



# 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)
Xtriage (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

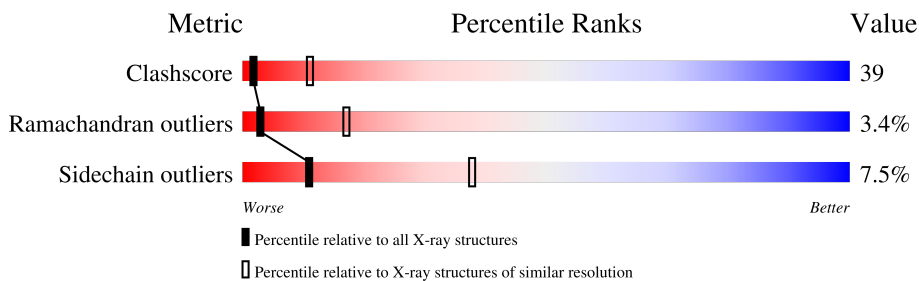
# 1 Overall quality at a glance

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	<div> <div>41%</div> <div>52%</div> <div>6%</div> </div>
1	B	438	<div> <div>41%</div> <div>51%</div> <div>8%</div> </div>
2	C	633	<div> <div>37%</div> <div>38%</div> <div>5%</div> <div>20%</div> </div>
2	D	633	<div> <div>37%</div> <div>39%</div> <div>.</div> <div>20%</div> </div>

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

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
1	A	437	Total	C	N	O	S	Se	0	0	0
			3406	2159	578	650	5	14			
1	B	437	Total	C	N	O	S	Se	0	0	0
			3406	2162	575	650	5	14			

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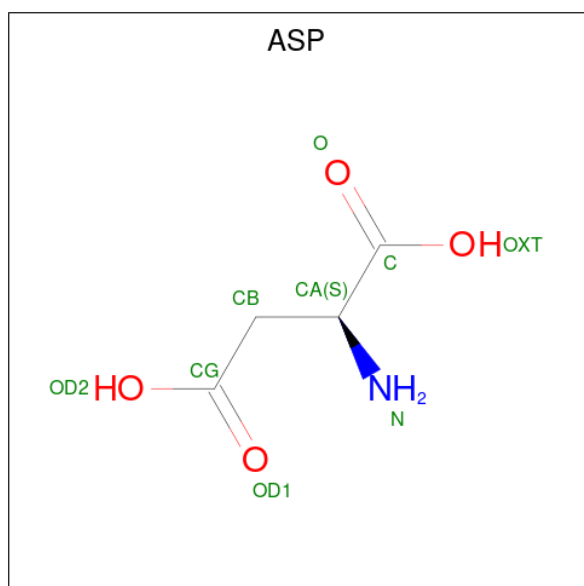
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Chain	Residue	Modelled	Actual	Comment	Reference
B	237	MSE	MET	modified residue	UNP Q9V0T9
B	257	MSE	MET	modified residue	UNP Q9V0T9
B	362	MSE	MET	modified residue	UNP Q9V0T9
B	393	MSE	MET	modified residue	UNP Q9V0T9
B	403	MSE	MET	modified residue	UNP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

