



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:18 am BST

PDB ID : 5U0K  
Title : C-terminal ankyrin repeats from human liver-type glutaminase (GAB/LGA)  
Authors : Ferreira, I.M.; Pasquali, C.C.; Gonzalez, A.; Dias, S.M.G.; Ambrosio, A.L.B.  
Deposited on : 2016-11-24  
Resolution : 2.55 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](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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

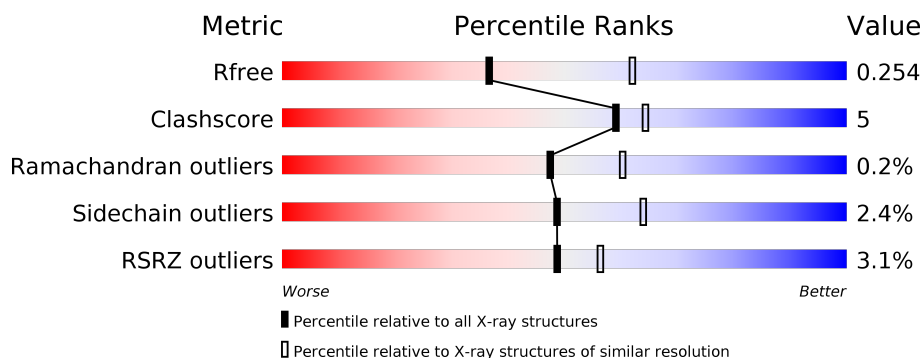
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	141	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 63%, green 30%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>63%</span> <span>6%</span> <span>30%</span> </div> </div>
1	B	141	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 63%, green 33%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>63%</span> <span>.</span> <span>33%</span> </div> </div>
1	C	141	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 60%, green 33%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>60%</span> <span>6%</span> <span>33%</span> </div> </div>
1	D	141	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 56%, green 33%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>56%</span> <span>11%</span> <span>33%</span> </div> </div>
1	E	141	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 57%, green 32%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>57%</span> <span>11%</span> <span>32%</span> </div> </div>
1	F	141	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 60%, green 33%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>60%</span> <span>6%</span> <span>33%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	141	<div><div></div><div>6%</div><div>56%</div><div>12%</div><div>32%</div></div>
1	H	141	<div><div></div><div>3%</div><div>57%</div><div>10%</div><div>33%</div></div>
1	I	141	<div><div></div><div>3%</div><div>60%</div><div>8%</div><div>31%</div></div>
1	J	141	<div><div></div><div>4%</div><div>57%</div><div>12%</div><div>30%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7725 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 Glutaminase liver isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			777	495	131	147	4			
1	B	95	Total	C	N	O	S	0	0	0
			756	483	128	142	3			
1	C	94	Total	C	N	O	S	0	0	0
			747	477	126	141	3			
1	D	94	Total	C	N	O	S	0	0	0
			747	477	126	141	3			
1	E	96	Total	C	N	O	S	0	0	0
			761	486	129	143	3			
1	F	95	Total	C	N	O	S	0	0	0
			754	481	127	143	3			
1	G	96	Total	C	N	O	S	0	0	0
			763	487	129	144	3			
1	H	95	Total	C	N	O	S	0	0	0
			754	481	127	143	3			
1	I	97	Total	C	N	O	S	0	0	0
			771	492	130	145	4			
1	J	98	Total	C	N	O	S	0	0	0
			777	495	131	147	4			

There are 230 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	462	MET	-	initiating methionine	UNP Q9UI32
A	463	HIS	-	expression tag	UNP Q9UI32
A	464	HIS	-	expression tag	UNP Q9UI32
A	465	HIS	-	expression tag	UNP Q9UI32
A	466	HIS	-	expression tag	UNP Q9UI32
A	467	HIS	-	expression tag	UNP Q9UI32
A	468	HIS	-	expression tag	UNP Q9UI32
A	469	SER	-	expression tag	UNP Q9UI32
A	470	SER	-	expression tag	UNP Q9UI32

