



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 06:22 AM UTC

PDB ID : 8ENH / pdb_00008enh
Title : Cross-reactive 3180 TCR recognition of HLA-B*35:01-NP7 epitope from 2002 H3N2 influenza strain
Authors : Littler, D.R.; Rossjohn, J.
Deposited on : 2022-09-30
Resolution : 2.50 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

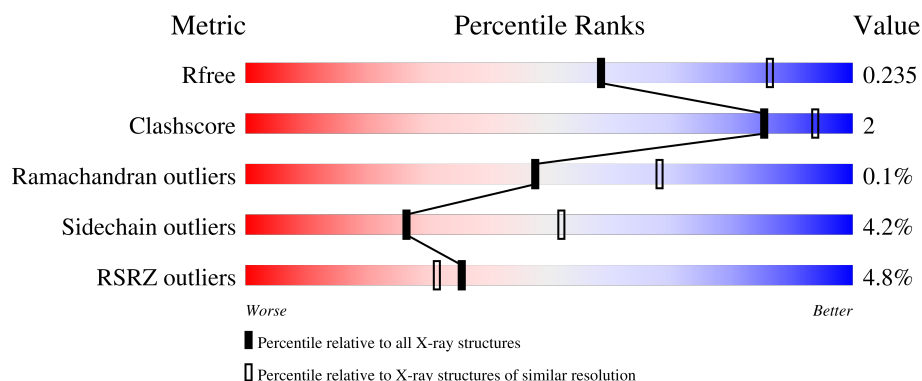
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



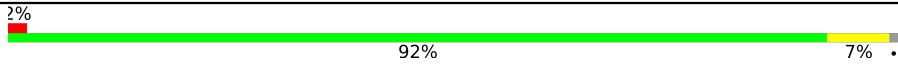
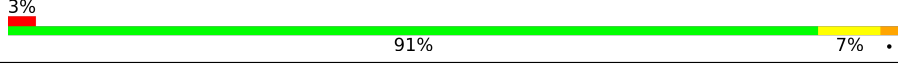
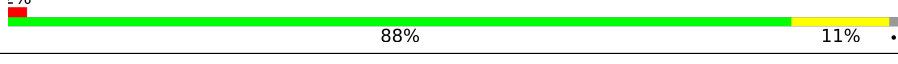
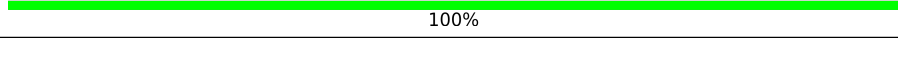
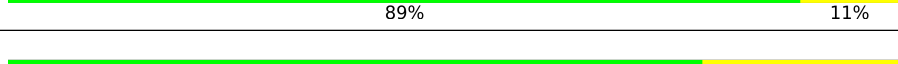
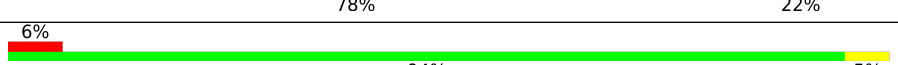
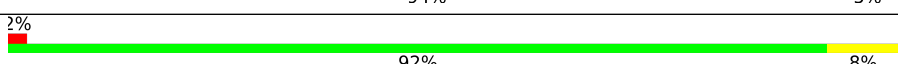
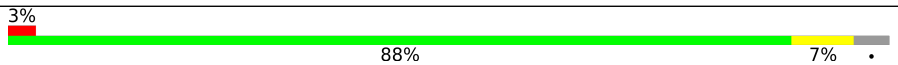
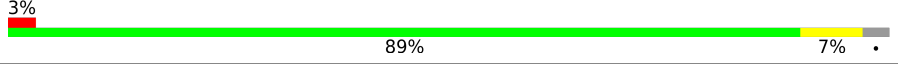
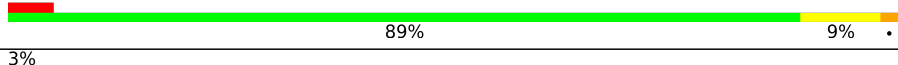
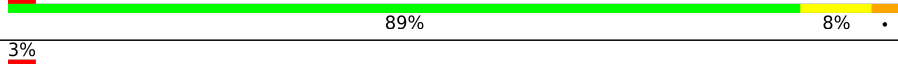
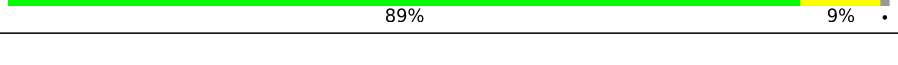
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	7% 90% 8% .
1	F	276	% 92% 7%
1	K	276	10% 84% 7% 9%
1	P	276	5% 90% 9% .
2	B	100	% 88% 9% ..

