



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:46 AM GMT

PDB ID : 2IAN  
Title : Structural basis for recognition of mutant self by a tumor-specific, MHC class II-restricted TCR  
Authors : Deng, L.; Langley, R.J.; Mariuzza, R.A.  
Deposited on : 2006-09-08  
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

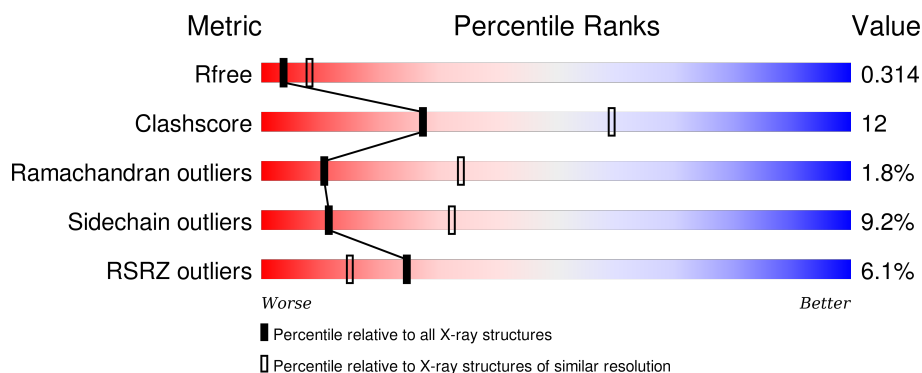
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	182	<div> <div>4%</div> <div>66% 25% 7% .</div> </div>
1	F	182	<div> <div>3%</div> <div>70% 25% . . .</div> </div>
1	K	182	<div> <div>19%</div> <div>69% 25% . . .</div> </div>
1	P	182	<div> <div>11%</div> <div>74% 23% . .</div> </div>
2	B	190	<div> <div>6%</div> <div>63% 28% . 5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	190	
2	L	190	
2	Q	190	
3	C	15	
3	H	15	
3	M	15	
3	R	15	
4	D	202	
4	I	202	
4	N	202	
4	S	202	
5	E	240	
5	J	240	
5	O	240	
5	T	240	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26209 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 II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1464	949	238	272	5			
1	F	179	Total	C	N	O	S	0	0	0
			1473	954	239	275	5			
1	K	179	Total	C	N	O	S	0	0	0
			1473	954	239	275	5			
1	P	179	Total	C	N	O	S	0	0	0
			1473	954	239	275	5			

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1-1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	0	0
			1485	936	265	278	6			
2	G	182	Total	C	N	O	S	0	0	0
			1493	940	266	281	6			
2	L	188	Total	C	N	O	S	0	0	0
			1544	973	277	288	6			
2	Q	188	Total	C	N	O	S	0	0	0
			1544	973	277	288	6			

- Molecule 3 is a protein called 15-mer peptide from Triosephosphate isomerase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	15	Total	C	N	O	0	0	0
			103	64	17	22			
3	H	15	Total	C	N	O	0	0	0
			103	64	17	22			
3	M	15	Total	C	N	O	0	0	0
			103	64	17	22			
3	R	15	Total	C	N	O	0	0	0
			103	64	17	22			

- Molecule 4 is a protein called CD4+ T cell receptor E8 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	198	Total	C	N	O	S	0	0	0
			1546	967	260	312	7			
4	I	198	Total	C	N	O	S	0	0	0
			1546	967	260	312	7			
4	N	198	Total	C	N	O	S	0	0	0
			1546	967	260	312	7			
4	S	198	Total	C	N	O	S	0	0	0
			1546	967	260	312	7			

- Molecule 5 is a protein called CD4+ T cell receptor E8 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	238	Total	C	N	O	S	0	0	0
			1896	1203	323	361	9			
5	J	239	Total	C	N	O	S	0	0	0
			1901	1206	324	362	9			
5	O	238	Total	C	N	O	S	0	0	0
			1895	1203	323	360	9			
5	T	238	Total	C	N	O	S	0	0	0
			1896	1203	323	361	9			

- Molecule 6 is water.

