Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 07:02 AM GMT

PDB ID	:	2Z8G
Title	:	Aspergillus niger ATCC9642 isopullulanase complexed with isopanose
Authors	:	Mizuno, M.; Koide, A.; Yamamura, A.; Akeboshi, H.; Yoshida, H.; Kamitori, S.; Sakano, Y.; Nishikawa, A.; Tonozuka, T.
Deposited on	:	2007-09-05
Resolution	:	1.70 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:

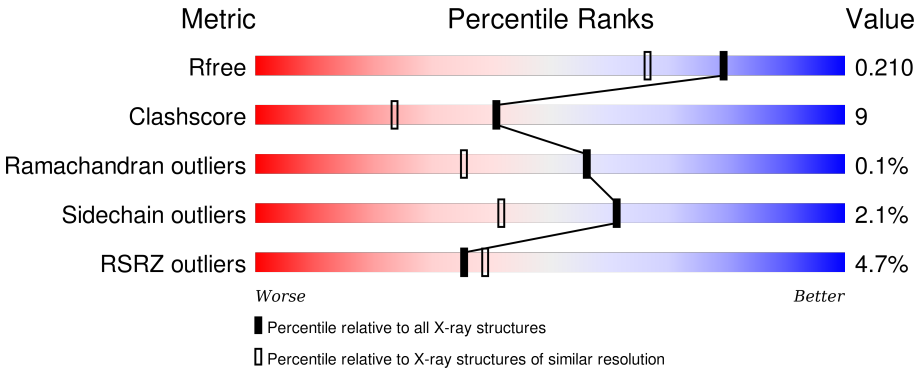
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	549	5% 85% 14%
1	B	549	5% 81% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1000	-	-	-	X
2	NAG	A	1006	-	-	-	X
2	NAG	A	1007	-	-	-	X
2	NAG	A	1011	-	-	-	X
2	NAG	B	1000	-	-	-	X
2	NAG	B	1002	-	-	-	X
2	NAG	B	1003	-	-	-	X
2	NAG	B	1005	-	-	-	X
2	NAG	B	1007	-	-	-	X
2	NAG	B	1008	-	-	-	X
2	NAG	B	1009	-	-	-	X
3	GLC	A	2002	-	-	-	X
3	BGC	A	2003	-	-	-	X
3	BGC	B	2003	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10037 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.

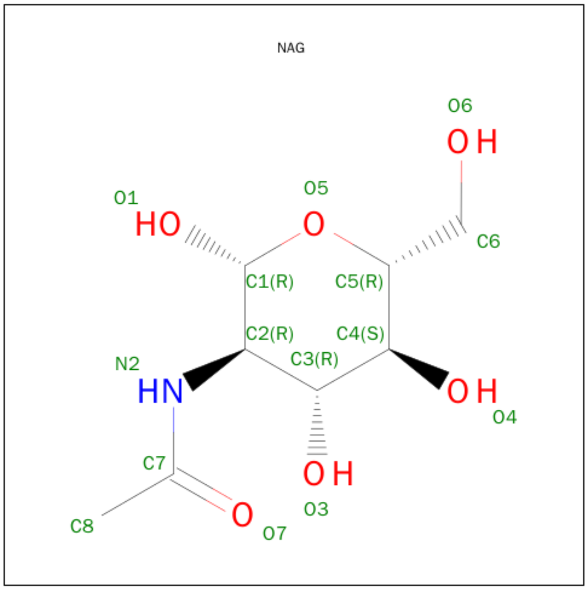
- Molecule 1 is a protein called Isopullulanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4242	2676	710	845	11			
1	B	549	Total	C	N	O	S	0	0	0
			4242	2676	710	845	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ARG	-	EXPRESSION TAG	UNP O00105
A	17	GLU	-	EXPRESSION TAG	UNP O00105
A	18	PHE	-	EXPRESSION TAG	UNP O00105
A	19	MET	-	EXPRESSION TAG	UNP O00105
B	16	ARG	-	EXPRESSION TAG	UNP O00105
B	17	GLU	-	EXPRESSION TAG	UNP O00105
B	18	PHE	-	EXPRESSION TAG	UNP O00105
B	19	MET	-	EXPRESSION TAG	UNP O00105

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total C O 34 18 16	0	0
3	B	3	Total C O 34 18 16	0	0

- Molecule 4 is water.

