



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:26 PM GMT

PDB ID : 4GX1  
Title : Crystal structure of the GsuK bound to ADP  
Authors : Kong, C.; Zeng, W.; Ye, S.; Chen, L.; Sauer, D.B.; Lam, Y.; Derebe, M.G.;  
Jiang, Y.  
Deposited on : 2012-09-03  
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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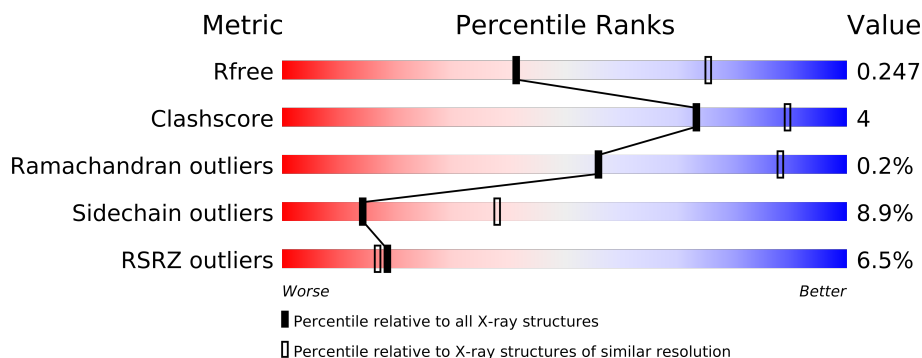
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	565	
1	B	565	
1	C	565	
1	D	565	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	K	A	603	-	X
2	K	B	602	-	X
2	K	D	601	-	X
2	K	D	602	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	ZN	B	604	-	X
3	ZN	D	603	-	X
4	CA	C	606	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14702 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TrkA domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2931	1885	507	528	11			
1	B	547	Total	C	N	O	S	0	0	0
			4197	2687	725	770	15			
1	C	546	Total	C	N	O	S	0	0	0
			4188	2682	723	768	15			
1	D	376	Total	C	N	O	S	0	0	0
			2928	1883	507	527	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	EXPRESSION TAG	UNP Q74FS9
A	5	GLN	-	EXPRESSION TAG	UNP Q74FS9
A	6	ARG	-	EXPRESSION TAG	UNP Q74FS9
A	7	GLY	-	EXPRESSION TAG	UNP Q74FS9
A	8	SER	-	EXPRESSION TAG	UNP Q74FS9
A	52	ALA	GLU	ENGINEERED MUTATION	UNP Q74FS9
A	77	GLU	GLN	ENGINEERED MUTATION	UNP Q74FS9
A	97	ASP	LEU	ENGINEERED MUTATION	UNP Q74FS9
A	565	LEU	-	EXPRESSION TAG	UNP Q74FS9
A	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
A	567	PRO	-	EXPRESSION TAG	UNP Q74FS9
A	568	ARG	-	EXPRESSION TAG	UNP Q74FS9
B	4	MET	-	EXPRESSION TAG	UNP Q74FS9
B	5	GLN	-	EXPRESSION TAG	UNP Q74FS9
B	6	ARG	-	EXPRESSION TAG	UNP Q74FS9
B	7	GLY	-	EXPRESSION TAG	UNP Q74FS9
B	8	SER	-	EXPRESSION TAG	UNP Q74FS9
B	52	ALA	GLU	ENGINEERED MUTATION	UNP Q74FS9
B	77	GLU	GLN	ENGINEERED MUTATION	UNP Q74FS9
B	97	ASP	LEU	ENGINEERED MUTATION	UNP Q74FS9
B	565	LEU	-	EXPRESSION TAG	UNP Q74FS9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
B	567	PRO	-	EXPRESSION TAG	UNP Q74FS9
B	568	ARG	-	EXPRESSION TAG	UNP Q74FS9
C	4	MET	-	EXPRESSION TAG	UNP Q74FS9
C	5	GLN	-	EXPRESSION TAG	UNP Q74FS9
C	6	ARG	-	EXPRESSION TAG	UNP Q74FS9
C	7	GLY	-	EXPRESSION TAG	UNP Q74FS9
C	8	SER	-	EXPRESSION TAG	UNP Q74FS9
C	52	ALA	GLU	ENGINEERED MUTATION	UNP Q74FS9
C	77	GLU	GLN	ENGINEERED MUTATION	UNP Q74FS9
C	97	ASP	LEU	ENGINEERED MUTATION	UNP Q74FS9
C	565	LEU	-	EXPRESSION TAG	UNP Q74FS9
C	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
C	567	PRO	-	EXPRESSION TAG	UNP Q74FS9
C	568	ARG	-	EXPRESSION TAG	UNP Q74FS9
D	4	MET	-	EXPRESSION TAG	UNP Q74FS9
D	5	GLN	-	EXPRESSION TAG	UNP Q74FS9
D	6	ARG	-	EXPRESSION TAG	UNP Q74FS9
D	7	GLY	-	EXPRESSION TAG	UNP Q74FS9
D	8	SER	-	EXPRESSION TAG	UNP Q74FS9
D	52	ALA	GLU	ENGINEERED MUTATION	UNP Q74FS9
D	77	GLU	GLN	ENGINEERED MUTATION	UNP Q74FS9
D	97	ASP	LEU	ENGINEERED MUTATION	UNP Q74FS9
D	565	LEU	-	EXPRESSION TAG	UNP Q74FS9
D	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
D	567	PRO	-	EXPRESSION TAG	UNP Q74FS9
D	568	ARG	-	EXPRESSION TAG	UNP Q74FS9

