Full wwPDB X-ray Structure Validation Report

Nov 13, 2016 – 04:51 AM EST

PDB ID	:	5KXD
Title	:	Wisteria floribunda lectin in complex with GalNAc(beta1-4)GlcNAc (LacdiNAc) at pH 6.5
Authors	:	Evans, S.V.; Haji-Ghassemi, O.
Deposited on	:	2016-07-20
Resolution	:	1.95 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 ⓘ symbol.

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

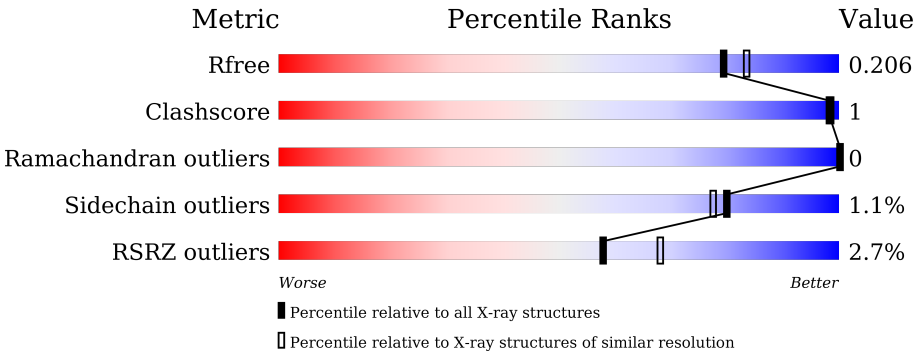
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

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 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	243	2% 94%
1	B	243	3% 96%
1	C	243	3% 92% 5%
1	D	243	2% 95%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	6Y2	A	306	-	-	-	X
7	6Y2	C	312	-	-	-	X

2 Entry composition

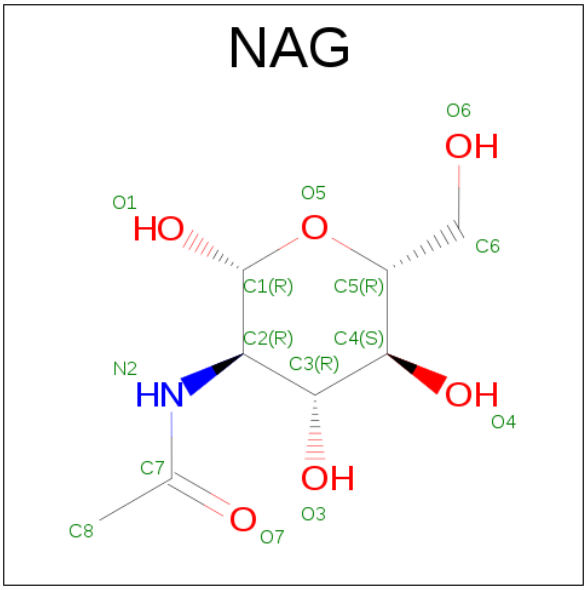
There are 11 unique types of molecules in this entry. The entry contains 8367 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Wisteria floribunda agglutinin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	0	0	0
			1851	1179	304	368			
1	B	238	Total	C	N	O	0	0	0
			1851	1179	304	368			
1	C	238	Total	C	N	O	0	0	0
			1851	1179	304	368			
1	D	238	Total	C	N	O	0	0	0
			1851	1179	304	368			

- Molecule 2 is 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	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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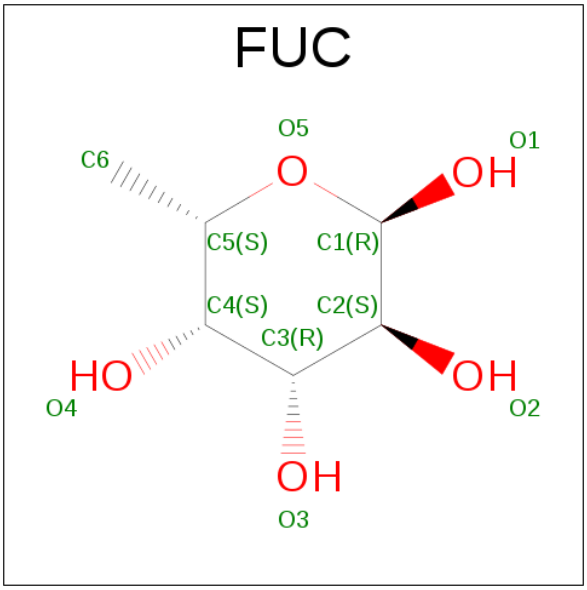
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 6 4	0	0
3	C	1	Total C O 10 6 4	0	0
3	D	1	Total C O 10 6 4	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0
4	A	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0

