



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:50 am BST

PDB ID : 3NIO  
Title : Crystal structure of Pseudomonas aeruginosa guanidinobutyrase  
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Deposited on : 2010-06-16  
Resolution : 2.00 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

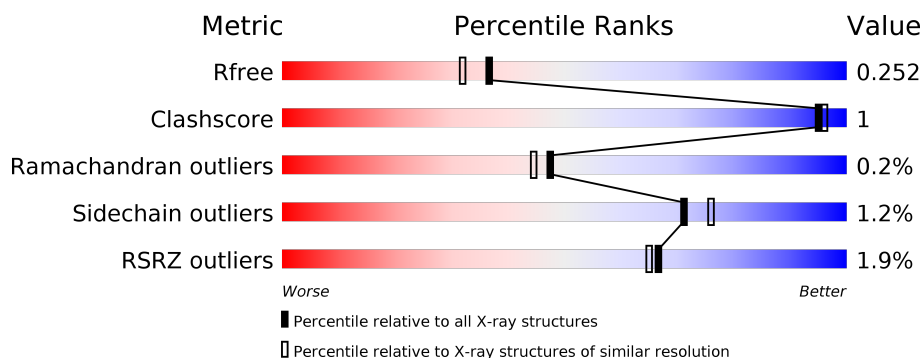
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	319	<div> <div>%</div> <div>96%</div> <div>..</div> </div>
1	B	319	<div> <div>%</div> <div>97%</div> <div>..</div> </div>
1	C	319	<div> <div>2%</div> <div>95%</div> <div>..</div> </div>
1	D	319	<div> <div>3%</div> <div>97%</div> <div>..</div> </div>
1	E	319	<div> <div>3%</div> <div>97%</div> <div>..</div> </div>
1	F	319	<div> <div>2%</div> <div>97%</div> <div>..</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15530 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 Guanidinobutyrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2420	1529	426	451	14			
1	B	316	Total	C	N	O	S	0	0	0
			2418	1527	426	451	14			
1	C	316	Total	C	N	O	S	0	0	0
			2420	1529	426	451	14			
1	D	316	Total	C	N	O	S	0	0	0
			2420	1529	426	451	14			
1	E	316	Total	C	N	O	S	0	0	0
			2414	1523	426	451	14			
1	F	316	Total	C	N	O	S	0	0	0
			2422	1531	426	451	14			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Mn	0	0
			2	2		
2	E	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		
2	F	2	Total	Mn	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	174	Total 174	O 174	0	0
3	B	181	Total 181	O 181	0	0
3	C	160	Total 160	O 160	0	0
3	D	180	Total 180	O 180	0	0
3	E	145	Total 145	O 145	0	0
3	F	164	Total 164	O 164	0	0

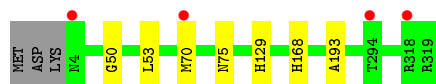
### 3 Residue-property plots [i](#)

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: Guanidinobutyrase



- Molecule 1: Guanidinobutyrase



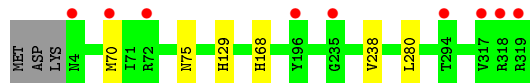
- Molecule 1: Guanidinobutyrase



- Molecule 1: Guanidinobutyrase



- Molecule 1: Guanidinobutyrase



- Molecule 1: Guanidinobutyrase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.05Å 158.95Å 84.55Å 90.00° 114.84° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.93 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.00) 99.9 (19.93-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.65 (at 2.01Å)	Xtriage
Refinement program	CNS, REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.233 , 0.251 0.235 , 0.252	Depositor DCC
$R_{free}$ test set	6635 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.9	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 93.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15530	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: MLY, MN

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	0.53	0/2398	0.59	0/3265
1	B	0.53	1/2398 (0.0%)	0.59	0/3265
1	C	0.49	0/2398	0.57	0/3265
1	D	0.52	0/2398	0.58	0/3265
1	E	0.48	0/2398	0.57	0/3265
1	F	0.50	0/2398	0.58	0/3265
All	All	0.51	1/14388 (0.0%)	0.58	0/19590

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	50	GLY	N-CA	5.25	1.53	1.46

There are no bond angle outliers.

