



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:44 AM GMT

PDB ID : 2NZT  
Title : Crystal structure of human hexokinase II  
Authors : Rabeh, W.M.; Zhu, H.; Nedyalkova, L.; Tempel, W.; Wasney, G.; Landry, R.; Vedadi, M.; Arrowsmith, C.H.; Edwards, A.M.; Sundstrom, M.; Weigelt, J.; Bochkarev, A.; Park, H.; Structural Genomics Consortium (SGC)  
Deposited on : 2006-11-25  
Resolution : 2.45 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

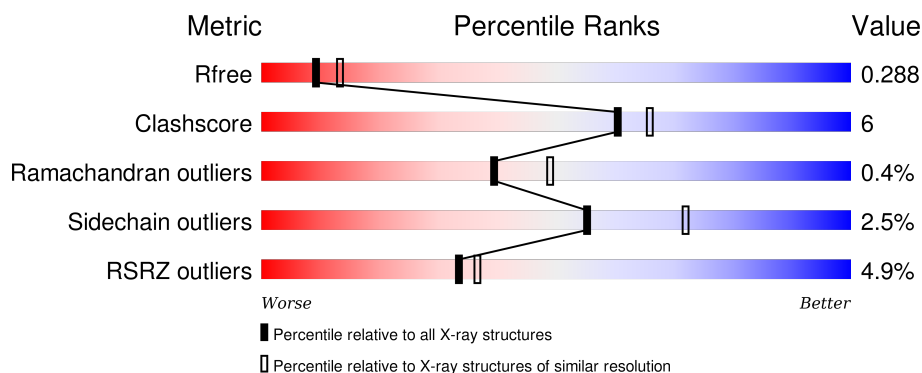
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
$R_{free}$	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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	A	902	<div> <div>4%</div> <div>82%</div> <div>14%</div> <div>• •</div> </div>
1	B	902	<div> <div>5%</div> <div>83%</div> <div>12%</div> <div>• •</div> </div>

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
4	UNX	A	1	-	-	-	X
4	UNX	A	10	-	-	-	X
4	UNX	A	1006	-	-	-	X
4	UNX	A	1007	-	-	-	X
4	UNX	A	1008	-	-	-	X
4	UNX	A	1009	-	-	-	X
4	UNX	A	11	-	-	-	X
4	UNX	A	4	-	-	-	X
4	UNX	A	6	-	-	-	X
4	UNX	A	8	-	-	-	X
4	UNX	A	9	-	-	-	X
4	UNX	B	1005	-	-	-	X
4	UNX	B	1006	-	-	-	X
4	UNX	B	1009	-	-	-	X
4	UNX	B	1012	-	-	-	X
4	UNX	B	1013	-	-	-	X
4	UNX	B	12	-	-	-	X
4	UNX	B	13	-	-	-	X
4	UNX	B	14	-	-	-	X
4	UNX	B	2	-	-	-	X
4	UNX	B	3	-	-	-	X
4	UNX	B	5	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13546 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.

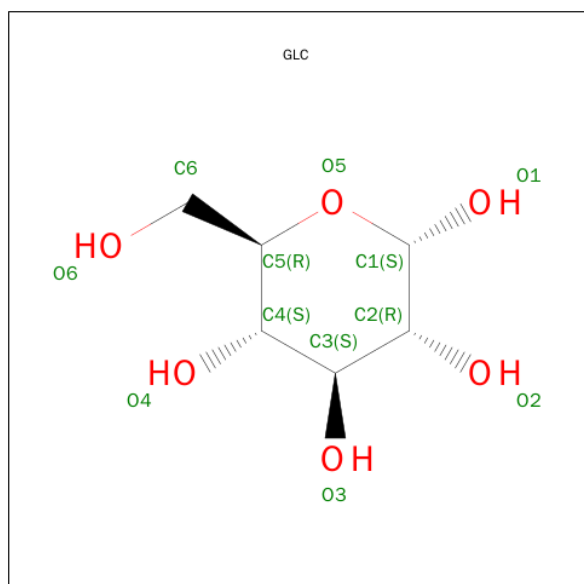
- Molecule 1 is a protein called Hexokinase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	871	Total	C	N	O	S	0	0	0
			6653	4181	1157	1253	62			
1	B	867	Total	C	N	O	S	0	0	0
			6656	4181	1157	1256	62			

There are 4 discrepancies between the modelled and reference sequences:

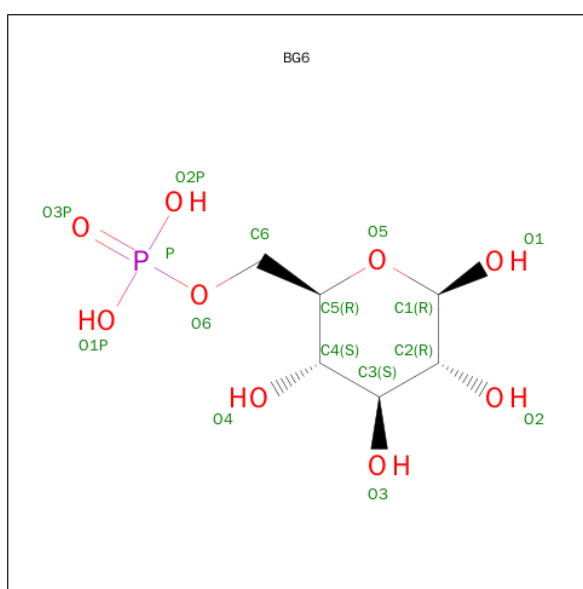
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	-	CLONING ARTIFACT	UNP P52789
A	16	SER	-	CLONING ARTIFACT	UNP P52789
B	15	GLY	-	CLONING ARTIFACT	UNP P52789
B	16	SER	-	CLONING ARTIFACT	UNP P52789

- 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		
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 (BETA-D-GLUCOSE-6-PHOSPHATE) (three-letter code: BG6) (formula: C<sub>6</sub>H<sub>13</sub>O<sub>9</sub>P).



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 UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	16	Total	X	0	0
			16	16		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	X	0	0
			12	12		

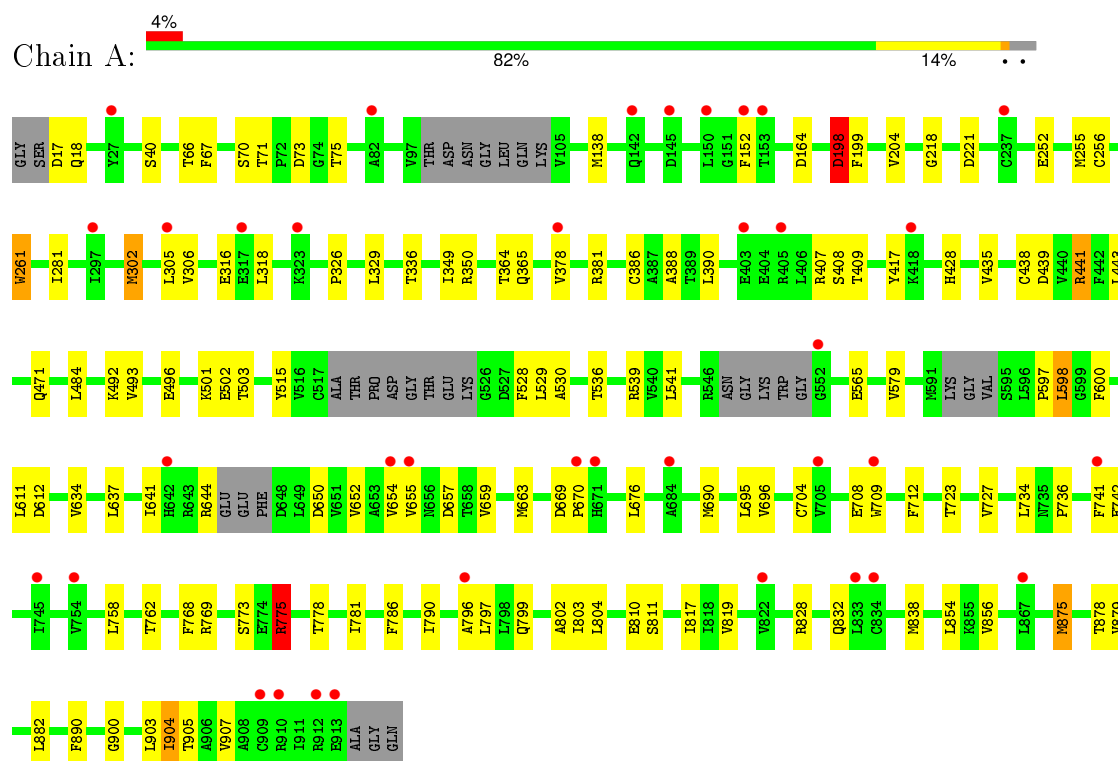
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	49	Total	O	0	0
			49	49		
5	B	48	Total	O	0	0
			48	48		

