



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:44 AM UTC

PDB ID : 6NCA / pdb_00006nca
Title : HLA-A2 (A*02:01) bound to a peptide from the Epstein-Barr virus BRLF1 protein
Authors : Stern, L.J.; Selin, L.K.; Song, I.Y.
Deposited on : 2018-12-11
Resolution : 3.30 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 Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

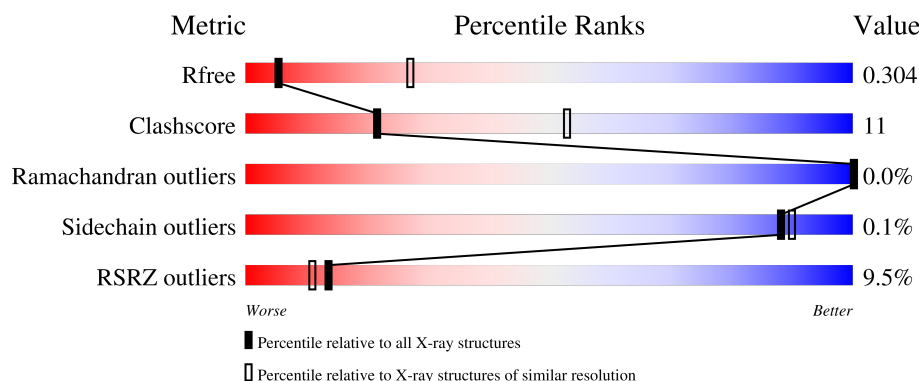
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	9	22% 56% 44%
1	2	9	67% 33%
1	3	9	33% 33% 67%
1	4	9	56% 44%
1	5	9	33% 67% 33%

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Mol	Chain	Length	Quality of chain
1	6	9	11% 78% 22%
1	7	9	44% 100%
1	8	9	22% 78% 22%
1	U	9	44% 56%
1	V	9	22% 44% 56%
1	W	9	22% 67% 33%
1	X	9	22% 44% 56%
1	Y	9	22% 89% 11%
1	Z	9	44% 56%
1	u	9	11% 67% 33%
1	v	9	11% 56% 44%
1	w	9	22% 78% 22%
1	x	9	11% 78% 22%
1	y	9	11% 78% 22%
1	z	9	11% 89% 11%
2	A	275	12% 76% 24%
2	B	275	10% 71% 29%
2	C	275	16% 67% 33%
2	D	275	6% 75% 25%
2	E	275	14% 70% 30%
2	F	275	12% 68% 32%
2	G	275	11% 65% 35%
2	H	275	8% 63% 37%
2	I	275	5% 71% 29%
2	J	275	5% 74% 26%

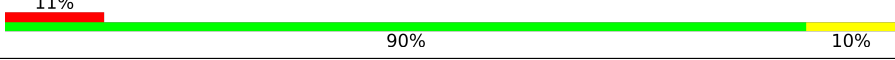
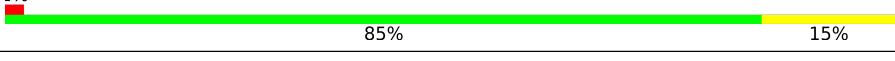
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Mol	Chain	Length	Quality of chain
2	K	275	9% 70% 30%
2	L	275	5% 73% 27%
2	M	275	9% 78% 22%
2	N	275	6% 72% 28%
2	O	275	11% 73% 27%
2	P	275	8% 65% 35%
2	Q	275	12% 73% 27%
2	R	275	12% 63% 37%
2	S	275	7% 73% 27%
2	T	275	5% 77% 23%
3	a	100	14% 80% 20%
3	b	100	3% 76% 24%
3	c	100	20% 73% 27%
3	d	100	3% 82% 18%
3	e	100	20% 85% 14%
3	f	100	16% 87% 13%
3	g	100	16% 78% 22%
3	h	100	5% 87% 13%
3	i	100	3% 88% 12%
3	j	100	3% 83% 17%
3	k	100	11% 83% 17%
3	l	100	8% 87% 12%
3	m	100	12% 86% 14%
3	n	100	2% 89% 11%
3	o	100	15% 85% 15%

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Mol	Chain	Length	Quality of chain
3	p	100	
3	q	100	
3	r	100	
3	s	100	
3	t	100	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 63200 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 Replication and transcription activator.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Y	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	u	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	z	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	y	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	8	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	w	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	4	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	3	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	W	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	6	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	x	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	5	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	X	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	v	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	2	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	U	9	Total	C	N	O	0	0	0
			76	52	11	13			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Z	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	V	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	7	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	1	9	Total	C	N	O	0	0	0
			76	52	11	13			

- Molecule 2 is a protein called HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	B	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	C	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	D	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	E	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	F	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	G	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	H	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	S	275	Total	C	N	O	S	17	0	0
			2247	1403	409	426	9			
2	J	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	K	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	L	275	Total	C	N	O	S	17	0	0
			2247	1403	409	426	9			
2	M	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	N	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	O	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	Q	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	R	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	I	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	T	275	Total	C	N	O	S	17	0	0
			2247	1403	409	426	9			

- Molecule 3 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	a	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	b	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	c	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	d	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	f	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	g	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	h	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	s	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	j	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	k	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	l	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	m	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	n	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	o	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	p	100	Total 837	C 533	N 141	O 159	S 4	5	0	0
3	q	100	Total 837	C 533	N 141	O 159	S 4	5	0	0
3	r	100	Total 837	C 533	N 141	O 159	S 4	5	0	0
3	i	100	Total 837	C 533	N 141	O 159	S 4	5	0	0
3	t	100	Total 837	C 533	N 141	O 159	S 4	5	0	0
3	e	100	Total 837	C 533	N 141	O 159	S 4	5	0	0

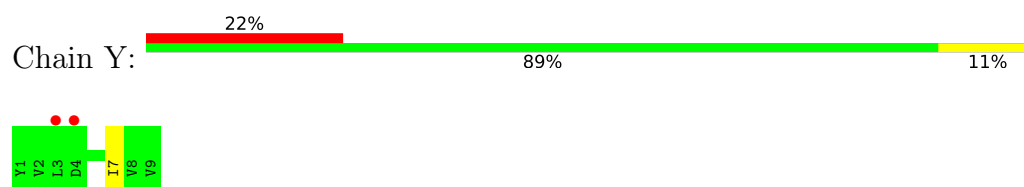
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1	MET	-	initiating methionine	UNP P61769
b	1	MET	-	initiating methionine	UNP P61769
c	1	MET	-	initiating methionine	UNP P61769
d	1	MET	-	initiating methionine	UNP P61769
f	1	MET	-	initiating methionine	UNP P61769
g	1	MET	-	initiating methionine	UNP P61769
h	1	MET	-	initiating methionine	UNP P61769
s	1	MET	-	initiating methionine	UNP P61769
j	1	MET	-	initiating methionine	UNP P61769
k	1	MET	-	initiating methionine	UNP P61769
l	1	MET	-	initiating methionine	UNP P61769
m	1	MET	-	initiating methionine	UNP P61769
n	1	MET	-	initiating methionine	UNP P61769
o	1	MET	-	initiating methionine	UNP P61769
p	1	MET	-	initiating methionine	UNP P61769
q	1	MET	-	initiating methionine	UNP P61769
r	1	MET	-	initiating methionine	UNP P61769
i	1	MET	-	initiating methionine	UNP P61769
t	1	MET	-	initiating methionine	UNP P61769
e	1	MET	-	initiating methionine	UNP P61769

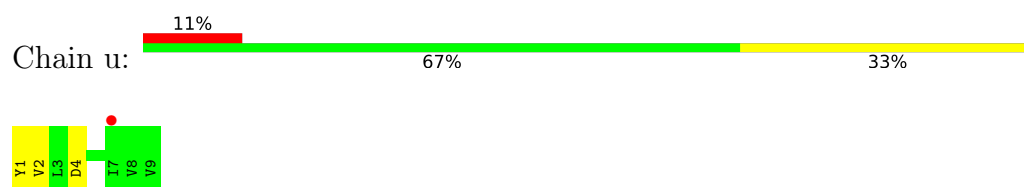
3 Residue-property plots [i](#)

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.

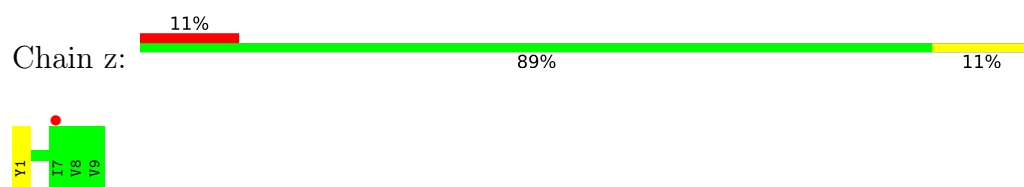
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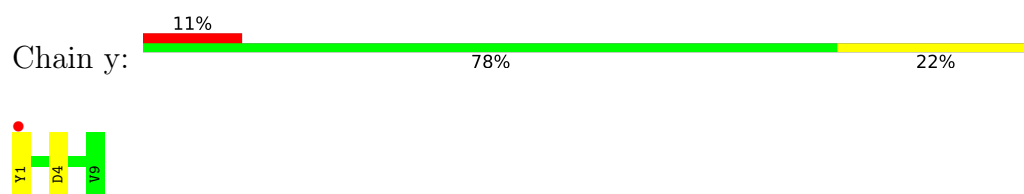
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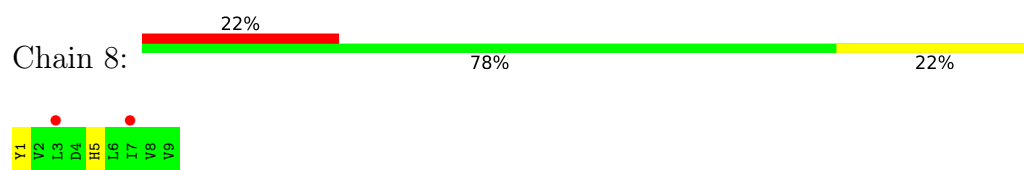
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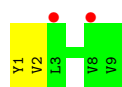
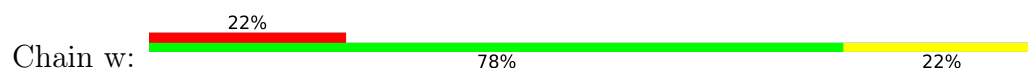
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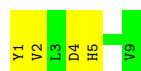
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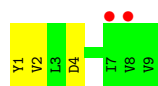
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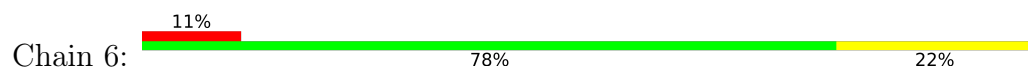
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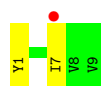
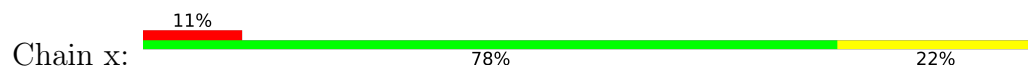
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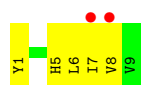
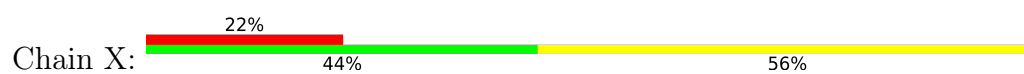
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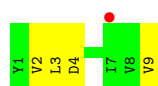
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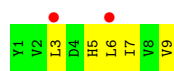
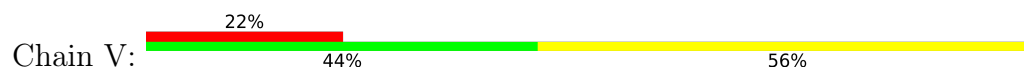
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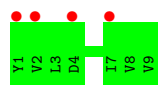
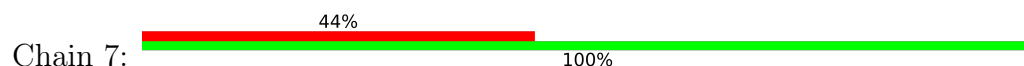
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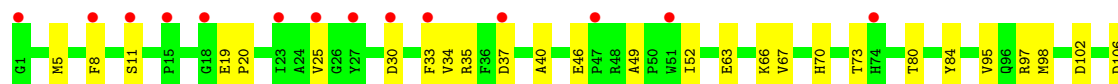
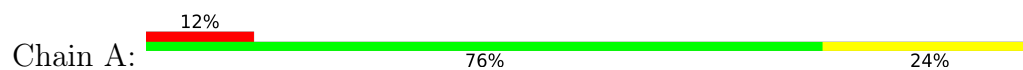
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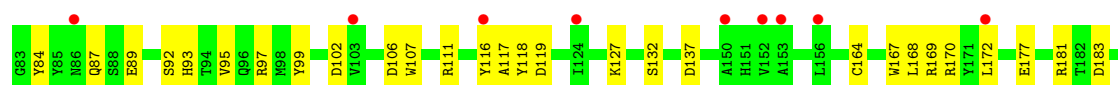
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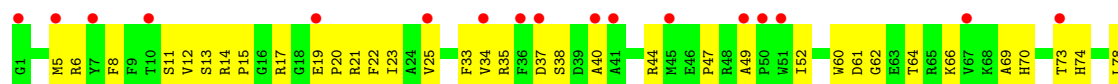
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



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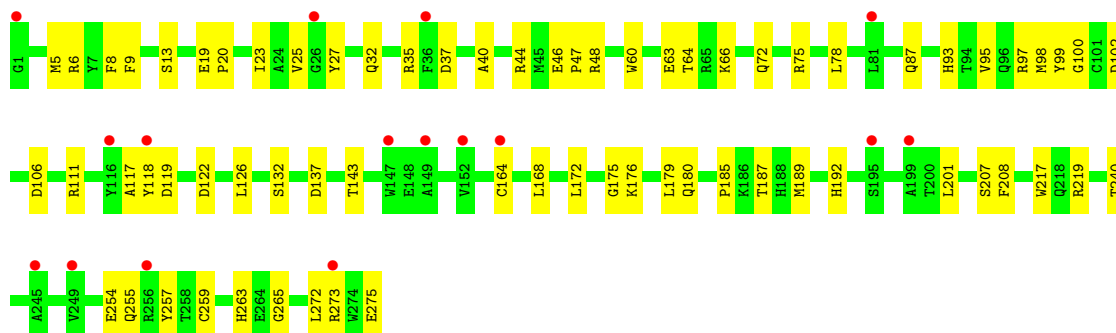
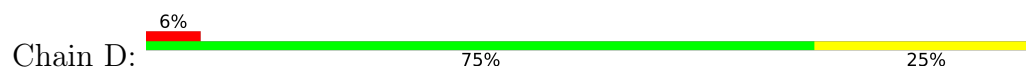


- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

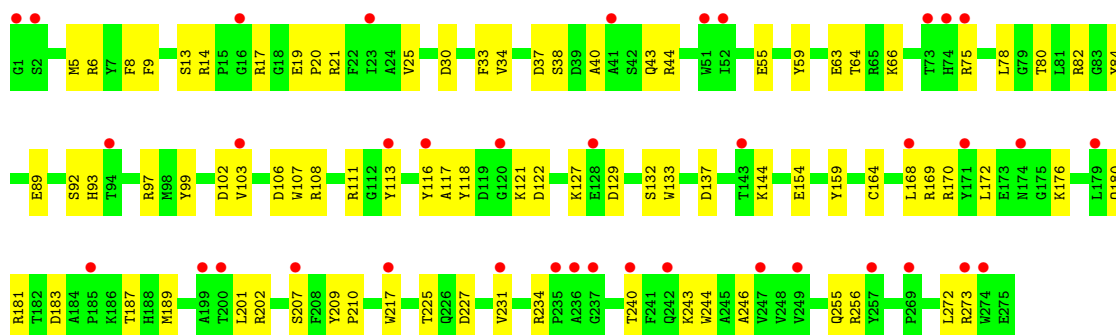




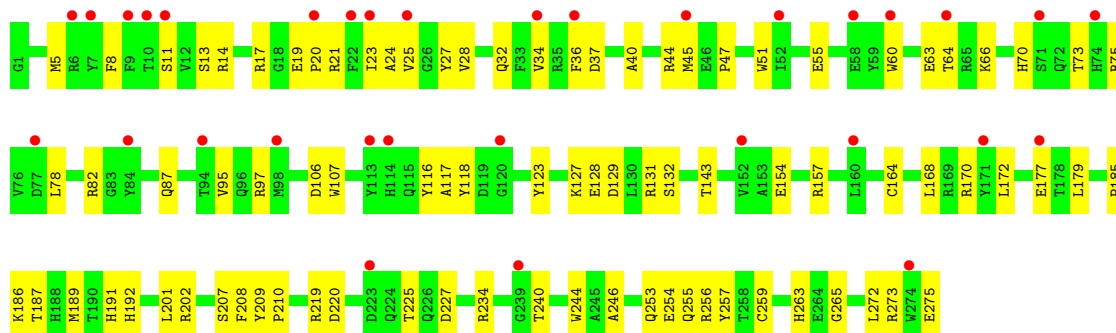
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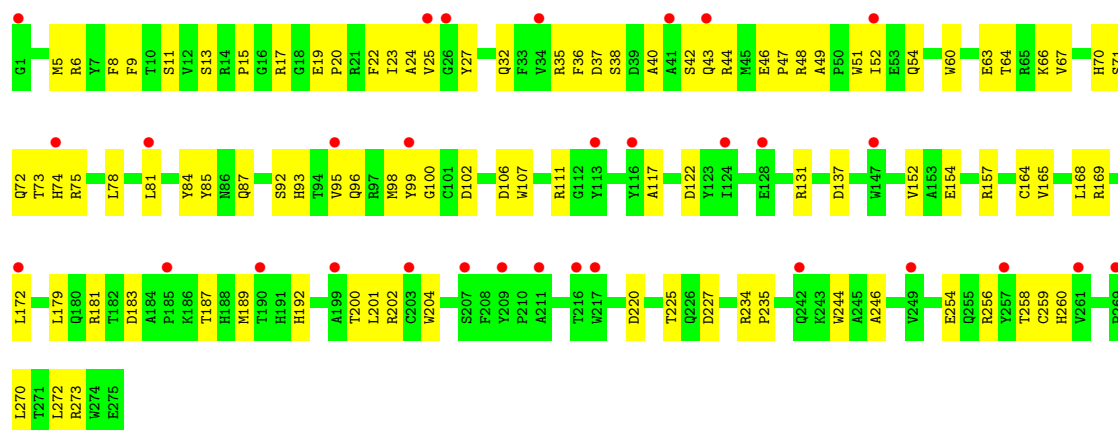


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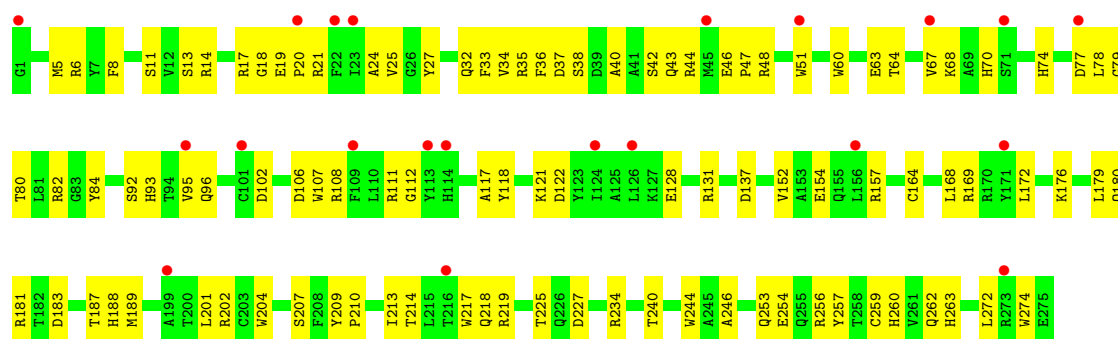


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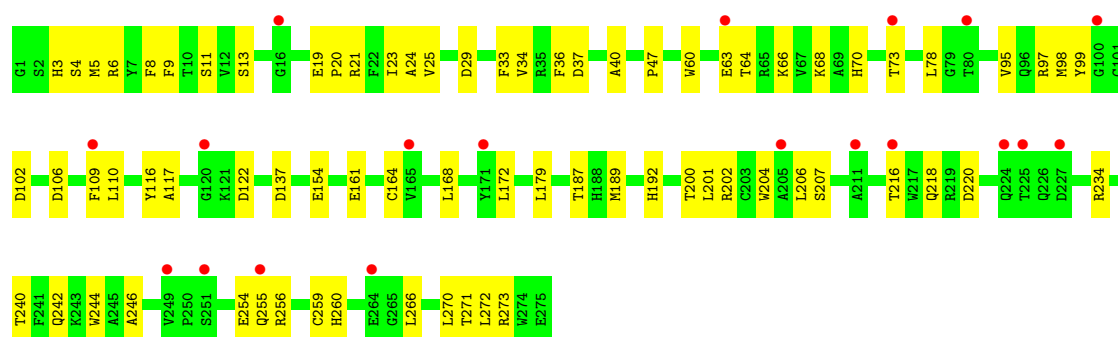




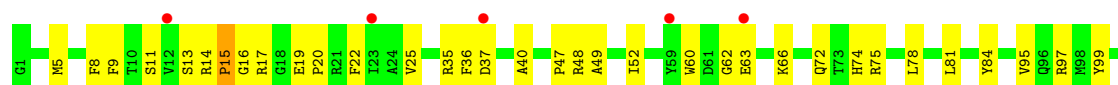
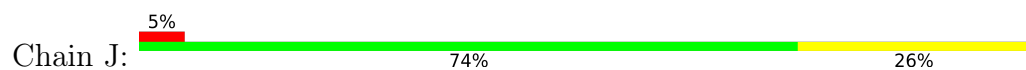
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

