



# wwPDB X-ray Structure Validation Summary Report

Mar 20, 2024 – 12:08 PM EDT

PDB ID : 8ENH  
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](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 : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

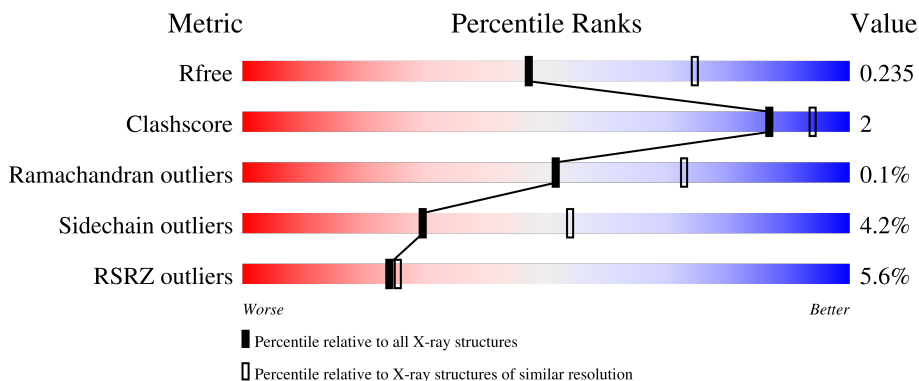
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	 11% 90% 9%
1	F	276	 4% 93% 7%
1	K	276	 10% 87% 9%
1	P	276	 11% 92% 7%
2	B	100	 90% 7%

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Mol	Chain	Length	Quality of chain
2	G	100	 % 92% 7%
2	L	100	 2% 91% 7%
2	Q	100	 4% 88% 11%
3	C	9	 78% 22%
3	H	9	 100%
3	M	9	 89% 11%
3	R	9	 78% 22%
4	D	206	 5% 94% 5%
4	I	206	 2% 91% 8%
4	N	206	 3% 89% 7%
4	S	206	 5% 91% 5%
5	E	246	 7% 89% 11%
5	J	246	 4% 91% 8%
5	O	246	 4% 89% 10%
5	T	246	 4% 89% 10%

## 2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	275	Total 2258	C 1408	N 411	O 431	S 8	0	1	0
1	F	275	Total 2250	C 1403	N 410	O 430	S 7	0	0	0
1	K	252	Total 2069	C 1299	N 379	O 384	S 7	0	0	0
1	P	275	Total 2250	C 1403	N 410	O 430	S 7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	Total 829	C 528	N 140	O 158	S 3	0	0	0
2	G	99	Total 829	C 528	N 140	O 158	S 3	0	0	0
2	L	100	Total 837	C 533	N 141	O 159	S 4	0	0	0
2	Q	99	Total 829	C 528	N 140	O 158	S 3	0	0	0

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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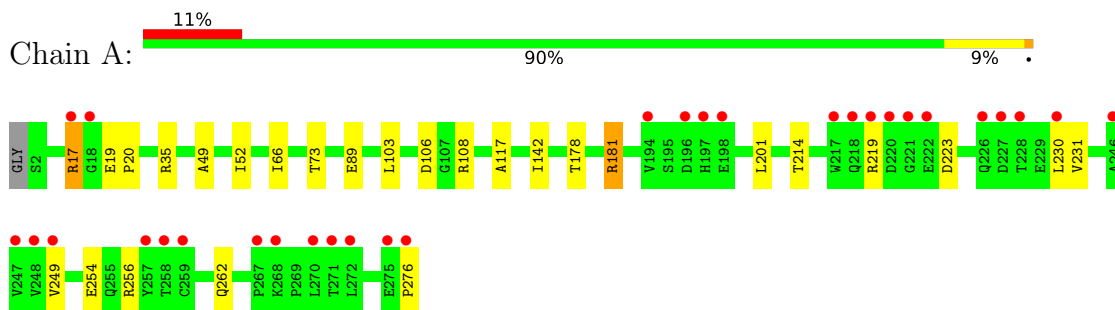
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	39	Total 39	O 39	0	0
6	E	70	Total 70	O 70	0	0
6	F	138	Total 138	O 138	0	0
6	G	66	Total 66	O 66	0	0
6	H	6	Total 6	O 6	0	0
6	I	57	Total 57	O 57	0	0
6	J	78	Total 78	O 78	0	0
6	K	118	Total 118	O 118	0	0
6	L	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