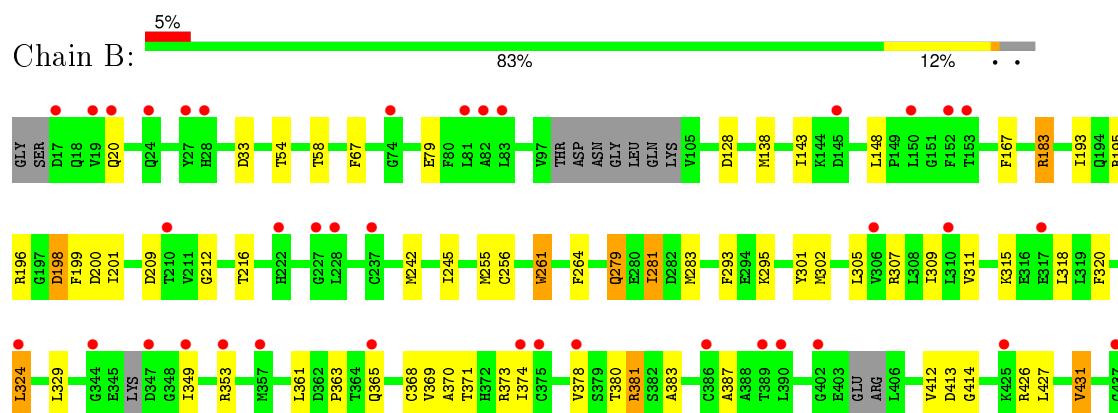
### 3 Residue-property plots [i](#)

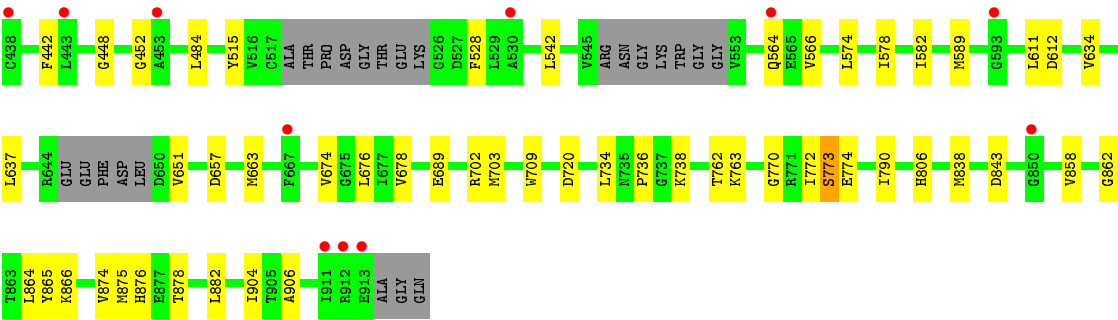
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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-2



#### • Molecule 1: Hexokinase-2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.89Å 129.34Å 187.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.45 24.74 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.2 (25.00-2.45) 98.2 (24.74-2.45)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 2.44Å)	Xtriage
Refinement program	REFMAC 5.2.0019, COOT, PRODRG, MOLPROBITY	Depositor
R, $R_{free}$	0.230 , 0.287 0.234 , 0.288	Depositor DCC
$R_{free}$ test set	2083 reflections (2.55%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 83669 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13546	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 2.89% 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: UNX, GLC, BG6

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	0.79	1/6751 (0.0%)	0.74	2/9091 (0.0%)
1	B	0.82	2/6755 (0.0%)	0.74	2/9095 (0.0%)
All	All	0.80	3/13506 (0.0%)	0.74	4/18186 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	256	CYS	CB-SG	-5.29	1.73	1.81
1	A	810	GLU	CG-CD	5.07	1.59	1.51
1	B	773	SER	CB-OG	5.03	1.48	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	775	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	B	183	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	381	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	539	ARG	NE-CZ-NH1	5.04	122.82	120.30

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	6653	0	6557	78	0
1	B	6656	0	6565	73	0
2	A	24	0	23	1	0
2	B	24	0	24	0	0
3	A	32	0	22	0	0
3	B	32	0	22	1	0
4	A	12	0	0	0	0
4	B	16	0	0	0	0
5	A	49	0	0	0	0
5	B	48	0	0	0	0
All	All	13546	0	13213	149	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 6.

