



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 03:13 pm GMT

PDB ID : 2HG8
Title : Crystal Structure of Cys315Ala mutant of human mitochondrial branched chain aminotransferase complexed with its substrate mimic, N-methyl leucine.
Authors : Yennawar, N.H.; Hutson, S.M.
Deposited on : 2006-06-26
Resolution : 1.80 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

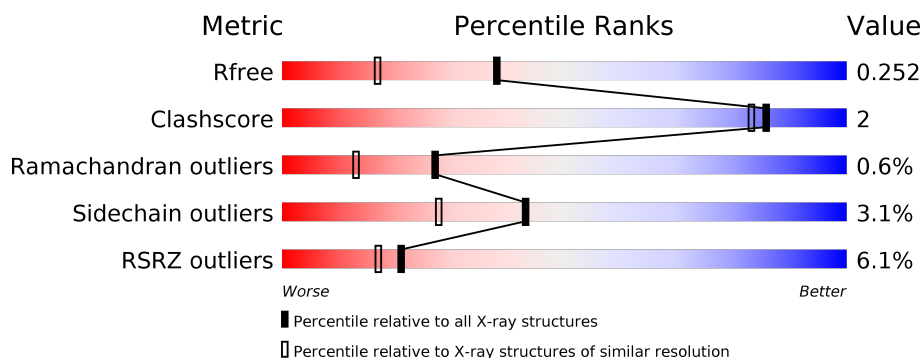
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	111664	5253 (1.80-1.80)
Clashscore	122126	6077 (1.80-1.80)
Ramachandran outliers	120053	6011 (1.80-1.80)
Sidechain outliers	120020	6010 (1.80-1.80)
RSRZ outliers	108989	5157 (1.80-1.80)

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 $\leq 5\%$. 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	365	<div> <div>6%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>••</div> </div> </div>
1	B	365	<div> <div>6%</div> <div> <div></div> <div>93%</div> <div>7%</div> <div>•</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6131 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.

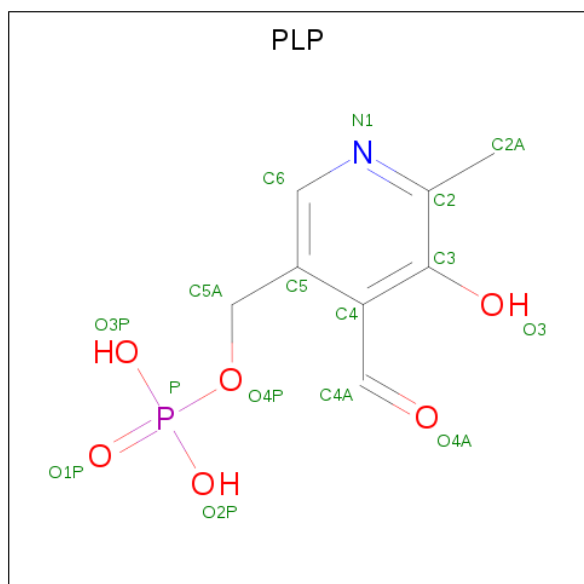
- Molecule 1 is a protein called Branched-chain-amino-acid aminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	1	0	1
			2846	1833	498	498	17			
1	B	363	Total	C	N	O	S	0	0	0
			2894	1866	504	507	17			

There are 4 discrepancies between the modelled and reference sequences:

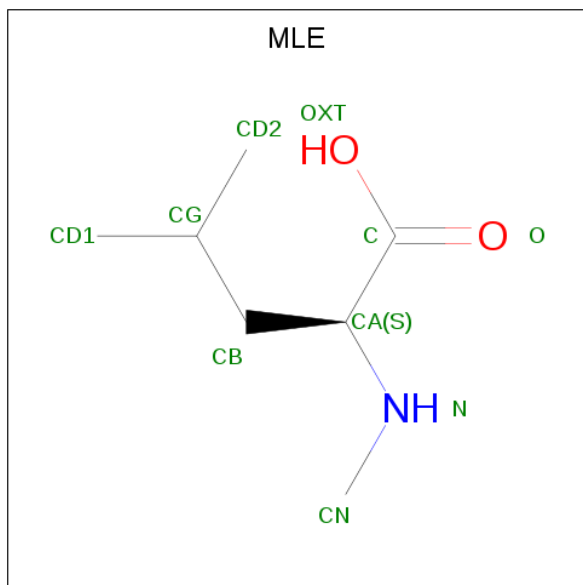
Chain	Residue	Modelled	Actual	Comment	Reference
A	159	ARG	THR	CONFLICT	UNP O15382
A	315	ALA	CYS	ENGINEERED	UNP O15382
B	659	ARG	THR	CONFLICT	UNP O15382
B	815	ALA	CYS	ENGINEERED	UNP O15382

