



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:59 PM GMT

PDB ID : 4B56  
Title : Structure of ectonucleotide pyrophosphatase-phosphodiesterase-1 (NPP1)  
Authors : Jansen, S.; Perrakis, A.; Ulens, C.; Winkler, C.; Andries, M.; Joosten, R.P.;  
Van Acker, M.; Luyten, F.P.; Moolenaar, W.H.; Bollen, M.  
Deposited on : 2012-08-02  
Resolution : 3.00 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

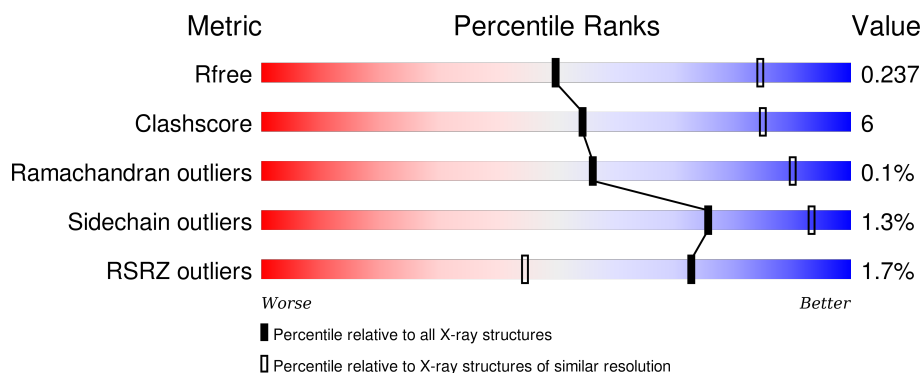
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	820	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 86%, yellow 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>86%</span> <span>13%</span> </div> </div>
1	B	820	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 77%, yellow 12%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>77%</span> <span>12%</span> <span>• 10%</span> </div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12834 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 ECTONUCLEOTIDE PYROPHOSPHATASE/PHOSPHODIESTERASE FAMILY MEMBER 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	816	Total	C	N	O	S	0	0	0
			6592	4209	1114	1224	45			
1	B	737	Total	C	N	O	S	0	0	0
			5981	3843	1001	1108	29			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 5 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	5	Total	C	N	O	0	0
			61	34	2	25		
5	B	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

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

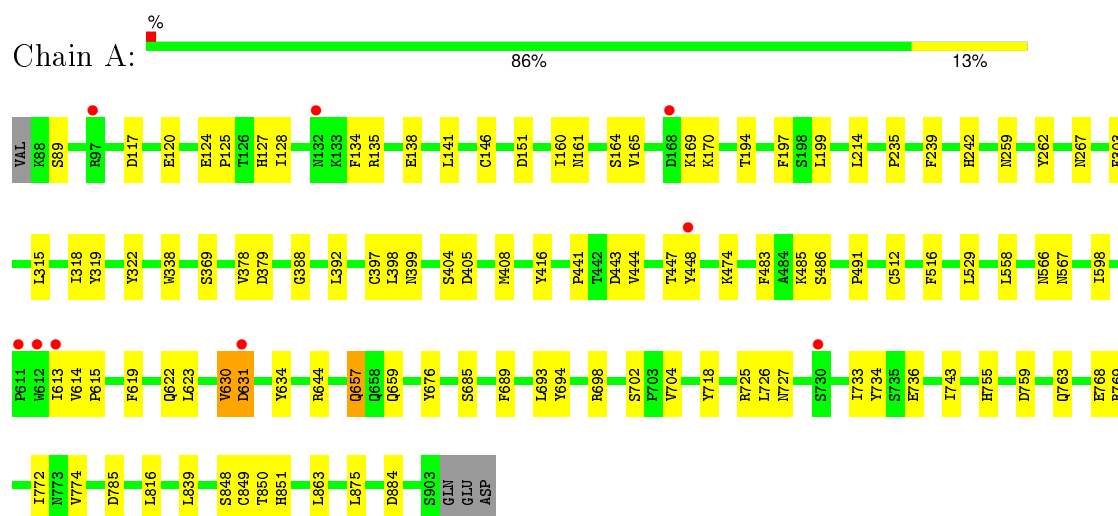
- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	3	Total	C	N	O	0	0
			39	22	2	15		

