



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:02 pm GMT

PDB ID : 2DTY  
Title : Crystal structure of basic winged bean lectin complexed with N-acetyl-D-galactosamine  
Authors : Kulkarni, K.A.; Katiyar, S.; Surolia, A.; Vijayan, M.; Suguna, K.  
Deposited on : 2006-07-19  
Resolution : 2.65 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](mailto: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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

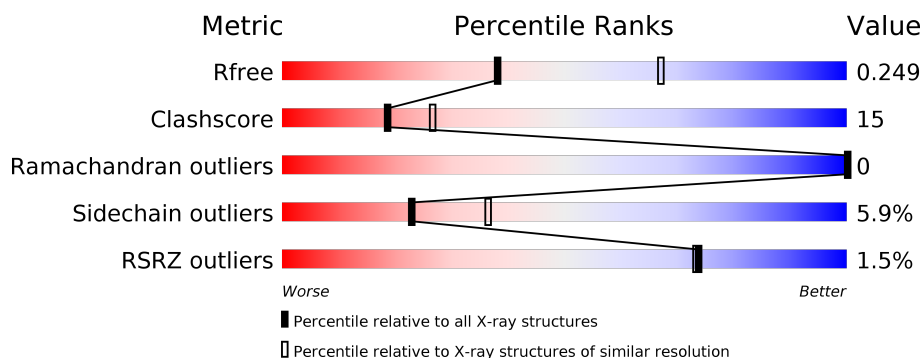
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	100719	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	241	<div> <div>2%</div> <div>71% 24%</div> <div>• •</div> </div>
1	B	241	<div> <div>2%</div> <div>76% 19%</div> <div>• •</div> </div>
1	C	241	<div> <div>73% 22%</div> <div>• •</div> </div>
1	D	241	<div> <div>2%</div> <div>74% 22%</div> <div>• •</div> </div>

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
3	NAG	B	603	-	-	X	-
3	NAG	D	501	-	-	-	X
4	BMA	C	504	-	-	-	X

## 2 Entry composition [i](#)

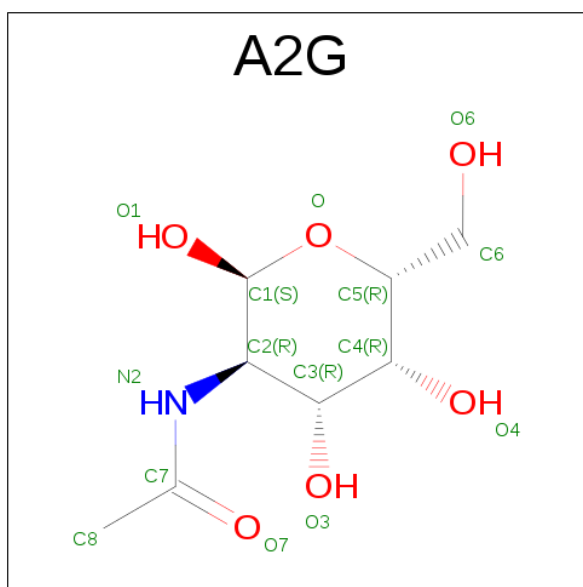
There are 8 unique types of molecules in this entry. The entry contains 7989 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Basic agglutinin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	0	0	0
			1838	1182	308	348			
1	B	237	Total	C	N	O	0	0	0
			1833	1179	307	347			
1	C	237	Total	C	N	O	0	0	0
			1829	1177	305	347			
1	D	237	Total	C	N	O	0	0	0
			1830	1178	305	347			

- Molecule 2 is SUGAR (N-ACETYL-D-GALACTOSAMINE) (three-letter code: A2G) (formula:  $C_8H_{15}NO_6$ ).



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

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			38	22	2	14		
3	A	3	Total	C	N	O	0	0
			38	22	2	14		
3	B	3	Total	C	N	O	0	0
			38	22	2	14		
3	B	3	Total	C	N	O	0	0
			38	22	2	14		
3	D	3	Total	C	N	O	0	0
			38	22	2	14		
3	D	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total 1	Mn 1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

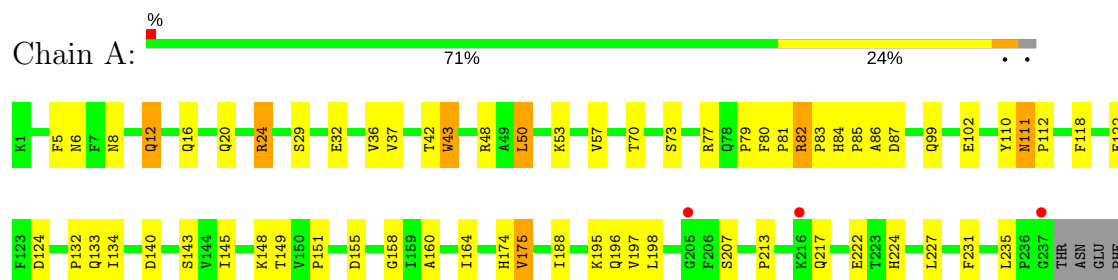
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	85	Total 85	O 85	0	0
8	B	72	Total 72	O 72	0	0
8	C	65	Total 65	O 65	0	0
8	D	54	Total 54	O 54	0	0

