



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:58 PM GMT

PDB ID : 1DGK  
Title : MUTANT MONOMER OF RECOMBINANT HUMAN HEXOKINASE  
TYPE I WITH GLUCOSE AND ADP IN THE ACTIVE SITE  
Authors : Aleshin, A.E.; Liu, X.; Kirby, C.; Bourenkov, G.P.; Bartunik, H.D.; Fromm,  
H.J.; Honzatko, R.B.  
Deposited on : 1999-11-24  
Resolution : 2.80 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

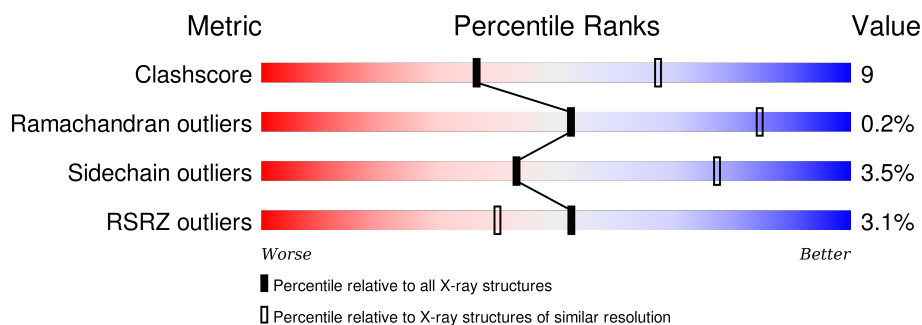
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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. 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	N	917	

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	GLC	N	919	-	-	-	X
4	ADP	N	921	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7256 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.

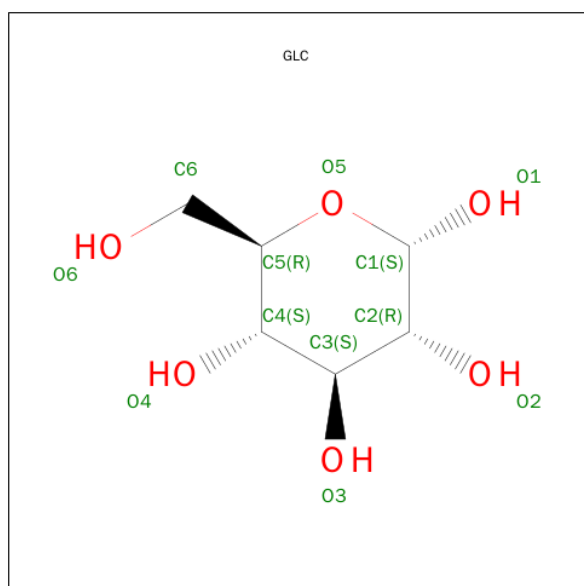
- Molecule 1 is a protein called HEXOKINASE TYPE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	N	898	7079	4435	1257	1333	54	0	13	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	240	GLU	ALA	ENGINEERED	UNP P19367
N	243	ARG	ALA	ENGINEERED	UNP P19367
N	284	TYR	GLY	ENGINEERED	UNP P19367
N	536	ALA	THR	ENGINEERED	UNP P19367
N	730	ASP	ASN	CONFLICT	UNP P19367
N	776	LEU	MET	CONFLICT	UNP P19367

- Molecule 2 is GLUCOSE (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	N	1	Total	C	O	0	0
			12	6	6		
2	N	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