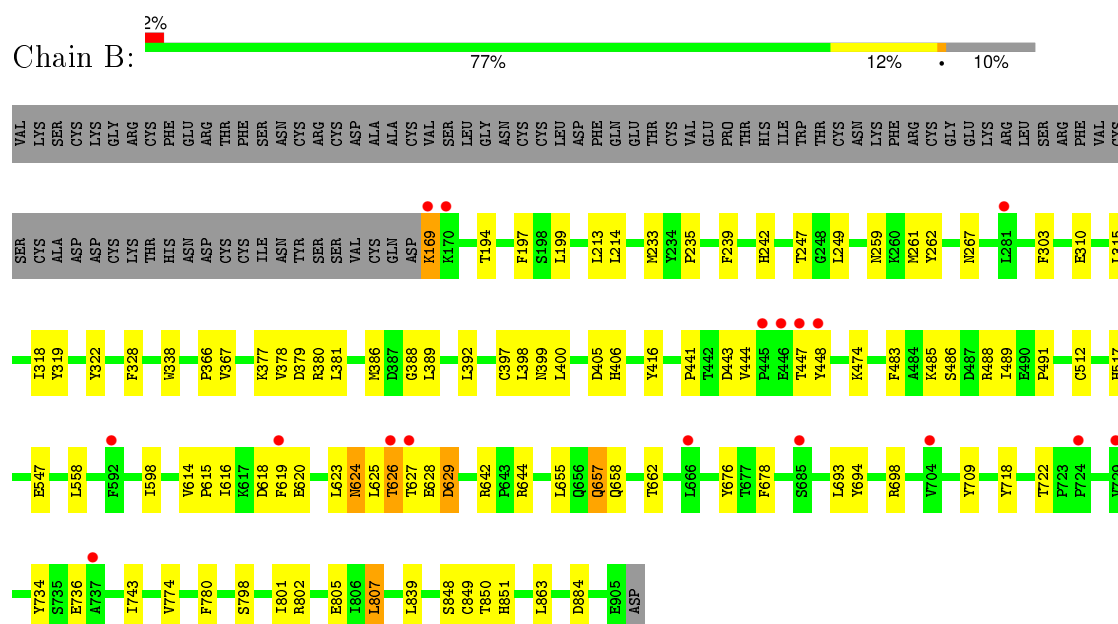
### 3 Residue-property plots

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: ECTONUCLEOTIDE PYROPHOSPHATASE/PHOSPHODIESTERASE FAMILY MEMBER 1



#### • Molecule 1: ECTONUCLEOTIDE PYROPHOSPHATASE/PHOSPHODIESTERASE FAMILY MEMBER 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.39Å 105.41Å 245.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.47 – 3.00 48.42 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.47-3.00) 99.8 (48.42-3.00)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.200 , 0.234 0.206 , 0.237	Depositor DCC
$R_{free}$ test set	2763 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	96.4	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 73.1	EDS
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 54361 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12834	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, PO4, CA, 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	0.39	0/6779	0.60	0/9207
1	B	0.36	0/6157	0.59	1/8371 (0.0%)
All	All	0.38	0/12936	0.60	1/17578 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	807	LEU	CA-CB-CG	5.23	127.32	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	6592	0	6377	77	0
1	B	5981	0	5820	84	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	61	0	52	3	0
5	B	61	0	52	0	0
6	A	28	0	26	0	0
6	B	28	0	26	0	0
7	A	28	0	25	2	0
8	B	39	0	34	1	0
All	All	12834	0	12412	161	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 (161) 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:615:PRO:HG2	1:B:618:ASP:OD2	1.72	0.89
1:B:625:LEU:O	1:B:626:THR:HG22	1.75	0.86
1:A:615:PRO:HB3	1:A:694:TYR:OH	1.76	0.85
1:A:875:LEU:HD13	5:A:2001:NAG:H81	1.59	0.82
1:B:303:PHE:CE1	1:B:322:TYR:HA	2.14	0.82
1:A:303:PHE:CE1	1:A:322:TYR:HA	2.16	0.80
1:B:615:PRO:CG	1:B:618:ASP:OD2	2.30	0.78
1:A:615:PRO:HB3	1:A:694:TYR:CZ	2.20	0.75
1:B:625:LEU:HD12	1:B:625:LEU:O	1.87	0.73
1:A:443:ASP:HB2	1:A:447:THR:CG2	2.19	0.73
1:A:485:LYS:HG2	1:A:485:LYS:O	1.90	0.71
1:B:443:ASP:HB2	1:B:447:THR:CG2	2.19	0.71
1:B:623:LEU:O	1:B:627:THR:HB	1.94	0.67
1:A:615:PRO:CB	1:A:694:TYR:OH	2.41	0.67
1:B:623:LEU:HD21	1:B:658:GLN:NE2	2.10	0.66
