



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:22 PM UTC

PDB ID : 5IRO / pdb\_00005iro  
Title : Crystal structure of a complex between the Human adenovirus type 4 E3-19K protein and MHC class molecule HLA-A2/TAX  
Authors : Li, L.; Bouvier, M.  
Deposited on : 2016-03-14  
Resolution : 2.64 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

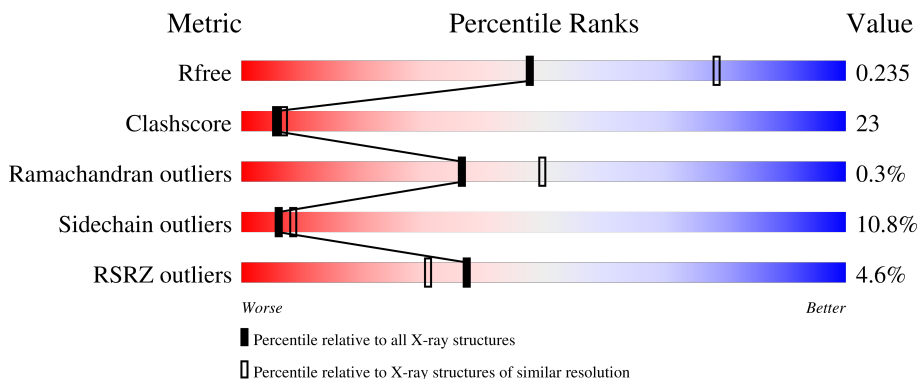
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	275	
1	E	275	
1	I	275	
1	M	275	
1	Q	275	

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Mol	Chain	Length	Quality of chain
1	U	275	
2	B	9	
2	F	9	
2	J	9	
2	N	9	
2	R	9	
2	V	9	
3	C	100	
3	G	100	
3	K	100	
3	O	100	
3	S	100	
3	W	100	
4	D	108	
4	H	108	
4	L	108	
4	P	108	
4	T	108	
4	X	108	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 23039 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-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	Total 2144	C 1338	N 389	O 408	S 9	0	0	0
1	E	268	Total 2183	C 1363	N 398	O 413	S 9	0	0	0
1	I	252	Total 2053	C 1282	N 376	O 386	S 9	0	0	0
1	M	265	Total 2160	C 1351	N 392	O 408	S 9	0	0	0
1	Q	259	Total 2111	C 1315	N 385	O 402	S 9	0	0	0
1	U	246	Total 2007	C 1259	N 363	O 376	S 9	0	0	0

- Molecule 2 is a protein called TAX protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	9	Total 76	C 56	N 9	O 11	0	0	0
2	F	9	Total 76	C 56	N 9	O 11	0	0	0
2	J	9	Total 76	C 56	N 9	O 11	0	0	0
2	N	9	Total 76	C 56	N 9	O 11	0	0	0
2	R	9	Total 76	C 56	N 9	O 11	0	0	0
2	V	9	Total 76	C 56	N 9	O 11	0	0	0

- Molecule 3 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	96	802	513	136	150	3	0	0	0
3	G	98	820	524	139	154	3	0	0	0
3	K	98	820	524	139	154	3	0	0	0
3	O	98	820	524	139	154	3	0	0	0
3	S	98	820	524	139	154	3	0	0	0
3	W	98	820	524	139	154	3	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769
K	0	MET	-	initiating methionine	UNP P61769
O	0	MET	-	initiating methionine	UNP P61769
S	0	MET	-	initiating methionine	UNP P61769
W	0	MET	-	initiating methionine	UNP P61769

- Molecule 4 is a protein called E3 19 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	102	823	520	144	149	10	0	0	0
4	H	103	832	526	146	150	10	0	0	0
4	L	103	832	526	146	150	10	0	0	0
4	P	103	832	526	146	150	10	0	0	0
4	T	103	832	526	146	150	10	0	0	0
4	X	103	832	526	146	150	10	0	0	0