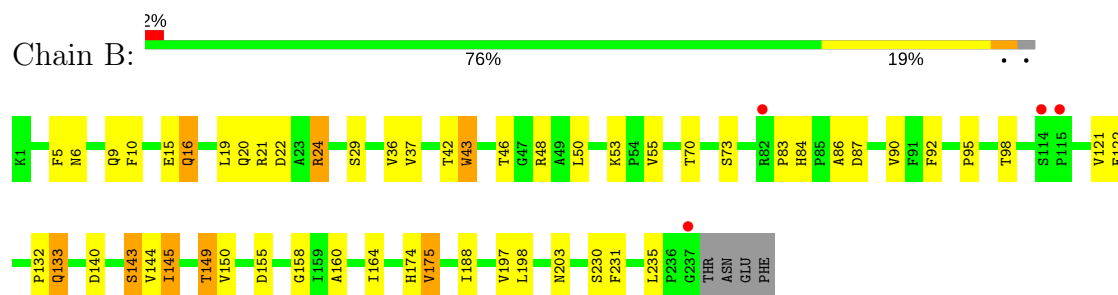
### 3 Residue-property plots

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 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.

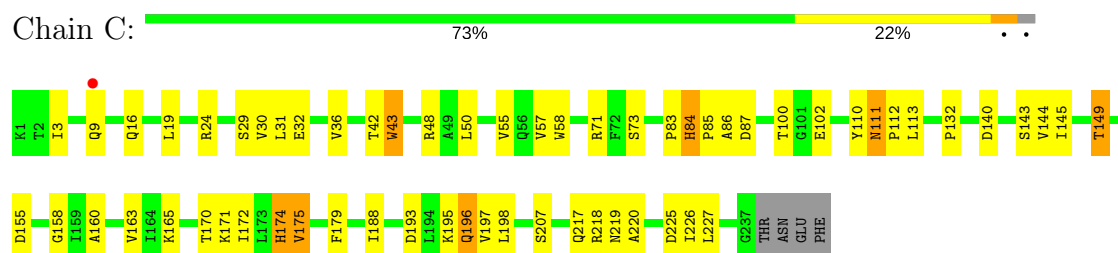
#### • Molecule 1: Basic agglutinin



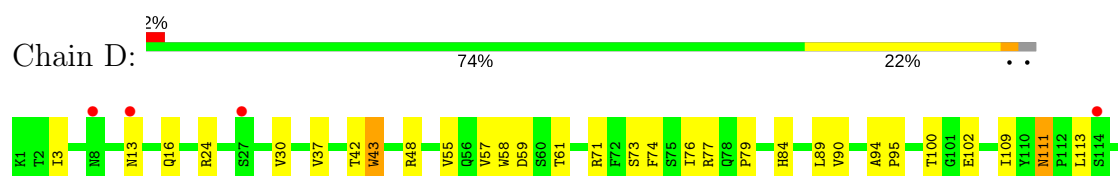
#### • Molecule 1: Basic agglutinin

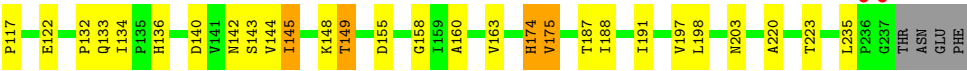


#### • Molecule 1: Basic agglutinin



#### • Molecule 1: Basic agglutinin







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.72Å 91.86Å 73.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.65 21.48 – 2.66	Depositor EDS
% Data completeness (in resolution range)	97.9 (25.00-2.65) 98.0 (21.48-2.66)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 2.67Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.196 , 0.239 0.211 , 0.249	Depositor DCC
$R_{free}$ test set	1629 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.4	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 61.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7989	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CA, MN, FUC, A2G, FUL

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	0.39	0/1891	0.68	1/2589 (0.0%)
1	B	0.41	0/1886	0.66	0/2583
1	C	0.39	0/1882	0.66	1/2576 (0.0%)
1	D	0.39	0/1882	0.66	0/2577
All	All	0.39	0/7541	0.66	2/10325 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	SER	N-CA-C	5.66	126.28	111.00
1	C	29	SER	N-CA-C	5.34	125.43	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	1838	0	1785	63	0
1	B	1833	0	1773	39	0
1	C	1829	0	1771	61	0
1	D	1830	0	1776	53	0
2	A	15	0	15	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	15	0	0
2	C	15	0	15	0	0
2	D	15	0	15	0	0
3	A	76	0	68	4	0
3	B	76	0	68	9	0
3	D	76	0	68	7	0
4	C	49	0	43	2	0
5	C	38	0	34	3	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	85	0	0	2	0
8	B	72	0	0	1	0
8	C	65	0	0	2	0
8	D	54	0	0	2	0
All	All	7989	0	7446	225	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 15.

