



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:59 am BST

PDB ID : 1EKF  
Title : CRYSTALLOGRAPHIC STRUCTURE OF HUMAN BRANCHED CHAIN AMINO ACID AMINOTRANSFERASE (MITOCHONDRIAL) COMPLEXED WITH PYRIDOXAL-5'-PHOSPHATE AT 1.95 ANGSTROMS (ORTHORHOMBIC FORM)  
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Deposited on : 2000-03-08  
Resolution : 1.95 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](mailto: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.

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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

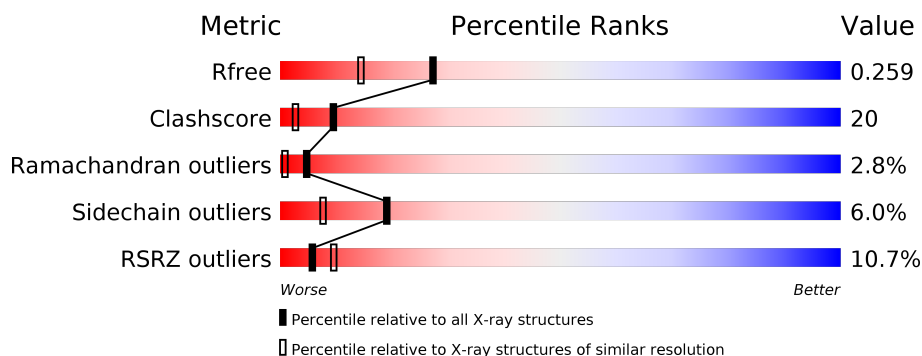
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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  $\geq 3$ , 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	365	<div> <div>11%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>5%</div> </div> </div>
1	B	365	<div> <div>11%</div> <div> <div></div> <div>67%</div> <div>27%</div> <div>5%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6123 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	365	Total	C	N	O	S	0	0	0
			2910	1875	507	510	18			
1	B	365	Total	C	N	O	S	0	0	0
			2910	1875	507	510	18			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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		

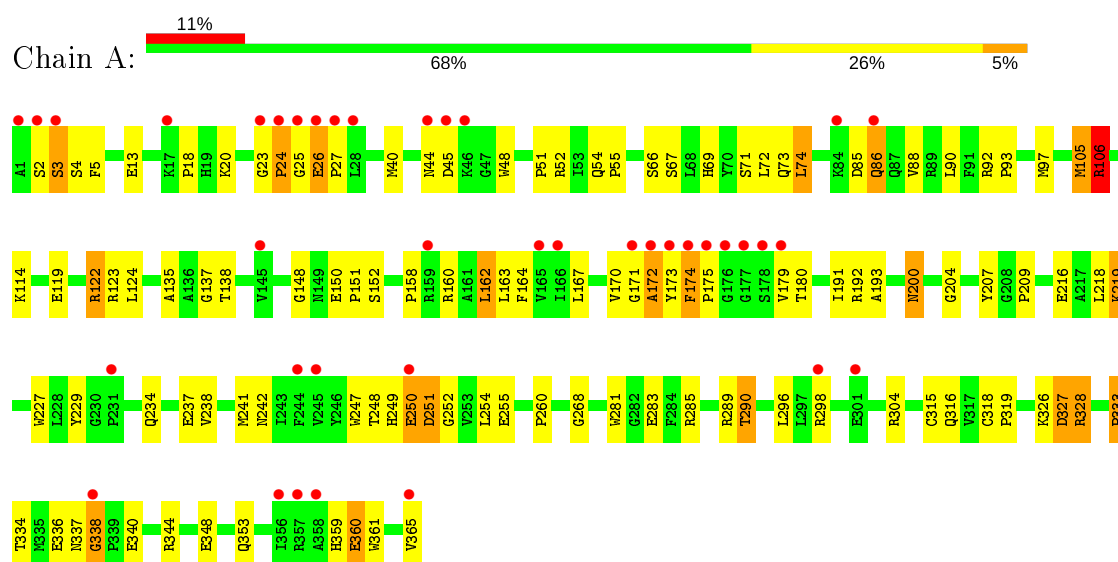
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	143	Total 143	O 143	0	0
3	B	130	Total 130	O 130	0	0