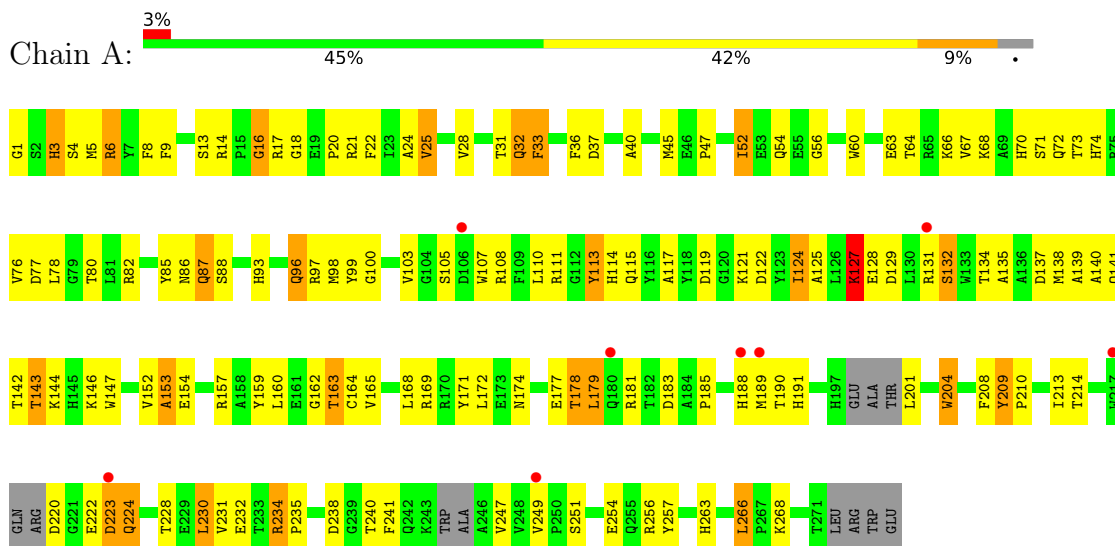
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total O 3 3	0	0
5	D	2	Total O 2 2	0	0
5	E	3	Total O 3 3	0	0
5	G	1	Total O 1 1	0	0
5	I	5	Total O 5 5	0	0
5	J	1	Total O 1 1	0	0
5	K	2	Total O 2 2	0	0
5	L	1	Total O 1 1	0	0
5	M	4	Total O 4 4	0	0
5	O	2	Total O 2 2	0	0
5	P	3	Total O 3 3	0	0
5	Q	3	Total O 3 3	0	0
5	S	3	Total O 3 3	0	0
5	T	3	Total O 3 3	0	0
5	U	3	Total O 3 3	0	0
5	W	1	Total O 1 1	0	0

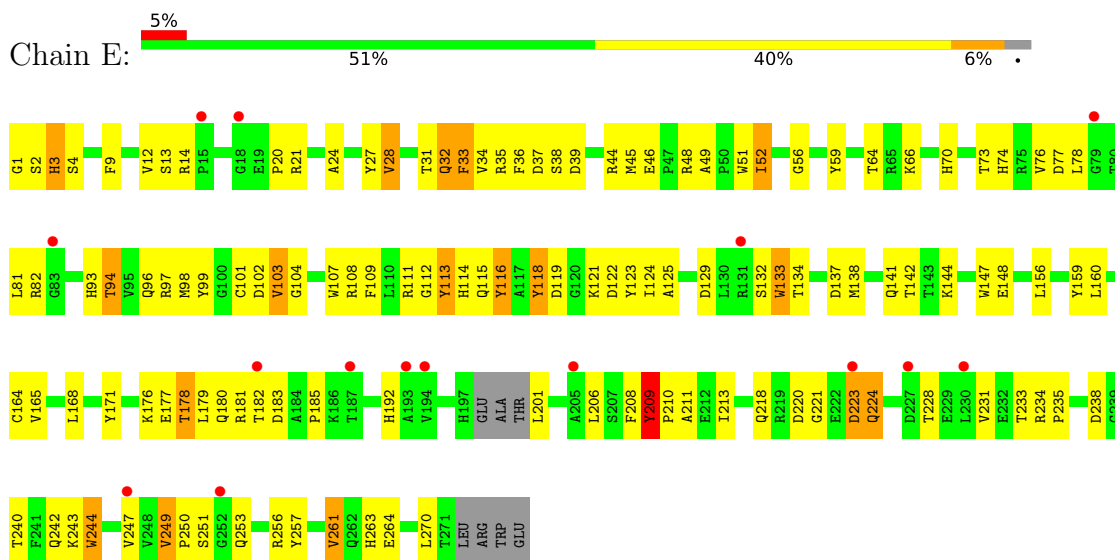
### 3 Residue-property plots [i](#)

