WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 04:07 AM GMT

PDB ID : 2HGX

Title : Crystal structure of Cys315Ala mutant of human mitochondrial branched chain aminotransferase

Authors : Yennawar, N.H.; Hutson, S.M.

Deposited on : 2006-06-27

Resolution : 1.80 Å(reported)

---

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.209
Clashscore		2
Ramachandran outliers		0.4%
Sidechain outliers		1.4%
RSRZ outliers		5.6%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
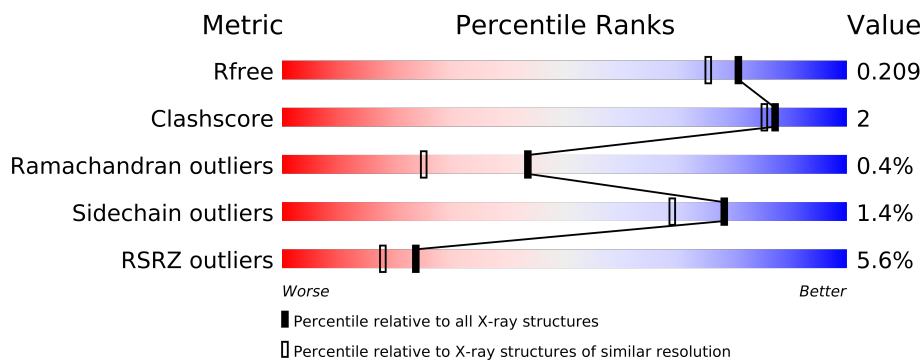
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	365	
1	B	365	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	EPE	B	1004	-	X
4	ACY	A	1001	-	X
4	ACY	B	1002	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 6203 atoms, of which 0 are hydrogen and 0 are deuterium.

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-acidaminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total 2853	C 1837	N 499	O 500	S 17	0	1	1
1	B	363	Total 2930	C 1890	N 509	O 513	S 18	0	5	0

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: $C_8H_{10}NO_6P$).
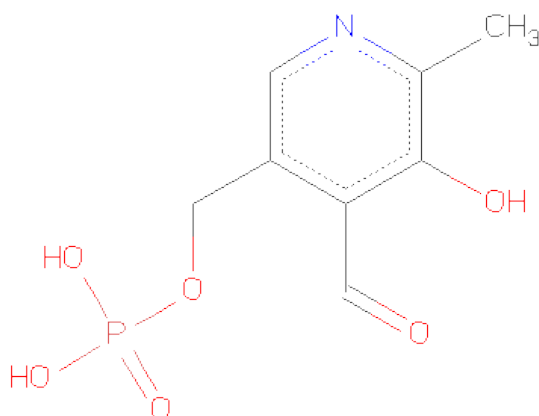
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 15	C 8	N 1	O 5	P 1	0	0
2	B	1	Total 15	C 8	N 1	O 5	P 1	0	0

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).
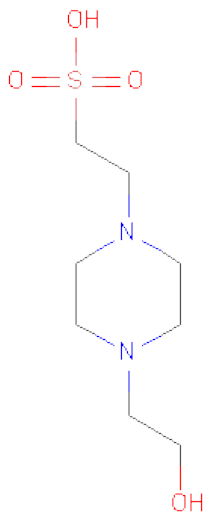
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 15	C 8	N 2	O 4	S 1	0	0

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).
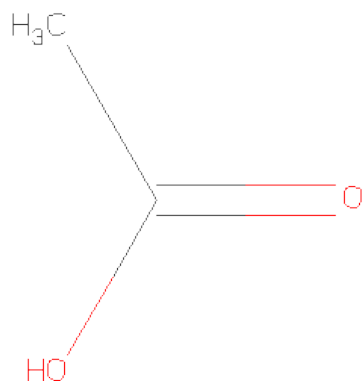
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	163	Total 163	O 163	0	0
5	B	200	Total 200	O 200	0	0