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	2420	0	2403	8	0
1	B	2418	0	2397	8	0
1	C	2420	0	2403	8	0
1	D	2420	0	2403	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2414	0	2384	6	0
1	F	2422	0	2408	16	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	174	0	0	1	0
3	B	181	0	0	1	0
3	C	160	0	0	0	0
3	D	180	0	0	4	0
3	E	145	0	0	0	0
3	F	164	0	0	0	0
All	All	15530	0	14398	34	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 1.

All (34) 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:D:53:LEU:HD22	1:F:70:MET:CE	1.77	1.15
1:D:53:LEU:CD2	1:F:70:MET:SD	2.36	1.13
1:D:53:LEU:HD22	1:F:70:MET:SD	1.95	1.05
1:D:53:LEU:HD21	1:F:70:MET:SD	1.98	1.04
3:D:748:HOH:O	1:F:70:MET:HE3	1.57	1.02
1:D:53:LEU:CD2	1:F:70:MET:CE	2.50	0.90
1:E:70:MET:SD	1:F:53:LEU:HD22	2.12	0.88
1:E:70:MET:CE	1:F:53:LEU:HD22	2.03	0.87
1:D:53:LEU:HD22	1:F:70:MET:HE1	1.63	0.80
1:B:70:MET:SD	1:C:53:LEU:HD22	2.22	0.80
1:E:70:MET:SD	1:F:53:LEU:CD2	2.70	0.80
3:D:748:HOH:O	1:F:70:MET:CE	2.18	0.79
1:A:70:MET:SD	3:B:350:HOH:O	2.39	0.79
1:A:70:MET:CE	1:B:53:LEU:HD21	2.18	0.73
1:E:70:MET:HE1	1:F:53:LEU:HD22	1.74	0.69
3:D:433:HOH:O	1:F:70:MET:HE2	1.94	0.66
1:D:53:LEU:CD2	1:F:70:MET:HE2	2.28	0.63
1:A:70:MET:HE1	1:B:53:LEU:HD21	1.82	0.61
1:B:70:MET:CE	1:C:53:LEU:HD22	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:MET:HE2	1:B:53:LEU:HD21	1.84	0.58
1:E:70:MET:SD	1:F:53:LEU:HD21	2.46	0.55
1:B:70:MET:HE2	1:C:53:LEU:HD22	1.88	0.55
1:C:238:VAL:HG13	1:C:280:LEU:HD23	1.91	0.53
1:A:70:MET:HE1	1:B:53:LEU:CD2	2.39	0.53
3:D:433:HOH:O	1:F:70:MET:CE	2.55	0.50
1:B:70:MET:SD	1:C:53:LEU:CD2	2.96	0.49
1:E:238:VAL:HG13	1:E:280:LEU:HD23	1.94	0.48
1:A:70:MET:CE	3:A:955:HOH:O	2.62	0.48
1:C:199:GLU:HA	1:C:202:ASN:HB2	2.00	0.43
1:D:238:VAL:HG13	1:D:280:LEU:HD23	2.00	0.43
1:C:96:ILE:H	1:C:96:ILE:HG13	1.72	0.43
1:A:96:ILE:H	1:A:96:ILE:HG13	1.75	0.42
1:C:121:LEU:HA	1:C:122:PRO:HD3	1.92	0.42
1:A:238:VAL:HG13	1:A:280:LEU:HD23	2.02	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	307/319 (96%)	300 (98%)	6 (2%)	1 (0%)	41	37
1	B	307/319 (96%)	296 (96%)	10 (3%)	1 (0%)	41	37
1	C	307/319 (96%)	298 (97%)	8 (3%)	1 (0%)	41	37
1	D	307/319 (96%)	295 (96%)	11 (4%)	1 (0%)	41	37
1	E	307/319 (96%)	297 (97%)	10 (3%)	0	100	100
1	F	307/319 (96%)	299 (97%)	8 (3%)	0	100	100
All	All	1842/1914 (96%)	1785 (97%)	53 (3%)	4 (0%)	47	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ALA
1	B	193	ALA
1	C	193	ALA
1	D	193	ALA