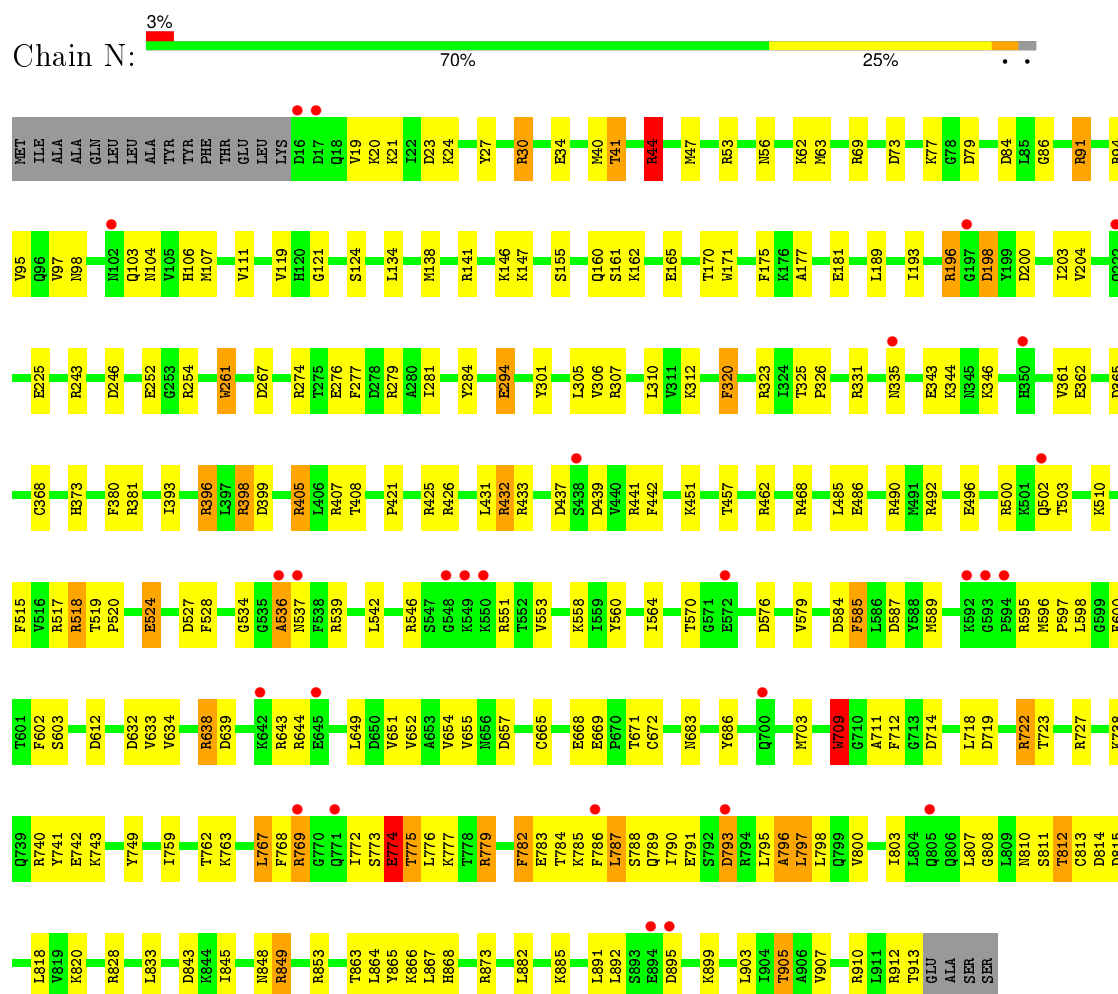
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	N	94	Total	O	0	0
			94	94		

### 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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: HEXOKINASE TYPE I



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.78Å 146.83Å 58.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 14.97 – 2.80	Depositor EDS
% Data completeness (in resolution range)	78.0 (8.00-2.80) 79.7 (14.97-2.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.258 , 0.308 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	64.7	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.4	EDS
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25141 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7256	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PO4, GLC, ADP

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	N	0.54	0/7247	1.75	156/9750 (1.6%)

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	N	0	1

There are no bond length outliers.

