Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:58 PM GMT

PDB ID	:	4GTW
Title	:	Crystal structure of mouse Enpp1 in complex with AMP
Authors	:	Kato, K.; Nishimasu, H.; Ishitani, R.; Nureki, O.
Deposited on	:	2012-08-29
Resolution	:	2.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

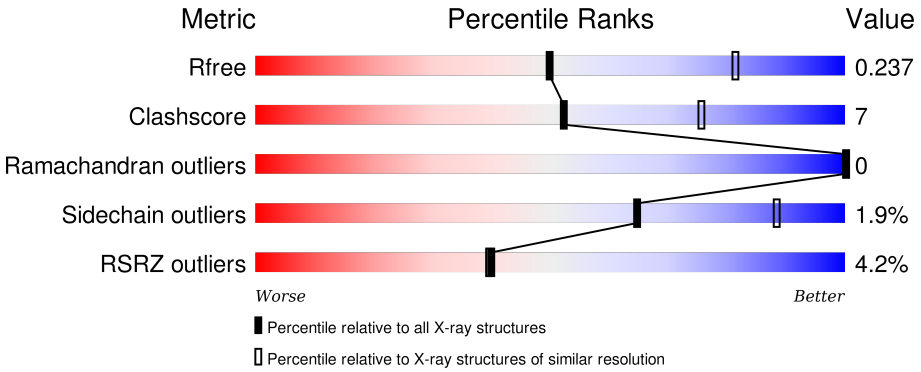
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	823	2% 70% 15% • 14%
1	B	823	5% 71% 12% • 15%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11346 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 2, Alkaline phosphodiesterase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	706	Total	C	N	O	S	Se	0	0	0
			5536	3564	916	1027	17	12			
1	B	697	Total	C	N	O	S	Se	0	0	0
			5481	3527	902	1023	17	12			

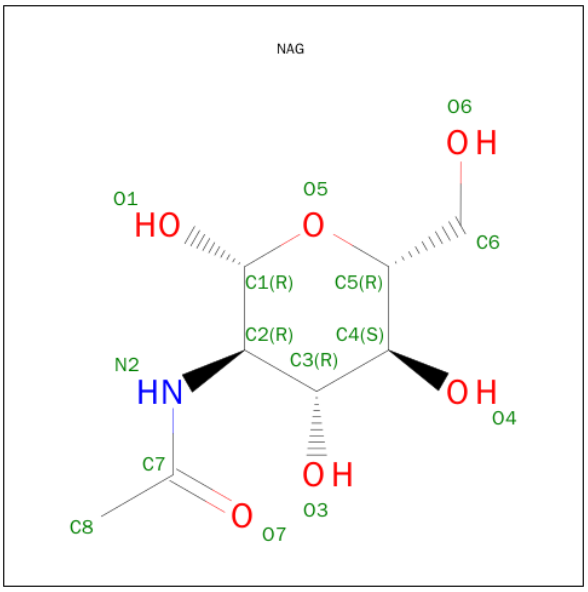
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	ARG	LYS	ENGINEERED MUTATION	UNP Q9R1E6
B	59	ARG	LYS	ENGINEERED MUTATION	UNP Q9R1E6

- Molecule 2 is a polymer of unknown type called SUGAR (6-MER).

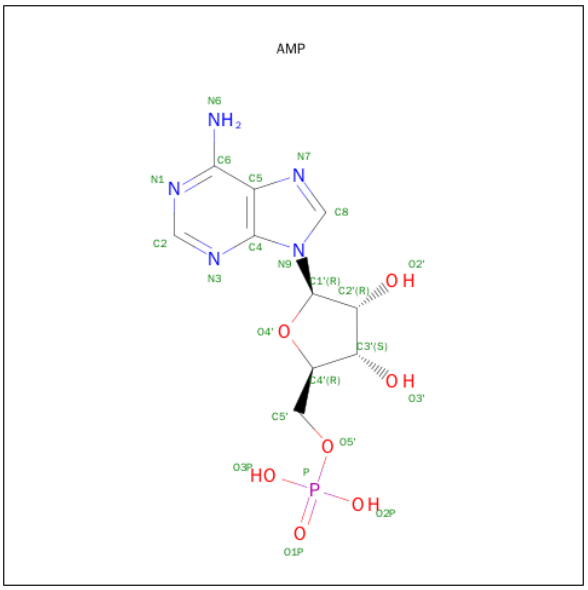
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

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

- Molecule 8 is water.

