



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:39 AM UTC

PDB ID : 9WVE / pdb_00009wve
Title : Crystal structure of HLA-A*11:01 in complex with KRAS G12A 10-mer peptide (VVVGAAGVGK)
Authors : Jiali, Z.; Linlin, Z.
Deposited on : 2025-09-19
Resolution : 2.80 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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

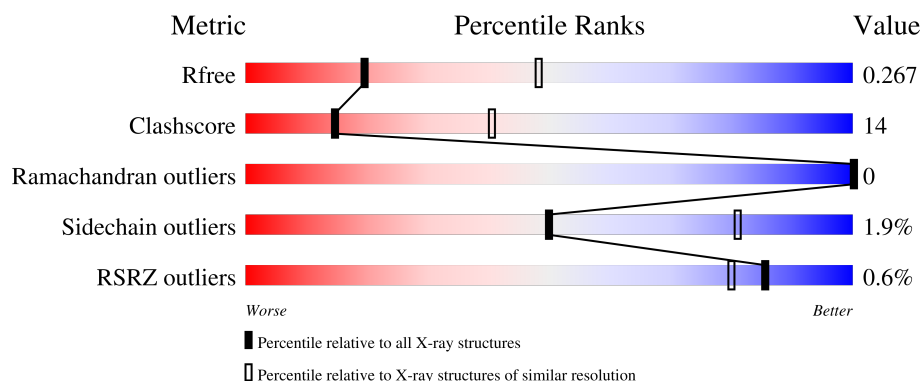
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 ≥ 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	% 70% 28% .
1	D	276	72% 26% .
1	G	276	% 73% 26%
1	J	276	77% 22%
2	B	122	% 57% 24% . 19%

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Mol	Chain	Length	Quality of chain
2	E	122	53% 28% 19%
2	H	122	% 55% 26% 19%
2	K	122	52% 30% 19%
3	C	10	10% 70% 20% 10%
3	F	10	10% 70% 30%
3	I	10	70% 30%
3	L	10	70% 30%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12456 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	0	0
			2218	1378	401	430	9			
1	D	275	Total	C	N	O	S	0	0	0
			2234	1388	404	433	9			
1	G	275	Total	C	N	O	S	0	0	0
			2238	1391	405	433	9			
1	J	275	Total	C	N	O	S	0	0	0
			2169	1347	391	422	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P04439
A	9	TYR	PHE	variant	UNP P04439
A	90	ASP	ALA	variant	UNP P04439
A	105	PRO	SER	variant	UNP P04439
D	0	MET	-	initiating methionine	UNP P04439
D	9	TYR	PHE	variant	UNP P04439
D	90	ASP	ALA	variant	UNP P04439
D	105	PRO	SER	variant	UNP P04439
G	0	MET	-	initiating methionine	UNP P04439
G	9	TYR	PHE	variant	UNP P04439
G	90	ASP	ALA	variant	UNP P04439
G	105	PRO	SER	variant	UNP P04439
J	0	MET	-	initiating methionine	UNP P04439
J	9	TYR	PHE	variant	UNP P04439
J	90	ASP	ALA	variant	UNP P04439
J	105	PRO	SER	variant	UNP P04439

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			815	520	137	155	3			
2	E	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	H	99	Total	C	N	O	S	0	0	0
			822	525	137	157	3			
2	K	99	Total	C	N	O	S	0	0	0
			824	526	140	155	3			

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 VAL-VAL-VAL-GLY-ALA-ALA-GLY-VAL-GLY-LYS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			60	38	11	11			
3	F	10	Total	C	N	O	0	0	0
			60	38	11	11			
3	I	10	Total	C	N	O	0	0	0
			60	38	11	11			
3	L	10	Total	C	N	O	0	0	0
			56	34	11	11			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	3	Total	O	0	0
			3	3		
4	D	9	Total	O	0	0
			9	9		
4	E	10	Total	O	0	0
			10	10		

