



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:34 AM GMT

PDB ID : 2WCG  
Title : X-RAY STRUCTURE OF ACID-BETA-GLUCOSIDASE WITH N-OCTYL(CYCLIC GUANIDINE)-NOJIRIMYCININ THE ACTIVE SITE  
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Deposited on : 2009-03-12  
Resolution : 2.30 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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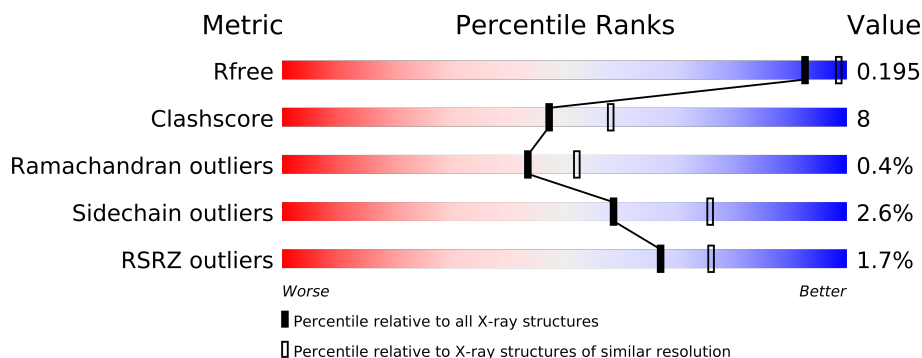
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	505	
1	B	505	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	FU4	B	1501	-	X
5	SO4	A	1505	-	X
5	SO4	A	1506	-	X
5	SO4	A	1507	-	X
5	SO4	A	1508	-	X
5	SO4	B	1504	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	SO4	B	1505	-	X
5	SO4	B	1506	-	X
5	SO4	B	1507	-	X
6	MT5	A	1509	-	X
6	MT5	B	1508	-	X

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 8672 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.

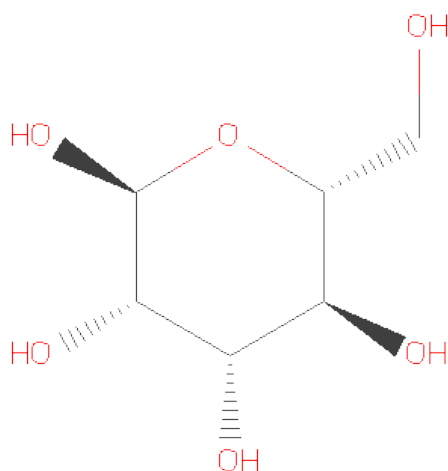
- Molecule 1 is a protein called GLUCOSYLCERAMIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3865	2494	660	695	16			
1	B	495	Total	C	N	O	S	0	0	0
			3878	2501	661	700	16			

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

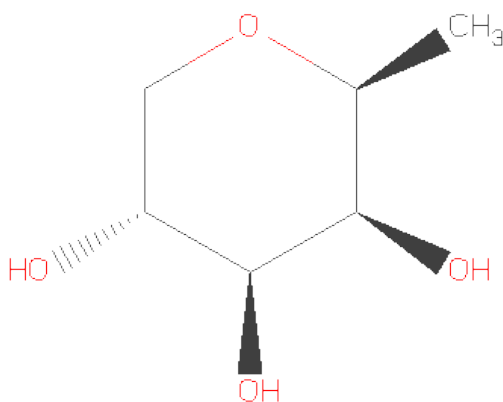
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



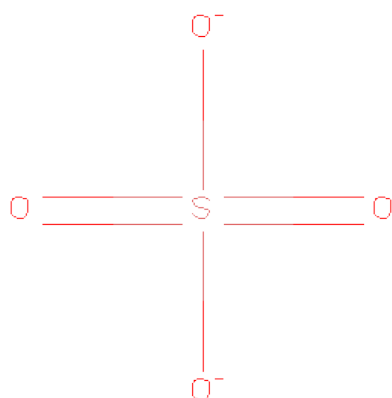
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is SUGAR (2,6-ANHYDRO-1-DEOXY-D-GALACTITOL) (three-letter code: FU4) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>4</sub>).



