



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:59 am GMT

PDB ID : 4HG6  
Title : Structure of a cellulose synthase - cellulose translocation intermediate  
Authors : Zimmer, J.  
Deposited on : 2012-10-07  
Resolution : 3.25 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

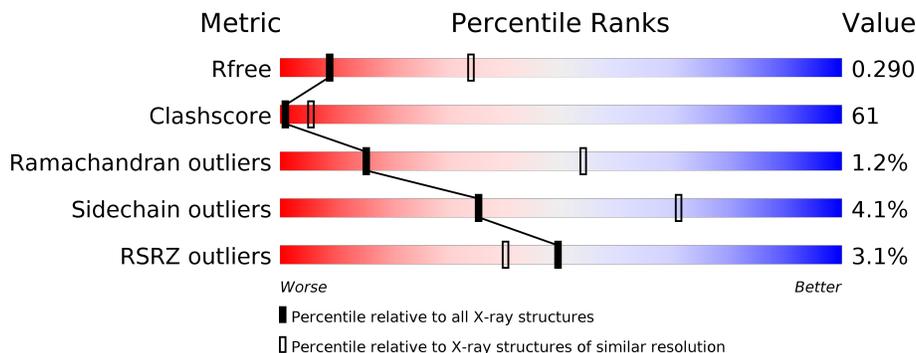
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1852 (3.32-3.20)
Clashscore	112137	2036 (3.32-3.20)
Ramachandran outliers	110173	2000 (3.32-3.20)
Sidechain outliers	110143	1998 (3.32-3.20)
RSRZ outliers	101464	1861 (3.32-3.20)

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	802	
2	B	707	

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	BGC	A	905	-	-	X	-
3	BGC	A	912	-	-	-	X
3	BGC	A	913	-	-	-	X
3	BGC	A	914	-	-	-	X
4	UDP	A	919	-	-	-	X
5	LDA	A	921	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11029 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 Cellulose Synthase Subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	747	5893	3822	1029	1011	31	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	789	HIS	-	EXPRESSION TAG	UNP Q3J125
A	790	HIS	-	EXPRESSION TAG	UNP Q3J125
A	791	HIS	-	EXPRESSION TAG	UNP Q3J125
A	792	HIS	-	EXPRESSION TAG	UNP Q3J125
A	793	HIS	-	EXPRESSION TAG	UNP Q3J125
A	794	HIS	-	EXPRESSION TAG	UNP Q3J125
A	795	LYS	-	EXPRESSION TAG	UNP Q3J125
A	796	LEU	-	EXPRESSION TAG	UNP Q3J125
A	797	HIS	-	EXPRESSION TAG	UNP Q3J125
A	798	HIS	-	EXPRESSION TAG	UNP Q3J125
A	799	HIS	-	EXPRESSION TAG	UNP Q3J125
A	800	HIS	-	EXPRESSION TAG	UNP Q3J125
A	801	HIS	-	EXPRESSION TAG	UNP Q3J125
A	802	HIS	-	EXPRESSION TAG	UNP Q3J125

- Molecule 2 is a protein called Cellulose Synthase Subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	655	4887	3100	864	907	16	0	0	0

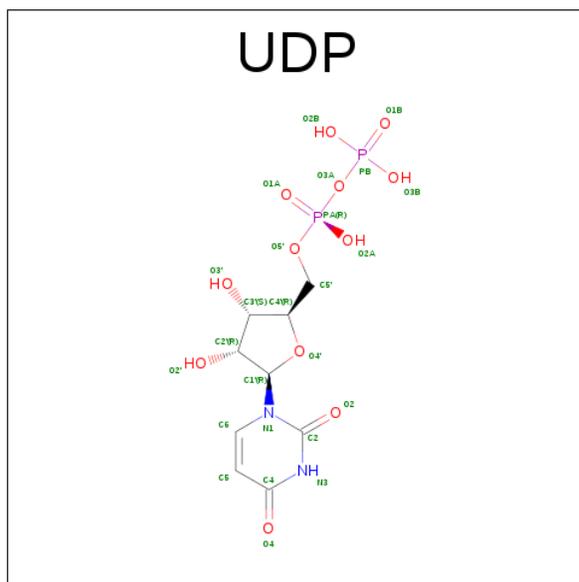
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	19	MET	-	EXPRESSION TAG	UNP Q3J126
B	20	GLY	-	EXPRESSION TAG	UNP Q3J126

- Molecule 3 is a polymer of unknown type called SUGAR (18-MER).

