



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 23, 2025 – 04:39 PM JST

PDB ID : 8K4V  
Title : Crystal structure of HLA-A\*11:01 in complex with KRAS G12R peptide (VVVGARGVGK)  
Authors : Xu, Y.  
Deposited on : 2023-07-20  
Resolution : 3.10 Å(reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<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
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

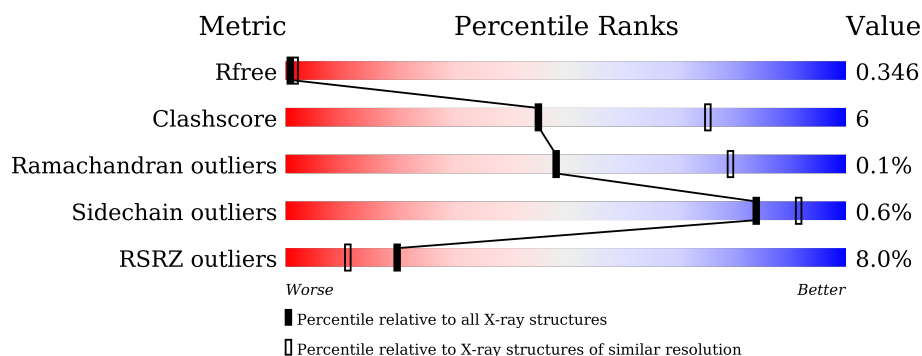
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

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  $\leq 5\%$ . 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	276	<div> <div>7%</div> <div>82%</div> <div>17%</div> </div>
1	D	276	<div> <div>8%</div> <div>85%</div> <div>15%</div> </div>
1	G	276	<div> <div>8%</div> <div>85%</div> <div>15%</div> </div>
1	J	276	<div> <div>10%</div> <div>86%</div> <div>14%</div> </div>
2	B	122	<div> <div>9%</div> <div>65%</div> <div>17%</div> <div>18%</div> </div>
2	E	122	<div> <div>6%</div> <div>63%</div> <div>19%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	122	
2	K	122	
3	C	10	
3	F	10	
3	I	10	
3	L	10	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12560 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 HLA class I histocompatibility antigen, A alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	1	0
			2250	1398	409	434	9			
1	D	275	Total	C	N	O	S	0	1	0
			2250	1398	409	434	9			
1	G	275	Total	C	N	O	S	0	1	0
			2250	1398	409	434	9			
1	J	275	Total	C	N	O	S	0	1	0
			2250	1398	409	434	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	initiating methionine	UNP P04439
A	33	TYR	PHE	variant	UNP P04439
A	114	ASP	ALA	variant	UNP P04439
A	129	PRO	SER	variant	UNP P04439
D	24	MET	-	initiating methionine	UNP P04439
D	33	TYR	PHE	variant	UNP P04439
D	114	ASP	ALA	variant	UNP P04439
D	129	PRO	SER	variant	UNP P04439
G	24	MET	-	initiating methionine	UNP P04439
G	33	TYR	PHE	variant	UNP P04439
G	114	ASP	ALA	variant	UNP P04439
G	129	PRO	SER	variant	UNP P04439
J	24	MET	-	initiating methionine	UNP P04439
J	33	TYR	PHE	variant	UNP P04439
J	114	ASP	ALA	variant	UNP P04439
J	129	PRO	SER	variant	UNP P04439

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total 836	C 533	N 141	O 158	S 4	0	0	0
2	E	100	Total 836	C 533	N 141	O 158	S 4	0	0	0
2	H	100	Total 836	C 533	N 141	O 158	S 4	0	0	0
2	K	100	Total 836	C 533	N 141	O 158	S 4	0	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
B	100	GLY	-	expression tag	UNP P61769
B	101	SER	-	expression tag	UNP P61769
B	102	GLY	-	expression tag	UNP P61769
B	103	GLY	-	expression tag	UNP P61769
B	104	SER	-	expression tag	UNP P61769
B	105	GLY	-	expression tag	UNP P61769
B	106	ALA	-	expression tag	UNP P61769
B	107	GLY	-	expression tag	UNP P61769
B	108	LEU	-	expression tag	UNP P61769
B	109	ASN	-	expression tag	UNP P61769
B	110	ASP	-	expression tag	UNP P61769
B	111	ILE	-	expression tag	UNP P61769
B	112	PHE	-	expression tag	UNP P61769
B	113	GLU	-	expression tag	UNP P61769
B	114	ALA	-	expression tag	UNP P61769
B	115	GLN	-	expression tag	UNP P61769
B	116	LYS	-	expression tag	UNP P61769
B	117	ILE	-	expression tag	UNP P61769
B	118	GLU	-	expression tag	UNP P61769
B	119	TRP	-	expression tag	UNP P61769
B	120	HIS	-	expression tag	UNP P61769
B	121	GLU	-	expression tag	UNP P61769
E	0	MET	-	initiating methionine	UNP P61769
E	100	GLY	-	expression tag	UNP P61769
E	101	SER	-	expression tag	UNP P61769
E	102	GLY	-	expression tag	UNP P61769
E	103	GLY	-	expression tag	UNP P61769
E	104	SER	-	expression tag	UNP P61769
E	105	GLY	-	expression tag	UNP P61769
E	106	ALA	-	expression tag	UNP P61769