All (225) 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:143:SER:OG	1:A:145:ILE:HG22	1.64	0.97
3:D:601:NAG:H5	3:D:603:NAG:H82	1.50	0.92
3:B:602:FUC:H3	3:B:603:NAG:H82	1.53	0.90
1:C:143:SER:OG	1:C:145:ILE:HG22	1.74	0.88
1:A:196:GLN:HE22	1:D:145:ILE:HG23	1.38	0.88
1:B:197:VAL:HG23	1:B:198:LEU:HG	1.55	0.87
1:A:16:GLN:HA	1:A:16:GLN:HE21	1.42	0.84
1:A:6:ASN:HD21	1:A:8:ASN:HD21	1.25	0.81
1:D:24:ARG:HB3	1:D:24:ARG:NH1	1.96	0.79
1:A:12:GLN:HE21	1:A:12:GLN:H	1.31	0.78
1:A:24:ARG:HH11	1:A:24:ARG:HB3	1.49	0.77
3:D:601:NAG:H3	3:D:602:FUC:H5	1.67	0.76
1:A:6:ASN:HD21	1:A:8:ASN:ND2	1.81	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:VAL:HG22	1:C:188:ILE:HG22	1.68	0.76
1:A:197:VAL:HG23	1:A:198:LEU:HG	1.68	0.75
1:A:16:GLN:HA	1:A:16:GLN:NE2	2.03	0.74
1:C:197:VAL:HG23	1:C:198:LEU:HG	1.68	0.74
1:A:99:GLN:HA	1:A:99:GLN:HE21	1.53	0.73
1:D:197:VAL:HG23	1:D:198:LEU:HG	1.71	0.72
1:D:175:VAL:HG22	1:D:188:ILE:HG22	1.72	0.71
1:A:24:ARG:NH1	1:A:24:ARG:HB3	2.05	0.71
1:C:42:THR:HG22	1:C:43:TRP:O	1.91	0.71
1:B:24:ARG:HB3	1:B:24:ARG:HH11	1.58	0.69
1:B:83:PRO:HD3	3:B:501:NAG:H82	1.75	0.68
1:A:196:GLN:NE2	1:D:145:ILE:HG23	2.08	0.68
1:C:145:ILE:HG23	1:C:145:ILE:O	1.94	0.67
1:B:143:SER:OG	1:B:145:ILE:HG23	1.94	0.67
1:A:110:TYR:CE2	1:A:112:PRO:HG3	2.29	0.66
1:C:140:ASP:HB3	1:C:143:SER:O	1.96	0.66
3:B:602:FUC:C3	3:B:603:NAG:H82	2.24	0.66
1:C:24:ARG:HB3	1:C:24:ARG:CZ	2.25	0.66
5:C:601:NAG:H62	5:C:603:NAG:C1	2.27	0.65
1:D:57:VAL:HG23	1:D:58:TRP:HD1	1.61	0.64
1:A:140:ASP:HB3	1:A:143:SER:O	1.97	0.64
3:B:602:FUC:H5	3:B:603:NAG:C1	2.26	0.64
1:C:24:ARG:HB3	1:C:24:ARG:NH1	2.11	0.64
1:B:145:ILE:HD11	1:C:195:LYS:HE2	1.80	0.64
1:B:150:VAL:HG12	1:B:188:ILE:HD12	1.80	0.64
1:D:59:ASP:OD2	1:D:61:THR:HB	1.98	0.64
1:D:140:ASP:HB3	1:D:143:SER:O	1.99	0.63
1:A:196:GLN:NE2	1:D:143:SER:OG	2.30	0.63
3:D:601:NAG:O4	3:D:602:FUC:H3	1.98	0.63
1:B:145:ILE:O	1:B:145:ILE:HG13	1.98	0.63
1:C:16:GLN:HE21	1:C:16:GLN:HA	1.64	0.63
3:B:601:NAG:H4	3:B:603:NAG:HN2	1.65	0.62
1:C:16:GLN:NE2	1:C:16:GLN:HA	2.14	0.62
1:B:24:ARG:HB3	1:B:24:ARG:NH1	2.14	0.62
1:C:3:ILE:HD13	1:C:55:VAL:HG12	1.81	0.62
1:A:132:PRO:HG3	1:A:149:THR:HG21	1.81	0.62
1:D:24:ARG:HB3	1:D:24:ARG:CZ	2.26	0.62
3:B:601:NAG:H4	3:B:603:NAG:N2	2.14	0.62
1:A:110:TYR:HE2	1:A:112:PRO:HG3	1.63	0.62
1:C:111:ASN:HD22	1:C:111:ASN:C	2.02	0.61
1:D:175:VAL:HG22	1:D:188:ILE:CG2	2.30	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ARG:HD3	1:C:163:VAL:HG22	1.83	0.61
1:A:83:PRO:HB2	1:A:84:HIS:ND1	2.15	0.60
3:D:601:NAG:H61	3:D:603:NAG:C1	2.30	0.60
1:D:71:ARG:HG2	1:D:163:VAL:HG22	1.84	0.60
1:C:175:VAL:HG22	1:C:188:ILE:CG2	2.33	0.58
1:A:145:ILE:O	1:A:145:ILE:HG23	2.04	0.58
1:B:145:ILE:HG23	1:C:196:GLN:HE22	1.69	0.58
1:C:19:LEU:HD23	1:C:24:ARG:HA	1.85	0.58
1:A:6:ASN:ND2	1:A:8:ASN:ND2	2.51	0.57
1:C:111:ASN:ND2	1:C:111:ASN:C	2.57	0.57
1:A:217:GLN:HE22	3:A:501:NAG:H82	1.70	0.57
1:C:132:PRO:HG3	1:C:149:THR:HG21	1.87	0.57
1:A:213:PRO:HB3	3:A:601:NAG:H82	1.84	0.57
1:A:195:LYS:HG2	1:D:145:ILE:HD11	1.85	0.56
1:B:145:ILE:HG23	1:C:196:GLN:NE2	2.20	0.56
1:D:3:ILE:HD13	1:D:55:VAL:HG12	1.87	0.56
1:A:12:GLN:HE21	1:A:12:GLN:N	2.01	0.56
1:D:155:ASP:OD2	1:D:158:GLY:HA3	2.06	0.56
1:A:99:GLN:HA	1:A:99:GLN:NE2	2.19	0.56
1:A:175:VAL:HG13	1:A:188:ILE:HG23	1.88	0.55
1:A:83:PRO:HB2	1:A:84:HIS:CE1	2.42	0.54
1:A:5:PHE:CZ	1:A:231:PHE:HB3	2.43	0.54
1:A:16:GLN:HE22	1:A:53:LYS:HE3	1.71	0.54
