



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 10, 2017 – 09:45 AM EDT

PDB ID : 5E84  
Title : ATP-bound state of BiP  
Authors : Liu, Q.; Yang, J.; Nune, M.; Zong, Y.; Zhou, L.  
Deposited on : unknown  
Resolution : 2.99 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.

---

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 : rb-20029824  
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) : rb-20029824

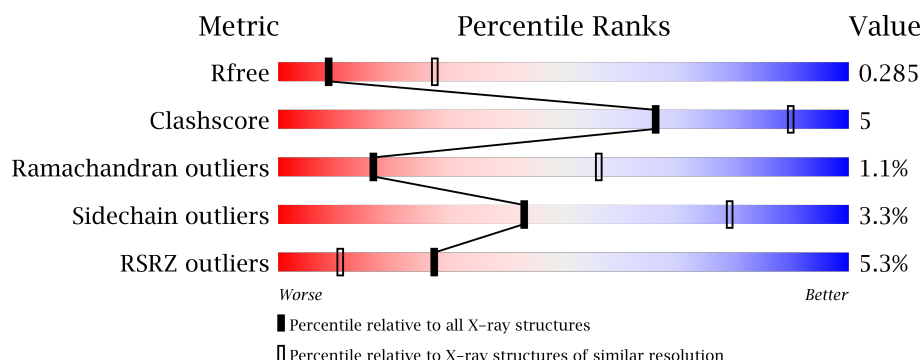
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	606	<div> <div>4%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	B	606	<div> <div>7%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
1	C	606	<div> <div>7%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	D	606	<div> <div>4%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	E	606	<div> <div>5%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	606	

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
4	MG	A	805	-	-	-	X
4	MG	D	804	-	-	X	-
5	SO4	A	808	-	-	X	-
5	SO4	C	806	-	-	X	-
5	SO4	D	808	-	-	X	-
5	SO4	E	806	-	-	X	-
5	SO4	F	806	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28484 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 78 kDa glucose-regulated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	606	Total	C	N	O	S	8	0	0
			4710	2955	806	938	11			
1	B	606	Total	C	N	O	S	8	0	0
			4700	2948	806	935	11			
1	C	606	Total	C	N	O	S	8	0	0
			4700	2948	806	935	11			
1	D	606	Total	C	N	O	S	8	0	0
			4700	2948	806	935	11			
1	E	606	Total	C	N	O	S	8	0	0
			4696	2945	805	935	11			
1	F	606	Total	C	N	O	S	8	0	0
			4700	2948	806	935	11			

There are 54 discrepancies between the modelled and reference sequences:

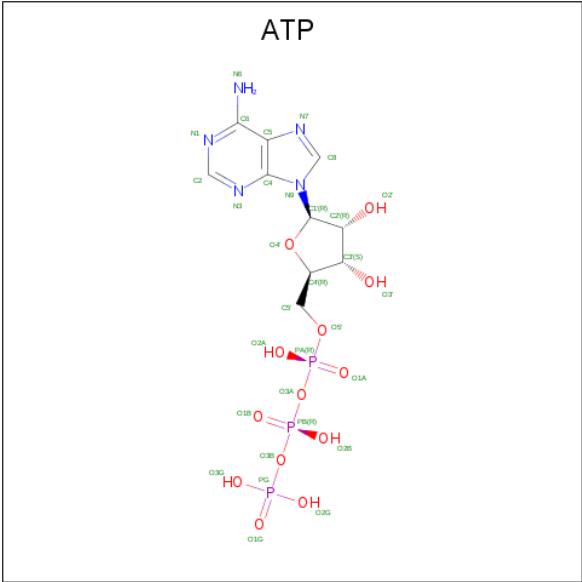
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	SER	-	expression tag	UNP P11021
A	229	ALA	THR	conflict	UNP P11021
A	?	-	THR	deletion	UNP P11021
A	?	-	ALA	deletion	UNP P11021
A	?	-	SER	deletion	UNP P11021
A	?	-	ASP	deletion	UNP P11021
A	453	VAL	ASN	conflict	UNP P11021
A	454	GLY	GLN	conflict	UNP P11021
A	455	GLY	PRO	conflict	UNP P11021
B	24	SER	-	expression tag	UNP P11021
B	229	ALA	THR	conflict	UNP P11021
B	?	-	THR	deletion	UNP P11021
B	?	-	ALA	deletion	UNP P11021
B	?	-	SER	deletion	UNP P11021
B	?	-	ASP	deletion	UNP P11021
B	453	VAL	ASN	conflict	UNP P11021
B	454	GLY	GLN	conflict	UNP P11021

