Full wwPDB X-ray Structure Validation Report ⓘ

Jun 9, 2025 – 02:42 PM JST

PDB ID	:	9IKY / pdb_00009iky
Title	:	Crystal structure of 1-2C-T96F TCR in complex with HLA-A*11:01 bound to KRAS-G12V peptide (VVGAVGVGK)
Authors	:	Ma, K.K.; Tan, S.G.; Gao, G.F.; Chai, Y.
Deposited on	:	2024-06-29
Resolution	:	3.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

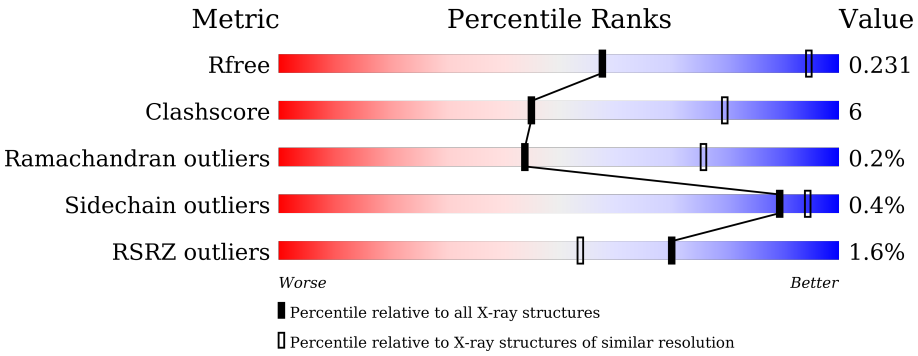
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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}	164625	1597 (3.52-3.40)
Clashscore	180529	1041 (3.50-3.42)
Ramachandran outliers	177936	1026 (3.50-3.42)
Sidechain outliers	177891	1027 (3.50-3.42)
RSRZ outliers	164620	1596 (3.52-3.40)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	275	88% 12%
1	F	275	% 84% 16%
1	K	275	% 84% 15%
1	P	275	80% 20%
1	U	275	% 86% 14%
1	Z	275	% 79% 7% 14%

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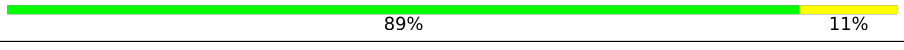
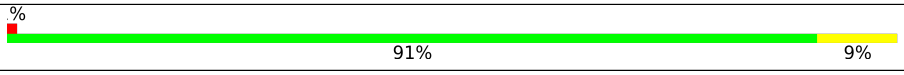
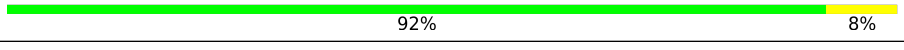
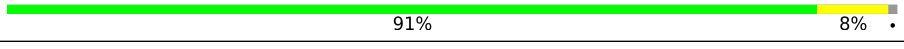
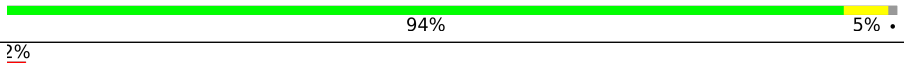
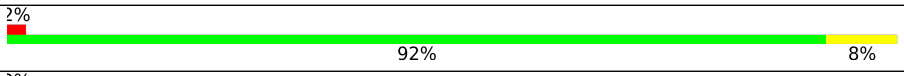
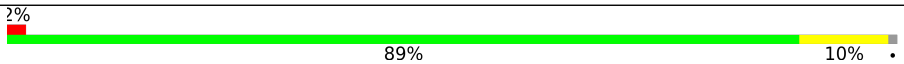
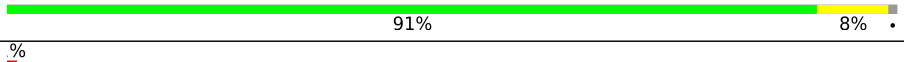
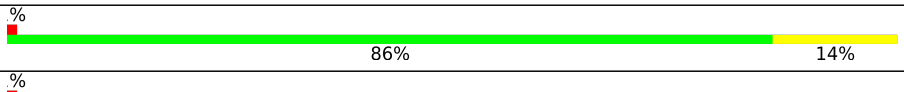
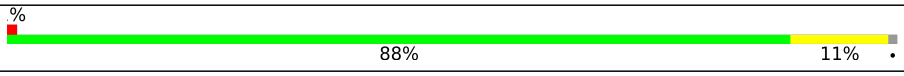
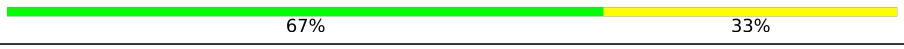
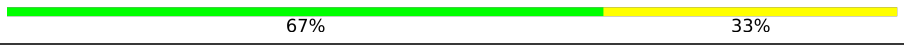
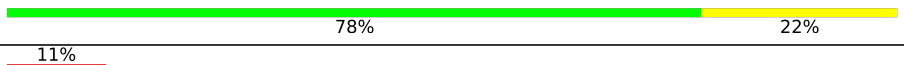
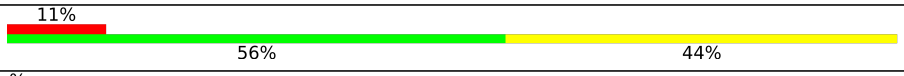
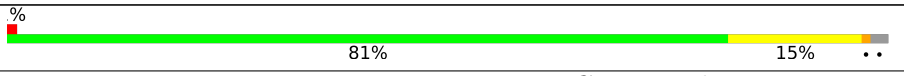
Mol	Chain	Length	Quality of chain
1	e	275	
1	j	275	
1	o	275	
1	t	275	
2	B	100	
2	G	100	
2	L	100	
2	Q	100	
2	V	100	
2	a	100	
2	f	100	
2	k	100	
2	p	100	
2	u	100	
3	C	9	
3	H	9	
3	M	9	
3	R	9	
3	W	9	
3	b	9	
3	g	9	
3	l	9	
3	q	9	
3	v	9	
4	D	204	

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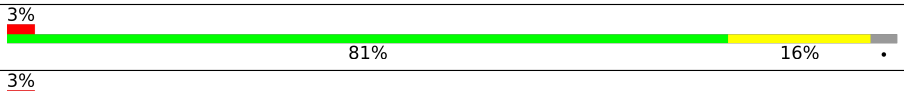
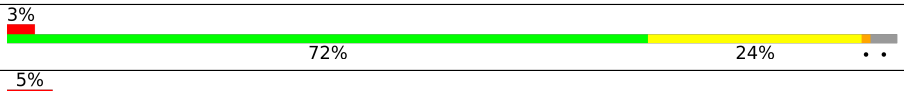
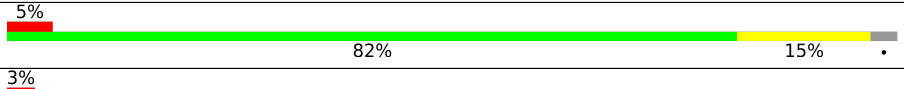
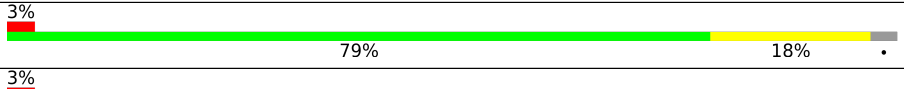
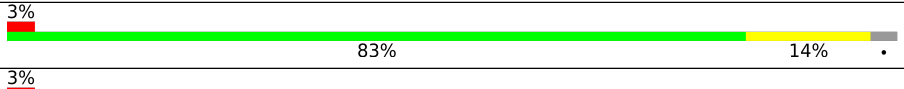
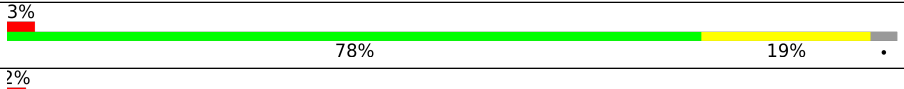
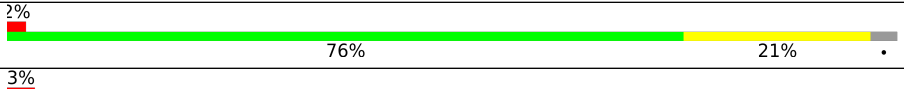
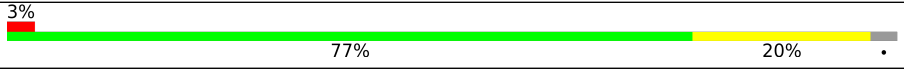
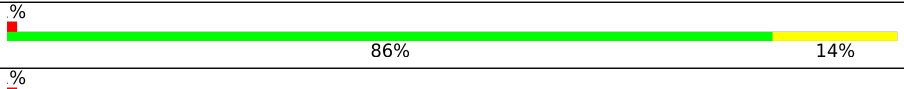
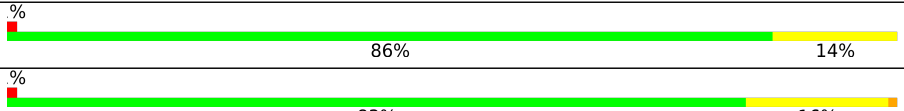
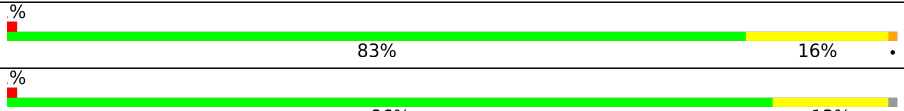
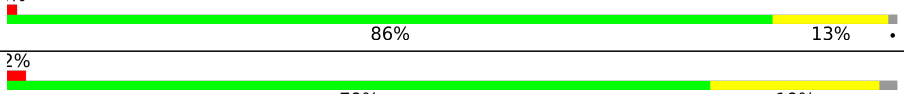
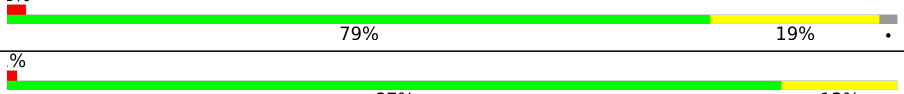
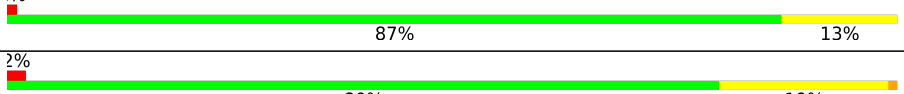
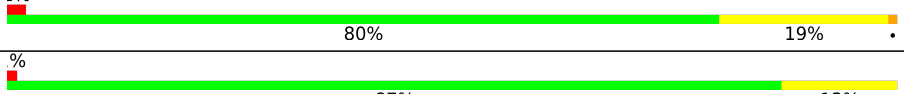
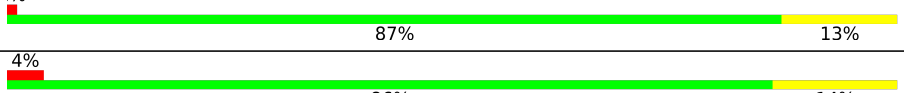
Mol	Chain	Length	Quality of chain
4	I	204	
4	N	204	
4	S	204	
4	X	204	
4	c	204	
4	h	204	
4	m	204	
4	r	204	
4	w	204	
5	E	242	
5	J	242	
5	O	242	
5	T	242	
5	Y	242	
5	d	242	
5	i	242	
5	n	242	
5	s	242	
5	x	242	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 65289 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	o	274	Total	C	N	O	S	0	0	0
			2235	1389	407	430	9			
1	A	274	Total	C	N	O	S	0	0	0
			2235	1389	407	430	9			
1	F	274	Total	C	N	O	S	0	0	0
			2235	1389	407	430	9			
1	K	274	Total	C	N	O	S	0	0	0
			2235	1389	407	430	9			
1	P	274	Total	C	N	O	S	0	0	0
			2235	1389	407	430	9			
1	U	274	Total	C	N	O	S	0	0	0
			2235	1389	407	430	9			
1	Z	236	Total	C	N	O	S	0	0	0
			1927	1207	350	363	7			
1	e	243	Total	C	N	O	S	0	0	0
			1979	1237	360	373	9			
1	j	274	Total	C	N	O	S	0	0	0
			2235	1389	407	430	9			
1	t	274	Total	C	N	O	S	0	0	0
			2235	1389	407	430	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	p	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	B	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	G	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	L	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	V	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	a	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	f	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	k	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	u	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p	0	MET	-	initiating methionine	UNP P61769
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
V	0	MET	-	initiating methionine	UNP P61769
a	0	MET	-	initiating methionine	UNP P61769
f	0	MET	-	initiating methionine	UNP P61769
k	0	MET	-	initiating methionine	UNP P61769
u	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called VAL-VAL-GLY-ALA-VAL-GLY-VAL-GLY-LYS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	q	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	C	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	H	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	M	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	R	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	W	9	Total	C	N	O	0	0	0
			55	35	10	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	b	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	g	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	l	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	v	9	Total	C	N	O	0	0	0
			55	35	10	10			

- Molecule 4 is a protein called 1-2C-T96F TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	r	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	D	199	Total	C	N	O	S	0	0	0
			1571	979	268	314	10			
4	I	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	N	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	S	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	X	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	c	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	h	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	m	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	w	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			

- Molecule 5 is a protein called 1-2C-T96F TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	s	242	Total	C	N	O	S	0	0	0
			1910	1199	334	371	6			
5	E	242	Total	C	N	O	S	0	0	0
			1910	1199	334	371	6			
5	J	242	Total	C	N	O	S	0	0	0
			1910	1199	334	371	6			

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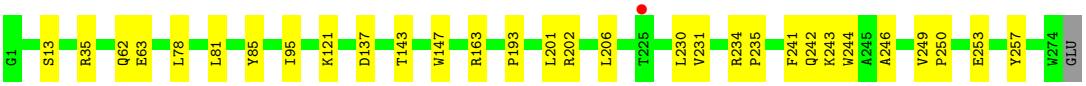
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	O	242	Total	C	N	O	S	0	0	0
			1910	1199	334	371	6			
5	T	241	Total	C	N	O	S	0	0	0
			1901	1194	333	368	6			
5	Y	239	Total	C	N	O	S	0	0	0
			1888	1187	331	364	6			
5	d	237	Total	C	N	O	S	0	0	0
			1872	1178	326	362	6			
5	i	241	Total	C	N	O	S	0	0	0
			1901	1194	333	368	6			
5	n	241	Total	C	N	O	S	0	0	0
			1901	1194	333	368	6			
5	x	241	Total	C	N	O	S	0	0	0
			1901	1194	333	368	6			

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.