1:A:315:LEU:HD23	1:A:319:TYR:CE1	2.32	0.65
1:B:624:ASN:N	1:B:624:ASN:HD22	1.94	0.64
1:A:614:VAL:HG13	1:A:614:VAL:O	1.98	0.64
1:B:315:LEU:HD23	1:B:319:TYR:CE1	2.33	0.63
1:B:247:THR:HG21	1:B:249:LEU:HD12	1.81	0.62
1:A:630:VAL:O	1:A:631:ASP:C	2.38	0.61
1:B:386:MET:CE	1:B:400:LEU:HD22	2.31	0.60
1:A:615:PRO:CG	1:A:694:TYR:OH	2.50	0.60
1:A:315:LEU:HD23	1:A:319:TYR:CZ	2.38	0.59
1:B:615:PRO:CD	1:B:618:ASP:OD2	2.51	0.59
1:B:315:LEU:HD23	1:B:319:TYR:CZ	2.38	0.58
1:B:318:ILE:HG21	1:B:338:TRP:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:ILE:HD11	1:A:816:LEU:HD13	1.86	0.58
1:B:386:MET:HE1	1:B:400:LEU:HD22	1.85	0.58
1:A:676:TYR:CE1	1:A:774:VAL:HB	2.40	0.57
1:B:801:ILE:HG22	1:B:802:ARG:HG2	1.86	0.57
1:B:620:GLU:O	1:B:623:LEU:HB3	2.05	0.56
1:A:239:PHE:HB2	1:A:259:ASN:OD1	2.05	0.56
1:A:875:LEU:CD1	5:A:2001:NAG:H81	2.34	0.56
7:A:2032:NAG:H83	7:A:2032:NAG:H3	1.88	0.56
1:B:443:ASP:HB2	1:B:447:THR:HG22	1.88	0.55
1:A:443:ASP:HB2	1:A:447:THR:HG22	1.87	0.55
1:A:619:PHE:CE2	1:A:694:TYR:HD2	2.23	0.55
1:B:239:PHE:HB2	1:B:259:ASN:OD1	2.06	0.55
1:A:318:ILE:HG21	1:A:338:TRP:CE2	2.41	0.55
1:B:676:TYR:CE1	1:B:774:VAL:HB	2.40	0.55
1:B:780:PHE:CE1	1:B:807:LEU:HD12	2.43	0.54
1:B:397:CYS:SG	1:B:397:CYS:O	2.66	0.53
1:B:261:MET:CE	1:B:488:ARG:HD2	2.38	0.53
1:A:615:PRO:HG3	1:A:694:TYR:OH	2.09	0.53
1:A:397:CYS:O	1:A:397:CYS:SG	2.66	0.53
1:A:839:LEU:HD21	1:A:863:LEU:HD23	1.90	0.52
1:B:624:ASN:ND2	1:B:624:ASN:N	2.57	0.52
1:B:839:LEU:HD21	1:B:863:LEU:HD23	1.92	0.52
1:B:598:ILE:O	1:B:598:ILE:HG23	2.10	0.51
1:A:199:LEU:HD13	1:A:378:VAL:HG11	1.93	0.51
1:B:734:TYR:OH	1:B:736:GLU:OE1	2.14	0.51
1:A:598:ILE:O	1:A:598:ILE:HG23	2.10	0.51
1:A:135:ARG:O	1:A:138:GLU:HB2	2.10	0.51
1:B:199:LEU:HD13	1:B:378:VAL:HG11	1.92	0.51
1:B:693:LEU:HD11	1:B:743:ILE:HG21	1.94	0.50
1:B:485:LYS:HG3	1:B:485:LYS:O	2.12	0.50
1:B:261:MET:HE1	1:B:488:ARG:HD2	1.94	0.50
1:A:702:SER:OG	1:A:704:VAL:HG22	2.12	0.50
1:B:262:TYR:OH	1:B:444:VAL:HG23	2.12	0.50
1:A:398:LEU:HD23	1:A:399:ASN:N	2.27	0.49
1:B:619:PHE:O	1:B:623:LEU:HB2	2.12	0.49
1:B:655:LEU:HB2	1:B:662:THR:HG23	1.94	0.49
1:A:262:TYR:OH	1:A:444:VAL:HG23	2.12	0.49
1:A:689:PHE:HZ	1:A:733:ILE:HG12	1.78	0.49
1:A:89:SER:HB2	1:A:117:ASP:OD2	2.13	0.49
