



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:31 am BST

PDB ID : 1TZK  
Title : Crystal structure of 1-aminocyclopropane-1-carboxylate-deaminase complexed with alpha-keto-butyrate  
Authors : Karthikeyan, S.; Zhou, Q.; Zhao, Z.; Kao, C.L.; Tao, Z.; Robinson, H.; Liu, H.W.; Zhang, H.  
Deposited on : 2004-07-10  
Resolution : 2.00 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.

---

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

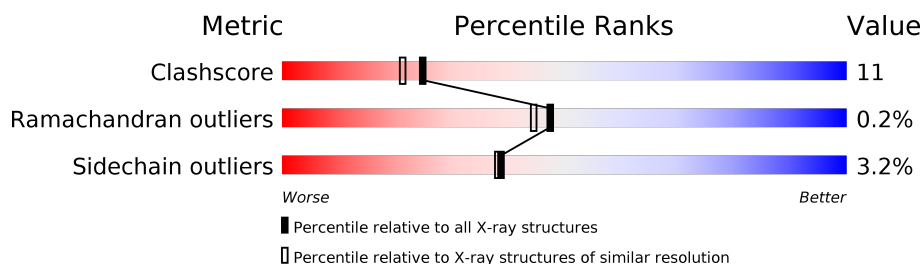
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	338	
1	B	338	
1	C	338	
1	D	338	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	2KT	A	501	-	-	X	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	2KT	C	502	-	-	X	-

## 2 Entry composition [i](#)

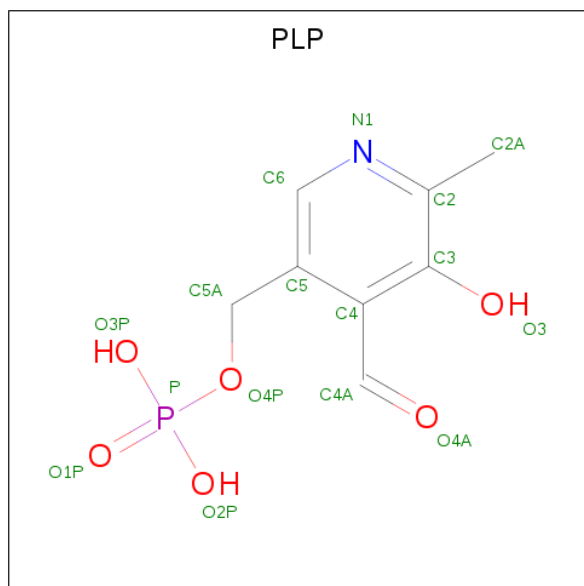
There are 5 unique types of molecules in this entry. The entry contains 10661 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1-aminocyclopropane-1-carboxylate deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2514	1576	451	472	15			
1	B	329	Total	C	N	O	S	0	0	0
			2499	1567	449	468	15			
1	C	335	Total	C	N	O	S	0	0	0
			2554	1600	461	478	15			
1	D	329	Total	C	N	O	S	0	0	0
			2495	1565	449	466	15			

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



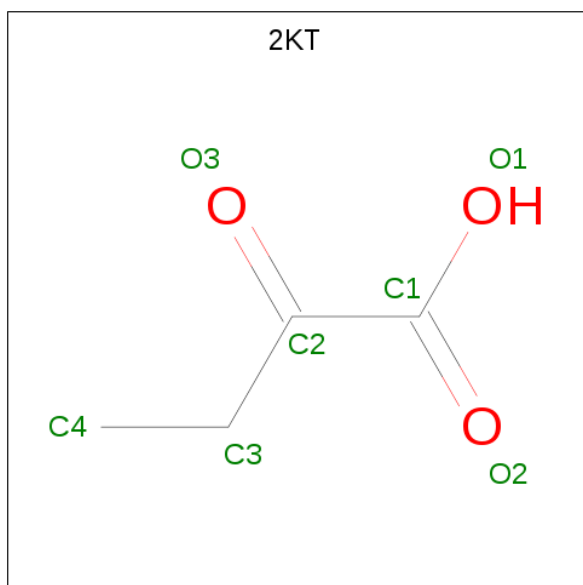
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is 2-KETOBUTYRIC ACID (three-letter code: 2KT) (formula:  $C_4H_6O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

