



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:01 am BST

PDB ID : 3NF0  
Title : mPlum-TTN  
Authors : Mayo, S.L.; Chica, R.A.; Moore, M.M.  
Deposited on : 2010-06-09  
Resolution : 1.75 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

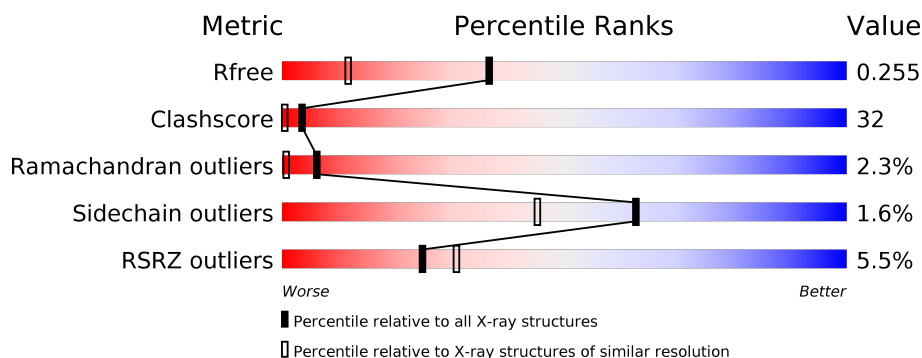
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
$R_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 respectively. 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	232	<div> <div>5%</div> <div> <div></div> <div>60%</div> <div>27%</div> <div>6% • 6%</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
2	MLT	A	228	-	-	X	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1935 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.

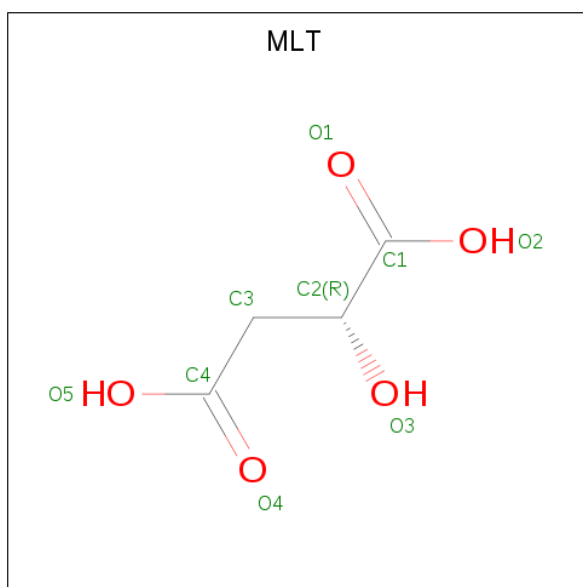
- Molecule 1 is a protein called Fluorescent protein plum.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	218	1799	1134	304	351	10	27	9	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	EXPRESSION TAG	UNP Q5S3G7
A	-7	GLY	-	EXPRESSION TAG	UNP Q5S3G7
A	-6	HIS	-	EXPRESSION TAG	UNP Q5S3G7
A	-5	HIS	-	EXPRESSION TAG	UNP Q5S3G7
A	-4	HIS	-	EXPRESSION TAG	UNP Q5S3G7
A	-3	HIS	-	EXPRESSION TAG	UNP Q5S3G7
A	-2	HIS	-	EXPRESSION TAG	UNP Q5S3G7
A	-1	HIS	-	EXPRESSION TAG	UNP Q5S3G7
A	0	GLY	-	EXPRESSION TAG	UNP Q5S3G7
A	67	CH6	MET	CHROMOPHORE	UNP Q5S3G7
A	67	CH6	TYR	CHROMOPHORE	UNP Q5S3G7
A	67	CH6	GLY	CHROMOPHORE	UNP Q5S3G7
A	197	THR	ILE	ENGINEERED MUTATION	UNP Q5S3G7
A	217	ASN	ALA	ENGINEERED MUTATION	UNP Q5S3G7

- Molecule 2 is D-MALATE (three-letter code: MLT) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		
2	A	1	Total	C	O	0	0
			9	4	5		
2	A	1	Total	C	O	0	0
			9	4	5		

