



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 21, 2016 – 10:22 PM EDT

PDB ID : 5E9T  
Title : Crystal structure of GtfA/B complex  
Authors : Chen, Y.; Rapoport, T.A.  
Deposited on : 2015-10-15  
Resolution : 2.92 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

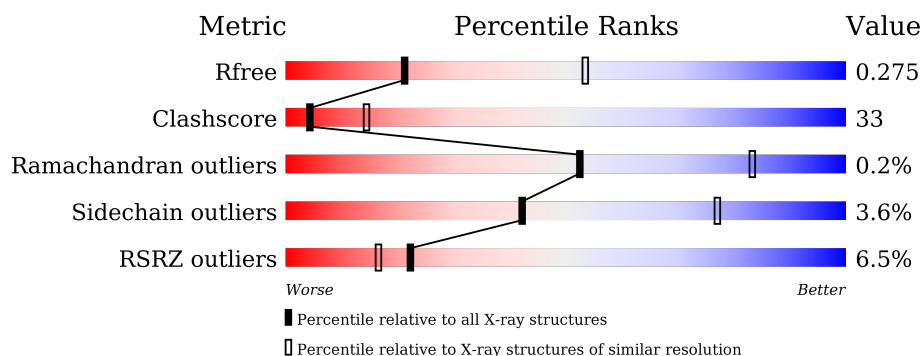
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.92 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	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)

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	503	<div> <div>5%</div> <div> <div></div> <div>60%</div> <div>36%</div> <div>..</div> </div> </div>
1	C	503	<div> <div>7%</div> <div> <div></div> <div>55%</div> <div>40%</div> <div>5%</div> </div> </div>
2	B	447	<div> <div>4%</div> <div> <div></div> <div>53%</div> <div>44%</div> <div>.</div> </div> </div>
2	D	447	<div> <div>9%</div> <div> <div></div> <div>50%</div> <div>45%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15474 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 Glycosyltransferase Gtf1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	Se	0	0	0
			4108	2624	687	789	2	6			
1	C	503	Total	C	N	O	S	Se	0	0	0
			4108	2624	687	789	2	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q9AET5
A	124	PHE	SER	engineered mutation	UNP Q9AET5
C	1	SER	-	expression tag	UNP Q9AET5
C	124	PHE	SER	engineered mutation	UNP Q9AET5

- Molecule 2 is a protein called Glycosyltransferase-stabilizing protein Gtf2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	447	Total	C	N	O	S	Se	0	0	0
			3615	2302	615	687	3	8			
2	D	445	Total	C	N	O	S	Se	0	0	0
			3607	2298	613	685	3	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MSE	-	initiating methionine	UNP Q79T00
D	1	MSE	-	initiating methionine	UNP Q79T00

- 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		

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

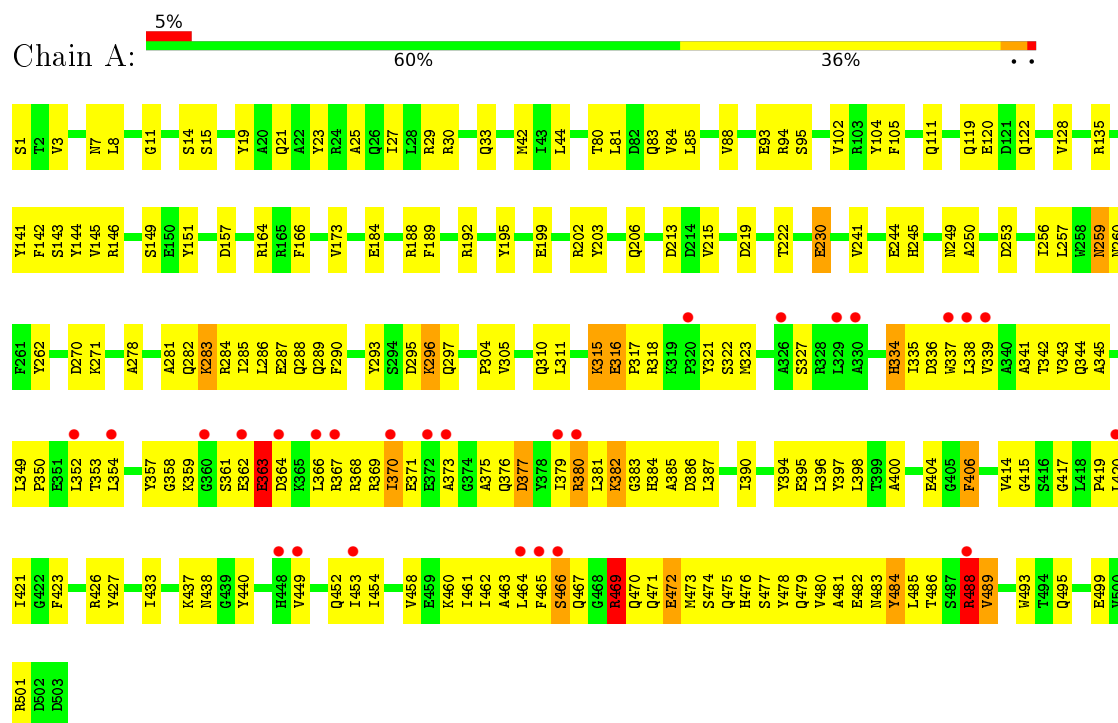
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	9	Total	O	0	0
			9	9		
4	C	8	Total	O	0	0
			8	8		
4	D	7	Total	O	0	0
			7	7		