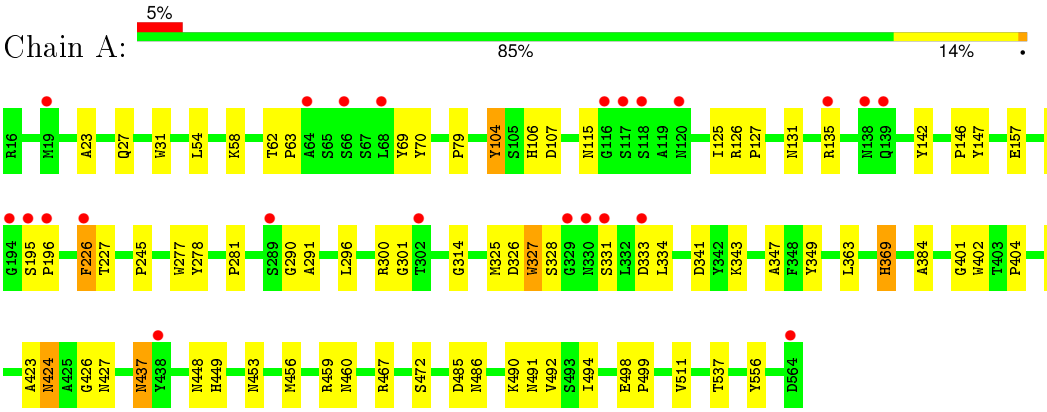
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	645	Total O 645 645	0	0
4	B	518	Total O 518 518	0	0

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.

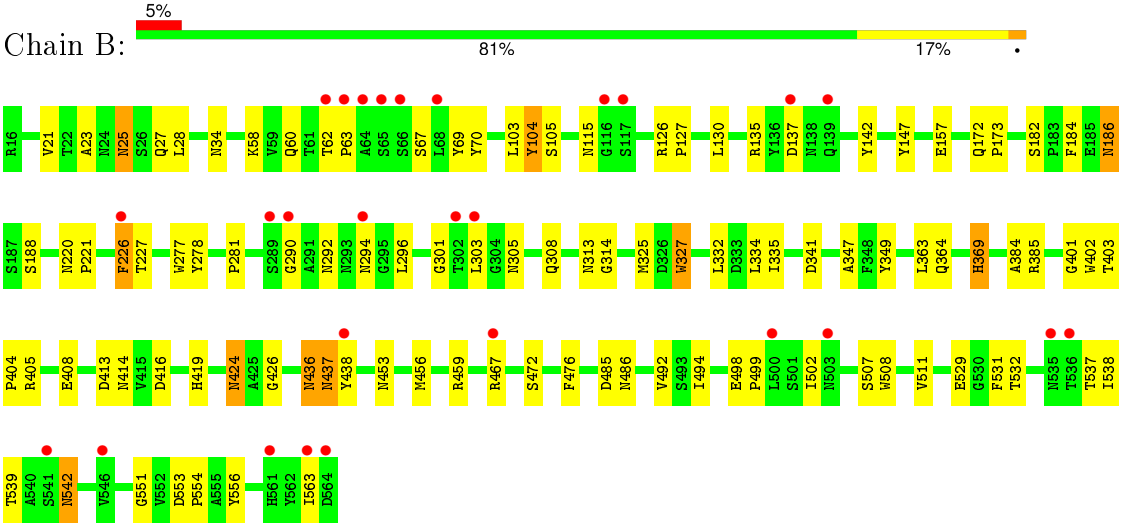
- Molecule 1: Isopullulanase

Chain A:



- Molecule 1: Isopullulanase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.67Å 99.39Å 134.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.69 – 1.70 49.69 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.69-1.70) 99.2 (49.69-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.187 , 0.211 0.185 , 0.210	Depositor DCC
R_{free} test set	12328 reflections (11.13%)	DCC
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	4 of 123129 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10037	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.70 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.0029e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GLC, BGC, NAG

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	0.33	0/4357	0.66	2/5962 (0.0%)
1	B	0.31	0/4357	0.63	2/5962 (0.0%)
All	All	0.32	0/8714	0.64	4/11924 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	226	PHE	N-CA-C	-5.93	94.99	111.00
1	B	226	PHE	N-CA-C	-5.46	96.27	111.00
1	A	369	HIS	N-CA-C	-5.32	96.64	111.00
1	B	369	HIS	N-CA-C	-5.07	97.30	111.00

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	4242	0	3978	57	0
1	B	4242	0	3979	88	0
2	A	168	0	156	7	0
2	B	154	0	143	5	0
3	A	34	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	34	0	30	0	0
4	A	645	0	0	6	0
4	B	518	0	0	5	0
All	All	10037	0	8316	147	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 9.

