Full wwPDB X-ray Structure Validation Report (i)

May 27, 2019 – 01:07 PM EDT

PDB ID	:	6JYN
Title	:	GII.13/21 noroviruses recognize glycans with a terminal beta-galactose via an unconventional glycan binding site
Authors	:	Duan, Z.; Xin, C.
Deposited on	:	2019-04-26
Resolution	:	1.60 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 (i) symbol.

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

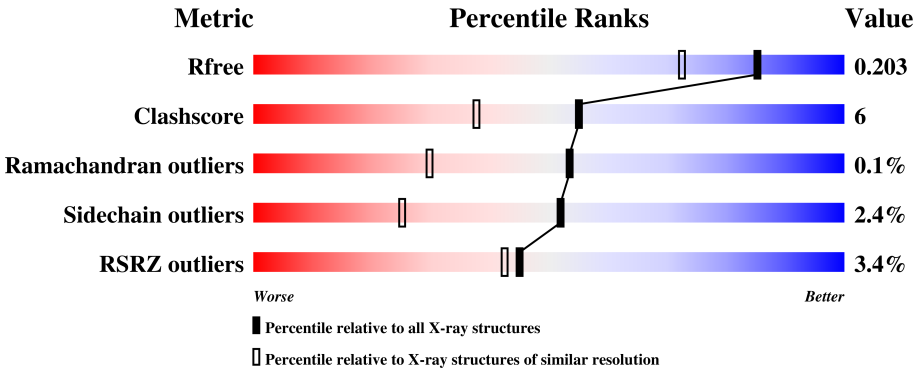
MolProbity	:	4.02b-467
Mogul	:	1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031633
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

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 1.60 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}	111664	2957 (1.60-1.60)
Clashscore	122126	3202 (1.60-1.60)
Ramachandran outliers	120053	3117 (1.60-1.60)
Sidechain outliers	120020	3116 (1.60-1.60)
RSRZ outliers	108989	2883 (1.60-1.60)

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	309	4% 86% 13%
1	B	309	3% 90% 10%
1	C	309	4% 87% 12%
1	D	309	3% 88% 11%

2 Entry composition

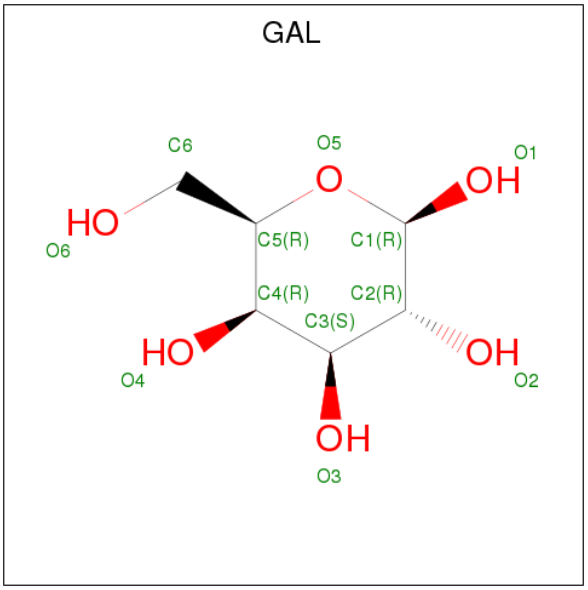
There are 4 unique types of molecules in this entry. The entry contains 11264 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 human norovirus P domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	2	0
			2405	1525	411	463	6			
1	B	309	Total	C	N	O	S	0	3	0
			2411	1527	412	466	6			
1	C	309	Total	C	N	O	S	0	0	0
			2392	1517	409	460	6			
1	D	309	Total	C	N	O	S	0	0	0
			2392	1517	409	460	6			

- Molecule 2 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		

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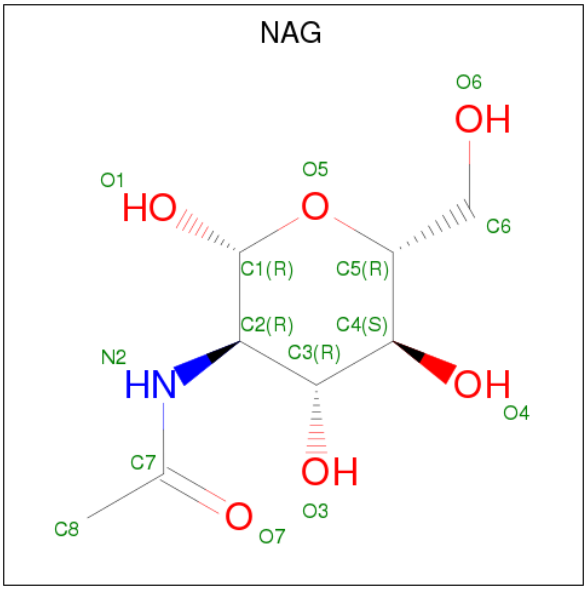
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 11 6 5	0	0
2	D	1	Total C O 11 6 5	0	0

