



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:52 am GMT

PDB ID : 4FCC  
Title : Glutamate dehydrogenase from E. coli  
Authors : Bilokapic, S.; Schwartz, T.U.  
Deposited on : 2012-05-24  
Resolution : 2.00 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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

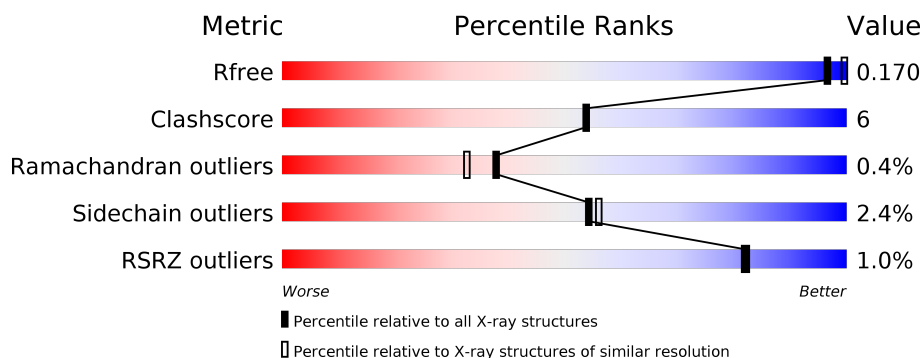
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	450	<div> <div>88%</div> <div>10% ..</div> </div>
1	B	450	<div> <div>2%</div> <div>84%</div> <div>14% ..</div> </div>
1	C	450	<div> <div>4%</div> <div>80%</div> <div>16% ..</div> </div>
1	D	450	<div> <div>2%</div> <div>85%</div> <div>13% ..</div> </div>
1	E	450	<div> <div>87%</div> <div>10% ..</div> </div>
1	F	450	<div> <div>87%</div> <div>11% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	450	 88% 10% ..
1	H	450	 2% 79% 18% .
1	I	450	 2% 82% 14% ..
1	J	450	 86% 12% .
1	K	450	 84% 13% ..
1	L	450	 89% 9% ..

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 44159 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 Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3366	2119	594	632	21			
1	B	442	Total	C	N	O	S	0	1	0
			3370	2122	594	633	21			
1	C	435	Total	C	N	O	S	0	1	0
			3318	2094	582	621	21			
1	D	442	Total	C	N	O	S	0	0	0
			3366	2119	594	632	21			
1	E	442	Total	C	N	O	S	0	0	0
			3366	2119	594	632	21			
1	F	442	Total	C	N	O	S	0	1	0
			3373	2124	596	632	21			
1	G	442	Total	C	N	O	S	0	0	0
			3366	2119	594	632	21			
1	H	438	Total	C	N	O	S	0	0	0
			3337	2104	587	625	21			
1	I	442	Total	C	N	O	S	0	0	0
			3366	2119	594	632	21			
1	J	442	Total	C	N	O	S	0	0	0
			3366	2119	594	632	21			
1	K	442	Total	C	N	O	S	0	0	0
			3366	2119	594	632	21			
1	L	442	Total	C	N	O	S	0	0	0
			3366	2119	594	632	21			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
A	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
A	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
B	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
B	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
C	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
C	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
C	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
D	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
D	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
D	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
E	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
E	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
E	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
F	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
F	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
F	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
G	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
G	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
G	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
H	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
H	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
H	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
I	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
I	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
I	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
J	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
J	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
J	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
K	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
K	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
K	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
L	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
L	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
L	0	SER	-	EXPRESSION TAG	UNP Q8XDW9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	409	Total O 409 409	0	0
2	B	277	Total O 277 277	0	0
2	C	300	Total O 300 300	0	0
2	D	254	Total O 254 254	0	0

