



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:01 PM EDT

PDB ID : 6JZ8 / pdb_00006jz8
Title : b-glucuronidase from Ruminococcus gnavus in complex with D-glucaro 1,5-lactone
Authors : Dashnyam, P.; Lin, H.Y.
Deposited on : 2019-04-30
Resolution : 1.58 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

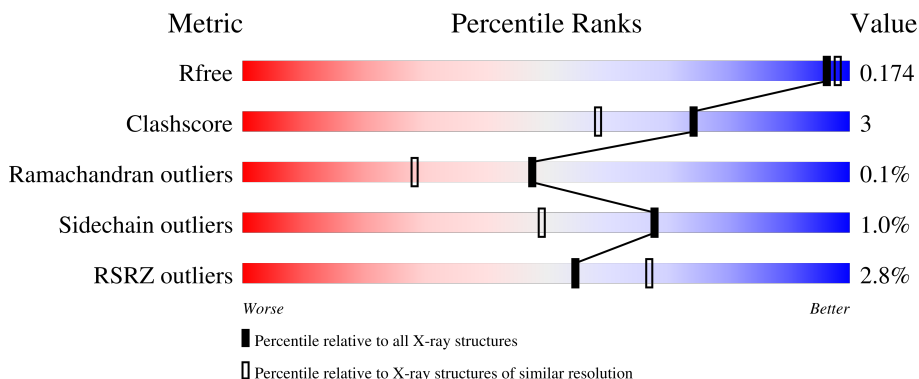
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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}	180053	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	603	 2% 90% 6% •
1	B	603	 3% 88% 7% •

2 Entry composition [i](#)

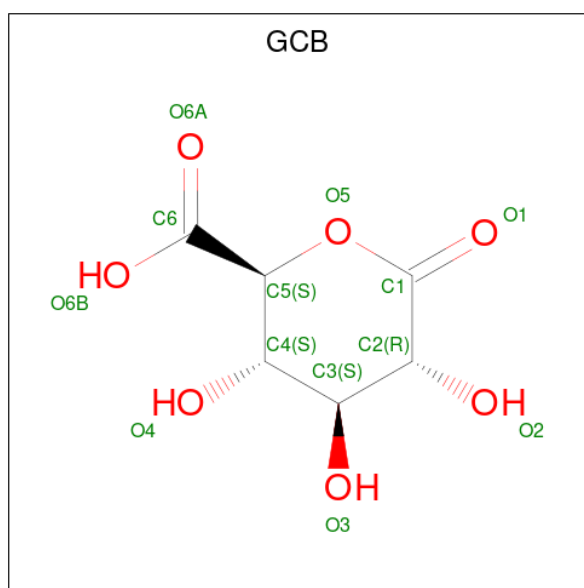
There are 3 unique types of molecules in this entry. The entry contains 10614 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4769	3071	779	895	24			
1	B	576	Total	C	N	O	S	0	0	0
			4717	3042	767	885	23			

- Molecule 2 is (2S,3S,4S,5R)-3,4,5-trihydroxy-6-oxo-oxane-2-carboxylic acid (CCD ID: GCB) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

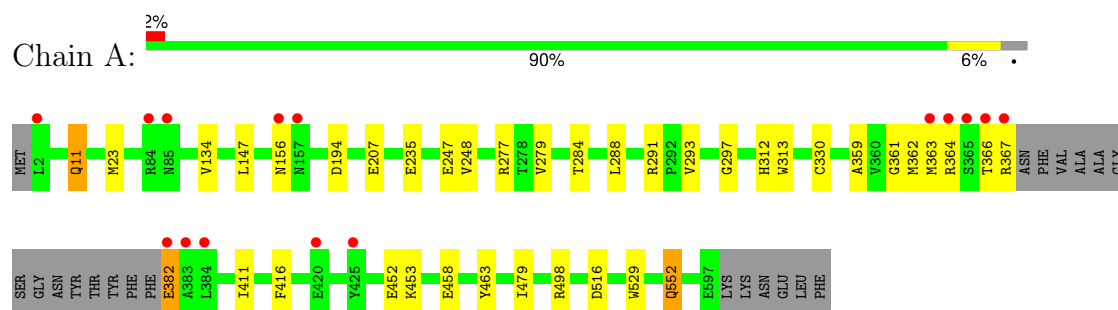
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	581	Total 581	O 581	0	0
3	B	521	Total 521	O 521	0	0

