Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 12:41 PM BST

PDB ID	:	1X0C
Title	:	Improved Crystal Structure of Isopullulanase from Aspergillus niger ATCC 9642
Authors	:	Mizuno, M.; Tonozuka, T.; Yamamura, A.; Miyasaka, Y.; Akeboshi, H.; Kamitori, S.; Nishikawa, A.; Sakano, Y.
Deposited on	:	2005-03-17
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

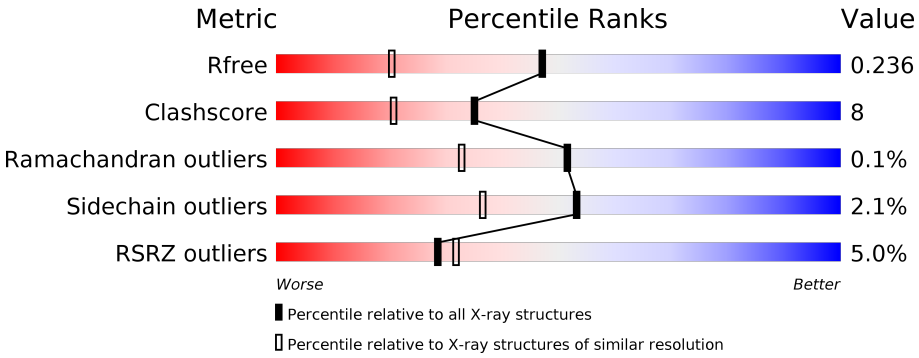
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 respectively. 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	2% 84% 15%
1	B	549	8% 83% 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10079 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.

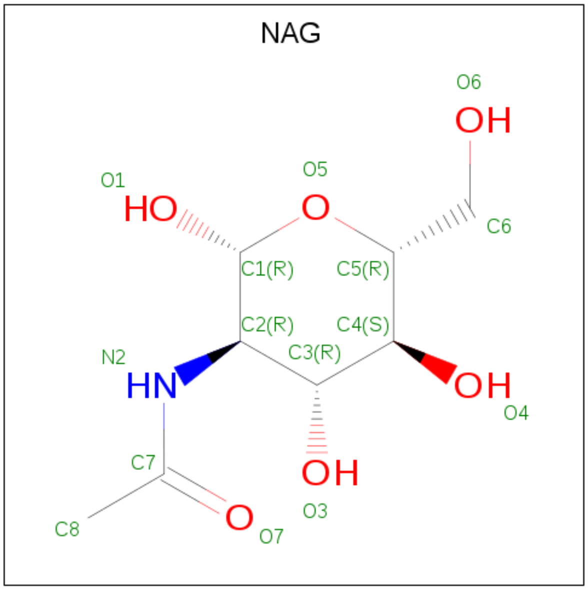
- Molecule 1 is a protein called Isopullulanase.

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 2-acetamido-2-deoxy-beta-D-glucopyranose (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	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

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

- Molecule 3 is water.

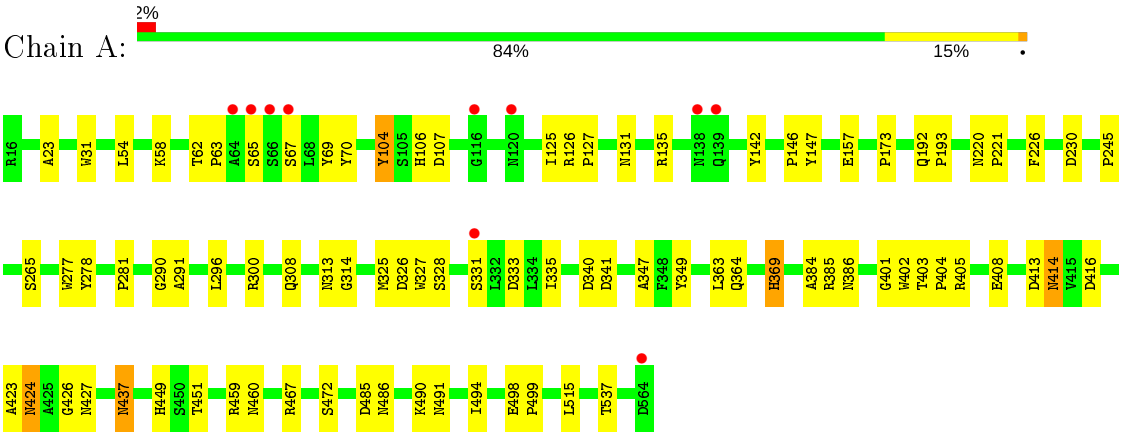
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	731	Total 731	O 731	0	0
3	B	542	Total 542	O 542	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