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 15 8 1 6	0	0
3	B	1	Total C N O 15 8 1 6	0	0
3	C	1	Total C N O 15 8 1 6	0	0
3	D	1	Total C N O 15 8 1 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	407	Total O 407 407	0	0
4	B	362	Total O 362 362	0	0
4	C	404	Total O 404 404	0	0

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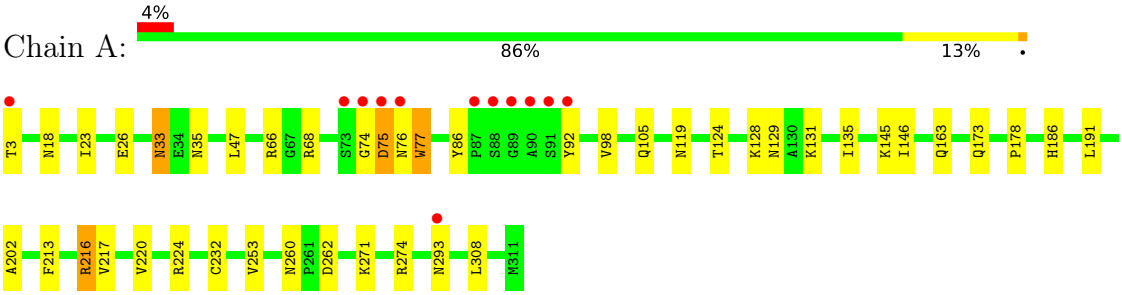
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	387	Total O 387 387	0	0

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometryand 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.

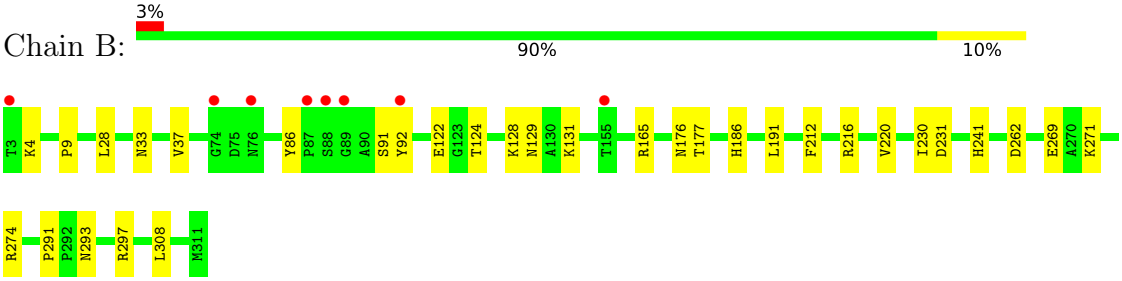
• Molecule 1: human norovirus P domain protein

Chain A:



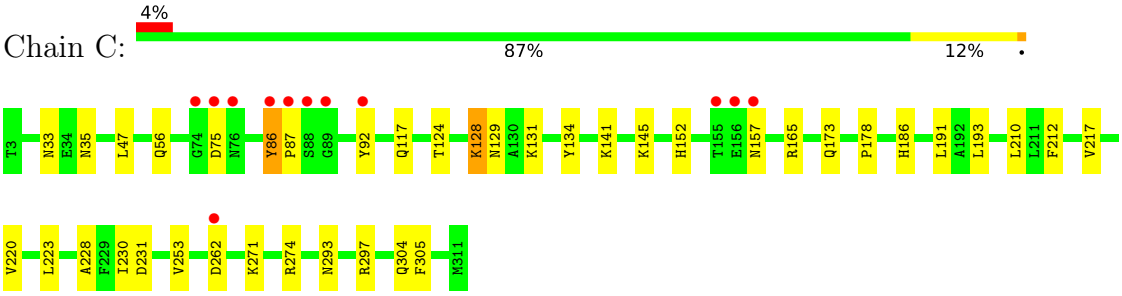
• Molecule 1: human norovirus P domain protein