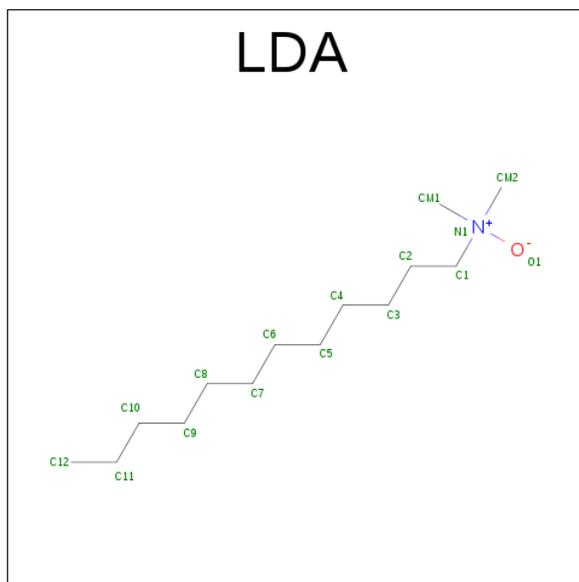
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	18	199	108	91	0	0

- Molecule 4 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula:  $C_9H_{14}N_2O_{12}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	25	9	2	12	2	0	0

- Molecule 5 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).

