



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 06:14 AM GMT

PDB ID : 4L3Q  
Title : Crystal structure of glucokinase-activatorcomplex  
Authors : Gajiwala, K.S.; Filipski, K.J.  
Deposited on : 2013-06-06  
Resolution : 2.70 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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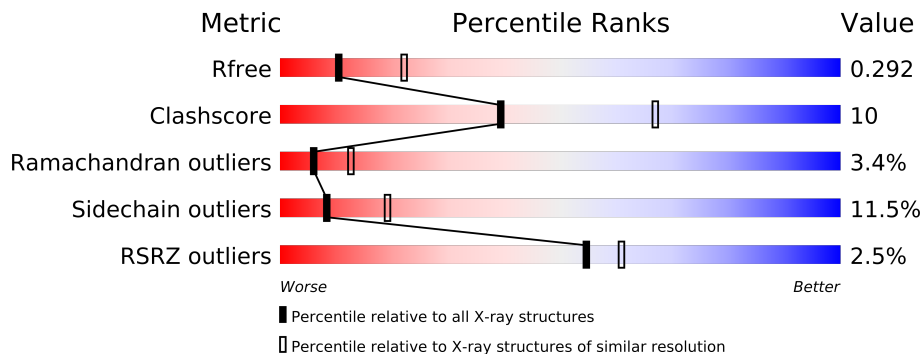
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 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	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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	457	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 3537 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.

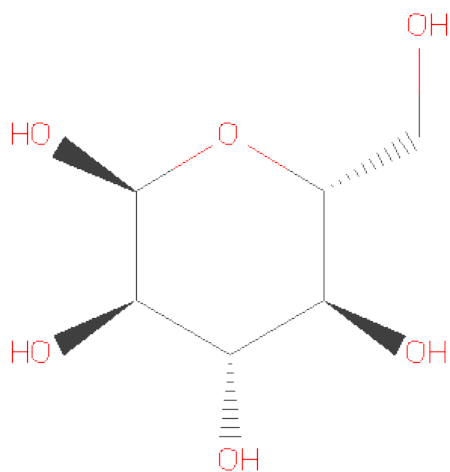
- Molecule 1 is a protein called Glucokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	447	3499	2175	608	685	31	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

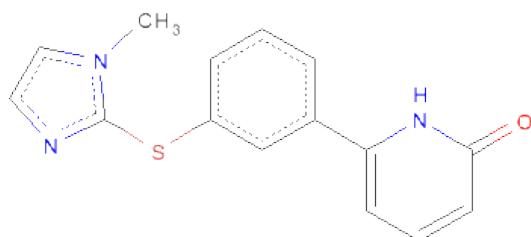
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLY	-	EXPRESSION TAG	UNP P35557
A	10	PRO	-	EXPRESSION TAG	UNP P35557
A	11	MET	-	EXPRESSION TAG	UNP P35557
A	12	ALA	-	EXPRESSION TAG	UNP P35557
A	13	LEU	-	EXPRESSION TAG	UNP P35557
A	14	THR	-	EXPRESSION TAG	UNP P35557
A	15	LEU	-	EXPRESSION TAG	UNP P35557

- Molecule 2 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
2	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is 6-{3-[(1-METHYL-1H-IMIDAZOL-2-YL)SULFANYL]PHENYL}PYRIDIN-2 (1H)-ONE (three-letter code: 926) (formula: C<sub>15</sub>H<sub>13</sub>N<sub>3</sub>OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			20	15	3	1	1		

- Molecule 4 is water.