1:C:84:HIS:HD2	1:C:84:HIS:O	1.89	0.54
1:D:16:GLN:HA	1:D:16:GLN:NE2	2.23	0.53
1:B:16:GLN:HE21	1:B:16:GLN:HA	1.74	0.53
1:D:24:ARG:CB	1:D:24:ARG:NH1	2.69	0.53
1:B:143:SER:OG	1:C:196:GLN:NE2	2.43	0.52
1:C:84:HIS:CD2	1:C:84:HIS:O	2.62	0.52
1:D:16:GLN:HA	1:D:16:GLN:HE21	1.75	0.52
1:C:217:GLN:HE22	4:C:501:NAG:H81	1.75	0.51
1:B:140:ASP:HB3	1:B:143:SER:O	2.10	0.51
1:A:37:VAL:HG23	1:A:37:VAL:O	2.11	0.51
1:B:164:ILE:HG12	1:B:175:VAL:HB	1.93	0.51
1:C:111:ASN:ND2	1:C:113:LEU:H	2.09	0.51
1:B:20:GLN:OE1	1:B:48:ARG:NH1	2.38	0.51
1:D:24:ARG:HH11	1:D:24:ARG:CB	2.24	0.51
1:C:227:LEU:HD22	1:C:227:LEU:N	2.27	0.50
1:A:151:PRO:HD3	8:A:1447:HOH:O	2.11	0.50
3:B:603:NAG:H83	3:B:603:NAG:H3	1.94	0.50
1:B:84:HIS:HD2	1:B:84:HIS:O	1.95	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:ILE:O	1:D:134:ILE:HD12	2.11	0.50
1:C:32:GLU:HG2	1:C:225:ASP:OD1	2.12	0.49
1:B:42:THR:HG22	1:B:43:TRP:N	2.27	0.49
1:D:134:ILE:HD12	1:D:134:ILE:C	2.33	0.49
1:D:132:PRO:HG3	1:D:149:THR:HG21	1.95	0.49
1:B:155:ASP:OD2	1:B:158:GLY:HA3	2.12	0.49
1:A:134:ILE:HD12	1:A:134:ILE:O	2.13	0.48
1:D:113:LEU:N	1:D:113:LEU:HD22	2.28	0.48
1:A:42:THR:HG22	1:A:43:TRP:N	2.27	0.48
3:B:603:NAG:O3	3:B:603:NAG:C7	2.61	0.48
1:B:132:PRO:HG3	1:B:149:THR:HG21	1.94	0.48
1:C:110:TYR:CE2	1:C:112:PRO:HG3	2.48	0.48
1:A:122:GLU:OE2	1:A:124:ASP:HB2	2.14	0.48
1:A:48:ARG:HG2	1:A:207:SER:OG	2.13	0.48
1:A:70:THR:HG22	1:A:164:ILE:HB	1.95	0.48
1:A:82:ARG:HE	1:A:82:ARG:HA	1.79	0.48
1:C:218:ARG:HG3	1:C:218:ARG:HH21	1.79	0.47
1:D:122:GLU:OE1	1:D:140:ASP:OD2	2.32	0.47
1:B:16:GLN:HE22	1:B:53:LYS:HE3	1.79	0.47
1:B:150:VAL:HG11	1:B:188:ILE:HB	1.96	0.47
1:B:90:VAL:HG12	1:B:122:GLU:HA	1.97	0.47
1:B:121:VAL:HG21	1:B:164:ILE:HD13	1.97	0.47
1:A:16:GLN:NE2	1:A:53:LYS:HE3	2.29	0.47
1:A:32:GLU:OE2	1:A:36:VAL:HG11	2.15	0.47
1:B:37:VAL:HG23	1:B:37:VAL:O	2.13	0.47
1:B:84:HIS:CD2	1:B:84:HIS:O	2.67	0.47
1:D:90:VAL:HG21	1:D:109:ILE:HD13	1.97	0.47
1:C:155:ASP:OD2	1:C:158:GLY:HA3	2.15	0.47
1:C:217:GLN:HA	1:C:217:GLN:HE21	1.80	0.47
1:D:48:ARG:NH1	1:D:100:THR:HA	2.30	0.46
1:A:43:TRP:CZ3	1:A:213:PRO:HA	2.50	0.46
1:B:95:PRO:O	1:B:98:THR:HG23	2.15	0.46
1:C:73:SER:HA	1:C:160:ALA:O	2.15	0.46
1:A:111:ASN:HD22	1:A:111:ASN:C	2.18	0.46
1:D:48:ARG:HH11	1:D:100:THR:HA	1.80	0.46
1:D:117:PRO:HA	1:D:142:ASN:OD1	2.15	0.46
1:D:74:PHE:C	1:D:74:PHE:CD1	2.89	0.46
1:D:48:ARG:HH11	1:D:100:THR:CA	2.29	0.46
3:D:601:NAG:H3	3:D:602:FUC:C5	2.42	0.46
1:C:217:GLN:HA	1:C:217:GLN:NE2	2.31	0.46
1:A:149:THR:HG22	8:A:1447:HOH:O	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ASP:OD2	1:A:158:GLY:HA3	2.16	0.46
1:B:22:ASP:O	1:B:24:ARG:HG2	2.16	0.46
1:B:203:ASN:HA	8:B:2425:HOH:O	2.15	0.46
1:C:145:ILE:CG2	1:C:145:ILE:O	2.64	0.46
1:D:48:ARG:NH1	1:D:100:THR:N	2.64	0.46
1:D:76:ILE:HG23	1:D:223:THR:O	2.16	0.45
1:A:50:LEU:N	1:A:50:LEU:HD22	2.31	0.45
1:C:83:PRO:O	1:C:84:HIS:HB3	2.16	0.45
1:D:42:THR:HG22	1:D:43:TRP:N	2.32	0.45
3:D:601:NAG:C5	3:D:603:NAG:H82	2.33	0.45
1:C:42:THR:HG22	1:C:43:TRP:N	2.31	0.45
1:D:148:LYS:HB3	1:D:188:ILE:HD11	1.99	0.45
1:D:43:TRP:C	1:D:43:TRP:CD1	2.88	0.45
3:D:501:NAG:C6	3:D:503:NAG:H82	2.45	0.45
1:D:37:VAL:HG23	1:D:37:VAL:O	2.16	0.45
1:C:193:ASP:HB2	8:C:3433:HOH:O	2.16	0.45
1:D:174:HIS:HB2	8:D:4450:HOH:O	2.15	0.45
1:A:42:THR:HG22	1:A:43:TRP:O	2.17	0.45
1:C:43:TRP:C	1:C:43:TRP:CD1	2.89	0.45
1:D:174:HIS:CD2	1:D:174:HIS:H	2.35	0.45
1:B:21:ARG:HB3	1:B:46:THR:O	2.16	0.44
1:C:16:GLN:NE2	1:C:16:GLN:CA	2.78	0.44