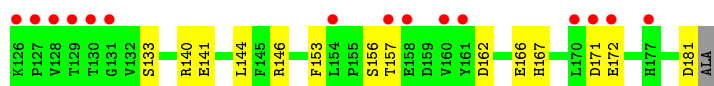
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	O	0	0
			4	4		
6	B	8	Total	O	0	0
			8	8		
6	D	6	Total	O	0	0
			6	6		
6	E	6	Total	O	0	0
			6	6		
6	F	5	Total	O	0	0
			5	5		
6	G	10	Total	O	0	0
			10	10		
6	I	6	Total	O	0	0
			6	6		
6	J	10	Total	O	0	0
			10	10		
6	L	4	Total	O	0	0
			4	4		

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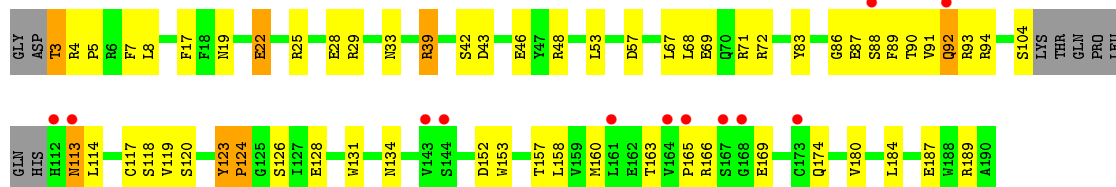
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	N	4	Total 4	O 4	0	0
6	O	1	Total 1	O 1	0	0
6	P	2	Total 2	O 2	0	0
6	Q	2	Total 2	O 2	0	0
6	S	2	Total 2	O 2	0	0
6	T	6	Total 6	O 6	0	0

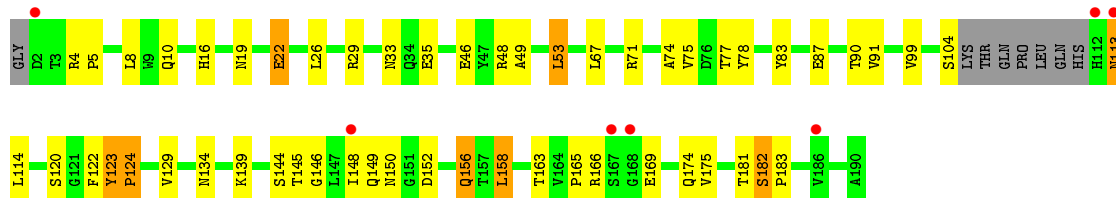




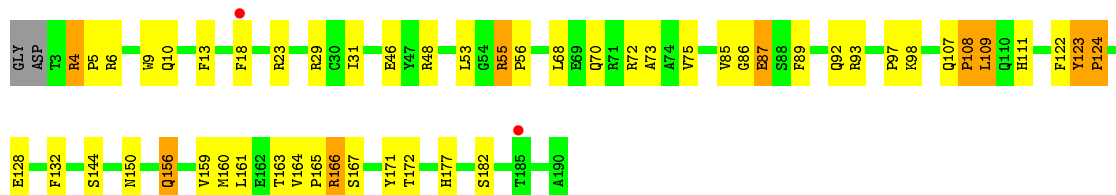
- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain



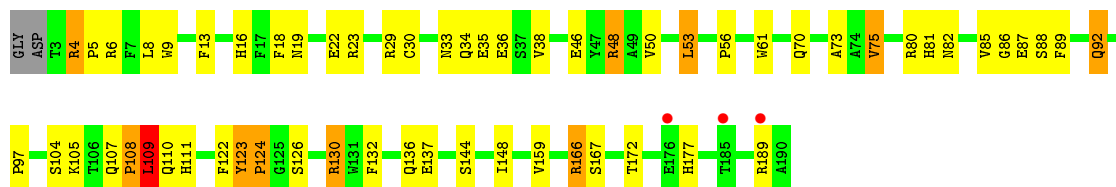
- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain



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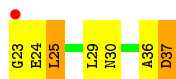


- Molecule 3: 15-mer peptide from Triosephosphate isomerase

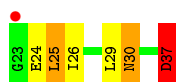




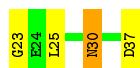
- Molecule 3: 15-mer peptide from Triosephosphate isomerase



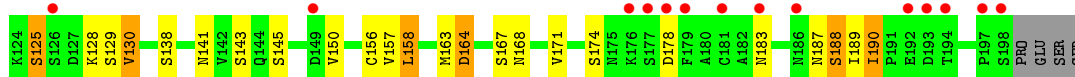
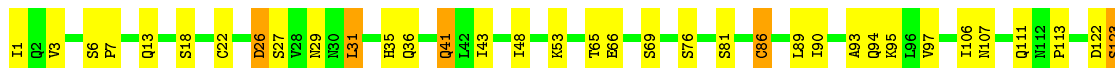
- Molecule 3: 15-mer peptide from Triosephosphate isomerase



