



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:30 PM GMT

PDB ID : 4CFP  
Title : Crystal structure of MltC in complex with tetrasaccharide at 2.15 Å resolution  
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Deposited on : 2013-11-19  
Resolution : 2.15 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

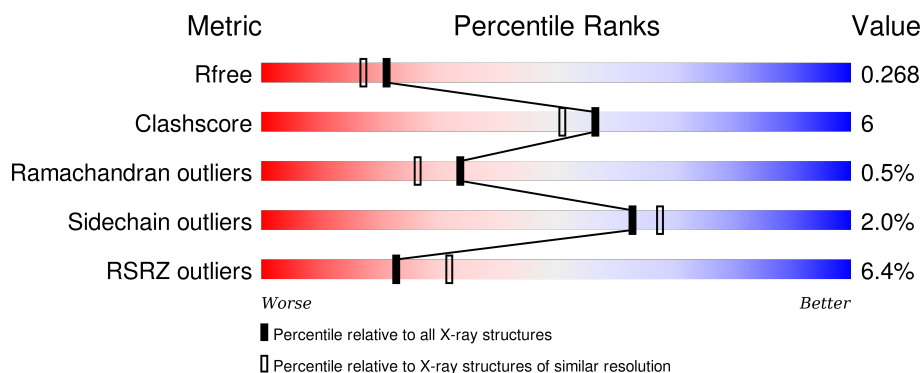
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	341	<div> <div>11%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
1	B	341	<div> <div>%</div> <div>85%</div> <div>11%</div> <div>•</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AMV	B	1363	-	-	-	X
4	P6G	A	1365	-	-	-	X
5	CIT	B	1364	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5525 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 MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2577	1616	461	492	8			
1	B	327	Total	C	N	O	S	0	0	0
			2577	1616	461	492	8			

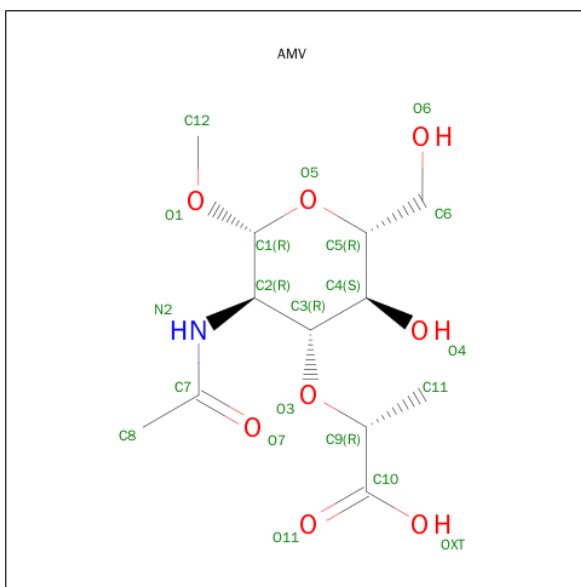
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	EXPRESSION TAG	UNP C5A0N2
A	217	GLN	GLU	ENGINEERED MUTATION	UNP C5A0N2
B	19	MET	-	EXPRESSION TAG	UNP C5A0N2
B	217	GLN	GLU	ENGINEERED MUTATION	UNP C5A0N2

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

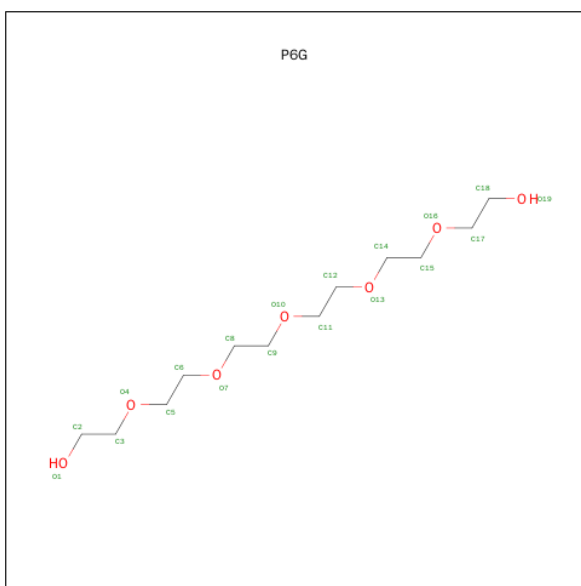
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			47	27	3	17		
2	B	3	Total	C	N	O	0	0
			47	27	3	17		

