

wwPDB X-ray Structure Validation Summary Report (i)

May 17, 2020 – 06:32 pm BST

PDB ID 3C8G

> Title Crystal structure of a possible transciptional regulator YggD from Shigella

> > flexneri 2a str. 2457T

Authors : Tan, K.; Borovilos, M.; Clancy, S.; Joachimiak, A.; Midwest Center for Struc-

tural Genomics (MCSG)

2008-02-12 Deposited on

Resolution 2.50 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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 EDS 2.11

20191225.v01 (using entries in the PDB archive December 25th 2019) Percentile statistics

> Refmac 5.8.0158

CCP4 7.0.044 (Gargrove) Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

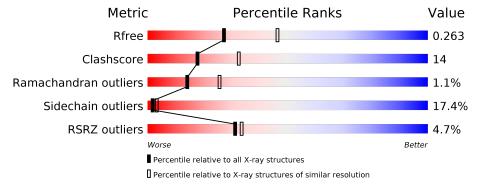
Validation Pipeline (wwPDB-VP) 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$egin{aligned} ext{Similar resolution} \ (\# ext{Entries, resolution range}(ext{\AA})) \end{aligned}$		
R_{free}	130704	4661 (2.50-2.50)		
Clashscore	141614	5346 (2.50-2.50)		
Ramachandran outliers	138981	5231 (2.50-2.50)		
Sidechain outliers	138945	5233 (2.50-2.50)		
RSRZ outliers	127900	4559 (2.50-2.50)		

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 >=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 <=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	172	63%	27%	6% •				
	71		2%	2170	070 •				
1	С	172	66% 7%	27%	5% •				
2	В	172	59%	30%	8% •				
3	D	172	64%	22%	8% 6%				



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5350 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 Putative transcriptional regulator.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	A	166	Total 1341	C 869	N 209	O 258	Se 5	0	0	0
1	С	167	Total 1349	C 873		O 261	Se 5	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual		Reference
A	-2	SER	_	EXPRESSION TAG	UNP Q83Q96
A	-1	ASN		EXPRESSION TAG	
A	0	ALA		EXPRESSION TAG	• •
С	-2	SER	_	EXPRESSION TAG	UNP Q83Q96
С	-1	ASN		EXPRESSION TAG	
С	0	ALA	-	EXPRESSION TAG	UNP Q83Q96

• Molecule 2 is a protein called Putative transcriptional regulator.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	166	Total 1347	C 874	N 209	O 260	Se 4	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	-2	SER	-	EXPRESSION TAG	UNP Q83Q96
В	-1	ASN	-	EXPRESSION TAG	UNP Q83Q96
В	0	ALA	-	EXPRESSION TAG	UNP Q83Q96

• Molecule 3 is a protein called Putative transcriptional regulator.

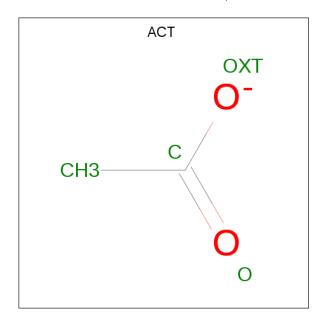


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	D	161	Total 1297	C 838	N 203	O 252	Se 4	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	_	EXPRESSION TAG	UNP Q83Q96
D	-1	ASN	-	EXPRESSION TAG	UNP Q83Q96
D	0	ALA	-	EXPRESSION TAG	UNP Q83Q96

• Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

 \bullet Molecule 5 is water.

