Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:58 PM GMT

PDB ID	:	4GTZ
Title	:	Crystal structure of mouse Enpp1 in complex with CMP
Authors	:	Kato, K.; Nishimasu, H.; Ishitani, R.; Nureki, O.
Deposited on	:	2012-08-29
Resolution	:	3.19 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:

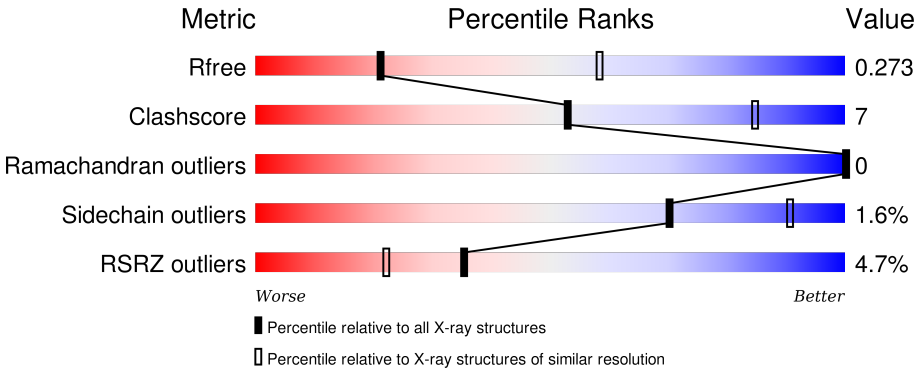
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.19 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	3%, 72%, 13%, •, 14%
1	B	823	5%, 69%, 15%, 15%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11156 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	0	0	0
			5502	3540	907	1026	29			
1	B	697	Total	C	N	O	S	0	0	0
			5450	3509	894	1018	29			

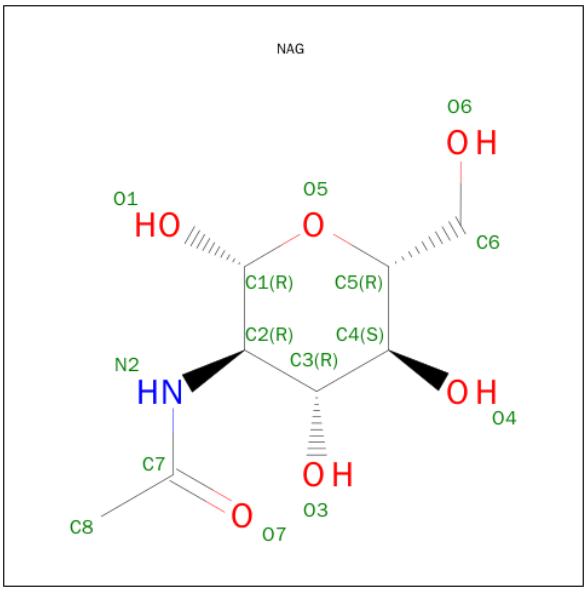
There are 2 discrepancies between the modelled and reference sequences:

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).

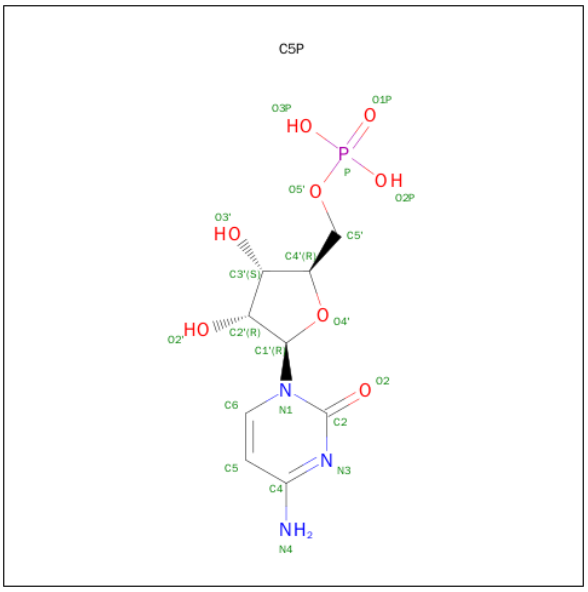
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	6	Total	C	N	O	0	0
			72	40	2	30		

- 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 CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C5P) (formula: $C_9H_{14}N_3O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			21	9	3	8	1		
4	B	1	Total	C	N	O	P	0	0
			21	9	3	8	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).