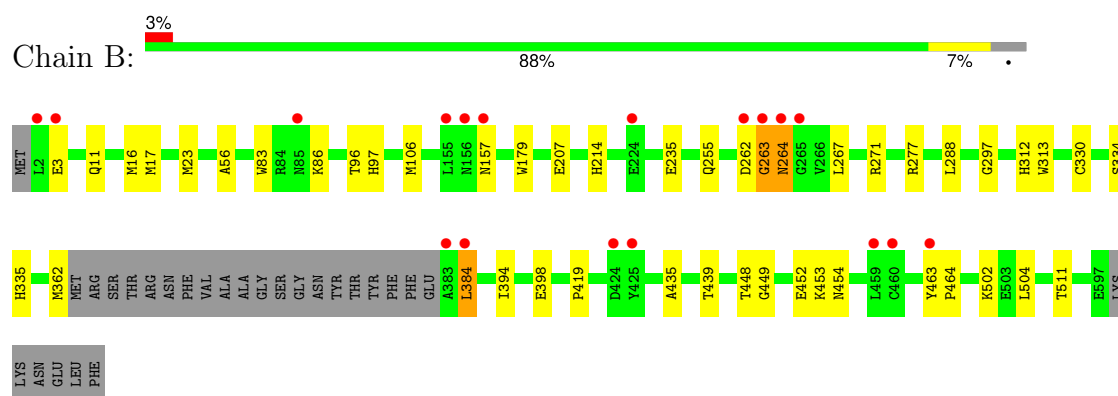
3 Residue-property plots [i](#)

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

• Molecule 1: Beta-glucuronidase



• Molecule 1: Beta-glucuronidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.56Å 103.34Å 112.28Å 90.00° 130.99° 90.00°	Depositor
Resolution (Å)	29.95 – 1.58 29.95 – 1.58	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.95-1.58) 96.2 (29.95-1.58)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.58Å)	Xtriage
Refinement program	PHENIX 1.9 1692	Depositor
R, R_{free}	0.163 , 0.174 0.162 , 0.174	Depositor DCC
R_{free} test set	1996 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10614	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GCB

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	0.65	3/4903 (0.1%)	0.81	3/6647 (0.0%)
1	B	0.63	4/4851 (0.1%)	0.82	4/6579 (0.1%)
All	All	0.64	7/9754 (0.1%)	0.82	7/13226 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	449	GLY	C-O	-7.30	1.16	1.23
1	A	552	GLN	CD-OE1	-7.26	1.09	1.23
1	B	277	ARG	C-O	-6.73	1.15	1.23
1	A	11	GLN	C-O	-6.63	1.16	1.24
1	B	448	THR	C-O	-5.56	1.18	1.23
1	B	288	LEU	C-O	-5.31	1.18	1.24
1	A	277	ARG	C-O	-5.10	1.17	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	263	GLY	CA-C-N	6.17	132.81	121.70
1	B	263	GLY	C-N-CA	6.17	132.81	121.70
1	B	86	LYS	N-CA-C	-5.69	102.04	110.46
1	A	463	TYR	CA-C-N	-5.25	114.41	119.87
1	A	463	TYR	C-N-CA	-5.25	114.41	119.87
1	A	361	GLY	N-CA-C	-5.18	107.89	115.72
1	B	56	ALA	N-CA-C	5.04	116.78	111.28

There are no chirality outliers.

There are no planarity outliers.

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	4769	0	4559	30	0
1	B	4717	0	4506	33	0
2	A	13	0	0	0	0
2	B	13	0	0	0	0
3	A	581	0	0	6	0
3	B	521	0	0	1	0
All	All	10614	0	9065	58	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 3.

