



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:29 PM GMT

PDB ID : 1TW1  
Title : beta-1,4-galactosyltransferase mutant Met344His (m344H-Gal-T1) complex with UDP-galactose and magnesium  
Authors : Ramakrishnan, B.; Boeggeman, E.; Qasba, P.K.  
Deposited on : 2004-06-30  
Resolution : 2.30 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

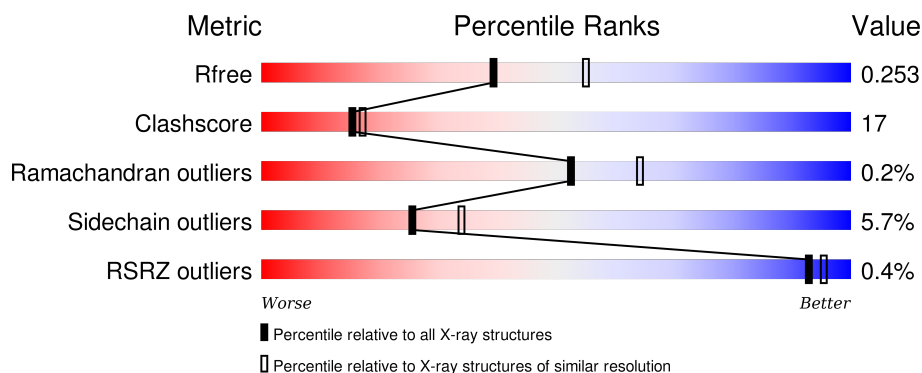
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	286	 63% 29% • 5%
1	B	286	 66% 25% • 5%

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
2	GDU	A	2	X	-	-	-
2	GDU	B	404	X	-	-	-
6	MES	B	870	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5087 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-1,4-galactosyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2221	1426	384	399	12			
1	B	272	Total	C	N	O	S	0	0	0
			2221	1426	384	399	12			

There are 30 discrepancies between the modelled and reference sequences:

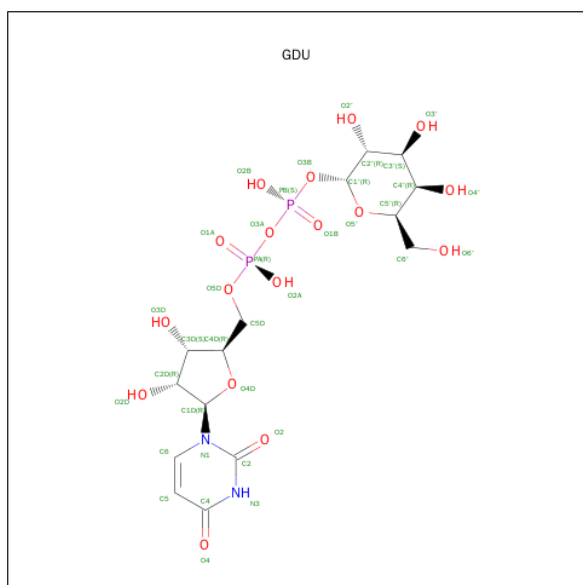
Chain	Residue	Modelled	Actual	Comment	Reference
A	117	ALA	-	SEE REMARK 999	UNP P08037
A	118	SER	-	SEE REMARK 999	UNP P08037
A	119	MET	-	SEE REMARK 999	UNP P08037
A	120	THR	-	SEE REMARK 999	UNP P08037
A	121	GLY	-	SEE REMARK 999	UNP P08037
A	122	GLY	-	SEE REMARK 999	UNP P08037
A	123	GLN	-	SEE REMARK 999	UNP P08037
A	124	GLN	-	SEE REMARK 999	UNP P08037
A	125	MET	-	SEE REMARK 999	UNP P08037
A	126	GLY	-	SEE REMARK 999	UNP P08037
A	127	ARG	-	SEE REMARK 999	UNP P08037
A	128	GLY	-	SEE REMARK 999	UNP P08037
A	129	SER	-	SEE REMARK 999	UNP P08037
A	342	THR	CYS	ENGINEERED	UNP P08037
A	344	HIS	MET	ENGINEERED	UNP P08037
B	117	ALA	-	SEE REMARK 999	UNP P08037
B	118	SER	-	SEE REMARK 999	UNP P08037
B	119	MET	-	SEE REMARK 999	UNP P08037
B	120	THR	-	SEE REMARK 999	UNP P08037
B	121	GLY	-	SEE REMARK 999	UNP P08037
B	122	GLY	-	SEE REMARK 999	UNP P08037
B	123	GLN	-	SEE REMARK 999	UNP P08037
B	124	GLN	-	SEE REMARK 999	UNP P08037
B	125	MET	-	SEE REMARK 999	UNP P08037
B	126	GLY	-	SEE REMARK 999	UNP P08037

