



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 24, 2024 – 12:26 AM EDT

PDB ID : 1ZQ1  
Title : Structure of GatDE tRNA-Dependent Amidotransferase from *Pyrococcus abyssi*  
Authors : Schmitt, E.; Panvert, M.; Blanquet, S.; Mechulam, Y.  
Deposited on : 2005-05-18  
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

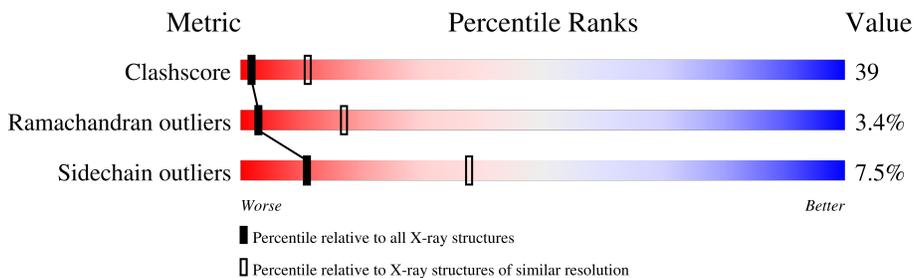
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)

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 of 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	438	41% (green), 52% (yellow), 6% (orange)
1	B	438	41% (green), 51% (yellow), 8% (orange)
2	C	633	37% (green), 38% (yellow), 5% (orange), 20% (grey)
2	D	633	37% (green), 39% (yellow), . (orange), 20% (grey)

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	ASP	A	1000	-	-	X	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 14869 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 Glutamyl-tRNA(Gln) amidotransferase subunit D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	437	3406	2159	578	650	5	14	0	0	0
1	B	437	3406	2162	575	650	5	14	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q9V0T9
A	36	MSE	MET	modified residue	UNP Q9V0T9
A	127	LEU	VAL	conflict	UNP Q9V0T9
A	149	MSE	MET	modified residue	UNP Q9V0T9
A	181	MSE	MET	modified residue	UNP Q9V0T9
A	191	MSE	MET	modified residue	UNP Q9V0T9
A	217	MSE	MET	modified residue	UNP Q9V0T9
A	225	MSE	MET	modified residue	UNP Q9V0T9
A	234	MSE	MET	modified residue	UNP Q9V0T9
A	237	MSE	MET	modified residue	UNP Q9V0T9
A	257	MSE	MET	modified residue	UNP Q9V0T9
A	362	MSE	MET	modified residue	UNP Q9V0T9
A	393	MSE	MET	modified residue	UNP Q9V0T9
A	403	MSE	MET	modified residue	UNP Q9V0T9
A	418	MSE	MET	modified residue	UNP Q9V0T9
A	419	MSE	MET	modified residue	UNP Q9V0T9
B	1	MSE	MET	modified residue	UNP Q9V0T9
B	36	MSE	MET	modified residue	UNP Q9V0T9
B	127	LEU	VAL	conflict	UNP Q9V0T9
B	149	MSE	MET	modified residue	UNP Q9V0T9
B	181	MSE	MET	modified residue	UNP Q9V0T9
B	191	MSE	MET	modified residue	UNP Q9V0T9
B	217	MSE	MET	modified residue	UNP Q9V0T9
B	225	MSE	MET	modified residue	UNP Q9V0T9
B	234	MSE	MET	modified residue	UNP Q9V0T9

