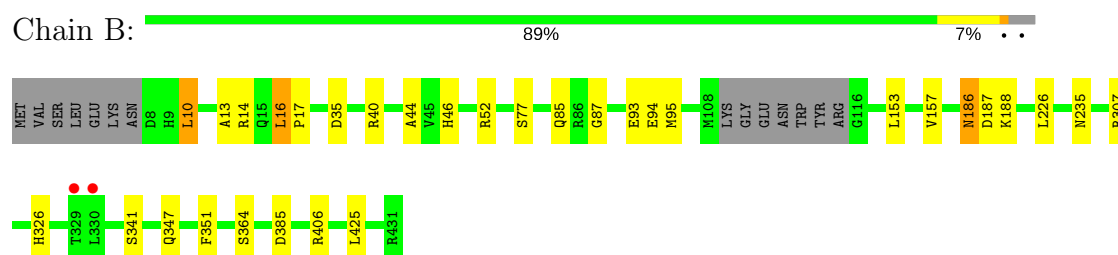
### 3 Residue-property plots [i](#)

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.

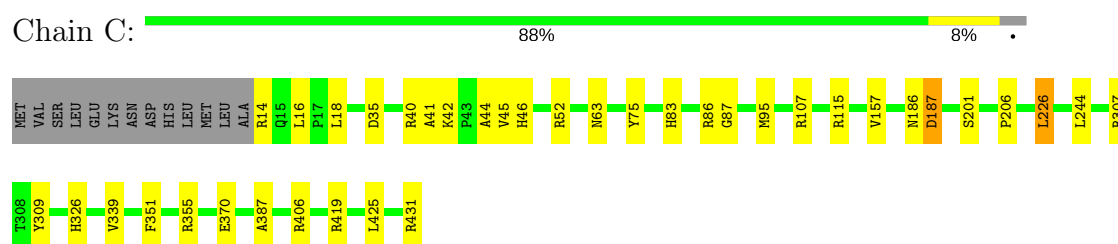
- Molecule 1: Glucose-1-phosphate adenylyltransferase



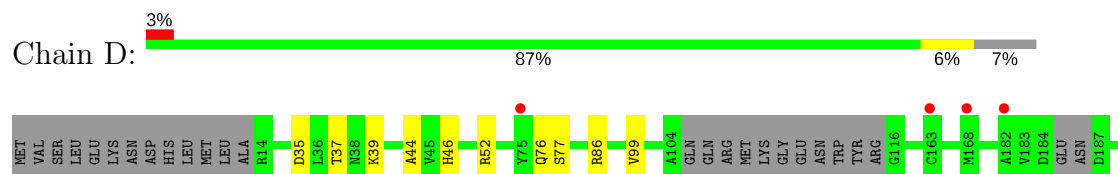
- Molecule 1: Glucose-1-phosphate adenylyltransferase



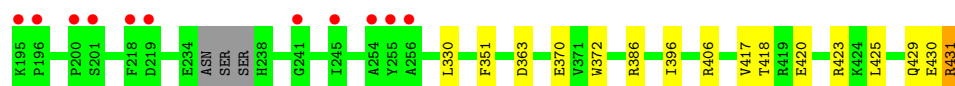
- Molecule 1: Glucose-1-phosphate adenylyltransferase



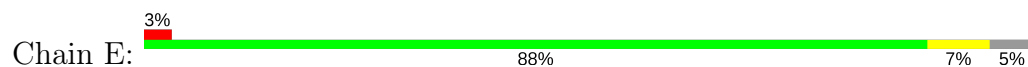
- Molecule 1: Glucose-1-phosphate adenylyltransferase



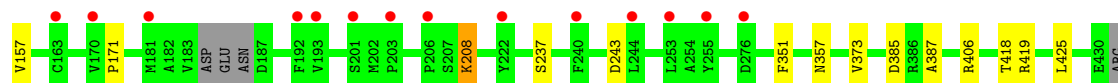
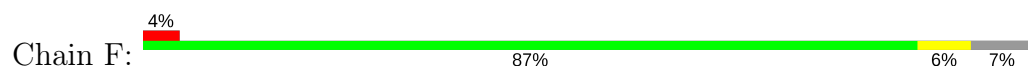