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Chain	Residue	Modelled	Actual	Comment	Reference
B	127	ARG	-	SEE REMARK 999	UNP P08037
B	128	GLY	-	SEE REMARK 999	UNP P08037
B	129	SER	-	SEE REMARK 999	UNP P08037
B	342	THR	CYS	ENGINEERED	UNP P08037
B	344	HIS	MET	ENGINEERED	UNP P08037

- Molecule 2 is SUGAR (GALACTOSE-URIDINE-5'-DIPHOSPHATE) (three-letter code: GDU) (formula:  $C_{15}H_{24}N_2O_{17}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

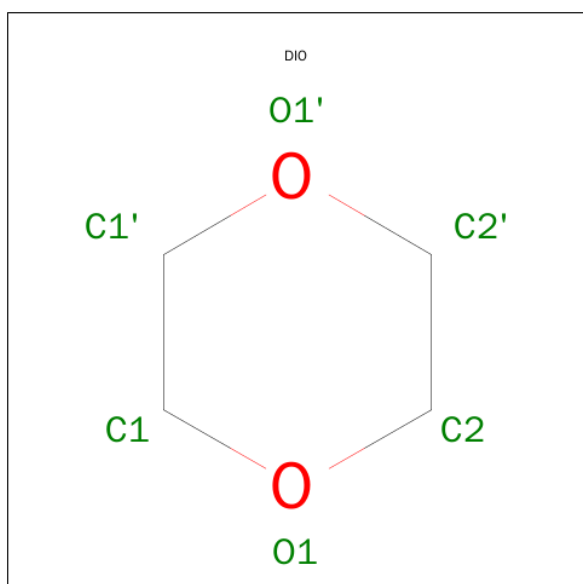
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



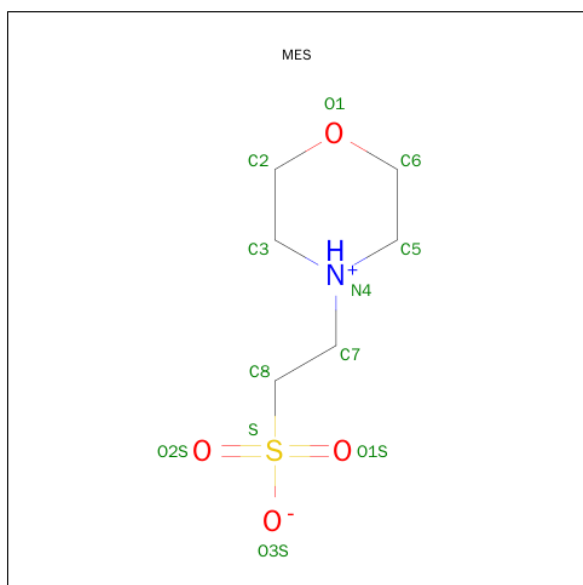
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>).



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

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is water.

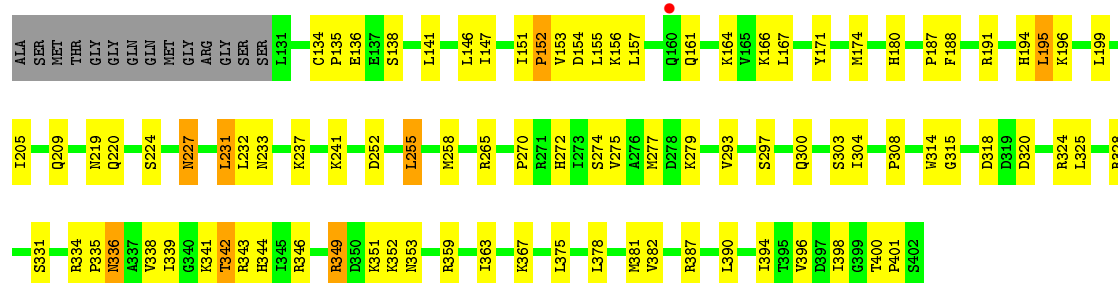
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	262	Total	O	0	0
			262	262		
7	B	260	Total	O	0	0
			260	260		

### 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 ( $\text{RSRZ} > 2$ ). 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.

