



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:15 AM GMT

PDB ID : 1GC3
Title : THERMUS THERMOPHILUS ASPARTATE AMINOTRANSFERASE
TETRA MUTANT 2 COMPLEXED WITH TRYPTOPHAN
Authors : Ura, H.; Nakai, T.; Hirotsu, K.; Kuramitsu, S.
Deposited on : 2000-07-18
Resolution : 3.30 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

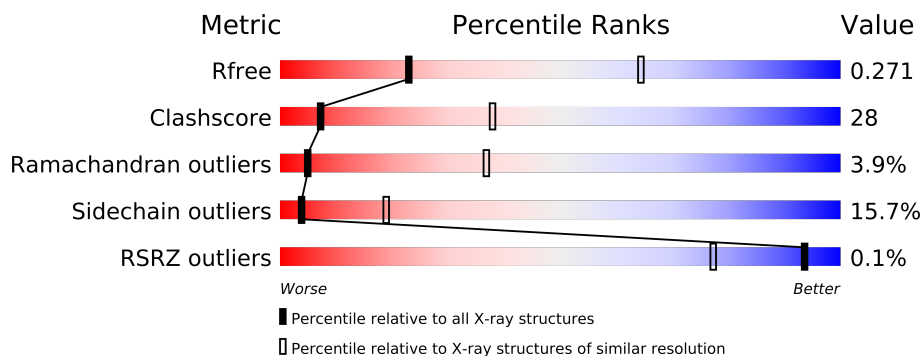
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.30 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}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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 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	385	
1	B	385	
1	C	385	
1	D	385	
1	E	385	
1	F	385	
1	G	385	
1	H	385	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	TRP	A	414	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	TRP	A	914	-	X
2	TRP	C	1414	-	X
2	TRP	D	1914	-	X
2	TRP	E	2414	-	X
2	TRP	E	2914	-	X
2	TRP	G	3414	-	X
2	TRP	H	3914	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23824 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 ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			
1	B	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			
1	C	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			
1	D	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			
1	E	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			
1	F	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			
1	G	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			
1	H	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			

There are 32 discrepancies between the modelled and reference sequences:

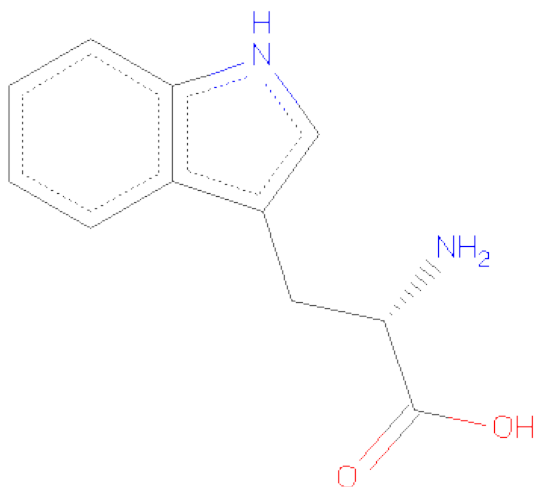
Chain	Residue	Modelled	Actual	Comment	Reference
A	14	ASP	SER	ENGINEERED	UNP Q56232
A	16	VAL	THR	ENGINEERED	UNP Q56232
A	101	SER	LYS	ENGINEERED	UNP Q56232
A	261	ARG	SER	ENGINEERED	UNP Q56232
B	514	ASP	SER	ENGINEERED	UNP Q56232
B	516	VAL	THR	ENGINEERED	UNP Q56232
B	601	SER	LYS	ENGINEERED	UNP Q56232
B	761	ARG	SER	ENGINEERED	UNP Q56232
C	1014	ASP	SER	ENGINEERED	UNP Q56232
C	1016	VAL	THR	ENGINEERED	UNP Q56232
C	1101	SER	LYS	ENGINEERED	UNP Q56232
C	1261	ARG	SER	ENGINEERED	UNP Q56232
D	1514	ASP	SER	ENGINEERED	UNP Q56232