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Chain	Residue	Modelled	Actual	Comment	Reference
E	107	GLY	-	expression tag	UNP P61769
E	108	LEU	-	expression tag	UNP P61769
E	109	ASN	-	expression tag	UNP P61769
E	110	ASP	-	expression tag	UNP P61769
E	111	ILE	-	expression tag	UNP P61769
E	112	PHE	-	expression tag	UNP P61769
E	113	GLU	-	expression tag	UNP P61769
E	114	ALA	-	expression tag	UNP P61769
E	115	GLN	-	expression tag	UNP P61769
E	116	LYS	-	expression tag	UNP P61769
E	117	ILE	-	expression tag	UNP P61769
E	118	GLU	-	expression tag	UNP P61769
E	119	TRP	-	expression tag	UNP P61769
E	120	HIS	-	expression tag	UNP P61769
E	121	GLU	-	expression tag	UNP P61769
H	0	MET	-	initiating methionine	UNP P61769
H	100	GLY	-	expression tag	UNP P61769
H	101	SER	-	expression tag	UNP P61769
H	102	GLY	-	expression tag	UNP P61769
H	103	GLY	-	expression tag	UNP P61769
H	104	SER	-	expression tag	UNP P61769
H	105	GLY	-	expression tag	UNP P61769
H	106	ALA	-	expression tag	UNP P61769
H	107	GLY	-	expression tag	UNP P61769
H	108	LEU	-	expression tag	UNP P61769
H	109	ASN	-	expression tag	UNP P61769
H	110	ASP	-	expression tag	UNP P61769
H	111	ILE	-	expression tag	UNP P61769
H	112	PHE	-	expression tag	UNP P61769
H	113	GLU	-	expression tag	UNP P61769
H	114	ALA	-	expression tag	UNP P61769
H	115	GLN	-	expression tag	UNP P61769
H	116	LYS	-	expression tag	UNP P61769
H	117	ILE	-	expression tag	UNP P61769
H	118	GLU	-	expression tag	UNP P61769
H	119	TRP	-	expression tag	UNP P61769
H	120	HIS	-	expression tag	UNP P61769
H	121	GLU	-	expression tag	UNP P61769
K	0	MET	-	initiating methionine	UNP P61769
K	100	GLY	-	expression tag	UNP P61769
K	101	SER	-	expression tag	UNP P61769
K	102	GLY	-	expression tag	UNP P61769

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Chain	Residue	Modelled	Actual	Comment	Reference
K	103	GLY	-	expression tag	UNP P61769
K	104	SER	-	expression tag	UNP P61769
K	105	GLY	-	expression tag	UNP P61769
K	106	ALA	-	expression tag	UNP P61769
K	107	GLY	-	expression tag	UNP P61769
K	108	LEU	-	expression tag	UNP P61769
K	109	ASN	-	expression tag	UNP P61769
K	110	ASP	-	expression tag	UNP P61769
K	111	ILE	-	expression tag	UNP P61769
K	112	PHE	-	expression tag	UNP P61769
K	113	GLU	-	expression tag	UNP P61769
K	114	ALA	-	expression tag	UNP P61769
K	115	GLN	-	expression tag	UNP P61769
K	116	LYS	-	expression tag	UNP P61769
K	117	ILE	-	expression tag	UNP P61769
K	118	GLU	-	expression tag	UNP P61769
K	119	TRP	-	expression tag	UNP P61769
K	120	HIS	-	expression tag	UNP P61769
K	121	GLU	-	expression tag	UNP P61769