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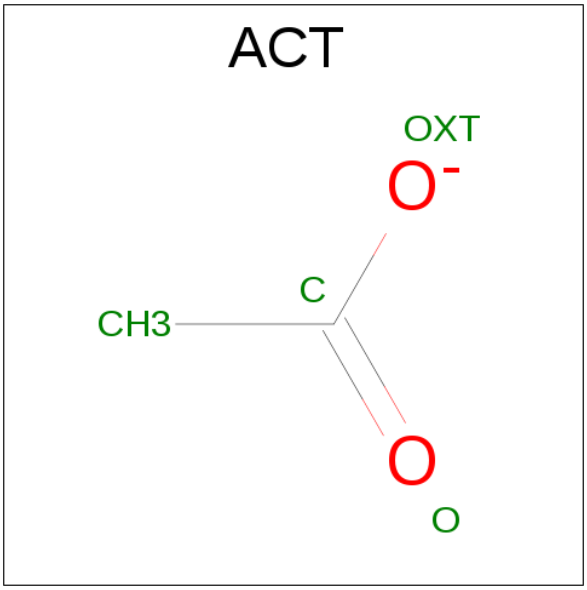
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Ca 1 1	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mn 1 1	0	0
5	A	1	Total Mn 1 1	0	0
5	D	1	Total Mn 1 1	0	0
5	C	1	Total Mn 1 1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0

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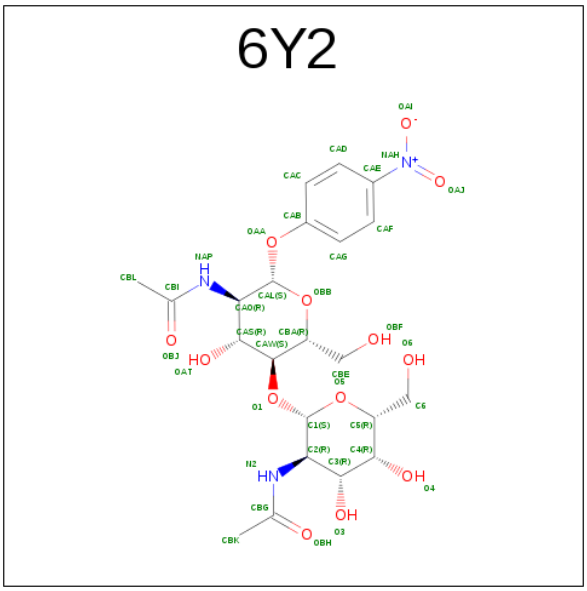
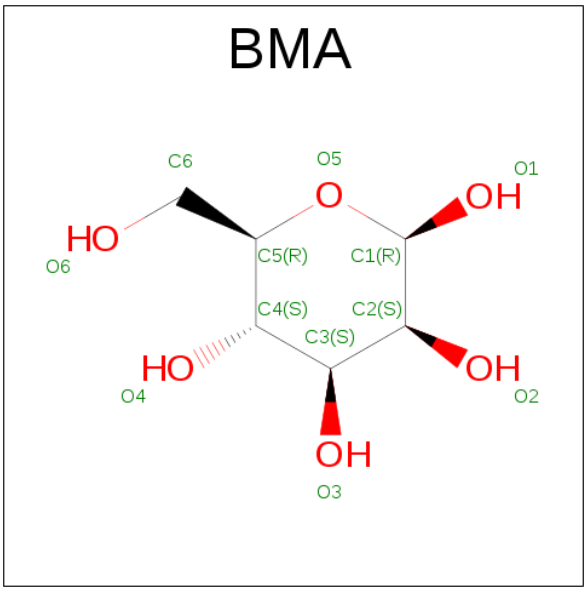
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0

- Molecule 7 is {N}-[(2 {S},3 {R},4 {R},5 {R},6 {R})-2-[(2 {R},3 {S},4 {R},5 {R},6 {S})-5-acetamido-2-(hydroxymethyl)-6-(4-nitrophenoxy)-4-oxidanyl-oxan-3-yl]oxy-6-(hydroxymethyl)-4,5-bis(oxidanyl)oxan-3-yl]ethanamide (three-letter code: 6Y2) (formula: $C_{22}H_{31}N_3O_{13}$).