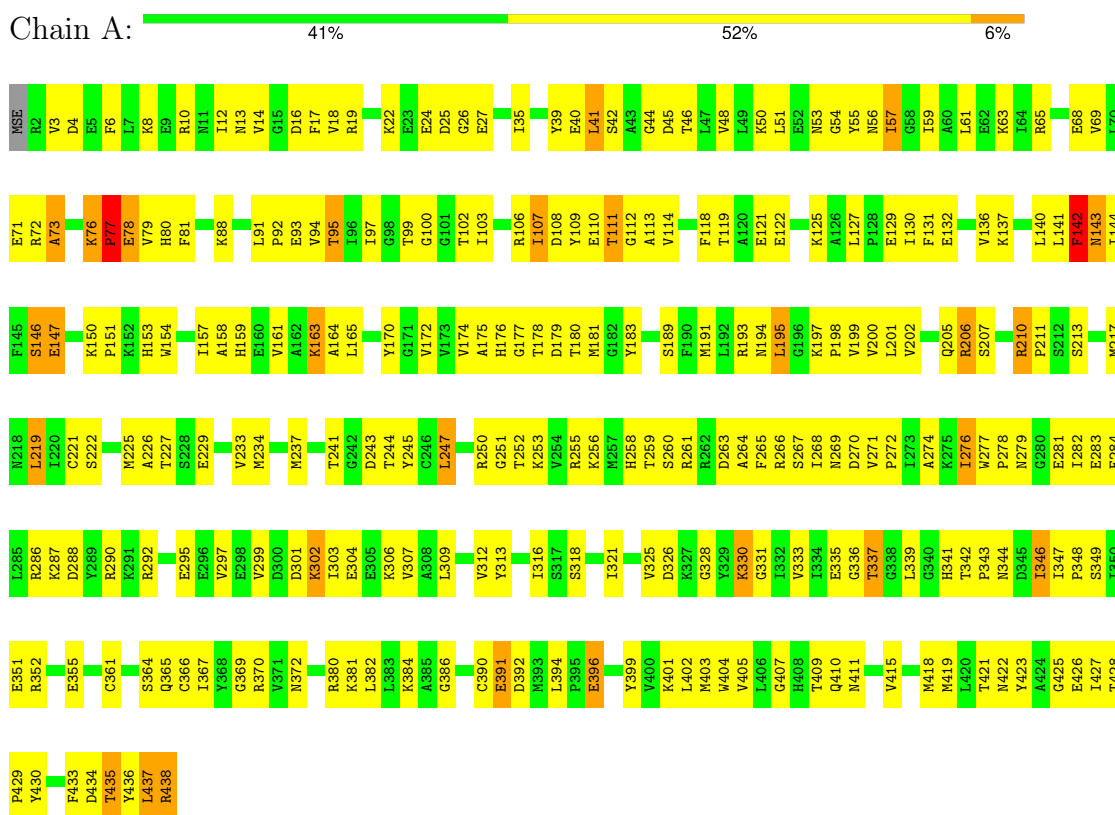
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total 12	O 12	0	0
4	B	24	Total 24	O 24	0	0
4	C	22	Total 22	O 22	0	0
4	D	10	Total 10	O 10	0	0

### 3 Residue-property plots

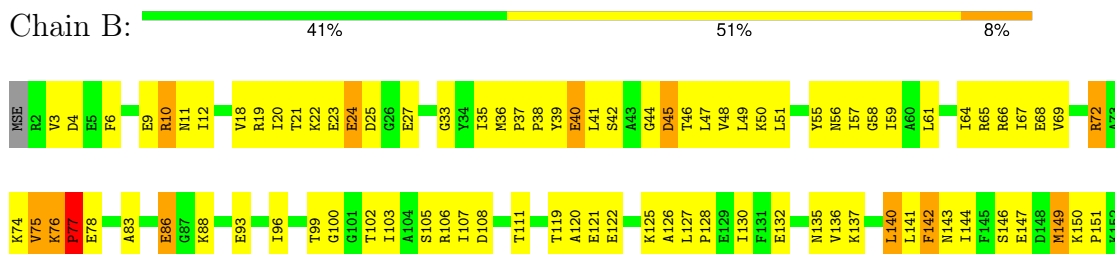
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