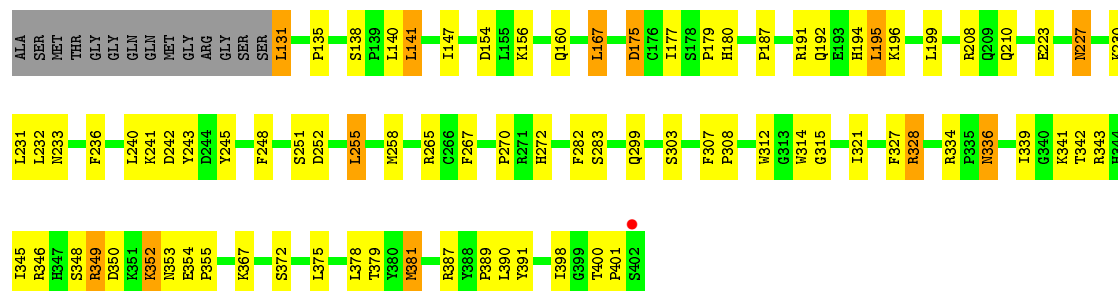
- Molecule 1: Beta-1,4-galactosyltransferase 1

Chain A: 



- Molecule 1: Beta-1,4-galactosyltransferase 1

Chain B: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.01Å 91.52Å 142.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.38 – 2.30 42.22 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (37.38-2.30) 98.6 (42.22-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.29Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.196 , 0.261 0.191 , 0.253	Depositor DCC
$R_{free}$ test set	1451 reflections (4.92%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.6	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 53.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 29656 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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: MG, DIO, GDU, MES, SO4

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	0.47	0/2282	0.74	0/3092
1	B	0.51	0/2282	0.76	1/3092 (0.0%)
All	All	0.49	0/4564	0.75	1/6184 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	GLY	N-CA-C	5.52	126.90	113.10

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	2221	0	2185	90	0
1	B	2221	0	2185	70	0
2	A	36	0	21	2	0
2	B	36	0	21	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	0	0	0
4	B	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	12	0	16	2	0
6	B	12	0	13	1	0
7	A	262	0	0	4	0
7	B	260	0	0	6	0
All	All	5087	0	4441	156	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 17.