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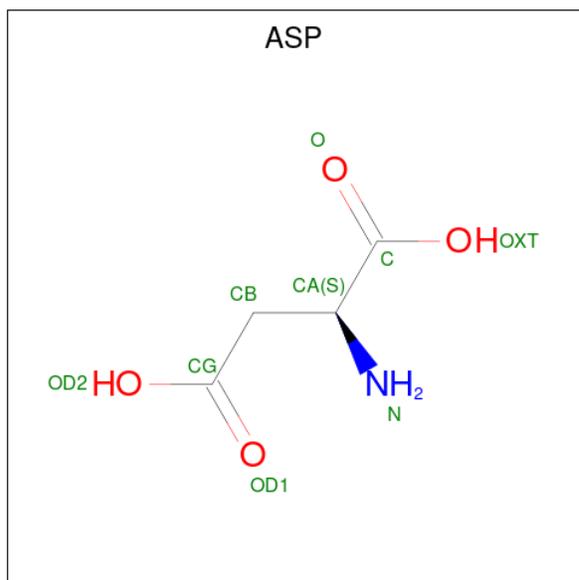
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Chain	Residue	Modelled	Actual	Comment	Reference
B	237	MSE	MET	modified residue	UNP Q9V0T9
B	257	MSE	MET	modified residue	UNP Q9V0T9
B	362	MSE	MET	modified residue	UNP Q9V0T9
B	393	MSE	MET	modified residue	UNP Q9V0T9
B	403	MSE	MET	modified residue	UNP Q9V0T9
B	418	MSE	MET	modified residue	UNP Q9V0T9
B	419	MSE	MET	modified residue	UNP Q9V0T9

- Molecule 2 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	508	Total	C	N	O	S	0	0	0
			4005	2543	700	755	7			
2	D	508	Total	C	N	O	S	0	0	0
			3966	2523	693	743	7			

- Molecule 3 is ASPARTIC ACID (three-letter code: ASP) (formula: C<sub>4</sub>H<sub>7</sub>NO<sub>4</sub>).

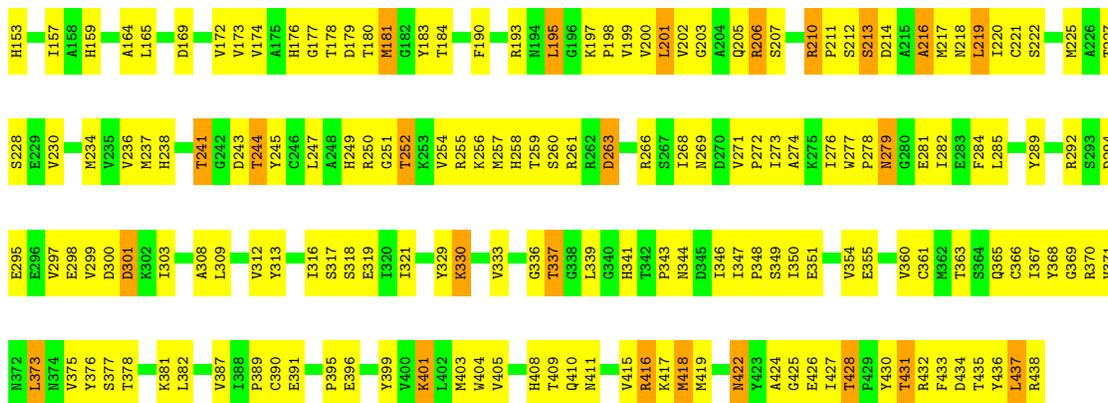


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total	C	N	O	0	0
			9	4	1	4		
3	B	1	Total	C	N	O	0	0
			9	4	1	4		