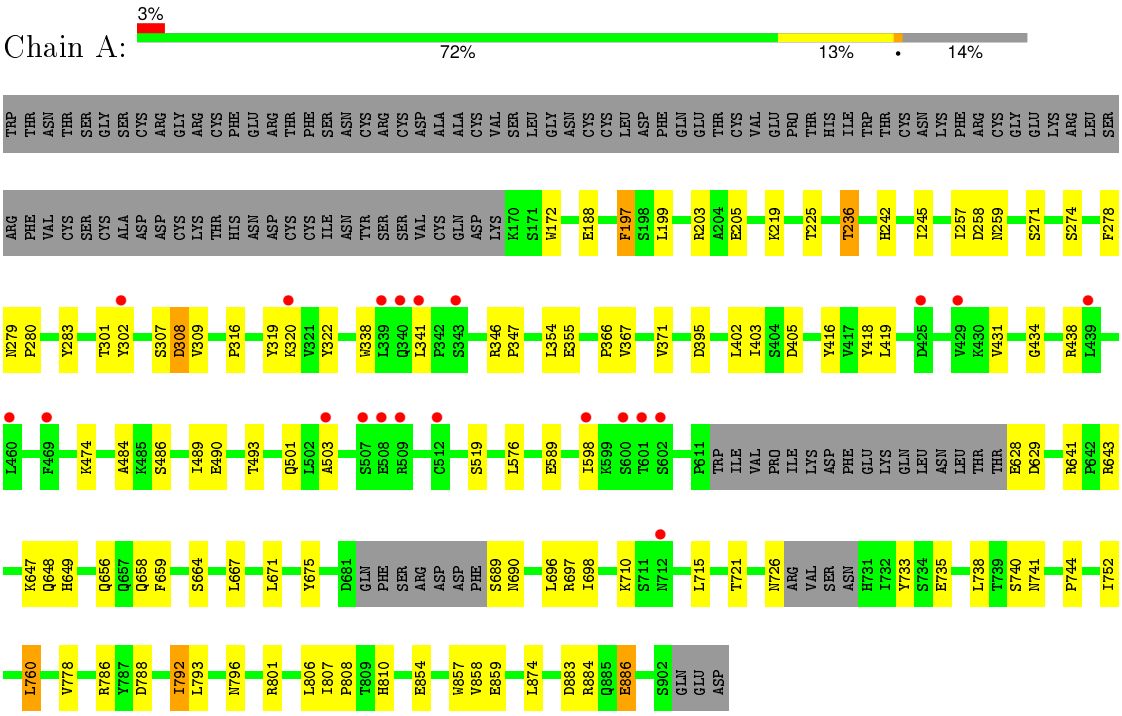
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	2	Total	C	N	O	0	0
			28	16	2	10		

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.

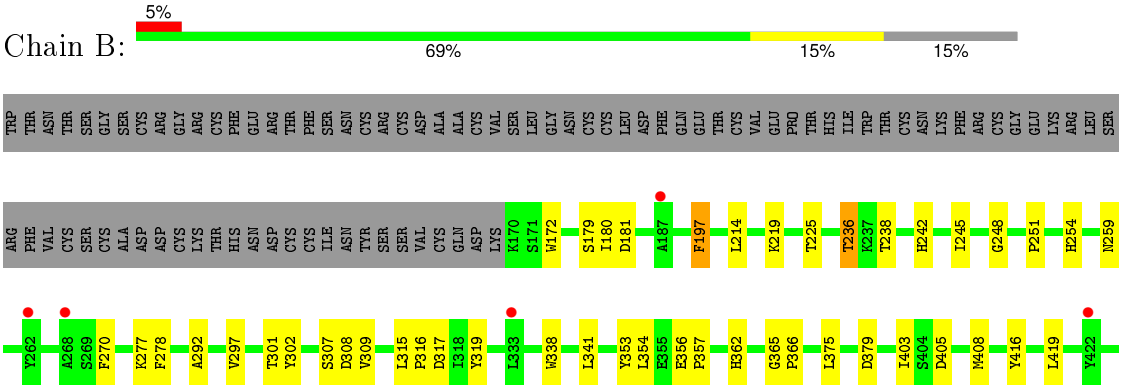
• Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2, Alkaline phosphodiesterase I