Chain B:



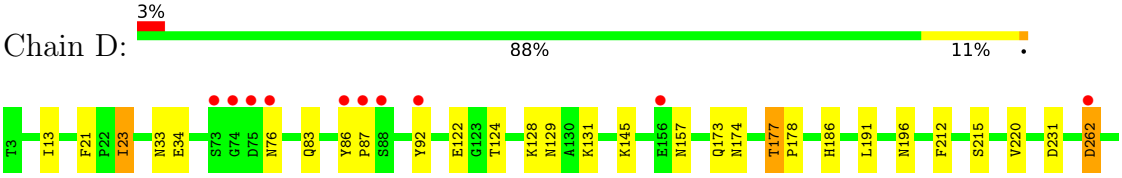
• Molecule 1: human norovirus P domain protein

Chain C:



• Molecule 1: human norovirus P domain protein

Chain D:




R265
K271
R274
N293
D299
Q304
L308
M311

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.94Å 122.94Å 83.28Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	49.45 – 1.60 49.46 – 1.60	Depositor EDS
% Data completeness (in resolution range)	92.4 (49.45-1.60) 92.1 (49.46-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.19 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.181 , 0.201 0.183 , 0.203	Depositor DCC
R_{free} test set	8462 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	13.5	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 26.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.457 for h,-k,-l	Xtriage
Reported twinning fraction	0.470 for h,-k,-l	Depositor
Outliers	0 of 171051 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11264	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6107e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: GAL, 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	0.26	0/2471	0.49	0/3384
1	B	0.27	0/2477	0.48	0/3392
1	C	0.26	0/2458	0.48	0/3365
1	D	0.26	0/2458	0.49	0/3365
All	All	0.26	0/9864	0.48	0/13506

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	1
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	33	ASN	Peptide
1	B	33	ASN	Peptide
1	C	33	ASN	Peptide
1	D	33	ASN	Peptide
1	D	76	ASN	Peptide

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	2405	0	2317	35	0
1	B	2411	0	2319	24	0
1	C	2392	0	2304	31	0
1	D	2392	0	2304	23	0
2	A	11	0	10	1	0
2	B	11	0	10	1	0
2	C	11	0	10	0	0
2	D	11	0	10	1	0
3	A	15	0	14	0	0
3	B	15	0	14	0	0
3	C	15	0	14	0	0
3	D	15	0	14	0	0
4	A	407	0	0	18	0
4	B	362	0	0	11	0
4	C	404	0	0	13	0
4	D	387	0	0	5	0
All	All	11264	0	9340	106	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 6.