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-2 alpha chain

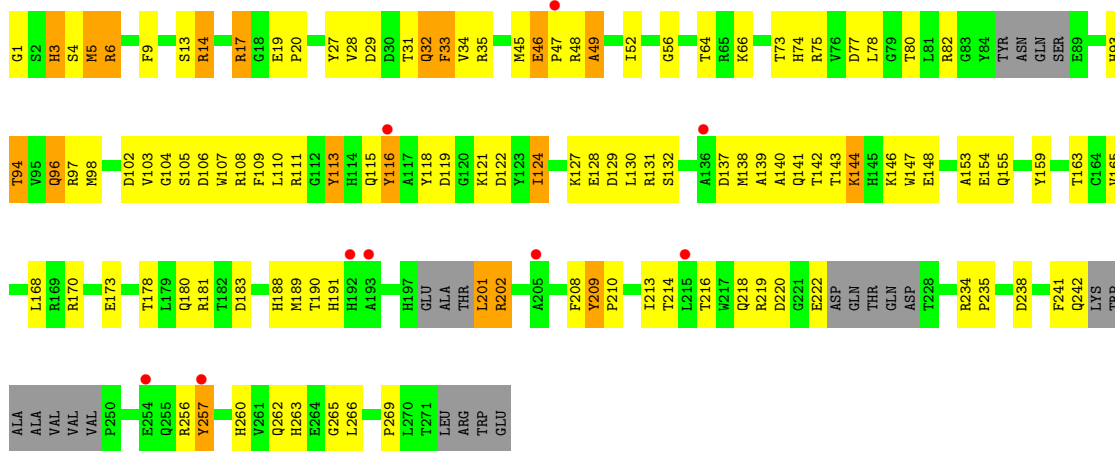


- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

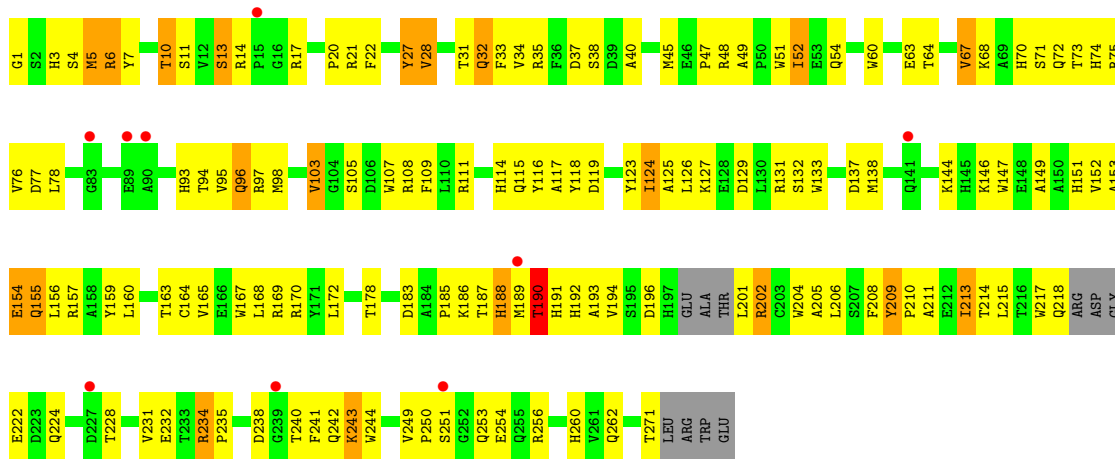


- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

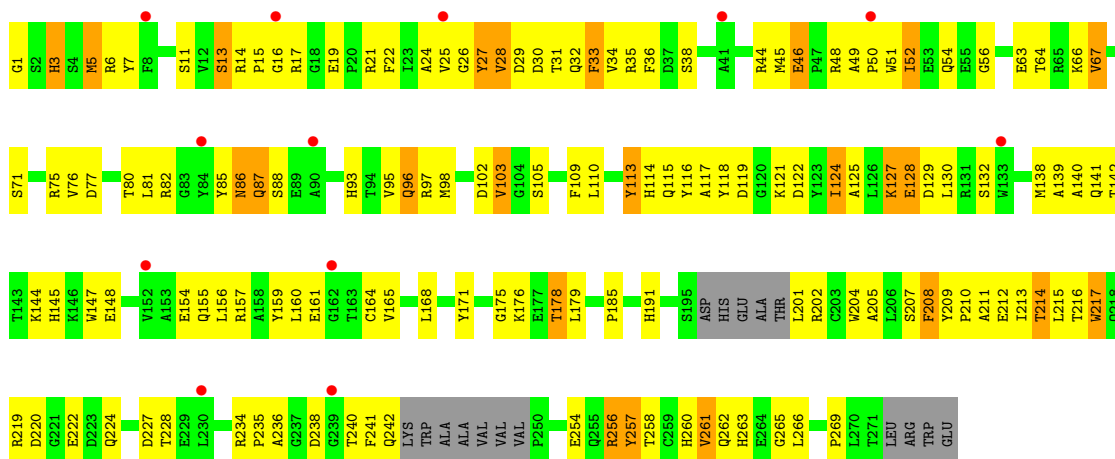




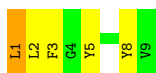
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



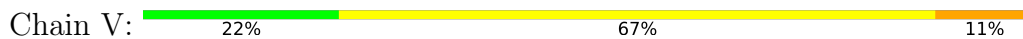
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



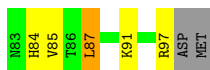
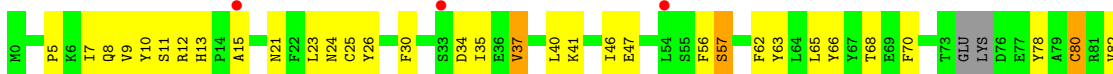




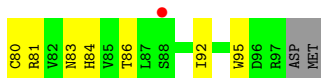
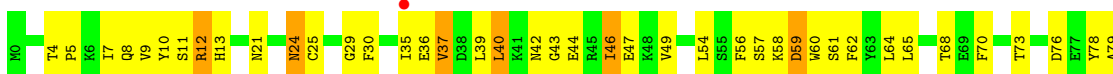