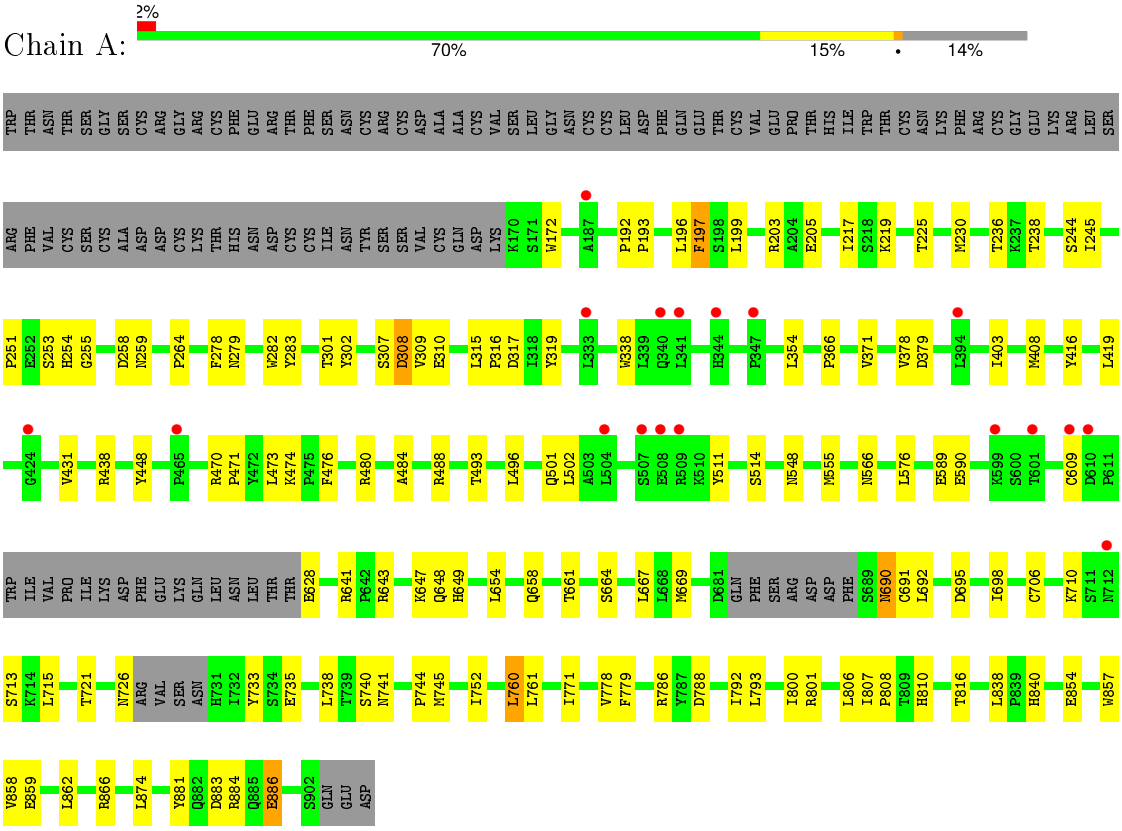
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	70	Total	O	0	0
			70	70		
8	B	51	Total	O	0	0
			51	51		

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.

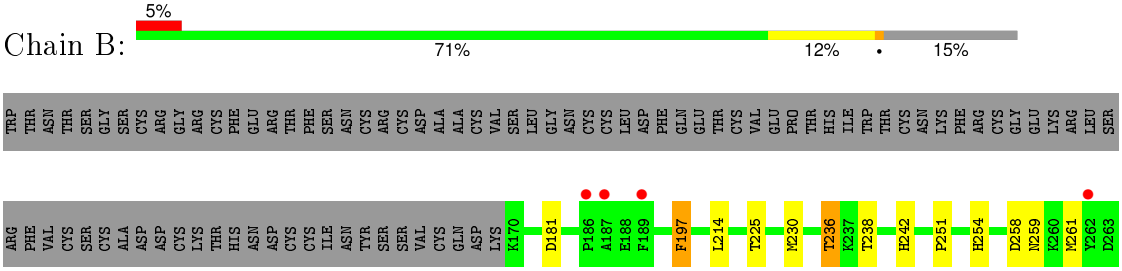
• Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2, Alkaline phosphodiesterase I