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total K 3 3	0	0
2	A	3	Total K 3 3	0	0
2	D	2	Total K 2 2	0	0
2	C	3	Total K 3 3	0	0

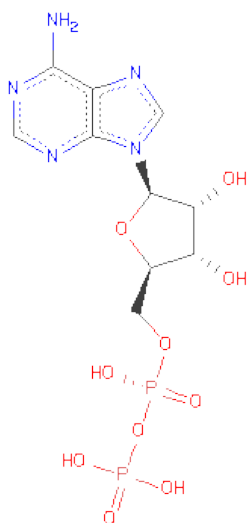
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	C	2	Total	Ca	0	0
			2	2		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



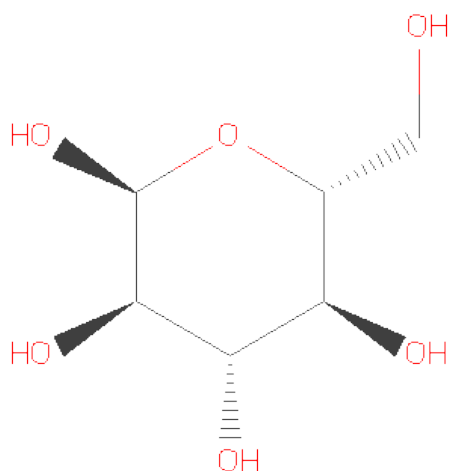
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
5	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

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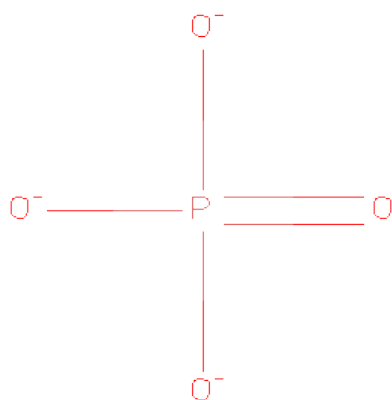
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is SUGAR (ALPHA-D-GLUCOSE) (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			12	6	6		
6	C	1	Total	C	O	0	0
			12	6	6		
6	C	1	Total	C	O	0	0
			12	6	6		
6	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



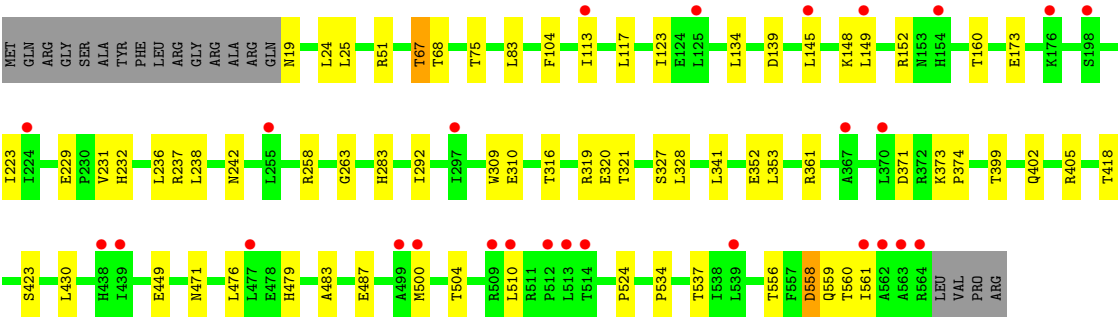
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	P	0	0
			5	4	1		
7	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	49	Total	O	0	0
			49	49		
8	B	91	Total	O	0	0
			91	91		
8	C	83	Total	O	0	0
			83	83		
8	D	50	Total	O	0	0
			50	50		