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	N	722	ARG	NE-CZ-NH2	23.00	131.80	120.30
1	N	576	ASP	CB-CG-OD2	-17.67	102.39	118.30
1	N	727	ARG	NE-CZ-NH1	-15.78	112.41	120.30
1	N	576	ASP	CB-CG-OD1	15.05	131.85	118.30
1	N	727	ARG	NE-CZ-NH2	14.92	127.76	120.30
1	N	468	ARG	NE-CZ-NH1	-14.49	113.06	120.30
1	N	828	ARG	NE-CZ-NH2	-13.83	113.38	120.30
1	N	539	ARG	NE-CZ-NH2	-13.17	113.71	120.30
1	N	517	ARG	NE-CZ-NH2	-12.29	114.15	120.30
1	N	468	ARG	NE-CZ-NH2	12.00	126.30	120.30
1	N	849	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	N	539	ARG	NE-CZ-NH1	10.90	125.75	120.30
1	N	657	ASP	CB-CG-OD1	-10.64	108.72	118.30
1	N	30	ARG	NE-CZ-NH1	10.55	125.58	120.30
1	N	643	ARG	NE-CZ-NH1	-10.53	115.03	120.30
1	N	243	ARG	NE-CZ-NH1	10.36	125.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	639	ASP	CB-CG-OD2	-10.35	108.98	118.30
1	N	243	ARG	CD-NE-CZ	10.25	137.96	123.60
1	N	524	GLU	OE1-CD-OE2	-10.03	111.27	123.30
1	N	492	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	N	722	ARG	NH1-CZ-NH2	-9.77	108.66	119.40
1	N	742	GLU	OE1-CD-OE2	-9.67	111.70	123.30
1	N	91	ARG	NE-CZ-NH2	-9.53	115.54	120.30
1	N	279[A]	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	N	279[B]	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	N	492	ARG	NE-CZ-NH1	-9.38	115.61	120.30
1	N	405[A]	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	N	405[B]	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	N	769	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	N	343	GLU	OE1-CD-OE2	9.21	134.36	123.30
1	N	243	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	N	407	ARG	NE-CZ-NH2	9.07	124.84	120.30
1	N	632	ASP	CB-CG-OD2	-9.07	110.14	118.30
1	N	585	PHE	CB-CG-CD1	-8.95	114.54	120.80
1	N	492	ARG	NH1-CZ-NH2	8.81	129.09	119.40
1	N	396	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	N	307	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	N	79	ASP	CB-CG-OD1	8.53	125.98	118.30
1	N	779	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	N	200	ASP	CB-CG-OD1	8.38	125.84	118.30
1	N	94	ARG	NE-CZ-NH1	-8.38	116.11	120.30
1	N	905	THR	CA-CB-CG2	-8.38	100.67	112.40
1	N	381	ARG	NE-CZ-NH2	8.37	124.49	120.30
1	N	181	GLU	OE1-CD-OE2	-8.30	113.34	123.30
1	N	432	ARG	NE-CZ-NH2	8.30	124.45	120.30
1	N	294	GLU	OE1-CD-OE2	8.27	133.22	123.30
1	N	44[A]	ARG	CD-NE-CZ	8.26	135.17	123.60
1	N	44[B]	ARG	CD-NE-CZ	8.26	135.17	123.60
1	N	719	ASP	CB-CG-OD2	8.26	125.73	118.30
1	N	769	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	N	307	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	N	849	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	N	828	ARG	NH1-CZ-NH2	8.04	128.24	119.40
1	N	141	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	N	277	PHE	CB-CG-CD2	-7.87	115.29	120.80
1	N	912	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	N	225	GLU	OE1-CD-OE2	7.66	132.49	123.30
1	N	595	ARG	NE-CZ-NH2	-7.55	116.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	279[A]	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	N	279[B]	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	N	284	TYR	CB-CG-CD2	-7.49	116.51	121.00
1	N	585	PHE	CB-CG-CD2	7.43	126.00	120.80
1	N	912	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	N	441	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	N	517	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	N	91	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	N	426	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	N	27	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	N	462	ARG	NE-CZ-NH2	7.15	123.88	120.30
1	N	510	LYS	CD-CE-NZ	7.08	127.99	111.70
1	N	873[A]	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	N	873[B]	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	N	686	TYR	CB-CG-CD1	7.07	125.24	121.00
1	N	527	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	N	895	ASP	CB-CG-OD1	7.00	124.60	118.30
1	N	811	SER	CA-C-N	-6.98	101.85	117.20