3 Residue-property plots ⓘ

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: Branched-chain-amino-acidaminotransferase, mitochondrial
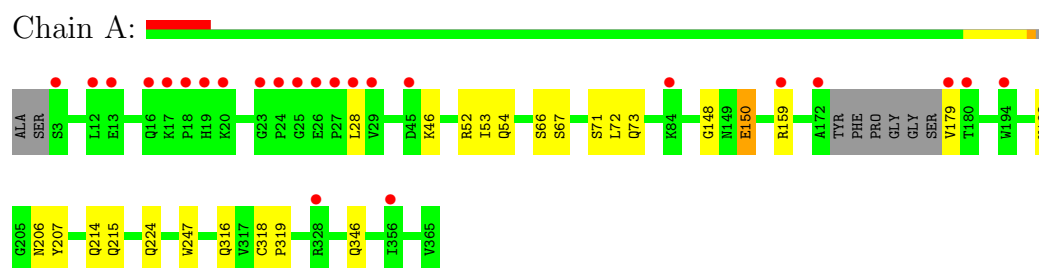
Chain A:

- Molecule 1: Branched-chain-amino-acidaminotransferase, mitochondrial

Chain B:
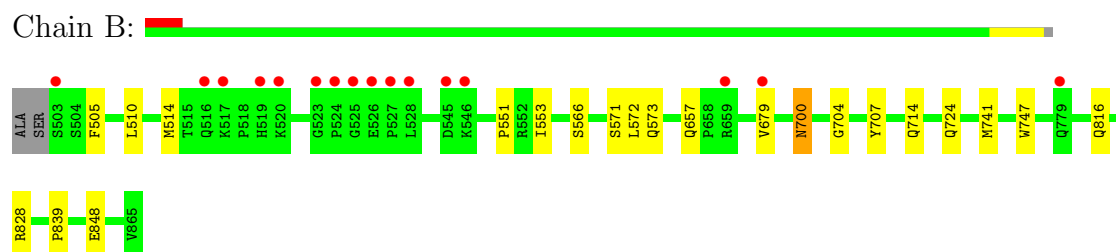
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.74Å　　109.90Å　　59.59Å 90.00°　　96.51°　　90.00°	Depositor
Resolution (Å)	25.00　–　1.80 29.18　–　1.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (25.00-1.80) 99.4 (29.18-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.90 (at 1.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.208　,　0.231 0.209　,　0.209	Depositor DCC
R_{free} test set	3470 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	17.2	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 31.1	EDS
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
L-test for twinning	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 69848 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6203	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, EPE, 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	0.61	0/2926	0.73	1/3971 (0.0%)
1	B	0.62	0/3007	0.72	0/4083
All	All	0.62	0/5933	0.72	1/8054 (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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	ILE	N-CA-C	-5.22	96.91	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	TYR	Sidechain
1	B	707	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2853	0	2877	17	0
1	B	2930	0	2952	16	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
3	B	15	0	17	1	0
4	A	4	0	3	0	0
4	B	8	0	6	0	0
5	A	163	0	0	0	0
5	B	200	0	0	2	0