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	455	GLY	PRO	conflict	UNP P11021
C	24	SER	-	expression tag	UNP P11021
C	229	ALA	THR	conflict	UNP P11021
C	?	-	THR	deletion	UNP P11021
C	?	-	ALA	deletion	UNP P11021
C	?	-	SER	deletion	UNP P11021
C	?	-	ASP	deletion	UNP P11021
C	453	VAL	ASN	conflict	UNP P11021
C	454	GLY	GLN	conflict	UNP P11021
C	455	GLY	PRO	conflict	UNP P11021
D	24	SER	-	expression tag	UNP P11021
D	229	ALA	THR	conflict	UNP P11021
D	?	-	THR	deletion	UNP P11021
D	?	-	ALA	deletion	UNP P11021
D	?	-	SER	deletion	UNP P11021
D	?	-	ASP	deletion	UNP P11021
D	453	VAL	ASN	conflict	UNP P11021
D	454	GLY	GLN	conflict	UNP P11021
D	455	GLY	PRO	conflict	UNP P11021
E	24	SER	-	expression tag	UNP P11021
E	229	ALA	THR	conflict	UNP P11021
E	?	-	THR	deletion	UNP P11021
E	?	-	ALA	deletion	UNP P11021
E	?	-	SER	deletion	UNP P11021
E	?	-	ASP	deletion	UNP P11021
E	453	VAL	ASN	conflict	UNP P11021
E	454	GLY	GLN	conflict	UNP P11021
E	455	GLY	PRO	conflict	UNP P11021
F	24	SER	-	expression tag	UNP P11021
F	229	ALA	THR	conflict	UNP P11021
F	?	-	THR	deletion	UNP P11021
F	?	-	ALA	deletion	UNP P11021
F	?	-	SER	deletion	UNP P11021
F	?	-	ASP	deletion	UNP P11021
F	453	VAL	ASN	conflict	UNP P11021
F	454	GLY	GLN	conflict	UNP P11021
F	455	GLY	PRO	conflict	UNP P11021

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

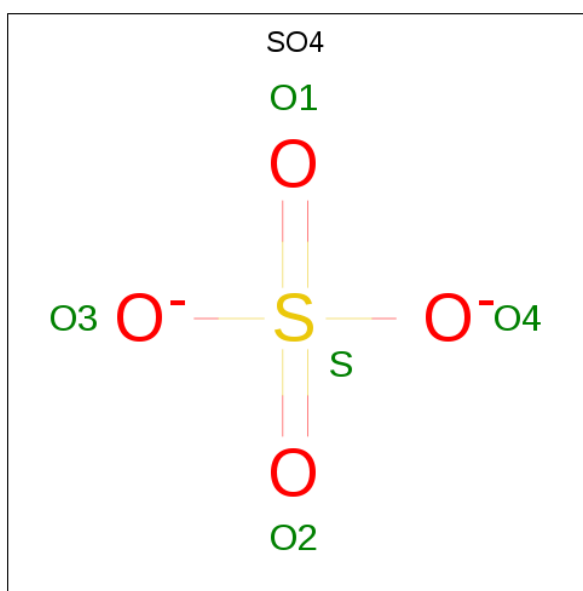
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	3	Total	Zn	0	0
			3	3		
3	E	3	Total	Zn	0	0
			3	3		
3	B	3	Total	Zn	0	0
			3	3		
3	C	3	Total	Zn	0	0
			3	3		
3	A	3	Total	Zn	0	0
			3	3		
3	F	3	Total	Zn	0	0
			3	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total	Mg	0	0
			3	3		
4	E	1	Total	Mg	0	0
			1	1		
4	B	3	Total	Mg	0	0
			3	3		
4	C	1	Total	Mg	0	0
			1	1		
4	A	3	Total	Mg	0	0
			3	3		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

