



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:06 PM GMT

PDB ID : 3W5G  
Title : Crystal structure of tomato beta-galactosidase 4 in complex with galactose  
Authors : Eda, M.; Tada, T.  
Deposited on : 2013-01-29  
Resolution : 3.00 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

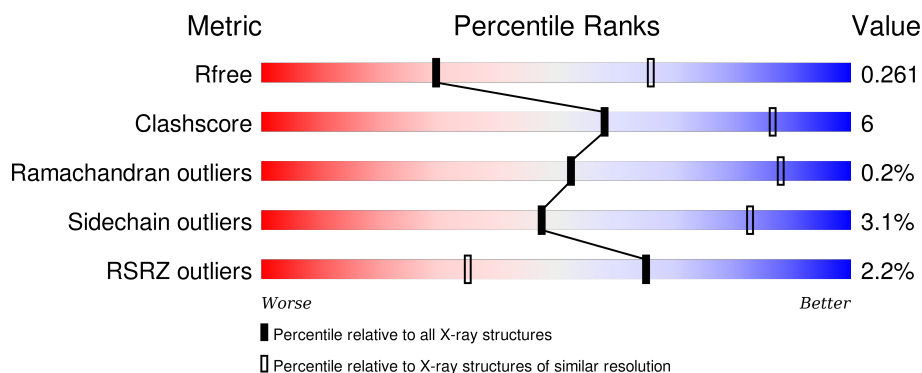
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	718	
1	B	718	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GAL	A	804	-	-	-	X
3	GAL	B	801	-	-	-	X
3	GAL	B	806	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11426 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	705	Total	C	N	O	S	0	0	0
			5531	3535	944	1025	27			
1	B	705	Total	C	N	O	S	0	0	0
			5531	3535	944	1025	27			

There are 34 discrepancies between the modelled and reference sequences:

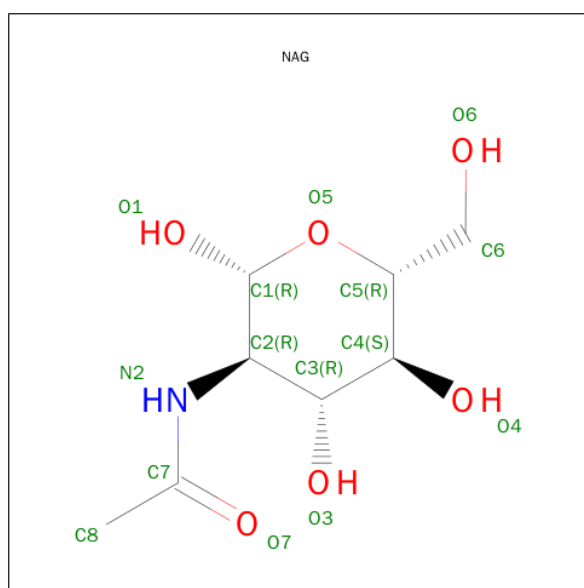
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLU	-	EXPRESSION TAG	UNP O81100
A	19	ALA	-	EXPRESSION TAG	UNP O81100
A	20	GLU	-	EXPRESSION TAG	UNP O81100
A	21	ALA	-	EXPRESSION TAG	UNP O81100
A	22	GLU	-	EXPRESSION TAG	UNP O81100
A	23	PHE	-	EXPRESSION TAG	UNP O81100
A	725	SER	-	EXPRESSION TAG	UNP O81100
A	726	ALA	-	EXPRESSION TAG	UNP O81100
A	727	ALA	-	EXPRESSION TAG	UNP O81100
A	728	ALA	-	EXPRESSION TAG	UNP O81100
A	729	ALA	-	EXPRESSION TAG	UNP O81100
A	730	SER	-	EXPRESSION TAG	UNP O81100
A	731	PHE	-	EXPRESSION TAG	UNP O81100
A	732	LEU	-	EXPRESSION TAG	UNP O81100
A	733	GLU	-	EXPRESSION TAG	UNP O81100
A	734	GLN	-	EXPRESSION TAG	UNP O81100
A	735	LYS	-	EXPRESSION TAG	UNP O81100
B	18	GLU	-	EXPRESSION TAG	UNP O81100
B	19	ALA	-	EXPRESSION TAG	UNP O81100
B	20	GLU	-	EXPRESSION TAG	UNP O81100
B	21	ALA	-	EXPRESSION TAG	UNP O81100
B	22	GLU	-	EXPRESSION TAG	UNP O81100
B	23	PHE	-	EXPRESSION TAG	UNP O81100
B	725	SER	-	EXPRESSION TAG	UNP O81100
B	726	ALA	-	EXPRESSION TAG	UNP O81100