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Chain	Residue	Modelled	Actual	Comment	Reference
A	471	GLY	-	expression tag	UNP Q9UI32
A	472	VAL	-	expression tag	UNP Q9UI32
A	473	ASP	-	expression tag	UNP Q9UI32
A	474	LEU	-	expression tag	UNP Q9UI32
A	475	GLY	-	expression tag	UNP Q9UI32
A	476	THR	-	expression tag	UNP Q9UI32
A	477	GLU	-	expression tag	UNP Q9UI32
A	478	ASN	-	expression tag	UNP Q9UI32
A	479	LEU	-	expression tag	UNP Q9UI32
A	480	TYR	-	expression tag	UNP Q9UI32
A	481	PHE	-	expression tag	UNP Q9UI32
A	482	GLN	-	expression tag	UNP Q9UI32
A	483	SER	-	expression tag	UNP Q9UI32
A	484	MET	-	expression tag	UNP Q9UI32
B	462	MET	-	initiating methionine	UNP Q9UI32
B	463	HIS	-	expression tag	UNP Q9UI32
B	464	HIS	-	expression tag	UNP Q9UI32
B	465	HIS	-	expression tag	UNP Q9UI32
B	466	HIS	-	expression tag	UNP Q9UI32
B	467	HIS	-	expression tag	UNP Q9UI32
B	468	HIS	-	expression tag	UNP Q9UI32
B	469	SER	-	expression tag	UNP Q9UI32
B	470	SER	-	expression tag	UNP Q9UI32
B	471	GLY	-	expression tag	UNP Q9UI32
B	472	VAL	-	expression tag	UNP Q9UI32
B	473	ASP	-	expression tag	UNP Q9UI32
B	474	LEU	-	expression tag	UNP Q9UI32
B	475	GLY	-	expression tag	UNP Q9UI32
B	476	THR	-	expression tag	UNP Q9UI32
B	477	GLU	-	expression tag	UNP Q9UI32
B	478	ASN	-	expression tag	UNP Q9UI32
B	479	LEU	-	expression tag	UNP Q9UI32
B	480	TYR	-	expression tag	UNP Q9UI32
B	481	PHE	-	expression tag	UNP Q9UI32
B	482	GLN	-	expression tag	UNP Q9UI32
B	483	SER	-	expression tag	UNP Q9UI32
B	484	MET	-	expression tag	UNP Q9UI32
C	462	MET	-	initiating methionine	UNP Q9UI32
C	463	HIS	-	expression tag	UNP Q9UI32
C	464	HIS	-	expression tag	UNP Q9UI32
C	465	HIS	-	expression tag	UNP Q9UI32
C	466	HIS	-	expression tag	UNP Q9UI32

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Chain	Residue	Modelled	Actual	Comment	Reference
C	467	HIS	-	expression tag	UNP Q9UI32
C	468	HIS	-	expression tag	UNP Q9UI32
C	469	SER	-	expression tag	UNP Q9UI32
C	470	SER	-	expression tag	UNP Q9UI32
C	471	GLY	-	expression tag	UNP Q9UI32
C	472	VAL	-	expression tag	UNP Q9UI32
C	473	ASP	-	expression tag	UNP Q9UI32
C	474	LEU	-	expression tag	UNP Q9UI32
C	475	GLY	-	expression tag	UNP Q9UI32
C	476	THR	-	expression tag	UNP Q9UI32
C	477	GLU	-	expression tag	UNP Q9UI32
C	478	ASN	-	expression tag	UNP Q9UI32
C	479	LEU	-	expression tag	UNP Q9UI32
C	480	TYR	-	expression tag	UNP Q9UI32
C	481	PHE	-	expression tag	UNP Q9UI32
C	482	GLN	-	expression tag	UNP Q9UI32
C	483	SER	-	expression tag	UNP Q9UI32
C	484	MET	-	expression tag	UNP Q9UI32
D	462	MET	-	initiating methionine	UNP Q9UI32
D	463	HIS	-	expression tag	UNP Q9UI32
D	464	HIS	-	expression tag	UNP Q9UI32
D	465	HIS	-	expression tag	UNP Q9UI32
D	466	HIS	-	expression tag	UNP Q9UI32
D	467	HIS	-	expression tag	UNP Q9UI32
D	468	HIS	-	expression tag	UNP Q9UI32
D	469	SER	-	expression tag	UNP Q9UI32
D	470	SER	-	expression tag	UNP Q9UI32
D	471	GLY	-	expression tag	UNP Q9UI32
D	472	VAL	-	expression tag	UNP Q9UI32
D	473	ASP	-	expression tag	UNP Q9UI32
D	474	LEU	-	expression tag	UNP Q9UI32
D	475	GLY	-	expression tag	UNP Q9UI32
D	476	THR	-	expression tag	UNP Q9UI32
D	477	GLU	-	expression tag	UNP Q9UI32
D	478	ASN	-	expression tag	UNP Q9UI32
D	479	LEU	-	expression tag	UNP Q9UI32
D	480	TYR	-	expression tag	UNP Q9UI32
D	481	PHE	-	expression tag	UNP Q9UI32
D	482	GLN	-	expression tag	UNP Q9UI32
D	483	SER	-	expression tag	UNP Q9UI32
D	484	MET	-	expression tag	UNP Q9UI32
E	462	MET	-	initiating methionine	UNP Q9UI32