### 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	249/252 (99%)	245 (98%)	4 (2%)	62	67
1	B	249/252 (99%)	246 (99%)	3 (1%)	71	76
1	C	249/252 (99%)	246 (99%)	3 (1%)	71	76
1	D	249/252 (99%)	247 (99%)	2 (1%)	81	86
1	E	249/252 (99%)	246 (99%)	3 (1%)	71	76
1	F	249/252 (99%)	246 (99%)	3 (1%)	71	76
All	All	1494/1512 (99%)	1476 (99%)	18 (1%)	71	76

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	128	ASP
1	A	129	HIS
1	A	168	HIS
1	B	75	ASN
1	B	129	HIS
1	B	168	HIS
1	C	75	ASN
1	C	129	HIS
1	C	168	HIS
1	D	75	ASN
1	D	129	HIS
1	E	75	ASN
1	E	129	HIS
1	E	168	HIS

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Mol	Chain	Res	Type
1	F	75	ASN
1	F	129	HIS
1	F	168	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	87	ASN
1	A	276	GLN
1	B	75	ASN
1	B	87	ASN
1	B	297	ASN
1	C	75	ASN
1	C	87	ASN
1	C	276	GLN
1	D	75	ASN
1	E	75	ASN
1	E	87	ASN
1	E	276	GLN
1	F	75	ASN
1	F	87	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