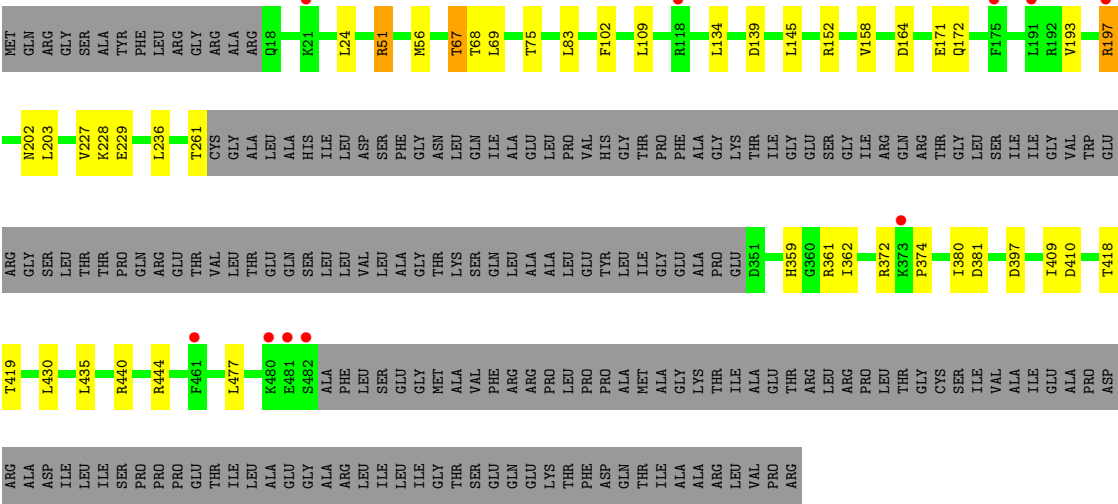






● Molecule 1: TrkA domain protein

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	234.32Å 111.44Å 164.74Å 90.00° 134.93° 90.00°	Depositor
Resolution (Å)	41.47 – 2.80 49.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.7 (41.47-2.80) 96.8 (49.53-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.212 , 0.255 0.205 , 0.247	Depositor DCC
$R_{free}$ test set	3621 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.7	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 47.4	EDS
Estimated twinning fraction	0.089 for -h-2*k,l,h+1 0.015 for -h,-k,h+1 0.023 for -h-2*k,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 71620 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14702	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.14 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3762e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ADP, K, GLC, PO4, CA

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	0.34	0/2991	0.49	0/4072
1	B	0.31	0/4280	0.47	0/5829
1	C	0.28	0/4271	0.47	0/5817
1	D	0.29	0/2988	0.47	0/4068
All	All	0.31	0/14530	0.48	0/19786