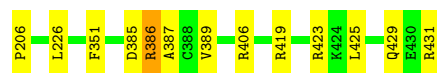
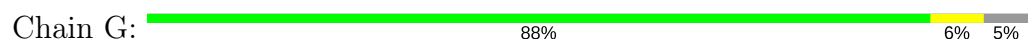
- Molecule 1: Glucose-1-phosphate adenylyltransferase



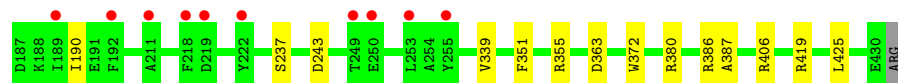
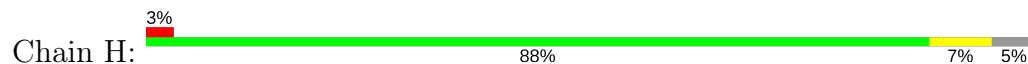
- Molecule 1: Glucose-1-phosphate adenylyltransferase



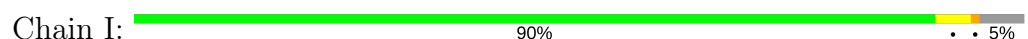
- Molecule 1: Glucose-1-phosphate adenylyltransferase

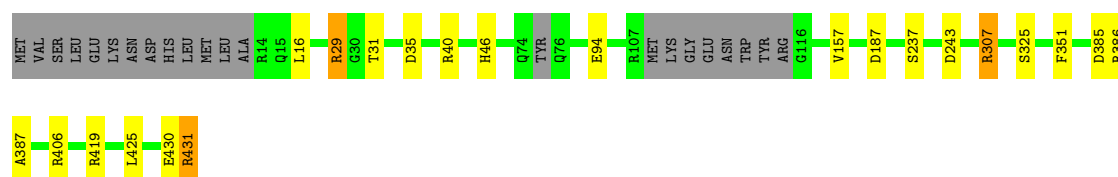


- Molecule 1: Glucose-1-phosphate adenylyltransferase

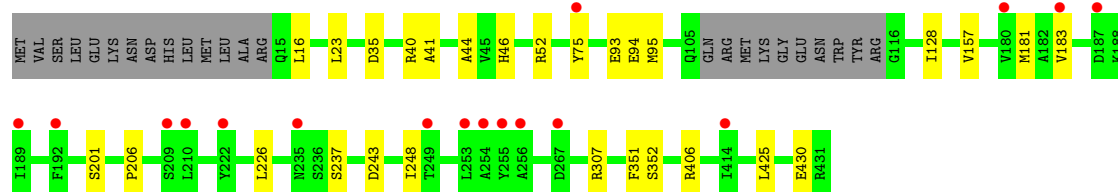
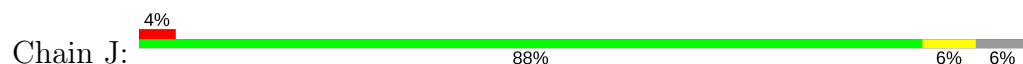


- Molecule 1: Glucose-1-phosphate adenylyltransferase

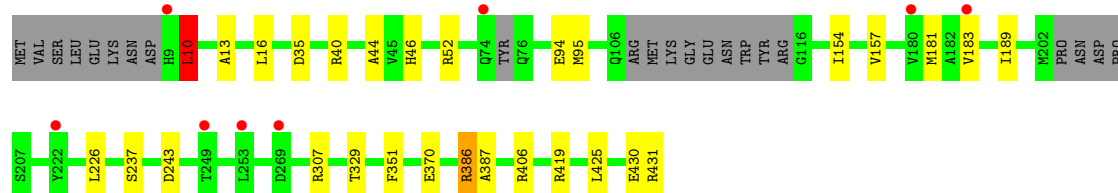




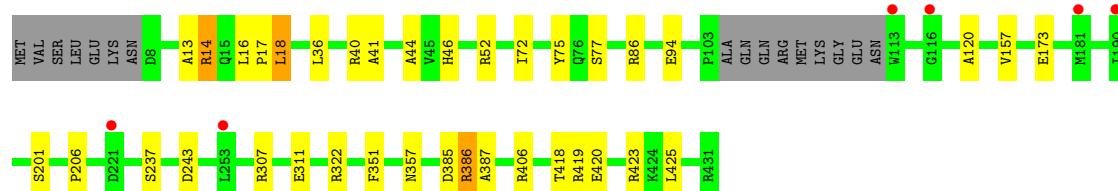
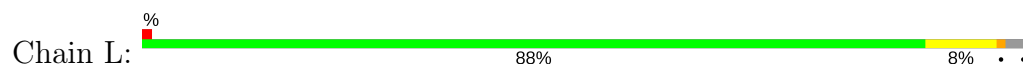
- Molecule 1: Glucose-1-phosphate adenylyltransferase