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: 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 N-METHYLLEUCINE (three-letter code: MLE) (formula: $C_7H_{15}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	7	1	2		
3	A	1	Total	C	N	O	0	0
			10	7	1	2		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

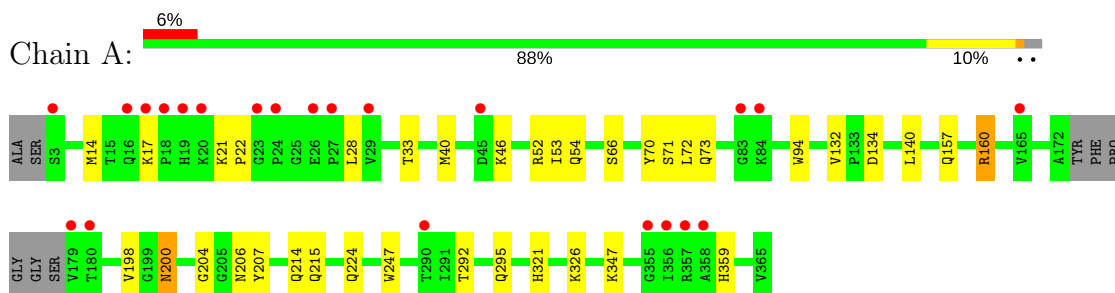
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	152	Total	O	0	0
			152	152		
5	B	185	Total	O	0	0
			185	185		

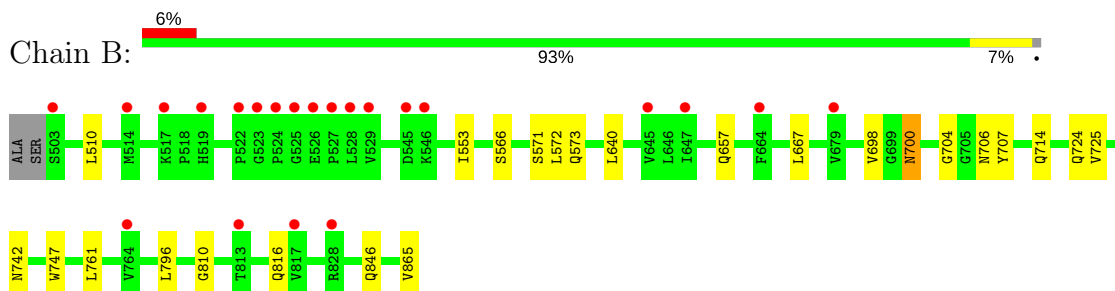
3 Residue-property plots [i](#)

