



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2017 – 04:30 PM EST

PDB ID : 2ZML  
Title : Crystal structure of basic winged bean lectin in complex with Gal-ALPHA 1,4 Gal  
Authors : Kulkarni, K.A.; Katiyar, S.; Surolia, A.; Vijayan, M.; Suguna, K.  
Deposited on : 2008-04-19  
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.

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The following versions of software and data (see [references ⓘ](#)) 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-20028442  
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-20028442

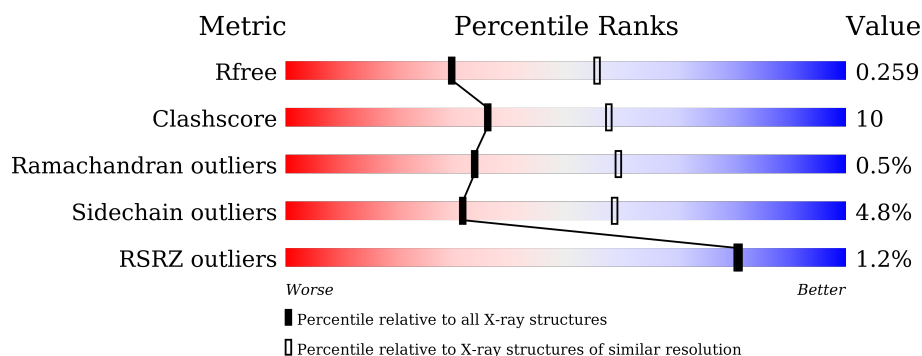
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (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>%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>..</div> </div> </div>
1	B	241	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>..</div> </div> </div>
1	C	241	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>..</div> </div> </div>
1	D	241	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>22%</div> <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	501	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7715 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
			1820	1172	304	344			
1	B	237	Total	C	N	O	0	0	0
			1821	1173	303	345			
1	C	237	Total	C	N	O	0	0	0
			1819	1172	305	342			
1	D	237	Total	C	N	O	0	0	0
			1791	1153	295	343			

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	2	Total	C	O	0	0
			23	12	11		
2	B	2	Total	C	O	0	0
			23	12	11		
2	C	2	Total	C	O	0	0
			23	12	11		
2	D	2	Total	C	O	0	0
			23	12	11		

- 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	B	3	Total	C	N	O	0	0
			38	22	2	14		
3	C	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			24	14	1	9		

- 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		
6	C	1	Total	Mn	0	0
			1	1		

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

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

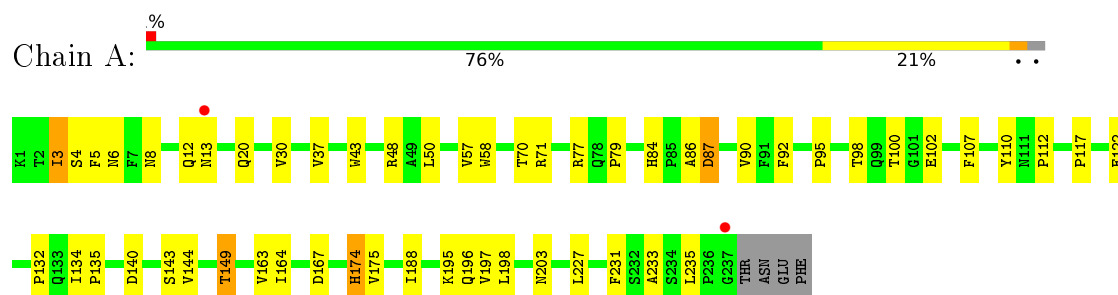
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	58	Total O 58 58	0	0
8	B	45	Total O 45 45	0	0
8	C	37	Total O 37 37	0	0
8	D	44	Total O 44 44	0	0