All (58) 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:364:ARG:HG3	1:A:367:ARG:HH12	1.12	1.06
1:A:364:ARG:HG3	1:A:367:ARG:NH1	1.90	0.87
1:B:255:GLN:HE21	1:B:271:ARG:HD3	1.44	0.83
1:A:312:HIS:HD2	1:B:312:HIS:HD2	1.31	0.77
1:B:263:GLY:HA3	1:B:264:ASN:CB	2.15	0.76
1:A:363:MET:HE3	1:A:366:THR:OG1	1.87	0.75
1:A:248:VAL:HG23	1:A:288:LEU:HD22	1.73	0.70
1:A:312:HIS:HD2	1:B:312:HIS:CD2	2.11	0.68
1:A:364:ARG:CG	1:A:367:ARG:HH12	2.01	0.66
1:B:384:LEU:HD12	1:B:384:LEU:H	1.61	0.65
1:A:312:HIS:CD2	1:B:312:HIS:HD2	2.12	0.65
1:B:263:GLY:HA3	1:B:264:ASN:HB3	1.77	0.65
1:A:382:GLU:OE1	1:A:382:GLU:N	2.31	0.64
1:B:384:LEU:H	1:B:384:LEU:CD1	2.13	0.62
1:B:255:GLN:NE2	1:B:271:ARG:HD3	2.12	0.62
1:A:247:GLU:OE2	1:A:291:ARG:NH2	2.33	0.60
1:A:453:LYS:HD2	1:A:479:ILE:HD11	1.83	0.60
1:B:362:MET:HE2	1:B:419:PRO:HB3	1.83	0.60
1:B:255:GLN:NE2	1:B:271:ARG:HH21	2.00	0.60
1:B:214:HIS:CD2	1:B:262:ASP:HB2	2.37	0.59
1:A:147:LEU:HD21	1:A:362:MET:HE3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ASN:ND2	3:B:801:HOH:O	2.21	0.57
1:A:284:THR:O	1:A:552:GLN:HG3	2.06	0.55
1:A:293:VAL:HG22	3:A:966:HOH:O	2.07	0.55
1:A:458:GLU:OE2	1:A:498:ARG:HD2	2.07	0.54
1:B:263:GLY:HA3	1:B:264:ASN:HB2	1.88	0.54
1:B:452:GLU:OE1	1:B:454:ASN:ND2	2.40	0.54
1:A:279:VAL:HG21	1:A:411:ILE:HG22	1.89	0.53
1:A:363:MET:HB2	3:A:960:HOH:O	2.09	0.52
1:B:502:LYS:HB2	1:B:504:LEU:HD11	1.90	0.52
1:B:502:LYS:HB2	1:B:504:LEU:CD1	2.39	0.52
1:A:23:MET:HG2	1:B:313:TRP:CD2	2.46	0.51
1:A:248:VAL:CG2	1:A:288:LEU:HD22	2.38	0.51
1:B:463:TYR:OH	1:B:502:LYS:NZ	2.40	0.50
1:A:156:ASN:HB3	3:A:1118:HOH:O	2.11	0.49
1:B:435:ALA:O	1:B:439:THR:HG23	2.13	0.48
1:A:207:GLU:HG2	1:A:235:GLU:HG2	1.94	0.48
1:A:362:MET:HB2	3:A:1136:HOH:O	2.14	0.47
1:B:504:LEU:HD12	1:B:504:LEU:N	2.30	0.47
1:A:279:VAL:HG22	1:A:288:LEU:HD12	1.96	0.47
1:A:194:ASP:OD2	3:A:801:HOH:O	2.21	0.45
1:A:552:GLN:OE1	3:A:802:HOH:O	2.21	0.43
1:A:297:GLY:HA3	1:A:330:CYS:O	2.19	0.42
1:B:16:MET:HE2	1:B:83:TRP:CD1	2.54	0.42
1:B:263:GLY:CA	1:B:264:ASN:CB	2.94	0.42
1:B:96:THR:HA	1:B:97:HIS:HA	1.84	0.42
1:B:463:TYR:CG	1:B:464:PRO:HD3	2.55	0.42
1:B:384:LEU:HD12	1:B:384:LEU:N	2.32	0.41
1:B:297:GLY:HA3	1:B:330:CYS:O	2.20	0.41
1:B:334:SER:HA	1:B:335:HIS:HA	1.81	0.41
1:B:394:ILE:O	1:B:398:GLU:HG3	2.21	0.41
1:A:359:ALA:HB3	1:A:416:PHE:HA	2.03	0.41
1:B:106:MET:HE3	1:B:106:MET:HB3	1.97	0.41
1:A:313:TRP:CD2	1:B:23:MET:HG2	2.56	0.40
1:A:364:ARG:HH11	1:A:364:ARG:HD2	1.73	0.40
1:A:516:ASP:O	1:A:529:TRP:HA	2.22	0.40
1:B:17:MET:HE2	1:B:179:TRP:CZ3	2.57	0.40
1:B:207:GLU:HG2	1:B:235:GLU:HG2	2.03	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	A	578/603 (96%)	563 (97%)	15 (3%)	0	100	100
1	B	572/603 (95%)	552 (96%)	19 (3%)	1 (0%)	43	26
All	All	1150/1206 (95%)	1115 (97%)	34 (3%)	1 (0%)	48	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	264	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	508/525 (97%)	504 (99%)	4 (1%)	73	57
1	B	502/525 (96%)	496 (99%)	6 (1%)	63	40
All	All	1010/1050 (96%)	1000 (99%)	10 (1%)	68	49