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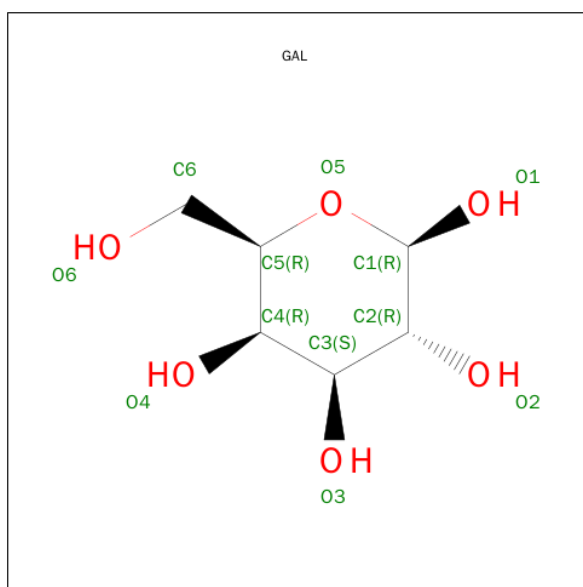
Chain	Residue	Modelled	Actual	Comment	Reference
B	727	ALA	-	EXPRESSION TAG	UNP O81100
B	728	ALA	-	EXPRESSION TAG	UNP O81100
B	729	ALA	-	EXPRESSION TAG	UNP O81100
B	730	SER	-	EXPRESSION TAG	UNP O81100
B	731	PHE	-	EXPRESSION TAG	UNP O81100
B	732	LEU	-	EXPRESSION TAG	UNP O81100
B	733	GLU	-	EXPRESSION TAG	UNP O81100
B	734	GLN	-	EXPRESSION TAG	UNP O81100
B	735	LYS	-	EXPRESSION TAG	UNP O81100

- Molecule 2 is SUGAR (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	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		

- Molecule 3 is SUGAR (BETA-D-GALACTOSE) (three-letter code: GAL) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