1	N	671	THR	CA-CB-CG2	-6.95	102.67	112.40
1	N	84	ASP	CB-CG-OD1	6.82	124.44	118.30
1	N	246	ASP	CB-CG-OD1	6.78	124.40	118.30
1	N	261	TRP	CA-CB-CG	6.74	126.50	113.70
1	N	584	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	N	246	ASP	CB-CG-OD2	-6.66	112.30	118.30
1	N	774	GLU	CA-C-N	6.66	131.86	117.20
1	N	433	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	N	546	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	N	767	LEU	CB-CA-C	-6.48	97.88	110.20
1	N	196[A]	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	N	196[B]	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	N	600	PHE	CB-CG-CD2	6.45	125.32	120.80
1	N	686	TYR	CB-CG-CD2	-6.45	117.13	121.00
1	N	843	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	N	517	ARG	CG-CD-NE	6.37	125.17	111.80
1	N	267	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	N	274	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	N	669	GLU	OE1-CD-OE2	6.33	130.90	123.30
1	N	774	GLU	CA-C-O	-6.33	106.81	120.10
1	N	284	TYR	CB-CG-CD1	6.27	124.76	121.00
1	N	749	TYR	CB-CG-CD2	6.26	124.76	121.00
1	N	515	PHE	CB-CG-CD2	6.25	125.17	120.80
1	N	41	THR	CA-CB-CG2	6.24	121.13	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	528	PHE	CB-CG-CD2	-6.23	116.44	120.80
1	N	527	ASP	CB-CG-OD1	6.23	123.91	118.30
1	N	405[A]	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	N	405[B]	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	N	709	TRP	CA-CB-CG	6.18	125.44	113.70
1	N	742	GLU	CG-CD-OE2	6.07	130.45	118.30
1	N	587	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	N	30	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	N	518	ARG	CD-NE-CZ	5.99	131.99	123.60
1	N	301	TYR	CB-CG-CD1	5.98	124.59	121.00
1	N	23	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	N	399	ASP	CB-CG-OD1	-5.93	112.96	118.30
1	N	865	TYR	CB-CG-CD2	5.93	124.56	121.00
1	N	873[A]	ARG	CD-NE-CZ	5.93	131.90	123.60
1	N	873[B]	ARG	CD-NE-CZ	5.93	131.90	123.60
1	N	612	ASP	CB-CG-OD2	5.91	123.62	118.30
1	N	528	PHE	CB-CG-CD1	5.91	124.94	120.80
1	N	27	TYR	CB-CG-CD1	5.81	124.49	121.00
1	N	398	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	N	537	ASN	CB-CG-OD1	-5.73	110.15	121.60
1	N	518	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	N	774	GLU	OE1-CD-OE2	-5.66	116.51	123.30
1	N	34	GLU	CG-CD-OE2	-5.65	107.00	118.30
1	N	69	ARG	NE-CZ-NH1	-5.63	117.49	120.30
1	N	331	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	N	56	ASN	CB-CG-OD1	-5.62	110.36	121.60
1	N	848	ASN	CB-CG-OD1	-5.58	110.44	121.60
1	N	396	ARG	NH1-CZ-NH2	5.47	125.42	119.40
1	N	639	ASP	CB-CG-OD1	5.44	123.20	118.30
1	N	546	ARG	NH1-CZ-NH2	5.42	125.36	119.40
1	N	254	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	N	546	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	N	408	THR	O-C-N	5.35	131.26	122.70
1	N	73	ASP	CB-CG-OD2	5.35	123.11	118.30
1	N	719	ASP	CB-CG-OD1	-5.33	113.51	118.30
1	N	432	ARG	NH1-CZ-NH2	-5.32	113.55	119.40
1	N	53	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	N	426	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	N	425	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	N	40	MET	O-C-N	-5.25	114.30	122.70
1	N	462	ARG	CD-NE-CZ	5.22	130.90	123.60
1	N	741	TYR	CB-CG-CD1	5.20	124.12	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	638	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	N	655	VAL	N-CA-CB	-5.19	100.09	111.50
1	N	274	ARG	O-C-N	-5.18	114.41	122.70
1	N	536	ALA	N-CA-CB	5.17	117.34	110.10
1	N	654	VAL	CG1-CB-CG2	-5.17	102.63	110.90
1	N	30	ARG	N-CA-CB	-5.16	101.32	110.60
1	N	595	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	N	723	THR	CA-CB-CG2	-5.09	105.28	112.40
1	N	23	ASP	CB-CG-OD1	5.08	122.87	118.30
1	N	181	GLU	CG-CD-OE1	5.07	128.44	118.30
1	N	812	THR	N-CA-C	-5.06	97.34	111.00
1	N	346	LYS	CA-CB-CG	5.04	124.48	113.40
1	N	703	MET	N-CA-CB	5.04	119.66	110.60
1	N	94	ARG	NH1-CZ-NH2	5.01	124.91	119.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	796	ALA	Mainchain