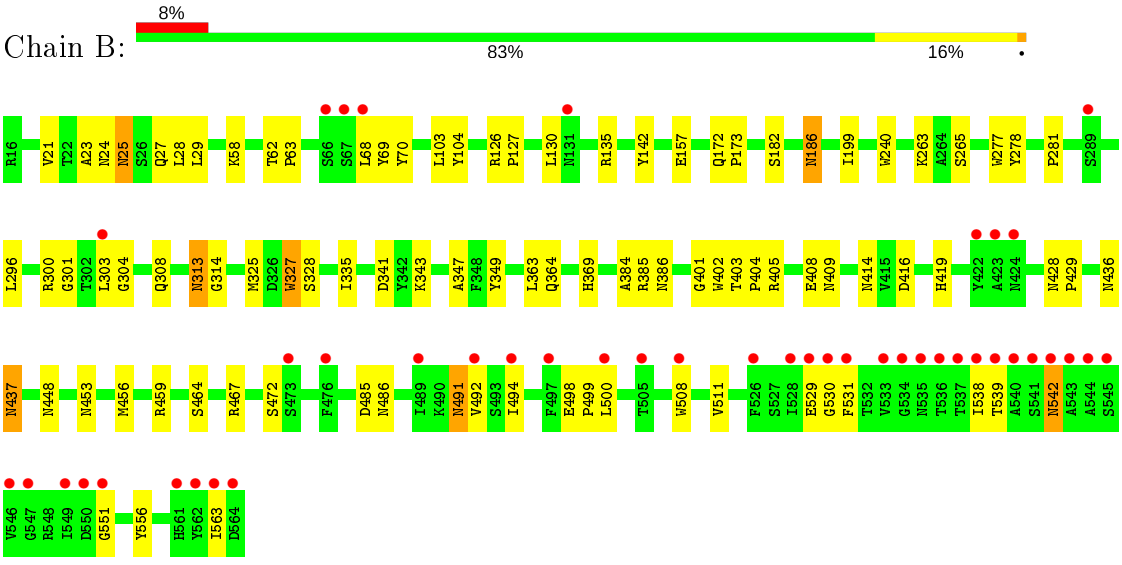
- Molecule 1: Isopullulanase

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	99.72Å 136.16Å 84.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.86 – 1.70 49.86 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.86-1.70) 99.1 (49.86-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.13 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.195 , 0.229 0.206 , 0.236	Depositor DCC
R_{free} test set	12531 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å^2)	15.0	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 48.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10079	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.32% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.32	0/4357	0.64	1/5962 (0.0%)
1	B	0.30	0/4357	0.61	0/5962
All	All	0.31	0/8714	0.63	1/11924 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	369	HIS	N-CA-C	-5.39	96.44	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	3979	58	0
1	B	4242	0	3978	78	0
2	A	154	0	143	5	0
2	B	168	0	156	9	0
3	A	731	0	0	8	0
3	B	542	0	0	7	0
All	All	10079	0	8256	140	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 8.