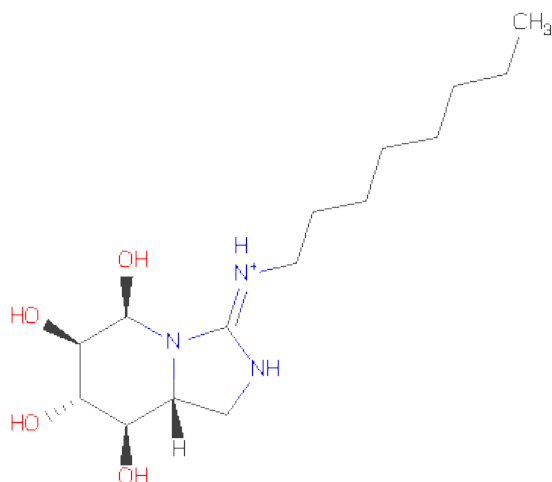
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is N-[(3E,5R,6R,7S,8R,8AR)-5,6,7,8-TETRAHYDROXYHEXAHYDROIMIDAZO[1,5-A]PYRIDIN-3(2H)-YLIDENE]OCTAN-1-AMINIUM (three-letter code: MT5) (formula: C<sub>15</sub>H<sub>30</sub>N<sub>3</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	7	3	4		
6	B	1	Total	C	N	O	0	0
			14	7	3	4		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		
7	A	1	Total	Cl	0	0
			1	1		

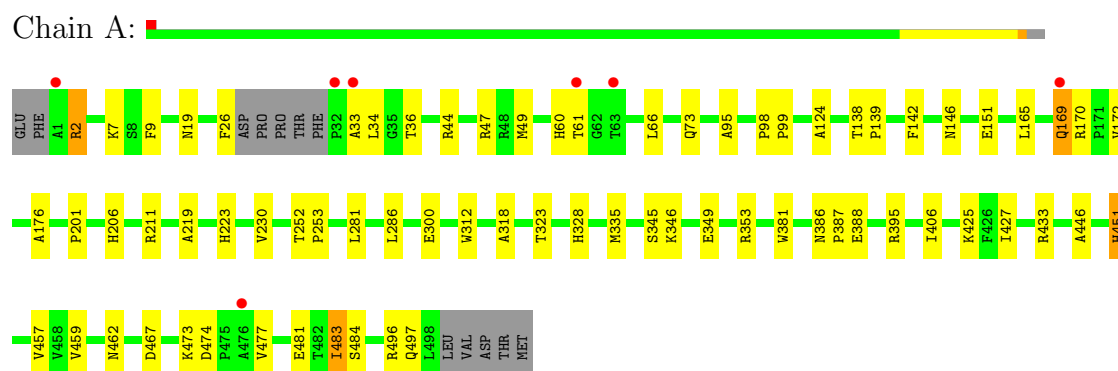
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	369	Total	O	0	0
			369	369		
8	B	372	Total	O	0	0
			372	372		