- Molecule 3: 15-mer peptide from Triosephosphate isomerase



- Molecule 4: CD4+ T cell receptor E8 alpha chain

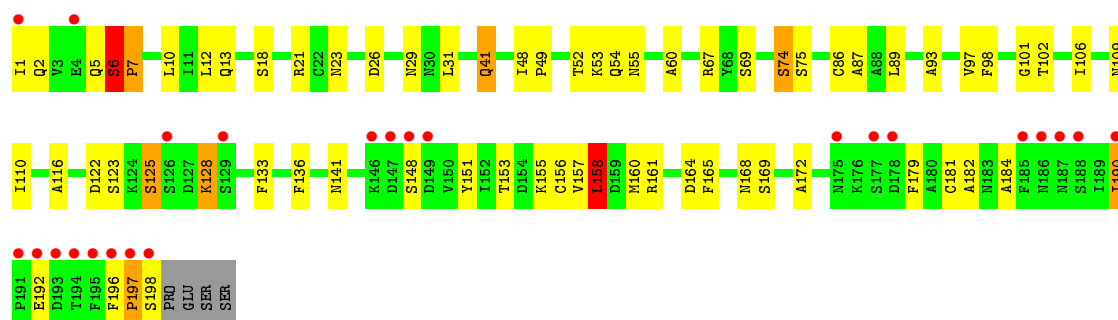


- Molecule 4: CD4+ T cell receptor E8 alpha chain

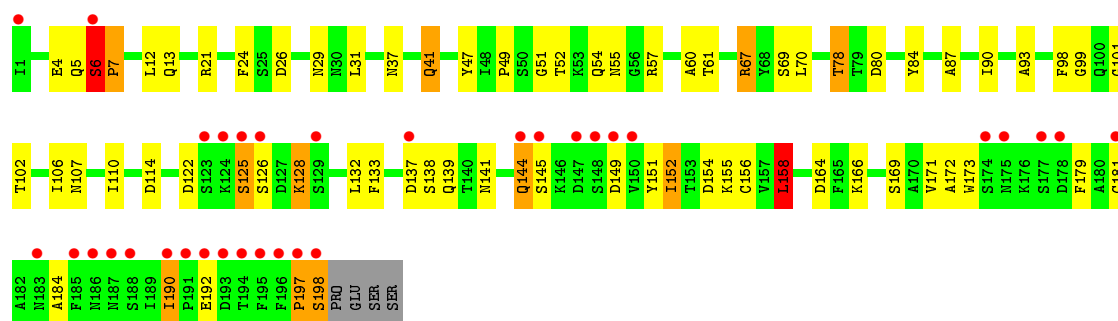


- Molecule 4: CD4+ T cell receptor E8 alpha chain

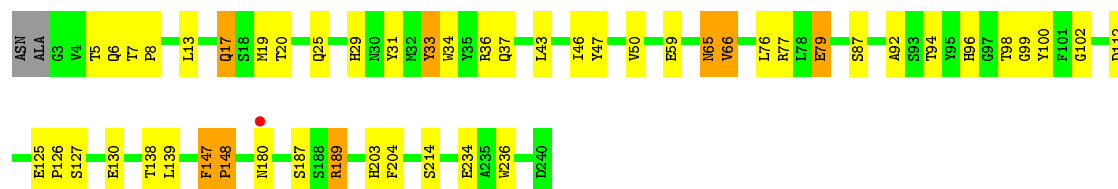
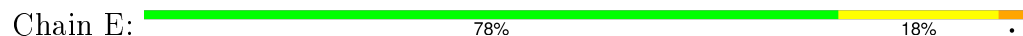