All (140) 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:54:LEU:HD11	2:A:1002:NAG:H61	1.53	0.91
1:B:539:THR:H	1:B:542:ASN:HD21	1.16	0.91
1:A:414:ASN:ND2	1:A:467:ARG:HH22	1.72	0.87
1:B:539:THR:H	1:B:542:ASN:ND2	1.76	0.82
1:B:25:ASN:HD22	1:B:27:GLN:H	1.27	0.79
1:B:347:ALA:H	1:B:369:HIS:HD2	1.29	0.79
1:B:157:GLU:OE2	1:B:419:HIS:HE1	1.66	0.78
1:A:347:ALA:H	1:A:369:HIS:HD2	1.29	0.77
1:B:127:PRO:HG2	1:B:130:LEU:CD1	2.17	0.75
1:B:529:GLU:HB2	1:B:563:ILE:HB	1.73	0.70
1:B:127:PRO:HG2	1:B:130:LEU:HD13	1.74	0.69
1:B:25:ASN:ND2	1:B:28:LEU:H	1.91	0.68
1:B:303:LEU:HD23	1:B:304:GLY:O	1.93	0.68
1:B:308:GLN:NE2	1:B:327:TRP:HE1	1.93	0.65
1:A:414:ASN:HD21	1:A:467:ARG:HH22	1.42	0.65
1:A:192:GLN:HB3	1:A:193:PRO:HD2	1.79	0.64
1:A:135:ARG:HG2	1:A:142:TYR:HB2	1.78	0.63
1:A:386:ASN:HB3	3:A:1284:HOH:O	1.98	0.63
1:B:308:GLN:HE21	1:B:327:TRP:HE1	1.47	0.63
1:B:539:THR:N	1:B:542:ASN:HD21	1.94	0.60
1:B:25:ASN:ND2	1:B:27:GLN:H	1.97	0.60
1:B:157:GLU:HB3	1:B:173:PRO:HG3	1.83	0.60
1:B:436:ASN:ND2	1:B:437:ASN:H	1.99	0.60
1:B:453:ASN:HA	2:B:1008:NAG:H82	1.84	0.60
1:A:146:PRO:HG3	3:A:1498:HOH:O	2.01	0.59
1:B:186:ASN:HD22	1:B:186:ASN:C	2.05	0.59
1:B:472:SER:HB3	1:B:494:ILE:HG23	1.84	0.58
1:A:58:LYS:HB3	1:A:69:TYR:HB3	1.85	0.58
1:B:416:ASP:HB2	1:B:467:ARG:NH2	2.18	0.58
1:B:127:PRO:HG2	1:B:130:LEU:HD11	1.86	0.57
1:B:135:ARG:HG2	1:B:142:TYR:HB2	1.85	0.57
1:A:54:LEU:HD12	3:A:1364:HOH:O	2.04	0.57
1:B:436:ASN:HD22	1:B:437:ASN:H	1.53	0.57
2:A:1007:NAG:H81	3:A:1362:HOH:O	2.03	0.57
1:B:511:VAL:HA	1:B:556:TYR:CE1	2.40	0.57
2:A:1000:NAG:H81	3:A:1669:HOH:O	2.05	0.56
2:B:1003:NAG:H83	3:B:1392:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PRO:HB3	1:A:416:ASP:OD2	2.06	0.56
1:B:542:ASN:HD22	1:B:542:ASN:C	2.09	0.56
1:A:423:ALA:H	1:A:427:ASN:ND2	2.03	0.56
1:B:23:ALA:HB2	1:B:70:TYR:CG	2.41	0.56
1:A:404:PRO:HG2	3:A:1398:HOH:O	2.06	0.56
1:A:537:THR:HG23	3:A:1320:HOH:O	2.06	0.56
1:A:424:ASN:H	1:A:427:ASN:ND2	2.04	0.55
1:A:125:ILE:HD12	1:A:125:ILE:N	2.21	0.55
1:B:498:GLU:HB3	1:B:499:PRO:HD2	1.88	0.54
1:B:281:PRO:HG3	1:B:296:LEU:HD13	1.89	0.54
