



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:48 AM UTC

PDB ID : 3CO8 / pdb_00003co8
Title : Crystal structure of alanine racemase from *Oenococcus oeni*
Authors : Palani, K.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center
for Structural Genomics (NYSGXRC)
Deposited on : 2008-03-27
Resolution : 1.70 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

<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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

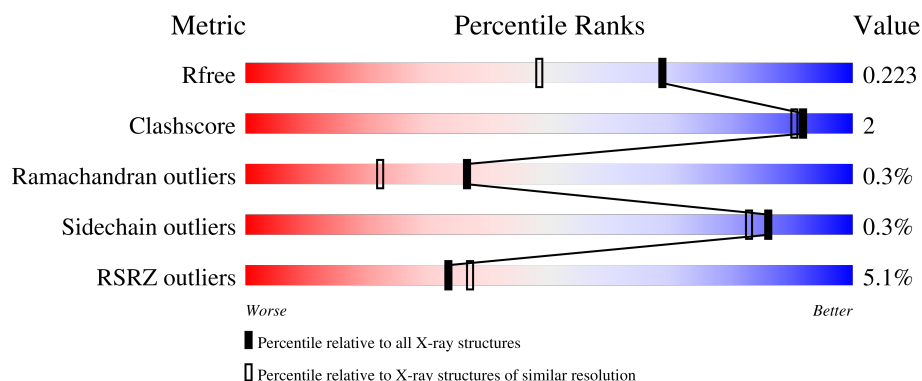
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

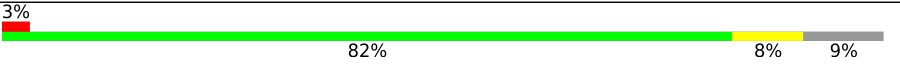
The reported resolution of this entry is 1.70 Å.

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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 ≥ 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	380	
1	B	380	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6204 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.

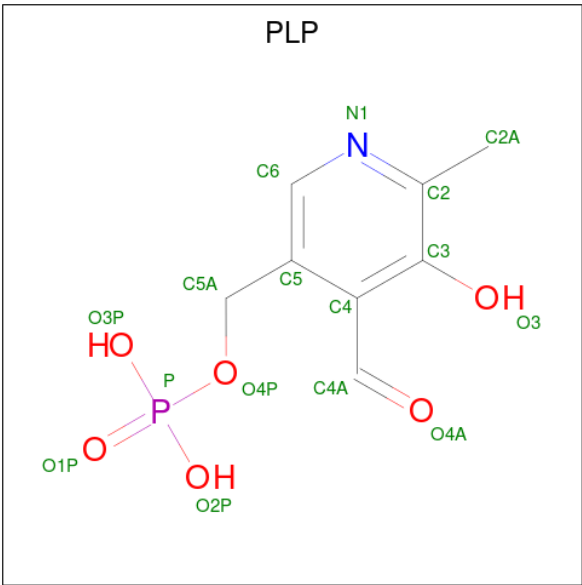
- Molecule 1 is a protein called Alanine racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	Se	0	0	0
			2827	1819	479	518	3	8			
1	B	345	Total	C	N	O	S	Se	0	0	0
			2721	1748	461	501	3	8			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MSE	-	expression tag	UNP Q04HB7
A	1	SER	-	expression tag	UNP Q04HB7
A	2	LEU	-	expression tag	UNP Q04HB7
A	372	GLU	-	expression tag	UNP Q04HB7
A	373	GLY	-	expression tag	UNP Q04HB7
A	374	HIS	-	expression tag	UNP Q04HB7
A	375	HIS	-	expression tag	UNP Q04HB7
A	376	HIS	-	expression tag	UNP Q04HB7
A	377	HIS	-	expression tag	UNP Q04HB7
A	378	HIS	-	expression tag	UNP Q04HB7
A	379	HIS	-	expression tag	UNP Q04HB7
B	0	MSE	-	expression tag	UNP Q04HB7
B	1	SER	-	expression tag	UNP Q04HB7
B	2	LEU	-	expression tag	UNP Q04HB7
B	372	GLU	-	expression tag	UNP Q04HB7
B	373	GLY	-	expression tag	UNP Q04HB7
B	374	HIS	-	expression tag	UNP Q04HB7
B	375	HIS	-	expression tag	UNP Q04HB7
B	376	HIS	-	expression tag	UNP Q04HB7
B	377	HIS	-	expression tag	UNP Q04HB7
B	378	HIS	-	expression tag	UNP Q04HB7
B	379	HIS	-	expression tag	UNP Q04HB7