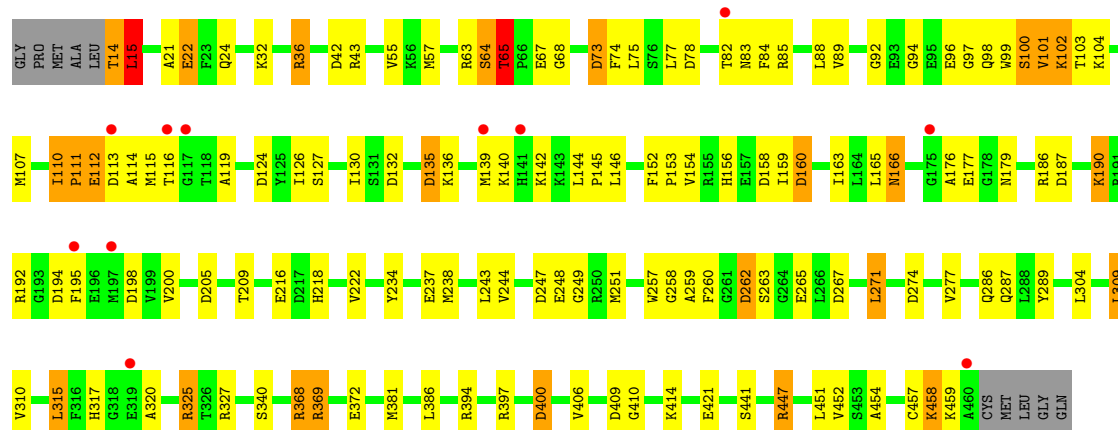
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		

### 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 ( $\text{RSRZ} > 2$ ). 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: Glucokinase

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.51Å 79.51Å 321.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.84 – 2.70 39.45 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.84-2.70) 99.6 (39.45-2.70)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	10.05 (at 2.69Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.254 , 0.304 0.244 , 0.292	Depositor DCC
$R_{free}$ test set	1769 reflections (11.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.5	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 24.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 17435 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3537	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: GLC, 926

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	0.61	0/3552	0.88	16/4775 (0.3%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ASP	CB-CG-OD2	8.11	125.60	118.30
1	A	247	ASP	CB-CG-OD2	7.60	125.14	118.30
1	A	262	ASP	CB-CG-OD2	7.57	125.11	118.30
1	A	158	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	132	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	267	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	124	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	42	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	315	LEU	CA-CB-CG	5.92	128.92	115.30
1	A	274	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	160	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	135	ASP	CB-CG-OD2	5.43	123.18	118.30
1	A	113	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	15	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	400	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	78	ASP	CB-CG-OD2	5.18	122.97	118.30

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	3499	0	3438	67	0
2	A	12	0	12	0	0
3	A	20	0	13	2	0
4	A	6	0	0	0	0
All	All	3537	0	3463	67	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 10.

