Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:56 AM 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/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:

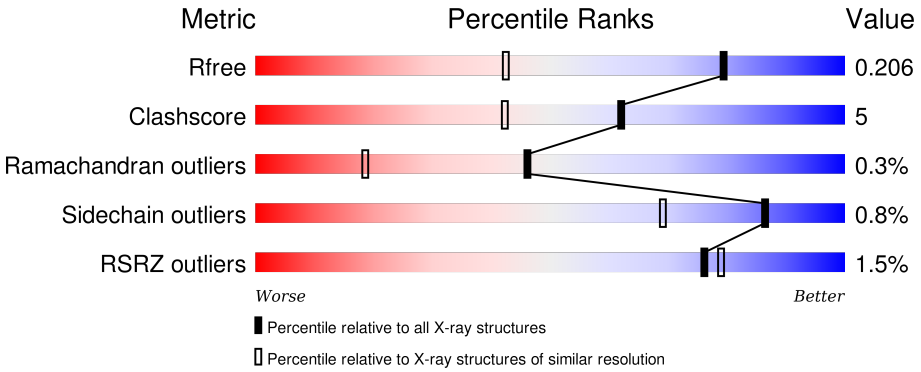
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

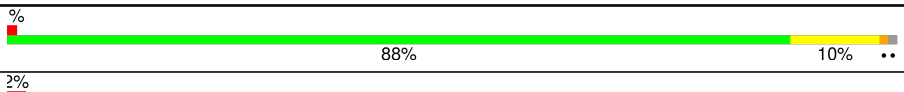
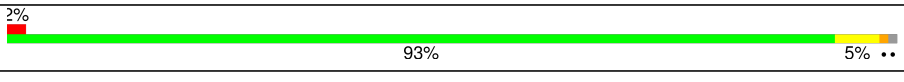
The reported resolution of this entry is 1.47 Å.

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}	91344	3129 (1.50-1.46)
Clashscore	102246	3380 (1.50-1.46)
Ramachandran outliers	100387	3310 (1.50-1.46)
Sidechain outliers	100360	3308 (1.50-1.46)
RSRZ outliers	91569	3133 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	
1	B	391	

2 Entry composition

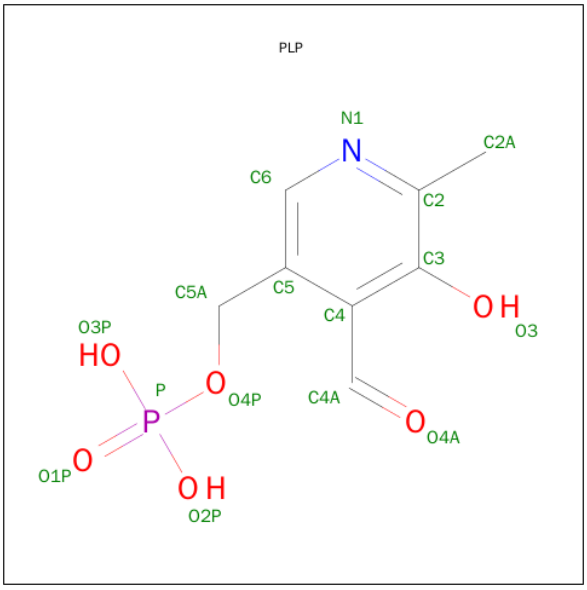
There are 5 unique types of molecules in this entry. The entry contains 7335 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	387	Total	C	N	O	S	0	4	0
			3135	2043	516	570	6			
1	B	386	Total	C	N	O	S	0	6	0
			3143	2046	520	571	6			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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

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

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

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

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

- Molecule 5 is water.