1:A:141:LEU:HD22	1:B:169:LYS:HE2	1.95	0.49
1:A:267:ASN:OD1	1:A:444:VAL:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:LEU:HD11	1:A:743:ILE:HG21	1.95	0.48
1:B:627:THR:O	1:B:627:THR:HG22	2.13	0.48
1:B:267:ASN:OD1	1:B:444:VAL:HG22	2.13	0.48
1:A:733:ILE:HD12	1:A:733:ILE:N	2.28	0.48
1:B:398:LEU:HD23	1:B:399:ASN:N	2.28	0.48
1:B:618:ASP:OD1	1:B:619:PHE:N	2.46	0.48
1:B:318:ILE:HG21	1:B:338:TRP:CZ2	2.49	0.48
1:B:235:PRO:HD3	1:B:483:PHE:CE1	2.49	0.48
1:A:164:SER:HB3	1:A:170:LYS:HG2	1.95	0.48
1:B:247:THR:CG2	1:B:249:LEU:HD12	2.43	0.48
1:A:659:GLN:HB3	1:A:725:ARG:NH2	2.28	0.48
1:A:768:GLU:OE1	1:A:769:ARG:NH1	2.47	0.48
1:A:631:ASP:O	1:A:634:TYR:N	2.47	0.47
1:A:318:ILE:HG21	1:A:338:TRP:CZ2	2.49	0.47
7:A:2032:NAG:C8	7:A:2032:NAG:H3	2.44	0.47
1:A:161:ASN:HB2	1:A:165:VAL:HG23	1.96	0.47
1:B:624:ASN:ND2	1:B:624:ASN:H	2.12	0.47
1:B:389:LEU:HD13	1:B:398:LEU:HD13	1.97	0.47
1:B:389:LEU:CD1	1:B:398:LEU:HD13	2.45	0.47
1:A:127:HIS:HA	1:B:380:ARG:HD3	1.97	0.47
1:B:444:VAL:HG13	1:B:444:VAL:O	2.15	0.47
1:A:235:PRO:HD3	1:A:483:PHE:CE1	2.49	0.47
1:A:615:PRO:HB3	1:A:694:TYR:CE2	2.50	0.47
1:A:444:VAL:HG13	1:A:444:VAL:O	2.16	0.46
1:A:567:ASN:HD22	5:A:2001:NAG:H83	1.81	0.46
1:A:727:ASN:HB2	1:A:734:TYR:CE1	2.51	0.46
1:A:693:LEU:HD21	1:A:718:TYR:CE2	2.51	0.45
1:B:262:TYR:CZ	1:B:444:VAL:HG23	2.51	0.45
1:B:483:PHE:O	1:B:489:ILE:HD13	2.17	0.45
1:A:644:ARG:NH2	1:A:884:ASP:OD1	2.50	0.45
1:B:623:LEU:O	1:B:627:THR:CB	2.63	0.44
1:B:448:TYR:OH	1:B:491:PRO:HD3	2.17	0.44
8:B:2012:NAG:O3	8:B:2013:BMA:H2	2.17	0.44
1:A:685:SER:CB	1:A:733:ILE:HD11	2.47	0.44
1:B:194:THR:HG21	1:B:558:LEU:HB3	1.99	0.44
1:A:262:TYR:CZ	1:A:444:VAL:HG23	2.52	0.44
1:B:233:MET:HE3	1:B:547:GLU:HB3	2.00	0.44
1:B:644:ARG:NH2	1:B:884:ASP:OD1	2.50	0.44
1:B:386:MET:HE3	1:B:400:LEU:HD22	2.00	0.44
1:A:848:SER:O	1:A:849:CYS:C	2.56	0.44
1:A:124:GLU:HG2	1:A:125:PRO:HD3	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:LYS:O	1:B:381:LEU:HD13	2.18	0.43
1:B:247:THR:HG22	1:B:249:LEU:HG	1.99	0.43
1:A:194:THR:HG21	1:A:558:LEU:HB3	2.00	0.43
1:A:448:TYR:OH	1:A:491:PRO:HD3	2.18	0.43
1:B:443:ASP:HB2	1:B:447:THR:HB	2.01	0.43
1:B:366:PRO:O	1:B:367:VAL:CG2	2.67	0.43
1:B:693:LEU:HD21	1:B:718:TYR:CE2	2.54	0.43
