



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:53 am BST

PDB ID : 6JIF
Title : Crystal Structures of Branched-Chain Aminotransferase from *Pseudomonas* sp. UW4
Authors : Zheng, X.; Guo, L.; Li, D.F.; Wu, B.
Deposited on : 2019-02-21
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

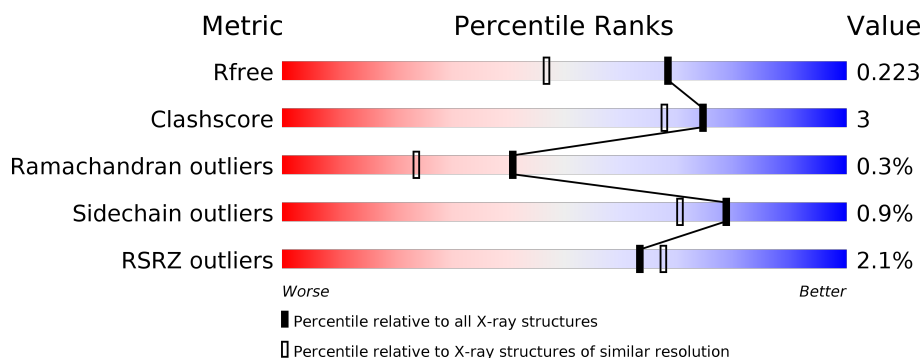
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 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 $\leq 5\%$. 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	359	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 85%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 85% 6% • 7% </div> </div>
1	B	359	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 1%, green 87%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 87% 6% 7% </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5987 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 Branched-chain-amino-acid aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2575	1644	439	480	12			
1	B	334	Total	C	N	O	S	0	0	0
			2583	1650	440	481	12			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP K9NJ94
A	-17	GLY	-	expression tag	UNP K9NJ94
A	-16	SER	-	expression tag	UNP K9NJ94
A	-15	SER	-	expression tag	UNP K9NJ94
A	-14	HIS	-	expression tag	UNP K9NJ94
A	-13	HIS	-	expression tag	UNP K9NJ94
A	-12	HIS	-	expression tag	UNP K9NJ94
A	-11	HIS	-	expression tag	UNP K9NJ94
A	-10	HIS	-	expression tag	UNP K9NJ94
A	-9	HIS	-	expression tag	UNP K9NJ94
A	-8	SER	-	expression tag	UNP K9NJ94
A	-7	SER	-	expression tag	UNP K9NJ94
A	-6	GLY	-	expression tag	UNP K9NJ94
A	-5	LEU	-	expression tag	UNP K9NJ94
A	-4	VAL	-	expression tag	UNP K9NJ94
A	-3	PRO	-	expression tag	UNP K9NJ94
A	-2	ARG	-	expression tag	UNP K9NJ94
A	-1	GLY	-	expression tag	UNP K9NJ94
A	0	SER	-	expression tag	UNP K9NJ94
A	1	HIS	-	expression tag	UNP K9NJ94
B	-18	MET	-	initiating methionine	UNP K9NJ94
B	-17	GLY	-	expression tag	UNP K9NJ94
B	-16	SER	-	expression tag	UNP K9NJ94
B	-15	SER	-	expression tag	UNP K9NJ94
B	-14	HIS	-	expression tag	UNP K9NJ94

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP K9NJ94
B	-12	HIS	-	expression tag	UNP K9NJ94
B	-11	HIS	-	expression tag	UNP K9NJ94
B	-10	HIS	-	expression tag	UNP K9NJ94
B	-9	HIS	-	expression tag	UNP K9NJ94
B	-8	SER	-	expression tag	UNP K9NJ94
B	-7	SER	-	expression tag	UNP K9NJ94
B	-6	GLY	-	expression tag	UNP K9NJ94
B	-5	LEU	-	expression tag	UNP K9NJ94
B	-4	VAL	-	expression tag	UNP K9NJ94
B	-3	PRO	-	expression tag	UNP K9NJ94
B	-2	ARG	-	expression tag	UNP K9NJ94
B	-1	GLY	-	expression tag	UNP K9NJ94
B	0	SER	-	expression tag	UNP K9NJ94
B	1	HIS	-	expression tag	UNP K9NJ94

- PLP
-
- The diagram shows the chemical structure of PLP (Pyridoxal phosphate). The central pyridine ring is labeled with N1 for the nitrogen atom. The ring carbons are labeled C2, C3, C4, C5, and C6. A hydroxyl group (OH) is attached to C3, with the oxygen labeled O3. A hydroxymethyl group (CH2OH) is attached to C5, with the ring carbon labeled C5A and the hydroxyl oxygen labeled O4P. An aldehyde group (CHO) is attached to C4, with the carbonyl carbon labeled C4A and the oxygen labeled O4A. A phosphate group is attached to the hydroxymethyl group, with the phosphorus atom labeled P. The phosphate group consists of the phosphorus atom bonded to four oxygen atoms: one double-bonded to O1P, one single-bonded to O2P, one single-bonded to O3P, and one single-bonded to the hydroxymethyl group's oxygen (O4P).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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