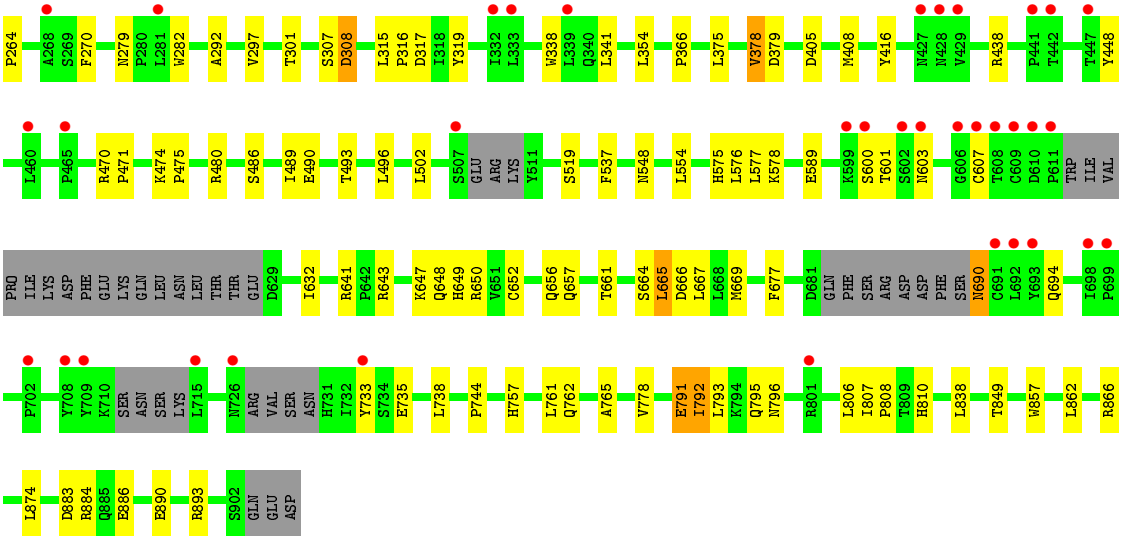
Chain A:



• Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2, Alkaline phosphodiesterase I

Chain B:




P264 A268 S269 F270 N279 P280 L281 W282 A292 V297 T301 S307 D308 L315 P316 D317 I318 Y319 I332 L333 W338 L339 Q340 L341 L354 P366 L375 V378 D379 D405 M408 Y416 N427 N428 V429 R438 P441 T442 T447 Y448
L460 P465 R470 P471 K474 P475 R480 S486 I489 E490 T493 L496 L502 S507 GLU ARG LYS Y511 S519 F537 N548 L554 H575 L576 L577 K578 E589 K599 S600 T601 S602 N603 G606 C607 T608 C609 D610 P611 TRP ILE VAL
PRO ILE LYS ASP PHE GLU LYS GLN LEU ASN LEU THR THR GLU D629 I632 R641 P642 R643 K647 Q648 H649 R650 V651 C652 Q656 Q657 T661 S664 L665 D666 L667 L668 M669 F677 D681 GLN PHE SER ARG ASP ASP PHE SER N690 C691 L692 Y693 Q694 I698 P699
P702 Y708 Y709 K710 SER ASN SER LYS L715 N726 ARG VAL SER ASN H731 I732 Y733 S734 E735 L738 P744 H757 L761 Q762 A765 V778 E791 I792 L793 K794 Q795 N796 R801 L806 I807 P808 T809 H810 L838 T849 W857 L862 R866
L874 D883 R884 Q885 E886 E890 R893 S902 GLN GLU ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	105.28Å 105.28Å 173.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.88 – 2.70 48.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.88-2.70) 98.4 (48.87-2.70)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.231 , 0.276 0.237 , 0.237	Depositor DCC
R_{free} test set	2914 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.6	EDS
Estimated twinning fraction	0.049 for -h,-k,l 0.073 for h,-h-k,-l 0.049 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 58182 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	11346	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, BMA, NAG, CA, AMP, 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	0.22	0/5688	0.42	0/7747
1	B	0.22	0/5630	0.41	0/7668
All	All	0.22	0/11318	0.42	0/15415

There are no bond length outliers.

There are no bond angle outliers.