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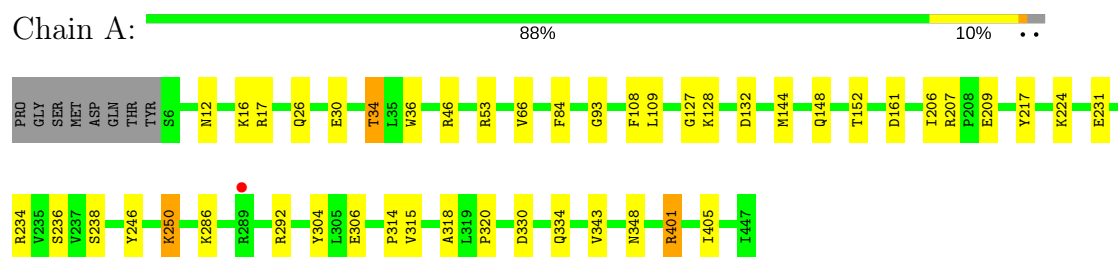
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	351	Total 351	O 351	0	0
2	F	323	Total 323	O 323	0	0
2	G	370	Total 370	O 370	0	0
2	H	288	Total 288	O 288	0	0
2	I	276	Total 276	O 276	0	0
2	J	325	Total 325	O 325	0	0
2	K	335	Total 335	O 335	0	0
2	L	325	Total 325	O 325	0	0

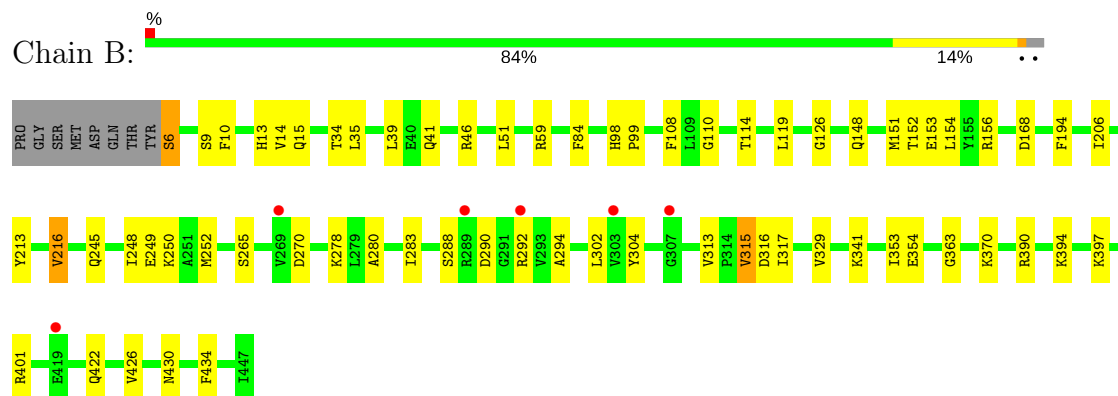
### 3 Residue-property plots [i](#)

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.