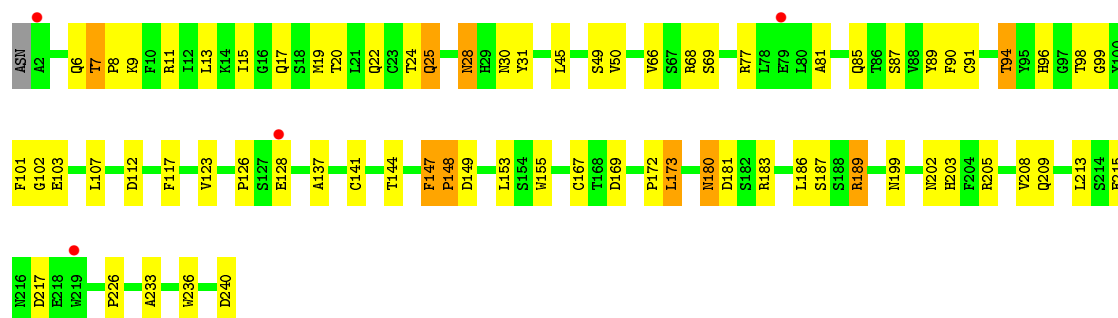
- Molecule 4: CD4+ T cell receptor E8 alpha chain



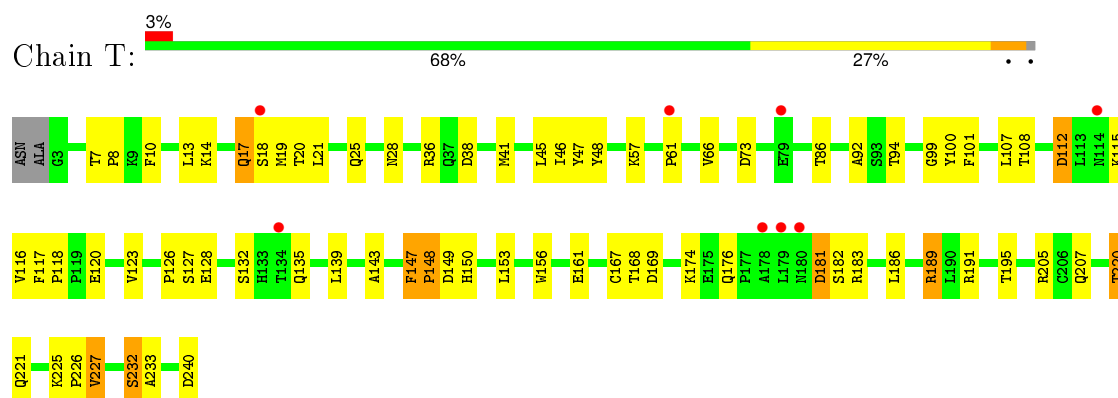
- Molecule 5: CD4+ T cell receptor E8 beta chain



- Molecule 5: CD4+ T cell receptor E8 beta chain



- Molecule 5: CD4+ T cell receptor E8 beta chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.47Å 242.87Å 105.22Å 90.00° 111.32° 90.00°	Depositor
Resolution (Å)	45.45 – 2.80 45.45 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.8 (45.45-2.80) 93.8 (45.45-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.87 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.221 , 0.296 0.254 , 0.314	Depositor DCC
$R_{free}$ test set	5054 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.3	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 18.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 100442 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	26209	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	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 22.19 % 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 6.0021e-03. 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.59	0/1509	0.71	0/2058
1	F	0.62	0/1518	0.73	0/2070
1	K	0.54	0/1518	0.69	1/2070 (0.0%)
1	P	0.57	0/1518	0.69	0/2070
2	B	0.67	0/1522	0.79	3/2066 (0.1%)
2	G	0.67	0/1530	0.79	1/2077 (0.0%)
2	L	0.59	0/1584	0.72	0/2152
2	Q	0.61	0/1584	0.71	1/2152 (0.0%)
3	C	0.82	0/103	0.98	0/138
3	H	0.76	0/103	0.95	0/138
3	M	0.71	0/103	0.97	1/138 (0.7%)
3	R	0.73	0/103	0.78	0/138
4	D	0.63	0/1579	0.78	1/2148 (0.0%)
4	I	0.65	0/1579	0.82	3/2148 (0.1%)
4	N	0.62	1/1579 (0.1%)	0.75	1/2148 (0.0%)
4	S	0.61	0/1579	0.74	1/2148 (0.0%)
5	E	0.67	0/1951	0.75	0/2659
5	J	0.68	1/1956 (0.1%)	0.75	1/2666 (0.0%)
5	O	0.60	0/1950	0.69	1/2658 (0.0%)
5	T	0.60	0/1951	0.68	0/2659
All	All	0.63	2/26819 (0.0%)	0.74	15/36501 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	F	0	2
1	K	0	2
1	P	0	2
2	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	1
2	L	0	1
2	Q	0	1
4	D	0	1
4	I	0	1
4	N	0	1
4	S	0	1
5	E	0	2
5	J	0	2
5	O	0	2
5	T	0	2
All	All	0	24