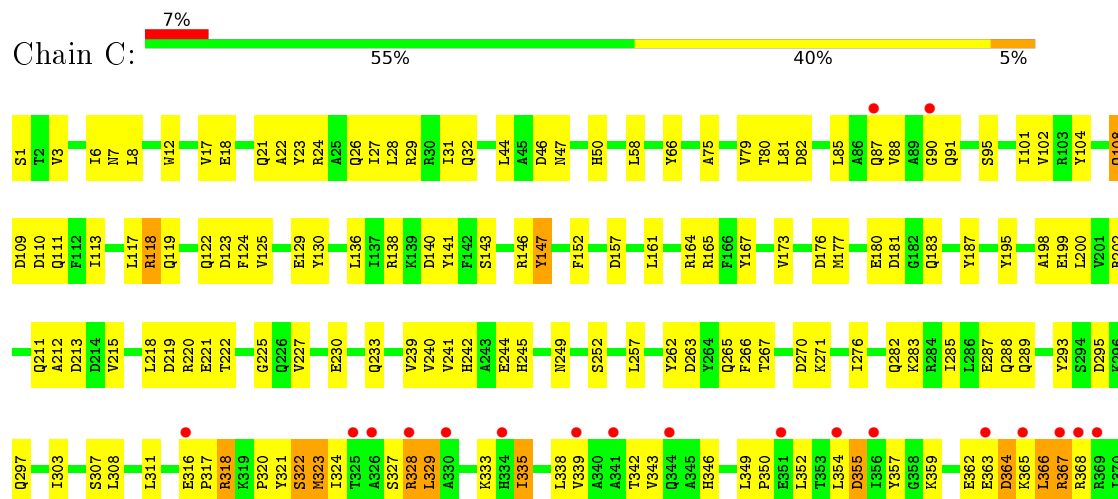
### 3 Residue-property plots

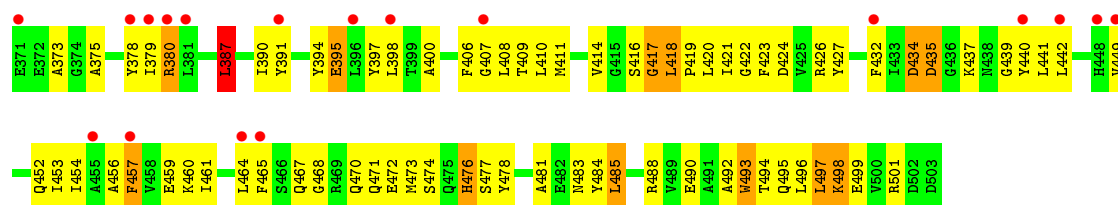
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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: Glycosyltransferase Gtf1