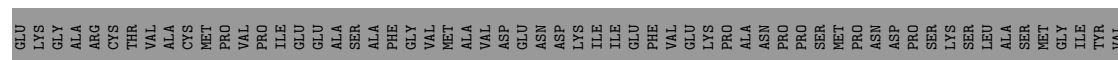
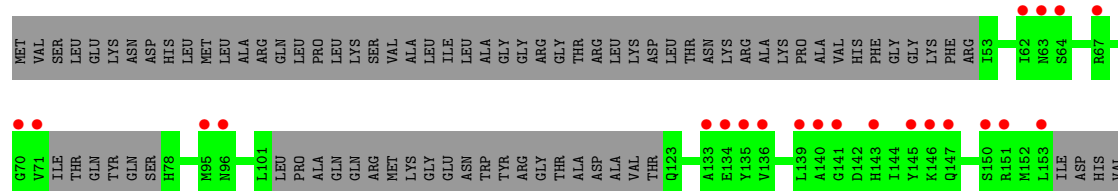
- Molecule 1: Glucose-1-phosphate adenylyltransferase

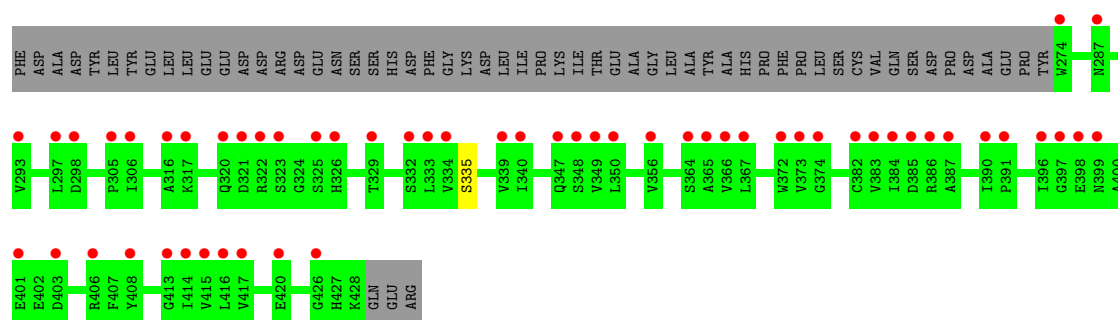


- Molecule 1: Glucose-1-phosphate adenylyltransferase