- Molecule 3 is METHYL 2-(ACETYLAMINO)-3-O-[(1R)-1-CARBOXYETHYL]-2-DEOXY-BETA-D-GLUCOPYRANOSIDE (three-letter code: AMV) (formula: C<sub>12</sub>H<sub>21</sub>NO<sub>8</sub>).



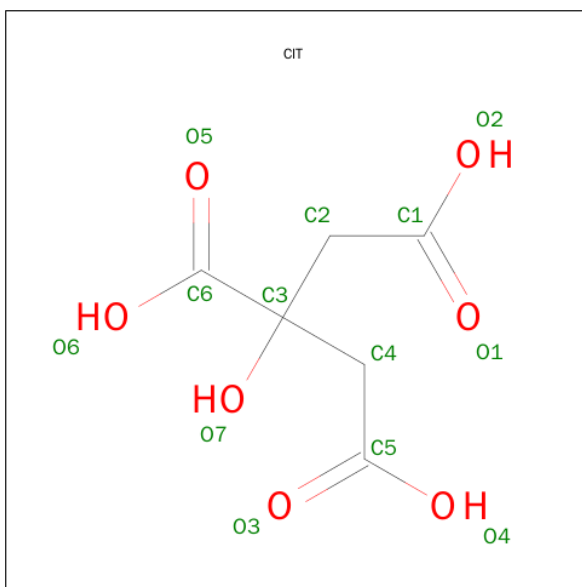
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	12	1	8		
3	B	1	Total	C	N	O	0	0
			21	12	1	8		

- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	6	7		

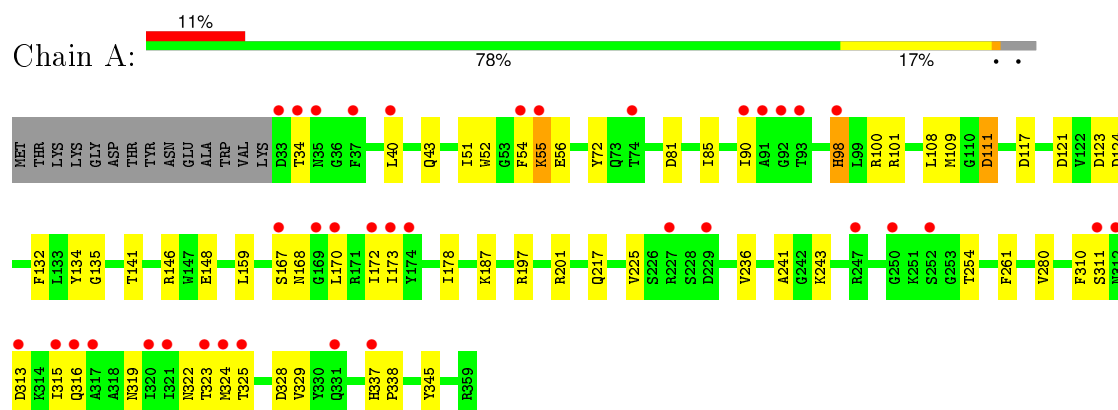
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	85	Total	O	0	0
			85	85		
6	B	118	Total	O	0	0
			118	118		

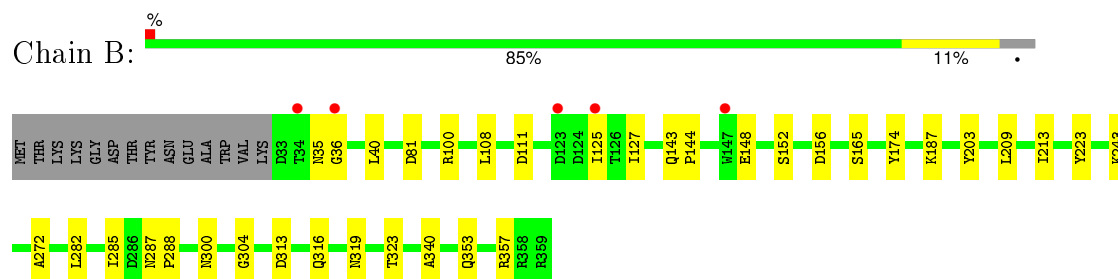
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE C



#### • Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.51Å 114.33Å 61.77Å 90.00° 93.28° 90.00°	Depositor
Resolution (Å)	49.43 – 2.15 57.17 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.43-2.15) 94.8 (57.17-2.15)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.14Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.191 , 0.268 0.203 , 0.268	Depositor DCC
$R_{free}$ test set	1858 reflections (5.53%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 59.9	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 37143 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5525	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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: AMV, AMU, NAG, P6G, CIT

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	0.39	0/2628	0.58	0/3559
1	B	0.42	0/2628	0.55	0/3559
All	All	0.40	0/5256	0.56	0/7118

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	HIS	Peptide

### 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	2577	0	2547	45	0
1	B	2577	0	2547	17	0
2	A	47	0	40	2	0
2	B	47	0	40	3	0
3	A	21	0	19	0	0
3	B	21	0	19	2	0
4	A	19	0	26	3	0
5	B	13	0	5	1	0
6	A	85	0	0	1	0
6	B	118	0	0	1	0
All	All	5525	0	5243	64	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 (64) 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:167:SER:HB2	1:A:172:ILE:HD12	1.61	0.83
1:A:55:LYS:HE3	1:A:168:ASN:HB2	1.60	0.82
1:B:100:ARG:NH1	1:B:156:ASP:OD1	2.22	0.73
1:A:111:ASP:HB3	1:A:132:PHE:HB2	1.74	0.69
1:A:197:ARG:HB3	1:A:201:ARG:HH12	1.58	0.69
1:A:236:VAL:HA	2:A:1362:NAG:H83	1.77	0.67
1:A:90:ILE:HG22	1:A:173:ILE:HG12	1.77	0.66
1:A:337:HIS:HD2	1:A:338:PRO:CD	2.09	0.66
1:A:319:ASN:O	1:A:323:THR:HG23	2.00	0.61
1:A:337:HIS:CD2	1:A:338:PRO:HD2	2.35	0.61
1:A:337:HIS:CD2	1:A:338:PRO:CD	2.84	0.60
1:B:340:ALA:HB3	5:B:1364:CIT:H22	1.84	0.59
1:A:187:LYS:HD2	4:A:1365:P6G:H121	1.84	0.59
1:A:51:ILE:HD12	1:A:72:TYR:HB2	1.86	0.58
1:A:101:ARG:NH2	1:A:123:ASP:OD2	2.36	0.57
1:A:315:ILE:HG13	1:A:316:GLN:N	2.19	0.56
1:B:353:GLN:O	1:B:357:ARG:HG3	2.07	0.55
2:B:1360:NAG:O6	2:B:1361:AMU:H111	2.09	0.53
1:A:40:LEU:HA	1:A:43:GLN:HB2	1.91	0.53
1:A:217:GLN:NE2	1:A:345:TYR:HE2	2.06	0.53
1:A:168:ASN:OD1	1:A:170:LEU:N	2.41	0.52
1:B:304:GLY:HA3	2:B:1361:AMU:H112	1.91	0.52
1:A:324:MET:HB2	1:A:328:ASP:HB2	1.90	0.52
1:A:319:ASN:HA	1:A:322:ASN:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ASN:O	3:B:1363:AMV:H111	2.10	0.51
1:A:117:ASP:N	1:A:124:ASP:OD2	2.42	0.50