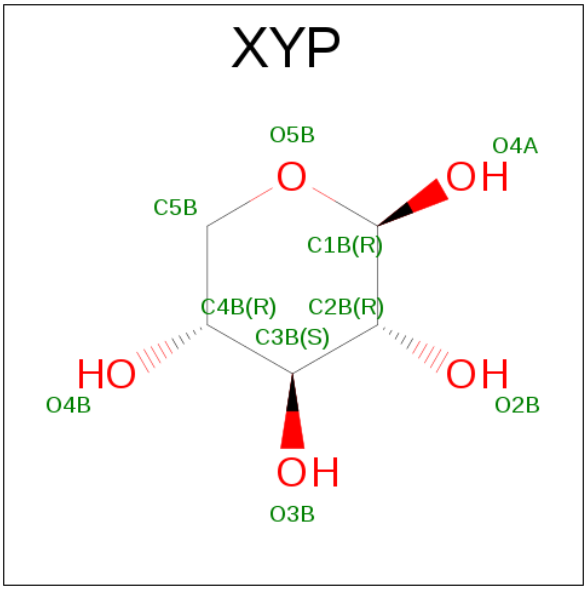
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 38 22 3 13	0	0
7	B	1	Total C N O 38 22 3 13	0	0
7	C	1	Total C N O 38 22 3 13	0	0
7	D	1	Total C N O 38 22 3 13	0	0

- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



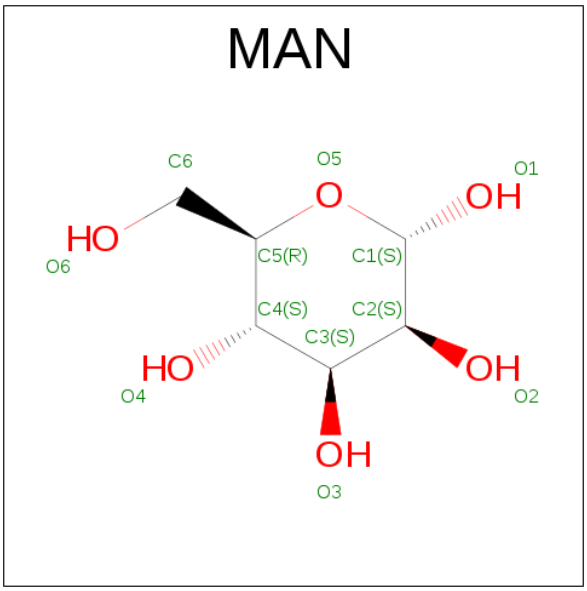
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 11 6 5	0	0

- Molecule 9 is BETA-D-XYLOPYRANOSE (three-letter code: XYP) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O 9 5 4	0	0

- Molecule 10 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total C O 11 6 5	0	0
10	C	1	Total C O 11 6 5	0	0

- Molecule 11 is water.

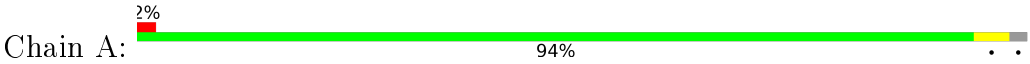
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	179	Total O 179 179	0	0
11	B	165	Total O 165 165	0	0
11	C	163	Total O 163 163	0	0
11	D	130	Total O 130 130	0	0

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.