All (106) 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:135:ILE:O	4:A:701:HOH:O	1.99	0.81
1:D:262:ASP:OD1	1:D:293:ASN:ND2	2.19	0.74
1:A:213:PHE:O	4:A:702:HOH:O	2.05	0.74
1:D:196:ASN:ND2	4:D:702:HOH:O	2.22	0.73
1:C:56:GLN:NE2	4:C:705:HOH:O	2.20	0.73
1:C:210:LEU:O	4:C:701:HOH:O	2.06	0.72
1:A:105:GLN:NE2	4:A:708:HOH:O	2.22	0.72
1:B:216:ARG:NH2	4:B:704:HOH:O	2.24	0.69
1:A:26:GLU:OE2	4:A:703:HOH:O	2.11	0.69
1:A:18:ASN:ND2	4:A:702:HOH:O	2.26	0.68
1:A:119:ASN:ND2	4:A:709:HOH:O	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ASN:O	4:B:701:HOH:O	2.13	0.66
1:C:193:LEU:O	4:C:702:HOH:O	2.14	0.65
1:C:141:LYS:NZ	4:C:709:HOH:O	2.30	0.65
1:B:262:ASP:OD2	1:B:293:ASN:ND2	2.29	0.65
1:C:262:ASP:OD2	1:C:293:ASN:ND2	2.31	0.64
1:A:163:GLN:NE2	4:A:714:HOH:O	2.30	0.63
1:C:165:ARG:NH1	4:C:707:HOH:O	2.25	0.63
1:B:186:HIS:O	1:B:186:HIS:ND1	2.29	0.63
1:C:186:HIS:O	1:C:186:HIS:ND1	2.29	0.62
1:C:220:VAL:HA	1:D:129:ASN:HB3	1.80	0.61
1:A:26:GLU:OE1	1:A:216:ARG:NH2	2.31	0.61
1:B:28:LEU:O	4:B:702:HOH:O	2.16	0.61
1:D:186:HIS:O	1:D:186:HIS:ND1	2.33	0.60
1:A:186:HIS:O	1:A:186:HIS:ND1	2.34	0.60
1:D:293:ASN:OD1	4:D:701:HOH:O	2.17	0.60
1:A:262:ASP:OD2	1:A:293:ASN:ND2	2.35	0.59
1:B:37:VAL:N	4:B:708:HOH:O	2.31	0.59
1:B:124:THR:HG22	1:B:128:LYS:HG2	1.84	0.58
1:A:124:THR:HG22	1:A:128:LYS:HG2	1.85	0.57
1:A:260:ASN:OD1	1:A:293:ASN:ND2	2.38	0.56
1:A:35:ASN:OD1	4:A:704:HOH:O	2.18	0.56
1:C:117:GLN:O	4:C:703:HOH:O	2.17	0.56
1:C:165:ARG:NH2	4:C:703:HOH:O	2.21	0.56
1:D:124:THR:HG22	1:D:128:LYS:HG2	1.87	0.56
1:D:174:ASN:OD1	1:D:177:THR:HG23	2.06	0.56
1:B:4:LYS:NZ	4:B:714:HOH:O	2.38	0.56
4:B:722:HOH:O	1:C:191:LEU:HB3	2.06	0.55
1:A:224:ARG:NH1	4:A:730:HOH:O	2.39	0.55
1:A:220:VAL:HA	1:B:129:ASN:HB3	1.88	0.55
1:C:217:VAL:HG11	1:C:230:ILE:HD12	1.90	0.54
1:C:124:THR:HG22	1:C:128:LYS:HG2	1.87	0.54
1:A:3:THR:N	4:A:729:HOH:O	2.39	0.54
4:A:703:HOH:O	1:B:165:ARG:NH1	2.41	0.54
1:C:35:ASN:ND2	4:C:723:HOH:O	2.40	0.53
1:A:202:ALA:N	4:A:731:HOH:O	2.40	0.53
1:C:304:GLN:OE1	4:C:704:HOH:O	2.19	0.53
1:A:253:VAL:HG11	1:A:271:LYS:HG2	1.90	0.52
1:B:269:GLU:HG3	1:B:308:LEU:HD22	1.92	0.52
1:C:297:ARG:NH2	4:C:713:HOH:O	2.31	0.52
1:C:86:TYR:CG	1:C:87:PRO:HD2	2.44	0.52
1:A:76:ASN:OD1	4:A:705:HOH:O	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:GLN:HG3	1:D:178:PRO:HA	1.93	0.51
1:D:271:LYS:HG3	1:D:308:LEU:HD21	1.93	0.51
1:B:271:LYS:HG3	1:B:308:LEU:HD21	1.91	0.51
1:B:269:GLU:N	4:B:722:HOH:O	2.44	0.50