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Chain	Residue	Modelled	Actual	Comment	Reference
E	463	HIS	-	expression tag	UNP Q9UI32
E	464	HIS	-	expression tag	UNP Q9UI32
E	465	HIS	-	expression tag	UNP Q9UI32
E	466	HIS	-	expression tag	UNP Q9UI32
E	467	HIS	-	expression tag	UNP Q9UI32
E	468	HIS	-	expression tag	UNP Q9UI32
E	469	SER	-	expression tag	UNP Q9UI32
E	470	SER	-	expression tag	UNP Q9UI32
E	471	GLY	-	expression tag	UNP Q9UI32
E	472	VAL	-	expression tag	UNP Q9UI32
E	473	ASP	-	expression tag	UNP Q9UI32
E	474	LEU	-	expression tag	UNP Q9UI32
E	475	GLY	-	expression tag	UNP Q9UI32
E	476	THR	-	expression tag	UNP Q9UI32
E	477	GLU	-	expression tag	UNP Q9UI32
E	478	ASN	-	expression tag	UNP Q9UI32
E	479	LEU	-	expression tag	UNP Q9UI32
E	480	TYR	-	expression tag	UNP Q9UI32
E	481	PHE	-	expression tag	UNP Q9UI32
E	482	GLN	-	expression tag	UNP Q9UI32
E	483	SER	-	expression tag	UNP Q9UI32
E	484	MET	-	expression tag	UNP Q9UI32
F	462	MET	-	initiating methionine	UNP Q9UI32
F	463	HIS	-	expression tag	UNP Q9UI32
F	464	HIS	-	expression tag	UNP Q9UI32
F	465	HIS	-	expression tag	UNP Q9UI32
F	466	HIS	-	expression tag	UNP Q9UI32
F	467	HIS	-	expression tag	UNP Q9UI32
F	468	HIS	-	expression tag	UNP Q9UI32
F	469	SER	-	expression tag	UNP Q9UI32
F	470	SER	-	expression tag	UNP Q9UI32
F	471	GLY	-	expression tag	UNP Q9UI32
F	472	VAL	-	expression tag	UNP Q9UI32
F	473	ASP	-	expression tag	UNP Q9UI32
F	474	LEU	-	expression tag	UNP Q9UI32
F	475	GLY	-	expression tag	UNP Q9UI32
F	476	THR	-	expression tag	UNP Q9UI32
F	477	GLU	-	expression tag	UNP Q9UI32
F	478	ASN	-	expression tag	UNP Q9UI32
F	479	LEU	-	expression tag	UNP Q9UI32
F	480	TYR	-	expression tag	UNP Q9UI32
F	481	PHE	-	expression tag	UNP Q9UI32

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Chain	Residue	Modelled	Actual	Comment	Reference
F	482	GLN	-	expression tag	UNP Q9UI32
F	483	SER	-	expression tag	UNP Q9UI32
F	484	MET	-	expression tag	UNP Q9UI32
G	462	MET	-	initiating methionine	UNP Q9UI32
G	463	HIS	-	expression tag	UNP Q9UI32
G	464	HIS	-	expression tag	UNP Q9UI32
G	465	HIS	-	expression tag	UNP Q9UI32
G	466	HIS	-	expression tag	UNP Q9UI32
G	467	HIS	-	expression tag	UNP Q9UI32
G	468	HIS	-	expression tag	UNP Q9UI32
G	469	SER	-	expression tag	UNP Q9UI32
G	470	SER	-	expression tag	UNP Q9UI32
G	471	GLY	-	expression tag	UNP Q9UI32
G	472	VAL	-	expression tag	UNP Q9UI32
G	473	ASP	-	expression tag	UNP Q9UI32
G	474	LEU	-	expression tag	UNP Q9UI32
G	475	GLY	-	expression tag	UNP Q9UI32
G	476	THR	-	expression tag	UNP Q9UI32
G	477	GLU	-	expression tag	UNP Q9UI32
G	478	ASN	-	expression tag	UNP Q9UI32
G	479	LEU	-	expression tag	UNP Q9UI32
G	480	TYR	-	expression tag	UNP Q9UI32
G	481	PHE	-	expression tag	UNP Q9UI32
G	482	GLN	-	expression tag	UNP Q9UI32
G	483	SER	-	expression tag	UNP Q9UI32
G	484	MET	-	expression tag	UNP Q9UI32
H	462	MET	-	initiating methionine	UNP Q9UI32
H	463	HIS	-	expression tag	UNP Q9UI32
H	464	HIS	-	expression tag	UNP Q9UI32
H	465	HIS	-	expression tag	UNP Q9UI32
H	466	HIS	-	expression tag	UNP Q9UI32
H	467	HIS	-	expression tag	UNP Q9UI32
H	468	HIS	-	expression tag	UNP Q9UI32
H	469	SER	-	expression tag	UNP Q9UI32
H	470	SER	-	expression tag	UNP Q9UI32
H	471	GLY	-	expression tag	UNP Q9UI32
H	472	VAL	-	expression tag	UNP Q9UI32
H	473	ASP	-	expression tag	UNP Q9UI32
H	474	LEU	-	expression tag	UNP Q9UI32
H	475	GLY	-	expression tag	UNP Q9UI32
H	476	THR	-	expression tag	UNP Q9UI32
H	477	GLU	-	expression tag	UNP Q9UI32