1:B:491:ASN:HD22	2:B:1010:NAG:H82	1.71	0.54
1:A:347:ALA:H	1:A:369:HIS:CD2	2.18	0.54
1:A:331:SER:HB3	1:A:333:ASP:OD1	2.07	0.54
1:B:404:PRO:HG2	3:B:1207:HOH:O	2.07	0.54
1:A:449:HIS:HD2	3:A:1692:HOH:O	1.91	0.53
1:B:404:PRO:HG2	1:B:456:MET:HE1	1.91	0.53
1:A:157:GLU:HB3	1:A:173:PRO:HG3	1.90	0.53
1:A:23:ALA:HB2	1:A:70:TYR:CG	2.44	0.53
1:B:172:GLN:HG2	1:B:419:HIS:CD2	2.45	0.52
1:B:401:GLY:O	1:B:402:TRP:HB2	2.09	0.52
1:A:460:ASN:ND2	2:A:1007:NAG:C7	2.72	0.52
1:A:308:GLN:O	1:A:335:ILE:HD12	2.09	0.52
1:A:472:SER:HB3	1:A:494:ILE:HG23	1.91	0.51
1:B:419:HIS:HD2	3:B:1223:HOH:O	1.93	0.51
2:B:1002:NAG:H81	3:B:1395:HOH:O	2.11	0.51
1:B:21:VAL:HG11	1:B:68:LEU:HD21	1.93	0.50
1:A:423:ALA:H	1:A:427:ASN:HD22	1.58	0.50
1:A:62:THR:HB	1:A:63:PRO:HA	1.94	0.49
1:B:459:ARG:HA	1:B:485:ASP:O	2.13	0.49
1:B:492:VAL:HG13	1:B:531:PHE:CD1	2.48	0.49
1:B:21:VAL:O	1:B:21:VAL:HG13	2.12	0.49
1:B:62:THR:HB	1:B:63:PRO:HA	1.95	0.48
1:B:29:LEU:HD23	1:B:103:LEU:HD12	1.96	0.48
1:B:103:LEU:HA	1:B:182:SER:O	2.14	0.48
1:B:437:ASN:HD22	1:B:437:ASN:C	2.16	0.48
1:B:347:ALA:N	1:B:369:HIS:HD2	2.03	0.47
1:A:106:HIS:HD2	1:A:107:ASP:O	1.97	0.47
1:A:340:ASP:OD1	1:A:364:GLN:HG3	2.14	0.47
1:B:126:ARG:HA	1:B:127:PRO:C	2.34	0.47
1:B:25:ASN:HD22	1:B:27:GLN:N	2.06	0.47
1:B:58:LYS:HB3	1:B:69:TYR:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:LYS:O	1:A:491:ASN:HB2	2.15	0.47
1:B:25:ASN:ND2	1:B:28:LEU:N	2.63	0.47
1:A:126:ARG:HA	1:A:127:PRO:C	2.35	0.47
1:B:464:SER:HB2	2:B:1010:NAG:H81	1.95	0.47
1:A:408:GLU:HA	1:A:459:ARG:O	2.15	0.46
1:B:24:ASN:HD22	2:B:1000:NAG:C8	2.29	0.46
1:B:277:TRP:CD1	1:B:349:TYR:HB3	2.50	0.46
1:B:492:VAL:O	1:B:492:VAL:HG13	2.16	0.46
1:B:542:ASN:ND2	1:B:542:ASN:C	2.70	0.45
1:A:424:ASN:HD22	1:A:426:GLY:N	2.13	0.45
1:B:265:SER:HA	1:B:313:ASN:O	2.16	0.45
1:A:265:SER:HA	1:A:313:ASN:O	2.17	0.45
1:A:363:LEU:O	1:A:384:ALA:HA	2.16	0.45
1:B:467:ARG:HH11	1:B:467:ARG:HG3	1.82	0.45
1:A:401:GLY:O	1:A:402:TRP:HB2	2.17	0.44
1:B:508:TRP:HB3	1:B:551:GLY:HA3	1.99	0.44
1:B:301:GLY:HA3	1:B:327:TRP:CE2	2.53	0.44
1:A:281:PRO:HG3	1:A:296:LEU:HD13	1.99	0.44
1:B:186:ASN:ND2	1:B:186:ASN:C	2.70	0.44