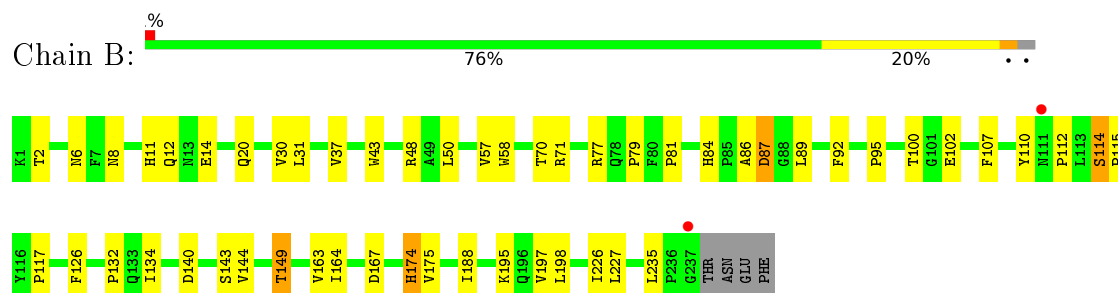
### 3 Residue-property plots [i](#)

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: Basic agglutinin



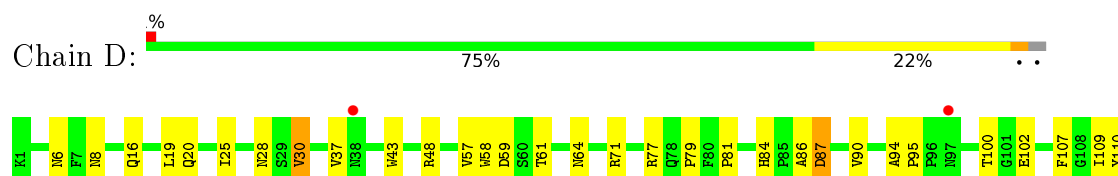
#### • Molecule 1: Basic agglutinin



#### • Molecule 1: Basic agglutinin



#### • Molecule 1: Basic agglutinin



N111	P112	L113	S114	P115	Y116	P117	F126	P132	Q133	I134	P135	D140	V141	N142	S143	V144	I145	T149	V163	D167	H174	V175	I188	V197	L198	L227	L235	P236	G237	THR	ASN	GLU	PHE
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.93 Å 91.52 Å 73.65 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.55 – 2.65 26.55 – 2.65	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.55-2.65) 96.6 (26.55-2.65)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.29 (at 2.64 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.206 , 0.247 0.219 , 0.259	Depositor DCC
$R_{free}$ test set	1468 reflections (4.77%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtriage
Anisotropy	1.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 43.8	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	0.93	EDS
Total number of atoms	7715	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: GLA, CA, MN, NAG, FUC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.38	0/1873	0.65	0/2566
1	B	0.39	0/1874	0.65	0/2568
1	C	0.37	0/1872	0.66	0/2565
1	D	0.37	0/1843	0.65	0/2530
All	All	0.38	0/7462	0.65	0/10229

There are no bond length outliers.

There are no bond angle outliers.

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	1820	0	1753	34	0
1	B	1821	0	1752	35	0
1	C	1819	0	1753	36	0
1	D	1791	0	1697	38	0
2	A	23	0	21	0	0
2	B	23	0	21	1	0
2	C	23	0	21	1	0
2	D	23	0	21	1	0
3	A	38	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	38	0	34	1	0
3	C	38	0	34	2	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	B	24	0	22	0	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	58	0	0	1	0
8	B	45	0	0	3	0
8	C	37	0	0	1	0
8	D	44	0	0	0	0
All	All	7715	0	7202	142	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 10.