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	215	GLU	CB-CG	5.20	1.62	1.52
4	N	86	CYS	CB-SG	-5.03	1.73	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	15	ASN	C-N-CD	-6.80	105.64	120.60
4	I	158	LEU	CA-CB-CG	6.76	130.84	115.30
5	O	147	PHE	C-N-CD	-6.64	106.00	120.60
4	D	31	LEU	CA-CB-CG	-6.41	100.56	115.30
4	N	158	LEU	CA-CB-CG	6.39	130.00	115.30

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	THR	Peptide
1	A	14	LEU	Peptide
2	B	123	TYR	Peptide
4	D	6	SER	Peptide
5	E	7	THR	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	1464	0	1401	47	1
1	F	1473	0	1407	38	0
1	K	1473	0	1407	32	1
1	P	1473	0	1407	29	0
2	B	1485	0	1416	43	0
2	G	1493	0	1420	38	0
2	L	1544	0	1478	39	0
2	Q	1544	0	1478	50	0
3	C	103	0	105	2	0
3	H	103	0	105	5	0
3	M	103	0	105	7	0
3	R	103	0	105	3	0
4	D	1546	0	1474	36	0
4	I	1546	0	1474	43	0
4	N	1546	0	1474	58	0
4	S	1546	0	1474	57	0
5	E	1896	0	1795	33	0
5	J	1901	0	1800	44	0
5	O	1895	0	1795	37	0
5	T	1896	0	1795	42	0
6	A	4	0	0	0	0
6	B	8	0	0	1	0
6	D	6	0	0	0	0
6	E	6	0	0	0	0
6	F	5	0	0	1	0
6	G	10	0	0	0	0
6	I	6	0	0	0	0
6	J	10	0	0	0	0
6	L	4	0	0	0	0
6	N	4	0	0	0	0
6	O	1	0	0	0	0
6	P	2	0	0	0	0
6	Q	2	0	0	0	0
6	S	2	0	0	0	0
6	T	6	0	0	0	0
All	All	26209	0	24915	608	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 12.

The worst 5 of 608 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:A:82:ILE:HD13	1:A:114:PRO:HD3	1.23	1.12
2:Q:124:PRO:HD2	2:Q:177:HIS:HE2	1.15	1.09
1:F:55:GLU:HG2	4:I:93:ALA:HB2	1.38	1.05
2:Q:124:PRO:HD2	2:Q:177:HIS:NE2	1.75	1.01
4:D:1:ILE:N	4:D:27:SER:HB2	1.75	1.00

All (1) 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:A:126:LYS:NZ	1:K:120:THR:CG2[1_656]	1.76	0.44

## 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	176/182 (97%)	162 (92%)	9 (5%)	5 (3%)	6	21
1	F	177/182 (97%)	165 (93%)	9 (5%)	3 (2%)	11	36
1	K	177/182 (97%)	165 (93%)	10 (6%)	2 (1%)	17	50
1	P	177/182 (97%)	160 (90%)	14 (8%)	3 (2%)	11	36
2	B	177/190 (93%)	161 (91%)	13 (7%)	3 (2%)	11	36
2	G	178/190 (94%)	161 (90%)	13 (7%)	4 (2%)	8	28
2	L	186/190 (98%)	172 (92%)	10 (5%)	4 (2%)	8	28
2	Q	186/190 (98%)	169 (91%)	13 (7%)	4 (2%)	8	28
3	C	13/15 (87%)	13 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	13/15 (87%)	13 (100%)	0	0	100	100
3	M	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
3	R	13/15 (87%)	13 (100%)	0	0	100	100
4	D	196/202 (97%)	178 (91%)	15 (8%)	3 (2%)	13	40
4	I	196/202 (97%)	175 (89%)	16 (8%)	5 (3%)	7	22
4	N	196/202 (97%)	177 (90%)	15 (8%)	4 (2%)	9	30
4	S	196/202 (97%)	176 (90%)	14 (7%)	6 (3%)	5	17
5	E	236/240 (98%)	221 (94%)	13 (6%)	2 (1%)	24	58
5	J	237/240 (99%)	217 (92%)	16 (7%)	4 (2%)	11	36
5	O	236/240 (98%)	218 (92%)	14 (6%)	4 (2%)	11	36
5	T	236/240 (98%)	219 (93%)	14 (6%)	3 (1%)	15	44
All	All	3215/3316 (97%)	2947 (92%)	209 (6%)	59 (2%)	11	34