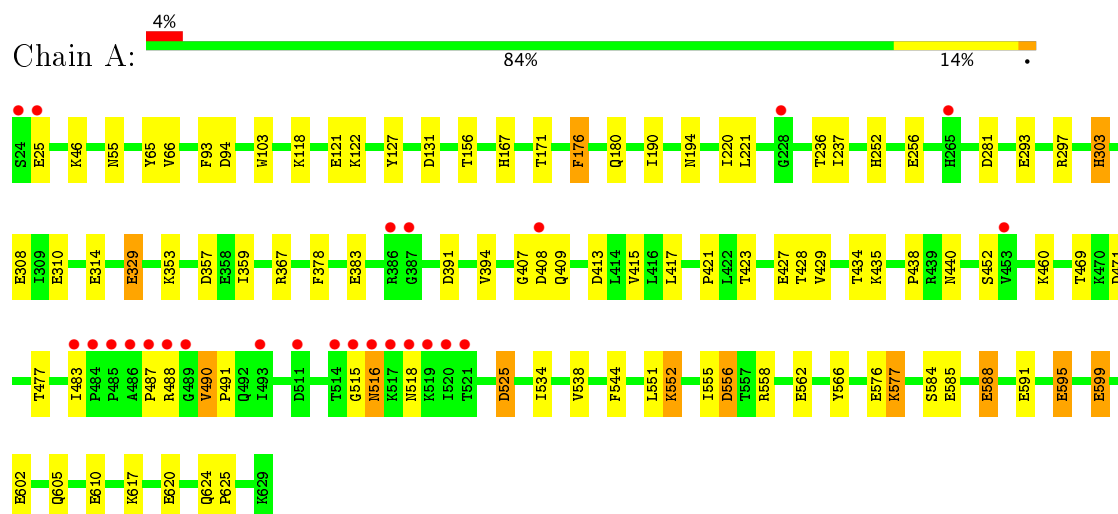
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	5	Total	O	0	0
			5	5		
6	C	4	Total	O	0	0
			4	4		
6	D	4	Total	O	0	0
			4	4		
6	E	9	Total	O	0	0
			9	9		
6	F	3	Total	O	0	0
			3	3		



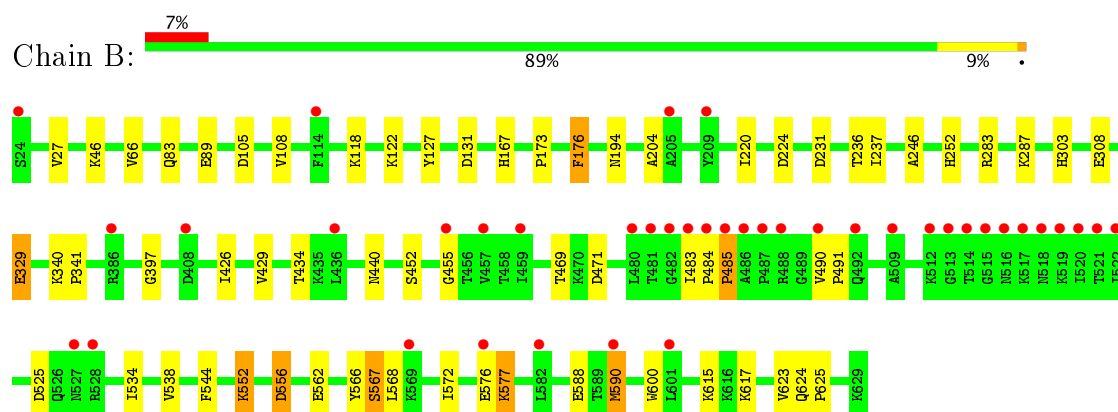
### 3 Residue-property plots

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.