1:B:850:THR:O	1:B:851:HIS:C	2.56	0.43
1:B:628:GLU:O	1:B:629:ASP:C	2.57	0.43
1:A:369:SER:HB3	1:B:213:LEU:HD13	2.00	0.42
1:A:124:GLU:N	1:A:125:PRO:CD	2.82	0.42
1:A:120:GLU:HG3	1:A:134:PHE:CE2	2.54	0.42
1:B:798:SER:OG	1:B:805:GLU:HG2	2.18	0.42
1:B:214:LEU:HD22	1:B:379:ASP:HB2	2.01	0.42
1:B:616:ILE:O	1:B:619:PHE:HB3	2.20	0.42
1:B:242:HIS:CE1	1:B:405:ASP:HB3	2.54	0.42
1:A:622:GLN:NE2	1:A:736:GLU:OE1	2.52	0.42
1:A:242:HIS:CE1	1:A:405:ASP:HB3	2.54	0.42
1:A:443:ASP:HB2	1:A:447:THR:HB	2.01	0.42
1:B:709:TYR:CE1	1:B:802:ARG:HB2	2.54	0.42
1:A:850:THR:O	1:A:851:HIS:C	2.58	0.42
1:B:614:VAL:HG12	1:B:618:ASP:OD1	2.19	0.42
1:A:613:ILE:HG22	1:A:615:PRO:HD3	2.01	0.42
1:B:388:GLY:O	1:B:392:LEU:HG	2.20	0.42
1:B:676:TYR:CD1	1:B:722:THR:HG22	2.55	0.41
1:B:406:HIS:NE2	1:B:517:HIS:CE1	2.88	0.41
1:B:657:GLN:OE1	1:B:698:ARG:NH2	2.52	0.41
1:B:848:SER:O	1:B:849:CYS:C	2.56	0.41
1:B:474:LYS:NZ	1:B:486:SER:O	2.52	0.41
1:B:616:ILE:HB	1:B:694:TYR:CD2	2.56	0.41
1:A:839:LEU:CD2	1:A:863:LEU:HD23	2.50	0.41
1:A:89:SER:CB	1:A:117:ASP:OD2	2.68	0.41
1:B:625:LEU:O	1:B:626:THR:CG2	2.57	0.41
1:A:214:LEU:HD22	1:A:379:ASP:HB2	2.01	0.41
1:A:657:GLN:OE1	1:A:698:ARG:NH2	2.53	0.41
1:A:443:ASP:HB2	1:A:447:THR:CB	2.51	0.41
1:A:135:ARG:NH2	1:A:146:CYS:O	2.50	0.41
1:B:310:GLU:HG2	1:B:315:LEU:HD13	2.03	0.41
1:A:598:ILE:HD12	1:A:623:LEU:HB2	2.01	0.41
1:A:474:LYS:NZ	1:A:486:SER:O	2.54	0.41
1:A:408:MET:HE3	1:A:516:PHE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:HIS:CE1	1:A:759:ASP:HB2	2.56	0.41
1:A:388:GLY:O	1:A:392:LEU:HG	2.20	0.41
1:A:404:SER:HB3	1:A:529:LEU:H	1.86	0.41
1:A:485:LYS:HD2	1:A:785:ASP:HB2	2.02	0.41
1:B:642:ARG:O	1:B:644:ARG:NH1	2.54	0.41
1:A:124:GLU:O	1:A:128:ILE:HG12	2.20	0.41
1:B:615:PRO:O	1:B:618:ASP:OD1	2.38	0.40
1:A:441:PRO:HG2	1:A:447:THR:HG23	2.03	0.40
1:B:441:PRO:HG2	1:B:447:THR:HG23	2.03	0.40
1:B:328:PHE:HB3	1:B:381:LEU:HD23	2.02	0.40
1:B:625:LEU:HD12	1:B:625:LEU:C	2.41	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	814/820 (99%)	765 (94%)	48 (6%)	1 (0%)	56	90
1	B	735/820 (90%)	697 (95%)	37 (5%)	1 (0%)	56	90
All	All	1549/1640 (94%)	1462 (94%)	85 (6%)	2 (0%)	56	90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	629	ASP
1	A	631	ASP