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	5536	0	5222	79	0
1	B	5481	0	5156	66	0
2	A	72	0	61	1	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
4	A	23	0	12	2	0
4	B	23	0	12	2	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	28	0	25	0	0
8	A	70	0	0	3	0
8	B	51	0	0	1	0
All	All	11346	0	10540	146	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 7.

All (146) 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:715:LEU:O	1:A:801:ARG:NH2	2.12	0.83
1:B:650:ARG:NH1	1:B:666:ASP:OD1	2.16	0.78
1:B:230:MSE:HE2	1:B:548:ASN:HA	1.70	0.72
1:B:603:ASN:H	1:B:694:GLN:HE22	1.41	0.69
1:B:225:THR:HG21	1:B:576:LEU:HG	1.75	0.68
1:A:316:PRO:HG2	1:A:319:TYR:HB3	1.75	0.68
1:A:230:MSE:HE2	1:A:548:ASN:HA	1.74	0.68
1:A:225:THR:HG21	1:A:576:LEU:HG	1.78	0.66
1:B:238:THR:OG1	4:B:1005:AMP:P	2.54	0.65
1:A:308:ASP:OD2	1:A:308:ASP:N	2.31	0.64
1:A:838:LEU:HD21	1:A:862:LEU:HD13	1.80	0.63
1:A:238:THR:OG1	4:A:1009:AMP:P	2.57	0.62
1:A:196:LEU:HD22	1:A:555:MSE:HE1	1.80	0.62
1:B:838:LEU:HD11	1:B:862:LEU:HD13	1.81	0.62
1:B:496:LEU:HD21	1:B:502:LEU:HB2	1.81	0.61
1:A:649:HIS:NE2	1:A:664:SER:OG	2.25	0.61
1:B:438:ARG:HG2	1:B:493:THR:HG22	1.82	0.61
1:B:733:TYR:CZ	1:B:735:GLU:HB2	2.35	0.61
1:B:316:PRO:HG2	1:B:319:TYR:HB3	1.82	0.60
1:B:643:ARG:NH2	1:B:883:ASP:OD2	2.34	0.60
1:A:733:TYR:CZ	1:A:735:GLU:HB2	2.37	0.59
1:B:575:HIS:CE1	1:B:893:ARG:HD3	2.37	0.59
1:A:438:ARG:HG2	1:A:493:THR:HG22	1.84	0.59
1:B:792:ILE:O	1:B:796:ASN:ND2	2.32	0.59
1:A:197:PHE:HE1	1:A:354:LEU:HD13	1.67	0.58
1:B:315:LEU:HD12	1:B:316:PRO:HD2	1.85	0.58
1:B:438:ARG:HB3	1:B:490:GLU:HB2	1.86	0.58
1:A:721:THR:HB	1:A:741:ASN:HD21	1.69	0.57
1:B:649:HIS:HE2	1:B:664:SER:HG	1.51	0.57
1:B:600:SER:OG	1:B:601:THR:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:LYS:H	1:A:801:ARG:NH1	2.02	0.57
1:B:735:GLU:HA	1:B:738:LEU:HD13	1.86	0.57
1:A:496:LEU:HD21	1:A:502:LEU:HB2	1.86	0.57
1:A:793:LEU:HD22	1:A:806:LEU:HD21	1.86	0.57
1:A:690:ASN:O	1:A:690:ASN:ND2	2.38	0.57
1:A:643:ARG:NH2	1:A:883:ASP:OD2	2.38	0.56
1:B:264:PRO:HG3	1:B:448:TYR:CZ	2.41	0.56
1:A:698:ILE:HD13	1:A:740:SER:HB3	1.87	0.56
1:B:301:THR:HG21	1:B:307:SER:HB2	1.88	0.55
1:A:501:GLN:NE2	8:A:1138:HOH:O	2.35	0.55
1:A:196:LEU:HD13	1:A:555:MSE:HE1	1.89	0.55
1:A:258:ASP:OD1	1:A:259:ASN:N	2.39	0.54
1:B:258:ASP:OD1	1:B:259:ASN:N	2.40	0.54
1:B:667:LEU:HB3	1:B:669:MSE:HG2	1.89	0.54
1:A:778:VAL:HB	1:A:810:HIS:HB2	1.89	0.54