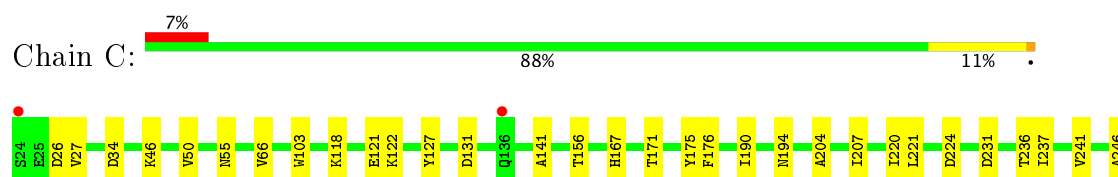
- Molecule 1: 78 kDa glucose-regulated protein

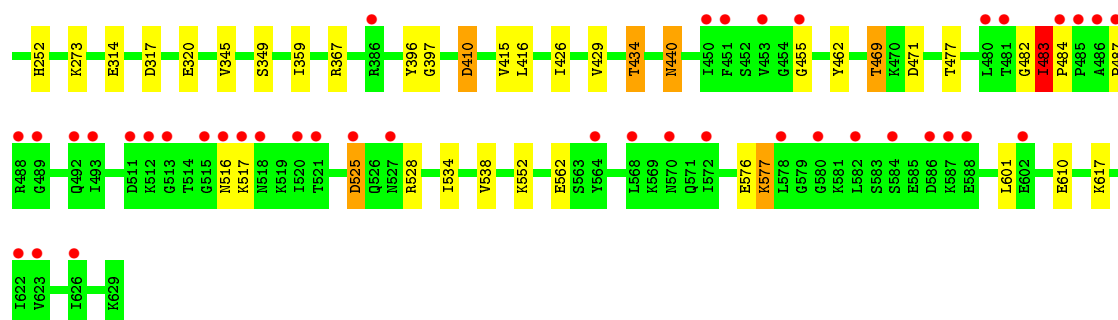


- Molecule 1: 78 kDa glucose-regulated protein

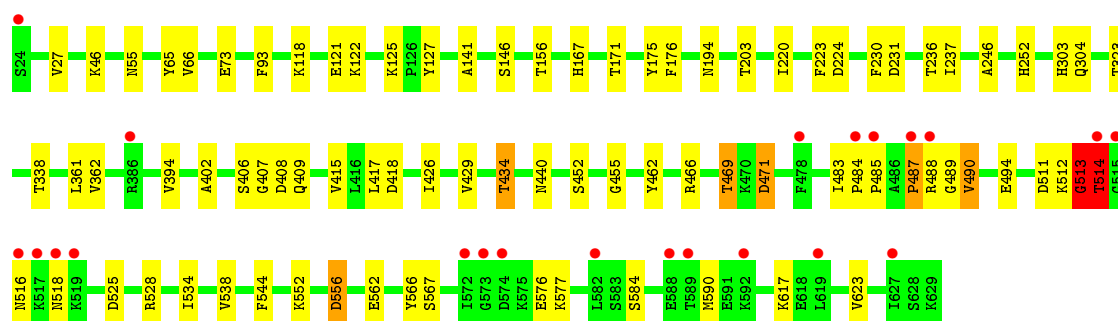
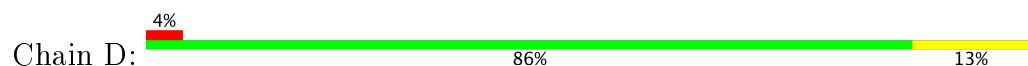