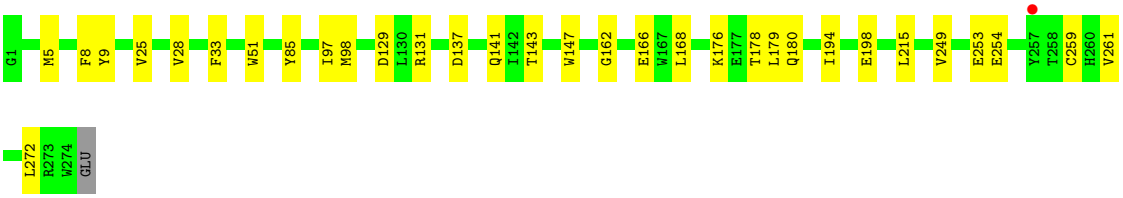
- Molecule 1: MHC class I antigen

Chain o:



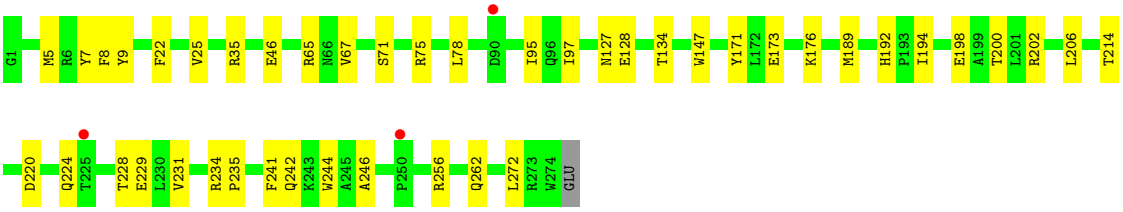
- Molecule 1: MHC class I antigen

Chain A:



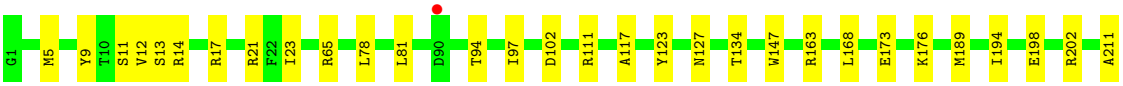
- Molecule 1: MHC class I antigen

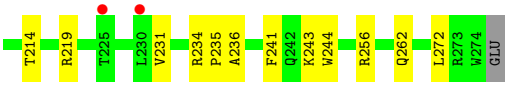
Chain F:



- Molecule 1: MHC class I antigen

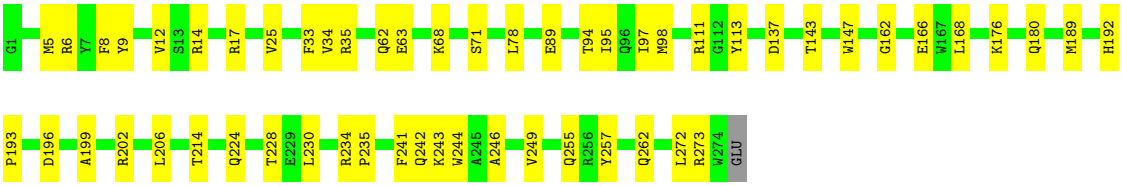
Chain K:





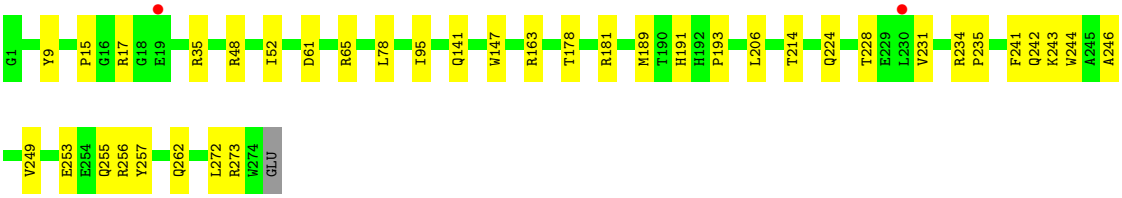
• Molecule 1: MHC class I antigen

Chain P:



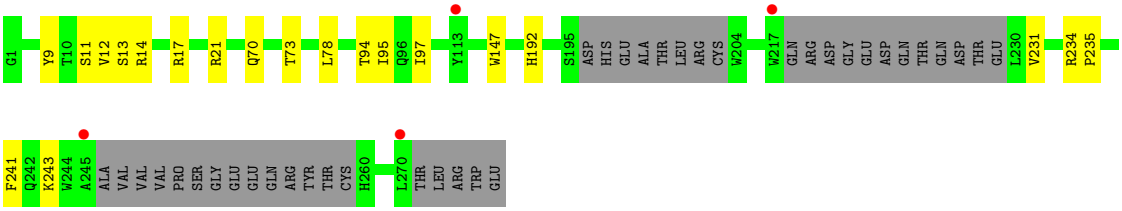
• Molecule 1: MHC class I antigen

Chain U:



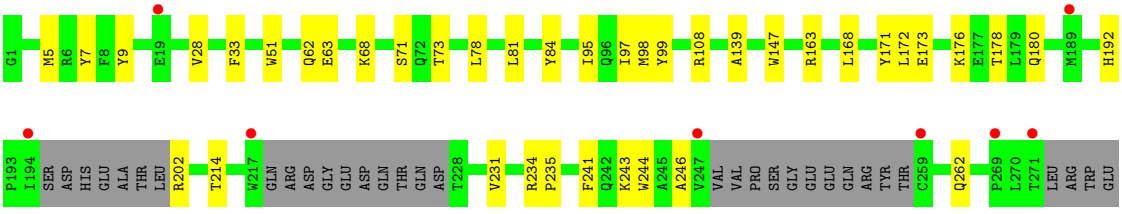
• Molecule 1: MHC class I antigen

Chain Z:



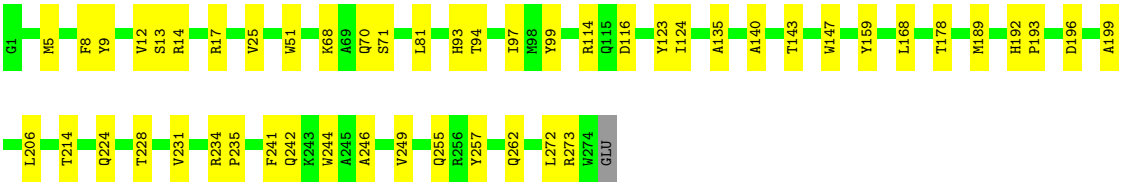
• Molecule 1: MHC class I antigen

Chain e:

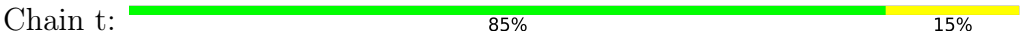


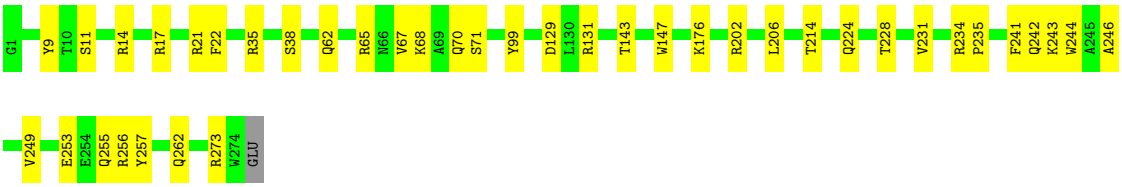
• Molecule 1: MHC class I antigen

Chain j:

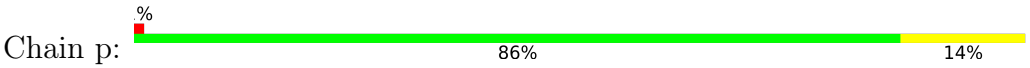


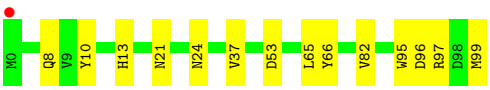
• Molecule 1: MHC class I antigen



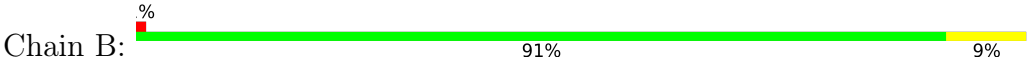


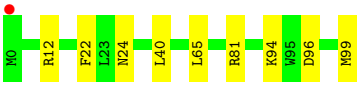
• Molecule 2: Beta-2-microglobulin



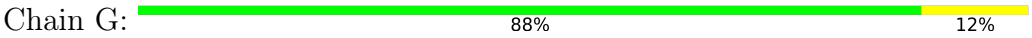


• Molecule 2: Beta-2-microglobulin

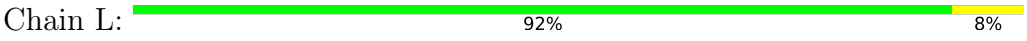




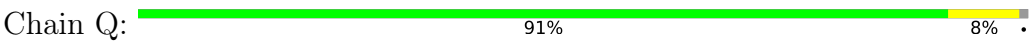
• Molecule 2: Beta-2-microglobulin

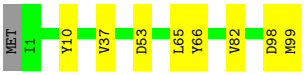


• Molecule 2: Beta-2-microglobulin



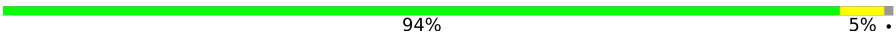
• Molecule 2: Beta-2-microglobulin

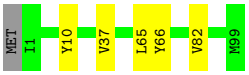




• Molecule 2: Beta-2-microglobulin

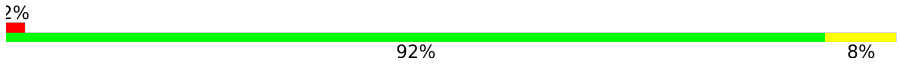
Chain V:

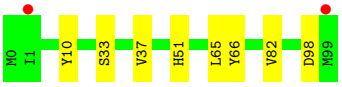




• Molecule 2: Beta-2-microglobulin

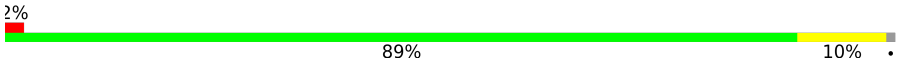
Chain a:

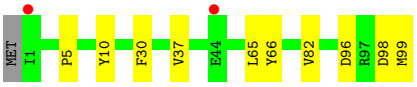




• Molecule 2: Beta-2-microglobulin

Chain f:



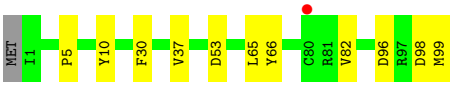


• Molecule 2: Beta-2-microglobulin

Chain k:

• Molecule 2: Beta-2-microglobulin

Chain u:



• Molecule 3: VAL-VAL-GLY-ALA-VAL-GLY-VAL-GLY-LYS

Chain q:

• Molecule 3: VAL-VAL-GLY-ALA-VAL-GLY-VAL-GLY-LYS

Chain C:

• Molecule 3: VAL-VAL-GLY-ALA-VAL-GLY-VAL-GLY-LYS

Chain H:

• Molecule 3: VAL-VAL-GLY-ALA-VAL-GLY-VAL-GLY-LYS

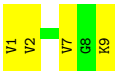
Chain M:

• Molecule 3: VAL-VAL-GLY-ALA-VAL-GLY-VAL-GLY-LYS

Chain R:

• Molecule 3: VAL-VAL-GLY-ALA-VAL-GLY-VAL-GLY-LYS

Chain W:

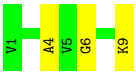


• Molecule 3: VAL-VAL-GLY-ALA-VAL-GLY-VAL-GLY-LYS

Chain b:

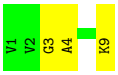
• Molecule 3: VAL-VAL-GLY-ALA-VAL-GLY-VAL-GLY-LYS

Chain g:



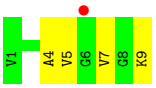
• Molecule 3: VAL-VAL-GLY-ALA-VAL-GLY-VAL-GLY-LYS

Chain l:



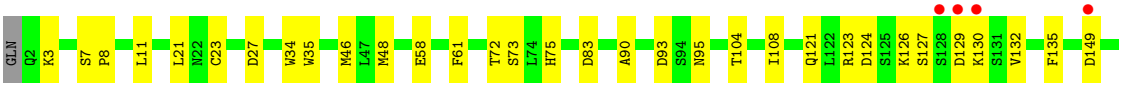
• Molecule 3: VAL-VAL-GLY-ALA-VAL-GLY-VAL-GLY-LYS

Chain v:



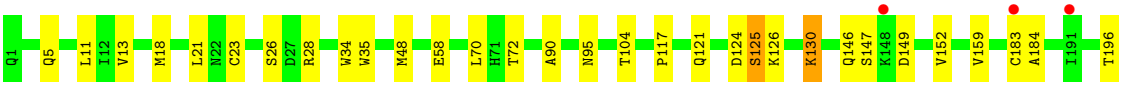
• Molecule 4: 1-2C-T96F TCR alpha chain

Chain r:



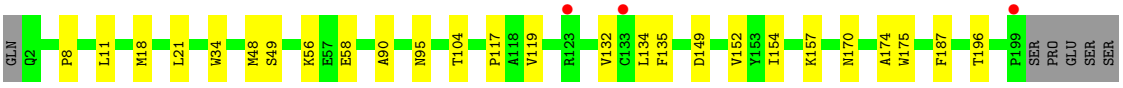
• Molecule 4: 1-2C-T96F TCR alpha chain

Chain D:



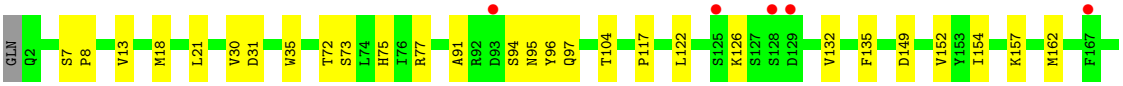
• Molecule 4: 1-2C-T96F TCR alpha chain

Chain I:



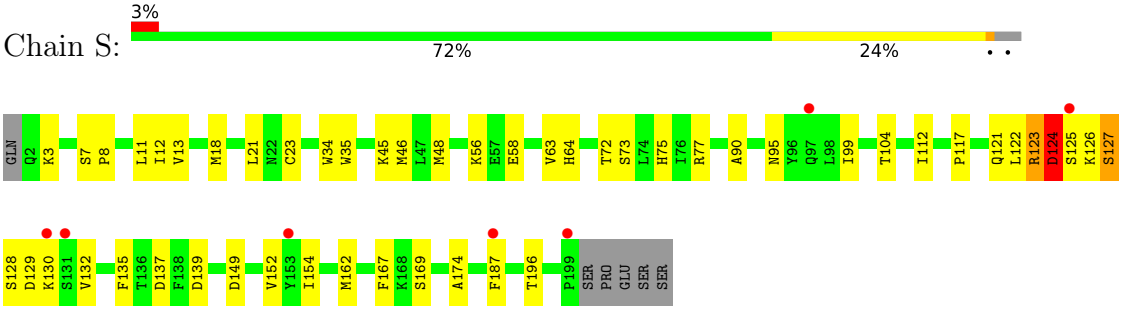
• Molecule 4: 1-2C-T96F TCR alpha chain

Chain N:



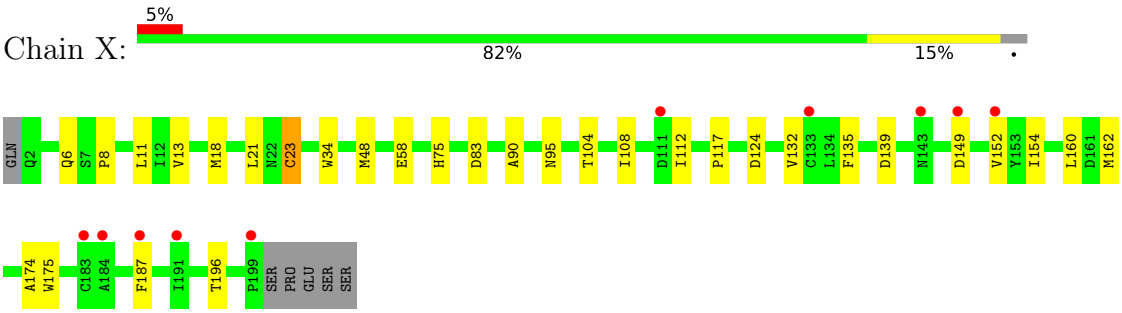
• Molecule 4: 1-2C-T96F TCR alpha chain

Chain S:



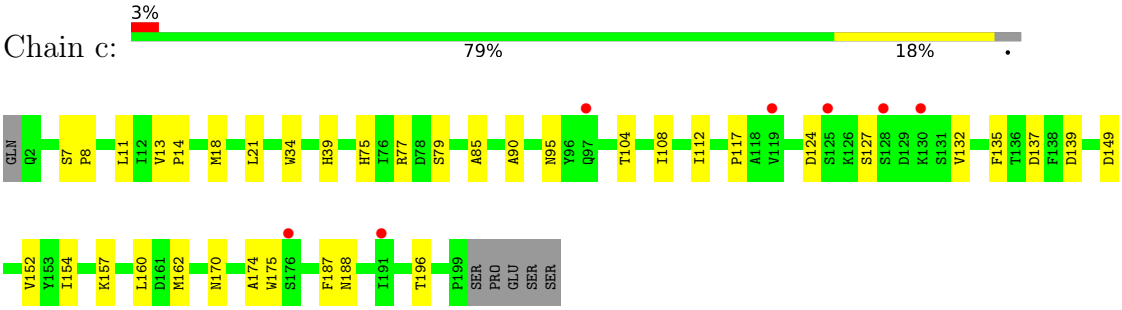
• Molecule 4: 1-2C-T96F TCR alpha chain

Chain X:



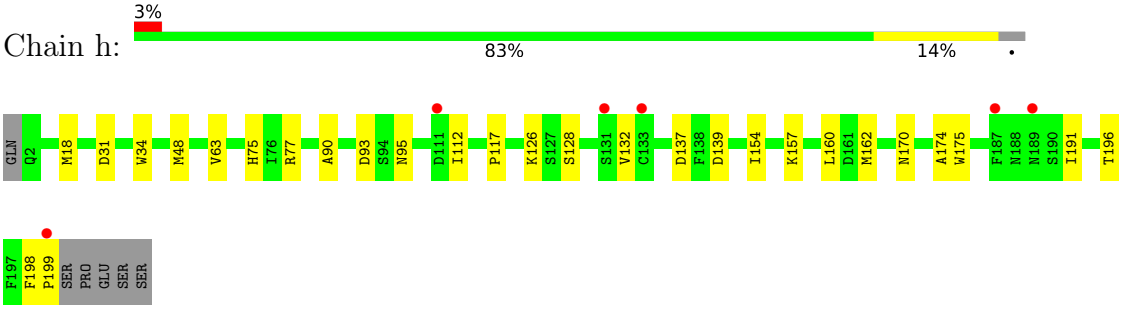
• Molecule 4: 1-2C-T96F TCR alpha chain

Chain c:



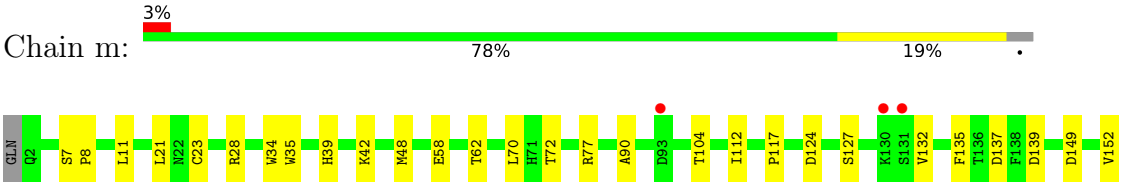
• Molecule 4: 1-2C-T96F TCR alpha chain

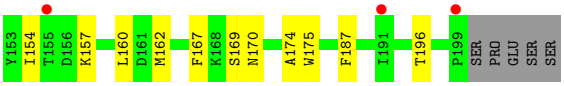
Chain h:



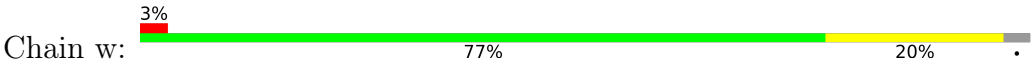
• Molecule 4: 1-2C-T96F TCR alpha chain

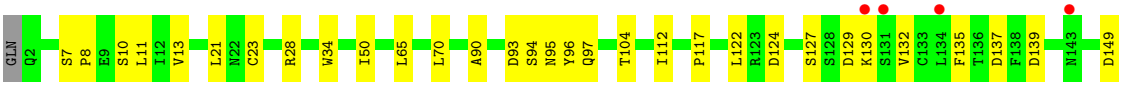
Chain m:

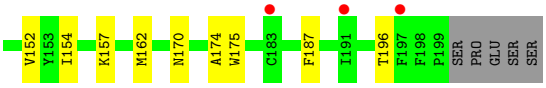




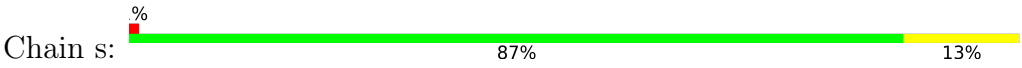
• Molecule 4: 1-2C-T96F TCR alpha chain

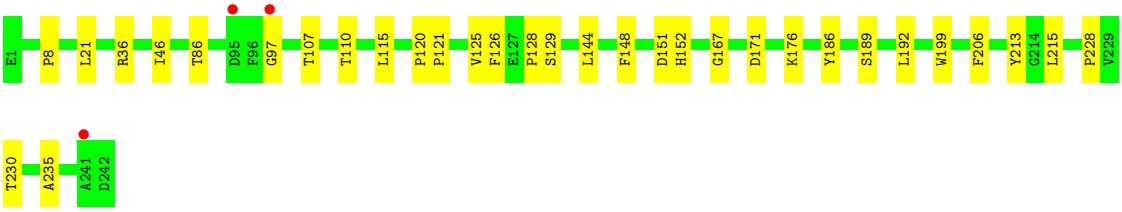




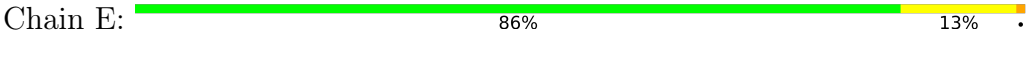


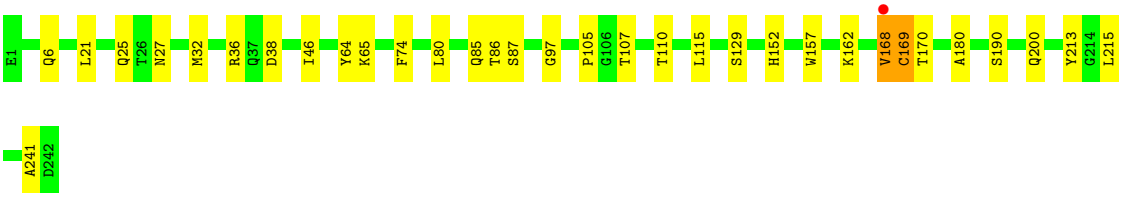
• Molecule 5: 1-2C-T96F TCR beta chain



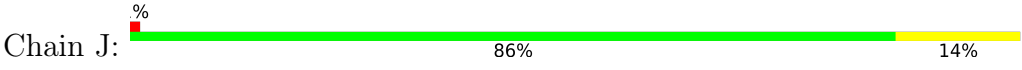


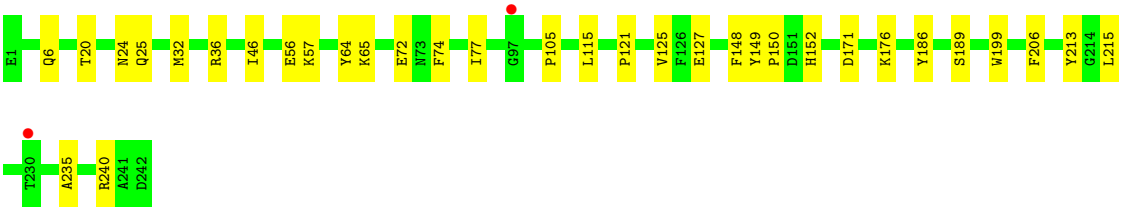
• Molecule 5: 1-2C-T96F TCR beta chain



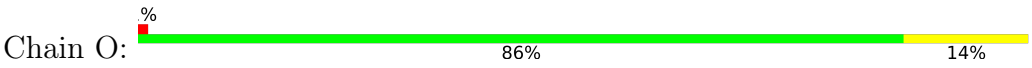


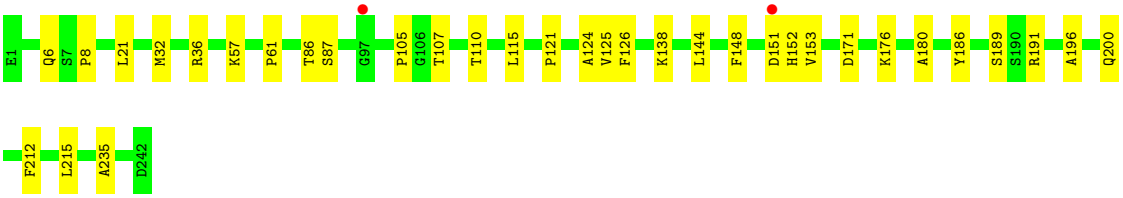
• Molecule 5: 1-2C-T96F TCR beta chain





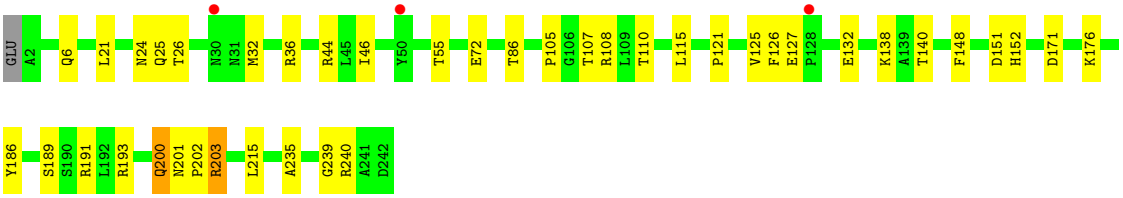
• Molecule 5: 1-2C-T96F TCR beta chain





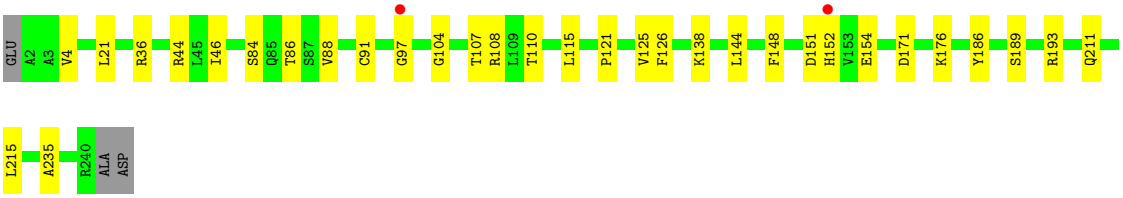
• Molecule 5: 1-2C-T96F TCR beta chain

Chain T:



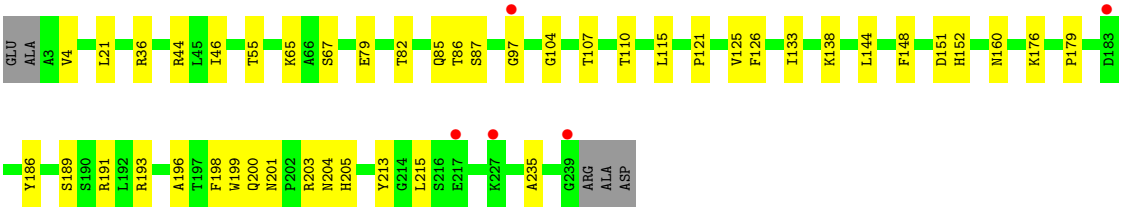
• Molecule 5: 1-2C-T96F TCR beta chain

Chain Y:



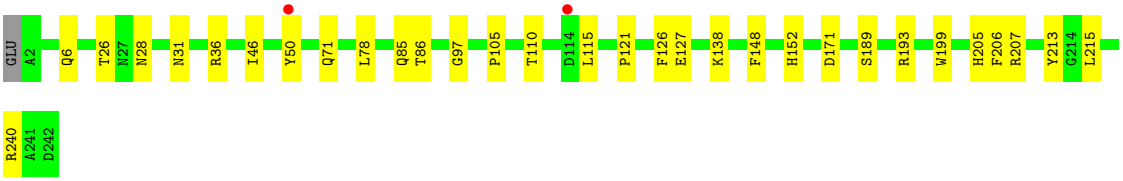
• Molecule 5: 1-2C-T96F TCR beta chain

Chain d:



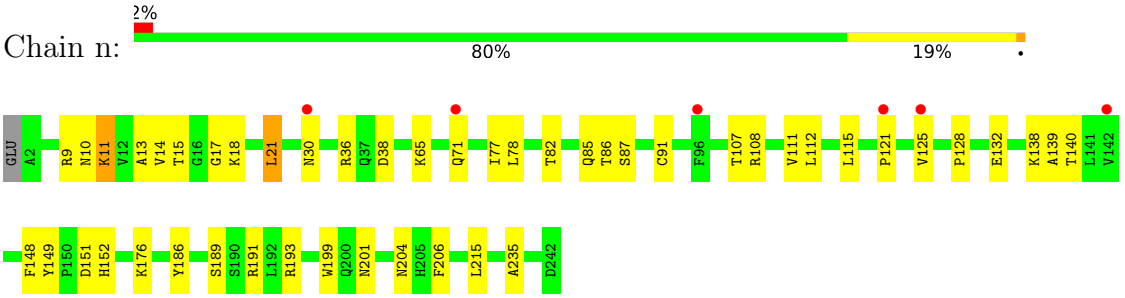
• Molecule 5: 1-2C-T96F TCR beta chain

Chain i:



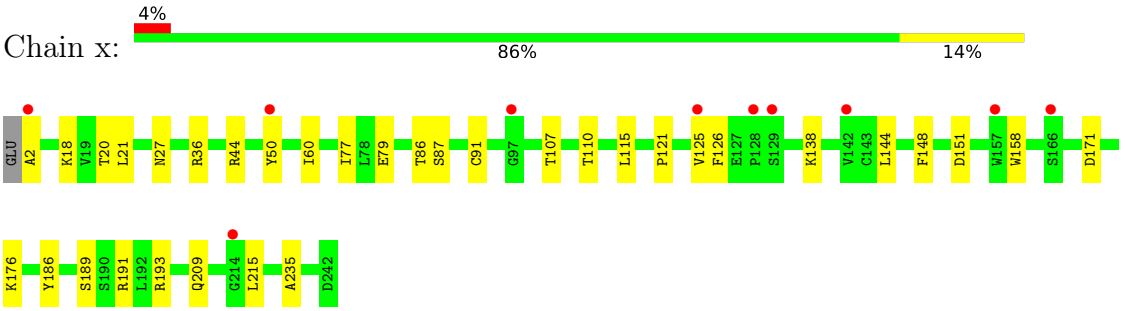
• Molecule 5: 1-2C-T96F TCR beta chain

Chain n:



• Molecule 5: 1-2C-T96F TCR beta chain

Chain x:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	157.78Å 157.77Å 193.02Å 103.03° 101.92° 82.17°	Depositor
Resolution (Å)	35.00 – 3.45 35.00 – 3.45	Depositor EDS
% Data completeness (in resolution range)	98.0 (35.00-3.45) 98.1 (35.00-3.45)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.209 , 0.234 0.206 , 0.231	Depositor DCC
R_{free} test set	11414 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	94.6	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	65289	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.19	0/2296	0.35	0/3117
1	F	0.13	0/2296	0.31	0/3117
1	K	0.12	0/2296	0.28	0/3117
1	P	0.14	0/2296	0.30	0/3117
1	U	0.11	0/2296	0.28	0/3117
1	Z	0.12	0/1980	0.31	0/2682
1	e	0.14	0/2032	0.30	0/2753
1	j	0.12	0/2296	0.29	0/3117
1	o	0.12	0/2296	0.33	0/3117
1	t	0.11	0/2296	0.31	0/3117
2	B	0.10	0/859	0.25	0/1162
2	G	0.11	0/859	0.32	0/1162
2	L	0.11	0/859	0.30	0/1162
2	Q	0.10	0/851	0.29	0/1152
2	V	0.11	0/851	0.29	0/1152
2	a	0.10	0/859	0.29	0/1162
2	f	0.10	0/851	0.29	0/1152
2	k	0.10	0/851	0.28	0/1152
2	p	0.11	0/859	0.31	0/1162
2	u	0.11	0/851	0.29	0/1152
3	C	0.14	0/54	0.38	0/70
3	H	0.13	0/54	0.51	0/70
3	M	0.16	0/54	0.49	0/70
3	R	0.15	0/54	0.43	0/70
3	W	0.17	0/54	0.51	0/70
3	b	0.13	0/54	0.45	0/70
3	g	0.13	0/54	0.48	0/70
3	l	0.17	0/54	0.56	0/70
3	q	0.54	0/54	0.91	0/70
3	v	0.18	0/54	0.56	0/70
4	D	0.20	0/1607	0.38	0/2175
4	I	0.11	0/1598	0.30	0/2163
4	N	0.11	0/1598	0.27	0/2163
4	S	0.32	0/1598	0.47	1/2163 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
4	X	0.11	0/1598	0.29	0/2163
4	c	0.10	0/1598	0.28	0/2163
4	h	0.12	0/1598	0.32	0/2163
4	m	0.09	0/1598	0.27	0/2163
4	r	0.22	0/1598	0.39	0/2163
4	w	0.17	0/1598	0.33	0/2163
5	E	0.17	0/1963	0.32	0/2675
5	J	0.14	0/1963	0.33	0/2675
5	O	0.12	0/1963	0.29	0/2675
5	T	0.25	0/1954	0.41	0/2663
5	Y	0.11	0/1941	0.30	0/2645
5	d	0.20	0/1925	0.35	0/2624
5	i	0.11	0/1954	0.29	0/2663
5	n	0.23	0/1954	0.39	0/2663
5	s	0.12	0/1963	0.30	0/2675
5	x	0.12	0/1954	0.27	0/2663
All	All	0.15	0/66993	0.32	1/90904 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	S	124	ASP	CA-CB-CG	5.19	117.79	112.60

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	2235	0	2085	22	0
1	F	2235	0	2085	33	0
1	K	2235	0	2085	30	0
1	P	2235	0	2085	37	0
1	U	2235	0	2085	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z	1927	0	1806	17	0
1	e	1979	0	1856	32	0
1	j	2235	0	2085	39	0
1	o	2235	0	2085	25	0
1	t	2235	0	2085	37	0
2	B	836	0	803	5	0
2	G	836	0	803	11	0
2	L	836	0	803	8	0
2	Q	828	0	794	7	0
2	V	828	0	794	4	0
2	a	836	0	803	7	0
2	f	828	0	794	7	0
2	k	828	0	794	6	0
2	p	836	0	803	11	0
2	u	828	0	794	10	0
3	C	55	0	65	4	0
3	H	55	0	65	2	0
3	M	55	0	65	2	0
3	R	55	0	65	4	0
3	W	55	0	65	6	0
3	b	55	0	65	3	0
3	g	55	0	65	3	0
3	l	55	0	65	11	0
3	q	55	0	65	4	0
3	v	55	0	65	7	0
4	D	1571	0	1495	17	0
4	I	1562	0	1484	14	0
4	N	1562	0	1484	24	0
4	S	1562	0	1484	40	0
4	X	1562	0	1484	20	0
4	c	1562	0	1484	24	0
4	h	1562	0	1484	19	0
4	m	1562	0	1484	22	0
4	r	1562	0	1485	25	0
4	w	1562	0	1484	27	0
5	E	1910	0	1797	22	0
5	J	1910	0	1797	17	0
5	O	1910	0	1797	22	0
5	T	1901	0	1788	34	0
5	Y	1888	0	1779	21	0
5	d	1872	0	1761	27	0
5	i	1901	0	1788	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	n	1901	0	1788	32	0
5	s	1910	0	1798	20	0
5	x	1901	0	1788	21	0
All	All	65289	0	61710	740	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 6.

