



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:34 PM GMT

PDB ID : 1BG3
Title : RAT BRAIN HEXOKINASE TYPE I COMPLEX WITH GLUCOSE AND
INHIBITOR GLUCOSE-6-PHOSPHATE
Authors : Mulichak, A.M.; Garavito, R.M.
Deposited on : 1998-06-04
Resolution : 2.80 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
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 (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

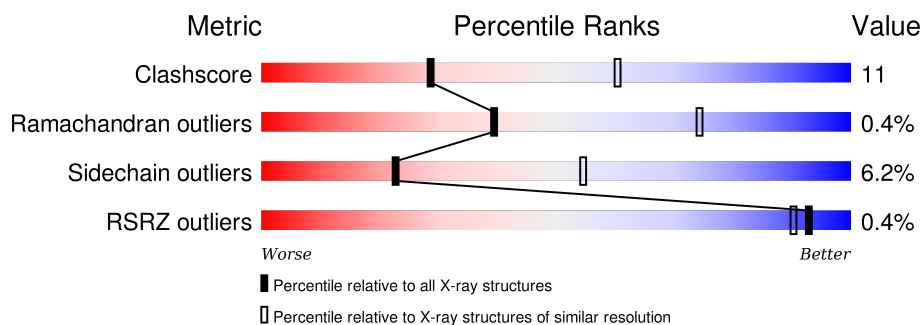
1 Overall quality at a glance

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 ≥ 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	918	
1	B	918	

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
3	G6P	A	1002	X	-	-	-
3	G6P	A	1004	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	G6P	B	1002	X	-	-	-
3	G6P	B	1004	X	-	-	-

2 Entry composition [i](#)

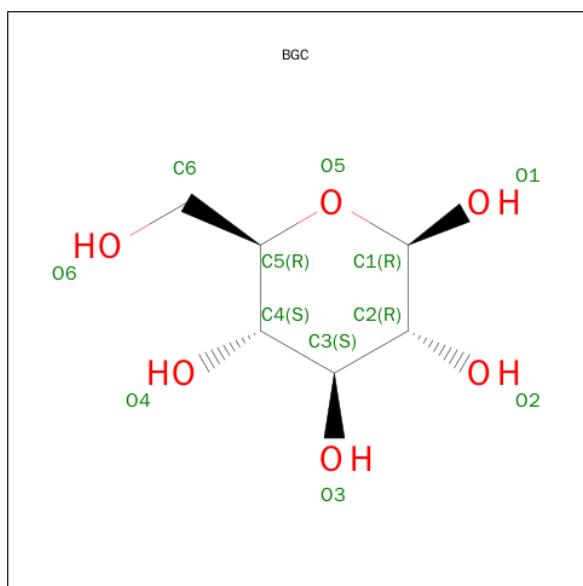
There are 5 unique types of molecules in this entry. The entry contains 13962 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

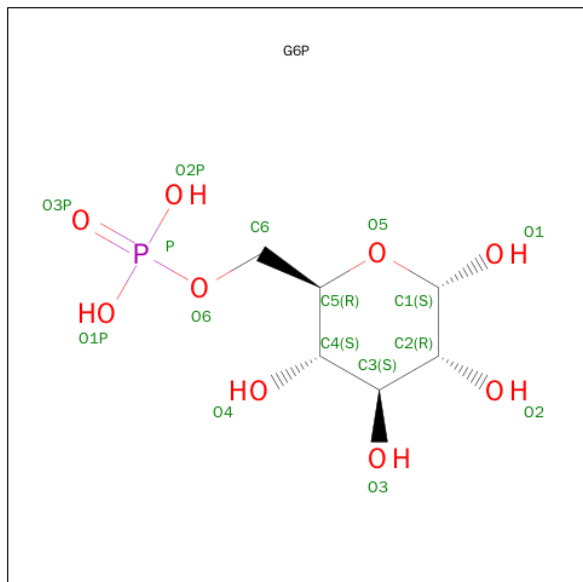
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	902	Total	C	N	O	S	0	0	0
			6832	4304	1177	1296	55			
1	B	902	Total	C	N	O	S	0	0	0
			6783	4276	1157	1295	55			

- Molecule 2 is SUGAR (GLUCOSE) (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