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1516	VAL	THR	ENGINEERED	UNP Q56232
D	1601	SER	LYS	ENGINEERED	UNP Q56232
D	1761	ARG	SER	ENGINEERED	UNP Q56232
E	2014	ASP	SER	ENGINEERED	UNP Q56232
E	2016	VAL	THR	ENGINEERED	UNP Q56232
E	2101	SER	LYS	ENGINEERED	UNP Q56232
E	2261	ARG	SER	ENGINEERED	UNP Q56232
F	2514	ASP	SER	ENGINEERED	UNP Q56232
F	2516	VAL	THR	ENGINEERED	UNP Q56232
F	2601	SER	LYS	ENGINEERED	UNP Q56232
F	2761	ARG	SER	ENGINEERED	UNP Q56232
G	3014	ASP	SER	ENGINEERED	UNP Q56232
G	3016	VAL	THR	ENGINEERED	UNP Q56232
G	3101	SER	LYS	ENGINEERED	UNP Q56232
G	3261	ARG	SER	ENGINEERED	UNP Q56232
H	3514	ASP	SER	ENGINEERED	UNP Q56232
H	3516	VAL	THR	ENGINEERED	UNP Q56232
H	3601	SER	LYS	ENGINEERED	UNP Q56232
H	3761	ARG	SER	ENGINEERED	UNP Q56232

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



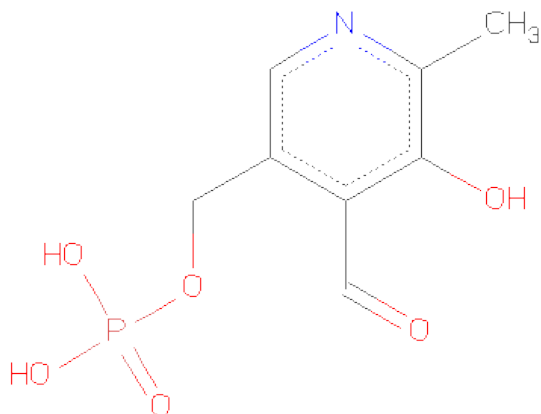
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	A	1	Total	C	N	O	0	0
			15	11	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			15	11	2	2		
2	D	1	Total	C	N	O	0	0
			15	11	2	2		
2	E	1	Total	C	N	O	0	0
			15	11	2	2		
2	E	1	Total	C	N	O	0	0
			15	11	2	2		
2	G	1	Total	C	N	O	0	0
			15	11	2	2		
2	H	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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

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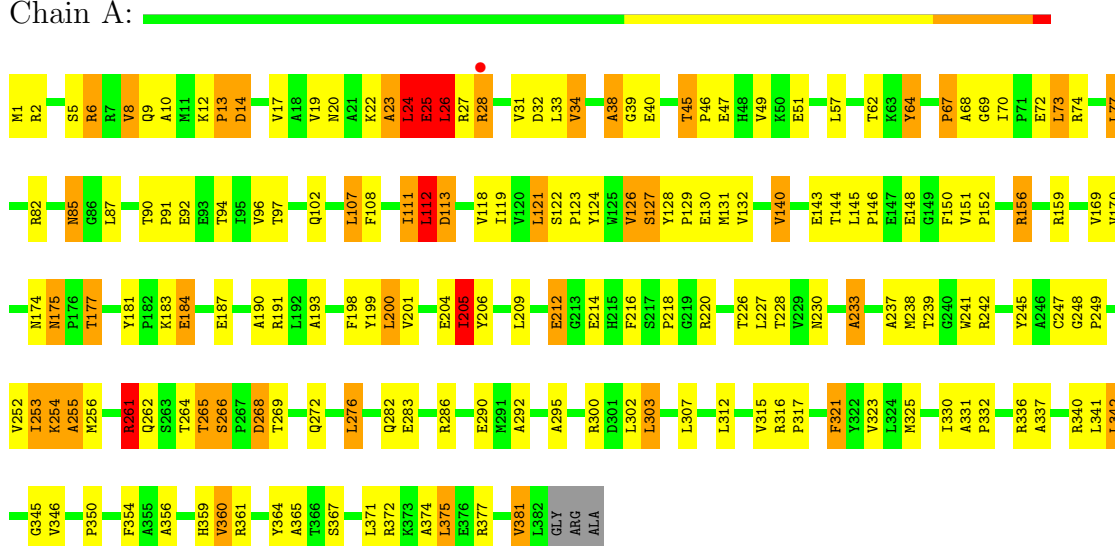
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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.