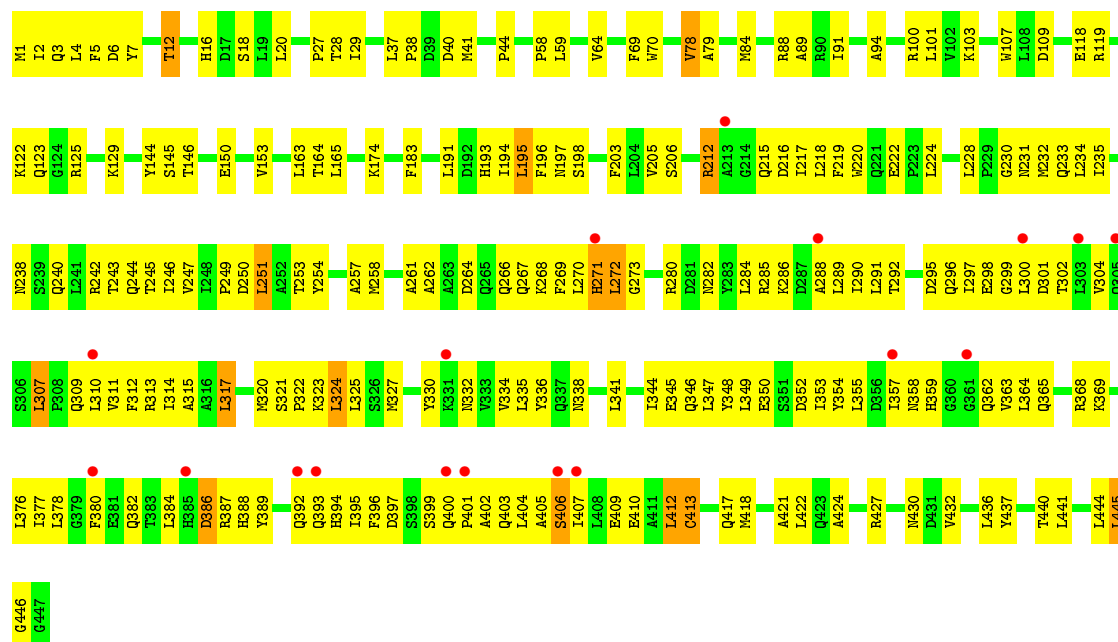


#### • Molecule 1: Glycosyltransferase Gtf1

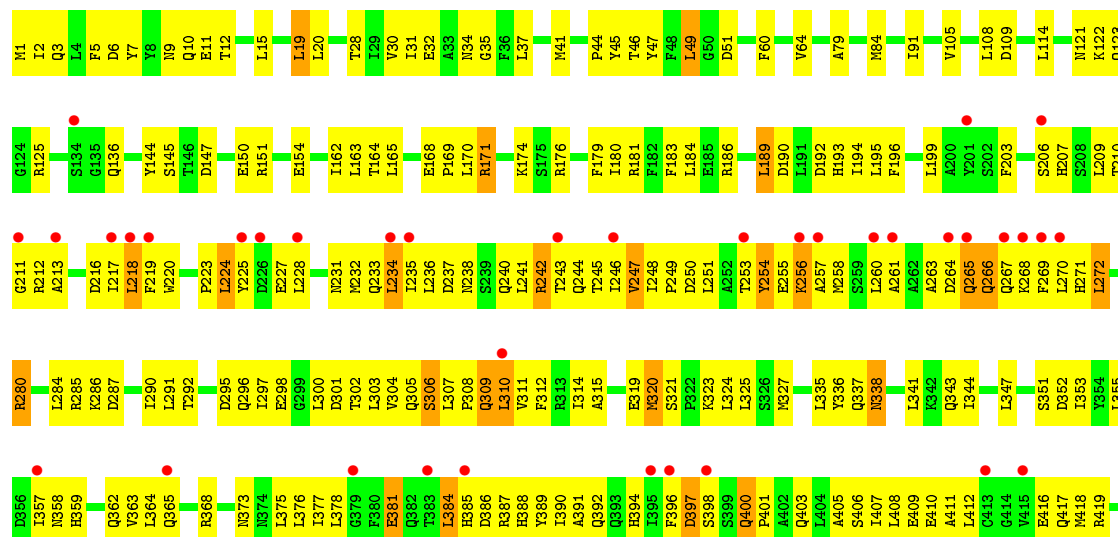




• Molecule 2: Glycosyltransferase-stabilizing protein Gtf2



• Molecule 2: Glycosyltransferase-stabilizing protein Gtf2





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.93Å 196.41Å 220.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.12 – 2.92 122.12 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.9 (122.12-2.92) 94.8 (122.12-2.62)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.95 (at 2.62Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.217 , 0.275 0.214 , 0.275	Depositor DCC
$R_{free}$ test set	3569 reflections (4.85%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 33.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 95954 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	15474	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.64	14/4196 (0.3%)	0.81	11/5678 (0.2%)
1	C	0.49	2/4196 (0.0%)	0.78	12/5678 (0.2%)
2	B	0.39	0/3686	0.67	8/4986 (0.2%)
2	D	0.54	5/3678 (0.1%)	0.87	19/4976 (0.4%)
All	All	0.53	21/15756 (0.1%)	0.79	50/21318 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	5
2	D	0	3
All	All	0	10