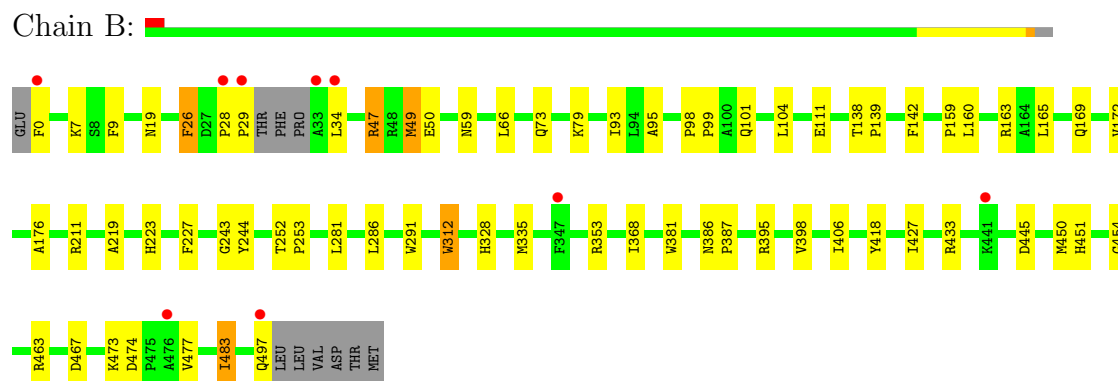
### 3 Residue-property plots

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: GLUCOSYLCERAMIDASE



#### • Molecule 1: GLUCOSYLCERAMIDASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.31Å 96.83Å 83.23Å 90.00° 104.34° 90.00°	Depositor
Resolution (Å)	19.74 – 2.30 19.74 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.74-2.30) 99.7 (19.74-2.30)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.27 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, $R_{free}$	0.135 , 0.194 0.136 , 0.195	Depositor DCC
$R_{free}$ test set	2346 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 37.8	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 46531 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8672	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% 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: FU4, NAG, CL, MT5, SO4, MAN

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	0.90	0/3982	0.86	6/5431 (0.1%)
1	B	0.90	3/3996 (0.1%)	0.84	4/5451 (0.1%)
All	All	0.90	3/7978 (0.0%)	0.85	10/10882 (0.1%)

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
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	26	PHE	CB-CG	-6.10	1.41	1.51
1	B	433	ARG	CZ-NH1	-5.40	1.26	1.33
1	B	398	VAL	CB-CG1	5.26	1.63	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	B	433	ARG	NE-CZ-NH2	9.18	124.89	120.30
1	A	433	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	A	47	ARG	NE-CZ-NH1	8.37	124.49	120.30
1	B	353	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	47	ARG	NE-CZ-NH1	-6.42	117.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	A	353	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	A	353	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	353	ARG	NH1-CZ-NH2	-5.18	113.70	119.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	LEU	Peptide
1	B	34	LEU	Peptide

## 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	3865	0	3759	51	0
1	B	3878	0	3763	58	0
2	A	28	0	24	12	0
2	B	28	0	24	15	0
3	A	11	0	10	0	0
3	B	11	0	10	0	0
4	A	10	0	12	6	0
4	B	10	0	12	8	0
5	A	30	0	0	1	0
5	B	30	0	0	1	0
6	A	14	0	11	0	0
6	B	14	0	12	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	369	0	0	7	0
8	B	372	0	0	12	0
All	All	8672	0	7637	123	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 8.