All	All	6203	0	5867	29	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (29) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:200:ASN:HD22	1:A:200:ASN:H	1.15	0.88
1:B:700:ASN:HD22	1:B:700:ASN:H	1.20	0.87
1:A:150:GLU:HG3	1:A:159:ARG:H	1.58	0.68
1:A:215:GLN:HE22	1:B:657:GLN:NE2	1.98	0.61
1:A:73:GLN:HE22	1:B:571:SER:H	1.48	0.59
1:A:200:ASN:ND2	1:A:200:ASN:H	1.95	0.58
1:A:71:SER:H	1:B:573:GLN:HE22	1.52	0.55
1:A:214:GLN:HE22	1:A:224:GLN:HA	1.73	0.53
1:B:714:GLN:HE22	1:B:724:GLN:HA	1.74	0.53
1:A:179:VAL:HG11	1:A:346:GLN:HE22	1.75	0.51
1:B:700:ASN:ND2	1:B:700:ASN:H	1.99	0.51
1:B:573:GLN:HE21	1:B:704:GLY:HA3	1.77	0.49
1:B:566:SER:HB2	1:B:572:LEU:HD12	1.96	0.48
1:A:66:SER:HB2	1:A:72:LEU:HD12	1.97	0.47
1:A:73:GLN:HE21	1:A:204:GLY:HA3	1.79	0.47
1:A:198:VAL:HG23	1:A:206:ASN:HD21	1.80	0.47
1:A:52:ARG:HE	1:A:54:GLN:NE2	2.11	0.46
1:B:700:ASN:HD22	1:B:700:ASN:N	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:200:ASN:N	1:A:200:ASN:HD22	1.94	0.46
1:A:179:VAL:HG11	1:A:346:GLN:NE2	2.32	0.45
1:B:679[B]:VAL:HG22	5:B:272:HOH:O	2.17	0.44
1:A:73:GLN:NE2	1:B:571:SER:H	2.14	0.43
1:B:848:GLU:OE1	3:B:1004:EPE:H81	2.18	0.43
1:B:505:PHE:HB2	1:B:551:PRO:HD3	2.01	0.43
1:B:714:GLN:NE2	5:B:16:HOH:O	2.51	0.42
1:A:67:SER:HB3	1:A:148:GLY:O	2.19	0.42
1:B:724:GLN:HE22	1:B:741:MET:CE	2.33	0.42
1:A:318:CYS:HA	1:A:319:PRO:HD3	1.94	0.41
1:B:510:LEU:HD11	1:B:553:ILE:HG13	2.03	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	354/365 (97%)	341 (96%)	12 (3%)	1 (0%)	50	31
1	B	366/365 (100%)	357 (98%)	7 (2%)	2 (0%)	38	19
All	All	720/730 (99%)	698 (97%)	19 (3%)	3 (0%)	43	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	GLN
1	B	816	GLN
1	B	839	PRO