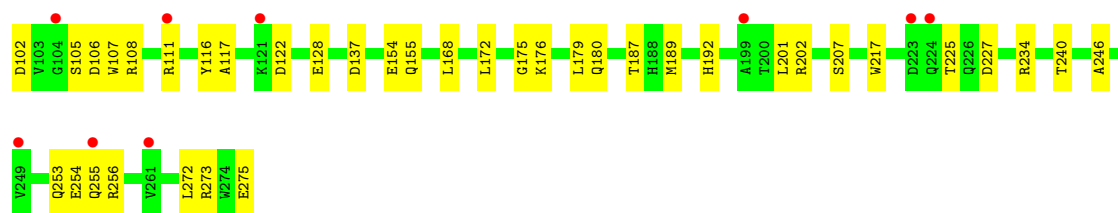


- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

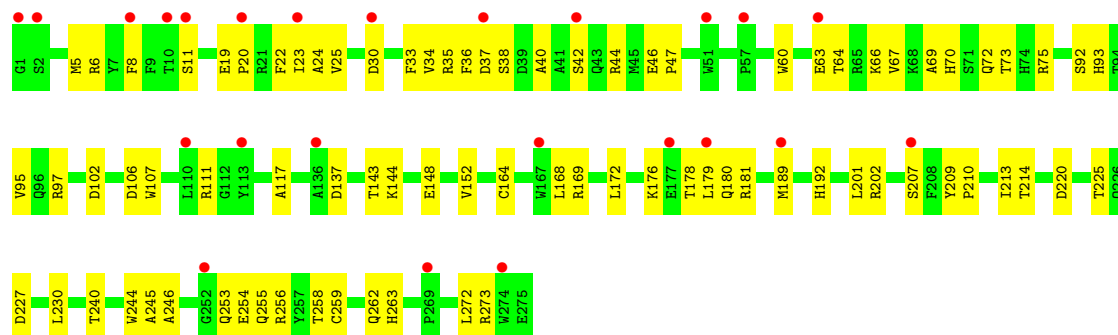


- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

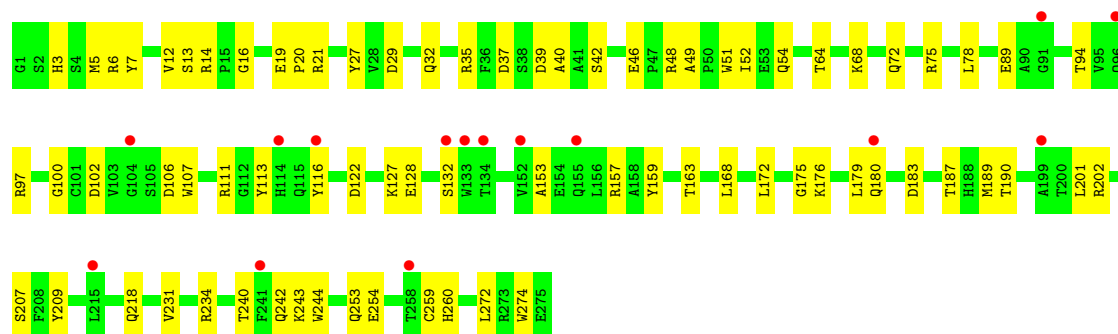




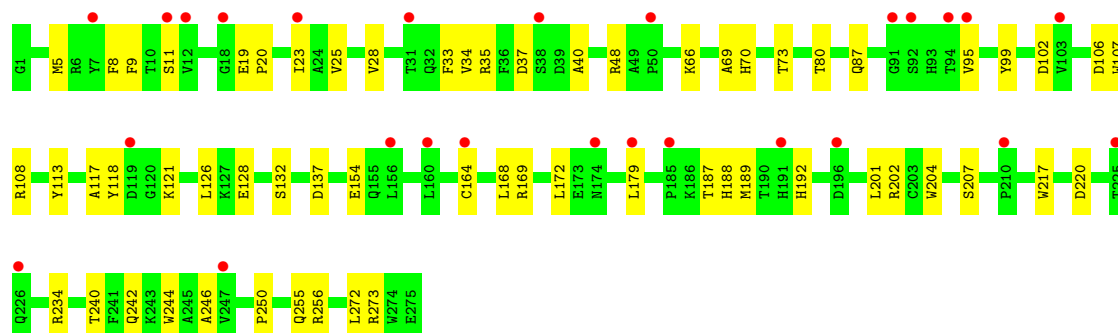
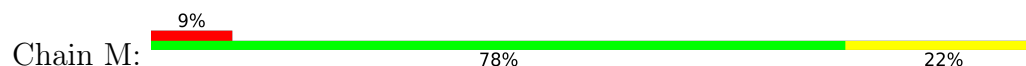
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



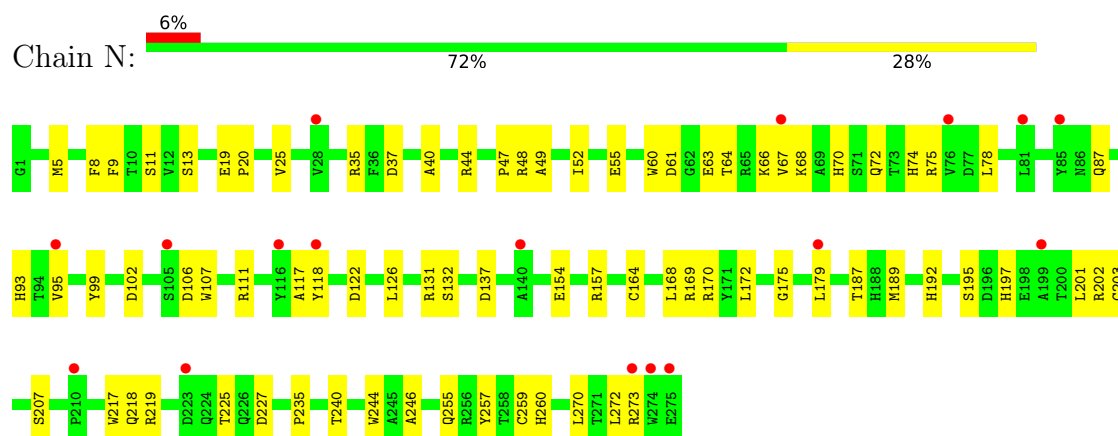
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



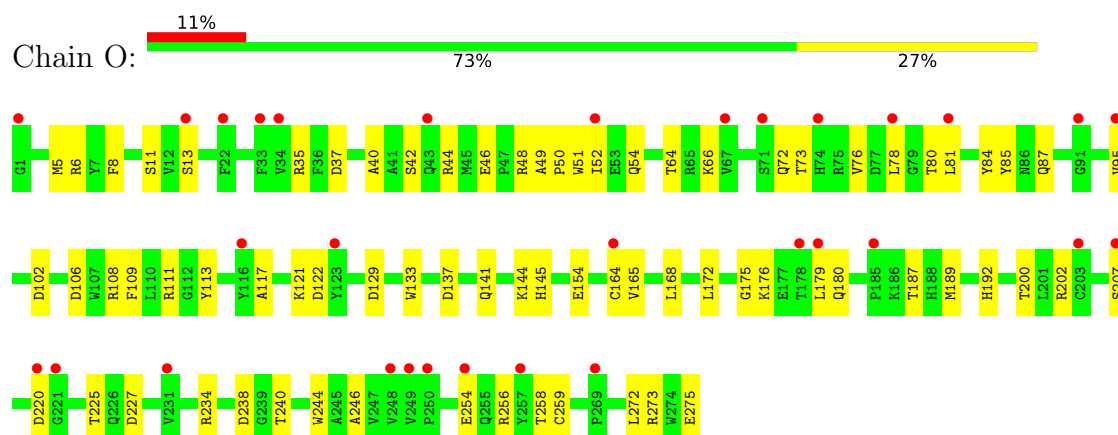
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



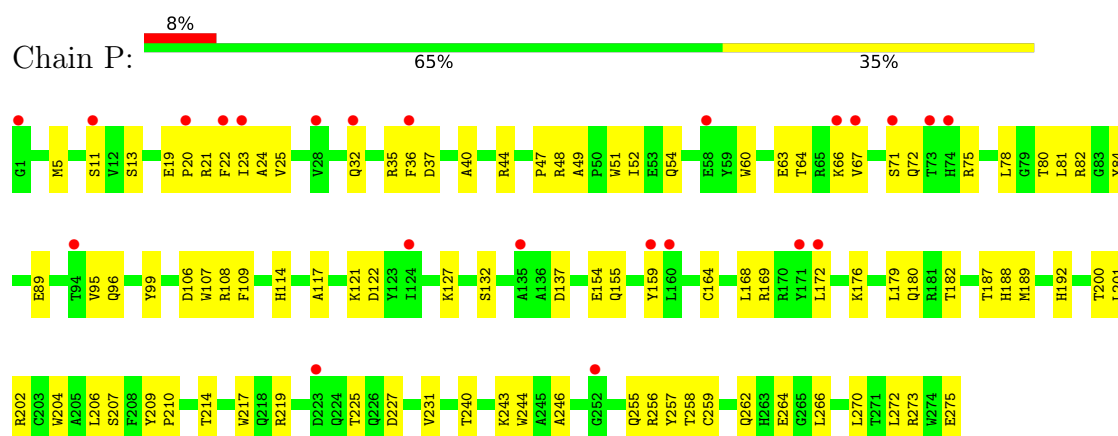
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



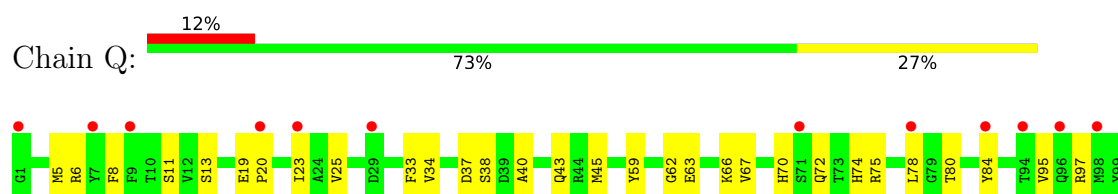
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

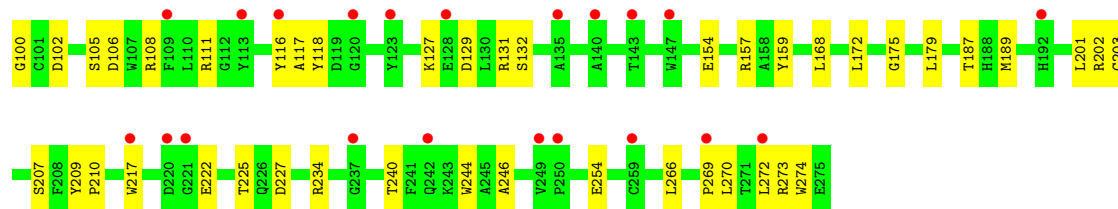


- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

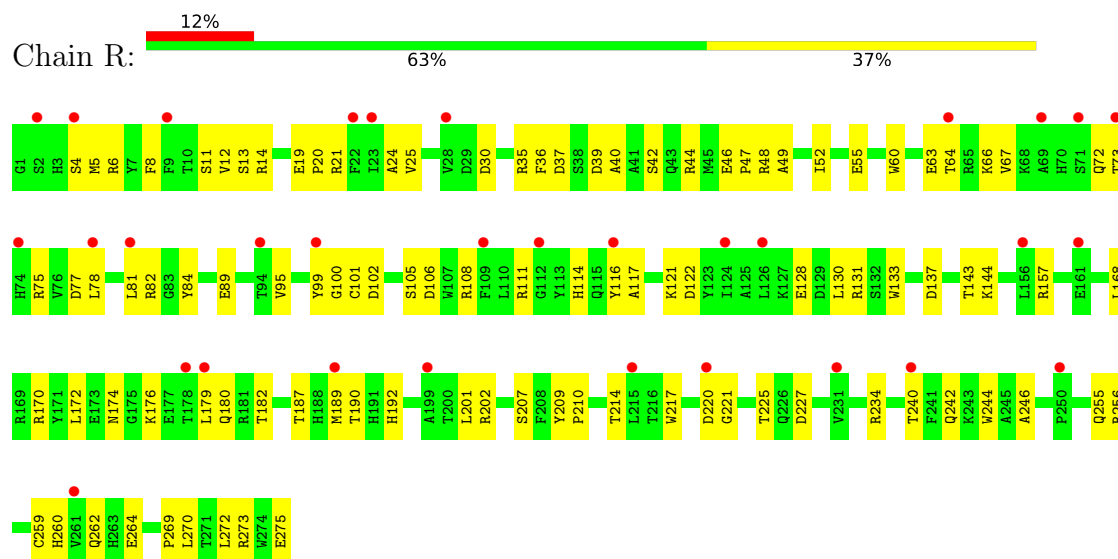


- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

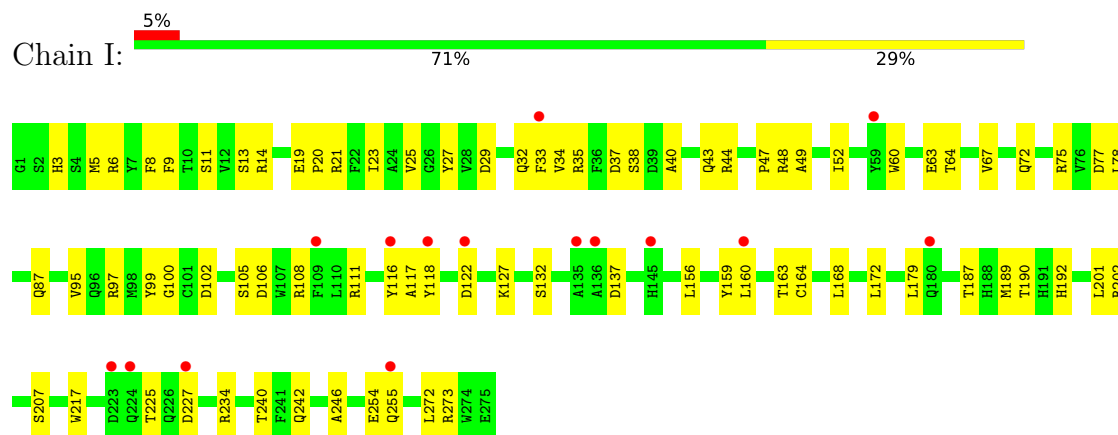




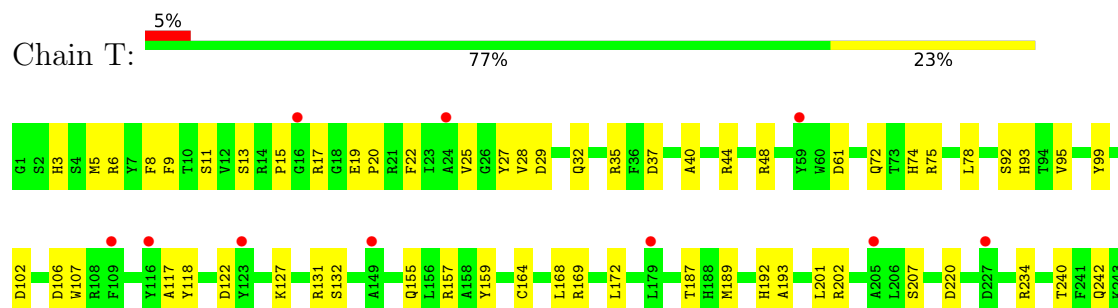
• Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



• Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

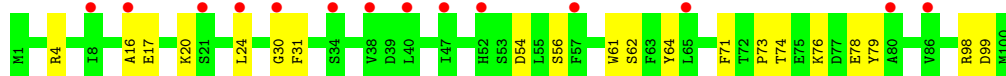
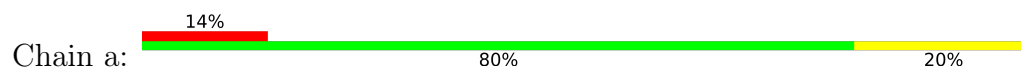


• Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

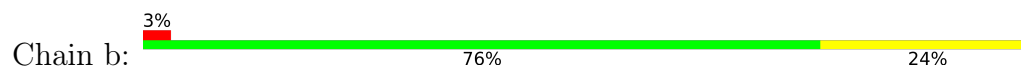




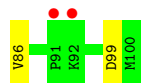
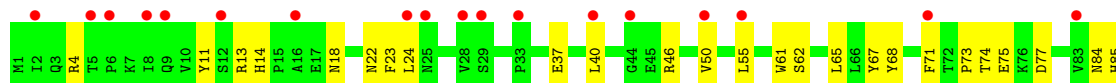
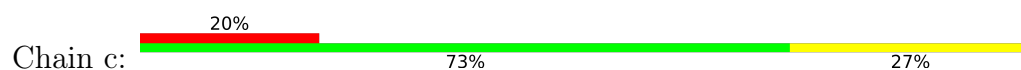
- Molecule 3: Beta-2-microglobulin



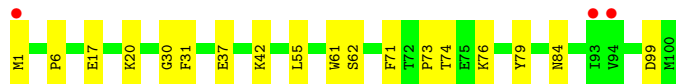
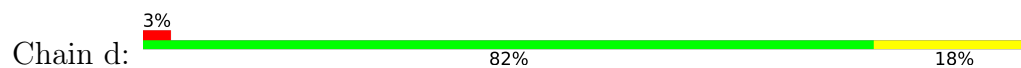
- Molecule 3: Beta-2-microglobulin



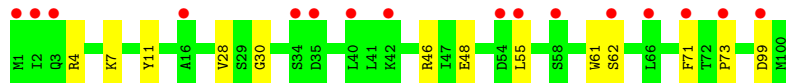
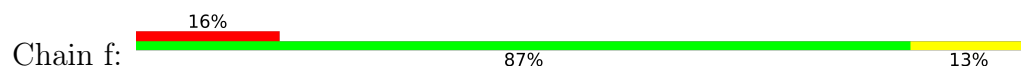
- Molecule 3: Beta-2-microglobulin



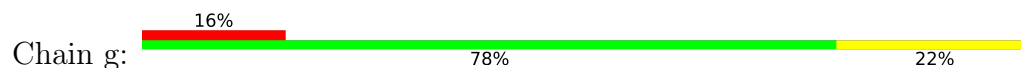
- Molecule 3: Beta-2-microglobulin

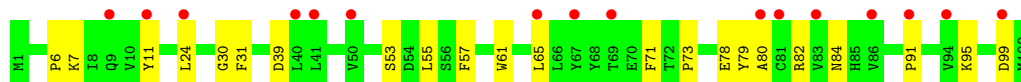


- Molecule 3: Beta-2-microglobulin

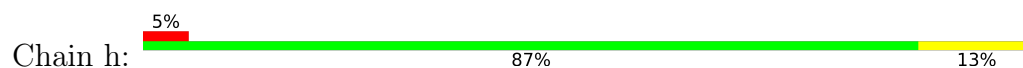


- Molecule 3: Beta-2-microglobulin

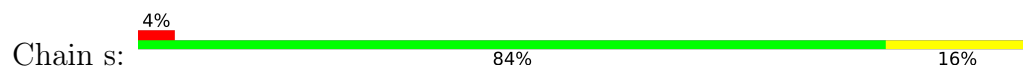




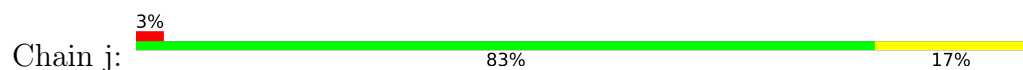
- Molecule 3: Beta-2-microglobulin



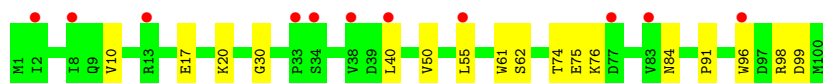
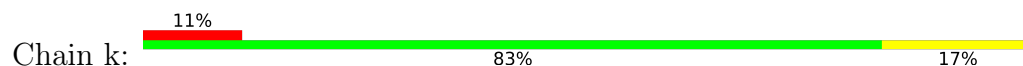
- Molecule 3: Beta-2-microglobulin



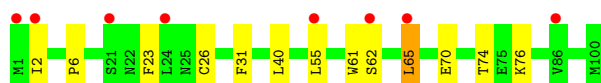
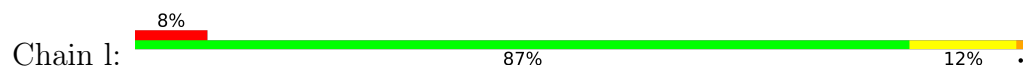
- Molecule 3: Beta-2-microglobulin



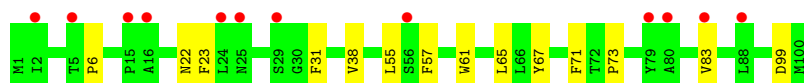
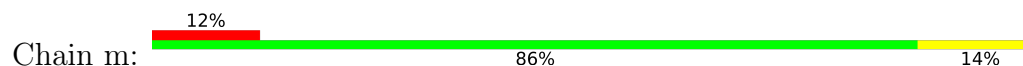
- Molecule 3: Beta-2-microglobulin



