Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2021 – 07:04 pm GMT

PDB ID	:	5E25
Title	:	Crystal structure of branched-chain aminotransferase from thermophilic archaea Geoglobus acetivorans complexed with alpha-ketoglutarate
Authors	:	Boyko, K.M.; Nikolaeva, A.Y.; Stekhanova, T.N.; Mardanov, A.V.; Rakitin, A.L.; Ravin, N.V.; Popov, V.O.
Deposited on	:	2015-09-30
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

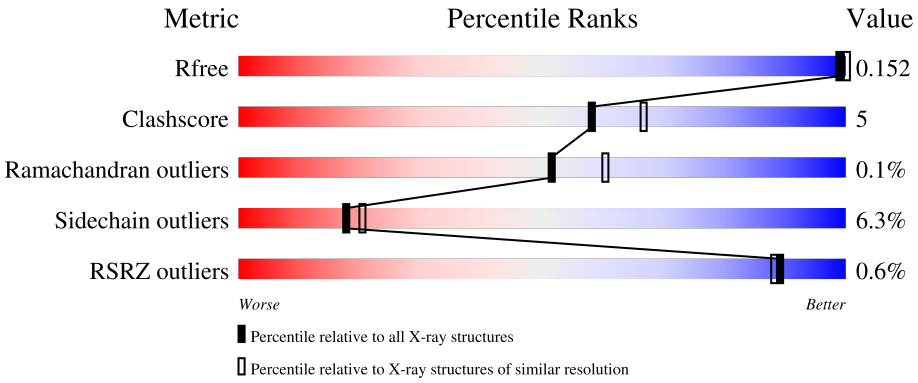
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17.2.dev2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.2.dev2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	291	81% 15%
1	B	291	88% 9%
1	C	291	87% 10%

2 Entry composition

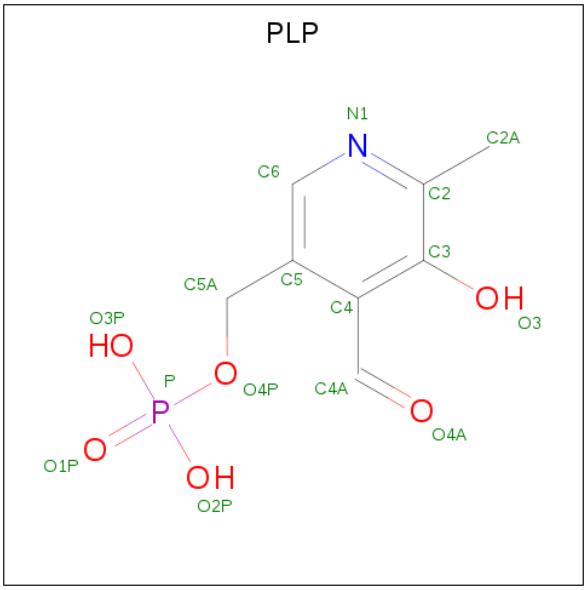
There are 4 unique types of molecules in this entry. The entry contains 7354 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 aminotransferase.

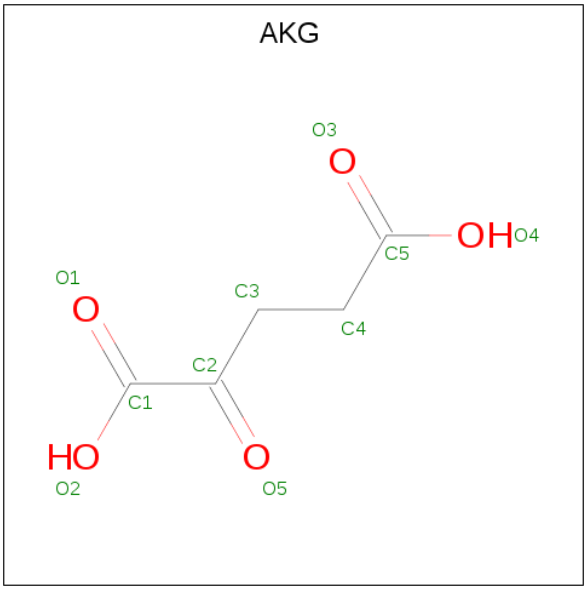
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	4	0
			2262	1450	380	427	5			
1	B	289	Total	C	N	O	S	0	8	0
			2289	1460	386	438	5			
1	C	285	Total	C	N	O	S	0	7	0
			2240	1429	382	424	5			

- 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	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		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 5 5	0	0

- Molecule 4 is water.