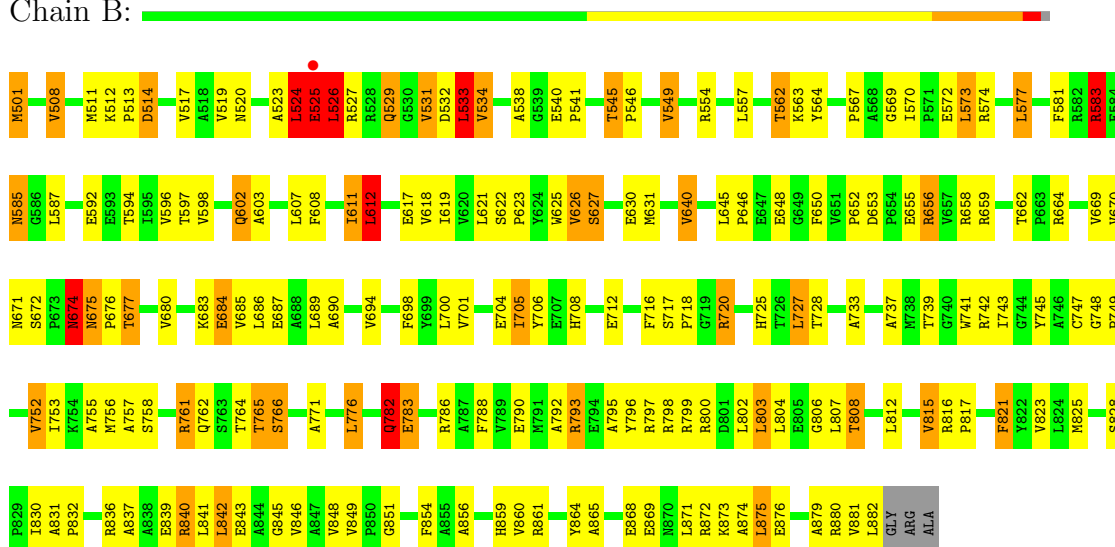
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain A:



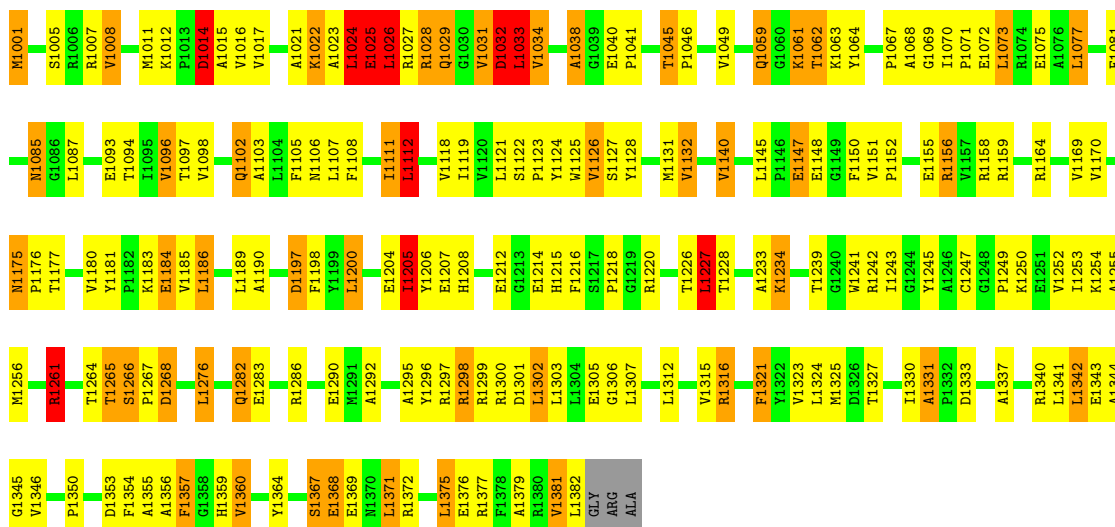
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain B:



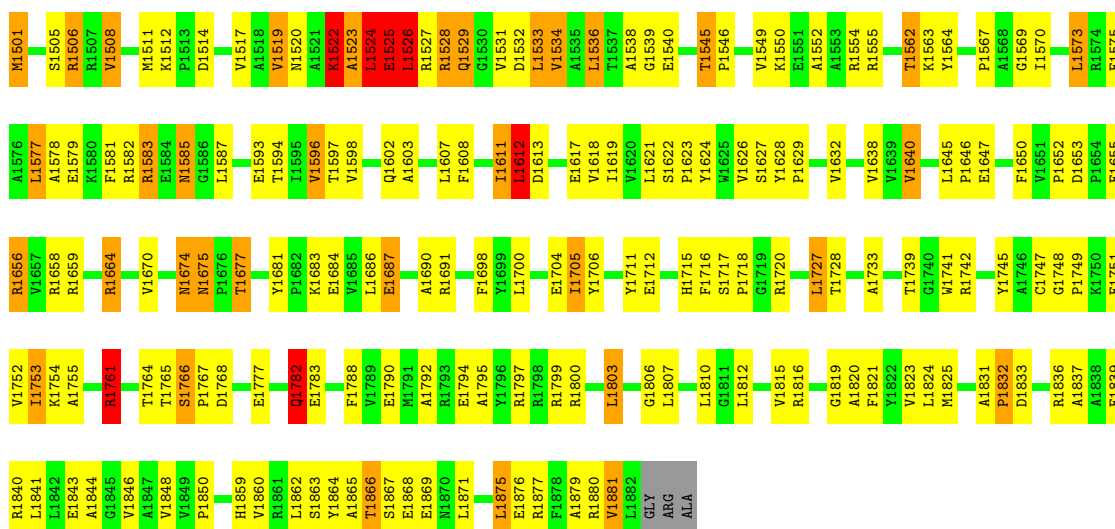
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain C:



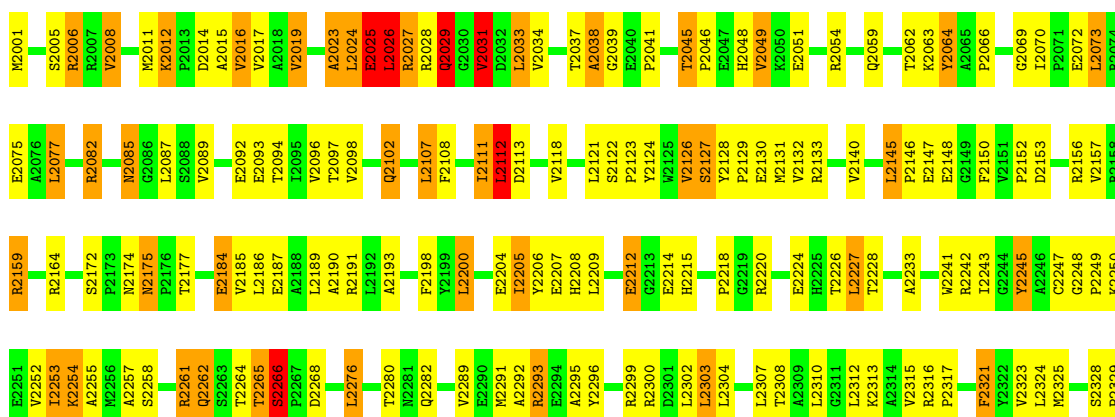
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain D:



• Molecule 1: ASPARTATE AMINOTRANSFERASE

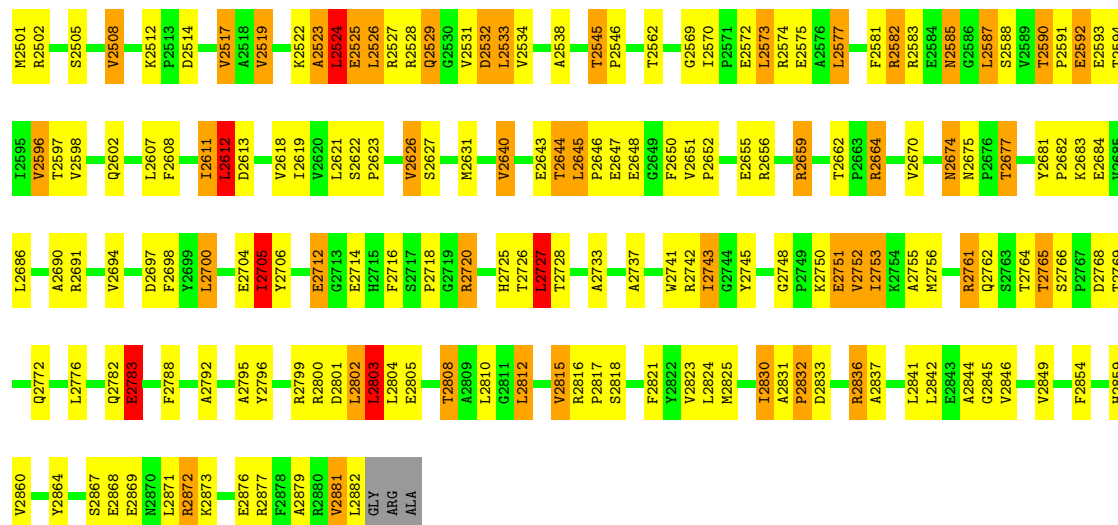
Chain E:





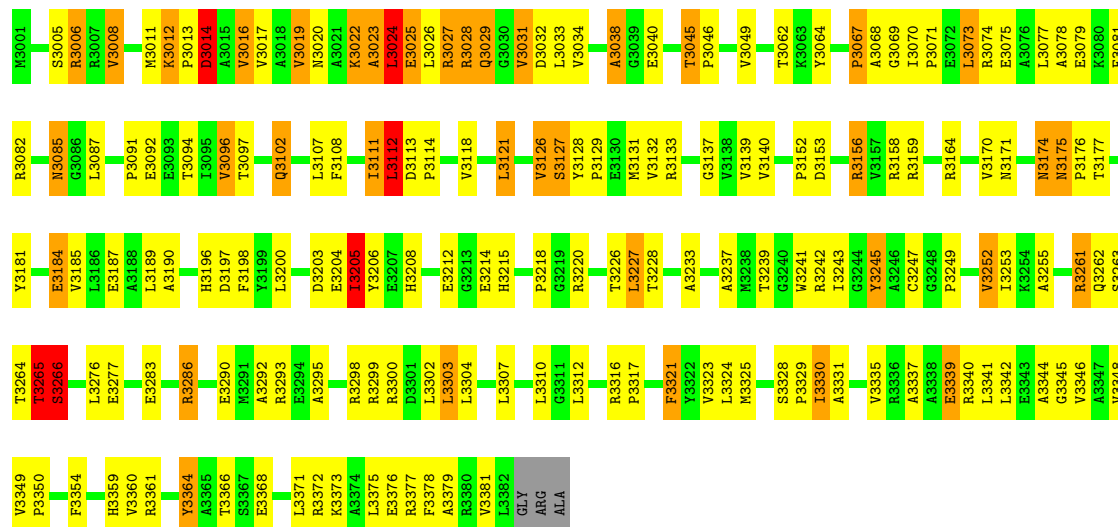
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain F:



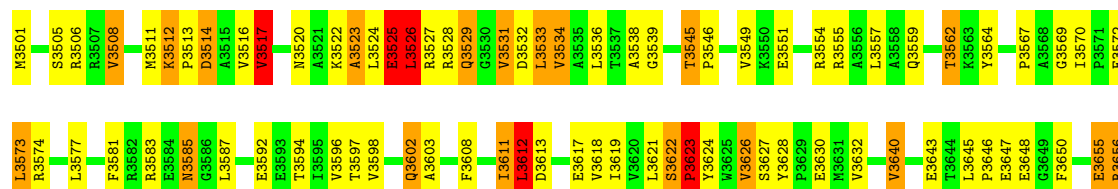
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain G:



• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain H:



E3839	R3840	L3841	L3842	E3843	A3844	G3845	V3846		F3854		H3859	V3860	R3861	L3862	S3863	Y3864	A3865		E3868		L3871	R3872	K3873	A3874	L3875	E3876	R3877	F3878	A3879	R3880	V3881	L3882	GLY	ARG	ALA																								
G3748	P3749	K3750	E3751	V3752	I3753	K3754	A3755		R3761	Q3762	S3763	T3764	T3765	S3766	P3767	D3768		L3776		Q3782	E3783		R3786		E3790	P3791	A3792		A3795	Y3796		R3799	R3800	D3801	L3802	L3803	L3804		L3807		L3812		P3817		F3821	Y3822	V3823	L3824	M3825	D3826	T3827	S3828	P3829	I3830	A3831	P3832		A3837	A3838
V3657	R3658	R3659		R3664		V3670		N3674	N3675	P3676	T3677	G3678		Y3681	P3682	K3683	E3684	V3685	L3686	E3687	A3688	L3689	A3690	R3691	L3692	A3693		F3698	Y3699	L3700		E3704	I3705	Y3706	E3707	H3708	L3709		E3714	H3715	F3716	S3717	P3718	G3719	R3720		T3726	L3727	T3728		A3733		W3741	R3742	I3743	G3744	Y3745	A3746	C3747

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.50Å 98.40Å 187.00Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	8.00 – 3.30 47.58 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (8.00-3.30) 94.9 (47.58-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.33Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.203 , 0.282 0.196 , 0.271	Depositor DCC
R_{free} test set	3992 reflections (10.11%)	DCC
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 31.2	EDS
Estimated twinning fraction	0.049 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	1 of 42518 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23824	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.65 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.0780e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities 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: 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	0.49	4/3009 (0.1%)	1.07	23/4092 (0.6%)
1	B	0.43	1/3009 (0.0%)	1.04	22/4092 (0.5%)
1	C	0.48	2/3009 (0.1%)	1.09	25/4092 (0.6%)
1	D	0.45	1/3009 (0.0%)	1.07	19/4092 (0.5%)
1	E	0.43	0/3009	0.98	12/4092 (0.3%)
1	F	0.42	0/3009	0.98	21/4092 (0.5%)
1	G	0.43	0/3009	0.97	17/4092 (0.4%)
1	H	0.48	3/3009 (0.1%)	0.98	21/4092 (0.5%)
All	All	0.45	11/24072 (0.0%)	1.02	160/32736 (0.5%)

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	2
1	C	0	1
1	D	0	1
1	E	0	1
1	H	0	1
All	All	0	6

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1261	ARG	CG-CD	-10.02	1.26	1.51
1	A	261	ARG	NE-CZ	7.27	1.42	1.33
1	H	3517	VAL	CB-CG2	-7.10	1.38	1.52
1	H	3761	ARG	CG-CD	6.76	1.68	1.51
1	H	3761	ARG	CZ-NH2	6.39	1.41	1.33

The worst 5 of 160 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1261	ARG	NE-CZ-NH2	22.81	131.70	120.30
1	A	261	ARG	NE-CZ-NH1	22.08	131.34	120.30
1	D	1761	ARG	NE-CZ-NH2	21.92	131.26	120.30
1	B	761	ARG	NE-CZ-NH2	18.72	129.66	120.30
1	C	1261	ARG	NH1-CZ-NH2	-15.26	102.62	119.40

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	ARG	Sidechain
1	A	64	TYR	Sidechain
1	C	1261	ARG	Sidechain
1	D	1761	ARG	Sidechain
1	E	2064	TYR	Sidechain

5.2 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 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	2948	0	2965	166	0
1	B	2948	0	2962	207	0
1	C	2948	0	2962	186	0
1	D	2948	0	2962	172	0
1	E	2948	0	2962	193	0
1	F	2948	0	2962	141	0
1	G	2948	0	2962	176	0
1	H	2948	0	2962	181	0
2	A	30	0	18	10	0
2	C	15	0	9	8	0
2	D	15	0	9	11	0
2	E	30	0	18	14	0
2	G	15	0	9	6	0
2	H	15	0	9	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	15	0	6	2	0
3	B	15	0	7	3	0
3	C	15	0	6	4	0
3	D	15	0	6	2	0
3	E	15	0	7	2	0
3	F	15	0	7	0	0
3	G	15	0	6	2	0
3	H	15	0	6	2	0
All	All	23824	0	23822	1342	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 28.