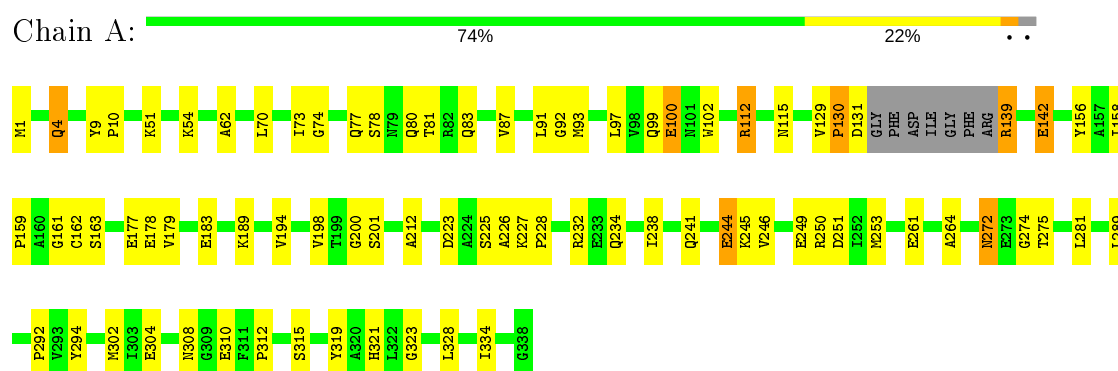
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	131	Total	O	0	0
			131	131		
5	B	118	Total	O	0	0
			118	118		
5	C	144	Total	O	0	0
			144	144		
5	D	122	Total	O	0	0
			122	122		

### 3 Residue-property plots [i](#)

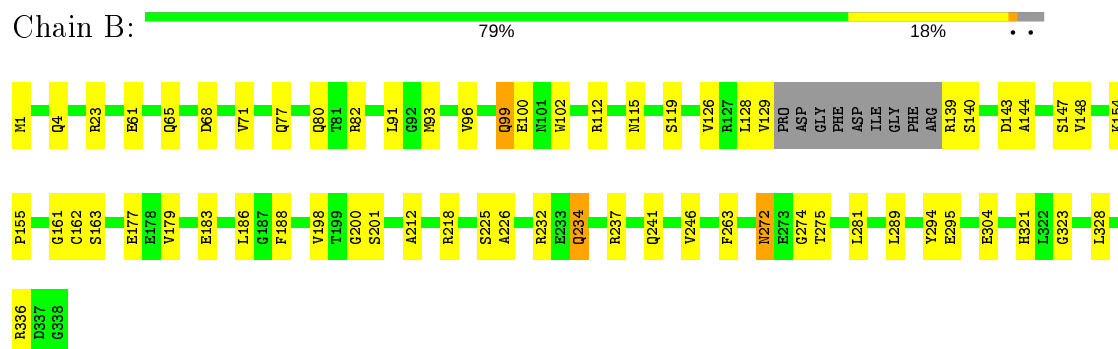
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

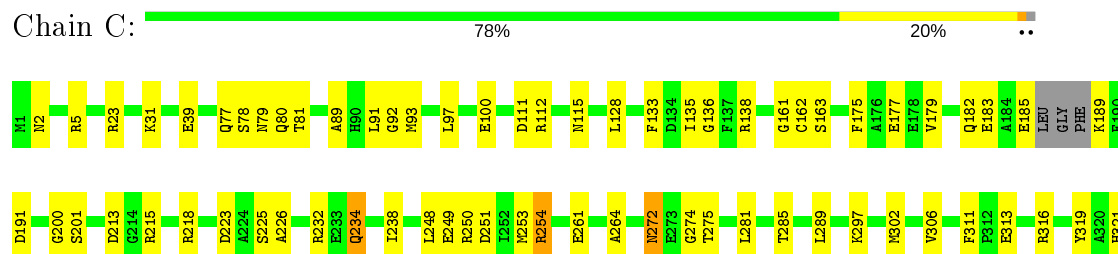
- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase



- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

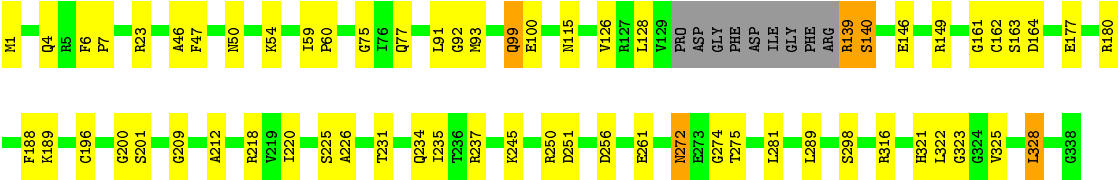
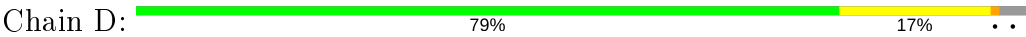


- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase





- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.66 Å 68.45 Å 350.17 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.89 – 2.00	Depositor
% Data completeness (in resolution range)	99.4 (29.89-2.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.218 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10661	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

## 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: 2KT, SO4, 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	0.51	0/2561	0.72	2/3461 (0.1%)
1	B	0.49	0/2545	0.71	1/3438 (0.0%)
1	C	0.51	0/2602	0.74	1/3514 (0.0%)
1	D	0.49	0/2541	0.72	1/3433 (0.0%)
All	All	0.50	0/10249	0.72	5/13846 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	GLY	N-CA-C	7.85	132.73	113.10
1	D	200	GLY	N-CA-C	6.72	129.91	113.10
1	A	200	GLY	N-CA-C	6.64	129.69	113.10
1	B	200	GLY	N-CA-C	6.59	129.58	113.10
1	A	112	ARG	NE-CZ-NH1	-5.23	117.69	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	2514	0	2486	73	0
1	B	2499	0	2474	43	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2554	0	2526	57	0
1	D	2495	0	2471	47	0
2	A	15	0	7	1	0
2	B	15	0	7	1	0
2	C	15	0	7	0	0
2	D	15	0	7	0	0
3	A	7	0	5	7	0
3	C	7	0	5	5	0
4	B	5	0	0	1	0
4	D	5	0	0	0	0
5	A	131	0	0	9	0
5	B	118	0	0	1	0
5	C	144	0	0	9	0
5	D	122	0	0	5	0
All	All	10661	0	9995	218	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 11.