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Chain	Residue	Modelled	Actual	Comment	Reference
H	478	ASN	-	expression tag	UNP Q9UI32
H	479	LEU	-	expression tag	UNP Q9UI32
H	480	TYR	-	expression tag	UNP Q9UI32
H	481	PHE	-	expression tag	UNP Q9UI32
H	482	GLN	-	expression tag	UNP Q9UI32
H	483	SER	-	expression tag	UNP Q9UI32
H	484	MET	-	expression tag	UNP Q9UI32
I	462	MET	-	initiating methionine	UNP Q9UI32
I	463	HIS	-	expression tag	UNP Q9UI32
I	464	HIS	-	expression tag	UNP Q9UI32
I	465	HIS	-	expression tag	UNP Q9UI32
I	466	HIS	-	expression tag	UNP Q9UI32
I	467	HIS	-	expression tag	UNP Q9UI32
I	468	HIS	-	expression tag	UNP Q9UI32
I	469	SER	-	expression tag	UNP Q9UI32
I	470	SER	-	expression tag	UNP Q9UI32
I	471	GLY	-	expression tag	UNP Q9UI32
I	472	VAL	-	expression tag	UNP Q9UI32
I	473	ASP	-	expression tag	UNP Q9UI32
I	474	LEU	-	expression tag	UNP Q9UI32
I	475	GLY	-	expression tag	UNP Q9UI32
I	476	THR	-	expression tag	UNP Q9UI32
I	477	GLU	-	expression tag	UNP Q9UI32
I	478	ASN	-	expression tag	UNP Q9UI32
I	479	LEU	-	expression tag	UNP Q9UI32
I	480	TYR	-	expression tag	UNP Q9UI32
I	481	PHE	-	expression tag	UNP Q9UI32
I	482	GLN	-	expression tag	UNP Q9UI32
I	483	SER	-	expression tag	UNP Q9UI32
I	484	MET	-	expression tag	UNP Q9UI32
J	462	MET	-	initiating methionine	UNP Q9UI32
J	463	HIS	-	expression tag	UNP Q9UI32
J	464	HIS	-	expression tag	UNP Q9UI32
J	465	HIS	-	expression tag	UNP Q9UI32
J	466	HIS	-	expression tag	UNP Q9UI32
J	467	HIS	-	expression tag	UNP Q9UI32
J	468	HIS	-	expression tag	UNP Q9UI32
J	469	SER	-	expression tag	UNP Q9UI32
J	470	SER	-	expression tag	UNP Q9UI32
J	471	GLY	-	expression tag	UNP Q9UI32
J	472	VAL	-	expression tag	UNP Q9UI32
J	473	ASP	-	expression tag	UNP Q9UI32

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Chain	Residue	Modelled	Actual	Comment	Reference
J	474	LEU	-	expression tag	UNP Q9UI32
J	475	GLY	-	expression tag	UNP Q9UI32
J	476	THR	-	expression tag	UNP Q9UI32
J	477	GLU	-	expression tag	UNP Q9UI32
J	478	ASN	-	expression tag	UNP Q9UI32
J	479	LEU	-	expression tag	UNP Q9UI32
J	480	TYR	-	expression tag	UNP Q9UI32
J	481	PHE	-	expression tag	UNP Q9UI32
J	482	GLN	-	expression tag	UNP Q9UI32
J	483	SER	-	expression tag	UNP Q9UI32
J	484	MET	-	expression tag	UNP Q9UI32

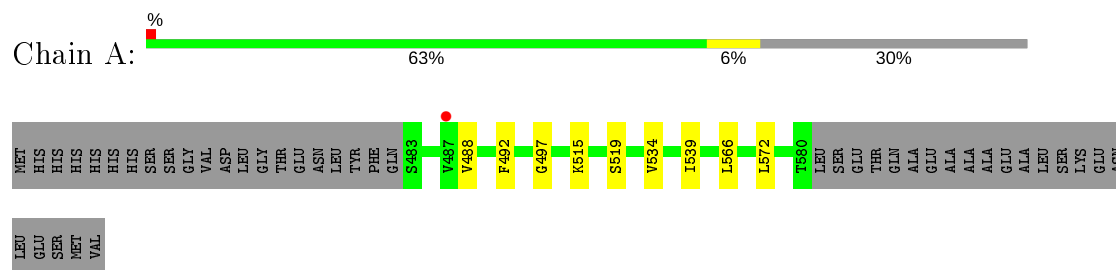
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	11	Total O 11 11	0	0
2	B	19	Total O 19 19	0	0
2	C	21	Total O 21 21	0	0
2	D	13	Total O 13 13	0	0
2	E	6	Total O 6 6	0	0
2	F	19	Total O 19 19	0	0
2	G	6	Total O 6 6	0	0
2	H	13	Total O 13 13	0	0
2	I	6	Total O 6 6	0	0
2	J	4	Total O 4 4	0	0

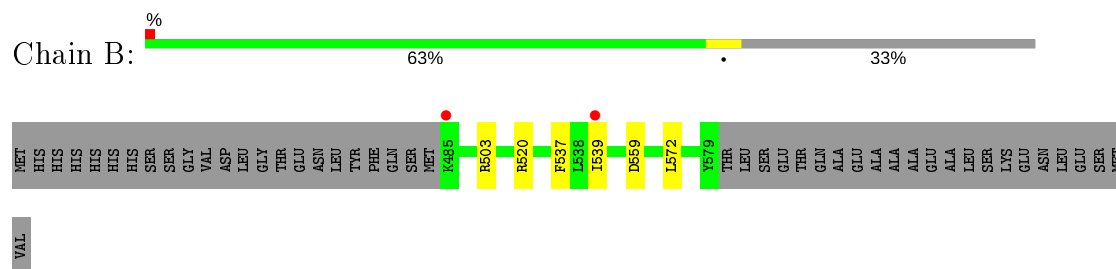
### 3 Residue-property plots [i](#)

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 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.