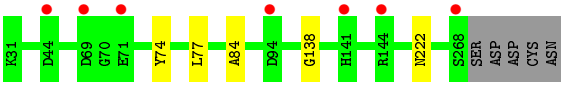
- Molecule 1: Wisteria floribunda agglutinin

Chain A:



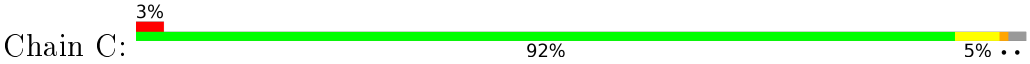
- Molecule 1: Wisteria floribunda agglutinin

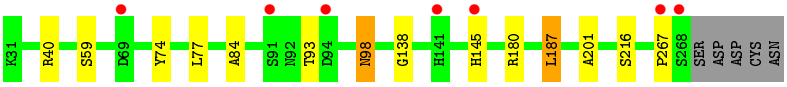
Chain B:



- Molecule 1: Wisteria floribunda agglutinin

Chain C:





- Molecule 1: Wisteria floribunda agglutinin

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.10Å 104.27Å 148.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95 24.85 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-1.95) 98.2 (24.85-1.95)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.77 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.179 , 0.198 0.188 , 0.206	Depositor DCC
R_{free} test set	4358 reflections (5.19%)	DCC
Wilson B-factor (Å^2)	19.0	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.0	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	8367	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: 6Y2, XYP, BMA, NAG, CA, MN, FUC, ACT, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.55	0/1899	0.75	2/2599 (0.1%)
1	B	0.54	0/1899	0.71	0/2599
1	C	0.55	0/1899	0.78	3/2599 (0.1%)
1	D	0.52	0/1899	0.72	1/2599 (0.0%)
All	All	0.54	0/7596	0.74	6/10396 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	180	ARG	CG-CD-NE	-7.58	95.88	111.80
1	C	187	LEU	CB-CG-CD1	-7.26	98.66	111.00
1	C	40	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	C	180	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	D	40	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	180	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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	1851	0	1781	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1851	0	1781	4	0
1	C	1851	0	1781	7	0
1	D	1851	0	1781	2	0
2	A	14	0	12	0	0
2	B	14	0	13	0	0
2	C	28	0	23	0	0
2	D	14	0	12	0	0
3	A	10	0	10	0	0
3	C	10	0	10	0	0
3	D	10	0	10	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	4	0	3	0	0
6	B	4	0	3	0	0
6	C	8	0	6	0	0
6	D	8	0	6	1	0
7	A	38	0	0	0	0
7	B	38	0	0	0	0
7	C	38	0	0	0	0
7	D	38	0	0	0	0
8	C	11	0	7	0	0
9	C	9	0	8	0	0
10	C	22	0	20	0	0
11	A	179	0	0	1	1
11	B	165	0	0	0	0
11	C	163	0	0	0	2
11	D	130	0	0	1	0
All	All	8367	0	7267	14	2

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 1.

All (14) 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:C:93:THR:HB	1:C:267:PRO:HG3	1.82	0.61
6:D:305:ACT:H1	11:D:509:HOH:O	2.06	0.55
1:A:186:ASP:OD2	11:A:401:HOH:O	2.19	0.52
1:A:84:ALA:HB2	1:B:84:ALA:HB2	1.92	0.52
1:A:98:ASN:ND2	1:A:201:ALA:H	2.09	0.50
1:C:84:ALA:HB2	1:D:84:ALA:HB2	1.94	0.49
1:C:98:ASN:ND2	1:C:201:ALA:H	2.11	0.48
1:B:77:LEU:HD11	1:B:138:GLY:HA3	1.97	0.47
1:C:77:LEU:HD11	1:C:138:GLY:HA3	1.97	0.47
1:B:222:ASN:HD21	1:C:216:SER:HA	1.79	0.47
1:A:77:LEU:HD11	1:A:138:GLY:HA3	1.97	0.46
1:B:222:ASN:ND2	1:C:216:SER:HA	2.33	0.43
1:D:77:LEU:HD11	1:D:138:GLY:HA3	2.00	0.43
1:C:145:HIS:O	1:C:145:HIS:ND1	2.54	0.41

All (2) 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)
11:C:496:HOH:O	11:C:535:HOH:O[4_555]	2.04	0.16
11:A:420:HOH:O	11:C:409:HOH:O[3_544]	2.13	0.07