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2931	0	0	16	0
1	B	4197	0	0	17	0
1	C	4188	0	0	17	0
1	D	2928	0	0	10	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	27	0	0	3	0
5	B	27	0	0	2	0
5	C	27	0	0	1	0
5	D	27	0	0	3	0
6	B	12	0	11	0	0
6	C	24	0	22	0	0
6	D	12	0	11	0	0
7	B	5	0	0	0	0
7	C	5	0	0	2	0
8	A	49	0	0	1	0
8	B	91	0	0	1	0
8	C	83	0	0	3	0
8	D	50	0	0	0	0
All	All	14702	0	44	60	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (60) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:139:ASP:OD2	1:B:202:ASN:ND2	2.24	0.71
1:B:361:ARG:NH1	8:B:728:HOH:O	2.22	0.70
1:A:359:HIS:ND1	8:A:737:HOH:O	2.24	0.70
1:A:444:ARG:NH1	5:A:606:ADP:O1B	2.29	0.66
1:C:402:GLN:OE1	1:C:405:ARG:NE	2.29	0.66
1:C:361:ARG:N	5:C:607:ADP:O3B	2.29	0.65
1:D:397:ASP:OD1	5:D:604:ADP:N6	2.29	0.65
1:A:433:ARG:NH1	1:A:439:ILE:O	2.30	0.65
1:D:229:GLU:OE1	1:D:361:ARG:NE	2.30	0.65
1:B:172:GLN:NE2	1:B:172:GLN:O	2.30	0.65
1:B:298:ARG:NH2	1:B:523:ALA:O	2.31	0.64
1:D:51:ARG:NH2	1:D:75:THR:O	2.30	0.64
1:C:67:THR:O	1:C:68:THR:OG1	2.17	0.62
1:D:444:ARG:NH2	5:D:604:ADP:O2B	2.32	0.62
1:C:19:ASN:N	8:C:710:HOH:O	2.32	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:362:ILE:N	5:D:604:ADP:O1B	2.33	0.60
1:D:139:ASP:OD2	1:D:202:ASN:ND2	2.34	0.60
1:B:67:THR:O	1:B:68:THR:OG1	2.20	0.59
1:A:363:GLY:N	5:A:606:ADP:O3B	2.35	0.59
1:C:310:GLU:OE1	1:C:327:SER:OG	2.21	0.59
1:D:197:ARG:NH1	1:D:477:LEU:O	2.36	0.58
1:D:67:THR:O	1:D:68:THR:OG1	2.19	0.58
7:C:610:PO4:O1	8:C:748:HOH:O	2.17	0.57
1:B:552:GLU:O	1:B:556:THR:OG1	2.22	0.57
1:B:297:ILE:O	1:B:301:THR:OG1	2.23	0.55
1:C:556:THR:O	1:C:560:THR:OG1	2.25	0.55
1:A:51:ARG:NH2	1:A:75:THR:O	2.40	0.54
1:C:51:ARG:NH2	1:C:75:THR:O	2.42	0.52
1:B:270:ASP:OD1	1:B:276:GLN:NE2	2.43	0.52
1:B:492:PHE:O	1:B:547:LEU:N	2.42	0.51
1:A:229:GLU:O	1:A:232:HIS:N	2.44	0.51
1:B:471:ASN:O	1:B:475:ASN:ND2	2.44	0.51
1:B:521:ILE:O	1:B:530:LEU:N	2.44	0.51
1:B:51:ARG:NH2	1:B:75:THR:O	2.44	0.50
1:A:425:ASN:ND2	1:A:444:ARG:O	2.43	0.50
1:B:216:ARG:NH1	1:B:242:ASN:OD1	2.45	0.49
1:A:67:THR:O	1:A:68:THR:OG1	2.29	0.49
1:C:309:TRP:NE1	7:C:610:PO4:O2	2.45	0.49
1:B:444:ARG:NH2	5:B:606:ADP:O2B	2.46	0.49
1:A:203:LEU:O	1:A:228:LYS:NZ	2.46	0.49
1:C:449:GLU:OE1	1:C:449:GLU:N	2.46	0.48
1:D:203:LEU:O	1:D:228:LYS:NZ	2.48	0.47
1:A:397:ASP:OD2	5:A:606:ADP:N6	2.48	0.47
1:C:113:ILE:O	1:C:117:LEU:N	2.48	0.46
1:A:388:CYS:SG	1:A:389:ASN:N	2.89	0.45
1:A:99:ILE:O	1:A:103:GLY:N	2.50	0.44
1:C:237:ARG:NH2	8:C:745:HOH:O	2.49	0.44
1:B:362:ILE:N	5:B:606:ADP:O1B	2.51	0.43
1:C:479:HIS:O	1:C:483:ALA:N	2.51	0.43
1:B:99:ILE:O	1:B:103:GLY:N	2.51	0.43
1:D:359:HIS:N	1:D:381:ASP:OD1	2.51	0.43
1:C:229:GLU:O	1:C:232:HIS:N	2.52	0.43
1:C:534:PRO:O	1:C:537:THR:OG1	2.37	0.43
1:C:263:GLY:N	1:C:283:HIS:O	2.52	0.43
1:A:197:ARG:NH2	1:A:477:LEU:O	2.51	0.42
1:C:558:ASP:N	1:C:558:ASP:OD1	2.52	0.42
1:C:223:ILE:N	1:C:242:ASN:OD1	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:359:HIS:N	1:A:381:ASP:OD1	2.53	0.42
1:A:216:ARG:NH1	1:A:221:THR:O	2.53	0.41
1:A:69:LEU:CD2	1:B:70:GLY:CA	2.99	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	372/565 (66%)	356 (96%)	15 (4%)	1 (0%)	50	84
1	B	545/565 (96%)	527 (97%)	18 (3%)	0	100	100
1	C	544/565 (96%)	522 (96%)	20 (4%)	2 (0%)	43	80
1	D	372/565 (66%)	357 (96%)	14 (4%)	1 (0%)	50	84
All	All	1833/2260 (81%)	1762 (96%)	67 (4%)	4 (0%)	56	88

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	524	PRO
1	C	374	PRO
1	D	374	PRO
1	A	230	PRO

### 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	314/463 (68%)	286 (91%)	28 (9%)	14	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	448/463 (97%)	411 (92%)	37 (8%)	16	42
1	C	447/463 (96%)	405 (91%)	42 (9%)	13	34
1	D	314/463 (68%)	285 (91%)	29 (9%)	13	36
All	All	1523/1852 (82%)	1387 (91%)	136 (9%)	14	38