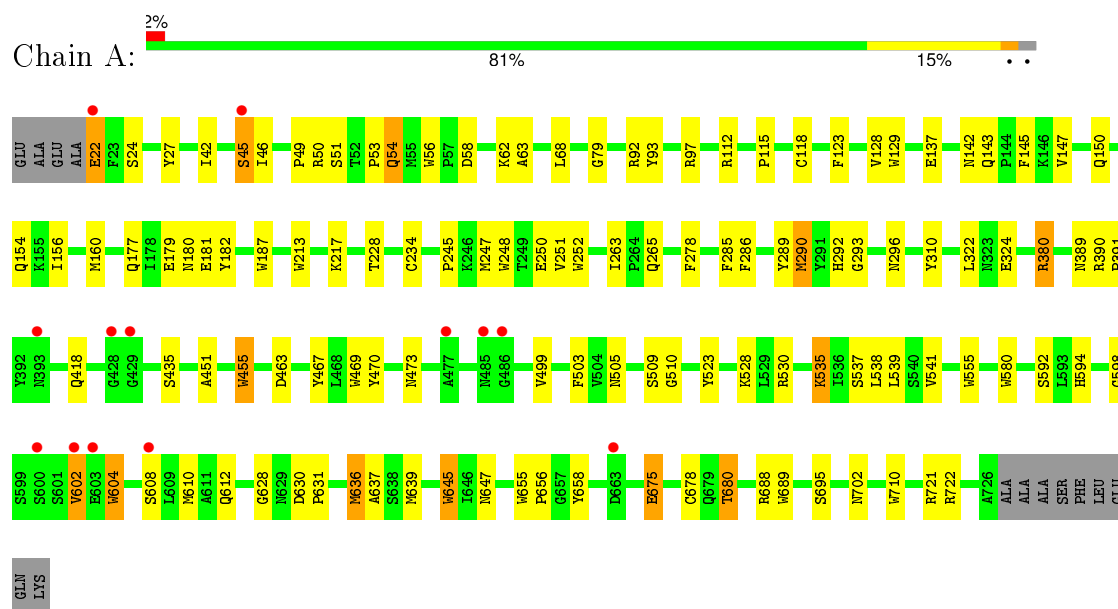
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	103	Total 103	O 103	0	0
5	B	95	Total 95	O 95	0	0

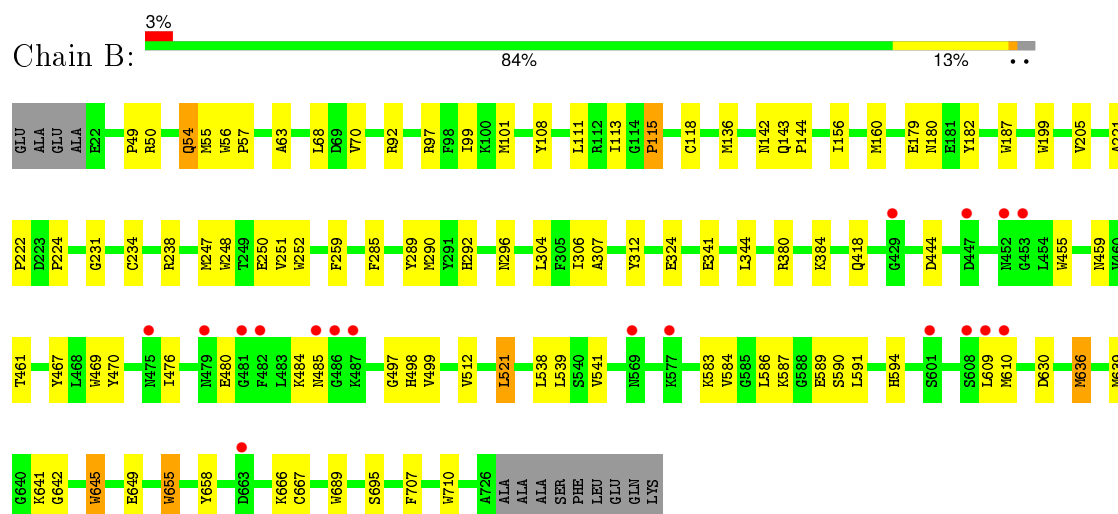
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Beta-galactosidase



#### • Molecule 1: Beta-galactosidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.93Å 106.38Å 162.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.06 – 3.00 31.06 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (31.06-3.00) 98.8 (31.06-3.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.81 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.200 , 0.259 0.201 , 0.261	Depositor DCC
$R_{free}$ test set	1653 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.8	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 34.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 32721 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11426	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.54	12/5694 (0.2%)	0.52	0/7739
1	B	0.54	7/5694 (0.1%)	0.52	0/7739
All	All	0.54	19/11388 (0.2%)	0.52	0/15478