All (149) 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:B:216:THR:HG22	1:B:452:GLY:H	1.13	1.13
1:B:216:THR:HG22	1:B:452:GLY:N	1.83	0.93
1:A:655:VAL:HG11	1:A:904:ILE:HD12	1.52	0.91
1:B:542:LEU:HD23	1:B:589:MET:CE	2.06	0.85
1:B:542:LEU:HD23	1:B:589:MET:HE2	1.57	0.84
1:B:365:GLN:O	1:B:369:VAL:HG23	1.80	0.80
1:B:216:THR:HG21	1:B:448:GLY:O	1.88	0.74
1:A:875:MET:HE1	1:A:890:PHE:CZ	2.31	0.66
1:A:435:VAL:CG1	1:A:438:CYS:SG	2.85	0.65
1:A:435:VAL:HG11	1:A:438:CYS:SG	2.37	0.64
1:A:281:ILE:HG13	1:A:305:LEU:HD13	1.79	0.64
1:A:758:LEU:O	1:A:762:THR:HG23	1.98	0.63
1:A:775:ARG:HH11	1:A:775:ARG:CG	2.12	0.63
1:A:652:VAL:HB	1:A:905:THR:HG23	1.81	0.62
1:A:501:LYS:HB3	1:A:695:LEU:HD23	1.80	0.62
1:A:796:ALA:O	1:A:799:GLN:HB2	1.99	0.62
1:A:612:ASP:O	1:A:634:VAL:HG21	1.99	0.61
1:A:306:VAL:HG22	1:A:378:VAL:HG21	1.82	0.61
1:B:387:ALA:HB2	1:B:427:LEU:HD12	1.83	0.61
1:A:306:VAL:CG2	1:A:378:VAL:HG21	2.30	0.60
1:A:903:LEU:O	1:A:907:VAL:HG23	2.02	0.59
1:B:542:LEU:HD23	1:B:589:MET:HE3	1.84	0.59
1:A:676:LEU:HD13	1:A:838:MET:CE	2.33	0.58
1:B:763:LYS:HB3	1:B:772:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:TYR:O	1:A:611:LEU:HD13	2.05	0.57
1:B:862:GLY:O	1:B:866:LYS:HG2	2.04	0.57
1:B:412:VAL:HG12	1:B:413:ASP:N	2.20	0.57
1:B:515:TYR:O	1:B:611:LEU:HD13	2.05	0.57
1:A:73:ASP:HB3	1:A:75:THR:HG23	1.86	0.56
1:B:637:LEU:HD23	1:B:651:VAL:HG21	1.88	0.56
1:A:797:LEU:HD11	1:A:817:ILE:HG23	1.87	0.55
1:B:307:ARG:O	1:B:311:VAL:HG23	2.05	0.55
1:B:663:MET:HG3	1:B:904:ILE:HD11	1.87	0.55
1:A:799:GLN:O	1:A:802:ALA:HB3	2.06	0.55
1:B:515:TYR:CD2	1:B:703:MET:HE1	2.42	0.55
1:B:874:VAL:O	1:B:878:THR:OG1	2.21	0.55
1:A:786:PHE:O	1:A:790:ILE:HD12	2.06	0.55
1:B:320:PHE:CE2	1:B:361:LEU:HD13	2.42	0.55
1:A:778:THR:HG22	1:A:781:ILE:HG23	1.89	0.54
1:B:79:GLU:O	1:B:148:LEU:HD22	2.08	0.54
1:B:542:LEU:CD2	1:B:589:MET:HE3	2.38	0.53
1:B:383:ALA:O	1:B:427:LEU:HD13	2.08	0.53
1:A:797:LEU:HD11	1:A:817:ILE:CG2	2.39	0.53
1:B:678:VAL:HG12	1:B:864:LEU:HD23	1.90	0.53
1:B:216:THR:CG2	1:B:452:GLY:H	2.01	0.53
1:B:138:MET:SD	1:B:199:PHE:CD2	3.02	0.53
1:A:854:LEU:HD21	1:A:856:VAL:HG21	1.89	0.53
1:B:353:ARG:NH2	1:B:363:PRO:O	2.42	0.53
1:B:875:MET:HE2	1:B:876:HIS:CD2	2.44	0.53
1:A:407:ARG:HD3	1:A:439:ASP:OD2	2.08	0.52
1:A:854:LEU:HG	1:A:856:VAL:HG23	1.91	0.52