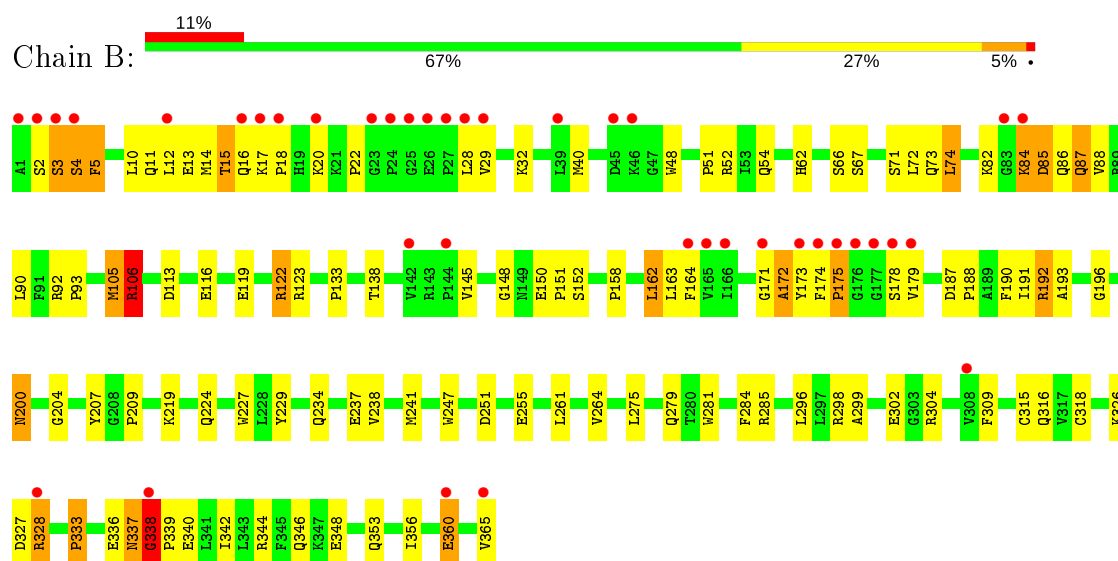
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.39 Å 105.03 Å 107.02 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.29 – 1.95 24.29 – 1.90	Depositor EDS
% Data completeness (in resolution range)	83.8 (24.29-1.95) 88.9 (24.29-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 1.89 Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.222 , 0.260 0.224 , 0.259	Depositor DCC
$R_{free}$ test set	4542 reflections (8.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.1	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6123	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.46	0/2987	0.73	2/4053 (0.0%)
1	B	0.46	0/2987	0.74	5/4053 (0.1%)
All	All	0.46	0/5974	0.74	7/8106 (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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	LEU	CA-CB-CG	7.17	131.79	115.30
1	A	74	LEU	CA-CB-CG	7.03	131.47	115.30
1	B	106	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	338	GLY	N-CA-C	-5.58	99.15	113.10
1	B	337	ASN	N-CA-C	-5.46	96.25	111.00
1	A	106	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	11	GLN	N-CA-C	-5.00	97.49	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	207	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	2910	0	2938	125	0
1	B	2910	0	2938	117	0
2	A	15	0	6	3	0
2	B	15	0	6	1	0
3	A	143	0	0	8	0
3	B	130	0	0	6	0
All	All	6123	0	5888	230	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 20.