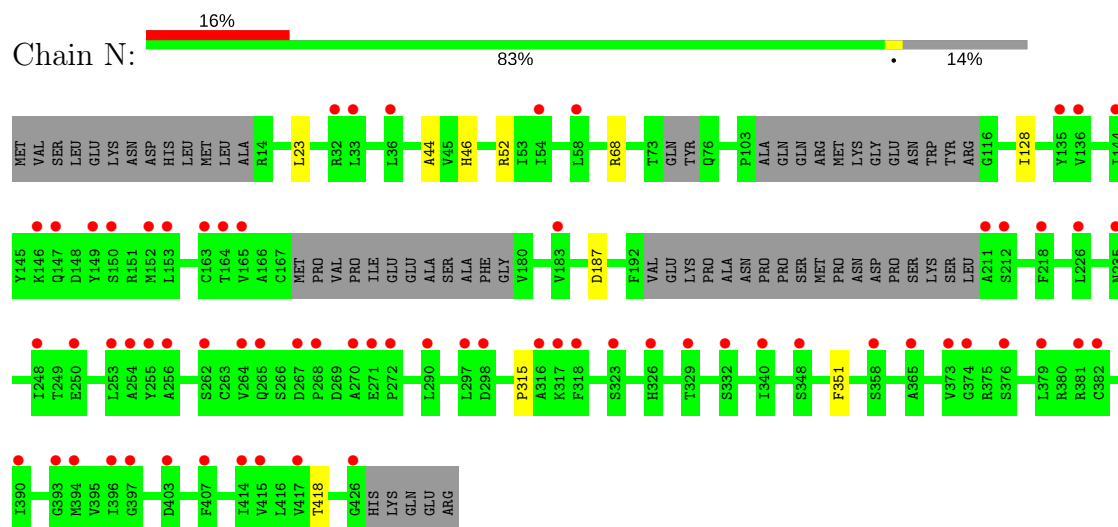


- Molecule 1: Glucose-1-phosphate adenylyltransferase

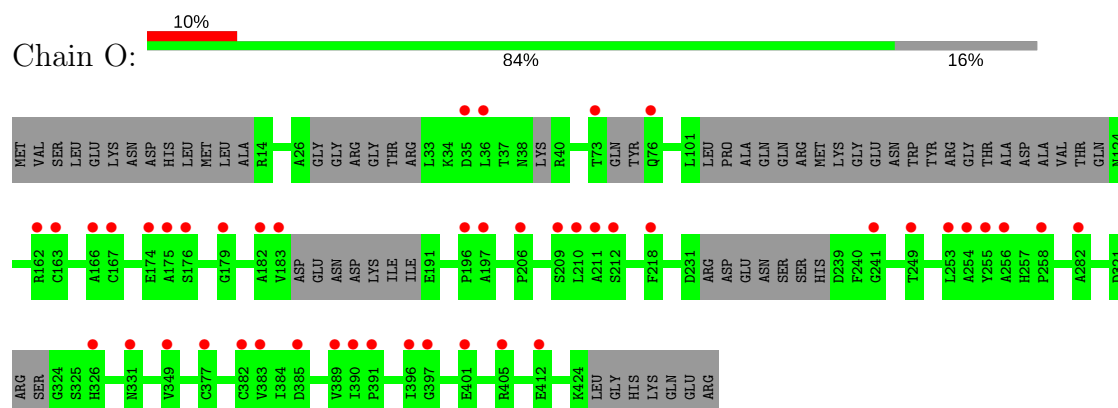




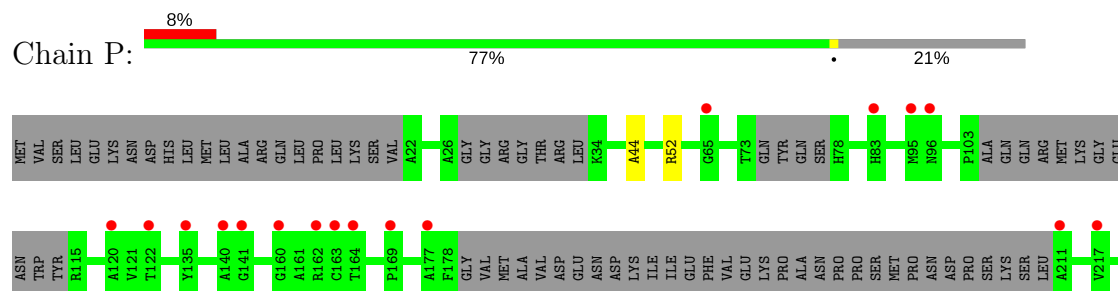
- Molecule 1: Glucose-1-phosphate adenylyltransferase