All (740) 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:S:132:VAL:HG11	5:T:126:PHE:HE2	1.44	0.82
4:S:132:VAL:HG11	5:T:126:PHE:CE2	2.17	0.79
1:j:147:TRP:HE1	3:l:9:LYS:H	1.28	0.79
1:U:65:ARG:NH2	4:X:95:ASN:OD1	2.17	0.77
5:n:86:THR:HG22	5:n:111:VAL:H	1.49	0.77
5:x:20:THR:HG23	5:x:77:ILE:HG12	1.68	0.75
1:o:13:SER:HB3	1:o:78:LEU:HD13	1.66	0.74
1:Z:12:VAL:HG12	1:Z:94:THR:HG22	1.68	0.74
4:w:162:MET:HE1	5:x:138:LYS:HD3	1.69	0.74
1:K:13:SER:HB3	1:K:78:LEU:HD13	1.70	0.73
5:d:21:LEU:HD22	5:d:107:THR:HG21	1.70	0.73
1:j:147:TRP:CZ2	3:l:9:LYS:HG3	2.24	0.73
1:e:5:MET:HE2	1:e:7:TYR:HE1	1.54	0.72
4:c:162:MET:HE1	5:d:138:LYS:HD3	1.72	0.72
5:Y:36:ARG:NH2	5:Y:84:SER:O	2.21	0.71
4:S:132:VAL:CG1	5:T:126:PHE:CE2	2.74	0.70
5:n:21:LEU:HD22	5:n:107:THR:HG21	1.73	0.70
5:n:36:ARG:HH21	5:n:87:SER:HB3	1.56	0.70
1:o:250:PRO:HG2	1:o:253:GLU:OE1	1.92	0.70
1:P:147:TRP:HE1	3:R:9:LYS:H	1.38	0.69
4:h:162:MET:HE1	5:i:138:LYS:HD3	1.75	0.69
4:m:8:PRO:HG3	4:m:11:LEU:HD12	1.74	0.69
4:m:62:THR:OG1	4:m:77:ARG:NH2	2.25	0.68
4:X:162:MET:HE1	5:Y:138:LYS:HD3	1.74	0.68
4:S:13:VAL:HG23	4:w:7:SER:HB2	1.76	0.68
1:Z:192:HIS:NE2	2:a:98:ASP:OD2	2.27	0.68
1:o:201:LEU:HD22	1:o:249:VAL:HG11	1.76	0.67
1:t:253:GLU:HB3	1:t:256:ARG:HD3	1.75	0.67
4:r:21:LEU:HD22	4:r:104:THR:HG21	1.77	0.67
4:S:124:ASP:HB2	5:T:126:PHE:CE1	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:162:MET:HE1	5:T:138:LYS:HD3	1.77	0.67
1:Z:147:TRP:HE1	3:b:9:LYS:H	1.41	0.67
4:I:117:PRO:HB2	4:I:196:THR:HG22	1.77	0.67
1:U:178:THR:O	1:U:181:ARG:NH1	2.26	0.67
4:c:21:LEU:HD22	4:c:104:THR:HG21	1.76	0.67
4:m:162:MET:HE1	5:n:138:LYS:HD3	1.75	0.67
4:X:48:MET:HE1	4:X:58:GLU:HB2	1.76	0.66
4:S:124:ASP:HB2	5:T:126:PHE:HE1	1.60	0.66
4:m:117:PRO:HB2	4:m:196:THR:HG22	1.78	0.66
4:I:49:SER:O	4:I:56:LYS:NZ	2.21	0.66
5:O:21:LEU:HD22	5:O:107:THR:HG21	1.77	0.66
1:t:147:TRP:CZ2	3:v:9:LYS:HG3	2.30	0.66
4:w:21:LEU:HD22	4:w:104:THR:HG21	1.77	0.66
4:m:21:LEU:HD22	4:m:104:THR:HG21	1.78	0.66
4:X:21:LEU:HD22	4:X:104:THR:HG21	1.78	0.66
1:j:147:TRP:HZ2	3:l:9:LYS:HG3	1.62	0.65
1:t:65:ARG:HG2	5:x:50:TYR:HE2	1.59	0.65
1:P:192:HIS:NE2	2:Q:98:ASP:OD2	2.29	0.65
4:h:18:MET:HE3	4:h:77:ARG:HG2	1.77	0.65
4:N:132:VAL:HG12	4:N:175:TRP:HB3	1.78	0.65
4:I:21:LEU:HD22	4:I:104:THR:HG21	1.77	0.65
4:I:132:VAL:HG12	4:I:175:TRP:HB3	1.79	0.65
4:N:30:VAL:HG11	4:N:91:ALA:HB1	1.79	0.65
1:U:253:GLU:HB3	1:U:256:ARG:HD3	1.77	0.64
4:X:117:PRO:HB2	4:X:196:THR:HG22	1.80	0.64
5:E:36:ARG:HB2	5:E:46:ILE:HD11	1.78	0.64
4:c:117:PRO:HB2	4:c:196:THR:HG22	1.79	0.64
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.79	0.64
5:O:36:ARG:HH21	5:O:87:SER:HB2	1.62	0.64
1:o:147:TRP:HE1	3:q:9:LYS:H	1.44	0.63
4:D:34:TRP:HB2	4:D:90:ALA:HB3	1.81	0.63
1:t:14:ARG:HB3	1:t:17:ARG:HB2	1.80	0.63
1:e:51:TRP:CD1	1:e:178:THR:HG21	2.34	0.63
1:F:5:MET:HE2	1:F:7:TYR:HE1	1.64	0.62
4:N:18:MET:SD	4:N:77:ARG:NH1	2.72	0.62
1:A:143:THR:HG23	3:C:9:LYS:HA	1.80	0.62
4:D:117:PRO:HB2	4:D:196:THR:HG22	1.81	0.62
1:P:111:ARG:NE	1:P:113:TYR:OH	2.23	0.62
1:U:255:GLN:O	1:U:273:ARG:NH1	2.34	0.61
5:Y:44:ARG:HG3	5:Y:44:ARG:HH11	1.64	0.61
4:N:13:VAL:HG23	4:c:7:SER:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:36:ARG:HB2	5:Y:46:ILE:HD11	1.82	0.61
5:d:36:ARG:HH21	5:d:87:SER:HB2	1.66	0.61
5:x:21:LEU:HD22	5:x:107:THR:HG21	1.83	0.61
1:F:147:TRP:HE1	3:H:9:LYS:H	1.47	0.61
5:Y:108:ARG:HE	5:Y:152:HIS:HB3	1.65	0.61
5:x:36:ARG:HH21	5:x:87:SER:HB2	1.64	0.61
4:r:149:ASP:HB3	4:r:152:VAL:HG12	1.83	0.61
1:U:214:THR:HB	1:U:262:GLN:HB2	1.82	0.61
4:S:12:ILE:HD12	4:w:10:SER:HB3	1.82	0.60
5:E:25:GLN:HG2	5:E:32:MET:HE3	1.83	0.60
4:h:117:PRO:HB2	4:h:196:THR:HG22	1.83	0.60
1:t:65:ARG:HH21	4:w:95:ASN:CG	2.10	0.60
4:r:132:VAL:HG12	4:r:175:TRP:HB3	1.84	0.60
5:T:108:ARG:HD2	5:T:152:HIS:HB3	1.82	0.60
1:F:35:ARG:HH12	1:F:46:GLU:CD	2.08	0.60
1:P:244:TRP:HZ3	1:P:246:ALA:HB2	1.66	0.60
4:w:8:PRO:HG3	4:w:11:LEU:HD12	1.84	0.60
1:K:5:MET:HB2	1:K:168:LEU:HD13	1.83	0.60
5:x:86:THR:HG23	5:x:110:THR:HA	1.84	0.60
1:e:192:HIS:NE2	2:f:98:ASP:OD2	2.33	0.59
4:w:95:ASN:O	4:w:97:GLN:N	2.35	0.59
1:P:193:PRO:HA	1:P:199:ALA:HA	1.83	0.59
1:t:99:TYR:CE1	3:v:4:ALA:HB2	2.37	0.59
5:x:171:ASP:OD2	5:x:189:SER:OG	2.20	0.59
1:e:163:ARG:NH2	4:h:31:ASP:OD1	2.35	0.59
5:x:2:ALA:N	5:x:27:ASN:OD1	2.36	0.59
5:s:86:THR:HG23	5:s:110:THR:HA	1.85	0.59
4:S:117:PRO:HB2	4:S:196:THR:HG22	1.84	0.59
5:i:36:ARG:HB2	5:i:46:ILE:HD11	1.85	0.58
2:p:37:VAL:HB	2:p:66:TYR:CE2	2.38	0.58
4:S:132:VAL:CG1	5:T:126:PHE:HE2	2.11	0.58
5:s:21:LEU:HD22	5:s:107:THR:HG21	1.86	0.58
5:E:21:LEU:HD22	5:E:107:THR:HG21	1.86	0.58
2:B:96:ASP:HB3	2:B:99:MET:HB3	1.86	0.58
4:I:149:ASP:HB3	4:I:152:VAL:HG12	1.86	0.58
1:P:214:THR:HB	1:P:262:GLN:HB2	1.86	0.58
4:S:18:MET:HE2	4:S:75:HIS:HB3	1.85	0.58
4:S:132:VAL:HG21	5:T:126:PHE:HD2	1.69	0.58
1:j:13:SER:HG	1:j:93:HIS:H	1.52	0.58
4:r:188:ASN:HB3	5:E:180:ALA:HA	1.86	0.58
1:j:12:VAL:HG12	1:j:94:THR:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:HD22	1:A:261:VAL:HG22	1.85	0.57
1:e:147:TRP:HE1	3:g:9:LYS:H	1.50	0.57
4:r:48:MET:HE1	4:r:58:GLU:HB2	1.85	0.57
2:G:37:VAL:HB	2:G:66:TYR:CE2	2.39	0.57
2:V:37:VAL:HB	2:V:66:TYR:CE2	2.38	0.57
1:Z:235:PRO:HG2	2:a:65:LEU:HD22	1.85	0.57
1:e:214:THR:HB	1:e:262:GLN:HB2	1.85	0.57
1:j:14:ARG:HH11	1:j:17:ARG:HD3	1.69	0.57
4:r:35:TRP:HE1	4:r:72:THR:HG22	1.70	0.57
4:N:117:PRO:HB2	4:N:196:THR:HG22	1.86	0.57
1:F:35:ARG:HD2	2:G:53:ASP:CG	2.29	0.57
2:u:37:VAL:HB	2:u:66:TYR:CE2	2.38	0.57
4:r:126:LYS:HG3	4:r:127:SER:H	1.68	0.57
4:S:124:ASP:CG	4:S:128:SER:H	2.13	0.57
4:S:21:LEU:HD22	4:S:104:THR:HG21	1.87	0.57
1:e:5:MET:HE2	1:e:7:TYR:CE1	2.38	0.57
5:J:121:PRO:HB3	5:J:148:PHE:HB3	1.86	0.57
4:r:73:SER:OG	4:r:75:HIS:NE2	2.37	0.57
2:Q:37:VAL:HB	2:Q:66:TYR:CE2	2.40	0.57
4:c:132:VAL:HG12	4:c:175:TRP:HB3	1.87	0.57
1:t:202:ARG:HH22	2:u:99:MET:HE2	1.70	0.56
1:o:163:ARG:NH2	4:r:93:ASP:O	2.38	0.56
5:T:86:THR:HG23	5:T:110:THR:HA	1.86	0.56
1:Z:9:TYR:OH	3:b:2:VAL:HG13	2.05	0.56
5:n:121:PRO:HB3	5:n:148:PHE:HB3	1.86	0.56
2:L:37:VAL:HB	2:L:66:TYR:CE2	2.40	0.56
5:d:4:VAL:HG13	5:d:104:GLY:HA2	1.87	0.56
1:j:68:LYS:O	1:j:71:SER:OG	2.22	0.56
4:r:8:PRO:HG3	4:r:11:LEU:HD12	1.86	0.56
5:E:152:HIS:HB3	5:E:213:TYR:HB2	1.86	0.56
4:X:18:MET:HE2	4:X:75:HIS:HB3	1.86	0.56
1:j:147:TRP:HE1	3:l:9:LYS:N	2.01	0.56
4:D:124:ASP:OD1	4:D:130:LYS:HG2	2.05	0.56
5:J:25:GLN:HG2	5:J:32:MET:SD	2.46	0.56
5:n:9:ARG:O	5:n:107:THR:HA	2.05	0.56
5:T:171:ASP:OD2	5:T:189:SER:OG	2.22	0.56
1:U:189:MET:HE3	1:U:272:LEU:HB3	1.88	0.56
5:d:176:LYS:HE3	5:d:179:PRO:HA	1.87	0.56
1:t:147:TRP:HE1	3:v:9:LYS:H	1.54	0.55
5:O:86:THR:HG23	5:O:110:THR:HA	1.88	0.55
5:Y:86:THR:HG23	5:Y:110:THR:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:235:PRO:HG2	2:p:65:LEU:HD22	1.88	0.55
5:E:169:CYS:O	5:E:169:CYS:SG	2.61	0.55
5:Y:171:ASP:OD2	5:Y:189:SER:OG	2.22	0.55
1:Z:14:ARG:HB3	1:Z:17:ARG:HB2	1.87	0.55
4:w:117:PRO:HB2	4:w:196:THR:HG22	1.87	0.55
5:J:64:TYR:C	5:J:65:LYS:HD3	2.32	0.55
1:P:12:VAL:HG22	1:P:94:THR:HG22	1.88	0.55
1:U:78:LEU:HD22	1:U:95:ILE:HD12	1.89	0.55
4:r:135:PHE:HB2	4:r:187:PHE:CE2	2.42	0.55
4:N:149:ASP:HB3	4:N:152:VAL:HG12	1.89	0.55
4:S:126:LYS:O	4:S:127:SER:C	2.50	0.55
2:k:37:VAL:HB	2:k:66:TYR:CE2	2.40	0.55
4:S:48:MET:HE1	4:S:58:GLU:HB2	1.88	0.55
2:G:37:VAL:HG22	2:G:82:VAL:HG22	1.89	0.55
4:N:162:MET:HE1	5:O:138:LYS:HD3	1.89	0.55
5:i:171:ASP:OD2	5:i:189:SER:OG	2.24	0.55
1:j:143:THR:HG23	3:l:9:LYS:HA	1.88	0.55
4:I:8:PRO:HG3	4:I:11:LEU:HD12	1.89	0.54
4:c:149:ASP:HB3	4:c:152:VAL:HG12	1.89	0.54
4:r:121:GLN:HB3	4:r:123:ARG:HH21	1.72	0.54
1:t:68:LYS:O	1:t:71:SER:OG	2.24	0.54
5:J:171:ASP:OD2	5:J:189:SER:OG	2.25	0.54
1:K:234:ARG:HD2	2:L:10:TYR:CE1	2.42	0.54
1:U:9:TYR:OH	3:W:2:VAL:HG13	2.07	0.54
1:K:235:PRO:HG2	2:L:65:LEU:HD22	1.88	0.54
4:N:73:SER:OG	4:N:75:HIS:NE2	2.38	0.54
1:e:5:MET:HE1	1:e:171:TYR:HE2	1.72	0.54
1:j:189:MET:HE3	1:j:272:LEU:HB3	1.89	0.54
5:Y:21:LEU:HD22	5:Y:107:THR:HG21	1.88	0.54
1:o:35:ARG:HD2	2:p:53:ASP:CG	2.33	0.54
1:o:244:TRP:HZ3	1:o:246:ALA:HB2	1.71	0.54
1:K:81:LEU:HD11	1:K:123:TYR:CZ	2.43	0.54
4:c:18:MET:HE3	4:c:77:ARG:HG2	1.90	0.54
1:j:81:LEU:HD11	1:j:123:TYR:CZ	2.42	0.54
4:N:7:SER:HB2	4:c:14:PRO:HD2	1.89	0.54
5:d:36:ARG:HB3	5:d:46:ILE:HD11	1.89	0.54
2:f:37:VAL:HB	2:f:66:TYR:CE2	2.43	0.54
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.91	0.53
1:P:14:ARG:HB3	1:P:17:ARG:HB2	1.89	0.53
1:P:162:GLY:O	1:P:166:GLU:HG3	2.08	0.53
4:S:3:LYS:HD2	4:S:99:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:w:34:TRP:HB2	4:w:90:ALA:HB3	1.90	0.53
2:L:37:VAL:HG22	2:L:82:VAL:HG22	1.89	0.53
1:U:231:VAL:O	1:U:243:LYS:NZ	2.35	0.53
4:w:132:VAL:HG12	4:w:175:TRP:HB3	1.90	0.53
4:h:137:ASP:OD1	5:i:193:ARG:NH1	2.37	0.53
4:m:39:HIS:HB2	4:m:42:LYS:HD3	1.91	0.53
1:F:127:ASN:OD1	1:F:134:THR:OG1	2.22	0.53
4:m:48:MET:HE1	4:m:58:GLU:HB3	1.91	0.53
4:m:157:LYS:HD2	4:m:170:ASN:HD22	1.72	0.53
1:e:231:VAL:O	1:e:243:LYS:NZ	2.39	0.53
5:J:20:THR:HG23	5:J:77:ILE:HG12	1.91	0.53
4:S:149:ASP:HB3	4:S:152:VAL:HG12	1.91	0.53
4:S:34:TRP:HB2	4:S:90:ALA:HB3	1.90	0.53
1:U:147:TRP:HZ2	3:W:9:LYS:HG3	1.74	0.53
1:Z:78:LEU:HD23	1:Z:95:ILE:HD12	1.90	0.53
1:e:244:TRP:HZ3	1:e:246:ALA:HB2	1.74	0.53
1:t:62:GLN:HG3	4:w:95:ASN:OD1	2.09	0.53
1:F:8:PHE:HB2	1:F:25:VAL:HG23	1.91	0.52
1:o:202:ARG:HH22	2:p:99:MET:HE2	1.74	0.52
1:P:189:MET:HE3	1:P:272:LEU:HB3	1.91	0.52
1:P:9:TYR:OH	3:R:2:VAL:HG13	2.09	0.52
4:X:132:VAL:HG12	4:X:175:TRP:HB3	1.91	0.52
5:x:115:LEU:HD22	5:x:215:LEU:HD21	1.91	0.52
4:I:154:ILE:HG12	4:I:174:ALA:HB2	1.91	0.52
1:K:127:ASN:OD1	1:K:134:THR:OG1	2.25	0.52
4:h:18:MET:HE2	4:h:75:HIS:HB3	1.91	0.52
1:A:259:CYS:HB3	1:A:272:LEU:HB2	1.91	0.52
5:E:38:ASP:OD1	5:E:87:SER:OG	2.24	0.52
1:F:235:PRO:HG2	2:G:65:LEU:HD22	1.92	0.52
1:P:9:TYR:HB2	1:P:97:ILE:HB	1.90	0.52
1:U:206:LEU:HD13	1:U:242:GLN:HG2	1.91	0.52
4:I:34:TRP:HB2	4:I:90:ALA:HB3	1.91	0.52
4:N:21:LEU:HD23	4:N:104:THR:HG21	1.91	0.52
1:U:147:TRP:HE1	3:W:9:LYS:H	1.56	0.52
2:a:37:VAL:HB	2:a:66:TYR:CE2	2.44	0.52
5:n:78:LEU:HD23	5:n:85:GLN:OE1	2.10	0.52
1:t:22:PHE:H	1:t:38:SER:HB3	1.74	0.52
1:t:65:ARG:NH2	4:w:95:ASN:ND2	2.58	0.52
5:s:152:HIS:HD2	5:s:213:TYR:HB2	1.74	0.52
5:E:200:GLN:HG3	5:E:241:ALA:HA	1.92	0.52
1:F:71:SER:O	1:F:75:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:143:THR:HG23	3:v:9:LYS:HA	1.91	0.52
4:w:149:ASP:HB3	4:w:152:VAL:HG12	1.91	0.52
2:p:13:HIS:O	2:p:21:ASN:ND2	2.42	0.51
1:P:235:PRO:HG2	2:Q:65:LEU:HD22	1.90	0.51
5:i:86:THR:HG23	5:i:110:THR:HA	1.92	0.51
5:n:176:LYS:HG2	5:n:186:TYR:CE1	2.45	0.51
5:s:8:PRO:HD2	5:s:21:LEU:HD23	1.92	0.51
4:N:157:LYS:HD2	4:N:170:ASN:HD22	1.76	0.51
5:s:171:ASP:OD2	5:s:189:SER:OG	2.24	0.51
4:h:160:LEU:HD13	5:i:193:ARG:HG3	1.92	0.51
1:j:99:TYR:CE1	3:l:4:ALA:HB2	2.45	0.51
4:w:28:ARG:HA	4:w:70:LEU:HD11	1.92	0.51
1:U:224:GLN:O	1:U:228:THR:OG1	2.24	0.51
1:e:9:TYR:HB2	1:e:97:ILE:HB	1.91	0.51
5:E:25:GLN:CG	5:E:32:MET:HE3	2.41	0.51
1:F:214:THR:HB	1:F:262:GLN:HB2	1.93	0.51
1:F:224:GLN:O	1:F:228:THR:HG23	2.10	0.51
1:U:35:ARG:HD3	1:U:48:ARG:NE	2.25	0.51
1:j:249:VAL:HG12	1:j:257:TYR:CD2	2.46	0.51
1:F:5:MET:HE2	1:F:7:TYR:CE1	2.46	0.51
5:T:176:LYS:HG2	5:T:186:TYR:CE1	2.46	0.51
1:e:73:THR:HG21	3:g:6:GLY:HA3	1.92	0.51
1:e:78:LEU:HD22	1:e:95:ILE:HD12	1.93	0.51
4:I:48:MET:HE1	4:I:58:GLU:HB2	1.93	0.51
1:U:244:TRP:HZ3	1:U:246:ALA:HB2	1.76	0.51
1:e:5:MET:CE	1:e:171:TYR:HE2	2.24	0.51
4:h:128:SER:HB2	5:i:126:PHE:HE1	1.76	0.51
4:h:132:VAL:HG12	4:h:175:TRP:HB3	1.93	0.51
4:h:157:LYS:HD2	4:h:170:ASN:HD22	1.77	0.51
5:d:55:THR:HG21	5:d:67:SER:HA	1.93	0.50
1:P:249:VAL:HG12	1:P:257:TYR:CD2	2.46	0.50
5:d:151:ASP:HB3	5:d:186:TYR:HE2	1.75	0.50
1:P:78:LEU:HD22	1:P:95:ILE:HD12	1.92	0.50
1:t:244:TRP:HZ3	1:t:246:ALA:HB2	1.76	0.50
1:U:147:TRP:NE1	3:W:7:VAL:HG23	2.26	0.50
5:d:65:LYS:HE3	5:d:79:GLU:HG3	1.93	0.50
1:F:194:ILE:HD11	1:F:198:GLU:HB3	1.94	0.50
5:T:121:PRO:HB3	5:T:148:PHE:HB3	1.93	0.50
1:U:235:PRO:HG2	2:V:65:LEU:HD22	1.91	0.50
4:X:154:ILE:HG12	4:X:174:ALA:HB2	1.92	0.50
5:Y:154:GLU:HB2	5:Y:211:GLN:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:n:112:LEU:HD11	5:n:149:TYR:CE2	2.47	0.50
4:X:13:VAL:HG23	4:m:7:SER:HB2	1.93	0.50
1:F:35:ARG:NH1	1:F:46:GLU:OE1	2.42	0.50
4:N:154:ILE:HG12	4:N:174:ALA:HB2	1.93	0.50
5:n:108:ARG:CZ	5:n:152:HIS:HB2	2.42	0.50
1:A:85:TYR:OH	1:A:137:ASP:OD2	2.27	0.49
4:c:112:ILE:HG13	4:c:139:ASP:HA	1.94	0.49
1:e:173:GLU:HA	1:e:176:LYS:HG3	1.93	0.49
1:F:220:ASP:OD1	1:F:256:ARG:HG2	2.12	0.49
4:I:135:PHE:HB2	4:I:187:PHE:CE2	2.47	0.49
5:T:21:LEU:HD22	5:T:107:THR:HG21	1.94	0.49
4:c:157:LYS:HD2	4:c:170:ASN:HD22	1.77	0.49
5:i:127:GLU:OE1	5:i:240:ARG:NH2	2.45	0.49
1:t:249:VAL:HG12	1:t:257:TYR:CD2	2.47	0.49
5:n:132:GLU:OE2	5:n:140:THR:OG1	2.26	0.49
5:E:168:VAL:O	5:E:169:CYS:C	2.54	0.49
4:S:154:ILE:HG12	4:S:174:ALA:HB2	1.95	0.49
4:X:34:TRP:HB2	4:X:90:ALA:HB3	1.94	0.49
5:Y:176:LYS:HG2	5:Y:186:TYR:CE1	2.48	0.49
1:F:128:GLU:OE1	1:F:128:GLU:N	2.30	0.49
4:m:28:ARG:HA	4:m:70:LEU:HD11	1.95	0.49
1:K:214:THR:HB	1:K:262:GLN:HB2	1.93	0.49
5:T:200:GLN:O	5:T:201:ASN:C	2.55	0.49
5:d:126:PHE:HE2	5:d:144:LEU:HD12	1.78	0.49
2:k:37:VAL:HG22	2:k:82:VAL:HG22	1.93	0.49
1:t:214:THR:HB	1:t:262:GLN:HB2	1.93	0.49
5:T:202:PRO:HA	5:T:239:GLY:O	2.13	0.49
4:c:135:PHE:HB2	4:c:187:PHE:CE2	2.48	0.49
5:d:151:ASP:HB3	5:d:186:TYR:CE2	2.48	0.49
5:J:152:HIS:HB3	5:J:213:TYR:HB2	1.94	0.49
4:N:95:ASN:O	4:N:97:GLN:N	2.45	0.49
4:S:45:LYS:HB2	4:S:45:LYS:NZ	2.28	0.49
4:S:121:GLN:HG3	4:S:123:ARG:HH22	1.78	0.49
1:U:234:ARG:HD2	2:V:10:TYR:CE1	2.47	0.49
4:h:48:MET:HB2	4:h:63:VAL:HG21	1.95	0.49
1:j:244:TRP:HZ3	1:j:246:ALA:HB2	1.78	0.49
4:m:35:TRP:HE1	4:m:72:THR:HG22	1.78	0.49
4:r:3:LYS:HD2	4:r:27:ASP:HB2	1.95	0.49
2:Q:37:VAL:HG22	2:Q:82:VAL:HG22	1.94	0.49
5:E:86:THR:HG23	5:E:110:THR:HA	1.95	0.49
5:O:176:LYS:HG2	5:O:186:TYR:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:83:ASP:HB2	4:X:108:ILE:HD11	1.95	0.49
2:a:37:VAL:HG22	2:a:82:VAL:HG22	1.95	0.49
1:t:129:ASP:O	1:t:131:ARG:NH1	2.46	0.49
1:F:234:ARG:HD2	2:G:10:TYR:CE1	2.48	0.48
1:F:244:TRP:HZ3	1:F:246:ALA:HB2	1.78	0.48
1:P:35:ARG:HD3	2:Q:53:ASP:CG	2.38	0.48
4:S:132:VAL:HG21	5:T:126:PHE:CD2	2.46	0.48
5:x:121:PRO:HB3	5:x:148:PHE:HB3	1.95	0.48
1:o:235:PRO:HA	1:o:241:PHE:HD1	1.78	0.48
1:K:102:ASP:HB2	1:K:111:ARG:HG2	1.96	0.48
5:O:121:PRO:HB3	5:O:148:PHE:HB3	1.94	0.48
1:Z:234:ARG:HD2	2:a:10:TYR:CE1	2.48	0.48
5:x:176:LYS:HG2	5:x:186:TYR:CE1	2.48	0.48
4:D:121:GLN:O	5:E:129:SER:HB2	2.13	0.48
5:O:6:GLN:HB2	5:O:105:PRO:HG2	1.95	0.48
5:T:151:ASP:HB3	5:T:186:TYR:CE2	2.49	0.48
1:U:235:PRO:HA	1:U:241:PHE:HD1	1.78	0.48
1:e:235:PRO:HA	1:e:241:PHE:HD1	1.78	0.48
1:t:131:ARG:HG3	1:t:131:ARG:HH11	1.77	0.48
4:w:112:ILE:HG13	4:w:139:ASP:HA	1.95	0.48
5:s:151:ASP:HB3	5:s:186:TYR:CE2	2.47	0.48
4:D:48:MET:HE1	4:D:58:GLU:HB2	1.96	0.48
4:D:125:SER:O	4:D:126:LYS:HD3	2.14	0.48
1:U:61:ASP:O	1:U:65:ARG:HG3	2.13	0.48
4:c:34:TRP:HB2	4:c:90:ALA:HB3	1.94	0.48
4:h:112:ILE:HG13	4:h:139:ASP:HA	1.95	0.48
2:p:37:VAL:HG22	2:p:82:VAL:HG22	1.95	0.48
5:J:6:GLN:HB2	5:J:105:PRO:HG2	1.95	0.48
1:K:219:ARG:HE	1:K:256:ARG:HH21	1.60	0.48
5:d:121:PRO:HB3	5:d:148:PHE:HB3	1.95	0.48
4:w:157:LYS:HD2	4:w:170:ASN:HD22	1.77	0.48
5:E:162:LYS:HE2	2:G:1:ILE:HD11	1.95	0.48
5:O:115:LEU:HD22	5:O:215:LEU:HD21	1.95	0.48
1:F:9:TYR:HB2	1:F:97:ILE:HB	1.96	0.48
5:O:57:LYS:HE2	5:O:61:PRO:HB2	1.95	0.48
4:S:132:VAL:HG13	5:T:126:PHE:CE2	2.47	0.48
1:A:194:ILE:HD11	1:A:198:GLU:HB3	1.95	0.48
4:c:18:MET:HE2	4:c:75:HIS:HB3	1.95	0.48
5:n:30:ASN:HA	5:n:71:GLN:OE1	2.14	0.48
1:t:129:ASP:O	1:t:131:ARG:HG3	2.14	0.48
4:D:21:LEU:HD22	4:D:104:THR:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:125:VAL:HG23	5:J:235:ALA:HB3	1.96	0.48
1:K:231:VAL:O	1:K:243:LYS:NZ	2.38	0.48
4:X:160:LEU:HD13	5:Y:193:ARG:HG3	1.96	0.48
4:m:124:ASP:HB3	4:m:127:SER:O	2.14	0.48
4:h:128:SER:HB2	5:i:126:PHE:CE1	2.49	0.47
4:h:154:ILE:HG12	4:h:174:ALA:HB2	1.95	0.47
5:i:28:ASN:HA	5:i:71:GLN:OE1	2.14	0.47
4:w:135:PHE:HB2	4:w:187:PHE:CE2	2.49	0.47
1:A:162:GLY:O	1:A:166:GLU:HG3	2.14	0.47
4:X:135:PHE:HB2	4:X:187:PHE:CE2	2.50	0.47