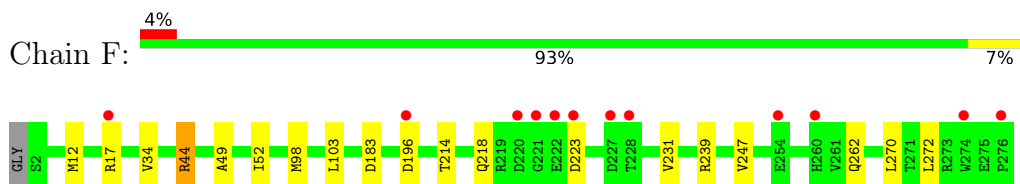
### 3 Residue-property plots [i](#)

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.

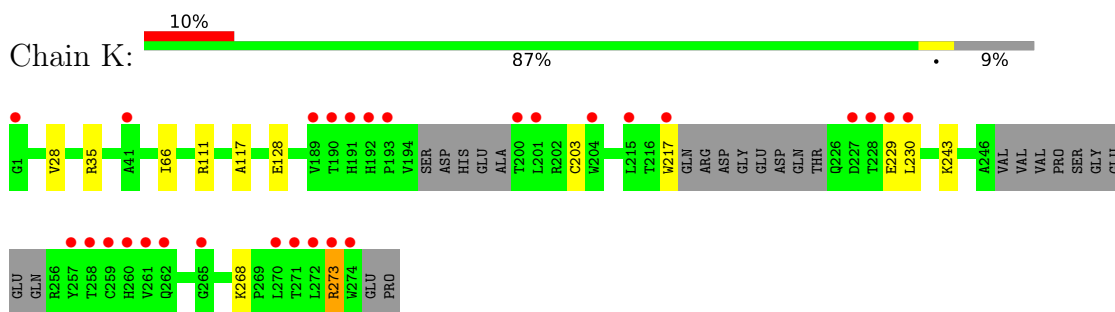
- Molecule 1: MHC class I antigen



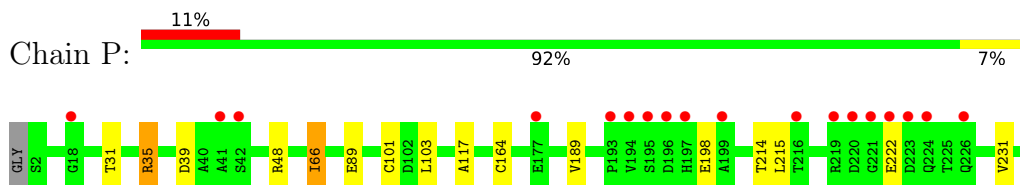
- Molecule 1: MHC class I antigen

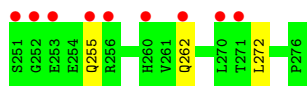


- Molecule 1: MHC class I antigen

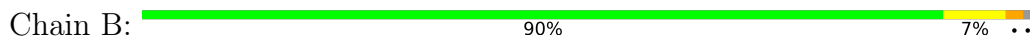


- Molecule 1: MHC class I antigen

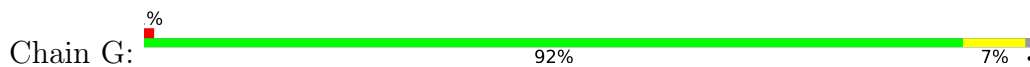




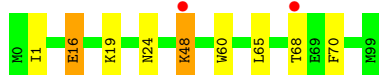
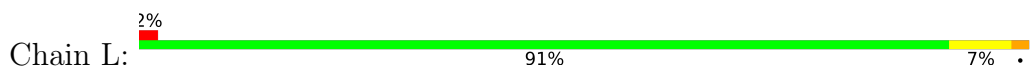
- Molecule 2: Beta-2-microglobulin