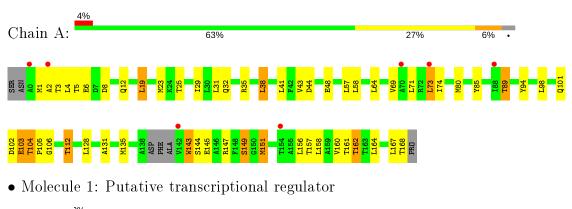
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0
5	С	4	$\begin{array}{cc} \text{Total} & \text{O} \\ 4 & 4 \end{array}$	0	0
5	D	4	$\begin{array}{cc} \text{Total} & \text{O} \\ 4 & 4 \end{array}$	0	0

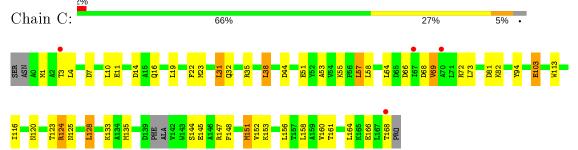


3 Residue-property plots (i)

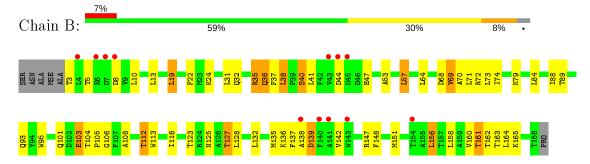
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Putative transcriptional regulator





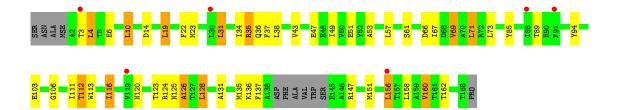
• Molecule 2: Putative transcriptional regulator



• Molecule 3: Putative transcriptional regulator









4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	$71.36 ext{Å}$ $70.95 ext{Å}$ $159.04 ext{Å}$	Denesiten
a, b, c, α , β , γ	90.00° 90.43° 90.00°	Depositor
Resolution (Å)	31.81 - 2.50	Depositor
Resolution (A)	31.81 - 2.50	EDS
% Data completeness	93.9 (31.81-2.50)	Depositor
(in resolution range)	93.9 (31.81-2.50)	EDS
R_{merge}	0.07	Depositor
R_{sum}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.14 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.270	Depositor
$\Pi,\ \Pi free$	0.204 , 0.263	DCC
R_{free} test set	2020 reflections (7.74%)	wwPDB-VP
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33,65.3	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
	0.019 for k,h,-l	
Estimated twinning fraction	0.020 for -k,-h,-l	Xtriage
	0.020 for -h,-k,l	
F_o, F_c correlation	0.95	EDS
Total number of atoms	5350	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.42% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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, ACT

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		
IVIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.76	0/1298	0.86	$1/1765 \ (0.1\%)$	
1	С	0.65	0/1306	0.74	0/1776	
2	В	0.66	0/1307	0.79	0/1781	
3	D	0.67	0/1275	0.82	0/1732	
All	All	0.69	0/5186	0.80	$1/7054 \ (0.0\%)$	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	73	LEU	CA-CB-CG	5.77	128.58	115.30

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	1341	0	1318	29	0
1	С	1349	0	1322	31	0
2	В	1347	0	1315	47	0
3	D	1297	0	1271	42	0
4	A	4	0	3	0	0
5	A	4	0	0	0	0

Continued on next page...



Continued from previous page...

Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
5	С	4	0	0	0	0
5	D	4	0	0	0	0
All	All	5350	0	5229	144	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 14.

The worst 5 of 144 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	Clash overlap (Å)
1:C:135:MSE:HE1	1:C:151:MSE:HG3	1.40	1.04
2:B:35:ARG:HG2	2:B:35:ARG:HH21	1.33	0.92
1:A:151:MSE:SE	2:B:151:MSE:HE1	2.24	0.87
1:C:22:PHE:HD2	1:C:23:MSE:HE2	1.39	0.86
1:C:22:PHE:CD2	1:C:23:MSE:CE	2.59	0.85

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	156/172 (91%)	151 (97%)	4 (3%)	1 (1%)	25 43	
1	С	157/172 (91%)	145 (92%)	9 (6%)	3 (2%)	8 13	
2	В	$158/172 \ (92\%)$	147 (93%)	10 (6%)	1 (1%)	25 43	
3	D	153/172~(89%)	142 (93%)	9 (6%)	2 (1%)	12 21	
All	All	624/688 (91%)	585 (94%)	32 (5%)	7 (1%)	14 26	

5 of 7 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
2	В	138	ALA
1	A	2	ALA
1	С	3	THR
3	D	61	SER
1	С	123	THR

