



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 8, 2026 – 07:35 AM JST

PDB ID : 9K2I / pdb_00009k2i
Title : Rac1 epitope specific TCR 5934 binding to Rac1P29S-HLA-A2
Authors : Yang, D.D.; Wu, D.C.
Deposited on : 2024-10-17
Resolution : 3.05 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

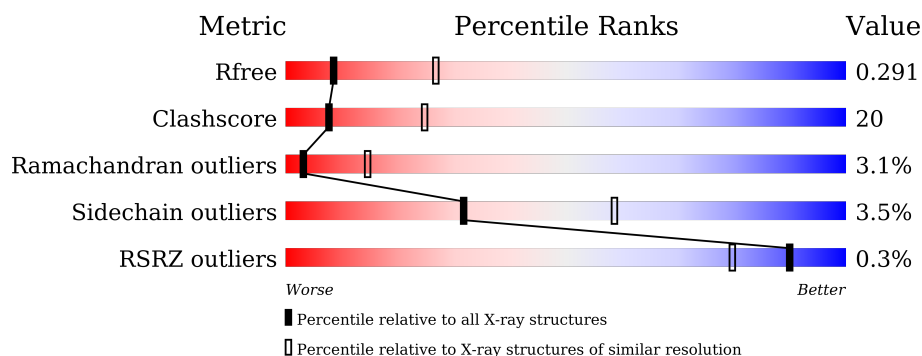
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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.



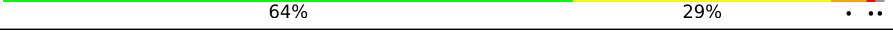
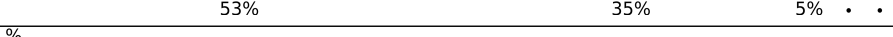
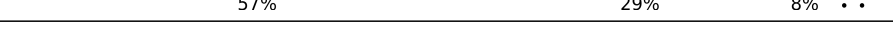
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	67% 28% ..
1	F	276	61% 36% .
1	K	276	% 57% 33% 7% .
1	P	276	70% 26% ..
2	B	100	70% 27% .
2	G	100	% 79% 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	L	100	 66% 32% .
2	Q	100	 79% 21%
3	C	9	 89% 11%
3	H	9	 44% 44% 11%
3	M	9	 67% 22% 11%
3	R	9	 56% 33% 11%
4	E	247	 61% 34% . .
4	J	247	 68% 28% . .
4	O	247	 64% 29% . .
4	T	247	 61% 34% . .
5	D	207	 % 53% 35% 5% . .
5	I	207	 % 46% 40% 7% . .
5	N	207	 50% 39% 5% . .
5	S	207	 57% 29% 8% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26756 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			
1	F	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			
1	K	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			
1	P	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q8WLS4
F	0	MET	-	initiating methionine	UNP Q8WLS4
K	0	MET	-	initiating methionine	UNP Q8WLS4
P	0	MET	-	initiating methionine	UNP Q8WLS4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	4	3	0
			848	541	142	161	4			
2	G	100	Total	C	N	O	S	4	3	0
			848	541	142	161	4			
2	L	100	Total	C	N	O	S	3	3	0
			848	541	142	161	4			
2	Q	100	Total	C	N	O	S	4	3	0
			848	541	142	161	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769
L	0	MET	-	initiating methionine	UNP P61769
Q	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called PHE-SER-GLY-GLU-TYR-ILE-PRO-THR-VAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			72	48	9	15			
3	H	9	Total	C	N	O	0	0	0
			72	48	9	15			
3	M	9	Total	C	N	O	0	0	0
			72	48	9	15			
3	R	9	Total	C	N	O	0	0	0
			72	48	9	15			

- Molecule 4 is a protein called T cell receptor 5934 chain beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	245	Total	C	N	O	S	0	0	0
			1962	1245	336	373	8			
4	E	245	Total	C	N	O	S	0	0	0
			1962	1245	336	373	8			
4	T	245	Total	C	N	O	S	0	0	0
			1962	1245	336	373	8			
4	O	245	Total	C	N	O	S	0	0	0
			1962	1245	336	373	8			