## 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	N	7079	0	7138	134	0
2	N	24	0	22	1	0
3	N	5	0	0	0	0
4	N	54	0	23	14	0
5	N	94	0	0	2	0
All	All	7256	0	7183	134	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 9.

All (134) 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:N:196[A]:ARG:HG2	1:N:198:ASP:HB2	1.31	1.13
1:N:361:VAL:HG12	1:N:362:GLU:H	1.36	0.90
1:N:323[A]:ARG:HD3	1:N:361:VAL:HG13	1.55	0.87
1:N:553:VAL:HG11	1:N:899:LYS:HG3	1.62	0.81
1:N:536:ALA:HB3	4:N:921:ADP:O2B	1.83	0.78
1:N:772:ILE:HG22	1:N:777:LYS:HG3	1.64	0.78
1:N:103:GLN:HE21	1:N:106:HIS:HB2	1.47	0.78
1:N:867:LEU:HD12	4:N:921:ADP:C5	2.19	0.77
1:N:524:GLU:HA	1:N:910:ARG:HH22	1.49	0.77
1:N:867:LEU:HD12	4:N:921:ADP:C6	2.21	0.76
1:N:320:PHE:HB3	1:N:361:VAL:HG11	1.66	0.75
1:N:784:THR:HA	1:N:787:LEU:HB2	1.68	0.75
1:N:789:GLN:HB3	1:N:803:ILE:HD11	1.69	0.75
1:N:863:THR:HB	4:N:921:ADP:O4'	1.88	0.73
1:N:41:THR:HG23	1:N:44[B]:ARG:HH21	1.54	0.73
1:N:431:LEU:HD22	1:N:442:PHE:HZ	1.56	0.71
1:N:323[A]:ARG:CD	1:N:361:VAL:HG13	2.23	0.69
1:N:788:SER:HB2	4:N:921:ADP:HN62	1.57	0.68
1:N:718:LEU:O	1:N:722:ARG:HG3	1.94	0.68
1:N:323[B]:ARG:NH1	1:N:362:GLU:HB2	2.09	0.68
1:N:325:THR:HB	1:N:326:PRO:HD2	1.79	0.64
1:N:812:THR:H	1:N:815:ASP:HB2	1.63	0.63
1:N:95:VAL:HG22	1:N:107:MET:HE2	1.82	0.61
1:N:119:VAL:HG13	1:N:175:PHE:HA	1.81	0.61
1:N:162:LYS:HG2	1:N:165[A]:GLU:HG2	1.81	0.61
1:N:519:THR:HB	1:N:520:PRO:HD2	1.84	0.59
1:N:866:LYS:HG2	1:N:892:LEU:HD21	1.85	0.59
1:N:536:ALA:HB3	4:N:921:ADP:PB	2.42	0.58
1:N:570:THR:HB	5:N:973:HOH:O	2.01	0.58
1:N:323[B]:ARG:HH12	1:N:362:GLU:HB2	1.68	0.57
1:N:767:LEU:HG	1:N:818:LEU:HD23	1.86	0.57
1:N:773:SER:O	1:N:774:GLU:C	2.39	0.57
1:N:773:SER:O	1:N:775:THR:N	2.38	0.56
1:N:783:GLU:HB2	1:N:786:PHE:HD2	1.71	0.56
1:N:107:MET:HE3	1:N:451:LYS:HB2	1.86	0.56
1:N:486:GLU:O	1:N:490:ARG:HG3	2.04	0.56
1:N:793:ASP:OD1	1:N:820:LYS:HE3	2.06	0.56
1:N:161:SER:N	1:N:165[A]:GLU:OE1	2.36	0.56
1:N:790:ILE:HG13	1:N:803:ILE:HD13	1.87	0.55
1:N:170[B]:THR:HG22	1:N:171:TRP:O	2.06	0.54
1:N:785:LYS:HA	4:N:921:ADP:C5	2.43	0.53
1:N:598:LEU:HD23	1:N:598:LEU:C	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:759:ILE:HG22	1:N:763:LYS:HE3	1.90	0.53
1:N:773:SER:O	1:N:776:LEU:N	2.39	0.53
1:N:281:ILE:HG21	1:N:305:LEU:HD21	1.91	0.53
1:N:788:SER:OG	1:N:868:HIS:HA	2.10	0.52
1:N:189:LEU:HD23	1:N:203:ILE:HD13	1.91	0.52
1:N:47:MET:HE3	1:N:393:ILE:HG12	1.92	0.52
1:N:344:LYS:HG2	1:N:421:PRO:HG3	1.91	0.51
1:N:596:MET:HB3	1:N:597:PRO:HD2	1.92	0.51
1:N:524:GLU:HA	1:N:910:ARG:NH2	2.20	0.51
1:N:853:ARG:HA	1:N:885:LYS:O	2.10	0.51
1:N:634:VAL:O	1:N:638:ARG:HG3	2.10	0.51
1:N:496:GLU:OE2	1:N:500:ARG:NH1	2.43	0.51
1:N:19:VAL:HG13	1:N:373:HIS:CE1	2.46	0.51
1:N:665:CYS:SG	1:N:672:CYS:SG	3.06	0.50
1:N:294:GLU:OE2	2:N:918:GLC:O1	2.30	0.50
1:N:759:ILE:HG23	1:N:772:ILE:HD12	1.94	0.50
1:N:785:LYS:HA	4:N:921:ADP:N7	2.28	0.49
1:N:767:LEU:CD2	1:N:818:LEU:HD23	2.43	0.49
1:N:103:GLN:NE2	1:N:106:HIS:HB2	2.20	0.49
1:N:518:ARG:NH2	1:N:907:VAL:HG22	2.27	0.49
1:N:20:LYS:O	1:N:24:LYS:HG3	2.13	0.48
1:N:845:ILE:O	1:N:849:ARG:HG3	2.12	0.48
1:N:431:LEU:HD22	1:N:442:PHE:CZ	2.44	0.48