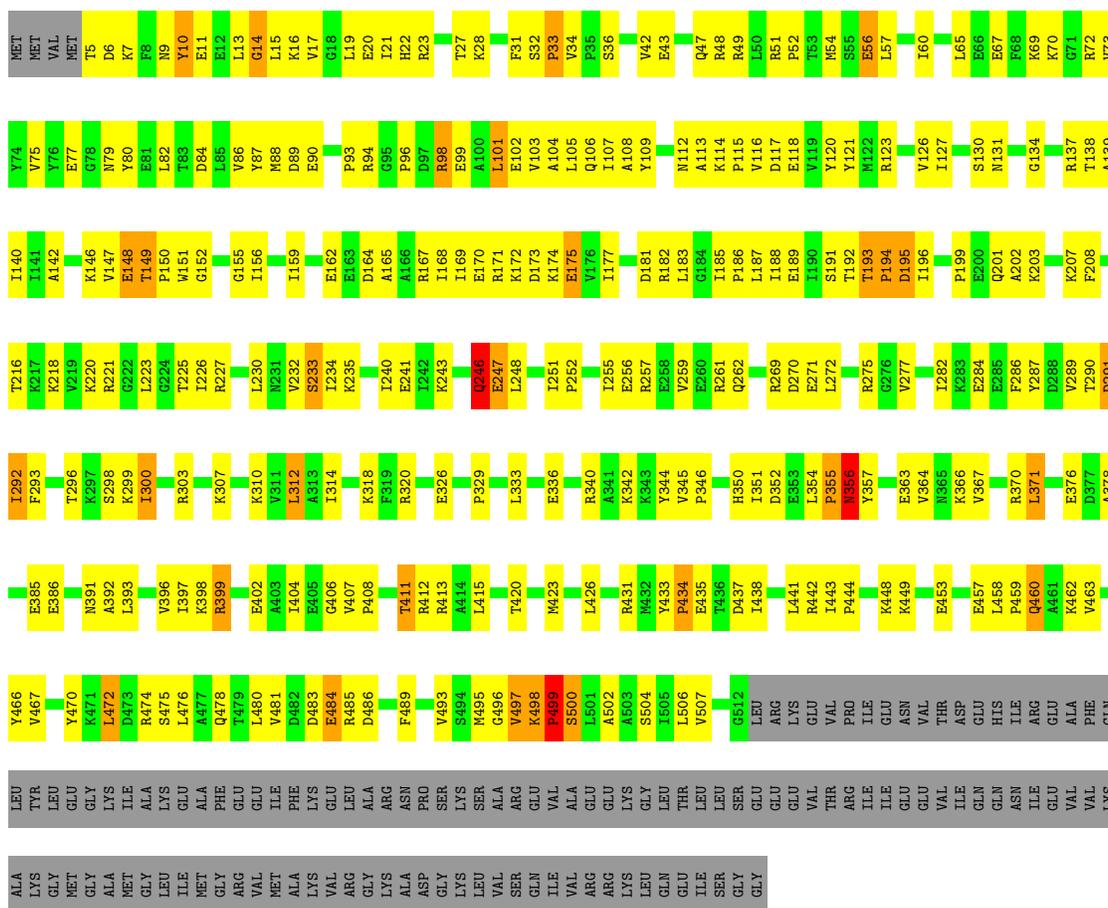
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	B	24	Total O 24 24	0	0
4	C	22	Total O 22 22	0	0
4	D	10	Total O 10 10	0	0