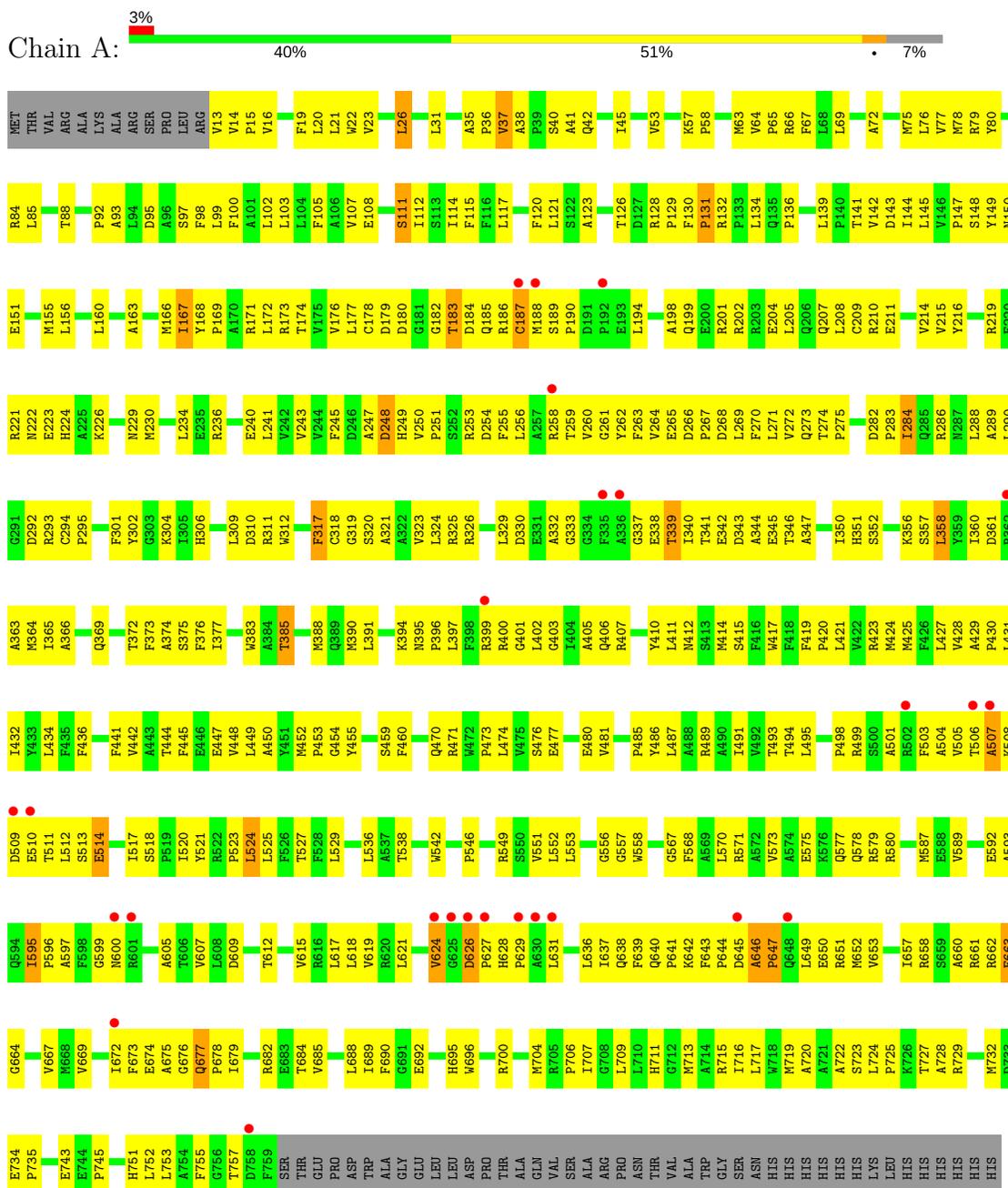


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			9	7	1	1		
5	A	1	Total	C	N	O	0	0
			16	14	1	1		

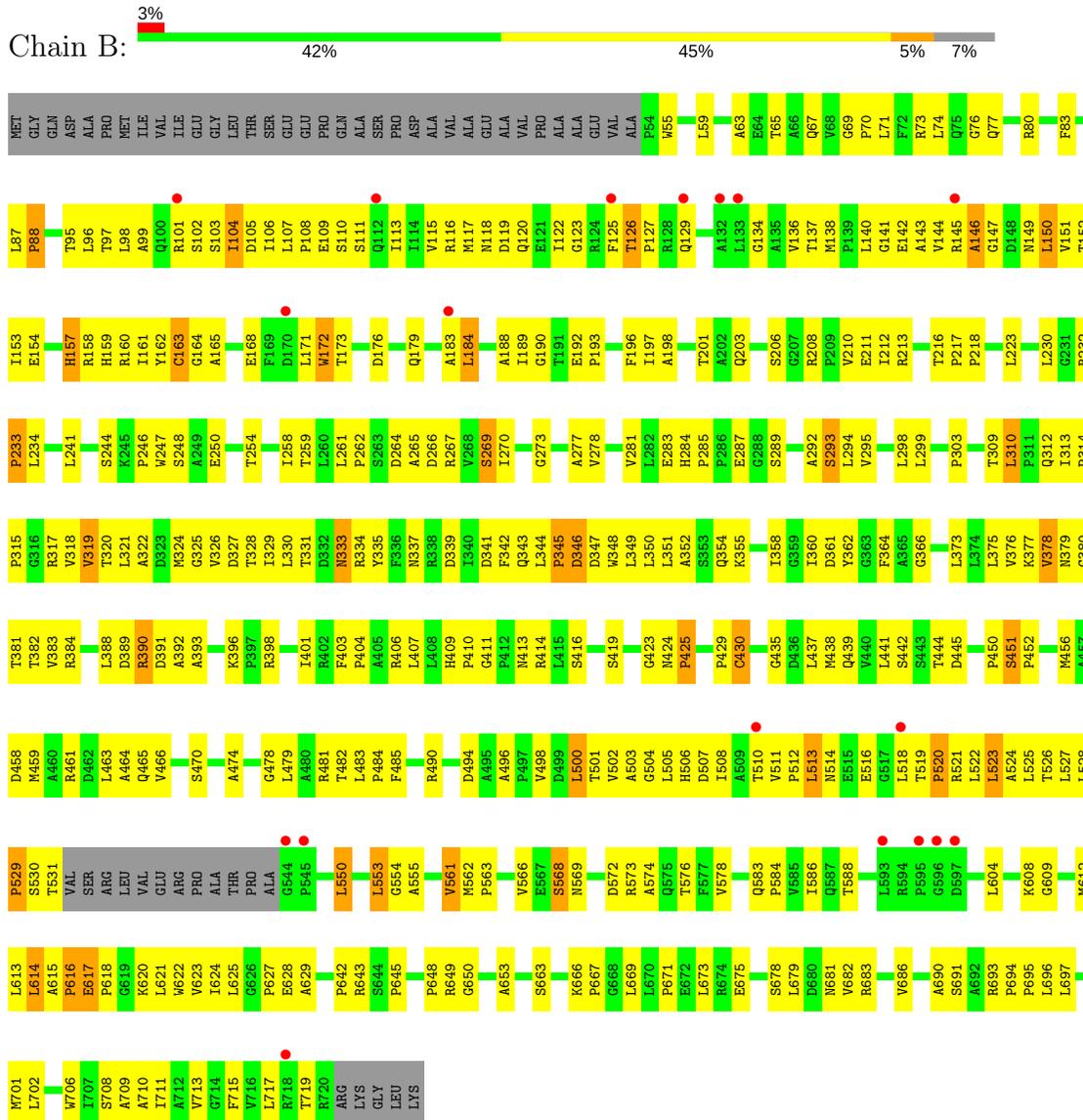
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Cellulose Synthase Subunit A