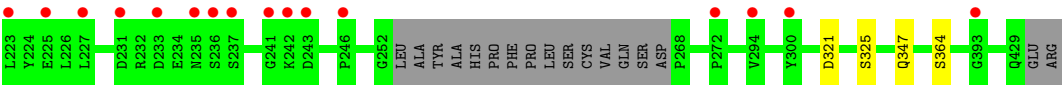


- Molecule 1: Glucose-1-phosphate adenylyltransferase



- 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, $\alpha$ , $\beta$ , $\gamma$	161.16Å 148.90Å 177.49Å 90.00° 113.10° 90.00°	Depositor
Resolution (Å)	70.75 – 3.04 70.75 – 3.04	Depositor EDS
% Data completeness (in resolution range)	98.7 (70.75-3.04) 98.6 (70.75-3.04)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 3.01Å)	Xtriage
Refinement program	PHENIX (dev_2219: ???)	Depositor
R, $R_{free}$	0.234 , 0.272 0.229 , 0.267	Depositor DCC
$R_{free}$ test set	7261 reflections (4.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	81.6	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 79.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	45056	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: FBP, 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	0.24	0/3083	0.42	0/4212
1	B	0.24	0/3261	0.42	0/4428
1	C	0.25	0/3354	0.42	0/4546
1	D	0.25	0/2997	0.43	0/4083
1	E	0.25	0/3174	0.42	0/4311
1	F	0.24	0/3121	0.42	0/4240
1	G	0.25	0/3208	0.43	1/4353 (0.0%)
1	H	0.24	0/3142	0.42	0/4276
1	I	0.25	0/3203	0.43	0/4349
1	J	0.24	0/3140	0.42	0/4277
1	K	0.25	0/3176	0.44	1/4314 (0.0%)
1	L	0.25	0/3263	0.42	0/4431
1	M	0.23	0/1186	0.43	0/1642
1	N	0.24	0/2312	0.43	0/3186
1	O	0.25	0/2186	0.42	0/3030
1	P	0.24	0/1841	0.43	0/2542
All	All	0.24	0/45647	0.43	2/62220 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	10	LEU	CA-CB-CG	7.33	132.16	115.30
1	G	10	LEU	CA-CB-CG	5.11	127.05	115.30

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	3016	0	2779	9	0
1	B	3194	0	3112	20	0
1	C	3283	0	3215	23	0
1	D	2938	0	2718	16	0
1	E	3108	0	2996	17	1
1	F	3059	0	2944	18	0
1	G	3144	0	3050	17	0
1	H	3076	0	2942	13	0
1	I	3138	0	3038	12	1
1	J	3074	0	2918	15	0
1	K	3115	0	2991	15	0
1	L	3196	0	3093	21	0
1	M	1185	0	606	1	0
1	N	2278	0	1714	4	0
1	O	2145	0	1418	0	0
1	P	1832	0	1096	3	0
2	A	15	0	0	1	0
2	B	15	0	0	1	0
2	C	15	0	0	1	0
2	D	20	0	0	1	0
2	E	15	0	0	3	0
2	F	10	0	0	3	0
2	G	15	0	0	1	0
2	H	20	0	0	0	0
2	I	15	0	0	2	0
2	J	15	0	0	2	0
2	K	15	0	0	2	0
2	L	15	0	0	2	0
2	P	10	0	0	0	0
3	C	20	0	10	0	0
3	G	20	0	10	1	0
3	I	20	0	10	0	0
3	L	20	0	10	1	0
All	All	45056	0	40670	186	1

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 2.

The worst 5 of 186 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:B:87:GLY:O	1:B:307:ARG:NH1	2.18	0.75
1:B:186:ASN:O	1:B:188:LYS:N	2.20	0.74
1:C:87:GLY:O	1:C:307:ARG:NH2	2.21	0.74
1:B:307:ARG:HB3	1:C:95:MET:HE3	1.70	0.73
1:G:36:LEU:O	1:G:40:ARG:NH1	2.21	0.73

All (1) 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)
1:E:392:GLU:OE1	1:I:325:SER:OG[2_445]	2.19	0.01

## 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	405/431 (94%)	387 (96%)	17 (4%)	1 (0%)	51	85
1	B	413/431 (96%)	397 (96%)	15 (4%)	1 (0%)	51	85
1	C	416/431 (96%)	403 (97%)	13 (3%)	0	100	100
1	D	394/431 (91%)	381 (97%)	13 (3%)	0	100	100
1	E	402/431 (93%)	388 (96%)	14 (4%)	0	100	100
1	F	394/431 (91%)	383 (97%)	11 (3%)	0	100	100
1	G	401/431 (93%)	391 (98%)	10 (2%)	0	100	100
1	H	402/431 (93%)	387 (96%)	14 (4%)	1 (0%)	51	85
1	I	403/431 (94%)	390 (97%)	13 (3%)	0	100	100
1	J	403/431 (94%)	392 (97%)	11 (3%)	0	100	100
1	K	401/431 (93%)	388 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	411/431 (95%)	396 (96%)	15 (4%)	0	100	100
1	M	221/431 (51%)	216 (98%)	5 (2%)	0	100	100
1	N	359/431 (83%)	348 (97%)	10 (3%)	1 (0%)	44	79
1	O	348/431 (81%)	338 (97%)	10 (3%)	0	100	100
1	P	327/431 (76%)	318 (97%)	9 (3%)	0	100	100
All	All	6100/6896 (88%)	5903 (97%)	193 (3%)	4 (0%)	55	88

