Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:02 PM GMT

PDB ID	:	1N7R
Title	:	Streptococcus pneumoniae Hyaluronate Lyase W291A/W292A/F343V Mutant complex with hexasaccharide hyaluronan
Authors	:	Nukui, M.; Taylor, K.B.; McPherson, D.T.; Shigenaga, M.; Jedrzejas, M.J.
Deposited on	:	2002-11-16
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:

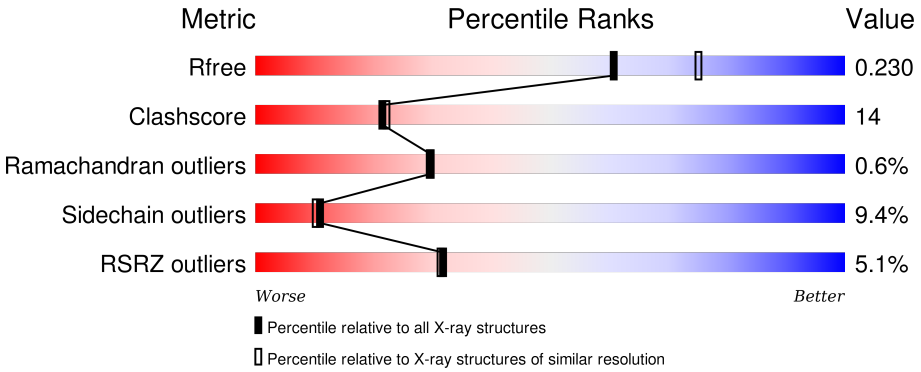
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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	721	5% 74% 21%

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BDP	A	1001	-	-	-	X
2	NAG	A	1002	-	-	X	X
2	BDP	A	1003	-	-	-	X
2	NAG	A	1004	-	-	X	X
2	BDP	A	1005	X	-	X	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6332 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 HYALURONIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	721	Total	C	N	O	S	0	0	0
			5762	3618	966	1156	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	ALA	TRP	ENGINEERED	GB 437705
A	292	ALA	TRP	ENGINEERED	GB 437705
A	343	VAL	PHE	ENGINEERED	GB 437705
A	731	VAL	GLY	SEE REMARK 999	GB 437705

- 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.

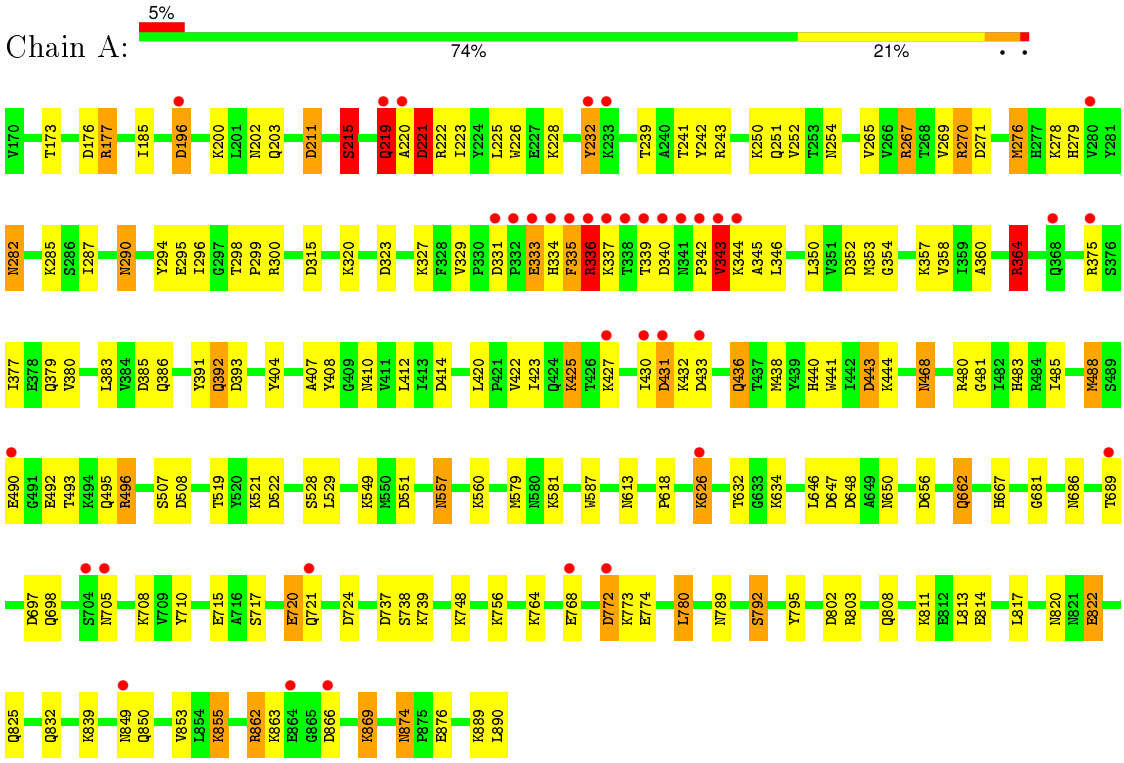
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	491	Total	O	0	0
			491	491		