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	138/138 (100%)	111 (80%)	27 (20%)		1	2	
1	С	139/138 (101%)	115 (83%)	24 (17%)		2	3	
2	В	139/138 (101%)	115 (83%)	24 (17%)		2	3	
3	D	136/140 (97%)	115 (85%)	21 (15%)		2	5	
All	All	552/554~(100%)	456 (83%)	96 (17%)		2	3	

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	123	THR
1	С	10	LEU
3	D	111	ILE
2	В	127	THR
2	В	160	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	В	99	ASN
3	D	36	GLN
1	С	99	ASN
2	В	45	ASN
3	D	32	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)

22 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).

Mal	T	Chain	Chain Res	T :1-	В	ond leng	gths	В	ond ang	gles
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MLY	D	24	3	9,10,11	0.64	0	6,11,13	2.12	3 (50%)
1	MLY	С	133	1	9,10,11	0.44	0	6,11,13	2.11	2 (33%)
1	MLY	A	136	1	9,10,11	0.57	0	6,11,13	2.60	5 (83%)
2	MLY	В	133	2	9,10,11	0.49	0	6,11,13	2.27	2 (33%)
1	MLY	С	136	1	9,10,11	0.47	0	6,11,13	2.54	4 (66%)
2	MLY	В	165	2	9,10,11	0.57	0	6,11,13	2.17	3 (50%)
2	MLY	В	24	2	9,10,11	0.74	0	6,11,13	2.34	4 (66%)
3	MLY	D	79	3	9,10,11	0.69	0	6,11,13	2.05	3 (50%)
1	MLY	A	79	1	9,10,11	0.70	0	6,11,13	2.00	3 (50%)
1	MLY	С	55	1	9,10,11	0.50	0	6,11,13	2.21	4 (66%)
1	MLY	С	24	1	9,10,11	0.31	0	6,11,13	2.15	2 (33%)
2	MLY	В	153	2	9,10,11	0.61	0	6,11,13	2.34	3 (50%)
1	MLY	С	82	1	9,10,11	0.49	0	6,11,13	2.09	3 (50%)
1	MLY	A	82	1	9,10,11	0.54	0	6,11,13	2.33	4 (66%)
2	MLY	В	55	2	9,10,11	0.52	0	6,11,13	2.01	3 (50%)
1	MLY	A	55	1	9,10,11	0.57	0	6,11,13	2.77	4 (66%)
1	MLY	A	133	1	9,10,11	0.51	0	6,11,13	2.35	4 (66%)
2	MLY	В	136	2	9,10,11	0.47	0	6,11,13	2.35	4 (66%)
3	MLY	D	55	3	9,10,11	0.83	0	6,11,13	2.02	2 (33%)
1	MLY	С	79	1	9,10,11	0.44	0	6,11,13	2.26	3 (50%)
3	MLY	D	136	3	9,10,11	0.54	0	6,11,13	2.46	4 (66%)
1	MLY	A	24	1	9,10,11	0.57	0	6,11,13	2.26	4 (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
3	MLY	D	24	3	-	1/8/9/11	-
1	MLY	С	133	1	-	4/8/9/11	-
1	MLY	A	136	1	-	4/8/9/11	-
2	MLY	В	133	2	-	3/8/9/11	-
1	MLY	С	136	1	-	2/8/9/11	-
2	MLY	В	165	2	-	5/8/9/11	-
2	MLY	В	24	2	-	7/8/9/11	-
3	MLY	D	79	3	-	5/8/9/11	-
1	MLY	A	79	1	-	4/8/9/11	-
1	MLY	С	55	1	-	2/8/9/11	-
1	MLY	С	24	1	-	2/8/9/11	-
2	MLY	В	153	2	-	3/8/9/11	-
1	MLY	С	82	1	-	4/8/9/11	-
1	MLY	A	82	1	-	3/8/9/11	-
2	MLY	В	55	2	-	1/8/9/11	-
1	MLY	A	55	1	-	4/8/9/11	-
1	MLY	A	133	1	-	1/8/9/11	-
2	MLY	В	136	2	-	3/8/9/11	_
3	MLY	D	55	3	-	6/8/9/11	-
1	MLY	С	79	1	-	3/8/9/11	-
3	MLY	D	136	3		5/8/9/11	-
1	MLY	A	24	1	-	1/8/9/11	-

There are no bond length outliers.