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	236/243 (97%)	232 (98%)	4 (2%)	0	100	100
1	B	236/243 (97%)	232 (98%)	4 (2%)	0	100	100
1	C	236/243 (97%)	231 (98%)	5 (2%)	0	100	100
1	D	236/243 (97%)	232 (98%)	4 (2%)	0	100	100
All	All	944/972 (97%)	927 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	210/215 (98%)	208 (99%)	2 (1%)	82 80
1	B	210/215 (98%)	209 (100%)	1 (0%)	92 91
1	C	210/215 (98%)	206 (98%)	4 (2%)	65 58
1	D	210/215 (98%)	208 (99%)	2 (1%)	82 80
All	All	840/860 (98%)	831 (99%)	9 (1%)	80 77

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	TYR
1	A	222	ASN
1	B	74	TYR
1	C	59	SER
1	C	74	TYR
1	C	98	ASN
1	C	187	LEU
1	D	74	TYR
1	D	92	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	145	HIS
1	A	222	ASN
1	B	175	ASN
1	B	222	ASN
1	C	61	HIS
1	C	98	ASN
1	D	173	ASN

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Mol	Chain	Res	Type
1	D	175	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 8 are monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	301	1,3	14,14,15	0.48	0	15,19,21	1.34	1 (6%)
3	FUC	A	302	2	10,10,11	0.31	0	13,14,16	0.77	0
6	ACT	A	305	-	0,3,3	0.00	-	0,3,3	0.00	-
7	6Y2	A	306	-	38,40,40	2.29	3 (7%)	50,57,57	1.09	6 (12%)
2	NAG	B	301	1	14,14,15	0.78	1 (7%)	15,19,21	2.43	7 (46%)
6	ACT	B	304	-	0,3,3	0.00	-	0,3,3	0.00	-
7	6Y2	B	305	-	38,40,40	1.92	1 (2%)	50,57,57	1.20	4 (8%)
2	NAG	C	301	1,3,2	14,14,15	0.41	0	15,19,21	1.00	1 (6%)
3	FUC	C	302	2	10,10,11	1.21	1 (10%)	13,14,16	1.38	2 (15%)
2	NAG	C	303	8,2	14,14,15	0.46	0	15,19,21	1.09	1 (6%)
8	BMA	C	304	9,10,2	11,11,12	0.62	0	15,15,17	1.46	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	XYP	C	305	8	9,9,10	0.37	0	12,12,14	0.82	0
10	MAN	C	306	8	11,11,12	0.48	0	15,15,17	0.88	0
10	MAN	C	307	8	11,11,12	0.61	0	15,15,17	1.40	2 (13%)
6	ACT	C	310	-	0,3,3	0.00	-	0,3,3	0.00	-
6	ACT	C	311	-	0,3,3	0.00	-	0,3,3	0.00	-
7	6Y2	C	312	-	38,40,40	2.61	5 (13%)	50,57,57	1.06	2 (4%)
2	NAG	D	301	1,3	14,14,15	0.30	0	15,19,21	1.17	2 (13%)
3	FUC	D	302	2	10,10,11	0.29	0	13,14,16	0.77	0
6	ACT	D	305	-	0,3,3	0.00	-	0,3,3	0.00	-
6	ACT	D	306	-	0,3,3	0.00	-	0,3,3	0.00	-
7	6Y2	D	307	-	38,40,40	2.53	4 (10%)	50,57,57	1.10	3 (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	301	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	302	2	-	0/0/17/20	0/1/1/1
6	ACT	A	305	-	-	0/0/0/0	0/0/0/0
7	6Y2	A	306	-	-	0/24/64/64	0/3/3/3
2	NAG	B	301	1	-	0/6/23/26	0/1/1/1
6	ACT	B	304	-	-	0/0/0/0	0/0/0/0
7	6Y2	B	305	-	-	0/24/64/64	0/3/3/3
2	NAG	C	301	1,3,2	-	0/6/23/26	0/1/1/1
3	FUC	C	302	2	-	0/0/17/20	0/1/1/1
2	NAG	C	303	8,2	-	0/6/23/26	0/1/1/1
8	BMA	C	304	9,10,2	-	0/2/19/22	0/1/1/1
9	XYP	C	305	8	-	0/0/14/17	0/1/1/1
10	MAN	C	306	8	-	0/2/19/22	0/1/1/1
10	MAN	C	307	8	-	0/2/19/22	0/1/1/1
6	ACT	C	310	-	-	0/0/0/0	0/0/0/0
6	ACT	C	311	-	-	0/0/0/0	0/0/0/0
7	6Y2	C	312	-	-	0/24/64/64	0/3/3/3
2	NAG	D	301	1,3	-	0/6/23/26	0/1/1/1
3	FUC	D	302	2	-	0/0/17/20	0/1/1/1
6	ACT	D	305	-	-	0/0/0/0	0/0/0/0
6	ACT	D	306	-	-	0/0/0/0	0/0/0/0
7	6Y2	D	307	-	-	0/24/64/64	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	306	6Y2	CAL-CAO	-2.95	1.47	1.53
7	D	307	6Y2	CAL-CAO	-2.79	1.48	1.53
3	C	302	FUC	O5-C1	-2.52	1.39	1.43
7	D	307	6Y2	OAT-CAS	-2.00	1.38	1.43
7	C	312	6Y2	CBK-CBG	2.05	1.54	1.50
7	C	312	6Y2	CAO-NAP	2.08	1.49	1.45
2	B	301	NAG	C1-C2	2.09	1.55	1.52
7	C	312	6Y2	CBL-CBI	2.22	1.55	1.50
7	D	307	6Y2	C4-C5	2.27	1.58	1.53
7	C	312	6Y2	OAA-CAL	2.87	1.45	1.41
7	A	306	6Y2	OAA-CAL	3.15	1.46	1.41
7	B	305	6Y2	OAJ-NAH	10.32	1.43	1.22
7	A	306	6Y2	OAJ-NAH	12.39	1.47	1.22
7	D	307	6Y2	OAJ-NAH	14.35	1.51	1.22
7	C	312	6Y2	OAJ-NAH	14.75	1.52	1.22