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	689	TRP	CD2-CE2	5.51	1.48	1.41
1	A	689	TRP	CD2-CE2	5.43	1.47	1.41
1	B	187	TRP	CD2-CE2	5.38	1.47	1.41
1	A	710	TRP	CD2-CE2	5.22	1.47	1.41
1	A	213	TRP	CD2-CE2	5.19	1.47	1.41
1	A	555	TRP	CD2-CE2	5.17	1.47	1.41
1	A	469	TRP	CD2-CE2	5.15	1.47	1.41
1	A	604	TRP	CD2-CE2	5.13	1.47	1.41
1	A	129	TRP	CD2-CE2	5.11	1.47	1.41
1	B	655	TRP	CD2-CE2	5.10	1.47	1.41
1	A	455	TRP	CD2-CE2	5.09	1.47	1.41
1	B	710	TRP	CD2-CE2	5.09	1.47	1.41
1	A	580	TRP	CD2-CE2	5.08	1.47	1.41
1	A	645	TRP	CD2-CE2	5.06	1.47	1.41
1	B	56	TRP	CD2-CE2	5.05	1.47	1.41
1	B	199	TRP	CD2-CE2	5.05	1.47	1.41
1	A	187	TRP	CD2-CE2	5.04	1.47	1.41
1	B	645	TRP	CD2-CE2	5.01	1.47	1.41
1	A	56	TRP	CD2-CE2	5.01	1.47	1.41

There are no bond angle outliers.