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Mol	Chain	Length	Quality of chain
2	G	100	
2	L	100	
2	Q	100	
3	C	9	
3	H	9	
3	M	9	
3	R	9	
4	D	206	
4	I	206	
4	N	206	
4	S	206	
5	E	246	
5	J	246	
5	O	246	
5	T	246	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27676 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	1	0
			2258	1408	411	431	8			
1	F	275	Total	C	N	O	S	0	0	0
			2250	1403	410	430	7			
1	K	252	Total	C	N	O	S	0	0	0
			2069	1299	379	384	7			
1	P	275	Total	C	N	O	S	0	0	0
			2250	1403	410	430	7			

- 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
			829	528	140	158	3			
2	G	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	L	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	Q	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

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 Nucleoprotein NP7 epitope.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			74	49	10	14	1			
3	H	9	Total	C	N	O	S	0	0	0
			74	49	10	14	1			
3	M	9	Total	C	N	O	S	0	0	0
			74	49	10	14	1			
3	R	9	Total	C	N	O	S	0	0	0
			74	49	10	14	1			

- Molecule 4 is a protein called 3180 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	205	Total	C	N	O	S	0	0	0
			1591	992	266	326	7			
4	I	205	Total	C	N	O	S	0	0	0
			1591	992	266	326	7			
4	N	198	Total	C	N	O	S	0	0	0
			1530	951	259	313	7			
4	S	199	Total	C	N	O	S	0	0	0
			1539	956	260	316	7			

- Molecule 5 is a protein called 3180 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	245	Total	C	N	O	S	0	0	0
			1937	1219	334	375	9			
5	J	246	Total	C	N	O	S	0	0	0
			1942	1222	335	376	9			
5	O	246	Total	C	N	O	S	0	0	0
			1942	1222	335	376	9			
5	T	244	Total	C	N	O	S	0	0	0
			1928	1215	333	371	9			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	102	Total	O	0	0
			102	102		
6	B	48	Total	O	0	0
			48	48		
6	C	8	Total	O	0	0
			8	8		