1:B:744:PRO:HG2	1:B:808:PRO:HD3	1.89	0.54
1:A:589:GLU:OE2	1:A:641:ARG:NH2	2.41	0.54
1:B:649:HIS:NE2	1:B:664:SER:OG	2.32	0.53
1:A:301:THR:HG21	1:A:307:SER:HB3	1.89	0.53
1:B:757:HIS:HA	1:B:761:LEU:HB2	1.90	0.53
1:B:589:GLU:OE2	1:B:641:ARG:NH2	2.42	0.52
1:B:261:MSE:HG3	1:B:270:PHE:HB3	1.90	0.52
1:B:338:TRP:HA	1:B:341:LEU:HD13	1.91	0.52
1:A:760:LEU:HD21	1:A:859:GLU:HG2	1.91	0.52
1:A:649:HIS:HE1	1:A:667:LEU:HD13	1.76	0.51
1:B:890:GLU:HG2	1:B:893:ARG:HH21	1.75	0.51
1:A:735:GLU:HA	1:A:738:LEU:HD13	1.93	0.51
1:A:310:GLU:HB3	1:A:315:LEU:HG	1.91	0.51
1:A:511:TYR:HD2	1:A:514:SER:HG	1.60	0.50
1:B:537:PHE:O	1:B:578:LYS:NZ	2.36	0.50
1:B:366:PRO:HG3	1:B:408:MSE:HG3	1.92	0.50
1:A:172:TRP:O	1:A:219:LYS:NZ	2.41	0.50
1:A:744:PRO:HG2	1:A:808:PRO:HD3	1.94	0.50
1:A:255:GLY:O	1:A:488:ARG:NH2	2.44	0.49
1:B:197:PHE:HE1	1:B:354:LEU:HD13	1.77	0.49
1:A:278:PHE:HA	1:A:309:VAL:HG22	1.94	0.49
1:A:203:ARG:NH2	1:A:205:GLU:OE1	2.46	0.49
1:A:283:TYR:CE2	1:A:309:VAL:HG21	2.48	0.49
1:A:366:PRO:HG3	1:A:408:MSE:HG3	1.94	0.49
1:A:647:LYS:HA	1:A:648:GLN:HA	1.54	0.48
1:A:199:LEU:HD13	1:A:378:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:CYS:HB3	1:B:690:ASN:O	2.13	0.48
1:A:264:PRO:HG3	1:A:448:TYR:CZ	2.48	0.48
1:B:778:VAL:HB	1:B:810:HIS:HB2	1.94	0.48
1:B:486:SER:HB3	1:B:489:ILE:HG13	1.95	0.48
1:A:419:LEU:HD12	1:A:431:VAL:HG21	1.96	0.48
1:B:308:ASP:OD2	1:B:308:ASP:N	2.47	0.47
1:A:566:ASN:ND2	8:A:1108:HOH:O	2.48	0.47
1:B:791:GLU:O	1:B:795:GLN:HG3	2.15	0.47
1:B:292:ALA:HB1	1:B:297:VAL:HB	1.97	0.47
1:B:649:HIS:HE1	1:B:667:LEU:HD13	1.80	0.46
1:A:695:ASP:OD2	1:A:740:SER:OG	2.28	0.46
1:A:282:TRP:HA	1:A:488:ARG:NH1	2.30	0.46
1:B:214:LEU:HD22	1:B:379:ASP:HB2	1.96	0.46
1:B:793:LEU:HD22	1:B:806:LEU:HD21	1.97	0.46
1:B:554:LEU:HD11	1:B:577:LEU:HD21	1.97	0.46
1:A:752:ILE:HG23	1:A:858:VAL:HG13	1.97	0.46
1:A:816:THR:HG1	1:A:881:TYR:HH	1.56	0.46
1:A:302:TYR:HD2	1:A:338:TRP:CH2	2.33	0.46
1:A:695:ASP:HB3	1:A:698:ILE:HG12	1.97	0.46
1:B:279:ASN:HB3	1:B:282:TRP:CD1	2.51	0.46
1:B:656:GLN:HE22	1:B:661:THR:HG22	1.81	0.46
1:B:632:ILE:HG12	1:B:657:GLN:HA	1.98	0.45
1:B:251:PRO:HA	1:B:254:HIS:CE1	2.51	0.45
1:B:677:PHE:HE2	1:B:762:GLN:HA	1.81	0.45
1:A:854:GLU:HA	1:A:857:TRP:NE1	2.31	0.45
1:A:884:ARG:HG3	1:A:886:GLU:HG2	1.97	0.45
1:A:473:LEU:HB2	1:A:476:PHE:CD2	2.51	0.45
1:A:788:ASP:HB3	1:A:792:ILE:HG23	1.98	0.45
1:B:242:HIS:CE1	1:B:405:ASP:HB3	2.51	0.45