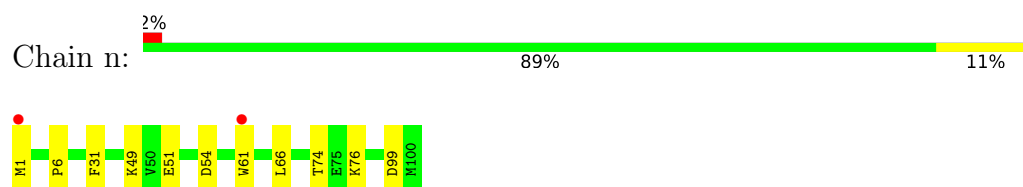
- Molecule 3: Beta-2-microglobulin



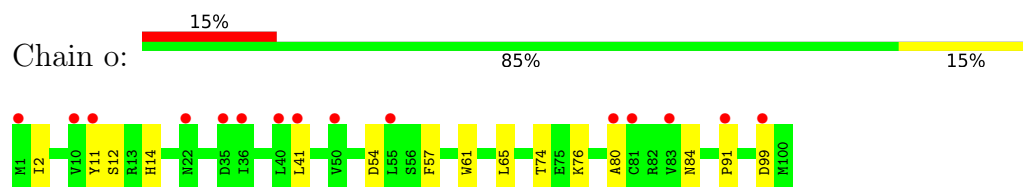
- Molecule 3: Beta-2-microglobulin



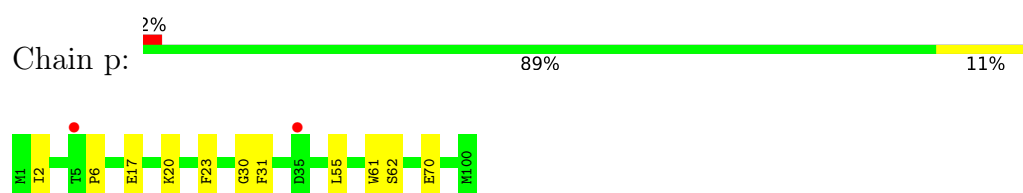
- Molecule 3: Beta-2-microglobulin



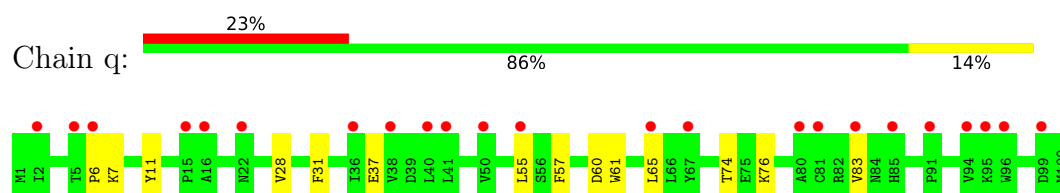
- Molecule 3: Beta-2-microglobulin



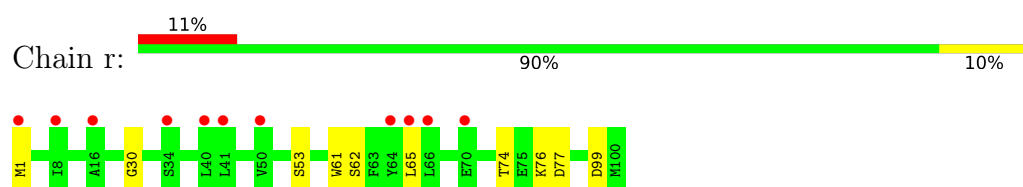
- Molecule 3: Beta-2-microglobulin



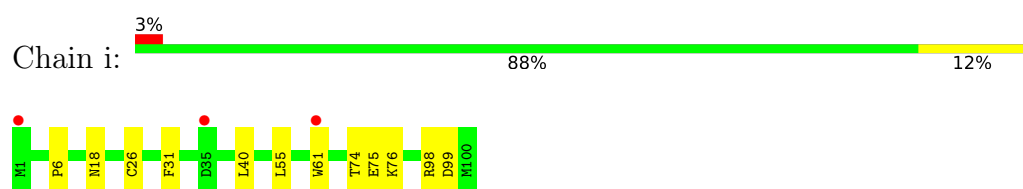
- Molecule 3: Beta-2-microglobulin



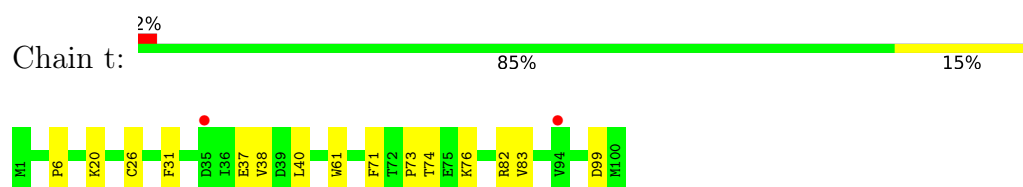
- Molecule 3: Beta-2-microglobulin



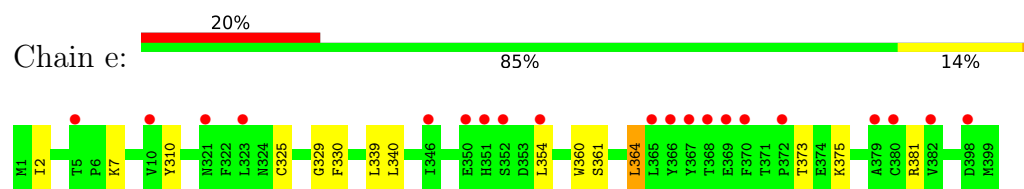
- Molecule 3: Beta-2-microglobulin



- Molecule 3: Beta-2-microglobulin



● Molecule 3: Beta-2-microglobulin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	189.91Å 100.17Å 292.41Å 90.00° 94.43° 90.00°	Depositor
Resolution (Å)	111.42 – 3.30 111.42 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (111.42-3.30) 92.6 (111.42-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.79 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.285 , 0.303 0.285 , 0.304	Depositor DCC
R_{free} test set	1516 reflections (0.69%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	63200	wwPDB-VP
Average B, all atoms (Å ²)	58.0	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 36.73 % 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 4.7800e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.15	0/77	0.48	0/104
1	2	0.12	0/77	0.44	0/104
1	3	0.19	0/77	0.50	0/104
1	4	0.16	0/77	0.56	0/104
1	5	0.20	0/77	0.61	0/104
1	6	0.19	0/77	0.69	0/104
1	7	0.12	0/77	0.45	0/104
1	8	0.16	0/77	0.56	0/104
1	U	0.17	0/77	0.49	0/104
1	V	0.20	0/77	0.59	0/104
1	W	0.12	0/77	0.42	0/104
1	X	0.16	0/77	0.46	0/104
1	Y	0.14	0/77	0.43	0/104
1	Z	0.17	0/77	0.54	0/104
1	u	0.15	0/77	0.42	0/104
1	v	0.14	0/77	0.43	0/104
1	w	0.15	0/77	0.48	0/104
1	x	0.17	0/77	0.39	0/104
1	y	0.13	0/77	0.36	0/104
1	z	0.12	0/77	0.46	0/104
2	A	0.18	0/2312	0.48	0/3137
2	B	0.13	0/2312	0.42	0/3137
2	C	0.16	0/2312	0.45	0/3137
2	D	0.14	0/2312	0.42	0/3137
2	E	0.14	0/2312	0.40	0/3137
2	F	0.14	0/2312	0.44	0/3137
2	G	0.14	0/2312	0.44	0/3137
2	H	0.13	0/2312	0.44	0/3137
2	I	0.13	0/2312	0.41	0/3137
2	J	0.13	0/2312	0.43	0/3137
2	K	0.15	0/2312	0.45	0/3137
2	L	0.13	0/2312	0.42	0/3137
2	M	0.13	0/2312	0.43	0/3137
2	N	0.13	0/2312	0.42	0/3137

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	O	0.14	0/2312	0.44	0/3137
2	P	0.13	0/2312	0.43	0/3137
2	Q	0.15	0/2312	0.42	0/3137
2	R	0.15	0/2312	0.44	0/3137
2	S	0.13	0/2312	0.41	0/3137
2	T	0.13	0/2312	0.41	0/3137
3	a	0.16	0/860	0.47	0/1162
3	b	0.14	0/860	0.44	0/1162
3	c	0.17	0/860	0.53	0/1162
3	d	0.14	0/860	0.43	0/1162
3	e	0.13	0/860	0.42	0/1162
3	f	0.14	0/860	0.46	0/1162
3	g	0.16	0/860	0.46	0/1162
3	h	0.14	0/860	0.42	0/1162
3	i	0.14	0/860	0.44	0/1162
3	j	0.14	0/860	0.42	0/1162
3	k	0.15	0/860	0.45	0/1162
3	l	0.13	0/860	0.43	0/1162
3	m	0.14	0/860	0.43	0/1162
3	n	0.14	0/860	0.41	0/1162
3	o	0.13	0/860	0.46	0/1162
3	p	0.13	0/860	0.42	0/1162
3	q	0.14	0/860	0.45	0/1162
3	r	0.14	0/860	0.44	0/1162
3	s	0.13	0/860	0.43	0/1162
3	t	0.14	0/860	0.42	0/1162
All	All	0.14	0/64980	0.44	0/88060

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	76	0	82	5	0
1	2	76	0	82	2	0
1	3	76	0	82	8	0
1	4	76	0	82	6	0
1	5	76	0	82	5	0
1	6	76	0	82	2	0
1	7	76	0	82	0	0
1	8	76	0	82	2	0
1	U	76	0	82	6	0
1	V	76	0	82	5	0
1	W	76	0	82	6	0
1	X	76	0	82	9	0
1	Y	76	0	82	1	0
1	Z	76	0	82	8	0
1	u	76	0	82	4	0
1	v	76	0	82	4	0
1	w	76	0	82	4	0
1	x	76	0	82	3	0
1	y	76	0	82	3	0
1	z	76	0	82	1	0
2	A	2247	0	2096	50	2
2	B	2247	0	2096	57	0
2	C	2247	0	2096	64	0
2	D	2247	0	2096	49	2
2	E	2247	0	2096	62	0
2	F	2247	0	2096	69	1
2	G	2247	0	2096	73	0
2	H	2247	0	2096	74	0
2	I	2247	0	2096	55	0
2	J	2247	0	2096	57	0
2	K	2247	0	2096	60	0
2	L	2247	0	2096	45	1
2	M	2247	0	2096	44	1
2	N	2247	0	2096	60	0
2	O	2247	0	2096	64	0
2	P	2247	0	2096	65	0
2	Q	2247	0	2096	62	0
2	R	2247	0	2096	84	0
2	S	2247	0	2096	46	0
2	T	2247	0	2096	44	0
3	a	837	0	803	17	0
3	b	837	0	803	17	1
3	c	837	0	803	21	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	d	837	0	803	14	0
3	e	837	0	803	11	0
3	f	837	0	803	10	0
3	g	837	0	803	17	0
3	h	837	0	803	15	0
3	i	837	0	803	12	0
3	j	837	0	803	14	0
3	k	837	0	803	11	0
3	l	837	0	803	8	0
3	m	837	0	803	9	0
3	n	837	0	803	12	0
3	o	837	0	803	11	0
3	p	837	0	803	8	0
3	q	837	0	803	11	0
3	r	837	0	803	12	0
3	s	837	0	803	13	1
3	t	837	0	803	13	0
All	All	63200	0	59620	1309	5

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 11.