1:A:23:ILE:HD11	1:A:217[A]:VAL:HG12	1.93	0.49
1:A:129:ASN:HB3	1:B:220:VAL:HA	1.93	0.49
1:D:177:THR:HG21	2:D:601:GAL:O3	2.12	0.49
1:A:76:ASN:ND2	4:A:741:HOH:O	2.46	0.49
1:A:47:LEU:HG	1:A:274:ARG:HA	1.96	0.48
1:A:271:LYS:HG3	1:A:308:LEU:HD21	1.96	0.47
1:C:274:ARG:NH2	4:C:742:HOH:O	2.48	0.47
1:B:212:PHE:HB3	1:B:231:ASP:HB3	1.97	0.47
1:C:129:ASN:HB3	1:D:220:VAL:HA	1.97	0.47
1:C:86:TYR:CD1	1:C:87:PRO:HD2	2.49	0.47
1:B:165:ARG:NH2	4:B:709:HOH:O	2.33	0.47
1:C:165:ARG:NH2	4:C:743:HOH:O	2.48	0.46
1:A:68:ARG:HD2	1:C:305:PHE:CD1	2.50	0.46
1:B:177[A]:THR:HG22	4:B:748:HOH:O	2.16	0.46
1:D:21:PHE:HB3	4:D:725:HOH:O	2.16	0.45
1:B:86:TYR:CE2	1:B:92:TYR:HA	2.52	0.45
1:D:83:GLN:NE2	4:D:715:HOH:O	2.36	0.44
1:B:297:ARG:NE	4:B:729:HOH:O	2.50	0.44
1:B:177[A]:THR:HG21	2:B:601:GAL:O3	2.18	0.44
1:A:77:TRP:HB2	2:A:601:GAL:H5	2.00	0.43
1:D:177:THR:OG1	1:D:177:THR:O	2.34	0.43
1:A:74:GLY:HA2	1:A:75:ASP:HA	1.74	0.43
1:B:291:PRO:O	4:B:703:HOH:O	2.21	0.43
1:D:191:LEU:N	4:D:740:HOH:O	2.51	0.43
1:A:92:TYR:HE2	1:A:145:LYS:O	2.01	0.43
1:A:86:TYR:CE1	1:A:92:TYR:HA	2.54	0.42
1:A:173:GLN:HG3	1:A:178:PRO:HA	2.01	0.42
1:C:173:GLN:HG3	1:C:178:PRO:HA	2.01	0.42
1:C:212:PHE:HB3	1:C:231:ASP:HB3	2.01	0.42
1:C:217:VAL:HG22	1:C:228:ALA:O	2.19	0.42
1:A:146:ILE:HD11	4:A:907:HOH:O	2.19	0.42
1:A:33:ASN:OD1	4:A:707:HOH:O	2.22	0.42
1:D:212:PHE:HB3	1:D:231:ASP:HB3	2.02	0.42
1:C:47:LEU:HG	1:C:274:ARG:HA	2.02	0.42
1:D:23:ILE:HD11	1:D:215:SER:HB3	2.02	0.42
1:D:304:GLN:N	1:D:304:GLN:OE1	2.41	0.42
1:C:92:TYR:HE2	1:C:145:LYS:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:GLN:O	1:B:122:GLU:HG3	2.20	0.41
1:D:262:ASP:N	1:D:262:ASP:OD1	2.53	0.41
1:C:173:GLN:O	1:D:122:GLU:HG3	2.20	0.41
1:C:253:VAL:HG11	1:C:271:LYS:HG2	2.02	0.41
1:D:13:ILE:HA	1:D:13:ILE:HD13	1.93	0.41
1:B:9:PRO:HD3	1:B:241:HIS:CD2	2.56	0.41
1:A:232:CYS:N	4:A:702:HOH:O	2.52	0.41
1:C:297:ARG:NE	4:C:728:HOH:O	2.53	0.41
1:C:134:TYR:HB2	1:C:152:HIS:HB3	2.03	0.41
1:D:86:TYR:CD1	1:D:87:PRO:HD2	2.56	0.41
1:A:76:ASN:N	4:A:755:HOH:O	2.54	0.40
1:D:92:TYR:HE2	1:D:145:LYS:O	2.04	0.40
1:B:230:ILE:HA	1:B:230:ILE:HD13	1.95	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	309/309 (100%)	295 (96%)	13 (4%)	1 (0%)	43	22
1	B	310/309 (100%)	299 (96%)	11 (4%)	0	100	100
1	C	307/309 (99%)	295 (96%)	12 (4%)	0	100	100
1	D	307/309 (99%)	292 (95%)	15 (5%)	0	100	100
All	All	1233/1236 (100%)	1181 (96%)	51 (4%)	1 (0%)	53	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	TRP