- Molecule 3 is a protein called KRAS G12R peptide (VVVGARGVGK).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			66	41	14	11			
3	F	8	Total	C	N	O	0	0	0
			50	32	9	9			
3	I	8	Total	C	N	O	0	0	0
			50	32	9	9			
3	L	8	Total	C	N	O	0	0	0
			50	32	9	9			

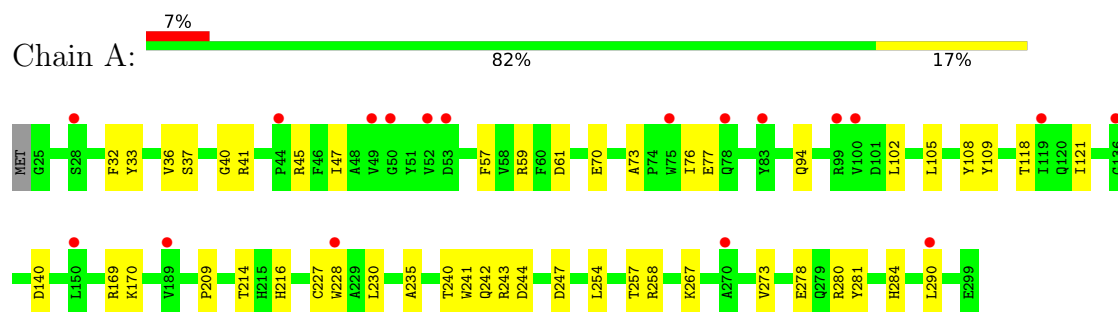
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	6	ARG	GLY	engineered mutation	UNP P01116
F	6	ARG	GLY	engineered mutation	UNP P01116
I	6	ARG	GLY	engineered mutation	UNP P01116
L	6	ARG	GLY	engineered mutation	UNP P01116

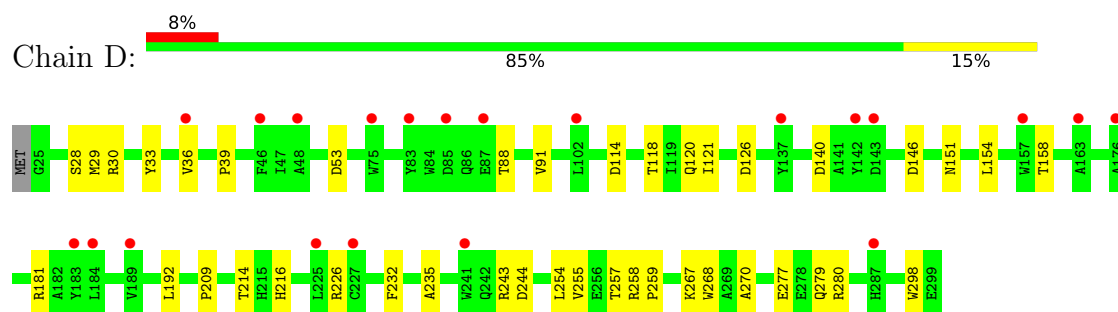
### 3 Residue-property plots [i](#)

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 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.

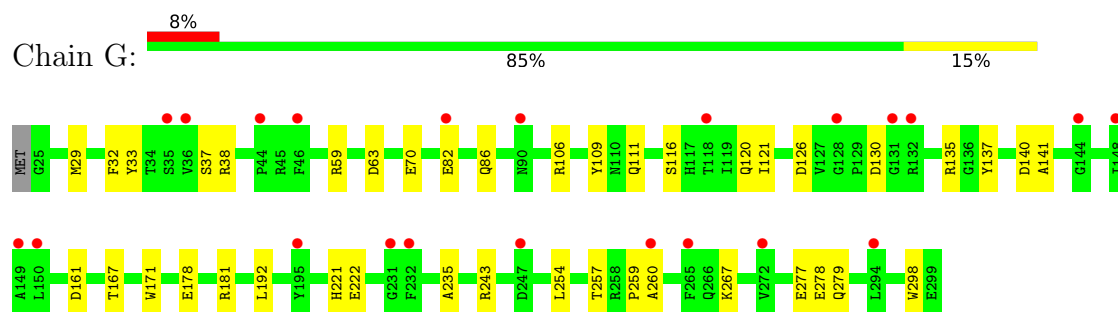
- Molecule 1: HLA class I histocompatibility antigen, A alpha chain



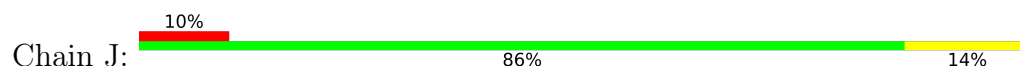
- Molecule 1: HLA class I histocompatibility antigen, A alpha chain