All (1309) 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)
2:R:170:ARG:CZ	2:R:174:ASN:HD21	1.58	1.16
2:R:170:ARG:NH2	2:R:174:ASN:ND2	1.92	1.16
2:E:181:ARG:NH1	2:E:183:ASP:OD2	1.78	1.14
2:E:102:ASP:OD2	2:E:111:ARG:NH1	1.84	1.09
2:R:55:GLU:OE2	2:R:170:ARG:NH2	1.86	1.08
2:O:102:ASP:OD2	2:O:111:ARG:NH1	1.84	1.08
2:B:181:ARG:NH1	2:B:183:ASP:OD2	1.87	1.04
1:X:7:ILE:HD13	2:G:152:VAL:CG1	1.87	1.03
2:K:102:ASP:OD2	2:K:111:ARG:NH1	1.93	1.01
3:k:17:GLU:OE2	3:k:20:LYS:NZ	1.93	1.00
2:K:19:GLU:OE2	2:K:75:ARG:NH1	1.98	0.97
1:X:7:ILE:HD13	2:G:152:VAL:HG11	1.44	0.96
2:N:107:TRP:O	2:N:169:ARG:NH1	1.99	0.94
2:R:170:ARG:CZ	2:R:174:ASN:ND2	2.24	0.94
2:N:255:GLN:O	2:N:273:ARG:NH1	1.99	0.94
3:h:20:LYS:NZ	2:J:275:GLU:OXT	2.00	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:48:ARG:NH1	3:n:54:ASP:OD2	2.01	0.93
2:T:131:ARG:HH21	2:T:157:ARG:HH12	1.09	0.93
2:G:102:ASP:OD2	2:G:111:ARG:NH1	2.02	0.92
2:A:127:LYS:NZ	2:A:134:THR:OG1	2.01	0.92
2:H:102:ASP:OD2	2:H:111:ARG:NH1	2.03	0.92
2:R:255:GLN:O	2:R:273:ARG:NH1	2.02	0.91
2:S:255:GLN:O	2:S:273:ARG:NH1	2.03	0.89
2:L:3:HIS:ND1	2:L:29:ASP:OD2	2.05	0.89
2:G:192:HIS:HE1	3:g:99:ASP:HB3	1.38	0.88
2:N:131:ARG:HH21	2:N:157:ARG:HH12	1.18	0.88
2:N:55:GLU:OE2	2:N:170:ARG:NH1	2.07	0.88
2:G:131:ARG:HH21	2:G:157:ARG:HH12	1.19	0.85
2:N:102:ASP:OD2	2:N:111:ARG:NH1	2.09	0.85
1:3:1:TYR:HE2	2:O:66:LYS:HZ1	1.19	0.84
2:G:51:TRP:O	2:G:54:GLN:NE2	2.10	0.83
2:E:107:TRP:O	2:E:169:ARG:NH1	2.10	0.83
2:A:70:HIS:CE1	2:A:97:ARG:HH12	1.97	0.83
2:F:255:GLN:O	2:F:273:ARG:NH1	2.13	0.82
3:e:373:THR:HG22	3:e:375:LYS:H	1.44	0.82
2:D:255:GLN:O	2:D:273:ARG:NH1	2.13	0.81
2:C:5:MET:HB2	2:C:168:LEU:HD13	1.62	0.81
2:O:6:ARG:NH1	2:O:102:ASP:OD1	2.13	0.81
2:O:50:PRO:O	2:O:54:GLN:NE2	2.15	0.80
2:C:15:PRO:O	2:C:17:ARG:NH1	2.15	0.80
2:K:255:GLN:O	2:K:273:ARG:NH1	2.15	0.79
2:F:189:MET:HE2	2:F:201:LEU:HD22	1.63	0.79
2:G:220:ASP:OD2	2:G:256:ARG:NH2	2.12	0.79
2:L:6:ARG:NH2	2:L:102:ASP:OD1	2.16	0.79
3:d:17:GLU:OE1	3:d:20:LYS:NZ	2.12	0.79
2:Q:131:ARG:HE	2:Q:157:ARG:NH1	1.82	0.78
2:T:5:MET:HB2	2:T:168:LEU:HD13	1.65	0.78
2:S:19:GLU:HG3	2:S:20:PRO:HD2	1.65	0.78
2:M:187:THR:HB	2:M:272:LEU:HD11	1.63	0.78
2:L:5:MET:HB2	2:L:168:LEU:HD13	1.66	0.78
2:K:6:ARG:NH2	2:K:102:ASP:OD1	2.17	0.77
1:X:7:ILE:CD1	2:G:152:VAL:CG1	2.60	0.77
2:J:255:GLN:O	2:J:273:ARG:NH1	2.17	0.77
2:A:102:ASP:OD2	2:A:111:ARG:NH1	2.19	0.76
2:C:102:ASP:OD2	2:C:111:ARG:NH1	2.18	0.76
2:I:255:GLN:O	2:I:273:ARG:NH1	2.19	0.76
2:G:6:ARG:HD3	2:G:100:GLY:HA3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:13:SER:HB3	2:J:78:LEU:HD13	1.69	0.75
2:O:220:ASP:OD2	2:O:256:ARG:NH2	2.20	0.75
2:C:224:GLN:NE2	2:C:227:ASP:OD2	2.20	0.75
2:K:220:ASP:OD2	2:K:256:ARG:NH2	2.15	0.75
1:V:3:LEU:HD13	1:V:5:HIS:H	1.51	0.75
2:G:189:MET:HE2	2:G:201:LEU:HD22	1.68	0.74
2:S:266:LEU:HD13	2:S:270:LEU:HD13	1.69	0.74
2:F:192:HIS:CE1	3:f:99:ASP:HB3	2.22	0.74
2:F:23:ILE:HG21	3:f:55:LEU:HB3	1.68	0.73
2:C:220:ASP:OD2	2:C:256:ARG:NE	2.19	0.73
2:O:35:ARG:HG2	2:O:48:ARG:HD3	1.68	0.73
2:S:220:ASP:OD2	2:S:256:ARG:NH2	2.19	0.73
2:F:131:ARG:NH2	2:F:157:ARG:HH12	1.87	0.73
3:j:37:GLU:OE2	3:j:39:ASP:OD2	2.06	0.72
2:I:3:HIS:ND1	2:I:29:ASP:OD2	2.20	0.72
2:A:253:GLN:OE1	2:A:256:ARG:NH1	2.22	0.72
3:n:74:THR:HG22	3:n:76:LYS:H	1.52	0.72
2:M:23:ILE:HG21	3:m:55:LEU:HB3	1.72	0.72
2:T:131:ARG:HH21	2:T:157:ARG:NH1	1.87	0.72
2:Q:254:GLU:HB3	2:Q:274:TRP:HD1	1.55	0.72
1:V:7:ILE:O	2:C:73:THR:OG1	2.07	0.72
2:C:14:ARG:NE	2:C:19:GLU:O	2.22	0.72
2:F:187:THR:HB	2:F:272:LEU:HD11	1.72	0.72
1:Z:6:LEU:HD11	2:K:69:ALA:HB1	1.70	0.71
2:I:102:ASP:OD2	2:I:111:ARG:NH1	2.23	0.71
2:T:3:HIS:ND1	2:T:29:ASP:OD2	2.23	0.71
2:F:192:HIS:HE1	3:f:99:ASP:HB3	1.53	0.71
2:F:5:MET:HB2	2:F:168:LEU:HD13	1.71	0.71
2:G:258:THR:HG22	2:G:273:ARG:HG2	1.73	0.71
2:H:42:SER:OG	2:H:46:GLU:OE2	2.06	0.71
2:O:192:HIS:O	2:O:200:THR:N	2.19	0.71
2:Q:189:MET:HE2	2:Q:201:LEU:HD22	1.72	0.70
2:D:19:GLU:OE1	2:D:75:ARG:NH1	2.23	0.70
2:K:192:HIS:HE1	3:k:99:ASP:HB3	1.55	0.70
3:s:82:ARG:NH1	2:I:105:SER:HB2	2.05	0.70
3:f:46:ARG:HH21	3:f:48:GLU:HA	1.55	0.70
2:P:188:HIS:HD2	2:P:204:TRP:HB2	1.56	0.70
2:G:259:CYS:HB3	2:G:272:LEU:HB2	1.74	0.70
2:I:19:GLU:OE2	2:I:75:ARG:NH2	2.24	0.70
1:6:1:TYR:HE2	2:R:66:LYS:HE2	1.57	0.70
2:P:172:LEU:HA	2:P:179:LEU:HD11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:35:ARG:HD3	3:a:54:ASP:OD2	1.92	0.69
3:a:24:LEU:HD22	3:a:79:TYR:HD1	1.57	0.69
2:G:131:ARG:NH2	2:G:157:ARG:HH12	1.91	0.69
2:R:172:LEU:HA	2:R:179:LEU:HD11	1.74	0.69
2:A:192:HIS:HE1	3:a:99:ASP:HB3	1.56	0.69
2:C:151:HIS:HB3	2:C:154:GLU:OE2	1.91	0.69
2:F:259:CYS:HB3	2:F:272:LEU:HB2	1.74	0.69
2:R:6:ARG:HE	2:R:100:GLY:HA3	1.56	0.69
2:R:42:SER:OG	2:R:46:GLU:OE2	2.09	0.69
2:D:13:SER:HB3	2:D:78:LEU:HD13	1.73	0.69
2:H:121:LYS:HE2	3:h:2:ILE:HG13	1.73	0.69
2:I:189:MET:HE2	2:I:201:LEU:HD22	1.73	0.69
2:B:3:HIS:ND1	2:B:29:ASP:OD2	2.24	0.69
2:D:189:MET:HE3	2:D:217:TRP:HH2	1.58	0.69
2:J:5:MET:HB2	2:J:168:LEU:HD13	1.73	0.69
2:R:170:ARG:NH2	2:R:174:ASN:HD21	1.68	0.69
2:K:5:MET:HB2	2:K:168:LEU:HD13	1.75	0.69
2:Q:108:ARG:NH2	2:R:275:GLU:OE1	2.26	0.69
2:B:21:ARG:HD2	2:B:39:ASP:OD2	1.93	0.69
2:N:48:ARG:HH12	3:n:54:ASP:CG	2.00	0.69
2:O:172:LEU:HA	2:O:179:LEU:HD11	1.75	0.69
2:H:187:THR:HB	2:H:272:LEU:HD11	1.74	0.68
2:A:102:ASP:HB2	2:A:111:ARG:HB3	1.76	0.68
2:A:192:HIS:CE1	3:a:99:ASP:HB3	2.29	0.68
2:A:189:MET:HE2	2:A:201:LEU:HD22	1.74	0.68
2:D:189:MET:HE2	2:D:201:LEU:HD22	1.75	0.68
2:S:5:MET:HB2	2:S:168:LEU:HD13	1.76	0.68
2:N:187:THR:HB	2:N:272:LEU:HD11	1.75	0.68
2:J:253:GLN:OE1	2:J:256:ARG:NH1	2.27	0.67
2:B:235:PRO:O	3:b:11:TYR:OH	2.12	0.67
2:Q:6:ARG:NH2	2:Q:102:ASP:OD1	2.25	0.67
2:D:187:THR:HB	2:D:272:LEU:HD11	1.75	0.67
2:S:189:MET:HE2	2:S:201:LEU:HD22	1.75	0.67
2:E:108:ARG:NH2	2:F:275:GLU:OE1	2.28	0.67
2:O:273:ARG:NH2	2:P:109:PHE:O	2.28	0.67
2:R:170:ARG:NH2	2:R:174:ASN:HD22	1.92	0.67
3:e:7:LYS:NZ	3:e:329:GLY:HA3	2.09	0.67
2:J:172:LEU:HA	2:J:179:LEU:HD11	1.77	0.66
2:C:6:ARG:NH2	2:C:102:ASP:OD1	2.25	0.66
2:H:35:ARG:NH1	3:h:54:ASP:OD1	2.29	0.66
2:E:55:GLU:OE2	2:E:170:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:ASP:OD2	2:B:111:ARG:NH1	2.28	0.66
2:N:172:LEU:HA	2:N:179:LEU:HD11	1.77	0.66
2:Q:102:ASP:HB2	2:Q:111:ARG:HG2	1.76	0.66
2:Q:172:LEU:HA	2:Q:179:LEU:HD11	1.77	0.66
2:R:77:ASP:OD2	2:R:116:TYR:OH	2.11	0.66
2:I:187:THR:HB	2:I:272:LEU:HD11	1.78	0.66
2:I:172:LEU:HA	2:I:179:LEU:HD11	1.78	0.66
2:F:55:GLU:OE2	2:F:170:ARG:NH2	2.28	0.66
2:H:6:ARG:NH2	2:H:102:ASP:OD1	2.29	0.66
2:O:108:ARG:NH2	2:P:275:GLU:OE1	2.29	0.66
2:T:93:HIS:ND1	2:T:118:TYR:OH	2.23	0.66
2:F:131:ARG:HH21	2:F:157:ARG:HH12	1.44	0.66
2:J:63:GLU:OE2	2:J:66:LYS:NZ	2.29	0.66
2:N:5:MET:HB2	2:N:168:LEU:HD13	1.77	0.65
2:F:13:SER:HB3	2:F:78:LEU:HD13	1.77	0.65
2:P:107:TRP:O	2:P:169:ARG:NH1	2.27	0.65
2:R:170:ARG:HH21	2:R:174:ASN:ND2	1.88	0.65
2:C:197:HIS:O	2:C:251:SER:N	2.19	0.65
2:D:87:GLN:OE1	2:D:118:TYR:OH	2.12	0.65
1:5:1:TYR:CE2	2:Q:66:LYS:HE2	2.31	0.65
2:R:13:SER:HB3	2:R:78:LEU:HD13	1.77	0.65
2:G:172:LEU:HA	2:G:179:LEU:HD11	1.76	0.65
2:C:172:LEU:HA	2:C:179:LEU:HD11	1.78	0.65
2:L:111:ARG:HD3	2:L:128:GLU:OE2	1.96	0.65
2:L:12:VAL:HG22	2:L:94:THR:HG23	1.78	0.64
2:F:70:HIS:O	2:F:73:THR:OG1	2.14	0.64
2:R:187:THR:HB	2:R:272:LEU:HD11	1.79	0.64
2:G:131:ARG:HE	2:G:157:ARG:NH1	1.95	0.64
2:D:172:LEU:HA	2:D:179:LEU:HD11	1.80	0.64
2:N:189:MET:HE2	2:N:201:LEU:HD22	1.79	0.64
2:K:189:MET:HE2	2:K:201:LEU:HD22	1.79	0.64
2:C:8:PHE:HB2	2:C:25:VAL:HG23	1.79	0.64
2:L:187:THR:HB	2:L:272:LEU:HD11	1.79	0.64
2:I:156:LEU:O	2:I:160:LEU:HD12	1.98	0.64
2:C:195:SER:OG	2:C:196:ASP:N	2.29	0.64
3:i:74:THR:HG22	3:i:76:LYS:H	1.63	0.64
1:V:6:LEU:HD11	2:C:69:ALA:HB1	1.79	0.63
2:A:202:ARG:HD3	2:A:246:ALA:HB2	1.80	0.63
3:g:24:LEU:HD22	3:g:79:TYR:HD1	1.63	0.63
2:K:192:HIS:CE1	3:k:99:ASP:HB3	2.33	0.63
2:R:214:THR:HB	2:R:262:GLN:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:LYS:HD2	2:B:132:SER:HB2	1.80	0.63
3:d:74:THR:HG22	3:d:76:LYS:H	1.63	0.63
2:E:154:GLU:OE2	2:E:154:GLU:N	2.29	0.63
3:s:37:GLU:OE1	2:I:108:ARG:HD3	1.98	0.63
2:K:172:LEU:HA	2:K:179:LEU:HD11	1.80	0.63
2:P:214:THR:HB	2:P:262:GLN:HB2	1.80	0.63
1:Z:7:ILE:HG13	2:K:97:ARG:HH22	1.63	0.63
2:T:22:PHE:HE1	2:T:74:HIS:HD2	1.45	0.63
1:X:7:ILE:HD13	2:G:152:VAL:HG13	1.79	0.63
2:M:66:LYS:NZ	1:I:1:TYR:CZ	2.67	0.63
2:I:6:ARG:NH2	2:I:102:ASP:OD1	2.30	0.63
2:S:64:THR:HG22	2:S:68:LYS:HE3	1.81	0.63
1:3:7:ILE:O	2:O:73:THR:HG23	1.99	0.62
2:R:259:CYS:HB3	2:R:272:LEU:HB2	1.80	0.62
2:L:42:SER:OG	2:L:46:GLU:OE2	2.12	0.62
2:Q:187:THR:HB	2:Q:272:LEU:HD11	1.81	0.62
3:q:74:THR:HG22	3:q:76:LYS:H	1.64	0.62
2:L:172:LEU:HA	2:L:179:LEU:HD11	1.80	0.62
2:L:259:CYS:HB3	2:L:272:LEU:HB2	1.81	0.62
3:r:74:THR:HG22	3:r:76:LYS:H	1.64	0.62
3:l:74:THR:HG22	3:l:76:LYS:H	1.65	0.62
2:N:9:PHE:HE2	2:N:99:TYR:HE2	1.47	0.62
2:N:131:ARG:NH2	2:N:157:ARG:HH12	1.93	0.62
2:K:37:ASP:HB3	2:K:40:ALA:HB2	1.81	0.62
2:Q:37:ASP:HB3	2:Q:40:ALA:HB2	1.81	0.61
1:5:1:TYR:HE2	2:Q:66:LYS:HE2	1.65	0.61
2:B:192:HIS:CE1	3:b:99:ASP:HB3	2.35	0.61
2:N:189:MET:HE3	2:N:217:TRP:HH2	1.64	0.61
2:Q:5:MET:HB2	2:Q:168:LEU:HD13	1.81	0.61
2:G:13:SER:HB3	2:G:78:LEU:HD13	1.82	0.61
2:K:42:SER:OG	2:K:46:GLU:OE2	2.11	0.61
2:T:189:MET:HE2	2:T:201:LEU:HD22	1.81	0.61
1:U:7:ILE:HG21	2:A:152:VAL:HG13	1.83	0.61
2:Q:273:ARG:NE	2:R:106:ASP:OD2	2.33	0.61
2:R:275:GLU:OXT	3:t:20:LYS:HE2	2.00	0.61
2:T:187:THR:HB	2:T:272:LEU:HD11	1.82	0.61
2:H:14:ARG:HB2	2:H:17:ARG:O	1.99	0.61
2:J:106:ASP:OD2	3:t:37:GLU:OE2	2.19	0.61
1:3:4:ASP:HA	2:O:66:LYS:HD3	1.81	0.61
2:A:11:SER:HB3	2:A:95:VAL:HG22	1.82	0.61
2:E:30:ASP:HB2	2:E:209:TYR:HE1	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:37:ASP:HB3	2:F:40:ALA:HB2	1.83	0.61
2:I:35:ARG:HG2	2:I:48:ARG:HD3	1.82	0.61
1:v:4:ASP:HA	2:D:66:LYS:HD3	1.83	0.60
2:B:37:ASP:HB3	2:B:40:ALA:HB2	1.82	0.60
2:K:22:PHE:HB3	2:K:38:SER:HB3	1.83	0.60
2:K:70:HIS:O	2:K:73:THR:OG1	2.20	0.60
2:L:159:TYR:HA	2:L:163:THR:HB	1.83	0.60
2:P:189:MET:HE2	2:P:201:LEU:HD22	1.83	0.60
2:R:122:ASP:OD1	3:r:61:TRP:NE1	2.28	0.60
2:L:234:ARG:NH2	2:L:242:GLN:OE1	2.32	0.60
2:P:259:CYS:HB3	2:P:272:LEU:HB2	1.82	0.60
2:R:4:SER:HB2	2:R:6:ARG:NH1	2.16	0.60
2:R:189:MET:HE2	2:R:201:LEU:HD22	1.81	0.60
2:G:37:ASP:HB3	2:G:40:ALA:HB2	1.82	0.60
2:C:70:HIS:O	2:C:73:THR:HG22	2.02	0.60
2:G:24:ALA:HB3	2:G:36:PHE:HB3	1.83	0.60
2:G:202:ARG:HD3	2:G:246:ALA:HB2	1.82	0.60
2:M:35:ARG:HG2	2:M:48:ARG:HD3	1.82	0.60
2:G:122:ASP:OD1	3:g:61:TRP:NE1	2.24	0.60
2:H:122:ASP:OD1	3:h:61:TRP:NE1	2.26	0.60
2:L:37:ASP:HB3	2:L:40:ALA:HB2	1.82	0.60
2:B:218:GLN:OE1	2:B:260:HIS:NE2	2.35	0.60
3:c:65:LEU:HD21	3:c:67:TYR:CD1	2.37	0.60
2:S:70:HIS:O	2:S:73:THR:OG1	2.18	0.60
3:l:6:PRO:HB3	3:l:31:PHE:HB3	1.83	0.60
2:I:11:SER:HB3	2:I:95:VAL:HG23	1.84	0.60
2:E:129:ASP:CB	2:F:256:ARG:HH12	2.15	0.60
2:H:64:THR:HG22	2:H:68:LYS:HE2	1.82	0.60
2:A:37:ASP:HB3	2:A:40:ALA:HB2	1.83	0.59
2:H:37:ASP:HB3	2:H:40:ALA:HB2	1.84	0.59
2:N:35:ARG:HD3	2:N:48:ARG:NH1	2.17	0.59
2:T:37:ASP:HB3	2:T:40:ALA:HB2	1.83	0.59
3:a:74:THR:HG22	3:a:76:LYS:H	1.67	0.59
2:S:13:SER:HB3	2:S:78:LEU:HD13	1.84	0.59
2:M:102:ASP:OD2	2:M:113:TYR:HE1	1.85	0.59
2:R:202:ARG:HD3	2:R:246:ALA:HB2	1.83	0.59
1:X:7:ILE:CD1	2:G:152:VAL:HG13	2.32	0.59
2:D:23:ILE:HG21	3:d:55:LEU:HB3	1.84	0.59
2:L:127:LYS:HD2	2:L:132:SER:HB2	1.84	0.59
3:h:74:THR:HG22	3:h:76:LYS:H	1.66	0.59
2:Q:131:ARG:HE	2:Q:157:ARG:HH12	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:187:THR:HB	2:C:272:LEU:HD11	1.85	0.59
2:H:189:MET:HE3	2:H:217:TRP:HH2	1.67	0.59
2:H:259:CYS:HB3	2:H:272:LEU:HB2	1.84	0.59
2:R:202:ARG:HD2	2:R:244:TRP:CE3	2.38	0.59
2:E:255:GLN:O	2:E:273:ARG:NH1	2.36	0.59
2:H:154:GLU:OE1	2:H:154:GLU:N	2.36	0.59
2:B:266:LEU:HD13	2:B:270:LEU:HG	1.84	0.59
2:C:106:ASP:OD2	2:C:108:ARG:HD3	2.02	0.59
3:h:30:GLY:HA2	3:h:62:SER:HB3	1.84	0.59
2:E:189:MET:HE2	2:E:201:LEU:HD22	1.84	0.59
2:P:13:SER:HB3	2:P:78:LEU:HD13	1.85	0.59
2:I:37:ASP:HB3	2:I:40:ALA:HB2	1.83	0.59
2:P:188:HIS:CD2	2:P:204:TRP:HB2	2.36	0.58
2:B:119:ASP:OD2	3:b:1:MET:HG2	2.03	0.58
2:D:122:ASP:OD1	3:d:61:TRP:NE1	2.25	0.58
2:R:182:THR:HG21	2:R:264:GLU:HG2	1.85	0.58
2:C:23:ILE:HG21	3:c:55:LEU:HB3	1.86	0.58
2:E:37:ASP:HB3	2:E:40:ALA:HB2	1.84	0.58
2:B:6:ARG:NH2	2:B:102:ASP:OD1	2.36	0.58
2:B:82:ARG:HH21	2:B:89:GLU:HB2	1.67	0.58
2:G:63:GLU:CD	2:G:66:LYS:HZ1	2.12	0.58
2:L:14:ARG:NE	2:L:19:GLU:O	2.36	0.58
2:N:55:GLU:CD	2:N:170:ARG:HH11	2.10	0.58
3:p:30:GLY:HA2	3:p:62:SER:HB3	1.85	0.58
2:I:13:SER:HB3	2:I:78:LEU:HD13	1.85	0.58
3:t:74:THR:HG22	3:t:76:LYS:H	1.69	0.58
2:P:121:LYS:HE2	3:p:2:ILE:HG13	1.85	0.58
2:Q:95:VAL:HG12	2:Q:118:TYR:HD1	1.68	0.58
3:b:24:LEU:HD22	3:b:79:TYR:HD1	1.67	0.58
2:S:63:GLU:OE2	2:S:66:LYS:NZ	2.36	0.58
1:5:1:TYR:O	2:Q:159:TYR:OH	2.14	0.58
2:E:121:LYS:HE2	3:e:2:ILE:HG13	1.85	0.58
2:P:122:ASP:OD1	3:p:61:TRP:NE1	2.32	0.58
3:c:65:LEU:HD21	3:c:67:TYR:CE1	2.39	0.58
2:H:189:MET:HE2	2:H:201:LEU:HD22	1.84	0.58
2:K:107:TRP:O	2:K:169:ARG:NH1	2.34	0.58
2:K:30:ASP:HB2	2:K:209:TYR:HE1	1.68	0.58
2:K:207:SER:HA	2:K:240:THR:HB	1.86	0.58
2:M:192:HIS:HE1	3:m:99:ASP:HB3	1.68	0.58
2:I:5:MET:HB2	2:I:168:LEU:HD13	1.85	0.58
2:A:172:LEU:HA	2:A:179:LEU:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:234:ARG:HG3	2:A:242:GLN:HB2	1.84	0.58
3:j:6:PRO:HB3	3:j:31:PHE:HB3	1.86	0.57
3:j:26:CYS:HB2	3:j:40:LEU:HD21	1.85	0.57
2:R:82:ARG:HH21	2:R:89:GLU:HB2	1.69	0.57
2:R:99:TYR:HB3	2:R:114:HIS:CD2	2.38	0.57
2:I:192:HIS:HE1	3:i:99:ASP:HB3	1.70	0.57
2:M:220:ASP:OD2	2:M:256:ARG:NH2	2.31	0.57
1:Z:9:VAL:HG13	2:K:143:THR:HG21	1.87	0.57
2:B:187:THR:HB	2:B:272:LEU:HD11	1.86	0.57
2:F:14:ARG:NH1	2:F:21:ARG:HB2	2.20	0.57
2:R:108:ARG:HH11	2:R:108:ARG:HG2	1.69	0.57
2:D:259:CYS:HB3	2:D:272:LEU:HB2	1.85	0.57
2:F:127:LYS:HD2	2:F:132:SER:HB2	1.85	0.57
2:H:253:GLN:HG2	2:H:256:ARG:NH1	2.20	0.57
2:O:207:SER:HA	2:O:240:THR:HB	1.86	0.57
3:b:74:THR:HG22	3:b:76:LYS:H	1.70	0.57
2:B:5:MET:HB2	2:B:168:LEU:HD13	1.85	0.57
2:Q:269:PRO:O	2:R:105:SER:OG	2.15	0.57
2:F:207:SER:HA	2:F:240:THR:HB	1.86	0.57
2:Q:70:HIS:O	2:Q:74:HIS:ND1	2.37	0.57
2:E:189:MET:HE3	2:E:217:TRP:HH2	1.70	0.56
2:H:214:THR:HB	2:H:262:GLN:HB2	1.87	0.56
2:D:93:HIS:CE1	3:d:1:MET:HE2	2.40	0.56
1:Z:7:ILE:HG21	2:K:152:VAL:HG13	1.87	0.56
2:A:35:ARG:NE	2:A:46:GLU:OE1	2.36	0.56
2:F:177:GLU:OE1	2:F:177:GLU:N	2.35	0.56
2:L:13:SER:HB3	2:L:78:LEU:HD13	1.86	0.56
2:R:99:TYR:HB3	2:R:114:HIS:HD2	1.68	0.56
2:R:121:LYS:NZ	3:r:1:MET:HA	2.20	0.56
2:I:127:LYS:HD2	2:I:132:SER:HB2	1.86	0.56
1:8:5:HIS:HD2	2:T:155:GLN:HB3	1.70	0.56
2:A:95:VAL:HG12	2:A:118:TYR:HD1	1.69	0.56
3:d:30:GLY:HA2	3:d:62:SER:HB3	1.86	0.56
2:P:96:GLN:HB2	2:P:117:ALA:HB3	1.86	0.56
2:D:192:HIS:CE1	3:d:99:ASP:HB3	2.40	0.56
2:K:214:THR:HB	2:K:262:GLN:HB2	1.86	0.56
2:M:5:MET:HB2	2:M:168:LEU:HD13	1.87	0.56
2:R:11:SER:HB3	2:R:95:VAL:HG23	1.87	0.56
2:T:207:SER:HA	2:T:240:THR:HB	1.87	0.56
2:B:93:HIS:ND1	2:B:118:TYR:OH	2.37	0.56
2:G:11:SER:HB3	2:G:95:VAL:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:131:ARG:HE	2:N:157:ARG:NH1	2.04	0.56
3:r:53:SER:O	3:r:65:LEU:HD11	2.05	0.56
2:C:13:SER:HB3	2:C:78:LEU:HD13	1.88	0.56
2:C:127:LYS:HD2	2:C:132:SER:HB2	1.88	0.56
2:P:189:MET:HE3	2:P:217:TRP:HH2	1.71	0.56
2:R:189:MET:HE3	2:R:217:TRP:HH2	1.71	0.56
2:L:72:GLN:O	2:L:75:ARG:HG2	2.05	0.56
2:O:37:ASP:HB3	2:O:40:ALA:HB2	1.88	0.56
1:x:7:ILE:HG21	2:H:152:VAL:HG13	1.86	0.56
2:S:37:ASP:HB3	2:S:40:ALA:HB2	1.86	0.56
2:T:11:SER:HB3	2:T:95:VAL:HG23	1.87	0.56
1:u:4:ASP:HA	2:B:66:LYS:HD3	1.88	0.55
2:B:107:TRP:O	2:B:169:ARG:NH1	2.33	0.55
2:E:93:HIS:ND1	2:E:118:TYR:OH	2.37	0.55
2:E:129:ASP:HA	2:F:256:ARG:HH12	1.71	0.55
2:F:202:ARG:HD2	2:F:244:TRP:CE3	2.41	0.55
2:H:14:ARG:HB3	2:H:17:ARG:HG3	1.87	0.55
2:C:70:HIS:O	2:C:74:HIS:ND1	2.31	0.55
2:H:131:ARG:HE	2:H:157:ARG:NH1	2.04	0.55
2:E:256:ARG:HH22	2:F:129:ASP:HA	1.72	0.55
2:J:111:ARG:HD3	2:J:128:GLU:OE2	2.06	0.55
2:M:87:GLN:OE1	2:M:118:TYR:OH	2.13	0.55
2:T:13:SER:HB3	2:T:78:LEU:HD13	1.89	0.55
1:x:1:TYR:HB2	2:H:63:GLU:OE2	2.06	0.55
2:F:154:GLU:OE1	2:F:154:GLU:N	2.37	0.55
2:A:154:GLU:OE1	2:A:154:GLU:N	2.39	0.55
2:D:9:PHE:HE2	2:D:99:TYR:HE2	1.55	0.55
2:F:24:ALA:HB3	2:F:36:PHE:HB3	1.87	0.55
3:n:6:PRO:HB3	3:n:31:PHE:HB3	1.87	0.55
2:P:37:ASP:HB3	2:P:40:ALA:HB2	1.89	0.55
2:G:165:VAL:HG12	2:G:169:ARG:NH1	2.22	0.55
3:t:26:CYS:HB2	3:t:40:LEU:HD21	1.88	0.55
2:C:35:ARG:NH1	2:C:37:ASP:HB2	2.22	0.55
2:S:122:ASP:OD1	3:s:61:TRP:NE1	2.32	0.55
2:F:123:TYR:HH	2:F:143:THR:HG1	1.51	0.55
2:R:6:ARG:HH21	2:R:101:CYS:N	2.05	0.55
2:T:122:ASP:OD1	3:t:61:TRP:NE1	2.32	0.55
2:J:14:ARG:HD2	2:J:17:ARG:NH1	2.22	0.55
2:K:202:ARG:HD3	2:K:246:ALA:HB2	1.89	0.55
2:L:153:ALA:O	2:L:157:ARG:HG3	2.07	0.55
2:O:202:ARG:HD3	2:O:246:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:187:THR:HB	2:P:272:LEU:HD11	1.89	0.55
3:p:6:PRO:HB3	3:p:31:PHE:HB3	1.88	0.55
2:R:14:ARG:NH2	2:R:39:ASP:OD1	2.40	0.55
2:R:220:ASP:OD2	2:R:256:ARG:NH1	2.40	0.55
2:H:74:HIS:HA	2:H:77:ASP:OD2	2.06	0.54
2:K:11:SER:HB3	2:K:95:VAL:HG23	1.90	0.54
2:L:122:ASP:OD1	3:l:61:TRP:NE1	2.21	0.54
2:C:37:ASP:HB3	2:C:40:ALA:HB2	1.88	0.54
2:R:35:ARG:HG2	2:R:48:ARG:HD3	1.89	0.54
2:L:218:GLN:OE1	2:L:260:HIS:NE2	2.40	0.54
2:Q:23:ILE:HG21	3:q:55:LEU:HB3	1.88	0.54
1:y:1:TYR:CE2	2:J:66:LYS:HE2	2.42	0.54
2:A:259:CYS:HB3	2:A:272:LEU:HB2	1.89	0.54
2:N:225:THR:C	2:N:227:ASP:H	2.16	0.54
2:N:235:PRO:HG2	3:n:66:LEU:HD22	1.88	0.54
2:Q:38:SER:O	2:Q:43:GLN:NE2	2.41	0.54
3:k:84:ASN:ND2	3:k:91:PRO:HG3	2.23	0.54
2:L:35:ARG:HG2	2:L:48:ARG:HD3	1.88	0.54
2:G:117:ALA:HB2	3:g:61:TRP:CE2	2.42	0.54
2:M:234:ARG:NH2	2:M:242:GLN:OE1	2.40	0.54
2:O:5:MET:HB2	2:O:168:LEU:HD13	1.89	0.54
2:O:13:SER:HB3	2:O:78:LEU:HD13	1.90	0.54
2:F:47:PRO:HB3	2:F:60:TRP:CH2	2.42	0.54
2:K:102:ASP:HB2	2:K:111:ARG:HB3	1.90	0.54
2:A:19:GLU:OE1	2:A:19:GLU:HA	2.08	0.54
2:F:220:ASP:OD2	2:F:256:ARG:NH1	2.41	0.54
2:M:95:VAL:HG12	2:M:118:TYR:HD1	1.72	0.54
2:M:154:GLU:OE1	2:M:154:GLU:N	2.40	0.54
2:Q:13:SER:HB3	2:Q:78:LEU:HD13	1.90	0.54
3:i:18:ASN:HD22	3:i:75:GLU:HG2	1.73	0.54
3:c:37:GLU:HB3	3:c:84:ASN:HB3	1.89	0.54
2:G:96:GLN:HB2	2:G:117:ALA:HB3	1.90	0.54
2:H:48:ARG:NH1	3:h:54:ASP:OD2	2.40	0.54
3:s:37:GLU:CD	2:I:106:ASP:HB2	2.33	0.54
2:Q:117:ALA:HB2	3:q:61:TRP:CE2	2.43	0.54
2:R:176:LYS:O	2:R:180:GLN:HB2	2.08	0.54
2:R:192:HIS:CE1	3:r:99:ASP:HB3	2.43	0.53
2:T:127:LYS:HD2	2:T:132:SER:HB2	1.89	0.53
2:B:19:GLU:OE2	2:B:75:ARG:NH2	2.41	0.53
3:l:26:CYS:HB2	3:l:40:LEU:HD21	1.90	0.53
2:I:122:ASP:OD1	3:i:61:TRP:NE1	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:8:PHE:HB2	2:F:25:VAL:HG23	1.90	0.53
2:P:23:ILE:HG21	3:p:55:LEU:HB3	1.89	0.53
2:P:47:PRO:HB3	2:P:60:TRP:CH2	2.43	0.53
1:3:1:TYR:CD2	2:O:66:LYS:NZ	2.77	0.53
2:C:117:ALA:HB2	3:c:61:TRP:CE2	2.44	0.53
2:D:6:ARG:NH2	2:D:102:ASP:OD1	2.39	0.53
2:G:85:TYR:HB2	2:G:87:GLN:HG3	1.90	0.53
2:Q:222:GLU:HB2	2:R:128:GLU:OE1	2.08	0.53
2:R:170:ARG:HH21	2:R:174:ASN:HD22	1.52	0.53
3:i:18:ASN:OD1	3:i:98:ARG:NH1	2.32	0.53
2:T:72:GLN:O	2:T:75:ARG:HG2	2.08	0.53
3:b:22:ASN:OD1	3:b:23:PHE:N	2.34	0.53
2:J:17:ARG:HG3	2:J:17:ARG:HH11	1.74	0.53
2:K:259:CYS:HB3	2:K:272:LEU:HB2	1.90	0.53
2:P:225:THR:C	2:P:227:ASP:H	2.16	0.53
2:R:37:ASP:HB3	2:R:40:ALA:HB2	1.91	0.53
2:T:19:GLU:OE2	2:T:75:ARG:NH2	2.39	0.53
1:X:7:ILE:O	2:G:73:THR:HG23	2.08	0.53
3:g:84:ASN:ND2	3:g:91:PRO:HG3	2.24	0.53
2:O:102:ASP:HB2	2:O:111:ARG:HB3	1.91	0.53
2:Q:154:GLU:N	2:Q:154:GLU:OE1	2.41	0.53
2:R:44:ARG:HG2	2:R:64:THR:HG21	1.91	0.53
1:U:1:TYR:CE2	2:A:66:LYS:NZ	2.76	0.53
2:L:176:LYS:O	2:L:180:GLN:HB2	2.09	0.53
2:M:255:GLN:O	2:M:273:ARG:NH1	2.42	0.53
2:O:44:ARG:HA	2:O:64:THR:HG23	1.91	0.53
2:R:8:PHE:HB2	2:R:25:VAL:HG23	1.91	0.53
2:I:77:ASP:OD2	2:I:116:TYR:OH	2.25	0.53
3:a:17:GLU:OE2	3:a:20:LYS:HD2	2.09	0.53
3:c:71:PHE:CZ	3:c:73:PRO:HG3	2.43	0.53
2:O:121:LYS:HG2	3:o:2:ILE:HD12	1.89	0.53
2:O:129:ASP:HA	2:P:256:ARG:HH22	1.73	0.53
2:O:259:CYS:HB3	2:O:272:LEU:HB2	1.90	0.53
3:d:17:GLU:HG2	3:d:20:LYS:HD3	1.90	0.52
2:H:107:TRP:O	2:H:169:ARG:NH1	2.41	0.52
2:M:66:LYS:NZ	1:1:1:TYR:OH	2.42	0.52
2:T:117:ALA:HB2	3:t:61:TRP:CE2	2.44	0.52
2:A:122:ASP:OD1	3:a:61:TRP:NE1	2.31	0.52
2:C:44:ARG:HA	2:C:64:THR:HG23	1.91	0.52
2:E:129:ASP:CA	2:F:256:ARG:HH12	2.22	0.52
2:F:87:GLN:OE1	2:F:118:TYR:OH	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:202:ARG:HD3	2:M:246:ALA:HB2	1.89	0.52
2:P:11:SER:HB3	2:P:95:VAL:HG23	1.91	0.52
2:I:72:GLN:O	2:I:75:ARG:HG2	2.09	0.52
1:5:2:VAL:HG23	2:Q:63:GLU:OE1	2.10	0.52
1:5:9:VAL:OXT	2:Q:80:THR:HG21	2.09	0.52
2:J:102:ASP:OD2	2:J:111:ARG:NH1	2.42	0.52
2:O:141:GLN:O	2:O:145:HIS:ND1	2.40	0.52
3:s:6:PRO:HB3	3:s:31:PHE:HB3	1.91	0.52
2:L:6:ARG:HD3	2:L:100:GLY:HA3	1.91	0.52
2:H:176:LYS:O	2:H:180:GLN:HB2	2.10	0.52
2:M:37:ASP:HB3	2:M:40:ALA:HB2	1.91	0.52
2:N:102:ASP:HB2	2:N:111:ARG:HB3	1.91	0.52
2:P:127:LYS:HD2	2:P:132:SER:HB2	1.92	0.52
2:R:225:THR:C	2:R:227:ASP:H	2.18	0.52
2:G:70:HIS:O	2:G:74:HIS:ND1	2.38	0.52
2:G:187:THR:HB	2:G:272:LEU:HD11	1.90	0.52
2:J:37:ASP:HB3	2:J:40:ALA:HB2	1.91	0.52
2:M:11:SER:HB3	2:M:95:VAL:HG22	1.91	0.52
1:w:1:TYR:CE2	2:F:66:LYS:NZ	2.78	0.52
3:c:4:ARG:NH1	3:c:62:SER:OG	2.42	0.52
2:M:168:LEU:O	2:M:172:LEU:HG	2.10	0.52
2:Q:202:ARG:HD3	2:Q:246:ALA:HB2	1.92	0.52
1:4:1:TYR:O	2:P:159:TYR:OH	2.27	0.52
3:b:6:PRO:HB3	3:b:31:PHE:HB3	1.92	0.52
2:E:127:LYS:HD2	2:E:132:SER:HB2	1.92	0.52
2:E:187:THR:HB	2:E:272:LEU:HD11	1.91	0.52
2:M:8:PHE:HB2	2:M:25:VAL:HG23	1.92	0.52
2:O:11:SER:HB3	2:O:95:VAL:HG23	1.92	0.52
2:F:225:THR:C	2:F:227:ASP:H	2.17	0.51
2:H:225:THR:C	2:H:227:ASP:H	2.18	0.51
2:S:47:PRO:HB3	2:S:60:TRP:CH2	2.45	0.51
3:i:18:ASN:ND2	3:i:75:GLU:HG2	2.24	0.51
1:8:1:TYR:O	2:T:159:TYR:OH	2.23	0.51
2:B:168:LEU:O	2:B:172:LEU:HG	2.11	0.51
2:E:225:THR:C	2:E:227:ASP:H	2.19	0.51
2:J:14:ARG:HD2	2:J:17:ARG:HH11	1.75	0.51
2:N:19:GLU:OE1	2:N:75:ARG:NH2	2.43	0.51
2:P:82:ARG:HH21	2:P:89:GLU:HB2	1.75	0.51
2:R:63:GLU:O	2:R:67:VAL:HG12	2.11	0.51
2:G:38:SER:O	2:G:43:GLN:NE2	2.43	0.51
2:K:33:PHE:CD2	2:K:34:VAL:HG13	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:107:TRP:HB3	2:K:169:ARG:HD3	1.93	0.51
2:M:19:GLU:HB3	2:M:20:PRO:HD2	1.93	0.51
2:M:108:ARG:HA	2:M:169:ARG:HH21	1.75	0.51
2:J:11:SER:HB3	2:J:95:VAL:HG23	1.93	0.51
2:O:35:ARG:HD3	3:o:54:ASP:OD2	2.10	0.51
2:P:81:LEU:HA	2:P:84:TYR:HD2	1.75	0.51
2:I:192:HIS:CE1	3:i:99:ASP:HB3	2.45	0.51
2:T:5:MET:HE2	2:T:164:CYS:SG	2.51	0.51
2:T:15:PRO:HD2	2:T:17:ARG:HH12	1.76	0.51
2:J:35:ARG:HD2	2:J:48:ARG:HE	1.75	0.51
2:H:19:GLU:HB3	2:H:20:PRO:HD2	1.92	0.51
2:S:187:THR:HB	2:S:272:LEU:HD11	1.93	0.51
2:K:230:LEU:HD13	2:K:245:ALA:HB2	1.92	0.51
1:4:1:TYR:CE2	1:4:4:ASP:OD2	2.64	0.51
2:F:5:MET:HE2	2:F:164:CYS:SG	2.51	0.51
3:g:6:PRO:HB3	3:g:31:PHE:HB3	1.93	0.51
2:B:177:GLU:CD	2:B:177:GLU:H	2.19	0.51
2:D:47:PRO:HB3	2:D:60:TRP:CH2	2.46	0.51
2:E:13:SER:HB3	2:E:78:LEU:HD13	1.91	0.51
2:E:97:ARG:NH2	2:E:116:TYR:OH	2.38	0.51
2:G:72:GLN:O	2:G:75:ARG:HG2	2.10	0.51
3:s:26:CYS:HB2	3:s:40:LEU:HD21	1.91	0.51
3:i:6:PRO:HB3	3:i:31:PHE:HB3	1.93	0.51
2:D:219:ARG:HD3	2:D:257:TYR:CZ	2.46	0.51
2:F:51:TRP:CZ2	2:F:179:LEU:HD11	2.45	0.51
2:H:5:MET:HE2	2:H:164:CYS:SG	2.51	0.51
2:N:122:ASP:OD1	3:n:61:TRP:NE1	2.31	0.51
2:R:19:GLU:OE2	2:R:75:ARG:NH2	2.44	0.51
2:B:35:ARG:HG2	2:B:48:ARG:HD3	1.93	0.51
3:f:30:GLY:HA2	3:f:62:SER:HB3	1.92	0.51
2:J:108:ARG:HE	3:t:37:GLU:CD	2.18	0.51
2:J:192:HIS:CE1	3:j:99:ASP:HB3	2.46	0.51
2:G:92:SER:C	2:G:93:HIS:HD2	2.19	0.50
2:J:35:ARG:HG2	2:J:36:PHE:N	2.26	0.50
2:N:259:CYS:HB3	2:N:272:LEU:HB2	1.93	0.50
2:A:207:SER:HA	2:A:240:THR:HB	1.93	0.50
2:C:22:PHE:HB3	2:C:38:SER:HB2	1.92	0.50
2:G:192:HIS:HB2	2:G:200:THR:HB	1.92	0.50
2:H:111:ARG:HD3	2:H:128:GLU:OE2	2.11	0.50
2:P:182:THR:HG21	2:P:264:GLU:HG2	1.92	0.50
2:B:219:ARG:NH1	2:C:122:ASP:OD2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:8:PHE:HB3	3:s:57:PHE:CE1	2.46	0.50
2:P:11:SER:HA	2:P:21:ARG:O	2.11	0.50
2:G:63:GLU:OE1	2:G:66:LYS:NZ	2.44	0.50
2:H:202:ARG:HD3	2:H:246:ALA:HB2	1.92	0.50
2:E:6:ARG:NH1	2:E:113:TYR:CD2	2.79	0.50
2:E:122:ASP:OD1	3:e:360:TRP:NE1	2.24	0.50
3:r:74:THR:HG23	2:T:193:ALA:HB3	1.93	0.50
3:b:31:PHE:HZ	3:b:65:LEU:HD23	1.77	0.50
2:E:9:PHE:HE2	2:E:99:TYR:CE2	2.29	0.50
2:P:154:GLU:N	2:P:154:GLU:OE1	2.44	0.50
2:R:19:GLU:OE2	2:R:75:ARG:NH1	2.45	0.50
2:I:189:MET:HE3	2:I:217:TRP:HH2	1.77	0.50
1:Z:1:TYR:CZ	2:K:66:LYS:NZ	2.76	0.50
2:B:19:GLU:HB3	2:B:20:PRO:HD2	1.93	0.50
2:E:209:TYR:CD1	2:E:210:PRO:HA	2.47	0.50
2:F:14:ARG:HB3	2:F:17:ARG:HG3	1.94	0.50
2:I:117:ALA:HB2	3:i:61:TRP:CE2	2.47	0.50
1:x:7:ILE:HG21	2:H:152:VAL:CG1	2.42	0.50
2:A:114:HIS:CE1	2:A:116:TYR:HE2	2.29	0.50
2:N:207:SER:HA	2:N:240:THR:HB	1.94	0.50
1:u:1:TYR:HB2	2:B:167:TRP:CD2	2.47	0.50
2:B:92:SER:C	2:B:93:HIS:HD2	2.20	0.50
2:E:5:MET:HE2	2:E:164:CYS:SG	2.52	0.50
2:F:186:LYS:HD2	2:F:207:SER:HB2	1.94	0.50
2:M:117:ALA:HB2	3:m:61:TRP:CE2	2.47	0.50
3:m:38:VAL:HG22	3:m:83:VAL:HG13	1.93	0.50
2:N:202:ARG:HD3	2:N:246:ALA:HB2	1.94	0.50
2:I:100:GLY:O	2:I:160:LEU:HD23	2.11	0.50
1:W:4:ASP:HA	2:E:66:LYS:HD3	1.94	0.49
2:G:225:THR:C	2:G:227:ASP:H	2.20	0.49
2:H:218:GLN:OE1	2:H:260:HIS:NE2	2.45	0.49
3:j:71:PHE:CZ	3:j:73:PRO:HG3	2.47	0.49
2:R:130:LEU:HB2	2:R:157:ARG:HH11	1.77	0.49
1:U:7:ILE:HG21	2:A:152:VAL:CG1	2.42	0.49
2:C:234:ARG:NH2	2:C:242:GLN:OE1	2.45	0.49
2:E:181:ARG:HH11	2:E:183:ASP:CG	2.13	0.49
3:k:74:THR:HG22	3:k:76:LYS:H	1.77	0.49
2:P:168:LEU:O	2:P:172:LEU:HG	2.12	0.49
2:Q:203:CYS:HB2	2:Q:217:TRP:CZ2	2.47	0.49
1:4:2:VAL:HG23	2:P:63:GLU:OE1	2.13	0.49
1:v:3:LEU:HD23	2:D:97:ARG:HH12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:35:ARG:HB2	3:a:54:ASP:OD2	2.12	0.49
2:C:12:VAL:O	2:C:21:ARG:N	2.45	0.49
2:E:20:PRO:HG3	2:E:75:ARG:HG3	1.95	0.49
2:S:9:PHE:HE2	2:S:99:TYR:CE2	2.31	0.49
2:R:12:VAL:O	2:R:21:ARG:N	2.44	0.49
2:R:133:TRP:HB2	2:R:144:LYS:HG3	1.95	0.49
3:i:26:CYS:HB2	3:i:40:LEU:HD21	1.94	0.49
2:H:63:GLU:O	2:H:67:VAL:HG12	2.12	0.49
2:J:97:ARG:NH2	2:J:116:TYR:OH	2.42	0.49
2:O:234:ARG:HD2	3:o:11:TYR:CE1	2.47	0.49
3:o:12:SER:OG	3:o:14:HIS:O	2.23	0.49
3:o:74:THR:HG22	3:o:76:LYS:H	1.78	0.49
2:R:47:PRO:HB3	2:R:60:TRP:CH2	2.47	0.49
2:R:117:ALA:HB2	3:r:61:TRP:CE2	2.47	0.49
2:I:38:SER:O	2:I:43:GLN:NE2	2.44	0.49
2:T:192:HIS:CE1	3:t:99:ASP:HB3	2.47	0.49
1:W:1:TYR:HD2	2:E:63:GLU:OE2	1.96	0.49
2:C:238:ASP:HB3	3:c:13:ARG:HH11	1.77	0.49
2:H:209:TYR:CD1	2:H:210:PRO:HA	2.47	0.49
2:N:87:GLN:OE1	2:N:118:TYR:OH	2.26	0.49
2:N:192:HIS:NE2	3:n:99:ASP:HB3	2.27	0.49
2:O:5:MET:HE2	2:O:164:CYS:SG	2.53	0.49
2:O:109:PHE:HB2	2:O:165:VAL:HG21	1.94	0.49
1:4:5:HIS:ND1	2:P:155:GLN:HG2	2.28	0.49
3:d:74:THR:HG22	3:d:76:LYS:N	2.28	0.49
2:H:202:ARG:HD2	2:H:244:TRP:CE3	2.48	0.49
3:s:16:ALA:HB3	3:s:98:ARG:HG3	1.93	0.49
2:J:106:ASP:OD1	2:J:106:ASP:N	2.45	0.49
2:L:168:LEU:O	2:L:172:LEU:HG	2.13	0.49
2:I:5:MET:HE2	2:I:164:CYS:SG	2.53	0.49
1:W:1:TYR:O	2:E:159:TYR:OH	2.26	0.49
2:A:19:GLU:HB3	2:A:20:PRO:HD2	1.94	0.49
2:F:19:GLU:HB3	2:F:20:PRO:HD2	1.93	0.49
2:F:97:ARG:NH2	2:F:116:TYR:OH	2.37	0.49
3:g:80:ALA:HB2	3:g:95:LYS:HG2	1.95	0.49
2:J:189:MET:HE2	2:J:201:LEU:HD13	1.95	0.49
2:O:117:ALA:HB2	3:o:61:TRP:CE2	2.48	0.49
2:Q:129:ASP:O	2:R:256:ARG:NH2	2.43	0.49
3:e:330:PHE:HZ	3:e:364:LEU:HD23	1.77	0.49
3:j:18:ASN:OD1	3:j:98:ARG:NH1	2.37	0.49
2:I:14:ARG:NH1	2:I:21:ARG:HB2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:ARG:NH2	2:B:116:TYR:OH	2.38	0.49
2:F:209:TYR:CD1	2:F:210:PRO:HA	2.48	0.49
2:J:105:SER:OG	3:t:82:ARG:NH1	2.45	0.49
2:M:80:THR:HG21	1:l:9:VAL:OXT	2.13	0.49
2:P:209:TYR:CD1	2:P:210:PRO:HA	2.48	0.49
2:Q:234:ARG:HD2	3:q:11:TYR:CE1	2.48	0.49
3:q:7:LYS:O	3:q:28:VAL:HA	2.12	0.49
2:R:44:ARG:HA	2:R:64:THR:HG23	1.93	0.49
2:E:202:ARG:HD3	2:E:246:ALA:HB2	1.95	0.48
2:H:48:ARG:NH1	3:h:54:ASP:CG	2.70	0.48
2:H:70:HIS:O	2:H:74:HIS:ND1	2.45	0.48
2:P:72:GLN:O	2:P:75:ARG:HG2	2.13	0.48
1:3:9:VAL:OXT	2:O:80:THR:HG21	2.13	0.48
2:D:37:ASP:HB3	2:D:40:ALA:HB2	1.95	0.48
2:J:72:GLN:O	2:J:75:ARG:HG2	2.13	0.48
2:Q:72:GLN:O	2:Q:75:ARG:HG2	2.13	0.48
1:U:2:VAL:HG23	2:A:63:GLU:OE1	2.14	0.48
2:C:192:HIS:O	2:C:200:THR:N	2.39	0.48
2:J:154:GLU:N	2:J:154:GLU:OE1	2.46	0.48