1:j:255:GLN:O	1:j:273:ARG:NH1	2.46	0.47
4:r:83:ASP:HB2	4:r:108:ILE:CD1	2.44	0.47
5:E:115:LEU:HD22	5:E:215:LEU:HD21	1.96	0.47
1:K:173:GLU:HA	1:K:176:LYS:HG3	1.96	0.47
1:o:62:GLN:HG3	1:o:63:GLU:N	2.29	0.47
5:s:125:VAL:HG23	5:s:235:ALA:HB3	1.96	0.47
5:Y:4:VAL:HG23	5:Y:104:GLY:HA2	1.97	0.47
4:D:35:TRP:HE1	4:D:72:THR:HG22	1.79	0.47
5:s:213:TYR:HA	5:s:230:THR:HG23	1.96	0.47
4:D:149:ASP:HB3	4:D:152:VAL:HG12	1.96	0.47
1:F:242:GLN:NE2	2:G:12:ARG:O	2.47	0.47
4:S:64:HIS:HB3	4:S:73:SER:OG	2.15	0.47
1:Z:235:PRO:HA	1:Z:241:PHE:HD1	1.79	0.47
1:j:99:TYR:HB3	1:j:114:ARG:HD2	1.96	0.47
1:A:147:TRP:HE1	3:C:9:LYS:H	1.62	0.47
5:E:32:MET:SD	5:E:74:PHE:HB2	2.54	0.47
1:F:202:ARG:HG2	1:F:246:ALA:HB2	1.97	0.47
1:F:235:PRO:HA	1:F:241:PHE:HD1	1.79	0.47
5:J:115:LEU:HD22	5:J:215:LEU:HD21	1.97	0.47
4:S:167:PHE:CE2	4:S:169:SER:HB3	2.49	0.47
2:V:37:VAL:HG22	2:V:82:VAL:HG22	1.97	0.47
5:Y:126:PHE:HE2	5:Y:144:LEU:HD12	1.79	0.47
1:Z:12:VAL:HG12	1:Z:94:THR:CG2	2.41	0.47
5:d:176:LYS:HG2	5:d:186:TYR:CE1	2.50	0.47
5:d:198:PHE:O	5:d:199:TRP:C	2.58	0.47
1:t:206:LEU:HD13	1:t:242:GLN:HG2	1.96	0.47
1:t:255:GLN:O	1:t:273:ARG:NH1	2.48	0.47
5:x:125:VAL:HG23	5:x:235:ALA:HB3	1.96	0.47
4:r:83:ASP:HB2	4:r:108:ILE:HD11	1.95	0.47
1:K:147:TRP:HE1	3:M:9:LYS:H	1.61	0.47
1:P:206:LEU:HD13	1:P:242:GLN:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:192:HIS:NE2	2:k:98:ASP:OD2	2.47	0.47
4:m:132:VAL:HG12	4:m:175:TRP:HB3	1.96	0.47
1:F:78:LEU:HD22	1:F:95:ILE:HD12	1.96	0.47
4:N:135:PHE:HB2	4:N:187:PHE:CE2	2.50	0.47
4:S:35:TRP:HE1	4:S:72:THR:HG22	1.80	0.47
1:e:98:MET:HE3	1:e:98:MET:HB3	1.73	0.47
1:e:172:LEU:HB3	1:e:180:GLN:HE21	1.80	0.47
1:A:9:TYR:HB2	1:A:97:ILE:HB	1.97	0.47
5:J:176:LYS:HG2	5:J:186:TYR:CE1	2.50	0.47
4:S:7:SER:HB2	4:w:13:VAL:HG23	1.97	0.47
4:w:154:ILE:HG12	4:w:174:ALA:HB2	1.97	0.47
1:o:206:LEU:HD13	1:o:242:GLN:HG2	1.97	0.46
1:K:12:VAL:HG13	1:K:94:THR:HG22	1.95	0.46
1:P:255:GLN:O	1:P:273:ARG:NH1	2.47	0.46
5:O:125:VAL:HG23	5:O:235:ALA:HB3	1.96	0.46
1:P:89:GLU:OE1	1:P:89:GLU:N	2.44	0.46
1:P:202:ARG:HH22	2:Q:99:MET:HE2	1.80	0.46
1:P:235:PRO:HA	1:P:241:PHE:HD1	1.80	0.46
5:d:201:ASN:HD21	5:d:203:ARG:HB2	1.79	0.46
1:j:147:TRP:NE1	3:l:9:LYS:H	2.05	0.46
2:B:40:LEU:HD11	2:B:81:ARG:HB2	1.97	0.46
1:Z:231:VAL:O	1:Z:243:LYS:NZ	2.43	0.46
5:i:121:PRO:HB3	5:i:148:PHE:HB3	1.96	0.46
4:S:135:PHE:HB2	4:S:187:PHE:CE2	2.50	0.46
1:e:84:TYR:HB3	1:e:139:ALA:HB1	1.97	0.46
5:i:26:THR:O	5:i:26:THR:OG1	2.30	0.46
1:j:235:PRO:HA	1:j:241:PHE:HD1	1.80	0.46
3:v:5:VAL:HG12	3:v:7:VAL:HG13	1.96	0.46
1:F:65:ARG:HE	4:I:95:ASN:HD21	1.64	0.46
4:S:112:ILE:HG13	4:S:139:ASP:HA	1.97	0.46
1:e:81:LEU:HD12	1:e:95:ILE:HD11	1.98	0.46
4:m:154:ILE:HG12	4:m:174:ALA:HB2	1.97	0.46
5:O:180:ALA:HA	4:c:188:ASN:HB3	1.98	0.46
5:x:126:PHE:HE2	5:x:144:LEU:HD12	1.81	0.46
2:B:94:LYS:HB3	2:B:94:LYS:HE2	1.67	0.46
5:E:157:TRP:CD1	5:E:168:VAL:HG22	2.51	0.46
1:U:15:PRO:HD2	1:U:17:ARG:NH2	2.31	0.46
5:d:152:HIS:CD2	5:d:213:TYR:HB2	2.51	0.46
4:w:124:ASP:HB3	4:w:127:SER:O	2.16	0.46
1:o:234:ARG:HD2	2:p:10:TYR:CE1	2.51	0.46
1:j:8:PHE:HB2	1:j:25:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:124:ASP:HA	5:T:126:PHE:CD1	2.51	0.46
4:r:154:ILE:HG12	4:r:174:ALA:HB2	1.98	0.46
5:d:125:VAL:HG23	5:d:235:ALA:HB3	1.97	0.46
1:t:231:VAL:O	1:t:243:LYS:NZ	2.40	0.46
1:t:235:PRO:HG2	2:u:65:LEU:HD22	1.97	0.46
1:P:224:GLN:O	1:P:228:THR:OG1	2.27	0.45
5:T:55:THR:O	5:T:55:THR:OG1	2.31	0.45
5:Y:125:VAL:HG23	5:Y:235:ALA:HB3	1.97	0.45
5:n:10:ASN:ND2	5:n:108:ARG:HH21	2.13	0.45
1:t:235:PRO:HA	1:t:241:PHE:HD1	1.81	0.45
1:A:147:TRP:CE2	3:C:7:VAL:HG23	2.50	0.45
1:K:236:ALA:HB1	2:L:12:ARG:HG3	1.98	0.45
4:N:122:LEU:HB2	4:N:132:VAL:HG23	1.98	0.45
1:P:234:ARG:HD2	2:Q:10:TYR:CE1	2.52	0.45
4:X:149:ASP:HB3	4:X:152:VAL:HG12	1.97	0.45
1:Z:9:TYR:HB2	1:Z:97:ILE:HB	1.97	0.45
5:d:86:THR:HG23	5:d:110:THR:HA	1.97	0.45
1:j:224:GLN:O	1:j:228:THR:OG1	2.26	0.45
4:w:137:ASP:OD1	5:x:193:ARG:NH1	2.45	0.45
1:o:230:LEU:HD11	1:o:243:LYS:HE3	1.98	0.45
1:A:28:VAL:HG23	1:A:33:PHE:CE1	2.52	0.45
5:J:199:TRP:HE3	5:J:206:PHE:HE2	1.65	0.45
1:t:9:TYR:CE2	1:t:70:GLN:HG2	2.52	0.45
4:r:132:VAL:HG12	4:r:175:TRP:CB	2.47	0.45
1:F:206:LEU:HD13	1:F:242:GLN:HG2	1.98	0.45
1:P:33:PHE:CD2	1:P:34:VAL:HG13	2.51	0.45
5:n:11:LYS:HA	5:n:11:LYS:HD2	1.60	0.45
1:t:147:TRP:HZ2	3:v:9:LYS:HG3	1.79	0.45
4:r:46:MET:HE2	4:r:46:MET:HB3	1.84	0.45
1:A:147:TRP:NE1	3:C:7:VAL:HG23	2.32	0.45
4:S:18:MET:HE3	4:S:77:ARG:HG2	1.99	0.45
5:i:6:GLN:HB2	5:i:105:PRO:HG2	1.98	0.45
4:w:122:LEU:HB3	5:x:126:PHE:HB3	1.98	0.45
1:U:191:HIS:HE1	1:U:193:PRO:HG3	1.80	0.45
5:E:170:THR:HG23	5:E:190:SER:HB2	1.98	0.45
1:F:173:GLU:O	1:F:176:LYS:HG3	2.17	0.45
1:Z:73:THR:HG21	3:b:6:GLY:HA3	1.99	0.45
4:c:124:ASP:HB3	4:c:127:SER:O	2.16	0.45
1:e:202:ARG:HG2	1:e:246:ALA:HB2	1.97	0.45
1:j:235:PRO:HG2	2:k:65:LEU:HD22	1.98	0.45
4:N:126:LYS:HD2	5:O:124:ALA:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:125:VAL:HG23	5:T:235:ALA:HB3	1.99	0.45
1:e:163:ARG:HE	4:h:31:ASP:HB3	1.81	0.45
5:n:18:LYS:HA	5:n:78:LEU:O	2.17	0.45
4:r:48:MET:HE3	4:r:61:PHE:HB2	1.98	0.45
2:p:96:ASP:HB3	2:p:99:MET:HB3	1.99	0.45
4:I:18:MET:HE3	4:I:18:MET:HB2	1.78	0.45
1:P:143:THR:HG23	3:R:9:LYS:HA	1.99	0.45
1:U:249:VAL:HG12	1:U:257:TYR:CD2	2.52	0.45
1:e:62:GLN:HG3	1:e:63:GLU:N	2.32	0.45
4:m:149:ASP:HB3	4:m:152:VAL:HG12	1.98	0.45
1:o:202:ARG:HG2	1:o:246:ALA:HB2	1.99	0.44
4:D:5:GLN:HE22	4:D:26:SER:HB3	1.81	0.44
1:F:189:MET:HE3	1:F:272:LEU:HB3	1.99	0.44
1:t:65:ARG:NH2	4:w:95:ASN:CG	2.75	0.44
1:A:249:VAL:HG21	1:A:254:GLU:HG3	1.98	0.44
1:U:163:ARG:HG2	3:W:1:VAL:HG21	2.00	0.44
1:j:5:MET:HB2	1:j:168:LEU:HG	1.99	0.44
5:s:176:LYS:HG2	5:s:186:TYR:CE1	2.52	0.44
1:K:235:PRO:HA	1:K:241:PHE:HD1	1.81	0.44
4:S:167:PHE:HE2	4:S:169:SER:HB3	1.81	0.44
4:c:137:ASP:OD1	5:d:193:ARG:NH1	2.42	0.44
1:e:163:ARG:NH2	4:h:93:ASP:O	2.37	0.44
5:O:171:ASP:OD2	5:O:189:SER:OG	2.27	0.44
1:P:196:ASP:N	1:P:196:ASP:OD1	2.44	0.44
4:S:137:ASP:OD1	5:T:193:ARG:NH1	2.40	0.44
5:T:25:GLN:HB3	5:T:32:MET:HE3	2.00	0.44
1:U:147:TRP:CZ2	3:W:9:LYS:HG3	2.52	0.44
5:Y:108:ARG:HE	5:Y:152:HIS:CB	2.30	0.44
4:c:154:ILE:HG12	4:c:174:ALA:HB2	1.98	0.44
1:t:11:SER:HA	1:t:21:ARG:O	2.17	0.44
5:E:80:LEU:HD23	5:E:80:LEU:HA	1.88	0.44
4:S:8:PRO:HB3	4:w:11:LEU:HD21	1.99	0.44
4:X:112:ILE:HG13	4:X:139:ASP:HA	1.99	0.44
4:c:79:SER:HB3	4:c:108:ILE:HD13	2.00	0.44
1:e:51:TRP:HD1	1:e:178:THR:HG21	1.81	0.44
5:n:36:ARG:NH2	5:n:87:SER:HB3	2.30	0.44
1:t:224:GLN:O	1:t:228:THR:OG1	2.26	0.44
1:A:253:GLU:O	1:A:254:GLU:C	2.60	0.44
1:F:147:TRP:CE2	3:H:7:VAL:HG23	2.53	0.44
4:N:35:TRP:HE1	4:N:72:THR:HG22	1.82	0.44
4:X:124:ASP:HA	5:Y:126:PHE:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:115:LEU:HD22	5:Y:215:LEU:HD21	2.00	0.44
1:j:97:ILE:HD11	3:l:9:LYS:HZ3	1.82	0.44
5:x:151:ASP:HB3	5:x:186:TYR:CE2	2.53	0.44
1:o:147:TRP:NE1	3:q:7:VAL:HG23	2.33	0.44
5:T:44:ARG:HG3	5:T:44:ARG:HH11	1.82	0.44
2:k:13:HIS:O	2:k:21:ASN:ND2	2.49	0.44
5:n:82:THR:O	5:n:85:GLN:N	2.47	0.44
5:O:151:ASP:OD1	5:O:152:HIS:N	2.51	0.44
5:T:115:LEU:HD22	5:T:215:LEU:HD21	1.99	0.44
4:X:6:GLN:HG2	4:X:23:CYS:HB2	2.00	0.44
5:Y:44:ARG:HG3	5:Y:44:ARG:NH1	2.32	0.44
5:n:125:VAL:HG23	5:n:235:ALA:HB3	1.99	0.44
5:s:167:GLY:O	5:s:192:LEU:HA	2.18	0.44
4:c:160:LEU:HD13	5:d:193:ARG:HG3	2.00	0.44
5:s:21:LEU:CD2	5:s:107:THR:HG21	2.48	0.43
5:s:115:LEU:HD22	5:s:215:LEU:HD21	1.99	0.43
1:P:111:ARG:HB3	1:P:111:ARG:CZ	2.47	0.43
4:X:8:PRO:HG3	4:X:11:LEU:HD12	1.99	0.43
4:h:191:ILE:O	4:h:191:ILE:HG13	2.18	0.43
1:A:141:GLN:HG3	1:j:193:PRO:HD2	2.00	0.43
5:E:27:ASN:OD1	5:E:27:ASN:N	2.51	0.43
5:E:64:TYR:C	5:E:65:LYS:HD3	2.43	0.43
5:O:151:ASP:HB3	5:O:186:TYR:CE2	2.53	0.43
5:T:26:THR:HG22	5:T:26:THR:O	2.18	0.43
5:i:115:LEU:HD22	5:i:215:LEU:HD21	2.00	0.43
1:o:85:TYR:OH	1:o:137:ASP:OD2	2.37	0.43
1:o:193:PRO:HD2	1:U:141:GLN:CG	2.48	0.43
2:p:24:ASN:HB3	2:p:65:LEU:HD11	1.99	0.43
1:K:189:MET:HE3	1:K:272:LEU:HB3	2.00	0.43
1:K:235:PRO:O	2:L:10:TYR:OH	2.28	0.43
4:m:135:PHE:HB2	4:m:187:PHE:CE2	2.53	0.43
5:n:128:PRO:HG2	5:n:139:ALA:HB1	2.00	0.43
5:n:151:ASP:HB3	5:n:186:TYR:CE2	2.53	0.43
1:o:143:THR:HG23	3:q:9:LYS:HA	2.00	0.43
1:o:231:VAL:HB	2:p:8:GLN:HE22	1.83	0.43
1:P:230:LEU:HD11	1:P:243:LYS:HE3	2.01	0.43
1:o:78:LEU:HD23	1:o:78:LEU:HA	1.68	0.43
1:o:249:VAL:HG12	1:o:257:TYR:CD2	2.53	0.43
5:J:127:GLU:OE1	5:J:240:ARG:NH2	2.50	0.43
1:P:6:ARG:HH11	1:P:6:ARG:HG2	1.83	0.43
1:Z:13:SER:HB3	1:Z:78:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:i:31:ASN:HD22	5:i:50:TYR:HD1	1.67	0.43
5:i:78:LEU:HD23	5:i:85:GLN:OE1	2.17	0.43
1:F:5:MET:HE1	1:F:171:TYR:HE2	1.84	0.43
5:T:127:GLU:OE1	5:T:240:ARG:NH2	2.51	0.43
4:m:137:ASP:OD1	5:n:193:ARG:NH1	2.42	0.43
5:s:126:PHE:HE2	5:s:144:LEU:HD12	1.83	0.43
1:F:22:PHE:HE2	1:F:67:VAL:HG22	1.82	0.43
5:Y:121:PRO:HB3	5:Y:148:PHE:HB3	2.01	0.43
5:Y:151:ASP:OD1	5:Y:152:HIS:N	2.52	0.43
1:e:68:LYS:O	1:e:71:SER:OG	2.27	0.43
2:f:5:PRO:HB3	2:f:30:PHE:HB3	2.01	0.43
1:j:234:ARG:HD2	2:k:10:TYR:CE1	2.54	0.43
1:o:81:LEU:HD12	1:o:95:ILE:HD11	2.00	0.43
4:r:73:SER:HG	4:r:75:HIS:CE1	2.36	0.43
4:I:119:VAL:HA	4:I:134:LEU:O	2.19	0.43
1:K:163:ARG:HE	4:N:31:ASP:CG	2.26	0.43
1:Z:9:TYR:CE2	1:Z:70:GLN:HG2	2.54	0.43
1:j:193:PRO:HA	1:j:199:ALA:HA	2.00	0.43
1:j:231:VAL:HG22	1:j:244:TRP:O	2.19	0.43
1:t:35:ARG:HD3	2:u:53:ASP:CG	2.43	0.43
4:r:34:TRP:HB2	4:r:90:ALA:HB3	2.00	0.43
1:j:116:ASP:HB2	1:j:124:ILE:HG22	2.01	0.43
1:t:35:ARG:HD3	2:u:53:ASP:OD2	2.18	0.43
1:t:202:ARG:NH1	2:u:98:ASP:O	2.52	0.43
4:w:129:ASP:OD1	4:w:130:LYS:N	2.52	0.43
1:K:9:TYR:HB2	1:K:97:ILE:HB	1.99	0.43
5:T:36:ARG:HB2	5:T:46:ILE:HD11	2.00	0.43
4:m:112:ILE:HG13	4:m:139:ASP:HA	2.00	0.43
5:n:36:ARG:HG3	5:n:38:ASP:OD1	2.19	0.43
5:s:120:PRO:HD3	5:s:228:PRO:HB3	2.01	0.42
5:J:36:ARG:HB2	5:J:46:ILE:HD11	2.00	0.42
5:O:151:ASP:HB3	5:O:186:TYR:HE2	1.83	0.42
1:P:176:LYS:HA	1:P:180:GLN:HG3	1.99	0.42
4:S:125:SER:O	4:S:126:LYS:C	2.62	0.42
5:T:6:GLN:HB2	5:T:105:PRO:HG2	2.01	0.42
5:T:132:GLU:OE2	5:T:140:THR:OG1	2.27	0.42
5:x:18:LYS:HG2	5:x:79:GLU:HA	2.00	0.42
4:r:129:ASP:HB3	4:r:130:LYS:H	1.64	0.42
2:f:37:VAL:HG22	2:f:82:VAL:HG22	2.01	0.42
1:t:176:LYS:HE3	1:t:176:LYS:HB2	1.76	0.42
4:D:146:GLN:HG3	4:D:147:SER:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:126:PHE:HE2	5:O:144:LEU:HD12	1.84	0.42
4:S:46:MET:HE2	4:S:46:MET:HB3	1.96	0.42
5:d:160:ASN:HA	5:d:205:HIS:HB3	2.01	0.42
4:h:34:TRP:HB2	4:h:90:ALA:HB3	2.02	0.42
5:n:115:LEU:HD22	5:n:215:LEU:HD21	2.02	0.42
1:t:234:ARG:HD2	2:u:10:TYR:CE1	2.53	0.42
1:A:129:ASP:O	1:A:131:ARG:HG3	2.19	0.42
1:K:211:ALA:HA	1:K:241:PHE:HD2	1.84	0.42
4:N:13:VAL:CG2	4:c:7:SER:HB2	2.49	0.42
1:j:135:ALA:HB1	1:j:140:ALA:HB3	2.00	0.42
1:j:249:VAL:HG12	1:j:257:TYR:CE2	2.53	0.42
5:n:189:SER:OG	5:n:191:ARG:NH1	2.53	0.42
2:G:95:TRP:CZ2	2:G:97:ARG:HG2	2.54	0.42
1:e:108:ARG:HA	1:e:108:ARG:HD3	1.69	0.42
5:n:65:LYS:HB2	5:n:77:ILE:HB	2.01	0.42
4:D:11:LEU:HA	4:D:11:LEU:HD23	1.82	0.42
4:r:7:SER:HB2	4:D:13:VAL:HG23	2.02	0.42
1:e:28:VAL:HG23	1:e:33:PHE:CE1	2.55	0.42
5:s:36:ARG:HB2	5:s:46:ILE:HD11	2.02	0.42
1:P:147:TRP:HE1	3:R:9:LYS:N	2.13	0.42
5:T:203:ARG:H	5:T:203:ARG:HG2	1.64	0.42
4:c:8:PRO:HG3	4:c:11:LEU:HD12	2.00	0.42
4:D:18:MET:HE3	4:D:18:MET:HB2	1.89	0.42
5:d:82:THR:OG1	5:d:85:GLN:HG3	2.20	0.42
5:d:115:LEU:HD22	5:d:215:LEU:HD21	2.01	0.42
1:e:235:PRO:HG2	2:f:65:LEU:HD22	2.01	0.42
1:j:196:ASP:OD1	1:j:196:ASP:N	2.46	0.42
1:Z:12:VAL:HG11	2:a:33:SER:OG	2.20	0.42
1:j:159:TYR:CD1	3:l:3:GLY:HA3	2.55	0.42
2:u:96:ASP:HB3	2:u:99:MET:HB3	2.02	0.42
1:K:11:SER:HA	1:K:21:ARG:O	2.19	0.41
2:u:5:PRO:HB3	2:u:30:PHE:HB3	2.01	0.41
5:T:189:SER:OG	5:T:191:ARG:NH1	2.53	0.41
1:e:234:ARG:HD2	2:f:10:TYR:CE1	2.55	0.41
2:f:96:ASP:HB3	2:f:99:MET:HB3	2.02	0.41
1:j:51:TRP:CD1	1:j:178:THR:HG1	2.38	0.41
1:j:206:LEU:HD13	1:j:242:GLN:HG2	2.02	0.41
4:m:160:LEU:HD13	5:n:193:ARG:HG3	2.03	0.41
5:x:44:ARG:HH21	5:x:60:ILE:HD13	1.85	0.41
2:p:95:TRP:CZ2	2:p:97:ARG:HG2	2.54	0.41
4:D:184:ALA:HA	4:D:198:PHE:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:6:GLN:HB2	5:E:105:PRO:HG2	2.01	0.41
1:P:6:ARG:HG2	1:P:6:ARG:NH1	2.35	0.41
1:U:52:ILE:HD12	1:U:52:ILE:HA	1.95	0.41
1:j:9:TYR:CE2	1:j:70:GLN:HG2	2.55	0.41
5:n:112:LEU:HD11	5:n:149:TYR:HE2	1.85	0.41
5:n:199:TRP:HE3	5:n:206:PHE:HE2	1.67	0.41
5:n:201:ASN:HB2	5:n:204:ASN:ND2	2.35	0.41
1:K:147:TRP:CE2	3:M:7:VAL:HG23	2.55	0.41
4:S:56:LYS:HB3	4:S:63:VAL:HG23	2.02	0.41
4:c:39:HIS:ND1	4:c:85:ALA:HB2	2.35	0.41
4:w:93:ASP:O	4:w:94:SER:C	2.64	0.41
1:K:163:ARG:HH12	4:N:94:SER:HA	1.84	0.41
5:Y:88:VAL:HG22	5:Y:108:ARG:HG3	2.03	0.41
2:a:51:HIS:HB2	2:a:66:TYR:CE1	2.55	0.41
5:d:189:SER:OG	5:d:191:ARG:NH1	2.46	0.41
4:m:34:TRP:HB2	4:m:90:ALA:HB3	2.02	0.41
1:A:51:TRP:CD1	1:A:178:THR:HG1	2.38	0.41
1:A:98:MET:HE3	1:A:98:MET:HB3	1.83	0.41
1:P:8:PHE:HB2	1:P:25:VAL:HG23	2.03	0.41
1:j:214:THR:HB	1:j:262:GLN:HB2	2.03	0.41
5:n:86:THR:HG22	5:n:111:VAL:N	2.27	0.41
5:E:64:TYR:CZ	5:E:85:GLN:HG2	2.56	0.41
1:F:220:ASP:OD2	1:F:256:ARG:NE	2.43	0.41
4:I:157:LYS:HD2	4:I:170:ASN:HD22	1.86	0.41
5:J:32:MET:HE2	5:J:74:PHE:CB	2.51	0.41
1:K:14:ARG:HB3	1:K:17:ARG:HB2	2.02	0.41
1:K:194:ILE:HD11	1:K:198:GLU:HB3	2.03	0.41
5:O:189:SER:OG	5:O:191:ARG:NH1	2.53	0.41
1:P:5:MET:HB2	1:P:168:LEU:HG	2.01	0.41
1:P:68:LYS:O	1:P:71:SER:OG	2.32	0.41
5:i:28:ASN:ND2	5:i:28:ASN:O	2.53	0.41
1:o:147:TRP:CE2	3:q:7:VAL:HG23	2.56	0.41
5:J:24:ASN:HA	5:J:72:GLU:O	2.21	0.41
4:N:7:SER:HB2	4:c:13:VAL:HG23	2.02	0.41
4:h:198:PHE:HA	4:h:199:PRO:HD3	1.94	0.41
5:i:199:TRP:HE3	5:i:206:PHE:HE2	1.68	0.41
5:i:205:HIS:CE1	5:i:207:ARG:HB2	2.56	0.41
5:n:15:THR:C	5:n:17:GLY:H	2.29	0.41
1:t:147:TRP:CE2	3:v:7:VAL:HG23	2.56	0.41
4:w:50:ILE:HG23	4:w:65:LEU:HD22	2.03	0.41
1:A:8:PHE:HB2	1:A:25:VAL:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LYS:HB2	1:A:176:LYS:HE2	1.79	0.41
5:J:149:TYR:CD1	5:J:150:PRO:HA	2.56	0.41
1:K:23:ILE:HG21	2:L:54:LEU:HB3	2.01	0.41
4:N:18:MET:HE3	4:N:18:MET:HB2	1.78	0.41
4:S:11:LEU:HD23	4:S:11:LEU:HA	1.83	0.41
5:d:160:ASN:OD1	5:d:204:ASN:HA	2.21	0.41
1:e:5:MET:HB2	1:e:168:LEU:HG	2.02	0.41
1:j:97:ILE:HD11	3:l:9:LYS:NZ	2.35	0.41
5:x:151:ASP:HB3	5:x:186:TYR:HE2	1.85	0.41
5:s:121:PRO:HB3	5:s:148:PHE:HB3	2.03	0.41
5:s:199:TRP:HE3	5:s:206:PHE:HE2	1.69	0.41
4:D:28:ARG:HA	4:D:70:LEU:HD11	2.03	0.41
1:K:78:LEU:HD23	1:K:78:LEU:HA	1.76	0.41
1:P:98:MET:HB3	1:P:98:MET:HE3	1.81	0.41
4:m:167:PHE:CE2	4:m:169:SER:HB3	2.56	0.41
1:t:249:VAL:HG12	1:t:257:TYR:CE2	2.56	0.41
4:D:198:PHE:HA	4:D:199:PRO:HD3	1.93	0.40
2:G:24:ASN:HB3	2:G:65:LEU:HD11	2.02	0.40
5:O:32:MET:HE2	5:O:32:MET:HB3	2.00	0.40
4:X:8:PRO:HB3	4:m:11:LEU:HD21	2.01	0.40
1:e:99:TYR:CE1	3:g:4:ALA:HB2	2.55	0.40
4:r:121:GLN:O	5:s:129:SER:HB2	2.22	0.40
1:A:51:TRP:CZ2	1:A:179:LEU:HD11	2.57	0.40
1:K:65:ARG:HE	4:N:95:ASN:ND2	2.19	0.40
5:O:8:PRO:HD2	5:O:21:LEU:HA	2.03	0.40
5:d:133:ILE:HG23	5:d:196:ALA:HB1	2.03	0.40
1:j:159:TYR:CE1	3:l:3:GLY:HA3	2.56	0.40
2:B:12:ARG:HB2	2:B:22:PHE:HB2	2.04	0.40
1:F:192:HIS:O	1:F:200:THR:OG1	2.38	0.40
1:F:231:VAL:HB	2:G:8:GLN:HE22	1.86	0.40
2:G:97:ARG:H	2:G:97:ARG:HG3	1.71	0.40
5:J:56:GLU:HG3	5:J:57:LYS:N	2.35	0.40
1:K:202:ARG:HD3	1:K:244:TRP:CE3	2.55	0.40
4:N:8:PRO:HB3	4:c:11:LEU:HD21	2.01	0.40
5:O:153:VAL:HG12	5:O:212:PHE:HA	2.03	0.40
5:n:13:ALA:HB3	5:n:111:VAL:HA	2.02	0.40
5:x:158:TRP:NE1	5:x:209:GLN:OE1	2.54	0.40
5:x:189:SER:OG	5:x:191:ARG:NH1	2.53	0.40
1:A:176:LYS:HA	1:A:180:GLN:HG3	2.02	0.40
1:F:229:GLU:HB3	1:F:246:ALA:HB3	2.03	0.40
1:K:117:ALA:HB2	2:L:60:TRP:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:24:ASN:HA	5:T:72:GLU:O	2.21	0.40
1:Z:11:SER:HA	1:Z:21:ARG:O	2.21	0.40
5:d:44:ARG:HE	5:d:44:ARG:HB2	1.75	0.40
1:t:22:PHE:HE2	1:t:67:VAL:HG22	1.87	0.40
1:o:121:LYS:HE2	1:o:121:LYS:HB2	1.91	0.40
4:r:124:ASP:HA	5:s:126:PHE:HD1	1.87	0.40
5:s:128:PRO:HD2	5:s:199:TRP:CZ2	2.57	0.40
5:O:196:ALA:O	5:O:200:GLN:HG3	2.20	0.40
1:P:62:GLN:HG3	1:P:63:GLU:N	2.36	0.40
4:S:11:LEU:HD12	4:S:21:LEU:HD23	2.03	0.40
4:X:21:LEU:CD2	4:X:104:THR:HG21	2.49	0.40
5:i:152:HIS:CD2	5:i:213:TYR:HB2	2.57	0.40
2:u:37:VAL:HG22	2:u:82:VAL:HG22	2.03	0.40

