wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 12:48 am BST

|		
PDB ID	:	1BKG
Title	:	ASPARTATE AMINOTRANSFERASE FROM THERMUS THER-MOPHILUS WITH MALEATE
Authors	:	Nakai, T.; Okada, K.; Kuramitsu, S.; Hirotsu, K.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	1998-07-07
Resolution	:	2.60 Å(reported)

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 2.60 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.
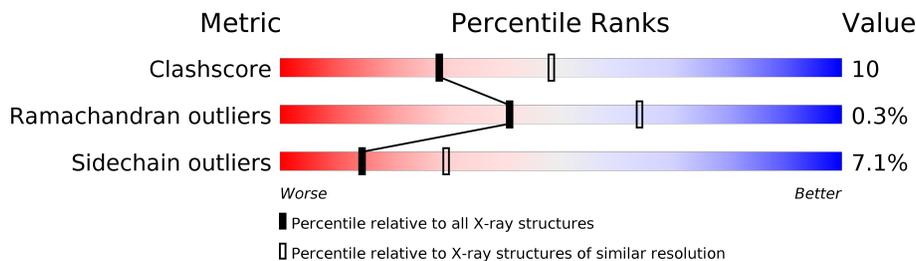
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	385	76% 21% ••
1	B	385	76% 21% ••
1	C	385	78% 19% ••
1	D	385	77% 20% ••

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
2	PMP	A	413	-	-	X	-

Continued on next page...

Continued from previous page...

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PMP	B	413	-	-	X	-
2	PMP	C	413	-	-	X	-
2	PMP	D	413	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12152 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 ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2944	1864	521	551	8			
1	B	382	Total	C	N	O	S	0	0	0
			2944	1864	521	551	8			
1	C	382	Total	C	N	O	S	0	0	0
			2944	1864	521	551	8			
1	D	382	Total	C	N	O	S	0	0	0
			2944	1864	521	551	8			

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: $C_8H_{13}N_2O_5P$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 16	C 8	N 2	O 5	P 1	0	0
2	D	1	Total 16	C 8	N 2	O 5	P 1	0	0

- Molecule 3 is MALEIC ACID (three-letter code: MAE) (formula: $C_4H_4O_4$).

MAE
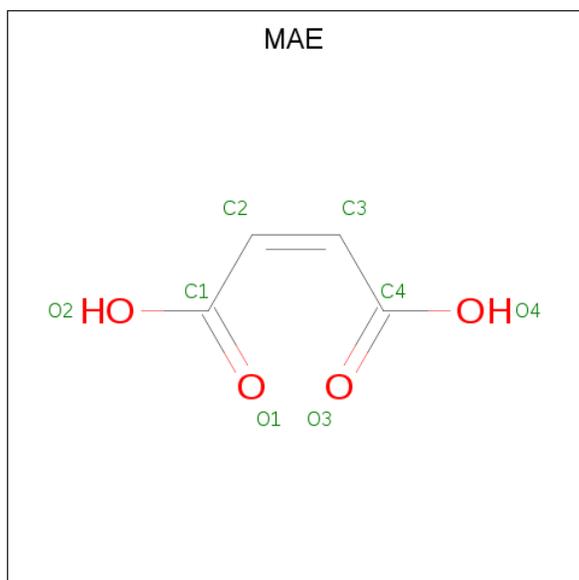
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 8	C 4	O 4	0	0
3	B	1	Total 8	C 4	O 4	0	0
3	C	1	Total 8	C 4	O 4	0	0
3	D	1	Total 8	C 4	O 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total 72	O 72	0	0
4	B	69	Total 69	O 69	0	0
4	C	68	Total 68	O 68	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	71	Total 71	O 71	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. 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: ASPARTATE AMINOTRANSFERASE
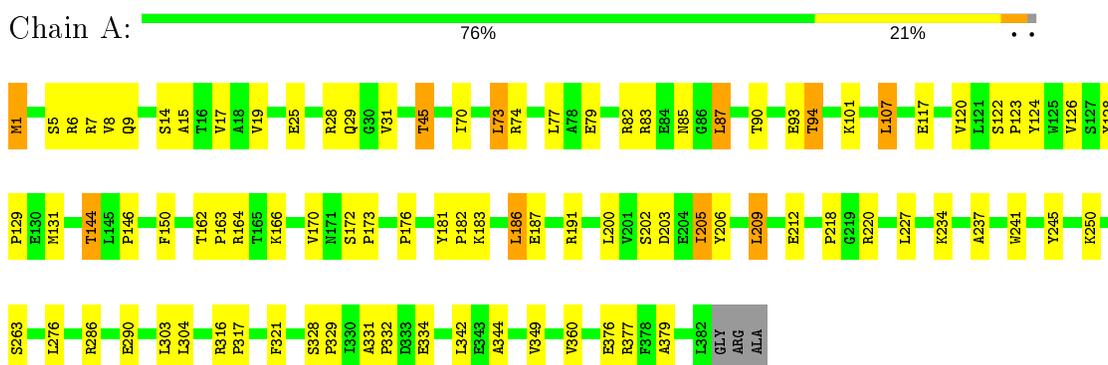
• Molecule 1: ASPARTATE AMINOTRANSFERASE