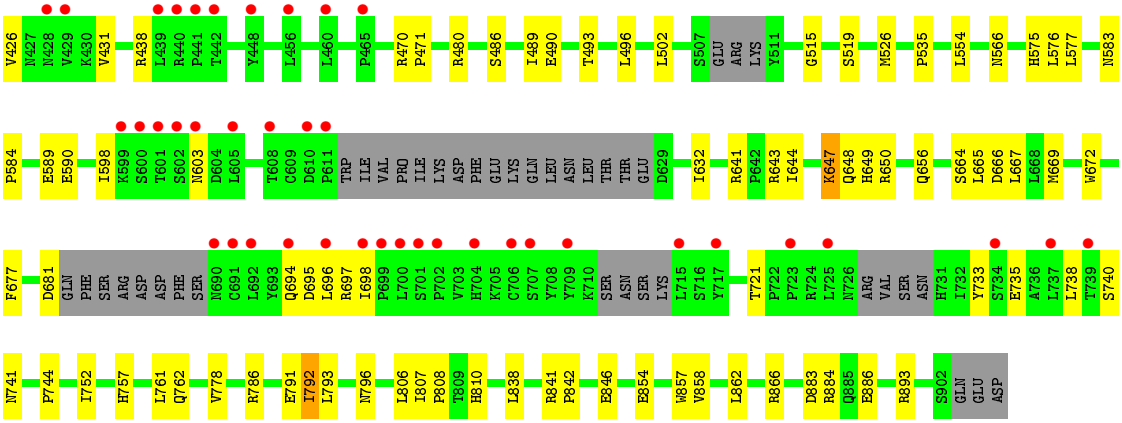
Chain A:



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

Chain B:




V426 N427 N428 V429 K430 V431 R438 L439 R440 P441 T442 Y448 L456 L460 P465 R470 P471 R480 S486 I489 E490 T493 L496 L502 S507 GLU ARG LYS Y511 G515 S519 M526 P535 L554 N566 H575 L576 L577 N583
P584 E589 E590 I598 K599 S600 T601 S602 N603 D604 L605 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 I644 K647 Q648 H649 R650 Q656 S664 L665 D666 L667 L668 M669 W672
F677 D681 GLN PHE SER ARG ASP ASP PHE SER N690 C691 L692 Y693 Q694 D695 L696 R697 I698 P699 L700 S701 P702 V703 H704 K705 C706 S707 Y708 Y709 K710 SER ASN SER LYS L715 S716 Y717 T721 P722 P723 R724 L725 N726 ARG VAL SER ASN H731 I732 Y733 S734 E735 A736 L737 L738 T739 S740
N741 P744 I752 H757 L761 Q762 V778 R786 E791 I792 L793 N796 L806 I807 P808 T809 H810 L838 R841 P842 E846 E854 W857 V858 L862 R866 D883 R884 Q885 E886 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	105.21Å 105.21Å 174.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.06 – 3.19 49.06 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.1 (49.06-3.19) 97.1 (49.06-3.19)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.233 , 0.263 0.241 , 0.273	Depositor DCC
R_{free} test set	1731 reflections (5.22%)	DCC
Wilson B-factor (Å^2)	64.5	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.9	EDS
Estimated twinning fraction	0.077 for -h,-k,l 0.086 for h,-h-k,-l 0.074 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 34900 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	11156	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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, C5P, 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	0.24	0/5666	0.42	0/7746
1	B	0.23	0/5611	0.42	0/7667
All	All	0.23	0/11277	0.42	0/15413