- Molecule 2: TAX protein



- Molecule 3: Beta-2-microglobulin



- Molecule 3: Beta-2-microglobulin

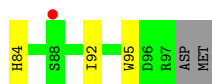


- Molecule 3: Beta-2-microglobulin

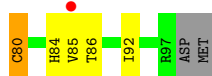
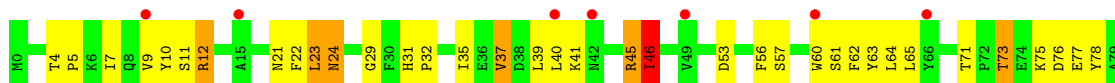


- Molecule 3: Beta-2-microglobulin

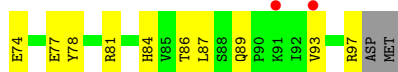




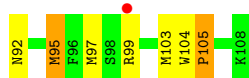
- Molecule 3: Beta-2-microglobulin



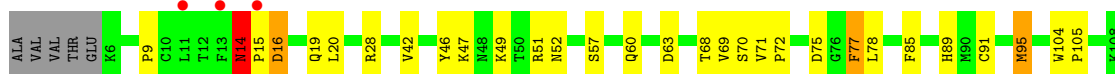
- Molecule 3: Beta-2-microglobulin



- Molecule 4: E3 19 kDa protein



- Molecule 4: E3 19 kDa protein



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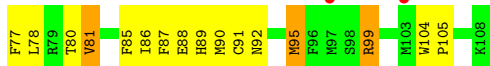