All (218) 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:131:ASP:HB3	5:A:961:HOH:O	1.68	0.92
1:D:1:MET:HE3	1:D:212:ALA:HB2	1.54	0.88
1:A:272:ASN:HD22	1:A:274:GLY:H	1.19	0.85
1:D:1:MET:CE	1:D:212:ALA:HB2	2.06	0.85
1:C:272:ASN:HD22	1:C:274:GLY:H	1.24	0.83
1:C:78:SER:OG	3:C:502:2KT:H31	1.78	0.81
1:B:1:MET:HE3	1:B:212:ALA:HB2	1.62	0.81
1:A:100:GLU:OE1	1:A:129:VAL:HG11	1.83	0.78
3:C:502:2KT:H32	5:C:805:HOH:O	1.85	0.77
1:D:100:GLU:HB3	5:D:970:HOH:O	1.83	0.77
1:B:272:ASN:HD22	1:B:274:GLY:H	1.32	0.76
1:A:228:PRO:HG3	5:A:955:HOH:O	1.85	0.76
1:C:272:ASN:HD22	1:C:274:GLY:N	1.84	0.74
1:B:1:MET:CE	1:B:212:ALA:HB2	2.17	0.73
1:A:161:GLY:O	1:A:162:CYS:HB2	1.86	0.73
1:B:77:GLN:HE22	1:B:115:ASN:H	1.37	0.73
1:C:182:GLN:O	1:C:185:GLU:HG2	1.91	0.71
1:B:91:LEU:HD13	1:B:93:MET:HE3	1.72	0.71
1:D:180:ARG:NH2	1:D:209:GLY:O	2.23	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLU:HG3	5:A:946:HOH:O	1.90	0.70
1:D:7:PRO:O	1:D:60:PRO:HG2	1.91	0.70
1:C:191:ASP:O	1:C:218:ARG:HD2	1.92	0.69
1:C:80:GLN:HG2	5:C:805:HOH:O	1.91	0.69
1:A:178:GLU:HG3	5:A:1052:HOH:O	1.94	0.68
1:D:77:GLN:HE22	1:D:115:ASN:H	1.40	0.68
1:A:272:ASN:HD22	1:A:274:GLY:N	1.92	0.67
1:D:272:ASN:HD22	1:D:274:GLY:H	1.43	0.66
1:C:272:ASN:ND2	1:C:275:THR:H	1.92	0.66
1:C:77:GLN:HE22	1:C:115:ASN:H	1.43	0.66
1:B:321:HIS:HD2	1:B:323:GLY:H	1.42	0.65
1:A:77:GLN:HE22	1:A:115:ASN:H	1.44	0.65
1:B:289:LEU:O	1:B:321:HIS:HE1	1.80	0.65
1:A:241:GLN:NE2	1:A:245:LYS:HD3	2.12	0.64
1:B:161:GLY:O	1:B:162:CYS:HB2	1.97	0.64
1:A:234:GLN:O	1:A:238:ILE:HG13	1.97	0.64
1:A:272:ASN:ND2	1:A:274:GLY:H	1.95	0.63
1:A:308:ASN:HB2	1:A:310:GLU:HG3	1.81	0.63
1:C:91:LEU:CD1	1:C:93:MET:HE2	2.29	0.63
1:C:311:PHE:HB2	5:C:1030:HOH:O	1.98	0.63
1:D:234:GLN:HG2	1:D:237:ARG:NH2	2.14	0.63
1:C:112:ARG:HD3	5:D:954:HOH:O	1.98	0.62
1:A:81:THR:HB	1:A:97:LEU:HD13	1.81	0.62
1:D:99:GLN:HB2	1:D:128:LEU:HD23	1.81	0.62
1:A:91:LEU:CD1	1:A:93:MET:HE2	2.30	0.61
1:D:161:GLY:O	1:D:162:CYS:HB2	2.00	0.61
1:C:161:GLY:O	1:C:162:CYS:HB2	2.00	0.61
1:B:272:ASN:HD22	1:B:274:GLY:N	1.98	0.61
3:C:502:2KT:H42	5:C:1163:HOH:O	1.99	0.61
1:D:188:PHE:HB2	1:D:316:ARG:NH1	2.15	0.61
1:C:175:PHE:O	1:C:179:VAL:HG23	2.01	0.60
1:A:289:LEU:O	1:A:321:HIS:HE1	1.83	0.60
1:A:80:GLN:HG2	3:A:501:2KT:H43	1.83	0.60
1:A:91:LEU:HD13	1:A:93:MET:HE2	1.84	0.60
1:B:91:LEU:CD1	1:B:93:MET:HE3	2.31	0.59
1:A:129:VAL:HG23	1:A:129:VAL:O	2.00	0.59
1:C:321:HIS:HD2	1:C:323:GLY:H	1.50	0.59
1:D:272:ASN:HD22	1:D:274:GLY:N	2.00	0.59
1:C:111:ASP:O	1:C:112:ARG:HG2	2.02	0.59
1:D:91:LEU:HD13	1:D:93:MET:HE2	1.84	0.59
1:A:74:GLY:HA2	1:A:102:TRP:CH2	2.39	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:GLU:HB2	1:B:102:TRP:NE1	2.19	0.58
1:A:1:MET:CE	1:A:212:ALA:HB2	2.33	0.57
1:D:139:ARG:HH11	1:D:140:SER:HB3	1.68	0.57
1:A:100:GLU:HB2	1:A:102:TRP:CD1	2.40	0.57
1:B:144:ALA:O	1:B:147:SER:HB3	2.05	0.57
1:C:183:GLU:C	1:C:185:GLU:H	2.08	0.57
1:C:183:GLU:CD	1:C:189:LYS:HD3	2.25	0.57
1:D:234:GLN:HG2	1:D:237:ARG:HH21	1.70	0.57
1:D:4:GLN:NE2	1:D:4:GLN:O	2.38	0.57
1:C:289:LEU:O	1:C:321:HIS:HE1	1.89	0.56
1:A:161:GLY:H	3:A:501:2KT:H42	1.71	0.56
1:D:321:HIS:HD2	1:D:323:GLY:H	1.51	0.56
1:C:91:LEU:HD12	1:C:93:MET:HE2	1.86	0.56
1:A:321:HIS:HD2	1:A:323:GLY:H	1.52	0.56
1:C:78:SER:HG	3:C:502:2KT:H31	1.71	0.56