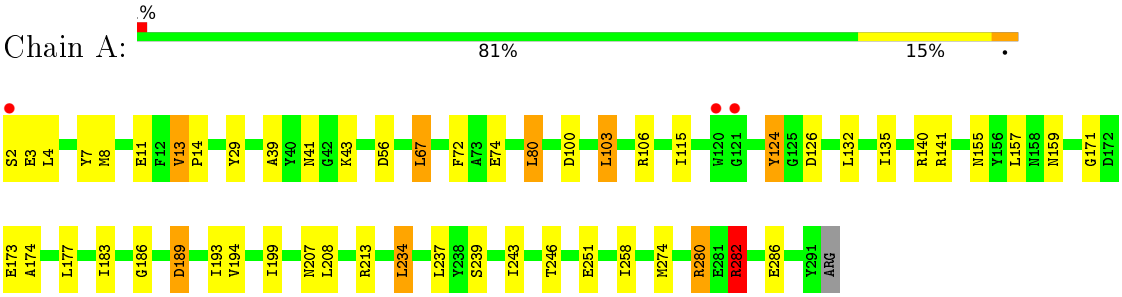
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	150	Total O 150 150	0	0
4	B	178	Total O 178 178	0	0
4	C	180	Total O 180 180	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

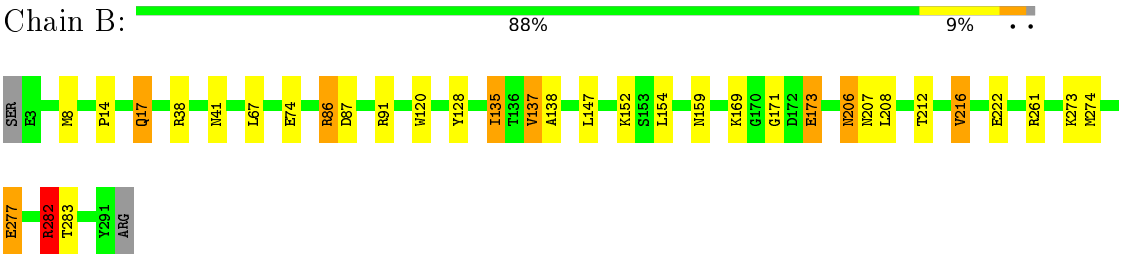
- Molecule 1: branched-chain aminotransferase

Chain A:



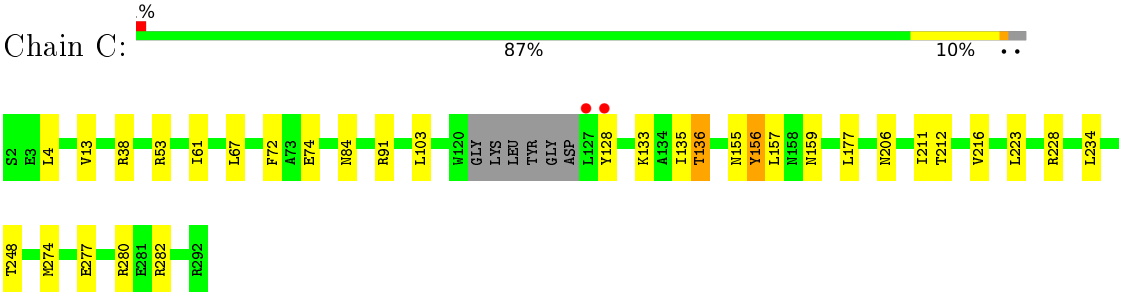
- Molecule 1: branched-chain aminotransferase

Chain B:



- Molecule 1: branched-chain aminotransferase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	117.31Å 117.31Å 135.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.65 – 2.20 58.66 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.65-2.20) 99.8 (58.66-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.25 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.150 , 0.208 0.154 , 0.152	Depositor DCC
R_{free} test set	2635 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7354	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, AKG

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	0.95	0/2326	1.06	14/3154 (0.4%)
1	B	0.97	2/2374 (0.1%)	1.07	11/3216 (0.3%)
1	C	0.97	0/2320	1.00	5/3142 (0.2%)
All	All	0.96	2/7020 (0.0%)	1.04	30/9512 (0.3%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	173[A]	GLU	CD-OE2	5.31	1.31	1.25
1	B	173[B]	GLU	CD-OE2	5.31	1.31	1.25