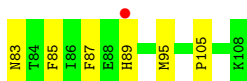
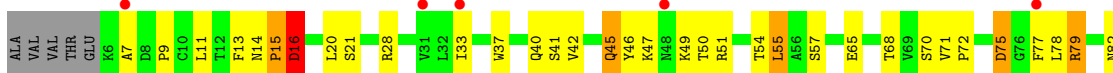
• Molecule 4: E3 19 kDa protein



• Molecule 4: E3 19 kDa protein



• Molecule 4: E3 19 kDa protein



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	165.73Å 165.73Å 122.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.62 – 2.64 49.62 – 2.64	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.62-2.64) 99.3 (49.62-2.64)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.257 , 0.288 0.217 , 0.235	Depositor DCC
$R_{free}$ test set	1983 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.6	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.31$ , $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	0.359 for -h,-k,l 0.390 for h,-h-k,-l 0.337 for -k,-h,-l	Xtriage
Reported twinning fraction	0.470 for -h,-k,l	Depositor
Outliers	0 of 110879 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	23039	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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	0.43	1/2202 (0.0%)	0.95	10/2983 (0.3%)
1	E	0.41	0/2245	0.98	9/3045 (0.3%)
1	I	0.34	0/2109	0.92	12/2852 (0.4%)
1	M	0.51	1/2221 (0.0%)	1.02	13/3012 (0.4%)
1	Q	0.43	0/2169	1.03	10/2937 (0.3%)
1	U	0.40	0/2061	1.01	16/2791 (0.6%)
2	B	0.33	0/79	0.79	0/108
2	F	0.41	0/79	0.79	0/108
2	J	0.29	0/79	0.56	0/108
2	N	0.30	0/79	0.55	0/108
2	R	0.28	0/79	0.54	0/108
2	V	0.45	0/79	0.84	0/108
3	C	0.37	0/824	0.95	4/1115 (0.4%)
3	G	0.34	0/843	0.91	3/1141 (0.3%)
3	K	0.34	0/843	0.85	1/1141 (0.1%)
3	O	0.37	0/843	0.85	1/1141 (0.1%)
3	S	0.36	0/843	0.90	5/1141 (0.4%)
3	W	0.37	0/843	0.93	3/1141 (0.3%)
4	D	0.34	0/849	0.95	3/1154 (0.3%)
4	H	0.42	0/858	1.00	4/1165 (0.3%)
4	L	0.34	0/858	0.96	7/1165 (0.6%)
4	P	0.39	0/858	0.98	6/1165 (0.5%)
4	T	0.36	0/858	0.93	5/1165 (0.4%)
4	X	0.37	0/858	1.02	3/1165 (0.3%)
All	All	0.40	2/23659 (0.0%)	0.96	115/32067 (0.4%)

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	M	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	190	THR	CA-C	8.89	1.63	1.52
1	A	153	ALA	CA-CB	-5.29	1.45	1.53

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	209	TYR	CA-C-N	-12.23	107.18	120.14
1	E	209	TYR	C-N-CA	-12.23	107.18	120.14
4	P	16	ASP	N-CA-C	-9.61	101.44	113.55
4	D	16	ASP	N-CA-C	-9.29	101.84	113.55
3	K	46	ILE	N-CA-C	9.12	115.97	106.21