1:D:144:VAL:O	1:D:144:VAL:CG1	2.64	0.44
1:A:73:SER:HA	1:A:160:ALA:O	2.17	0.44
1:A:77:ARG:O	1:A:79:PRO:HD3	2.17	0.44
1:C:197:VAL:CG2	1:C:198:LEU:HG	2.42	0.44
1:C:86:ALA:HA	1:C:87:ASP:HA	1.84	0.44
1:C:144:VAL:HG22	8:C:3402:HOH:O	2.16	0.44
1:C:50:LEU:HD22	1:C:50:LEU:N	2.32	0.44
1:C:219:ASN:ND2	4:C:501:NAG:H82	2.32	0.44
1:C:111:ASN:ND2	1:C:113:LEU:N	2.65	0.44
1:A:70:THR:CG2	1:A:164:ILE:HB	2.47	0.44
1:C:48:ARG:HG2	1:C:207:SER:OG	2.18	0.44
1:C:160:ALA:HB2	1:C:179:PHE:CE1	2.53	0.44
1:B:133:GLN:HB3	1:B:133:GLN:HE21	1.59	0.43
3:B:601:NAG:C4	3:B:603:NAG:HN2	2.30	0.43
1:A:24:ARG:HH11	1:A:24:ARG:CB	2.26	0.43
1:A:134:ILE:HD12	1:A:134:ILE:C	2.39	0.43
1:A:148:LYS:HB3	1:A:188:ILE:HD11	2.00	0.43
1:C:174:HIS:CD2	1:C:174:HIS:N	2.86	0.43
1:C:174:HIS:CD2	1:C:174:HIS:H	2.37	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ASN:OD1	1:B:230:SER:HB3	2.19	0.42
1:B:70:THR:CG2	1:B:164:ILE:HB	2.49	0.42
1:C:172:ILE:HD11	1:D:191:ILE:HG13	2.01	0.42
1:C:84:HIS:O	1:C:220:ALA:HA	2.19	0.42
1:B:10:PHE:HB2	1:B:29:SER:O	2.18	0.42
1:B:86:ALA:HA	1:B:87:ASP:HA	1.87	0.42
1:C:144:VAL:O	1:C:144:VAL:HG22	2.19	0.42
1:D:144:VAL:O	1:D:144:VAL:HG12	2.19	0.42
1:C:165:LYS:HD3	1:D:187:THR:HG23	2.02	0.42
1:A:99:GLN:CA	1:A:99:GLN:HE21	2.22	0.42
1:B:50:LEU:N	1:B:50:LEU:HD22	2.35	0.42
1:A:84:HIS:HA	1:A:85:PRO:HD3	1.89	0.42
1:B:5:PHE:CZ	1:B:231:PHE:HB3	2.54	0.42
1:D:111:ASN:C	1:D:111:ASN:HD22	2.22	0.42
1:A:164:ILE:HG12	1:A:175:VAL:HB	2.02	0.41
1:A:118:PHE:C	1:A:118:PHE:CD1	2.93	0.41
1:A:20:GLN:OE1	1:A:48:ARG:HD3	2.19	0.41
1:C:48:ARG:HD2	1:C:100:THR:HG23	2.01	0.41
1:A:16:GLN:CA	1:A:16:GLN:HE21	2.13	0.41
1:C:31:LEU:HB3	1:C:226:ILE:HB	2.01	0.41
1:D:113:LEU:H	1:D:113:LEU:HD22	1.85	0.41
1:D:13:ASN:N	1:D:13:ASN:HD22	2.17	0.41
1:D:84:HIS:O	1:D:220:ALA:HA	2.21	0.41
1:A:86:ALA:HA	1:A:87:ASP:HA	1.85	0.41
1:D:89:LEU:C	1:D:89:LEU:HD12	2.41	0.41
1:A:217:GLN:HE22	3:A:501:NAG:C8	2.32	0.41
1:C:48:ARG:HD2	1:C:100:THR:OG1	2.21	0.41
1:A:80:PHE:HA	1:A:81:PRO:HD2	1.87	0.41
1:D:57:VAL:HG23	1:D:58:TRP:CD1	2.49	0.41
1:A:222:GLU:OE2	1:A:224:HIS:NE2	2.47	0.41
3:A:601:NAG:O4	3:A:602:FUC:C1	2.69	0.41
1:A:6:ASN:ND2	1:A:8:ASN:HD21	2.05	0.41
1:C:36:VAL:O	1:C:36:VAL:HG13	2.20	0.41
1:D:203:ASN:HA	8:D:4417:HOH:O	2.20	0.41
1:B:50:LEU:HD11	1:B:92:PHE:CZ	2.55	0.41
1:C:57:VAL:HG23	1:C:58:TRP:HD1	1.85	0.41
1:B:73:SER:HA	1:B:160:ALA:O	2.20	0.41
1:B:9:GLN:HG2	1:B:10:PHE:N	2.35	0.41
1:C:84:HIS:HA	1:C:85:PRO:HD3	1.95	0.41
1:D:94:ALA:HB1	1:D:95:PRO:CD	2.51	0.41
1:A:175:VAL:HG13	1:A:188:ILE:CG2	2.51	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:GLN:HE21	1:C:217:GLN:CA	2.32	0.40
1:D:132:PRO:HD2	1:D:136:HIS:CE1	2.57	0.40
1:C:170:THR:O	1:C:171:LYS:HB2	2.22	0.40
1:D:77:ARG:O	1:D:79:PRO:HD3	2.21	0.40
5:C:601:NAG:H3	5:C:602:FUL:O2	2.21	0.40
5:C:602:FUL:HO2	5:C:603:NAG:H82	1.87	0.40
1:D:73:SER:HA	1:D:160:ALA:O	2.22	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	235/241 (98%)	224 (95%)	11 (5%)	0	100	100
1	B	235/241 (98%)	223 (95%)	12 (5%)	0	100	100
1	C	235/241 (98%)	224 (95%)	11 (5%)	0	100	100
1	D	235/241 (98%)	223 (95%)	12 (5%)	0	100	100
All	All	940/964 (98%)	894 (95%)	46 (5%)	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	204/210 (97%)	191 (94%)	13 (6%)	20	33
1	B	202/210 (96%)	187 (93%)	15 (7%)	16	26
1	C	202/210 (96%)	192 (95%)	10 (5%)	28	44
1	D	202/210 (96%)	192 (95%)	10 (5%)	28	44
All	All	810/840 (96%)	762 (94%)	48 (6%)	23	36