• Molecule 2: Glutamyl-tRNA(Gln) amidotransferase subunit E



• Molecule 2: Glutamyl-tRNA(Gln) amidotransferase subunit E



VAL	L82	A153	K220	T296	N454	PHE	VAL
LYS	V154	V154	R221	K297	E457	GLN	LYS
ALA	G155	G155	G222	S298	L373	LEU	ALA
LYS	I156	I156	L223	L458	P459	TYR	LYS
MET	P157	P157	G224	S374	M459	LEU	MET
GLY	M88	M88	T225	E375	K462	GLY	GLY
ALA	D89	D89	I226	E376	R465	ALA	ALA
ALA	E90	E90	R227	D377	Y466	ILE	MET
LYS	E91	E91	L230	A378	V467	LYS	GLY
LEU	P92	P92	M231	V382	Y470	GLU	LEU
LEU	P93	P93	K310	E385	K471	ALA	MET
ILE	R94	R94	V311	E386	L472	PHE	GLY
MET	G95	G95	L312	K390	L476	GLU	ARG
GLY	P96	P96	A313	N391	L480	GLU	VAL
ARG	A100	A100	I314	A392	E484	VAL	VAL
VAL	L101	L101	R320	L393	M495	VAL	VAL
VAL	A104	A104	F319	R394	G496	LEU	LYS
VAL	Q106	Q106	R320	E395	V497	LEU	ALA
GLY	I107	I107	G324	V396	K498	LEU	VAL
GLY	L110	L110	R325	K398	P499	LEU	LEU
GLY	L111	L111	E326	R399	S500	LEU	LEU
GLY	L116	L116	P329	A400	L501	LEU	LEU
GLY	V117	V117	R401	R401	A502	LEU	LEU
GLY	E118	E118	I404	I404	L506	LEU	LEU
GLY	V119	V119	E409	E409	V507	LEU	LEU
GLY	Y120	Y120	F410	F410	V508	LEU	LEU
GLY	M121	M121	T411	T411	V509	LEU	LEU
GLY	R123	R123	R412	R412	G612	LEU	LEU
GLY	K124	K124	I415	I415	LEU	LEU	LEU
GLY	I125	I125	P416	P416	ARG	LEU	LEU
GLY	V126	V126	D417	D417	GLY	LEU	LEU
GLY	I127	I127	E421	E421	GLY	LEU	LEU
GLY	D128	D128	Y422	Y422	GLY	LEU	LEU
GLY	G129	G129	M423	M423	GLY	LEU	LEU
GLY	S130	S130	R424	R424	GLY	LEU	LEU
GLY	N131	N131	P425	P425	GLY	LEU	LEU
GLY	V132	V132	L426	L426	GLY	LEU	LEU
GLY	F135	F135	R431	R431	GLY	LEU	LEU
GLY	Q136	Q136	E352	E352	GLY	LEU	LEU
GLY	R137	R137	L354	L354	GLY	LEU	LEU
GLY	T138	T138	P355	P355	GLY	LEU	LEU
GLY	A139	A139	X356	X356	GLY	LEU	LEU
GLY	I140	I140	Y357	Y357	GLY	LEU	LEU
GLY	I141	I141	S360	S360	GLY	LEU	LEU
GLY	D144	D144	Q361	Q361	GLY	LEU	LEU
GLY	V147	V147	E362	E362	GLY	LEU	LEU
GLY	E148	E148	P463	P463	GLY	LEU	LEU
GLY	T149	T149	L441	L441	GLY	LEU	LEU
GLY	P150	P150	R442	R442	GLY	LEU	LEU
GLY	W151	W151	I443	I443	GLY	LEU	LEU
GLY	G152	G152	V367	V367	GLY	LEU	LEU
GLY	A153	A153	I368	I368	GLY	LEU	LEU
GLY	V154	V154			GLY	LEU	LEU
GLY	G155	G155			GLY	LEU	LEU
GLY	I156	I156			GLY	LEU	LEU
GLY	P157	P157			GLY	LEU	LEU
GLY	M88	M88			GLY	LEU	LEU
GLY	D89	D89			GLY	LEU	LEU
GLY	E90	E90			GLY	LEU	LEU
GLY	E91	E91			GLY	LEU	LEU
GLY	P92	P92			GLY	LEU	LEU
GLY	R94	R94			GLY	LEU	LEU
GLY	G95	G95			GLY	LEU	LEU
GLY	P96	P96			GLY	LEU	LEU
GLY	A100	A100			GLY	LEU	LEU
GLY	L101	L101			GLY	LEU	LEU
GLY	A104	A104			GLY	LEU	LEU
GLY	Q106	Q106			GLY	LEU	LEU
GLY	I107	I107			GLY	LEU	LEU
GLY	L110	L110			GLY	LEU	LEU
GLY	L111	L111			GLY	LEU	LEU
GLY	L116	L116			GLY	LEU	LEU
GLY	V117	V117			GLY	LEU	LEU
GLY	E118	E118			GLY	LEU	LEU
GLY	V119	V119			GLY	LEU	LEU
GLY	Y120	Y120			GLY	LEU	LEU
GLY	M121	M121			GLY	LEU	LEU
GLY	R123	R123			GLY	LEU	LEU