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	5502	0	5138	66	0
1	B	5450	0	5099	77	0
2	A	72	0	61	1	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
4	A	21	0	12	1	0
4	B	21	0	12	5	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	1	0
All	All	11156	0	10399	142	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 (142) 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:301:THR:HG21	1:B:307:SER:HB2	1.66	0.77
1:A:225:THR:HG21	1:A:576:LEU:HG	1.69	0.75
1:B:470:ARG:NH1	1:B:846:GLU:O	2.20	0.74
1:B:225:THR:HG21	1:B:576:LEU:HG	1.74	0.70
1:B:603:ASN:H	1:B:694:GLN:HE22	1.43	0.66
1:A:752:ILE:HG23	1:A:858:VAL:HG13	1.80	0.64
1:A:316:PRO:HG2	1:A:319:TYR:HB3	1.80	0.64
1:A:760:LEU:HD21	1:A:859:GLU:HG2	1.80	0.63
1:A:438:ARG:HG2	1:A:493:THR:HG22	1.81	0.62
1:B:733:TYR:CZ	1:B:735:GLU:HB2	2.35	0.62
1:B:650:ARG:NH1	1:B:666:ASP:OD1	2.32	0.62
1:B:496:LEU:HD21	1:B:502:LEU:HB2	1.83	0.61
1:A:589:GLU:OE2	1:A:641:ARG:NH2	2.34	0.60
1:B:315:LEU:HD12	1:B:316:PRO:HD2	1.84	0.60
1:A:786:ARG:HH21	2:A:1002:NAG:H62	1.66	0.59
1:B:589:GLU:OE2	1:B:641:ARG:NH2	2.35	0.59
1:B:744:PRO:HG2	1:B:808:PRO:HD3	1.84	0.59
1:B:590:GLU:HB3	1:B:647:LYS:HB3	1.85	0.59
1:A:486:SER:HB3	1:A:489:ILE:HG13	1.84	0.58
1:A:733:TYR:CZ	1:A:735:GLU:HB2	2.38	0.58
1:A:308:ASP:OD1	1:A:308:ASP:N	2.35	0.58
1:A:735:GLU:HA	1:A:738:LEU:HD13	1.86	0.57
1:B:259:ASN:ND2	4:B:1005:C5P:O1P	2.38	0.57
1:A:259:ASN:ND2	4:A:1009:C5P:O3P	2.35	0.57
1:B:793:LEU:HD22	1:B:806:LEU:HD21	1.86	0.57
1:A:649:HIS:NE2	1:A:664:SER:OG	2.32	0.56
1:A:643:ARG:NH2	1:A:883:ASP:OD2	2.38	0.56
1:B:197:PHE:HE1	1:B:354:LEU:HD13	1.70	0.56
1:B:649:HIS:NE2	1:B:664:SER:OG	2.29	0.56
1:A:721:THR:HB	1:A:741:ASN:HD21	1.70	0.56
1:A:778:VAL:HB	1:A:810:HIS:HB2	1.88	0.55
1:B:486:SER:HB3	1:B:489:ILE:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:PHE:HA	1:A:309:VAL:HG22	1.88	0.54
1:B:735:GLU:HA	1:B:738:LEU:HD13	1.90	0.54
1:B:643:ARG:NH2	1:B:883:ASP:OD2	2.40	0.53
1:B:667:LEU:HB3	1:B:669:MET:HG2	1.90	0.53
1:B:575:HIS:CE1	1:B:893:ARG:HD3	2.44	0.53
1:B:238:THR:OG1	4:B:1005:C5P:O2P	2.27	0.52
1:B:338:TRP:HA	1:B:341:LEU:HD13	1.92	0.52
1:B:366:PRO:HG3	1:B:408:MET:HG3	1.90	0.52
1:B:238:THR:OG1	4:B:1005:C5P:P	2.67	0.52
1:B:438:ARG:HG2	1:B:493:THR:HG22	1.92	0.52
1:B:786:ARG:HH21	7:B:1002:NAG:H62	1.75	0.51