1:B:100:GLU:HB2	1:B:102:TRP:CD1	2.41	0.55
1:B:234:GLN:CD	1:B:237:ARG:HH22	2.08	0.55
1:B:179:VAL:O	1:B:183:GLU:HG3	2.06	0.54
1:B:100:GLU:HA	1:B:129:VAL:HG22	1.88	0.54
1:D:6:PHE:CZ	1:D:245:LYS:HG2	2.43	0.54
1:B:80:GLN:HB3	4:B:601:SO4:O2	2.08	0.54
1:C:232:ARG:NH2	1:C:261:GLU:OE2	2.40	0.54
1:B:186:LEU:HD13	1:B:188:PHE:CZ	2.43	0.53
1:D:250:ARG:HD2	1:D:251:ASP:O	2.07	0.53
1:A:302:MET:HE3	1:A:319:TYR:HD1	1.73	0.53
1:A:302:MET:CE	1:A:319:TYR:HB2	2.40	0.52
1:A:78:SER:OG	3:A:501:2KT:H32	2.09	0.52
1:D:99:GLN:HG3	1:D:126:VAL:HG13	1.91	0.52
1:B:91:LEU:HD13	1:B:93:MET:CE	2.39	0.52
1:C:213:ASP:OD1	1:C:215:ARG:HG3	2.10	0.52
1:B:198:VAL:HG21	1:B:294:TYR:HE1	1.75	0.52
1:C:248:LEU:CD1	1:C:250:ARG:HB3	2.40	0.52
1:D:289:LEU:O	1:D:321:HIS:HE1	1.93	0.52
1:B:99:GLN:HG3	1:B:126:VAL:HG13	1.92	0.51
1:C:112:ARG:CD	5:D:954:HOH:O	2.54	0.51
1:C:81:THR:HB	1:C:97:LEU:HD13	1.92	0.51
1:D:231:THR:O	1:D:235:ILE:HG13	2.10	0.51
1:A:161:GLY:H	3:A:501:2KT:C4	2.24	0.51
1:A:302:MET:HE1	1:A:319:TYR:HB2	1.92	0.51
1:A:1:MET:HB2	1:A:246:VAL:O	2.10	0.51
1:A:100:GLU:HA	1:A:129:VAL:HG22	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:HD3	5:C:850:HOH:O	2.11	0.51
1:C:234:GLN:O	1:C:238:ILE:HG13	2.11	0.50
1:A:334:ILE:HG13	5:A:1035:HOH:O	2.10	0.50
1:A:250:ARG:HG2	1:A:251:ASP:N	2.27	0.50
1:A:223:ASP:O	1:A:264:ALA:HB2	2.11	0.50
1:D:1:MET:HE2	1:D:212:ALA:HB2	1.90	0.49
1:C:111:ASP:C	1:C:112:ARG:HG2	2.32	0.49
1:A:163:SER:HA	1:A:201:SER:HB3	1.94	0.49
1:A:73:ILE:O	3:A:501:2KT:H41	2.12	0.49
1:B:321:HIS:CD2	1:B:323:GLY:H	2.28	0.48
1:B:71:VAL:HG22	1:B:96:VAL:HB	1.94	0.48
1:D:189:LYS:HE2	5:D:1169:HOH:O	2.14	0.48
1:D:188:PHE:HB2	1:D:316:ARG:HH12	1.77	0.48
1:B:99:GLN:HB2	1:B:128:LEU:HD23	1.94	0.48
1:B:198:VAL:HG21	1:B:294:TYR:CE1	2.49	0.48
1:C:163:SER:HA	1:C:201:SER:HB3	1.96	0.48
1:B:112:ARG:HD3	5:D:1080:HOH:O	2.13	0.48
1:D:272:ASN:ND2	1:D:275:THR:H	2.11	0.48
1:A:225:SER:O	1:A:226:ALA:HB3	2.13	0.48
1:A:232:ARG:HD2	5:A:1096:HOH:O	2.13	0.48
1:B:163:SER:HA	1:B:201:SER:HB3	1.94	0.48
1:C:248:LEU:HD13	1:C:250:ARG:HB3	1.94	0.48
1:C:297:LYS:HG2	5:C:817:HOH:O	2.12	0.48
1:A:54:LYS:NZ	2:A:401:PLP:O2P	2.41	0.47
1:C:78:SER:CB	3:C:502:2KT:H31	2.45	0.47
1:D:146:GLU:HA	1:D:149:ARG:NH1	2.30	0.47
1:B:225:SER:O	1:B:226:ALA:HB3	2.15	0.47
1:C:100:GLU:OE1	1:C:135:ILE:HG12	2.14	0.47
1:A:272:ASN:ND2	1:A:274:GLY:N	2.58	0.47
1:B:139:ARG:O	1:B:143:ASP:OD2	2.33	0.47
1:B:218:ARG:HG3	1:B:218:ARG:NH1	2.29	0.47
1:C:249:GLU:HG2	5:C:1012:HOH:O	2.14	0.46
1:D:91:LEU:CD1	1:D:93:MET:HE2	2.43	0.46
1:D:139:ARG:NH1	1:D:140:SER:HB3	2.30	0.46
1:A:244:GLU:C	1:A:244:GLU:OE1	2.53	0.46
1:A:4:GLN:HA	1:A:4:GLN:HE21	1.81	0.46
1:C:92:GLY:HA2	1:D:23:ARG:CZ	2.45	0.46
1:A:227:LYS:N	1:A:228:PRO:HD3	2.30	0.46
1:D:6:PHE:HZ	1:D:245:LYS:HG2	1.81	0.46
1:A:250:ARG:HD2	5:A:1173:HOH:O	2.15	0.46
1:B:336:ARG:HG2	1:B:336:ARG:HH11	1.79	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ARG:NH1	1:D:92:GLY:HA2	2.31	0.46
1:B:148:VAL:HG11	1:B:155:PRO:HB3	1.98	0.45
1:A:251:ASP:C	1:A:253:MET:HE2	2.37	0.45
1:A:92:GLY:HA2	1:B:23:ARG:CZ	2.46	0.45
1:C:272:ASN:ND2	1:C:274:GLY:N	2.59	0.45
1:C:250:ARG:HG2	1:C:251:ASP:N	2.32	0.45
1:D:321:HIS:CD2	1:D:323:GLY:H	2.33	0.45
1:A:272:ASN:ND2	1:A:275:THR:H	2.15	0.45