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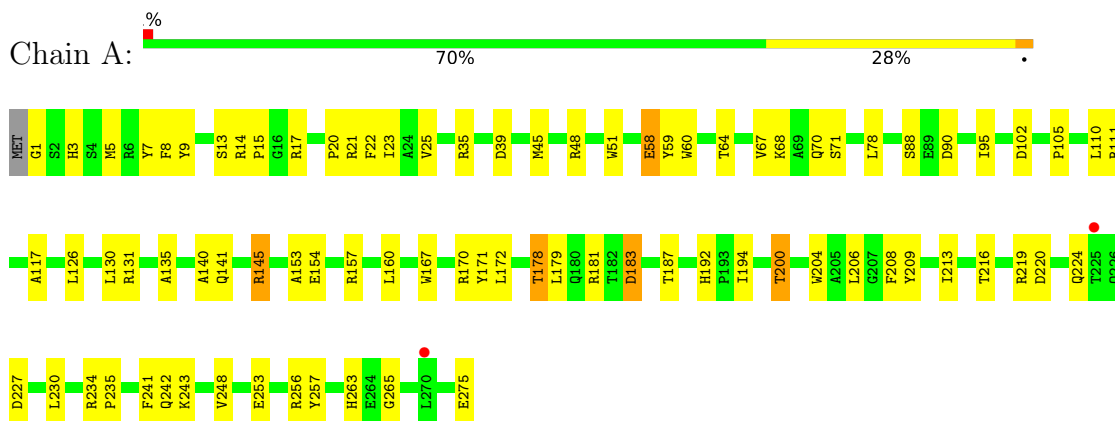
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total 1	O 1	0	0
4	G	11	Total 11	O 11	0	0
4	H	7	Total 7	O 7	0	0
4	J	12	Total 12	O 12	0	0
4	K	11	Total 11	O 11	0	0

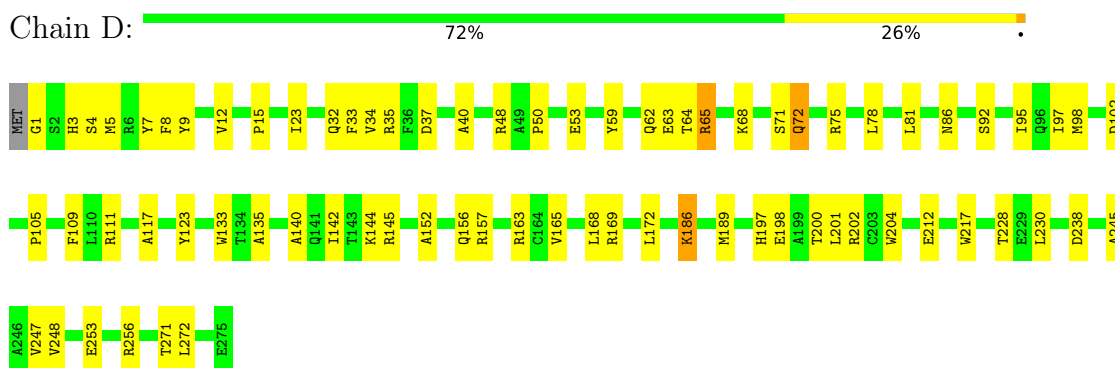
3 Residue-property plots

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 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.

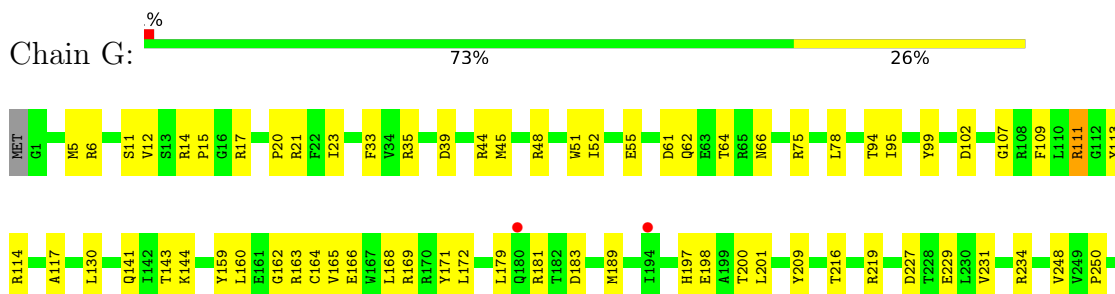
- Molecule 1: HLA class I histocompatibility antigen, A alpha chain