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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		

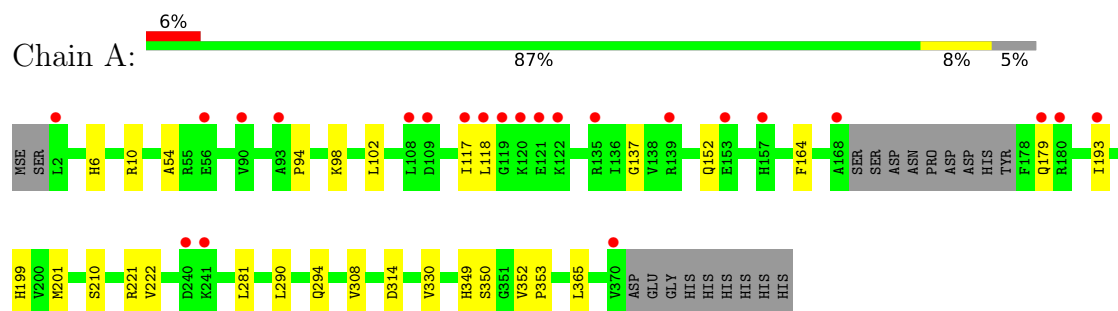
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	319	Total	O	0	0
			319	319		
3	B	307	Total	O	0	0
			307	307		

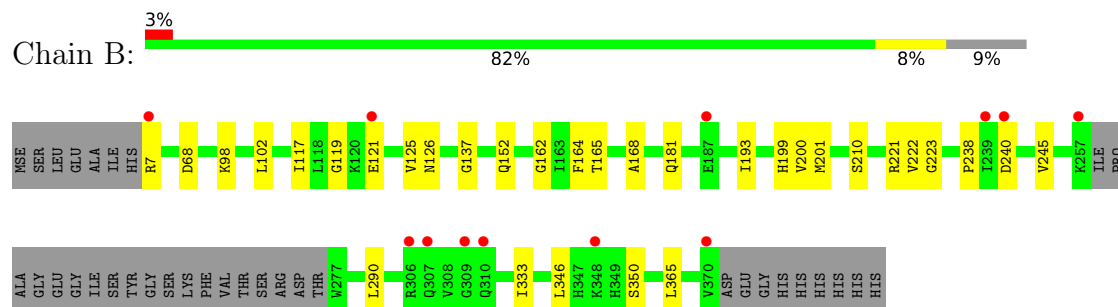
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Alanine racemase