1:A:300:ARG:NH1	1:A:328:SER:OG	2.49	0.44
1:B:448:ASN:ND2	2:B:1007:NAG:H82	2.33	0.44
1:A:104:TYR:CE2	1:A:147:TYR:HA	2.53	0.44
1:A:300:ARG:NE	1:A:328:SER:OG	2.50	0.44
1:A:65:SER:C	1:A:67:SER:H	2.19	0.44
1:A:424:ASN:HD22	1:A:426:GLY:H	1.65	0.43
1:B:303:LEU:HD13	1:B:335:ILE:HG13	1.98	0.43
1:B:363:LEU:O	1:B:384:ALA:HA	2.18	0.43
1:B:24:ASN:HD22	2:B:1000:NAG:H83	1.84	0.43
1:B:408:GLU:HG3	1:B:409:ASN:ND2	2.32	0.43
1:A:437:ASN:C	1:A:437:ASN:HD22	2.21	0.43
1:B:403:THR:O	1:B:405:ARG:HG3	2.18	0.43
1:B:491:ASN:ND2	2:B:1010:NAG:H82	2.33	0.43
1:B:343:LYS:HD2	1:B:343:LYS:N	2.34	0.43
1:A:498:GLU:HB3	1:A:499:PRO:HD2	2.01	0.43
1:A:300:ARG:HD2	1:A:326:ASP:O	2.19	0.43
1:A:414:ASN:HD21	1:A:467:ARG:NH2	2.14	0.42
1:A:451:THR:HA	1:A:515:LEU:HB2	2.00	0.42
1:A:403:THR:O	1:A:405:ARG:HG3	2.18	0.42
1:A:414:ASN:HD22	1:A:467:ARG:HH22	1.58	0.42
1:A:226:PHE:O	1:A:230:ASP:HB3	2.20	0.42
1:A:31:TRP:CZ3	1:A:245:PRO:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLY:HA2	1:A:341:ASP:O	2.19	0.42
1:A:459:ARG:HA	1:A:485:ASP:O	2.20	0.42
1:A:220:ASN:HB3	1:A:221:PRO:HD2	2.02	0.42
1:A:467:ARG:HG3	1:A:467:ARG:HH11	1.83	0.42
1:B:281:PRO:CG	1:B:296:LEU:HD13	2.50	0.41
1:B:314:GLY:HA2	1:B:341:ASP:O	2.20	0.41
1:B:240:TRP:CE2	1:B:263:LYS:HE3	2.54	0.41
1:B:364:GLN:HA	1:B:385:ARG:O	2.20	0.41
1:B:428:ASN:N	1:B:429:PRO:CD	2.84	0.41
1:B:500:LEU:HD21	3:B:1303:HOH:O	2.21	0.41
1:A:385:ARG:HA	1:A:413:ASP:O	2.21	0.40
1:B:199:ILE:HD12	3:B:1287:HOH:O	2.20	0.40
1:B:300:ARG:NH2	1:B:328:SER:HB2	2.36	0.40
1:B:511:VAL:HA	1:B:556:TYR:CZ	2.56	0.40
1:B:491:ASN:HA	1:B:530:GLY:O	2.21	0.40
1:A:277:TRP:CD1	1:A:349:TYR:HB3	2.56	0.40
1:B:386:ASN:HB3	3:B:1192:HOH:O	2.21	0.40
1:B:58:LYS:HA	1:B:70:TYR:O	2.22	0.40
1:A:221:PRO:HG2	2:A:1000:NAG:H83	2.04	0.40
1:A:290:GLY:O	1:A:291:ALA:C	2.60	0.40
1:B:538:ILE:HA	1:B:542:ASN:HD21	1.86	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	547/549 (100%)	517 (94%)	30 (6%)	0	100	100
1	B	547/549 (100%)	514 (94%)	32 (6%)	1 (0%)	47	30
All	All	1094/1098 (100%)	1031 (94%)	62 (6%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	491	ASN

