



# wwPDB X-ray Structure Validation Summary Report

Dec 3, 2023 – 04:01 pm GMT

PDB ID : 2VD8  
Title : The crystal structure of alanine racemase from Bacillus anthracis (BA0252)  
Authors : Au, K.; Ren, J.; Walter, T.S.; Harlos, K.; Nettleship, J.E.; Owens, R.J.; Stuart, D.I.; Esnouf, R.M.; Oxford Protein Production Facility (OPPF); Structural Proteomics in Europe (SPINE)  
Deposited on : 2007-10-01  
Resolution : 1.47 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

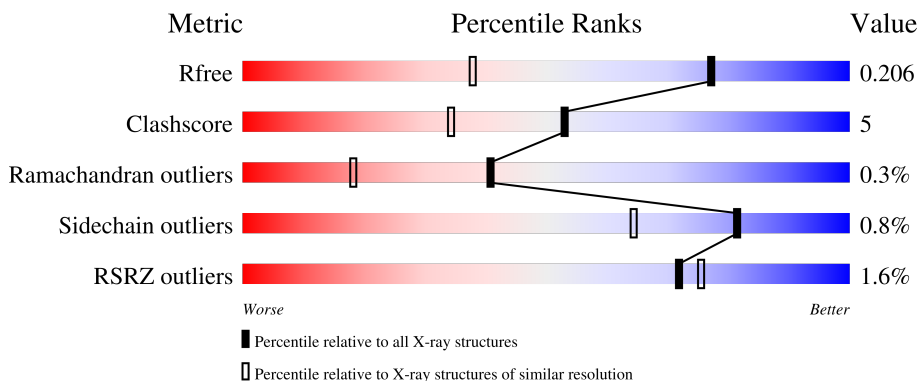
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.47 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	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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 of 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	391	 85% 11% ..
1	B	391	 3% 88% 9% ..

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7335 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 ALANINE RACEMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	387	Total 3135	C 2043	N 516	O 570	S 6	0	4	0
1	B	386	Total 3143	C 2046	N 520	O 571	S 6	0	6	0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 15	C 8	N 1	O 5	P 1	0	0
2	B	1	Total 15	C 8	N 1	O 5	P 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	3	Total Mg 3 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0
4	B	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	557	Total O 557 557	0	0
5	B	463	Total O 463 463	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.55Å 88.36Å 138.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.19 – 1.47 44.18 – 1.47	Depositor EDS
% Data completeness (in resolution range)	96.2 (44.19-1.47) 96.2 (44.18-1.47)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 1.47Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.168 , 0.199 0.174 , 0.206	Depositor DCC
$R_{free}$ test set	5826 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.5	Xtrriage
Anisotropy	0.056	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7335	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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: MG, MLY, CL, PLP

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	0.49	0/3010	0.68	2/4116 (0.0%)
1	B	0.46	0/3018	0.66	1/4127 (0.0%)
All	All	0.47	0/6028	0.67	3/8243 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	B	3	0
All	All	4	0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	177	THR	OG1-CB-CG2	7.31	126.81	110.00
1	A	363[A]	THR	CA-CB-CG2	5.38	119.93	112.40
1	A	363[B]	THR	CA-CB-CG2	5.38	119.93	112.40

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	363[A]	THR	CB
1	B	106[B]	THR	CB
1	B	177	THR	CB
1	B	212[B]	THR	CB

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	3135	0	3150	42	0
1	B	3143	0	3159	26	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
5	A	557	0	0	13	0
5	B	463	0	0	8	0
All	All	7335	0	6321	68	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 5.