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



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





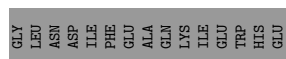
- Molecule 1: HLA class I histocompatibility antigen, A alpha chain

Chain J: 77% 22%



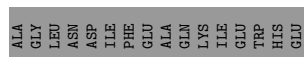
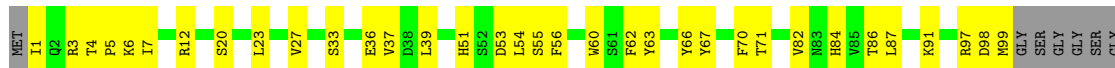
- Molecule 2: Beta-2-microglobulin

Chain B: 57% 24% 19%



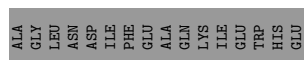
- Molecule 2: Beta-2-microglobulin

Chain E: 53% 28% 19%



- Molecule 2: Beta-2-microglobulin

Chain H: 55% 26% 19%



- Molecule 2: Beta-2-microglobulin

Chain K: 52% 30% 19%



SER GLY GLY SER GLY ALA GLY LEU ASN ASP ILE PHE GLU ALA GLN LYS ILE GLU TRP HIS GLU

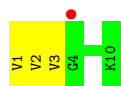
- Molecule 3: VAL-VAL-VAL-GLY-ALA-ALA-GLY-VAL-GLY-LYS

Chain C: 



- Molecule 3: VAL-VAL-VAL-GLY-ALA-ALA-GLY-VAL-GLY-LYS

Chain F: 



- Molecule 3: VAL-VAL-VAL-GLY-ALA-ALA-GLY-VAL-GLY-LYS

Chain I: 



- Molecule 3: VAL-VAL-VAL-GLY-ALA-ALA-GLY-VAL-GLY-LYS

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.88Å 121.57Å 132.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.80 – 2.80 44.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.80-2.80) 99.6 (44.80-2.80)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.247 , 0.267 0.247 , 0.267	Depositor DCC
R_{free} test set	2005 reflections (4.18%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12456	wwPDB-VP
Average B, all atoms (Å ²)	80.0	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 31.03 % 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 1.1849e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0.49	0/2277	0.74	0/3092
1	D	0.47	0/2295	0.75	0/3118
1	G	0.43	0/2299	0.68	0/3122
1	J	0.45	0/2227	0.70	1/3030 (0.0%)
2	B	0.45	0/838	0.71	0/1136
2	E	0.50	0/851	0.72	0/1152
2	H	0.51	0/845	0.71	0/1145
2	K	0.47	0/847	0.69	0/1147
3	C	1.00	0/59	1.50	1/77 (1.3%)
3	F	0.92	0/59	1.26	0/77
3	I	0.90	0/59	1.30	0/77
3	L	0.97	0/55	1.26	0/71
All	All	0.48	0/12711	0.73	2/17244 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	2
1	G	0	2
1	J	0	1
All	All	0	6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	8	VAL	N-CA-CB	-7.42	103.53	111.46
1	J	6	ARG	CG-CD-NE	-6.12	98.54	112.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	ARG	Sidechain
1	D	157	ARG	Sidechain
1	D	65	ARG	Sidechain
1	G	111	ARG	Sidechain
1	G	114	ARG	Sidechain

5.2 Too-close contacts

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	2218	0	2054	70	0
1	D	2234	0	2069	57	0
1	G	2238	0	2080	65	0
1	J	2169	0	1977	41	0
2	B	815	0	770	36	0
2	E	828	0	794	28	0
2	H	822	0	783	30	0
2	K	824	0	790	37	0
3	C	60	0	70	6	0
3	F	60	0	70	7	0
3	I	60	0	70	4	0
3	L	56	0	56	2	0
4	A	8	0	0	1	0
4	B	3	0	0	1	0
4	D	9	0	0	1	0
4	E	10	0	0	0	0
4	F	1	0	0	0	0
4	G	11	0	0	3	0
4	H	7	0	0	1	0
4	J	12	0	0	1	0
4	K	11	0	0	2	0
All	All	12456	0	11583	334	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 14.