- Molecule 1: 78 kDa glucose-regulated protein

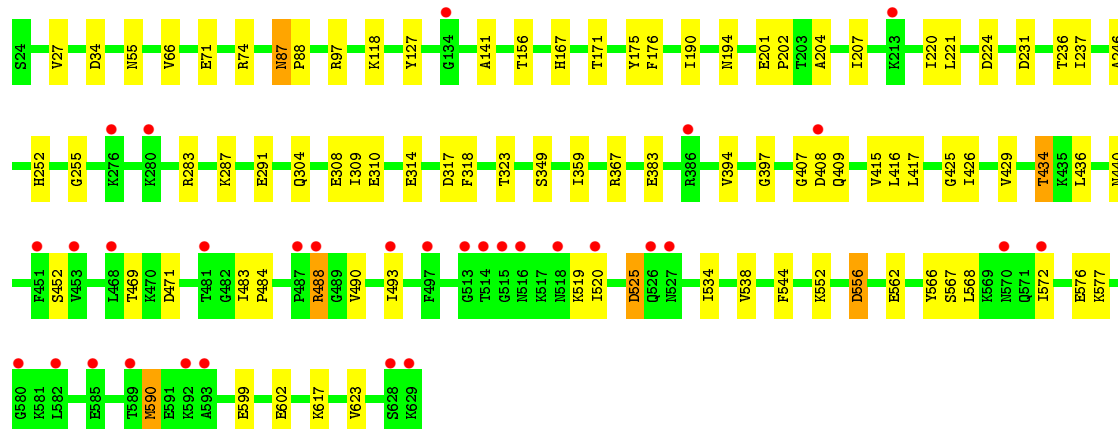
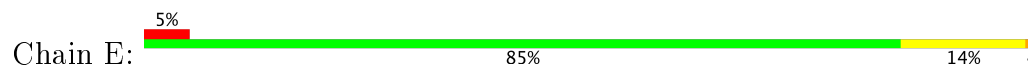




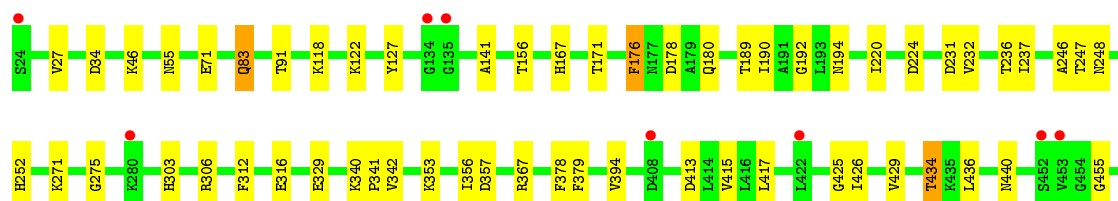
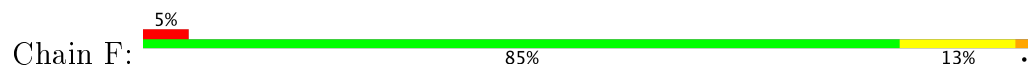
- Molecule 1: 78 kDa glucose-regulated protein

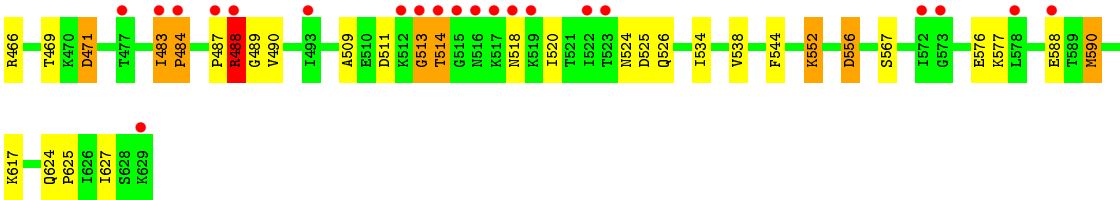


- Molecule 1: 78 kDa glucose-regulated protein



- Molecule 1: 78 kDa glucose-regulated protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	222.47Å 222.47Å 209.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.76 – 2.99 39.65 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.6 (40.76-2.99) 97.6 (39.65-2.99)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.42 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.243 , 0.287 0.241 , 0.285	Depositor DCC
$R_{free}$ test set	5907 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.3	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.309 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	28484	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: MG, ZN, ATP, 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	0.75	9/4777 (0.2%)	0.86	7/6446 (0.1%)
1	B	0.60	4/4767 (0.1%)	0.73	5/6432 (0.1%)
1	C	0.56	1/4767 (0.0%)	0.71	2/6432 (0.0%)
1	D	0.67	3/4767 (0.1%)	0.78	8/6432 (0.1%)
1	E	0.66	1/4763 (0.0%)	0.73	4/6428 (0.1%)
1	F	0.61	3/4767 (0.1%)	0.75	6/6432 (0.1%)
All	All	0.65	21/28608 (0.1%)	0.76	32/38602 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	3
1	D	2	2
1	F	0	3
All	All	2	9

