Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:45 PM GMT

PDB ID	:	1LXM
Title	:	Crystal Structure of Streptococcus agalactiae Hyaluronate Lyase Complexed with Hexasaccharide Unit of Hyaluronan
Authors	:	Mello, L.V.; de Groot, B.L.; Li, S.; Jedrzejas, M.J.
Deposited on	:	2002-06-05
Resolution	:	2.20 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:

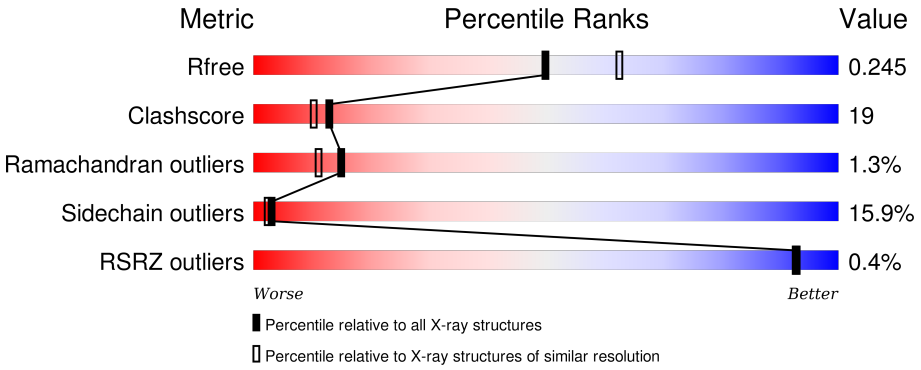
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	814	57% 34% 6% •

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	BDP	A	2001	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	2002	-	-	-	X
2	BDP	A	2003	-	-	-	X
2	BDP	A	2005	X	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6628 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 HYALURONATE Lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	794	Total	C	N	O	S	309	0	0
			6358	4008	1080	1253	17			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	ALA	GLY	SEE REMARK 999	UNP q53591
A	248	THR	PRO	SEE REMARK 999	UNP q53591
A	280	ASN	THR	SEE REMARK 999	UNP q53591
A	288	ALA	GLY	SEE REMARK 999	UNP q53591
A	583	THR	ALA	SEE REMARK 999	UNP q53591
A	688	PHE	LEU	SEE REMARK 999	UNP q53591
A	689	TRP	GLY	SEE REMARK 999	UNP q53591
A	882	GLN	LEU	SEE REMARK 999	UNP q53591
A	894	MET	LEU	SEE REMARK 999	UNP q53591

- Molecule 2 is a polymer of unknown type called SUGAR (NAG-GCU-NAG-GCU-NAG-GCU).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	6	Total	C	N	O	0	0
			79	42	3	34		

- Molecule 3 is water.

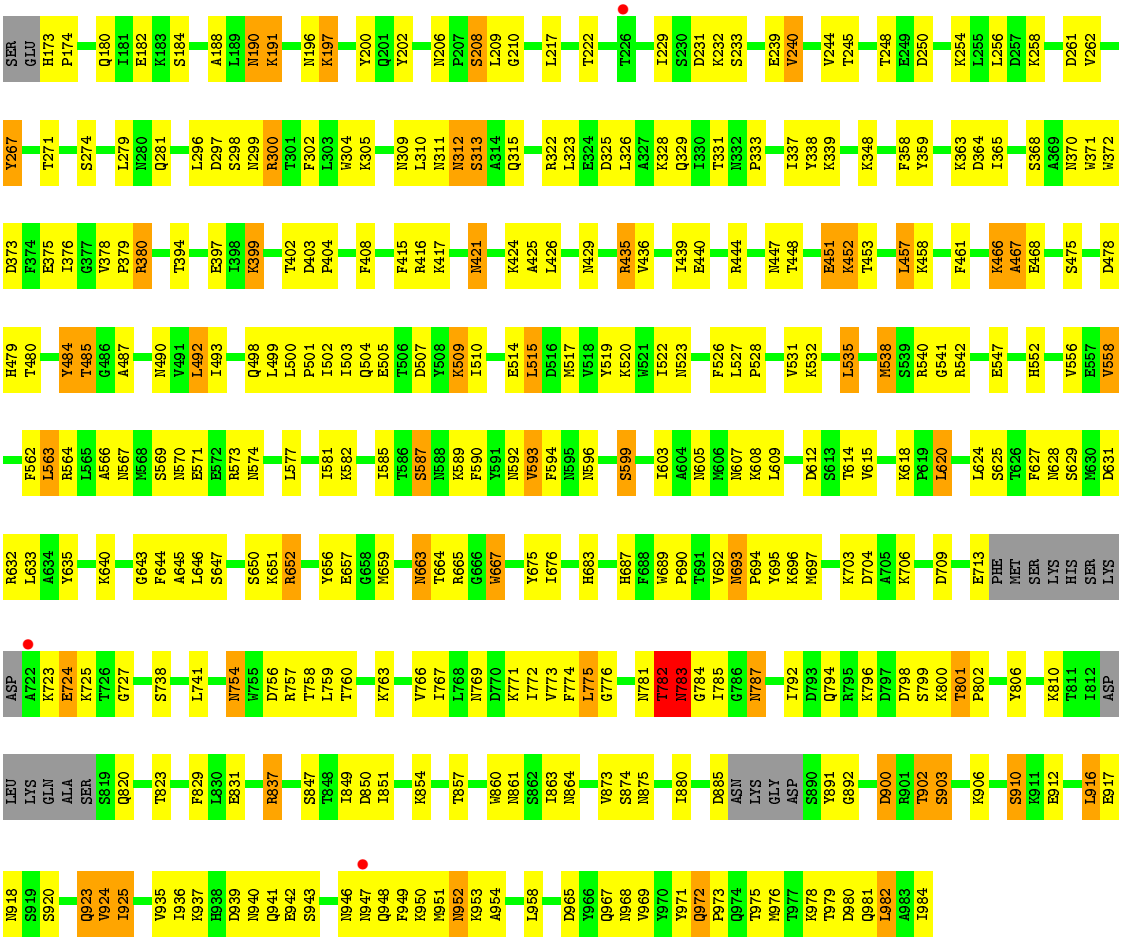
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	191	Total	O	0	0
			191	191		