1:A:282:TRP:HA	1:A:488:ARG:HH12	1.82	0.44
1:B:603:ASN:N	1:B:694:GLN:HE22	2.11	0.44
1:A:643:ARG:NH1	1:B:181:ASP:OD1	2.50	0.44
1:B:677:PHE:CE2	1:B:762:GLN:HA	2.53	0.44
1:A:658:GLN:NE2	1:A:726:ASN:HD22	2.16	0.44
1:B:470:ARG:HA	1:B:471:PRO:HD3	1.88	0.44
1:A:692:LEU:HD12	1:A:706:CYS:SG	2.58	0.44
1:A:366:PRO:O	1:A:371:VAL:HG21	2.18	0.43
1:A:474:LYS:HG2	1:A:484:ALA:HA	1.99	0.43
1:B:474:LYS:HG3	1:B:475:PRO:HD3	2.00	0.43
1:A:245:ILE:HD13	1:A:403:ILE:HD13	2.00	0.43
1:A:807:ILE:HA	1:A:808:PRO:HD3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:TYR:OH	1:A:735:GLU:OE1	2.25	0.43
1:B:279:ASN:HB3	1:B:282:TRP:HD1	1.83	0.43
1:A:649:HIS:CE1	1:A:667:LEU:HD13	2.54	0.43
1:B:647:LYS:HA	1:B:648:GLN:HA	1.53	0.43
1:B:375:LEU:O	1:B:378:VAL:HG12	2.19	0.43
1:B:251:PRO:HA	1:B:254:HIS:NE2	2.34	0.43
1:A:480:ARG:HD3	1:A:866:ARG:O	2.19	0.42
1:B:884:ARG:HA	1:B:884:ARG:HD2	1.88	0.42
4:A:1009:AMP:N6	8:A:1169:HOH:O	2.32	0.42
1:A:251:PRO:HA	1:A:254:HIS:CE1	2.54	0.42
1:B:807:ILE:HA	1:B:808:PRO:HD3	1.83	0.42
1:A:244:SER:OG	1:A:254:HIS:NE2	2.50	0.42
1:A:713:SER:HB3	1:A:801:ARG:NH1	2.35	0.42
1:A:217:ILE:HG12	1:A:379:ASP:OD1	2.20	0.42
1:A:669:MSE:SE	1:A:779:PHE:HZ	2.53	0.42
1:B:884:ARG:HG3	1:B:886:GLU:OE1	2.20	0.42
1:B:480:ARG:HD3	1:B:866:ARG:O	2.20	0.41
4:B:1005:AMP:N6	8:B:1149:HOH:O	2.42	0.41
1:A:761:LEU:HG	1:A:771:ILE:HD11	2.03	0.41
1:A:654:LEU:HB2	1:A:661:THR:HG23	2.01	0.41
1:A:172:TRP:CZ3	1:A:219:LYS:HD3	2.55	0.41
1:B:652:CYS:SG	1:B:665:LEU:HD21	2.60	0.41
1:A:470:ARG:HA	1:A:471:PRO:HD3	1.87	0.41
1:A:197:PHE:CE1	1:A:354:LEU:HD13	2.52	0.41
1:A:609:CYS:HA	1:A:691:CYS:HB2	2.03	0.41
1:A:715:LEU:HD23	1:A:800:ILE:HD13	2.02	0.41
1:B:849:THR:HG23	1:B:857:TRP:NE1	2.36	0.41
1:A:192:PRO:HA	1:A:193:PRO:HD3	1.92	0.41
1:A:786:ARG:HH21	2:A:1002:NAG:H62	1.86	0.41
1:B:643:ARG:HD3	1:B:643:ARG:HA	1.98	0.40
1:B:677:PHE:CD2	1:B:765:ALA:HB2	2.56	0.40
1:A:745:MSE:HA	1:A:840:HIS:CE1	2.56	0.40
1:B:236:THR:OG1	1:B:519:SER:O	2.39	0.40
1:A:279:ASN:HB3	1:A:282:TRP:CD1	2.57	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	698/823 (85%)	675 (97%)	23 (3%)	0	100	100
1	B	685/823 (83%)	660 (96%)	25 (4%)	0	100	100
All	All	1383/1646 (84%)	1335 (96%)	48 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	600/743 (81%)	588 (98%)	12 (2%)	63	87
1	B	596/743 (80%)	585 (98%)	11 (2%)	66	89
All	All	1196/1486 (80%)	1173 (98%)	23 (2%)	65	88