All (156) 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:351:LYS:HD2	1:A:352:LYS:HG2	1.54	0.88
1:B:349:ARG:H	1:B:349:ARG:HD3	1.42	0.82
1:A:224:SER:HB2	7:A:916:HOH:O	1.78	0.82
1:B:258:MET:HE3	1:B:341:LYS:HB3	1.61	0.81
1:A:336:ASN:HD22	1:A:336:ASN:C	1.86	0.80
1:A:349:ARG:H	1:A:349:ARG:NE	1.80	0.78
1:B:349:ARG:N	1:B:349:ARG:HD3	1.98	0.78
1:A:231:LEU:HD13	1:A:398:ILE:HD13	1.69	0.74
1:A:336:ASN:ND2	1:A:338:VAL:H	1.85	0.73
1:B:348:SER:HB2	1:B:349:ARG:NH1	2.03	0.73
1:B:349:ARG:CD	1:B:349:ARG:H	2.00	0.72
1:A:258:MET:HE3	1:A:341:LYS:HB3	1.74	0.68
1:A:336:ASN:HD21	1:A:339:ILE:H	1.39	0.68
1:A:191:ARG:HH21	1:A:194:HIS:HD2	1.42	0.68
1:A:336:ASN:HD22	1:A:338:VAL:N	1.92	0.67
1:A:336:ASN:ND2	1:A:338:VAL:N	2.42	0.67
1:A:336:ASN:ND2	1:A:339:ILE:H	1.93	0.67
1:A:154:ASP:OD1	1:A:156:LYS:HB2	1.95	0.66
1:A:336:ASN:HD22	1:A:338:VAL:H	1.43	0.66
1:B:336:ASN:HD22	1:B:336:ASN:C	1.99	0.66
1:B:336:ASN:ND2	1:B:339:ILE:H	1.94	0.65
1:B:154:ASP:OD1	1:B:156:LYS:HE2	1.96	0.65
1:A:270:PRO:HD2	1:A:331:SER:O	1.96	0.65
1:A:335:PRO:HB2	1:A:339:ILE:HG13	1.79	0.64
1:B:258:MET:HE2	1:B:342:THR:CA	2.28	0.64
1:B:314:TRP:CD1	2:B:404:GDU:H6'1	2.33	0.64
1:B:307:PHE:HB3	1:B:308:PRO:HD2	1.81	0.62
1:A:151:ILE:HG13	1:A:151:ILE:O	2.00	0.61
1:B:191:ARG:HH21	1:B:194:HIS:HD2	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ILE:O	1:A:209:GLN:HG3	2.01	0.61
1:A:336:ASN:C	1:A:336:ASN:ND2	2.55	0.60
1:A:351:LYS:O	1:A:352:LYS:HB2	2.01	0.59
1:A:157:LEU:O	1:A:161:GLN:HG3	2.01	0.59
1:B:258:MET:HE2	1:B:342:THR:N	2.18	0.59
1:A:349:ARG:CD	1:A:349:ARG:H	2.15	0.59
1:B:135:PRO:HD2	1:B:210:GLN:HE22	1.68	0.58
1:B:303:SER:O	1:B:328:ARG:HD3	2.03	0.58
1:A:304:ILE:HG22	1:A:328:ARG:HG3	1.86	0.57
1:B:195:LEU:HD22	1:B:199:LEU:HG	1.86	0.57
1:A:400:THR:H	5:A:861:DIO:H1'2	1.68	0.57
1:A:382:VAL:O	1:B:387:ARG:HD2	2.05	0.57
1:A:314:TRP:CD1	2:A:2:GDU:H6'1	2.40	0.56
1:A:272:HIS:HB3	1:A:334:ARG:HG2	1.88	0.56
1:A:154:ASP:HB3	1:A:157:LEU:HD13	1.88	0.56
1:A:191:ARG:HH21	1:A:194:HIS:CD2	2.24	0.55
1:A:167:LEU:HD11	1:A:387:ARG:HB3	1.87	0.55
1:B:227:ASN:C	1:B:227:ASN:HD22	2.10	0.55
1:B:233:ASN:HB3	1:B:378:LEU:HD22	1.90	0.54
1:B:252:ASP:HB2	1:B:255:LEU:HD22	1.89	0.54
1:B:230:LYS:HD3	1:B:398:ILE:HB	1.89	0.54
1:B:240:LEU:HD21	1:B:248:PHE:HZ	1.72	0.54
1:A:136:GLU:H	5:A:860:DIO:H22	1.74	0.53
1:B:258:MET:HE2	1:B:342:THR:C	2.29	0.53