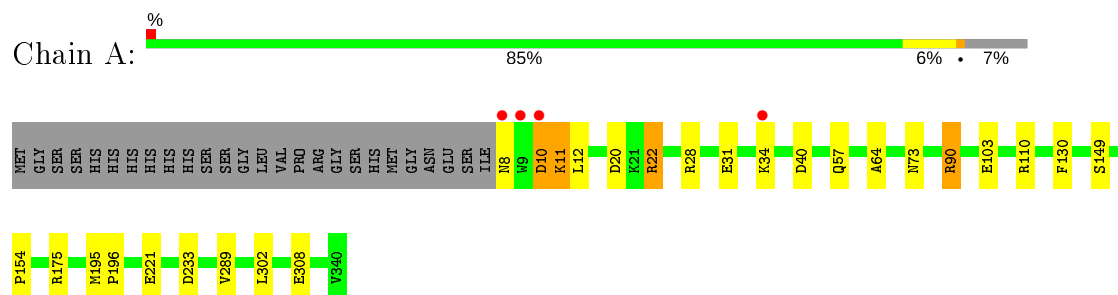
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	381	Total 381	O 381	0	0
3	B	418	Total 418	O 418	0	0

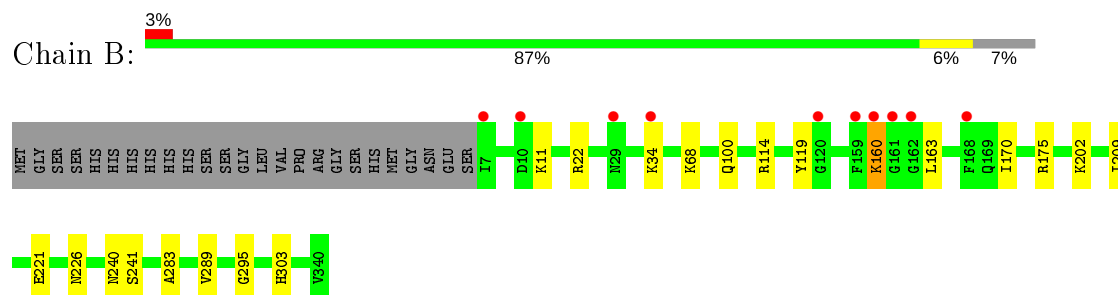
3 Residue-property plots [i](#)

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: Branched-chain-amino-acid aminotransferase



- Molecule 1: Branched-chain-amino-acid aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.83Å 95.72Å 109.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.86 – 1.70 47.86 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.86-1.70) 99.9 (47.86-1.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.182 , 0.223 0.182 , 0.223	Depositor DCC
R_{free} test set	2000 reflections (2.39%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5987	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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	0.67	0/2638	0.77	4/3574 (0.1%)
1	B	0.71	0/2646	0.80	4/3585 (0.1%)
All	All	0.69	0/5284	0.79	8/7159 (0.1%)

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	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	114	ARG	NE-CZ-NH1	-7.74	116.43	120.30
1	A	90	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	34	LYS	CA-CB-CG	-6.78	98.49	113.40
1	A	10	ASP	CB-CG-OD2	-6.63	112.34	118.30
1	A	233	ASP	CB-CG-OD2	5.67	123.41	118.30
1	B	160	LYS	CD-CE-NZ	5.61	124.60	111.70
1	B	163	LEU	CB-CG-CD1	-5.30	102.00	111.00
1	B	163	LEU	CA-CB-CG	5.29	127.47	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	ASP	Sidechain

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	2575	0	2527	20	0
1	B	2583	0	2538	12	0
2	A	15	0	6	2	0
2	B	15	0	7	0	0
3	A	381	0	0	11	4
3	B	418	0	0	7	3
All	All	5987	0	5078	33	4

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 3.