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

- Molecule 3 is SUGAR (ALPHA-D-GLUCOSE-6-PHOSPHATE) (three-letter code: G6P) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		

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

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

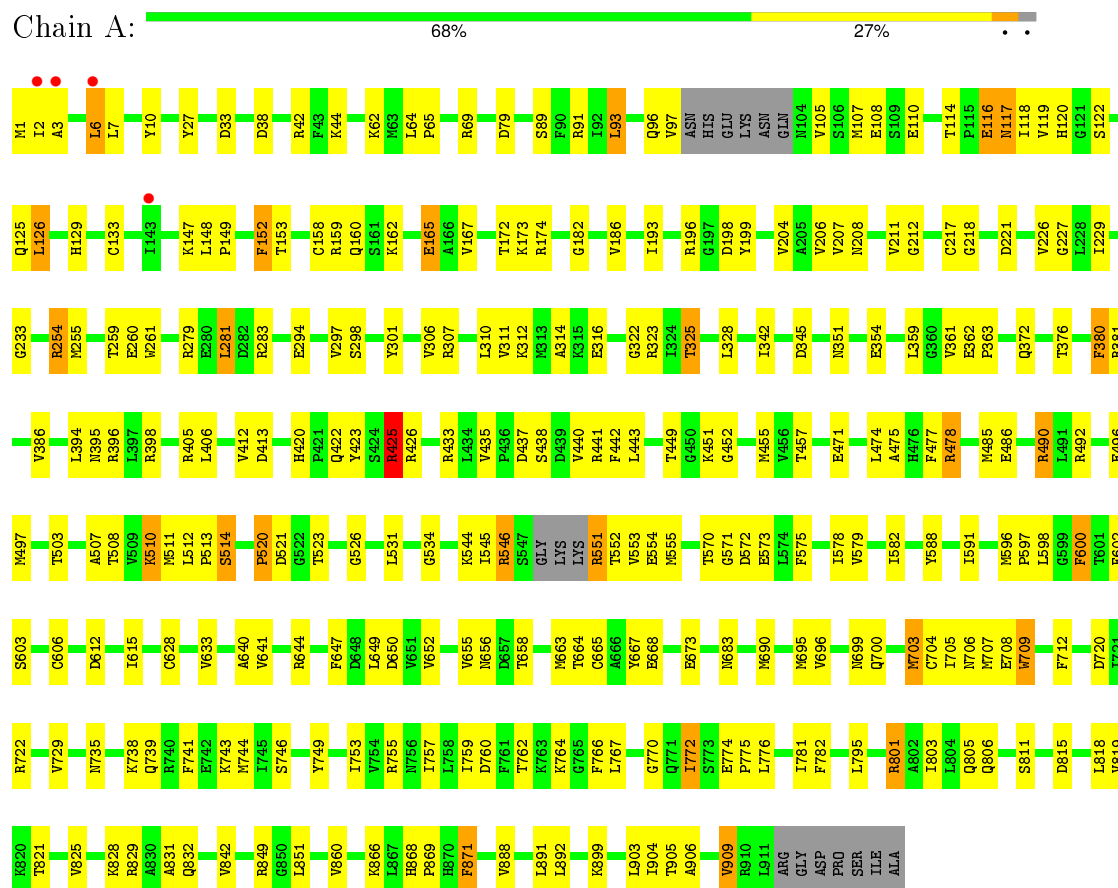
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	136	Total	O	0	0
			136	136		
5	B	98	Total	O	0	0
			98	98		