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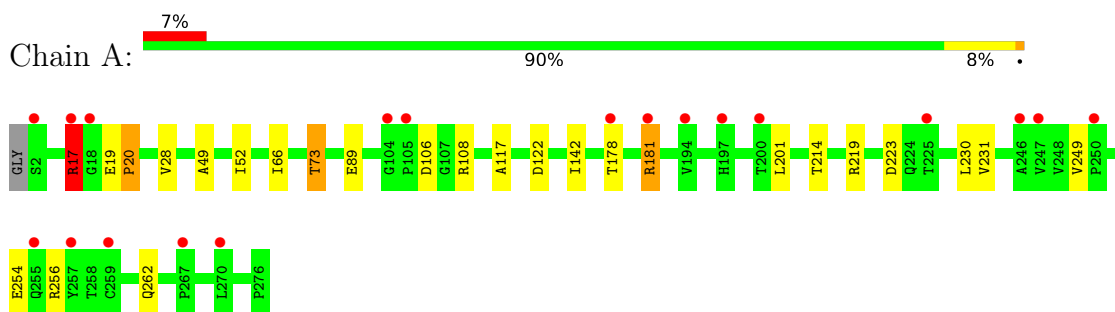
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	39	Total 39	O 39	0	0
6	E	70	Total 70	O 70	0	0
6	F	138	Total 138	O 138	0	0
6	G	66	Total 66	O 66	0	0
6	H	6	Total 6	O 6	0	0
6	I	57	Total 57	O 57	0	0
6	J	78	Total 78	O 78	0	0
6	K	118	Total 118	O 118	0	0
6	L	59	Total 59	O 59	0	0
6	M	5	Total 5	O 5	0	0
6	N	66	Total 66	O 66	0	0
6	O	78	Total 78	O 78	0	0
6	P	116	Total 116	O 116	0	0
6	Q	51	Total 51	O 51	0	0
6	R	4	Total 4	O 4	0	0
6	S	50	Total 50	O 50	0	0
6	T	70	Total 70	O 70	0	0

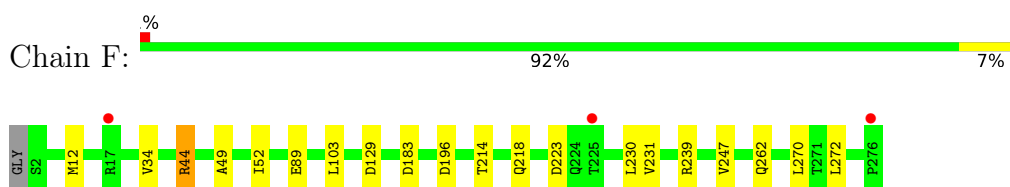
3 Residue-property plots [i](#)

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.