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	261	ARG	NE-CZ-NH1	-9.02	115.79	120.30
1	A	141	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	B	137	VAL	CG1-CB-CG2	7.57	123.00	110.90
1	B	274	MET	CG-SD-CE	7.46	112.14	100.20
1	A	282	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	B	216	VAL	CG1-CB-CG2	7.18	122.39	110.90
1	A	106	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	80	LEU	CA-CB-CG	6.79	130.92	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	137	VAL	CB-CA-C	6.78	124.29	111.40
1	B	91	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	C	280	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	141	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	274	MET	CG-SD-CE	6.17	110.07	100.20
1	A	213	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	213	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	C	177	LEU	CA-CB-CG	6.10	129.34	115.30
1	C	280	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	91	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	C	177	LEU	CB-CG-CD1	5.79	120.84	111.00
1	A	56	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	124	TYR	N-CA-C	5.58	126.06	111.00
1	A	140	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	67	LEU	CA-CB-CG	5.41	127.74	115.30
1	B	282[A]	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	B	282[B]	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	B	137	VAL	CA-CB-CG1	5.35	118.92	110.90
1	B	137	VAL	N-CA-CB	-5.31	99.83	111.50
1	C	91	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	234	LEU	CB-CG-CD1	5.19	119.82	111.00
1	A	237	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	TYR	Peptide

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	2262	0	2243	29	0
1	B	2289	0	2263	24	0
1	C	2240	0	2202	25	0
2	A	15	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	6	1	0
2	C	15	0	6	0	0
3	A	10	0	4	0	0
4	A	150	0	0	1	0
4	B	178	0	0	4	0
4	C	180	0	0	5	0
All	All	7354	0	6731	66	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 5.

All (66) 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:C:156[B]:TYR:HE1	4:C:540:HOH:O	0.96	1.28
1:C:156[B]:TYR:CE1	4:C:540:HOH:O	1.63	1.25
1:A:280[A]:ARG:HH11	1:A:280[A]:ARG:HG2	1.30	0.94
1:C:74[A]:GLU:OE1	4:C:401:HOH:O	1.86	0.94
1:A:280[A]:ARG:HG2	1:A:280[A]:ARG:NH1	1.86	0.88
1:C:84[A]:ASN:OD1	4:C:402:HOH:O	1.92	0.87
1:B:277[B]:GLU:OE1	4:B:401:HOH:O	1.96	0.83
1:B:138:ALA:CB	1:C:136:THR:HG23	2.10	0.81
1:A:155:ASN:HD21	1:C:157:LEU:H	1.26	0.80
1:A:157:LEU:H	1:C:155:ASN:HD21	1.30	0.78
1:B:207:ASN:HD22	1:B:208:LEU:H	1.32	0.77
1:A:207:ASN:HD22	1:A:208:LEU:H	1.35	0.75
1:B:138:ALA:HB2	1:C:136:THR:HG23	1.67	0.75
1:A:100:ASP:HB3	4:A:537:HOH:O	1.85	0.75
1:B:277[B]:GLU:CD	4:B:401:HOH:O	2.27	0.72
1:B:206:ASN:HD22	1:B:206:ASN:C	1.96	0.69
1:A:177:LEU:HD22	1:A:183:ILE:HD13	1.81	0.63
1:B:41:ASN:OD1	1:B:86:ARG:NH1	2.31	0.63
4:B:521:HOH:O	1:C:135:ILE:HD11	1.99	0.63
1:B:169:LYS:NZ	1:C:136:THR:HG22	2.15	0.62
1:A:282:ARG:HD2	1:A:286:GLU:OE1	2.02	0.60
1:A:3:GLU:OE1	1:A:14:PRO:HB3	2.02	0.59
1:A:207:ASN:ND2	1:A:208:LEU:H	2.00	0.59
1:B:169:LYS:HZ3	1:C:136:THR:HG22	1.67	0.59
1:B:135:ILE:HG12	1:B:171:GLY:HA3	1.84	0.59
1:B:207:ASN:ND2	1:B:208:LEU:H	2.00	0.58
1:A:155:ASN:ND2	1:C:157:LEU:H	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:HG12	1:A:171:GLY:HA3	1.85	0.57
1:C:212:THR:O	1:C:216:VAL:HG13	2.04	0.56
1:A:280[A]:ARG:HH11	1:A:280[A]:ARG:CG	2.05	0.55
1:B:138:ALA:HB3	1:C:136:THR:HG23	1.89	0.55
1:B:159:ASN:H	1:B:159:ASN:HD22	1.52	0.55
1:C:84[A]:ASN:CG	4:C:402:HOH:O	2.40	0.55
1:A:159:ASN:H	1:A:159:ASN:HD22	1.54	0.54
1:B:222:GLU:OE1	1:B:282[B]:ARG:NH2	2.35	0.54
1:B:277[B]:GLU:OE2	4:B:401:HOH:O	2.19	0.53
1:C:159:ASN:ND2	1:C:159:ASN:H	2.07	0.52
1:B:159:ASN:H	1:B:159:ASN:ND2	2.06	0.52
1:B:206:ASN:C	1:B:206:ASN:ND2	2.63	0.52
1:A:280[A]:ARG:NH1	1:A:280[A]:ARG:CG	2.62	0.51
1:B:212:THR:O	1:B:216:VAL:HG13	2.10	0.50
1:B:14:PRO:HG2	1:B:17:GLN:HB2	1.92	0.50
1:A:8:MET:HG3	1:A:13:VAL:HG13	1.94	0.48
1:B:128:TYR:HD1	1:B:273:LYS:HG2	1.79	0.48
1:C:223:LEU:HD13	1:C:274:MET:HE2	1.94	0.48
1:A:194:VAL:HG22	1:A:199:ILE:HG12	1.94	0.48
1:A:159:ASN:H	1:A:159:ASN:ND2	2.13	0.47
1:B:38[A]:ARG:NH2	1:B:120:TRP:HB3	2.31	0.45
1:A:174:ALA:O	1:A:186:GLY:HA2	2.17	0.45
1:A:39:ALA:HA	1:A:43:LYS:O	2.16	0.45
1:C:206:ASN:OD1	1:C:206:ASN:C	2.56	0.44
1:C:159:ASN:H	1:C:159:ASN:HD22	1.64	0.44
1:A:246:THR:HA	1:A:251:GLU:O	2.17	0.44
1:A:193:ILE:HG22	1:A:243:ILE:HG12	2.01	0.43
1:A:157:LEU:HD21	1:C:61:ILE:HG21	2.00	0.42
1:A:173:GLU:OE1	1:A:189:ASP:OD1	2.37	0.42
1:A:157:LEU:H	1:C:155:ASN:ND2	2.06	0.42
1:C:53:ARG:CZ	1:C:211:ILE:HD12	2.49	0.42
1:A:103:LEU:HD13	1:C:156[A]:TYR:HE2	1.85	0.42
1:A:29:TYR:HB3	1:C:156[A]:TYR:HB3	2.02	0.42
1:A:7:TYR:HB3	1:A:115:ILE:HB	2.02	0.41
1:B:152:LYS:NZ	2:B:301:PLP:O3	2.54	0.41
1:B:135:ILE:HG12	1:B:171:GLY:CA	2.48	0.41
1:A:177:LEU:HD22	1:A:183:ILE:CD1	2.49	0.41
1:C:38:ARG:HG2	1:C:248:THR:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	292/291 (100%)	279 (96%)	13 (4%)	0	100 100
1	B	295/291 (101%)	283 (96%)	12 (4%)	0	100 100
1	C	287/291 (99%)	275 (96%)	11 (4%)	1 (0%)	41 46
All	All	874/873 (100%)	837 (96%)	36 (4%)	1 (0%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	128	TYR