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	5531	0	5350	77	0
1	B	5531	0	5350	54	0
2	A	28	0	26	0	0
2	B	14	0	13	4	0
3	A	48	0	48	1	0
3	B	48	0	48	1	0
4	B	28	0	25	0	0
5	A	103	0	0	2	0
5	B	95	0	0	1	0
All	All	11426	0	10860	130	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 (130) 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:435:SER:HB3	1:A:610:MET:HE2	1.25	1.16
1:A:435:SER:HB3	1:A:610:MET:CE	1.82	1.07
1:A:45:SER:HB3	1:A:290:MET:CE	2.03	0.89
1:A:435:SER:CB	1:A:610:MET:HE2	2.10	0.79
1:A:602:VAL:HA	1:A:604:TRP:HD1	1.49	0.78
1:A:435:SER:CB	1:A:610:MET:CE	2.64	0.74
1:B:459:ASN:HD22	2:B:804:NAG:H83	1.60	0.66
1:A:50:ARG:HE	1:A:296:ASN:HD21	1.42	0.66
1:A:636:MET:CE	1:A:639:MET:HG3	2.27	0.65
1:A:45:SER:HB3	1:A:290:MET:HE2	1.79	0.65
1:B:499:VAL:HB	1:B:541:VAL:HB	1.78	0.64
1:A:50:ARG:HE	1:A:296:ASN:ND2	1.97	0.63
1:A:54:GLN:HG3	1:A:695:SER:HB2	1.83	0.61
1:A:435:SER:HB3	1:A:610:MET:HE1	1.78	0.59
1:A:293:GLY:HA3	1:A:310:TYR:O	2.03	0.59
1:B:469:TRP:HB2	1:B:583:LYS:HB3	1.85	0.59
1:B:455:TRP:CD1	2:B:804:NAG:H82	2.37	0.59
1:B:476:ILE:HG23	1:B:480:GLU:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:SER:HB3	1:A:290:MET:HE3	1.85	0.58
1:A:602:VAL:HA	1:A:604:TRP:CD1	2.36	0.57
1:B:179:GLU:HG3	1:B:180:ASN:N	2.19	0.57
1:A:22:GLU:HG2	1:B:380:ARG:HD2	1.86	0.57
1:A:470:TYR:HB2	1:A:538:LEU:HB2	1.87	0.56
1:B:250:GLU:OE1	3:B:805:GAL:H1	2.05	0.56
1:B:587:LYS:O	1:B:591:LEU:HD12	2.05	0.56
1:B:247:MET:HG2	1:B:285:PHE:HB3	1.86	0.56
1:B:179:GLU:HG3	1:B:180:ASN:H	1.70	0.56
1:A:63:ALA:HB1	1:A:68:LEU:HD12	1.87	0.55
1:A:435:SER:CB	1:A:610:MET:HE1	2.36	0.55
1:A:505:ASN:ND2	1:A:535:LYS:H	2.05	0.55
1:B:156:ILE:O	1:B:160:MET:HG2	2.09	0.53
1:B:205:VAL:HG21	1:B:224:PRO:HD2	1.90	0.52
1:B:259:PHE:CE2	1:B:307:ALA:HA	2.43	0.52
1:B:636:MET:CE	1:B:639:MET:HG3	2.40	0.52
1:A:234:CYS:HB2	1:A:248:TRP:CD2	2.45	0.52
1:A:252:TRP:HA	1:A:289:TYR:O	2.09	0.52
1:A:380:ARG:HB3	1:A:380:ARG:HH11	1.75	0.52
1:B:179:GLU:HG2	1:B:182:TYR:HB2	1.91	0.51
1:A:247:MET:HG2	1:A:285:PHE:HB3	1.93	0.51
1:A:647:ASN:HD21	1:A:702:ASN:HA	1.76	0.51
1:B:455:TRP:CZ2	2:B:804:NAG:H4	2.46	0.51
1:B:304:LEU:O	1:B:306:ILE:HD12	2.12	0.50
1:B:636:MET:HE3	1:B:639:MET:HG3	1.93	0.50
1:B:57:PRO:HG3	1:B:101:MET:SD	2.52	0.50
1:A:62:LYS:HD3	1:A:322:LEU:HD21	1.93	0.50
1:B:143:GLN:HB3	1:B:144:PRO:HD3	1.93	0.50
1:A:179:GLU:HG2	1:A:182:TYR:HB2	1.95	0.49
1:B:609:LEU:O	1:B:610:MET:C	2.49	0.48
1:B:231:GLY:HA2	1:B:252:TRP:CZ3	2.48	0.48
1:A:181:GLU:HG2	1:A:217:LYS:HB2	1.94	0.48
1:A:42:ILE:HG12	1:A:286:PHE:CZ	2.49	0.48
1:A:234:CYS:O	1:A:278:PHE:HD1	1.96	0.48
1:A:150:GLN:O	1:A:154:GLN:HB2	2.14	0.48
1:A:592:SER:O	1:A:598:GLY:HA3	2.14	0.48
1:A:630:ASP:HB2	1:A:721:ARG:HE	1.78	0.48
1:B:49:PRO:HA	1:B:92:ARG:HB3	1.95	0.48
1:B:99:ILE:HD11	1:B:111:LEU:HD13	1.96	0.47
1:A:142:ASN:HD22	1:A:145:PHE:H	1.62	0.47
1:B:609:LEU:HG	1:B:609:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ARG:CG	1:A:380:ARG:HH11	2.28	0.47
1:A:631:PRO:HG2	1:A:722:ARG:HB3	1.97	0.47
1:B:324:GLU:HB3	1:B:418:GLN:O	2.16	0.46
1:B:586:LEU:HB2	1:B:589:GLU:HG3	1.98	0.46