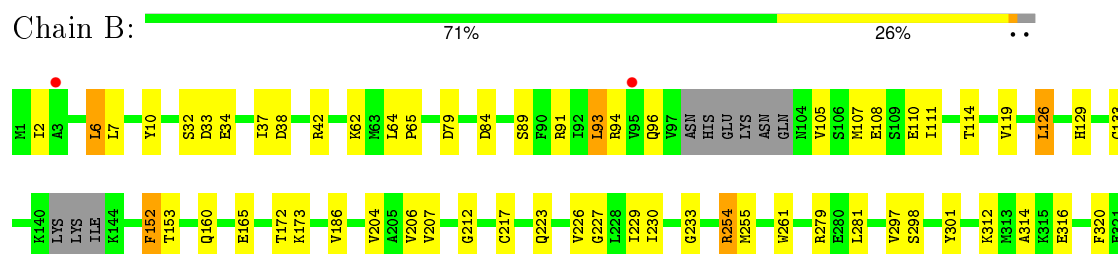
3 Residue-property plots

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: HEXOKINASE



• Molecule 1: HEXOKINASE



L892	L757	V651	V553	L443	G322
R899	I758	V652	E554	T449	R323
	D760	V655	M555	G450	I324
L903	F761	T658	H556	K451	T325
I904	T762		M557	G452	L328
T905	L767	M663	K558	M455	R331
A906	G770	T664	G569	H456	I342
	S773	C665	G571	T457	D345
ARG	L776	E668	D572	R468	
GLY	K777	E669	E573	E471	G348
ASP	I781	P670	L574		I349
PRO		T671	F575	A475	Q350
SER		M683	I578	H476	R351
ILE		E688	V579	F477	A352
ALA		E689	I582	R478	K353
	C813	M690	L586	K481	E354
	D814		L591	M485	R358
	D815	V693	K592	E486	L359
	L818	M695	G593	R492	G380
	V819	Q700			V361
	V825			E496	E362
		M703	M596	M497	P363
	K828	G704	P597	K501	
	R829	I705	L598		F380
		N706	G599		R381
	Q832	N707	F600	A507	V386
	V842	E708	T601	T508	L397
E843	E843	S603	F602	V509	
K844	K844	G710	S603	K510	K401
L845	K844	A711	F604	M511	G402
R846	L845	F712	C605		T403
E847	R846		C606	S514	P404
N848	N847	D720	D612		
B853	N848	I721	C613	P520	V412
		R722	G614	D521	D413
			I615	G522	
		V729	L616	T523	L416
	V860		I617	E524	
		N735	S618	H525	H420
	K866	S736	A625	G526	P421
	B870	G737	T626	L529	Q422
F871	F871	K738	R626	A530	Y423
S872	S872	Q739	D627	L531	S424
R873	R873	R740	C628	L531	R425
I874	I874	F741			R426
		E742	V633	G534	F427
		K743			H428
	L882	M744	A640	L541	
				L542	R433
	K885	I753	F647	V543	L434
C886	C886	V754	D648	K544	
T887	T887	L649	L649	I545	R441
V888	V888	N756	D650	R546	F442

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	132.10Å 77.10Å 137.10Å 90.00° 96.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 38.48 – 2.80	Depositor EDS
% Data completeness (in resolution range)	71.0 (20.00-2.80) 70.6 (38.48-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.81Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.196 , 0.251 0.195 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 74.7	EDS
Estimated twinning fraction	0.045 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 48013 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13962	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BGC, G6P

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	0.62	1/6935 (0.0%)	0.89	15/9367 (0.2%)
1	B	0.62	0/6885	0.90	15/9310 (0.2%)
All	All	0.62	1/13820 (0.0%)	0.90	30/18677 (0.2%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	CYS	CB-SG	-5.23	1.73	1.81

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	ARG	NE-CZ-NH2	-14.98	112.81	120.30
1	B	279	ARG	NE-CZ-NH2	-14.97	112.81	120.30
1	A	279	ARG	NE-CZ-NH2	-14.74	112.93	120.30
1	B	425	ARG	NE-CZ-NH2	-14.09	113.26	120.30
1	B	279	ARG	NE-CZ-NH1	14.07	127.34	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	490	ARG	Sidechain

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	6832	0	6711	177	0
1	B	6783	0	6623	136	0
2	A	24	0	23	2	0
2	B	24	0	24	1	0
3	A	32	0	22	0	0
3	B	32	0	22	0	0
4	A	1	0	0	0	0
5	A	136	0	0	6	0
5	B	98	0	0	0	0
All	All	13962	0	13425	311	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 11.