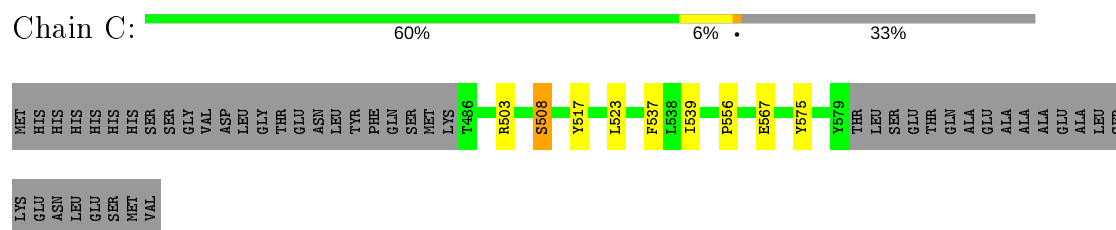
- Molecule 1: Glutaminase liver isoform, mitochondrial



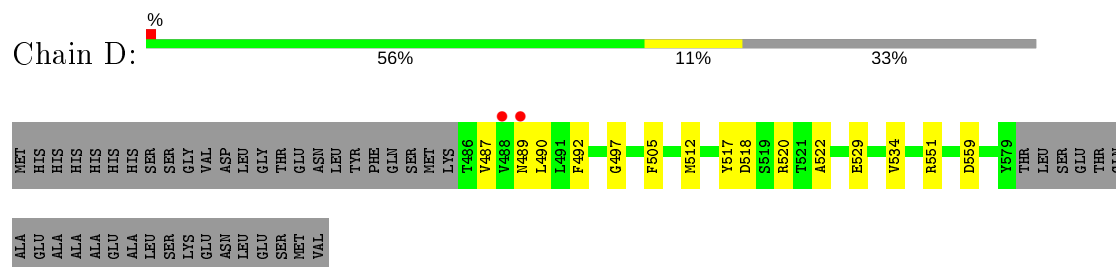
- Molecule 1: Glutaminase liver isoform, mitochondrial



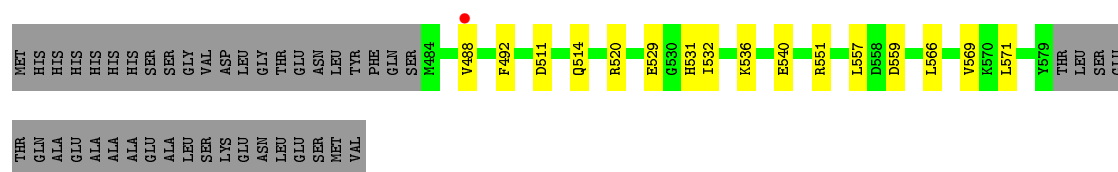
- Molecule 1: Glutaminase liver isoform, mitochondrial



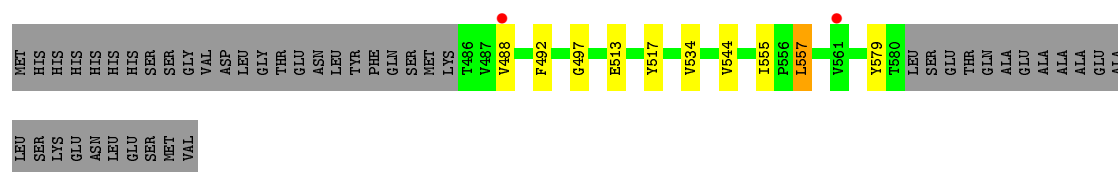
- Molecule 1: Glutaminase liver isoform, mitochondrial



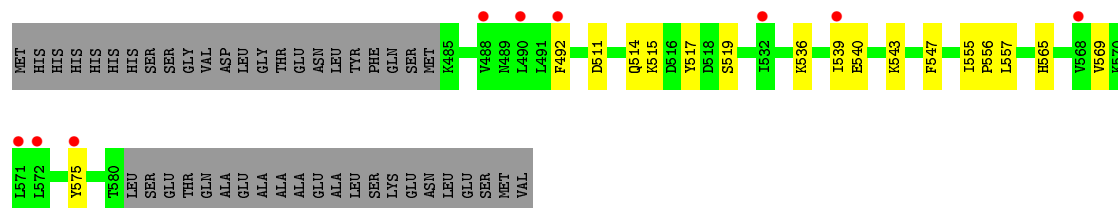
- Molecule 1: Glutaminase liver isoform, mitochondrial