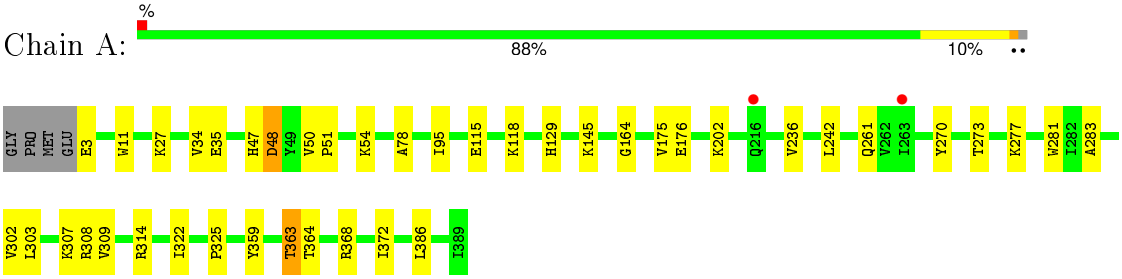
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	557	Total O 557 557	0	0
5	B	463	Total O 463 463	0	0

3 Residue-property plots (i)

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

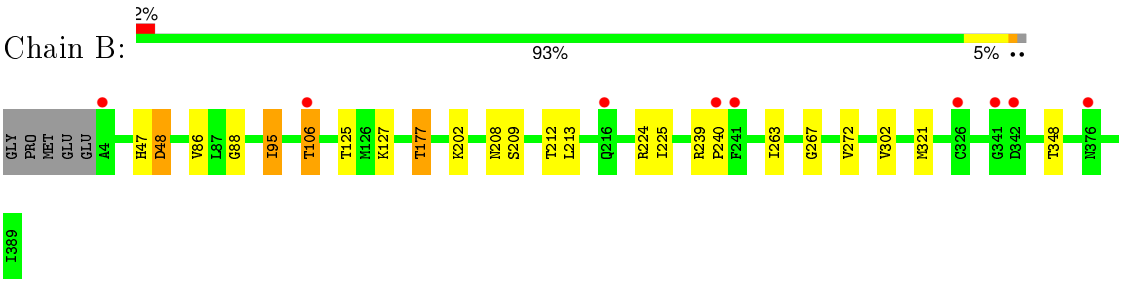
- Molecule 1: ALANINE RACEMASE

Chain A:



- Molecule 1: ALANINE RACEMASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.60 (at 1.47Å)	Xtriage
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 (5.29%)	DCC
Wilson B-factor (Å^2)	12.5	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 115958 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7335	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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(^{o})	Ideal(^{o})
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.