The worst 5 of 1342 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:1414:TRP:CZ3	1:D:1564:TYR:HB3	1.83	1.14
1:A:67:PRO:HB3	1:A:261:ARG:HG3	1.26	1.14
1:G:3261:ARG:CZ	1:H:3517:VAL:HG21	1.78	1.13
1:A:67:PRO:HG2	1:A:68:ALA:N	1.61	1.12
1:G:3067:PRO:HG3	1:G:3261:ARG:NH1	1.66	1.10

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%)	332 (87%)	36 (10%)	12 (3%)	6	43
1	B	380/385 (99%)	322 (85%)	42 (11%)	16 (4%)	4	34
1	C	380/385 (99%)	321 (84%)	41 (11%)	18 (5%)	4	30
1	D	380/385 (99%)	322 (85%)	41 (11%)	17 (4%)	4	32
1	E	380/385 (99%)	323 (85%)	42 (11%)	15 (4%)	5	37
1	F	380/385 (99%)	321 (84%)	45 (12%)	14 (4%)	5	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	380/385 (99%)	325 (86%)	41 (11%)	14 (4%)	5	39
1	H	380/385 (99%)	323 (85%)	43 (11%)	14 (4%)	5	39
All	All	3040/3080 (99%)	2589 (85%)	331 (11%)	120 (4%)	5	37

5 of 120 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	25	GLU
1	A	26	LEU
1	A	205	ILE
1	A	266	SER

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	305/306 (100%)	265 (87%)	40 (13%)	6	28
1	B	305/306 (100%)	263 (86%)	42 (14%)	5	25
1	C	305/306 (100%)	252 (83%)	53 (17%)	3	14
1	D	305/306 (100%)	259 (85%)	46 (15%)	4	21
1	E	305/306 (100%)	246 (81%)	59 (19%)	2	10
1	F	305/306 (100%)	250 (82%)	55 (18%)	2	13
1	G	305/306 (100%)	256 (84%)	49 (16%)	3	17
1	H	305/306 (100%)	269 (88%)	36 (12%)	8	34
All	All	2440/2448 (100%)	2060 (84%)	380 (16%)	4	19

5 of 380 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1803	LEU
1	E	2184	GLU
1	H	3545	THR
1	D	1866	THR

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Mol	Chain	Res	Type
1	E	2045	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	2106	ASN
1	E	2175	ASN
1	H	3782	GLN
1	E	2171	ASN
1	F	2671	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 ⓘ

16 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	PLP	A	413	2	14,15,16	2.02	3 (21%)	20,22,23	1.53	5 (25%)
2	TRP	A	414	3	16,16,16	1.07	1 (6%)	22,22,22	2.17	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TRP	A	914	3	16,16,16	1.37	2 (12%)	22,22,22	5.54	6 (27%)
3	PLP	B	913	2	14,15,16	3.03	5 (35%)	20,22,23	2.29	6 (30%)
3	PLP	C	1413	2	14,15,16	2.22	5 (35%)	20,22,23	2.76	9 (45%)
2	TRP	C	1414	3	16,16,16	1.52	3 (18%)	22,22,22	5.14	4 (18%)
3	PLP	D	1913	2	14,15,16	2.97	6 (42%)	20,22,23	2.53	6 (30%)
2	TRP	D	1914	3	16,16,16	2.17	3 (18%)	22,22,22	4.19	3 (13%)
3	PLP	E	2413	2	14,15,16	1.64	4 (28%)	20,22,23	1.83	7 (35%)
2	TRP	E	2414	3	16,16,16	1.69	2 (12%)	22,22,22	2.33	5 (22%)
2	TRP	E	2914	3	16,16,16	3.53	5 (31%)	22,22,22	3.43	2 (9%)
3	PLP	F	2913	2	14,15,16	3.13	4 (28%)	20,22,23	1.76	5 (25%)
3	PLP	G	3413	2	14,15,16	2.59	5 (35%)	20,22,23	2.24	9 (45%)
2	TRP	G	3414	3	16,16,16	1.38	2 (12%)	22,22,22	4.28	5 (22%)
3	PLP	H	3913	2	14,15,16	2.85	7 (50%)	20,22,23	1.61	3 (15%)
2	TRP	H	3914	3	16,16,16	2.47	2 (12%)	22,22,22	5.09	4 (18%)