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: HYALURONIDASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.49Å 102.49Å 103.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.21	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.20) 99.8 (20.00-2.21)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.21	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.21Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.177 , 0.222 0.189 , 0.230	Depositor DCC
R_{free} test set	937 reflections (2.09%)	DCC
Wilson B-factor (Å^2)	29.7	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.2	EDS
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 45691 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6332	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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	1.31	19/5876 (0.3%)	1.21	39/7935 (0.5%)

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
1	A	0	4
2	A	1	0
All	All	1	4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	792	SER	CB-OG	-9.85	1.29	1.42
1	A	267	ARG	CG-CD	8.57	1.73	1.51
1	A	267	ARG	NE-CZ	7.57	1.42	1.33
1	A	276	MET	SD-CE	-6.79	1.39	1.77
1	A	587	TRP	CB-CG	6.62	1.62	1.50
1	A	507	SER	CB-OG	6.41	1.50	1.42
1	A	795	TYR	CD2-CE2	-6.32	1.29	1.39
1	A	242	TYR	CD2-CE2	-6.10	1.30	1.39
1	A	632	THR	CA-CB	6.05	1.69	1.53
1	A	267	ARG	CB-CG	6.02	1.68	1.52
1	A	215	SER	CB-OG	-5.67	1.34	1.42
1	A	267	ARG	CD-NE	5.46	1.55	1.46
1	A	468	ASN	CB-CG	5.42	1.63	1.51
1	A	648	ASP	CG-OD1	5.35	1.37	1.25
1	A	221	ASP	CB-CG	5.34	1.62	1.51
1	A	270	ARG	CD-NE	-5.09	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	LYS	CD-CE	5.07	1.64	1.51
1	A	294	TYR	CE1-CZ	5.06	1.45	1.38
1	A	697	ASP	CB-CG	5.01	1.62	1.51

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	270	ARG	NE-CZ-NH2	-19.74	110.43	120.30
1	A	270	ARG	NE-CZ-NH1	14.16	127.38	120.30
1	A	737	ASP	CB-CG-OD2	12.57	129.61	118.30
1	A	431	ASP	CB-CG-OD2	9.62	126.96	118.30
1	A	323	ASP	CB-CG-OD2	8.84	126.25	118.30
1	A	772	ASP	CB-CG-OD2	8.42	125.88	118.30
1	A	211	ASP	CB-CG-OD2	8.25	125.73	118.30
1	A	267	ARG	NE-CZ-NH2	8.12	124.36	120.30
1	A	443	ASP	CB-CG-OD2	7.23	124.81	118.30
1	A	780	LEU	CA-CB-CG	7.12	131.68	115.30
1	A	364	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	529	LEU	CB-CG-CD2	-6.89	99.29	111.00
1	A	792	SER	N-CA-CB	-6.66	100.51	110.50
1	A	508	ASP	CB-CG-OD2	6.54	124.18	118.30
1	A	196	ASP	CB-CG-OD2	6.44	124.10	118.30
1	A	385	ASP	CB-CG-OD2	6.29	123.97	118.30
1	A	270	ARG	CD-NE-CZ	6.14	132.19	123.60
1	A	724	ASP	CB-CG-OD2	6.14	123.82	118.30
1	A	862	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	340	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	270	ARG	CG-CD-NE	-5.99	99.22	111.80
1	A	551	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	267	ARG	CA-CB-CG	5.63	125.79	113.40
1	A	331	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	176	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	221	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	648	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	802	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	866	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	656	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	352	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	393	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	648	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	647	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	271	ASP	CB-CG-OD2	5.25	123.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	697	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	780	LEU	CB-CG-CD1	5.19	119.82	111.00
1	A	522	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	315	ASP	CB-CG-OD2	5.00	122.80	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1005	BDP	C4