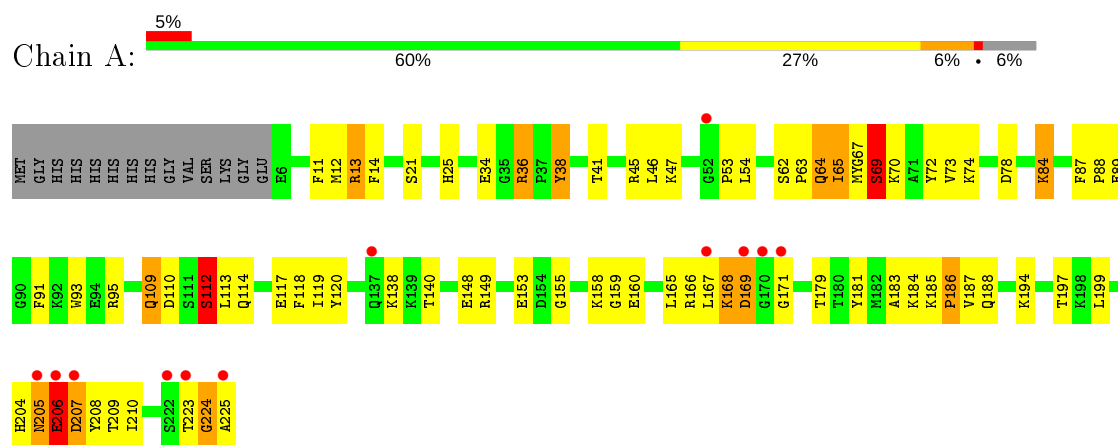
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total	O	0	2
			109	109		

### 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 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: Fluorescent protein plum



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.27Å 61.30Å 94.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.46 – 1.75 32.46 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.1 (32.46-1.75) 99.2 (32.46-1.75)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 1.75Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.208 , 0.256 0.208 , 0.255	Depositor DCC
$R_{free}$ test set	1170 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.9	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 64.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	1935	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLT, CH6

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	1.47	20/1842 (1.1%)	1.28	9/2476 (0.4%)

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	7

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	LYS	CE-NZ	8.15	1.69	1.49
1	A	72	TYR	CG-CD2	-6.79	1.30	1.39
1	A	72	TYR	CE1-CZ	-6.65	1.29	1.38
1	A	186	PRO	CB-CG	6.46	1.82	1.50
1	A	11	PHE	C-O	6.42	1.35	1.23
1	A	183	ALA	CA-CB	6.36	1.65	1.52
1	A	72	TYR	CE2-CZ	-6.32	1.30	1.38
1	A	155	GLY	C-O	6.16	1.33	1.23
1	A	112[A]	SER	CB-OG	-6.08	1.34	1.42
1	A	112[B]	SER	CB-OG	-6.08	1.34	1.42
1	A	36	ARG	C-O	5.90	1.34	1.23
1	A	34	GLU	CG-CD	5.85	1.60	1.51
1	A	12	MET	C-O	-5.80	1.12	1.23
1	A	187	VAL	C-O	-5.64	1.12	1.23
1	A	84	LYS	C-O	5.55	1.33	1.23
1	A	34	GLU	CD-OE2	5.49	1.31	1.25
1	A	187	VAL	CA-CB	-5.41	1.43	1.54
1	A	69	SER	CA-CB	5.14	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	ARG	CZ-NH1	5.11	1.39	1.33
1	A	185	LYS	CA-CB	-5.02	1.43	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	GLU	OE1-CD-OE2	7.32	132.08	123.30
1	A	41	THR	OG1-CB-CG2	-6.80	94.36	110.00
1	A	64	GLN	O-C-N	-6.59	112.16	122.70
1	A	13	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	A	112[A]	SER	CB-CA-C	-5.66	99.34	110.10
1	A	112[B]	SER	CB-CA-C	-5.66	99.34	110.10
1	A	65	ILE	CA-CB-CG2	5.44	121.77	110.90
1	A	166	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	38	TYR	CG-CD2-CE2	-5.12	117.20	121.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	GLN	Mainchain
1	A	205[B]	ASN	Peptide
1	A	206[A]	GLU	Peptide
1	A	206[B]	GLU	Peptide
1	A	207	ASP	Peptide
1	A	224	GLY	Peptide
1	A	64	GLN	Mainchain

## 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	1799	0	1710	111	0
2	A	27	0	11	13	0
3	A	109	0	0	5	0
All	All	1935	0	1721	112	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 32.