1:B:236:PHE:CE2	1:B:375:LEU:HD21	2.43	0.53
1:A:237:LYS:HE3	1:A:375:LEU:CD1	2.39	0.52
1:B:160:GLN:HB2	7:B:1081:HOH:O	2.09	0.52
1:B:349:ARG:HG2	1:B:349:ARG:HH11	1.75	0.52
1:A:394:ILE:HG22	1:A:396:VAL:HG13	1.91	0.52
1:B:390:LEU:O	1:B:391:TYR:HB3	2.10	0.51
1:A:147:ILE:HB	1:A:343:ARG:HD2	1.92	0.51
1:A:154:ASP:OD1	1:A:156:LYS:N	2.44	0.51
1:A:180:HIS:CE1	1:A:265:ARG:HD2	2.45	0.51
1:B:327:PHE:CE1	1:B:367:LYS:HB2	2.45	0.51
1:A:336:ASN:HD21	1:A:338:VAL:HB	1.76	0.51
1:A:258:MET:HE2	1:A:342:THR:C	2.30	0.51
1:A:191:ARG:NH2	1:A:194:HIS:HD2	2.07	0.50
1:B:191:ARG:HD2	1:B:194:HIS:CD2	2.46	0.50
1:A:277:MET:CE	1:A:279:LYS:HD3	2.42	0.50
1:B:342:THR:HG21	7:B:1386:HOH:O	2.10	0.50
1:B:187:PRO:HD2	1:B:251:SER:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ASP:HB3	2:B:404:GDU:O3D	2.11	0.50
1:B:223:GLU:HG2	7:B:1293:HOH:O	2.11	0.50
1:A:233:ASN:HB3	1:A:378:LEU:HD22	1.95	0.49
1:B:367:LYS:HE2	7:B:1039:HOH:O	2.13	0.49
1:A:167:LEU:CD1	1:A:387:ARG:HB3	2.43	0.49
1:A:381:MET:HE2	1:B:167:LEU:HD12	1.94	0.48
1:B:349:ARG:H	1:B:349:ARG:HH11	1.61	0.48
1:B:131:LEU:HD22	1:B:131:LEU:N	2.28	0.48
1:A:255:LEU:CD1	1:A:344:HIS:HD2	2.26	0.48
1:A:241:LYS:HB3	1:B:241:LYS:HD3	1.95	0.48
1:B:187:PRO:HD3	1:B:232:LEU:HD21	1.94	0.48
1:A:297:SER:OG	1:A:300:GLN:HG3	2.13	0.48
1:A:138:SER:HB3	1:A:141:LEU:HD13	1.95	0.48
1:A:346:ARG:HG3	1:A:346:ARG:HH21	1.79	0.48
1:A:255:LEU:HD23	1:A:293:VAL:HG23	1.96	0.48
1:A:151:ILE:O	1:A:152:PRO:C	2.53	0.47
1:B:227:ASN:ND2	1:B:230:LYS:H	2.11	0.47
1:B:131:LEU:HB2	1:B:177:ILE:HG12	1.96	0.47
1:B:147:ILE:HB	1:B:343:ARG:HD2	1.96	0.47
1:B:387:ARG:HH11	1:B:387:ARG:HG3	1.80	0.47
1:A:315:GLY:HA2	7:A:1297:HOH:O	2.15	0.47
1:B:346:ARG:HG3	1:B:346:ARG:HH21	1.80	0.47
1:B:349:ARG:HG2	1:B:349:ARG:NH1	2.29	0.47
1:A:270:PRO:HG2	1:A:325:LEU:HD22	1.97	0.46
1:B:175:ASP:N	1:B:175:ASP:OD2	2.45	0.46
1:A:349:ARG:CD	1:A:349:ARG:N	2.79	0.46
1:A:154:ASP:CB	1:A:157:LEU:HD13	2.44	0.46
1:B:167:LEU:HD23	1:B:389:PRO:HA	1.96	0.46
1:A:227:ASN:HD22	1:A:227:ASN:C	2.19	0.46
1:A:237:LYS:HE3	1:A:375:LEU:HD11	1.97	0.46
1:A:320:ASP:O	1:A:324:ARG:HG3	2.14	0.46
1:A:275:VAL:HG11	1:A:335:PRO:HD2	1.98	0.45
1:B:258:MET:CE	1:B:282:PHE:HE2	2.28	0.45
1:A:314:TRP:NE1	2:A:2:GDU:H6'1	2.32	0.45
1:A:164:LYS:HB3	1:A:171:TYR:HE1	1.81	0.45
1:A:166:LYS:HB2	1:A:166:LYS:HE3	1.75	0.45
1:B:299:GLN:CG	7:B:919:HOH:O	2.64	0.45
1:A:343:ARG:HH21	1:A:343:ARG:HG2	1.82	0.45