All (230) 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:160:ARG:HG3	1:A:160:ARG:HH11	1.25	0.99
1:A:150:GLU:HG3	1:A:158:PRO:HA	1.45	0.98
1:A:122:ARG:HG3	1:A:365:VAL:O	1.66	0.96
1:B:200:ASN:H	1:B:200:ASN:HD22	1.11	0.95
1:A:200:ASN:H	1:A:200:ASN:HD22	1.11	0.94
1:B:122:ARG:HG3	1:B:365:VAL:O	1.67	0.93
1:A:26:GLU:N	1:A:27:PRO:HD3	1.91	0.85
1:A:338:GLY:O	1:A:340:GLU:N	2.12	0.83
1:B:90:LEU:HB3	1:B:93:PRO:HG3	1.61	0.81
1:A:23:GLY:H	1:A:24:PRO:HD3	1.45	0.81
1:A:71:SER:H	1:B:73:GLN:HE22	1.27	0.81
1:A:106:ARG:NH2	1:B:209:PRO:O	2.15	0.80
1:B:3:SER:O	1:B:4:SER:HB2	1.80	0.79
1:B:337:ASN:O	1:B:338:GLY:C	2.19	0.79
1:B:84:LYS:H	1:B:84:LYS:HD3	1.47	0.78
1:B:122:ARG:HB3	1:B:122:ARG:HH11	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HB3	1:A:93:PRO:HG3	1.66	0.78
1:A:219:LYS:HB2	1:A:219:LYS:NZ	1.97	0.77
1:A:85:ASP:O	1:A:86:GLN:HB3	1.82	0.77
1:A:337:ASN:O	1:A:338:GLY:C	2.23	0.77
1:A:122:ARG:HH11	1:A:122:ARG:HB3	1.50	0.75
1:A:160:ARG:HG3	1:A:160:ARG:NH1	1.98	0.75
1:B:264:VAL:O	1:B:264:VAL:HG12	1.86	0.74
1:B:10:LEU:HD23	1:B:51:PRO:HB2	1.70	0.74
1:A:24:PRO:C	1:A:26:GLU:H	1.93	0.72
1:B:315:CYS:SG	1:B:318:CYS:HB2	2.29	0.72
1:A:20:LYS:NZ	1:A:20:LYS:HB3	2.05	0.71
1:A:365:VAL:HG12	3:A:474:HOH:O	1.90	0.70
1:B:84:LYS:HE3	1:B:356:ILE:HD13	1.73	0.70
1:B:73:GLN:HE21	1:B:204:GLY:HA3	1.57	0.69
1:B:20:LYS:HB3	1:B:20:LYS:NZ	2.08	0.69
1:A:52:ARG:NH1	1:A:54:GLN:NE2	2.40	0.69
1:B:52:ARG:NH1	1:B:54:GLN:NE2	2.41	0.68
1:A:73:GLN:HE21	1:A:204:GLY:HA3	1.60	0.67
1:A:315:CYS:SG	1:A:318:CYS:HB2	2.35	0.67
1:A:209:PRO:O	1:B:106:ARG:NH2	2.28	0.67
1:A:152:SER:HB2	1:B:32:LYS:HD3	1.78	0.66
1:A:73:GLN:HE22	1:B:71:SER:H	1.41	0.66
1:B:52:ARG:HH11	1:B:54:GLN:NE2	1.94	0.66
1:A:52:ARG:HH11	1:A:54:GLN:NE2	1.94	0.65
1:A:191:ILE:HD11	1:A:193:ALA:O	1.96	0.65
1:B:298:ARG:HD3	1:B:302:GLU:OE2	1.97	0.64
1:B:192:ARG:HH12	1:B:193:ALA:HB3	1.62	0.64
1:A:326:LYS:C	1:A:328:ARG:H	1.99	0.64
1:B:122:ARG:CG	1:B:365:VAL:O	2.44	0.64
1:B:192:ARG:HB3	1:B:192:ARG:HH11	1.61	0.63
1:A:191:ILE:HG22	1:B:196:GLY:O	1.98	0.63
1:B:275:LEU:O	1:B:279:GLN:HG3	1.99	0.63
1:B:238:VAL:O	1:B:238:VAL:HG23	1.99	0.62
1:A:359:HIS:HD2	1:A:361:TRP:H	1.46	0.62
1:B:200:ASN:HD22	1:B:200:ASN:N	1.89	0.62
1:B:316:GLN:HE22	1:B:353:GLN:HE22	1.46	0.62
1:B:2:SER:HB3	3:B:493:HOH:O	1.99	0.62
1:B:4:SER:HB3	1:B:48:TRP:HD1	1.63	0.62
1:A:200:ASN:N	1:A:200:ASN:HD22	1.89	0.61
1:A:249:HIS:CD2	1:A:250:GLU:H	2.18	0.61
1:A:337:ASN:O	1:A:338:GLY:O	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:VAL:O	1:A:179:VAL:HG12	2.00	0.61