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	GLN	Peptide
1	A	220	ALA	Peptide
1	A	221	ASP	Peptide
1	A	270	ARG	Sidechain

5.2 Too-close contacts (i)

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	5762	0	5585	155	0
2	A	79	0	51	49	0
3	A	491	0	0	60	1
All	All	6332	0	5636	161	1

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 14.

All (161) 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:408:TYR:CE1	2:A:1002:NAG:H82	1.44	1.52
1:A:579:MET:SD	1:A:579:MET:CE	2.02	1.48
1:A:408:TYR:CZ	2:A:1002:NAG:H82	1.82	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ARG:NH2	2:A:1004:NAG:H83	1.64	1.12
1:A:358:VAL:HG22	3:A:1472:HOH:O	1.58	1.03
1:A:408:TYR:CE1	2:A:1002:NAG:C8	2.41	1.03
2:A:1002:NAG:H62	3:A:1404:HOH:O	1.55	1.02
1:A:613:ASN:H	1:A:698:GLN:HE22	1.07	1.02
1:A:243:ARG:CZ	2:A:1004:NAG:H83	1.91	0.99
1:A:243:ARG:HH12	2:A:1003:BDP:C6	1.77	0.97
1:A:483:HIS:HE1	3:A:1317:HOH:O	1.50	0.93
1:A:408:TYR:CD1	2:A:1002:NAG:H82	2.04	0.93
1:A:822:GLU:HG3	3:A:1391:HOH:O	1.70	0.90
1:A:488:MET:HB3	3:A:1435:HOH:O	1.73	0.88
1:A:243:ARG:NH1	2:A:1003:BDP:O6A	2.08	0.86
1:A:250:LYS:HZ1	2:A:1005:BDP:C3	1.88	0.86
1:A:773:LYS:HE3	3:A:1462:HOH:O	1.75	0.86
1:A:243:ARG:HD3	2:A:1004:NAG:C8	2.07	0.84
1:A:267:ARG:HD2	3:A:1280:HOH:O	1.76	0.84
1:A:278:LYS:HG3	1:A:279:HIS:HD2	1.44	0.82
1:A:408:TYR:CZ	2:A:1002:NAG:C8	2.62	0.81
1:A:267:ARG:CD	3:A:1280:HOH:O	2.27	0.81
1:A:243:ARG:HD3	2:A:1004:NAG:H82	1.65	0.79
1:A:243:ARG:CZ	2:A:1004:NAG:C8	2.64	0.76
1:A:890:LEU:CB	3:A:1470:HOH:O	2.33	0.75
1:A:811:LYS:HG3	3:A:1433:HOH:O	1.86	0.75
1:A:241:THR:HG21	1:A:276:MET:HE3	1.68	0.75
1:A:278:LYS:HG3	1:A:279:HIS:CD2	2.21	0.74
1:A:336:ARG:HH12	2:A:1000:NAG:H4	1.52	0.73
1:A:626:LYS:NZ	3:A:1452:HOH:O	2.15	0.73
1:A:185:ILE:O	2:A:1005:BDP:O4	2.06	0.72
1:A:890:LEU:C	3:A:1363:HOH:O	2.26	0.72
1:A:241:THR:HG21	1:A:276:MET:CE	2.20	0.72
1:A:414:ASP:OD2	2:A:1004:NAG:C6	2.38	0.72
1:A:243:ARG:CD	2:A:1004:NAG:H82	2.23	0.68
1:A:221:ASP:HB3	3:A:1425:HOH:O	1.93	0.68
1:A:440:HIS:HE1	3:A:1434:HOH:O	1.77	0.67
1:A:557:ASN:C	1:A:557:ASN:HD22	1.98	0.67
1:A:414:ASP:OD2	2:A:1004:NAG:H61	1.95	0.67
1:A:720:GLU:HG3	3:A:1412:HOH:O	1.94	0.67
2:A:1004:NAG:O4	3:A:1486:HOH:O	2.12	0.66
1:A:243:ARG:HH21	2:A:1004:NAG:H83	1.60	0.66
1:A:650:ASN:HD21	1:A:832:GLN:HE22	1.43	0.66
1:A:360:ALA:O	1:A:364:ARG:HG3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ARG:HH22	2:A:1004:NAG:H4	1.61	0.65
1:A:354:GLY:HA3	1:A:377:ILE:HD11	1.79	0.65
1:A:243:ARG:NH1	2:A:1003:BDP:C6	2.56	0.65