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	576	GLU	CB-CG	25.85	2.01	1.52
1	D	577	LYS	CB-CG	-17.80	1.04	1.52
1	F	577	LYS	CB-CG	-13.61	1.15	1.52
1	B	577	LYS	CB-CG	-13.20	1.17	1.52
1	D	576	GLU	CB-CG	-12.78	1.27	1.52

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	556	ASP	CB-CG-OD1	11.50	128.65	118.30
1	A	556	ASP	CB-CG-OD1	11.41	128.57	118.30
1	D	577	LYS	CA-CB-CG	9.73	134.82	113.40
1	A	599	GLU	OE1-CD-OE2	-9.65	111.72	123.30
1	E	576	GLU	CA-CB-CG	-9.10	93.39	113.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	488	ARG	CA
1	D	514	THR	CA

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	488	ARG	Peptide
1	C	482	GLY	Peptide
1	C	483	ILE	Peptide
1	C	484	PRO	Peptide
1	D	487	PRO	Peptide

## 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	4710	0	4736	47	4
1	B	4700	0	4713	33	2
1	C	4700	0	4713	37	1
1	D	4700	0	4713	52	0
1	E	4696	0	4702	51	4
1	F	4700	0	4713	58	1
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
2	D	31	0	12	1	0
2	E	31	0	12	1	0
2	F	31	0	12	1	0
3	A	3	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
4	A	3	0	0	1	2
4	B	3	0	0	0	0
4	C	1	0	0	0	1
4	D	3	0	0	0	2
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	5	0	0	6	0
5	B	5	0	0	1	0
5	C	5	0	0	6	0
5	D	5	0	0	5	0
5	E	5	0	0	7	0
5	F	5	0	0	5	0
6	A	7	0	0	2	0
6	B	5	0	0	4	1
6	C	4	0	0	0	0
6	D	4	0	0	1	0
6	E	9	0	0	3	0
6	F	3	0	0	1	0
All	All	28484	0	28362	262	12

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 5.

The worst 5 of 262 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:D:303:HIS:ND1	1:F:556:ASP:OD1	1.97	0.95
1:D:556:ASP:OD2	1:F:303:HIS:CE1	2.26	0.89
1:B:552:LYS:HE2	1:B:556:ASP:OD2	1.75	0.87
1:D:556:ASP:OD2	1:F:303:HIS:ND1	2.12	0.82
1:A:415:VAL:HG11	1:D:417:LEU:HD21	1.63	0.81

The worst 5 of 12 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:317:ASP:OD2	4:D:804:MG:MG[6_654]	1.44	0.76
4:A:803:MG:MG	4:C:803:MG:MG[2_554]	1.48	0.72
1:C:317:ASP:OD2	4:A:804:MG:MG[6_554]	1.50	0.70
1:A:303:HIS:ND1	1:A:556:ASP:OD1[6_554]	1.54	0.66
1:A:595:GLU:OE2	1:A:595:GLU:OE2[5_554]	1.62	0.58

## 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	604/606 (100%)	566 (94%)	29 (5%)	9 (2%)	12	48
1	B	604/606 (100%)	569 (94%)	32 (5%)	3 (0%)	32	74
1	C	604/606 (100%)	562 (93%)	36 (6%)	6 (1%)	18	59
1	D	604/606 (100%)	561 (93%)	34 (6%)	9 (2%)	12	48
1	E	604/606 (100%)	560 (93%)	38 (6%)	6 (1%)	18	59
1	F	604/606 (100%)	564 (93%)	32 (5%)	8 (1%)	14	51
All	All	3624/3636 (100%)	3382 (93%)	201 (6%)	41 (1%)	17	56

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	408	ASP
1	A	516	ASN
1	C	483	ILE
1	C	517	LYS
1	D	408	ASP

### 5.3.2 Protein sidechains [i](#)

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



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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	515/518 (99%)	498 (97%)	17 (3%)	43	79
1	B	511/518 (99%)	495 (97%)	16 (3%)	45	80
1	C	511/518 (99%)	490 (96%)	21 (4%)	35	73
1	D	511/518 (99%)	494 (97%)	17 (3%)	43	79
1	E	510/518 (98%)	495 (97%)	15 (3%)	48	82
1	F	511/518 (99%)	495 (97%)	16 (3%)	45	80
All	All	3069/3108 (99%)	2967 (97%)	102 (3%)	43	79

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	471	ASP
1	D	146	SER
1	F	434	THR
1	C	483	ILE
1	C	577	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	167	HIS
1	C	194	ASN
1	E	492	GLN
1	B	194	ASN
1	E	167	HIS

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 30 are monoatomic - leaving 12 for Mogul analysis.