• Molecule 1: ASPARTATE AMINOTRANSFERASE

R316 P317 F321 S328 P329 I330 A331 P332 D333 E334 L342 E343 A344 V349 V360 E376 R377 F378 A379 R380 V381 L382 GLY ARG ALA
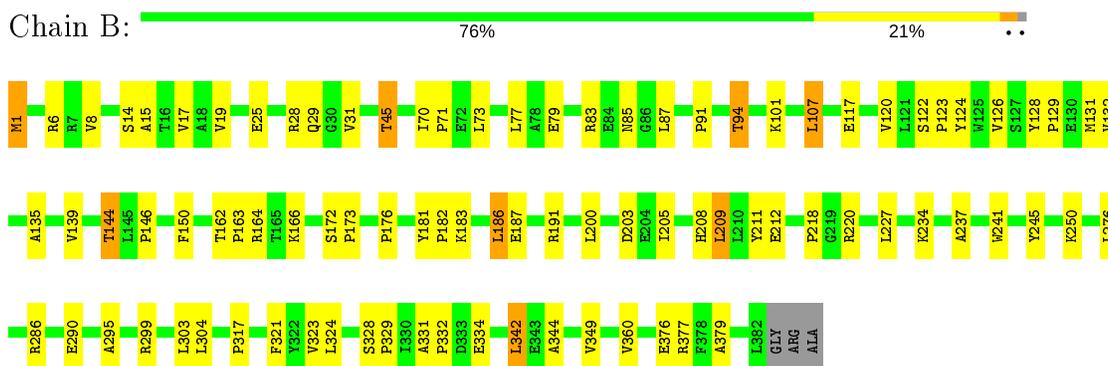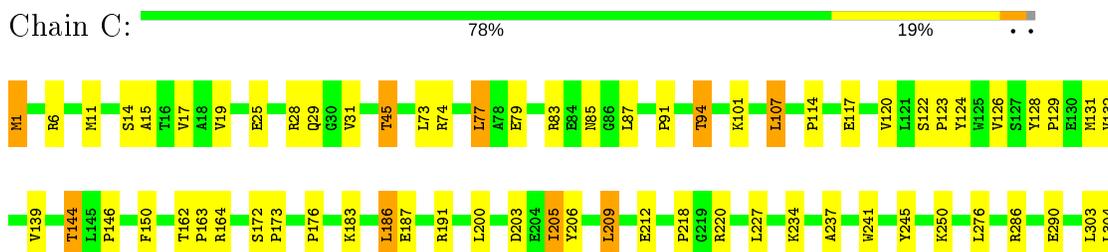
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain D: 77%   20%

M1 R6 R7 V8 S14 A15 T16 V17 A18 V19 E25 R28 Q29 G30 V31 T45 L73 L77 A78 E79 R83 E84 N85 G86 L87 T94 K101 L107 P114 E117 V120 L121 S122 P123 Y124 W125 V126 S127 Y128 P129 E130 M131 V132 T144 L145

P146 F150 T162 P163 R164 T165 K166 V170 N171 S172 P173 P176 Y181 P182 K183 L186 E187 R191 L200 V201 S202 D203 E204 I205 Y206 L209 E212 P218 G219 R220 I227 K234 A237 W241 Y245 K250 Q262 L276 R286

E290 L303 L304 R316 P317 F321 Y322 V323 S328 P329 I330 A331 P332 D333 E334 L342 V349 V360 E376 A379 L382 GLY ARG ALA

4   Data and refinement statistics (i)

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, α, β, γ	80.25Å 109.71Å 197.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	94.3 (8.00-2.60)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.197 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12152	wwPDB-VP
Average B, all atoms (Å^2)	24.0	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: PMP, MAE

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	0.52	0/3005	0.72	0/4086
1	B	0.53	0/3005	0.72	0/4086
1	C	0.52	0/3005	0.72	0/4086
1	D	0.53	0/3005	0.72	0/4086
All	All	0.53	0/12020	0.72	0/16344

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	211	TYR	Sidechain

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	2944	0	2964	63	0
1	B	2944	0	2964	59	0
1	C	2944	0	2964	57	0
1	D	2944	0	2964	58	0
2	A	16	0	11	8	0
2	B	16	0	11	7	0
2	C	16	0	11	8	0
2	D	16	0	11	8	0
3	A	8	0	2	0	0
3	B	8	0	2	0	0
3	C	8	0	2	0	0
3	D	8	0	2	0	0
4	A	72	0	0	1	0
4	B	69	0	0	2	0
4	C	68	0	0	0	0
4	D	71	0	0	0	0
All	All	12152	0	11908	233	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 10.