All (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
1:A:27:MLY:HH12	5:A:2052:HOH:O	1.73	0.86
1:A:27:MLY:HH23	1:A:34:VAL:O	1.76	0.84
1:B:125[B]:THR:HG21	5:B:2229:HOH:O	1.77	0.84
1:B:302:VAL:HG12	5:B:2398:HOH:O	1.79	0.83
1:A:145:MLY:HH22	5:A:2247:HOH:O	1.83	0.78
1:A:3:GLU:N	5:A:2001:HOH:O	2.16	0.77
1:A:309:VAL:HG23	1:A:322[B]:ILE:CD1	2.13	0.74
1:A:283:ALA:HB3	1:A:322[B]:ILE:HG22	1.70	0.73
1:B:212[A]:THR:HG21	1:B:225:ILE:CD1	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:MET:HE2	5:B:2372:HOH:O	1.95	0.66
1:A:202:MLY:HH12	5:A:2332:HOH:O	1.95	0.66
1:A:309:VAL:CG2	1:A:322[B]:ILE:HD11	2.20	0.65
1:A:283:ALA:HB3	1:A:322[B]:ILE:CG2	2.27	0.64
1:A:302:VAL:CG2	1:A:322[B]:ILE:CD1	2.77	0.62
1:B:125[A]:THR:HG22	1:B:127:MLY:CH1	2.29	0.62
1:B:208:ASN:O	1:B:212[A]:THR:HG22	2.00	0.61
1:A:27:MLY:HH22	1:A:35:GLU:HA	1.83	0.61
1:A:202:MLY:CH1	5:A:2275:HOH:O	2.34	0.60
1:B:125[A]:THR:HG21	5:B:2229:HOH:O	2.01	0.59
1:A:302:VAL:CG2	1:A:322[B]:ILE:HD12	2.33	0.58
1:B:212[A]:THR:HG21	1:B:225:ILE:HD11	1.86	0.57
1:A:54:MLY:HH23	5:A:2086:HOH:O	2.03	0.57
1:B:125[A]:THR:HG22	1:B:127:MLY:HH13	1.87	0.56
1:B:348[B]:THR:HG21	5:B:2415:HOH:O	2.06	0.56
1:B:88:GLY:O	1:B:106[A]:THR:CG2	2.54	0.56
1:B:202:MLY:HH22	5:B:2230:HOH:O	2.05	0.55
1:A:242:LEU:HD23	5:A:2368:HOH:O	2.07	0.55
1:A:54:MLY:HH22	1:A:78:ALA:O	2.08	0.54
1:A:302:VAL:CG2	1:A:322[B]:ILE:HD11	2.38	0.53
1:A:118:MLY:HH13	5:A:2205:HOH:O	2.10	0.51
1:A:175:VAL:HG23	1:A:176:GLU:N	2.26	0.50
1:A:307:MLY:HH13	1:A:325:PRO:HG3	1.93	0.50
1:A:47:HIS:O	1:A:48:ASP:HB2	2.12	0.50
1:A:277:MLY:HH12	5:A:2418:HOH:O	2.11	0.49
1:B:212[B]:THR:HG21	1:B:225:ILE:HD11	1.93	0.49
1:A:11:TRP:CD1	1:A:372:ILE:HD12	2.49	0.48
1:B:239:ARG:N	1:B:240:PRO:HD2	2.29	0.48
1:A:115:GLU:OE2	1:A:118:MLY:HH22	2.14	0.48
1:A:236:VAL:HG22	5:A:2361:HOH:O	2.13	0.47
1:B:47:HIS:O	1:B:48:ASP:HB2	2.15	0.47
1:B:106[B]:THR:HG22	5:B:2112:HOH:O	2.14	0.46
1:A:302:VAL:HG21	1:A:322[B]:ILE:HD12	1.98	0.45
1:B:125[A]:THR:HG22	1:B:127:MLY:HH11	1.98	0.45
1:B:209:SER:O	1:B:212[A]:THR:HG22	2.16	0.45
1:A:309:VAL:CG2	1:A:322[B]:ILE:CD1	2.89	0.44
1:B:212[B]:THR:HG21	1:B:225:ILE:CD1	2.48	0.43
1:B:209:SER:O	1:B:212[A]:THR:CG2	2.66	0.43
1:B:86:VAL:O	1:B:106[A]:THR:HG22	2.19	0.43
1:A:273:THR:HG21	1:A:314:ARG:CZ	2.47	0.43
1:A:308:ARG:NH1	5:A:2459:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:GLN:HG3	1:A:281:TRP:CZ3	2.55	0.42
1:B:208:ASN:HA	1:B:224:ARG:O	2.19	0.42
1:A:359:TYR:O	1:A:363[B]:THR:HG22	2.20	0.42
1:A:363[B]:THR:HG23	1:A:364:THR:HG23	2.01	0.42
1:A:270:TYR:OH	5:A:2410:HOH:O	2.19	0.41
1:A:129:HIS:HA	1:A:164:GLY:O	2.20	0.41
1:A:368:ARG:HB2	1:A:386:LEU:HD11	2.02	0.41
1:A:50:VAL:HB	1:A:51:PRO:HD3	2.02	0.41
1:B:267:GLY:HA3	1:B:272:VAL:HG13	2.02	0.41
1:A:261:GLN:HG3	1:A:281:TRP:CH2	2.56	0.41
1:A:303:LEU:HD23	1:A:308:ARG:HD2	2.03	0.40
1:B:95:ILE:C	1:B:95:ILE:HD13	2.42	0.40
1:B:212[B]:THR:HG22	1:B:213:LEU:HG	2.03	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	371/391 (95%)	361 (97%)	9 (2%)	1 (0%)	46 18
1	B	372/391 (95%)	360 (97%)	11 (3%)	1 (0%)	46 18
All	All	743/782 (95%)	721 (97%)	20 (3%)	2 (0%)	46 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