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	24	ARG
1	A	43	TRP
1	A	50	LEU
1	A	57	VAL
1	A	82	ARG
1	A	102	GLU
1	A	111	ASN
1	A	133	GLN
1	A	174	HIS
1	A	175	VAL
1	A	227	LEU
1	A	235	LEU
1	B	15	GLU
1	B	16	GLN
1	B	19	LEU
1	B	24	ARG
1	B	36	VAL
1	B	43	TRP
1	B	55	VAL
1	B	133	GLN
1	B	143	SER
1	B	144	VAL
1	B	145	ILE
1	B	149	THR
1	B	174	HIS
1	B	175	VAL
1	B	235	LEU
1	C	9	GLN
1	C	30	VAL
1	C	43	TRP
1	C	84	HIS
1	C	102	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	111	ASN
1	C	149	THR
1	C	174	HIS
1	C	175	VAL
1	C	196	GLN
1	D	30	VAL
1	D	43	TRP
1	D	102	GLU
1	D	111	ASN
1	D	133	GLN
1	D	145	ILE
1	D	149	THR
1	D	174	HIS
1	D	175	VAL
1	D	235	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	12	GLN
1	A	16	GLN
1	A	38	ASN
1	A	78	GLN
1	A	97	ASN
1	A	99	GLN
1	A	111	ASN
1	A	133	GLN
1	A	196	GLN
1	A	217	GLN
1	B	8	ASN
1	B	12	GLN
1	B	16	GLN
1	B	38	ASN
1	B	56	GLN
1	B	64	ASN
1	B	78	GLN
1	B	84	HIS
1	B	97	ASN
1	B	99	GLN
1	B	111	ASN
1	B	133	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	203	ASN
1	B	217	GLN
1	C	8	ASN
1	C	16	GLN
1	C	38	ASN
1	C	64	ASN
1	C	78	GLN
1	C	84	HIS
1	C	97	ASN
1	C	99	GLN
1	C	111	ASN
1	C	133	GLN
1	C	196	GLN
1	C	217	GLN
1	D	12	GLN
1	D	13	ASN
1	D	16	GLN
1	D	38	ASN
1	D	64	ASN
1	D	78	GLN
1	D	99	GLN
1	D	111	ASN
1	D	133	GLN
1	D	203	ASN
1	D	217	GLN