1:A:598:ILE:HG23	1:A:696:LEU:HB3	1.92	0.51
1:A:197:PHE:HE1	1:A:354:LEU:HD13	1.75	0.51
1:A:793:LEU:HD22	1:A:806:LEU:HD21	1.94	0.50
1:B:353:TYR:CE2	4:B:1005:C5P:H5	2.47	0.50
1:A:338:TRP:HA	1:A:341:LEU:HD13	1.94	0.50
1:B:677:PHE:HE2	1:B:762:GLN:HA	1.77	0.49
1:A:188:GLU:O	1:A:346:ARG:NH2	2.35	0.49
1:B:721:THR:HB	1:B:741:ASN:HD21	1.77	0.49
1:B:214:LEU:HD22	1:B:379:ASP:HB2	1.93	0.49
1:A:257:ILE:HG12	1:A:489:ILE:HG12	1.95	0.49
1:B:838:LEU:HD11	1:B:862:LEU:HD13	1.94	0.49
1:A:434:GLY:HA2	1:A:501:GLN:HE21	1.76	0.49
1:A:438:ARG:HB3	1:A:490:GLU:HB2	1.94	0.49
1:B:554:LEU:HD11	1:B:577:LEU:HD21	1.94	0.49
1:B:438:ARG:HB3	1:B:490:GLU:HB2	1.94	0.48
4:B:1005:C5P:H2'1	4:B:1005:C5P:H6	1.55	0.48
1:B:778:VAL:HB	1:B:810:HIS:HB2	1.94	0.48
1:A:656:GLN:OE1	1:A:697:ARG:NH2	2.46	0.48
1:A:302:TYR:CE2	1:A:320:LYS:HD2	2.47	0.48
1:A:698:ILE:HD13	1:A:740:SER:HB3	1.96	0.48
1:A:245:ILE:HD13	1:A:403:ILE:HD13	1.96	0.48
1:A:710:LYS:H	1:A:801:ARG:NH1	2.12	0.48
1:A:854:GLU:HA	1:A:857:TRP:NE1	2.28	0.48
1:A:649:HIS:HE1	1:A:667:LEU:HD13	1.78	0.48
1:B:752:ILE:HG23	1:B:858:VAL:HG13	1.96	0.47
1:A:884:ARG:HG3	1:A:886:GLU:HG2	1.95	0.47
1:A:419:LEU:HD12	1:A:431:VAL:HG21	1.96	0.47
1:B:647:LYS:HA	1:B:648:GLN:HA	1.51	0.47
1:B:278:PHE:HA	1:B:309:VAL:HG22	1.97	0.47
1:A:788:ASP:HB3	1:A:792:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:SER:O	1:A:690:ASN:HB3	2.15	0.46
1:A:647:LYS:HA	1:A:648:GLN:HA	1.55	0.46
1:B:598:ILE:HG23	1:B:696:LEU:HB3	1.98	0.46
1:A:258:ASP:OD1	1:A:259:ASN:N	2.48	0.46
1:B:214:LEU:HD21	1:B:375:LEU:HB3	1.98	0.46
1:A:172:TRP:O	1:A:219:LYS:NZ	2.40	0.46
1:A:236:THR:OG1	1:A:519:SER:O	2.34	0.45
1:B:649:HIS:HE1	1:B:667:LEU:HD13	1.82	0.45
1:B:236:THR:OG1	1:B:519:SER:O	2.34	0.45
1:B:792:ILE:O	1:B:796:ASN:ND2	2.41	0.45
1:A:320:LYS:HE3	1:A:338:TRP:HZ2	1.81	0.45
1:B:236:THR:HG21	1:B:526:MET:HB3	1.99	0.45
1:A:659:PHE:HB3	1:A:675:TYR:HB3	1.99	0.45
1:B:698:ILE:HD13	1:B:740:SER:HB3	1.99	0.45
1:B:419:LEU:HD12	1:B:431:VAL:HG21	1.99	0.44
1:A:366:PRO:O	1:A:371:VAL:HG21	2.17	0.44
1:B:245:ILE:HD13	1:B:403:ILE:HD13	1.99	0.44
1:A:744:PRO:HG2	1:A:808:PRO:HD3	1.99	0.44
1:B:172:TRP:CZ3	1:B:219:LYS:HD3	2.52	0.44
1:A:283:TYR:CE1	1:A:309:VAL:HG21	2.53	0.44
1:A:715:LEU:O	1:A:801:ARG:NH2	2.51	0.44
1:B:302:TYR:HD1	1:B:338:TRP:HH2	1.65	0.44