5.3.2 Protein sidechains (i)

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	238/246 (97%)	218 (92%)	20 (8%)	11 11
1	B	245/246 (100%)	228 (93%)	17 (7%)	15 16
1	C	238/246 (97%)	225 (94%)	13 (6%)	21 26
All	All	721/738 (98%)	671 (93%)	50 (7%)	18 16

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	4	LEU

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Mol	Chain	Res	Type
1	A	11	GLU
1	A	13	VAL
1	A	41	ASN
1	A	67	LEU
1	A	72	PHE
1	A	74	GLU
1	A	80	LEU
1	A	103	LEU
1	A	126	ASP
1	A	132	LEU
1	A	189	ASP
1	A	234	LEU
1	A	239[A]	SER
1	A	239[B]	SER
1	A	258	ILE
1	A	280[A]	ARG
1	A	280[B]	ARG
1	A	282	ARG
1	B	8	MET
1	B	17	GLN
1	B	67	LEU
1	B	74[A]	GLU
1	B	74[B]	GLU
1	B	86	ARG
1	B	87	ASP
1	B	135	ILE
1	B	137	VAL
1	B	147	LEU
1	B	154	LEU
1	B	206	ASN
1	B	277[A]	GLU
1	B	277[B]	GLU
1	B	282[A]	ARG
1	B	282[B]	ARG
1	B	283	THR
1	C	4	LEU
1	C	13	VAL
1	C	67	LEU
1	C	72	PHE
1	C	103	LEU
1	C	133	LYS
1	C	136	THR