1:A:756:LYS:HE3	3:A:1442:HOH:O	1.97	0.64
1:A:708:LYS:HE3	1:A:715:GLU:OE2	1.98	0.64
1:A:839:LYS:HD2	1:A:853:VAL:HG23	1.79	0.63
1:A:560:LYS:HD3	3:A:1054:HOH:O	1.98	0.63
1:A:243:ARG:CD	2:A:1004:NAG:C8	2.75	0.62
1:A:203:GLN:HG2	3:A:1438:HOH:O	1.99	0.62
1:A:232:TYR:HB3	3:A:1314:HOH:O	1.99	0.62
1:A:408:TYR:CD1	2:A:1002:NAG:C8	2.79	0.61
1:A:519:THR:CG2	2:A:1005:BDP:C6	2.80	0.59
2:A:1002:NAG:H4	3:A:1404:HOH:O	2.02	0.58
1:A:243:ARG:NE	2:A:1004:NAG:C8	2.67	0.58
1:A:444:LYS:NZ	3:A:1118:HOH:O	2.36	0.57
1:A:219:GLN:C	3:A:1339:HOH:O	2.42	0.57
1:A:392:GLN:HG2	3:A:1099:HOH:O	2.05	0.57
1:A:243:ARG:NH1	2:A:1004:NAG:HN2	2.03	0.57
1:A:221:ASP:HB3	3:A:1455:HOH:O	2.05	0.57
1:A:850:GLN:HE21	1:A:863:LYS:HE3	1.70	0.56
1:A:278:LYS:HB3	3:A:1451:HOH:O	2.06	0.56
1:A:225:LEU:HD12	1:A:276:MET:HE3	1.86	0.56
1:A:557:ASN:ND2	1:A:560:LYS:H	2.03	0.56
1:A:290:ASN:ND2	3:A:1250:HOH:O	2.39	0.55
1:A:215:SER:HB3	1:A:226:TRP:CD1	2.42	0.55
1:A:436:GLN:HE21	1:A:436:GLN:N	2.03	0.55
1:A:414:ASP:OD2	2:A:1004:NAG:O6	2.25	0.55
1:A:423:ILE:HG21	1:A:430:ILE:HD12	1.88	0.55
2:A:1002:NAG:C5	3:A:1404:HOH:O	2.56	0.54
1:A:391:TYR:CD2	1:A:549:LYS:HG3	2.42	0.54
1:A:519:THR:HG23	2:A:1005:BDP:O6B	2.07	0.54
1:A:336:ARG:HH22	2:A:1000:NAG:H62	1.73	0.54
1:A:483:HIS:CE1	3:A:1408:HOH:O	2.60	0.54
1:A:243:ARG:CZ	2:A:1004:NAG:HN2	2.21	0.54
1:A:336:ARG:NH1	2:A:1000:NAG:H4	2.22	0.53
1:A:250:LYS:NZ	3:A:1181:HOH:O	2.25	0.52
1:A:343:VAL:HG13	1:A:344:LYS:N	2.24	0.52
1:A:443:ASP:OD2	1:A:496:ARG:NH2	2.43	0.52
1:A:855:LYS:CG	3:A:1465:HOH:O	2.57	0.52
1:A:285:LYS:O	1:A:327:LYS:NZ	2.43	0.51
2:A:1002:NAG:C6	3:A:1404:HOH:O	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:LEU:CB	3:A:1454:HOH:O	2.59	0.51
1:A:521:LYS:HD2	3:A:1479:HOH:O	2.11	0.51
1:A:689:THR:HA	3:A:1474:HOH:O	2.10	0.51
1:A:720:GLU:CG	3:A:1412:HOH:O	2.55	0.51
1:A:820:ASN:HD22	1:A:825:GLN:HG2	1.75	0.50
1:A:200:LYS:CE	3:A:1453:HOH:O	2.59	0.50
1:A:579:MET:CE	1:A:579:MET:CG	2.89	0.50
1:A:296:ILE:HD11	1:A:335:PHE:CZ	2.47	0.50
1:A:343:VAL:HG21	3:A:1480:HOH:O	2.11	0.49
1:A:557:ASN:ND2	1:A:557:ASN:C	2.64	0.49
1:A:350:LEU:HD21	1:A:379:GLN:HG2	1.93	0.49
1:A:874:ASN:HD22	1:A:874:ASN:C	2.15	0.49
1:A:689:THR:HG22	3:A:1474:HOH:O	2.13	0.49
1:A:354:GLY:CA	1:A:377:ILE:HD11	2.42	0.49
1:A:581:LYS:HB3	1:A:768:GLU:HB2	1.95	0.49
1:A:686:ASN:H	1:A:789:ASN:ND2	2.11	0.49
1:A:346:LEU:HD21	3:A:1244:HOH:O	2.12	0.48
1:A:822:GLU:CG	3:A:1391:HOH:O	2.45	0.48
1:A:334:HIS:O	3:A:1212:HOH:O	2.20	0.48
1:A:295:GLU:OE2	1:A:336:ARG:HA	2.13	0.48