2:O:6:ARG:NH1	2:O:113:TYR:CE1	2.81	0.48
2:G:23:ILE:HG21	3:g:55:LEU:HB3	1.95	0.48
2:S:168:LEU:O	2:S:172:LEU:HG	2.13	0.48
2:Q:168:LEU:O	2:Q:172:LEU:HG	2.14	0.48
3:t:6:PRO:HB3	3:t:31:PHE:HB3	1.95	0.48
3:d:6:PRO:HB3	3:d:31:PHE:HB3	1.95	0.48
2:E:5:MET:HB2	2:E:168:LEU:HD13	1.94	0.48
2:H:48:ARG:HH22	3:h:54:ASP:H	1.61	0.48
2:S:21:ARG:HE	2:S:23:ILE:HD11	1.78	0.48
2:T:202:ARG:HD2	2:T:244:TRP:CE3	2.48	0.48
1:Z:7:ILE:HG21	2:K:152:VAL:CG1	2.44	0.48
2:H:35:ARG:HH11	3:h:54:ASP:CG	2.21	0.48
2:H:92:SER:C	2:H:93:HIS:HD2	2.22	0.48
2:O:44:ARG:HG2	2:O:64:THR:HG21	1.96	0.48
2:O:154:GLU:N	2:O:154:GLU:OE1	2.46	0.48
2:B:72:GLN:O	2:B:75:ARG:HG2	2.13	0.48
2:H:111:ARG:HG2	2:H:112:GLY:H	1.79	0.48
2:H:254:GLU:HB3	2:H:274:TRP:HD1	1.79	0.48
2:K:63:GLU:O	2:K:67:VAL:HG12	2.14	0.48
2:M:5:MET:HE2	2:M:164:CYS:SG	2.54	0.48
2:P:82:ARG:HE	2:P:89:GLU:HA	1.79	0.48
2:R:72:GLN:O	2:R:75:ARG:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:176:LYS:O	2:A:180:GLN:HB2	2.13	0.48
2:B:55:GLU:OE2	2:B:170:ARG:NH2	2.46	0.48
2:H:207:SER:HA	2:H:240:THR:HB	1.94	0.48
2:S:154:GLU:N	2:S:154:GLU:OE1	2.45	0.48
2:J:122:ASP:OD1	3:j:61:TRP:NE1	2.39	0.48
2:J:187:THR:HB	2:J:272:LEU:HD11	1.95	0.48
2:K:253:GLN:HG2	2:K:256:ARG:HD3	1.96	0.48
2:O:51:TRP:HA	2:O:54:GLN:HE22	1.79	0.48
3:f:7:LYS:O	3:f:28:VAL:HA	2.13	0.48
2:S:172:LEU:HA	2:S:179:LEU:HD11	1.94	0.48
2:N:5:MET:HE2	2:N:164:CYS:SG	2.53	0.48
2:N:219:ARG:HB2	2:N:257:TYR:CE2	2.49	0.48
2:O:133:TRP:HB2	2:O:144:LYS:HG3	1.96	0.48
3:c:13:ARG:HE	3:c:23:PHE:HB2	1.79	0.48
2:D:8:PHE:HB2	2:D:25:VAL:HG23	1.96	0.48
2:J:9:PHE:HE2	2:J:99:TYR:CE2	2.31	0.48
2:N:154:GLU:N	2:N:154:GLU:OE1	2.47	0.48
2:D:5:MET:HE2	2:D:164:CYS:SG	2.54	0.47
2:E:82:ARG:HD2	2:E:89:GLU:HA	1.96	0.47
2:E:117:ALA:HB2	3:e:360:TRP:CE2	2.49	0.47
2:G:5:MET:HB2	2:G:168:LEU:HD13	1.96	0.47
2:G:9:PHE:HE2	2:G:99:TYR:CE2	2.32	0.47
2:G:154:GLU:N	2:G:154:GLU:OE1	2.44	0.47
2:S:202:ARG:HD2	2:S:244:TRP:CE3	2.49	0.47
2:K:176:LYS:O	2:K:180:GLN:HB2	2.15	0.47
3:c:40:LEU:HD12	3:c:50:VAL:HG12	1.96	0.47
2:F:13:SER:HA	2:F:20:PRO:HB3	1.95	0.47
2:S:106:ASP:N	2:S:106:ASP:OD1	2.47	0.47
2:J:207:SER:HA	2:J:240:THR:HB	1.96	0.47
2:K:8:PHE:HB2	2:K:25:VAL:HG23	1.96	0.47
2:R:19:GLU:OE2	2:R:75:ARG:CZ	2.62	0.47
2:F:219:ARG:HD3	2:F:257:TYR:CZ	2.49	0.47
2:H:79:GLY:HA2	2:H:82:ARG:CZ	2.44	0.47
2:Q:62:GLY:C	2:Q:66:LYS:HZ2	2.23	0.47
2:B:8:PHE:HB2	2:B:25:VAL:HG23	1.97	0.47
2:C:234:ARG:HD2	3:c:11:TYR:CE1	2.50	0.47
3:c:65:LEU:HD23	3:c:65:LEU:C	2.40	0.47
2:G:63:GLU:CD	2:G:66:LYS:NZ	2.73	0.47
2:H:96:GLN:HB2	2:H:117:ALA:HB3	1.97	0.47
2:S:23:ILE:HG21	3:s:55:LEU:HB3	1.97	0.47
2:L:27:TYR:CE2	2:L:32:GLN:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9:PHE:HE2	2:D:99:TYR:CE2	2.33	0.47
2:S:11:SER:HB3	2:S:95:VAL:HG23	1.97	0.47
2:N:218:GLN:OE1	2:N:260:HIS:NE2	2.47	0.47
2:P:258:THR:HG22	2:P:273:ARG:HG2	1.96	0.47
2:A:225:THR:C	2:A:227:ASP:H	2.23	0.47
2:B:63:GLU:O	2:B:67:VAL:HG12	2.15	0.47
2:B:117:ALA:HB2	3:b:61:TRP:CE2	2.49	0.47
2:E:133:TRP:HB2	2:E:144:LYS:HG3	1.96	0.47
2:E:168:LEU:O	2:E:172:LEU:HG	2.15	0.47
2:G:44:ARG:HA	2:G:64:THR:HG23	1.97	0.47
2:G:181:ARG:NH1	2:G:183:ASP:OD2	2.48	0.47
2:H:21:ARG:HH21	2:H:37:ASP:CG	2.23	0.47
2:J:8:PHE:HB2	2:J:25:VAL:HG23	1.96	0.47
2:J:155:GLN:HA	2:J:155:GLN:HE21	1.80	0.47
2:N:70:HIS:O	2:N:74:HIS:ND1	2.46	0.47
2:O:81:LEU:HD23	2:O:84:TYR:HD2	1.79	0.47
2:P:207:SER:HA	2:P:240:THR:HB	1.96	0.47
2:Q:105:SER:OG	2:R:269:PRO:O	2.22	0.47
2:I:234:ARG:NH2	2:I:242:GLN:OE1	2.47	0.47
2:T:8:PHE:HB2	2:T:25:VAL:HG23	1.96	0.47
1:w:2:VAL:HG23	2:F:63:GLU:OE1	2.15	0.47
2:F:202:ARG:HD3	2:F:246:ALA:HB2	1.97	0.47
2:J:192:HIS:HE1	3:j:99:ASP:HB3	1.79	0.47
2:M:95:VAL:HG12	2:M:118:TYR:CD1	2.50	0.47
2:O:85:TYR:HB2	2:O:87:GLN:HG3	1.97	0.47
3:a:30:GLY:HA2	3:a:62:SER:OG	2.15	0.47
3:c:71:PHE:CE2	3:c:73:PRO:HG3	2.50	0.47
3:g:7:LYS:HD2	3:g:30:GLY:HA3	1.96	0.47
2:S:8:PHE:HB2	2:S:25:VAL:HG23	1.97	0.47
2:K:92:SER:C	2:K:93:HIS:HD2	2.22	0.47
2:N:47:PRO:HB3	2:N:60:TRP:CH2	2.49	0.47
2:N:202:ARG:HD2	2:N:244:TRP:CE3	2.50	0.47
3:e:329:GLY:HA2	3:e:361:SER:HB3	1.97	0.47
2:A:219:ARG:NH1	2:A:256:ARG:HH22	2.13	0.47
2:K:44:ARG:HA	2:K:64:THR:HG23	1.96	0.47
3:k:40:LEU:HD12	3:k:50:VAL:HG13	1.97	0.47
2:O:8:PHE:HB3	3:o:57:PHE:CE1	2.50	0.47
2:O:168:LEU:O	2:O:172:LEU:HG	2.15	0.47
2:O:273:ARG:NE	2:P:106:ASP:OD2	2.43	0.47
2:F:117:ALA:HB2	3:f:61:TRP:CE2	2.50	0.46
2:G:5:MET:HE2	2:G:164:CYS:SG	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:15:PRO:HD2	2:G:17:ARG:HH12	1.80	0.46
2:K:213:ILE:HG13	2:K:263:HIS:HB2	1.97	0.46
1:4:1:TYR:CE2	2:P:66:LYS:HE2	2.49	0.46
2:E:92:SER:C	2:E:93:HIS:HD2	2.22	0.46
2:F:5:MET:HG3	2:F:28:VAL:HG22	1.97	0.46
2:F:254:GLU:OE1	2:F:254:GLU:N	2.46	0.46
2:H:13:SER:HB3	2:H:78:LEU:HD13	1.97	0.46
2:M:189:MET:HE3	2:M:217:TRP:HH2	1.80	0.46
2:I:47:PRO:HB3	2:I:60:TRP:CH2	2.50	0.46
3:a:78:GLU:C	3:a:79:TYR:HD2	2.24	0.46
2:C:49:ALA:O	2:C:52:ILE:HG22	2.15	0.46
2:C:207:SER:HA	2:C:240:THR:HB	1.97	0.46
2:J:47:PRO:HB3	2:J:60:TRP:CH2	2.50	0.46
3:r:30:GLY:HA2	3:r:62:SER:HB3	1.96	0.46
2:T:131:ARG:NH2	2:T:157:ARG:HH12	1.92	0.46
1:W:1:TYR:CD2	2:E:63:GLU:OE2	2.68	0.46
1:Z:1:TYR:CE2	2:K:66:LYS:NZ	2.82	0.46
2:C:259:CYS:HB3	2:C:272:LEU:HB2	1.98	0.46
2:E:8:PHE:HB2	2:E:25:VAL:HG23	1.98	0.46
2:E:9:PHE:HE2	2:E:99:TYR:HE2	1.64	0.46
2:S:218:GLN:OE1	2:S:260:HIS:NE2	2.48	0.46
3:l:23:PHE:CE2	3:l:70:GLU:HG2	2.50	0.46
2:P:202:ARG:HD2	2:P:244:TRP:CE3	2.50	0.46
2:R:207:SER:HA	2:R:240:THR:HB	1.97	0.46
2:D:35:ARG:NE	2:D:46:GLU:OE1	2.49	0.46
2:N:55:GLU:CD	2:N:170:ARG:NH1	2.73	0.46
2:O:225:THR:C	2:O:227:ASP:H	2.23	0.46
3:q:37:GLU:O	3:q:83:VAL:HA	2.16	0.46
3:b:2:ILE:HD11	2:C:250:PRO:HG3	1.97	0.46
2:F:82:ARG:HG3	2:F:87:GLN:HE21	1.81	0.46
2:G:81:LEU:HD23	2:G:84:TYR:HD2	1.81	0.46
2:S:117:ALA:HB2	3:s:61:TRP:CE2	2.50	0.46
2:J:117:ALA:HB2	3:j:61:TRP:CE2	2.50	0.46
2:K:24:ALA:HB3	2:K:36:PHE:HB3	1.98	0.46
2:L:254:GLU:OE1	2:L:254:GLU:N	2.48	0.46
2:P:106:ASP:OD1	2:P:106:ASP:N	2.48	0.46
3:p:23:PHE:CE2	3:p:70:GLU:HG2	2.50	0.46
2:R:24:ALA:HB3	2:R:36:PHE:HB3	1.97	0.46
2:I:106:ASP:N	2:I:106:ASP:OD1	2.48	0.46
1:v:9:VAL:HG23	2:D:143:THR:HG21	1.97	0.46
2:A:5:MET:HE2	2:A:164:CYS:SG	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:186:LYS:HD2	2:C:207:SER:HB2	1.97	0.46
2:S:6:ARG:NH1	2:S:102:ASP:OD1	2.47	0.46
2:N:37:ASP:HB3	2:N:40:ALA:HB2	1.98	0.46
2:I:168:LEU:O	2:I:172:LEU:HG	2.15	0.46
2:T:106:ASP:OD1	2:T:106:ASP:N	2.48	0.46
2:T:234:ARG:HG3	2:T:242:GLN:HB2	1.97	0.46
2:B:5:MET:HE2	2:B:164:CYS:SG	2.56	0.46
2:J:189:MET:HE3	2:J:217:TRP:HH2	1.81	0.46
2:M:8:PHE:HB3	3:m:57:PHE:CE1	2.50	0.46
2:M:107:TRP:O	2:M:169:ARG:NE	2.46	0.46
2:R:5:MET:HB2	2:R:168:LEU:HD13	1.96	0.46
2:R:121:LYS:HZ2	3:r:1:MET:HA	1.81	0.46
2:B:8:PHE:HB3	3:b:57:PHE:CE1	2.51	0.46
3:f:4:ARG:NH1	3:f:62:SER:OG	2.49	0.46
2:J:72:GLN:CD	2:J:75:ARG:HD3	2.40	0.46
2:J:168:LEU:O	2:J:172:LEU:HG	2.16	0.46
2:L:183:ASP:HB2	2:L:209:TYR:H	1.81	0.46
2:P:25:VAL:HG13	2:P:32:GLN:HE21	1.81	0.46
2:I:23:ILE:HG21	3:i:55:LEU:HB3	1.98	0.46
1:W:2:VAL:HG13	2:E:66:LYS:HD2	1.98	0.46
3:b:71:PHE:CE2	3:b:73:PRO:HG3	2.51	0.46
2:D:5:MET:HB2	2:D:168:LEU:HD13	1.98	0.46
2:G:19:GLU:HB3	2:G:20:PRO:HD2	1.98	0.46
2:H:106:ASP:OD1	2:H:106:ASP:N	2.49	0.46
2:N:9:PHE:HE2	2:N:99:TYR:CE2	2.30	0.46
2:T:35:ARG:HG2	2:T:48:ARG:HD3	1.98	0.46
1:3:6:LEU:HD12	2:O:73:THR:OG1	2.16	0.45
2:D:27:TYR:CE2	2:D:32:GLN:HB2	2.52	0.45
2:H:11:SER:HB3	2:H:95:VAL:HG22	1.98	0.45
2:J:137:ASP:OD1	2:J:137:ASP:N	2.48	0.45
3:k:10:VAL:HG13	3:k:96:TRP:HA	1.97	0.45
2:L:49:ALA:O	2:L:52:ILE:HG22	2.16	0.45
2:L:64:THR:HG22	2:L:68:LYS:HE3	1.98	0.45
2:T:92:SER:C	2:T:93:HIS:HD2	2.23	0.45
1:v:2:VAL:HG23	2:D:63:GLU:OE1	2.16	0.45
2:N:13:SER:HB3	2:N:78:LEU:HD13	1.97	0.45
2:P:219:ARG:HD3	2:P:257:TYR:CZ	2.51	0.45
2:Q:207:SER:HA	2:Q:240:THR:HB	1.97	0.45
2:B:106:ASP:OD1	2:B:106:ASP:N	2.50	0.45
2:C:107:TRP:O	2:C:169:ARG:HD2	2.16	0.45
2:E:19:GLU:HB3	2:E:20:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:253:GLN:HG2	2:F:256:ARG:HG3	1.99	0.45
2:G:235:PRO:O	3:g:11:TYR:OH	2.23	0.45
2:S:4:SER:HB2	2:S:6:ARG:NH1	2.31	0.45
2:K:178:THR:O	2:K:181:ARG:NE	2.48	0.45
2:M:69:ALA:HB1	1:1:6:LEU:HD11	1.99	0.45
2:R:106:ASP:OD1	2:R:106:ASP:N	2.49	0.45
2:I:63:GLU:O	2:I:67:VAL:HG12	2.16	0.45
1:y:1:TYR:OH	1:y:4:ASP:OD2	2.20	0.45
1:U:5:HIS:CE1	2:A:155:GLN:HG3	2.52	0.45
2:C:192:HIS:NE2	3:c:99:ASP:HB3	2.31	0.45
2:G:202:ARG:HD2	2:G:244:TRP:CE3	2.51	0.45
2:J:19:GLU:HB3	2:J:20:PRO:HD2	1.97	0.45
2:K:258:THR:HG22	2:K:273:ARG:HG3	1.99	0.45
2:L:111:ARG:HD2	2:L:113:TYR:CE2	2.52	0.45
2:P:202:ARG:HD3	2:P:246:ALA:HB2	1.97	0.45
2:R:131:ARG:HH21	2:R:157:ARG:NH2	2.14	0.45
2:R:170:ARG:NE	2:R:174:ASN:ND2	2.60	0.45
2:D:207:SER:HA	2:D:240:THR:HB	1.98	0.45
3:g:53:SER:O	3:g:65:LEU:HD11	2.16	0.45
2:N:35:ARG:HD3	3:n:54:ASP:OD2	2.16	0.45
2:N:72:GLN:O	2:N:75:ARG:HG2	2.17	0.45
2:N:106:ASP:N	2:N:106:ASP:OD1	2.49	0.45
2:N:126:LEU:HD12	2:N:132:SER:O	2.16	0.45
2:T:9:PHE:HE2	2:T:99:TYR:CE2	2.34	0.45
2:D:95:VAL:HG22	2:D:118:TYR:HD1	1.80	0.45
2:G:49:ALA:O	2:G:52:ILE:HG22	2.17	0.45
2:S:204:TRP:HE3	2:S:206:LEU:HD21	1.82	0.45
2:J:35:ARG:HD2	2:J:48:ARG:NE	2.32	0.45
2:K:225:THR:C	2:K:227:ASP:H	2.25	0.45
2:M:172:LEU:HA	2:M:179:LEU:HD11	1.99	0.45
2:O:137:ASP:O	2:O:141:GLN:HG2	2.16	0.45
2:P:35:ARG:HG2	2:P:48:ARG:HD3	1.99	0.45
3:a:71:PHE:CZ	3:a:73:PRO:HG3	2.51	0.45
2:P:192:HIS:O	2:P:200:THR:N	2.32	0.45
2:Q:225:THR:C	2:Q:227:ASP:H	2.24	0.45
2:R:209:TYR:CD1	2:R:210:PRO:HA	2.51	0.45
2:T:155:GLN:HA	2:T:155:GLN:HE21	1.81	0.45
3:b:78:GLU:C	3:b:79:TYR:HD2	2.25	0.45
2:G:35:ARG:HG2	2:G:48:ARG:HD3	1.99	0.45
2:H:95:VAL:HG12	2:H:118:TYR:HD1	1.82	0.45
2:K:254:GLU:OE1	2:K:254:GLU:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:64:THR:HG22	2:N:68:LYS:HE2	1.99	0.45
2:Q:97:ARG:HE	2:Q:116:TYR:HE2	1.63	0.45
2:A:8:PHE:HB2	2:A:25:VAL:HG22	1.99	0.45
2:B:47:PRO:HB3	2:B:60:TRP:CH2	2.51	0.45
2:E:103:VAL:HG13	2:E:108:ARG:O	2.17	0.45
2:F:11:SER:HB3	2:F:95:VAL:HG23	1.99	0.45
2:I:207:SER:HA	2:I:240:THR:HB	1.98	0.45
2:T:19:GLU:HB3	2:T:20:PRO:HD2	1.98	0.45
2:A:106:ASP:OD1	2:A:106:ASP:N	2.50	0.45
2:B:13:SER:O	2:B:15:PRO:HD3	2.17	0.45
2:C:33:PHE:CD2	2:C:34:VAL:HG13	2.52	0.45
2:S:207:SER:HA	2:S:240:THR:HB	1.98	0.45
2:J:254:GLU:OE1	2:J:254:GLU:N	2.48	0.45
2:K:35:ARG:HH21	2:K:46:GLU:CD	2.25	0.45
2:K:202:ARG:HD2	2:K:244:TRP:CE3	2.51	0.45
3:k:30:GLY:HA2	3:k:62:SER:OG	2.17	0.45
2:M:33:PHE:CD2	2:M:34:VAL:HG13	2.52	0.45
3:m:38:VAL:HB	3:m:67:TYR:CE2	2.51	0.45
2:Q:266:LEU:HD13	2:Q:270:LEU:HG	1.98	0.45
1:w:1:TYR:HD2	2:F:63:GLU:OE2	2.00	0.44
2:C:141:GLN:O	2:C:145:HIS:ND1	2.50	0.44
2:G:234:ARG:NH1	3:g:11:TYR:HB3	2.33	0.44
2:S:192:HIS:O	2:S:200:THR:N	2.30	0.44
2:L:231:VAL:O	2:L:243:LYS:HE3	2.17	0.44
2:M:137:ASP:OD1	2:M:137:ASP:N	2.49	0.44
2:O:254:GLU:OE1	2:O:254:GLU:N	2.46	0.44
2:P:22:PHE:CD2	2:P:71:SER:HB2	2.52	0.44
2:P:80:THR:HG22	2:P:84:TYR:CE2	2.52	0.44
2:I:9:PHE:HE2	2:I:99:TYR:CE2	2.35	0.44
2:I:254:GLU:OE1	2:I:254:GLU:N	2.48	0.44
1:X:1:TYR:HD2	2:G:63:GLU:OE2	2.00	0.44
2:A:117:ALA:HB2	3:a:61:TRP:CE2	2.52	0.44
2:B:49:ALA:O	2:B:52:ILE:HG22	2.17	0.44
2:B:189:MET:HE2	2:B:201:LEU:HD22	1.99	0.44
3:g:71:PHE:CE2	3:g:73:PRO:HG3	2.52	0.44
3:g:78:GLU:C	3:g:79:TYR:HD2	2.25	0.44
2:H:47:PRO:HB3	2:H:60:TRP:CH2	2.52	0.44
2:L:254:GLU:HB3	2:L:274:TRP:CD1	2.51	0.44
2:R:108:ARG:HG2	2:R:108:ARG:NH1	2.31	0.44
2:G:22:PHE:CD2	2:G:71:SER:HB2	2.53	0.44
2:K:106:ASP:OD1	2:K:106:ASP:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:51:TRP:O	2:L:54:GLN:NE2	2.50	0.44
3:l:31:PHE:N	3:l:62:SER:OG	2.50	0.44
2:P:19:GLU:HB3	2:P:20:PRO:HD2	1.99	0.44
2:Q:62:GLY:O	2:Q:66:LYS:NZ	2.44	0.44
1:3:2:VAL:HG13	2:O:66:LYS:HD2	1.99	0.44
2:E:106:ASP:OD1	2:E:106:ASP:N	2.49	0.44
2:N:260:HIS:HA	2:N:270:LEU:O	2.18	0.44
2:O:6:ARG:NH1	2:O:113:TYR:HE1	2.15	0.44
2:R:190:THR:OG1	2:R:202:ARG:HB3	2.18	0.44
2:C:228:THR:HG22	2:C:247:VAL:HG23	1.98	0.44
2:G:98:MET:HE3	2:G:98:MET:HB3	1.94	0.44
3:h:7:LYS:O	3:h:28:VAL:HA	2.17	0.44
2:L:253:GLN:HE21	2:M:121:LYS:HE3	1.83	0.44
2:Q:19:GLU:HB3	2:Q:20:PRO:HD2	2.00	0.44
2:I:202:ARG:HD3	2:I:246:ALA:HB2	2.00	0.44
2:A:209:TYR:CD1	2:A:210:PRO:HA	2.52	0.44
3:d:71:PHE:CZ	3:d:73:PRO:HG3	2.53	0.44
3:n:74:THR:HG22	3:n:76:LYS:N	2.27	0.44
2:P:51:TRP:O	2:P:54:GLN:HG2	2.18	0.44
1:2:5:HIS:HD2	1:2:6:LEU:N	2.15	0.44
2:B:80:THR:HG22	2:B:84:TYR:CE2	2.52	0.44
2:C:15:PRO:HD2	2:C:17:ARG:NH2	2.32	0.44
2:D:117:ALA:HB2	3:d:61:TRP:CE2	2.53	0.44
2:E:59:TYR:O	2:E:63:GLU:HG2	2.18	0.44
2:S:259:CYS:O	2:S:271:THR:HA	2.17	0.44
2:N:137:ASP:N	2:N:137:ASP:OD1	2.50	0.44
2:O:42:SER:OG	2:O:46:GLU:OE2	2.32	0.44
2:R:102:ASP:OD2	2:R:111:ARG:NH1	2.51	0.44
2:R:234:ARG:NH2	2:R:242:GLN:OE1	2.50	0.44
2:T:22:PHE:CE1	2:T:74:HIS:HD2	2.29	0.44
2:T:168:LEU:O	2:T:172:LEU:HG	2.18	0.44
1:Y:7:ILE:HD11	2:I:156:LEU:HD21	2.00	0.44
2:B:207:SER:HA	2:B:240:THR:HB	1.99	0.44
3:c:18:ASN:HA	3:c:73:PRO:O	2.18	0.44
2:K:5:MET:HE2	2:K:164:CYS:SG	2.58	0.44
2:O:106:ASP:OD1	2:O:106:ASP:N	2.49	0.44
2:Q:129:ASP:CB	2:R:256:ARG:HH12	2.31	0.44
2:I:137:ASP:OD1	2:I:137:ASP:N	2.50	0.44
3:a:16:ALA:HB3	3:a:98:ARG:HG3	2.00	0.44
3:c:74:THR:HG23	3:c:77:ASP:H	1.83	0.44
2:D:126:LEU:HD12	2:D:132:SER:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:21:ARG:NH2	2:E:37:ASP:OD2	2.45	0.44
2:F:21:ARG:NH2	2:F:37:ASP:OD2	2.51	0.44
2:H:24:ALA:HB3	2:H:36:PHE:HB3	2.00	0.44
2:L:190:THR:OG1	2:L:202:ARG:HB3	2.17	0.44
1:u:2:VAL:HG13	2:B:66:LYS:HD2	1.99	0.43
1:U:8:VAL:HG22	2:A:73:THR:HG23	1.99	0.43
2:A:192:HIS:O	2:A:199:ALA:HB1	2.18	0.43
2:F:27:TYR:CE2	2:F:32:GLN:HB2	2.53	0.43
2:H:93:HIS:ND1	2:H:118:TYR:OH	2.36	0.43
2:K:209:TYR:CD1	2:K:210:PRO:HA	2.53	0.43
2:L:19:GLU:HB3	2:L:20:PRO:HD2	2.00	0.43
2:N:63:GLU:O	2:N:67:VAL:HG12	2.18	0.43
2:P:176:LYS:O	2:P:180:GLN:HB2	2.18	0.43
2:Q:127:LYS:HD2	2:Q:132:SER:HB2	2.00	0.43
2:R:52:ILE:O	2:R:55:GLU:HG2	2.18	0.43
2:I:44:ARG:HG2	2:I:64:THR:HG21	1.99	0.43
2:T:44:ARG:NH2	2:T:61:ASP:OD1	2.51	0.43
2:C:47:PRO:HB3	2:C:60:TRP:CH2	2.53	0.43
3:c:24:LEU:O	3:c:68:TYR:HA	2.18	0.43
3:n:49:LYS:HE2	3:n:51:GLU:OE2	2.19	0.43
2:P:49:ALA:O	2:P:52:ILE:HG22	2.17	0.43
2:Q:8:PHE:HB2	2:Q:25:VAL:HG23	2.00	0.43
2:I:225:THR:C	2:I:227:ASP:H	2.27	0.43
2:B:9:PHE:HE2	2:B:99:TYR:CE2	2.36	0.43
3:c:14:HIS:HB2	3:c:22:ASN:ND2	2.33	0.43
2:D:20:PRO:HG3	2:D:75:ARG:HB2	1.99	0.43
2:F:34:VAL:HB	2:F:45:MET:SD	2.58	0.43
2:H:14:ARG:CB	2:H:17:ARG:HG3	2.48	0.43
2:S:33:PHE:CD2	2:S:34:VAL:HG13	2.52	0.43
2:J:176:LYS:O	2:J:180:GLN:HB2	2.18	0.43
2:M:207:SER:HA	2:M:240:THR:HB	2.00	0.43
2:A:127:LYS:HD2	2:A:132:SER:HB2	2.00	0.43
2:G:8:PHE:HB2	2:G:25:VAL:HG23	2.00	0.43
2:J:81:LEU:HD23	2:J:84:TYR:HD2	1.82	0.43
2:N:168:LEU:O	2:N:172:LEU:HG	2.18	0.43
2:O:122:ASP:OD1	3:o:61:TRP:NE1	2.40	0.43
2:O:187:THR:HB	2:O:272:LEU:HD11	2.00	0.43
3:o:41:LEU:HG	3:o:80:ALA:HB3	2.00	0.43
2:Q:234:ARG:HD2	3:q:11:TYR:CD1	2.53	0.43
3:r:74:THR:HG22	3:r:77:ASP:H	1.83	0.43
2:T:201:LEU:O	2:T:246:ALA:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:1:TYR:CE2	2:O:66:LYS:NZ	2.64	0.43
2:C:62:GLY:O	2:C:66:LYS:HG3	2.19	0.43
2:E:33:PHE:CD2	2:E:34:VAL:HG13	2.53	0.43
2:H:80:THR:HG22	2:H:84:TYR:CE2	2.52	0.43
2:A:30:ASP:HB2	2:A:209:TYR:HE1	1.83	0.43
2:A:49:ALA:O	2:A:52:ILE:HG22	2.17	0.43
3:a:71:PHE:CE2	3:a:73:PRO:HG3	2.53	0.43
2:B:95:VAL:HG12	2:B:118:TYR:HD1	1.83	0.43
2:E:129:ASP:HB2	2:F:256:ARG:HH12	1.83	0.43
3:s:38:VAL:HG22	3:s:83:VAL:HG13	2.01	0.43
2:J:105:SER:OG	3:t:82:ARG:NH2	2.51	0.43
3:l:2:ILE:HD11	2:M:250:PRO:HG3	2.00	0.43
2:N:8:PHE:HB2	2:N:25:VAL:HG23	1.99	0.43
2:O:275:GLU:OE1	2:P:108:ARG:NH2	2.51	0.43
2:Q:62:GLY:C	2:Q:66:LYS:NZ	2.76	0.43
2:R:19:GLU:HB3	2:R:20:PRO:HD2	2.00	0.43
2:I:27:TYR:CE2	2:I:32:GLN:HB2	2.53	0.43
3:t:38:VAL:HG22	3:t:83:VAL:HG13	2.01	0.43
3:e:340:LEU:HD21	3:e:381:ARG:HH21	1.84	0.43
2:A:5:MET:HB2	2:A:168:LEU:HD13	2.01	0.43
2:D:254:GLU:OE1	2:D:254:GLU:N	2.50	0.43
2:F:19:GLU:HG2	2:F:75:ARG:NH1	2.34	0.43
2:G:47:PRO:HB3	2:G:60:TRP:CH2	2.54	0.43
3:g:39:ASP:OD2	3:g:82:ARG:NH2	2.51	0.43
2:H:51:TRP:CE2	2:H:179:LEU:HD11	2.54	0.43
3:j:41:LEU:HD11	3:j:82:ARG:HB2	2.01	0.43
2:K:11:SER:HB3	2:K:95:VAL:CG2	2.49	0.43
2:M:106:ASP:OD1	2:M:106:ASP:N	2.49	0.43
2:O:189:MET:HG3	2:O:202:ARG:O	2.18	0.43
2:O:238:ASP:OD1	2:O:240:THR:OG1	2.31	0.43
2:P:22:PHE:HE2	2:P:67:VAL:HG22	1.84	0.43
2:P:117:ALA:HB2	3:p:61:TRP:CE2	2.53	0.43
2:Q:222:GLU:OE2	2:R:128:GLU:OE1	2.36	0.43
2:I:19:GLU:HB3	2:I:20:PRO:HD2	2.00	0.43
1:W:4:ASP:OD1	1:W:4:ASP:N	2.45	0.43
2:F:44:ARG:HA	2:F:64:THR:HG23	2.00	0.43
2:G:42:SER:OG	2:G:46:GLU:OE2	2.32	0.43
2:S:5:MET:HE2	2:S:164:CYS:SG	2.59	0.43
2:J:17:ARG:NH1	2:J:17:ARG:HG3	2.34	0.43
3:k:75:GLU:HA	3:k:98:ARG:HH22	1.83	0.43
2:L:12:VAL:O	2:L:21:ARG:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:66:LYS:HD3	1:I:4:ASP:HA	2.00	0.43
2:M:70:HIS:O	2:M:73:THR:HB	2.19	0.43
1:2:4:ASP:HA	2:N:66:LYS:HD3	2.00	0.43
2:A:35:ARG:CD	3:a:54:ASP:OD2	2.63	0.43
2:B:254:GLU:OE1	2:B:254:GLU:N	2.47	0.43
2:C:106:ASP:OD1	2:C:106:ASP:N	2.50	0.43
2:C:220:ASP:CG	2:C:256:ARG:HG2	2.43	0.43
2:H:38:SER:O	2:H:43:GLN:NE2	2.52	0.43
2:S:137:ASP:N	2:S:137:ASP:OD1	2.52	0.43
2:Q:59:TYR:O	2:Q:63:GLU:HG2	2.19	0.43
2:Q:209:TYR:CD1	2:Q:210:PRO:HA	2.53	0.43
2:I:87:GLN:OE1	2:I:118:TYR:OH	2.22	0.43
2:C:11:SER:HB3	2:C:95:VAL:HG23	2.00	0.43
2:C:147:TRP:O	2:C:152:VAL:HG22	2.18	0.43
2:N:117:ALA:HB2	3:n:61:TRP:CE2	2.54	0.43
2:O:258:THR:HG22	2:O:273:ARG:HG2	2.00	0.43
2:Q:111:ARG:HB3	2:R:221:GLY:HA3	2.01	0.43
2:R:260:HIS:HA	2:R:270:LEU:O	2.17	0.43
2:I:6:ARG:HD3	2:I:100:GLY:HA3	2.00	0.43
1:V:3:LEU:HD13	1:V:5:HIS:N	2.28	0.42
2:A:63:GLU:O	2:A:67:VAL:HG12	2.19	0.42
2:A:80:THR:HG22	2:A:84:TYR:CE2	2.53	0.42
2:B:202:ARG:HD3	2:B:246:ALA:HB2	2.00	0.42
2:S:216:THR:OG1	2:S:260:HIS:HB2	2.19	0.42
3:m:6:PRO:HB3	3:m:31:PHE:HB3	2.01	0.42
2:N:93:HIS:CE1	3:n:1:MET:HE2	2.54	0.42
2:P:99:TYR:HB3	2:P:114:HIS:ND1	2.34	0.42
2:I:159:TYR:CD1	2:I:163:THR:HB	2.54	0.42
2:I:190:THR:OG1	2:I:202:ARG:HB3	2.19	0.42
2:E:176:LYS:O	2:E:180:GLN:HB2	2.19	0.42
2:G:260:HIS:HA	2:G:270:LEU:O	2.20	0.42
2:H:8:PHE:HB2	2:H:25:VAL:HG23	2.01	0.42
3:s:20:LYS:O	3:s:73:PRO:HD2	2.19	0.42
2:Q:6:ARG:HD3	2:Q:100:GLY:HA3	2.00	0.42
2:T:220:ASP:OD2	2:T:256:ARG:NE	2.47	0.42
1:6:9:VAL:HG13	2:R:143:THR:HG21	2.01	0.42
1:Z:2:VAL:HG23	2:K:63:GLU:OE1	2.20	0.42
2:C:176:LYS:O	2:C:180:GLN:HB2	2.19	0.42
2:C:219:ARG:HD3	2:C:257:TYR:CZ	2.54	0.42
2:D:44:ARG:HA	2:D:64:THR:HG23	2.02	0.42
2:F:19:GLU:N	2:F:19:GLU:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:9:PHE:HE2	2:G:99:TYR:HE2	1.67	0.42
2:G:106:ASP:OD1	2:G:106:ASP:N	2.51	0.42
2:S:24:ALA:HB3	2:S:36:PHE:HB3	2.02	0.42
2:K:19:GLU:HB3	2:K:20:PRO:HD2	2.02	0.42
2:K:23:ILE:HG21	3:k:55:LEU:HB3	2.00	0.42
2:Q:8:PHE:HB3	3:q:57:PHE:CE1	2.54	0.42
2:Q:202:ARG:HD2	2:Q:244:TRP:CE3	2.54	0.42
2:T:107:TRP:O	2:T:169:ARG:NH1	2.51	0.42
2:A:33:PHE:CD2	2:A:34:VAL:HG13	2.54	0.42
2:C:14:ARG:HB3	2:C:17:ARG:HG3	2.01	0.42
2:C:44:ARG:NH2	2:C:61:ASP:OD1	2.43	0.42
3:c:18:ASN:ND2	3:c:75:GLU:HB2	2.34	0.42
2:D:106:ASP:N	2:D:106:ASP:OD1	2.50	0.42
2:F:168:LEU:O	2:F:172:LEU:HG	2.19	0.42
2:G:92:SER:C	2:G:93:HIS:CD2	2.98	0.42
2:J:225:THR:C	2:J:227:ASP:H	2.27	0.42
2:K:144:LYS:O	2:K:148:GLU:HG3	2.19	0.42
2:E:102:ASP:HB2	2:E:111:ARG:HB3	2.02	0.42
2:F:106:ASP:O	2:F:107:TRP:HB2	2.20	0.42
2:F:185:PRO:HA	2:F:208:PHE:HB3	2.02	0.42
2:H:108:ARG:HH11	2:H:108:ARG:HG2	1.83	0.42
2:S:254:GLU:OE1	2:S:254:GLU:N	2.50	0.42
2:P:231:VAL:O	2:P:243:LYS:HE3	2.20	0.42
3:q:6:PRO:HB3	3:q:31:PHE:HB3	2.01	0.42
2:B:202:ARG:HD2	2:B:244:TRP:CE3	2.55	0.42
2:E:80:THR:HG22	2:E:84:TYR:CE2	2.55	0.42
2:F:106:ASP:OD1	2:F:106:ASP:N	2.51	0.42
2:G:106:ASP:O	2:G:107:TRP:HB2	2.19	0.42
3:h:23:PHE:CE2	3:h:70:GLU:HG2	2.54	0.42
2:S:97:ARG:NH2	2:S:116:TYR:OH	2.40	0.42
2:J:202:ARG:HD3	2:J:246:ALA:HB2	2.02	0.42
2:K:47:PRO:HB3	2:K:60:TRP:CH2	2.55	0.42
2:I:72:GLN:CD	2:I:75:ARG:HD3	2.45	0.42
1:y:1:TYR:CE2	1:y:4:ASP:OD2	2.73	0.42
1:X:5:HIS:HD2	1:X:6:LEU:N	2.18	0.42
3:b:26:CYS:HB2	3:b:40:LEU:HD21	2.02	0.42
3:b:71:PHE:CZ	3:b:73:PRO:HG3	2.55	0.42
2:C:81:LEU:HD23	2:C:84:TYR:HD2	1.84	0.42
2:C:254:GLU:OE1	2:C:254:GLU:N	2.50	0.42
3:d:42:LYS:HE3	3:d:79:TYR:OH	2.20	0.42
2:H:27:TYR:CE2	2:H:32:GLN:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:137:ASP:OD1	2:H:137:ASP:N	2.53	0.42
2:J:8:PHE:HB3	3:j:57:PHE:CE1	2.55	0.42
2:M:188:HIS:CD2	2:M:204:TRP:HB2	2.55	0.42
2:N:49:ALA:O	2:N:52:ILE:HG22	2.20	0.42
2:O:49:ALA:O	2:O:52:ILE:HG22	2.20	0.42
2:P:137:ASP:OD1	2:P:137:ASP:N	2.53	0.42
2:Q:106:ASP:OD1	2:Q:106:ASP:N	2.50	0.42
2:Q:175:GLY:O	2:Q:179:LEU:HG	2.20	0.42
2:B:192:HIS:O	2:B:200:THR:N	2.39	0.42
2:D:72:GLN:O	2:D:75:ARG:HG2	2.19	0.42
2:L:21:ARG:HH21	2:L:39:ASP:HB2	1.84	0.42
2:P:266:LEU:HD13	2:P:270:LEU:HG	2.02	0.42
2:I:33:PHE:CD2	2:I:34:VAL:HG13	2.54	0.42
2:C:35:ARG:HH11	2:C:37:ASP:HB2	1.85	0.42
2:C:137:ASP:N	2:C:137:ASP:OD1	2.52	0.42
3:c:85:HIS:CE1	3:c:86:VAL:HG12	2.54	0.42
2:D:93:HIS:ND1	2:D:119:ASP:OD2	2.38	0.42
2:E:234:ARG:HD2	3:e:310:TYR:CE1	2.55	0.42
2:F:128:GLU:H	2:F:128:GLU:CD	2.26	0.42
2:G:131:ARG:NE	2:G:157:ARG:NH1	2.67	0.42
2:H:48:ARG:HH12	3:h:54:ASP:CG	2.27	0.42
2:H:168:LEU:O	2:H:172:LEU:HG	2.20	0.42
2:H:188:HIS:CD2	2:H:204:TRP:HB2	2.55	0.42
2:L:202:ARG:HD2	2:L:244:TRP:CE3	2.55	0.42
2:L:207:SER:HA	2:L:240:THR:HB	2.01	0.42
2:M:5:MET:HG3	2:M:28:VAL:HG22	2.02	0.42
2:N:13:SER:HA	2:N:20:PRO:HB3	2.02	0.42
2:P:44:ARG:HA	2:P:64:THR:HG23	2.02	0.42
2:P:255:GLN:C	2:P:273:ARG:HH12	2.26	0.42
2:R:11:SER:HA	2:R:21:ARG:O	2.19	0.42
2:R:49:ALA:O	2:R:52:ILE:HG22	2.20	0.42
1:u:1:TYR:HB2	2:B:167:TRP:CG	2.55	0.42
3:f:71:PHE:CZ	3:f:73:PRO:HG3	2.53	0.42
2:M:202:ARG:HD2	2:M:244:TRP:CE3	2.54	0.42
2:O:192:HIS:CE1	3:o:99:ASP:HB3	2.55	0.42
2:P:5:MET:HE2	2:P:164:CYS:SG	2.60	0.42
1:X:7:ILE:HG22	1:X:8:VAL:N	2.35	0.41
2:C:172:LEU:HD23	2:C:179:LEU:HD13	2.01	0.41
2:E:14:ARG:HB3	2:E:17:ARG:NE	2.35	0.41
3:g:39:ASP:HB2	3:g:82:ARG:CZ	2.51	0.41
2:H:33:PHE:CD2	2:H:34:VAL:HG13	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:22:PHE:HE1	2:J:74:HIS:ND1	2.17	0.41
2:K:19:GLU:HA	2:K:19:GLU:OE1	2.19	0.41
2:M:9:PHE:HE2	2:M:99:TYR:CE2	2.37	0.41
2:O:137:ASP:OD1	2:O:137:ASP:N	2.53	0.41
2:T:19:GLU:CD	2:T:75:ARG:HH22	2.26	0.41
2:A:98:MET:HE3	2:A:98:MET:HB3	1.93	0.41
3:a:56:SER:HB3	3:a:64:TYR:CZ	2.56	0.41
2:B:214:THR:HB	2:B:262:GLN:CG	2.50	0.41
2:F:191:HIS:C	2:F:192:HIS:HD2	2.27	0.41
2:F:263:HIS:HD1	2:F:265:GLY:H	1.68	0.41
2:G:8:PHE:HB3	3:g:57:PHE:CE1	2.55	0.41
2:H:234:ARG:HD2	3:h:11:TYR:CE1	2.55	0.41
2:Q:33:PHE:CD2	2:Q:34:VAL:HG13	2.55	0.41
2:E:207:SER:HA	2:E:240:THR:HB	2.02	0.41
2:H:181:ARG:NH1	2:H:183:ASP:OD2	2.52	0.41
3:s:31:PHE:N	3:s:62:SER:OG	2.53	0.41
2:K:137:ASP:OD1	2:K:137:ASP:N	2.53	0.41
2:E:38:SER:O	2:E:43:GLN:NE2	2.54	0.41
2:E:137:ASP:N	2:E:137:ASP:OD1	2.53	0.41
2:H:78:LEU:O	2:H:82:ARG:HG3	2.19	0.41
2:J:175:GLY:O	2:J:179:LEU:HG	2.20	0.41
2:N:11:SER:HB3	2:N:95:VAL:HG22	2.03	0.41
3:r:74:THR:HG22	3:r:76:LYS:N	2.31	0.41
2:T:202:ARG:HD3	2:T:246:ALA:HB2	2.02	0.41
1:w:1:TYR:CD2	2:F:66:LYS:NZ	2.88	0.41
2:B:44:ARG:HA	2:B:64:THR:HG23	2.01	0.41
2:D:176:LYS:O	2:D:180:GLN:HB2	2.21	0.41
3:d:37:GLU:HB3	3:d:84:ASN:HB3	2.02	0.41
2:G:27:TYR:CE2	2:G:32:GLN:HB2	2.56	0.41
2:G:63:GLU:O	2:G:67:VAL:HG12	2.20	0.41
2:S:109:PHE:CD1	2:S:161:GLU:HA	2.55	0.41
2:S:202:ARG:HD3	2:S:246:ALA:HB2	2.02	0.41
2:L:97:ARG:NH2	2:L:116:TYR:OH	2.54	0.41
2:Q:11:SER:HB3	2:Q:95:VAL:HG22	2.02	0.41
2:Q:63:GLU:O	2:Q:67:VAL:HG12	2.20	0.41
3:i:74:THR:HG22	3:i:76:LYS:N	2.31	0.41
2:F:20:PRO:CG	2:F:75:ARG:HG2	2.51	0.41
2:G:202:ARG:HG2	2:G:204:TRP:NE1	2.35	0.41
3:m:22:ASN:C	3:m:23:PHE:HD1	2.28	0.41
3:m:71:PHE:CZ	3:m:73:PRO:HG3	2.56	0.41
2:P:24:ALA:HB3	2:P:36:PHE:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:204:TRP:HE3	2:P:206:LEU:HD21	1.84	0.41
2:T:27:TYR:CE2	2:T:32:GLN:HB2	2.56	0.41
2:B:260:HIS:CE1	2:B:271:THR:HG23	2.55	0.41
3:c:74:THR:HG22	3:c:77:ASP:HB2	2.02	0.41
2:H:44:ARG:HA	2:H:64:THR:HG23	2.02	0.41
3:b:38:VAL:HB	3:b:67:TYR:CZ	2.56	0.41
2:G:168:LEU:O	2:G:172:LEU:HG	2.21	0.41
2:G:254:GLU:OE1	2:G:254:GLU:N	2.49	0.41
2:K:72:GLN:O	2:K:75:ARG:HG2	2.20	0.41
2:L:106:ASP:O	2:L:107:TRP:HB2	2.21	0.41
2:L:175:GLY:O	2:L:179:LEU:HG	2.21	0.41
2:O:6:ARG:HH12	2:O:102:ASP:CG	2.28	0.41
2:O:202:ARG:HD2	2:O:244:TRP:CE3	2.55	0.41
3:o:84:ASN:ND2	3:o:91:PRO:HG3	2.36	0.41
2:P:106:ASP:O	2:P:107:TRP:HB2	2.21	0.41
3:r:65:LEU:HD12	3:r:65:LEU:HA	1.80	0.41
1:V:9:VAL:OXT	2:C:80:THR:HG21	2.21	0.41
3:a:4:ARG:O	3:a:31:PHE:HA	2.21	0.41
2:C:262:GLN:N	2:C:262:GLN:OE1	2.53	0.41
2:D:6:ARG:HD3	2:D:100:GLY:HA3	2.02	0.41
2:D:102:ASP:HB2	2:D:111:ARG:HG2	2.03	0.41
2:D:137:ASP:OD1	2:D:137:ASP:N	2.54	0.41
2:D:175:GLY:O	2:D:179:LEU:HG	2.21	0.41
2:D:185:PRO:HA	2:D:208:PHE:HB3	2.02	0.41
2:E:202:ARG:HD2	2:E:244:TRP:CE3	2.56	0.41
2:F:234:ARG:HD2	3:f:11:TYR:CE1	2.56	0.41
2:G:220:ASP:O	2:H:128:GLU:HG2	2.20	0.41
2:S:3:HIS:ND1	2:S:29:ASP:OD2	2.39	0.41
2:S:98:MET:HE3	2:S:98:MET:HB3	1.95	0.41
2:S:234:ARG:NH2	2:S:242:GLN:OE1	2.54	0.41
2:J:49:ALA:O	2:J:52:ILE:HG22	2.21	0.41
2:J:106:ASP:O	2:J:107:TRP:HB2	2.21	0.41
2:J:234:ARG:HD2	3:j:11:TYR:CE1	2.56	0.41
3:j:31:PHE:N	3:j:62:SER:OG	2.54	0.41
2:K:117:ALA:HB2	3:k:61:TRP:CE2	2.56	0.41
2:L:89:GLU:OE1	2:L:89:GLU:N	2.51	0.41
2:N:175:GLY:O	2:N:179:LEU:HG	2.21	0.41
2:N:195:SER:OG	2:N:197:HIS:CE1	2.74	0.41
2:N:203:CYS:SG	2:N:272:LEU:HD12	2.61	0.41
2:O:175:GLY:O	2:O:179:LEU:HG	2.20	0.41
2:O:176:LYS:O	2:O:180:GLN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:234:ARG:NH1	3:q:11:TYR:HB3	2.36	0.41
3:q:60:ASP:OD1	3:q:60:ASP:N	2.54	0.41
2:R:168:LEU:O	2:R:172:LEU:HG	2.21	0.41
3:e:325:CYS:HB2	3:e:339:LEU:HD21	2.03	0.41
2:B:82:ARG:HE	2:B:89:GLU:HA	1.86	0.41
2:C:8:PHE:HB2	2:C:25:VAL:CG2	2.49	0.41
2:D:263:HIS:HD1	2:D:265:GLY:H	1.65	0.41
2:K:30:ASP:HB2	2:K:209:TYR:CE1	2.54	0.41
2:L:189:MET:HE2	2:L:201:LEU:HD22	2.02	0.41
2:M:189:MET:HE2	2:M:201:LEU:HD22	2.03	0.41
2:Q:34:VAL:HB	2:Q:45:MET:SD	2.61	0.41
2:Q:189:MET:HE3	2:Q:217:TRP:HH2	1.86	0.41
2:I:97:ARG:HE	2:I:116:TYR:HE2	1.69	0.41
2:T:6:ARG:NH2	2:T:102:ASP:OD1	2.52	0.41
1:4:1:TYR:HE2	1:4:4:ASP:OD2	2.03	0.40
2:A:168:LEU:O	2:A:172:LEU:HG	2.21	0.40
2:B:137:ASP:N	2:B:137:ASP:OD1	2.53	0.40
2:D:35:ARG:HG2	2:D:48:ARG:HD3	2.02	0.40
2:D:168:LEU:O	2:D:172:LEU:HG	2.20	0.40
2:D:189:MET:HE3	2:D:217:TRP:CH2	2.47	0.40
2:N:44:ARG:NH2	2:N:61:ASP:OD1	2.52	0.40
2:R:81:LEU:HD23	2:R:84:TYR:HD2	1.87	0.40
1:z:1:TYR:N	2:L:7:TYR:OH	2.33	0.40
2:C:93:HIS:CD2	2:C:119:ASP:OD2	2.74	0.40
2:N:35:ARG:CD	2:N:48:ARG:HH11	2.34	0.40
2:R:30:ASP:HB2	2:R:209:TYR:HE1	1.87	0.40
2:I:49:ALA:O	2:I:52:ILE:HG22	2.21	0.40
2:B:87:GLN:OE1	2:B:118:TYR:OH	2.25	0.40
2:B:106:ASP:O	2:B:107:TRP:HB2	2.22	0.40
2:D:98:MET:HE3	2:D:98:MET:HB3	1.90	0.40
2:E:231:VAL:O	2:E:243:LYS:HE3	2.22	0.40
2:H:35:ARG:NH1	3:h:54:ASP:CG	2.79	0.40
2:H:253:GLN:HG2	2:H:256:ARG:HH11	1.87	0.40
2:M:126:LEU:HD12	2:M:132:SER:O	2.21	0.40
2:O:72:GLN:O	2:O:76:VAL:HG23	2.21	0.40
2:P:107:TRP:HB3	2:P:169:ARG:HD3	2.03	0.40
2:R:137:ASP:OD1	2:R:137:ASP:N	2.54	0.40
3:b:31:PHE:N	3:b:62:SER:OG	2.54	0.40
2:C:191:HIS:HB2	2:C:274:TRP:CH2	2.56	0.40
2:E:106:ASP:O	2:E:107:TRP:HB2	2.21	0.40
2:F:123:TYR:OH	2:F:143:THR:OG1	2.26	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:187:THR:HA	2:S:204:TRP:O	2.21	0.40
2:J:15:PRO:HA	2:J:16:GLY:HA2	1.51	0.40
3:l:55:LEU:HA	3:l:65:LEU:HD11	2.03	0.40
2:N:19:GLU:HB3	2:N:20:PRO:HD2	2.03	0.40
2:Q:270:LEU:HD23	2:Q:270:LEU:HA	1.90	0.40
2:I:8:PHE:HB2	2:I:25:VAL:HG23	2.04	0.40
2:I:44:ARG:HA	2:I:64:THR:HG23	2.02	0.40
2:A:219:ARG:HD3	2:A:257:TYR:CZ	2.56	0.40
2:B:21:ARG:HE	2:B:23:ILE:HD11	1.85	0.40
2:C:19:GLU:HB3	2:C:20:PRO:HD2	2.03	0.40
2:E:44:ARG:HA	2:E:64:THR:HG23	2.02	0.40
2:G:137:ASP:N	2:G:137:ASP:OD1	2.52	0.40
2:H:92:SER:C	2:H:93:HIS:CD2	3.00	0.40
2:H:213:ILE:HG13	2:H:263:HIS:HB2	2.03	0.40
2:H:219:ARG:HD3	2:H:257:TYR:CZ	2.56	0.40
2:J:62:GLY:O	2:J:66:LYS:HG3	2.21	0.40
2:J:234:ARG:HD2	3:j:11:TYR:CD1	2.57	0.40
3:p:17:GLU:OE2	3:p:20:LYS:HD2	2.22	0.40
2:Q:80:THR:HG22	2:Q:84:TYR:CE2	2.57	0.40
2:T:5:MET:HG3	2:T:28:VAL:HG22	2.03	0.40
3:t:71:PHE:CZ	3:t:73:PRO:HG3	2.57	0.40
3:e:354:LEU:HD13	3:e:364:LEU:HD21	2.04	0.40