1:A:344:ARG:HD2	3:A:479:HOH:O	2.00	0.61
1:B:200:ASN:ND2	1:B:200:ASN:H	1.91	0.61
1:B:255:GLU:OE1	1:B:285:ARG:HD2	2.00	0.61
1:A:175:PRO:HB3	1:A:180:THR:HG23	1.82	0.61
1:B:326:LYS:C	1:B:328:ARG:H	2.02	0.61
1:B:338:GLY:O	1:B:340:GLU:N	2.29	0.61
1:B:299:ALA:HA	1:B:304:ARG:NH1	2.16	0.60
1:A:122:ARG:CG	1:A:365:VAL:O	2.44	0.60
1:A:71:SER:N	1:B:73:GLN:HE22	2.00	0.60
1:A:200:ASN:H	1:A:200:ASN:ND2	1.91	0.59
1:B:138:THR:HA	1:B:171:GLY:O	2.02	0.59
1:A:24:PRO:HB2	1:A:27:PRO:CD	2.33	0.59
1:A:23:GLY:N	1:A:24:PRO:HD3	2.15	0.59
1:A:216:GLU:HA	1:A:219:LYS:HG2	1.84	0.58
1:A:122:ARG:HH11	1:A:122:ARG:CB	2.15	0.58
1:A:219:LYS:HZ3	1:A:219:LYS:HB2	1.67	0.58
1:B:12:LEU:HD21	1:B:14:MET:SD	2.44	0.58
1:B:251:ASP:OD2	1:B:285:ARG:NH2	2.35	0.58
1:B:122:ARG:HH11	1:B:122:ARG:CB	2.15	0.57
1:A:316:GLN:HE22	1:A:353:GLN:HE22	1.51	0.57
1:B:138:THR:HG22	1:B:171:GLY:O	2.03	0.57
1:B:315:CYS:HG	1:B:318:CYS:HB2	1.68	0.57
1:A:238:VAL:HG23	1:A:238:VAL:O	2.03	0.57
1:B:82:LYS:HD3	1:B:86:GLN:NE2	2.19	0.57
1:A:26:GLU:N	1:A:27:PRO:CD	2.67	0.57
1:A:105:MET:HA	1:A:105:MET:CE	2.35	0.56
1:A:150:GLU:HG3	1:A:158:PRO:CA	2.29	0.56
1:A:137:GLY:O	1:A:172:ALA:HB2	2.04	0.56
1:B:174:PHE:HB3	1:B:178:SER:HB2	1.88	0.56
1:A:20:LYS:HZ3	1:A:20:LYS:HB3	1.70	0.56
1:A:326:LYS:C	1:A:328:ARG:N	2.60	0.56
1:B:105:MET:CE	1:B:105:MET:HA	2.36	0.55
1:B:15:THR:HG21	1:B:18:PRO:HG3	1.89	0.55
1:B:264:VAL:O	1:B:264:VAL:CG1	2.53	0.55
1:A:304:ARG:NH2	3:A:398:HOH:O	2.40	0.55
1:B:22:PRO:HB3	1:B:28:LEU:HD22	1.89	0.55
1:A:23:GLY:N	1:A:24:PRO:CD	2.71	0.54
1:A:4:SER:HA	1:A:48:TRP:HD1	1.74	0.53
1:B:3:SER:O	1:B:4:SER:CB	2.55	0.53
1:A:180:THR:HG21	3:A:457:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:SER:H	1:B:73:GLN:NE2	2.03	0.52
1:B:72:LEU:HD13	1:B:158:PRO:HG3	1.91	0.52
1:A:333:PRO:HA	1:A:336:GLU:OE1	2.09	0.52
1:A:250:GLU:C	1:A:252:GLY:H	2.13	0.52
1:B:66:SER:HB2	1:B:72:LEU:HD12	1.92	0.52
1:B:192:ARG:HB2	1:B:227:TRP:CE3	2.45	0.51
1:A:179:VAL:HG12	1:A:319:PRO:HG2	1.92	0.51
1:B:333:PRO:HA	1:B:336:GLU:OE1	2.09	0.51
1:A:72:LEU:HD13	1:A:158:PRO:HG3	1.93	0.51
1:A:163:LEU:C	1:A:163:LEU:HD23	2.31	0.51
1:A:24:PRO:C	1:A:26:GLU:N	2.62	0.51
1:B:187:ASP:HB3	1:B:190:PHE:CE1	2.46	0.51
1:B:88:VAL:O	1:B:365:VAL:N	2.44	0.51
1:A:66:SER:HB2	1:A:72:LEU:HD12	1.93	0.50
1:A:92:ARG:N	1:A:93:PRO:HD3	2.26	0.50
1:A:249:HIS:HD2	3:A:398:HOH:O	1.93	0.50
1:A:238:VAL:HG23	1:A:241:MET:HB2	1.92	0.50
1:A:13:GLU:O	1:A:55:PRO:HD3	2.12	0.50
1:A:289:ARG:HG2	1:A:290:THR:N	2.27	0.50