All (147) 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:25:ASN:HD22	1:B:27:GLN:H	1.08	0.96
1:B:539:THR:H	1:B:542:ASN:HD21	1.27	0.80
1:A:226:PHE:O	1:A:227:THR:HG23	1.82	0.79
1:B:226:PHE:O	1:B:227:THR:HG23	1.84	0.76
1:B:539:THR:H	1:B:542:ASN:ND2	1.83	0.75
1:B:436:ASN:HD22	1:B:437:ASN:H	1.33	0.75
1:A:347:ALA:H	1:A:369:HIS:HD2	1.34	0.75
1:A:192:GLN:HB3	1:A:193:PRO:HD2	1.69	0.74
1:B:25:ASN:ND2	1:B:27:GLN:H	1.85	0.74
1:B:347:ALA:H	1:B:369:HIS:HD2	1.34	0.72
1:B:303:LEU:HD21	1:B:334:LEU:HB2	1.71	0.71
1:B:303:LEU:HD22	1:B:335:ILE:HG13	1.72	0.69
1:B:157:GLU:OE2	1:B:419:HIS:HE1	1.75	0.69
1:B:436:ASN:ND2	1:B:437:ASN:H	1.91	0.68
1:B:135:ARG:HG2	1:B:142:TYR:HB2	1.76	0.67
1:B:308:GLN:NE2	1:B:327:TRP:HE1	1.92	0.67
1:A:146:PRO:HG3	4:A:1290:HOH:O	1.95	0.66
1:B:186:ASN:HD22	1:B:186:ASN:C	1.99	0.66
1:A:135:ARG:HG2	1:A:142:TYR:HB2	1.76	0.66
1:A:331:SER:HB3	1:A:333:ASP:OD1	1.97	0.65
1:A:423:ALA:H	1:A:427:ASN:ND2	1.96	0.63
1:B:308:GLN:HE21	1:B:327:TRP:HE1	1.45	0.63
1:B:414:ASN:ND2	1:B:467:ARG:HH12	1.96	0.63
1:B:25:ASN:ND2	1:B:28:LEU:H	1.97	0.62
1:B:127:PRO:HG2	1:B:130:LEU:HD13	1.82	0.62
1:B:127:PRO:HG2	1:B:130:LEU:CD1	2.30	0.61
1:B:34:ASN:HB2	4:B:1355:HOH:O	2.01	0.59
1:A:226:PHE:O	1:A:227:THR:CG2	2.49	0.59
1:A:460:ASN:ND2	2:A:1007:NAG:H83	2.18	0.59
1:B:226:PHE:O	1:B:227:THR:CG2	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ALA:HB2	1:B:70:TYR:CG	2.39	0.58
1:B:498:GLU:HB3	1:B:499:PRO:HD2	1.85	0.57
1:A:424:ASN:H	1:A:427:ASN:ND2	2.02	0.56
1:B:538:ILE:HA	1:B:542:ASN:HD21	1.70	0.56
1:A:192:GLN:HG2	4:A:1366:HOH:O	2.06	0.56
1:A:23:ALA:HB2	1:A:70:TYR:CG	2.42	0.55
1:B:539:THR:N	1:B:542:ASN:HD21	2.01	0.55
1:B:115:ASN:ND2	2:B:1002:NAG:H82	2.22	0.55
1:A:62:THR:HB	1:A:63:PRO:HA	1.90	0.54
1:B:529:GLU:HB2	1:B:563:ILE:HB	1.90	0.54
1:A:424:ASN:HD22	1:A:426:GLY:H	1.56	0.54
1:A:453:ASN:ND2	2:A:1011:NAG:H83	2.23	0.54
1:B:332:LEU:HD12	1:B:332:LEU:N	2.22	0.53
1:B:332:LEU:HD13	4:B:1204:HOH:O	2.07	0.53
1:A:347:ALA:H	1:A:369:HIS:CD2	2.23	0.53
1:B:127:PRO:HB3	1:B:416:ASP:OD2	2.08	0.53
1:A:300:ARG:HD2	1:A:326:ASP:O	2.08	0.53
1:B:436:ASN:HD22	1:B:437:ASN:N	2.04	0.53
1:A:423:ALA:H	1:A:427:ASN:HD22	1.57	0.53
1:A:424:ASN:HD22	1:A:426:GLY:N	2.06	0.53