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	ATP	A	801	3	27,33,33	0.92	1 (3%)	25,52,52	2.05	6 (24%)
5	SO4	A	808	-	4,4,4	0.48	0	6,6,6	0.37	0
2	ATP	B	801	3	27,33,33	0.89	1 (3%)	25,52,52	1.90	5 (20%)
5	SO4	B	808	-	4,4,4	0.48	0	6,6,6	0.41	0
2	ATP	C	801	3	27,33,33	0.87	1 (3%)	25,52,52	2.12	5 (20%)
5	SO4	C	806	-	4,4,4	0.37	0	6,6,6	0.35	0
2	ATP	D	801	3	27,33,33	0.82	1 (3%)	25,52,52	1.87	4 (16%)
5	SO4	D	808	-	4,4,4	0.46	0	6,6,6	0.26	0
2	ATP	E	801	3	27,33,33	1.05	1 (3%)	25,52,52	1.81	4 (16%)
5	SO4	E	806	-	4,4,4	0.45	0	6,6,6	0.54	0
2	ATP	F	801	3	27,33,33	1.18	2 (7%)	25,52,52	1.77	5 (20%)
5	SO4	F	806	-	4,4,4	0.42	0	6,6,6	0.34	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	ATP	A	801	3	-	0/18/38/38	0/3/3/3
5	SO4	A	808	-	-	0/0/0/0	0/0/0/0
2	ATP	B	801	3	-	0/18/38/38	0/3/3/3
5	SO4	B	808	-	-	0/0/0/0	0/0/0/0
2	ATP	C	801	3	-	0/18/38/38	0/3/3/3
5	SO4	C	806	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	D	801	3	-	0/18/38/38	0/3/3/3
5	SO4	D	808	-	-	0/0/0/0	0/0/0/0
2	ATP	E	801	3	-	0/18/38/38	0/3/3/3
5	SO4	E	806	-	-	0/0/0/0	0/0/0/0
2	ATP	F	801	3	-	0/18/38/38	0/3/3/3
5	SO4	F	806	-	-	0/0/0/0	0/0/0/0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	ATP	PG-O3B	2.21	1.63	1.60
2	D	801	ATP	C5-C4	2.46	1.46	1.40
2	B	801	ATP	C5-C4	2.47	1.46	1.40
2	A	801	ATP	C5-C4	2.47	1.46	1.40
2	C	801	ATP	C5-C4	2.51	1.46	1.40

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	ATP	N3-C2-N1	-8.40	121.54	128.86
2	B	801	ATP	N3-C2-N1	-7.00	122.77	128.86
2	F	801	ATP	N3-C2-N1	-6.62	123.09	128.86
2	D	801	ATP	N3-C2-N1	-6.49	123.20	128.86
2	A	801	ATP	N3-C2-N1	-6.42	123.27	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	808	SO4	6	0
5	B	808	SO4	1	0
5	C	806	SO4	6	0
2	D	801	ATP	1	0
5	D	808	SO4	5	0
2	E	801	ATP	1	0
5	E	806	SO4	7	0
2	F	801	ATP	1	0
5	F	806	SO4	5	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	606/606 (100%)	0.46	25 (4%)	38 15	30, 56, 111, 166	2 (0%)
1	B	606/606 (100%)	0.55	40 (6%)	19 7	47, 79, 144, 221	2 (0%)
1	C	606/606 (100%)	0.61	43 (7%)	17 6	45, 74, 148, 197	2 (0%)
1	D	606/606 (100%)	0.42	22 (3%)	43 18	40, 70, 131, 201	2 (0%)
1	E	606/606 (100%)	0.47	32 (5%)	27 11	48, 77, 131, 177	2 (0%)
1	F	606/606 (100%)	0.48	29 (4%)	31 12	47, 76, 129, 183	2 (0%)
All	All	3636/3636 (100%)	0.50	191 (5%)	27 11	30, 72, 134, 221	12 (0%)