1:B:229:TYR:O	1:B:234:GLN:HG2	2.12	0.50
1:B:92:ARG:N	1:B:93:PRO:HD3	2.27	0.50
1:B:40:MET:SD	1:B:162:LEU:HD11	2.51	0.49
1:A:229:TYR:O	1:A:234:GLN:HG2	2.11	0.49
1:A:326:LYS:O	1:A:327:ASP:HB2	2.13	0.49
1:A:255:GLU:HB3	1:A:285:ARG:HD2	1.94	0.49
1:B:337:ASN:C	1:B:338:GLY:O	2.49	0.49
1:B:326:LYS:C	1:B:328:ARG:N	2.64	0.49
1:A:219:LYS:HZ2	1:A:219:LYS:HB2	1.75	0.49
1:B:171:GLY:O	1:B:172:ALA:HB2	2.13	0.49
1:B:122:ARG:NH2	3:B:431:HOH:O	2.46	0.49
1:A:191:ILE:CG2	1:B:196:GLY:O	2.61	0.49
1:B:192:ARG:HB2	1:B:227:TRP:CD2	2.48	0.48
1:B:342:ILE:O	1:B:346:GLN:HG3	2.13	0.48
1:B:163:LEU:HD23	1:B:163:LEU:C	2.34	0.48
1:B:192:ARG:HH11	1:B:192:ARG:CB	2.25	0.48
1:B:150:GLU:HG3	1:B:152:SER:HB3	1.94	0.48
1:B:15:THR:CG2	1:B:18:PRO:HG3	2.42	0.48
1:A:151:PRO:HD3	1:A:160:ARG:HD2	1.96	0.48
1:B:337:ASN:O	1:B:338:GLY:O	2.31	0.48
1:A:250:GLU:HG2	1:A:298:ARG:HH12	1.78	0.48
1:A:283:GLU:CD	1:A:344:ARG:HH22	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:PHE:HB3	1:B:342:ILE:HD11	1.95	0.48
1:A:40:MET:SD	1:A:162:LEU:HD11	2.54	0.47
1:B:20:LYS:HB3	1:B:20:LYS:HZ3	1.78	0.47
1:A:359:HIS:CD2	1:A:361:TRP:H	2.30	0.47
1:B:17:LYS:O	1:B:17:LYS:HD2	2.14	0.47
1:B:67:SER:HB3	1:B:148:GLY:O	2.15	0.47
1:B:22:PRO:HB3	1:B:28:LEU:CD2	2.44	0.47
1:A:281:TRP:CH2	1:A:344:ARG:HG2	2.50	0.47
1:B:90:LEU:CB	1:B:93:PRO:HG3	2.40	0.47
1:A:174:PHE:H	1:A:175:PRO:HD2	1.79	0.47
1:A:25:GLY:N	1:A:27:PRO:HD3	2.29	0.47
1:B:281:TRP:CH2	1:B:344:ARG:HG2	2.49	0.47
1:A:4:SER:HA	1:A:48:TRP:CD1	2.49	0.47
1:B:72:LEU:HD13	1:B:158:PRO:CG	2.44	0.47
1:A:124:LEU:HG	1:A:167:LEU:HD11	1.98	0.46
1:B:238:VAL:HG23	1:B:241:MET:HB2	1.97	0.46
1:A:135:ALA:HB3	1:A:138:THR:HG21	1.97	0.46
1:A:237:GLU:OE1	2:A:370:PLP:N1	2.48	0.46
1:B:192:ARG:HH12	1:B:193:ALA:CB	2.27	0.46
1:A:2:SER:O	1:A:3:SER:C	2.53	0.46
1:B:315:CYS:HG	1:B:318:CYS:CB	2.27	0.46
1:A:72:LEU:HD13	1:A:158:PRO:CG	2.46	0.46
1:A:337:ASN:C	1:A:338:GLY:O	2.53	0.46
1:A:85:ASP:O	1:A:86:GLN:CB	2.57	0.46
1:B:224:GLN:HE21	1:B:224:GLN:HB3	1.59	0.45
1:B:133:PRO:HB2	1:B:138:THR:OG1	2.16	0.45
1:B:85:ASP:CG	1:B:87:GLN:HB2	2.36	0.45
1:A:334:THR:O	1:A:337:ASN:O	2.34	0.45
1:B:123:ARG:NH1	1:B:123:ARG:HB3	2.31	0.45
1:B:192:ARG:NH1	3:B:389:HOH:O	2.49	0.45
1:A:260:PRO:HD3	1:A:289:ARG:C	2.36	0.45
1:A:45:ASP:HA	3:A:507:HOH:O	2.17	0.45
1:B:84:LYS:C	1:B:86:GLN:H	2.19	0.45
1:B:187:ASP:HA	1:B:188:PRO:HD3	1.85	0.45
1:B:29:VAL:HB	1:B:32:LYS:HG3	1.97	0.45
1:A:365:VAL:HG23	1:A:365:VAL:O	2.17	0.44
1:A:69:HIS:CE1	1:B:145:VAL:HG21	2.52	0.44