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: HYALURONATE Lyase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	51.11Å 155.04Å 238.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 44.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.20) 93.3 (44.95-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.218 , 0.271 0.228 , 0.245	Depositor DCC
R_{free} test set	2269 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	34.9	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 73.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	2 of 45244 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6628	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: NAG, BDP

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	0.38	0/6480	0.62	0/8771

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2005	BDP	C4

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	6358	0	6254	224	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	79	0	51	7	0
3	A	191	0	0	4	0
All	All	6628	0	6305	226	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 19.

All (226) 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:416:ARG:HH12	2:A:2000:NAG:H2	1.25	1.02
1:A:188:ALA:HB3	1:A:191:LYS:HG3	1.42	1.01
1:A:628:ASN:HD21	1:A:738:SER:H	1.08	0.97
1:A:952:ASN:HD22	1:A:953:LYS:H	0.99	0.96
1:A:421:ASN:H	1:A:421:ASN:HD22	1.01	0.94
1:A:946:ASN:HD22	1:A:948:GLN:HE21	1.16	0.93
1:A:312:ASN:HD22	1:A:312:ASN:C	1.74	0.91
1:A:421:ASN:N	1:A:421:ASN:HD22	1.66	0.90
1:A:782:THR:O	1:A:783:ASN:HB3	1.71	0.89
1:A:952:ASN:HD22	1:A:953:LYS:N	1.70	0.89
1:A:504:GLN:HE22	1:A:510:ILE:H	1.22	0.83
1:A:952:ASN:ND2	1:A:953:LYS:H	1.77	0.82
1:A:754:ASN:HD21	1:A:758:THR:H	1.25	0.81
1:A:946:ASN:ND2	1:A:948:GLN:HE21	1.80	0.80
1:A:946:ASN:HD22	1:A:948:GLN:NE2	1.79	0.78
1:A:190:ASN:HD21	1:A:248:THR:H	1.32	0.77
1:A:756:ASP:O	1:A:758:THR:HG23	1.85	0.76
1:A:258:LYS:HE3	1:A:505:GLU:HG3	1.66	0.76
1:A:421:ASN:N	1:A:421:ASN:ND2	2.33	0.76
1:A:421:ASN:H	1:A:421:ASN:ND2	1.83	0.74
1:A:394:THR:OG1	1:A:397:GLU:HG2	1.86	0.74
1:A:190:ASN:ND2	1:A:248:THR:H	1.87	0.72
1:A:416:ARG:NH1	2:A:2000:NAG:H2	2.04	0.71
1:A:628:ASN:HD21	1:A:738:SER:N	1.85	0.71
1:A:190:ASN:H	1:A:190:ASN:HD22	1.40	0.69
1:A:773:VAL:HG11	1:A:925:ILE:HD12	1.72	0.69
1:A:258:LYS:O	1:A:262:VAL:HG23	1.92	0.69
1:A:683:HIS:CE1	1:A:796:LYS:H	2.12	0.68
1:A:949:PHE:HB3	1:A:984:ILE:HG12	1.76	0.68
1:A:517:MET:HE3	3:A:1161:HOH:O	1.94	0.68
1:A:547:GLU:HG3	1:A:860:TRP:CE2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:MET:HG3	3:A:1017:HOH:O	1.95	0.66
1:A:312:ASN:ND2	1:A:312:ASN:C	2.49	0.66
1:A:458:LYS:HE2	1:A:510:ILE:HA	1.77	0.65
1:A:754:ASN:HD21	1:A:758:THR:N	1.94	0.64
1:A:582:LYS:NZ	1:A:612:ASP:O	2.30	0.64