All (142) 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:6:ASN:HD21	1:A:8:ASN:ND2	1.84	0.76
1:D:77:ARG:O	1:D:79:PRO:HD3	1.85	0.76
1:A:77:ARG:O	1:A:79:PRO:HD3	1.86	0.75
1:B:77:ARG:O	1:B:79:PRO:HD3	1.85	0.75
1:A:132:PRO:HG3	1:A:149:THR:HG21	1.71	0.72
1:A:197:VAL:HG23	1:A:198:LEU:HG	1.70	0.72
1:A:196:GLN:HE22	1:D:145:ILE:HB	1.52	0.72
1:D:197:VAL:HG23	1:D:198:LEU:HG	1.72	0.71
1:B:197:VAL:HG23	1:B:198:LEU:HG	1.71	0.71
1:A:6:ASN:HD21	1:A:8:ASN:HD21	1.36	0.71
1:C:197:VAL:HG23	1:C:198:LEU:HG	1.70	0.71
1:C:77:ARG:O	1:C:79:PRO:HD3	1.88	0.71
1:D:132:PRO:HG3	1:D:149:THR:HG21	1.73	0.70
1:C:132:PRO:HG3	1:C:149:THR:HG21	1.74	0.69
1:B:132:PRO:HG3	1:B:149:THR:HG21	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLN:NE2	1:D:145:ILE:HB	2.07	0.68
1:A:140:ASP:HB3	1:A:143:SER:O	1.94	0.67
1:D:6:ASN:HD21	1:D:8:ASN:ND2	1.93	0.67
1:D:140:ASP:HB3	1:D:143:SER:O	1.96	0.65
1:C:140:ASP:HB3	1:C:143:SER:O	1.96	0.65
1:B:140:ASP:HB3	1:B:143:SER:O	1.97	0.65
1:C:6:ASN:HD21	1:C:8:ASN:ND2	1.98	0.61
1:C:175:VAL:HG22	1:C:188:ILE:HG22	1.82	0.61
1:D:175:VAL:HG22	1:D:188:ILE:HG22	1.82	0.61
1:B:81:PRO:HG3	8:B:670:HOH:O	2.00	0.60
1:B:149:THR:HB	8:B:663:HOH:O	2.00	0.60
1:A:175:VAL:HG22	1:A:188:ILE:HG22	1.84	0.59
1:B:175:VAL:HG22	1:B:188:ILE:HG22	1.84	0.59
1:D:20:GLN:OE1	1:D:48:ARG:HD3	2.03	0.58
1:A:110:TYR:CE2	1:A:112:PRO:HG3	2.39	0.58
1:C:110:TYR:CE2	1:C:112:PRO:HG3	2.40	0.57
1:A:3:ILE:HD13	1:A:4:SER:N	2.19	0.57
1:D:90:VAL:HG21	1:D:109:ILE:HD13	1.87	0.56
1:B:110:TYR:CE2	1:B:112:PRO:HG3	2.39	0.56
1:D:110:TYR:CE2	1:D:112:PRO:HG3	2.41	0.56
1:B:84:HIS:HD2	1:B:84:HIS:O	1.90	0.54
1:C:3:ILE:C	1:C:3:ILE:HD13	2.29	0.53
1:C:95:PRO:O	1:C:98:THR:HG23	2.09	0.53
1:B:114:SER:N	1:B:115:PRO:HD3	2.23	0.52
1:B:84:HIS:O	1:B:84:HIS:CD2	2.63	0.52
1:C:89:LEU:C	1:C:89:LEU:HD12	2.30	0.52
1:B:2:THR:O	1:B:2:THR:HG23	2.10	0.51
1:D:126:PHE:CE2	2:D:400:GLA:H3	2.45	0.51
1:C:48:ARG:HD2	1:C:100:THR:OG1	2.09	0.51
1:B:89:LEU:C	1:B:89:LEU:HD12	2.31	0.51
3:B:501:NAG:O4	3:B:502:FUC:H5	2.11	0.51
1:C:3:ILE:HD13	1:C:4:SER:N	2.25	0.50
1:D:113:LEU:C	1:D:115:PRO:HD3	2.31	0.50
1:D:84:HIS:O	1:D:84:HIS:HD2	1.95	0.50
1:C:83:PRO:HD3	3:C:501:NAG:C8	2.43	0.49