All (123) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:19:ASN:HD21	2:B:1498:NAG:C1	0.98	1.63
1:A:19:ASN:HD21	2:A:1499:NAG:C1	0.97	1.54
1:B:19:ASN:ND2	2:B:1498:NAG:C1	1.80	1.43
2:B:1498:NAG:O3	4:B:1501:FU4:H1C2	1.30	1.29
1:A:169:GLN:HG3	1:A:170:ARG:HG3	1.39	1.05
1:A:2:ARG:HG3	1:A:2:ARG:HH11	1.23	1.02
1:A:474:ASP:HB3	1:A:477:VAL:HG12	1.40	1.01
2:B:1498:NAG:O3	4:B:1501:FU4:C1	2.10	0.99
1:A:474:ASP:HB3	1:A:477:VAL:CG1	1.93	0.97
1:B:474:ASP:HB3	1:B:477:VAL:CG1	1.97	0.95
1:B:95:ALA:HB1	1:B:406:ILE:HD12	1.51	0.92
2:B:1498:NAG:C3	4:B:1501:FU4:H1C2	2.02	0.90
1:A:95:ALA:HB1	1:A:406:ILE:HD12	1.56	0.87
1:A:19:ASN:HD21	2:A:1499:NAG:C2	1.89	0.83
1:A:169:GLN:CG	1:A:170:ARG:HG3	2.09	0.82
2:A:1499:NAG:O3	4:A:1502:FU4:H1C2	1.80	0.82
1:B:474:ASP:HB3	1:B:477:VAL:HG12	1.60	0.80
1:B:19:ASN:HD21	2:B:1498:NAG:C2	1.93	0.80
1:B:0:PHE:CB	8:B:2097:HOH:O	2.31	0.79
1:A:19:ASN:CG	2:A:1499:NAG:C1	2.53	0.77
1:B:19:ASN:CG	2:B:1498:NAG:C1	2.54	0.76
2:A:1499:NAG:O3	4:A:1502:FU4:H3	1.87	0.74
1:A:474:ASP:CB	1:A:477:VAL:HG12	2.16	0.72
1:A:142:PHE:O	1:A:211:ARG:NH2	2.23	0.71
1:B:497:GLN:CG	8:B:2352:HOH:O	2.37	0.71
1:A:2:ARG:HG3	1:A:2:ARG:NH1	2.01	0.70
2:A:1499:NAG:C3	4:A:1502:FU4:H1C2	2.23	0.69
1:B:474:ASP:CB	1:B:477:VAL:HG12	2.21	0.69
1:B:467:ASP:HB3	1:B:483:ILE:HD11	1.74	0.69
1:A:26:PHE:CG	1:A:425:LYS:HE2	2.29	0.67
1:A:7:LYS:HE3	1:A:9:PHE:CZ	2.29	0.67
1:A:328:HIS:HD2	8:A:2259:HOH:O	1.78	0.67
1:A:151:GLU:HG3	8:A:2143:HOH:O	1.95	0.67
1:A:60:HIS:HD2	1:A:481:GLU:OE2	1.79	0.66
1:B:7:LYS:HE3	1:B:9:PHE:CZ	2.30	0.65
1:B:328:HIS:HD2	8:B:2259:HOH:O	1.80	0.64
1:B:474:ASP:CB	1:B:477:VAL:CG1	2.73	0.64
1:B:59:ASN:CB	8:B:2058:HOH:O	2.46	0.63
1:A:346:LYS:HB2	1:A:349:GLU:CD	2.20	0.63
1:A:474:ASP:CB	1:A:477:VAL:CG1	2.74	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:47:ARG:HD3	8:B:2046:HOH:O	1.98	0.62
2:A:1499:NAG:O3	4:A:1502:FU4:C1	2.48	0.61
1:A:386:ASN:HB2	1:A:387:PRO:CD	2.30	0.61
1:B:142:PHE:O	1:B:211:ARG:NH2	2.34	0.60
1:B:395:ARG:NH1	8:B:2295:HOH:O	2.26	0.60
1:A:467:ASP:HB3	1:A:483:ILE:HD11	1.83	0.59
1:B:111:GLU:HA	8:B:2368:HOH:O	2.02	0.59
1:A:19:ASN:ND2	2:A:1499:NAG:C2	2.58	0.58
2:A:1499:NAG:O3	4:A:1502:FU4:C3	2.53	0.57
1:A:26:PHE:CD2	1:A:425:LYS:HE2	2.40	0.57
1:B:26:PHE:HZ	1:B:49:MET:HE2	1.71	0.54
1:B:474:ASP:CG	1:B:477:VAL:HG12	2.27	0.54
1:A:60:HIS:CD2	1:A:481:GLU:OE2	2.59	0.54
1:B:19:ASN:ND2	2:B:1498:NAG:C2	2.62	0.53
1:A:406:ILE:HG22	8:A:2304:HOH:O	2.09	0.53
1:A:19:ASN:ND2	2:A:1499:NAG:O5	2.32	0.52
1:A:300:GLU:CG	8:A:2235:HOH:O	2.56	0.52
1:B:95:ALA:HB1	1:B:406:ILE:CD1	2.32	0.52
1:A:318:ALA:HB1	1:A:323:THR:HG21	1.92	0.51
1:A:451:HIS:HD2	1:A:457:VAL:HG23	1.76	0.51
1:A:36:THR:HG22	8:A:2058:HOH:O	2.10	0.51
1:B:386:ASN:HB2	1:B:387:PRO:CD	2.40	0.51
2:B:1498:NAG:HO3	4:B:1501:FU4:H1C2	1.63	0.51
1:B:450:MET:HE3	1:B:454:GLY:HA2	1.93	0.51