All (67) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:263:SER:HB2	1:A:265:GLU:OE2	1.79	0.81
1:A:457:CYS:C	1:A:459:LYS:H	1.99	0.64
1:A:75:LEU:HD23	1:A:146:LEU:HD13	1.80	0.63
1:A:111:PRO:HD2	1:A:114:ALA:HB3	1.78	0.63
1:A:126:ILE:O	1:A:130:ILE:HG13	2.00	0.61
1:A:73:ASP:HB3	1:A:88:LEU:HD11	1.83	0.59
1:A:92:GLY:HA3	1:A:99:TRP:CE2	2.40	0.57
1:A:103:THR:O	1:A:104:LYS:HG3	2.04	0.56
1:A:238:MET:HB2	1:A:249:GLY:O	2.06	0.56
1:A:111:PRO:O	1:A:112:GLU:HB3	2.05	0.56
1:A:244:VAL:HG11	1:A:251:MET:HE1	1.88	0.56
1:A:36:ARG:HG2	1:A:36:ARG:HH11	1.69	0.56
1:A:166:ASN:HA	1:A:177:GLU:HG2	1.88	0.55
1:A:409:ASP:OD1	1:A:414:LYS:HE3	2.09	0.53
1:A:259:ALA:HB2	1:A:287:GLN:OE1	2.10	0.52
1:A:447:ARG:O	1:A:451:LEU:HD12	2.09	0.51
1:A:209:THR:HG23	1:A:441:SER:HB3	1.94	0.50
1:A:452:VAL:HG13	3:A:501:926:H2	1.93	0.50
1:A:92:GLY:HA3	1:A:99:TRP:CZ2	2.46	0.50
1:A:100:SER:HB2	1:A:447:ARG:HG2	1.93	0.50
1:A:111:PRO:HD2	1:A:114:ALA:CB	2.42	0.50
1:A:277:VAL:HG23	1:A:304:LEU:HD22	1.94	0.49
1:A:369:ARG:NH1	1:A:369:ARG:HA	2.27	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:119:ALA:HB2	1:A:176:ALA:HB2	1.93	0.49
1:A:165:LEU:O	1:A:166:ASN:HB3	2.13	0.49
1:A:74:PHE:CD2	1:A:145:PRO:HB2	2.48	0.48
1:A:154:VAL:HG12	1:A:156:HIS:HD2	1.80	0.47
1:A:22:GLU:O	1:A:271:LEU:HD21	2.15	0.47
1:A:64:SER:O	1:A:65:THR:C	2.52	0.47
1:A:368:ARG:O	1:A:372:GLU:HG3	2.15	0.47
1:A:457:CYS:C	1:A:459:LYS:N	2.67	0.47
1:A:63:ARG:H	3:A:501:926:C3	2.28	0.47
1:A:77:LEU:HG	1:A:146:LEU:HD11	1.98	0.46
1:A:85:ARG:HG2	1:A:107:MET:HG2	1.98	0.46
1:A:238:MET:HE2	1:A:244:VAL:CG1	2.46	0.45
1:A:152:PHE:HB3	1:A:153:PRO:HD2	1.96	0.45
1:A:260:PHE:O	1:A:289:TYR:HB2	2.17	0.45
1:A:14:THR:O	1:A:14:THR:HG23	2.17	0.45
1:A:163:ILE:HA	1:A:179:ASN:O	2.17	0.45
1:A:258:GLY:O	1:A:287:GLN:HA	2.17	0.44
1:A:139:MET:HG2	1:A:142:LYS:NZ	2.32	0.44
1:A:194:ASP:HB2	1:A:195:PHE:HD2	1.82	0.44
1:A:57:MET:CE	1:A:234:TYR:OH	2.65	0.44
1:A:84:PHE:CZ	1:A:126:ILE:HG23	2.53	0.44
1:A:36:ARG:HG2	1:A:36:ARG:NH1	2.32	0.43
1:A:110:ILE:HG13	1:A:110:ILE:H	1.60	0.43
1:A:262:ASP:OD2	1:A:286:GLN:HA	2.18	0.43
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.73	0.43
1:A:447:ARG:HH11	1:A:447:ARG:CB	2.31	0.43
1:A:15:LEU:HD12	1:A:15:LEU:H	1.84	0.43
1:A:222:VAL:HB	1:A:406:VAL:HG22	2.00	0.43
1:A:101:VAL:HG22	1:A:102:LYS:O	2.18	0.42
1:A:251:MET:HE3	1:A:251:MET:HB2	1.90	0.42
1:A:410:GLY:O	1:A:414:LYS:HG3	2.20	0.42
1:A:21:ALA:HB1	1:A:24:GLN:NE2	2.34	0.42
1:A:94:GLY:N	1:A:97:GLY:O	2.52	0.42
1:A:369:ARG:HH12	1:A:372:GLU:HB2	1.85	0.42
1:A:21:ALA:CB	1:A:24:GLN:HE21	2.32	0.41
1:A:192:ARG:C	1:A:194:ASP:H	2.23	0.41
1:A:21:ALA:HB1	1:A:24:GLN:HE21	1.86	0.41
1:A:160:ASP:HB3	1:A:200:VAL:O	2.21	0.41
1:A:237:GLU:HA	1:A:237:GLU:OE2	2.21	0.41
1:A:43:ARG:HH11	1:A:43:ARG:HG2	1.86	0.41
1:A:320:ALA:HB3	1:A:325:ARG:HH11	1.86	0.40
1:A:309:LEU:HD12	1:A:309:LEU:HA	1.85	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:186:ARG:O	1:A:190:LYS:HD2	2.21	0.40
1:A:55:VAL:O	1:A:57:MET:HG2	2.20	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	445/457 (97%)	402 (90%)	28 (6%)	15 (3%)	6	12

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	GLU
1	A	101	VAL
1	A	111	PRO
1	A	116	THR
1	A	136	LYS
1	A	166	ASN
1	A	454	ALA
1	A	458	LYS
1	A	22	GLU
1	A	67	GLU
1	A	135	ASP
1	A	115	MET
1	A	65	THR
1	A	68	GLY
1	A	159	ILE