All (112) 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:84:LYS:NZ	1:A:84:LYS:CE	1.69	1.54
1:A:186:PRO:CB	1:A:186:PRO:CG	1.82	1.45
1:A:70[B]:LYS:HD2	3:A:290:HOH:O	1.11	1.26
1:A:93:TRP:NE1	1:A:109[B]:GLN:OE1	1.83	1.11
1:A:207:ASP:CB	2:A:228:MLT:O1	2.15	0.94
1:A:207:ASP:N	1:A:209:THR:H	1.67	0.93
1:A:207:ASP:HB2	2:A:228:MLT:O1	1.71	0.91
1:A:206[A]:GLU:OE1	1:A:210:ILE:HG13	1.72	0.88
1:A:169:ASP:OD2	1:A:171:GLY:N	2.09	0.86
1:A:93:TRP:CD1	1:A:109[B]:GLN:OE1	2.28	0.86
1:A:87:PHE:HE2	1:A:112[B]:SER:O	1.59	0.85
1:A:207:ASP:CA	2:A:228:MLT:O1	2.26	0.83
1:A:87:PHE:CE2	1:A:112[B]:SER:O	2.31	0.83
1:A:206[A]:GLU:N	2:A:228:MLT:O4	2.12	0.83
1:A:109[B]:GLN:HE21	1:A:110:ASP:C	1.83	0.82
1:A:206[B]:GLU:N	2:A:228:MLT:O4	2.16	0.79
1:A:109[B]:GLN:NE2	1:A:110:ASP:C	2.36	0.79
1:A:207:ASP:HA	2:A:228:MLT:O1	1.82	0.78
1:A:149:ARG:NH2	1:A:160:GLU:CD	2.36	0.78
1:A:207:ASP:HA	2:A:227:MLT:O5	1.86	0.76
1:A:70[B]:LYS:H	1:A:70[B]:LYS:CD	2.01	0.74
1:A:206[A]:GLU:OE2	3:A:323:HOH:O	2.06	0.73
1:A:70[B]:LYS:HE3	1:A:93:TRP:NE1	2.04	0.72
1:A:95:ARG:HE	1:A:179[B]:THR:HG21	1.54	0.71
1:A:206[A]:GLU:CA	2:A:228:MLT:O4	2.40	0.70
1:A:206[B]:GLU:CA	2:A:228:MLT:O4	2.40	0.69
1:A:70[B]:LYS:HE2	1:A:91:PHE:CZ	2.29	0.68
1:A:95:ARG:HE	1:A:179[B]:THR:CG2	2.06	0.68
1:A:205[A]:ASN:O	1:A:206[A]:GLU:HB2	1.95	0.67
1:A:206[A]:GLU:HA	2:A:228:MLT:O4	1.94	0.67
1:A:206[B]:GLU:OE2	1:A:206[B]:GLU:N	2.28	0.67
1:A:206[A]:GLU:CD	1:A:210:ILE:HG13	2.16	0.65
1:A:205[B]:ASN:CB	1:A:206[B]:GLU:OE2	2.45	0.65
1:A:109[A]:GLN:C	1:A:109[A]:GLN:HE21	2.02	0.63
1:A:206[B]:GLU:CD	1:A:206[B]:GLU:N	2.53	0.61
1:A:205[B]:ASN:HB2	1:A:206[B]:GLU:OE2	2.01	0.61
1:A:47:LYS:HB3	1:A:210:ILE:HD13	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70[B]:LYS:HE3	1:A:93:TRP:CD1	2.36	0.61
1:A:167:LEU:CB	1:A:169:ASP:HB3	2.31	0.60
1:A:70[B]:LYS:H	1:A:70[B]:LYS:HD3	1.65	0.60
1:A:205[A]:ASN:O	1:A:206[A]:GLU:CB	2.49	0.60
1:A:69:SER:HB2	1:A:120:TYR:CE2	2.35	0.60
1:A:149:ARG:O	1:A:159:GLY:HA2	2.00	0.60
1:A:167:LEU:HB2	1:A:169:ASP:HB3	1.84	0.60
1:A:95:ARG:HG3	1:A:179[B]:THR:HG22	1.82	0.59
1:A:53:PRO:HG3	1:A:207:ASP:OD2	2.02	0.59
1:A:149:ARG:HH22	1:A:160:GLU:CD	2.03	0.59
1:A:38:TYR:O	1:A:74:LYS:HG3	2.04	0.58
1:A:206[B]:GLU:HA	2:A:228:MLT:O4	2.02	0.57
1:A:70[B]:LYS:HE2	1:A:91:PHE:HZ	1.68	0.57
1:A:109[A]:GLN:NE2	1:A:110:ASP:C	2.57	0.56
1:A:36:ARG:NE	3:A:243:HOH:O	2.29	0.56
1:A:179[A]:THR:HG21	1:A:181:TYR:CZ	2.40	0.56