1:B:542:ASN:HD22	1:B:542:ASN:C	2.12	0.53
1:B:424:ASN:HD22	1:B:426:GLY:N	2.06	0.52
1:A:79:PRO:HG2	4:A:1543:HOH:O	2.08	0.52
1:A:404:PRO:HG2	1:A:456:MET:HE1	1.92	0.52
1:B:437:ASN:HD22	1:B:437:ASN:C	2.14	0.51
1:B:104:TYR:CE2	1:B:147:TYR:HA	2.46	0.51
1:B:453:ASN:HA	2:B:1008:NAG:H82	1.92	0.51
1:B:327:TRP:CD1	1:B:335:ILE:HD13	2.46	0.51
2:B:1003:NAG:H83	2:B:1003:NAG:O3	2.11	0.50
1:A:498:GLU:HB3	1:A:499:PRO:HD2	1.94	0.50
1:A:125:ILE:HD12	1:A:125:ILE:N	2.27	0.50
1:B:62:THR:HB	1:B:63:PRO:HA	1.93	0.49
1:A:157:GLU:HB3	1:A:173:PRO:HG3	1.94	0.49
1:A:363:LEU:O	1:A:384:ALA:HA	2.12	0.49
1:B:424:ASN:HD22	1:B:426:GLY:H	1.60	0.49
1:B:437:ASN:HD22	1:B:438:TYR:N	2.09	0.49
1:B:172:GLN:HG2	1:B:419:HIS:CD2	2.47	0.49
1:B:58:LYS:HB3	1:B:69:TYR:HB3	1.95	0.49
1:A:437:ASN:C	1:A:437:ASN:HD22	2.16	0.48
1:A:281:PRO:HG3	1:A:296:LEU:HD13	1.96	0.48
1:B:157:GLU:HB3	1:B:173:PRO:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ARG:HA	1:A:127:PRO:C	2.33	0.48
1:B:459:ARG:HA	1:B:485:ASP:O	2.13	0.48
1:B:499:PRO:O	1:B:502:ILE:HG12	2.14	0.47
1:B:103:LEU:HA	1:B:182:SER:O	2.14	0.47
1:A:467:ARG:HD2	4:A:1343:HOH:O	2.13	0.47
1:B:414:ASN:HD22	1:B:467:ARG:HH12	1.61	0.47
1:B:508:TRP:HB3	1:B:551:GLY:HA3	1.96	0.47
1:B:301:GLY:HA3	1:B:327:TRP:CE2	2.49	0.47
1:B:419:HIS:HD2	4:B:1322:HOH:O	1.98	0.47
1:A:127:PRO:HB3	1:A:416:ASP:OD2	2.14	0.47
1:A:449:HIS:HD2	4:A:1078:HOH:O	1.98	0.47
2:A:1005:NAG:H62	1:B:184:PHE:CD1	2.49	0.47
1:A:314:GLY:HA2	1:A:341:ASP:O	2.14	0.47
1:A:58:LYS:HB3	1:A:69:TYR:HB3	1.97	0.47
1:A:104:TYR:CE2	1:A:147:TYR:HA	2.50	0.46
1:A:54:LEU:HD11	2:A:1002:NAG:H61	1.97	0.46
1:A:277:TRP:CD1	1:A:349:TYR:HB3	2.51	0.46
1:B:472:SER:HB3	1:B:494:ILE:HG23	1.96	0.46
1:B:186:ASN:ND2	1:B:188:SER:H	2.14	0.46
1:B:511:VAL:HA	1:B:556:TYR:CE1	2.50	0.46
1:B:21:VAL:O	1:B:21:VAL:HG13	2.15	0.46
1:A:347:ALA:N	1:A:369:HIS:HD2	2.09	0.45
1:A:460:ASN:CG	2:A:1007:NAG:H83	2.36	0.45
1:B:281:PRO:HG3	1:B:296:LEU:HD13	1.97	0.45
1:B:459:ARG:NH1	1:B:485:ASP:OD2	2.41	0.45
1:A:490:LYS:O	1:A:491:ASN:HB2	2.16	0.45
1:B:532:THR:HG22	1:B:537:THR:HA	1.99	0.45
1:B:363:LEU:O	1:B:384:ALA:HA	2.17	0.45
1:A:27:GLN:NE2	2:B:1005:NAG:O3	2.49	0.45
1:B:303:LEU:HD22	1:B:335:ILE:CG1	2.43	0.45