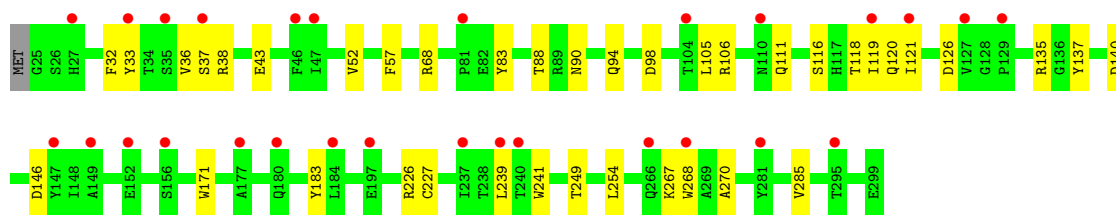
- Molecule 1: HLA class I histocompatibility antigen, A alpha chain



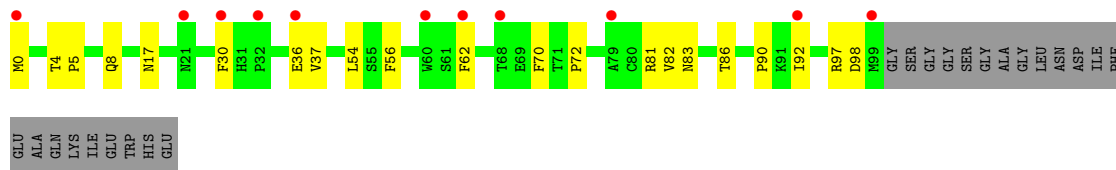
- Molecule 1: HLA class I histocompatibility antigen, A alpha chain



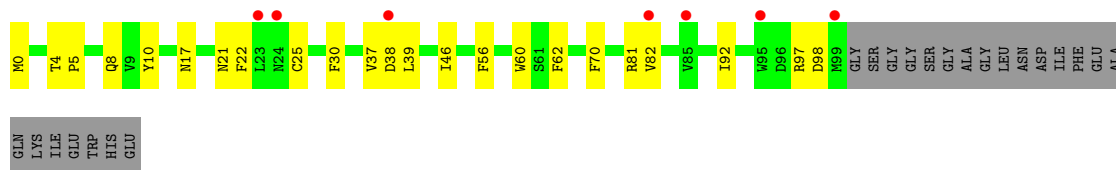




● Molecule 2: Beta-2-microglobulin



● Molecule 2: Beta-2-microglobulin



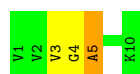
● Molecule 2: Beta-2-microglobulin




● Molecule 2: Beta-2-microglobulin

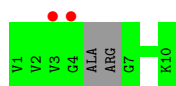


● Molecule 3: KRAS G12R peptide (VVVGARGVGK)



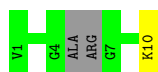
- Molecule 3: KRAS G12R peptide (VVVGARGVGK)

Chain F: 



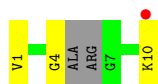
- Molecule 3: KRAS G12R peptide (VVVGARGVGK)

Chain I: 



- Molecule 3: KRAS G12R peptide (VVVGARGVGK)

Chain L: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.65Å 121.60Å 155.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.39 – 3.10 25.39 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (25.39-3.10) 79.6 (25.39-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	-0.21 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.296 , 0.347 0.297 , 0.346	Depositor DCC
$R_{free}$ test set	39660 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.4	Xtriage
Anisotropy	1.215	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.029 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	12560	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	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 26.41 % 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 2.6469e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.24	0/2314	0.46	0/3141
1	D	0.24	0/2314	0.46	0/3141
1	G	0.24	0/2314	0.45	0/3141
1	J	0.24	0/2314	0.44	0/3141
2	B	0.24	0/859	0.44	0/1162
2	E	0.24	0/859	0.45	0/1162
2	H	0.24	0/859	0.45	0/1162
2	K	0.23	0/859	0.45	0/1162
3	C	0.23	0/65	0.39	0/84
3	F	0.21	0/48	0.38	0/60
3	I	0.23	0/48	0.40	0/60
3	L	0.20	0/48	0.39	0/60
All	All	0.24	0/12901	0.45	0/17476