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	466/466 (100%)	457 (98%)	9 (2%)	57	41
1	B	466/466 (100%)	455 (98%)	11 (2%)	49	31
All	All	932/932 (100%)	912 (98%)	20 (2%)	53	36

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
1	A	414	ASN
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	414	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 (32) 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	120	ASN
1	A	122	ASN
1	A	131	ASN
1	A	139	GLN
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	186	ASN
1	B	192	GLN
1	B	286	GLN
1	B	308	GLN
1	B	330	ASN
1	B	369	HIS
1	B	386	ASN
1	B	414	ASN
1	B	419	HIS
1	B	436	ASN
1	B	437	ASN
1	B	486	ASN
1	B	542	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	B	1009	1	14,14,15	0.47	0	17,19,21	0.69	1 (5%)
2	NAG	A	1005	1	14,14,15	0.50	0	17,19,21	0.63	0
2	NAG	B	1005	1	14,14,15	0.50	0	17,19,21	0.62	0
2	NAG	A	1004	1	14,14,15	0.50	0	17,19,21	0.56	0
2	NAG	A	1000	1	14,14,15	0.54	0	17,19,21	0.72	1 (5%)
2	NAG	A	1001	1	14,14,15	0.44	0	17,19,21	0.61	0
2	NAG	B	1007	1	14,14,15	0.51	0	17,19,21	0.69	1 (5%)
2	NAG	B	1010	1	14,14,15	0.48	0	17,19,21	0.67	1 (5%)
2	NAG	B	1011	1	14,14,15	0.50	0	17,19,21	0.71	1 (5%)
2	NAG	A	1002	1	14,14,15	0.53	0	17,19,21	0.62	0
2	NAG	A	1007	1	14,14,15	0.59	0	17,19,21	0.53	0
2	NAG	A	1010	1	14,14,15	0.51	0	17,19,21	0.63	0
2	NAG	B	1001	1	14,14,15	0.51	0	17,19,21	0.66	0
2	NAG	B	1006	1	14,14,15	0.51	0	17,19,21	0.65	0
2	NAG	B	1008	1	14,14,15	0.46	0	17,19,21	0.70	1 (5%)
2	NAG	B	1004	1	14,14,15	0.50	0	17,19,21	0.77	1 (5%)
2	NAG	B	1003	1	14,14,15	0.49	0	17,19,21	0.70	1 (5%)
2	NAG	B	1002	1	14,14,15	0.47	0	17,19,21	0.66	1 (5%)
2	NAG	A	1003	1	14,14,15	0.60	0	17,19,21	0.65	0
2	NAG	B	1000	1	14,14,15	0.51	0	17,19,21	0.63	0
2	NAG	A	1008	1	14,14,15	0.43	0	17,19,21	0.64	0
2	NAG	A	1006	1	14,14,15	0.48	0	17,19,21	0.70	1 (5%)
2	NAG	A	1009	1	14,14,15	0.53	0	17,19,21	0.73	1 (5%)