1:N:768:PHE:O	1:N:769:ARG:HB2	2.14	0.48
1:N:867:LEU:HD12	4:N:921:ADP:N7	2.29	0.48
1:N:107:MET:CE	1:N:451:LYS:HB2	2.44	0.47
1:N:683:ASN:HA	1:N:709:TRP:CD1	2.49	0.47
1:N:551:ARG:HH21	1:N:668:GLU:CD	2.18	0.47
1:N:812:THR:HG22	1:N:814:ASP:H	1.79	0.47
1:N:524:GLU:HA	1:N:910:ARG:HH12	1.79	0.47
1:N:44[A]:ARG:HH11	1:N:44[A]:ARG:HG2	1.79	0.47
1:N:519:THR:HB	1:N:520:PRO:CD	2.45	0.47
1:N:864:LEU:HD12	4:N:921:ADP:H2	1.80	0.46
1:N:431:LEU:HG	1:N:431:LEU:O	2.16	0.46
1:N:344:LYS:HE3	1:N:421:PRO:HB3	1.97	0.46
1:N:204:VAL:CG2	1:N:457:THR:HG23	2.46	0.46
1:N:714:ASP:OD1	1:N:740:ARG:HG3	2.16	0.46
1:N:649:LEU:HA	1:N:649:LEU:HD23	1.83	0.45
1:N:867:LEU:HD12	4:N:921:ADP:N6	2.31	0.45
1:N:774:GLU:HA	1:N:774:GLU:OE1	2.17	0.45
1:N:405[A]:ARG:NH1	1:N:439:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:398:ARG:NH2	1:N:437:ASP:HB2	2.32	0.45
1:N:432:ARG:HD2	5:N:939:HOH:O	2.14	0.45
1:N:793:ASP:N	1:N:793:ASP:OD1	2.48	0.45
1:N:791:GLU:OE2	1:N:868:HIS:NE2	2.45	0.45
1:N:864:LEU:HA	4:N:921:ADP:N3	2.32	0.44
1:N:585:PHE:CZ	1:N:589:MET:HG3	2.52	0.44
1:N:520:PRO:HG3	1:N:903:LEU:HD13	1.99	0.44
1:N:652:VAL:HB	1:N:905:THR:HG23	1.99	0.44
1:N:665:CYS:HG	1:N:672:CYS:CB	2.29	0.44
1:N:193:ILE:O	1:N:196[B]:ARG:HB2	2.18	0.44
1:N:866:LYS:HE3	1:N:892:LEU:HD11	2.00	0.44
1:N:19:VAL:HG13	1:N:373:HIS:NE2	2.32	0.44
1:N:306:VAL:O	1:N:310:LEU:HG	2.18	0.43
1:N:772:ILE:CG2	1:N:777:LYS:HG3	2.44	0.43
1:N:782:PHE:O	1:N:783:GLU:C	2.56	0.43
1:N:790:ILE:HG23	1:N:800:VAL:HG22	2.00	0.43
1:N:767:LEU:HD21	1:N:818:LEU:HB3	2.01	0.43
1:N:398:ARG:HH21	1:N:437:ASP:HB2	1.84	0.43
1:N:62:LYS:O	1:N:63:MET:C	2.56	0.43
1:N:121:GLY:O	1:N:177:ALA:HA	2.18	0.43
1:N:864:LEU:HA	4:N:921:ADP:C2	2.54	0.42
1:N:365:ASP:O	1:N:368:CYS:HB2	2.19	0.42
1:N:762:THR:HB	1:N:772:ILE:HD13	2.01	0.42
1:N:789:GLN:HB3	1:N:803:ILE:CD1	2.45	0.42
1:N:485:LEU:HD23	1:N:882:LEU:HD22	2.00	0.42
1:N:579:VAL:HG12	1:N:644:ARG:HD2	2.01	0.42
1:N:189:LEU:HD23	1:N:203:ILE:CD1	2.50	0.42
1:N:711:ALA:O	1:N:712:PHE:C	2.58	0.42
1:N:788:SER:OG	4:N:921:ADP:N1	2.39	0.42
1:N:134:LEU:HD11	1:N:138:MET:HE2	2.02	0.42
1:N:98:ASN:ND2	1:N:104:ASN:HA	2.35	0.42
1:N:91:ARG:HG2	1:N:111:VAL:HG22	2.02	0.42
1:N:634:VAL:HG13	1:N:651:VAL:HG11	2.02	0.41
1:N:553:VAL:HG21	1:N:899:LYS:HD3	2.02	0.41
1:N:276:GLU:OE1	1:N:312:LYS:HE3	2.21	0.41
1:N:796:ALA:O	1:N:797:LEU:C	2.56	0.41
1:N:602:PHE:CE1	1:N:633:VAL:HG11	2.54	0.41
1:N:518:ARG:HH22	1:N:907:VAL:HG22	1.86	0.41
1:N:534:GLY:HA3	1:N:603:SER:OG	2.20	0.41
1:N:558:LYS:HE2	1:N:560:TYR:CE2	2.56	0.41
1:N:738:LYS:O	1:N:743:LYS:NZ	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:323[A]:ARG:HD3	1:N:361:VAL:HA	2.03	0.40
1:N:796:ALA:O	1:N:798:LEU:N	2.54	0.40
1:N:146:LYS:O	1:N:147:LYS:HB2	2.21	0.40
1:N:598:LEU:HD13	1:N:649:LEU:HD13	2.02	0.40
1:N:119:VAL:CG1	1:N:175:PHE:HA	2.49	0.40
1:N:502:GLN:HG2	1:N:503:THR:HG23	2.04	0.40
1:N:833:LEU:HA	1:N:833:LEU:HD23	1.93	0.40
1:N:86:GLY:HA3	1:N:155:SER:OG	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	N	909/917 (99%)	878 (97%)	29 (3%)	2 (0%)	52	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	774	GLU
1	N	808	GLY