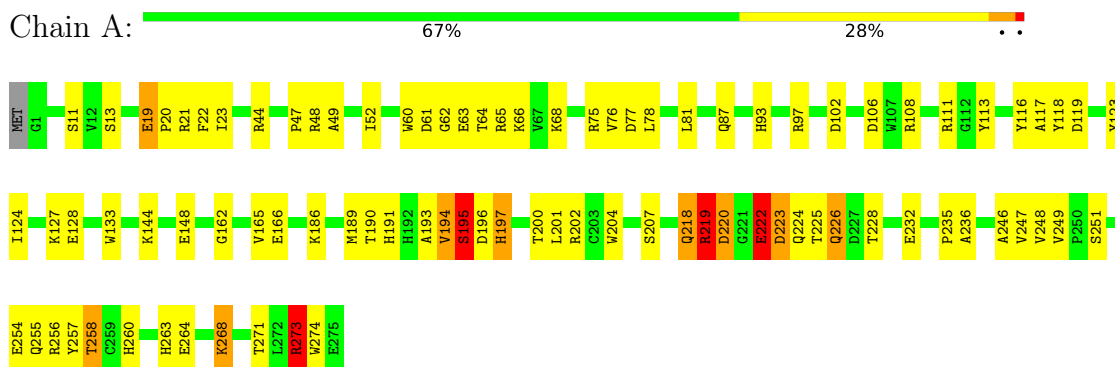
- Molecule 5 is a protein called T cell receptor5934 chain alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	200	Total	C	N	O	S	0	0	0
			1561	972	265	317	7			
5	D	200	Total	C	N	O	S	0	0	0
			1561	972	265	317	7			
5	S	200	Total	C	N	O	S	0	0	0
			1561	972	265	317	7			
5	N	200	Total	C	N	O	S	0	0	0
			1561	972	265	317	7			

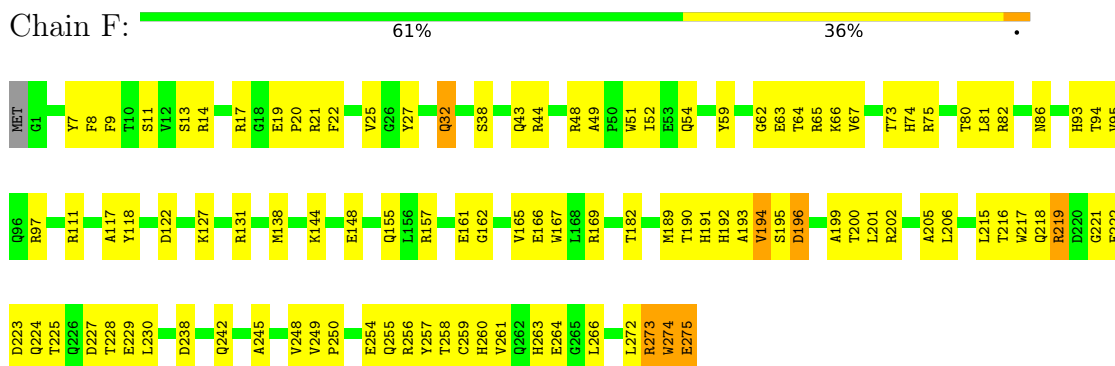
3 Residue-property plots

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.