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%)	94 86
1	B	314/312 (101%)	309 (98%)	5 (2%)	70 39
All	All	627/624 (100%)	621 (99%)	6 (1%)	86 60

All (6) residues with a non-rotameric sidechain are listed below:

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

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

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	A	110	1	9,10,11	0.51	0	9,11,13	1.84	2 (22%)
1	MLY	A	118	1	9,10,11	0.41	0	9,11,13	1.86	3 (33%)
1	MLY	A	127	1	9,10,11	0.43	0	9,11,13	1.87	2 (22%)
1	MLY	A	145	1	9,10,11	0.45	0	9,11,13	2.08	2 (22%)
1	MLY	A	148	1	9,10,11	0.64	0	9,11,13	1.99	2 (22%)
1	MLY	A	152	1	9,10,11	0.40	0	9,11,13	2.03	4 (44%)
1	MLY	A	182	1	9,10,11	0.51	0	9,11,13	1.94	3 (33%)
1	MLY	A	195	1	9,10,11	0.48	0	9,11,13	1.88	3 (33%)
1	MLY	A	202	1	9,10,11	0.45	0	9,11,13	1.90	3 (33%)
1	MLY	A	245	1	9,10,11	0.40	0	9,11,13	1.99	4 (44%)
1	MLY	A	255	1	9,10,11	0.34	0	9,11,13	1.92	2 (22%)
1	MLY	A	264	1	9,10,11	0.39	0	9,11,13	1.88	2 (22%)
1	MLY	A	27	1	9,10,11	0.50	0	9,11,13	1.99	3 (33%)
1	MLY	A	277	1	9,10,11	0.60	0	9,11,13	1.90	3 (33%)
1	MLY	A	307	1	9,10,11	0.40	0	9,11,13	1.85	4 (44%)
1	MLY	A	333	1	9,10,11	0.69	0	9,11,13	1.84	2 (22%)
1	MLY	A	378	1	9,10,11	0.46	0	9,11,13	1.94	3 (33%)
1	MLY	A	54	1	9,10,11	0.47	0	9,11,13	1.95	4 (44%)
1	MLY	B	110	1	9,10,11	0.49	0	9,11,13	1.89	3 (33%)
1	MLY	B	118	1	9,10,11	0.46	0	9,11,13	1.88	3 (33%)
1	MLY	B	127	1	9,10,11	0.50	0	9,11,13	1.76	3 (33%)
1	MLY	B	145	1	9,10,11	0.40	0	9,11,13	1.98	4 (44%)
1	MLY	B	148	1	9,10,11	0.44	0	9,11,13	1.88	2 (22%)
1	MLY	B	152	1	9,10,11	0.34	0	9,11,13	1.78	2 (22%)
1	MLY	B	182	1	9,10,11	0.35	0	9,11,13	1.90	2 (22%)
1	MLY	B	195	1	9,10,11	0.43	0	9,11,13	1.92	4 (44%)
1	MLY	B	202	1	9,10,11	0.43	0	9,11,13	1.88	2 (22%)
1	MLY	B	245	1	9,10,11	0.37	0	9,11,13	1.93	4 (44%)
1	MLY	B	255	1	9,10,11	0.39	0	9,11,13	1.95	2 (22%)
1	MLY	B	264	1	9,10,11	0.51	0	9,11,13	2.19	4 (44%)
1	MLY	B	27	1	9,10,11	0.37	0	9,11,13	1.89	2 (22%)
1	MLY	B	277	1	9,10,11	0.49	0	9,11,13	1.79	3 (33%)
1	MLY	B	307	1	9,10,11	0.46	0	9,11,13	1.85	2 (22%)
1	MLY	B	333	1	9,10,11	0.42	0	9,11,13	1.90	2 (22%)
1	MLY	B	378	1	9,10,11	0.51	0	9,11,13	1.87	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MLY	B	54	1	9,10,11	0.48	0	9,11,13	1.82	2 (22%)