1:A:172:TRP:CZ3	1:A:219:LYS:HD3	2.53	0.44
1:A:628:GLU:HG3	1:A:629:ASP:H	1.83	0.43
1:A:649:HIS:CE1	1:A:667:LEU:HD13	2.53	0.43
1:B:695:ASP:HB3	1:B:698:ILE:HG12	2.00	0.43
1:A:418:TYR:HA	1:A:503:ALA:O	2.19	0.43
1:A:664:SER:HB2	1:A:671:LEU:HG	2.01	0.43
1:A:395:ASP:N	1:A:395:ASP:OD1	2.50	0.43
1:B:480:ARG:HD3	1:B:866:ARG:O	2.19	0.43
1:A:474:LYS:HG2	1:A:484:ALA:HA	2.01	0.42
1:A:792:ILE:O	1:A:796:ASN:ND2	2.47	0.42
1:B:681:ASP:N	1:B:681:ASP:OD1	2.51	0.42
1:B:884:ARG:HG3	1:B:886:GLU:OE1	2.18	0.42
1:B:251:PRO:HA	1:B:254:HIS:NE2	2.35	0.42
1:A:203:ARG:NH2	1:A:205:GLU:OE1	2.52	0.42
1:B:248:GLY:O	1:B:566:ASN:HB2	2.20	0.42
1:B:884:ARG:HA	1:B:884:ARG:HD2	1.82	0.42
1:B:644:ILE:HD11	1:B:672:TRP:HE1	1.85	0.42
1:B:854:GLU:HA	1:B:857:TRP:NE1	2.35	0.42
1:A:279:ASN:HA	1:A:280:PRO:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:LEU:HA	1:B:315:LEU:HD12	1.96	0.42
1:A:301:THR:HG21	1:A:307:SER:HB3	2.02	0.42
1:A:807:ILE:HA	1:A:808:PRO:HD3	1.84	0.41
1:B:356:GLU:OE2	1:B:357:PRO:HA	2.20	0.41
1:B:292:ALA:HB1	1:B:297:VAL:HB	2.02	0.41
1:B:242:HIS:CE1	1:B:405:ASP:HB3	2.56	0.41
1:B:757:HIS:HA	1:B:761:LEU:HB2	2.01	0.41
1:B:470:ARG:HA	1:B:471:PRO:HD3	1.90	0.41
1:A:643:ARG:NH1	1:B:181:ASP:OD1	2.53	0.41
1:B:362:HIS:ND1	1:B:515:GLY:O	2.50	0.41
1:B:841:ARG:HA	1:B:842:PRO:HD3	1.86	0.41
1:B:270:PHE:CE1	1:B:277:LYS:HA	2.55	0.41
1:A:346:ARG:HA	1:A:347:PRO:HD3	1.95	0.41
1:A:322:TYR:OH	1:A:355:GLU:OE2	2.30	0.41
1:B:438:ARG:NH1	1:B:490:GLU:OE1	2.51	0.41
1:B:365:GLY:HA2	1:B:366:PRO:HD3	1.92	0.41
1:B:656:GLN:OE1	1:B:697:ARG:NH2	2.47	0.41
1:A:199:LEU:HD11	1:A:402:LEU:HD11	2.03	0.41
1:B:632:ILE:HD12	1:B:632:ILE:HA	1.94	0.41
1:A:658:GLN:NE2	1:A:726:ASN:HD22	2.19	0.41
1:B:316:PRO:HG2	1:B:319:TYR:HB3	2.01	0.40
1:B:643:ARG:HD3	1:B:643:ARG:HA	1.97	0.40
1:A:271:SER:HB2	1:A:274:SER:HB2	2.03	0.40
1:A:641:ARG:NH1	1:B:179:SER:OG	2.54	0.40
1:B:807:ILE:HA	1:B:808:PRO:HD3	1.86	0.40
1:A:242:HIS:CE1	1:A:405:ASP:HB3	2.57	0.40
1:B:583:ASN:HA	1:B:584:PRO:HD2	1.99	0.40
1:B:180:ILE:HB	1:B:535:PRO:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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	592/755 (78%)	583 (98%)	9 (2%)	72	91
1	B	589/755 (78%)	579 (98%)	10 (2%)	68	90
All	All	1181/1510 (78%)	1162 (98%)	19 (2%)	70	91