1:D:64:ASN:HB3	1:D:236:PRO:HG2	1.94	0.49
1:D:79:PRO:O	1:D:81:PRO:HD3	2.11	0.49
1:B:6:ASN:HD21	1:B:8:ASN:ND2	2.11	0.49
1:D:84:HIS:CD2	1:D:84:HIS:O	2.66	0.48
1:A:5:PHE:CZ	1:A:231:PHE:HB3	2.49	0.48
1:B:57:VAL:HG23	1:B:58:TRP:HD1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:GLN:NE2	1:C:16:GLN:HA	2.29	0.47
1:C:86:ALA:O	1:C:210:THR:HA	2.14	0.47
1:D:57:VAL:HG23	1:D:58:TRP:HD1	1.79	0.47
8:C:616:HOH:O	1:D:174:HIS:HB2	2.14	0.47
1:C:57:VAL:HG23	1:C:58:TRP:HD1	1.79	0.47
1:B:174:HIS:CD2	1:B:174:HIS:N	2.83	0.47
1:B:48:ARG:HD2	1:B:100:THR:OG1	2.15	0.47
1:A:57:VAL:HG23	1:A:58:TRP:HD1	1.81	0.46
1:B:126:PHE:CE2	2:B:400:GLA:H3	2.50	0.46
1:D:113:LEU:O	1:D:115:PRO:HD3	2.15	0.46
1:A:71:ARG:HG2	1:A:163:VAL:HG22	1.97	0.46
1:B:58:TRP:CE3	1:B:195:LYS:HG3	2.50	0.46
1:B:95:PRO:HD3	1:B:117:PRO:O	2.16	0.46
1:C:84:HIS:O	1:C:220:ALA:HA	2.16	0.46
1:C:71:ARG:HG2	1:C:163:VAL:HG22	1.98	0.46
1:D:174:HIS:CD2	1:D:174:HIS:N	2.83	0.46
1:A:3:ILE:HG22	1:A:233:ALA:HB3	1.98	0.46
1:A:70:THR:HG22	1:A:164:ILE:HB	1.98	0.46
1:A:20:GLN:OE1	1:A:48:ARG:HD3	2.16	0.45
1:C:174:HIS:CD2	1:C:174:HIS:N	2.84	0.45
1:D:227:LEU:CD1	1:D:227:LEU:N	2.79	0.45
1:B:227:LEU:CD1	1:B:227:LEU:N	2.80	0.45
1:B:144:VAL:HG13	8:B:646:HOH:O	2.16	0.45
1:B:71:ARG:HG2	1:B:163:VAL:HG22	1.99	0.45
1:C:20:GLN:OE1	1:C:48:ARG:HD3	2.16	0.45
1:A:174:HIS:CD2	1:A:174:HIS:N	2.85	0.45
1:D:134:ILE:HD12	1:D:134:ILE:O	2.17	0.45
1:A:86:ALA:HB1	1:A:87:ASP:OD1	2.17	0.45
1:D:134:ILE:HD12	1:D:134:ILE:C	2.38	0.45
1:C:83:PRO:HD3	3:C:501:NAG:H81	1.99	0.44
1:D:48:ARG:HD2	1:D:100:THR:OG1	2.16	0.44
1:B:70:THR:HG22	1:B:164:ILE:HB	1.99	0.44
1:C:134:ILE:O	1:C:134:ILE:HD12	2.17	0.44
1:A:95:PRO:HD3	1:A:117:PRO:O	2.16	0.44
1:C:95:PRO:HD3	1:C:117:PRO:O	2.18	0.44
1:A:37:VAL:HG23	1:A:37:VAL:O	2.18	0.44
1:D:28:ASN:OD1	1:D:30:VAL:HG13	2.18	0.44
1:C:80:PHE:HA	1:C:81:PRO:HD2	1.90	0.43
1:A:227:LEU:N	1:A:227:LEU:CD1	2.81	0.43
1:B:144:VAL:CG1	1:B:144:VAL:O	2.66	0.43
1:C:134:ILE:HD12	1:C:134:ILE:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:VAL:CG1	1:D:144:VAL:O	2.66	0.43
1:A:90:VAL:HG12	1:A:122:GLU:HA	1.99	0.43
1:A:58:TRP:CE3	1:A:195:LYS:HG3	2.53	0.43