### 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	N	784/786 (100%)	756 (96%)	28 (4%)	42 76

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	21	LYS
1	N	30	ARG
1	N	44[A]	ARG
1	N	44[B]	ARG
1	N	77	LYS
1	N	97	VAL
1	N	124	SER
1	N	198	ASP
1	N	252	GLU
1	N	261	TRP
1	N	320	PHE
1	N	380	PHE
1	N	396	ARG
1	N	542	LEU
1	N	564	ILE
1	N	709	TRP
1	N	775	THR
1	N	779	ARG
1	N	782	PHE
1	N	787	LEU
1	N	793	ASP
1	N	795	LEU
1	N	797	LEU
1	N	807	LEU
1	N	810	ASN
1	N	813	CYS
1	N	891	LEU
1	N	913	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	18	GLN
1	N	98	ASN
1	N	384	ASN
1	N	504	HIS
1	N	506	ASN

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Mol	Chain	Res	Type
1	N	608	GLN
1	N	700	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 ⓘ

5 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	GLC	N	918	-	12,12,12	0.79	0	17,17,17	1.90	4 (23%)
2	GLC	N	919	-	12,12,12	0.56	0	17,17,17	2.23	7 (41%)
3	PO4	N	920	-	4,4,4	1.52	1 (25%)	6,6,6	0.34	0
4	ADP	N	921	-	22,29,29	1.22	4 (18%)	27,45,45	1.61	7 (25%)
4	ADP	N	922	-	22,29,29	1.34	4 (18%)	27,45,45	2.15	6 (22%)