1:B:35:ASN:ND2	6:B:2001:HOH:O	2.44	0.50
1:A:241:ALA:HB3	2:A:1362:NAG:H82	1.94	0.49
1:B:282:LEU:HB3	1:B:285:ILE:HD12	1.93	0.49
1:A:313:ASP:OD2	1:A:315:ILE:HG12	2.12	0.49
1:A:337:HIS:HD2	1:A:338:PRO:N	2.11	0.49
1:B:313:ASP:HB3	1:B:316:GLN:HB2	1.95	0.48
1:A:225:VAL:CG1	1:A:261:PHE:HZ	2.27	0.46
1:A:197:ARG:HB3	1:A:201:ARG:NH1	2.26	0.46
1:A:100:ARG:HB2	1:A:159:LEU:HD11	1.96	0.46
1:B:319:ASN:O	1:B:323:THR:HG23	2.15	0.46
1:A:134:TYR:CE1	1:A:146:ARG:HB2	2.51	0.45
1:A:324:MET:HB2	1:A:328:ASP:CB	2.47	0.45
1:A:325:THR:O	1:A:328:ASP:HB2	2.16	0.45
1:A:337:HIS:HD2	1:A:338:PRO:CG	2.29	0.45
1:B:36:GLY:O	1:B:40:LEU:HG	2.17	0.45
1:B:111:ASP:HA	1:B:223:TYR:OH	2.18	0.44
1:B:203:TYR:CZ	1:B:272:ALA:HB2	2.52	0.44
1:A:187:LYS:NZ	4:A:1365:P6G:O7	2.50	0.44
1:A:337:HIS:CD2	1:A:338:PRO:HG2	2.52	0.44
1:B:108:LEU:HD11	1:B:148:GLU:HA	2.00	0.43
1:B:165:SER:HB3	1:B:174:TYR:CD1	2.53	0.43
1:A:337:HIS:HD2	1:A:338:PRO:HG2	1.84	0.43
1:B:287:ASN:HA	1:B:288:PRO:HD3	1.86	0.43
1:A:90:ILE:CG2	1:A:173:ILE:HG12	2.48	0.43
1:A:108:LEU:HD11	1:A:148:GLU:HA	2.00	0.43
1:A:135:GLY:HA2	4:A:1365:P6G:H32	2.01	0.42
1:A:72:TYR:CE1	1:A:121:ASP:HB3	2.54	0.42
1:A:85:ILE:HB	1:A:178:ILE:HB	2.01	0.42
1:A:52:TRP:HB3	1:A:56:GLU:HB2	2.02	0.42
1:B:143:GLN:HA	1:B:144:PRO:HD3	1.90	0.41
1:A:337:HIS:CD2	1:A:337:HIS:C	2.93	0.41
1:B:209:LEU:O	1:B:213:ILE:HG12	2.20	0.41
1:A:109:MET:HE2	6:A:2024:HOH:O	2.19	0.41
2:B:1362:NAG:O5	3:B:1363:AMV:H9	2.21	0.41
1:A:310:PHE:O	1:A:311:SER:HB2	2.21	0.41
1:A:325:THR:O	1:A:329:VAL:HG23	2.20	0.40
1:A:225:VAL:HG13	1:A:261:PHE:HZ	1.86	0.40
1:A:243:LYS:HD3	1:A:254:THR:HG22	2.04	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	325/341 (95%)	306 (94%)	17 (5%)	2 (1%)	30	21
1	B	325/341 (95%)	320 (98%)	4 (1%)	1 (0%)	46	42
All	All	650/682 (95%)	626 (96%)	21 (3%)	3 (0%)	34	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	ASP
1	A	280	VAL
1	B	125	ILE

### 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	279/291 (96%)	273 (98%)	6 (2%)	60	63
1	B	279/291 (96%)	274 (98%)	5 (2%)	66	71
All	All	558/582 (96%)	547 (98%)	11 (2%)	63	67

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	54	PHE
1	A	55	LYS

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Mol	Chain	Res	Type
1	A	81	ASP
1	A	98	HIS
1	A	141	THR
1	B	81	ASP
1	B	127	ILE
1	B	152	SER
1	B	187	LYS
1	B	243	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	337	HIS
1	B	331	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](#)