1:A:773:VAL:HG11	1:A:925:ILE:CD1	2.27	0.64
1:A:693:ASN:H	1:A:794:GLN:HE22	1.45	0.64
1:A:504:GLN:HE22	1:A:510:ILE:N	1.96	0.62
1:A:365:ILE:HD13	1:A:371:TRP:HA	1.81	0.62
1:A:829:PHE:CE2	1:A:831:GLU:HB2	2.35	0.61
1:A:683:HIS:HE1	1:A:796:LYS:H	1.48	0.60
1:A:967:GLN:HA	1:A:981:GLN:NE2	2.15	0.60
1:A:297:ASP:O	1:A:300:ARG:HD2	2.02	0.60
1:A:946:ASN:O	1:A:948:GLN:HG2	2.02	0.60
1:A:587:SER:O	1:A:589:LYS:HG2	2.01	0.60
1:A:325:ASP:HA	1:A:328:LYS:HD2	1.84	0.59
1:A:504:GLN:HA	1:A:509:LYS:HB3	1.85	0.59
1:A:376:ILE:O	1:A:380:ARG:HB2	2.03	0.59
1:A:916:LEU:HB2	1:A:924:VAL:HG22	1.84	0.59
1:A:861:ASN:HA	1:A:864:ASN:O	2.03	0.59
1:A:313:SER:HB3	1:A:373:ASP:OD2	2.03	0.58
1:A:693:ASN:C	1:A:693:ASN:HD22	2.06	0.58
1:A:952:ASN:ND2	1:A:953:LYS:N	2.45	0.58
1:A:656:TYR:CE1	1:A:667:TRP:HA	2.39	0.57
1:A:484:TYR:CD1	1:A:487:ALA:HB3	2.39	0.57
1:A:552:HIS:O	1:A:556:VAL:HG23	2.04	0.57
1:A:829:PHE:HE2	1:A:831:GLU:HB2	1.68	0.57
1:A:520:LYS:HE2	3:A:1117:HOH:O	2.03	0.57
1:A:942:GLU:HA	1:A:952:ASN:HA	1.87	0.57
1:A:949:PHE:HB3	1:A:984:ILE:CG1	2.34	0.57
1:A:900:ASP:OD2	1:A:903:SER:HB2	2.03	0.57
1:A:312:ASN:HD22	1:A:313:SER:N	2.02	0.57
1:A:503:ILE:HG22	1:A:504:GLN:HE21	1.69	0.57
1:A:582:LYS:HD3	1:A:615:VAL:HG12	1.88	0.56
1:A:566:ALA:HB2	1:A:577:LEU:HD23	1.88	0.56
1:A:492:LEU:HD12	1:A:492:LEU:C	2.27	0.56
1:A:766:VAL:HB	1:A:773:VAL:HB	1.88	0.55
1:A:967:GLN:HA	1:A:981:GLN:HE22	1.70	0.55
1:A:563:LEU:HD13	1:A:605:ASN:HB3	1.87	0.55
1:A:403:ASP:N	1:A:404:PRO:HD2	2.21	0.55
1:A:527:LEU:HB2	1:A:528:PRO:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:917:GLU:HB3	1:A:924:VAL:HG13	1.89	0.54
1:A:447:ASN:O	1:A:451:GLU:HB3	2.08	0.54
1:A:693:ASN:ND2	1:A:695:TYR:H	2.06	0.54
1:A:690:PRO:HG3	1:A:860:TRP:CE2	2.42	0.54
1:A:250:ASP:O	1:A:254:LYS:HG2	2.07	0.54
1:A:599:SER:O	1:A:603:ILE:HG13	2.07	0.54
1:A:906:LYS:O	1:A:910:SER:HB3	2.09	0.53
1:A:202:TYR:CE2	1:A:229:ILE:HG12	2.44	0.53
1:A:380:ARG:NH1	1:A:380:ARG:HG2	2.24	0.53
1:A:519:TYR:CE1	1:A:573:ARG:HD2	2.44	0.53
1:A:504:GLN:NE2	1:A:510:ILE:H	2.00	0.52
1:A:371:TRP:O	1:A:375:GLU:HG3	2.10	0.52
1:A:624:LEU:HG	1:A:635:TYR:CD1	2.45	0.52
1:A:522:ILE:HG12	1:A:562:PHE:CE1	2.45	0.52
1:A:918:ASN:HA	1:A:923:GLN:HG3	1.91	0.52
1:A:415:PHE:HE2	1:A:429:ASN:HB3	1.75	0.51
1:A:633:LEU:HB3	1:A:646:LEU:HB2	1.92	0.51
1:A:479:HIS:O	1:A:480:THR:HB	2.11	0.51
1:A:783:ASN:O	1:A:785:ILE:N	2.44	0.51
1:A:190:ASN:ND2	1:A:190:ASN:H	2.06	0.51
1:A:475:SER:OG	1:A:627:PHE:HB3	2.11	0.51
1:A:323:LEU:O	1:A:326:LEU:HB2	2.11	0.51
1:A:531:VAL:HG22	1:A:532:LYS:HG3	1.91	0.50
1:A:364:ASP:HA	1:A:408:PHE:HE1	1.75	0.50
1:A:484:TYR:CE1	1:A:541:GLY:HA3	2.47	0.50
1:A:683:HIS:HE1	1:A:796:LYS:N	2.10	0.50
1:A:547:GLU:HG3	1:A:860:TRP:NE1	2.26	0.50
1:A:924:VAL:HB	1:A:935:VAL:HG22	1.93	0.50