1:B:86:ALA:HA	1:B:87:ASP:HA	1.85	0.43
1:D:111:ASN:ND2	1:D:114:SER:H	2.17	0.43
1:B:37:VAL:HG23	1:B:37:VAL:O	2.19	0.43
1:A:144:VAL:CG1	1:A:144:VAL:O	2.67	0.42
1:B:50:LEU:HD11	1:B:92:PHE:CZ	2.54	0.42
1:C:37:VAL:O	1:C:37:VAL:HG23	2.19	0.42
1:B:11:HIS:O	1:B:14:GLU:HG2	2.18	0.42
1:B:20:GLN:OE1	1:B:48:ARG:HD3	2.18	0.42
1:D:71:ARG:HG2	1:D:163:VAL:HG22	2.01	0.42
1:A:12:GLN:O	1:A:13:ASN:HB2	2.19	0.42
1:A:203:ASN:HA	8:A:612:HOH:O	2.18	0.42
1:A:50:LEU:HD11	1:A:92:PHE:CZ	2.55	0.42
1:D:134:ILE:HB	1:D:135:PRO:HA	2.01	0.42
1:A:134:ILE:HD12	1:A:134:ILE:O	2.20	0.42
1:D:37:VAL:O	1:D:37:VAL:HG23	2.19	0.42
1:C:134:ILE:HB	1:C:135:PRO:HA	2.01	0.42
1:B:134:ILE:C	1:B:134:ILE:HD12	2.40	0.42
1:B:134:ILE:O	1:B:134:ILE:HD12	2.20	0.42
1:C:227:LEU:CD1	1:C:227:LEU:N	2.82	0.42
1:A:134:ILE:HD12	1:A:134:ILE:C	2.41	0.42
1:B:31:LEU:HB3	1:B:226:ILE:HB	2.01	0.42
1:C:48:ARG:HD2	1:C:100:THR:HA	2.01	0.41
1:A:134:ILE:HB	1:A:135:PRO:HA	2.01	0.41
1:A:86:ALA:HB1	1:A:87:ASP:CG	2.40	0.41
1:B:174:HIS:CD2	1:B:174:HIS:H	2.38	0.41
1:C:144:VAL:O	1:C:144:VAL:CG1	2.67	0.41
1:C:84:HIS:HA	1:C:85:PRO:HD3	1.88	0.41
1:D:94:ALA:HB1	1:D:95:PRO:CD	2.50	0.41
1:C:126:PHE:CE2	2:C:400:GLA:H3	2.55	0.41
1:D:235:LEU:O	1:D:236:PRO:C	2.59	0.41
1:D:86:ALA:HA	1:D:87:ASP:HA	1.91	0.41
1:C:70:THR:HG22	1:C:164:ILE:HB	2.02	0.41
1:D:174:HIS:H	1:D:174:HIS:CD2	2.39	0.41
1:B:70:THR:CG2	1:B:164:ILE:HB	2.51	0.41
1:D:117:PRO:HA	1:D:142:ASN:OD1	2.20	0.41
1:D:19:LEU:HD21	1:D:25:ILE:HG13	2.03	0.41
1:D:59:ASP:OD2	1:D:61:THR:HB	2.21	0.41
1:C:174:HIS:H	1:C:174:HIS:CD2	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ARG:HD2	1:A:100:THR:OG1	2.22	0.40
1:A:95:PRO:O	1:A:98:THR:HG23	2.22	0.40
1:C:3:ILE:CG2	1:C:233:ALA:HB3	2.52	0.40
1:C:44:ASN:HB2	1:C:213:PRO:HG3	2.03	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%)	225 (96%)	9 (4%)	1 (0%)	39	65
1	B	235/241 (98%)	224 (95%)	9 (4%)	2 (1%)	21	44
1	C	235/241 (98%)	225 (96%)	9 (4%)	1 (0%)	39	65
1	D	235/241 (98%)	221 (94%)	13 (6%)	1 (0%)	39	65
All	All	940/964 (98%)	895 (95%)	40 (4%)	5 (0%)	34	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	114	SER
1	D	107	PHE
1	A	107	PHE
1	B	107	PHE
1	C	107	PHE