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	24	LEU
1	A	30	LEU
1	A	67	THR
1	A	69	LEU
1	A	83	LEU
1	A	115	ARG
1	A	123	ILE
1	A	134	LEU
1	A	143	ARG
1	A	145	LEU
1	A	153	ASN
1	A	158	VAL
1	A	160	THR
1	A	172	GLN
1	A	236	LEU
1	A	238	LEU
1	A	243	GLN
1	A	351	ASP
1	A	353	LEU
1	A	355	PHE
1	A	390	ASP
1	A	411	ARG
1	A	418	THR
1	A	433	ARG
1	A	440	ARG
1	A	476	LEU
1	A	480	LYS
1	B	23	LEU
1	B	24	LEU
1	B	30	LEU
1	B	67	THR
1	B	69	LEU

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Mol	Chain	Res	Type
1	B	83	LEU
1	B	105	VAL
1	B	107	MET
1	B	116	ARG
1	B	118	ARG
1	B	123	ILE
1	B	125	LEU
1	B	134	LEU
1	B	145	LEU
1	B	167	LEU
1	B	172	GLN
1	B	235	LEU
1	B	236	LEU
1	B	238	LEU
1	B	258	ARG
1	B	265	LEU
1	B	310	GLU
1	B	316	THR
1	B	328	LEU
1	B	352	GLU
1	B	353	LEU
1	B	371	ASP
1	B	399	THR
1	B	410	ASP
1	B	417	VAL
1	B	430	LEU
1	B	435	LEU
1	B	476	LEU
1	B	504	THR
1	B	509	ARG
1	B	536	GLU
1	B	556	THR
1	C	24	LEU
1	C	25	LEU
1	C	67	THR
1	C	83	LEU
1	C	104	PHE
1	C	123	ILE
1	C	134	LEU
1	C	139	ASP
1	C	145	LEU
1	C	148	LYS

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Mol	Chain	Res	Type
1	C	149	LEU
1	C	152	ARG
1	C	160	THR
1	C	173	GLU
1	C	231	VAL
1	C	236	LEU
1	C	238	LEU
1	C	258	ARG
1	C	292	ILE
1	C	316	THR
1	C	319	ARG
1	C	320	GLU
1	C	321	THR
1	C	328	LEU
1	C	341	LEU
1	C	352	GLU
1	C	353	LEU
1	C	371	ASP
1	C	373	LYS
1	C	399	THR
1	C	418	THR
1	C	423	SER
1	C	430	LEU
1	C	471	ASN
1	C	476	LEU
1	C	487	GLU
1	C	500	MET
1	C	504	THR
1	C	510	LEU
1	C	558	ASP
1	C	559	GLN
1	C	561	ILE
1	D	24	LEU
1	D	51	ARG
1	D	56	MET
1	D	67	THR
1	D	69	LEU
1	D	83	LEU
1	D	102	PHE
1	D	109	LEU
1	D	134	LEU
1	D	145	LEU

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Mol	Chain	Res	Type
1	D	152	ARG
1	D	158	VAL
1	D	164	ASP
1	D	171	GLU
1	D	172	GLN
1	D	193	VAL
1	D	197	ARG
1	D	227	VAL
1	D	236	LEU
1	D	261	THR
1	D	372	ARG
1	D	380	ILE
1	D	409	ILE
1	D	410	ASP
1	D	418	THR
1	D	419	THR
1	D	430	LEU
1	D	435	LEU
1	D	440	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 29 ligands modelled in this entry, 19 are monoatomic - leaving 10 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
5	ADP	A	606	-	29,29,29	1.44	5 (17%)	45,45,45	2.37	8 (17%)
5	ADP	B	606	-	29,29,29	1.64	7 (24%)	45,45,45	2.49	12 (26%)
6	GLC	B	607	-	12,12,12	1.73	2 (16%)	17,17,17	1.27	1 (5%)
7	PO4	B	608	-	4,4,4	0.33	0	6,6,6	0.31	0
5	ADP	C	607	-	29,29,29	1.53	5 (17%)	45,45,45	2.36	9 (20%)
6	GLC	C	608	-	12,12,12	1.69	2 (16%)	17,17,17	1.24	2 (11%)
6	GLC	C	609	-	12,12,12	1.70	2 (16%)	17,17,17	1.23	3 (17%)
7	PO4	C	610	-	4,4,4	0.29	0	6,6,6	0.30	0
5	ADP	D	604	-	29,29,29	1.58	6 (20%)	45,45,45	2.46	12 (26%)
6	GLC	D	605	-	12,12,12	1.68	2 (16%)	17,17,17	1.24	1 (5%)