1:A:261:TRP:HH2	1:A:390:LEU:HD13	1.73	0.52
1:B:193:ILE:HG23	1:B:199:PHE:CE1	2.45	0.52
1:A:723:THR:O	1:A:727:VAL:HG23	2.10	0.52
1:A:435:VAL:HG12	1:A:438:CYS:SG	2.50	0.52
1:B:264:PHE:O	1:B:293:PHE:HB2	2.10	0.52
1:A:875:MET:HE1	1:A:879:VAL:HG21	1.92	0.51
1:B:564:GLN:HA	1:B:564:GLN:OE1	2.10	0.51
1:B:431:VAL:HG11	1:B:442:PHE:HZ	1.76	0.51
1:B:295:LYS:HA	1:B:301:TYR:CD2	2.45	0.51
1:A:17:ASP:CG	1:A:18:GLN:H	2.13	0.51
1:B:128:ASP:OD1	1:B:195:ARG:NH1	2.43	0.51
1:B:309:ILE:HG22	1:B:374:ILE:HD13	1.91	0.51
1:A:67:PHE:HA	1:A:255:MET:HE2	1.92	0.51
1:A:875:MET:O	1:A:879:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:GLY:HA2	3:B:1002:BG6:O6	2.11	0.50
1:B:196:ARG:HB3	1:B:198:ASP:HB2	1.92	0.50
1:A:734:LEU:C	1:A:736:PRO:HD3	2.32	0.50
1:B:212:GLY:O	1:B:216:THR:HG23	2.11	0.49
1:B:305:LEU:HD21	1:B:381:ARG:NH2	2.26	0.49
1:B:528:PHE:CZ	1:B:906:ALA:HB2	2.47	0.49
1:B:311:VAL:O	1:B:315:LYS:HG3	2.12	0.49
1:A:326:PRO:HA	1:A:329:LEU:HD12	1.94	0.49
1:A:762:THR:HG21	1:A:768:PHE:HD1	1.78	0.49
1:A:138:MET:SD	1:A:199:PHE:CD2	3.06	0.48
1:A:775:ARG:HH11	1:A:775:ARG:HG3	1.78	0.48
1:A:712:PHE:HB3	1:A:741:PHE:HB2	1.95	0.48
1:B:865:TYR:HE1	1:B:875:MET:HE1	1.78	0.48
1:A:690:MET:CE	1:A:696:VAL:HG12	2.44	0.48
1:B:566:VAL:HG13	1:B:574:LEU:HA	1.96	0.48
1:A:502:GLU:HG2	1:A:503:THR:HG23	1.96	0.47
1:B:689:GLU:OE2	1:B:702:ARG:HG2	2.14	0.47
1:A:349:ILE:HG13	1:A:350:ARG:N	2.28	0.47
1:B:242:MET:HA	1:B:245:ILE:HD12	1.95	0.47
1:A:484:LEU:HB3	1:A:882:LEU:HD11	1.97	0.47
1:B:578:ILE:O	1:B:582:ILE:HG13	2.15	0.47
1:B:200:ASP:OD1	1:B:201:ILE:N	2.44	0.47
1:B:657:ASP:OD1	1:B:657:ASP:N	2.48	0.47
1:B:674:VAL:HB	1:B:858:VAL:HG22	1.96	0.47
1:A:364:THR:O	1:A:365:GLN:C	2.52	0.47
1:B:279:GLN:O	1:B:283:MET:HG2	2.15	0.47
1:B:209:ASP:N	1:B:209:ASP:OD1	2.45	0.46
1:B:676:LEU:HD13	1:B:838:MET:CE	2.44	0.46
1:A:492:LYS:O	1:A:496:GLU:HG3	2.14	0.46
1:B:542:LEU:CD2	1:B:589:MET:CE	2.87	0.46
1:A:409:THR:HG23	1:A:441:ARG:HG2	1.97	0.46
1:B:515:TYR:HA	1:B:703:MET:CE	2.46	0.45
1:A:164:ASP:HA	1:A:204:VAL:O	2.16	0.45
1:B:309:ILE:CG2	1:B:374:ILE:HD13	2.46	0.45
1:A:878:THR:HG22	1:A:882:LEU:HD12	1.99	0.44
1:A:530:ALA:HB3	1:A:541:LEU:HB2	1.98	0.44
1:A:676:LEU:HD13	1:A:838:MET:HE1	1.99	0.44
1:A:690:MET:HE1	1:A:696:VAL:HG12	2.00	0.44
1:A:659:VAL:HG22	1:A:704:CYS:SG	2.58	0.44