2:B:1498:NAG:O3	4:B:1501:FU4:H5	2.11	0.50
1:B:66:LEU:HD11	1:B:473:LYS:HB2	1.94	0.50
1:A:252:THR:HB	1:A:253:PRO:HD2	1.95	0.48
1:B:47:ARG:CD	8:B:2046:HOH:O	2.58	0.48
1:B:463:ARG:HD3	8:B:2325:HOH:O	2.14	0.48
1:A:19:ASN:OD1	2:A:1499:NAG:C1	2.62	0.48
1:B:98:PRO:N	1:B:99:PRO:CD	2.77	0.48
1:B:19:ASN:OD1	2:B:1498:NAG:C1	2.62	0.47
1:A:446:ALA:HA	1:A:459:VAL:O	2.15	0.47
1:B:26:PHE:CZ	1:B:49:MET:HE2	2.49	0.47
1:B:427:ILE:O	1:B:427:ILE:HG22	2.13	0.47
1:B:169:GLN:CB	5:B:1507:SO4:O1	2.63	0.47
1:B:474:ASP:CG	1:B:477:VAL:CG1	2.84	0.46
1:B:497:GLN:CG	8:B:2330:HOH:O	2.63	0.46
1:A:451:HIS:HD2	1:A:457:VAL:CG2	2.28	0.46
1:A:44:ARG:HB3	5:A:1506:SO4:O2	2.16	0.46
1:A:395:ARG:HD3	8:A:2299:HOH:O	2.15	0.46
1:B:368:ILE:HG21	1:B:445:ASP:HB3	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:138:THR:HA	1:B:139:PRO:HD3	1.84	0.45
1:A:66:LEU:HD11	1:A:473:LYS:HB2	1.98	0.45
1:B:165:LEU:CD2	1:B:172:VAL:HB	2.47	0.45
1:B:286:LEU:HD12	1:B:286:LEU:C	2.36	0.45
1:B:159:PRO:O	1:B:163:ARG:HG3	2.17	0.45
1:B:211:ARG:HD2	8:B:2169:HOH:O	2.15	0.45
1:B:176:ALA:HB2	1:B:227:PHE:CE2	2.52	0.45
1:A:219:ALA:O	1:A:223:HIS:HD2	2.00	0.45
1:B:243:GLY:O	1:B:244:TYR:C	2.55	0.43
1:A:386:ASN:HB2	1:A:387:PRO:HD3	1.98	0.43
2:B:1498:NAG:O3	4:B:1501:FU4:H3	2.18	0.43
1:A:98:PRO:N	1:A:99:PRO:CD	2.81	0.43
1:B:219:ALA:O	1:B:223:HIS:HD2	2.02	0.43
1:A:451:HIS:CD2	1:A:457:VAL:CG2	3.01	0.42
1:A:95:ALA:HB1	1:A:406:ILE:CD1	2.40	0.42
1:A:427:ILE:O	1:A:427:ILE:HG22	2.19	0.42
1:A:26:PHE:HZ	1:A:49:MET:HE2	1.85	0.42
1:B:79:LYS:HA	1:B:79:LYS:HD2	1.86	0.42
2:A:1499:NAG:O3	4:A:1502:FU4:H5	2.19	0.42
1:B:395:ARG:NH1	8:B:2294:HOH:O	2.36	0.42
1:B:93:ILE:O	1:B:101:GLN:HG2	2.19	0.42
1:B:28:PRO:HA	1:B:29:PRO:HD3	1.89	0.42
1:B:312:TRP:CD1	1:B:312:TRP:C	2.93	0.42
1:A:176:ALA:HB3	1:A:230:VAL:HG12	2.02	0.41
1:B:26:PHE:HZ	1:B:49:MET:SD	2.43	0.41
1:A:60:HIS:HE1	8:A:2070:HOH:O	2.03	0.41
2:B:1498:NAG:O3	4:B:1501:FU4:C3	2.69	0.41
1:B:49:MET:HG3	1:B:418:TYR:HD2	1.85	0.41
1:A:165:LEU:CD2	1:A:172:VAL:HB	2.51	0.41
1:B:104:LEU:HD23	1:B:104:LEU:C	2.40	0.41
1:B:253:PRO:HB3	1:B:291:TRP:CD2	2.55	0.41
2:B:1498:NAG:O3	4:B:1501:FU4:C2	2.67	0.41
1:B:160:LEU:HA	1:B:160:LEU:HD23	1.88	0.41
1:A:201:PRO:HA	1:A:206:HIS:CG	2.55	0.41
1:B:47:ARG:HD2	1:B:50:GLU:OE1	2.21	0.41
1:B:252:THR:HB	1:B:253:PRO:HD2	2.03	0.41
1:A:138:THR:HA	1:A:139:PRO:HD3	1.88	0.41
1:B:26:PHE:HZ	1:B:49:MET:CE	2.33	0.40
1:B:19:ASN:ND2	2:B:1498:NAG:O5	2.44	0.40
1:A:462:ASN:HB2	1:A:484:SER:OG	2.22	0.40
1:A:286:LEU:C	1:A:286:LEU:HD12	2.42	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	489/505 (97%)	464 (95%)	22 (4%)	3 (1%)	33	39
1	B	491/505 (97%)	468 (95%)	22 (4%)	1 (0%)	56	68
All	All	980/1010 (97%)	932 (95%)	44 (4%)	4 (0%)	43	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ALA
1	A	281	LEU
1	B	281	LEU
1	A	124	ALA