● Molecule 2: Cellulose Synthase Subunit B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.12Å 103.12Å 468.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.81 – 3.25 34.81 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.81-3.25) 99.9 (34.81-3.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.91 (at 3.25Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.213 , 0.282 0.229 , 0.290	Depositor DCC
$R_{free}$ test set	2055 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	117.9	Xtrriage
Anisotropy	0.057	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 95.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11029	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	140.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: LDA, BGC, UDP

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	0.41	0/6044	0.63	2/8217 (0.0%)
2	B	0.39	1/5006 (0.0%)	0.63	2/6865 (0.0%)
All	All	0.40	1/11050 (0.0%)	0.63	4/15082 (0.0%)

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
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	345	PRO	N-CD	-10.24	1.33	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	346	ASP	CB-CA-C	-7.15	96.10	110.40
2	B	345	PRO	CA-N-CD	6.14	120.30	111.70
1	A	646	ALA	C-N-CD	-6.03	107.33	120.60
1	A	663	GLU	N-CA-C	-5.53	96.06	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	390	ARG	Sidechain

## 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	5893	0	5996	742	0
2	B	4887	0	4966	603	0
3	A	199	0	165	29	0
4	A	25	0	11	2	0
5	A	25	0	45	7	0
All	All	11029	0	11183	1350	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 61.

The worst 5 of 1350 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:B:330:LEU:CD2	2:B:439:GLN:HG3	1.33	1.58
2:B:377:LYS:CG	2:B:382:THR:HG22	1.32	1.56
1:A:643:PHE:HB3	1:A:646:ALA:CB	1.42	1.49
2:B:107:LEU:CD1	2:B:160:ARG:HA	1.47	1.41
1:A:317:PHE:CE2	1:A:347:ALA:HB2	1.58	1.38

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	745/802 (93%)	674 (90%)	64 (9%)	7 (1%)	20	60
2	B	651/707 (92%)	574 (88%)	67 (10%)	10 (2%)	12	49
All	All	1396/1509 (92%)	1248 (89%)	131 (9%)	17 (1%)	15	54