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

Mol	Chain	Res	Type
1	A	197	PHE
1	A	236	THR
1	A	308	ASP
1	A	367	VAL
1	A	416	TYR
1	A	760	LEU
1	A	792	ILE
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	416	TYR
1	B	426	VAL
1	B	647	LYS
1	B	665	LEU
1	B	791	GLU

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Mol	Chain	Res	Type
1	B	792	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	452	ASN
1	A	501	GLN
1	A	525	ASN
1	A	634	HIS
1	A	658	GLN
1	A	741	ASN
1	A	769	ASN
1	A	820	GLN
1	B	229	ASN
1	B	694	GLN
1	B	820	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	1002	2	14,14,15	0.52	0	15,19,21	0.59	0
2	BMA	A	1003	2	11,11,12	0.59	0	14,15,17	0.68	0
2	MAN	A	1004	2	11,11,12	0.59	0	14,15,17	0.50	0
2	MAN	A	1005	2	11,11,12	0.59	0	14,15,17	1.44	2 (14%)
2	MAN	A	1006	2	11,11,12	0.57	0	14,15,17	0.77	0
7	NAG	B	1001	1,7	14,14,15	0.57	0	15,19,21	1.11	1 (6%)
7	NAG	B	1002	7	14,14,15	0.51	0	15,19,21	0.57	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	0/1/1/1
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})
7	B	1001	NAG	C3-C4-C5	2.47	114.51	110.20
2	A	1005	MAN	C1-C2-C3	2.85	112.92	109.54
2	A	1005	MAN	C1-O5-C5	3.25	116.37	112.25

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	1002	NAG	1	0
7	B	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	0.49	0	15,19,21	0.80	0
3	NAG	A	1008	1	14,14,15	0.47	0	15,19,21	0.82	1 (6%)
4	C5P	A	1009	5	17,22,22	2.11	4 (23%)	22,33,33	1.35	3 (13%)
3	NAG	B	1003	1	14,14,15	0.52	0	15,19,21	0.60	0
3	NAG	B	1004	1	14,14,15	0.47	0	15,19,21	1.00	1 (6%)
4	C5P	B	1005	5	17,22,22	2.06	4 (23%)	22,33,33	1.33	2 (9%)