1:A:764:LYS:HD2	1:A:772:ASP:HB3	1.95	0.48
1:A:874:ASN:HD22	1:A:876:GLU:H	1.63	0.47
1:A:241:THR:HG21	1:A:276:MET:HE1	1.97	0.47
1:A:483:HIS:CE1	3:A:1317:HOH:O	2.39	0.47
1:A:250:LYS:NZ	2:A:1005:BDP:C3	2.70	0.47
1:A:329:VAL:HG12	1:A:357:LYS:HD2	1.95	0.47
1:A:335:PHE:CZ	1:A:353:MET:HB2	2.49	0.47
1:A:689:THR:CB	3:A:1474:HOH:O	2.62	0.47
1:A:243:ARG:NE	2:A:1004:NAG:H83	2.26	0.47
1:A:890:LEU:CA	3:A:1363:HOH:O	2.62	0.47
1:A:667:HIS:O	1:A:681:GLY:HA2	2.15	0.46
2:A:1002:NAG:C4	3:A:1404:HOH:O	2.63	0.46
1:A:855:LYS:CD	3:A:1465:HOH:O	2.63	0.46
1:A:412:LEU:C	1:A:412:LEU:HD23	2.36	0.46
1:A:282:ASN:HD22	1:A:282:ASN:C	2.19	0.46
1:A:243:ARG:NE	2:A:1004:NAG:H82	2.29	0.46
1:A:667:HIS:HE1	3:A:1326:HOH:O	1.99	0.45
1:A:250:LYS:NZ	2:A:1005:BDP:C4	2.80	0.45
1:A:869:LYS:HE2	3:A:1487:HOH:O	2.16	0.45
1:A:412:LEU:HD21	1:A:441:TRP:CZ3	2.52	0.45
1:A:346:LEU:HB2	3:A:1342:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLU:C	1:A:296:ILE:HD13	2.36	0.45
1:A:267:ARG:HD3	3:A:1280:HOH:O	2.06	0.45
1:A:646:LEU:HD21	1:A:862:ARG:HB2	1.99	0.44
1:A:221:ASP:OD1	1:A:222:ARG:NH1	2.51	0.44
1:A:634:LYS:HD3	3:A:1209:HOH:O	2.17	0.44
1:A:739:LYS:HE2	3:A:1289:HOH:O	2.18	0.44
1:A:480:ARG:NH2	2:A:1004:NAG:H61	2.33	0.44
1:A:343:VAL:HG21	2:A:1000:NAG:H61	2.00	0.44
1:A:425:LYS:HE2	3:A:1491:HOH:O	2.18	0.43
1:A:440:HIS:CE1	3:A:1434:HOH:O	2.60	0.43
1:A:265:VAL:O	1:A:269:VAL:HG23	2.19	0.43
1:A:408:TYR:CZ	2:A:1002:NAG:C7	3.01	0.43
1:A:343:VAL:CG2	3:A:1480:HOH:O	2.67	0.43
1:A:407:ALA:O	1:A:410:ASN:HB2	2.18	0.43
1:A:211:ASP:O	1:A:215:SER:HB2	2.19	0.43
1:A:618:PRO:HG3	3:A:1037:HOH:O	2.19	0.42
1:A:173:THR:HG22	3:A:1359:HOH:O	2.18	0.42
1:A:202:ASN:ND2	1:A:251:GLN:HE22	2.16	0.42
1:A:386:GLN:NE2	3:A:1396:HOH:O	2.52	0.42
1:A:298:THR:HB	1:A:299:PRO:HD3	2.02	0.42
1:A:480:ARG:HH21	2:A:1004:NAG:H61	1.83	0.42
1:A:333:GLU:O	1:A:345:ALA:HB3	2.20	0.42
1:A:710:TYR:CE2	1:A:803:ARG:NH1	2.87	0.42
1:A:177:ARG:HG3	1:A:422:VAL:HG13	2.02	0.42
1:A:243:ARG:NH1	2:A:1004:NAG:N2	2.68	0.41
1:A:243:ARG:CD	2:A:1004:NAG:H83	2.49	0.41
1:A:287:ILE:HD12	1:A:339:THR:CG2	2.51	0.41
1:A:481:GLY:O	1:A:485:ILE:HG12	2.21	0.41
1:A:250:LYS:HE3	2:A:1005:BDP:O3	2.21	0.41
1:A:549:LYS:HE2	3:A:1426:HOH:O	2.21	0.41
1:A:343:VAL:HG11	2:A:1000:NAG:H62	2.02	0.41
1:A:420:LEU:HD23	1:A:420:LEU:HA	1.93	0.41
1:A:241:THR:CG2	1:A:276:MET:HE3	2.46	0.41
1:A:874:ASN:ND2	1:A:876:GLU:H	2.18	0.40
1:A:662:GLN:HE21	1:A:662:GLN:HB2	1.63	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1240:HOH:O	3:A:1480:HOH:O[4_446]	2.05	0.15