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	PRO
1	A	514	GLU
1	A	647	PRO
2	B	146	ALA
2	B	529	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	614/661 (93%)	595 (97%)	19 (3%)	45	77
2	B	520/559 (93%)	492 (95%)	28 (5%)	26	63
All	All	1134/1220 (93%)	1087 (96%)	47 (4%)	35	71

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	163	CYS
2	B	289	SER
2	B	568	SER
2	B	184	LEU
2	B	309	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	412	ASN

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Mol	Chain	Res	Type
1	A	515	ASN
2	B	337	ASN
1	A	306	HIS
2	B	67	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

18 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	BGC	A	901	3	12,12,12	0.50	0	17,17,17	1.89	3 (17%)
3	BGC	A	902	3	11,11,12	0.67	0	13,15,17	2.15	2 (15%)
3	BGC	A	903	3	11,11,12	0.59	0	13,15,17	1.16	0
3	BGC	A	904	3	11,11,12	0.62	0	13,15,17	0.83	0
3	BGC	A	905	3	11,11,12	0.65	0	13,15,17	0.98	1 (7%)
3	BGC	A	906	3	11,11,12	0.84	0	13,15,17	2.11	4 (30%)
3	BGC	A	907	3	11,11,12	0.75	0	13,15,17	2.02	3 (23%)
3	BGC	A	908	3	11,11,12	0.62	0	13,15,17	1.29	2 (15%)
3	BGC	A	909	3	11,11,12	0.57	0	13,15,17	1.75	3 (23%)
3	BGC	A	910	3	11,11,12	0.64	0	13,15,17	1.19	2 (15%)
3	BGC	A	911	3	11,11,12	0.85	0	13,15,17	1.45	2 (15%)
3	BGC	A	912	3	11,11,12	0.98	0	13,15,17	2.03	3 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BGC	A	913	3	11,11,12	0.80	0	13,15,17	1.75	4 (30%)
3	BGC	A	914	3	11,11,12	0.65	0	13,15,17	3.07	6 (46%)
3	BGC	A	915	3	11,11,12	0.59	0	13,15,17	1.44	2 (15%)
3	BGC	A	916	3	11,11,12	0.62	0	13,15,17	1.59	2 (15%)
3	BGC	A	917	3	11,11,12	0.74	0	13,15,17	2.66	4 (30%)
3	BGC	A	918	3	11,11,12	0.71	0	13,15,17	2.24	4 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	A	901	3	-	0/2/22/22	0/1/1/1
3	BGC	A	902	3	-	0/2/19/22	0/1/1/1
3	BGC	A	903	3	-	0/2/19/22	0/1/1/1
3	BGC	A	904	3	-	0/2/19/22	0/1/1/1
3	BGC	A	905	3	-	0/2/19/22	0/1/1/1
3	BGC	A	906	3	-	0/2/19/22	0/1/1/1
3	BGC	A	907	3	-	0/2/19/22	0/1/1/1
3	BGC	A	908	3	-	0/2/19/22	0/1/1/1
3	BGC	A	909	3	-	0/2/19/22	0/1/1/1
3	BGC	A	910	3	-	0/2/19/22	0/1/1/1
3	BGC	A	911	3	-	0/2/19/22	0/1/1/1
3	BGC	A	912	3	-	0/2/19/22	0/1/1/1
3	BGC	A	913	3	-	0/2/19/22	0/1/1/1
3	BGC	A	914	3	-	0/2/19/22	0/1/1/1
3	BGC	A	915	3	-	0/2/19/22	0/1/1/1
3	BGC	A	916	3	-	0/2/19/22	0/1/1/1
3	BGC	A	917	3	-	0/2/19/22	0/1/1/1
3	BGC	A	918	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	916	BGC	O5-C1-C2	-3.90	104.68	110.79
3	A	914	BGC	O4-C4-C5	-3.89	99.49	109.28
3	A	911	BGC	O4-C4-C5	-3.79	99.74	109.28
3	A	912	BGC	C1-O5-C5	-3.64	107.15	112.17
3	A	912	BGC	O4-C4-C5	-3.32	100.93	109.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	905	BGC	6	0
3	A	906	BGC	1	0
3	A	907	BGC	1	0
3	A	908	BGC	2	0
3	A	909	BGC	3	0
3	A	910	BGC	4	0
3	A	911	BGC	5	0
3	A	912	BGC	4	0
3	A	913	BGC	3	0
3	A	916	BGC	1	0
3	A	917	BGC	4	0
3	A	918	BGC	3	0