1:B:484:LYS:HG3	1:B:485:ASN:N	2.30	0.46
1:B:54:GLN:CG	1:B:695:SER:CB	2.94	0.46
1:B:54:GLN:HG3	1:B:695:SER:CB	2.45	0.46
1:A:248:TRP:CD2	1:A:251:VAL:HG22	2.51	0.46
1:B:70:VAL:HG22	1:B:108:TYR:HB2	1.97	0.46
1:B:497:GLY:HA3	1:B:498:HIS:CD2	2.51	0.46
1:A:156:ILE:O	1:A:160:MET:HG2	2.16	0.46
1:B:470:TYR:HB2	1:B:538:LEU:HB2	1.97	0.46
1:B:289:TYR:HA	1:B:290:MET:HA	1.76	0.45
1:A:637:ALA:HB2	1:A:688:ARG:HG3	1.98	0.45
1:B:455:TRP:CE2	2:B:804:NAG:H4	2.51	0.45
1:A:636:MET:HE3	1:A:639:MET:HG3	1.97	0.45
1:A:54:GLN:CG	1:A:695:SER:HB2	2.45	0.45
1:A:499:VAL:HB	1:A:541:VAL:HB	1.98	0.45
1:A:250:GLU:OE1	3:A:803:GAL:H1	2.16	0.45
1:B:252:TRP:HA	1:B:289:TYR:O	2.17	0.45
1:B:248:TRP:CD2	1:B:251:VAL:HG22	2.52	0.45
1:A:451:ALA:HB2	1:A:455:TRP:CZ2	2.52	0.45
1:B:136:MET:HA	1:B:142:ASN:HD21	1.82	0.45
1:B:467:TYR:HB3	1:B:539:LEU:HD11	1.99	0.45
1:A:265:GLN:O	1:A:678:CYS:HB2	2.17	0.45
1:A:46:ILE:HG12	1:A:292:HIS:HB3	1.99	0.45
1:B:54:GLN:HG3	1:B:695:SER:HB3	1.99	0.45
1:A:467:TYR:HB3	1:A:539:LEU:HD11	1.99	0.45
1:A:263:ILE:O	1:A:680:THR:HG23	2.17	0.45
1:A:675:GLU:H	1:A:675:GLU:HG3	1.46	0.45
1:A:234:CYS:O	1:A:278:PHE:CD1	2.69	0.45
1:A:228:THR:HG22	1:A:247:MET:HB2	1.99	0.44
1:A:112:ARG:HA	1:A:177:GLN:HB3	1.99	0.44
1:A:473:ASN:OD1	1:A:535:LYS:HE2	2.18	0.44
1:B:221:ALA:HA	1:B:222:PRO:HD3	1.86	0.44
1:A:58:ASP:O	1:A:62:LYS:HG3	2.18	0.44
1:A:636:MET:HE2	1:A:639:MET:HG3	1.98	0.43
1:A:324:GLU:HB3	1:A:418:GLN:O	2.18	0.43
1:A:24:SER:HA	5:A:936:HOH:O	2.18	0.43
1:A:179:GLU:HG3	1:A:180:ASN:N	2.33	0.43
1:A:594:HIS:HB2	1:A:645:TRP:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:VAL:HG21	1:A:463:ASP:HB3	1.99	0.43
1:B:642:GLY:HA3	1:B:707:PHE:O	2.18	0.43
1:B:63:ALA:HB1	1:B:68:LEU:HD12	2.00	0.43
1:B:113:ILE:O	1:B:115:PRO:HA	2.18	0.43
1:A:289:TYR:HA	1:A:290:MET:HA	1.71	0.43
1:A:79:GLY:HA3	1:A:93:TYR:CE2	2.55	0.42
1:A:53:PRO:HD3	1:A:92:ARG:HB3	2.01	0.42
1:A:115:PRO:HD2	5:A:914:HOH:O	2.18	0.42
1:A:655:TRP:N	1:A:656:PRO:HD3	2.35	0.42
1:A:628:GLY:HA3	1:A:721:ARG:HH22	1.85	0.42
1:B:641:LYS:HB2	1:B:655:TRP:CD1	2.55	0.42
1:B:50:ARG:HH21	1:B:296:ASN:HD21	1.67	0.42
1:B:341:GLU:HA	1:B:344:LEU:HD12	2.01	0.42
1:B:594:HIS:HB2	1:B:645:TRP:CG	2.55	0.42
1:A:234:CYS:HB2	1:A:248:TRP:CE2	2.54	0.42
1:A:27:TYR:CD1	1:A:245:PRO:HD3	2.56	0.41
1:A:42:ILE:HG22	1:A:68:LEU:HD23	2.03	0.41
1:A:143:GLN:HE21	1:A:143:GLN:HA	1.84	0.41
1:A:503:PHE:HB2	1:A:537:SER:HB2	2.03	0.41
1:B:461:THR:HG22	1:B:584:VAL:HG13	2.01	0.41
1:B:497:GLY:HA2	1:B:498:HIS:HA	1.76	0.41
1:A:137:GLU:H	1:A:142:ASN:ND2	2.18	0.41
1:A:143:GLN:O	1:A:147:VAL:HG23	2.20	0.41
1:B:292:HIS:HD2	5:B:916:HOH:O	2.04	0.41
1:B:512:VAL:HB	1:B:521:LEU:HD12	2.03	0.41
1:A:510:GLY:HA3	1:A:523:TYR:HE1	1.86	0.40
1:A:380:ARG:CB	1:A:380:ARG:HH11	2.32	0.40
1:B:54:GLN:CG	1:B:695:SER:HB3	2.52	0.40
1:A:390:ARG:HA	1:A:391:PRO:HD3	1.89	0.40
1:A:179:GLU:CG	1:A:182:TYR:HB2	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	703/718 (98%)	670 (95%)	31 (4%)	2 (0%)	46	84
1	B	703/718 (98%)	678 (96%)	24 (3%)	1 (0%)	56	90
All	All	1406/1436 (98%)	1348 (96%)	55 (4%)	3 (0%)	52	88