### 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	199/210 (95%)	189 (95%)	10 (5%)	30	56
1	B	199/210 (95%)	190 (96%)	9 (4%)	34	61
1	C	198/210 (94%)	188 (95%)	10 (5%)	29	55
1	D	193/210 (92%)	184 (95%)	9 (5%)	32	60
All	All	789/840 (94%)	751 (95%)	38 (5%)	31	59

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	30	VAL
1	A	43	TRP
1	A	84	HIS
1	A	87	ASP
1	A	102	GLU
1	A	149	THR
1	A	167	ASP
1	A	174	HIS
1	A	235	LEU
1	B	12	GLN
1	B	30	VAL
1	B	43	TRP
1	B	87	ASP
1	B	102	GLU
1	B	149	THR
1	B	167	ASP
1	B	174	HIS
1	B	235	LEU
1	C	3	ILE
1	C	14	GLU
1	C	30	VAL
1	C	43	TRP
1	C	87	ASP
1	C	102	GLU
1	C	149	THR
1	C	167	ASP
1	C	174	HIS
1	C	235	LEU
1	D	16	GLN

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Mol	Chain	Res	Type
1	D	30	VAL
1	D	43	TRP
1	D	87	ASP
1	D	102	GLU
1	D	149	THR
1	D	167	ASP
1	D	174	HIS
1	D	235	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	12	GLN
1	A	64	ASN
1	A	78	GLN
1	A	84	HIS
1	A	97	ASN
1	A	196	GLN
1	A	203	ASN
1	B	8	ASN
1	B	9	GLN
1	B	12	GLN
1	B	38	ASN
1	B	64	ASN
1	B	78	GLN
1	B	84	HIS
1	B	97	ASN
1	B	203	ASN
1	C	8	ASN
1	C	16	GLN
1	C	38	ASN
1	C	64	ASN
1	C	78	GLN
1	C	97	ASN
1	C	196	GLN
1	D	8	ASN
1	D	16	GLN
1	D	38	ASN
1	D	78	GLN
1	D	84	HIS
1	D	99	GLN

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Mol	Chain	Res	Type
1	D	111	ASN
1	D	203	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 ⓘ

19 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	GLA	A	400	2	11,11,12	0.87	0	15,15,17	0.72	0
2	GLA	A	401	2	12,12,12	0.98	0	17,17,17	0.91	0
3	NAG	A	501	1,3	14,14,15	0.49	0	15,19,21	0.88	1 (6%)
3	FUC	A	502	3	10,10,11	0.63	0	13,14,16	0.64	0
3	NAG	A	503	3	14,14,15	0.48	0	15,19,21	0.84	1 (6%)
2	GLA	B	400	2	11,11,12	0.79	0	15,15,17	0.81	0
2	GLA	B	401	2	12,12,12	0.88	1 (8%)	17,17,17	0.83	0
3	NAG	B	501	1,3	14,14,15	0.47	0	15,19,21	0.73	1 (6%)
3	FUC	B	502	3	10,10,11	0.52	0	13,14,16	0.38	0
3	NAG	B	503	3	14,14,15	0.55	0	15,19,21	0.76	1 (6%)
5	NAG	B	601	1,5	14,14,15	0.72	0	15,19,21	0.81	1 (6%)
5	FUC	B	602	5	10,10,11	0.50	0	13,14,16	0.36	0
2	GLA	C	400	2	11,11,12	0.79	0	15,15,17	0.76	0
2	GLA	C	401	2	12,12,12	0.92	0	17,17,17	0.88	0
3	NAG	C	501	1,3	14,14,15	0.64	0	15,19,21	0.78	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FUC	C	502	3	10,10,11	0.53	0	13,14,16	0.32	0
3	NAG	C	503	3	14,14,15	0.45	0	15,19,21	0.77	1 (6%)
2	GLA	D	400	2	11,11,12	1.08	0	15,15,17	0.78	0
2	GLA	D	401	2	12,12,12	1.14	0	17,17,17	0.91	1 (5%)

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	GLA	A	400	2	-	0/2/19/22	0/1/1/1
2	GLA	A	401	2	-	0/2/22/22	0/1/1/1
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
2	GLA	B	400	2	-	0/2/19/22	0/1/1/1
2	GLA	B	401	2	-	0/2/22/22	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
5	NAG	B	601	1,5	-	0/6/23/26	0/1/1/1
5	FUC	B	602	5	-	0/0/17/20	0/1/1/1
2	GLA	C	400	2	-	0/2/19/22	0/1/1/1
2	GLA	C	401	2	-	0/2/22/22	0/1/1/1
3	NAG	C	501	1,3	-	0/6/23/26	0/1/1/1
3	FUC	C	502	3	-	0/0/17/20	0/1/1/1
3	NAG	C	503	3	-	0/6/23/26	0/1/1/1
2	GLA	D	400	2	-	0/2/19/22	0/1/1/1
2	GLA	D	401	2	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	GLA	O5-C1	2.05	1.47	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NAG	C2-N2-C7	-2.85	119.40	123.11
3	A	503	NAG	C2-N2-C7	-2.58	119.75	123.11
3	C	503	NAG	C2-N2-C7	-2.49	119.87	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	NAG	C2-N2-C7	-2.37	120.02	123.11
3	B	501	NAG	C2-N2-C7	-2.16	120.29	123.11
2	D	401	GLA	C3-C4-C5	-2.07	106.53	110.23
5	B	601	NAG	C2-N2-C7	-2.06	120.43	123.11
3	C	501	NAG	C2-N2-C7	-2.05	120.44	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	GLA	1	0
3	B	501	NAG	1	0
3	B	502	FUC	1	0
2	C	400	GLA	1	0
3	C	501	NAG	2	0
2	D	400	GLA	1	0