6 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	1360	2	14,14,15	1.07	1 (7%)	15,19,21	1.24	1 (6%)
2	AMU	A	1361	2	16,19,20	1.67	4 (25%)	15,26,28	1.53	2 (13%)
2	NAG	A	1362	3,2	14,14,15	1.19	2 (14%)	15,19,21	2.29	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	1360	2	14,14,15	1.07	2 (14%)	15,19,21	1.43	2 (13%)
2	AMU	B	1361	2	16,19,20	1.75	4 (25%)	15,26,28	2.47	3 (20%)
2	NAG	B	1362	3,2	14,14,15	1.45	3 (21%)	15,19,21	1.15	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	1360	2	-	0/6/23/26	0/1/1/1
2	AMU	A	1361	2	-	0/10/31/34	0/1/1/1
2	NAG	A	1362	3,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1360	2	-	0/6/23/26	0/1/1/1
2	AMU	B	1361	2	-	0/10/31/34	0/1/1/1
2	NAG	B	1362	3,2	-	0/6/23/26	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1361	AMU	O5-C1	-3.31	1.38	1.43
2	A	1361	AMU	C2-N2	-2.90	1.41	1.46
2	B	1361	AMU	C2-N2	-2.87	1.41	1.46
2	A	1361	AMU	O5-C1	-2.68	1.39	1.43
2	B	1362	NAG	O5-C1	-2.55	1.39	1.43
2	B	1362	NAG	C2-N2	-2.28	1.42	1.46
2	B	1360	NAG	C2-N2	-2.23	1.42	1.46
2	A	1362	NAG	O5-C1	-2.02	1.40	1.43
2	B	1361	AMU	C7-N2	2.35	1.43	1.34
2	B	1360	NAG	C7-N2	2.42	1.43	1.34
2	A	1362	NAG	C7-N2	2.43	1.43	1.34
2	A	1360	NAG	C7-N2	2.44	1.43	1.34
2	A	1361	AMU	C3-C2	2.52	1.56	1.52
2	B	1361	AMU	C3-C2	2.64	1.56	1.52
2	A	1361	AMU	C7-N2	2.73	1.44	1.34
2	B	1362	NAG	C7-N2	2.79	1.45	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1361	AMU	C11-C9-C10	-8.27	102.60	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1362	NAG	C4-C3-C2	-4.17	104.75	111.23
2	B	1360	NAG	C2-N2-C7	-2.11	120.32	123.04
2	A	1362	NAG	O7-C7-C8	-2.10	118.20	122.06
2	A	1361	AMU	C11-C9-C10	-2.08	110.51	113.18
2	B	1361	AMU	C3-C4-C5	2.00	114.15	109.61
2	A	1362	NAG	O3-C3-C4	2.02	114.89	110.34
2	A	1360	NAG	O5-C5-C6	2.06	111.80	107.35
2	B	1361	AMU	C1-O5-C5	2.34	115.22	112.25
2	A	1362	NAG	C3-C2-N2	3.25	118.35	110.56
2	A	1362	NAG	C8-C7-N2	3.53	122.86	116.11
2	B	1360	NAG	C1-O5-C5	3.63	116.85	112.25
2	A	1361	AMU	C1-O5-C5	4.08	117.43	112.25
2	A	1362	NAG	C1-O5-C5	4.77	118.30	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1362	NAG	2	0
2	B	1360	NAG	1	0
2	B	1361	AMU	2	0
2	B	1362	NAG	1	0

## 5.6 Ligand geometry

4 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	$\# Z  > 2$
3	AMV	A	1363	2	18,21,21	1.35	1 (5%)	22,29,29	1.40	2 (9%)
4	P6G	A	1365	-	18,18,18	0.75	0	17,17,17	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AMV	B	1363	2	18,21,21	1.43	4 (22%)	22,29,29	2.23	8 (36%)
5	CIT	B	1364	-	3,12,12	1.22	0	3,17,17	2.62	1 (33%)