1:D:218:ARG:O	1:D:220:ILE:HD12	2.17	0.45
1:A:179:VAL:O	1:A:183:GLU:HG3	2.16	0.45
1:D:163:SER:HA	1:D:201:SER:HB3	1.98	0.45
1:D:46:ALA:O	1:D:47:PHE:HB2	2.16	0.45
1:B:272:ASN:ND2	1:B:275:THR:H	2.15	0.44
1:C:23:ARG:HD3	1:C:285:THR:O	2.17	0.44
1:D:225:SER:O	1:D:226:ALA:HB3	2.18	0.44
1:C:2:ASN:ND2	1:C:5:ARG:HB2	2.32	0.44
1:A:194:VAL:HG21	1:A:302:MET:HE2	1.99	0.44
1:A:70:LEU:HD21	1:A:93:MET:HE1	1.99	0.44
1:B:61:GLU:O	1:B:65:GLN:HG3	2.17	0.44
1:C:302:MET:O	1:C:306:VAL:HG23	2.17	0.44
1:C:31:LYS:HB3	1:C:313:GLU:HG3	1.99	0.44
1:D:54:LYS:HD3	1:D:162:CYS:HB2	1.98	0.44
1:A:289:LEU:O	1:A:321:HIS:CE1	2.68	0.44
1:C:302:MET:SD	1:C:319:TYR:HB2	2.57	0.44
1:A:194:VAL:HB	1:A:302:MET:CE	2.48	0.44
1:D:75:GLY:HA2	1:D:100:GLU:O	2.17	0.44
1:D:54:LYS:NZ	1:D:161:GLY:O	2.45	0.44
1:B:82:ARG:HA	1:B:119:SER:OG	2.19	0.43
1:A:129:VAL:O	1:A:129:VAL:CG2	2.65	0.43
1:B:295:GLU:OE2	2:B:401:PLP:N1	2.51	0.43
1:C:223:ASP:O	1:C:264:ALA:HB2	2.19	0.43
1:A:194:VAL:CG2	1:A:302:MET:HE2	2.49	0.43
1:C:89:ALA:O	1:D:23:ARG:NH1	2.52	0.43
1:A:198:VAL:HG21	1:A:294:TYR:CE1	2.54	0.43
1:C:135:ILE:HG13	1:C:136:GLY:N	2.33	0.43
1:C:183:GLU:C	1:C:185:GLU:N	2.72	0.43
1:D:196:CYS:HB2	1:D:298:SER:HB3	2.01	0.43
1:D:188:PHE:CB	1:D:316:ARG:NH1	2.82	0.43
1:A:304:GLU:HG3	5:A:1213:HOH:O	2.19	0.42
1:A:91:LEU:HD12	1:A:93:MET:HE2	2.00	0.42
1:A:80:GLN:CB	3:A:501:2KT:H43	2.50	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ASN:ND2	1:C:275:THR:N	2.65	0.42
1:A:158:ILE:HA	1:A:159:PRO:HD2	1.91	0.42
1:B:68:ASP:OD1	1:B:154:LYS:N	2.50	0.42
1:C:91:LEU:HD13	1:C:93:MET:HE2	2.00	0.42
1:D:325:VAL:O	1:D:328:LEU:HB2	2.19	0.42
1:C:225:SER:O	1:C:226:ALA:HB3	2.20	0.42
1:A:62:ALA:HA	1:A:156:TYR:CD1	2.54	0.42
1:D:50:ASN:HB3	1:D:322:LEU:HD22	2.01	0.42
1:B:263:PHE:HE1	1:B:304:GLU:HG2	1.84	0.42
1:A:198:VAL:HG21	1:A:294:TYR:HE1	1.85	0.42
1:D:250:ARG:NH1	1:D:256:ASP:OD2	2.47	0.42
1:C:39:GLU:HB2	1:C:321:HIS:O	2.20	0.42
1:B:234:GLN:HB2	1:B:234:GLN:HE21	1.64	0.41
1:B:237:ARG:O	1:B:241:GLN:HG3	2.20	0.41
1:A:312:PRO:HD2	1:A:315:SER:OG	2.21	0.41
1:A:161:GLY:N	3:A:501:2KT:H42	2.34	0.41
1:C:79:ASN:OD1	1:C:324:GLY:HA2	2.20	0.41
1:C:133:PHE:CE1	1:C:138:ARG:NH1	2.88	0.41
1:C:251:ASP:HB2	1:C:253:MET:CE	2.50	0.41
1:D:59:ILE:HD12	1:D:91:LEU:CD1	2.50	0.41
1:B:232:ARG:NE	5:B:1004:HOH:O	2.25	0.41
1:A:100:GLU:HB2	1:A:102:TRP:NE1	2.36	0.41
1:A:9:TYR:HA	1:A:10:PRO:HD3	1.91	0.41
1:B:1:MET:HB2	1:B:246:VAL:O	2.21	0.41
1:A:244:GLU:OE1	1:A:245:LYS:N	2.54	0.41
1:C:272:ASN:ND2	1:C:274:GLY:H	2.04	0.41
1:C:316:ARG:NE	5:C:1112:HOH:O	2.53	0.41
1:A:51:LYS:HD2	1:A:80:GLN:OE1	2.20	0.41
1:A:139:ARG:HB3	1:A:142:GLU:HB2	2.04	0.40
1:A:292:PRO:HD3	1:A:328:LEU:HD23	2.02	0.40
1:A:189:LYS:HE2	5:A:1013:HOH:O	2.21	0.40
1:A:83:GLN:O	1:A:87:VAL:HG23	2.22	0.40
1:C:254:ARG:HD3	5:C:1088:HOH:O	2.22	0.40
1:C:91:LEU:HD12	1:C:93:MET:CE	2.51	0.40
1:A:139:ARG:HD3	1:A:139:ARG:HA	1.94	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	327/338 (97%)	311 (95%)	14 (4%)	2 (1%)	25	19
1	B	325/338 (96%)	316 (97%)	9 (3%)	0	100	100
1	C	331/338 (98%)	315 (95%)	16 (5%)	0	100	100
1	D	325/338 (96%)	312 (96%)	12 (4%)	1 (0%)	41	37
All	All	1308/1352 (97%)	1254 (96%)	51 (4%)	3 (0%)	47	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	PRO
1	D	140	SER
1	A	249	GLU