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	272/275 (99%)	262 (96%)	10 (4%)	0	100	100
1	F	272/275 (99%)	261 (96%)	11 (4%)	0	100	100
1	K	272/275 (99%)	264 (97%)	8 (3%)	0	100	100
1	P	272/275 (99%)	260 (96%)	12 (4%)	0	100	100
1	U	272/275 (99%)	262 (96%)	10 (4%)	0	100	100
1	Z	228/275 (83%)	218 (96%)	10 (4%)	0	100	100
1	e	235/275 (86%)	223 (95%)	12 (5%)	0	100	100
1	j	272/275 (99%)	264 (97%)	8 (3%)	0	100	100
1	o	272/275 (99%)	261 (96%)	11 (4%)	0	100	100
1	t	272/275 (99%)	263 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	G	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	L	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	Q	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
2	V	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
2	a	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	f	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
2	k	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
2	p	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	u	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
3	C	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	H	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	M	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	R	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	W	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	b	7/9 (78%)	4 (57%)	3 (43%)	0	100	100
3	g	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	l	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	q	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	v	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	197/204 (97%)	187 (95%)	7 (4%)	3 (2%)	8	38
4	I	196/204 (96%)	192 (98%)	4 (2%)	0	100	100
4	N	196/204 (96%)	188 (96%)	7 (4%)	1 (0%)	25	59
4	S	196/204 (96%)	188 (96%)	6 (3%)	2 (1%)	13	46
4	X	196/204 (96%)	190 (97%)	6 (3%)	0	100	100
4	c	196/204 (96%)	189 (96%)	6 (3%)	1 (0%)	25	59
4	h	196/204 (96%)	190 (97%)	4 (2%)	2 (1%)	13	46
4	m	196/204 (96%)	191 (97%)	5 (3%)	0	100	100
4	r	196/204 (96%)	181 (92%)	13 (7%)	2 (1%)	13	46
4	w	196/204 (96%)	188 (96%)	7 (4%)	1 (0%)	25	59
5	E	240/242 (99%)	229 (95%)	10 (4%)	1 (0%)	30	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	J	240/242 (99%)	230 (96%)	10 (4%)	0	100	100
5	O	240/242 (99%)	235 (98%)	5 (2%)	0	100	100
5	T	239/242 (99%)	231 (97%)	8 (3%)	0	100	100
5	Y	237/242 (98%)	231 (98%)	5 (2%)	1 (0%)	30	64
5	d	235/242 (97%)	226 (96%)	8 (3%)	1 (0%)	30	64
5	i	239/242 (99%)	233 (98%)	5 (2%)	1 (0%)	30	64
5	n	239/242 (99%)	228 (95%)	11 (5%)	0	100	100
5	s	240/242 (99%)	232 (97%)	7 (3%)	1 (0%)	30	64
5	x	239/242 (99%)	232 (97%)	7 (3%)	0	100	100
All	All	8033/8300 (97%)	7727 (96%)	289 (4%)	17 (0%)	44	76