42 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	MLY	C	220	1	9,10,11	0.46	0	6,11,13	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	F	142	1	9,10,11	0.49	0	6,11,13	0.69	0
1	MLY	B	165	1	7,8,11	0.46	0	3,8,13	0.27	0
1	MLY	A	145	1	9,10,11	0.53	0	6,11,13	0.51	0
1	MLY	E	165	1	7,8,11	0.46	0	3,8,13	0.33	0
1	MLY	F	220	1	9,10,11	0.40	0	6,11,13	0.79	0
1	MLY	D	140	1	9,10,11	0.48	0	6,11,13	0.65	0
1	MLY	D	220	1	9,10,11	0.42	0	6,11,13	0.84	0
1	MLY	B	220	1	9,10,11	0.45	0	6,11,13	0.61	0
1	MLY	C	142	1	7,8,11	0.55	0	3,8,13	0.29	0
1	MLY	C	232	1	7,8,11	0.56	0	3,8,13	0.19	0
1	MLY	A	232	1	7,8,11	0.53	0	3,8,13	0.20	0
1	MLY	F	232	1	9,10,11	0.47	0	6,11,13	0.61	0
1	MLY	E	220	1	7,8,11	0.45	0	3,8,13	0.43	0
1	MLY	D	165	1	7,8,11	0.51	0	3,8,13	0.31	0
1	MLY	B	142	1	7,8,11	0.52	0	3,8,13	0.30	0
1	MLY	F	165	1	7,8,11	0.49	0	3,8,13	0.32	0
1	MLY	D	142	1	7,8,11	0.50	0	3,8,13	0.33	0
1	MLY	B	145	1	7,8,11	0.44	0	3,8,13	0.25	0
1	MLY	E	206	1	7,8,11	0.45	0	3,8,13	0.39	0
1	MLY	A	140	1	9,10,11	0.46	0	6,11,13	0.68	0
1	MLY	B	206	1	9,10,11	0.47	0	6,11,13	0.66	0
1	MLY	A	206	1	9,10,11	0.47	0	6,11,13	0.63	0
1	MLY	D	145	1	9,10,11	0.53	0	6,11,13	0.40	0
1	MLY	E	142	1	7,8,11	0.50	0	3,8,13	0.35	0
1	MLY	A	142	1	7,8,11	0.54	0	3,8,13	0.28	0
1	MLY	D	232	1	9,10,11	0.56	0	6,11,13	0.35	0
1	MLY	E	232	1	7,8,11	0.56	0	3,8,13	0.20	0
1	MLY	A	165	1	9,10,11	0.50	0	6,11,13	0.43	0
1	MLY	E	140	1	7,8,11	0.44	0	3,8,13	0.36	0
1	MLY	A	220	1	7,8,11	0.45	0	3,8,13	0.50	0
1	MLY	F	206	1	7,8,11	0.45	0	3,8,13	0.42	0
1	MLY	B	140	1	9,10,11	0.45	0	6,11,13	0.62	0
1	MLY	F	145	1	9,10,11	0.55	0	6,11,13	0.44	0
1	MLY	E	145	1	9,10,11	0.53	0	6,11,13	0.42	0
1	MLY	C	145	1	9,10,11	0.45	0	6,11,13	0.73	0
1	MLY	C	165	1	7,8,11	0.46	0	3,8,13	0.28	0
1	MLY	B	232	1	7,8,11	0.61	0	3,8,13	0.15	0
1	MLY	F	140	1	9,10,11	0.52	0	6,11,13	0.43	0
1	MLY	C	206	1	9,10,11	0.48	0	6,11,13	0.73	0
1	MLY	C	140	1	9,10,11	0.47	0	6,11,13	0.72	0
1	MLY	D	206	1	7,8,11	0.47	0	3,8,13	0.36	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
1	MLY	C	220	1	-	7/8/9/11	-
1	MLY	F	142	1	-	3/8/9/11	-
1	MLY	B	165	1	-	3/6/7/11	-
1	MLY	A	145	1	-	2/8/9/11	-
1	MLY	E	165	1	-	0/6/7/11	-
1	MLY	F	220	1	-	5/8/9/11	-
1	MLY	D	140	1	-	5/8/9/11	-
1	MLY	D	220	1	-	5/8/9/11	-
1	MLY	B	220	1	-	5/8/9/11	-
1	MLY	C	142	1	-	0/6/7/11	-
1	MLY	C	232	1	-	1/6/7/11	-
1	MLY	A	232	1	-	2/6/7/11	-
1	MLY	F	232	1	-	3/8/9/11	-
1	MLY	E	220	1	-	0/6/7/11	-
1	MLY	D	165	1	-	0/6/7/11	-
1	MLY	B	142	1	-	0/6/7/11	-
1	MLY	F	165	1	-	1/6/7/11	-
1	MLY	D	142	1	-	0/6/7/11	-
1	MLY	B	145	1	-	0/6/7/11	-
1	MLY	E	206	1	-	0/6/7/11	-
1	MLY	A	140	1	-	5/8/9/11	-
1	MLY	B	206	1	-	5/8/9/11	-
1	MLY	A	206	1	-	5/8/9/11	-
1	MLY	D	145	1	-	2/8/9/11	-
1	MLY	E	142	1	-	0/6/7/11	-
1	MLY	A	142	1	-	0/6/7/11	-
1	MLY	D	232	1	-	4/8/9/11	-
1	MLY	E	232	1	-	2/6/7/11	-
1	MLY	A	165	1	-	5/8/9/11	-
1	MLY	E	140	1	-	1/6/7/11	-
1	MLY	A	220	1	-	0/6/7/11	-
1	MLY	F	206	1	-	0/6/7/11	-
1	MLY	B	140	1	-	7/8/9/11	-
1	MLY	F	145	1	-	2/8/9/11	-