1:A:372:TRP:CD1	1:A:376:ILE:HD12	2.47	0.50
1:A:380:ARG:HH11	1:A:380:ARG:HG2	1.77	0.50
1:A:502:ILE:N	1:A:502:ILE:HD12	2.27	0.49
1:A:440:GLU:O	1:A:444:ARG:HG3	2.12	0.49
1:A:380:ARG:HH12	2:A:2004:NAG:C8	2.25	0.49
1:A:979:THR:HG21	1:A:982:LEU:HB2	1.94	0.49
1:A:687:HIS:C	1:A:690:PRO:HD2	2.33	0.49
1:A:902:THR:O	1:A:906:LYS:HG3	2.12	0.49
1:A:776:GLY:HA3	1:A:891:TYR:CE2	2.48	0.49
1:A:500:LEU:HB2	1:A:501:PRO:HD3	1.93	0.49
1:A:504:GLN:NE2	1:A:509:LYS:HB3	2.28	0.49
1:A:635:TYR:O	1:A:643:GLY:HA2	2.12	0.48
1:A:468:GLU:HG2	1:A:478:ASP:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:HIS:N	1:A:174:PRO:CD	2.77	0.48
2:A:2003:BDP:H4	3:A:1026:HOH:O	2.13	0.48
1:A:631:ASP:O	1:A:632:ARG:HD3	2.13	0.48
1:A:939:ASP:C	1:A:940:ASN:HD22	2.16	0.48
1:A:182:GLU:HG3	1:A:196:ASN:ND2	2.29	0.48
1:A:581:ILE:O	1:A:585:ILE:HG12	2.13	0.48
1:A:918:ASN:OD1	1:A:923:GLN:CG	2.62	0.48
1:A:979:THR:CG2	1:A:982:LEU:HB2	2.44	0.48
1:A:310:LEU:HB2	1:A:358:PHE:CZ	2.49	0.48
1:A:757:ARG:HD3	1:A:757:ARG:H	1.79	0.47
1:A:402:THR:CB	1:A:444:ARG:HH11	2.27	0.47
1:A:563:LEU:HD22	1:A:567:ASN:ND2	2.29	0.47
1:A:971:TYR:OH	1:A:976:MET:HG2	2.15	0.47
1:A:693:ASN:HD22	1:A:695:TYR:H	1.61	0.47
1:A:359:TYR:OH	1:A:379:PRO:HG3	2.14	0.47
1:A:359:TYR:CE2	1:A:404:PRO:HB2	2.50	0.47
1:A:297:ASP:O	1:A:300:ARG:HB3	2.15	0.47
1:A:380:ARG:HH12	2:A:2004:NAG:H82	1.80	0.47
1:A:946:ASN:ND2	1:A:948:GLN:NE2	2.51	0.47
1:A:664:THR:HB	1:A:709:ASP:HB3	1.97	0.47
1:A:182:GLU:O	1:A:240:VAL:HG21	2.15	0.46
1:A:950:LYS:N	1:A:984:ILE:OXT	2.39	0.46
1:A:475:SER:HB2	1:A:629:SER:HB2	1.96	0.46
1:A:940:ASN:HD21	1:A:954:ALA:H	1.62	0.46
1:A:415:PHE:CE2	1:A:429:ASN:HB3	2.51	0.46
1:A:466:LYS:HG3	1:A:467:ALA:N	2.30	0.46
1:A:485:THR:HG22	1:A:526:PHE:CE1	2.51	0.46
1:A:798:ASP:OD1	1:A:837:ARG:NH2	2.45	0.46
1:A:969:VAL:HG12	1:A:980:ASP:OD2	2.16	0.46
1:A:510:ILE:HD11	1:A:515:LEU:HG	1.97	0.45
1:A:645:ALA:HB3	1:A:675:TYR:HB2	1.98	0.45
1:A:593:VAL:HG13	1:A:594:PHE:N	2.30	0.45
1:A:338:TYR:O	1:A:339:LYS:HB2	2.16	0.45
1:A:725:LYS:C	1:A:727:GLY:H	2.19	0.45
1:A:972:GLN:OE1	1:A:975:THR:N	2.36	0.45
1:A:399:LYS:HD3	1:A:444:ARG:NH2	2.32	0.45
1:A:309:ASN:N	1:A:315:GLN:OE1	2.48	0.45
1:A:329:GLN:HB2	1:A:337:ILE:HD11	1.97	0.45
1:A:704:ASP:CG	1:A:787:ASN:HD22	2.20	0.45
1:A:436:VAL:O	1:A:440:GLU:HB2	2.17	0.45
1:A:939:ASP:O	1:A:940:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ARG:HH22	2:A:2004:NAG:H82	1.82	0.45
1:A:435:ARG:O	1:A:439:ILE:HG12	2.16	0.44
1:A:594:PHE:CZ	1:A:607:ASN:ND2	2.86	0.44
1:A:767:ILE:HG12	1:A:772:ILE:CD1	2.48	0.44
1:A:493:ILE:CG2	1:A:558:VAL:HG12	2.47	0.44
1:A:783:ASN:ND2	1:A:783:ASN:C	2.71	0.44
1:A:594:PHE:HZ	1:A:607:ASN:ND2	2.15	0.44
1:A:425:ALA:O	1:A:426:LEU:HD23	2.18	0.44
1:A:806:TYR:HE1	1:A:831:GLU:HB3	1.82	0.44
1:A:523:ASN:O	1:A:528:PRO:HD3	2.17	0.44