The worst 5 of 68 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:27:MLY:CH2	1:A:34:VAL:O	2.00	1.10
1:A:309:VAL:HG23	1:A:322[B]:ILE:HD11	1.33	1.05
1:A:202:MLY:HH13	5:A:2275:HOH:O	1.63	0.99
1:B:348[B]:THR:HG22	5:B:2416:HOH:O	1.69	0.93
1:A:27:MLY:HH21	1:A:34:VAL:O	1.74	0.87

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	371/391 (95%)	361 (97%)	9 (2%)	1 (0%)	41	18
1	B	372/391 (95%)	360 (97%)	11 (3%)	1 (0%)	41	18
All	All	743/782 (95%)	721 (97%)	20 (3%)	2 (0%)	41	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	B	48	ASP

### 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	313/312 (100%)	312 (100%)	1 (0%)	92	84
1	B	314/312 (101%)	309 (98%)	5 (2%)	62	34
All	All	627/624 (100%)	621 (99%)	6 (1%)	81	54

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	106[B]	THR
1	B	177	THR
1	B	263	ILE
1	B	95	ILE
1	A	95	ILE

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

36 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	B	307	1	9,10,11	0.51	0	6,11,13	2.06	2 (33%)
1	MLY	A	148	1	9,10,11	0.57	0	6,11,13	2.28	2 (33%)
1	MLY	A	202	1	9,10,11	0.46	0	6,11,13	2.11	2 (33%)
1	MLY	B	110	1	9,10,11	0.52	0	6,11,13	2.23	3 (50%)
1	MLY	A	118	1	9,10,11	0.44	0	6,11,13	2.16	3 (50%)
1	MLY	B	27	1	9,10,11	0.37	0	6,11,13	2.21	2 (33%)
1	MLY	B	148	1	9,10,11	0.47	0	6,11,13	2.21	2 (33%)
1	MLY	B	277	1	9,10,11	0.50	0	6,11,13	2.10	3 (50%)
1	MLY	B	333	1	9,10,11	0.43	0	6,11,13	2.24	2 (33%)
1	MLY	A	127	1	9,10,11	0.45	0	6,11,13	2.20	2 (33%)
1	MLY	A	54	1	9,10,11	0.52	0	6,11,13	2.26	4 (66%)
1	MLY	B	245	1	9,10,11	0.41	0	6,11,13	2.22	3 (50%)
1	MLY	A	255	1	9,10,11	0.36	0	6,11,13	2.25	2 (33%)
1	MLY	B	378	1	9,10,11	0.49	0	6,11,13	2.17	2 (33%)
1	MLY	A	27	1	9,10,11	0.48	0	6,11,13	2.28	2 (33%)
1	MLY	B	145	1	9,10,11	0.44	0	6,11,13	2.34	4 (66%)
1	MLY	B	118	1	9,10,11	0.50	0	6,11,13	2.17	3 (50%)
1	MLY	B	182	1	9,10,11	0.35	0	6,11,13	2.20	3 (50%)
1	MLY	A	110	1	9,10,11	0.52	0	6,11,13	2.17	2 (33%)
1	MLY	A	245	1	9,10,11	0.37	0	6,11,13	2.31	4 (66%)
1	MLY	B	152	1	9,10,11	0.37	0	6,11,13	2.08	2 (33%)
1	MLY	B	127	1	9,10,11	0.52	0	6,11,13	2.04	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	A	277	1	9,10,11	0.50	0	6,11,13	2.21	3 (50%)
1	MLY	A	378	1	9,10,11	0.44	0	6,11,13	2.18	3 (50%)
1	MLY	A	307	1	9,10,11	0.44	0	6,11,13	2.14	3 (50%)
1	MLY	B	202	1	9,10,11	0.42	0	6,11,13	2.17	2 (33%)
1	MLY	B	264	1	9,10,11	0.56	0	6,11,13	2.53	4 (66%)
1	MLY	B	195	1	9,10,11	0.48	0	6,11,13	2.15	3 (50%)
1	MLY	A	145	1	9,10,11	0.48	0	6,11,13	2.38	2 (33%)
1	MLY	B	54	1	9,10,11	0.45	0	6,11,13	2.13	2 (33%)
1	MLY	A	152	1	9,10,11	0.39	0	6,11,13	2.37	4 (66%)
1	MLY	A	182	1	9,10,11	0.45	0	6,11,13	2.25	3 (50%)
1	MLY	A	264	1	9,10,11	0.43	0	6,11,13	2.17	2 (33%)
1	MLY	B	255	1	9,10,11	0.38	0	6,11,13	2.29	2 (33%)
1	MLY	A	333	1	9,10,11	0.59	0	6,11,13	2.16	2 (33%)
1	MLY	A	195	1	9,10,11	0.46	0	6,11,13	2.20	3 (50%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	307	1	-	2/8/9/11	-
1	MLY	A	148	1	-	5/8/9/11	-
1	MLY	A	202	1	-	1/8/9/11	-
1	MLY	B	110	1	-	2/8/9/11	-
1	MLY	A	118	1	-	2/8/9/11	-
1	MLY	B	27	1	-	2/8/9/11	-
1	MLY	B	148	1	-	1/8/9/11	-
1	MLY	B	277	1	-	3/8/9/11	-
1	MLY	B	333	1	-	1/8/9/11	-
1	MLY	A	127	1	-	1/8/9/11	-
1	MLY	A	54	1	-	2/8/9/11	-
1	MLY	B	245	1	-	3/8/9/11	-
1	MLY	A	255	1	-	1/8/9/11	-
1	MLY	B	378	1	-	3/8/9/11	-
1	MLY	A	27	1	-	3/8/9/11	-
1	MLY	B	145	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	118	1	-	2/8/9/11	-
1	MLY	B	182	1	-	1/8/9/11	-
1	MLY	A	110	1	-	1/8/9/11	-
1	MLY	A	245	1	-	2/8/9/11	-
1	MLY	B	152	1	-	2/8/9/11	-
1	MLY	B	127	1	-	3/8/9/11	-
1	MLY	A	277	1	-	4/8/9/11	-
1	MLY	A	378	1	-	3/8/9/11	-
1	MLY	A	307	1	-	1/8/9/11	-
1	MLY	B	202	1	-	1/8/9/11	-
1	MLY	B	264	1	-	2/8/9/11	-
1	MLY	B	195	1	-	1/8/9/11	-
1	MLY	A	145	1	-	1/8/9/11	-
1	MLY	B	54	1	-	2/8/9/11	-
1	MLY	A	152	1	-	2/8/9/11	-
1	MLY	A	182	1	-	2/8/9/11	-
1	MLY	A	264	1	-	1/8/9/11	-
1	MLY	B	255	1	-	1/8/9/11	-
1	MLY	A	333	1	-	1/8/9/11	-
1	MLY	A	195	1	-	3/8/9/11	-