### 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	258/264 (98%)	247 (96%)	11 (4%)	29	26
1	B	256/264 (97%)	248 (97%)	8 (3%)	40	40
1	C	262/264 (99%)	256 (98%)	6 (2%)	50	53
1	D	255/264 (97%)	247 (97%)	8 (3%)	40	40
All	All	1031/1056 (98%)	998 (97%)	33 (3%)	39	38

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	99	GLN
1	A	100	GLU
1	A	130	PRO
1	A	139	ARG
1	A	142	GLU
1	A	177	GLU
1	A	244	GLU
1	A	261	GLU
1	A	272	ASN
1	A	281	LEU
1	B	4	GLN
1	B	99	GLN
1	B	140	SER
1	B	177	GLU
1	B	234	GLN
1	B	272	ASN
1	B	281	LEU
1	B	328	LEU
1	C	128	LEU
1	C	177	GLU
1	C	234	GLN
1	C	254	ARG
1	C	272	ASN
1	C	281	LEU
1	D	99	GLN
1	D	139	ARG
1	D	164	ASP
1	D	177	GLU
1	D	261	GLU
1	D	272	ASN
1	D	281	LEU
1	D	328	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	77	GLN
1	A	99	GLN
1	A	230	GLN
1	A	234	GLN
1	A	241	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	272	ASN
1	A	308	ASN
1	A	321	HIS
1	B	77	GLN
1	B	99	GLN
1	B	230	GLN
1	B	234	GLN
1	B	272	ASN
1	B	321	HIS
1	C	77	GLN
1	C	230	GLN
1	C	234	GLN
1	C	272	ASN
1	C	321	HIS
1	D	4	GLN
1	D	77	GLN
1	D	99	GLN
1	D	272	ASN
1	D	321	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