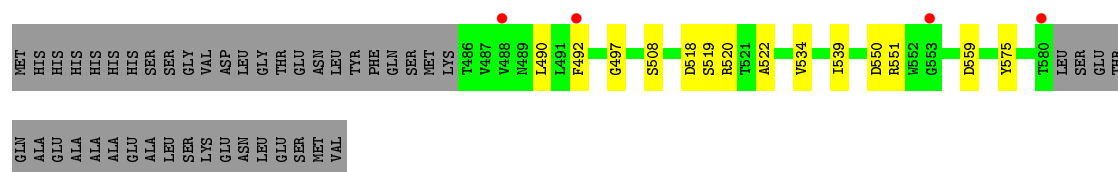
- Molecule 1: Glutaminase liver isoform, mitochondrial



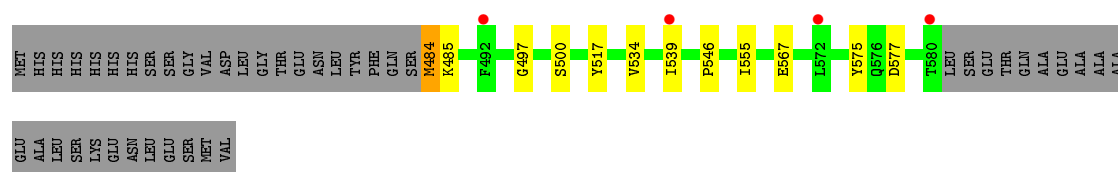
- Molecule 1: Glutaminase liver isoform, mitochondrial



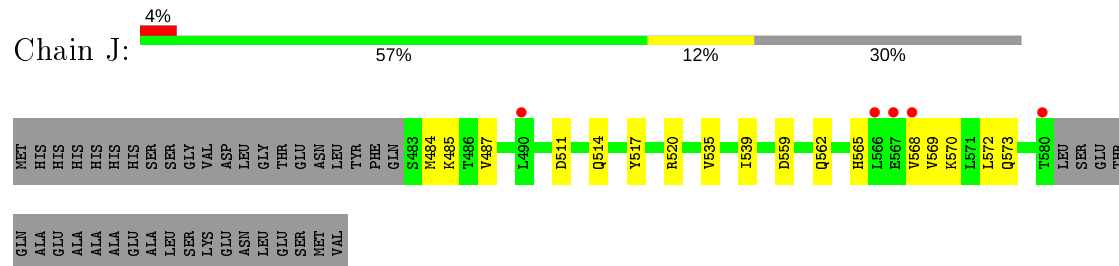
- Molecule 1: Glutaminase liver isoform, mitochondrial



- Molecule 1: Glutaminase liver isoform, mitochondrial



- Molecule 1: Glutaminase liver isoform, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.26 Å 85.26 Å 336.78 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.03 – 2.55 73.84 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.03-2.55) 99.8 (73.84-2.55)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 2.55 Å)	Xtriage
Refinement program	PHENIX (dev_2733: ???)	Depositor
R, $R_{free}$	0.218 , 0.257 0.216 , 0.254	Depositor DCC
$R_{free}$ test set	2369 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.5	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.075 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7725	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	0.25	0/792	0.40	0/1072
1	B	0.24	0/771	0.38	0/1044
1	C	0.24	0/762	0.37	0/1033
1	D	0.25	0/762	0.37	0/1033
1	E	0.25	0/776	0.36	0/1051
1	F	0.25	0/769	0.39	0/1043
1	G	0.25	0/778	0.38	0/1054
1	H	0.28	0/769	0.41	0/1043
1	I	0.24	0/786	0.41	0/1064
1	J	0.25	0/792	0.38	0/1072
All	All	0.25	0/7757	0.39	0/10509

There are no bond length outliers.

There are no bond angle outliers.