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	187	ASP
1	A	187	ASP
1	H	76	GLN
1	N	187	ASP

### 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	296/373 (79%)	291 (98%)	5 (2%)	66	89
1	B	335/373 (90%)	327 (98%)	8 (2%)	54	83
1	C	352/373 (94%)	348 (99%)	4 (1%)	78	93
1	D	286/373 (77%)	281 (98%)	5 (2%)	66	89
1	E	322/373 (86%)	317 (98%)	5 (2%)	68	89
1	F	319/373 (86%)	315 (99%)	4 (1%)	73	91
1	G	331/373 (89%)	326 (98%)	5 (2%)	70	90
1	H	313/373 (84%)	307 (98%)	6 (2%)	62	87
1	I	330/373 (88%)	323 (98%)	7 (2%)	59	86
1	J	317/373 (85%)	311 (98%)	6 (2%)	62	87
1	K	324/373 (87%)	317 (98%)	7 (2%)	57	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	337/373 (90%)	330 (98%)	7 (2%)	59	86
1	M	19/373 (5%)	19 (100%)	0	100	100
1	N	150/373 (40%)	148 (99%)	2 (1%)	73	91
1	O	102/373 (27%)	102 (100%)	0	100	100
1	P	57/373 (15%)	57 (100%)	0	100	100
All	All	4190/5968 (70%)	4119 (98%)	71 (2%)	66	89

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	94	GLU
1	H	190	ILE
1	L	173	GLU
1	G	187	ASP
1	H	35	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	78	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