1:B:174:PHE:CE1	1:B:179:VAL:HA	2.52	0.44
1:A:191:ILE:O	1:A:191:ILE:HG23	2.17	0.44
1:A:67:SER:HB3	1:A:148:GLY:O	2.16	0.44
1:A:170:VAL:HG12	1:A:171:GLY:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ARG:HB2	1:A:227:TRP:CE3	2.52	0.44
1:A:348:GLU:HG3	3:A:479:HOH:O	2.18	0.43
1:A:192:ARG:HH21	2:A:370:PLP:H2A3	1.83	0.43
1:B:174:PHE:CD1	1:B:179:VAL:HA	2.53	0.43
1:A:122:ARG:HH11	1:A:122:ARG:CG	2.31	0.43
1:B:237:GLU:OE1	2:B:370:PLP:N1	2.51	0.43
1:A:250:GLU:O	1:A:252:GLY:N	2.52	0.43
1:A:86:GLN:CD	1:A:86:GLN:C	2.76	0.43
1:B:316:GLN:NE2	1:B:353:GLN:HE22	2.14	0.43
1:B:40:MET:HG2	1:B:52:ARG:HH12	1.83	0.43
1:A:218:LEU:HD12	3:A:492:HOH:O	2.19	0.43
1:A:251:ASP:OD1	1:A:285:ARG:NH2	2.39	0.43
1:A:192:ARG:NH2	2:A:370:PLP:H2A3	2.34	0.43
1:B:238:VAL:O	1:B:238:VAL:CG2	2.67	0.43
1:A:360:GLU:O	1:A:360:GLU:OE1	2.37	0.42
1:A:90:LEU:CB	1:A:93:PRO:HG3	2.44	0.42
1:A:163:LEU:HD23	1:A:164:PHE:N	2.34	0.42
1:A:250:GLU:C	1:A:252:GLY:N	2.72	0.42
1:B:163:LEU:HD23	1:B:164:PHE:N	2.33	0.42
1:B:304:ARG:NH2	3:B:489:HOH:O	2.52	0.42
1:B:326:LYS:O	1:B:328:ARG:N	2.52	0.42
1:A:123:ARG:HB3	1:A:123:ARG:NH1	2.34	0.42
1:B:84:LYS:CD	1:B:84:LYS:H	2.20	0.42
1:A:338:GLY:C	1:A:340:GLU:N	2.72	0.42
1:B:360:GLU:O	1:B:360:GLU:OE1	2.38	0.42
1:A:44:ASN:HB3	1:A:45:ASP:H	1.67	0.41
1:A:71:SER:N	1:B:73:GLN:NE2	2.66	0.41
1:B:122:ARG:HH12	1:B:123:ARG:HG2	1.84	0.41
1:A:250:GLU:O	1:A:250:GLU:OE1	2.37	0.41
1:B:105:MET:HE2	1:B:105:MET:HA	2.01	0.41
1:A:88:VAL:O	1:A:365:VAL:N	2.51	0.41
1:B:12:LEU:HD23	1:B:13:GLU:N	2.35	0.41
1:B:14:MET:O	1:B:15:THR:O	2.37	0.41
1:B:284:PHE:HA	3:B:406:HOH:O	2.19	0.41
1:A:242:ASN:ND2	1:A:268:GLY:HA3	2.35	0.41
1:A:97:MET:HB3	1:A:114:LYS:HB3	2.02	0.41
1:A:122:ARG:HH12	1:A:123:ARG:HG2	1.85	0.41
1:A:248:THR:HA	1:A:254:LEU:HA	2.03	0.41
1:B:365:VAL:HG23	1:B:365:VAL:O	2.21	0.41
1:A:40:MET:HG2	1:A:52:ARG:HH12	1.86	0.41
1:A:5:PHE:HB2	1:A:51:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLN:NE2	1:B:71:SER:H	2.13	0.41
1:B:2:SER:O	1:B:3:SER:O	2.38	0.41
1:A:122:ARG:HH12	1:A:123:ARG:CD	2.34	0.40
1:B:62:HIS:CD2	1:B:151:PRO:HB3	2.57	0.40
1:A:283:GLU:OE1	1:A:344:ARG:NH2	2.55	0.40
1:B:122:ARG:HH12	1:B:123:ARG:CD	2.34	0.40
1:B:113:ASP:HB3	1:B:116:GLU:CG	2.52	0.40
1:B:264:VAL:HG12	3:B:389:HOH:O	2.21	0.40
1:B:281:TRP:NE1	1:B:348:GLU:OE2	2.53	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	363/365 (100%)	335 (92%)	19 (5%)	9 (2%)	5	1
1	B	363/365 (100%)	329 (91%)	23 (6%)	11 (3%)	4	0
All	All	726/730 (100%)	664 (92%)	42 (6%)	20 (3%)	5	1