The worst 5 of 233 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:D:45:THR:HG21	1:D:241:TRP:HE1	1.31	0.93
1:C:45:THR:HG21	1:C:241:TRP:HE1	1.32	0.93
1:B:45:THR:HG21	1:B:241:TRP:HE1	1.32	0.92
1:A:45:THR:HG21	1:A:241:TRP:HE1	1.34	0.91
1:A:6:ARG:HD3	4:A:572:HOH:O	1.77	0.85

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	380/385 (99%)	364 (96%)	15 (4%)	1 (0%)	41	64
1	B	380/385 (99%)	364 (96%)	15 (4%)	1 (0%)	41	64
1	C	380/385 (99%)	364 (96%)	15 (4%)	1 (0%)	41	64
1	D	380/385 (99%)	364 (96%)	15 (4%)	1 (0%)	41	64
All	All	1520/1540 (99%)	1456 (96%)	60 (4%)	4 (0%)	41	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	VAL
1	B	126	VAL
1	C	126	VAL
1	D	126	VAL

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	305/306 (100%)	283 (93%)	22 (7%)	14	29
1	B	305/306 (100%)	283 (93%)	22 (7%)	14	29
1	C	305/306 (100%)	284 (93%)	21 (7%)	15	31
1	D	305/306 (100%)	283 (93%)	22 (7%)	14	29
All	All	1220/1224 (100%)	1133 (93%)	87 (7%)	14	29

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	303	LEU
1	C	87	LEU
1	D	245	TYR
1	B	321	PHE
1	C	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	208	HIS
1	C	59	GLN
1	D	59	GLN
1	B	106	ASN
1	C	208	HIS

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)

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	$\#|Z| > 2$
3	MAE	D	414	-	1,7,7	0.52	0	2,8,8	1.21	0
3	MAE	B	414	-	1,7,7	0.51	0	2,8,8	1.14	0
2	PMP	C	413	-	16,16,16	1.47	2 (12%)	21,23,23	1.63	4 (19%)
2	PMP	D	413	-	16,16,16	1.68	6 (37%)	21,23,23	1.57	3 (14%)
2	PMP	A	413	-	16,16,16	1.68	4 (25%)	21,23,23	1.54	3 (14%)
2	PMP	B	413	-	16,16,16	1.70	4 (25%)	21,23,23	1.62	4 (19%)
3	MAE	C	414	-	1,7,7	0.59	0	2,8,8	1.24	0
3	MAE	A	414	-	1,7,7	0.43	0	2,8,8	1.47	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
3	MAE	D	414	-	-	0/0/5/5	-
3	MAE	B	414	-	-	0/0/5/5	-
2	PMP	C	413	-	-	6/8/8/8	0/1/1/1
2	PMP	D	413	-	-	6/8/8/8	0/1/1/1
2	PMP	A	413	-	-	6/8/8/8	0/1/1/1
2	PMP	B	413	-	-	6/8/8/8	0/1/1/1
3	MAE	C	414	-	-	0/0/5/5	-
3	MAE	A	414	-	-	0/0/5/5	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	413	PMP	C3-C2	-4.29	1.36	1.40
2	A	413	PMP	C3-C2	-3.43	1.37	1.40
2	D	413	PMP	C3-C2	-3.19	1.37	1.40
2	C	413	PMP	P-O3P	-3.01	1.43	1.54
2	D	413	PMP	C2A-C2	2.78	1.55	1.50

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	413	PMP	O3P-P-O4P	4.03	117.46	106.73
2	D	413	PMP	O3P-P-O4P	3.78	116.79	106.73
2	B	413	PMP	O3P-P-O4P	3.55	116.18	106.73
2	B	413	PMP	O4P-C5A-C5	3.42	115.87	109.35
2	A	413	PMP	O4P-C5A-C5	3.39	115.81	109.35

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	413	PMP	C3-C4-C4A-N4A
2	C	413	PMP	C5-C4-C4A-N4A
2	C	413	PMP	C4-C5-C5A-O4P
2	C	413	PMP	C6-C5-C5A-O4P
2	C	413	PMP	C5A-O4P-P-O1P

There are no ring outliers.

4 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	413	PMP	8	0
2	D	413	PMP	8	0
2	A	413	PMP	8	0
2	B	413	PMP	7	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.