The worst 5 of 311 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:A:361:VAL:O	1:A:363:PRO:HD3	1.62	1.00
1:B:361:VAL:O	1:B:363:PRO:HD3	1.67	0.93
1:A:312:LYS:O	1:A:316:GLU:HG3	1.80	0.81
1:A:162:LYS:HG3	1:A:165:GLU:HB2	1.62	0.81
1:A:849:ARG:HB2	1:A:851:LEU:HD11	1.62	0.81

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	896/918 (98%)	829 (92%)	65 (7%)	2 (0%)	52	84
1	B	896/918 (98%)	835 (93%)	55 (6%)	6 (1%)	26	62
All	All	1792/1836 (98%)	1664 (93%)	120 (7%)	8 (0%)	39	74

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	345	ASP
1	A	345	ASP
1	A	871	PHE
1	B	871	PHE
1	B	404	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	722/791 (91%)	676 (94%)	46 (6%)	22	52
1	B	714/791 (90%)	671 (94%)	43 (6%)	24	56
All	All	1436/1582 (91%)	1347 (94%)	89 (6%)	23	54

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	772	ILE
1	B	126	LEU
1	B	736	SER
1	A	795	LEU
1	A	909	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	125	GLN
1	B	853	HIS
1	B	384	ASN
1	A	384	ASN
1	B	692	ASN

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 ⓘ

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	BGC	A	1001	-	12,12,12	0.61	0	17,17,17	1.23	1 (5%)
3	G6P	A	1002	-	16,16,16	0.79	0	23,24,24	0.70	0
2	BGC	A	1003	-	12,12,12	0.39	0	17,17,17	0.67	1 (5%)
3	G6P	A	1004	-	16,16,16	0.71	0	23,24,24	0.68	0
2	BGC	B	1001	-	12,12,12	0.48	0	17,17,17	1.14	1 (5%)
3	G6P	B	1002	-	16,16,16	0.74	0	23,24,24	0.83	0
2	BGC	B	1003	-	12,12,12	0.37	0	17,17,17	0.73	1 (5%)
3	G6P	B	1004	-	16,16,16	0.76	0	23,24,24	0.72	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	BGC	A	1001	-	-	0/2/22/22	0/1/1/1
3	G6P	A	1002	-	1/1/6/6	0/6/26/26	0/1/1/1
2	BGC	A	1003	-	-	0/2/22/22	0/1/1/1
3	G6P	A	1004	-	1/1/6/6	0/6/26/26	0/1/1/1
2	BGC	B	1001	-	-	0/2/22/22	0/1/1/1
3	G6P	B	1002	-	1/1/6/6	0/6/26/26	0/1/1/1
2	BGC	B	1003	-	-	0/2/22/22	0/1/1/1
3	G6P	B	1004	-	1/1/6/6	0/6/26/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	BGC	C1-C2-C3	-4.26	104.09	110.43
2	B	1001	BGC	C1-C2-C3	-3.75	104.85	110.43
2	A	1003	BGC	C1-C2-C3	-2.37	106.91	110.43
2	B	1003	BGC	C1-C2-C3	-2.31	106.99	110.43

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1002	G6P	C1
3	A	1002	G6P	C1
3	A	1004	G6P	C1
3	B	1004	G6P	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	BGC	2	0
2	B	1001	BGC	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	902/918 (98%)	-0.43	4 (0%) 93 90	14, 33, 47, 59	0
1	B	902/918 (98%)	-0.46	3 (0%) 94 92	15, 33, 47, 59	0
All	All	1804/1836 (98%)	-0.44	7 (0%) 93 90	14, 33, 47, 59	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ALA	3.3
1	B	95	VAL	3.2
1	A	3	ALA	3.0
1	A	2	ILE	2.9
1	A	6	LEU	2.8

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, 95th 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(\AA^2)	Q<0.9
2	BGC	B	1003	12/12	0.96	0.23	1.22	21,26,29,31	0
2	BGC	B	1001	12/12	0.96	0.18	1.16	23,29,31,31	0
2	BGC	A	1003	12/12	0.96	0.25	0.84	21,26,31,33	0
2	BGC	A	1001	12/12	0.97	0.18	0.56	25,27,29,29	0
3	G6P	B	1004	16/16	0.98	0.19	0.40	35,37,42,43	0
3	G6P	A	1002	16/16	0.97	0.14	0.17	28,31,36,37	0
3	G6P	A	1004	16/16	0.97	0.19	-0.42	36,38,41,45	0
3	G6P	B	1002	16/16	0.97	0.11	-0.71	30,34,42,44	0
4	CA	A	1005	1/1	0.96	0.18	-	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.