There are no bond length outliers.

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	MLY	CH2-NZ-CH1	4.38	121.06	109.73
1	A	145	MLY	CH2-NZ-CH1	4.33	120.91	109.73
1	B	255	MLY	CH2-NZ-CH1	4.16	120.48	109.73
1	B	264	MLY	CH2-NZ-CH1	4.08	120.28	109.73
1	B	145	MLY	CH2-NZ-CH1	3.99	120.05	109.73

There are no chirality outliers.

5 of 71 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	148	MLY	N-CA-CB-CG
1	A	148	MLY	C-CA-CB-CG
1	A	378	MLY	O-C-CA-CB
1	B	127	MLY	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	B	277	MLY	O-C-CA-CB

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	202	MLY	3	0
1	A	118	MLY	2	0
1	A	54	MLY	2	0
1	A	27	MLY	5	0
1	B	127	MLY	3	0
1	A	277	MLY	1	0
1	A	307	MLY	1	0
1	B	202	MLY	1	0
1	A	145	MLY	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 for Mogul analysis.

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	PLP	A	1041	1	15,15,16	1.61	2 (13%)	20,22,23	1.27	2 (10%)
2	PLP	B	1041	1	15,15,16	1.71	2 (13%)	20,22,23	1.36	3 (15%)

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	PLP	A	1041	1	-	0/6/6/8	0/1/1/1
2	PLP	B	1041	1	-	0/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1041	PLP	O3-C3	-5.01	1.25	1.37
2	A	1041	PLP	O3-C3	-4.38	1.26	1.37
2	A	1041	PLP	C2-N1	2.53	1.38	1.33
2	B	1041	PLP	C2-N1	2.45	1.38	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1041	PLP	C5-C6-N1	-2.70	119.32	123.82
2	B	1041	PLP	C5-C6-N1	-2.47	119.70	123.82
2	A	1041	PLP	O3-C3-C2	2.18	122.24	117.49
2	B	1041	PLP	C6-N1-C2	2.16	123.17	119.17
2	B	1041	PLP	C4A-C4-C5	-2.14	118.73	120.94