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	AMV	A	1363	2	-	0/12/36/36	0/1/1/1
4	P6G	A	1365	-	-	0/16/16/16	0/0/0/0
3	AMV	B	1363	2	-	0/12/36/36	0/1/1/1
5	CIT	B	1364	-	-	0/6/16/16	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1363	AMV	C1-C2	-2.37	1.48	1.53
3	B	1363	AMV	O3-C3	-2.11	1.38	1.43
3	B	1363	AMV	C8-C7	2.31	1.55	1.50
3	B	1363	AMV	C7-N2	2.97	1.45	1.34
3	A	1363	AMV	C7-N2	3.02	1.45	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1363	AMV	C11-C9-C10	-4.51	107.41	113.18
5	B	1364	CIT	C3-C4-C5	-4.38	107.96	114.96
3	B	1363	AMV	C1-C2-C3	-3.31	103.79	110.13
3	A	1363	AMV	C11-C9-C10	-3.14	109.15	113.18
3	B	1363	AMV	O5-C1-C2	-2.85	104.59	110.78
3	B	1363	AMV	C3-C4-C5	-2.80	103.27	109.61
3	A	1363	AMV	C1-C2-C3	-2.09	106.12	110.13
3	B	1363	AMV	C3-C2-N2	2.03	114.60	111.07
3	B	1363	AMV	O1-C1-C2	2.05	111.36	108.03
3	B	1363	AMV	O3-C3-C4	4.16	117.92	107.17
3	B	1363	AMV	O3-C9-C11	5.24	119.71	107.17

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
4	A	1365	P6G	3	0
3	B	1363	AMV	2	0
5	B	1364	CIT	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	327/341 (95%)	0.69	37 (11%) 7 11	21, 44, 97, 140	0
1	B	327/341 (95%)	0.13	5 (1%) 76 82	17, 31, 60, 97	0
All	All	654/682 (95%)	0.41	42 (6%) 23 32	17, 36, 87, 140	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	320	ILE	5.6
1	A	90	ILE	4.7
1	A	323	THR	4.5
1	A	35	ASN	4.4
1	A	34	THR	4.3
1	A	93	THR	4.2
1	A	316	GLN	4.1
1	A	312	ASN	4.1
1	A	315	ILE	4.0
1	A	169	GLY	3.8
1	A	54	PHE	3.7
1	A	324	MET	3.6
1	A	40	LEU	3.4
1	A	92	GLY	3.4
1	A	33	ASP	3.2
1	A	311	SER	3.1
1	A	174	TYR	3.0
1	B	147	TRP	3.0
1	A	167	SER	2.9
1	A	252	SER	2.9
1	A	317	ALA	2.8
1	A	250	GLY	2.8
1	A	173	ILE	2.8
1	A	337	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	325	THR	2.7
1	A	321	ILE	2.5
1	A	313	ASP	2.5
1	A	91	ALA	2.4
1	B	125	ILE	2.4
1	A	331	GLN	2.4
1	A	37	PHE	2.4
1	B	36	GLY	2.3
1	A	170	LEU	2.3
1	A	98	HIS	2.3
1	A	227	ARG	2.2
1	A	74	THR	2.2
1	A	229	ASP	2.1
1	A	247	ARG	2.1
1	A	172	ILE	2.0
1	B	34	THR	2.0
1	B	123	ASP	2.0
1	A	55	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
2	AMU	B	1361	19/20	0.94	0.14	1.11	16,24,57,66	0
2	NAG	A	1362	14/15	0.91	0.15	0.29	20,33,45,52	0
2	NAG	B	1362	14/15	0.96	0.12	-0.33	9,27,32,41	0
2	AMU	A	1361	19/20	0.92	0.13	-0.43	26,33,53,57	0
2	NAG	A	1360	14/15	0.88	0.14	-0.48	38,44,48,49	0
2	NAG	B	1360	14/15	0.94	0.11	-0.63	21,27,39,41	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
5	CIT	B	1364	13/13	0.85	0.27	3.10	57,71,85,86	0
4	P6G	A	1365	19/19	0.83	0.19	2.80	43,55,74,76	0
3	AMV	B	1363	21/21	0.92	0.15	2.08	16,25,54,56	0
3	AMV	A	1363	21/21	0.94	0.17	0.26	15,36,54,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.