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	118	CYS
1	A	118	CYS
1	A	602	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	591/599 (99%)	571 (97%)	20 (3%)	44	81
1	B	591/599 (99%)	574 (97%)	17 (3%)	50	84
All	All	1182/1198 (99%)	1145 (97%)	37 (3%)	47	83

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	45	SER
1	A	49	PRO
1	A	51	SER
1	A	54	GLN
1	A	97	ARG
1	A	123	PHE
1	A	290	MET
1	A	380	ARG
1	A	389	ASN

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Mol	Chain	Res	Type
1	A	509	SER
1	A	528	LYS
1	A	530	ARG
1	A	535	LYS
1	A	608	SER
1	A	612	GLN
1	A	636	MET
1	A	658	TYR
1	A	675	GLU
1	A	680	THR
1	B	54	GLN
1	B	55	MET
1	B	97	ARG
1	B	115	PRO
1	B	234	CYS
1	B	238	ARG
1	B	312	TYR
1	B	384	LYS
1	B	444	ASP
1	B	521	LEU
1	B	590	SER
1	B	630	ASP
1	B	636	MET
1	B	649	GLU
1	B	658	TYR
1	B	666	LYS
1	B	667	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	143	GLN
1	A	296	ASN
1	A	389	ASN
1	A	411	ASN
1	A	418	GLN
1	A	505	ASN
1	A	647	ASN
1	A	713	ASN
1	B	142	ASN
1	B	154	GLN

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Mol	Chain	Res	Type
1	B	292	HIS
1	B	296	ASN
1	B	388	GLN
1	B	393	ASN
1	B	411	ASN
1	B	418	GLN
1	B	437	ASN
1	B	505	ASN
1	B	574	ASN
1	B	647	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 ⓘ

2 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	$\# Z  > 2$
4	NAG	B	802	1,4	14,14,15	0.30	0	15,19,21	0.52	0
4	NAG	B	803	4	14,14,15	0.28	0	15,19,21	0.54	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
4	NAG	B	802	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	803	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

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.