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	189	MET	Peptide

## 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	2144	0	1999	136	1
1	E	2183	0	2037	108	0
1	I	2053	0	1916	105	0
1	M	2160	0	2016	151	0
1	Q	2111	0	1966	120	0
1	U	2007	0	1881	116	0
2	B	76	0	79	13	0
2	F	76	0	79	9	0
2	J	76	0	79	6	0
2	N	76	0	79	11	0
2	R	76	0	79	9	0
2	V	76	0	79	9	0
3	C	802	0	770	27	0
3	G	820	0	790	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	820	0	790	31	0
3	O	820	0	790	32	0
3	S	820	0	790	36	0
3	W	820	0	790	42	0
4	D	823	0	773	29	0
4	H	832	0	786	16	0
4	L	832	0	786	23	0
4	P	832	0	786	27	0
4	T	832	0	786	40	0
4	X	832	0	786	28	0
5	A	3	0	0	0	0
5	D	2	0	0	0	0
5	E	3	0	0	0	0
5	G	1	0	0	0	0
5	I	5	0	0	0	0
5	J	1	0	0	0	0
5	K	2	0	0	0	0
5	L	1	0	0	0	0
5	M	4	0	0	0	0
5	O	2	0	0	1	0
5	P	3	0	0	0	0
5	Q	3	0	0	0	0
5	S	3	0	0	0	0
5	T	3	0	0	0	0
5	U	3	0	0	0	0
5	W	1	0	0	0	0
All	All	23039	0	21712	1042	1

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 23.

The worst 5 of 1042 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:I:32:GLN:HB2	1:I:48:ARG:HH12	1.24	1.01
1:M:205:ALA:HB3	1:M:243:LYS:HE2	1.45	0.99
1:Q:5:MET:HG3	1:Q:6:ARG:HG3	1.47	0.96
1:U:250:PRO:O	1:U:253:GLN:NE2	2.01	0.93
1:E:59:TYR:HH	1:E:171:TYR:HH	1.12	0.91

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:SER:OG	1:A:129:ASP:OD1[3_555]	2.13	0.07

## 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	256/275 (93%)	229 (90%)	27 (10%)	0	100	100
1	E	264/275 (96%)	233 (88%)	31 (12%)	0	100	100
1	I	242/275 (88%)	216 (89%)	26 (11%)	0	100	100
1	M	259/275 (94%)	230 (89%)	29 (11%)	0	100	100
1	Q	253/275 (92%)	225 (89%)	27 (11%)	1 (0%)	30	42
1	U	238/275 (86%)	214 (90%)	23 (10%)	1 (0%)	30	42
2	B	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	J	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	N	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	R	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	V	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	C	92/100 (92%)	82 (89%)	10 (11%)	0	100	100
3	G	96/100 (96%)	85 (88%)	11 (12%)	0	100	100
3	K	96/100 (96%)	84 (88%)	12 (12%)	0	100	100
3	O	96/100 (96%)	86 (90%)	10 (10%)	0	100	100
3	S	96/100 (96%)	86 (90%)	10 (10%)	0	100	100
3	W	96/100 (96%)	85 (88%)	11 (12%)	0	100	100
4	D	100/108 (93%)	88 (88%)	11 (11%)	1 (1%)	12	18
4	H	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	12	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	12	18
4	P	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	12	18
4	T	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	12	18
4	X	101/108 (94%)	89 (88%)	10 (10%)	2 (2%)	6	8
All	All	2731/2952 (92%)	2424 (89%)	298 (11%)	9 (0%)	36	50

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	9	PRO
4	P	9	PRO
4	X	9	PRO
4	H	9	PRO
4	T	9	PRO