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	B	1009	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1005	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1005	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1004	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1000	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1007	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1010	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1011	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1002	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1007	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1010	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	1006	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1008	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1004	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1003	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1002	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1000	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1008	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1006	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1009	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1004	NAG	C2-N2-C7	-2.34	119.56	122.90
2	A	1000	NAG	C2-N2-C7	-2.28	119.65	122.90
2	A	1009	NAG	C2-N2-C7	-2.19	119.78	122.90
2	A	1006	NAG	C2-N2-C7	-2.16	119.83	122.90
2	B	1008	NAG	C2-N2-C7	-2.12	119.88	122.90
2	B	1009	NAG	C2-N2-C7	-2.11	119.90	122.90
2	B	1010	NAG	C2-N2-C7	-2.08	119.94	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1007	NAG	C2-N2-C7	-2.06	119.97	122.90
2	B	1011	NAG	C2-N2-C7	-2.06	119.97	122.90
2	B	1003	NAG	C2-N2-C7	-2.05	119.98	122.90
2	B	1002	NAG	C2-N2-C7	-2.05	119.99	122.90

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1009	NAG	C8-C7-N2-C2
2	B	1009	NAG	O7-C7-N2-C2
2	B	1005	NAG	C8-C7-N2-C2
2	B	1005	NAG	O7-C7-N2-C2
2	A	1000	NAG	O7-C7-N2-C2
2	B	1007	NAG	C8-C7-N2-C2
2	B	1007	NAG	O7-C7-N2-C2
2	B	1010	NAG	C8-C7-N2-C2
2	B	1010	NAG	O7-C7-N2-C2
2	B	1011	NAG	C8-C7-N2-C2
2	B	1011	NAG	O7-C7-N2-C2
2	A	1002	NAG	C8-C7-N2-C2
2	A	1002	NAG	O7-C7-N2-C2
2	A	1007	NAG	C1-C2-N2-C7
2	A	1007	NAG	C8-C7-N2-C2
2	A	1007	NAG	O7-C7-N2-C2
2	B	1004	NAG	C8-C7-N2-C2
2	B	1004	NAG	O7-C7-N2-C2
2	B	1000	NAG	C8-C7-N2-C2
2	B	1000	NAG	O7-C7-N2-C2
2	A	1009	NAG	C8-C7-N2-C2
2	A	1009	NAG	O7-C7-N2-C2
2	A	1000	NAG	C8-C7-N2-C2
2	B	1002	NAG	C8-C7-N2-C2
2	A	1006	NAG	C8-C7-N2-C2
2	B	1002	NAG	O7-C7-N2-C2
2	A	1006	NAG	O7-C7-N2-C2
2	B	1006	NAG	O5-C5-C6-O6
2	B	1006	NAG	C4-C5-C6-O6
2	A	1008	NAG	O5-C5-C6-O6
2	B	1003	NAG	C8-C7-N2-C2
2	B	1006	NAG	C8-C7-N2-C2
2	B	1009	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	1003	NAG	O7-C7-N2-C2
2	B	1006	NAG	O7-C7-N2-C2
2	A	1009	NAG	C4-C5-C6-O6
2	B	1009	NAG	O5-C5-C6-O6
2	A	1009	NAG	O5-C5-C6-O6
2	A	1004	NAG	C8-C7-N2-C2
2	B	1008	NAG	C8-C7-N2-C2
2	A	1004	NAG	O7-C7-N2-C2
2	A	1005	NAG	C4-C5-C6-O6
2	B	1004	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	NAG	2	0
2	B	1007	NAG	1	0
2	B	1010	NAG	3	0
2	A	1002	NAG	1	0
2	A	1007	NAG	2	0
2	B	1008	NAG	1	0
2	B	1003	NAG	1	0
2	B	1002	NAG	1	0
2	B	1000	NAG	2	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	549/549 (100%)	-0.14	10 (1%)	68	72	7, 13, 27, 48	0
1	B	549/549 (100%)	0.43	45 (8%)	11	13	9, 20, 34, 62	0
All	All	1098/1098 (100%)	0.14	55 (5%)	28	32	7, 16, 32, 62	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	564	ASP	6.4
1	B	538	ILE	6.2
1	B	500	LEU	6.0
1	B	563	ILE	4.6
1	B	530	GLY	4.6
1	B	540	ALA	4.6
1	B	535	ASN	4.4
1	B	546	VAL	4.3
1	B	541	SER	4.2
1	B	66	SER	4.1
1	B	528	ILE	4.0
1	B	539	THR	4.0
1	B	561	HIS	3.7
1	B	543	ALA	3.7
1	B	68	LEU	3.6
1	B	549	ILE	3.6
1	A	64	ALA	3.5
1	B	537	THR	3.4
1	B	533	VAL	3.4
1	A	65	SER	3.4
1	B	492	VAL	3.4
1	A	138	ASN	3.2
1	A	116	GLY	3.0
1	B	67	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	531	PHE	2.9
1	B	508	TRP	2.9
1	B	505	THR	2.8
1	B	526	PHE	2.8
1	A	564	ASP	2.8
1	B	551	GLY	2.7
1	A	66	SER	2.6
1	B	303	LEU	2.6
1	B	542	ASN	2.6
1	B	476	PHE	2.6
1	A	139	GLN	2.5
1	B	562	TYR	2.5
1	B	497	PHE	2.5
1	B	550	ASP	2.4
1	B	547	GLY	2.4
1	A	331	SER	2.4
1	A	120	ASN	2.4
1	B	424	ASN	2.3
1	A	67	SER	2.3
1	B	536	THR	2.3
1	B	534	GLY	2.2
1	B	473	SER	2.2
1	B	529	GLU	2.2
1	B	131	ASN	2.2
1	B	489	ILE	2.2
1	B	494	ILE	2.2
1	B	545	SER	2.2
1	B	544	ALA	2.1
1	B	423	ALA	2.1
1	B	289	SER	2.0
1	B	422	TYR	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)