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	24	PRO
1	A	173	TYR
1	B	3	SER
1	B	4	SER
1	B	15	THR
1	A	338	GLY
1	B	172	ALA
1	A	174	PHE

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Mol	Chain	Res	Type
1	A	251	ASP
1	B	5	PHE
1	B	175	PRO
1	B	85	ASP
1	A	18	PRO
1	A	172	ALA
1	B	191	ILE
1	A	333	PRO
1	B	333	PRO
1	B	339	PRO
1	B	338	GLY

### 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	316/316 (100%)	299 (95%)	17 (5%)	22	10
1	B	316/316 (100%)	295 (93%)	21 (7%)	16	6
All	All	632/632 (100%)	594 (94%)	38 (6%)	19	8

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	74	LEU
1	A	86	GLN
1	A	105	MET
1	A	106	ARG
1	A	119	GLU
1	A	122	ARG
1	A	162	LEU
1	A	200	ASN
1	A	219	LYS
1	A	247	TRP
1	A	250	GLU

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Mol	Chain	Res	Type
1	A	290	THR
1	A	296	LEU
1	A	327	ASP
1	A	328	ARG
1	A	360	GLU
1	B	5	PHE
1	B	16	GLN
1	B	74	LEU
1	B	84	LYS
1	B	87	GLN
1	B	105	MET
1	B	106	ARG
1	B	119	GLU
1	B	122	ARG
1	B	162	LEU
1	B	173	TYR
1	B	175	PRO
1	B	192	ARG
1	B	200	ASN
1	B	219	LYS
1	B	247	TRP
1	B	261	LEU
1	B	296	LEU
1	B	327	ASP
1	B	328	ARG
1	B	360	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	54	GLN
1	A	73	GLN
1	A	86	GLN
1	A	200	ASN
1	A	206	ASN
1	A	215	GLN
1	A	224	GLN
1	A	242	ASN
1	A	249	HIS
1	A	321	HIS
1	A	353	GLN

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Mol	Chain	Res	Type
1	A	359	HIS
1	B	19	HIS
1	B	54	GLN
1	B	73	GLN
1	B	86	GLN
1	B	200	ASN
1	B	206	ASN
1	B	215	GLN
1	B	224	GLN
1	B	242	ASN
1	B	337	ASN
1	B	353	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 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	B	370	1	15,15,16	1.57	2 (13%)	20,22,23	1.79	6 (30%)
2	PLP	A	370	1	15,15,16	1.65	2 (13%)	20,22,23	1.86	8 (40%)