All (5) 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)
3:b:84:ASN:OD1	2:L:176:LYS:NZ[1_565]	2.00	0.20
2:A:221:GLY:O	2:D:111:ARG:NH2[1_455]	2.08	0.12
2:F:275:GLU:OXT	3:s:20:LYS:NZ[2_455]	2.08	0.12
2:A:108:ARG:NH2	2:D:275:GLU:OE2[1_455]	2.15	0.05
3:c:46:ARG:NH2	2:M:128:GLU:OE2[1_565]	2.15	0.05

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	1	7/9 (78%)	7 (100%)	0	0	100	100
1	2	7/9 (78%)	7 (100%)	0	0	100	100
1	3	7/9 (78%)	7 (100%)	0	0	100	100
1	4	7/9 (78%)	7 (100%)	0	0	100	100
1	5	7/9 (78%)	7 (100%)	0	0	100	100
1	6	7/9 (78%)	7 (100%)	0	0	100	100
1	7	7/9 (78%)	7 (100%)	0	0	100	100
1	8	7/9 (78%)	7 (100%)	0	0	100	100
1	U	7/9 (78%)	7 (100%)	0	0	100	100
1	V	7/9 (78%)	7 (100%)	0	0	100	100
1	W	7/9 (78%)	7 (100%)	0	0	100	100
1	X	7/9 (78%)	7 (100%)	0	0	100	100
1	Y	7/9 (78%)	7 (100%)	0	0	100	100
1	Z	7/9 (78%)	7 (100%)	0	0	100	100
1	u	7/9 (78%)	7 (100%)	0	0	100	100
1	v	7/9 (78%)	7 (100%)	0	0	100	100
1	w	7/9 (78%)	7 (100%)	0	0	100	100
1	x	7/9 (78%)	7 (100%)	0	0	100	100
1	y	7/9 (78%)	7 (100%)	0	0	100	100
1	z	7/9 (78%)	7 (100%)	0	0	100	100
2	A	273/275 (99%)	262 (96%)	11 (4%)	0	100	100
2	B	273/275 (99%)	263 (96%)	10 (4%)	0	100	100
2	C	273/275 (99%)	263 (96%)	10 (4%)	0	100	100
2	D	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
2	E	273/275 (99%)	265 (97%)	8 (3%)	0	100	100
2	F	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
2	G	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
2	H	273/275 (99%)	264 (97%)	8 (3%)	1 (0%)	30	60
2	I	273/275 (99%)	263 (96%)	10 (4%)	0	100	100
2	J	273/275 (99%)	264 (97%)	8 (3%)	1 (0%)	30	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	273/275 (99%)	263 (96%)	10 (4%)	0	100	100
2	L	273/275 (99%)	264 (97%)	8 (3%)	1 (0%)	30	60
2	M	273/275 (99%)	263 (96%)	10 (4%)	0	100	100
2	N	273/275 (99%)	266 (97%)	7 (3%)	0	100	100
2	O	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
2	P	273/275 (99%)	263 (96%)	10 (4%)	0	100	100
2	Q	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
2	R	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
2	S	273/275 (99%)	266 (97%)	7 (3%)	0	100	100
2	T	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
3	a	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	b	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
3	c	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	d	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	e	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
3	f	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	g	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	h	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	i	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	j	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	k	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	l	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
3	m	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	n	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	o	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	p	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	q	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	r	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	s	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	t	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
All	All	7560/7680 (98%)	7335 (97%)	222 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	16	GLY
2	H	18	GLY
2	J	15	PRO