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	A	110	1	-	0/7/9/11	0/0/0/0
1	MLY	A	118	1	-	0/7/9/11	0/0/0/0
1	MLY	A	127	1	-	0/7/9/11	0/0/0/0
1	MLY	A	145	1	-	0/7/9/11	0/0/0/0
1	MLY	A	148	1	-	0/7/9/11	0/0/0/0
1	MLY	A	152	1	-	0/7/9/11	0/0/0/0
1	MLY	A	182	1	-	0/7/9/11	0/0/0/0
1	MLY	A	195	1	-	0/7/9/11	0/0/0/0
1	MLY	A	202	1	-	0/7/9/11	0/0/0/0
1	MLY	A	245	1	-	0/7/9/11	0/0/0/0
1	MLY	A	255	1	-	0/7/9/11	0/0/0/0
1	MLY	A	264	1	-	0/7/9/11	0/0/0/0
1	MLY	A	27	1	-	0/7/9/11	0/0/0/0
1	MLY	A	277	1	-	0/7/9/11	0/0/0/0
1	MLY	A	307	1	-	0/7/9/11	0/0/0/0
1	MLY	A	333	1	-	0/7/9/11	0/0/0/0
1	MLY	A	378	1	-	0/7/9/11	0/0/0/0
1	MLY	A	54	1	-	0/7/9/11	0/0/0/0
1	MLY	B	110	1	-	0/7/9/11	0/0/0/0
1	MLY	B	118	1	-	0/7/9/11	0/0/0/0
1	MLY	B	127	1	-	0/7/9/11	0/0/0/0
1	MLY	B	145	1	-	0/7/9/11	0/0/0/0
1	MLY	B	148	1	-	0/7/9/11	0/0/0/0
1	MLY	B	152	1	-	0/7/9/11	0/0/0/0
1	MLY	B	182	1	-	0/7/9/11	0/0/0/0
1	MLY	B	195	1	-	0/7/9/11	0/0/0/0
1	MLY	B	202	1	-	0/7/9/11	0/0/0/0
1	MLY	B	245	1	-	0/7/9/11	0/0/0/0
1	MLY	B	255	1	-	0/7/9/11	0/0/0/0
1	MLY	B	264	1	-	0/7/9/11	0/0/0/0
1	MLY	B	27	1	-	0/7/9/11	0/0/0/0
1	MLY	B	277	1	-	0/7/9/11	0/0/0/0
1	MLY	B	307	1	-	0/7/9/11	0/0/0/0
1	MLY	B	333	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	378	1	-	0/7/9/11	0/0/0/0
1	MLY	B	54	1	-	0/7/9/11	0/0/0/0

There are no bond length outliers.