### 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	222/231 (96%)	196 (88%)	26 (12%)	5	7
1	E	225/231 (97%)	203 (90%)	22 (10%)	7	11
1	I	211/231 (91%)	186 (88%)	25 (12%)	5	6
1	M	223/231 (96%)	199 (89%)	24 (11%)	6	8
1	Q	218/231 (94%)	188 (86%)	30 (14%)	3	4
1	U	206/231 (89%)	179 (87%)	27 (13%)	4	5
2	B	8/8 (100%)	6 (75%)	2 (25%)	0	0
2	F	8/8 (100%)	5 (62%)	3 (38%)	0	0
2	J	8/8 (100%)	8 (100%)	0	100	100
2	N	8/8 (100%)	7 (88%)	1 (12%)	4	6
2	R	8/8 (100%)	7 (88%)	1 (12%)	4	6
2	V	8/8 (100%)	6 (75%)	2 (25%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	91/95 (96%)	85 (93%)	6 (7%)	15	25
3	G	93/95 (98%)	84 (90%)	9 (10%)	8	11
3	K	93/95 (98%)	81 (87%)	12 (13%)	4	5
3	O	93/95 (98%)	85 (91%)	8 (9%)	10	15
3	S	93/95 (98%)	84 (90%)	9 (10%)	8	11
3	W	93/95 (98%)	88 (95%)	5 (5%)	20	33
4	D	91/96 (95%)	85 (93%)	6 (7%)	15	25
4	H	92/96 (96%)	84 (91%)	8 (9%)	9	15
4	L	92/96 (96%)	82 (89%)	10 (11%)	6	8
4	P	92/96 (96%)	82 (89%)	10 (11%)	6	8
4	T	92/96 (96%)	84 (91%)	8 (9%)	9	15
4	X	92/96 (96%)	80 (87%)	12 (13%)	4	5
All	All	2460/2580 (95%)	2194 (89%)	266 (11%)	6	8

5 of 266 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	114	HIS
1	U	182	THR
4	X	55	LEU
1	I	130	LEU
1	I	113	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
3	O	42	ASN
1	Q	224	GLN
4	P	52	ASN
1	Q	87	GLN
1	Q	262	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, 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	264/275 (96%)	0.22	8 (3%) 52 47	20, 49, 98, 218	0
1	E	268/275 (97%)	0.33	15 (5%) 30 25	18, 49, 126, 173	0
1	I	252/275 (91%)	0.20	9 (3%) 46 40	14, 41, 85, 176	0
1	M	265/275 (96%)	0.36	9 (3%) 48 42	18, 51, 117, 161	0
1	Q	259/275 (94%)	0.64	12 (4%) 37 31	22, 61, 134, 238	0
1	U	246/275 (89%)	0.70	28 (11%) 10 8	27, 59, 131, 224	0
2	B	9/9 (100%)	0.07	0 100 100	29, 33, 52, 58	0
2	F	9/9 (100%)	0.26	0 100 100	34, 53, 82, 85	0
2	J	9/9 (100%)	0.15	0 100 100	22, 33, 49, 83	0
2	N	9/9 (100%)	0.13	0 100 100	20, 39, 61, 77	0
2	R	9/9 (100%)	0.66	0 100 100	33, 41, 70, 75	0
2	V	9/9 (100%)	0.51	0 100 100	41, 51, 77, 80	0
3	C	96/100 (96%)	0.26	3 (3%) 51 45	30, 54, 130, 166	0
3	G	98/100 (98%)	0.07	2 (2%) 65 61	16, 42, 73, 218	0
3	K	98/100 (98%)	0.07	2 (2%) 65 61	15, 40, 74, 180	0
3	O	98/100 (98%)	0.18	3 (3%) 51 45	26, 48, 121, 147	0
3	S	98/100 (98%)	0.66	8 (8%) 17 14	23, 57, 142, 203	0
3	W	98/100 (98%)	0.69	8 (8%) 17 14	20, 57, 115, 186	0
4	D	102/108 (94%)	0.06	2 (1%) 65 61	15, 42, 79, 193	0
4	H	103/108 (95%)	0.09	3 (2%) 53 48	22, 38, 76, 132	0
4	L	103/108 (95%)	0.05	2 (1%) 66 62	17, 36, 81, 129	0
4	P	103/108 (95%)	0.08	2 (1%) 66 62	16, 44, 115, 147	0
4	T	103/108 (95%)	0.37	7 (6%) 23 19	19, 54, 114, 160	0
4	X	103/108 (95%)	0.47	6 (5%) 29 24	18, 49, 92, 186	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	2811/2952 (95%)	0.34	129 (4%) 37 31	14, 49, 118, 238	0

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	W	93	VAL	6.7
3	W	20	SER	6.0
1	E	223	ASP	5.7
1	I	254	GLU	5.0
1	M	90	ALA	4.8

## 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 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.