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
5	ADP	A	606	-	-	0/16/32/32	0/1/3/3
5	ADP	B	606	-	-	0/16/32/32	0/1/3/3
6	GLC	B	607	-	-	0/2/22/22	0/1/1/1
7	PO4	B	608	-	-	0/0/0/0	0/0/0/0
5	ADP	C	607	-	-	0/16/32/32	0/1/3/3
6	GLC	C	608	-	-	0/2/22/22	0/1/1/1
6	GLC	C	609	-	-	0/2/22/22	0/1/1/1
7	PO4	C	610	-	-	0/0/0/0	0/0/0/0
5	ADP	D	604	-	-	0/16/32/32	0/1/3/3
6	GLC	D	605	-	-	0/2/22/22	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	607	GLC	C4-C3	-3.81	1.42	1.52
6	C	609	GLC	C4-C3	-3.80	1.42	1.52
6	D	605	GLC	C4-C3	-3.74	1.42	1.52
6	C	608	GLC	C4-C3	-3.72	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	606	ADP	C2'-C1'	-3.56	1.48	1.53
5	A	606	ADP	C2'-C3'	-3.55	1.43	1.53
5	B	606	ADP	C2'-C3'	-3.52	1.43	1.53
5	C	607	ADP	C2'-C3'	-3.48	1.43	1.53
5	D	604	ADP	C2'-C3'	-3.43	1.43	1.53
5	C	607	ADP	C2'-C1'	-3.36	1.48	1.53
6	C	608	GLC	C3-C2	-3.30	1.43	1.52
6	B	607	GLC	C3-C2	-3.27	1.43	1.52
6	C	609	GLC	C3-C2	-3.18	1.43	1.52
5	D	604	ADP	C2'-C1'	-3.17	1.49	1.53
5	B	606	ADP	PB-O3A	-3.16	1.54	1.60
6	D	605	GLC	C3-C2	-3.11	1.44	1.52
5	D	604	ADP	PB-O3A	-3.03	1.54	1.60
5	A	606	ADP	C2'-C1'	-2.87	1.49	1.53
5	C	607	ADP	O4'-C4'	-2.64	1.38	1.45
5	D	604	ADP	O4'-C4'	-2.61	1.38	1.45
5	A	606	ADP	C6-N6	2.47	1.43	1.35
5	C	607	ADP	PB-O3A	-2.45	1.55	1.60
5	B	606	ADP	C6-N6	2.45	1.42	1.35
5	D	604	ADP	PA-O3A	-2.44	1.55	1.59
5	C	607	ADP	C6-N6	2.43	1.42	1.35
5	D	604	ADP	C6-N6	2.42	1.42	1.35
5	B	606	ADP	O4'-C4'	-2.40	1.39	1.45
5	B	606	ADP	PA-O3A	-2.39	1.55	1.59
5	A	606	ADP	O4'-C4'	-2.27	1.39	1.45
5	A	606	ADP	O4'-C1'	2.14	1.44	1.41
5	B	606	ADP	O4'-C1'	2.08	1.44	1.41