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	125	SER
4	h	126	LYS
4	w	96	TYR
4	S	127	SER
4	r	95	ASN
4	D	95	ASN
4	D	130	LYS
4	S	95	ASN
5	Y	97	GLY
4	h	95	ASN
4	N	96	TYR
4	c	95	ASN
5	i	97	GLY
4	r	193	PRO
5	s	97	GLY
5	d	97	GLY
5	E	97	GLY

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	231/232 (100%)	231 (100%)	0	100 100
1	F	231/232 (100%)	231 (100%)	0	100 100
1	K	231/232 (100%)	231 (100%)	0	100 100
1	P	231/232 (100%)	230 (100%)	1 (0%)	89 94
1	U	231/232 (100%)	231 (100%)	0	100 100
1	Z	197/232 (85%)	197 (100%)	0	100 100
1	e	203/232 (88%)	203 (100%)	0	100 100
1	j	231/232 (100%)	231 (100%)	0	100 100
1	o	231/232 (100%)	231 (100%)	0	100 100
1	t	231/232 (100%)	231 (100%)	0	100 100
2	B	95/95 (100%)	95 (100%)	0	100 100
2	G	95/95 (100%)	95 (100%)	0	100 100
2	L	95/95 (100%)	95 (100%)	0	100 100
2	Q	94/95 (99%)	94 (100%)	0	100 100
2	V	94/95 (99%)	94 (100%)	0	100 100
2	a	95/95 (100%)	95 (100%)	0	100 100
2	f	94/95 (99%)	94 (100%)	0	100 100
2	k	94/95 (99%)	94 (100%)	0	100 100
2	p	95/95 (100%)	95 (100%)	0	100 100
2	u	94/95 (99%)	94 (100%)	0	100 100
3	C	5/5 (100%)	5 (100%)	0	100 100
3	H	5/5 (100%)	5 (100%)	0	100 100
3	M	5/5 (100%)	5 (100%)	0	100 100
3	R	5/5 (100%)	5 (100%)	0	100 100
3	W	5/5 (100%)	5 (100%)	0	100 100
3	b	5/5 (100%)	5 (100%)	0	100 100
3	g	5/5 (100%)	5 (100%)	0	100 100
3	l	5/5 (100%)	5 (100%)	0	100 100
3	q	5/5 (100%)	5 (100%)	0	100 100
3	v	5/5 (100%)	5 (100%)	0	100 100
4	D	181/186 (97%)	178 (98%)	3 (2%)	56 75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	I	180/186 (97%)	180 (100%)	0	100 100
4	N	180/186 (97%)	180 (100%)	0	100 100
4	S	180/186 (97%)	174 (97%)	6 (3%)	33 62
4	X	180/186 (97%)	179 (99%)	1 (1%)	84 91
4	c	180/186 (97%)	180 (100%)	0	100 100
4	h	180/186 (97%)	180 (100%)	0	100 100
4	m	180/186 (97%)	179 (99%)	1 (1%)	84 91
4	r	180/186 (97%)	176 (98%)	4 (2%)	47 71
4	w	180/186 (97%)	179 (99%)	1 (1%)	84 91
5	E	206/206 (100%)	204 (99%)	2 (1%)	73 84
5	J	206/206 (100%)	206 (100%)	0	100 100
5	O	206/206 (100%)	206 (100%)	0	100 100
5	T	205/206 (100%)	203 (99%)	2 (1%)	73 84
5	Y	204/206 (99%)	203 (100%)	1 (0%)	86 92
5	d	203/206 (98%)	202 (100%)	1 (0%)	86 92
5	i	205/206 (100%)	205 (100%)	0	100 100
5	n	205/206 (100%)	201 (98%)	4 (2%)	50 73
5	s	206/206 (100%)	206 (100%)	0	100 100
5	x	205/206 (100%)	204 (100%)	1 (0%)	86 92
All	All	7095/7240 (98%)	7067 (100%)	28 (0%)	89 94