• Molecule 1: Alanine racemase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.40 Å 99.64 Å 84.67 Å 90.00° 103.26° 90.00°	Depositor
Resolution (Å)	38.08 – 1.70 38.08 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.3 (38.08-1.70) 96.5 (38.08-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.29 (at 1.70 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.259 0.204 , 0.223	Depositor DCC
R_{free} test set	4092 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6204	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.64	1/2882 (0.0%)	1.08	16/3882 (0.4%)
1	B	0.62	0/2775	1.04	13/3739 (0.3%)
All	All	0.63	1/5657 (0.0%)	1.06	29/7621 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	PRO	CA-C	5.87	1.55	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	LEU	N-CA-C	11.19	127.27	113.17
1	B	201	MSE	N-CA-C	8.36	122.61	108.23
1	A	117	ILE	N-CA-C	8.30	120.06	112.43
1	A	201	MSE	N-CA-C	7.71	121.50	108.23
1	A	179	GLN	N-CA-C	7.29	118.87	111.07
1	B	222	VAL	N-CA-C	6.71	119.46	108.99
1	A	137	GLY	N-CA-C	6.70	118.31	111.95
1	A	290	LEU	N-CA-C	6.66	119.41	110.35
1	A	222	VAL	N-CA-C	6.65	119.36	108.99
1	A	210	SER	N-CA-C	6.53	118.39	111.28
1	B	102	LEU	N-CA-C	-6.20	99.07	108.67
1	A	350	SER	N-CA-C	6.18	120.95	113.41
1	B	125	VAL	N-CA-C	6.14	117.14	108.36
1	A	352	VAL	CA-C-N	6.13	124.14	119.66
1	A	352	VAL	C-N-CA	6.13	124.14	119.66
1	A	102	LEU	N-CA-C	-6.10	99.21	108.67
1	B	240	ASP	N-CA-C	5.94	119.63	112.38
1	B	164	PHE	N-CA-C	5.81	117.08	108.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ARG	N-CA-C	5.78	118.06	108.99
1	B	137	GLY	N-CA-C	5.63	117.30	111.95
1	B	290	LEU	N-CA-C	5.57	117.48	110.24
1	B	350	SER	N-CA-C	5.52	120.29	113.50
1	A	164	PHE	N-CA-C	5.43	116.53	108.60
1	A	308	VAL	N-CA-C	5.43	116.80	108.71
1	B	238	PRO	N-CA-C	5.36	118.89	110.80
1	A	54	ALA	N-CA-C	5.27	117.44	111.11
1	B	210	SER	N-CA-C	5.21	116.96	111.28
1	B	117	ILE	N-CA-C	5.06	118.95	113.43
1	B	245	VAL	N-CA-C	5.05	118.61	112.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2827	0	2852	7	0
1	B	2721	0	2728	12	0
2	A	15	0	7	1	0
2	B	15	0	7	0	0
3	A	319	0	0	0	0
3	B	307	0	0	2	0
All	All	6204	0	5594	18	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 2.

All (18) 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:B:168:ALA:H	1:B:181:GLN:HE22	1.15	0.89
1:A:152:GLN:HE22	1:A:193:ILE:HD13	1.62	0.65
1:B:199:HIS:HD1	1:B:221:ARG:HH11	1.48	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LEU:HD21	1:A:330:VAL:HG21	1.82	0.61
1:A:199:HIS:HD2	1:A:221:ARG:HD3	1.65	0.60
1:B:199:HIS:HD1	1:B:221:ARG:HD3	1.67	0.58
1:B:168:ALA:H	1:B:181:GLN:NE2	1.97	0.52
1:B:152:GLN:HE22	1:B:193:ILE:HD13	1.75	0.50
1:A:6:HIS:HD2	1:B:68:ASP:OD1	1.96	0.49
1:B:121:GLU:HG3	3:B:646:HOH:O	2.13	0.48
1:B:126:ASN:HD22	1:B:162:GLY:HA3	1.80	0.47
1:A:221:ARG:NE	2:A:401:PLP:N1	2.54	0.46
1:B:7:ARG:NH2	1:B:365:LEU:HD23	2.31	0.45
1:B:98:LYS:HG3	3:B:646:HOH:O	2.17	0.45
1:A:94:PRO:O	1:A:98:LYS:HG2	2.18	0.43
1:B:333:ILE:HD11	1:B:346:LEU:HD22	2.02	0.42
1:B:165:THR:HG22	1:B:200:VAL:HG12	2.02	0.41
1:A:294:GLN:O	1:A:349:HIS:HE1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	356/380 (94%)	346 (97%)	10 (3%)	0	100	100
1	B	341/380 (90%)	330 (97%)	9 (3%)	2 (1%)	21	9
All	All	697/760 (92%)	676 (97%)	19 (3%)	2 (0%)	36	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	119	GLY
1	B	223	GLY

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	305/315 (97%)	303 (99%)	2 (1%)	76	69
1	B	295/315 (94%)	295 (100%)	0	100	100
All	All	600/630 (95%)	598 (100%)	2 (0%)	86	83