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	ADP	N3-C2-N1	-10.67	119.79	128.71
5	D	604	ADP	N3-C2-N1	-10.62	119.83	128.71
5	C	607	ADP	N3-C2-N1	-10.27	120.12	128.71
5	A	606	ADP	N3-C2-N1	-10.10	120.27	128.71
5	A	606	ADP	O4'-C1'-N9	6.76	114.73	108.44
5	B	606	ADP	O4'-C1'-N9	6.55	114.53	108.44
5	D	604	ADP	O4'-C1'-N9	5.59	113.64	108.44
5	D	604	ADP	PA-O3A-PB	-5.41	115.83	131.68
5	B	606	ADP	PA-O3A-PB	-5.34	116.01	131.68
5	C	607	ADP	O4'-C1'-N9	5.14	113.22	108.44
5	A	606	ADP	N3-C4-N9	4.97	134.41	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	607	ADP	PA-O3A-PB	-4.83	117.51	131.68
5	C	607	ADP	N3-C4-N9	4.70	133.92	125.43
5	B	606	ADP	N3-C4-N9	4.66	133.84	125.43
5	D	604	ADP	N3-C4-N9	4.48	133.52	125.43
5	A	606	ADP	C4'-O4'-C1'	-4.07	105.33	109.75
5	C	607	ADP	C4'-O4'-C1'	-3.73	105.70	109.75
5	D	604	ADP	C8-N9-C4	3.37	109.47	106.90
5	D	604	ADP	C4'-O4'-C1'	-3.26	106.21	109.75
5	A	606	ADP	C5-C4-N3	-3.07	119.02	125.70
5	C	607	ADP	C5-C4-N3	-2.94	119.31	125.70
5	B	606	ADP	C5-C4-N3	-2.83	119.53	125.70
5	B	606	ADP	O5'-C5'-C4'	2.76	119.06	108.94
5	D	604	ADP	C5-C4-N3	-2.64	119.95	125.70
6	D	605	GLC	O5-C1-C2	2.62	113.91	109.86
5	D	604	ADP	O5'-C5'-C4'	2.58	118.40	108.94
5	C	607	ADP	O5'-C5'-C4'	2.54	118.24	108.94
5	B	606	ADP	C8-N9-C4	2.48	108.79	106.90
5	B	606	ADP	C2-N3-C4	2.46	121.01	114.01
5	A	606	ADP	C2-N3-C4	2.45	120.99	114.01
5	C	607	ADP	C2-N3-C4	2.43	120.94	114.01
5	D	604	ADP	C2-N3-C4	2.42	120.89	114.01
5	B	606	ADP	C4'-O4'-C1'	-2.38	107.16	109.75
5	D	604	ADP	C1'-N9-C4	-2.36	122.56	126.64
6	C	608	GLC	O5-C1-C2	2.33	113.47	109.86
6	C	608	GLC	O6-C6-C5	2.28	119.22	111.36
5	B	606	ADP	C3'-C2'-C1'	2.24	104.41	100.91
5	D	604	ADP	N7-C8-N9	-2.20	108.12	114.36
6	B	607	GLC	O5-C1-C2	2.17	113.22	109.86
5	C	607	ADP	C8-N9-C4	2.16	108.55	106.90
5	A	606	ADP	O2B-PB-O3A	2.15	115.33	105.14
5	B	606	ADP	C2'-C3'-C4'	2.10	106.84	102.65
5	D	604	ADP	C4-C5-N7	-2.09	107.73	109.52
5	A	606	ADP	C8-N9-C4	2.09	108.49	106.90
6	C	609	GLC	O6-C6-C5	2.07	118.49	111.36
6	C	609	GLC	O3-C3-C4	-2.06	105.74	110.35
6	C	609	GLC	O5-C1-C2	2.04	113.02	109.86
5	B	606	ADP	C4-C5-N7	-2.03	107.78	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	376/565 (66%)	0.12	10 (2%) 52 52	45, 68, 135, 186	0
1	B	547/565 (96%)	0.54	73 (13%) 4 3	49, 81, 190, 249	0
1	C	546/565 (96%)	0.23	27 (4%) 28 29	50, 79, 150, 217	0
1	D	376/565 (66%)	0.11	10 (2%) 52 52	45, 70, 138, 197	0
All	All	1845/2260 (81%)	0.28	120 (6%) 18 17	45, 75, 159, 249	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	516	CYS	9.9
1	B	561	ILE	9.4
1	A	481	GLU	7.0
1	B	563	ALA	6.6
1	B	518	ILE	6.2
1	B	508	THR	6.2
1	D	480	LYS	6.1
1	D	482	SER	6.0
1	B	564	ARG	5.9
1	B	496	LEU	5.9
1	B	509	ARG	5.7
1	B	510	LEU	5.6
1	B	519	VAL	5.5
1	D	481	GLU	5.4
1	A	480	LYS	5.4
1	B	484	PHE	5.3
1	C	561	ILE	5.3
1	B	512	PRO	5.1
1	D	175	PHE	5.0
1	B	483	ALA	4.9
1	B	543	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	155	LEU	4.5
1	B	506	ALA	4.5
1	B	517	SER	4.4
1	C	513	LEU	4.2
1	A	117	LEU	4.2
1	B	507	GLU	4.2
1	B	497	PRO	4.2
1	C	154	HIS	4.2
1	C	477	LEU	3.9
1	B	505	ILE	3.8
1	B	492	PHE	3.8
1	B	18	GLN	3.7
1	B	438	HIS	3.6
1	C	510	LEU	3.5
1	B	175	PHE	3.5
1	B	560	THR	3.5
1	B	19	ASN	3.5
1	B	463	VAL	3.4
1	C	145	LEU	3.4
1	C	509	ARG	3.4
1	B	495	PRO	3.3
1	B	520	ALA	3.3
1	B	557	PHE	3.3
1	B	545	LEU	3.3
1	B	255	LEU	3.3
1	C	438	HIS	3.3
1	C	500	MET	3.2
1	B	513	LEU	3.2
1	C	564	ARG	3.2
1	B	120	HIS	3.2
1	C	512	PRO	3.2
1	C	499	ALA	3.2
1	B	477	LEU	3.2
1	B	416	ILE	3.2
1	C	149	LEU	3.2
1	B	156	PHE	3.1
1	B	151	SER	3.1
1	A	118	ARG	3.1
1	C	539	LEU	3.1
1	B	473	LEU	3.1
1	B	529	ILE	3.0
1	C	562	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	439	ILE	2.9
1	C	370	LEU	2.9
1	D	21	LYS	2.9
1	B	218	LEU	2.9
1	A	478	GLU	2.8
1	B	154	HIS	2.8
1	B	356	ILE	2.7
1	B	500	MET	2.7
1	C	514	THR	2.7
1	B	555	LYS	2.7
1	D	461	PHE	2.7
1	B	117	LEU	2.7
1	B	514	THR	2.6
1	C	176	LYS	2.6
1	A	21	LYS	2.6
1	B	134	LEU	2.6
1	D	118	ARG	2.5
1	B	499	ALA	2.5
1	B	257	ILE	2.5
1	B	174	GLY	2.5
1	B	104	PHE	2.5
1	B	480	LYS	2.5
1	B	157	VAL	2.4
1	B	178	VAL	2.4
1	B	465	ASN	2.4
1	B	439	ILE	2.4
1	A	149	LEU	2.4
1	C	367	ALA	2.4
1	B	562	ALA	2.4
1	C	224	ILE	2.4
1	C	113	ILE	2.4
1	B	236	LEU	2.3
1	C	563	ALA	2.4
1	D	373	LYS	2.3
1	B	189	ALA	2.3
1	B	521	ILE	2.3
1	A	18	GLN	2.3
1	B	113	ILE	2.3
1	C	255	LEU	2.3
1	B	549	GLY	2.2
1	B	404	LEU	2.2
1	C	198	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	511	ARG	2.1
1	D	191	LEU	2.1
1	A	461	PHE	2.1
1	B	108	PHE	2.1
1	B	355	PHE	2.1
1	B	243	GLN	2.1
1	A	168	HIS	2.1
1	B	150	GLU	2.1
1	B	487	GLU	2.1
1	C	125	LEU	2.1
1	D	197	ARG	2.0
1	B	193	VAL	2.0
1	B	546	ILE	2.0
1	C	297	ILE	2.0
1	B	436	HIS	2.0