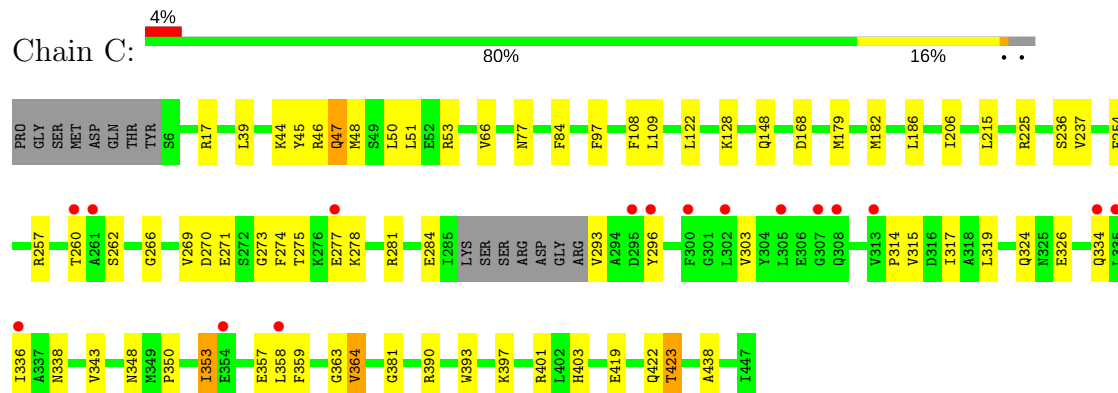
- Molecule 1: Glutamate dehydrogenase



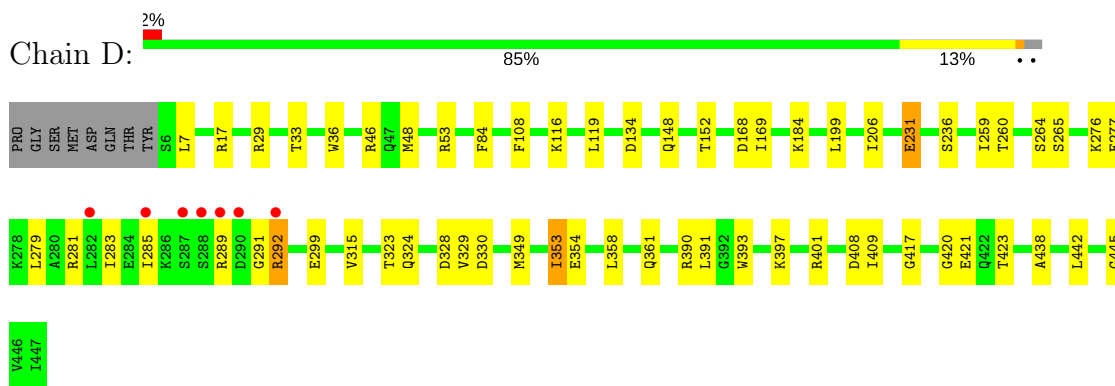
- Molecule 1: Glutamate dehydrogenase



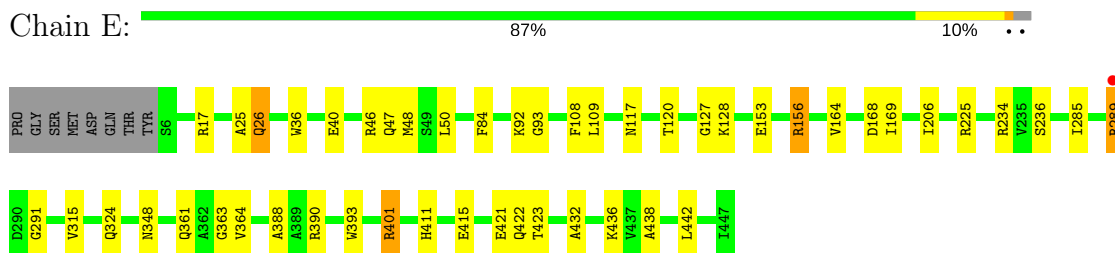
- Molecule 1: Glutamate dehydrogenase



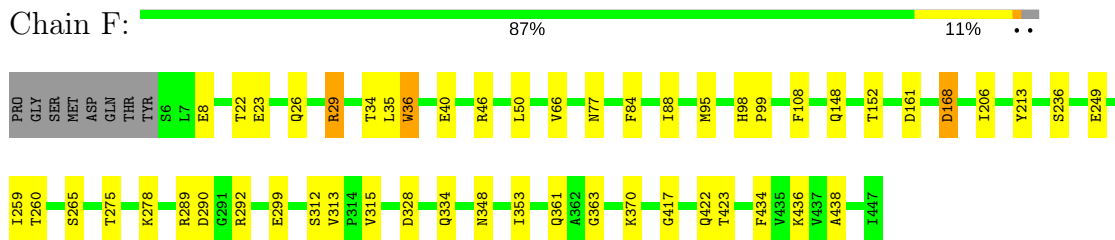
- Molecule 1: Glutamate dehydrogenase



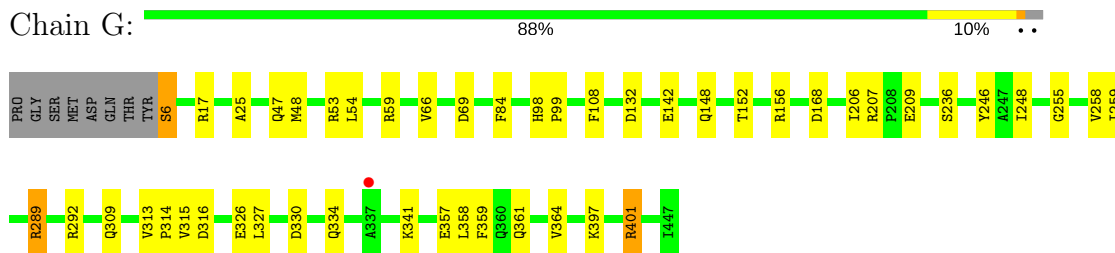
- Molecule 1: Glutamate dehydrogenase



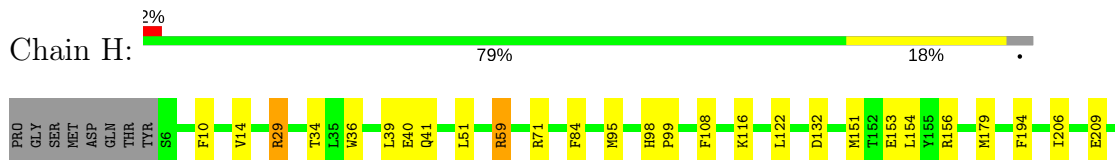
- Molecule 1: Glutamate dehydrogenase



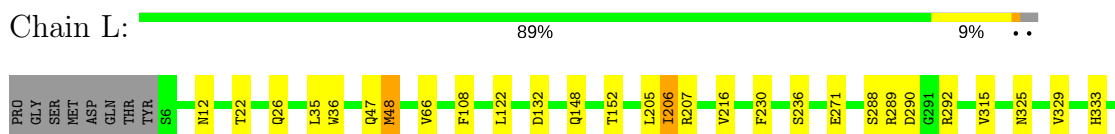
- Molecule 1: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase







E345	G346	A347	M348	M349	P350	T351	T352	T353		L358	F359	Q360	Q361		F366	G381		R401	V426	M430		V446	T447
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.22Å 176.26Å 150.25Å 90.00° 89.94° 90.00°	Depositor
Resolution (Å)	49.65 – 2.00 49.67 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.65-2.00) 98.9 (49.67-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.181 , 0.229 0.141 , 0.170	Depositor DCC