43 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	A	501	-	4,4,4	0.15	0	6,6,6	0.08	0
2	SO4	A	502	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	B	501	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	502	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	503	-	4,4,4	0.12	0	6,6,6	0.08	0
2	SO4	C	501	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	C	502	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	C	503	-	4,4,4	0.14	0	6,6,6	0.07	0
3	FBP	C	504	-	18,20,20	0.52	0	23,32,32	0.74	0
2	SO4	D	501	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	D	502	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	D	503	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	D	504	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	E	501	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	E	502	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	E	503	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	F	501	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	F	502	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	G	501	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	G	502	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	G	503	-	4,4,4	0.15	0	6,6,6	0.11	0
3	FBP	G	504	-	18,20,20	0.40	0	23,32,32	0.80	1 (4%)
2	SO4	H	501	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	H	502	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	H	503	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	H	504	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	I	501	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	I	502	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	I	503	-	4,4,4	0.15	0	6,6,6	0.06	0
3	FBP	I	504	-	18,20,20	0.41	0	23,32,32	0.78	1 (4%)
2	SO4	J	501	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	J	502	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	J	503	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	K	501	-	4,4,4	0.14	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	K	502	-	4,4,4	0.16	0	6,6,6	0.06	0
2	SO4	K	503	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	L	501	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	L	502	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	L	503	-	4,4,4	0.13	0	6,6,6	0.07	0
3	FBP	L	504	-	18,20,20	0.53	0	23,32,32	0.81	0
2	SO4	P	501	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	P	502	-	4,4,4	0.13	0	6,6,6	0.09	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	SO4	A	501	-	-	0/0/0/0	0/0/0/0
2	SO4	A	502	-	-	0/0/0/0	0/0/0/0
2	SO4	A	503	-	-	0/0/0/0	0/0/0/0
2	SO4	B	501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	502	-	-	0/0/0/0	0/0/0/0
2	SO4	B	503	-	-	0/0/0/0	0/0/0/0
2	SO4	C	501	-	-	0/0/0/0	0/0/0/0
2	SO4	C	502	-	-	0/0/0/0	0/0/0/0
2	SO4	C	503	-	-	0/0/0/0	0/0/0/0
3	FBP	C	504	-	-	0/13/32/32	0/1/1/1
2	SO4	D	501	-	-	0/0/0/0	0/0/0/0
2	SO4	D	502	-	-	0/0/0/0	0/0/0/0
2	SO4	D	503	-	-	0/0/0/0	0/0/0/0
2	SO4	D	504	-	-	0/0/0/0	0/0/0/0
2	SO4	E	501	-	-	0/0/0/0	0/0/0/0
2	SO4	E	502	-	-	0/0/0/0	0/0/0/0
2	SO4	E	503	-	-	0/0/0/0	0/0/0/0
2	SO4	F	501	-	-	0/0/0/0	0/0/0/0
2	SO4	F	502	-	-	0/0/0/0	0/0/0/0
2	SO4	G	501	-	-	0/0/0/0	0/0/0/0
2	SO4	G	502	-	-	0/0/0/0	0/0/0/0
2	SO4	G	503	-	-	0/0/0/0	0/0/0/0
3	FBP	G	504	-	-	0/13/32/32	0/1/1/1
2	SO4	H	501	-	-	0/0/0/0	0/0/0/0
2	SO4	H	502	-	-	0/0/0/0	0/0/0/0
2	SO4	H	503	-	-	0/0/0/0	0/0/0/0
2	SO4	H	504	-	-	0/0/0/0	0/0/0/0
2	SO4	I	501	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	I	502	-	-	0/0/0/0	0/0/0/0
2	SO4	I	503	-	-	0/0/0/0	0/0/0/0
3	FBP	I	504	-	-	0/13/32/32	0/1/1/1
2	SO4	J	501	-	-	0/0/0/0	0/0/0/0
2	SO4	J	502	-	-	0/0/0/0	0/0/0/0
2	SO4	J	503	-	-	0/0/0/0	0/0/0/0
2	SO4	K	501	-	-	0/0/0/0	0/0/0/0
2	SO4	K	502	-	-	0/0/0/0	0/0/0/0
2	SO4	K	503	-	-	0/0/0/0	0/0/0/0
2	SO4	L	501	-	-	0/0/0/0	0/0/0/0
2	SO4	L	502	-	-	0/0/0/0	0/0/0/0
2	SO4	L	503	-	-	0/0/0/0	0/0/0/0
3	FBP	L	504	-	-	0/13/32/32	0/1/1/1
2	SO4	P	501	-	-	0/0/0/0	0/0/0/0
2	SO4	P	502	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	504	FBP	P2-O6-C6	2.16	124.23	118.30
3	G	504	FBP	P2-O6-C6	2.22	124.42	118.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	SO4	1	0
2	B	503	SO4	1	0
2	C	502	SO4	1	0
2	D	503	SO4	1	0
2	E	501	SO4	3	0
2	F	501	SO4	3	0
2	G	501	SO4	1	0
3	G	504	FBP	1	0
2	I	501	SO4	2	0
2	J	501	SO4	2	0
2	K	503	SO4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	501	SO4	1	0
2	L	502	SO4	1	0
3	L	504	FBP	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	409/431 (94%)	0.11	16 (3%) 40 17	59, 96, 145, 179	0
1	B	417/431 (96%)	-0.24	2 (0%) 90 74	44, 78, 119, 152	0
1	C	418/431 (96%)	-0.33	0 100 100	25, 53, 97, 129	0
1	D	402/431 (93%)	0.02	15 (3%) 42 18	24, 75, 160, 187	0
1	E	408/431 (94%)	0.08	12 (2%) 52 24	39, 90, 166, 193	0
1	F	402/431 (93%)	0.10	16 (3%) 39 17	44, 84, 155, 187	0
1	G	409/431 (94%)	-0.22	1 (0%) 94 86	35, 69, 113, 136	0
1	H	408/431 (94%)	0.06	13 (3%) 48 22	31, 84, 148, 180	0
1	I	409/431 (94%)	-0.19	0 100 100	36, 68, 113, 154	0
1	J	407/431 (94%)	0.14	17 (4%) 37 16	41, 88, 156, 179	0
1	K	409/431 (94%)	-0.07	8 (1%) 65 36	32, 78, 130, 170	0
1	L	415/431 (96%)	-0.16	6 (1%) 75 49	30, 67, 124, 168	0
1	M	229/431 (53%)	1.60	78 (34%) 0 0	120, 197, 256, 270	0
1	N	369/431 (85%)	0.84	68 (18%) 1 0	85, 153, 207, 239	0
1	O	364/431 (84%)	0.51	45 (12%) 4 1	70, 147, 196, 211	0
1	P	339/431 (78%)	0.47	33 (9%) 8 3	67, 141, 202, 244	0
All	All	6214/6896 (90%)	0.12	330 (5%) 27 11	24, 89, 186, 270	0