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	2250	0	2096	30	0
1	D	2250	0	2096	25	0
1	G	2250	0	2096	26	0
1	J	2250	0	2096	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	836	0	803	20	0
2	E	836	0	803	18	0
2	H	836	0	803	15	0
2	K	836	0	803	16	0
3	C	66	0	78	1	0
3	F	50	0	59	0	0
3	I	50	0	59	3	0
3	L	50	0	59	4	0
All	All	12560	0	11851	142	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 142 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:B:92:ILE:HG12	2:H:75:LYS:HD2	1.62	0.82
1:G:279:GLN:NE2	1:G:298:TRP:O	2.18	0.76
1:A:169:ARG:NH1	1:J:249:THR:OG1	2.19	0.75
1:G:120:GLN:NE2	2:H:60:TRP:O	2.21	0.74
1:A:216:HIS:NE2	2:B:98:ASP:OD2	2.21	0.73

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	274/276 (99%)	268 (98%)	6 (2%)	0	100	100
1	D	274/276 (99%)	269 (98%)	5 (2%)	0	100	100
1	G	274/276 (99%)	269 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	274/276 (99%)	268 (98%)	6 (2%)	0	100	100
2	B	98/122 (80%)	95 (97%)	3 (3%)	0	100	100
2	E	98/122 (80%)	95 (97%)	3 (3%)	0	100	100
2	H	98/122 (80%)	95 (97%)	3 (3%)	0	100	100
2	K	98/122 (80%)	95 (97%)	3 (3%)	0	100	100
3	C	8/10 (80%)	5 (62%)	1 (12%)	2 (25%)	0	0
3	F	4/10 (40%)	4 (100%)	0	0	100	100
3	I	4/10 (40%)	4 (100%)	0	0	100	100
3	L	4/10 (40%)	4 (100%)	0	0	100	100
All	All	1508/1632 (92%)	1471 (98%)	35 (2%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	4	GLY
3	C	5	ALA

### 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	233/233 (100%)	232 (100%)	1 (0%)	89	94
1	D	233/233 (100%)	232 (100%)	1 (0%)	89	94
1	G	233/233 (100%)	232 (100%)	1 (0%)	89	94
1	J	233/233 (100%)	232 (100%)	1 (0%)	89	94
2	B	95/110 (86%)	94 (99%)	1 (1%)	70	84
2	E	95/110 (86%)	94 (99%)	1 (1%)	70	84
2	H	95/110 (86%)	94 (99%)	1 (1%)	70	84
2	K	95/110 (86%)	94 (99%)	1 (1%)	70	84
3	C	6/6 (100%)	6 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	5/6 (83%)	5 (100%)	0	100	100
3	I	5/6 (83%)	5 (100%)	0	100	100
3	L	5/6 (83%)	5 (100%)	0	100	100
All	All	1333/1396 (96%)	1325 (99%)	8 (1%)	84	91

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	70	PHE
1	J	140	ASP
1	G	140	ASP
2	E	70	PHE
2	H	70	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

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 ⓘ

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	275/276 (99%)	0.90	18 (6%)	26	16	27, 54, 73, 86	1 (0%)
1	D	275/276 (99%)	0.78	21 (7%)	21	12	19, 47, 72, 85	1 (0%)
1	G	275/276 (99%)	0.82	22 (8%)	20	11	23, 50, 74, 96	1 (0%)
1	J	275/276 (99%)	0.99	28 (10%)	13	8	30, 70, 95, 107	1 (0%)
2	B	100/122 (81%)	0.99	11 (11%)	12	7	26, 48, 66, 87	0
2	E	100/122 (81%)	0.81	7 (7%)	24	14	25, 43, 62, 75	0
2	H	100/122 (81%)	0.81	5 (5%)	35	21	26, 44, 63, 71	0
2	K	100/122 (81%)	1.03	7 (7%)	24	14	40, 63, 85, 111	0
3	C	10/10 (100%)	0.67	0	100	100	48, 62, 80, 82	0
3	F	8/10 (80%)	0.82	2 (25%)	2	1	34, 49, 57, 58	0
3	I	8/10 (80%)	0.54	0	100	100	31, 40, 48, 50	0
3	L	8/10 (80%)	1.49	1 (12%)	9	6	75, 83, 95, 104	0
All	All	1534/1632 (93%)	0.88	122 (7%)	20	11	19, 52, 84, 111	4 (0%)

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	68	THR	6.2
2	B	32	PRO	4.8
2	K	31	HIS	4.6
1	G	247	ASP	4.5
2	E	23	LEU	4.5

### 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 monosaccharides 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.