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	PLP	A	413	2	-	0/6/6/8	0/1/1/1
2	TRP	A	414	3	-	0/8/8/8	0/0/2/2
2	TRP	A	914	3	-	0/8/8/8	0/0/2/2
3	PLP	B	913	2	-	0/6/6/8	0/1/1/1
3	PLP	C	1413	2	-	0/6/6/8	0/1/1/1
2	TRP	C	1414	3	-	0/8/8/8	0/0/2/2
3	PLP	D	1913	2	-	0/6/6/8	0/1/1/1
2	TRP	D	1914	3	-	0/8/8/8	0/0/2/2
3	PLP	E	2413	2	-	0/6/6/8	0/1/1/1
2	TRP	E	2414	3	-	0/8/8/8	0/0/2/2
2	TRP	E	2914	3	-	0/8/8/8	0/0/2/2
3	PLP	F	2913	2	-	0/6/6/8	0/1/1/1
3	PLP	G	3413	2	-	0/6/6/8	0/1/1/1
2	TRP	G	3414	3	-	0/8/8/8	0/0/2/2
3	PLP	H	3913	2	-	0/6/6/8	0/1/1/1
2	TRP	H	3914	3	-	0/8/8/8	0/0/2/2

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	913	PLP	C4-C5	9.76	1.56	1.39
2	H	3914	TRP	CB-CG	9.17	1.64	1.51
2	E	2914	TRP	CB-CG	-9.00	1.38	1.51
3	D	1913	PLP	C4-C5	7.40	1.52	1.39
3	H	3913	PLP	C4-C5	7.33	1.52	1.39

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	914	TRP	C-CA-N	24.38	149.72	109.36
2	H	3914	TRP	C-CA-N	23.10	147.61	109.36
2	C	1414	TRP	C-CA-N	22.34	146.35	109.36
2	D	1914	TRP	C-CA-N	18.89	140.64	109.36
2	G	3414	TRP	C-CA-N	18.38	139.78	109.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	382/385 (99%)	-0.31	1 (0%) 91 63	3, 17, 38, 57	0
1	B	382/385 (99%)	-0.30	1 (0%) 91 63	3, 18, 40, 66	0
1	C	382/385 (99%)	-0.31	0 100 100	2, 17, 38, 50	0
1	D	382/385 (99%)	-0.33	0 100 100	2, 16, 33, 50	0
1	E	382/385 (99%)	-0.36	0 100 100	2, 16, 37, 53	0
1	F	382/385 (99%)	-0.36	0 100 100	2, 15, 33, 56	0
1	G	382/385 (99%)	-0.37	0 100 100	3, 15, 34, 54	0
1	H	382/385 (99%)	-0.32	0 100 100	3, 17, 37, 60	0
All	All	3056/3080 (99%)	-0.33	2 (0%) 93 77	2, 17, 37, 66	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	ARG	2.1
1	B	525	GLU	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(Å ²)	Q<0.9
2	TRP	D	1914	15/15	0.50	11.58	32,43,59,61	0
2	TRP	G	3414	15/15	0.69	9.35	32,53,59,59	0
2	TRP	C	1414	15/15	0.73	9.20	41,64,68,70	0
2	TRP	E	2414	15/15	0.47	6.83	21,50,56,57	0
2	TRP	E	2914	15/15	0.56	6.70	29,61,76,77	0
2	TRP	A	914	15/15	0.48	6.32	26,59,74,75	0
2	TRP	A	414	15/15	0.53	5.49	35,41,47,49	0
2	TRP	H	3914	15/15	0.37	4.93	23,43,48,49	0
3	PLP	A	413	15/16	0.19	0.98	8,24,34,40	0
3	PLP	C	1413	15/16	0.19	0.90	8,18,24,34	0
3	PLP	E	2413	15/16	0.16	0.62	2,7,23,33	0
3	PLP	H	3913	15/16	0.17	0.13	7,17,27,30	0
3	PLP	D	1913	15/16	0.14	-0.44	2,14,19,26	0
3	PLP	B	913	15/16	0.15	-0.48	2,7,13,20	0
3	PLP	G	3413	15/16	0.14	-0.78	2,5,17,27	0
3	PLP	F	2913	15/16	0.13	-1.05	2,5,16,21	0

6.5 Other polymers

There are no such residues in this entry.