The worst 5 of 334 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:156:GLN:NE2	4:D:301:HOH:O	1.81	1.13
2:B:58:LYS:H	2:B:58:LYS:HD2	1.15	1.10
2:K:4:THR:HA	2:K:86:THR:HG21	1.48	0.96
2:B:8:GLN:HE21	2:B:99:MET:HE2	1.32	0.93
1:G:45:MET:H	1:G:64:THR:HG22	1.38	0.89

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	273/276 (99%)	267 (98%)	6 (2%)	0	100	100
1	D	273/276 (99%)	266 (97%)	7 (3%)	0	100	100
1	G	273/276 (99%)	268 (98%)	5 (2%)	0	100	100
1	J	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
2	B	97/122 (80%)	90 (93%)	7 (7%)	0	100	100
2	E	97/122 (80%)	96 (99%)	1 (1%)	0	100	100
2	H	97/122 (80%)	87 (90%)	10 (10%)	0	100	100
2	K	97/122 (80%)	95 (98%)	2 (2%)	0	100	100
3	C	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
3	F	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
3	I	8/10 (80%)	5 (62%)	3 (38%)	0	100	100
3	L	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
All	All	1512/1632 (93%)	1454 (96%)	58 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	227/233 (97%)	220 (97%)	7 (3%)	35	70
1	D	230/233 (99%)	226 (98%)	4 (2%)	53	83
1	G	231/233 (99%)	227 (98%)	4 (2%)	53	83
1	J	217/233 (93%)	215 (99%)	2 (1%)	70	89
2	B	91/110 (83%)	89 (98%)	2 (2%)	45	78
2	E	94/110 (86%)	91 (97%)	3 (3%)	34	70
2	H	93/110 (84%)	93 (100%)	0	100	100
2	K	93/110 (84%)	93 (100%)	0	100	100
3	C	5/5 (100%)	4 (80%)	1 (20%)	1	4
3	F	5/5 (100%)	4 (80%)	1 (20%)	1	4
3	I	5/5 (100%)	5 (100%)	0	100	100
3	L	3/5 (60%)	3 (100%)	0	100	100
All	All	1294/1392 (93%)	1270 (98%)	24 (2%)	50	81

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	70	PHE
3	F	3	VAL
2	E	98	ASP
1	G	113	TYR
1	A	275	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	180	GLN
1	J	255	GLN
2	K	42	ASN
1	D	66	ASN

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Mol	Chain	Res	Type
1	D	43	GLN

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 [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, 95th 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 ²)	Q<0.9
1	A	275/276 (99%)	0.24	2 (0%) 84 77	66, 90, 121, 145	0
1	D	275/276 (99%)	0.08	0 100 100	48, 79, 108, 130	0
1	G	275/276 (99%)	0.02	2 (0%) 84 77	56, 80, 112, 142	0
1	J	275/276 (99%)	0.27	1 (0%) 88 84	49, 78, 111, 139	0
2	B	99/122 (81%)	0.20	1 (1%) 79 72	58, 79, 106, 142	0
2	E	99/122 (81%)	-0.05	0 100 100	48, 64, 92, 162	0
2	H	99/122 (81%)	0.14	1 (1%) 79 72	58, 78, 105, 130	0
2	K	99/122 (81%)	-0.19	0 100 100	45, 58, 79, 108	0
3	C	10/10 (100%)	0.89	1 (10%) 12 9	88, 102, 120, 124	0
3	F	10/10 (100%)	0.83	1 (10%) 12 9	83, 103, 108, 119	0
3	I	10/10 (100%)	0.66	0 100 100	72, 82, 103, 108	0
3	L	10/10 (100%)	0.57	0 100 100	79, 91, 105, 128	0
All	All	1536/1632 (94%)	0.13	9 (0%) 85 80	45, 80, 113, 162	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1	ILE	2.5
3	C	8	VAL	2.5
2	B	99	MET	2.5
1	A	270	LEU	2.3
1	A	225	THR	2.2

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 oligosaccharides 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.