### 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	749/753 (100%)	738 (98%)	11 (2%)	72	92
1	B	676/753 (90%)	668 (99%)	8 (1%)	78	94
All	All	1425/1506 (95%)	1406 (99%)	19 (1%)	76	93

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	ASP
1	A	160	ILE
1	A	169	LYS
1	A	197	PHE
1	A	416	TYR
1	A	512	CYS
1	A	566	ASN
1	A	630	VAL
1	A	657	GLN
1	A	726	LEU
1	A	763	GLN
1	B	169	LYS
1	B	197	PHE
1	B	416	TYR
1	B	512	CYS
1	B	624	ASN
1	B	626	THR
1	B	657	GLN
1	B	678	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	603	ASN
1	A	763	GLN
1	B	624	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 ⓘ

15 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	$\# Z  > 2$
5	NAG	A	2001	1,5	14,14,15	0.75	0	15,19,21	1.90	5 (33%)
5	NAG	A	2002	5	14,14,15	0.69	0	15,19,21	1.46	4 (26%)
5	BMA	A	2003	5	11,11,12	0.66	0	14,15,17	1.19	2 (14%)
5	MAN	A	2004	5	11,11,12	0.59	0	14,15,17	1.64	2 (14%)
5	MAN	A	2005	5	11,11,12	0.56	0	14,15,17	1.23	1 (7%)
7	NAG	A	2031	1,7	14,14,15	0.60	0	15,19,21	1.64	1 (6%)
7	NAG	A	2032	7	14,14,15	0.70	0	15,19,21	2.07	4 (26%)
5	NAG	B	2001	1,5	14,14,15	0.60	0	15,19,21	1.22	3 (20%)
5	NAG	B	2002	5	14,14,15	0.67	0	15,19,21	0.97	0
5	BMA	B	2003	5	11,11,12	0.55	0	14,15,17	1.52	2 (14%)
5	MAN	B	2004	5	11,11,12	0.52	0	14,15,17	1.25	1 (7%)
5	MAN	B	2005	5	11,11,12	0.59	0	14,15,17	0.90	1 (7%)
8	NAG	B	2011	1,8	14,14,15	0.63	0	15,19,21	1.75	4 (26%)
8	NAG	B	2012	8	14,14,15	0.70	0	15,19,21	1.77	3 (20%)
8	BMA	B	2013	8	11,11,12	0.51	0	14,15,17	1.62	3 (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
5	NAG	A	2001	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2002	5	-	0/6/23/26	0/1/1/1
5	BMA	A	2003	5	-	0/2/19/22	0/1/1/1
5	MAN	A	2004	5	-	0/2/19/22	0/1/1/1
5	MAN	A	2005	5	-	0/2/19/22	0/1/1/1
7	NAG	A	2031	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	2032	7	-	0/6/23/26	0/1/1/1
5	NAG	B	2001	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2002	5	-	0/6/23/26	0/1/1/1
5	BMA	B	2003	5	-	0/2/19/22	0/1/1/1
5	MAN	B	2004	5	-	0/2/19/22	0/1/1/1
5	MAN	B	2005	5	-	0/2/19/22	0/1/1/1
8	NAG	B	2011	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	2012	8	-	0/6/23/26	0/1/1/1
8	BMA	B	2013	8	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	2013	BMA	O5-C1-C2	-3.39	105.35	110.86
5	A	2001	NAG	O7-C7-C8	-2.93	116.68	122.06
7	A	2032	NAG	O7-C7-C8	-2.91	116.72	122.06
8	B	2012	NAG	O7-C7-C8	-2.78	116.96	122.06
5	A	2001	NAG	O4-C4-C3	-2.71	104.24	110.34
8	B	2011	NAG	C4-C3-C2	-2.33	107.61	111.23