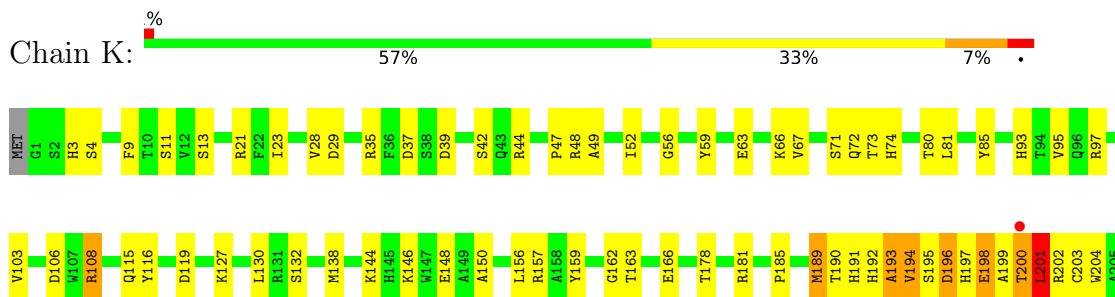
• Molecule 1: MHC class I antigen

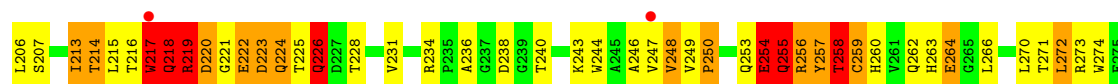


• Molecule 1: MHC class I antigen



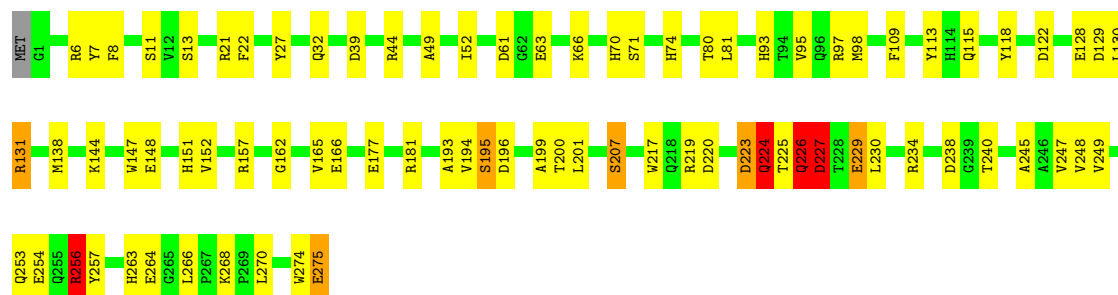
• Molecule 1: MHC class I antigen





• Molecule 1: MHC class I antigen

Chain P: 70% 26% ..



• Molecule 2: Beta-2-microglobulin

Chain B: 70% 27% .



• Molecule 2: Beta-2-microglobulin

Chain G: 79% 21%



• Molecule 2: Beta-2-microglobulin

Chain L: 66% 32% .



• Molecule 2: Beta-2-microglobulin

Chain Q: 79% 21%



• Molecule 3: PHE-SER-GLY-GLU-TYR-ILE-PRO-THR-VAL

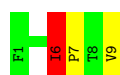
Chain C: 89% 11%



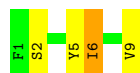
- Molecule 3: PHE-SER-GLY-GLU-TYR-ILE-PRO-THR-VAL



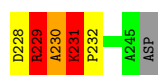
- Molecule 3: PHE-SER-GLY-GLU-TYR-ILE-PRO-THR-VAL