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<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	369/391 (94%)	-0.23	2 (0%) 91 93	7, 10, 18, 31	0
1	B	368/391 (94%)	-0.03	10 (2%) 54 58	7, 12, 22, 35	0
All	All	737/782 (94%)	-0.13	12 (1%) 72 75	7, 11, 20, 35	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	241	PHE	3.7
1	B	240	PRO	2.6
1	B	326	CYS	2.5
1	B	342	ASP	2.4
1	B	106[A]	THR	2.4

### 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<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	B	195	11/12	0.78	0.22	19,25,36,36	0
1	MLY	B	378	11/12	0.80	0.16	22,30,35,35	0
1	MLY	A	277	11/12	0.84	0.24	14,21,39,40	0
1	MLY	B	277	11/12	0.85	0.19	20,25,35,36	0
1	MLY	B	118	11/12	0.86	0.20	13,19,36,36	0
1	MLY	B	245	11/12	0.86	0.25	17,22,37,37	0
1	MLY	B	202	11/12	0.87	0.15	14,19,30,31	0
1	MLY	B	145	11/12	0.87	0.22	18,25,40,41	0
1	MLY	B	152	11/12	0.90	0.19	12,17,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	A	145	11/12	0.90	0.17	11,15,31,31	0
1	MLY	B	27	11/12	0.90	0.17	16,20,36,37	0
1	MLY	A	152	11/12	0.91	0.17	10,17,36,37	0
1	MLY	A	245	11/12	0.91	0.20	9,13,37,38	0
1	MLY	A	264	11/12	0.91	0.12	13,16,31,32	0
1	MLY	B	264	11/12	0.91	0.13	15,21,32,33	0
1	MLY	B	148	11/12	0.91	0.16	14,18,31,32	0
1	MLY	A	148	11/12	0.91	0.17	9,18,38,38	0
1	MLY	B	54	11/12	0.92	0.12	11,14,28,31	0
1	MLY	A	27	11/12	0.92	0.14	9,13,31,32	0
1	MLY	B	127	11/12	0.92	0.16	8,12,31,31	0
1	MLY	B	255	11/12	0.92	0.09	8,10,19,19	0
1	MLY	A	307	11/12	0.92	0.19	11,18,30,32	0
1	MLY	A	378	11/12	0.92	0.14	12,14,28,30	0
1	MLY	B	333	11/12	0.92	0.11	9,13,23,25	0
1	MLY	A	195	11/12	0.92	0.13	10,15,34,34	0
1	MLY	B	110	11/12	0.93	0.13	11,14,29,29	0
1	MLY	A	118	11/12	0.93	0.14	12,15,31,31	0
1	MLY	A	110	11/12	0.93	0.16	8,12,30,32	0
1	MLY	B	182	11/12	0.93	0.11	12,16,27,30	0
1	MLY	A	54	11/12	0.94	0.13	8,12,30,33	0
1	MLY	B	307	11/12	0.94	0.12	12,17,22,24	0
1	MLY	A	202	11/12	0.94	0.09	10,11,21,24	0
1	MLY	A	333	11/12	0.94	0.11	8,11,22,23	0
1	MLY	A	182	11/12	0.95	0.14	8,14,32,32	0
1	MLY	A	255	11/12	0.96	0.08	9,10,17,19	0
1	MLY	A	127	11/12	0.96	0.08	7,10,20,22	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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
3	MG	A	1390	1/1	0.95	0.26	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	B	1003	1/1	0.95	0.16	27,27,27,27	0
3	MG	B	1002	1/1	0.97	0.23	18,18,18,18	0
2	PLP	B	1041	15/16	0.97	0.07	9,9,12,13	0
2	PLP	A	1041	15/16	0.98	0.06	6,8,11,12	0
3	MG	B	1001	1/1	0.99	0.14	18,18,18,18	0
4	CL	A	1391	1/1	0.99	0.04	13,13,13,13	0
4	CL	A	1392	1/1	1.00	0.04	8,8,8,8	0
4	CL	B	1390	1/1	1.00	0.04	10,10,10,10	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.