1:A:472:SER:HB3	1:A:494:ILE:HG23	1.99	0.44
1:B:553:ASP:CG	1:B:554:PRO:HD2	2.38	0.44
1:A:106:HIS:HD2	1:A:107:ASP:O	1.99	0.44
1:A:300:ARG:NE	1:A:328:SER:OG	2.48	0.44
1:A:31:TRP:CZ3	1:A:245:PRO:HB3	2.53	0.44
1:A:492:VAL:O	1:A:492:VAL:HG13	2.18	0.44
1:B:277:TRP:CD1	1:B:349:TYR:HB3	2.52	0.44
1:B:369:HIS:HE1	4:B:1321:HOH:O	2.00	0.44
1:B:290:GLY:O	1:B:292:ASN:N	2.42	0.44
1:A:195:SER:OG	1:A:196:PRO:HD2	2.18	0.43
1:A:343:LYS:N	1:A:343:LYS:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:GLY:HA2	1:B:341:ASP:O	2.17	0.43
1:B:126:ARG:HA	1:B:127:PRO:C	2.39	0.43
1:A:511:VAL:HA	1:A:556:TYR:CE1	2.54	0.43
1:B:60:GLN:NE2	1:B:67:SER:OG	2.52	0.43
1:B:305:ASN:ND2	2:B:1005:NAG:H82	2.33	0.43
1:A:401:GLY:O	1:A:402:TRP:HB2	2.18	0.43
1:B:220:ASN:HB3	1:B:221:PRO:HD2	2.01	0.42
1:B:385:ARG:HA	1:B:413:ASP:O	2.18	0.42
1:B:294:ASN:HB2	4:B:1337:HOH:O	2.18	0.42
1:B:137:ASP:HB3	1:B:142:TYR:HE2	1.85	0.42
1:B:403:THR:O	1:B:405:ARG:HG3	2.20	0.42
1:A:537:THR:HG23	4:A:1576:HOH:O	2.19	0.42
1:B:105:SER:HA	1:B:147:TYR:CE1	2.55	0.42
1:B:347:ALA:N	1:B:369:HIS:HD2	2.09	0.41
1:B:492:VAL:HG13	1:B:531:PHE:CD1	2.55	0.41
1:B:364:GLN:HA	1:B:385:ARG:O	2.20	0.41
1:B:408:GLU:HA	1:B:459:ARG:O	2.21	0.41
1:B:186:ASN:ND2	1:B:186:ASN:C	2.70	0.41
1:B:25:ASN:ND2	1:B:28:LEU:N	2.68	0.41
1:B:542:ASN:ND2	1:B:542:ASN:C	2.75	0.41
1:B:476:PHE:O	1:B:507:SER:HA	2.21	0.41
1:A:334:LEU:HD12	1:A:334:LEU:N	2.36	0.41
1:A:408:GLU:HG3	1:A:409:ASN:ND2	2.36	0.41
2:A:1002:NAG:H83	2:A:1002:NAG:O3	2.21	0.41
1:A:459:ARG:HA	1:A:485:ASP:O	2.21	0.41
1:B:499:PRO:HG2	1:B:502:ILE:HG12	2.03	0.40
1:B:220:ASN:HB3	1:B:221:PRO:CD	2.51	0.40
1:B:401:GLY:O	1:B:402:TRP:HB2	2.20	0.40
1:B:332:LEU:N	1:B:332:LEU:CD1	2.84	0.40
1:B:404:PRO:HG2	1:B:456:MET:HE1	2.02	0.40
1:A:301:GLY:HA3	1:A:327:TRP:CE2	2.56	0.40
1:A:448:ASN:CG	2:A:1006:NAG:H82	2.42	0.40
1:B:127:PRO:HG2	1:B:130:LEU:HD11	2.04	0.40
1:A:408:GLU:HA	1:A:459:ARG:O	2.21	0.40
1:A:290:GLY:O	1:A:291:ALA:C	2.59	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	547/549 (100%)	517 (94%)	29 (5%)	1 (0%)	52 32
1	B	547/549 (100%)	513 (94%)	34 (6%)	0	100 100
All	All	1094/1098 (100%)	1030 (94%)	63 (6%)	1 (0%)	56 35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	ASN