All (33) 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:11:LYS:NZ	3:A:504:HOH:O	2.09	0.84
1:A:40:ASP:OD2	3:A:501:HOH:O	1.98	0.80
1:A:103:GLU:OE1	3:A:503:HOH:O	2.06	0.74
1:B:119:TYR:O	3:B:503:HOH:O	2.15	0.64
1:A:20:ASP:OD2	3:A:505:HOH:O	2.15	0.63
1:A:110:ARG:NH1	3:A:508:HOH:O	2.22	0.61
1:B:11:LYS:HA	1:B:160:LYS:HE2	1.85	0.59
1:B:202:LYS:HE2	3:B:622:HOH:O	2.02	0.58
1:B:202:LYS:HG2	3:B:622:HOH:O	2.03	0.58
1:A:31:GLU:OE1	3:A:506:HOH:O	2.18	0.56
1:A:12:LEU:HD21	1:A:154:PRO:HB2	1.91	0.53
1:A:175:ARG:HD3	1:A:221:GLU:HG3	1.92	0.51
1:A:28:ARG:NH1	3:A:509:HOH:O	2.24	0.50
1:B:240:ASN:ND2	3:B:502:HOH:O	2.11	0.50
1:B:175:ARG:HD3	1:B:221:GLU:HG3	1.94	0.50
1:B:100:GLN:NE2	3:B:501:HOH:O	2.03	0.50
1:B:226:ASN:O	1:B:283:ALA:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:PLP:H2A1	3:A:559:HOH:O	2.14	0.47
1:A:57:GLN:HG3	3:B:695:HOH:O	2.15	0.46
1:A:90:ARG:NE	3:A:502:HOH:O	2.01	0.46
1:A:195:MET:HB3	1:A:196:PRO:HD3	1.97	0.46
1:B:68:LYS:NZ	3:B:505:HOH:O	2.27	0.45
1:A:31:GLU:CD	3:A:506:HOH:O	2.56	0.44
1:B:170:ILE:HD13	1:B:209:ILE:HB	2.00	0.44
1:A:22:ARG:HD3	1:A:40:ASP:O	2.18	0.43
1:A:8:ASN:N	3:A:525:HOH:O	2.52	0.43
1:A:130:PHE:CE1	1:A:149:SER:HB3	2.54	0.42
1:A:64:ALA:HA	1:A:73:ASN:O	2.19	0.42
1:B:68:LYS:HD3	1:B:119:TYR:CE2	2.53	0.42
1:A:221:GLU:OE1	2:A:401:PLP:N1	2.52	0.42
1:B:295:GLY:HA2	1:B:303:HIS:O	2.20	0.41
1:A:302:LEU:HD21	1:A:308:GLU:OE2	2.21	0.40
1:A:130:PHE:CZ	1:A:149:SER:HB3	2.56	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:794:HOH:O	3:B:793:HOH:O[2_665]	1.93	0.27
3:A:798:HOH:O	3:B:514:HOH:O[1_455]	1.97	0.23
3:A:798:HOH:O	3:B:873:HOH:O[1_455]	2.10	0.10
3:A:518:HOH:O	3:A:777:HOH:O[3_646]	2.15	0.05

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	331/359 (92%)	320 (97%)	10 (3%)	1 (0%)	41 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	332/359 (92%)	325 (98%)	6 (2%)	1 (0%)	41	24
All	All	663/718 (92%)	645 (97%)	16 (2%)	2 (0%)	41	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	289	VAL
1	A	289	VAL

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	271/293 (92%)	269 (99%)	2 (1%)	84	77
1	B	272/293 (93%)	269 (99%)	3 (1%)	73	63
All	All	543/586 (93%)	538 (99%)	5 (1%)	78	70

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	22	ARG
1	B	22	ARG
1	B	34	LYS
1	B	241	SER

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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	1.30	2 (13%)	20,22,23	1.40	3 (15%)
2	PLP	B	401	1	15,15,16	0.78	0	20,22,23	1.35	2 (10%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PLP	C3-C2	-3.08	1.37	1.40
2	A	401	PLP	C2-N1	2.20	1.38	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PLP	O4P-C5A-C5	3.55	116.11	109.35
2	B	401	PLP	C6-C5-C4	3.07	120.57	118.16
2	B	401	PLP	C5A-C5-C6	-2.69	114.95	119.37
2	A	401	PLP	C5A-C5-C6	-2.08	115.95	119.37
2	A	401	PLP	C4A-C4-C5	2.07	123.06	120.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PLP	2	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 [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, 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	333/359 (92%)	0.04	4 (1%) 79 82	14, 23, 41, 69	0
1	B	334/359 (93%)	0.10	10 (2%) 50 54	13, 19, 38, 60	0
All	All	667/718 (92%)	0.07	14 (2%) 63 67	13, 21, 40, 69	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	161	GLY	4.8
1	A	10	ASP	3.8
1	B	120	GLY	2.9
1	B	160	LYS	2.7
1	A	9	TRP	2.4
1	B	159	PHE	2.2
1	B	168	PHE	2.2
1	B	7	ILE	2.2
1	B	162	GLY	2.1
1	A	34	LYS	2.1
1	B	10	ASP	2.1
1	B	34	LYS	2.0
1	A	8	ASN	2.0
1	B	29	ASN	2.0

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 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, 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(Å ²)	Q<0.9
2	PLP	B	401	15/16	0.96	0.11	15,21,26,27	0
2	PLP	A	401	15/16	0.97	0.09	17,20,26,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.