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	55	MLY	CH2-NZ-CH1	4.85	122.26	109.73
1	С	136	MLY	CH2-NZ-CH1	4.09	120.30	109.73
2	В	153	MLY	CH2-NZ-CH1	4.09	120.30	109.73
1	С	79	MLY	CH2-NZ-CH1	4.08	120.27	109.73
1	A	136	MLY	CH2-NZ-CH1	4.01	120.10	109.73

There are no chirality outliers.



5 of 73 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	С	133	MLY	C-CA-CB-CG
1	A	136	MLY	O-C-CA-CB
2	В	133	MLY	C-CA-CB-CG
1	С	136	MLY	C-CA-CB-CG
3	D	79	MLY	O-C-CA-CB

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	С	133	MLY	1	0
2	В	165	MLY	1	0
2	В	24	MLY	3	0
1	С	55	MLY	1	0
1	С	82	MLY	1	0
2	В	136	MLY	2	0
3	D	136	MLY	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand 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		
MIOI		Chain			Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	A	201	-	1,3,3	2.09	1 (100%)	0,3,3	0.00	-

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$Ideal(\AA)$
4	A	201	ACT	СН3-С	2.09	1.51	1.48

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 (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^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$		$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	155/172~(90%)	0.28	7 (4%) 33	36	51, 61, 83, 96	0
1	С	$156/172 \ (90\%)$	0.18	4 (2%) 56	59	51, 62, 86, 107	0
2	В	156/172 (90%)	0.34	12 (7%) 13	13	54, 63, 85, 90	0
3	D	153/172 (88%)	0.31	6 (3%) 39	42	52, 62, 76, 89	0
All	All	620/688 (90%)	0.28	29 (4%) 31	33	51, 62, 83, 107	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	140	PHE	5.2
2	В	141	ALA	3.7
1	A	142	VAL	3.7
2	В	4	LEU	3.5
2	В	138	ALA	3.4

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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	MLY	В	165	11/12	0.84	0.32	70,72,80,81	0
1	MLY	С	82	11/12	0.89	0.32	64,65,70,71	0
3	MLY	D	79	11/12	0.91	0.22	57,60,65,65	0
2	MLY	В	55	11/12	0.91	0.23	58,59,69,70	0
1	MLY	С	133	11/12	0.93	0.12	62,64,69,69	0
1	MLY	A	82	11/12	0.93	0.21	64,66,78,78	0
1	MLY	С	136	11/12	0.93	0.17	69,70,75,76	0

Continued on next page...



Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
1	MLY	A	55	11/12	0.93	0.18	53,56,69,69	0
3	MLY	D	55	11/12	0.93	0.23	54,57,70,70	0
2	MLY	В	153	11/12	0.94	0.28	59,61,77,78	0
1	MLY	A	133	11/12	0.94	0.17	53,54,57,58	0
1	MLY	A	79	11/12	0.94	0.13	64,64,66,66	0
1	MLY	С	79	11/12	0.94	0.18	62,65,74,74	0
1	MLY	С	24	11/12	0.95	0.17	44,49,55,56	0
2	MLY	В	136	11/12	0.95	0.14	69,73,76,76	0
1	MLY	A	136	11/12	0.96	0.15	61,62,71,73	0
2	MLY	В	24	11/12	0.96	0.17	58,59,62,65	0
2	MLY	В	133	11/12	0.96	0.14	59,61,67,68	0
3	MLY	D	24	11/12	0.96	0.23	54,58,60,61	0
1	MLY	С	55	11/12	0.96	0.15	52,54,58,60	0
3	MLY	D	136	11/12	0.96	0.18	61,63,65,65	0
1	MLY	A	24	11/12	0.97	0.18	52,54,56,56	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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	ACT	A	201	4/4	0.92	0.15	85,85,85,85	0

6.5 Other polymers (i)

There are no such residues in this entry.