### 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](#)

25 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
3	NAG	A	501	1,3	14,14,15	0.54	0	15,19,21	0.74	0
3	FUC	A	502	3	9,10,11	0.55	0	13,14,16	0.72	0
3	NAG	A	503	3	14,14,15	0.50	0	15,19,21	0.76	1 (6%)
3	NAG	A	601	1,3	14,14,15	0.78	0	15,19,21	0.90	0
3	FUC	A	602	3	9,10,11	0.58	0	13,14,16	0.56	0
3	NAG	A	603	3	14,14,15	0.45	0	15,19,21	0.86	1 (6%)
3	NAG	B	501	1,3	14,14,15	0.56	0	15,19,21	0.87	1 (6%)
3	FUC	B	502	3	9,10,11	0.55	0	13,14,16	0.50	0
3	NAG	B	503	3	14,14,15	0.58	0	15,19,21	0.67	0
3	NAG	B	601	1,3	14,14,15	0.66	0	15,19,21	0.87	0
3	FUC	B	602	3	9,10,11	0.45	0	13,14,16	0.43	0
3	NAG	B	603	3	14,14,15	0.70	0	15,19,21	0.67	0
4	NAG	C	501	1,4	14,14,15	0.53	0	15,19,21	0.72	0
4	FUC	C	502	4	9,10,11	0.52	0	13,14,16	0.42	0
4	NAG	C	503	4	14,14,15	0.63	0	15,19,21	0.65	0
4	BMA	C	504	4	11,11,12	0.64	0	13,15,17	1.04	1 (7%)
5	NAG	C	601	1,5	14,14,15	0.68	0	15,19,21	0.90	1 (6%)
5	FUL	C	602	5	9,10,11	0.53	0	13,14,16	0.80	1 (7%)
5	NAG	C	603	5	14,14,15	0.60	0	15,19,21	0.83	0
3	NAG	D	501	1,3	14,14,15	0.74	0	15,19,21	0.71	0
3	FUC	D	502	3	9,10,11	0.52	0	13,14,16	0.38	0
3	NAG	D	503	3	14,14,15	0.72	0	15,19,21	0.63	0
3	NAG	D	601	1,3	14,14,15	0.95	0	15,19,21	0.86	0
3	FUC	D	602	3	9,10,11	0.39	0	13,14,16	0.79	0
3	NAG	D	603	3	14,14,15	0.60	0	15,19,21	0.79	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
3	NAG	A	501	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	502	3	-	0/0/17/20	0/1/1/1
3	NAG	A	503	3	-	0/6/23/26	0/1/1/1
3	NAG	A	601	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	602	3	-	0/0/17/20	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	603	3	-	0/6/23/26	0/1/1/1
3	NAG	B	501	1,3	-	0/6/23/26	0/1/1/1
3	FUC	B	502	3	-	0/0/17/20	0/1/1/1
3	NAG	B	503	3	-	0/6/23/26	0/1/1/1
3	NAG	B	601	1,3	-	0/6/23/26	0/1/1/1
3	FUC	B	602	3	-	0/0/17/20	0/1/1/1
3	NAG	B	603	3	-	0/6/23/26	0/1/1/1
4	NAG	C	501	1,4	-	0/6/23/26	0/1/1/1
4	FUC	C	502	4	-	0/0/17/20	0/1/1/1
4	NAG	C	503	4	-	0/6/23/26	0/1/1/1
4	BMA	C	504	4	-	0/2/19/22	1/1/1/1
5	NAG	C	601	1,5	-	0/6/23/26	0/1/1/1
5	FUL	C	602	5	-	0/0/17/20	0/1/1/1
5	NAG	C	603	5	-	0/6/23/26	0/1/1/1
3	NAG	D	501	1,3	-	0/6/23/26	0/1/1/1
3	FUC	D	502	3	-	0/0/17/20	0/1/1/1
3	NAG	D	503	3	-	0/6/23/26	0/1/1/1
3	NAG	D	601	1,3	-	2/6/23/26	0/1/1/1
3	FUC	D	602	3	-	0/0/17/20	0/1/1/1
3	NAG	D	603	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	NAG	C2-N2-C7	-2.38	119.48	122.94
3	A	603	NAG	C2-N2-C7	-2.31	119.58	122.94
3	A	503	NAG	C2-N2-C7	-2.19	119.75	122.94
5	C	601	NAG	C4-C3-C2	2.05	114.02	111.02
5	C	602	FUL	C1-C2-C3	2.23	112.47	109.65
4	C	504	BMA	C1-O5-C5	2.78	116.00	112.17

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	601	NAG	C8-C7-N2-C2
3	D	601	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	504	BMA	C1-C2-C3-C4-C5-O5

16 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	NAG	2	0
3	A	601	NAG	2	0
3	A	602	FUC	1	0
3	B	501	NAG	1	0
3	B	601	NAG	3	0
3	B	602	FUC	3	0
3	B	603	NAG	8	0
4	C	501	NAG	2	0
5	C	601	NAG	2	0
5	C	602	FUL	2	0
5	C	603	NAG	2	0
3	D	501	NAG	1	0
3	D	503	NAG	1	0
3	D	601	NAG	6	0
3	D	602	FUC	3	0
3	D	603	NAG	3	0