$R_{free}$ test set	3641 reflections (1.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 35.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.346 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	44159	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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	0.40	0/3431	0.53	0/4630
1	B	0.35	0/3438	0.52	0/4640
1	C	0.38	0/3386	0.53	0/4571
1	D	0.35	0/3431	0.51	0/4630
1	E	0.39	0/3431	0.52	0/4630
1	F	0.38	0/3442	0.51	0/4645
1	G	0.41	0/3431	0.54	0/4630
1	H	0.36	0/3401	0.52	1/4589 (0.0%)
1	I	0.36	0/3431	0.50	0/4630
1	J	0.38	0/3431	0.52	0/4630
1	K	0.38	0/3431	0.54	0/4630
1	L	0.38	0/3431	0.51	0/4630
All	All	0.38	0/41115	0.52	1/55485 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	59	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	3366	0	3324	37	0
1	B	3370	0	3331	49	0
1	C	3318	0	3274	55	0
1	D	3366	0	3324	43	0
1	E	3366	0	3324	30	0
1	F	3373	0	3331	37	0
1	G	3366	0	3324	32	0
1	H	3337	0	3298	59	0
1	I	3366	0	3324	48	0
1	J	3366	0	3324	46	0
1	K	3366	0	3324	41	0
1	L	3366	0	3324	32	0
2	A	409	0	0	16	0
2	B	277	0	0	14	0
2	C	300	0	0	12	0
2	D	254	0	0	18	0
2	E	351	0	0	8	0
2	F	323	0	0	12	0
2	G	370	0	0	10	0
2	H	288	0	0	16	0
2	I	276	0	0	4	0
2	J	325	0	0	14	0
2	K	335	0	0	11	0
2	L	325	0	0	12	0
All	All	44159	0	39826	485	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 6.