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, mitochondrial



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.18Å 109.28Å 59.45Å 90.00° 97.23° 90.00°	Depositor
Resolution (Å)	25.00 – 1.80 29.49 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.5 (25.00-1.80) 92.0 (29.49-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 1.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.282 0.247 , 0.252	Depositor DCC
R_{free} test set	3293 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6131	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 4.64% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, MLE, 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	0.62	0/2919	0.73	1/3961 (0.0%)
1	B	0.63	0/2971	0.73	0/4033
All	All	0.62	0/5890	0.73	1/7994 (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	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	53	ILE	N-CA-C	-5.03	97.42	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	TYR	Sidechain
1	A	70	TYR	Sidechain
1	B	707	TYR	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	2846	0	2872	17	0
1	B	2894	0	2914	16	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
3	A	20	0	28	0	0
4	A	4	0	3	0	0
5	A	152	0	0	1	0
5	B	185	0	0	2	0
All	All	6131	0	5829	28	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 (28) 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:200:ASN:HD22	1:A:200:ASN:H	1.16	0.89
1:B:700:ASN:HD22	1:B:700:ASN:H	1.26	0.81
1:A:215:GLN:HE22	1:B:657:GLN:NE2	1.81	0.79
1:A:292:THR:H	1:A:295:GLN:HE21	1.45	0.63
1:A:73:GLN:HE22	1:B:571:SER:H	1.46	0.61
1:A:200:ASN:ND2	1:A:200:ASN:H	1.95	0.59
1:A:215:GLN:HE22	1:B:657:GLN:HE21	1.52	0.58
1:A:66:SER:HB2	1:A:72:LEU:HD12	1.86	0.57
1:A:71:SER:H	1:B:573:GLN:HE22	1.52	0.55
1:B:714:GLN:HE22	1:B:724:GLN:HA	1.70	0.55
1:B:698:VAL:HG23	1:B:706:ASN:HD21	1.73	0.53
1:B:640:LEU:HD21	1:B:667:LEU:HD13	1.92	0.52
1:A:200:ASN:N	1:A:200:ASN:HD22	1.96	0.50
1:A:73:GLN:HE21	1:A:204:GLY:HA3	1.76	0.50
1:A:52:ARG:HE	1:A:54:GLN:NE2	2.10	0.49
1:B:700:ASN:ND2	1:B:700:ASN:H	2.01	0.49
1:A:214:GLN:HE22	1:A:224:GLN:HA	1.78	0.48
1:B:573:GLN:HE21	1:B:704:GLY:HA3	1.80	0.47
1:B:725:VAL:HG12	5:B:72:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLN:NE2	1:B:571:SER:H	2.13	0.45
1:A:198:VAL:HG23	1:A:206:ASN:HD21	1.81	0.45
1:A:160:ARG:NH1	5:A:2521:HOH:O	2.46	0.44
1:B:714:GLN:NE2	5:B:72:HOH:O	2.52	0.43
1:A:132:VAL:HG22	1:A:140:LEU:HD22	1.99	0.42
1:B:566:SER:HB2	1:B:572:LEU:HD12	2.01	0.42
1:B:510:LEU:HD11	1:B:553:ILE:HG13	2.01	0.42
1:A:22:PRO:HG2	1:A:33:THR:HG21	2.03	0.41
1:B:742:ASN:O	1:B:810:GLY:HA2	2.21	0.41

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	353/365 (97%)	334 (95%)	16 (4%)	3 (1%)	21	8
1	B	361/365 (99%)	351 (97%)	9 (2%)	1 (0%)	43	28
All	All	714/730 (98%)	685 (96%)	25 (4%)	4 (1%)	27	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	MET
1	A	28	LEU
1	B	816	GLN
1	A	17	LYS

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	309/315 (98%)	296 (96%)	13 (4%)	32	16
1	B	313/315 (99%)	307 (98%)	6 (2%)	60	49
All	All	622/630 (99%)	603 (97%)	19 (3%)	43	28

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	40	MET
1	A	46	LYS
1	A	94	TRP
1	A	134	ASP
1	A	157	GLN
1	A	160	ARG
1	A	200	ASN
1	A	247	TRP
1	A	321	HIS
1	A	326	LYS
1	A	347	LYS
1	A	359	HIS
1	B	700	ASN
1	B	747	TRP
1	B	761	LEU
1	B	796	LEU
1	B	846	GLN
1	B	865	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	73	GLN
1	A	96	ASN

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Mol	Chain	Res	Type
1	A	200	ASN
1	A	206	ASN
1	A	214	GLN
1	A	295	GLN
1	A	337	ASN
1	B	550	GLN
1	B	573	GLN
1	B	657	GLN
1	B	700	ASN
1	B	706	ASN
1	B	714	GLN
1	B	724	GLN
1	B	734	GLN
1	B	742	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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
4	ACY	A	1001	-	1,3,3	3.05	1 (100%)	0,3,3	0.00	-
3	MLE	A	1414	-	6,9,9	0.90	0	6,11,11	2.17	3 (50%)
3	MLE	A	2414	-	6,9,9	0.71	0	6,11,11	2.04	3 (50%)
2	PLP	A	400	1	15,15,16	1.41	1 (6%)	20,22,23	1.64	6 (30%)
2	PLP	B	401	1	15,15,16	1.47	1 (6%)	20,22,23	1.66	5 (25%)