1:A:803:ILE:CG1	1:B:58:THR:HG21	2.47	0.44
1:A:828:ARG:O	1:A:832:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:LEU:HD21	1:A:819:VAL:HG11	1.99	0.44
1:B:167:PHE:HA	1:B:183:ARG:O	2.18	0.44
1:B:324:LEU:HD22	1:B:329:LEU:HD21	1.99	0.43
1:B:370:ALA:O	1:B:373:ARG:N	2.50	0.43
1:A:316:GLU:HB3	1:A:318:LEU:HD13	1.99	0.43
1:A:316:GLU:HB3	1:A:318:LEU:CD1	2.48	0.43
1:B:349:ILE:HD13	1:B:369:VAL:HG22	2.00	0.43
1:A:579:VAL:HG12	1:A:644:ARG:HD3	2.00	0.43
1:A:302:MET:CE	1:A:336:THR:HG23	2.49	0.42
1:B:281:ILE:HD12	1:B:305:LEU:HD13	2.01	0.42
1:A:803:ILE:HG13	1:B:58:THR:HG21	2.01	0.42
1:A:40:SER:CB	1:A:388:ALA:O	2.67	0.42
1:B:720:ASP:OD1	1:B:720:ASP:N	2.51	0.42
1:A:708:GLU:OE2	2:A:1003:GLC:O3	2.30	0.42
1:A:600:PHE:HB3	1:A:654:VAL:HG22	2.01	0.42
1:A:218:GLY:HA2	1:A:221:ASP:O	2.19	0.42
1:B:612:ASP:O	1:B:634:VAL:HG21	2.20	0.42
1:B:380:THR:OG1	1:B:426:ARG:CZ	2.67	0.42
1:B:67:PHE:HA	1:B:255:MET:HE2	2.02	0.42
1:B:281:ILE:CD1	1:B:305:LEU:HD13	2.50	0.42
1:A:66:THR:OG1	1:A:256:CYS:HB3	2.20	0.42
1:A:650:ASP:O	1:A:652:VAL:HG23	2.20	0.41
1:A:529:LEU:HB3	1:A:598:LEU:HD12	2.01	0.41
1:A:528:PHE:CD2	1:A:597:PRO:HG2	2.55	0.41
1:A:663:MET:HB2	1:A:900:GLY:HA3	2.02	0.41
1:B:349:ILE:HG23	1:B:368:CYS:HB3	2.02	0.41
1:A:669:ASP:OD1	1:A:669:ASP:C	2.59	0.41
1:A:612:ASP:HB3	1:A:652:VAL:O	2.21	0.41
1:A:637:LEU:O	1:A:641:ILE:HG13	2.21	0.41
1:B:734:LEU:C	1:B:736:PRO:HD3	2.40	0.41
1:A:305:LEU:HD21	1:A:381:ARG:NH2	2.35	0.41
1:A:417:TYR:OH	1:A:428:HIS:NE2	2.33	0.41
1:B:875:MET:CE	1:B:876:HIS:CD2	3.04	0.40
1:A:386:CYS:O	1:A:390:LEU:HB2	2.21	0.40
1:A:198:ASP:HB3	1:A:199:PHE:HD1	1.86	0.40
1:A:70:SER:OG	1:A:71:THR:O	2.38	0.40
1:B:302:MET:HG2	1:B:378:VAL:HG12	2.02	0.40
1:B:261:TRP:CD1	1:B:261:TRP:C	2.94	0.40
1:B:484:LEU:HB3	1:B:882:LEU:HD11	2.03	0.40
1:B:370:ALA:O	1:B:371:THR:C	2.60	0.40
1:A:797:LEU:CD1	1:A:817:ILE:HG22	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:ASP:N	1:A:657:ASP:OD1	2.52	0.40
1:B:762:THR:O	1:B:770:GLY:HA2	2.20	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	859/902 (95%)	825 (96%)	30 (4%)	4 (0%)	34	41
1	B	853/902 (95%)	815 (96%)	36 (4%)	2 (0%)	52	64
All	All	1712/1804 (95%)	1640 (96%)	66 (4%)	6 (0%)	39	49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	565	GLU
1	B	198	ASP
1	A	198	ASP
1	A	670	PRO
1	A	769	ARG
1	B	143	ILE