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	265/263 (101%)	259 (98%)	6 (2%)	53	27
1	B	266/263 (101%)	262 (98%)	4 (2%)	67	46
1	C	263/263 (100%)	257 (98%)	6 (2%)	53	27
1	D	263/263 (100%)	254 (97%)	9 (3%)	40	15
All	All	1057/1052 (100%)	1032 (98%)	25 (2%)	52	25

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	75	ASP
1	A	98	VAL
1	A	131	LYS
1	A	191	LEU
1	A	216	ARG
1	B	91	SER
1	B	131	LYS
1	B	191	LEU
1	B	274	ARG
1	C	75	ASP
1	C	86	TYR
1	C	128	LYS
1	C	131	LYS
1	C	157	ASN
1	C	223	LEU
1	D	23	ILE
1	D	34	GLU
1	D	131	LYS
1	D	157	ASN
1	D	177	THR
1	D	262	ASP
1	D	265	ARG
1	D	274	ARG
1	D	299	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	35	ASN
1	D	293	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 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	GAL	A	601	3	11,11,12	0.58	0	15,15,17	0.92	0
3	NAG	A	602	2	15,15,15	0.25	0	21,21,21	0.50	0
2	GAL	B	601	3	11,11,12	0.96	0	15,15,17	1.06	1 (6%)
3	NAG	B	602	2	15,15,15	0.29	0	21,21,21	0.32	0
2	GAL	C	601	3	11,11,12	0.79	0	15,15,17	1.02	1 (6%)
3	NAG	C	602	2	15,15,15	0.35	0	21,21,21	0.30	0
2	GAL	D	601	3	11,11,12	0.71	0	15,15,17	1.10	1 (6%)
3	NAG	D	602	2	15,15,15	0.43	0	21,21,21	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	A	601	3	-	0/2/19/22	0/1/1/1
3	NAG	A	602	2	-	0/6/26/26	0/1/1/1
2	GAL	B	601	3	-	0/2/19/22	0/1/1/1
3	NAG	B	602	2	-	0/6/26/26	0/1/1/1
2	GAL	C	601	3	-	0/2/19/22	0/1/1/1
3	NAG	C	602	2	-	0/6/26/26	0/1/1/1
2	GAL	D	601	3	-	0/2/19/22	0/1/1/1
3	NAG	D	602	2	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	GAL	C1-C2-C3	2.04	112.16	109.66
2	C	601	GAL	C1-C2-C3	2.11	112.26	109.66
2	B	601	GAL	C1-C2-C3	2.43	112.65	109.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	GAL	1	0
2	B	601	GAL	1	0
2	D	601	GAL	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	309/309 (100%)	-0.11	12 (3%)	39	37	7, 12, 27, 85	0
1	B	309/309 (100%)	-0.13	8 (2%)	56	54	7, 12, 28, 93	0
1	C	309/309 (100%)	-0.10	12 (3%)	39	37	8, 13, 29, 106	0
1	D	309/309 (100%)	-0.09	10 (3%)	47	45	7, 12, 29, 90	0
All	All	1236/1236 (100%)	-0.11	42 (3%)	45	42	7, 12, 29, 106	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	76	ASN	6.8
1	C	86	TYR	6.3
1	A	74	GLY	6.0
1	C	76	ASN	5.9
1	B	88	SER	5.8
1	A	87	PRO	5.3
1	D	75	ASP	5.2
1	C	87	PRO	5.1
1	A	88	SER	5.1
1	A	76	ASN	4.8
1	B	87	PRO	4.6
1	B	89	GLY	4.6
1	D	87	PRO	4.5
1	C	156	GLU	4.4
1	D	88	SER	4.4
1	B	155	THR	4.3
1	A	75	ASP	4.1
1	C	88	SER	4.1
1	D	86	TYR	4.0
1	B	74	GLY	4.0
1	A	89	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	74	GLY	3.7
1	B	92	TYR	3.6
1	D	92	TYR	3.5
1	C	89	GLY	3.3
1	C	74	GLY	3.2
1	C	155	THR	3.0
1	D	156	GLU	3.0
1	A	3	THR	2.8
1	A	90	ALA	2.8
1	C	157	ASN	2.8
1	C	75	ASP	2.6
1	A	293	ASN	2.6
1	B	76	ASN	2.5
1	D	73	SER	2.5
1	A	91	SER	2.4
1	A	92	TYR	2.4
1	B	3	THR	2.4
1	A	73	SER	2.3
1	C	92	TYR	2.2
1	C	262	ASP	2.1
1	D	262	ASP	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. 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
3	NAG	C	602	15/15	0.58	0.23	48,48,50,50	0
3	NAG	A	602	15/15	0.70	0.22	34,35,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	B	602	15/15	0.78	0.19	47,48,49,49	0
3	NAG	D	602	15/15	0.78	0.25	42,42,44,44	0
2	GAL	D	601	11/12	0.80	0.14	18,19,20,20	0
2	GAL	A	601	11/12	0.80	0.15	19,20,20,20	0
2	GAL	C	601	11/12	0.85	0.12	20,21,21,22	0
2	GAL	B	601	11/12	0.86	0.12	17,18,19,19	0

6.5 Other polymers

There are no such residues in this entry.