GLY	K124	K124			GLY	LEU	LEU
GLY	I125	I125			GLY	LEU	LEU
GLY	V126	V126			GLY	LEU	LEU
GLY	I127	I127			GLY	LEU	LEU
GLY	D128	D128			GLY	LEU	LEU
GLY	G129	G129			GLY	LEU	LEU
GLY	S130	S130			GLY	LEU	LEU
GLY	N131	N131			GLY	LEU	LEU
GLY	V132	V132			GLY	LEU	LEU
GLY	F135	F135			GLY	LEU	LEU
GLY	Q136	Q136			GLY	LEU	LEU
GLY	R137	R137			GLY	LEU	LEU
GLY	T138	T138			GLY	LEU	LEU
GLY	A139	A139			GLY	LEU	LEU
GLY	I140	I140			GLY	LEU	LEU
GLY	I141	I141			GLY	LEU	LEU
GLY	D144	D144			GLY	LEU	LEU
GLY	V147	V147			GLY	LEU	LEU
GLY	E148	E148			GLY	LEU	LEU
GLY	T149	T149			GLY	LEU	LEU
GLY	P150	P150			GLY	LEU	LEU
GLY	W151	W151			GLY	LEU	LEU
GLY	G152	G152			GLY	LEU	LEU
GLY	A153	A153			GLY	LEU	LEU
GLY	V154	V154			GLY	LEU	LEU
GLY	G155	G155			GLY	LEU	LEU
GLY	I156	I156			GLY	LEU	LEU
GLY	P157	P157			GLY	LEU	LEU
GLY	M88	M88			GLY	LEU	LEU
GLY	D89	D89			GLY	LEU	LEU
GLY	E90	E90			GLY	LEU	LEU
GLY	E91	E91			GLY	LEU	LEU
GLY	P92	P92			GLY	LEU	LEU
GLY	R94	R94			GLY	LEU	LEU
GLY	G95	G95			GLY	LEU	LEU
GLY	P96	P96			GLY	LEU	LEU
GLY	A100	A100			GLY	LEU	LEU
GLY	L101	L101			GLY	LEU	LEU
GLY	A104	A104			GLY	LEU	LEU
GLY	Q106	Q106			GLY	LEU	LEU
GLY	I107	I107			GLY	LEU	LEU
GLY	L110	L110			GLY	LEU	LEU
GLY	L111	L111			GLY	LEU	LEU
GLY	L116	L116			GLY	LEU	LEU
GLY	V117	V117			GLY	LEU	LEU
GLY	E118	E118			GLY	LEU	LEU
GLY	V119	V119			GLY	LEU	LEU
GLY	Y120	Y120			GLY	LEU	LEU
GLY	M121	M121			GLY	LEU	LEU
GLY	R123	R123			GLY	LEU	LEU
GLY	K124	K124			GLY	LEU	LEU
GLY	I125	I125			GLY	LEU	LEU
GLY	V126	V126			GLY	LEU	LEU
GLY	I127	I127			GLY	LEU	LEU
GLY	D128	D128			GLY	LEU	LEU
GLY	G129	G129			GLY	LEU	LEU
GLY	S130	S130			GLY	LEU	LEU
GLY	N131	N131			GLY	LEU	LEU
GLY	V132	V132			GLY	LEU	LEU
GLY	F135	F135			GLY	LEU	LEU
GLY	Q136	Q136			GLY	LEU	LEU
GLY	R137	R137			GLY	LEU	LEU
GLY	T138	T138			GLY	LEU	LEU
GLY	A139	A139			GLY	LEU	LEU
GLY	I140	I140			GLY	LEU	LEU
GLY	I141	I141			GLY	LEU	LEU
GLY	D144	D144			GLY	LEU	LEU
GLY	V147	V147			GLY	LEU	LEU
GLY	E148	E148			GLY	LEU	LEU
GLY	T149	T149			GLY	LEU	LEU
GLY	P150	P150			GLY	LEU	LEU
GLY	W151	W151			GLY	LEU	LEU
GLY	G152	G152			GLY	LEU	LEU
GLY	A153	A153			GLY	LEU	LEU
GLY	V154	V154			GLY	LEU	LEU
GLY	G155	G155			GLY	LEU	LEU
GLY	I156	I156			GLY	LEU	LEU
GLY	P157	P157			GLY	LEU	LEU
GLY	M88	M88			GLY	LEU	LEU
GLY	D89	D89			GLY	LEU	LEU
GLY	E90	E90			GLY	LEU	LEU
GLY	E91	E91			GLY	LEU	LEU
GLY	P92	P92			GLY	LEU	LEU
GLY	R94	R94			GLY	LEU	LEU
GLY	G95	G95			GLY	LEU	LEU
GLY	P96	P96			GLY	LEU	LEU
GLY	A100	A100			GLY	LEU	LEU
GLY	L101	L101			GLY	LEU	LEU
GLY	A104	A104			GLY	LEU	LEU
GLY	Q106	Q106			GLY	LEU	LEU
GLY	I107	I107			GLY	LEU	LEU
GLY	L110	L110			GLY	LEU	LEU
GLY	L111	L111			GLY	LEU	LEU
GLY	L116	L116			GLY	LEU	LEU
GLY	V117	V117			GLY	LEU	LEU
GLY	E118	E118			GLY	LEU	LEU
GLY	V119	V119			GLY	LEU	LEU
GLY	Y120	Y120			GLY	LEU	LEU
GLY	M121	M121			GLY	LEU	LE