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	GLC	N	918	-	-	0/2/22/22	0/1/1/1
2	GLC	N	919	-	-	0/2/22/22	0/1/1/1
3	PO4	N	920	-	-	0/0/0/0	0/0/0/0
4	ADP	N	921	-	-	0/12/32/32	0/3/3/3
4	ADP	N	922	-	-	0/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	922	ADP	C8-N7	-3.36	1.28	1.34
4	N	921	ADP	C8-N7	-2.99	1.28	1.34
4	N	922	ADP	C5-N7	-2.24	1.31	1.39
4	N	921	ADP	PA-O2A	-2.22	1.45	1.54
4	N	921	ADP	C5-N7	-2.10	1.32	1.39
4	N	922	ADP	PB-O3B	-2.04	1.47	1.54
4	N	921	ADP	C2-N1	2.10	1.37	1.33
4	N	922	ADP	C2-N1	2.14	1.38	1.33
3	N	920	PO4	P-O4	2.15	1.61	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	919	GLC	O2-C2-C3	-6.02	96.78	110.34
4	N	922	ADP	N3-C2-N1	-5.92	124.36	128.89
2	N	918	GLC	O3-C3-C2	-4.33	100.58	110.34
4	N	922	ADP	PA-O3A-PB	-3.36	121.41	132.67
2	N	918	GLC	O5-C5-C6	-2.78	99.34	106.36
2	N	919	GLC	C1-O5-C5	-2.77	108.34	113.47
4	N	922	ADP	O3A-PA-O5'	-2.76	95.61	102.94
2	N	919	GLC	O4-C4-C5	-2.47	102.70	109.24
2	N	919	GLC	C1-C2-C3	-2.44	106.80	110.43
4	N	921	ADP	O2B-PB-O1B	-2.43	102.75	110.58
2	N	919	GLC	O3-C3-C2	-2.22	105.34	110.34
4	N	921	ADP	O2A-PA-O1A	-2.07	101.29	112.53
2	N	919	GLC	O1-C1-O5	2.25	116.42	110.25
2	N	919	GLC	O2-C2-C1	2.29	114.86	109.82
4	N	921	ADP	O2A-PA-O3A	2.43	116.12	105.09
4	N	921	ADP	O5'-C5'-C4'	2.45	118.13	109.12
2	N	918	GLC	O6-C6-C5	2.85	120.75	111.33
4	N	921	ADP	C4-C5-N7	3.02	112.25	109.48
4	N	921	ADP	O4'-C4'-C5'	3.19	120.74	109.32
4	N	922	ADP	C2'-C1'-N9	3.22	119.20	114.29
4	N	921	ADP	N3-C2-N1	3.43	131.52	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	922	ADP	O2A-PA-O5'	3.44	125.82	108.46
2	N	918	GLC	O1-C1-C2	3.82	119.44	109.21
4	N	922	ADP	C4-C5-N7	4.96	114.05	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	918	GLC	1	0
4	N	921	ADP	14	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	N	898/917 (97%)	-0.20	28 (3%)	52 40	28, 45, 84, 116	21 (2%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	102	ASN	5.6
1	N	645	GLU	4.4
1	N	549	LYS	4.1
1	N	548	GLY	4.0
1	N	894	GLU	3.9
1	N	793	ASP	3.7
1	N	895	ASP	3.5
1	N	771	GLN	3.4
1	N	594	PRO	3.4
1	N	700	GLN	3.1
1	N	537	ASN	3.0
1	N	572	GLU	2.8
1	N	350	HIS	2.8
1	N	536	ALA	2.6
1	N	786	PHE	2.6
1	N	222	GLN	2.5
1	N	593	GLY	2.5
1	N	197	GLY	2.5
1	N	335[A]	ASN	2.4
1	N	592	LYS	2.3
1	N	769	ARG	2.3
1	N	16	ASP	2.3
1	N	438	SER	2.3
1	N	642	LYS	2.2
1	N	17	ASP	2.1
1	N	805	GLN	2.0
1	N	502	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	N	550	LYS	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
2	GLC	N	919	12/12	0.96	0.19	2.25	29,33,37,37	0
2	GLC	N	918	12/12	0.96	0.18	1.17	32,34,36,39	0
4	ADP	N	921	27/27	0.88	0.32	1.08	62,64,70,71	0
4	ADP	N	922	27/27	0.97	0.15	-0.40	41,47,59,60	0
3	PO4	N	920	5/5	0.91	0.12	-0.83	37,38,40,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.