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	264	MLY	CD-CE-NZ	-3.21	105.66	113.92
1	B	145	MLY	CD-CE-NZ	-2.55	107.35	113.92
1	A	245	MLY	CD-CE-NZ	-2.47	107.56	113.92
1	A	152	MLY	CD-CE-NZ	-2.40	107.75	113.92
1	B	195	MLY	O-C-CA	-2.23	119.69	125.49
1	A	27	MLY	O-C-CA	-2.17	119.82	125.49
1	A	54	MLY	CD-CE-NZ	-2.16	108.36	113.92
1	A	378	MLY	O-C-CA	-2.14	119.92	125.49
1	B	245	MLY	CD-CE-NZ	-2.09	108.54	113.92
1	A	202	MLY	O-C-CA	-2.04	120.17	125.49
1	A	307	MLY	O-C-CA	-2.01	120.26	125.49
1	B	110	MLY	CH1-NZ-CE	2.02	118.83	110.79
1	B	127	MLY	CH2-NZ-CE	2.02	118.84	110.79
1	A	307	MLY	CH2-NZ-CE	2.03	118.89	110.79
1	A	277	MLY	CH2-NZ-CE	2.04	118.89	110.79
1	A	118	MLY	CH2-NZ-CE	2.04	118.90	110.79
1	A	182	MLY	CH2-NZ-CE	2.05	118.94	110.79
1	B	195	MLY	CH2-NZ-CE	2.07	119.03	110.79
1	B	118	MLY	CH2-NZ-CE	2.10	119.15	110.79
1	B	277	MLY	CH2-NZ-CE	2.10	119.15	110.79
1	A	152	MLY	CH1-NZ-CE	2.10	119.17	110.79
1	A	54	MLY	CH2-NZ-CE	2.11	119.19	110.79
1	A	195	MLY	CH1-NZ-CE	2.21	119.59	110.79
1	A	245	MLY	CH2-NZ-CE	2.24	119.71	110.79
1	B	264	MLY	CH2-NZ-CE	2.25	119.74	110.79
1	B	145	MLY	CH2-NZ-CE	2.26	119.80	110.79
1	B	264	MLY	CH1-NZ-CE	2.31	119.98	110.79
1	B	245	MLY	CH2-NZ-CE	2.31	119.98	110.79
1	B	145	MLY	CH1-NZ-CE	2.35	120.15	110.79
1	A	255	MLY	CH1-NZ-CE	2.39	120.29	110.79
1	A	245	MLY	CH1-NZ-CE	2.43	120.45	110.79
1	A	152	MLY	CH2-NZ-CE	2.51	120.80	110.79
1	A	54	MLY	CH1-NZ-CE	2.55	120.95	110.79
1	B	245	MLY	CH1-NZ-CE	2.57	121.03	110.79
1	B	110	MLY	CH2-NZ-CE	2.64	121.29	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	277	MLY	CH1-NZ-CE	2.65	121.33	110.79
1	A	145	MLY	CH1-NZ-CE	2.68	121.47	110.79
1	A	118	MLY	CH1-NZ-CE	2.69	121.51	110.79
1	A	195	MLY	CH2-NZ-CE	2.72	121.61	110.79
1	A	182	MLY	CH1-NZ-CE	2.73	121.67	110.79
1	A	378	MLY	CH1-NZ-CE	2.74	121.70	110.79
1	B	148	MLY	CH1-NZ-CE	2.76	121.76	110.79
1	B	195	MLY	CH1-NZ-CE	2.77	121.80	110.79
1	B	118	MLY	CH1-NZ-CE	2.85	122.13	110.79
1	A	148	MLY	CH1-NZ-CE	2.89	122.29	110.79
1	B	182	MLY	CH1-NZ-CE	2.92	122.41	110.79
1	B	277	MLY	CH1-NZ-CE	2.92	122.43	110.79
1	B	378	MLY	CH1-NZ-CE	2.93	122.46	110.79
1	B	127	MLY	CH2-NZ-CH1	2.96	117.64	109.72
1	A	264	MLY	CH1-NZ-CE	3.00	122.73	110.79