8 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	SO4	B	601	-	4,4,4	0.24	0	6,6,6	0.16	0
2	PLP	C	401	1	15,15,16	1.50	3 (20%)	20,22,23	1.04	1 (5%)
2	PLP	D	401	1	15,15,16	1.49	3 (20%)	20,22,23	1.00	0
3	2KT	A	501	-	3,6,6	1.20	0	2,7,7	1.42	1 (50%)
4	SO4	D	602	-	4,4,4	0.23	0	6,6,6	0.20	0
2	PLP	B	401	1	15,15,16	1.73	4 (26%)	20,22,23	0.96	0
2	PLP	A	401	1	15,15,16	1.75	4 (26%)	20,22,23	1.02	1 (5%)
3	2KT	C	502	-	3,6,6	1.12	0	2,7,7	1.09	0

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	C	401	1	-	0/6/6/8	0/1/1/1
2	PLP	D	401	1	-	0/6/6/8	0/1/1/1
3	2KT	A	501	-	-	0/2/6/6	-
2	PLP	B	401	1	-	0/6/6/8	0/1/1/1
2	PLP	A	401	1	-	0/6/6/8	0/1/1/1
3	2KT	C	502	-	-	2/2/6/6	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PLP	C5-C4	3.93	1.44	1.40
2	B	401	PLP	C2A-C2	3.29	1.56	1.50
2	A	401	PLP	C2A-C2	3.19	1.55	1.50
2	B	401	PLP	C5-C4	3.13	1.44	1.40
2	B	401	PLP	C3-C2	3.12	1.44	1.40
2	C	401	PLP	C5-C4	3.10	1.43	1.40
2	D	401	PLP	C5-C4	2.97	1.43	1.40
2	D	401	PLP	C2A-C2	2.86	1.55	1.50
2	A	401	PLP	C3-C4	2.77	1.45	1.40
2	C	401	PLP	C3-C2	2.57	1.43	1.40
2	D	401	PLP	C3-C4	2.45	1.45	1.40
2	B	401	PLP	C4A-C4	2.14	1.56	1.51
2	C	401	PLP	C6-C5	2.13	1.42	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PLP	C6-C5	2.11	1.42	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PLP	C6-N1-C2	2.07	123.01	119.17
2	C	401	PLP	C6-N1-C2	2.06	122.99	119.17
3	A	501	2KT	C4-C3-C2	-2.01	111.07	114.03

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	502	2KT	O3-C2-C3-C4
3	C	502	2KT	C1-C2-C3-C4

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	SO4	1	0
3	A	501	2KT	7	0
2	B	401	PLP	1	0
2	A	401	PLP	1	0
3	C	502	2KT	5	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.