- Molecule 3: PHE-SER-GLY-GLU-TYR-ILE-PRO-THR-VAL



- Molecule 4: T cell receptor 5934 chain beta

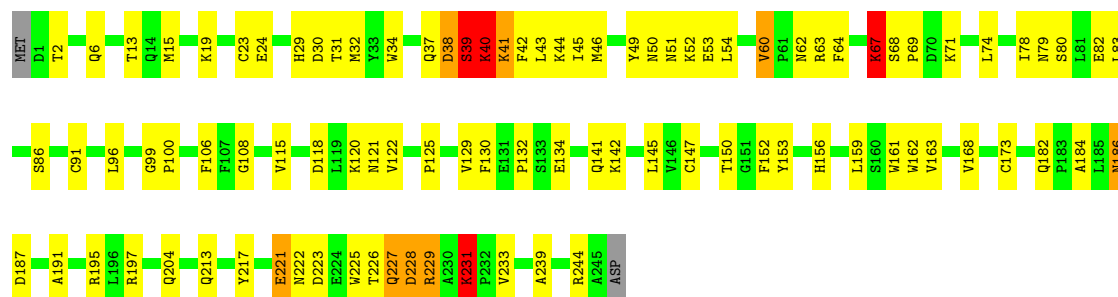


- Molecule 4: T cell receptor 5934 chain beta



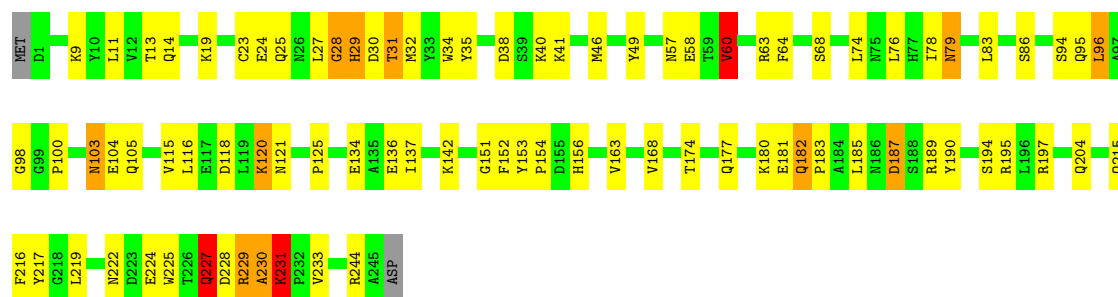
• Molecule 4: T cell receptor 5934 chain beta

Chain T:  61% 34% . . .



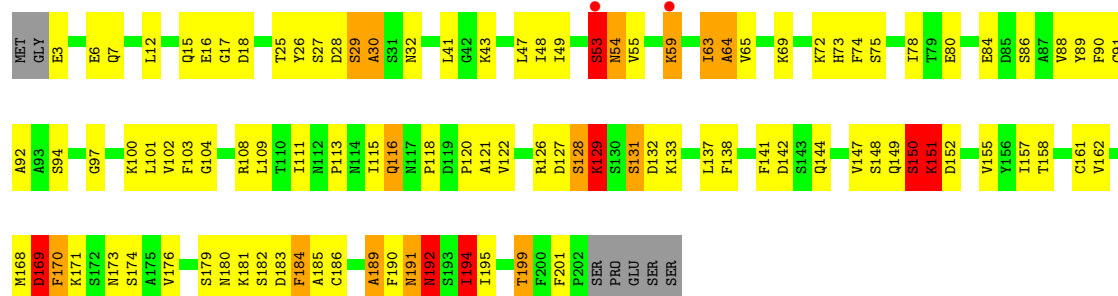
• Molecule 4: T cell receptor 5934 chain beta

Chain O:  64% 29% . . .



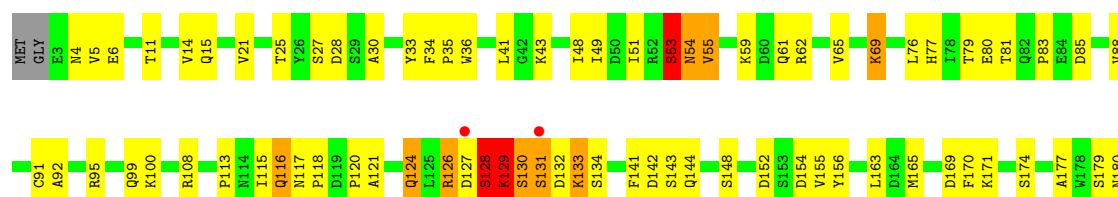
• Molecule 5: T cell receptor5934 chain alpha

Chain I:  % 46% 40% 7% . .



• Molecule 5: T cell receptor5934 chain alpha

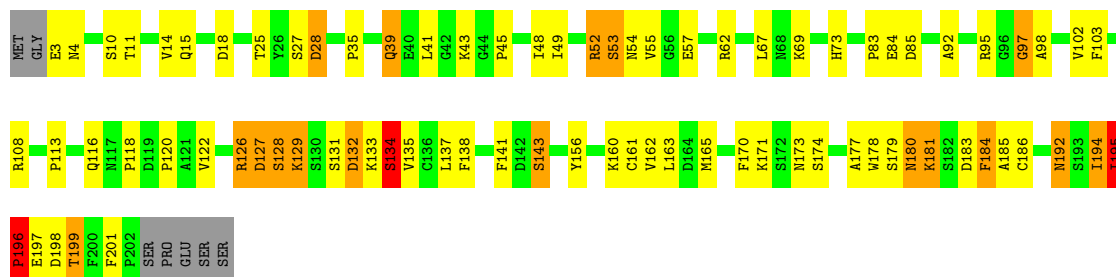
Chain D:  % 53% 35% 5% . . .