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	777	0	762	5	0
1	B	756	0	741	3	0
1	C	747	0	728	5	0
1	D	747	0	728	13	0
1	E	761	0	743	14	0
1	F	754	0	735	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	763	0	748	11	0
1	H	754	0	735	7	0
1	I	771	0	757	7	0
1	J	777	0	762	9	0
2	A	11	0	0	0	0
2	B	19	0	0	0	0
2	C	21	0	0	0	0
2	D	13	0	0	0	0
2	E	6	0	0	0	0
2	F	19	0	0	0	0
2	G	6	0	0	0	0
2	H	13	0	0	0	0
2	I	6	0	0	0	0
2	J	4	0	0	0	0
All	All	7725	0	7439	71	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 (71) 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:490:LEU:HD22	1:D:522:ALA:HB2	1.55	0.89
1:D:518:ASP:OD1	1:D:551:ARG:NH1	2.17	0.78
1:A:488:VAL:HG21	1:F:488:VAL:HG21	1.68	0.75
1:D:490:LEU:CD2	1:D:522:ALA:HB2	2.21	0.70
1:D:487:VAL:HG21	1:E:492:PHE:HE2	1.60	0.66
1:G:547:PHE:HA	1:G:555:ILE:HD11	1.77	0.66
1:E:532:ILE:HD11	1:E:571:LEU:HD12	1.80	0.63
1:G:511:ASP:HB3	1:G:514:GLN:HE21	1.63	0.62
1:D:551:ARG:NH2	1:E:529:GLU:OE2	2.36	0.59
1:H:539:ILE:HD12	1:H:575:TYR:CE2	2.38	0.58
1:A:488:VAL:HG11	1:F:488:VAL:HG21	1.85	0.58
1:J:569:VAL:O	1:J:573:GLN:HG3	2.04	0.58
1:H:520:ARG:NH1	1:H:559:ASP:OD2	2.34	0.58
1:J:520:ARG:NH1	1:J:559:ASP:OD2	2.30	0.57
1:G:555:ILE:HG13	1:G:556:PRO:HD2	1.86	0.57
1:H:518:ASP:HA	1:H:551:ARG:HH21	1.70	0.56
1:I:484:MET:CG	1:I:485:LYS:H	2.18	0.56
1:E:536:LYS:NZ	1:E:540:GLU:OE1	2.36	0.56
1:E:566:LEU:HD22	1:E:566:LEU:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:518:ASP:OD2	1:J:520:ARG:NE	2.30	0.55
1:D:529:GLU:OE2	1:E:551:ARG:NH1	2.37	0.54
1:I:484:MET:HG2	1:I:485:LYS:H	1.73	0.54
1:J:539:ILE:HD11	1:J:572:LEU:HD23	1.90	0.53
1:G:515:LYS:HB3	1:G:519:SER:HA	1.92	0.51
1:G:555:ILE:HG23	1:G:557:LEU:H	1.76	0.51
1:B:520:ARG:NH1	1:B:559:ASP:OD2	2.29	0.50
1:E:566:LEU:HD22	1:E:566:LEU:N	2.27	0.50
1:D:520:ARG:NH1	1:D:559:ASP:OD2	2.31	0.50
1:B:539:ILE:HD11	1:B:572:LEU:HD23	1.92	0.49
1:C:508:SER:O	1:C:508:SER:OG	2.30	0.49
1:F:555:ILE:HG22	1:F:557:LEU:H	1.78	0.49
1:H:519:SER:HB3	1:H:550:ASP:HA	1.95	0.49
1:D:490:LEU:CD2	1:D:522:ALA:CB	2.89	0.48
1:E:520:ARG:NH1	1:E:559:ASP:OD2	2.35	0.48
1:D:487:VAL:HG23	1:E:488:VAL:HG11	1.96	0.48
1:J:511:ASP:HB3	1:J:514:GLN:HG3	1.95	0.47
1:H:497:GLY:HA2	1:H:534:VAL:HG21	1.96	0.47
1:A:539:ILE:HD11	1:A:572:LEU:HD23	1.96	0.46
1:G:543:LYS:HG3	1:G:575:TYR:OH	2.15	0.46
1:D:489:ASN:HB3	1:D:505:PHE:CZ	2.51	0.46
1:D:497:GLY:HA2	1:D:534:VAL:HG21	1.98	0.45
1:I:567:GLU:N	1:I:567:GLU:OE1	2.39	0.45
1:J:565:HIS:O	1:J:569:VAL:HG23	2.16	0.45
1:H:490:LEU:HG	1:H:522:ALA:HB2	1.98	0.45
1:G:539:ILE:HD12	1:G:575:TYR:CD2	2.52	0.45
1:G:536:LYS:O	1:G:540:GLU:HG2	2.17	0.45
1:G:547:PHE:CA	1:G:555:ILE:HD11	2.46	0.45
1:G:565:HIS:O	1:G:569:VAL:HG23	2.17	0.44
1:I:539:ILE:HD12	1:I:575:TYR:CD2	2.52	0.44
1:E:511:ASP:HB3	1:E:514:GLN:HG3	1.99	0.44
1:I:539:ILE:HG23	1:I:575:TYR:CD1	2.53	0.44
1:G:557:LEU:HD21	1:G:569:VAL:HG13	1.99	0.44
1:D:490:LEU:HD11	1:D:512:MET:HA	2.00	0.43
1:F:513:GLU:HG2	1:F:544:VAL:HG12	1.99	0.43
1:J:535:VAL:HG11	1:J:568:VAL:HG23	2.01	0.43
1:D:517:TYR:HE2	1:E:488:VAL:HG13	1.83	0.43
1:J:562:GLN:HE21	1:J:562:GLN:HB2	1.61	0.43
1:I:497:GLY:HA2	1:I:534:VAL:HG21	2.01	0.42
1:C:503:ARG:HG2	1:C:537:PHE:CE1	2.55	0.42
1:F:497:GLY:HA2	1:F:534:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:GLY:HA2	1:A:534:VAL:HG21	2.02	0.42
1:J:484:MET:HA	1:J:487:VAL:HG12	2.01	0.42
1:E:532:ILE:O	1:E:536:LYS:HG3	2.20	0.42
1:A:515:LYS:HB2	1:A:519:SER:HA	2.02	0.41
1:C:567:GLU:H	1:C:567:GLU:CD	2.24	0.41
1:E:566:LEU:CD2	1:E:566:LEU:H	2.33	0.41
1:I:546:PRO:O	1:I:555:ILE:HG23	2.20	0.41
1:B:503:ARG:HG2	1:B:537:PHE:CE1	2.55	0.41
1:E:557:LEU:HD11	1:E:569:VAL:HG13	2.02	0.41
1:C:523:LEU:HD23	1:C:556:PRO:HG2	2.04	0.40
1:C:539:ILE:HG23	1:C:575:TYR:CD1	2.56	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	96/141 (68%)	91 (95%)	5 (5%)	0	100	100
1	B	93/141 (66%)	90 (97%)	3 (3%)	0	100	100
1	C	92/141 (65%)	88 (96%)	4 (4%)	0	100	100
1	D	92/141 (65%)	89 (97%)	3 (3%)	0	100	100
1	E	94/141 (67%)	90 (96%)	3 (3%)	1 (1%)	14	19
1	F	93/141 (66%)	88 (95%)	4 (4%)	1 (1%)	14	19
1	G	94/141 (67%)	89 (95%)	5 (5%)	0	100	100
1	H	93/141 (66%)	87 (94%)	6 (6%)	0	100	100
1	I	95/141 (67%)	91 (96%)	4 (4%)	0	100	100
1	J	96/141 (68%)	91 (95%)	5 (5%)	0	100	100
All	All	938/1410 (66%)	894 (95%)	42 (4%)	2 (0%)	47	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	579	TYR
1	E	531	HIS