1	MLY	E	145	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	C	145	1	-	6/8/9/11	-
1	MLY	C	165	1	-	3/6/7/11	-
1	MLY	B	232	1	-	1/6/7/11	-
1	MLY	F	140	1	-	1/8/9/11	-
1	MLY	C	206	1	-	4/8/9/11	-
1	MLY	C	140	1	-	5/8/9/11	-
1	MLY	D	206	1	-	0/6/7/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	220	MLY	N-CA-CB-CG
1	C	220	MLY	C-CA-CB-CG
1	B	165	MLY	C-CA-CB-CG
1	B	165	MLY	O-C-CA-CB
1	D	140	MLY	O-C-CA-CB
1	B	206	MLY	O-C-CA-CB
1	E	232	MLY	C-CA-CB-CG
1	B	140	MLY	C-CA-CB-CG
1	C	145	MLY	N-CA-CB-CG
1	C	145	MLY	C-CA-CB-CG
1	C	165	MLY	C-CA-CB-CG
1	C	165	MLY	O-C-CA-CB
1	F	142	MLY	CD-CE-NZ-CH1
1	F	142	MLY	CD-CE-NZ-CH2
1	F	220	MLY	CD-CE-NZ-CH1
1	D	220	MLY	CD-CE-NZ-CH1
1	D	220	MLY	CD-CE-NZ-CH2
1	F	232	MLY	CD-CE-NZ-CH1
1	F	232	MLY	CD-CE-NZ-CH2
1	A	206	MLY	CD-CE-NZ-CH1
1	A	206	MLY	CD-CE-NZ-CH2
1	A	165	MLY	CD-CE-NZ-CH1
1	B	140	MLY	CD-CE-NZ-CH1
1	C	145	MLY	CD-CE-NZ-CH1
1	C	206	MLY	CD-CE-NZ-CH1
1	D	232	MLY	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
1	B	140	MLY	CG-CD-CE-NZ
1	D	220	MLY	CG-CD-CE-NZ
1	C	206	MLY	CG-CD-CE-NZ
1	A	165	MLY	CG-CD-CE-NZ
1	F	220	MLY	CD-CE-NZ-CH2
1	A	165	MLY	CD-CE-NZ-CH2
1	B	140	MLY	CD-CE-NZ-CH2
1	C	145	MLY	CD-CE-NZ-CH2
1	C	206	MLY	CD-CE-NZ-CH2
1	E	145	MLY	CG-CD-CE-NZ
1	A	140	MLY	CG-CD-CE-NZ
1	D	140	MLY	CD-CE-NZ-CH1
1	B	220	MLY	CD-CE-NZ-CH2
1	B	220	MLY	CA-CB-CG-CD
1	C	140	MLY	CG-CD-CE-NZ
1	C	220	MLY	CD-CE-NZ-CH2
1	D	140	MLY	CD-CE-NZ-CH2
1	B	220	MLY	CD-CE-NZ-CH1
1	A	140	MLY	CD-CE-NZ-CH1
1	A	140	MLY	CD-CE-NZ-CH2
1	B	206	MLY	CD-CE-NZ-CH1
1	B	206	MLY	CD-CE-NZ-CH2
1	F	140	MLY	CA-CB-CG-CD
1	C	220	MLY	CG-CD-CE-NZ
1	C	220	MLY	CA-CB-CG-CD
1	C	220	MLY	CD-CE-NZ-CH1
1	F	145	MLY	CD-CE-NZ-CH2
1	F	220	MLY	CG-CD-CE-NZ
1	A	165	MLY	CA-CB-CG-CD
1	B	140	MLY	CA-CB-CG-CD
1	A	140	MLY	CE-CD-CG-CB
1	D	232	MLY	CA-CB-CG-CD
1	C	220	MLY	CE-CD-CG-CB
1	C	140	MLY	CE-CD-CG-CB
1	F	142	MLY	CE-CD-CG-CB
1	F	220	MLY	CE-CD-CG-CB
1	D	145	MLY	CE-CD-CG-CB
1	E	145	MLY	CE-CD-CG-CB
1	C	140	MLY	CD-CE-NZ-CH2
1	C	145	MLY	CE-CD-CG-CB
1	D	145	MLY	CG-CD-CE-NZ
1	D	140	MLY	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
1	E	140	MLY	CA-CB-CG-CD
1	A	232	MLY	C-CA-CB-CG
1	B	232	MLY	C-CA-CB-CG
1	B	220	MLY	CE-CD-CG-CB
1	B	206	MLY	CE-CD-CG-CB
1	D	232	MLY	CE-CD-CG-CB
1	A	206	MLY	CE-CD-CG-CB
1	A	165	MLY	CE-CD-CG-CB
1	B	220	MLY	CG-CD-CE-NZ
1	C	206	MLY	CE-CD-CG-CB
1	C	140	MLY	CD-CE-NZ-CH1
1	A	145	MLY	CE-CD-CG-CB
1	A	206	MLY	CG-CD-CE-NZ
1	F	232	MLY	CA-CB-CG-CD
1	F	165	MLY	CA-CB-CG-CD
1	A	145	MLY	CD-CE-NZ-CH2
1	D	232	MLY	CD-CE-NZ-CH1
1	D	140	MLY	N-CA-CB-CG
1	A	140	MLY	N-CA-CB-CG
1	B	140	MLY	N-CA-CB-CG
1	C	140	MLY	N-CA-CB-CG
1	C	145	MLY	CA-CB-CG-CD
1	A	206	MLY	C-CA-CB-CG
1	E	232	MLY	CE-CD-CG-CB
1	B	140	MLY	CE-CD-CG-CB
1	C	232	MLY	CE-CD-CG-CB
1	D	220	MLY	C-CA-CB-CG
1	B	206	MLY	C-CA-CB-CG
1	D	220	MLY	CE-CD-CG-CB
1	F	145	MLY	CG-CD-CE-NZ
1	F	220	MLY	CA-CB-CG-CD
1	A	232	MLY	CE-CD-CG-CB
1	B	165	MLY	N-CA-CB-CG
1	C	165	MLY	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 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