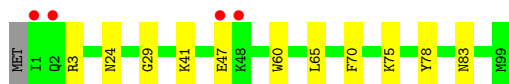
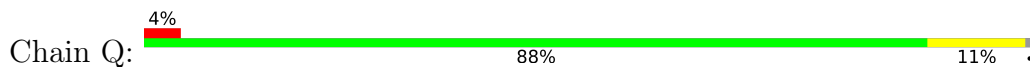
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: Nucleoprotein NP7 epitope

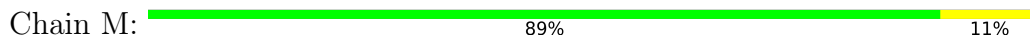


- Molecule 3: Nucleoprotein NP7 epitope



There are no outlier residues recorded for this chain.

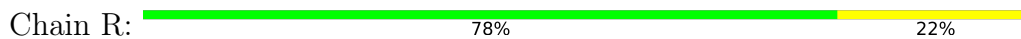
- Molecule 3: Nucleoprotein NP7 epitope



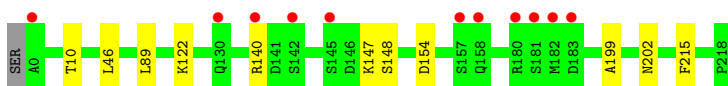




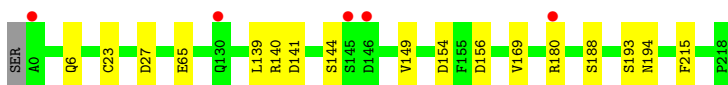
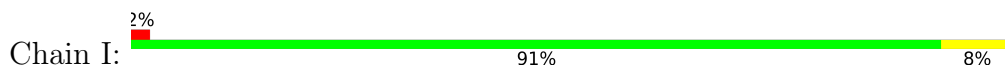
- Molecule 3: Nucleoprotein NP7 epitope



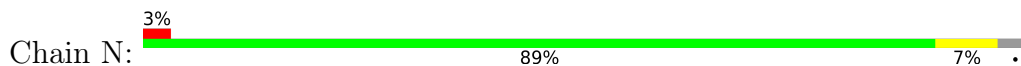
- Molecule 4: 3180 TCR alpha chain



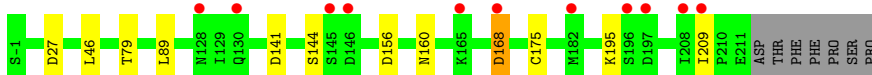
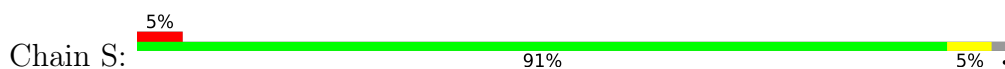
- Molecule 4: 3180 TCR alpha chain



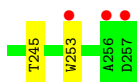
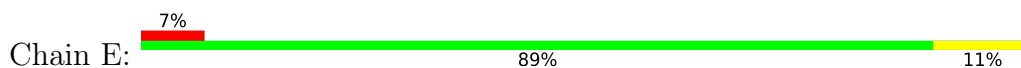
- Molecule 4: 3180 TCR alpha chain