### 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	702/763 (92%)	683 (97%)	19 (3%)	52	69
1	B	708/763 (93%)	692 (98%)	16 (2%)	58	74
All	All	1410/1526 (92%)	1375 (98%)	35 (2%)	55	72

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	PHE
1	A	198	ASP
1	A	252	GLU
1	A	261	TRP
1	A	302	MET
1	A	408	SER
1	A	441	ARG
1	A	443	LEU
1	A	471	GLN
1	A	493	VAL
1	A	536	THR
1	A	598	LEU
1	A	709	TRP
1	A	742	GLU
1	A	773	SER
1	A	775	ARG
1	A	811	SER
1	A	875	MET
1	A	904	ILE
1	B	20	GLN
1	B	33	ASP
1	B	54	THR
1	B	261	TRP
1	B	279	GLN
1	B	281	ILE
1	B	318	LEU
1	B	324	LEU
1	B	431	VAL
1	B	709	TRP
1	B	738	LYS
1	B	773	SER
1	B	774	GLU
1	B	790	ILE
1	B	806	HIS
1	B	843	ASP

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

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 28 are unknown - 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	GLC	A	1001	-	12,12,12	1.24	0	17,17,17	1.75	4 (23%)
3	BG6	A	1002	-	16,16,16	0.91	0	23,24,24	0.99	0
2	GLC	A	1003	-	12,12,12	0.92	0	17,17,17	0.94	1 (5%)
3	BG6	A	1004	-	16,16,16	0.91	0	23,24,24	1.57	5 (21%)
2	GLC	B	1001	-	12,12,12	0.72	0	17,17,17	0.66	0
3	BG6	B	1002	-	16,16,16	1.08	2 (12%)	23,24,24	1.30	2 (8%)
2	GLC	B	1003	-	12,12,12	0.78	0	17,17,17	1.22	2 (11%)
3	BG6	B	1004	-	16,16,16	0.67	0	23,24,24	1.59	5 (21%)

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	1001	-	-	0/2/22/22	0/1/1/1
3	BG6	A	1002	-	-	0/6/26/26	0/1/1/1
2	GLC	A	1003	-	-	0/2/22/22	0/1/1/1
3	BG6	A	1004	-	-	0/6/26/26	0/1/1/1
2	GLC	B	1001	-	-	0/2/22/22	0/1/1/1
3	BG6	B	1002	-	-	0/6/26/26	0/1/1/1
2	GLC	B	1003	-	-	0/2/22/22	0/1/1/1
3	BG6	B	1004	-	-	0/6/26/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	BG6	O3-C3	2.04	1.47	1.43
3	B	1002	BG6	P-O3P	2.27	1.58	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1004	BG6	O5-C1-C2	-4.49	102.63	109.80
2	A	1001	GLC	O5-C1-C2	-4.26	103.01	109.80
3	A	1004	BG6	O1-C1-O5	-3.95	99.44	110.25
3	B	1002	BG6	O6-P-O3P	-3.13	99.17	107.14
3	B	1004	BG6	C1-C2-C3	-3.05	105.89	110.43
2	B	1003	GLC	C6-C5-C4	-2.96	105.72	113.02
3	A	1004	BG6	O2P-P-O3P	-2.64	102.08	110.58
2	A	1001	GLC	O3-C3-C4	-2.41	104.91	110.34
3	B	1004	BG6	C4-C3-C2	-2.39	106.33	110.79
2	A	1003	GLC	C6-C5-C4	-2.13	107.76	113.02
3	A	1004	BG6	O6-P-O3P	-2.09	101.83	107.14
3	B	1004	BG6	O2P-P-O3P	-2.06	103.94	110.58
3	A	1004	BG6	O4-C4-C3	-2.02	105.78	110.34
2	B	1003	GLC	O5-C1-C2	2.06	113.09	109.80
2	A	1001	GLC	O3-C3-C2	2.41	115.77	110.34
2	A	1001	GLC	O5-C5-C4	2.46	114.31	109.68
3	A	1004	BG6	O2P-P-O6	2.66	114.22	106.56
3	B	1002	BG6	O1P-P-O6	2.69	114.31	106.56
3	B	1004	BG6	O2P-P-O1P	2.76	117.88	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1003	GLC	1	0
3	B	1002	BG6	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 ⓘ