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	306	6Y2	CAL-OBB-CBA	-3.08	107.69	113.74
7	B	305	6Y2	CAL-CAO-NAP	-3.03	105.31	111.01
7	B	305	6Y2	O1-C1-O5	-2.99	102.91	110.69
2	B	301	NAG	C4-C3-C2	-2.73	107.11	111.34
7	B	305	6Y2	C1-O5-C5	-2.71	108.43	113.74
8	C	304	BMA	C6-C5-C4	-2.67	106.30	112.99
7	D	307	6Y2	C1-O5-C5	-2.52	108.80	113.74
7	A	306	6Y2	CAS-CAO-NAP	-2.44	105.61	110.67
2	B	301	NAG	C3-C4-C5	-2.43	105.89	110.23
7	C	312	6Y2	C1-C2-N2	-2.41	106.48	111.01
7	D	307	6Y2	OBF-CBE-CBA	-2.38	103.35	111.30
10	C	307	MAN	O5-C5-C4	-2.37	106.21	110.13
3	C	302	FUC	O5-C1-C2	-2.24	107.31	110.89
2	B	301	NAG	O7-C7-C8	-2.22	117.98	122.07
2	D	301	NAG	O3-C3-C2	-2.17	104.73	109.37
2	C	303	NAG	O4-C4-C3	-2.14	105.53	110.36
7	A	306	6Y2	CAB-OAA-CAL	-2.12	114.79	117.87
7	D	307	6Y2	OBB-CAL-CAO	-2.10	106.26	110.76
7	A	306	6Y2	CAL-CAO-NAP	-2.02	107.20	111.01
2	B	301	NAG	O7-C7-N2	-2.02	117.73	121.84
3	C	302	FUC	C1-C2-C3	2.06	112.05	109.55
2	D	301	NAG	C1-O5-C5	2.11	115.24	112.14
8	C	304	BMA	C1-O5-C5	2.18	115.34	112.14
7	A	306	6Y2	O5-C5-C6	2.23	112.16	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	306	6Y2	CAD-CAE-NAH	2.26	121.14	119.51
7	C	312	6Y2	CAD-CAE-NAH	2.30	121.16	119.51
7	B	305	6Y2	OAJ-NAH-CAE	2.37	120.38	118.67
2	C	301	NAG	C1-O5-C5	2.42	115.70	112.14
8	C	304	BMA	O5-C5-C6	2.76	113.25	107.34
2	B	301	NAG	C1-O5-C5	2.94	116.46	112.14
2	A	301	NAG	C1-O5-C5	3.06	116.64	112.14
10	C	307	MAN	C1-C2-C3	3.53	113.82	109.55
2	B	301	NAG	C8-C7-N2	4.27	124.29	116.10
2	B	301	NAG	C2-N2-C7	5.62	130.42	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	305	ACT	1	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	238/243 (97%)	0.07	6 (2%) 61 71	13, 20, 35, 53	0
1	B	238/243 (97%)	0.09	7 (2%) 55 65	12, 20, 39, 57	0
1	C	238/243 (97%)	0.08	7 (2%) 55 65	12, 19, 37, 60	0
1	D	238/243 (97%)	0.08	6 (2%) 61 71	12, 20, 37, 61	0
All	All	952/972 (97%)	0.08	26 (2%) 58 68	12, 20, 37, 61	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	268	SER	6.2
1	B	268	SER	5.2
1	A	268	SER	4.0
1	D	268	SER	3.6
1	D	69	ASP	3.0
1	C	94	ASP	2.9
1	B	69	ASP	2.9
1	C	145	HIS	2.8
1	A	120	ALA	2.7
1	B	94	ASP	2.6
1	A	69	ASP	2.6
1	D	113	ALA	2.5
1	A	119	LEU	2.5
1	D	68	LYS	2.4
1	B	144	ARG	2.4
1	C	267	PRO	2.3
1	D	94	ASP	2.2
1	C	69	ASP	2.1
1	B	141	HIS	2.1
1	B	44	ASP	2.1
1	D	58	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	141	HIS	2.0
1	A	141	HIS	2.0
1	B	71	GLU	2.0
1	C	91	SER	2.0
1	A	144	ARG	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 carbohydrates in this entry.