The worst 5 of 330 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	383	VAL	8.6
1	P	237	SER	7.4
1	M	416	LEU	7.2
1	M	366	VAL	7.1
1	O	253	LEU	6.7

## 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	FBP	G	504	20/20	0.82	0.34	1.90	72,152,203,206	0
3	FBP	L	504	20/20	0.82	0.33	1.63	81,139,188,189	0
3	FBP	C	504	20/20	0.89	0.24	0.61	67,122,166,185	0
2	SO4	A	502	5/5	0.97	0.20	0.60	77,81,104,117	0
2	SO4	C	502	5/5	0.98	0.23	0.48	61,62,68,76	0
3	FBP	I	504	20/20	0.78	0.25	0.40	79,138,171,209	0
2	SO4	A	503	5/5	0.89	0.27	0.37	95,124,132,170	0
2	SO4	K	503	5/5	0.91	0.19	0.05	73,89,109,110	0
2	SO4	I	502	5/5	0.93	0.18	-0.30	69,80,89,98	0
2	SO4	B	503	5/5	0.96	0.19	-0.60	69,81,88,100	0
2	SO4	H	502	5/5	0.99	0.15	-0.66	42,46,49,52	0
2	SO4	L	503	5/5	0.95	0.15	-0.85	77,79,96,100	0
2	SO4	E	503	5/5	0.94	0.13	-0.92	96,97,118,122	0
2	SO4	L	501	5/5	0.99	0.18	-0.95	55,63,82,97	0
2	SO4	G	502	5/5	0.96	0.10	-1.04	79,79,104,106	0
2	SO4	E	502	5/5	0.98	0.12	-1.07	43,62,69,82	0
2	SO4	D	501	5/5	0.99	0.14	-1.18	33,41,44,47	0
2	SO4	I	503	5/5	0.93	0.15	-1.22	66,66,117,120	0
2	SO4	I	501	5/5	0.97	0.22	-1.28	58,62,89,97	0
2	SO4	B	502	5/5	0.94	0.12	-1.41	75,97,117,126	0
2	SO4	D	503	5/5	0.97	0.15	-1.42	60,80,95,96	0
2	SO4	P	502	5/5	0.86	0.20	-1.68	79,82,137,151	0
2	SO4	C	501	5/5	0.97	0.14	-1.68	53,73,81,108	0
2	SO4	C	503	5/5	0.98	0.15	-1.70	47,52,61,80	0
2	SO4	G	503	5/5	0.97	0.12	-1.74	48,60,70,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	J	502	5/5	0.97	0.08	-1.78	67,71,96,129	0
2	SO4	B	501	5/5	0.95	0.08	-1.86	102,128,135,146	0
2	SO4	L	502	5/5	0.99	0.15	-2.05	37,40,48,54	0
2	SO4	D	502	5/5	0.95	0.11	-2.06	83,105,110,111	0
2	SO4	K	501	5/5	0.93	0.09	-2.07	112,117,131,144	0
2	SO4	K	502	5/5	0.97	0.11	-2.32	62,73,85,93	0
2	SO4	J	501	5/5	0.98	0.12	-2.41	70,73,88,90	0
2	SO4	F	502	5/5	0.95	0.11	-2.42	67,68,94,100	0
2	SO4	H	501	5/5	0.94	0.12	-2.44	74,95,102,105	0
2	SO4	H	504	5/5	0.98	0.14	-2.70	60,61,81,113	0
2	SO4	P	501	5/5	0.95	0.09	-2.86	66,92,123,145	0
2	SO4	F	501	5/5	0.94	0.16	-2.88	77,78,105,111	0
2	SO4	E	501	5/5	0.97	0.14	-3.25	71,72,88,120	0
2	SO4	A	501	5/5	0.93	0.14	-3.32	92,101,111,132	0
2	SO4	G	501	5/5	0.99	0.10	-11.76	57,72,80,85	0
2	SO4	H	503	5/5	0.97	0.17	-	70,72,87,98	0
2	SO4	J	503	5/5	0.79	0.18	-	117,132,142,157	0
2	SO4	D	504	5/5	0.91	0.26	-	77,84,97,116	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.