### 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	410/432 (95%)	396 (97%)	14 (3%)	49	64
1	B	411/432 (95%)	404 (98%)	7 (2%)	73	87
All	All	821/864 (95%)	800 (97%)	21 (3%)	59	76

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	61	THR
1	A	73	GLN
1	A	146	ASN
1	A	169	GLN

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Mol	Chain	Res	Type
1	A	312	TRP
1	A	335	MET
1	A	345	SER
1	A	381	TRP
1	A	388	GLU
1	A	451	HIS
1	A	483	ILE
1	A	496	ARG
1	A	497	GLN
1	B	49	MET
1	B	73	GLN
1	B	312	TRP
1	B	335	MET
1	B	381	TRP
1	B	451	HIS
1	B	483	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	60	HIS
1	A	328	HIS
1	A	451	HIS
1	B	19	ASN
1	B	166	GLN
1	B	223	HIS
1	B	328	HIS
1	B	396	ASN

### 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 ⓘ

4 carbohydrates 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	NAG	A	1499	1,2	12,14,15	0.81	1 (8%)	15,19,21	1.42	3 (20%)
2	NAG	A	1500	3,2	12,14,15	0.60	0	15,19,21	1.39	3 (20%)
2	NAG	B	1498	2	12,14,15	0.73	0	15,19,21	1.42	2 (13%)
2	NAG	B	1499	3,2	12,14,15	0.68	0	15,19,21	1.67	4 (26%)