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
4	ACY	A	1001	-	-	0/0/0/0	0/0/0/0
3	MLE	A	1414	-	-	0/6/10/10	0/0/0/0
3	MLE	A	2414	-	-	0/6/10/10	0/0/0/0
2	PLP	A	400	1	-	0/6/6/8	0/1/1/1
2	PLP	B	401	1	-	0/6/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	PLP	C4A-C4	2.94	1.57	1.51
2	A	400	PLP	C4A-C4	2.95	1.57	1.51
4	A	1001	ACY	CH3-C	3.05	1.52	1.48

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1414	MLE	CB-CA-N	-3.52	103.67	110.67
3	A	2414	MLE	CB-CA-N	-2.86	104.97	110.67
2	B	401	PLP	O2P-P-O4P	-2.77	99.36	106.73
2	A	400	PLP	O2P-P-O4P	-2.28	100.66	106.73
2	B	401	PLP	C5A-C5-C6	-2.27	115.53	119.34
2	A	400	PLP	C5A-C5-C6	-2.11	115.80	119.34
2	B	401	PLP	O4P-P-O1P	2.12	112.41	106.47
2	A	400	PLP	C4A-C4-C5	2.24	123.11	120.85
2	A	400	PLP	C6-C5-C4	2.31	120.06	118.19
3	A	1414	MLE	CN-N-CA	2.36	121.31	113.60
3	A	2414	MLE	CN-N-CA	2.39	121.38	113.60
2	A	400	PLP	O3P-P-O1P	2.44	120.12	110.60
2	B	401	PLP	O3P-P-O1P	2.57	120.63	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1414	MLE	CG-CB-CA	3.10	122.69	114.78
3	A	2414	MLE	CG-CB-CA	3.27	123.13	114.78
2	B	401	PLP	O4P-C5A-C5	3.37	115.88	109.39
2	A	400	PLP	O4P-C5A-C5	3.39	115.92	109.39

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, 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	357/365 (97%)	0.49	22 (6%)	20 16	13, 26, 42, 49	2 (0%)
1	B	363/365 (99%)	0.41	22 (6%)	21 17	10, 22, 37, 47	5 (1%)
All	All	720/730 (98%)	0.45	44 (6%)	21 17	10, 24, 40, 49	7 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	356	ILE	8.7
1	B	817	VAL	8.1
1	B	813	THR	7.4
1	A	179	VAL	7.0
1	B	524	PRO	6.7
1	B	525	GLY	6.3
1	A	23	GLY	6.2
1	B	523	GLY	6.1
1	B	764	VAL	5.4
1	A	17	LYS	5.2
1	B	679	VAL	4.8
1	B	528	LEU	4.7
1	A	27	PRO	4.6
1	B	526	GLU	4.4
1	A	355	GLY	4.4
1	A	24	PRO	4.3
1	B	503	SER	4.2
1	A	180	THR	3.7
1	A	358	ALA	3.3
1	A	18	PRO	3.3
1	A	19	HIS	3.2
1	A	357	ARG	3.2
1	B	514	MET	3.2
1	A	290	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	519	HIS	3.0
1	A	45	ASP	2.9
1	A	16	GLN	2.9
1	A	84	LYS	2.9
1	B	527	PRO	2.9
1	A	3	SER	2.8
1	B	545	ASP	2.6
1	B	517	LYS	2.5
1	A	29	VAL	2.5
1	B	529	VAL	2.4
1	A	26	GLU	2.4
1	A	20	LYS	2.4
1	A	83	GLY	2.3
1	B	645	VAL	2.2
1	B	522	PRO	2.1
1	B	546	LYS	2.1
1	A	165	VAL	2.1
1	B	647	ILE	2.1
1	B	664	PHE	2.0
1	B	828	ARG	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(\AA^2)	Q<0.9
4	ACY	A	1001	4/4	0.54	0.31	41,42,42,43	0
3	MLE	A	1414	10/10	0.77	0.20	36,39,40,41	0
3	MLE	A	2414	10/10	0.85	0.17	26,30,31,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PLP	B	401	15/16	0.96	0.13	15,18,21,21	0
2	PLP	A	400	15/16	0.97	0.13	18,20,25,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.