5	A	2002	NAG	O7-C7-C8	-2.32	117.80	122.06
5	B	2001	NAG	O7-C7-C8	-2.20	118.02	122.06
5	B	2001	NAG	O4-C4-C3	-2.11	105.59	110.34
5	A	2002	NAG	C6-C5-C4	-2.03	108.00	113.02
8	B	2013	BMA	C1-O5-C5	2.01	114.80	112.25
5	B	2005	MAN	C1-C2-C3	2.03	111.94	109.54
5	A	2003	BMA	C1-O5-C5	2.11	114.92	112.25
5	B	2003	BMA	C2-C3-C4	2.45	115.21	111.04
5	A	2002	NAG	C1-O5-C5	2.46	115.38	112.25
5	B	2001	NAG	C1-O5-C5	2.54	115.47	112.25
5	A	2001	NAG	C3-C4-C5	2.65	114.82	110.20
8	B	2013	BMA	C3-C4-C5	2.77	115.02	110.20
5	A	2002	NAG	C3-C4-C5	2.78	115.04	110.20
8	B	2011	NAG	C2-N2-C7	2.99	126.88	123.04
8	B	2012	NAG	C3-C4-C5	3.00	115.42	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2001	NAG	C1-O5-C5	3.05	116.11	112.25
5	A	2003	BMA	C3-C4-C5	3.08	115.57	110.20
8	B	2011	NAG	C8-C7-N2	3.09	122.01	116.11
5	A	2001	NAG	C8-C7-N2	3.28	122.38	116.11
7	A	2032	NAG	C8-C7-N2	3.31	122.43	116.11
8	B	2011	NAG	C1-O5-C5	3.59	116.80	112.25
5	A	2005	MAN	C1-C2-C3	3.61	113.81	109.54
5	A	2004	MAN	C1-C2-C3	3.73	113.96	109.54
5	B	2003	BMA	C3-C4-C5	3.74	116.71	110.20
5	B	2004	MAN	C1-O5-C5	3.83	117.10	112.25
7	A	2032	NAG	C3-C2-N2	4.12	120.43	110.56
5	A	2004	MAN	C1-O5-C5	4.13	117.49	112.25
8	B	2012	NAG	C4-C3-C2	4.45	118.15	111.23
7	A	2032	NAG	C2-N2-C7	4.70	129.07	123.04
7	A	2031	NAG	C1-O5-C5	5.52	119.25	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2001	NAG	3	0
7	A	2032	NAG	2	0
8	B	2012	NAG	1	0
8	B	2013	BMA	1	0

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\# Z  > 2$
4	PO4	A	1007	2	4,4,4	0.35	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	2011	1	14,14,15	0.43	0	15,19,21	1.36	1 (6%)
6	NAG	A	2021	1	14,14,15	0.67	0	15,19,21	1.40	2 (13%)
4	PO4	B	1007	2	4,4,4	0.44	0	6,6,6	0.27	0
6	NAG	B	2021	1	14,14,15	0.42	0	15,19,21	1.54	5 (33%)
6	NAG	B	2026	1	14,14,15	0.46	0	15,19,21	1.06	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
4	PO4	A	1007	2	-	0/0/0/0	0/0/0/0
6	NAG	A	2011	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2021	1	-	0/6/23/26	0/1/1/1
4	PO4	B	1007	2	-	0/0/0/0	0/0/0/0
6	NAG	B	2021	1	-	0/6/23/26	0/1/1/1
6	NAG	B	2026	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2021	NAG	C4-C3-C2	-2.82	106.84	111.23
6	B	2021	NAG	O7-C7-C8	-2.06	118.28	122.06
6	B	2021	NAG	C1-O5-C5	2.25	115.10	112.25
6	B	2021	NAG	C3-C2-N2	2.40	116.32	110.56
6	B	2021	NAG	C8-C7-N2	2.47	120.83	116.11
6	A	2021	NAG	C3-C2-N2	3.02	117.80	110.56
6	A	2021	NAG	C2-N2-C7	3.47	127.50	123.04
6	A	2011	NAG	C1-O5-C5	4.53	118.00	112.25