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	134	VAL
1	A	382	GLU
1	A	452	GLU
1	B	3	GLU

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Mol	Chain	Res	Type
1	B	11	GLN
1	B	267	LEU
1	B	384	LEU
1	B	453	LYS
1	B	511	THR

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

Mol	Chain	Res	Type
1	A	18	GLN
1	A	130	GLN
1	A	584	GLN
1	B	18	GLN
1	B	255	GLN
1	B	454	ASN
1	B	584	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	GCB	B	701	-	13,13,13	2.43	6 (46%)	16,19,19	1.55	2 (12%)
2	GCB	A	701	-	13,13,13	2.42	7 (53%)	16,19,19	1.47	2 (12%)

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	GCB	B	701	-	-	0/4/24/24	0/1/1/1
2	GCB	A	701	-	-	0/4/24/24	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	GCB	C2-C1	-5.30	1.40	1.52
2	A	701	GCB	C2-C1	-5.19	1.40	1.52
2	B	701	GCB	O3-C3	-3.92	1.33	1.43
2	A	701	GCB	C4-C5	-3.56	1.47	1.53
2	B	701	GCB	C4-C5	-3.22	1.47	1.53
2	B	701	GCB	O6B-C6	-3.06	1.20	1.30
2	A	701	GCB	O5-C5	-2.93	1.41	1.46
2	B	701	GCB	O4-C4	-2.41	1.37	1.43
2	A	701	GCB	O4-C4	-2.40	1.37	1.43
2	B	701	GCB	C3-C2	2.30	1.56	1.53
2	A	701	GCB	O2-C2	-2.19	1.37	1.42
2	A	701	GCB	O6B-C6	-2.15	1.23	1.30
2	A	701	GCB	O3-C3	-2.14	1.37	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	GCB	C3-C4-C5	-4.34	101.83	109.30
2	A	701	GCB	C3-C4-C5	-4.25	101.99	109.30
2	B	701	GCB	O6A-C6-C5	-2.27	112.61	120.81
2	A	701	GCB	O5-C1-O1	2.06	121.50	118.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	582/603 (96%)	-0.13	15 (2%) 57 68	8, 14, 29, 53	0
1	B	576/603 (95%)	-0.05	18 (3%) 51 64	8, 14, 31, 53	0
All	All	1158/1206 (96%)	-0.09	33 (2%) 55 67	8, 14, 30, 53	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	156	ASN	6.1
1	B	384	LEU	6.0
1	B	425	TYR	4.7
1	A	367	ARG	4.5
1	B	383	ALA	4.4
1	A	425	TYR	4.3
1	A	363	MET	4.3
1	B	2	LEU	4.0
1	B	459	LEU	3.9
1	A	366	THR	3.8
1	B	263	GLY	3.5
1	A	384	LEU	3.5
1	B	264	ASN	3.4
1	B	262	ASP	3.3
1	A	364	ARG	3.3
1	A	85	ASN	3.0
1	A	2	LEU	3.0
1	A	382	GLU	2.9
1	A	383	ALA	2.7
1	B	85	ASN	2.7
1	A	84	ARG	2.7
1	B	155	LEU	2.6
1	B	157	ASN	2.5
1	B	463	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	365	SER	2.5
1	A	156	ASN	2.4
1	B	224	GLU	2.4
1	B	265	GLY	2.3
1	B	424	ASP	2.2
1	B	460	CYS	2.2
1	A	157	ASN	2.1
1	A	420	GLU	2.1
1	B	3	GLU	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	GCB	A	701	13/13	0.95	0.07	9,11,19,27	0
2	GCB	B	701	13/13	0.95	0.07	10,13,19,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.