### 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	871/902 (96%)	0.10	37 (4%)	40 43	31, 49, 68, 85	0
1	B	867/902 (96%)	0.17	49 (5%)	27 30	32, 49, 73, 87	0
All	All	1738/1804 (96%)	0.13	86 (4%)	33 36	31, 49, 71, 87	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	911	ILE	5.2
1	B	27	TYR	5.0
1	B	347	ASP	4.4
1	B	222	HIS	4.1
1	A	378	VAL	4.0
1	B	344	GLY	4.0
1	B	437	GLY	3.8
1	B	20	GLN	3.7
1	B	374	ILE	3.6
1	B	375	CYS	3.5
1	B	310	LEU	3.4
1	A	317	GLU	3.4
1	B	386	CYS	3.4
1	A	684	ALA	3.3
1	B	19	VAL	3.3
1	B	530	ALA	3.1
1	B	145	ASP	3.1
1	B	378	VAL	3.1
1	A	912	ARG	3.0
1	B	150	LEU	3.0
1	A	82	ALA	3.0
1	B	453	ALA	3.0
1	B	24	GLN	3.0
1	B	850	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	754	VAL	2.9
1	A	670	PRO	2.9
1	A	705	VAL	2.8
1	A	910	ARG	2.8
1	A	418	LYS	2.8
1	B	402	GLY	2.8
1	A	796	ALA	2.8
1	B	667	PHE	2.7
1	B	438	CYS	2.7
1	A	655	VAL	2.7
1	A	867	LEU	2.7
1	A	834	CYS	2.7
1	A	142	GLN	2.6
1	A	145	ASP	2.6
1	B	390	LEU	2.6
1	B	153	THR	2.6
1	A	405	ARG	2.5
1	B	593	GLY	2.5
1	A	305	LEU	2.5
1	A	153	THR	2.5
1	A	642	HIS	2.5
1	B	74	GLY	2.5
1	A	745	ILE	2.5
1	A	27	TYR	2.5
1	B	237	CYS	2.5
1	B	306	VAL	2.4
1	B	912	ARG	2.4
1	A	403	GLU	2.4
1	B	365	GLN	2.3
1	B	564	GLN	2.3
1	B	389	THR	2.3
1	A	709	TRP	2.3
1	B	83	LEU	2.3
1	A	909	CYS	2.3
1	B	324	LEU	2.3
1	A	822	VAL	2.3
1	B	228	LEU	2.3
1	B	317	GLU	2.3
1	B	82	ALA	2.3
1	A	297	ILE	2.2
1	B	81	LEU	2.2
1	A	913	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	357	MET	2.2
1	A	671	HIS	2.2
1	A	741	PHE	2.2
1	B	443	LEU	2.2
1	B	349	ILE	2.1
1	A	152	PHE	2.1
1	B	28	HIS	2.1
1	A	654	VAL	2.1
1	B	425	LYS	2.1
1	B	913	GLU	2.1
1	A	237	CYS	2.1
1	B	353	ARG	2.1
1	A	833	LEU	2.1
1	B	152	PHE	2.1
1	B	210	THR	2.1
1	B	17	ASP	2.0
1	B	227	GLY	2.0
1	A	552	GLY	2.0
1	A	150	LEU	2.0
1	A	323	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
4	UNX	A	1008	1/1	-0.33	6.18	301.01	2,2,2,2	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	UNX	B	1005	1/1	-0.28	2.88	198.97	2,2,2,2	1
4	UNX	B	2	1/1	0.42	2.58	145.11	2,2,2,2	1
4	UNX	A	11	1/1	-0.27	2.25	114.60	2,2,2,2	1
4	UNX	A	1007	1/1	-0.35	4.68	107.61	2,2,2,2	1
4	UNX	A	10	1/1	0.50	3.33	91.47	2,2,2,2	1
4	UNX	B	12	1/1	-0.49	3.13	67.05	2,2,2,2	1
4	UNX	A	1	1/1	0.63	1.42	64.68	2,2,2,2	1
4	UNX	A	4	1/1	0.26	1.17	59.54	2,2,2,2	1
4	UNX	B	1006	1/1	0.31	2.33	59.16	2,2,2,2	1
4	UNX	B	3	1/1	-0.13	2.43	57.16	2,2,2,2	1
4	UNX	B	14	1/1	0.28	2.63	52.11	2,2,2,2	1
4	UNX	A	1006	1/1	0.59	2.11	41.21	2,2,2,2	1
4	UNX	A	6	1/1	0.58	2.00	35.30	2,2,2,2	1
4	UNX	B	1012	1/1	0.19	2.07	34.50	2,2,2,2	1
4	UNX	B	1009	1/1	0.03	0.89	31.78	2,2,2,2	1
4	UNX	A	8	1/1	0.01	1.48	31.13	2,2,2,2	1
4	UNX	B	13	1/1	0.09	1.27	29.05	2,2,2,2	1
4	UNX	A	1009	1/1	0.23	1.34	26.06	2,2,2,2	1
4	UNX	B	1013	1/1	0.13	1.20	23.82	5,5,5,5	1
4	UNX	A	9	1/1	0.28	1.24	19.43	2,2,2,2	1
4	UNX	B	5	1/1	0.12	0.68	10.92	2,2,2,2	1
2	GLC	A	1001	12/12	0.96	0.19	0.67	29,32,34,34	0
2	GLC	B	1003	12/12	0.98	0.20	0.28	25,32,34,35	0
2	GLC	A	1003	12/12	0.97	0.16	-0.45	35,40,41,42	0
2	GLC	B	1001	12/12	0.98	0.13	-0.51	32,38,39,39	0
3	BG6	B	1004	16/16	0.97	0.10	-0.85	33,39,43,44	0
3	BG6	A	1002	16/16	0.98	0.09	-1.08	33,36,38,40	0
3	BG6	A	1004	16/16	0.97	0.10	-1.12	40,45,48,53	0
3	BG6	B	1002	16/16	0.97	0.09	-1.17	48,52,54,55	0
4	UNX	B	1008	1/1	0.46	4.38	-	2,2,2,2	1
4	UNX	B	1007	1/1	0.19	1.28	-	2,2,2,2	1
4	UNX	A	1005	1/1	0.32	2.28	-	2,2,2,2	1
4	UNX	B	1010	1/1	0.40	1.95	-	2,2,2,2	1
4	UNX	B	7	1/1	0.19	2.09	-	2,2,2,2	1
4	UNX	B	1011	1/1	0.32	4.14	-	2,2,2,2	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.