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	C5P	A	1009	5	-	0/6/26/26	0/2/2/2
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	C5P	B	1005	5	-	0/6/26/26	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1005	C5P	C5-C4	2.86	1.47	1.40
4	A	1009	C5P	C5-C4	3.01	1.47	1.40
4	B	1005	C5P	C6-C5	3.99	1.46	1.38
4	A	1009	C5P	C4-N3	4.06	1.43	1.35
4	B	1005	C5P	C4-N3	4.20	1.43	1.35
4	A	1009	C5P	C6-C5	4.24	1.47	1.38
4	B	1005	C5P	C6-N1	4.88	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1009	C5P	C6-N1	5.14	1.43	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1009	C5P	O3P-P-O1P	-2.05	103.97	110.58
3	A	1008	NAG	C1-O5-C5	2.23	115.08	112.25
4	B	1005	C5P	O2P-P-O1P	2.76	119.47	110.58
4	A	1009	C5P	O2P-P-O1P	2.82	119.65	110.58
4	B	1005	C5P	C2-N3-C4	2.95	119.77	115.61
3	B	1004	NAG	C1-O5-C5	2.97	116.01	112.25
4	A	1009	C5P	C2-N3-C4	3.58	120.66	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1009	C5P	1	0
4	B	1005	C5P	5	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^{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	706/823 (85%)	0.12	21 (2%)	54	39	54, 94, 139, 188	0
1	B	697/823 (84%)	0.25	45 (6%)	22	12	54, 97, 145, 180	0
All	All	1403/1646 (85%)	0.18	66 (4%)	35	22	54, 96, 143, 188	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	698	ILE	6.0
1	B	441	PRO	5.9
1	B	700	LEU	4.4
1	A	600	SER	4.4
1	B	439	LEU	4.0
1	B	715	LEU	3.7
1	A	508	GLU	3.6
1	B	704	HIS	3.5
1	A	712	ASN	3.4
1	B	600	SER	3.4
1	B	611	PRO	3.3
1	A	602	SER	3.2
1	B	707	SER	3.2
1	A	598	ILE	3.2
1	A	601	THR	3.1
1	B	610	ASP	3.0
1	B	709	TYR	2.9
1	B	602	SER	2.8
1	B	268	ALA	2.8
1	B	702	PRO	2.8
1	A	439	LEU	2.8
1	B	442	THR	2.8
1	B	448	TYR	2.8
1	B	422	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	737	LEU	2.7
1	B	428	ASN	2.7
1	A	340	GLN	2.7
1	B	692	LEU	2.6
1	A	429	VAL	2.6
1	B	601	THR	2.6
1	A	339	LEU	2.6
1	A	512	CYS	2.6
1	B	262	TYR	2.5
1	B	608	THR	2.5
1	A	341	LEU	2.5
1	B	694	GLN	2.5
1	A	509	ARG	2.4
1	B	440	ARG	2.4
1	B	723	PRO	2.4
1	A	302	TYR	2.4
1	A	469	PHE	2.3
1	B	333	LEU	2.3
1	B	734	SER	2.3
1	B	187	ALA	2.3
1	B	696	LEU	2.3
1	B	429	VAL	2.3
1	B	725	LEU	2.3
1	A	507	SER	2.3
1	A	460	LEU	2.3
1	A	425	ASP	2.2
1	B	739	THR	2.2
1	B	717	TYR	2.2
1	B	599	LYS	2.2
1	B	603	ASN	2.2
1	B	465	PRO	2.2
1	B	699	PRO	2.2
1	B	605	LEU	2.2
1	A	343	SER	2.1
1	B	456	LEU	2.1
1	B	460	LEU	2.1
1	B	691	CYS	2.1
1	A	320	LYS	2.1
1	A	503	ALA	2.1
1	B	706	CYS	2.1
1	B	701	SER	2.1
1	B	690	ASN	2.1

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	0.93	0.23	-0.50	80,84,93,104	0
2	NAG	A	1001	14/15	0.94	0.18	-1.02	64,69,74,84	0
2	BMA	A	1003	11/12	0.72	0.16	-	114,117,126,131	0
7	NAG	B	1002	14/15	0.77	0.32	-	112,117,121,122	0
2	MAN	A	1006	11/12	0.77	0.16	-	132,136,138,139	0
2	NAG	A	1002	14/15	0.91	0.19	-	78,98,105,111	0
2	MAN	A	1005	11/12	0.75	0.21	-	131,133,135,136	0
2	MAN	A	1004	11/12	0.89	0.13	-	106,111,115,116	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
6	CA	B	1008	1/1	0.93	0.23	-0.01	115,115,115,115	0
5	ZN	A	1010	1/1	0.99	0.17	-0.38	88,88,88,88	0
4	C5P	B	1005	21/21	0.94	0.20	-0.40	104,108,112,114	0
5	ZN	A	1011	1/1	0.98	0.15	-0.46	80,80,80,80	0
5	ZN	B	1006	1/1	0.96	0.19	-0.48	98,98,98,98	0
4	C5P	A	1009	21/21	0.95	0.19	-0.49	84,90,98,103	0
5	ZN	B	1007	1/1	0.98	0.15	-0.96	84,84,84,84	0
6	CA	A	1012	1/1	0.99	0.12	-2.72	96,96,96,96	0
3	NAG	B	1003	14/15	0.70	0.43	-	112,116,118,119	0
3	NAG	B	1004	14/15	0.73	0.25	-	97,103,106,108	0
3	NAG	A	1008	14/15	0.88	0.33	-	102,108,114,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	1007	14/15	0.79	0.40	-	109,115,116,116	0

6.5 Other polymers (i)

There are no such residues in this entry.