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	NAG	A	1499	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1500	3,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1498	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1499	3,2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1499	NAG	O5-C5	-2.31	1.41	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1498	NAG	O5-C5-C6	3.78	110.94	106.98
2	B	1499	NAG	C4-C3-C2	-3.48	102.79	111.32
2	B	1499	NAG	C3-C2-N2	3.33	116.84	111.76
2	A	1500	NAG	C4-C3-C2	-3.33	103.17	111.32
2	A	1499	NAG	O5-C5-C6	2.91	110.03	106.98
2	B	1499	NAG	O5-C5-C6	2.70	109.81	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	NAG	O5-C5-C6	2.66	109.77	106.98
2	A	1500	NAG	C3-C2-N2	2.60	115.72	111.76
2	B	1498	NAG	C2-N2-C7	-2.27	119.28	123.09
2	A	1499	NAG	C2-N2-C7	-2.25	119.31	123.09
2	A	1499	NAG	C3-C2-N2	2.11	114.97	111.76
2	B	1499	NAG	O3-C3-C2	2.03	113.36	109.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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
3	MAN	A	1501	2	10,11,12	0.68	0	11,15,17	1.87	3 (27%)
4	FU4	A	1502	-	10,10,10	0.79	0	14,14,14	1.42	3 (21%)
5	SO4	A	1503	-	4,4,4	0.38	0	6,6,6	0.45	0
5	SO4	A	1504	-	4,4,4	0.27	0	6,6,6	0.22	0
5	SO4	A	1505	-	4,4,4	0.31	0	6,6,6	0.54	0
5	SO4	A	1506	-	4,4,4	0.14	0	6,6,6	0.38	0
5	SO4	A	1507	-	4,4,4	0.18	0	6,6,6	0.40	0
5	SO4	A	1508	-	4,4,4	0.13	0	6,6,6	0.69	0
6	MT5	A	1509	-	15,15,23	1.52	3 (20%)	23,23,31	2.53	10 (43%)
3	MAN	B	1500	2	10,11,12	0.67	0	11,15,17	1.44	2 (18%)
4	FU4	B	1501	-	10,10,10	0.76	0	14,14,14	1.53	3 (21%)
5	SO4	B	1502	-	4,4,4	0.38	0	6,6,6	0.36	0
5	SO4	B	1503	-	4,4,4	0.32	0	6,6,6	0.26	0
5	SO4	B	1504	-	4,4,4	0.38	0	6,6,6	0.51	0
5	SO4	B	1505	-	4,4,4	0.17	0	6,6,6	0.22	0
5	SO4	B	1506	-	4,4,4	0.23	0	6,6,6	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	B	1507	-	4,4,4	0.14	0	6,6,6	0.45	0
6	MT5	B	1508	-	15,15,23	1.27	1 (6%)	23,23,31	3.01	10 (43%)

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
3	MAN	A	1501	2	1/1/4/5	0/2/19/22	0/1/1/1
4	FU4	A	1502	-	-	0/0/17/17	0/1/1/1
5	SO4	A	1503	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1504	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1505	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1506	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1507	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1508	-	-	0/0/0/0	0/0/0/0
6	MT5	A	1509	-	-	0/0/33/42	0/0/2/2
3	MAN	B	1500	2	-	0/2/19/22	0/1/1/1
4	FU4	B	1501	-	-	0/0/17/17	0/1/1/1
5	SO4	B	1502	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1503	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1504	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1505	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1506	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1507	-	-	0/0/0/0	0/0/0/0
6	MT5	B	1508	-	-	0/0/33/42	0/0/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1509	MT5	O16-C15	-3.55	1.36	1.41
6	B	1508	MT5	C13-N14	-2.85	1.43	1.47
6	A	1509	MT5	C21-C13	-2.62	1.47	1.53
6	A	1509	MT5	C15-N14	-2.31	1.41	1.47

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1508	MT5	C21-C13-N14	-9.36	99.76	109.64
6	A	1509	MT5	C21-C13-N14	-5.75	103.58	109.64
6	B	1508	MT5	C19-C21-C13	-5.11	103.50	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1508	MT5	O16-C15-N14	4.49	120.19	111.23
6	A	1509	MT5	O16-C15-N14	4.44	120.08	111.23
6	A	1509	MT5	C19-C21-C13	-4.16	105.00	111.62
6	B	1508	MT5	O18-C17-C15	3.96	117.97	109.34
3	A	1501	MAN	O5-C5-C6	3.86	111.03	106.98
6	A	1509	MT5	C19-C17-C15	3.45	115.29	109.11
3	A	1501	MAN	O5-C5-C4	-3.41	106.32	110.65
6	A	1509	MT5	C12-C13-N14	3.34	105.86	101.83
6	B	1508	MT5	C17-C15-N14	3.16	116.43	109.30
6	A	1509	MT5	C17-C15-N14	3.15	116.40	109.30
6	B	1508	MT5	N14-C10-N9	-3.08	118.03	126.52
6	B	1508	MT5	N11-C10-N9	3.08	129.96	122.57
6	A	1509	MT5	O18-C17-C15	2.99	115.85	109.34
3	B	1500	MAN	C4-C3-C2	2.94	114.45	110.50
6	A	1509	MT5	C15-N14-C10	2.86	129.42	125.13
3	B	1500	MAN	O5-C5-C6	2.81	109.93	106.98
4	A	1502	FU4	C1-C2-C3	2.78	113.20	109.71
3	A	1501	MAN	C4-C3-C2	2.72	114.15	110.50
4	B	1501	FU4	O5-C5-C6	2.59	110.72	106.20
6	B	1508	MT5	C19-C17-C15	2.38	113.37	109.11
4	B	1501	FU4	O2-C2-C3	-2.33	105.70	110.23
4	A	1502	FU4	O5-C5-C4	2.21	113.26	109.53
4	A	1502	FU4	O5-C5-C6	2.16	109.97	106.20
6	B	1508	MT5	N11-C10-N14	2.16	112.01	109.73
6	A	1509	MT5	N11-C10-N14	2.13	111.98	109.73
6	A	1509	MT5	O20-C19-C17	-2.06	105.74	110.35
6	B	1508	MT5	O20-C19-C21	-2.03	105.81	110.35
4	B	1501	FU4	O5-C5-C4	2.03	112.95	109.53