### 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	383/390 (98%)	339 (88%)	44 (12%)	8 19

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	15	LEU
1	A	32	LYS
1	A	36	ARG
1	A	64	SER
1	A	65	THR
1	A	73	ASP
1	A	82	THR
1	A	83	ASN
1	A	89	VAL
1	A	96	GLU
1	A	98	GLN
1	A	100	SER
1	A	102	LYS
1	A	110	ILE
1	A	127	SER
1	A	140	LYS
1	A	144	LEU
1	A	187	ASP
1	A	190	LYS
1	A	198	ASP
1	A	216	GLU
1	A	218	HIS
1	A	243	LEU
1	A	248	GLU
1	A	257	TRP
1	A	271	LEU
1	A	309	LEU
1	A	310	VAL
1	A	315	LEU
1	A	317	HIS
1	A	325	ARG
1	A	327	ARG
1	A	340	SER
1	A	368	ARG
1	A	369	ARG

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Mol	Chain	Res	Type
1	A	381	MET
1	A	386	LEU
1	A	394	ARG
1	A	397	ARG
1	A	400	ASP
1	A	421	GLU
1	A	447	ARG
1	A	458	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	156	HIS

### 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 ⓘ

2 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	A	500	-	12,12,12	0.82	0	17,17,17	3.27	11 (64%)
3	926	A	501	-	22,22,22	2.01	8 (36%)	28,30,30	2.15	11 (39%)

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	A	500	-	-	0/2/22/22	0/1/1/1
3	926	A	501	-	-	0/8/8/8	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	926	C15-N19	5.75	1.40	1.35
3	A	501	926	C4-C3	2.74	1.47	1.40
3	A	501	926	C12-C7	2.53	1.44	1.39
3	A	501	926	C12-C11	2.41	1.44	1.39
3	A	501	926	C15-N16	2.36	1.38	1.32
3	A	501	926	C5-C4	2.29	1.41	1.36
3	A	501	926	C10-C1	2.26	1.51	1.47
3	A	501	926	C7-C8	2.23	1.43	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	GLC	O5-C1-C2	6.58	120.05	109.86
3	A	501	926	C3-N2-C1	5.06	128.35	122.82
2	A	500	GLC	C4-C3-C2	4.86	119.79	110.82
2	A	500	GLC	C1-O5-C5	4.76	121.93	113.40
2	A	500	GLC	O5-C5-C4	4.04	117.25	109.76
3	A	501	926	C15-S14-C8	4.02	109.48	103.37
2	A	500	GLC	C3-C4-C5	3.80	116.99	110.20
2	A	500	GLC	O4-C4-C5	3.77	119.23	109.28
3	A	501	926	C9-C10-C1	-3.42	114.74	120.51
2	A	500	GLC	O1-C1-O5	-3.36	101.25	110.32
3	A	501	926	C10-C9-C8	3.25	123.20	120.06
3	A	501	926	C11-C10-C1	3.23	126.36	120.67
2	A	500	GLC	C1-C2-C3	3.05	115.36	110.53
3	A	501	926	C4-C5-C6	2.89	124.71	120.25
2	A	500	GLC	O2-C2-C1	2.80	115.85	109.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	926	C7-C8-S14	2.71	128.62	120.38
3	A	501	926	C6-C1-C10	2.63	127.22	122.68
3	A	501	926	C20-N19-C15	-2.46	123.31	125.63
3	A	501	926	C9-C8-S14	-2.37	112.69	119.66
2	A	500	GLC	O1-C1-C2	-2.34	102.83	109.47
2	A	500	GLC	O3-C3-C4	2.15	115.18	110.35
3	A	501	926	C20-N19-C18	2.04	128.78	124.93

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	447/457 (97%)	0.21	11 (2%) 54 61	25, 49, 90, 101	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	GLY	3.7
1	A	82	THR	3.3
1	A	139	MET	2.9
1	A	197	MET	2.7
1	A	141	HIS	2.7
1	A	113	ASP	2.6
1	A	116	THR	2.6
1	A	195	PHE	2.5
1	A	460	ALA	2.5
1	A	319	GLU	2.2
1	A	117	GLY	2.1

### 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	GLC	A	500	12/12	0.20	0.91	32,36,39,40	0
3	926	A	501	20/20	0.16	-0.62	37,40,44,44	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.