1:B:147:ILE:HB	1:B:343:ARG:CD	2.47	0.45
1:A:220:GLN:HB2	1:A:231:LEU:HD21	1.98	0.45
1:A:187:PRO:HD3	1:A:232:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:CYS:HB3	1:A:135:PRO:HD2	1.98	0.45
1:A:277:MET:HE1	7:A:982:HOH:O	2.16	0.44
1:B:227:ASN:HB2	1:B:312:TRP:CE3	2.52	0.44
1:A:154:ASP:CG	1:A:157:LEU:HD13	2.37	0.44
1:A:167:LEU:HD12	1:B:381:MET:CE	2.47	0.44
1:A:167:LEU:HD11	1:A:387:ARG:CB	2.48	0.44
1:A:188:PHE:O	1:A:219:ASN:HA	2.17	0.44
1:B:336:ASN:ND2	1:B:336:ASN:C	2.69	0.44
1:A:277:MET:HE2	1:A:279:LYS:HD3	2.00	0.44
1:A:335:PRO:HB2	1:A:339:ILE:CG1	2.48	0.43
1:B:379:THR:OG1	6:B:870:MES:H21	2.18	0.43
1:A:164:LYS:HB3	1:A:171:TYR:CE1	2.53	0.43
1:B:180:HIS:CE1	1:B:265:ARG:HD2	2.54	0.43
1:A:191:ARG:NH2	1:A:194:HIS:CD2	2.85	0.43
1:B:179:PRO:HG2	1:B:180:HIS:CE1	2.53	0.43
1:A:382:VAL:HA	1:A:396:VAL:HG12	2.01	0.42
1:A:195:LEU:HD22	1:A:199:LEU:HG	2.01	0.42
1:B:314:TRP:HB2	1:B:353:ASN:O	2.19	0.42
1:A:336:ASN:HD21	1:A:339:ILE:N	2.12	0.42
1:B:223:GLU:O	1:B:352:LYS:HE3	2.20	0.42
1:A:303:SER:O	1:A:328:ARG:HD3	2.20	0.41
1:B:138:SER:HB3	1:B:141:LEU:HD13	2.01	0.41
1:A:154:ASP:OD1	1:A:156:LYS:HE2	2.21	0.41
1:B:267:PHE:N	1:B:267:PHE:CD1	2.88	0.41
1:A:274:SER:HA	1:A:342:THR:HG21	2.02	0.41
1:A:167:LEU:C	1:A:167:LEU:HD13	2.41	0.41
1:A:252:ASP:HB2	1:A:255:LEU:HD22	2.02	0.41
1:A:155:LEU:HD22	1:A:390:LEU:HD12	2.03	0.41
1:B:243:TYR:HB3	1:B:245:TYR:CE1	2.55	0.41
1:B:272:HIS:HB3	1:B:334:ARG:HG2	2.01	0.41
1:A:318:ASP:OD2	1:A:318:ASP:N	2.54	0.41
1:A:308:PRO:HB3	1:A:324:ARG:NH1	2.35	0.41
1:A:367:LYS:NZ	7:A:1248:HOH:O	2.53	0.41
1:B:389:PRO:HG2	7:B:915:HOH:O	2.21	0.41
1:B:345:ILE:O	1:B:346:ARG:C	2.57	0.41
1:B:192:GLN:O	1:B:196:LYS:HG3	2.21	0.41
1:A:314:TRP:HB2	1:A:353:ASN:O	2.20	0.40
1:A:153:VAL:CG2	1:A:196:LYS:HB3	2.50	0.40
1:B:400:THR:HB	1:B:401:PRO:HD2	2.03	0.40
1:A:343:ARG:NH2	1:A:343:ARG:HG2	2.36	0.40
1:B:307:PHE:CD1	1:B:321:ILE:HG12	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ARG:O	1:A:363:ILE:HG23	2.21	0.40
1:B:312:TRP:NE1	1:B:401:PRO:HA	2.36	0.40
1:B:140:LEU:O	1:B:208:ARG:HD2	2.22	0.40
1:B:354:GLU:O	1:B:355:PRO:C	2.60	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	270/286 (94%)	254 (94%)	15 (6%)	1 (0%)	39	48
1	B	270/286 (94%)	259 (96%)	11 (4%)	0	100	100
All	All	540/572 (94%)	513 (95%)	26 (5%)	1 (0%)	52	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	PRO