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1501	MAN	C1

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	493/505 (97%)	-0.57	7 (1%) 72 80	14, 22, 36, 60	0
1	B	495/505 (98%)	-0.56	9 (1%) 65 74	13, 22, 36, 57	0
All	All	988/1010 (97%)	-0.56	16 (1%) 67 77	13, 22, 36, 60	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	497	GLN	5.0
1	A	33	ALA	3.9
1	B	347	PHE	3.4
1	B	34	LEU	3.2
1	A	32	PRO	3.1
1	B	476	ALA	3.0
1	B	33	ALA	2.8
1	B	28	PRO	2.7
1	B	29	PRO	2.6
1	A	61	THR	2.2
1	A	476	ALA	2.1
1	A	63	THR	2.1
1	B	441	LYS	2.1
1	A	1	ALA	2.1
1	B	0	PHE	2.0
1	A	169	GLN	2.0

### 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

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	NAG	B	1498	14/15	0.14	3.27	36,40,44,45	0
2	NAG	A	1499	14/15	0.16	1.81	36,40,44,45	0
2	NAG	B	1499	14/15	0.18	-	65,66,66,68	0
2	NAG	A	1500	14/15	0.26	-	65,66,67,68	0

### 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
4	FU4	B	1501	10/10	0.21	25.75	62,65,66,66	0
5	SO4	A	1507	5/5	0.27	22.41	76,78,78,79	0
5	SO4	A	1506	5/5	0.18	19.22	55,56,57,59	0
5	SO4	A	1508	5/5	0.37	14.30	88,89,90,91	0
5	SO4	B	1505	5/5	0.25	9.21	80,81,82,82	0
5	SO4	B	1504	5/5	0.17	4.50	46,48,51,53	0
5	SO4	A	1505	5/5	0.22	3.28	50,52,54,54	0
5	SO4	B	1507	5/5	0.17	2.99	64,65,67,70	0
6	MT5	A	1509	14/22	0.14	2.66	25,31,40,40	0
5	SO4	B	1506	5/5	0.19	2.47	61,62,63,64	0
6	MT5	B	1508	14/22	0.12	2.05	26,32,40,41	0
5	SO4	B	1503	5/5	0.11	1.74	45,45,46,47	0
5	SO4	A	1504	5/5	0.14	1.00	50,50,51,52	0
7	CL	B	1509	1/1	0.12	0.04	52,52,52,52	0
5	SO4	B	1502	5/5	0.04	-2.14	29,29,32,33	0
5	SO4	A	1503	5/5	0.05	-2.16	27,28,30,31	0
7	CL	A	1510	1/1	0.09	-3.80	59,59,59,59	0
3	MAN	B	1500	11/12	0.30	-	95,96,97,97	0
3	MAN	A	1501	11/12	0.34	-	95,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FU4	A	1502	10/10	0.39	-	62,65,66,66	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.