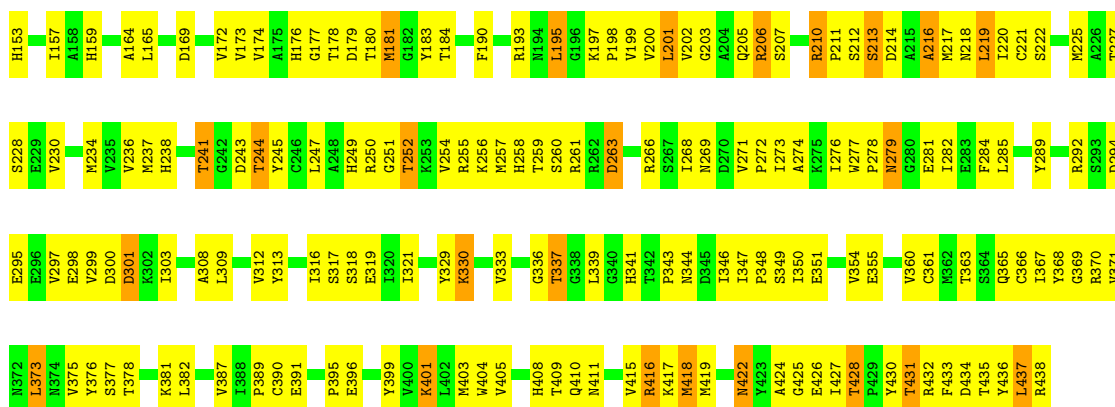
Note EDS was not executed.

#### • Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit D



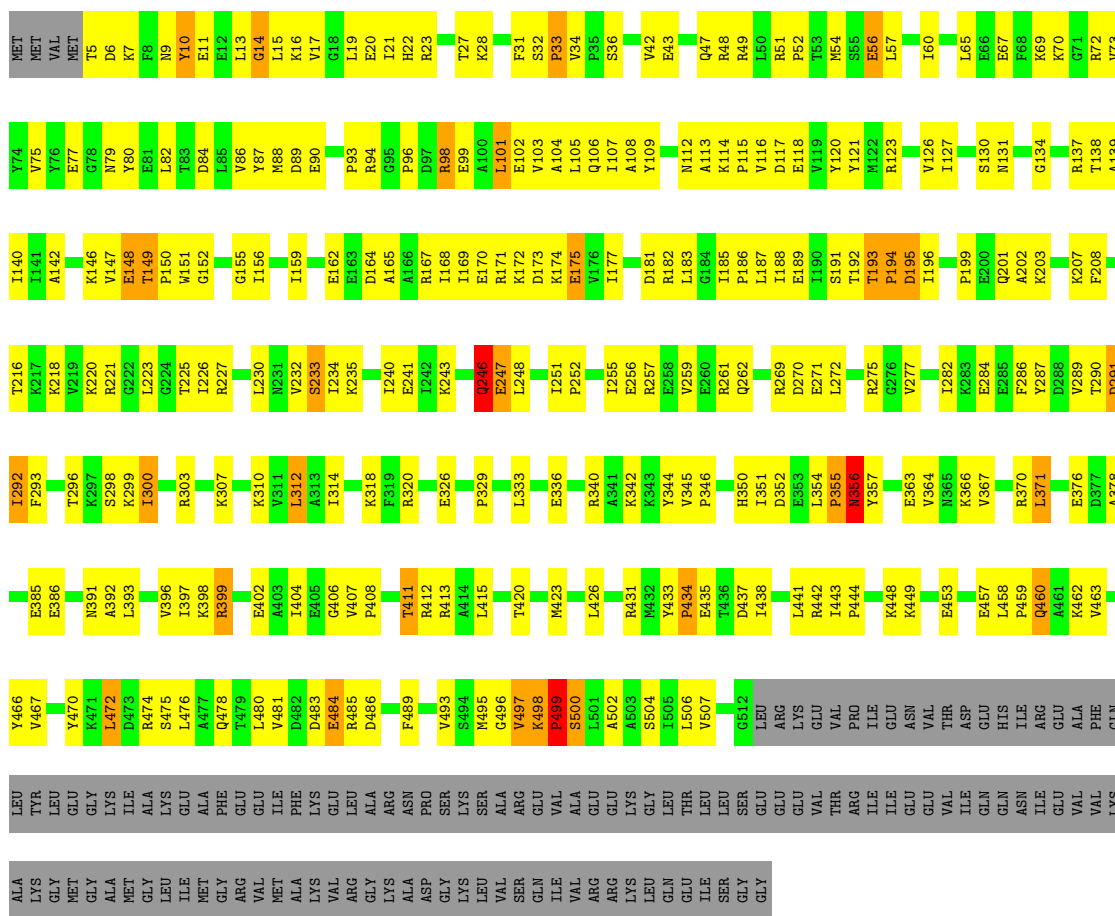
#### • Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit D