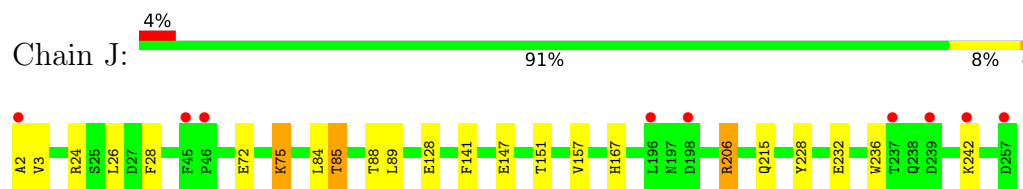
- Molecule 4: 3180 TCR alpha chain



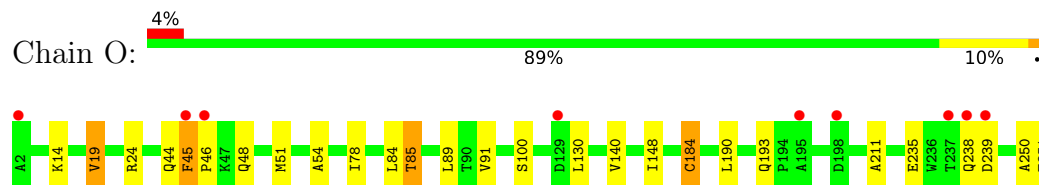
- Molecule 5: 3180 TCR alpha chain



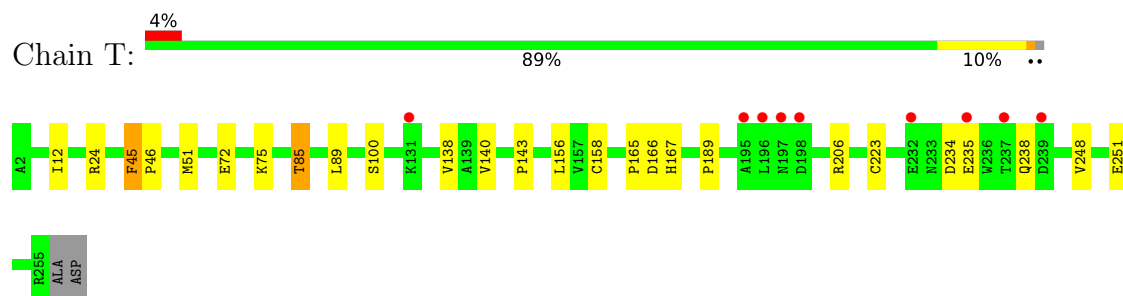
- Molecule 5: 3180 TCR alpha chain



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 2.51Å)	Xtrriage
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 (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.3	Xtrriage
Anisotropy	0.284	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	27676	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage'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.*

<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	0.45	0/2321	0.65	1/3155 (0.0%)
1	F	0.42	0/2313	0.62	0/3145
1	K	0.41	0/2126	0.61	1/2886 (0.0%)
1	P	0.49	0/2313	0.66	0/3145
2	B	0.47	0/852	0.64	0/1152
2	G	0.40	0/852	0.63	0/1152
2	L	0.40	0/860	0.63	0/1162
2	Q	0.41	0/852	0.61	0/1152
3	C	0.49	0/75	0.63	0/98
3	H	0.42	0/75	0.62	0/98
3	M	0.48	0/75	0.63	0/98
3	R	0.47	0/75	0.61	0/98
4	D	0.38	0/1625	0.61	0/2202
4	I	0.39	0/1625	0.64	0/2202
4	N	0.39	0/1560	0.62	0/2113
4	S	0.39	0/1569	0.62	0/2125
5	E	0.40	0/1988	0.64	0/2705
5	J	0.40	0/1993	0.62	0/2712
5	O	0.41	0/1993	0.63	0/2712
5	T	0.38	0/1979	0.61	0/2694
All	All	0.41	0/27121	0.63	2/36806 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	LEU	CA-CB-CG	6.57	130.41	115.30
1	K	28	VAL	N-CA-C	-5.23	96.87	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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	9	0
5	J	1942	0	1862	14	0
5	O	1942	0	1861	12	0
5	T	1928	0	1855	14	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	105	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 105 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:T:158:CYS:HG	5:T:223:CYS:HG	1.36	0.69

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	34	54
5	J	244/246 (99%)	235 (96%)	9 (4%)	0	100	100
5	O	244/246 (99%)	236 (97%)	7 (3%)	1 (0%)	34	54
5	T	242/246 (98%)	231 (96%)	10 (4%)	1 (0%)	34	54
All	All	3253/3348 (97%)	3152 (97%)	98 (3%)	3 (0%)	51	73