### 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	309/319 (96%)	0.01	3 (0%) 82 81	16, 20, 26, 29	0
1	B	309/319 (96%)	0.02	4 (1%) 77 76	16, 20, 26, 31	0
1	C	309/319 (96%)	0.09	7 (2%) 60 59	18, 23, 29, 35	0
1	D	309/319 (96%)	0.09	8 (2%) 56 54	16, 21, 27, 39	0
1	E	309/319 (96%)	0.13	9 (2%) 51 50	19, 24, 29, 37	0
1	F	309/319 (96%)	0.06	5 (1%) 72 70	17, 21, 27, 32	0
All	All	1854/1914 (96%)	0.07	36 (1%) 66 65	16, 22, 28, 39	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	294	THR	6.7
1	D	318	ARG	6.4
1	F	294	THR	5.4
1	B	70	MET	5.3
1	F	70	MET	5.0
1	E	294	THR	4.9
1	E	70	MET	4.9
1	E	4	ASN	4.4
1	C	294	THR	4.4
1	A	4	ASN	4.3
1	A	294	THR	4.2
1	D	319	ARG	4.1
1	E	318	ARG	4.0
1	D	4	ASN	4.0
1	B	294	THR	3.9
1	A	70	MET	3.9
1	C	114	ARG	3.3
1	C	4	ASN	3.3
1	B	4	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	269	MET	3.1
1	C	318	ARG	3.1
1	F	4	ASN	3.0
1	B	318	ARG	2.9
1	D	317	VAL	2.9
1	E	319	ARG	2.8
1	D	5	LEU	2.8
1	F	318	ARG	2.7
1	E	72	ARG	2.4
1	E	317	VAL	2.3
1	D	179	ASP	2.3
1	D	269	MET	2.3
1	C	319	ARG	2.2
1	E	235	GLY	2.2
1	E	196	TYR	2.1
1	C	72	ARG	2.1
1	C	196	TYR	2.0