1:A:692:VAL:O	1:A:694:PRO:HD3	2.18	0.44
1:A:519:TYR:CZ	1:A:573:ARG:HD2	2.53	0.43
1:A:620:LEU:HG	1:A:620:LEU:H	1.47	0.43
1:A:676:ILE:HD13	1:A:676:ILE:HA	1.90	0.43
1:A:300:ARG:HG3	1:A:302:PHE:O	2.19	0.43
1:A:304:TRP:CG	1:A:322:ARG:NH1	2.87	0.43
1:A:197:LYS:HB2	1:A:200:TYR:CD2	2.53	0.43
1:A:490:ASN:HD21	1:A:535:LEU:CD1	2.31	0.43
1:A:608:LYS:O	1:A:612:ASP:HB2	2.19	0.43
1:A:566:ALA:HA	1:A:574:ASN:OD1	2.19	0.43
1:A:378:VAL:HB	1:A:379:PRO:HD3	2.00	0.43
1:A:261:ASP:HB3	1:A:267:TYR:CE1	2.53	0.43
1:A:397:GLU:H	1:A:397:GLU:HG2	1.68	0.43
1:A:208:SER:O	1:A:210:GLY:N	2.52	0.43
1:A:940:ASN:HA	1:A:952:ASN:O	2.19	0.43
1:A:435:ARG:HA	1:A:499:LEU:HD21	2.01	0.42
1:A:453:THR:O	1:A:457:LEU:HB2	2.19	0.42
1:A:531:VAL:HG21	1:A:643:GLY:HA3	2.00	0.42
1:A:704:ASP:OD2	1:A:787:ASN:ND2	2.50	0.42
1:A:781:ASN:O	1:A:783:ASN:N	2.53	0.42
1:A:380:ARG:HH11	1:A:380:ARG:CG	2.32	0.42
1:A:723:LYS:O	1:A:724:GLU:C	2.58	0.42
1:A:329:GLN:HA	1:A:329:GLN:OE1	2.19	0.42
1:A:850:ASP:O	1:A:880:ILE:HA	2.18	0.42
2:A:2004:NAG:H4	2:A:2005:BDP:O5	2.20	0.42
1:A:632:ARG:CD	1:A:647:SER:HA	2.49	0.42
1:A:703:LYS:HE3	1:A:759:LEU:HB2	2.01	0.42
1:A:448:THR:O	1:A:452:LYS:HB2	2.20	0.42
1:A:774:PHE:O	1:A:892:GLY:HA2	2.20	0.42
1:A:461:PHE:CD2	1:A:514:GLU:HG2	2.54	0.42
1:A:971:TYR:O	1:A:973:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:SER:OG	1:A:652:ARG:HG3	2.20	0.42
1:A:633:LEU:O	1:A:645:ALA:HA	2.20	0.42
1:A:348:LYS:HE2	1:A:348:LYS:HB3	1.92	0.42
1:A:689:TRP:CZ3	1:A:697:MET:HE1	2.54	0.42
1:A:222:THR:HA	1:A:244:VAL:HB	2.01	0.41
1:A:592:ASN:O	1:A:593:VAL:C	2.58	0.41
1:A:958:LEU:O	1:A:968:ASN:HA	2.19	0.41
1:A:542:ARG:HD3	1:A:657:GLU:OE1	2.20	0.41
1:A:783:ASN:CG	1:A:783:ASN:O	2.59	0.41
1:A:635:TYR:O	1:A:644:PHE:N	2.52	0.41
1:A:775:LEU:HA	1:A:775:LEU:HD12	1.90	0.41
1:A:849:ILE:HD13	1:A:849:ILE:HA	1.86	0.41
1:A:663:ASN:HA	1:A:663:ASN:HD22	1.65	0.41
1:A:498:GLN:HG3	1:A:564:ARG:NH2	2.36	0.41
1:A:689:TRP:N	1:A:690:PRO:CD	2.83	0.41
1:A:364:ASP:HA	1:A:408:PHE:CE1	2.55	0.41
1:A:331:THR:O	1:A:333:PRO:HD3	2.21	0.41
1:A:801:THR:HA	1:A:802:PRO:HD2	1.85	0.41
1:A:723:LYS:O	1:A:725:LYS:O	2.39	0.41
1:A:820:GLN:HA	1:A:851:ILE:O	2.21	0.41
1:A:754:ASN:O	1:A:757:ARG:HD3	2.20	0.41
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.90	0.41
1:A:514:GLU:O	1:A:517:MET:HB2	2.21	0.40
1:A:923:GLN:HB2	1:A:936:ILE:HB	2.03	0.40
1:A:664:THR:HG23	1:A:863:ILE:O	2.21	0.40
1:A:197:LYS:HB2	1:A:200:TYR:HD2	1.87	0.40
1:A:504:GLN:NE2	1:A:504:GLN:HA	2.37	0.40
1:A:612:ASP:OD2	1:A:614:THR:N	2.54	0.40
1:A:693:ASN:C	1:A:693:ASN:ND2	2.74	0.40
1:A:333:PRO:HA	1:A:338:TYR:CD2	2.56	0.40
1:A:540:ARG:HH11	1:A:540:ARG:HD2	1.74	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	786/814 (97%)	726 (92%)	50 (6%)	10 (1%)	15 11