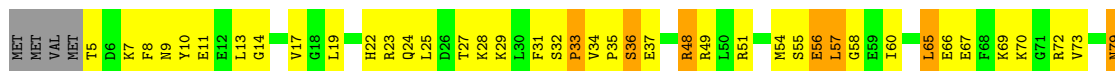
• Molecule 2: Glutamyl-tRNA(Gln) amidotransferase subunit E

Chain C: 37% 38% 5% 20%



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

Chain D: 37% 39% 20%





VAL	PHE	N454	L371	T296	K220	A153	L82
LYS	GLN	E457	N372	K297	R221	V154	L85
ALA	LEU	L458	L373	S298	G222	G155	M88
LYS	TYR	P459	S374	K299	G224	I156	D89
GLY	LEU		E375	I300	T225	T158	E90
MET	GLU	K462	E376	R303	I226	L161	P92
GLY	LYS		D377	V304	R227	E162	R94
ALA	ILE	R465	A378	G309	L230	D163	G95
ALA	LYS	Y466	V382	K310	L231	D164	P96
LEU	GLU	Y467		V311	N234	A165	A100
ILE	ALA	Y470	E385	L312	K235	A166	L101
MET	PHE	K471	E386	A313		R167	A104
GLY	GLU	L472	K390	I314	R239	E170	Q106
ARG	GLU	L476	N391	K318	I240	R171	L110
VAL	ILE	L480	A392	F319	E241	K172	L111
MET	ALA		L393	R320	I242	D173	
LYS	LYS	L484	R394	G324	K243	K174	A104
VAL	GLU	F489	E395	R325	G244		L105
GLY	ALA		V396	R326	Q245	R179	Q106
ALA	ASN	V493	I397	E326	Q246	D181	I107
ASP	PRO	S494	K398		E247	R182	L110
GLY	SER	N495	R399	P329	L248	L183	
LYS	LYS	G496	A400	R332	I251	G184	V116
LEU	SER	V497	R401	L333	P252	I185	D117
VAL	ALA	K498	I404	G334	I253	P186	E118
SER	ARG	P499	E409		I254	L187	V119
GLN	GLU	S500	E410	F337	I255	I188	Y120
ILE	VAL	L501	T411	A338	V259	E189	Y121
VAL	ALA	A502	R412	D339	E260	I190	M122
ARG	GLU			R340	R261	S191	R123
LYS	LYS	I506	I415	A341	Q262	T192	K124
LEU	GLY	L506	P416	K342	L263	T193	I125
LEU	LEU	V507	D417		N264	P194	V126
THR	THR	V508		V345	L265	D195	I127
LEU	LEU	V509	E421	P346	L266	I196	D128
SER	SER	G512	Y422	G347	K267	H197	G129
GLY	GLU	LEU	M423	I348	I268	H198	S130
	GLU	ARG	R424	F349	R269	P199	N131
	GLU	ARG	P425	H350	D270	E200	V132
	GLU	GLY	L426	I351	E271	Q201	
	GLU	THR		D352	L272	A202	F135
	THR	VAL	R431	E353		K203	Q136
	THR	VAL	M432	L354	R275	V204	R137
	ARG	PRO	Y433	P355	G276	V205	T138
	ILE	ILE	P434	K356	K207	A206	A139
	ILE	GLU	E435	Y357	V277	K207	I140
	GLU	ASN	T436		K278	F208	I141
	GLU	VAL	T436	S360	I282	D211	D144
	VAL	THR	D437	Q361	K283	A212	
	ILE	ASP	I438	E362	E284	L213	V147
	GLN	GLU	P439	E363			E148
	GLN	HIS	P440	V364	V289	T216	T149
	ASN	ILE	L441		T290	K217	P150
	ASN	ILE	R442		D291	K218	W151
	ILE	ARG	I443	V367	I292	G152	
	GLU	GLU		I368			
	VAL	ALA					

## 4 Data and refinement statistics

Xtriage (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.	Xtriage
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 ⓘ

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 ⓘ

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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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.