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

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	MLY	F	142	11/12	0.72	0.23	26,26,29,30	0
1	MLY	C	145	11/12	0.72	0.21	25,26,29,29	0
1	MLY	E	165	9/12	0.73	0.20	26,27,29,29	0
1	MLY	C	232	9/12	0.74	0.21	27,27,29,29	0
1	MLY	D	232	11/12	0.76	0.20	25,26,30,30	0
1	MLY	A	165	11/12	0.76	0.21	25,25,29,29	0
1	MLY	B	220	11/12	0.76	0.22	19,19,25,25	0
1	MLY	C	142	9/12	0.77	0.20	27,27,29,29	0
1	MLY	D	145	11/12	0.78	0.19	24,25,28,29	0
1	MLY	C	220	11/12	0.78	0.22	21,21,24,25	0
1	MLY	B	142	9/12	0.79	0.18	24,24,26,27	0
1	MLY	C	206	11/12	0.79	0.20	26,26,28,29	0
1	MLY	C	165	9/12	0.80	0.17	28,28,29,30	0
1	MLY	F	145	11/12	0.80	0.19	23,24,27,27	0
1	MLY	A	142	9/12	0.81	0.17	24,25,25,25	0
1	MLY	D	165	9/12	0.82	0.21	25,25,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	D	140	11/12	0.82	0.17	25,26,28,28	0
1	MLY	E	206	9/12	0.83	0.19	29,29,30,31	0
1	MLY	B	140	11/12	0.83	0.17	23,23,27,28	0
1	MLY	A	206	11/12	0.83	0.20	24,24,27,27	0
1	MLY	A	145	11/12	0.83	0.17	22,23,27,27	0
1	MLY	B	165	9/12	0.83	0.18	23,24,26,26	0
1	MLY	F	140	11/12	0.83	0.17	24,25,28,29	0
1	MLY	D	142	9/12	0.83	0.17	26,27,29,29	0
1	MLY	C	140	11/12	0.83	0.15	26,27,30,30	0
1	MLY	D	206	9/12	0.83	0.15	24,24,25,25	0
1	MLY	A	140	11/12	0.84	0.14	23,24,27,27	0
1	MLY	E	145	11/12	0.84	0.22	25,26,29,29	0
1	MLY	A	232	9/12	0.85	0.16	25,25,28,28	0
1	MLY	F	232	11/12	0.85	0.15	21,22,25,25	0
1	MLY	E	142	9/12	0.85	0.24	28,28,30,30	0
1	MLY	F	165	9/12	0.85	0.14	26,26,28,28	0
1	MLY	B	206	11/12	0.85	0.17	21,22,24,25	0
1	MLY	A	220	9/12	0.86	0.13	20,20,22,22	0
1	MLY	E	232	9/12	0.86	0.13	28,28,29,30	0
1	MLY	D	220	11/12	0.86	0.17	19,19,25,25	0
1	MLY	B	232	9/12	0.86	0.13	22,22,25,26	0
1	MLY	B	145	9/12	0.88	0.14	21,22,25,26	0
1	MLY	E	220	9/12	0.88	0.14	21,22,24,25	0
1	MLY	F	220	11/12	0.89	0.14	21,22,25,26	0
1	MLY	F	206	9/12	0.89	0.17	25,25,27,27	0
1	MLY	E	140	9/12	0.89	0.15	27,27,28,28	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	MN	E	1610	1/1	0.99	0.08	18,18,18,18	0
2	MN	A	1602	1/1	0.99	0.06	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	E	1609	1/1	0.99	0.05	20,20,20,20	0
2	MN	B	1604	1/1	0.99	0.09	14,14,14,14	0
2	MN	A	1601	1/1	0.99	0.07	19,19,19,19	0
2	MN	F	1612	1/1	0.99	0.06	17,17,17,17	0
2	MN	D	1608	1/1	0.99	0.08	16,16,16,16	0
2	MN	D	1607	1/1	1.00	0.05	16,16,16,16	0
2	MN	C	1606	1/1	1.00	0.06	17,17,17,17	0
2	MN	B	1603	1/1	1.00	0.05	15,15,15,15	0
2	MN	C	1605	1/1	1.00	0.06	19,19,19,19	0
2	MN	F	1611	1/1	1.00	0.03	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.