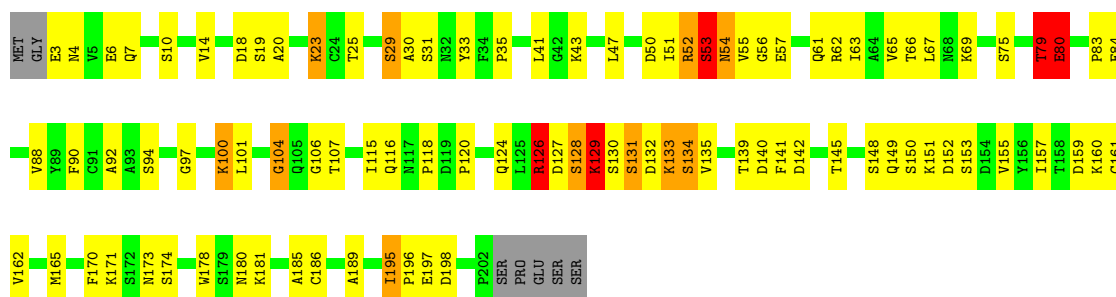
• Molecule 5: T cell receptor5934 chain alpha

Chain S: 57% 29% 8% ..



• Molecule 5: T cell receptor5934 chain alpha

Chain N: 50% 39% 5% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.30Å 147.50Å 122.17Å 90.00° 94.25° 90.00°	Depositor
Resolution (Å)	46.97 – 3.05 46.97 – 3.05	Depositor EDS
% Data completeness (in resolution range)	97.8 (46.97-3.05) 97.4 (46.97-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.222 , 0.290 0.227 , 0.291	Depositor DCC
R_{free} test set	1978 reflections (2.61%)	wwPDB-VP
Wilson B-factor (Å ²)	68.6	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	26756	wwPDB-VP
Average B, all atoms (Å ²)	75.0	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 19.82 % 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 9.9629e-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	0.72	0/2311	1.13	11/3137 (0.4%)
1	F	0.66	1/2311 (0.0%)	1.07	4/3137 (0.1%)
1	K	0.86	5/2311 (0.2%)	1.29	28/3137 (0.9%)
1	P	0.71	0/2311	1.17	7/3137 (0.2%)
2	B	0.52	0/884	0.94	0/1194
2	G	0.60	0/884	1.05	2/1194 (0.2%)
2	L	0.60	0/884	1.06	5/1194 (0.4%)
2	Q	0.57	0/884	1.01	0/1194
3	C	0.69	0/74	1.02	0/99
3	H	0.60	0/74	0.88	0/99
3	M	0.98	1/74 (1.4%)	1.03	0/99
3	R	0.82	0/74	0.94	0/99
4	E	0.67	1/2016 (0.0%)	1.14	14/2742 (0.5%)
4	J	0.62	0/2016	1.07	6/2742 (0.2%)
4	O	0.64	2/2016 (0.1%)	1.07	6/2742 (0.2%)
4	T	0.68	0/2016	1.14	13/2742 (0.5%)
5	D	0.77	2/1593 (0.1%)	1.37	19/2159 (0.9%)
5	I	0.74	0/1593	1.27	11/2159 (0.5%)
5	N	0.71	1/1593 (0.1%)	1.25	13/2159 (0.6%)
5	S	0.74	2/1593 (0.1%)	1.37	16/2159 (0.7%)
All	All	0.70	15/27512 (0.1%)	1.17	155/37324 (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	A	0	2
1	K	0	5
1	P	0	1
2	G	0	1
2	L	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
4	T	0	1
5	D	0	5
5	I	0	6
5	N	0	6
5	S	0	5
All	All	0	33