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	1	9/9 (100%)	9 (100%)	0	100	100
1	2	9/9 (100%)	9 (100%)	0	100	100
1	3	9/9 (100%)	9 (100%)	0	100	100
1	4	9/9 (100%)	9 (100%)	0	100	100
1	5	9/9 (100%)	9 (100%)	0	100	100
1	6	9/9 (100%)	9 (100%)	0	100	100
1	7	9/9 (100%)	9 (100%)	0	100	100
1	8	9/9 (100%)	9 (100%)	0	100	100
1	U	9/9 (100%)	9 (100%)	0	100	100
1	V	9/9 (100%)	9 (100%)	0	100	100
1	W	9/9 (100%)	9 (100%)	0	100	100
1	X	9/9 (100%)	9 (100%)	0	100	100
1	Y	9/9 (100%)	9 (100%)	0	100	100
1	Z	9/9 (100%)	9 (100%)	0	100	100
1	u	9/9 (100%)	9 (100%)	0	100	100
1	v	9/9 (100%)	9 (100%)	0	100	100
1	w	9/9 (100%)	9 (100%)	0	100	100
1	x	9/9 (100%)	9 (100%)	0	100	100
1	y	9/9 (100%)	9 (100%)	0	100	100
1	z	9/9 (100%)	9 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	231/231 (100%)	231 (100%)	0	100	100
2	B	231/231 (100%)	231 (100%)	0	100	100
2	C	231/231 (100%)	230 (100%)	1 (0%)	84	84
2	D	231/231 (100%)	231 (100%)	0	100	100
2	E	231/231 (100%)	231 (100%)	0	100	100
2	F	231/231 (100%)	231 (100%)	0	100	100
2	G	231/231 (100%)	231 (100%)	0	100	100
2	H	231/231 (100%)	231 (100%)	0	100	100
2	I	231/231 (100%)	231 (100%)	0	100	100
2	J	231/231 (100%)	231 (100%)	0	100	100
2	K	231/231 (100%)	231 (100%)	0	100	100
2	L	231/231 (100%)	231 (100%)	0	100	100
2	M	231/231 (100%)	231 (100%)	0	100	100
2	N	231/231 (100%)	231 (100%)	0	100	100
2	O	231/231 (100%)	231 (100%)	0	100	100
2	P	231/231 (100%)	231 (100%)	0	100	100
2	Q	231/231 (100%)	231 (100%)	0	100	100
2	R	231/231 (100%)	230 (100%)	1 (0%)	84	84
2	S	231/231 (100%)	230 (100%)	1 (0%)	84	84
2	T	231/231 (100%)	231 (100%)	0	100	100
3	a	95/95 (100%)	95 (100%)	0	100	100
3	b	95/95 (100%)	95 (100%)	0	100	100
3	c	95/95 (100%)	95 (100%)	0	100	100
3	d	95/95 (100%)	95 (100%)	0	100	100
3	e	95/95 (100%)	94 (99%)	1 (1%)	65	76
3	f	95/95 (100%)	95 (100%)	0	100	100
3	g	95/95 (100%)	95 (100%)	0	100	100
3	h	95/95 (100%)	95 (100%)	0	100	100
3	i	95/95 (100%)	95 (100%)	0	100	100
3	j	95/95 (100%)	95 (100%)	0	100	100
3	k	95/95 (100%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	l	95/95 (100%)	94 (99%)	1 (1%)	65	76
3	m	95/95 (100%)	94 (99%)	1 (1%)	65	76
3	n	95/95 (100%)	95 (100%)	0	100	100
3	o	95/95 (100%)	94 (99%)	1 (1%)	65	76
3	p	95/95 (100%)	95 (100%)	0	100	100
3	q	95/95 (100%)	94 (99%)	1 (1%)	65	76
3	r	95/95 (100%)	95 (100%)	0	100	100
3	s	95/95 (100%)	95 (100%)	0	100	100
3	t	95/95 (100%)	95 (100%)	0	100	100
All	All	6700/6700 (100%)	6692 (100%)	8 (0%)	88	90