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	PRO
4	D	7	PRO
5	E	8	PRO
5	E	148	PRO
1	F	16	PRO

### 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	163/166 (98%)	151 (93%)	12 (7%)	17	43
1	F	164/166 (99%)	157 (96%)	7 (4%)	35	70
1	K	164/166 (99%)	155 (94%)	9 (6%)	27	59
1	P	164/166 (99%)	152 (93%)	12 (7%)	17	44
2	B	163/171 (95%)	151 (93%)	12 (7%)	17	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	164/171 (96%)	152 (93%)	12 (7%)	17	44
2	L	170/171 (99%)	159 (94%)	11 (6%)	21	52
2	Q	170/171 (99%)	154 (91%)	16 (9%)	11	31
3	C	10/10 (100%)	7 (70%)	3 (30%)	0	1
3	H	10/10 (100%)	6 (60%)	4 (40%)	0	0
3	M	10/10 (100%)	7 (70%)	3 (30%)	0	1
3	R	10/10 (100%)	7 (70%)	3 (30%)	0	1
4	D	178/182 (98%)	155 (87%)	23 (13%)	5	16
4	I	178/182 (98%)	157 (88%)	21 (12%)	6	19
4	N	178/182 (98%)	161 (90%)	17 (10%)	10	29
4	S	178/182 (98%)	158 (89%)	20 (11%)	7	22
5	E	206/207 (100%)	191 (93%)	15 (7%)	17	44
5	J	206/207 (100%)	183 (89%)	23 (11%)	7	22
5	O	206/207 (100%)	183 (89%)	23 (11%)	7	22
5	T	206/207 (100%)	184 (89%)	22 (11%)	8	24
All	All	2898/2944 (98%)	2630 (91%)	268 (9%)	11	32

5 of 268 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	J	112	ASP
2	L	166	ARG
5	T	18	SER
5	J	173	LEU
1	K	97	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
5	J	22	GLN
2	L	111	HIS
4	S	168	ASN
2	L	33	ASN
3	M	30	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 carbohydrates 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, 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	178/182 (97%)	0.43	8 (4%) 37 26	6, 14, 20, 23	0
1	F	179/182 (98%)	0.54	6 (3%) 49 36	4, 15, 20, 30	0
1	K	179/182 (98%)	0.85	35 (19%) 1 1	10, 16, 22, 34	0
1	P	179/182 (98%)	0.72	20 (11%) 7 3	6, 16, 21, 28	0
2	B	181/190 (95%)	0.57	12 (6%) 22 13	3, 14, 18, 22	0
2	G	182/190 (95%)	0.51	7 (3%) 44 32	3, 13, 19, 28	0
2	L	188/190 (98%)	0.30	2 (1%) 82 74	4, 13, 19, 25	0
2	Q	188/190 (98%)	0.35	3 (1%) 74 66	4, 12, 18, 22	0
3	C	15/15 (100%)	0.22	0 100 100	2, 4, 15, 16	0
3	H	15/15 (100%)	0.43	1 (6%) 21 12	2, 7, 18, 19	0
3	M	15/15 (100%)	0.42	1 (6%) 21 12	3, 8, 21, 21	0
3	R	15/15 (100%)	0.24	0 100 100	4, 7, 17, 22	0
4	D	198/202 (98%)	0.58	14 (7%) 19 10	5, 15, 33, 35	0
4	I	198/202 (98%)	0.64	16 (8%) 15 7	4, 14, 41, 51	0
4	N	198/202 (98%)	0.64	24 (12%) 6 3	5, 14, 31, 35	0
4	S	198/202 (98%)	0.80	33 (16%) 2 1	5, 15, 31, 35	0
5	E	238/240 (99%)	0.21	1 (0%) 93 90	2, 12, 22, 24	0
5	J	239/240 (99%)	0.33	4 (1%) 73 63	3, 13, 24, 27	0
5	O	238/240 (99%)	0.22	4 (1%) 73 63	3, 13, 22, 27	0
5	T	238/240 (99%)	0.38	8 (3%) 49 36	5, 14, 21, 25	0
All	All	3259/3316 (98%)	0.49	199 (6%) 25 15	2, 14, 25, 51	0

The worst 5 of 199 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	177	SER	6.4
4	S	149	ASP	6.0
4	S	177	SER	5.8
4	N	192	GLU	5.1
4	N	193	ASP	4.9

## 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 carbohydrates 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.