## 5.6 Ligand geometry

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	$\# Z  > 2$
4	NAG	A	601	1	14,14,15	0.53	0	15,19,21	0.85	1 (6%)
4	NAG	C	601	1	14,14,15	0.56	0	15,19,21	0.70	0
4	NAG	D	601	1	14,14,15	0.57	0	15,19,21	0.78	1 (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
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1
4	NAG	C	601	1	-	0/6/23/26	0/1/1/1
4	NAG	D	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAG	C2-N2-C7	-2.35	120.04	123.11
4	D	601	NAG	C2-N2-C7	-2.28	120.14	123.11

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%)	-0.35	2 (0%) 87 87	8, 21, 39, 46	0
1	B	237/241 (98%)	-0.29	2 (0%) 87 87	10, 23, 44, 51	0
1	C	237/241 (98%)	-0.25	4 (1%) 73 72	13, 24, 46, 60	0
1	D	237/241 (98%)	-0.17	3 (1%) 79 79	13, 25, 47, 59	0
All	All	948/964 (98%)	-0.26	11 (1%) 81 80	8, 24, 45, 60	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	237	GLY	3.6
1	C	13	ASN	3.3
1	A	237	GLY	2.9
1	A	13	ASN	2.8
1	B	237	GLY	2.8
1	C	89	LEU	2.4
1	D	38	ASN	2.3
1	C	11	HIS	2.3
1	C	237	GLY	2.1
1	D	97	ASN	2.1
1	B	111	ASN	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<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
3	NAG	B	501	14/15	0.89	0.22	3.54	43,49,56,56	0
2	GLA	D	401	12/12	0.82	0.22	0.91	42,45,48,51	0
5	NAG	B	601	14/15	0.85	0.20	0.53	40,47,54,57	0
2	GLA	A	400	11/12	0.91	0.16	0.39	37,38,39,40	0
2	GLA	C	400	11/12	0.92	0.18	0.29	38,39,40,43	0
3	NAG	C	501	14/15	0.91	0.19	0.09	35,38,42,44	0
2	GLA	A	401	12/12	0.84	0.17	0.09	43,47,48,51	0
2	GLA	B	400	11/12	0.96	0.13	-0.62	23,26,28,28	0
2	GLA	D	400	11/12	0.93	0.13	-0.77	39,41,41,41	0
3	NAG	A	501	14/15	0.93	0.14	-1.04	36,38,40,43	0
3	FUC	C	502	10/11	0.87	0.29	-	46,47,48,50	0
2	GLA	B	401	12/12	0.90	0.18	-	30,32,35,41	0
3	FUC	A	502	10/11	0.92	0.21	-	39,41,42,43	0
3	NAG	A	503	14/15	0.89	0.28	-	47,49,51,51	0
5	FUC	B	602	10/11	0.91	0.26	-	44,47,48,48	0
3	NAG	B	503	14/15	0.79	0.31	-	61,63,65,66	0
3	NAG	C	503	14/15	0.87	0.19	-	47,48,51,53	0
2	GLA	C	401	12/12	0.84	0.20	-	41,42,44,48	0
3	FUC	B	502	10/11	0.84	0.24	-	57,58,60,61	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(Å <sup>2</sup> )	Q<0.9
4	NAG	A	601	14/15	0.89	0.24	1.42	41,44,46,49	0
7	CA	D	303	1/1	0.98	0.16	0.29	19,19,19,19	0
7	CA	A	303	1/1	0.96	0.17	0.22	16,16,16,16	0
7	CA	B	303	1/1	0.96	0.15	0.14	16,16,16,16	0
7	CA	C	303	1/1	0.93	0.12	-1.40	25,25,25,25	0
6	MN	A	300	1/1	0.99	0.04	-2.80	27,27,27,27	0
6	MN	B	300	1/1	0.99	0.03	-3.42	21,21,21,21	0
6	MN	D	300	1/1	0.98	0.06	-3.43	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MN	C	300	1/1	0.98	0.05	-3.44	30,30,30,30	0
4	NAG	D	601	14/15	0.84	0.21	-	41,45,47,47	0
4	NAG	C	601	14/15	0.86	0.29	-	52,57,62,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.