The worst 5 of 191 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	484	PRO	12.1
1	D	516	ASN	10.5
1	C	487	PRO	10.4
1	D	517	LYS	9.3
1	A	516	ASN	9.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
4	MG	A	805	1/1	0.99	0.25	3.12	38,38,38,38	0
3	ZN	B	802	1/1	0.96	0.24	1.84	68,68,68,68	0
3	ZN	F	802	1/1	0.85	0.25	1.08	71,71,71,71	0
3	ZN	B	803	1/1	0.98	0.21	0.81	87,87,87,87	0
2	ATP	D	801	31/31	0.98	0.22	0.67	42,48,59,61	0
3	ZN	C	802	1/1	0.97	0.21	0.63	68,68,68,68	0
2	ATP	B	801	31/31	0.97	0.21	0.35	47,54,61,65	0
2	ATP	F	801	31/31	0.97	0.21	0.34	43,53,61,66	0
2	ATP	A	801	31/31	0.97	0.23	0.34	35,42,51,57	0
2	ATP	C	801	31/31	0.97	0.21	-0.05	46,52,58,63	0
2	ATP	E	801	31/31	0.97	0.19	-0.39	45,52,59,62	0
5	SO4	D	808	5/5	0.90	0.17	-0.55	88,102,103,112	0
3	ZN	A	806	1/1	0.97	0.20	-0.93	65,65,65,65	0
5	SO4	F	806	5/5	0.96	0.16	-1.08	84,85,95,96	0
3	ZN	E	803	1/1	0.99	0.16	-1.12	65,65,65,65	0
3	ZN	C	804	1/1	0.99	0.19	-2.63	73,73,73,73	0
5	SO4	B	808	5/5	0.88	0.19	-	93,100,108,110	0
4	MG	A	804	1/1	0.91	0.27	-	41,41,41,41	0
3	ZN	D	806	1/1	0.98	0.18	-	74,74,74,74	0
4	MG	C	803	1/1	0.99	0.21	-	23,23,23,23	0
4	MG	E	802	1/1	0.83	0.28	-	67,67,67,67	0
4	MG	D	804	1/1	0.97	0.23	-	36,36,36,36	0
3	ZN	A	807	1/1	0.95	0.26	-	78,78,78,78	0
3	ZN	D	807	1/1	0.92	0.23	-	99,99,99,99	0
3	ZN	E	805	1/1	0.89	0.22	-	107,107,107,107	0
3	ZN	F	805	1/1	0.92	0.22	-	103,103,103,103	0
4	MG	B	804	1/1	0.81	0.22	-	58,58,58,58	0
4	MG	D	805	1/1	0.97	0.23	-	43,43,43,43	0
4	MG	A	803	1/1	0.99	0.21	-	54,54,54,54	0
5	SO4	E	806	5/5	0.94	0.17	-	74,92,94,98	0
3	ZN	D	802	1/1	0.96	0.23	-	71,71,71,71	0
4	MG	D	803	1/1	0.93	0.31	-	56,56,56,56	0
5	SO4	A	808	5/5	0.91	0.22	-	78,80,86,89	0
3	ZN	F	804	1/1	0.96	0.23	-	84,84,84,84	0
4	MG	B	805	1/1	0.78	0.22	-	96,96,96,96	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	F	803	1/1	0.98	0.25	-	55,55,55,55	0
3	ZN	C	805	1/1	0.95	0.24	-	81,81,81,81	0
3	ZN	E	804	1/1	0.94	0.19	-	84,84,84,84	0
4	MG	B	806	1/1	0.88	0.12	-	87,87,87,87	0
5	SO4	C	806	5/5	0.92	0.17	-	84,86,95,111	0
3	ZN	A	802	1/1	0.96	0.28	-	65,65,65,65	0
3	ZN	B	807	1/1	0.95	0.20	-	88,88,88,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.