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	PHE
1	A	236	THR
1	A	253	SER
1	A	308	ASP
1	A	317	ASP
1	A	416	TYR
1	A	590	GLU
1	A	628	GLU

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Mol	Chain	Res	Type
1	A	690	ASN
1	A	760	LEU
1	A	874	LEU
1	A	886	GLU
1	B	197	PHE
1	B	236	THR
1	B	308	ASP
1	B	317	ASP
1	B	378	VAL
1	B	416	TYR
1	B	665	LEU
1	B	690	ASN
1	B	791	GLU
1	B	792	ILE
1	B	874	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	A	525	ASN
1	A	553	ASN
1	A	570	HIS
1	A	595	GLN
1	A	634	HIS
1	A	658	GLN
1	A	690	ASN
1	A	769	ASN
1	A	820	GLN
1	A	850	HIS
1	B	229	ASN
1	B	570	HIS
1	B	694	GLN
1	B	820	GLN

5.3.3 RNA

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)

8 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	1001	1,2	14,14,15	0.53	0	15,19,21	0.78	0
2	NAG	A	1002	2	14,14,15	0.51	0	15,19,21	0.65	0
2	BMA	A	1003	2	11,11,12	0.62	0	14,15,17	0.73	0
2	MAN	A	1004	2	11,11,12	0.62	0	14,15,17	0.54	0
2	MAN	A	1005	2	11,11,12	0.61	0	14,15,17	1.42	3 (21%)
2	MAN	A	1006	2	11,11,12	0.56	0	14,15,17	0.81	0
7	NAG	B	1001	1,7	14,14,15	0.54	0	15,19,21	0.87	0
7	NAG	B	1002	7	14,14,15	0.48	0	15,19,21	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1003	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1004	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1005	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1006	2	-	0/2/19/22	1/1/1/1
7	NAG	B	1001	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	1002	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1005	MAN	C3-C4-C5	2.01	113.69	110.20
2	A	1005	MAN	C1-O5-C5	2.77	115.76	112.25
2	A	1005	MAN	C1-C2-C3	2.94	113.02	109.54

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1006	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	NAG	1	0

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	NAG	A	1007	1	14,14,15	0.50	0	15,19,21	0.71	0
3	NAG	A	1008	1	14,14,15	0.50	0	15,19,21	0.73	0
4	AMP	A	1009	5	20,25,25	0.94	1 (5%)	22,38,38	1.88	4 (18%)
3	NAG	B	1003	1	14,14,15	0.50	0	15,19,21	0.65	0
3	NAG	B	1004	1	14,14,15	0.50	0	15,19,21	0.69	0
4	AMP	B	1005	5	20,25,25	0.95	1 (5%)	22,38,38	1.88	4 (18%)

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	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1008	1	-	0/6/23/26	0/1/1/1
4	AMP	A	1009	5	-	0/6/26/26	0/3/3/3
3	NAG	B	1003	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1004	1	-	0/6/23/26	0/1/1/1
4	AMP	B	1005	5	-	0/6/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1009	AMP	C5-C4	3.10	1.47	1.40
4	B	1005	AMP	C5-C4	3.14	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1005	AMP	N3-C2-N1	-6.89	123.62	128.89
4	A	1009	AMP	N3-C2-N1	-6.83	123.67	128.89
4	A	1009	AMP	C4-C5-N7	-3.23	106.50	109.48
4	B	1005	AMP	C4-C5-N7	-3.11	106.62	109.48
4	B	1005	AMP	O3P-P-O5'	-2.49	99.41	106.56
4	A	1009	AMP	O3P-P-O5'	-2.32	99.88	106.56
4	B	1005	AMP	O2P-P-O1P	2.36	118.17	110.58
4	A	1009	AMP	O2P-P-O1P	2.37	118.20	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1009	AMP	2	0
4	B	1005	AMP	2	0