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	310/315 (98%)	305 (98%)	5 (2%)	75	63
1	B	318/315 (101%)	313 (98%)	5 (2%)	75	63
All	All	628/630 (100%)	618 (98%)	10 (2%)	78	63

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	46	LYS
1	A	150	GLU
1	A	200	ASN
1	A	247	TRP
1	B	514[A]	MET
1	B	514[B]	MET
1	B	700	ASN
1	B	747	TRP
1	B	828	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	73	GLN
1	A	96	ASN
1	A	200	ASN
1	A	206	ASN
1	A	214	GLN
1	A	242	ASN
1	A	249	HIS
1	A	295	GLN
1	A	346	GLN
1	B	516	GLN
1	B	573	GLN
1	B	586	GLN
1	B	657	GLN
1	B	700	ASN
1	B	706	ASN
1	B	714	GLN
1	B	715	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	724	GLN
1	B	734	GLN
1	B	742	ASN

5.3.3　RNA ⓘ

There are no RNA chains in this entry.

5.4　Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5　Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6　Ligand geometry ⓘ

6 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	-	3,3,3	1.03	0	3,3,3	1.50	1 (33%)
2	PLP	A	400	1	14,15,16	1.30	2 (14%)	20,22,23	1.60	4 (20%)
4	ACY	B	1002	-	3,3,3	1.06	0	3,3,3	1.46	0
4	ACY	B	1003	-	3,3,3	1.08	0	3,3,3	1.45	0
3	EPE	B	1004	-	15,15,15	1.40	4 (26%)	20,20,20	0.95	1 (5%)
2	PLP	B	401	1	14,15,16	1.34	2 (14%)	20,22,23	1.61	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
2	PLP	A	400	1	-	0/6/6/8	0/1/1/1
4	ACY	B	1002	-	-	0/0/0/0	0/0/0/0
4	ACY	B	1003	-	-	0/0/0/0	0/0/0/0
3	EPE	B	1004	-	-	0/9/19/19	0/1/1/1
2	PLP	B	401	1	-	0/6/6/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1004	EPE	C10-S	2.49	1.81	1.77
3	B	1004	EPE	C6-N1	2.43	1.53	1.47
3	B	1004	EPE	C9-N1	2.31	1.52	1.47
2	B	401	PLP	P-O1P	-2.24	1.43	1.51
2	B	401	PLP	C4-C5	2.24	1.43	1.39
2	A	400	PLP	P-O1P	-2.23	1.43	1.51
3	B	1004	EPE	C2-N1	2.19	1.53	1.47
2	A	400	PLP	C4-C5	2.06	1.42	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	400	PLP	O4P-C5A-C5	3.64	116.66	109.26
2	B	401	PLP	O4P-C5A-C5	3.36	116.10	109.26
2	B	401	PLP	O3P-P-O1P	3.02	120.30	110.44
2	A	400	PLP	O3P-P-O1P	2.90	119.92	110.44
2	B	401	PLP	O2P-P-O4P	-2.40	100.02	106.65
3	B	1004	EPE	C7-N4-C5	-2.38	105.17	111.32
2	A	400	PLP	O2P-P-O4P	-2.34	100.18	106.65
2	B	401	PLP	C3-C4-C5	-2.15	117.22	121.29
2	A	400	PLP	C3-C4-C5	-2.06	117.40	121.29
4	A	1001	ACY	O-C-CH3	-2.04	113.15	122.06
2	B	401	PLP	C5A-C5-C6	-2.02	115.46	119.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.37	24 (6%)	17	12	8, 17, 33, 48	0
1	B	363/365 (99%)	0.27	16 (4%)	33	26	8, 17, 31, 42	0
All	All	720/730 (98%)	0.32	40 (5%)	24	18	8, 17, 32, 48	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	ALA	12.7
1	B	524	PRO	9.3
1	A	25	GLY	9.2
1	A	3	SER	8.4
1	A	26	GLU	7.5
1	A	17	LYS	6.7
1	B	523	GLY	6.3
1	B	525	GLY	5.9
1	A	27	PRO	4.9
1	B	503	SER	4.5
1	B	546	LYS	4.3
1	A	19	HIS	4.3
1	B	526	GLU	4.2
1	A	28	LEU	3.9
1	A	20	LYS	3.8
1	B	527	PRO	3.8
1	A	12	LEU	3.5
1	A	179	VAL	3.5
1	A	84	LYS	3.4
1	A	24	PRO	3.3
1	A	16	GLN	3.3
1	B	545	ASP	3.3
1	B	520	LYS	3.2
1	A	29	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	18	PRO	3.1
1	B	517	LYS	3.0
1	A	194	TRP	3.0
1	A	23	GLY	2.8
1	B	679[A]	VAL	2.8
1	B	519	HIS	2.6
1	B	528	LEU	2.6
1	A	45	ASP	2.6
1	A	13	GLU	2.3
1	A	356	ILE	2.2
1	A	159	ARG	2.2
1	B	516	GLN	2.1
1	A	180	THR	2.1
1	A	328	ARG	2.1
1	B	779	GLN	2.1
1	B	659	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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, 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	RSR	LLDF	B-factors(Å²)	Q<0.9
3	EPE	B	1004	15/15	0.55	18.81	42,44,53,55	0
4	ACY	A	1001	4/4	0.27	7.47	38,39,39,39	0
4	ACY	B	1002	4/4	0.25	3.69	36,36,37,37	0
2	PLP	A	400	15/16	0.12	0.72	11,13,19,19	0
2	PLP	B	401	15/16	0.12	-0.13	10,13,16,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å²)	Q<0.9
4	ACY	B	1003	4/4	0.15	-0.36	37,37,38,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.