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	719/721 (100%)	679 (94%)	36 (5%)	4 (1%)	30 29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	GLN
1	A	342	PRO
1	A	336	ARG
1	A	343	VAL

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	636/638 (100%)	576 (91%)	60 (9%)	11 10

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	ARG
1	A	196	ASP
1	A	215	SER
1	A	219	GLN
1	A	223	ILE
1	A	232	TYR
1	A	239	THR

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Mol	Chain	Res	Type
1	A	252	VAL
1	A	254	ASN
1	A	282	ASN
1	A	290	ASN
1	A	320	LYS
1	A	333	GLU
1	A	335	PHE
1	A	336	ARG
1	A	337	LYS
1	A	343	VAL
1	A	364	ARG
1	A	375	ARG
1	A	380	VAL
1	A	383	LEU
1	A	392	GLN
1	A	404	TYR
1	A	425	LYS
1	A	427	LYS
1	A	431	ASP
1	A	432	LYS
1	A	433	ASP
1	A	436	GLN
1	A	438	MET
1	A	468	ASN
1	A	488	MET
1	A	490	GLU
1	A	492	GLU
1	A	493	THR
1	A	495	GLN
1	A	496	ARG
1	A	528	SER
1	A	557	ASN
1	A	626	LYS
1	A	662	GLN
1	A	705	ASN
1	A	717	SER
1	A	720	GLU
1	A	721	GLN
1	A	738	SER
1	A	748	LYS
1	A	774	GLU
1	A	780	LEU