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

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	816/820 (99%)	-0.18	9 (1%) 82 58	71, 105, 156, 198	0
1	B	737/820 (89%)	0.02	17 (2%) 64 33	78, 123, 173, 209	0
All	All	1553/1640 (94%)	-0.09	26 (1%) 73 45	71, 115, 167, 209	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	445	PRO	4.5
1	B	446	GLU	4.2
1	A	448	TYR	4.2
1	B	666	LEU	3.7
1	B	448	TYR	3.5
1	B	627	THR	3.0
1	B	704	VAL	2.9
1	B	169	LYS	2.9
1	B	592	PHE	2.9
1	B	724	PRO	2.8
1	A	97	ARG	2.6
1	A	168	ASP	2.5
1	A	612	TRP	2.5
1	A	631	ASP	2.3
1	B	447	THR	2.2
1	B	685	SER	2.2
1	A	611	PRO	2.2
1	B	281	LEU	2.2
1	A	613	ILE	2.2
1	B	626	THR	2.2
1	B	729	VAL	2.1
1	B	619	PHE	2.1
1	B	737	ALA	2.1
1	A	132	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	170	LYS	2.0
1	A	730	SER	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](#)

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
5	NAG	A	2001	14/15	0.92	0.22	0.50	86,90,94,99	0
5	NAG	B	2001	14/15	0.94	0.21	0.20	106,120,124,127	0
5	NAG	A	2002	14/15	0.95	0.15	-1.28	105,109,115,126	0
7	NAG	A	2031	14/15	0.94	0.15	-1.59	108,116,119,123	0
5	NAG	B	2002	14/15	0.90	0.23	-	126,135,142,148	0
5	MAN	A	2004	11/12	0.63	0.22	-	151,158,161,163	0
8	NAG	B	2011	14/15	0.92	0.16	-	126,134,137,138	0
5	BMA	B	2003	11/12	0.81	0.11	-	152,158,165,167	0
5	MAN	B	2005	11/12	0.84	0.22	-	165,166,172,173	0
5	MAN	A	2005	11/12	0.86	0.15	-	144,149,155,158	0
8	NAG	B	2012	14/15	0.87	0.21	-	145,148,156,159	0
8	BMA	B	2013	11/12	0.79	0.22	-	151,152,155,157	0
7	NAG	A	2032	14/15	0.73	0.35	-	132,139,146,146	0
5	MAN	B	2004	11/12	0.64	0.20	-	171,176,178,180	0
5	BMA	A	2003	11/12	0.82	0.17	-	133,143,148,153	0

## 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( $\text{\AA}^2$ )	Q<0.9
2	ZN	B	1001	1/1	0.99	0.18	0.46	96,96,96,96	0
2	ZN	A	1002	1/1	0.99	0.21	0.39	89,89,89,89	0
3	CA	A	1003	1/1	0.96	0.17	0.04	89,89,89,89	0
2	ZN	A	1001	1/1	0.99	0.19	-0.36	90,90,90,90	0
2	ZN	B	1002	1/1	0.99	0.17	-0.44	95,95,95,95	0
3	CA	B	1003	1/1	0.94	0.15	-1.18	124,124,124,124	0
4	PO4	B	1007	5/5	0.97	0.14	-1.80	149,150,156,158	0
4	PO4	A	1007	5/5	0.98	0.14	-2.61	133,137,141,143	0
6	NAG	A	2011	14/15	0.83	0.18	-	131,136,139,141	0
6	NAG	A	2021	14/15	0.81	0.45	-	142,147,154,155	0
6	NAG	B	2021	14/15	0.76	0.37	-	147,151,155,155	0
6	NAG	B	2026	14/15	0.78	0.33	-	168,175,178,181	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.