### 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	83/119 (70%)	81 (98%)	2 (2%)	49	64
1	B	80/119 (67%)	80 (100%)	0	100	100
1	C	79/119 (66%)	77 (98%)	2 (2%)	47	62
1	D	79/119 (66%)	78 (99%)	1 (1%)	69	80
1	E	80/119 (67%)	80 (100%)	0	100	100
1	F	80/119 (67%)	77 (96%)	3 (4%)	33	45
1	G	81/119 (68%)	79 (98%)	2 (2%)	47	62
1	H	80/119 (67%)	78 (98%)	2 (2%)	47	62
1	I	82/119 (69%)	78 (95%)	4 (5%)	25	34
1	J	83/119 (70%)	80 (96%)	3 (4%)	35	47
All	All	807/1190 (68%)	788 (98%)	19 (2%)	49	64

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	492	PHE
1	A	566	LEU
1	C	508	SER
1	C	517	TYR
1	D	492	PHE
1	F	492	PHE
1	F	517	TYR
1	F	557	LEU
1	G	492	PHE
1	G	517	TYR

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Mol	Chain	Res	Type
1	H	492	PHE
1	H	508	SER
1	I	484	MET
1	I	500	SER
1	I	517	TYR
1	I	577	ASP
1	J	485	LYS
1	J	517	TYR
1	J	570	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	514	GLN
1	I	573	GLN
1	J	562	GLN
1	J	573	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	98/141 (69%)	0.32	1 (1%) 82 86	32, 45, 66, 83	0
1	B	95/141 (67%)	0.39	2 (2%) 63 70	34, 42, 61, 71	0
1	C	94/141 (66%)	0.24	0 100 100	32, 40, 57, 68	0
1	D	94/141 (66%)	0.25	2 (2%) 63 70	32, 47, 67, 75	0
1	E	96/141 (68%)	0.41	1 (1%) 82 86	39, 54, 72, 78	0
1	F	95/141 (67%)	0.34	2 (2%) 63 70	34, 46, 70, 88	0
1	G	96/141 (68%)	0.51	9 (9%) 8 10	36, 61, 75, 82	1 (1%)
1	H	95/141 (67%)	0.47	4 (4%) 36 42	36, 54, 66, 78	1 (1%)
1	I	97/141 (68%)	0.51	4 (4%) 37 44	45, 68, 85, 100	2 (2%)
1	J	98/141 (69%)	0.47	5 (5%) 28 33	38, 60, 85, 95	1 (1%)
All	All	958/1410 (67%)	0.39	30 (3%) 49 56	32, 52, 76, 100	5 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	492	PHE	4.1
1	F	488	VAL	4.1
1	D	488	VAL	4.0
1	I	580	THR	3.0
1	G	539	ILE	2.9
1	H	488	VAL	2.8
1	G	490	LEU	2.7
1	I	539	ILE	2.7
1	G	492	PHE	2.6
1	J	567	GLU	2.5
1	G	568	VAL	2.4
1	E	488	VAL	2.4
1	I	492	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	568	VAL	2.3
1	D	489	ASN	2.2
1	G	575	TYR	2.2
1	A	487	VAL	2.2
1	B	539	ILE	2.1
1	H	553	GLY	2.1
1	I	572	LEU	2.1
1	G	488	VAL	2.1
1	J	580	THR	2.1
1	B	485	LYS	2.1
1	G	572	LEU	2.1
1	F	561	VAL	2.0
1	H	580	THR	2.0
1	G	571	LEU	2.0
1	J	566	LEU	2.0
1	G	532	ILE	2.0
1	J	490	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.