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	782	THR
1	A	783	ASN
1	A	784	GLY
1	A	209	LEU
1	A	800	LYS
1	A	368	SER
1	A	467	ALA
1	A	571	GLU
1	A	769	ASN
1	A	593	VAL

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	711/729 (98%)	598 (84%)	113 (16%)	3 2

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	184	SER
1	A	190	ASN
1	A	191	LYS
1	A	197	LYS
1	A	206	ASN
1	A	208	SER
1	A	217	LEU
1	A	231	ASP

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Mol	Chain	Res	Type
1	A	232	LYS
1	A	233	SER
1	A	239	GLU
1	A	240	VAL
1	A	245	THR
1	A	267	TYR
1	A	271	THR
1	A	274	SER
1	A	279	LEU
1	A	281	GLN
1	A	296	LEU
1	A	298	SER
1	A	299	ASN
1	A	300	ARG
1	A	305	LYS
1	A	311	ASN
1	A	312	ASN
1	A	313	SER
1	A	363	LYS
1	A	370	ASN
1	A	380	ARG
1	A	399	LYS
1	A	417	LYS
1	A	421	ASN
1	A	424	LYS
1	A	435	ARG
1	A	451	GLU
1	A	452	LYS
1	A	457	LEU
1	A	466	LYS
1	A	484	TYR
1	A	485	THR
1	A	492	LEU
1	A	507	ASP
1	A	509	LYS
1	A	515	LEU
1	A	535	LEU
1	A	538	MET
1	A	558	VAL
1	A	563	LEU
1	A	569	SER
1	A	570	ASN