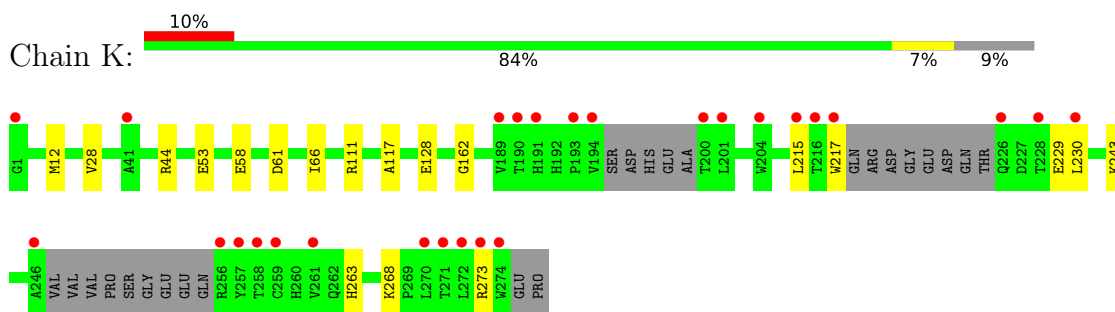
- Molecule 1: MHC class I antigen



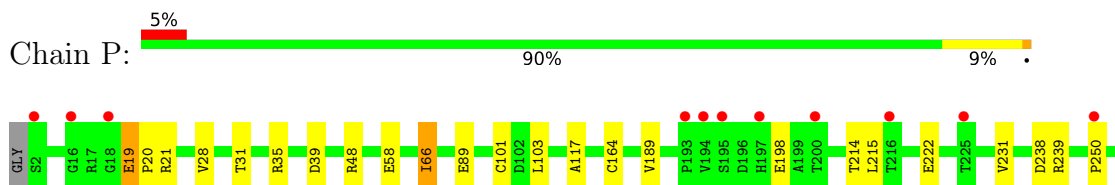
- Molecule 1: MHC class I antigen

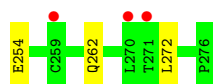


- Molecule 1: MHC class I antigen

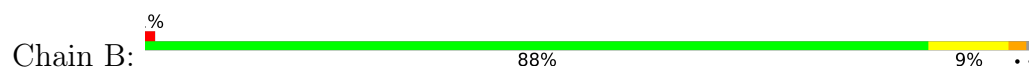


- Molecule 1: MHC class I antigen





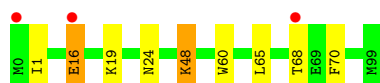
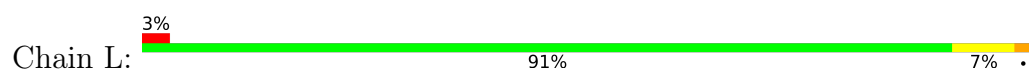
- Molecule 2: Beta-2-microglobulin



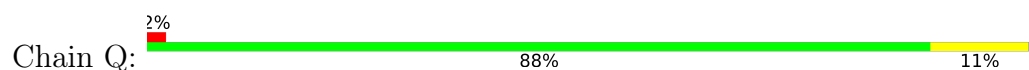
- Molecule 2: Beta-2-microglobulin



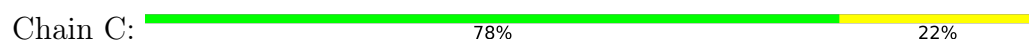
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: Nucleoprotein NP7 epitope



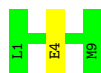
- Molecule 3: Nucleoprotein NP7 epitope



There are no outlier residues recorded for this chain.