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	r	23	CYS
4	r	191	ILE
4	r	195	ASP
4	r	196	THR
4	D	23	CYS
4	D	159	VAL
4	D	183	CYS
5	E	168	VAL
5	E	169	CYS
1	P	137	ASP
4	S	23	CYS

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Mol	Chain	Res	Type
4	S	122	LEU
4	S	123	ARG
4	S	124	ASP
4	S	129	ASP
4	S	130	LYS
5	T	200	GLN
5	T	203	ARG
4	X	23	CYS
5	Y	91	CYS
5	d	200	GLN
4	m	23	CYS
5	n	11	LYS
5	n	14	VAL
5	n	21	LEU
5	n	91	CYS
4	w	23	CYS
5	x	91	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	o	32	GLN
1	o	93	HIS
1	o	127	ASN
1	o	141	GLN
1	o	151	HIS
1	o	155	GLN
1	o	180	GLN
4	r	2	GLN
4	r	22	ASN
4	r	113	GLN
5	s	73	ASN
5	s	173	GLN
1	A	93	HIS
1	A	127	ASN
1	A	141	GLN
1	A	151	HIS
1	A	188	HIS
5	E	10	ASN
5	E	152	HIS
1	F	54	GLN
1	F	93	HIS

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Mol	Chain	Res	Type
1	F	151	HIS
1	F	260	HIS
4	I	22	ASN
4	I	146	GLN
5	J	24	ASN
5	J	27	ASN
5	J	41	HIS
5	J	73	ASN
5	J	173	GLN
5	J	231	GLN
1	K	93	HIS
1	K	151	HIS
4	N	2	GLN
5	O	29	HIS
5	O	173	GLN
1	P	93	HIS
1	P	96	GLN
1	P	141	GLN
1	P	151	HIS
4	S	22	ASN
4	S	64	HIS
4	S	97	GLN
5	T	6	GLN
5	T	10	ASN
5	T	24	ASN
5	T	135	HIS
5	T	173	GLN
5	T	201	ASN
5	T	204	ASN
1	U	93	HIS
1	U	141	GLN
1	U	151	HIS
1	U	155	GLN
1	U	191	HIS
2	V	31	HIS
4	X	22	ASN
4	X	29	ASN
4	X	64	HIS
4	X	80	GLN
4	X	146	GLN
5	Y	10	ASN
5	Y	27	ASN

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Mol	Chain	Res	Type
5	Y	173	GLN
1	Z	93	HIS
1	Z	141	GLN
1	Z	151	HIS
1	Z	155	GLN
1	Z	191	HIS
2	a	17	ASN
4	c	22	ASN
4	c	29	ASN
4	c	64	HIS
4	c	146	GLN
5	d	24	ASN
5	d	201	ASN
1	e	32	GLN
1	e	151	HIS
4	h	22	ASN
4	h	29	ASN
4	h	188	ASN
5	i	10	ASN
5	i	31	ASN
5	i	173	GLN
1	j	93	HIS
1	j	151	HIS
2	k	17	ASN
4	m	39	HIS
4	m	64	HIS
4	m	66	ASN
4	m	97	GLN
4	m	146	GLN
5	n	6	GLN
5	n	10	ASN
5	n	24	ASN
5	n	173	GLN
5	n	201	ASN
5	n	223	GLN
1	t	93	HIS
1	t	96	GLN
1	t	151	HIS
1	t	155	GLN
2	u	17	ASN
4	w	39	HIS
4	w	64	HIS

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Mol	Chain	Res	Type
5	x	24	ASN
5	x	28	ASN
5	x	47	HIS
5	x	173	GLN

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	274/275 (99%)	-0.15	1 (0%) 89 81	60, 88, 123, 156	0
1	F	274/275 (99%)	-0.15	3 (1%) 77 62	57, 84, 123, 154	0
1	K	274/275 (99%)	-0.16	3 (1%) 77 62	57, 85, 122, 158	0
1	P	274/275 (99%)	-0.12	0 100 100	65, 97, 131, 153	0
1	U	274/275 (99%)	-0.17	2 (0%) 84 71	61, 88, 130, 159	0
1	Z	236/275 (85%)	-0.04	4 (1%) 69 52	69, 98, 144, 169	0
1	e	243/275 (88%)	0.12	8 (3%) 49 36	69, 105, 152, 171	0
1	j	274/275 (99%)	-0.06	0 100 100	71, 94, 126, 151	0
1	o	274/275 (99%)	-0.15	1 (0%) 89 81	60, 84, 118, 150	0
1	t	274/275 (99%)	-0.11	0 100 100	67, 95, 127, 145	0
2	B	100/100 (100%)	-0.08	1 (1%) 79 64	66, 94, 131, 140	0
2	G	100/100 (100%)	-0.28	0 100 100	61, 84, 119, 133	0
2	L	100/100 (100%)	-0.13	0 100 100	62, 86, 124, 139	0
2	Q	99/100 (99%)	0.02	0 100 100	77, 110, 146, 161	0
2	V	99/100 (99%)	-0.10	0 100 100	69, 104, 147, 154	0
2	a	100/100 (100%)	0.13	2 (2%) 64 48	86, 118, 154, 165	0
2	f	99/100 (99%)	0.25	2 (2%) 64 48	88, 120, 163, 167	0
2	k	99/100 (99%)	-0.06	0 100 100	77, 101, 140, 150	0
2	p	100/100 (100%)	-0.03	1 (1%) 79 64	67, 95, 131, 143	0
2	u	99/100 (99%)	0.05	1 (1%) 79 64	78, 108, 144, 157	0
3	C	9/9 (100%)	0.48	0 100 100	71, 76, 79, 80	0
3	H	9/9 (100%)	0.30	0 100 100	66, 72, 82, 86	0
3	M	9/9 (100%)	0.33	0 100 100	65, 69, 85, 90	0
3	R	9/9 (100%)	0.70	0 100 100	74, 81, 96, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
3	W	9/9 (100%)	0.45	0	100	100	72, 75, 84, 93	0
3	b	9/9 (100%)	0.49	0	100	100	77, 83, 89, 95	0
3	g	9/9 (100%)	0.71	0	100	100	82, 89, 98, 107	0
3	l	9/9 (100%)	0.79	0	100	100	81, 84, 92, 93	0
3	q	9/9 (100%)	0.65	0	100	100	69, 73, 79, 82	0
3	v	9/9 (100%)	0.94	1 (11%)	12	11	80, 85, 100, 104	0
4	D	199/204 (97%)	0.05	3 (1%)	71	55	52, 89, 146, 163	0
4	I	198/204 (97%)	0.07	3 (1%)	71	55	57, 95, 149, 165	0
4	N	198/204 (97%)	0.27	7 (3%)	47	35	62, 95, 153, 162	0
4	S	198/204 (97%)	0.33	7 (3%)	47	35	68, 103, 170, 183	0
4	X	198/204 (97%)	0.29	10 (5%)	34	27	66, 99, 184, 201	0
4	c	198/204 (97%)	0.25	7 (3%)	47	35	63, 101, 170, 203	0
4	h	198/204 (97%)	0.26	6 (3%)	52	39	66, 102, 162, 168	0
4	m	198/204 (97%)	0.31	6 (3%)	52	39	66, 108, 195, 219	0
4	r	198/204 (97%)	0.16	5 (2%)	58	43	55, 91, 147, 162	0
4	w	198/204 (97%)	0.36	7 (3%)	47	35	71, 109, 186, 211	0
5	E	242/242 (100%)	-0.11	1 (0%)	89	81	59, 88, 126, 143	0
5	J	242/242 (100%)	0.13	2 (0%)	82	69	68, 98, 148, 165	0
5	O	242/242 (100%)	0.18	2 (0%)	82	69	65, 97, 147, 164	0
5	T	241/242 (99%)	0.10	3 (1%)	76	60	73, 109, 146, 161	0
5	Y	239/242 (98%)	0.18	2 (0%)	82	69	69, 112, 164, 173	0
5	d	237/242 (97%)	0.27	5 (2%)	63	47	69, 110, 159, 170	0
5	i	241/242 (99%)	0.10	2 (0%)	82	69	72, 101, 143, 172	0
5	n	241/242 (99%)	0.49	6 (2%)	58	43	84, 162, 200, 208	0
5	s	242/242 (100%)	-0.00	3 (1%)	76	60	60, 88, 132, 160	0
5	x	241/242 (99%)	0.50	10 (4%)	42	31	87, 155, 192, 201	0
All	All	8145/8300 (98%)	0.08	127 (1%)	70	54	52, 98, 166, 219	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	245	ALA	4.5
5	x	97	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	K	225	THR	3.7
2	a	99	MET	3.6
1	e	247	VAL	3.5
5	d	239	GLY	3.4
5	n	71	GLN	3.4
2	p	0	MET	3.4
4	c	191	ILE	3.4
5	i	50	TYR	3.3
1	F	225	THR	3.3
4	S	131	SER	3.3
1	U	19	GLU	3.2
4	N	167	PHE	3.2
4	c	130	LYS	3.1
4	w	130	LYS	3.1
4	N	199	PRO	3.1
4	X	199	PRO	3.0
4	X	133	CYS	3.0
4	h	133	CYS	3.0
4	m	130	LYS	2.9
5	x	125	VAL	2.9
4	D	183	CYS	2.9
4	X	183	CYS	2.9
5	x	2	ALA	2.9
4	m	131	SER	2.9
4	S	130	LYS	2.8
4	S	199	PRO	2.8
2	f	1	ILE	2.8
5	x	50	TYR	2.8
4	r	130	LYS	2.8
1	e	217	TRP	2.8
1	e	19	GLU	2.8
5	J	97	GLY	2.8
5	d	97	GLY	2.8
4	D	191	ILE	2.8
4	h	187	PHE	2.8
4	w	183	CYS	2.7
5	Y	97	GLY	2.7
5	x	214	GLY	2.7
1	o	225	THR	2.7
5	s	97	GLY	2.6
4	S	153	TYR	2.6
4	m	199	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
5	J	230	THR	2.5
1	F	90	ASP	2.5
4	S	187	PHE	2.5
4	c	97	GLN	2.5
5	x	157	TRP	2.5
5	s	241	ALA	2.5
4	w	191	ILE	2.5
5	x	166	SER	2.5
5	d	217	GLU	2.5
4	c	176	SER	2.5
5	n	96	PHE	2.4
4	S	125	SER	2.4
5	x	142	VAL	2.4
5	s	95	ASP	2.4
5	T	128	PRO	2.4
4	X	187	PHE	2.4
5	O	97	GLY	2.4
1	Z	113	TYR	2.4
4	r	199	PRO	2.4
4	w	131	SER	2.4
5	O	151	ASP	2.4
1	e	194	ILE	2.4
4	r	129	ASP	2.4
4	X	184	ALA	2.4
1	e	259	CYS	2.3
3	v	6	GLY	2.3
5	E	168	VAL	2.3
4	N	129	ASP	2.3
4	c	119	VAL	2.3
5	n	121	PRO	2.3
2	a	1	ILE	2.3
4	N	125	SER	2.3
1	K	90	ASP	2.3
4	r	149	ASP	2.3
4	X	149	ASP	2.3
4	m	93	ASP	2.3
5	i	114	ASP	2.3
4	I	133	CYS	2.3
4	N	183	CYS	2.3
4	D	148	LYS	2.3
1	K	230	LEU	2.3
5	Y	152	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
5	d	183	ASP	2.2
4	w	197	PHE	2.2
4	h	131	SER	2.2
5	x	129	SER	2.2
5	n	142	VAL	2.2
4	X	191	ILE	2.2
4	X	152	VAL	2.2
4	w	134	LEU	2.2
4	I	123	ARG	2.2
4	c	125	SER	2.2
4	m	155	THR	2.2
4	N	128	SER	2.2
4	c	128	SER	2.2
1	e	189	MET	2.2
1	e	271	THR	2.2
5	T	50	TYR	2.2
4	I	199	PRO	2.1
5	x	128	PRO	2.1
1	F	250	PRO	2.1
5	T	30	ASN	2.1
4	S	97	GLN	2.1
4	h	111	ASP	2.1
2	u	80	CYS	2.1
1	e	269	PRO	2.1
2	f	44	GLU	2.1
4	m	191	ILE	2.1
4	X	143	ASN	2.1
4	w	143	ASN	2.1
5	d	227	LYS	2.1
5	n	30	ASN	2.1
1	Z	270	LEU	2.1
1	Z	217	TRP	2.1
4	h	189	ASN	2.1
4	X	111	ASP	2.1
2	B	0	MET	2.1
5	n	125	VAL	2.1
1	A	257	TYR	2.0
4	r	128	SER	2.0
4	h	199	PRO	2.0
1	U	230	LEU	2.0
4	N	93	ASP	2.0

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.