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Mol	Chain	Res	Type
1	A	587	SER
1	A	590	PHE
1	A	596	ASN
1	A	599	SER
1	A	609	LEU
1	A	618	LYS
1	A	620	LEU
1	A	625	SER
1	A	640	LYS
1	A	651	LYS
1	A	652	ARG
1	A	659	MET
1	A	663	ASN
1	A	665	ARG
1	A	667	TRP
1	A	693	ASN
1	A	696	LYS
1	A	706	LYS
1	A	713	GLU
1	A	724	GLU
1	A	741	LEU
1	A	754	ASN
1	A	760	THR
1	A	763	LYS
1	A	771	LYS
1	A	775	LEU
1	A	782	THR
1	A	783	ASN
1	A	787	ASN
1	A	792	ILE
1	A	799	SER
1	A	801	THR
1	A	810	LYS
1	A	823	THR
1	A	837	ARG
1	A	847	SER
1	A	854	LYS
1	A	857	THR
1	A	873	VAL
1	A	874	SER
1	A	875	ASN
1	A	885	ASP

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Mol	Chain	Res	Type
1	A	900	ASP
1	A	902	THR
1	A	903	SER
1	A	910	SER
1	A	912	GLU
1	A	916	LEU
1	A	920	SER
1	A	923	GLN
1	A	924	VAL
1	A	925	ILE
1	A	937	LYS
1	A	941	GLN
1	A	943	SER
1	A	947	ASN
1	A	951	MET
1	A	952	ASN
1	A	965	ASP
1	A	972	GLN
1	A	978	LYS
1	A	982	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	A	206	ASN
1	A	266	ASN
1	A	311	ASN
1	A	312	ASN
1	A	355	HIS
1	A	356	GLN
1	A	370	ASN
1	A	391	ASN
1	A	407	HIS
1	A	421	ASN
1	A	447	ASN
1	A	455	HIS
1	A	504	GLN
1	A	567	ASN
1	A	570	ASN
1	A	596	ASN
1	A	605	ASN

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Mol	Chain	Res	Type
1	A	607	ASN
1	A	628	ASN
1	A	663	ASN
1	A	683	HIS
1	A	693	ASN
1	A	754	ASN
1	A	783	ASN
1	A	787	ASN
1	A	794	GLN
1	A	875	ASN
1	A	940	ASN
1	A	946	ASN
1	A	952	ASN
1	A	960	GLN
1	A	967	GLN
1	A	981	GLN

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

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	$\#\|Z\| > 2$
2	NAG	A	2000	2	15,15,15	2.75	8 (53%)	17,21,21	1.02	2 (11%)
2	BDP	A	2001	2	9,12,13	5.55	6 (66%)	13,17,19	2.35	5 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	2002	2	14,14,15	2.44	5 (35%)	15,19,21	1.55	6 (40%)
2	BDP	A	2003	2	9,12,13	5.55	5 (55%)	13,17,19	2.47	5 (38%)
2	NAG	A	2004	2	14,14,15	2.76	8 (57%)	15,19,21	1.00	1 (6%)
2	BDP	A	2005	2	9,12,13	6.50	3 (33%)	13,17,19	5.35	9 (69%)