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	466/466 (100%)	458 (98%)	8 (2%)	68 51
1	B	466/466 (100%)	454 (97%)	12 (3%)	54 32
All	All	932/932 (100%)	912 (98%)	20 (2%)	61 42

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	TYR
1	A	131	ASN
1	A	278	TYR
1	A	325	MET
1	A	327	TRP

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Mol	Chain	Res	Type
1	A	424	ASN
1	A	437	ASN
1	A	486	ASN
1	B	25	ASN
1	B	104	TYR
1	B	186	ASN
1	B	278	TYR
1	B	313	ASN
1	B	325	MET
1	B	327	TRP
1	B	424	ASN
1	B	436	ASN
1	B	437	ASN
1	B	486	ASN
1	B	542	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	41	GLN
1	A	51	GLN
1	A	106	HIS
1	A	122	ASN
1	A	131	ASN
1	A	330	ASN
1	A	369	HIS
1	A	386	ASN
1	A	414	ASN
1	A	424	ASN
1	A	427	ASN
1	A	437	ASN
1	A	449	HIS
1	A	486	ASN
1	A	516	ASN
1	B	25	ASN
1	B	41	GLN
1	B	60	GLN
1	B	186	ASN
1	B	192	GLN
1	B	286	GLN
1	B	308	GLN

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Mol	Chain	Res	Type
1	B	313	ASN
1	B	330	ASN
1	B	351	GLN
1	B	369	HIS
1	B	386	ASN
1	B	414	ASN
1	B	419	HIS
1	B	424	ASN
1	B	436	ASN
1	B	437	ASN
1	B	486	ASN
1	B	516	ASN
1	B	542	ASN
1	B	561	HIS

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)

6 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	$\#\|Z\| > 2$
3	GLC	A	2001	3	11,11,12	0.50	0	14,15,17	0.52	0
3	GLC	A	2002	3	11,11,12	0.43	0	14,15,17	0.69	1 (7%)
3	BGC	A	2003	3	12,12,12	0.32	0	17,17,17	0.43	0
3	GLC	B	2001	3	11,11,12	0.52	0	14,15,17	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GLC	B	2002	3	11,11,12	0.47	0	14,15,17	0.70	1 (7%)
3	BGC	B	2003	3	12,12,12	0.34	0	17,17,17	0.48	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
3	GLC	A	2001	3	-	0/2/19/22	0/1/1/1
3	GLC	A	2002	3	-	0/2/19/22	0/1/1/1
3	BGC	A	2003	3	-	0/2/22/22	0/1/1/1
3	GLC	B	2001	3	-	0/2/19/22	0/1/1/1
3	GLC	B	2002	3	-	0/2/19/22	0/1/1/1
3	BGC	B	2003	3	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2002	GLC	C1-O5-C5	2.17	115.00	112.25
3	B	2002	GLC	C1-O5-C5	2.27	115.13	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