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	258	THR	CA-C	9.75	1.63	1.52
1	K	218	GLN	CA-C	8.76	1.61	1.53
5	D	195	ILE	CA-C	7.50	1.60	1.52
5	S	127	ASP	CA-C	6.59	1.55	1.52
5	N	80	GLU	CA-C	6.38	1.61	1.52

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	195	ILE	CA-C-N	16.70	140.72	119.84
5	S	195	ILE	C-N-CA	16.70	140.72	119.84
1	A	218	GLN	N-CA-C	13.91	130.79	109.23
5	N	129	LYS	N-CA-C	12.11	127.44	108.67
5	D	195	ILE	CA-C-N	-11.99	104.85	119.84

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	SER	Peptide
1	A	197	HIS	Peptide
2	G	19	LYS	Peptide
1	K	108	ARG	Peptide
1	K	217	TRP	Peptide

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	2246	0	2096	105	0
1	F	2246	0	2096	97	1
1	K	2246	0	2096	141	1
1	P	2246	0	2096	95	0
2	B	848	0	817	26	0
2	G	848	0	817	15	0
2	L	848	0	817	27	0
2	Q	848	0	817	14	1
3	C	72	0	68	3	0
3	H	72	0	68	5	0
3	M	72	0	68	7	0
3	R	72	0	68	4	0
4	E	1962	0	1885	72	0
4	J	1962	0	1885	57	0
4	O	1962	0	1885	67	0
4	T	1962	0	1885	87	0
5	D	1561	0	1490	86	0
5	I	1561	0	1490	80	1
5	N	1561	0	1490	87	1
5	S	1561	0	1490	79	1
All	All	26756	0	25424	1044	3

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 20.

The worst 5 of 1044 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)
4:E:211:ARG:NH1	4:E:213:GLN:OE1	1.87	1.08
1:K:219:ARG:HG3	1:K:220:ASP:H	1.12	1.06
1:K:217:TRP:CZ2	1:K:257:TYR:HA	1.94	1.03
5:I:59:LYS:HZ3	5:I:64:ALA:HB3	1.21	1.00
5:N:100:LYS:NZ	4:O:58:GLU:OE2	1.94	1.00

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:MET:SD	5:I:151:LYS:NZ[2_647]	2.15	0.05
2:Q:89:GLN:NE2	5:N:197:GLU:OE2[2_556]	2.15	0.05
1:K:85:TYR:O	5:S:183:ASP:OD2[2_656]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	240 (88%)	28 (10%)	5 (2%)	6	24
1	F	273/276 (99%)	241 (88%)	26 (10%)	6 (2%)	5	20
1	K	273/276 (99%)	234 (86%)	35 (13%)	4 (2%)	8	28
1	P	273/276 (99%)	240 (88%)	28 (10%)	5 (2%)	6	24
2	B	101/100 (101%)	96 (95%)	5 (5%)	0	100	100
2	G	101/100 (101%)	96 (95%)	5 (5%)	0	100	100
2	L	101/100 (101%)	96 (95%)	5 (5%)	0	100	100
2	Q	101/100 (101%)	97 (96%)	4 (4%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	H	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	M	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	R	7/9 (78%)	7 (100%)	0	0	100	100
4	E	243/247 (98%)	207 (85%)	32 (13%)	4 (2%)	7	26
4	J	243/247 (98%)	207 (85%)	29 (12%)	7 (3%)	3	16
4	O	243/247 (98%)	205 (84%)	28 (12%)	10 (4%)	2	10
4	T	243/247 (98%)	209 (86%)	27 (11%)	7 (3%)	3	16
5	D	198/207 (96%)	159 (80%)	26 (13%)	13 (7%)	1	5
5	I	198/207 (96%)	154 (78%)	26 (13%)	18 (9%)	0	2
5	N	198/207 (96%)	154 (78%)	35 (18%)	9 (4%)	2	9
5	S	198/207 (96%)	157 (79%)	28 (14%)	13 (7%)	1	5
All	All	3288/3356 (98%)	2818 (86%)	369 (11%)	101 (3%)	3	14

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	222	GLU
1	F	194	VAL
1	F	228	THR
4	J	227	GLN