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	A2G	A	1401	-	15,15,15	1.68	3 (20%)	21,21,21	0.69	0
2	A2G	B	2401	-	15,15,15	1.67	2 (13%)	21,21,21	0.62	0
2	A2G	C	3401	-	15,15,15	1.71	3 (20%)	21,21,21	0.63	0
2	A2G	D	4401	-	15,15,15	1.69	2 (13%)	21,21,21	0.66	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	A2G	A	1401	-	-	0/6/26/26	0/1/1/1
2	A2G	B	2401	-	-	0/6/26/26	0/1/1/1
2	A2G	C	3401	-	-	0/6/26/26	0/1/1/1
2	A2G	D	4401	-	-	0/6/26/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3401	A2G	C3-C2	2.19	1.57	1.53
2	A	1401	A2G	C3-C2	2.39	1.57	1.53
2	A	1401	A2G	O-C1	3.56	1.49	1.43
2	B	2401	A2G	O-C1	3.61	1.49	1.43
2	D	4401	A2G	O-C1	3.68	1.49	1.43
2	C	3401	A2G	O-C1	3.77	1.50	1.43
2	C	3401	A2G	C1-C2	3.80	1.57	1.52
2	A	1401	A2G	C1-C2	3.86	1.57	1.52
2	D	4401	A2G	C1-C2	3.87	1.57	1.52
2	B	2401	A2G	C1-C2	3.91	1.57	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	237/241 (98%)	-0.20	3 (1%) 77 77	19, 33, 54, 67	0
1	B	237/241 (98%)	-0.24	4 (1%) 70 70	20, 33, 55, 63	0
1	C	237/241 (98%)	-0.26	1 (0%) 92 93	24, 35, 56, 71	0
1	D	237/241 (98%)	-0.21	6 (2%) 58 56	22, 37, 58, 77	0
All	All	948/964 (98%)	-0.23	14 (1%) 74 73	19, 34, 57, 77	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	GLY	4.0
1	D	237	GLY	3.7
1	B	115	PRO	3.5
1	D	114	SER	3.1
1	D	236	PRO	3.0
1	B	114	SER	2.7
1	B	237	GLY	2.5
1	B	82	ARG	2.3
1	C	9	GLN	2.3
1	D	8	ASN	2.3
1	A	216	LYS	2.2
1	D	27	SER	2.2
1	D	13	ASN	2.0
1	A	205	GLY	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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	BMA	C	504	11/12	0.84	0.35	5.98	71,72,73,73	0
3	NAG	D	501	14/15	0.82	0.34	2.69	71,74,79,84	0
3	NAG	A	501	14/15	0.95	0.23	1.51	50,53,58,60	0
3	NAG	B	601	14/15	0.88	0.20	0.58	47,56,64,65	0
4	NAG	C	501	14/15	0.92	0.15	0.31	45,52,57,58	0
3	NAG	B	501	14/15	0.89	0.14	-0.42	53,55,62,63	0
5	FUL	C	602	10/11	0.78	0.41	-	82,85,86,86	0
3	NAG	D	503	14/15	0.68	0.50	-	87,89,90,90	0
5	NAG	C	601	14/15	0.85	0.33	-	67,70,78,78	0
3	FUC	D	502	10/11	0.76	0.36	-	81,82,83,85	0
3	NAG	A	603	14/15	0.86	0.40	-	77,80,81,81	0
5	NAG	C	603	14/15	0.77	0.42	-	80,82,84,85	0
4	FUC	C	502	10/11	0.85	0.31	-	62,64,65,66	0
3	NAG	B	503	14/15	0.84	0.26	-	67,70,71,72	0
3	NAG	A	601	14/15	0.93	0.23	-	59,63,71,73	0
4	NAG	C	503	14/15	0.87	0.28	-	57,63,65,68	0
3	NAG	D	601	14/15	0.88	0.29	-	61,66,75,77	0
3	FUC	A	502	10/11	0.93	0.38	-	60,62,62,63	0
3	NAG	B	603	14/15	0.82	0.43	-	67,70,74,75	0
3	NAG	D	603	14/15	0.68	0.39	-	80,84,86,86	0
3	FUC	A	602	10/11	0.71	0.44	-	76,79,80,81	0
3	FUC	D	602	10/11	0.78	0.43	-	81,83,83,84	0
3	FUC	B	602	10/11	0.96	0.30	-	54,56,57,58	0
3	FUC	B	502	10/11	0.87	0.15	-	66,67,68,69	0
3	NAG	A	503	14/15	0.85	0.35	-	64,66,69,70	0

### 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	A2G	B	2401	15/15	0.95	0.15	-0.05	32,35,39,40	0
2	A2G	A	1401	15/15	0.94	0.17	-0.13	33,36,40,41	0
2	A2G	C	3401	15/15	0.93	0.15	-0.26	36,38,40,42	0
2	A2G	D	4401	15/15	0.95	0.13	-0.92	33,36,40,40	0
7	CA	D	4303	1/1	0.94	0.10	-1.76	27,27,27,27	0
7	CA	B	2303	1/1	1.00	0.10	-1.91	23,23,23,23	0
6	MN	B	2300	1/1	0.99	0.07	-2.59	31,31,31,31	0
6	MN	A	1300	1/1	0.98	0.06	-2.63	39,39,39,39	0
7	CA	C	3303	1/1	0.96	0.05	-3.20	32,32,32,32	0
7	CA	A	1303	1/1	0.99	0.05	-4.01	24,24,24,24	0
6	MN	C	3300	1/1	0.95	0.07	-4.01	43,43,43,43	0
6	MN	D	4300	1/1	0.99	0.03	-4.65	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.