1:A:207:ASP:HB3	1:A:209:THR:HG23	1.87	0.56
1:A:70[B]:LYS:H	1:A:70[B]:LYS:CE	2.17	0.56
1:A:87:PHE:HB3	1:A:88:PRO:HA	1.87	0.56
1:A:69:SER:N	1:A:70[B]:LYS:HD3	2.22	0.55
1:A:167:LEU:O	1:A:169:ASP:N	2.39	0.55
1:A:204:HIS:ND1	1:A:204:HIS:O	2.39	0.55
1:A:223:THR:H	1:A:224:GLY:HA3	1.71	0.55
1:A:179[B]:THR:HG23	3:A:272:HOH:O	2.06	0.54
1:A:179[B]:THR:OG1	1:A:181:TYR:CE1	2.56	0.54
1:A:223:THR:N	1:A:224:GLY:HA3	2.23	0.53
1:A:205[B]:ASN:N	1:A:206[B]:GLU:OE2	2.41	0.53
1:A:206[B]:GLU:O	1:A:208:TYR:N	2.43	0.52
1:A:70[B]:LYS:HE3	1:A:93:TRP:HE1	1.72	0.52
1:A:205[B]:ASN:CA	1:A:206[B]:GLU:OE2	2.57	0.52
1:A:54:LEU:O	1:A:138:LYS:CE	2.59	0.51
1:A:206[A]:GLU:O	1:A:208:TYR:N	2.43	0.51
1:A:87:PHE:CD2	1:A:112[B]:SER:O	2.65	0.50
1:A:204:HIS:CG	1:A:204:HIS:O	2.65	0.49
1:A:206[A]:GLU:HB2	1:A:210:ILE:HB	1.95	0.49
1:A:206[A]:GLU:OE1	1:A:210:ILE:CG1	2.55	0.49
1:A:194:LYS:NZ	1:A:225:ALA:O	2.44	0.49
1:A:21:SER:HA	1:A:25:HIS:O	2.13	0.48
1:A:70[B]:LYS:HE2	1:A:91:PHE:CE1	2.49	0.47
1:A:140:THR:HB	1:A:165:LEU:HD22	1.95	0.47
1:A:114:GLN:HG3	1:A:119:ILE:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205[B]:ASN:CB	1:A:206[B]:GLU:CD	2.83	0.46
1:A:206[B]:GLU:HG3	2:A:228:MLT:O4	2.15	0.46
1:A:67:CH6:CD2	1:A:197:THR:HG21	2.45	0.46
1:A:78:ASP:OD1	1:A:78:ASP:N	2.48	0.46
1:A:54:LEU:O	1:A:138:LYS:HE3	2.16	0.46
1:A:67:CH6:HE1	1:A:199:LEU:HD12	1.97	0.46
2:A:227:MLT:H2	2:A:228:MLT:O2	2.16	0.46
1:A:13:ARG:HB2	1:A:117:GLU:HG2	1.97	0.46
1:A:206[B]:GLU:CD	1:A:206[B]:GLU:H	2.19	0.46
1:A:209:THR:HB	3:A:323:HOH:O	2.15	0.46
1:A:67:CH6:HD1	1:A:199:LEU:HD12	1.97	0.46
1:A:149:ARG:HA	1:A:194:LYS:HD3	1.97	0.45
1:A:89:GLU:HG2	1:A:184:LYS:HD3	1.99	0.44
1:A:153:GLU:OE1	1:A:158:LYS:CE	2.65	0.44
1:A:149:ARG:NH2	1:A:160:GLU:CG	2.81	0.44
1:A:168[B]:LYS:O	1:A:169:ASP:HB2	2.18	0.43
1:A:206[B]:GLU:C	1:A:208:TYR:N	2.72	0.43
1:A:149:ARG:HB2	1:A:194:LYS:HE2	2.00	0.43
1:A:206[A]:GLU:CD	1:A:210:ILE:CG1	2.86	0.43
1:A:14:PHE:HA	1:A:118:PHE:O	2.18	0.43
1:A:73:VAL:O	1:A:84:LYS:NZ	2.52	0.41
1:A:167:LEU:O	1:A:169:ASP:HB3	2.21	0.41
1:A:205[B]:ASN:C	1:A:206[B]:GLU:OE2	2.59	0.41
1:A:67:CH6:C3	1:A:70[B]:LYS:HD3	2.51	0.41
1:A:62:SER:OG	1:A:63:PRO:HD3	2.21	0.41
1:A:46:LEU:HG	1:A:65:ILE:HD13	2.02	0.41
1:A:167:LEU:C	1:A:169:ASP:HB3	2.41	0.40
1:A:140:THR:HG21	1:A:165:LEU:HD13	2.04	0.40
1:A:62:SER:N	1:A:63:PRO:CD	2.85	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	222/232 (96%)	204 (92%)	9 (4%)	9 (4%)	3 0