- Molecule 3: Nucleoprotein NP7 epitope





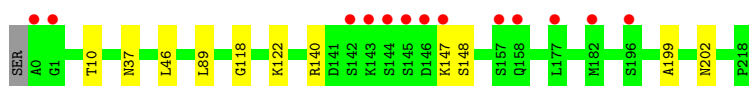
- Molecule 3: Nucleoprotein NP7 epitope

Chain R: 78% 22%



- Molecule 4: 3180 TCR alpha chain

Chain D: 6% 94% 5%



- Molecule 4: 3180 TCR alpha chain

Chain I: 2% 92% 8%



- Molecule 4: 3180 TCR alpha chain

Chain N: 3% 88% 7%



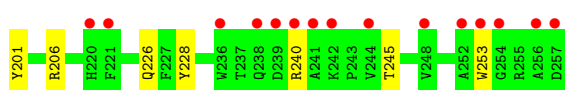
- Molecule 4: 3180 TCR alpha chain

Chain S: 3% 89% 7%

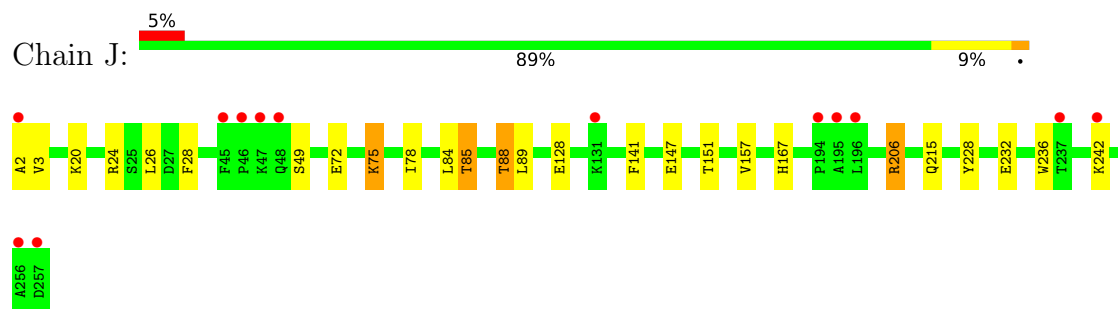


- Molecule 5: 3180 TCR alpha chain

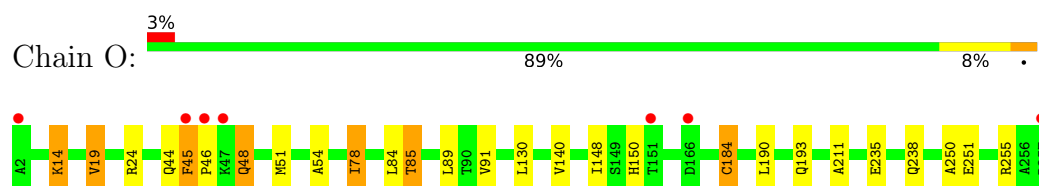
Chain E: 12% 86% 13%



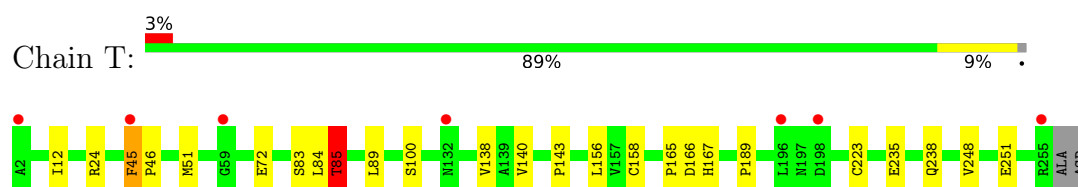
● Molecule 5: 3180 TCR alpha chain



● Molecule 5: 3180 TCR alpha chain



● Molecule 5: 3180 TCR alpha chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	168.15Å 79.55Å 172.19Å 90.00° 95.56° 90.00°	Depositor
Resolution (Å)	49.47 – 2.50 49.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.47-2.50) 99.7 (49.47-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.51Å)	Xtriage
Refinement program	BUSTER, PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.191 , 0.230 0.196 , 0.235	Depositor DCC
R_{free} test set	7850 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27676	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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 34.80 % 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 6.4455e-04. 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	0.77	0/2321	1.19	4/3155 (0.1%)
1	F	0.73	0/2313	1.16	1/3145 (0.0%)
1	K	0.71	0/2126	1.18	9/2886 (0.3%)
1	P	0.80	2/2313 (0.1%)	1.20	4/3145 (0.1%)
2	B	0.76	0/852	1.09	0/1152
2	G	0.69	0/852	1.09	0/1152
2	L	0.71	0/860	1.13	1/1162 (0.1%)
2	Q	0.72	0/852	1.10	0/1152
3	C	0.82	0/75	1.07	0/98
3	H	0.66	0/75	1.08	0/98
3	M	0.78	0/75	1.20	0/98
3	R	0.68	0/75	1.09	0/98
4	D	0.70	0/1625	1.11	2/2202 (0.1%)
4	I	0.70	0/1625	1.19	3/2202 (0.1%)
4	N	0.71	0/1560	1.08	1/2113 (0.0%)
4	S	0.71	0/1569	1.11	4/2125 (0.2%)
5	E	0.71	0/1988	1.13	3/2705 (0.1%)
5	J	0.69	0/1993	1.13	1/2712 (0.0%)
5	O	0.70	0/1993	1.13	2/2712 (0.1%)
5	T	0.69	0/1979	1.10	1/2694 (0.0%)
All	All	0.72	2/27121 (0.0%)	1.14	36/36806 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	58	GLU	C-O	-5.31	1.18	1.24
1	P	21	ARG	C-O	-5.05	1.17	1.24

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	28	VAL	N-CA-C	-7.10	96.87	107.37
4	I	81	ASN	CA-C-N	6.96	129.91	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	81	ASN	C-N-CA	6.96	129.91	120.38
1	K	162	GLY	N-CA-C	6.58	116.19	110.21
1	P	28	VAL	N-CA-C	-6.25	98.12	107.37

There are no chirality outliers.