## 5.6 Ligand geometry

11 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	NAG	A	801	1	14,14,15	0.28	0	15,19,21	0.53	0
2	NAG	A	802	1	14,14,15	0.29	0	15,19,21	0.53	0
3	GAL	A	803	-	12,12,12	0.42	0	17,17,17	0.52	0
3	GAL	A	804	-	12,12,12	0.42	0	17,17,17	0.51	0
3	GAL	A	805	-	12,12,12	0.43	0	17,17,17	0.51	0
3	GAL	A	806	-	12,12,12	0.43	0	17,17,17	0.52	0
3	GAL	B	801	-	12,12,12	0.43	0	17,17,17	0.52	0
2	NAG	B	804	1	14,14,15	0.28	0	15,19,21	0.53	0
3	GAL	B	805	-	12,12,12	0.42	0	17,17,17	0.51	0
3	GAL	B	806	-	12,12,12	0.42	0	17,17,17	0.51	0
3	GAL	B	807	-	12,12,12	0.43	0	17,17,17	0.51	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	NAG	A	801	1	-	0/6/23/26	0/1/1/1
2	NAG	A	802	1	-	0/6/23/26	0/1/1/1
3	GAL	A	803	-	-	0/2/22/22	0/1/1/1
3	GAL	A	804	-	-	0/2/22/22	0/1/1/1
3	GAL	A	805	-	-	0/2/22/22	0/1/1/1
3	GAL	A	806	-	-	0/2/22/22	0/1/1/1
3	GAL	B	801	-	-	0/2/22/22	0/1/1/1
2	NAG	B	804	1	-	0/6/23/26	0/1/1/1
3	GAL	B	805	-	-	0/2/22/22	0/1/1/1
3	GAL	B	806	-	-	0/2/22/22	0/1/1/1
3	GAL	B	807	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	GAL	1	0
2	B	804	NAG	4	0
3	B	805	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<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	705/718 (98%)	-0.18	13 (1%) 71 43	31, 44, 64, 88	0
1	B	705/718 (98%)	-0.19	18 (2%) 59 29	31, 44, 84, 117	0
All	All	1410/1436 (98%)	-0.18	31 (2%) 65 35	31, 44, 77, 117	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	608	SER	3.8
1	B	486	GLY	3.6
1	B	452	ASN	3.5
1	A	602	VAL	3.5
1	B	453	GLY	3.2
1	A	608	SER	3.1
1	A	429	GLY	3.0
1	B	485	ASN	3.0
1	B	479	ASN	2.9
1	B	481	GLY	2.7
1	A	600	SER	2.6
1	A	428	GLY	2.6
1	B	610	MET	2.6
1	B	577	LYS	2.6
1	A	486	GLY	2.5
1	B	429	GLY	2.5
1	B	609	LEU	2.5
1	A	393	ASN	2.4
1	B	663	ASP	2.4
1	A	45	SER	2.4
1	A	603	GLU	2.4
1	A	477	ALA	2.4
1	B	475	ASN	2.2
1	B	601	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	663	ASP	2.1
1	B	447	ASP	2.1
1	A	485	ASN	2.1
1	B	482	PHE	2.1
1	A	22	GLU	2.1
1	B	569	ASN	2.1
1	B	487	LYS	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
4	NAG	B	802	14/15	0.88	0.19	-0.07	42,49,52,56	0
4	NAG	B	803	14/15	0.86	0.46	-	59,62,64,65	0

## 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<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	GAL	B	806	12/12	0.87	0.25	3.82	48,54,56,59	0
3	GAL	A	804	12/12	0.83	0.30	2.62	50,55,57,57	0
3	GAL	B	801	12/12	0.86	0.24	2.24	81,84,87,88	0
3	GAL	A	805	12/12	0.88	0.36	1.96	68,69,70,71	0
3	GAL	A	806	12/12	0.82	0.35	1.90	61,65,67,67	0
3	GAL	B	807	12/12	0.83	0.35	1.38	62,69,70,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GAL	B	805	12/12	0.95	0.20	0.03	31,31,32,34	0
3	GAL	A	803	12/12	0.95	0.22	-0.19	34,36,37,38	0
2	NAG	A	801	14/15	0.92	0.17	-0.43	38,39,40,42	0
2	NAG	B	804	14/15	0.85	0.27	-	65,67,70,73	0
2	NAG	A	802	14/15	0.89	0.27	-	53,54,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.