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	314	ASP
1	A	365	LEU

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

Mol	Chain	Res	Type
1	A	6	HIS
1	A	152	GLN
1	A	181	GLN
1	A	199	HIS
1	A	315	GLN
1	A	349	HIS
1	B	45	HIS
1	B	126	ASN
1	B	152	GLN
1	B	157	HIS
1	B	181	GLN
1	B	294	GLN
1	B	297	GLN
1	B	303	GLN
1	B	310	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PLP	A	401	1	15,15,16	2.64	9 (60%)	21,22,23	1.45	3 (14%)
2	PLP	B	401	1	15,15,16	2.66	9 (60%)	21,22,23	1.41	3 (14%)

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	401	1	-	0/6/6/8	0/1/1/1
2	PLP	B	401	1	-	0/6/6/8	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	PLP	C2A-C2	4.16	1.57	1.50
2	B	401	PLP	C2-N1	4.12	1.41	1.33
2	A	401	PLP	C2A-C2	4.05	1.56	1.50
2	A	401	PLP	C2-N1	3.95	1.40	1.33
2	A	401	PLP	C5-C4	3.88	1.44	1.40
2	B	401	PLP	C4A-C4	3.76	1.59	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PLP	C4A-C4	3.68	1.59	1.51
2	B	401	PLP	C5-C4	3.64	1.44	1.40
2	B	401	PLP	C6-N1	3.27	1.41	1.34
2	A	401	PLP	C5A-C5	3.11	1.59	1.50
2	B	401	PLP	C5A-C5	3.09	1.59	1.50
2	A	401	PLP	C6-N1	3.09	1.40	1.34
2	A	401	PLP	C3-C4	2.98	1.45	1.40
2	B	401	PLP	C3-C4	2.41	1.44	1.40
2	B	401	PLP	C3-C2	2.21	1.43	1.41
2	A	401	PLP	P-O4P	2.11	1.67	1.60
2	A	401	PLP	C3-C2	2.07	1.43	1.41
2	B	401	PLP	P-O4P	2.06	1.66	1.60

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PLP	O2P-P-O4P	3.33	115.34	106.67
2	B	401	PLP	O4P-C5A-C5	-3.29	103.18	109.36
2	A	401	PLP	O4P-C5A-C5	-3.28	103.21	109.36
2	B	401	PLP	O2P-P-O4P	3.24	115.11	106.67
2	A	401	PLP	C5A-C5-C6	-2.27	115.66	119.36
2	B	401	PLP	C5A-C5-C6	-2.03	116.05	119.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PLP	1	0

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, 95th 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	352/380 (92%)	0.30	23 (6%) 25 27	5, 13, 26, 36	0
1	B	337/380 (88%)	0.26	12 (3%) 46 50	7, 14, 26, 31	0
All	All	689/760 (90%)	0.28	35 (5%) 33 37	5, 14, 26, 36	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	GLY	8.4
1	A	118	LEU	4.6
1	A	370	VAL	4.1
1	B	306	ARG	3.3
1	A	120	LYS	3.3
1	B	7	ARG	3.2
1	A	168	ALA	3.0
1	B	370	VAL	2.9
1	A	90	VAL	2.8
1	A	240	ASP	2.7
1	A	180	ARG	2.7
1	B	239	ILE	2.7
1	A	121	GLU	2.6
1	A	157	HIS	2.6
1	B	257	LYS	2.6
1	A	56	GLU	2.6
1	A	193	ILE	2.5
1	A	241	LYS	2.5
1	A	117	ILE	2.4
1	B	309	GLY	2.4
1	B	307	GLN	2.3
1	B	310	GLN	2.3
1	B	121	GLU	2.3
1	A	93	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	348	LYS	2.3
1	B	187	GLU	2.3
1	A	135	ARG	2.2
1	A	109	ASP	2.2
1	A	179	GLN	2.2
1	A	2	LEU	2.1
1	B	240	ASP	2.1
1	A	153	GLU	2.1
1	A	139	ARG	2.1
1	A	108	LEU	2.1
1	A	122	LYS	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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	PLP	A	401	15/16	0.95	0.11	10,23,26,26	0
2	PLP	B	401	15/16	0.95	0.09	10,16,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.