There are no planarity outliers.

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	2258	0	2121	12	0
1	F	2250	0	2111	5	0
1	K	2069	0	1959	5	0
1	P	2250	0	2115	11	0
2	B	829	0	794	3	0
2	G	829	0	794	4	0
2	L	837	0	803	4	0
2	Q	829	0	796	4	0
3	C	74	0	80	2	0
3	H	74	0	80	0	0
3	M	74	0	80	1	0
3	R	74	0	80	3	0
4	D	1591	0	1520	3	0
4	I	1591	0	1518	6	0
4	N	1530	0	1470	6	0
4	S	1539	0	1475	2	0
5	E	1937	0	1857	10	0
5	J	1942	0	1862	14	0
5	O	1942	0	1861	13	0
5	T	1928	0	1855	15	0
6	A	102	0	0	0	0
6	B	48	0	0	1	0
6	C	8	0	0	0	0
6	D	39	0	0	0	0
6	E	70	0	0	1	0
6	F	138	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	66	0	0	0	0
6	H	6	0	0	0	0
6	I	57	0	0	0	0
6	J	78	0	0	1	0
6	K	118	0	0	0	0
6	L	59	0	0	0	0
6	M	5	0	0	0	0
6	N	66	0	0	0	0
6	O	78	0	0	0	0
6	P	116	0	0	0	0
6	Q	51	0	0	0	0
6	R	4	0	0	0	0
6	S	50	0	0	0	0
6	T	70	0	0	0	0
All	All	27676	0	25231	108	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 2.

The worst 5 of 108 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)
5:O:45:PHE:HB3	5:O:46:PRO:CD	1.94	0.98
5:T:45:PHE:HB3	5:T:46:PRO:HD2	1.50	0.93
1:A:106:ASP:OD2	1:A:108:ARG:HB2	1.85	0.76
1:A:17:ARG:HG3	1:A:17:ARG:O	1.87	0.74
5:O:45:PHE:HB3	5:O:46:PRO:HD2	1.74	0.67

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%)	269 (98%)	5 (2%)	0	100	100
1	F	273/276 (99%)	264 (97%)	9 (3%)	0	100	100
1	K	244/276 (88%)	238 (98%)	6 (2%)	0	100	100
1	P	273/276 (99%)	266 (97%)	7 (3%)	0	100	100
2	B	97/100 (97%)	96 (99%)	1 (1%)	0	100	100
2	G	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
2	L	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	Q	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	H	7/9 (78%)	7 (100%)	0	0	100	100
3	M	7/9 (78%)	7 (100%)	0	0	100	100
3	R	7/9 (78%)	7 (100%)	0	0	100	100
4	D	203/206 (98%)	197 (97%)	6 (3%)	0	100	100
4	I	203/206 (98%)	197 (97%)	6 (3%)	0	100	100
4	N	196/206 (95%)	188 (96%)	8 (4%)	0	100	100
4	S	197/206 (96%)	189 (96%)	8 (4%)	0	100	100
5	E	243/246 (99%)	231 (95%)	11 (4%)	1 (0%)	30	49
5	J	244/246 (99%)	235 (96%)	9 (4%)	0	100	100
5	O	244/246 (99%)	236 (97%)	7 (3%)	1 (0%)	30	49
5	T	242/246 (98%)	231 (96%)	10 (4%)	1 (0%)	30	49
All	All	3253/3348 (97%)	3152 (97%)	98 (3%)	3 (0%)	48	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	48	GLN
5	O	45	PHE
5	T	45	PHE