The worst 5 of 485 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:H:151:MET:SD	2:H:508:HOH:O	2.07	1.10
1:C:179:MET:SD	2:C:639:HOH:O	2.17	1.01
1:H:153:GLU:O	1:H:156:ARG:NH1	1.93	1.00
1:J:153:GLU:O	1:J:156:ARG:NH1	1.98	0.96
1:J:406:MET:SD	2:J:542:HOH:O	2.23	0.95

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	440/450 (98%)	433 (98%)	6 (1%)	1 (0%)	51	48
1	B	441/450 (98%)	427 (97%)	12 (3%)	2 (0%)	32	26
1	C	432/450 (96%)	420 (97%)	11 (2%)	1 (0%)	51	48
1	D	440/450 (98%)	421 (96%)	15 (3%)	4 (1%)	20	12
1	E	440/450 (98%)	431 (98%)	8 (2%)	1 (0%)	51	48
1	F	441/450 (98%)	429 (97%)	10 (2%)	2 (0%)	32	26
1	G	440/450 (98%)	430 (98%)	8 (2%)	2 (0%)	32	26
1	H	434/450 (96%)	418 (96%)	15 (4%)	1 (0%)	51	48
1	I	440/450 (98%)	429 (98%)	9 (2%)	2 (0%)	32	26
1	J	440/450 (98%)	428 (97%)	10 (2%)	2 (0%)	32	26
1	K	440/450 (98%)	430 (98%)	8 (2%)	2 (0%)	32	26
1	L	440/450 (98%)	431 (98%)	8 (2%)	1 (0%)	51	48
All	All	5268/5400 (98%)	5127 (97%)	120 (2%)	21 (0%)	38	33

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ILE
1	B	206	ILE
1	C	206	ILE
1	D	206	ILE
1	E	206	ILE

### 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	347/354 (98%)	340 (98%)	7 (2%)	60	64
1	B	348/354 (98%)	340 (98%)	8 (2%)	56	58
1	C	342/354 (97%)	331 (97%)	11 (3%)	44	42
1	D	347/354 (98%)	340 (98%)	7 (2%)	60	64
1	E	347/354 (98%)	338 (97%)	9 (3%)	51	52
1	F	348/354 (98%)	342 (98%)	6 (2%)	66	70
1	G	347/354 (98%)	339 (98%)	8 (2%)	56	58
1	H	344/354 (97%)	336 (98%)	8 (2%)	56	58
1	I	347/354 (98%)	334 (96%)	13 (4%)	39	36
1	J	347/354 (98%)	342 (99%)	5 (1%)	71	76
1	K	347/354 (98%)	336 (97%)	11 (3%)	44	42
1	L	347/354 (98%)	340 (98%)	7 (2%)	60	64
All	All	4158/4248 (98%)	4058 (98%)	100 (2%)	54	56

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	84	PHE
1	G	401	ARG
1	K	401	ARG
1	F	108	PHE
1	G	108	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	422	GLN
1	F	422	GLN
1	L	26	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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](#)

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	442/450 (98%)	-0.57	1 (0%) 94 94	15, 26, 45, 79	0
1	B	442/450 (98%)	-0.38	6 (1%) 75 75	17, 32, 68, 129	0
1	C	435/450 (96%)	-0.14	16 (3%) 42 43	14, 31, 78, 104	0
1	D	442/450 (98%)	-0.36	7 (1%) 72 71	17, 33, 59, 108	0
1	E	442/450 (98%)	-0.56	1 (0%) 94 94	15, 28, 49, 80	0
1	F	442/450 (98%)	-0.58	0 100 100	15, 28, 47, 69	0
1	G	442/450 (98%)	-0.44	1 (0%) 94 94	14, 26, 48, 69	0
1	H	438/450 (97%)	-0.25	11 (2%) 58 57	17, 32, 75, 111	0
1	I	442/450 (98%)	-0.16	9 (2%) 65 65	14, 33, 81, 132	0
1	J	442/450 (98%)	-0.47	1 (0%) 94 94	15, 26, 48, 86	0
1	K	442/450 (98%)	-0.51	1 (0%) 94 94	15, 28, 50, 68	0
1	L	442/450 (98%)	-0.48	0 100 100	14, 29, 54, 77	0
All	All	5293/5400 (98%)	-0.41	54 (1%) 82 82	14, 29, 62, 132	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	289	ARG	7.0
1	H	302	LEU	5.2
1	H	281	ARG	4.7
1	D	288	SER	4.1
1	D	287	SER	3.8

### 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.