## 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	K	A	603	1/1	0.48	35.78	127,127,127,127	1
2	K	B	602	1/1	0.73	15.32	152,152,152,152	1
2	K	D	602	1/1	0.58	6.88	121,121,121,121	1
2	K	D	601	1/1	0.34	6.17	127,127,127,127	1
4	CA	C	606	1/1	0.20	2.86	68,68,68,68	0
3	ZN	B	604	1/1	0.22	2.22	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	D	603	1/1	0.22	2.20	68,68,68,68	0
2	K	C	603	1/1	0.28	1.75	71,71,71,71	1
3	ZN	A	604	1/1	0.22	1.26	70,70,70,70	0
6	GLC	C	609	12/12	0.23	0.89	120,127,129,129	0
2	K	C	602	1/1	0.24	0.69	55,55,55,55	1
2	K	B	601	1/1	0.19	0.42	75,75,75,75	1
6	GLC	C	608	12/12	0.21	0.26	118,127,128,128	0
3	ZN	C	604	1/1	0.19	0.22	68,68,68,68	0
4	CA	B	605	1/1	0.16	0.20	64,64,64,64	0
6	GLC	B	607	12/12	0.20	0.04	148,153,155,155	0
2	K	A	601	1/1	0.19	-0.14	55,55,55,55	1
5	ADP	D	604	27/27	0.17	-0.26	64,71,124,128	0
7	PO4	B	608	5/5	0.24	-0.37	80,81,87,87	0
2	K	C	601	1/1	0.17	-0.40	54,54,54,54	1
5	ADP	A	606	27/27	0.16	-0.50	65,71,203,203	0
5	ADP	C	607	27/27	0.16	-0.61	48,71,176,177	0
7	PO4	C	610	5/5	0.17	-0.62	86,91,92,93	0
5	ADP	B	606	27/27	0.14	-0.81	62,68,130,155	0
6	GLC	D	605	12/12	0.16	-0.86	133,138,139,139	0
4	CA	C	605	1/1	0.11	-1.67	62,62,62,62	0
2	K	A	602	1/1	0.13	-2.57	47,47,47,47	1
4	CA	A	605	1/1	0.09	-2.66	65,65,65,65	0
2	K	B	603	1/1	1.13	-	182,182,182,182	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.