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.70Å 138.20Å 134.40Å 90.00° 109.60° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	98.9 (50.00-3.00)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.217 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	14869	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.41	0/3455	0.72	2/4651 (0.0%)
1	B	0.42	0/3455	0.73	0/4652
2	C	0.39	0/4070	0.69	0/5497
2	D	0.33	0/4031	0.62	0/5450
All	All	0.39	0/15011	0.69	2/20250 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	PRO	N-CA-C	5.26	125.78	112.10
1	A	45	ASP	N-CA-C	-5.25	96.82	111.00

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	3406	0	3410	355	0
1	B	3406	0	3417	335	0
2	C	4005	0	4058	287	0
2	D	3966	0	4003	279	0
3	A	9	0	3	4	0
3	B	9	0	3	1	0
4	A	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	0	0	0
4	C	22	0	0	0	0
4	D	10	0	0	0	0
All	All	14869	0	14894	1160	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 39.

The worst 5 of 1160 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)
2:C:192:THR:HG22	2:C:193:THR:H	1.02	1.12
2:D:192:THR:HG22	2:D:193:THR:H	1.00	1.11
1:B:276:ILE:HG22	1:B:282:ILE:HG12	1.27	1.09
1:A:266:ARG:HD2	1:B:437:LEU:HD21	1.36	1.07
1:A:409:THR:HG22	1:A:411:ASN:H	1.18	1.05

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	435/438 (99%)	374 (86%)	49 (11%)	12 (3%)	4	21
1	B	435/438 (99%)	366 (84%)	56 (13%)	13 (3%)	3	20
2	C	506/633 (80%)	434 (86%)	54 (11%)	18 (4%)	3	16
2	D	506/633 (80%)	428 (85%)	57 (11%)	21 (4%)	2	13
All	All	1882/2142 (88%)	1602 (85%)	216 (12%)	64 (3%)	3	17

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	77	PRO
1	A	78	GLU
1	A	163	LYS
1	A	251	GLY

### 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	366/357 (102%)	338 (92%)	28 (8%)	10	37
1	B	367/357 (103%)	331 (90%)	36 (10%)	6	26
2	C	421/548 (77%)	395 (94%)	26 (6%)	15	45
2	D	412/548 (75%)	384 (93%)	28 (7%)	13	42
All	All	1566/1810 (86%)	1448 (92%)	118 (8%)	11	38

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	391	GLU
2	D	415	LEU
2	C	195	ASP
2	D	399	ARG
2	D	158	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	478	GLN
2	D	361	GLN
2	D	22	HIS
2	D	262	GLN
1	B	153	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 oligosaccharides 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
3	ASP	B	5000	-	7,8,8	1.19	1 (14%)	6,10,10	1.16	1 (16%)
3	ASP	A	1000	-	7,8,8	1.16	1 (14%)	6,10,10	1.02	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	ASP	B	5000	-	-	4/8/8/8	-
3	ASP	A	1000	-	-	4/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	ASP	OXT-C	-2.26	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5000	ASP	OXT-C	-2.24	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5000	ASP	OXT-C-O	-2.11	119.30	124.08

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1000	ASP	O-C-CA-N
3	B	5000	ASP	O-C-CA-N
3	A	1000	ASP	OXT-C-CA-N
3	B	5000	ASP	OXT-C-CA-N
3	A	1000	ASP	OXT-C-CA-CB

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5000	ASP	1	0
3	A	1000	ASP	4	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.