1	B	255	MLY	CH1-NZ-CE	3.01	122.77	110.79
1	A	202	MLY	CH1-NZ-CE	3.01	122.78	110.79
1	B	333	MLY	CH1-NZ-CE	3.01	122.78	110.79
1	A	307	MLY	CH1-NZ-CE	3.03	122.84	110.79
1	B	307	MLY	CH2-NZ-CH1	3.03	117.83	109.72
1	A	110	MLY	CH1-NZ-CE	3.06	122.96	110.79
1	B	54	MLY	CH1-NZ-CE	3.09	123.09	110.79
1	B	152	MLY	CH2-NZ-CH1	3.09	118.00	109.72
1	B	27	MLY	CH1-NZ-CE	3.10	123.13	110.79
1	B	202	MLY	CH1-NZ-CE	3.13	123.25	110.79
1	B	152	MLY	CH1-NZ-CE	3.18	123.46	110.79
1	A	307	MLY	CH2-NZ-CH1	3.19	118.26	109.72
1	B	127	MLY	CH1-NZ-CE	3.20	123.52	110.79
1	A	333	MLY	CH1-NZ-CE	3.22	123.60	110.79
1	A	127	MLY	CH1-NZ-CE	3.23	123.63	110.79
1	B	277	MLY	CH2-NZ-CH1	3.25	118.41	109.72
1	B	307	MLY	CH1-NZ-CE	3.25	123.74	110.79
1	B	54	MLY	CH2-NZ-CH1	3.30	118.55	109.72
1	B	27	MLY	CH2-NZ-CH1	3.35	118.69	109.72
1	B	118	MLY	CH2-NZ-CH1	3.36	118.72	109.72
1	A	195	MLY	CH2-NZ-CH1	3.39	118.80	109.72
1	A	202	MLY	CH2-NZ-CH1	3.40	118.81	109.72
1	B	182	MLY	CH2-NZ-CH1	3.41	118.84	109.72
1	A	27	MLY	CH2-NZ-CH1	3.41	118.85	109.72
1	A	110	MLY	CH2-NZ-CH1	3.41	118.85	109.72
1	A	333	MLY	CH2-NZ-CH1	3.42	118.87	109.72
1	B	245	MLY	CH2-NZ-CH1	3.46	118.99	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	378	MLY	CH2-NZ-CH1	3.52	119.13	109.72
1	B	195	MLY	CH2-NZ-CH1	3.53	119.17	109.72
1	B	333	MLY	CH2-NZ-CH1	3.53	119.17	109.72
1	A	264	MLY	CH2-NZ-CH1	3.59	119.33	109.72
1	B	202	MLY	CH2-NZ-CH1	3.60	119.34	109.72
1	A	27	MLY	CH1-NZ-CE	3.60	125.13	110.79
1	A	182	MLY	CH2-NZ-CH1	3.61	119.39	109.72
1	A	148	MLY	CH2-NZ-CH1	3.67	119.54	109.72
1	A	118	MLY	CH2-NZ-CH1	3.68	119.57	109.72
1	A	378	MLY	CH2-NZ-CH1	3.69	119.59	109.72
1	A	127	MLY	CH2-NZ-CH1	3.70	119.61	109.72
1	A	277	MLY	CH2-NZ-CH1	3.76	119.77	109.72
1	A	245	MLY	CH2-NZ-CH1	3.78	119.83	109.72
1	A	54	MLY	CH2-NZ-CH1	3.79	119.85	109.72
1	B	110	MLY	CH2-NZ-CH1	3.80	119.88	109.72
1	B	148	MLY	CH2-NZ-CH1	3.81	119.92	109.72
1	A	152	MLY	CH2-NZ-CH1	3.86	120.04	109.72
1	B	145	MLY	CH2-NZ-CH1	3.86	120.05	109.72
1	B	264	MLY	CH2-NZ-CH1	3.95	120.28	109.72
1	B	255	MLY	CH2-NZ-CH1	4.02	120.48	109.72
1	A	145	MLY	CH2-NZ-CH1	4.18	120.91	109.72
1	A	255	MLY	CH2-NZ-CH1	4.24	121.06	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 19 short contacts:

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

5.5 Carbohydrates (i)

There are no carbohydrates 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	1.58	3 (20%)	21,22,23	1.24	2 (9%)
2	PLP	B	1041	1	15,15,16	1.68	2 (13%)	21,22,23	1.34	2 (9%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1041	PLP	O3-C3	-4.99	1.25	1.37
2	A	1041	PLP	O3-C3	-4.37	1.26	1.37
2	A	1041	PLP	P-O2P	-2.04	1.47	1.54
2	B	1041	PLP	C2-N1	2.08	1.38	1.34
2	A	1041	PLP	C2-N1	2.15	1.38	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1041	PLP	C5-C6-N1	-2.62	119.32	123.86
2	B	1041	PLP	C5-C6-N1	-2.39	119.70	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1041	PLP	C4A-C4-C5	-2.07	118.73	120.88
2	A	1041	PLP	O3-C3-C2	2.63	122.24	117.66

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

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^{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>	#RSRZ>2		OWAB(Å^2)	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	9 (2%)	62 65	7, 12, 22, 35	0
All	All	737/782 (94%)	-0.13	11 (1%)	76 79	7, 11, 20, 35	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	241	PHE	3.7
1	B	326	CYS	2.6
1	B	240	PRO	2.5
1	B	342	ASP	2.4
1	B	4	ALA	2.4
1	A	263	ILE	2.4
1	B	106[A]	THR	2.4
1	B	341	GLY	2.3
1	B	376	ASN	2.3
1	A	216	GLN	2.1
1	B	216	GLN	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	LLDF	B-factors(Å^2)	Q<0.9
1	MLY	B	277	11/12	0.85	0.19	-	20,25,35,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	MLY	B	148	11/12	0.91	0.16	-	14,18,31,32	0
1	MLY	B	245	11/12	0.86	0.25	-	17,22,37,37	0
1	MLY	A	202	11/12	0.94	0.09	-	10,11,21,24	0
1	MLY	B	152	11/12	0.90	0.19	-	12,17,38,39	0
1	MLY	B	127	11/12	0.92	0.16	-	8,12,31,31	0
1	MLY	A	110	11/12	0.93	0.16	-	8,12,30,32	0
1	MLY	A	27	11/12	0.92	0.14	-	9,13,31,32	0
1	MLY	A	182	11/12	0.95	0.15	-	8,14,32,32	0
1	MLY	A	148	11/12	0.91	0.17	-	9,18,38,38	0
1	MLY	B	27	11/12	0.90	0.17	-	16,20,36,37	0
1	MLY	B	54	11/12	0.92	0.12	-	11,14,28,31	0
1	MLY	A	277	11/12	0.84	0.24	-	14,21,39,40	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	110	11/12	0.93	0.13	-	11,14,29,29	0
1	MLY	B	378	11/12	0.80	0.16	-	22,30,35,35	0
1	MLY	A	245	11/12	0.91	0.20	-	9,13,37,38	0
1	MLY	B	255	11/12	0.92	0.09	-	8,10,19,19	0
1	MLY	B	118	11/12	0.86	0.20	-	13,19,36,36	0
1	MLY	B	264	11/12	0.91	0.13	-	15,21,32,33	0
1	MLY	B	333	11/12	0.92	0.11	-	9,13,23,25	0
1	MLY	B	307	11/12	0.93	0.12	-	12,17,22,24	0
1	MLY	A	127	11/12	0.96	0.08	-	7,10,20,22	0
1	MLY	A	152	11/12	0.91	0.16	-	10,17,36,37	0
1	MLY	B	145	11/12	0.87	0.22	-	18,25,40,41	0
1	MLY	A	145	11/12	0.90	0.17	-	11,15,31,31	0
1	MLY	A	333	11/12	0.94	0.11	-	8,11,22,23	0
1	MLY	B	202	11/12	0.87	0.15	-	14,19,30,31	0
1	MLY	A	264	11/12	0.91	0.12	-	13,16,31,32	0
1	MLY	A	255	11/12	0.96	0.08	-	9,10,17,19	0
1	MLY	B	195	11/12	0.78	0.22	-	19,25,36,36	0
1	MLY	A	195	11/12	0.92	0.13	-	10,15,34,34	0
1	MLY	A	378	11/12	0.91	0.14	-	12,14,28,30	0
1	MLY	A	307	11/12	0.92	0.19	-	11,18,30,32	0
1	MLY	A	118	11/12	0.93	0.14	-	12,15,31,31	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	LLDF	B-factors(Å^2)	Q<0.9
2	PLP	B	1041	15/16	0.97	0.07	-0.48	9,9,12,13	0
2	PLP	A	1041	15/16	0.98	0.06	-0.88	6,8,11,12	0
3	MG	B	1003	1/1	0.95	0.16	-	27,27,27,27	0
4	CL	A	1391	1/1	0.99	0.04	-	13,13,13,13	0
4	CL	B	1390	1/1	1.00	0.04	-	10,10,10,10	0
3	MG	B	1002	1/1	0.97	0.23	-	18,18,18,18	0
4	CL	A	1392	1/1	1.00	0.05	-	8,8,8,8	0
3	MG	B	1001	1/1	0.99	0.14	-	18,18,18,18	0
3	MG	A	1390	1/1	0.95	0.26	-	23,23,23,23	0

6.5 Other polymers

There are no such residues in this entry.