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Mol	Chain	Res	Type
1	A	792	SER
1	A	808	GLN
1	A	813	LEU
1	A	814	GLU
1	A	817	LEU
1	A	822	GLU
1	A	849	ASN
1	A	855	LYS
1	A	869	LYS
1	A	874	ASN
1	A	889	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	254	ASN
1	A	279	HIS
1	A	282	ASN
1	A	341	ASN
1	A	349	ASN
1	A	436	GLN
1	A	557	ASN
1	A	580	ASN
1	A	662	GLN
1	A	667	HIS
1	A	698	GLN
1	A	759	GLN
1	A	789	ASN
1	A	820	ASN
1	A	825	GLN
1	A	832	GLN
1	A	850	GLN
1	A	874	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	1000	2	15,15,15	2.24	6 (40%)	17,21,21	0.90	0
2	BDP	A	1001	1,2	9,12,13	4.45	3 (33%)	13,17,19	2.66	7 (53%)
2	NAG	A	1002	2	14,14,15	2.29	6 (42%)	15,19,21	1.03	0
2	BDP	A	1003	2	9,12,13	4.35	5 (55%)	13,17,19	2.86	6 (46%)
2	NAG	A	1004	2	14,14,15	2.43	7 (50%)	15,19,21	1.21	3 (20%)
2	BDP	A	1005	2	9,12,13	6.85	3 (33%)	13,17,19	5.41	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	1000	2	-	0/6/26/26	0/1/1/1
2	BDP	A	1001	1,2	-	0/0/21/24	0/1/1/1
2	NAG	A	1002	2	-	0/6/23/26	0/1/1/1
2	BDP	A	1003	2	-	0/0/21/24	0/1/1/1
2	NAG	A	1004	2	-	0/6/23/26	0/1/1/1
2	BDP	A	1005	2	1/1/5/6	0/0/21/24	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1005	BDP	O4-C4	-14.99	1.07	1.43
2	A	1005	BDP	C4-C5	-7.87	1.36	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1004	NAG	O3-C3	2.01	1.47	1.43
2	A	1004	NAG	C4-C3	2.08	1.57	1.52
2	A	1002	NAG	C3-C2	2.13	1.57	1.52
2	A	1000	NAG	O5-C5	2.29	1.50	1.44
2	A	1000	NAG	C3-C2	2.29	1.57	1.53
2	A	1003	BDP	O4-C4	2.35	1.48	1.43
2	A	1002	NAG	C4-C5	2.50	1.58	1.53
2	A	1002	NAG	C2-N2	2.53	1.50	1.46
2	A	1000	NAG	C4-C5	2.77	1.59	1.53
2	A	1003	BDP	O5-C1	2.82	1.48	1.43
2	A	1002	NAG	O5-C5	2.92	1.49	1.43
2	A	1004	NAG	O5-C5	2.97	1.50	1.43
2	A	1000	NAG	C1-C2	3.05	1.56	1.53
2	A	1001	BDP	C2-C3	3.09	1.56	1.52
2	A	1002	NAG	C1-C2	3.11	1.56	1.52
2	A	1004	NAG	C4-C5	3.30	1.60	1.53
2	A	1003	BDP	C2-C3	3.41	1.57	1.52
2	A	1004	NAG	C1-C2	3.42	1.57	1.52
2	A	1004	NAG	C2-N2	3.49	1.52	1.46
2	A	1000	NAG	C2-N2	4.05	1.52	1.45
2	A	1004	NAG	O5-C1	4.57	1.51	1.43
2	A	1000	NAG	O5-C1	4.59	1.51	1.43
2	A	1003	BDP	C4-C5	4.77	1.63	1.53
2	A	1002	NAG	O5-C1	5.30	1.52	1.43
2	A	1001	BDP	C4-C5	6.23	1.66	1.53
2	A	1003	BDP	O5-C5	10.72	1.54	1.43
2	A	1001	BDP	O5-C5	10.85	1.54	1.43
2	A	1005	BDP	O5-C5	11.40	1.54	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1003	BDP	O4-C4-C5	-5.50	100.06	110.42
2	A	1005	BDP	O5-C1-C2	-4.74	103.16	110.86
2	A	1005	BDP	C1-C2-C3	-4.35	104.40	109.54
2	A	1001	BDP	O4-C4-C5	-4.09	102.72	110.42
2	A	1001	BDP	O5-C5-C4	-3.33	103.13	108.79
2	A	1003	BDP	O5-C5-C4	-2.97	103.74	108.79
2	A	1001	BDP	C2-C3-C4	-2.76	106.35	111.04
2	A	1005	BDP	O3-C3-C2	-2.55	105.39	110.00
2	A	1004	NAG	C4-C3-C2	-2.51	107.32	111.23
2	A	1004	NAG	C8-C7-N2	-2.15	111.99	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1003	BDP	C2-C3-C4	-2.00	107.64	111.04
2	A	1004	NAG	O7-C7-N2	2.18	126.31	121.86
2	A	1005	BDP	C1-O5-C5	2.35	115.47	111.84
2	A	1001	BDP	C3-C4-C5	2.59	113.68	108.66
2	A	1003	BDP	C3-C4-C5	2.69	113.87	108.66
2	A	1001	BDP	C6-C5-C4	2.80	120.90	113.00
2	A	1001	BDP	O4-C4-C3	2.95	116.99	110.34
2	A	1005	BDP	C6-C5-C4	3.01	121.50	113.00
2	A	1003	BDP	O4-C4-C3	3.77	118.83	110.34
2	A	1005	BDP	O4-C4-C5	4.71	119.28	110.42
2	A	1001	BDP	C1-O5-C5	5.66	120.56	111.84
2	A	1003	BDP	C1-O5-C5	5.78	120.75	111.84
2	A	1005	BDP	O4-C4-C3	7.61	127.46	110.34
2	A	1005	BDP	O5-C5-C4	8.86	123.82	108.79
2	A	1005	BDP	C2-C3-C4	12.50	132.27	111.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1005	BDP	C4