23 ligands 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	1000	1	14,14,15	0.52	0	15,19,21	0.72	1 (6%)
2	NAG	A	1001	1	14,14,15	0.49	0	15,19,21	0.82	1 (6%)
2	NAG	A	1002	1	14,14,15	0.47	0	15,19,21	0.76	1 (6%)
2	NAG	A	1003	1	14,14,15	0.52	0	15,19,21	0.74	1 (6%)
2	NAG	A	1004	1	14,14,15	0.46	0	15,19,21	0.70	1 (6%)
2	NAG	A	1005	1	14,14,15	0.48	0	15,19,21	0.75	1 (6%)
2	NAG	A	1006	1	14,14,15	0.49	0	15,19,21	0.75	1 (6%)
2	NAG	A	1007	1	14,14,15	0.52	0	15,19,21	0.65	0
2	NAG	A	1008	1	14,14,15	0.46	0	15,19,21	0.78	1 (6%)
2	NAG	A	1009	1	14,14,15	0.55	0	15,19,21	0.92	1 (6%)
2	NAG	A	1010	1	14,14,15	0.52	0	15,19,21	0.72	1 (6%)
2	NAG	A	1011	1	14,14,15	0.45	0	15,19,21	0.69	1 (6%)
2	NAG	B	1000	1	14,14,15	0.52	0	15,19,21	0.73	1 (6%)
2	NAG	B	1001	1	14,14,15	0.50	0	15,19,21	0.77	1 (6%)
2	NAG	B	1002	1	14,14,15	0.49	0	15,19,21	0.73	1 (6%)
2	NAG	B	1003	1	14,14,15	0.55	0	15,19,21	0.69	1 (6%)
2	NAG	B	1004	1	14,14,15	0.45	0	15,19,21	0.85	1 (6%)
2	NAG	B	1005	1	14,14,15	0.47	0	15,19,21	0.75	1 (6%)
2	NAG	B	1006	1	14,14,15	0.50	0	15,19,21	0.68	1 (6%)
2	NAG	B	1007	1	14,14,15	0.53	0	15,19,21	0.69	1 (6%)
2	NAG	B	1008	1	14,14,15	0.46	0	15,19,21	0.76	1 (6%)
2	NAG	B	1009	1	14,14,15	0.48	0	15,19,21	0.76	1 (6%)
2	NAG	B	1010	1	14,14,15	0.49	0	15,19,21	0.69	1 (6%)

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	1000	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1005	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1006	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1008	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1009	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1010	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1011	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1000	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1003	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1004	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1005	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1006	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1007	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1008	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1009	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1010	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1004	NAG	C2-N2-C7	-2.66	119.62	123.04
2	A	1009	NAG	C2-N2-C7	-2.59	119.71	123.04
2	B	1001	NAG	C2-N2-C7	-2.50	119.83	123.04
2	B	1009	NAG	C2-N2-C7	-2.47	119.86	123.04
2	A	1001	NAG	C2-N2-C7	-2.47	119.86	123.04
2	A	1002	NAG	C2-N2-C7	-2.47	119.87	123.04
2	B	1008	NAG	C2-N2-C7	-2.42	119.93	123.04
2	A	1008	NAG	C2-N2-C7	-2.41	119.94	123.04
2	B	1005	NAG	C2-N2-C7	-2.38	119.98	123.04
2	A	1006	NAG	C2-N2-C7	-2.34	120.03	123.04
2	A	1000	NAG	C2-N2-C7	-2.30	120.08	123.04
2	A	1005	NAG	C2-N2-C7	-2.27	120.13	123.04
2	B	1000	NAG	C2-N2-C7	-2.25	120.15	123.04
2	B	1002	NAG	C2-N2-C7	-2.24	120.17	123.04
2	A	1004	NAG	C2-N2-C7	-2.17	120.25	123.04
2	A	1010	NAG	C2-N2-C7	-2.15	120.27	123.04
2	A	1003	NAG	C2-N2-C7	-2.14	120.29	123.04
2	B	1003	NAG	C2-N2-C7	-2.08	120.37	123.04
2	A	1011	NAG	C2-N2-C7	-2.06	120.39	123.04
2	B	1010	NAG	C2-N2-C7	-2.06	120.40	123.04
2	B	1006	NAG	C2-N2-C7	-2.05	120.40	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1007	NAG	C2-N2-C7	-2.03	120.43	123.04

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1011	NAG	O7-C7-N2-C2
2	A	1011	NAG	C8-C7-N2-C2

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	NAG	2	0
2	A	1005	NAG	1	0
2	A	1006	NAG	1	0
2	A	1007	NAG	2	0
2	A	1011	NAG	1	0
2	B	1002	NAG	1	0
2	B	1003	NAG	1	0
2	B	1005	NAG	2	0
2	B	1008	NAG	1	0