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	472	GLU	CD-OE1	-10.31	1.14	1.25
1	A	316	GLU	CD-OE2	-9.69	1.15	1.25
1	A	469	ARG	NE-CZ	-9.68	1.20	1.33
1	A	316	GLU	CD-OE1	-9.50	1.15	1.25
2	D	247	VAL	CB-CG1	-7.63	1.36	1.52

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	488	ARG	NE-CZ-NH2	25.97	133.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	329	LEU	CA-CB-CG	16.30	152.78	115.30
1	A	488	ARG	NE-CZ-NH1	-14.02	113.29	120.30
2	D	256	LYS	CD-CE-NZ	-12.70	82.49	111.70
1	C	364	ASP	CB-CG-OD2	-12.15	107.37	118.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	363	GLU	Peptide
1	A	466	SER	Peptide
1	C	108	GLN	Peptide
1	C	322	SER	Peptide
1	C	328	ARG	Peptide

## 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	4108	0	3965	240	0
1	C	4108	0	3965	271	0
2	B	3615	0	3535	210	0
2	D	3607	0	3529	306	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	0	0	0
4	B	9	0	0	0	0
4	C	8	0	0	0	0
4	D	7	0	0	1	0
All	All	15474	0	14994	1005	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 33.

The worst 5 of 1005 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)
2:D:307:LEU:HA	2:D:309:GLN:NE2	1.64	1.12
2:B:345:GLU:OE2	2:B:369:LYS:NZ	1.83	1.12
1:A:470:GLN:HE21	1:A:471:GLN:HG3	1.06	1.12
2:D:307:LEU:HA	2:D:309:GLN:HE21	1.13	1.09
2:B:272:LEU:HD13	2:B:273:GLY:H	0.92	1.07

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	501/503 (100%)	482 (96%)	16 (3%)	3 (1%)	30	66
1	C	501/503 (100%)	480 (96%)	21 (4%)	0	100	100
2	B	445/447 (100%)	418 (94%)	26 (6%)	1 (0%)	52	83
2	D	443/447 (99%)	413 (93%)	30 (7%)	0	100	100
All	All	1890/1900 (100%)	1793 (95%)	93 (5%)	4 (0%)	52	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	GLU
1	A	474	SER
1	A	370	ILE
2	B	78	VAL

### 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	435/429 (101%)	414 (95%)	21 (5%)	31	67
1	C	435/429 (101%)	421 (97%)	14 (3%)	46	81
2	B	392/384 (102%)	381 (97%)	11 (3%)	51	83
2	D	392/384 (102%)	379 (97%)	13 (3%)	45	80
All	All	1654/1626 (102%)	1595 (96%)	59 (4%)	42	77

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	286	LYS
1	C	118	ARG
2	D	272	LEU
2	B	317	LEU
2	B	386	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	382	GLN
1	C	183	GLN
2	D	338	ASN
2	B	430	ASN
1	C	163	GLN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	497/503 (98%)	0.28	27 (5%) 29 24	11, 51, 121, 141	0
1	C	497/503 (98%)	0.53	37 (7%) 17 12	22, 71, 119, 141	0
2	B	439/447 (98%)	0.32	18 (4%) 41 35	14, 62, 105, 131	0
2	D	437/447 (97%)	0.48	39 (8%) 12 8	15, 77, 118, 161	0
All	All	1870/1900 (98%)	0.40	121 (6%) 22 16	11, 67, 117, 161	0

The worst 5 of 121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	354	LEU	6.8
1	C	448	HIS	6.7
1	C	379	ILE	6.4
1	C	325	THR	5.4
2	B	401	PRO	4.9

### 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( $\text{\AA}^2$ )	Q<0.9
3	MG	A	601	1/1	0.92	0.31	-	14,14,14,14	0
3	MG	B	501	1/1	0.98	0.33	-	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.