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
7	6Y2	A	306	38/38	0.87	0.20	5.20	20,39,92,98	0
7	6Y2	C	312	38/38	0.88	0.19	2.31	18,35,76,80	0
6	ACT	D	306	4/4	0.94	0.16	1.29	33,39,40,40	0
6	ACT	C	311	4/4	0.96	0.14	0.77	22,24,25,27	0
6	ACT	B	304	4/4	0.89	0.14	0.61	29,35,36,37	0
7	6Y2	B	305	38/38	0.94	0.10	0.18	16,19,38,42	0
7	6Y2	D	307	38/38	0.94	0.12	0.17	17,28,43,46	0
4	CA	A	303	1/1	1.00	0.07	-0.95	15,15,15,15	0
2	NAG	C	301	14/15	0.97	0.07	-1.05	19,21,23,23	0
4	CA	B	302	1/1	0.99	0.07	-1.46	14,14,14,14	0
4	CA	C	308	1/1	1.00	0.06	-1.96	15,15,15,15	0
4	CA	D	303	1/1	1.00	0.06	-2.28	15,15,15,15	0
5	MN	C	309	1/1	1.00	0.02	-3.48	19,19,19,19	0
5	MN	D	304	1/1	1.00	0.04	-3.57	19,19,19,19	0
5	MN	B	303	1/1	1.00	0.02	-3.63	19,19,19,19	0
5	MN	A	304	1/1	1.00	0.02	-4.23	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	BMA	C	304	11/12	0.71	0.23	-	53,59,65,67	0
3	FUC	D	302	10/11	0.79	0.45	-	68,71,72,73	0
10	MAN	C	306	11/12	0.74	0.45	-	70,74,81,83	0
2	NAG	A	301	14/15	0.88	0.25	-	37,44,53,53	0
6	ACT	D	305	4/4	0.95	0.11	-	32,35,36,39	0
2	NAG	B	301	14/15	0.75	0.28	-	53,61,66,66	0
6	ACT	A	305	4/4	0.80	0.17	-	31,34,37,40	0
3	FUC	A	302	10/11	0.77	0.28	-	53,56,59,61	0
3	FUC	C	302	10/11	0.95	0.08	-	20,22,23,23	0
2	NAG	D	301	14/15	0.88	0.26	-	44,49,52,58	0
9	XYP	C	305	9/10	0.76	0.38	-	61,66,70,74	0
10	MAN	C	307	11/12	0.66	0.35	-	69,74,76,76	0
2	NAG	C	303	14/15	0.93	0.15	-	27,33,39,45	0
6	ACT	C	310	4/4	0.81	0.25	-	32,40,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.