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	231/232 (100%)	226 (98%)	5 (2%)	45	67
1	F	231/232 (100%)	223 (96%)	8 (4%)	32	59
1	K	231/232 (100%)	219 (95%)	12 (5%)	21	48
1	P	231/232 (100%)	223 (96%)	8 (4%)	32	59
2	B	98/95 (103%)	91 (93%)	7 (7%)	13	37
2	G	98/95 (103%)	98 (100%)	0	100	100
2	L	98/95 (103%)	97 (99%)	1 (1%)	68	77
2	Q	98/95 (103%)	98 (100%)	0	100	100
3	C	8/8 (100%)	8 (100%)	0	100	100
3	H	8/8 (100%)	6 (75%)	2 (25%)	0	2
3	M	8/8 (100%)	7 (88%)	1 (12%)	4	16
3	R	8/8 (100%)	7 (88%)	1 (12%)	4	16
4	E	217/219 (99%)	210 (97%)	7 (3%)	34	60
4	J	217/219 (99%)	209 (96%)	8 (4%)	30	57
4	O	217/219 (99%)	207 (95%)	10 (5%)	24	52
4	T	217/219 (99%)	209 (96%)	8 (4%)	30	57
5	D	178/184 (97%)	174 (98%)	4 (2%)	45	67
5	I	178/184 (97%)	172 (97%)	6 (3%)	32	59
5	N	178/184 (97%)	168 (94%)	10 (6%)	19	45
5	S	178/184 (97%)	174 (98%)	4 (2%)	45	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2928/2952 (99%)	2826 (96%)	102 (4%)	32 59

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	I	194	ILE
5	S	57	GLU
4	O	185	LEU
5	D	69	LYS
4	E	60	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
5	D	124	GLN
4	T	6	GLN
5	D	192	ASN
4	E	121	ASN
4	T	139	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

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, 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%)	-0.17	0 100 100	44, 66, 127, 184	0
1	F	275/276 (99%)	-0.27	0 100 100	43, 62, 118, 164	0
1	K	275/276 (99%)	-0.01	3 (1%) 78 57	46, 71, 155, 172	0
1	P	275/276 (99%)	-0.24	0 100 100	43, 60, 117, 133	0
2	B	100/100 (100%)	-0.18	0 100 100	47, 77, 103, 117	3 (3%)
2	G	100/100 (100%)	-0.28	1 (1%) 79 59	44, 64, 87, 113	3 (3%)
2	L	100/100 (100%)	-0.24	0 100 100	46, 68, 93, 116	3 (3%)
2	Q	100/100 (100%)	-0.30	0 100 100	44, 65, 93, 99	3 (3%)
3	C	9/9 (100%)	-0.43	0 100 100	51, 55, 63, 63	0
3	H	9/9 (100%)	-0.16	0 100 100	52, 56, 66, 66	0
3	M	9/9 (100%)	-0.05	0 100 100	52, 54, 57, 60	0
3	R	9/9 (100%)	-0.21	0 100 100	49, 53, 57, 58	0
4	E	245/247 (99%)	-0.24	1 (0%) 88 75	41, 66, 106, 119	0
4	J	245/247 (99%)	-0.13	0 100 100	46, 72, 115, 131	0
4	O	245/247 (99%)	-0.18	0 100 100	47, 71, 106, 129	0
4	T	245/247 (99%)	-0.27	0 100 100	47, 65, 98, 123	0
5	D	200/207 (96%)	-0.01	2 (1%) 79 59	50, 78, 123, 154	0
5	I	200/207 (96%)	0.03	2 (1%) 79 59	52, 81, 133, 157	0
5	N	200/207 (96%)	-0.00	0 100 100	52, 82, 137, 159	0
5	S	200/207 (96%)	-0.06	0 100 100	45, 74, 123, 154	0
All	All	3316/3356 (98%)	-0.15	9 (0%) 90 80	41, 70, 121, 184	12 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	247	VAL	2.5
5	I	53	SER	2.5
5	I	59	LYS	2.4
5	D	127	ASP	2.3
1	K	200	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.