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113[A]	LEU
1	A	113[B]	LEU
1	A	206[A]	GLU
1	A	206[B]	GLU
1	A	168[A]	LYS
1	A	168[B]	LYS
1	A	169	ASP
1	A	112[A]	SER
1	A	112[B]	SER

### 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	193/196 (98%)	189 (98%)	4 (2%)	53 31

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	69	SER
1	A	109[A]	GLN
1	A	109[B]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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
1	CH6	A	67	1	24,24,25	3.63	6 (25%)	28,32,34	4.95	11 (39%)

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
1	CH6	A	67	1	-	3/12/31/32	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	CH6	CB2-CA2	15.46	1.48	1.35
1	A	67	CH6	C2-N3	-4.44	1.29	1.39
1	A	67	CH6	CA1-C1	-3.81	1.43	1.51
1	A	67	CH6	O2-C2	2.84	1.29	1.23
1	A	67	CH6	CA2-C2	-2.60	1.46	1.48
1	A	67	CH6	O3-C3	2.45	1.33	1.19

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	CH6	O2-C2-CA2	-20.11	119.67	130.96
1	A	67	CH6	CA2-C2-N3	9.62	107.92	103.37
1	A	67	CH6	CB2-CA2-N2	6.50	137.84	128.83
1	A	67	CH6	CE-SD-CG1	-6.18	79.18	100.40
1	A	67	CH6	CB2-CA2-C2	-5.10	116.18	122.28
1	A	67	CH6	C2-CA2-N2	-4.26	105.95	108.93
1	A	67	CH6	CG2-CB2-CA2	-4.16	124.85	129.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	CH6	O2-C2-N3	4.05	132.41	124.35
1	A	67	CH6	CD2-CE2-CZ	2.49	122.61	119.88
1	A	67	CH6	CE1-CZ-CE2	-2.49	115.58	119.77
1	A	67	CH6	CA2-N2-C1	2.30	107.47	105.77

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	67	CH6	N2-CA2-CB2-CG2
1	A	67	CH6	C2-CA2-CB2-CG2
1	A	67	CH6	C1-CA1-CB1-CG1

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	67	CH6	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 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
2	MLT	A	226	-	2,8,8	2.99	1 (50%)	3,10,10	3.59	2 (66%)
2	MLT	A	228	-	2,8,8	2.18	1 (50%)	3,10,10	3.47	1 (33%)
2	MLT	A	227	-	2,8,8	3.00	2 (100%)	3,10,10	7.14	2 (66%)

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	MLT	A	226	-	-	0/2/8/8	-
2	MLT	A	228	-	-	2/2/8/8	-
2	MLT	A	227	-	-	0/2/8/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	226	MLT	C3-C2	-4.20	1.47	1.53
2	A	227	MLT	O3-C2	-3.30	1.35	1.42
2	A	227	MLT	C3-C2	2.66	1.56	1.53
2	A	228	MLT	C3-C2	-2.62	1.49	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	227	MLT	C3-C2-C1	11.01	125.11	111.10
2	A	228	MLT	C3-C2-C1	-5.53	104.06	111.10
2	A	227	MLT	O3-C2-C1	-5.47	95.19	111.66
2	A	226	MLT	O3-C2-C3	-4.89	97.75	108.50
2	A	226	MLT	O3-C2-C1	3.57	122.42	111.66

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	228	MLT	C1-C2-C3-C4
2	A	228	MLT	O3-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	228	MLT	12	0
2	A	227	MLT	2	0

## 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	217/232 (93%)	0.30	12 (5%)	25 31	7, 24, 58, 82	9 (4%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	ALA	8.1
1	A	169	ASP	7.8
1	A	170	GLY	5.8
1	A	171	GLY	4.0
1	A	222	SER	3.4
1	A	207	ASP	3.1
1	A	206[A]	GLU	3.1
1	A	167	LEU	2.8
1	A	223	THR	2.6
1	A	205[A]	ASN	2.6
1	A	52	GLY	2.3
1	A	137	GLN	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	CH6	A	67	23/24	0.94	0.15	4,18,47,54	0

### 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MLT	A	228	9/9	0.77	0.47	48,53,57,60	9
2	MLT	A	227	9/9	0.84	0.26	48,50,52,53	9
2	MLT	A	226	9/9	0.86	0.16	25,32,40,41	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.