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	NAG	5	0
2	A	1002	NAG	12	0
2	A	1003	BDP	3	0
2	A	1004	NAG	22	0
2	A	1005	BDP	7	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

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	721/721 (100%)	-0.02	37 (5%) 32 31	20, 31, 56, 110	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	HIS	10.3
1	A	342	PRO	8.6
1	A	344	LYS	8.1
1	A	341	ASN	6.5
1	A	338	THR	6.0
1	A	335	PHE	5.8
1	A	339	THR	5.7
1	A	336	ARG	5.5
1	A	340	ASP	5.2
1	A	343	VAL	5.2
1	A	332	PRO	4.9
1	A	333	GLU	4.7
1	A	219	GLN	4.5
1	A	232	TYR	4.4
1	A	704	SER	4.3
1	A	337	LYS	4.2
1	A	431	ASP	3.3
1	A	427	LYS	3.3
1	A	721	GLN	3.0
1	A	849	ASN	3.0
1	A	866	ASP	2.7
1	A	705	ASN	2.5
1	A	490	GLU	2.5
1	A	233	LYS	2.5
1	A	220	ALA	2.4
1	A	768	GLU	2.4
1	A	196	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	433	ASP	2.3
1	A	689	THR	2.3
1	A	368	GLN	2.3
1	A	772	ASP	2.2
1	A	280	VAL	2.2
1	A	375	ARG	2.2
1	A	626	LYS	2.2
1	A	331	ASP	2.1
1	A	430	ILE	2.1
1	A	864	GLU	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
2	BDP	A	1003	12/13	0.00	0.73	23.75	88,91,94,95	0
2	NAG	A	1002	14/15	0.41	0.71	16.85	81,87,88,90	0
2	BDP	A	1005	12/13	0.78	0.48	13.97	92,94,94,95	0
2	NAG	A	1004	14/15	0.52	0.54	13.42	86,89,91,92	0
2	BDP	A	1001	12/13	0.44	0.48	6.04	81,87,90,91	0
2	NAG	A	1000	15/15	0.15	0.67	1.47	94,96,97,97	0

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.