### 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	245/254 (96%)	235 (96%)	10 (4%)	37	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	245/254 (96%)	227 (93%)	18 (7%)	17	22
All	All	490/508 (96%)	462 (94%)	28 (6%)	25	34

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	LEU
1	A	174	MET
1	A	195	LEU
1	A	227	ASN
1	A	231	LEU
1	A	255	LEU
1	A	336	ASN
1	A	342	THR
1	A	349	ARG
1	A	401	PRO
1	B	131	LEU
1	B	141	LEU
1	B	167	LEU
1	B	175	ASP
1	B	195	LEU
1	B	227	ASN
1	B	231	LEU
1	B	242	ASP
1	B	255	LEU
1	B	270	PRO
1	B	283	SER
1	B	328	ARG
1	B	336	ASN
1	B	349	ARG
1	B	350	ASP
1	B	352	LYS
1	B	372	SER
1	B	381	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	190	ASN
1	A	194	HIS

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Mol	Chain	Res	Type
1	A	207	GLN
1	A	210	GLN
1	A	227	ASN
1	A	336	ASN
1	B	161	GLN
1	B	190	ASN
1	B	194	HIS
1	B	207	GLN
1	B	210	GLN
1	B	227	ASN
1	B	336	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	GDU	A	2	3	29,38,38	1.52	4 (13%)	43,58,58	2.93	14 (32%)
4	SO4	A	858	-	4,4,4	3.25	2 (50%)	6,6,6	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	A	859	-	4,4,4	3.30	2 (50%)	6,6,6	1.02	0
5	DIO	A	860	-	6,6,6	0.68	0	6,6,6	1.46	2 (33%)
5	DIO	A	861	-	6,6,6	0.81	0	6,6,6	1.53	2 (33%)
2	GDU	B	404	3	29,38,38	1.58	5 (17%)	43,58,58	2.89	15 (34%)
4	SO4	B	855	-	4,4,4	3.27	2 (50%)	6,6,6	0.98	0
4	SO4	B	856	-	4,4,4	3.30	2 (50%)	6,6,6	0.94	0
4	SO4	B	857	-	4,4,4	3.33	2 (50%)	6,6,6	0.94	0
6	MES	B	870	-	11,12,12	1.41	2 (18%)	14,16,16	0.82	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	GDU	A	2	3	1/1/11/11	0/19/59/59	0/3/3/3
4	SO4	A	858	-	-	0/0/0/0	0/0/0/0
4	SO4	A	859	-	-	0/0/0/0	0/0/0/0
5	DIO	A	860	-	-	0/0/6/6	0/1/1/1
5	DIO	A	861	-	-	0/0/6/6	0/1/1/1
2	GDU	B	404	3	1/1/11/11	0/19/59/59	0/3/3/3
4	SO4	B	855	-	-	0/0/0/0	0/0/0/0
4	SO4	B	856	-	-	0/0/0/0	0/0/0/0
4	SO4	B	857	-	-	0/0/0/0	0/0/0/0
6	MES	B	870	-	-	0/6/14/14	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	859	SO4	O3-S	-4.62	1.30	1.47
4	B	855	SO4	O3-S	-4.60	1.30	1.47
4	A	858	SO4	O3-S	-4.45	1.31	1.47
4	B	857	SO4	O3-S	-4.44	1.31	1.47
4	B	856	SO4	O3-S	-4.36	1.31	1.47
2	B	404	GDU	PA-O2A	-2.21	1.45	1.54
2	B	404	GDU	PA-O1A	2.39	1.59	1.51
2	A	2	GDU	O5'-C1'	2.42	1.48	1.41
6	B	870	MES	C3-N4	2.47	1.53	1.46
2	A	2	GDU	PA-O1A	2.54	1.60	1.51
6	B	870	MES	C5-N4	2.70	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	404	GDU	O5'-C1'	3.02	1.49	1.41
2	A	2	GDU	C4-N3	3.65	1.39	1.33
2	B	404	GDU	C4-N3	4.11	1.40	1.33
2	A	2	GDU	C6-N1	4.33	1.41	1.35
2	B	404	GDU	C6-N1	4.48	1.42	1.35
4	B	855	SO4	O1-S	4.55	1.62	1.47
4	A	859	SO4	O1-S	4.63	1.63	1.47
4	A	858	SO4	O1-S	4.65	1.63	1.47
4	B	857	SO4	O1-S	4.89	1.63	1.47
4	B	856	SO4	O1-S	4.91	1.64	1.47