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Mol	Chain	Res	Type
1	C	156[A]	TYR
1	C	156[B]	TYR
1	C	228	ARG
1	C	234	LEU
1	C	277	GLU
1	C	282	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	150	ASN
1	A	155	ASN
1	A	159	ASN
1	A	167	ASN
1	A	196	ASN
1	A	207	ASN
1	B	112	ASN
1	B	155	ASN
1	B	159	ASN
1	B	180	ASN
1	B	196	ASN
1	B	206	ASN
1	B	207	ASN
1	C	142	ASN
1	C	155	ASN
1	C	159	ASN
1	C	180	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	301	1	15,15,16	3.59	3 (20%)	20,22,23	2.13	6 (30%)
3	AKG	A	302	-	3,9,9	1.29	1 (33%)	4,11,11	1.38	1 (25%)
2	PLP	A	301	1	15,15,16	3.50	3 (20%)	20,22,23	2.11	7 (35%)
2	PLP	C	301	1	15,15,16	4.03	4 (26%)	20,22,23	1.86	7 (35%)

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	301	1	-	1/6/6/8	0/1/1/1
3	AKG	A	302	-	-	0/3/9/9	-
2	PLP	A	301	1	-	0/6/6/8	0/1/1/1
2	PLP	C	301	1	-	1/6/6/8	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	PLP	C3-C2	11.25	1.52	1.40
2	B	301	PLP	C5-C4	9.33	1.50	1.40
2	C	301	PLP	C5-C4	8.80	1.50	1.40
2	A	301	PLP	C3-C2	8.73	1.49	1.40
2	A	301	PLP	C5-C4	8.70	1.50	1.40
2	B	301	PLP	C3-C2	8.27	1.49	1.40
2	C	301	PLP	C3-C4	5.30	1.51	1.40
2	B	301	PLP	C3-C4	4.71	1.49	1.40
2	A	301	PLP	C3-C4	4.31	1.49	1.40
3	A	302	AKG	C3-C2	2.22	1.54	1.51
2	C	301	PLP	C6-C5	2.01	1.41	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	PLP	O3P-P-O4P	-4.52	94.69	106.73
2	B	301	PLP	C6-C5-C4	4.02	121.32	118.16
2	C	301	PLP	C3-C4-C5	-3.89	114.53	118.74
2	C	301	PLP	O4P-P-O1P	-3.69	96.12	106.47
2	A	301	PLP	C6-N1-C2	3.64	125.90	119.17
2	A	301	PLP	O3P-P-O4P	-3.58	97.21	106.73
2	B	301	PLP	C3-C4-C5	-3.35	115.12	118.74
2	A	301	PLP	O3P-P-O2P	3.33	120.38	107.64
2	A	301	PLP	C6-C5-C4	3.21	120.69	118.16
2	B	301	PLP	C5A-C5-C6	-3.01	114.41	119.37
2	C	301	PLP	O4P-C5A-C5	2.94	114.96	109.35
2	A	301	PLP	C3-C4-C5	-2.84	115.67	118.74
2	B	301	PLP	C6-N1-C2	2.83	124.41	119.17
2	B	301	PLP	O4P-C5A-C5	2.80	114.69	109.35
2	A	301	PLP	O3P-P-O1P	2.73	121.36	110.68
2	C	301	PLP	C6-N1-C2	2.54	123.87	119.17
2	C	301	PLP	C3-C2-N1	-2.38	117.69	120.77
2	C	301	PLP	O2P-P-O1P	2.15	119.10	110.68
2	C	301	PLP	C4A-C4-C3	2.12	124.10	120.50
3	A	302	AKG	C3-C4-C5	2.11	116.21	112.67
2	A	301	PLP	C5-C6-N1	-2.02	120.46	123.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	PLP	C4-C5-C5A-O4P
2	C	301	PLP	C6-C5-C5A-O4P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	PLP	1	0

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, 95^{th} 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	290/291 (99%)	-0.56	3 (1%) 82 81	24, 38, 62, 82	0
1	B	289/291 (99%)	-0.64	0 100 100	23, 34, 58, 97	0
1	C	285/291 (97%)	-0.71	2 (0%) 87 86	22, 33, 51, 92	0
All	All	864/873 (98%)	-0.64	5 (0%) 89 88	22, 35, 59, 97	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	127	LEU	4.3
1	A	2	SER	2.7
1	A	120	TRP	2.7
1	A	121	GLY	2.4
1	C	128	TYR	2.2

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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	AKG	A	302	10/10	0.96	0.10	45,48,52,52	0
2	PLP	B	301	15/16	0.99	0.08	25,29,31,33	0
2	PLP	C	301	15/16	0.99	0.07	25,28,31,33	0
2	PLP	A	301	15/16	0.99	0.09	28,32,36,37	0

6.5 Other polymers (i)

There are no such residues in this entry.