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	2000	2	-	0/6/26/26	0/1/1/1
2	BDP	A	2001	2	-	0/0/21/24	0/1/1/1
2	NAG	A	2002	2	-	0/6/23/26	0/1/1/1
2	BDP	A	2003	2	-	0/0/21/24	0/1/1/1
2	NAG	A	2004	2	-	0/6/23/26	0/1/1/1
2	BDP	A	2005	2	1/1/5/6	0/0/21/24	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2005	BDP	O4-C4	-14.84	1.07	1.43
2	A	2005	BDP	C4-C5	-7.67	1.36	1.53
2	A	2003	BDP	C2-C3	2.06	1.55	1.52
2	A	2004	NAG	C4-C5	2.18	1.57	1.53
2	A	2004	NAG	C3-C2	2.25	1.57	1.52
2	A	2002	NAG	C2-N2	2.28	1.50	1.46
2	A	2000	NAG	C7-N2	2.32	1.43	1.34
2	A	2000	NAG	C4-C3	2.33	1.58	1.52
2	A	2002	NAG	O5-C5	2.36	1.48	1.43
2	A	2000	NAG	O5-C5	2.48	1.50	1.44
2	A	2001	BDP	C2-C3	2.60	1.56	1.52
2	A	2004	NAG	C4-C3	2.70	1.59	1.52
2	A	2001	BDP	C4-C3	2.78	1.59	1.52
2	A	2001	BDP	O5-C1	2.81	1.48	1.43
2	A	2001	BDP	O4-C4	2.97	1.50	1.43
2	A	2000	NAG	C3-C2	3.12	1.59	1.53
2	A	2004	NAG	O5-C5	3.14	1.50	1.43
2	A	2002	NAG	C3-C2	3.15	1.59	1.52
2	A	2000	NAG	C4-C5	3.23	1.59	1.53
2	A	2003	BDP	O4-C4	3.35	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2004	NAG	O3-C3	3.44	1.51	1.43
2	A	2004	NAG	C2-N2	3.61	1.52	1.46
2	A	2000	NAG	C1-C2	3.99	1.57	1.53
2	A	2004	NAG	C1-C2	4.20	1.58	1.52
2	A	2003	BDP	C4-C3	4.34	1.63	1.52
2	A	2002	NAG	C1-C2	4.56	1.58	1.52
2	A	2000	NAG	C2-N2	5.00	1.54	1.45
2	A	2002	NAG	O5-C1	5.17	1.52	1.43
2	A	2004	NAG	O5-C1	5.28	1.52	1.43
2	A	2000	NAG	O5-C1	5.34	1.53	1.43
2	A	2003	BDP	C4-C5	6.02	1.66	1.53
2	A	2001	BDP	C4-C5	7.00	1.68	1.53
2	A	2005	BDP	O5-C5	9.83	1.53	1.43
2	A	2001	BDP	O5-C5	13.88	1.57	1.43
2	A	2003	BDP	O5-C5	14.14	1.57	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2005	BDP	C1-C2-C3	-5.39	103.17	109.54
2	A	2003	BDP	O5-C5-C4	-4.03	101.95	108.79
2	A	2001	BDP	O5-C5-C4	-3.92	102.13	108.79
2	A	2003	BDP	O4-C4-C5	-3.61	103.62	110.42
2	A	2005	BDP	O5-C1-C2	-2.83	106.27	110.86
2	A	2002	NAG	C8-C7-N2	-2.60	111.14	116.11
2	A	2002	NAG	C4-C3-C2	-2.59	107.21	111.23
2	A	2005	BDP	O3-C3-C2	-2.40	105.66	110.00
2	A	2002	NAG	O3-C3-C4	-2.23	105.33	110.34
2	A	2004	NAG	C8-C7-N2	-2.20	111.90	116.11
2	A	2000	NAG	C8-C7-N2	-2.15	111.99	116.11
2	A	2003	BDP	O3-C3-C2	-2.14	106.13	110.00
2	A	2002	NAG	C2-N2-C7	-2.12	120.31	123.04
2	A	2001	BDP	C2-C3-C4	-2.02	107.62	111.04
2	A	2005	BDP	C1-O5-C5	2.15	115.15	111.84
2	A	2002	NAG	O7-C7-N2	2.16	126.26	121.86
2	A	2000	NAG	O7-C7-N2	2.31	126.58	121.86
2	A	2001	BDP	C6-C5-C4	2.38	119.73	113.00
2	A	2002	NAG	O3-C3-C2	2.42	113.90	109.11
2	A	2001	BDP	C3-C4-C5	2.62	113.75	108.66
2	A	2003	BDP	O4-C4-C3	2.97	117.03	110.34
2	A	2005	BDP	C6-C5-C4	3.61	123.20	113.00
2	A	2005	BDP	O4-C4-C5	4.36	118.62	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2003	BDP	C1-O5-C5	5.28	119.98	111.84
2	A	2001	BDP	C1-O5-C5	5.55	120.38	111.84
2	A	2005	BDP	O4-C4-C3	7.90	128.12	110.34
2	A	2005	BDP	O5-C5-C4	8.71	123.57	108.79
2	A	2005	BDP	C2-C3-C4	12.29	131.92	111.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2005	BDP	C4

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2000	NAG	2	0
2	A	2003	BDP	1	0
2	A	2004	NAG	4	0
2	A	2005	BDP	1	0

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	794/814 (97%)	-0.26	3 (0%)	93	93	17, 34, 53, 72	176 (22%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	722	ALA	2.3
1	A	226	THR	2.3
1	A	947	ASN	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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	BDP	A	2003	12/13	0.09	0.68	51.88	92,100,100,100	0
2	BDP	A	2005	12/13	0.38	0.54	28.07	91,100,100,100	0
2	BDP	A	2001	12/13	0.27	0.46	9.57	95,100,100,100	0
2	NAG	A	2002	14/15	0.61	0.43	9.18	90,98,100,100	0
2	NAG	A	2004	14/15	0.35	0.52	-	100,100,100,100	0
2	NAG	A	2000	15/15	0.32	0.45	-	75,97,100,100	0

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.