5.7 Other polymers (i)

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^{th} 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	694/823 (84%)	-0.04	18 (2%)	59	59	14, 45, 88, 128	0
1	B	685/823 (83%)	0.10	40 (5%)	26	25	16, 45, 86, 137	0
All	All	1379/1646 (83%)	0.03	58 (4%)	40	39	14, 45, 88, 137	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	507	SER	4.2
1	B	608	THR	4.0
1	B	427	ASN	4.0
1	B	611	PRO	3.9
1	B	609	CYS	3.6
1	B	333	LEU	3.6
1	B	801	ARG	3.6
1	A	712	ASN	3.5
1	B	187	ALA	3.4
1	A	509	ARG	3.4
1	B	600	SER	3.3
1	B	708	TYR	3.1
1	B	709	TYR	3.1
1	B	602	SER	3.0
1	B	603	ASN	2.9
1	B	702	PRO	2.9
1	B	428	ASN	2.9
1	B	715	LEU	2.9
1	B	465	PRO	2.8
1	A	187	ALA	2.8
1	B	186	PRO	2.7
1	B	599	LYS	2.7
1	A	424	GLY	2.6
1	A	465	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	508	GLU	2.6
1	A	601	THR	2.6
1	B	262	TYR	2.6
1	B	699	PRO	2.5
1	B	429	VAL	2.5
1	B	698	ILE	2.5
1	B	693	TYR	2.5
1	B	339	LEU	2.5
1	B	442	THR	2.5
1	B	460	LEU	2.5
1	B	607	CYS	2.5
1	B	610	ASP	2.5
1	B	189	PHE	2.4
1	A	333	LEU	2.4
1	A	504	LEU	2.4
1	B	281	LEU	2.4
1	B	441	PRO	2.3
1	B	507	SER	2.3
1	B	733	TYR	2.3
1	B	691	CYS	2.3
1	A	394	LEU	2.2
1	A	599	LYS	2.2
1	B	268	ALA	2.2
1	B	447	THR	2.2
1	A	344	HIS	2.1
1	B	606	GLY	2.1
1	B	726	ASN	2.1
1	A	610	ASP	2.1
1	B	692	LEU	2.1
1	A	609	CYS	2.1
1	A	341	LEU	2.0
1	A	347	PRO	2.0
1	B	332	ILE	2.0
1	A	340	GLN	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^{th} 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^2)	Q<0.9
7	NAG	B	1001	14/15	0.96	0.16	-0.23	24,36,50,61	0
2	NAG	A	1001	14/15	0.96	0.15	-0.38	17,25,36,45	0
2	NAG	A	1002	14/15	0.97	0.12	-	35,49,57,59	0
2	MAN	A	1004	11/12	0.87	0.11	-	44,68,81,88	0
2	MAN	A	1006	11/12	0.80	0.15	-	76,95,105,111	0
2	MAN	A	1005	11/12	0.79	0.18	-	53,64,76,88	0
7	NAG	B	1002	14/15	0.88	0.18	-	49,68,80,82	0
2	BMA	A	1003	11/12	0.85	0.16	-	41,58,69,73	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^{th} 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^2)	Q<0.9
4	AMP	B	1005	23/23	0.96	0.13	-0.90	34,50,69,73	0
4	AMP	A	1009	23/23	0.97	0.10	-1.39	31,43,54,68	0
5	ZN	A	1010	1/1	0.95	0.12	-1.57	38,38,38,38	0
6	CA	B	1008	1/1	0.99	0.10	-1.61	54,54,54,54	0
5	ZN	B	1006	1/1	0.97	0.10	-2.14	43,43,43,43	0
5	ZN	A	1011	1/1	0.98	0.09	-2.49	45,45,45,45	0
6	CA	A	1012	1/1	0.99	0.05	-4.38	44,44,44,44	0
5	ZN	B	1007	1/1	0.98	0.07	-6.94	39,39,39,39	0
3	NAG	B	1003	14/15	0.70	0.43	-	85,94,98,99	0
3	NAG	B	1004	14/15	0.78	0.24	-	59,76,84,85	0
3	NAG	A	1008	14/15	0.92	0.26	-	63,72,81,82	0
3	NAG	A	1007	14/15	0.84	0.32	-	54,72,85,86	0

6.5 Other polymers (i)

There are no such residues in this entry.