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^{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	549/549 (100%)	-0.06	25 (4%)	36	40	10, 16, 29, 46	0
1	B	549/549 (100%)	0.26	27 (4%)	33	36	11, 20, 35, 49	0
All	All	1098/1098 (100%)	0.10	52 (4%)	35	39	10, 18, 33, 49	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	64	ALA	7.7
1	B	289	SER	7.2
1	B	564	ASP	6.8
1	A	193	PRO	6.3
1	A	330	ASN	6.0
1	B	535	ASN	5.5
1	A	194	GLY	4.6
1	B	290	GLY	4.6
1	B	500	LEU	4.2
1	B	66	SER	4.2
1	A	329	GLY	4.0
1	B	303	LEU	3.9
1	B	65	SER	3.9
1	B	68	LEU	3.8
1	B	226	PHE	3.6
1	A	120	ASN	3.5
1	B	63	PRO	3.4
1	B	139	GLN	3.3
1	B	117	SER	3.3
1	B	503	ASN	3.2
1	A	331	SER	3.2
1	B	541	SER	3.2
1	A	226	PHE	3.1
1	A	192	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	564	ASP	3.0
1	A	68	LEU	2.9
1	B	116	GLY	2.8
1	A	138	ASN	2.8
1	B	563	ILE	2.8
1	A	116	GLY	2.7
1	A	139	GLN	2.6
1	A	302	THR	2.6
1	A	66	SER	2.6
1	B	536	THR	2.5
1	B	438	TYR	2.5
1	B	546	VAL	2.5
1	A	118	SER	2.5
1	A	195	SER	2.5
1	A	196	PRO	2.4
1	A	117	SER	2.4
1	B	302	THR	2.4
1	B	294	ASN	2.3
1	A	438	TYR	2.3
1	A	289	SER	2.1
1	A	333	ASP	2.1
1	B	467	ARG	2.1
1	A	135	ARG	2.1
1	B	62	THR	2.1
1	B	137	ASP	2.1
1	A	64	ALA	2.0
1	B	561	HIS	2.0
1	A	19	MET	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
3	BGC	B	2003	12/12	0.78	0.21	17.77	28,33,34,34	0
3	BGC	A	2003	12/12	0.86	0.19	11.18	22,27,27,27	0
3	GLC	A	2002	11/12	0.90	0.14	2.64	19,21,26,27	0
3	GLC	B	2002	11/12	0.89	0.13	0.43	23,24,29,33	0
3	GLC	B	2001	11/12	0.93	0.09	-0.57	19,20,22,24	0
3	GLC	A	2001	11/12	0.97	0.06	-1.60	16,16,19,20	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
2	NAG	B	1009	14/15	0.83	0.20	22.61	29,34,37,37	0
2	NAG	B	1000	14/15	0.66	0.23	19.11	43,45,49,50	0
2	NAG	A	1007	14/15	0.76	0.24	11.10	29,36,39,40	0
2	NAG	B	1008	14/15	0.76	0.20	9.25	34,36,39,40	0
2	NAG	A	1011	14/15	0.74	0.24	6.70	36,39,43,45	0
2	NAG	A	1000	14/15	0.89	0.14	4.35	24,26,29,31	0
2	NAG	B	1005	14/15	0.75	0.26	3.90	48,50,51,52	0
2	NAG	A	1006	14/15	0.90	0.11	3.63	26,30,36,36	0
2	NAG	B	1002	14/15	0.49	0.34	3.34	51,53,55,56	0
2	NAG	B	1003	14/15	0.61	0.34	2.94	54,55,56,57	0
2	NAG	B	1007	14/15	0.86	0.10	2.74	32,34,39,39	0
2	NAG	A	1010	14/15	0.83	0.20	1.66	35,37,40,40	0
2	NAG	A	1002	14/15	0.78	0.19	0.96	36,39,43,43	0
2	NAG	A	1005	14/15	0.87	0.12	0.58	28,33,37,38	0
2	NAG	B	1006	14/15	0.83	0.13	0.21	28,31,35,35	0
2	NAG	A	1001	14/15	0.92	0.08	-0.25	19,21,23,26	0
2	NAG	B	1004	14/15	0.90	0.12	-0.50	22,24,33,34	0
2	NAG	A	1003	14/15	0.95	0.07	-0.79	19,21,25,27	0
2	NAG	A	1004	14/15	0.88	0.13	-	32,35,38,42	0
2	NAG	A	1008	14/15	0.91	0.11	-	18,23,28,34	0
2	NAG	B	1010	14/15	0.91	0.14	-	24,28,32,35	0
2	NAG	A	1009	14/15	0.79	0.20	-	32,36,41,41	0
2	NAG	B	1001	14/15	0.84	0.16	-	30,32,37,38	0

6.5 Other polymers (i)

There are no such residues in this entry.