## 5.6 Ligand geometry [i](#)

3 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
4	UDP	A	919	-	21,26,26	1.03	1 (4%)	22,40,40	1.60	1 (4%)
5	LDA	A	920	-	6,8,15	3.58	2 (33%)	7,10,17	0.55	0
5	LDA	A	921	-	13,15,15	2.26	1 (7%)	14,17,17	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
4	UDP	A	919	-	-	0/12/32/32	0/2/2/2
5	LDA	A	920	-	-	0/6/6/13	0/0/0/0
5	LDA	A	921	-	-	0/13/13/13	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	920	LDA	O1-N1	-8.45	1.25	1.42
5	A	921	LDA	O1-N1	-7.85	1.26	1.42
5	A	920	LDA	C1-N1	-2.29	1.46	1.51
4	A	919	UDP	C4-N3	2.77	1.38	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	919	UDP	C4-N3-C2	6.47	119.69	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	919	UDP	2	0
5	A	920	LDA	5	0
5	A	921	LDA	2	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	747/802 (93%)	-0.11	26 (3%) 44 34	77, 127, 205, 236	0
2	B	655/707 (92%)	-0.10	18 (2%) 55 46	82, 143, 210, 235	0
All	All	1402/1509 (92%)	-0.10	44 (3%) 49 40	77, 135, 208, 236	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	544	GLY	7.2
2	B	183	ALA	5.0
2	B	545	PRO	4.6
1	A	627	PRO	3.8
2	B	596	GLY	3.8

### 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	BGC	A	913	11/12	0.95	0.39	5.32	88,107,120,127	0
3	BGC	A	912	11/12	0.95	0.34	3.45	86,103,140,157	0
3	BGC	A	914	11/12	0.98	0.32	2.84	97,114,126,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	BGC	A	915	11/12	0.97	0.33	1.70	108,116,170,173	0
3	BGC	A	917	11/12	0.92	0.32	1.68	97,106,119,140	0
3	BGC	A	911	11/12	0.99	0.22	0.76	83,93,108,111	0
3	BGC	A	916	11/12	0.97	0.26	0.34	90,104,129,158	0
3	BGC	A	918	11/12	0.96	0.28	0.33	116,121,136,142	0
3	BGC	A	907	11/12	0.97	0.17	0.25	79,109,137,143	0
3	BGC	A	909	11/12	0.99	0.18	-0.47	70,96,103,127	0
3	BGC	A	910	11/12	0.97	0.17	-0.50	82,97,109,114	0
3	BGC	A	906	11/12	0.96	0.15	-0.54	77,96,110,146	0
3	BGC	A	908	11/12	0.95	0.15	-0.69	78,92,104,118	0
3	BGC	A	905	11/12	0.95	0.15	-0.91	95,114,142,143	0
3	BGC	A	904	11/12	0.97	0.11	-1.83	97,115,128,142	0
3	BGC	A	901	12/12	0.90	0.38	-	176,192,196,198	0
3	BGC	A	902	11/12	0.96	0.20	-	149,170,193,198	0
3	BGC	A	903	11/12	0.98	0.09	-	100,112,144,154	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
4	UDP	A	919	25/25	0.79	0.70	5.00	57,85,113,131	25
5	LDA	A	921	16/16	0.79	0.36	2.84	105,128,177,182	0
5	LDA	A	920	9/16	0.92	0.31	1.93	92,109,143,144	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.