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	235/234 (100%)	227 (97%)	8 (3%)	32	60
1	F	234/234 (100%)	222 (95%)	12 (5%)	21	43
1	K	213/234 (91%)	208 (98%)	5 (2%)	44	72
1	P	234/234 (100%)	226 (97%)	8 (3%)	32	60
2	B	94/95 (99%)	85 (90%)	9 (10%)	8	17
2	G	94/95 (99%)	93 (99%)	1 (1%)	65	84
2	L	95/95 (100%)	92 (97%)	3 (3%)	34	62
2	Q	94/95 (99%)	90 (96%)	4 (4%)	26	51
3	C	9/9 (100%)	9 (100%)	0	100	100
3	H	9/9 (100%)	9 (100%)	0	100	100
3	M	9/9 (100%)	9 (100%)	0	100	100
3	R	9/9 (100%)	9 (100%)	0	100	100
4	D	181/182 (100%)	178 (98%)	3 (2%)	53	78
4	I	181/182 (100%)	176 (97%)	5 (3%)	38	66
4	N	174/182 (96%)	168 (97%)	6 (3%)	32	60
4	S	175/182 (96%)	166 (95%)	9 (5%)	21	43
5	E	216/216 (100%)	199 (92%)	17 (8%)	11	24
5	J	216/216 (100%)	205 (95%)	11 (5%)	21	43
5	O	216/216 (100%)	203 (94%)	13 (6%)	17	36
5	T	215/216 (100%)	206 (96%)	9 (4%)	26	52
All	All	2903/2944 (99%)	2780 (96%)	123 (4%)	26	52

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	J	78	ILE
4	S	160	ASN
2	L	1	ILE
4	S	156	ASP
5	T	89	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
5	J	44	GLN
5	T	116	GLN
1	K	113	HIS
5	T	57	ASN
5	T	226	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 ⓘ

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%)	0.22	19 (6%) 23 20	15, 40, 106, 119	1 (0%)
1	F	275/276 (99%)	-0.12	3 (1%) 78 75	18, 30, 88, 106	0
1	K	252/276 (91%)	0.21	27 (10%) 11 9	19, 35, 104, 127	0
1	P	275/276 (99%)	0.10	14 (5%) 33 29	17, 37, 102, 115	0
2	B	99/100 (99%)	0.06	1 (1%) 79 76	31, 48, 68, 77	0
2	G	99/100 (99%)	-0.21	2 (2%) 65 61	26, 39, 58, 64	0
2	L	100/100 (100%)	0.09	3 (3%) 52 48	28, 45, 66, 73	0
2	Q	99/100 (99%)	0.12	2 (2%) 65 61	27, 46, 69, 73	0
3	C	9/9 (100%)	-0.32	0 100 100	27, 27, 30, 31	0
3	H	9/9 (100%)	-0.83	0 100 100	19, 20, 23, 24	0
3	M	9/9 (100%)	-0.82	0 100 100	19, 20, 23, 24	0
3	R	9/9 (100%)	-0.33	0 100 100	19, 21, 24, 25	0
4	D	205/206 (99%)	0.35	13 (6%) 26 23	28, 53, 88, 100	0
4	I	205/206 (99%)	0.13	4 (1%) 65 61	23, 46, 75, 84	0
4	N	198/206 (96%)	0.17	6 (3%) 52 48	22, 45, 79, 90	0
4	S	199/206 (96%)	0.27	7 (3%) 47 42	23, 51, 90, 101	0
5	E	245/246 (99%)	0.63	29 (11%) 9 7	21, 60, 93, 117	0
5	J	246/246 (100%)	0.25	13 (5%) 32 28	20, 48, 81, 98	0
5	O	246/246 (100%)	0.10	7 (2%) 55 50	20, 44, 77, 93	1 (0%)
5	T	244/246 (99%)	0.25	7 (2%) 53 49	20, 51, 81, 96	1 (0%)
All	All	3298/3348 (98%)	0.18	157 (4%) 35 31	15, 44, 88, 127	3 (0%)

The worst 5 of 157 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	274	TRP	7.9
5	O	2	ALA	6.2
4	I	0	ALA	5.4
4	D	0	ALA	5.2
5	T	45	PHE	5.1

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.