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	B	370	1	-	0/6/6/8	0/1/1/1
2	PLP	A	370	1	-	0/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	370	PLP	C5-C4	3.54	1.44	1.40
2	B	370	PLP	C5-C4	3.04	1.43	1.40
2	A	370	PLP	C4A-C4	2.86	1.57	1.51
2	B	370	PLP	C4A-C4	2.53	1.56	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	370	PLP	O2P-P-O4P	-3.48	97.48	106.73
2	A	370	PLP	O4P-C5A-C5	3.37	115.76	109.35
2	A	370	PLP	O2P-P-O4P	-3.24	98.12	106.73
2	B	370	PLP	O4P-C5A-C5	3.22	115.48	109.35
2	A	370	PLP	C4A-C4-C5	3.17	124.20	120.94
2	B	370	PLP	C4A-C4-C5	2.86	123.88	120.94
2	A	370	PLP	C5A-C5-C6	-2.65	115.02	119.37
2	B	370	PLP	O3P-P-O1P	2.30	119.68	110.68
2	A	370	PLP	O3P-P-O1P	2.20	119.29	110.68
2	A	370	PLP	O4P-P-O1P	2.16	112.52	106.47
2	B	370	PLP	O4P-P-O1P	2.09	112.35	106.47
2	A	370	PLP	C5-C6-N1	-2.09	120.34	123.82
2	B	370	PLP	C5A-C5-C6	-2.07	115.96	119.37
2	A	370	PLP	C6-N1-C2	2.03	122.93	119.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	370	PLP	1	0
2	A	370	PLP	3	0

## 5.7 Other polymers

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	365/365 (100%)	0.68	39 (10%) 6 9	18, 30, 53, 73	0
1	B	365/365 (100%)	0.70	39 (10%) 6 9	17, 33, 55, 69	0
All	All	730/730 (100%)	0.69	78 (10%) 6 9	17, 32, 54, 73	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	PRO	14.3
1	B	3	SER	12.7
1	A	174	PHE	12.2
1	A	173	TYR	12.0
1	B	1	ALA	10.5
1	B	27	PRO	8.9
1	A	24	PRO	8.7
1	B	25	GLY	8.5
1	A	177	GLY	8.4
1	A	1	ALA	7.5
1	B	24	PRO	7.2
1	B	2	SER	7.0
1	A	2	SER	6.5
1	A	25	GLY	6.4
1	A	178	SER	6.4
1	A	176	GLY	5.7
1	B	84	LYS	5.6
1	A	172	ALA	5.5
1	B	176	GLY	5.5
1	A	179	VAL	5.0
1	B	174	PHE	4.9
1	B	173	TYR	4.8
1	A	3	SER	4.7
1	A	23	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	338	GLY	4.7
1	B	178	SER	4.1
1	A	358	ALA	4.1
1	B	20	LYS	4.1
1	A	357	ARG	4.0
1	B	177	GLY	4.0
1	A	171	GLY	3.9
1	B	175	PRO	3.9
1	A	45	ASP	3.9
1	B	83	GLY	3.7
1	B	28	LEU	3.4
1	A	84	LYS	3.4
1	A	26	GLU	3.3
1	A	28	LEU	3.3
1	B	165	VAL	3.3
1	A	86	GLN	3.3
1	A	250	GLU	3.0
1	B	16	GLN	3.0
1	B	45	ASP	3.0
1	A	27	PRO	2.9
1	A	244	PHE	2.9
1	B	179	VAL	2.8
1	B	4	SER	2.7
1	B	171	GLY	2.7
1	B	29	VAL	2.7
1	B	26	GLU	2.7
1	B	18	PRO	2.5
1	B	17	LYS	2.5
1	A	165	VAL	2.5
1	B	142	VAL	2.5
1	B	308	VAL	2.5
1	A	145	VAL	2.5
1	B	12	LEU	2.4
1	B	39	LEU	2.4
1	B	23	GLY	2.4
1	A	17	LYS	2.3
1	A	298	ARG	2.3
1	B	46	LYS	2.3
1	A	338	GLY	2.3
1	B	365	VAL	2.3
1	B	144	PRO	2.3
1	A	356	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	46	LYS	2.2
1	A	231	PRO	2.2
1	A	44	ASN	2.2
1	B	164	PHE	2.2
1	A	365	VAL	2.2
1	A	245	VAL	2.2
1	A	301	GLU	2.1
1	B	328	ARG	2.1
1	B	166	ILE	2.1
1	A	166	ILE	2.0
1	A	159	ARG	2.0
1	B	360	GLU	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, 95<sup>th</sup> 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	B	370	15/16	0.98	0.08	17,25,32,32	0
2	PLP	A	370	15/16	0.98	0.08	17,24,32,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.