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 [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	235/234 (100%)	226 (96%)	9 (4%)	33	58
1	F	234/234 (100%)	222 (95%)	12 (5%)	24	45
1	K	213/234 (91%)	208 (98%)	5 (2%)	50	76
1	P	234/234 (100%)	226 (97%)	8 (3%)	37	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	94/95 (99%)	87 (93%)	7 (7%)	13	27
2	G	94/95 (99%)	93 (99%)	1 (1%)	73	89
2	L	95/95 (100%)	91 (96%)	4 (4%)	30	54
2	Q	94/95 (99%)	90 (96%)	4 (4%)	29	53
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%)	176 (97%)	5 (3%)	43	70
4	I	181/182 (100%)	173 (96%)	8 (4%)	28	52
4	N	174/182 (96%)	169 (97%)	5 (3%)	42	69
4	S	175/182 (96%)	166 (95%)	9 (5%)	24	45
5	E	216/216 (100%)	204 (94%)	12 (6%)	21	40
5	J	216/216 (100%)	208 (96%)	8 (4%)	34	60
5	O	216/216 (100%)	203 (94%)	13 (6%)	19	37
5	T	215/216 (100%)	204 (95%)	11 (5%)	24	45
All	All	2903/2944 (99%)	2782 (96%)	121 (4%)	30	54

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	J	89	LEU
5	T	51	MET
4	N	17	ASP
4	S	209	ILE
5	T	235	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
4	N	90	HIS
2	Q	83	ASN
2	Q	84	HIS
1	F	218	GLN
4	I	37	ASN



### 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 monosaccharides 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	275/276 (99%)	0.42	30 (10%) 5 5	21, 40, 106, 119	0
1	F	275/276 (99%)	0.20	12 (4%) 34 37	18, 30, 88, 106	0
1	K	252/276 (91%)	0.30	28 (11%) 5 5	19, 35, 104, 127	0
1	P	275/276 (99%)	0.32	29 (10%) 6 6	17, 37, 102, 115	0
2	B	99/100 (99%)	-0.09	0 100 100	31, 48, 68, 77	0
2	G	99/100 (99%)	-0.23	1 (1%) 82 84	26, 39, 58, 64	0
2	L	100/100 (100%)	0.04	2 (2%) 65 68	28, 45, 66, 73	0
2	Q	99/100 (99%)	0.12	4 (4%) 38 41	27, 46, 69, 73	0
3	C	9/9 (100%)	0.21	0 100 100	27, 27, 30, 31	0
3	H	9/9 (100%)	-0.04	0 100 100	19, 20, 23, 24	0
3	M	9/9 (100%)	-0.03	0 100 100	19, 20, 23, 24	0
3	R	9/9 (100%)	0.13	0 100 100	19, 21, 24, 25	0
4	D	205/206 (99%)	0.18	11 (5%) 25 27	28, 53, 88, 100	0
4	I	205/206 (99%)	0.05	5 (2%) 59 62	23, 46, 75, 84	0
4	N	198/206 (96%)	0.05	6 (3%) 50 53	22, 45, 79, 90	0
4	S	199/206 (96%)	0.23	11 (5%) 25 26	23, 51, 90, 101	0
5	E	245/246 (99%)	0.44	18 (7%) 15 15	21, 60, 93, 117	0
5	J	246/246 (100%)	0.12	9 (3%) 41 45	20, 48, 81, 98	0
5	O	246/246 (100%)	0.13	10 (4%) 37 40	20, 44, 77, 93	1 (0%)
5	T	244/246 (99%)	0.12	9 (3%) 41 45	20, 51, 81, 96	1 (0%)
All	All	3298/3348 (98%)	0.19	185 (5%) 24 25	17, 44, 88, 127	2 (0%)

The worst 5 of 185 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	258	THR	6.1
4	S	197	ASP	5.7
5	E	239	ASP	5.6
5	O	2	ALA	5.5
5	T	195	ALA	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.