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	404	GDU	C5-C4-N3	-3.26	114.75	123.12
2	A	2	GDU	C5-C4-N3	-3.13	115.08	123.12
2	A	2	GDU	O4'-C4'-C3'	-2.93	103.74	110.34
2	A	2	GDU	O3A-PB-O3B	-2.89	95.30	103.63
2	B	404	GDU	O4'-C4'-C3'	-2.87	103.88	110.34
2	A	2	GDU	O3B-PB-O1B	-2.70	98.82	109.46
2	B	404	GDU	O3B-PB-O1B	-2.47	99.73	109.46
2	A	2	GDU	O5'-C1'-C2'	-2.31	105.53	110.28
2	B	404	GDU	O3A-PB-O3B	-2.15	97.44	103.63
2	B	404	GDU	O5'-C1'-C2'	-2.03	106.12	110.28
2	B	404	GDU	C6'-C5'-C4'	2.01	117.98	113.02
5	A	860	DIO	C2-O1-C1	2.03	116.73	109.89
2	A	2	GDU	C6'-C5'-C4'	2.07	118.12	113.02
5	A	861	DIO	C2-O1-C1	2.10	116.95	109.89
2	B	404	GDU	O5'-C5'-C6'	2.18	111.86	106.36
2	A	2	GDU	O5'-C5'-C6'	2.34	112.27	106.36
2	B	404	GDU	O3'-C3'-C4'	2.41	115.77	110.34
2	B	404	GDU	C1'-C2'-C3'	2.43	114.77	109.97
2	A	2	GDU	O3B-C1'-C2'	2.46	112.99	108.39
5	A	860	DIO	C2'-O1'-C1'	2.54	118.45	109.89
2	B	404	GDU	O3B-C1'-C2'	2.55	113.15	108.39
5	A	861	DIO	C2'-O1'-C1'	2.57	118.56	109.89
2	A	2	GDU	O3'-C3'-C4'	2.61	116.21	110.34
2	B	404	GDU	O2B-PB-O3A	3.03	118.84	105.09
2	A	2	GDU	O2B-PB-O3A	3.15	119.37	105.09
2	A	2	GDU	O4D-C1D-N1	3.24	114.90	108.08
2	B	404	GDU	O4D-C1D-N1	4.19	116.92	108.08
2	A	2	GDU	O3'-C3'-C2'	4.28	119.98	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	404	GDU	O3'-C3'-C2'	4.37	120.17	110.34
2	A	2	GDU	C4'-C3'-C2'	6.50	122.93	110.79
2	B	404	GDU	C4'-C3'-C2'	6.66	123.23	110.79
2	B	404	GDU	C4-N3-C2	13.19	127.20	114.14
2	A	2	GDU	C4-N3-C2	13.38	127.39	114.14

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	404	GDU	C3'
2	A	2	GDU	C3'

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2	GDU	2	0
5	A	860	DIO	1	0
5	A	861	DIO	1	0
2	B	404	GDU	2	0
6	B	870	MES	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 [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	272/286 (95%)	-0.14	1 (0%) 93 95	24, 33, 55, 63	0
1	B	272/286 (95%)	-0.19	1 (0%) 93 95	19, 31, 45, 60	0
All	All	544/572 (95%)	-0.16	2 (0%) 93 95	19, 32, 50, 63	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	GLN	2.9
1	B	402	SER	2.4

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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
6	MES	B	870	12/12	0.73	0.33	2.94	84,85,87,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GDU	A	2	36/36	0.97	0.12	0.09	23,26,32,34	0
2	GDU	B	404	36/36	0.97	0.11	-0.58	23,26,29,33	0
3	MG	A	1	1/1	0.98	0.10	-1.68	22,22,22,22	0
3	MG	B	403	1/1	0.99	0.04	-4.99	24,24,24,24	0
5	DIO	A	861	6/6	0.78	0.18	-	71,72,72,72	0
5	DIO	A	860	6/6	0.93	0.18	-	75,75,75,75	0
4	SO4	A	858	5/5	0.91	0.19	-	82,82,82,83	0
4	SO4	A	859	5/5	0.93	0.13	-	83,83,84,84	0
4	SO4	B	855	5/5	0.93	0.30	-	90,91,91,91	0
4	SO4	B	857	5/5	0.82	0.44	-	107,107,108,108	0
4	SO4	B	856	5/5	0.68	0.29	-	104,104,104,106	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.