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å^2)	Q<0.9
2	NAG	A	1000	14/15	0.70	0.21	32,34,39,42	0
2	NAG	A	1009	14/15	0.71	0.25	21,36,40,40	0
2	NAG	B	1006	14/15	0.75	0.19	33,38,43,47	0
2	NAG	B	1004	14/15	0.76	0.19	32,35,40,41	0
2	NAG	B	1002	14/15	0.77	0.25	31,40,47,47	0
2	NAG	B	1000	14/15	0.78	0.15	29,33,37,39	0
2	NAG	B	1008	14/15	0.78	0.20	38,41,43,45	0
2	NAG	A	1004	14/15	0.79	0.14	24,29,34,34	0
2	NAG	B	1009	14/15	0.79	0.16	37,41,47,49	0
2	NAG	B	1011	14/15	0.79	0.21	34,38,49,51	0
2	NAG	A	1007	14/15	0.80	0.17	30,36,41,43	0
2	NAG	B	1005	14/15	0.83	0.16	27,34,44,45	0
2	NAG	B	1010	14/15	0.83	0.24	42,46,48,48	0
2	NAG	A	1002	14/15	0.84	0.17	27,29,32,36	0
2	NAG	B	1007	14/15	0.84	0.12	33,35,42,43	0
2	NAG	A	1008	14/15	0.86	0.11	17,22,28,39	0
2	NAG	B	1003	14/15	0.86	0.22	31,33,40,40	0
2	NAG	B	1001	14/15	0.88	0.11	22,26,31,33	0
2	NAG	A	1010	14/15	0.89	0.15	24,27,31,34	0
2	NAG	A	1006	14/15	0.89	0.10	22,29,33,35	0
2	NAG	A	1005	14/15	0.89	0.12	22,28,33,37	0
2	NAG	A	1003	14/15	0.95	0.09	16,18,21,22	0
2	NAG	A	1001	14/15	0.96	0.08	13,15,17,17	0

6.5 Other polymers

There are no such residues in this entry.