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	183	ASP
2	S	110	LEU
3	l	65	LEU
3	m	65	LEU
3	o	65	LEU
3	q	65	LEU
2	R	73	THR
3	e	364	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	5	HIS
1	y	5	HIS
1	w	5	HIS
1	W	5	HIS
1	6	5	HIS
1	X	5	HIS
1	2	5	HIS
1	Z	5	HIS
1	7	5	HIS
2	A	70	HIS
2	A	115	GLN
2	A	192	HIS

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Mol	Chain	Res	Type
3	a	9	GLN
3	a	14	HIS
2	B	43	GLN
2	B	115	GLN
3	b	14	HIS
3	b	32	HIS
2	C	93	HIS
2	C	180	GLN
2	D	96	GLN
2	D	141	GLN
2	D	218	GLN
2	D	255	GLN
3	d	3	GLN
3	d	52	HIS
2	E	155	GLN
2	E	188	HIS
2	F	155	GLN
2	F	260	HIS
3	f	14	HIS
2	G	155	GLN
2	G	191	HIS
3	g	14	HIS
2	H	155	GLN
2	H	191	HIS
2	H	263	HIS
3	h	32	HIS
2	S	191	HIS
3	s	14	HIS
2	J	141	GLN
2	J	218	GLN
3	j	14	HIS
2	K	72	GLN
2	K	114	HIS
2	K	155	GLN
3	k	14	HIS
2	L	43	GLN
2	L	192	HIS
2	M	32	GLN
2	M	115	GLN
3	m	14	HIS
3	m	32	HIS
2	N	54	GLN

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Mol	Chain	Res	Type
2	N	115	GLN
2	N	155	GLN
3	n	25	ASN
2	O	54	GLN
2	O	188	HIS
2	O	218	GLN
3	o	14	HIS
2	P	188	HIS
2	P	218	GLN
3	p	14	HIS
3	p	32	HIS
2	Q	141	GLN
2	Q	155	GLN
3	q	14	HIS
2	R	151	HIS
2	R	174	ASN
2	R	192	HIS
3	r	14	HIS
3	r	52	HIS
2	I	192	HIS
3	i	14	HIS
2	T	96	GLN
2	T	155	GLN
2	T	192	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	1	9/9 (100%)	1.36	2 (22%) 2 2	58, 65, 74, 78	0
1	2	9/9 (100%)	1.17	0 100 100	45, 52, 60, 64	0
1	3	9/9 (100%)	1.67	3 (33%) 1 1	39, 42, 49, 56	0
1	4	9/9 (100%)	1.22	0 100 100	45, 50, 63, 66	0
1	5	9/9 (100%)	1.91	3 (33%) 1 1	52, 56, 59, 64	0
1	6	9/9 (100%)	1.01	1 (11%) 10 9	44, 50, 56, 66	0
1	7	9/9 (100%)	1.81	4 (44%) 0 0	39, 45, 49, 64	0
1	8	9/9 (100%)	1.25	2 (22%) 2 2	31, 36, 49, 54	0
1	U	9/9 (100%)	1.35	0 100 100	58, 62, 70, 72	0
1	V	9/9 (100%)	1.55	2 (22%) 2 2	62, 73, 86, 96	0
1	W	9/9 (100%)	1.63	2 (22%) 2 2	42, 45, 54, 57	0
1	X	9/9 (100%)	1.67	2 (22%) 2 2	44, 52, 64, 70	0
1	Y	9/9 (100%)	1.38	2 (22%) 2 2	36, 46, 52, 60	0
1	Z	9/9 (100%)	1.35	0 100 100	68, 69, 79, 84	0
1	u	9/9 (100%)	1.36	1 (11%) 10 9	53, 58, 65, 69	0
1	v	9/9 (100%)	0.95	1 (11%) 10 9	51, 55, 61, 61	0
1	w	9/9 (100%)	1.62	2 (22%) 2 2	52, 57, 68, 72	0
1	x	9/9 (100%)	1.32	1 (11%) 10 9	44, 49, 60, 63	0
1	y	9/9 (100%)	1.33	1 (11%) 10 9	32, 39, 49, 51	0
1	z	9/9 (100%)	1.57	1 (11%) 10 9	55, 57, 72, 76	0
2	A	275/275 (100%)	1.11	33 (12%) 9 7	36, 74, 90, 98	5 (1%)
2	B	275/275 (100%)	1.01	27 (9%) 13 10	24, 62, 76, 84	5 (1%)
2	C	275/275 (100%)	1.22	45 (16%) 4 4	39, 83, 98, 106	5 (1%)
2	D	275/275 (100%)	0.91	16 (5%) 29 19	26, 56, 75, 98	5 (1%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	E	275/275 (100%)	1.13	38 (13%) 6 5	27, 61, 82, 98	5 (1%)
2	F	275/275 (100%)	1.16	32 (11%) 9 8	28, 58, 79, 93	5 (1%)
2	G	275/275 (100%)	1.04	31 (11%) 10 8	27, 64, 84, 102	5 (1%)
2	H	275/275 (100%)	0.94	21 (7%) 20 14	22, 52, 71, 94	5 (1%)
2	I	275/275 (100%)	0.85	15 (5%) 30 21	15, 40, 58, 78	5 (1%)
2	J	275/275 (100%)	0.87	14 (5%) 33 22	17, 38, 54, 74	5 (1%)
2	K	275/275 (100%)	1.13	24 (8%) 16 12	35, 78, 95, 103	5 (1%)
2	L	275/275 (100%)	0.95	15 (5%) 30 21	27, 58, 75, 84	4 (1%)
2	M	275/275 (100%)	0.98	26 (9%) 14 11	31, 70, 88, 106	5 (1%)
2	N	275/275 (100%)	0.92	17 (6%) 26 18	23, 53, 77, 87	5 (1%)
2	O	275/275 (100%)	1.09	31 (11%) 10 8	22, 53, 80, 91	5 (1%)
2	P	275/275 (100%)	0.96	23 (8%) 17 13	17, 47, 67, 85	5 (1%)
2	Q	275/275 (100%)	1.09	33 (12%) 9 7	25, 61, 84, 100	5 (1%)
2	R	275/275 (100%)	1.12	32 (11%) 9 8	24, 51, 73, 88	5 (1%)
2	S	275/275 (100%)	0.92	19 (6%) 23 16	20, 44, 64, 89	4 (1%)
2	T	275/275 (100%)	0.71	13 (4%) 36 24	16, 37, 54, 74	4 (1%)
3	a	100/100 (100%)	1.26	14 (14%) 6 5	32, 85, 100, 108	1 (1%)
3	b	100/100 (100%)	0.87	3 (3%) 52 35	20, 55, 72, 80	1 (1%)
3	c	100/100 (100%)	1.45	20 (20%) 3 2	30, 88, 106, 114	1 (1%)
3	d	100/100 (100%)	0.80	3 (3%) 52 35	19, 51, 70, 76	1 (1%)
3	e	100/100 (100%)	1.40	20 (20%) 3 2	22, 72, 98, 102	1 (1%)
3	f	100/100 (100%)	1.23	16 (16%) 5 4	22, 58, 70, 80	1 (1%)
3	g	100/100 (100%)	1.30	16 (16%) 5 4	26, 76, 89, 94	1 (1%)
3	h	100/100 (100%)	0.78	5 (5%) 34 23	21, 44, 61, 74	1 (1%)
3	i	100/100 (100%)	0.65	3 (3%) 52 35	11, 31, 49, 57	1 (1%)
3	j	100/100 (100%)	0.59	3 (3%) 52 35	12, 31, 50, 59	1 (1%)
3	k	100/100 (100%)	1.23	11 (11%) 10 9	28, 88, 101, 109	1 (1%)
3	l	100/100 (100%)	1.01	8 (8%) 18 14	17, 54, 73, 81	1 (1%)
3	m	100/100 (100%)	1.09	12 (12%) 9 7	25, 72, 91, 101	1 (1%)
3	n	100/100 (100%)	0.89	2 (2%) 65 46	15, 54, 73, 86	1 (1%)
3	o	100/100 (100%)	1.33	15 (15%) 5 5	21, 69, 82, 93	1 (1%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	p	100/100 (100%)	0.76	2 (2%) 65 46	16, 40, 62, 76	1 (1%)
3	q	100/100 (100%)	1.46	23 (23%) 2 2	30, 78, 93, 97	1 (1%)
3	r	100/100 (100%)	1.12	11 (11%) 10 9	20, 49, 72, 92	1 (1%)
3	s	100/100 (100%)	0.76	4 (4%) 42 28	13, 35, 56, 62	1 (1%)
3	t	100/100 (100%)	0.66	2 (2%) 65 46	14, 32, 49, 57	1 (1%)
All	All	7680/7680 (100%)	1.02	728 (9%) 14 11	11, 57, 88, 114	117 (1%)

All (728) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	1	GLY	7.1
2	Q	1	GLY	6.5
2	O	249	VAL	6.3
3	e	368	THR	6.0
2	G	1	GLY	5.3
2	L	116	TYR	5.3
2	D	199	ALA	5.0
3	q	81	CYS	4.9
3	g	80	ALA	4.8
2	F	34	VAL	4.8
2	Q	78	LEU	4.7
2	E	1	GLY	4.6
2	C	34	VAL	4.5
2	N	81	LEU	4.5
2	I	116	TYR	4.4
2	E	23	ILE	4.3
2	T	116	TYR	4.2
2	E	249	VAL	4.2
3	g	94	VAL	4.2
2	M	94	THR	4.2
2	F	45	MET	4.1
3	q	41	LEU	4.0
2	K	11	SER	4.0
3	m	16	ALA	4.0
3	g	81	CYS	3.9
2	N	116	TYR	3.9
2	M	11	SER	3.9
3	a	8	ILE	3.9
3	l	86	VAL	3.9
2	Q	128	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
2	E	128	GLU	3.8
2	F	20	PRO	3.8
2	F	113	TYR	3.8
2	P	171	TYR	3.8
3	o	41	LEU	3.7
3	q	80	ALA	3.7
2	F	36	PHE	3.7
3	e	323	LEU	3.7
2	Q	217	TRP	3.7
3	j	35	ASP	3.6
2	R	261	VAL	3.6
3	q	55	LEU	3.6
2	C	245	ALA	3.6
3	e	398	ASP	3.6
3	g	41	LEU	3.5
3	r	41	LEU	3.5
2	E	217	TRP	3.5
2	K	177	GLU	3.5
2	Q	23	ILE	3.5
2	C	261	VAL	3.5
3	n	1	MET	3.5
2	M	95	VAL	3.4
3	o	81	CYS	3.4
3	i	61	TRP	3.4
2	A	30	ASP	3.4
3	q	16	ALA	3.4
2	C	37	ASP	3.4
3	e	366	TYR	3.4
2	Q	94	THR	3.4
2	L	199	ALA	3.3
3	e	354	LEU	3.3
1	5	4	ASP	3.3
2	Q	123	TYR	3.3
2	Q	249	VAL	3.3
2	R	124	ILE	3.3
2	A	37	ASP	3.3
2	H	114	HIS	3.3
2	L	104	GLY	3.3
3	e	372	PRO	3.2
1	V	3	LEU	3.2
3	e	346	ILE	3.2
2	A	1	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
2	P	74	HIS	3.2
3	o	22	ASN	3.2
2	N	118	TYR	3.2
2	P	71	SER	3.2
2	Q	71	SER	3.2
3	c	50	VAL	3.2
1	5	7	ILE	3.2
2	O	221	GLY	3.1
2	F	171	TYR	3.1
1	3	7	ILE	3.1
2	F	74	HIS	3.1
2	O	74	HIS	3.1
2	C	214	THR	3.1
2	D	81	LEU	3.1
2	T	179	LEU	3.1
2	C	259	CYS	3.1
3	l	1	MET	3.1
2	O	178	THR	3.1
2	D	36	PHE	3.1
2	H	109	PHE	3.1
2	C	40	ALA	3.1
2	S	205	ALA	3.1
2	F	22	PHE	3.1
3	e	370	PHE	3.1
2	T	227	ASP	3.1
2	P	124	ILE	3.1
2	B	266	LEU	3.0
3	k	40	LEU	3.0
2	B	261	VAL	3.0
3	f	1	MET	3.0
2	E	171	TYR	3.0
2	R	74	HIS	3.0
2	Q	96	GLN	3.0
2	K	207	SER	3.0
2	I	223	ASP	3.0
3	l	55	LEU	3.0
1	y	1	TYR	3.0
2	R	2	SER	3.0
3	f	55	LEU	3.0
2	E	236	ALA	3.0
2	S	165	VAL	3.0
2	N	28	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	O	248	VAL	3.0
2	P	28	VAL	3.0
2	F	52	ILE	3.0
3	h	1	MET	3.0
3	e	379	ALA	3.0
2	K	30	ASP	3.0
3	i	35	ASP	3.0
2	R	231	VAL	3.0
3	g	9	GLN	3.0
2	A	241	PHE	3.0
2	F	9	PHE	3.0
2	K	20	PRO	2.9
2	B	153	ALA	2.9
2	H	71	SER	2.9
2	R	71	SER	2.9
3	c	29	SER	2.9
2	C	231	VAL	2.9
2	F	120	GLY	2.9
2	P	1	GLY	2.9
2	R	109	PHE	2.9
3	b	25	ASN	2.9
2	K	10	THR	2.9
2	P	20	PRO	2.9
2	K	136	ALA	2.9
2	E	269	PRO	2.9
2	F	223	ASP	2.9
3	s	35	ASP	2.9
3	q	99	ASP	2.9
2	E	199	ALA	2.9
2	O	254	GLU	2.9
2	E	116	TYR	2.9
2	E	120	GLY	2.9
2	Q	84	TYR	2.9
2	E	207	SER	2.9
3	m	2	ILE	2.9
2	N	199	ALA	2.9
2	B	156	LEU	2.9
2	R	199	ALA	2.8
2	S	225	THR	2.8
3	f	73	PRO	2.8
2	G	34	VAL	2.8
3	m	25	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
3	c	55	LEU	2.8
2	C	5	MET	2.8
2	P	135	ALA	2.8
2	M	12	VAL	2.8
3	q	38	VAL	2.8
2	A	51	TRP	2.8
2	O	52	ILE	2.8
2	R	81	LEU	2.8
2	D	118	TYR	2.8
3	g	67	TYR	2.8
3	f	3	GLN	2.8
2	C	49	ALA	2.8
2	M	38	SER	2.8
2	H	67	VAL	2.8
3	m	83	VAL	2.8
2	K	37	ASP	2.8
3	e	350	GLU	2.8
3	c	71	PHE	2.8
2	T	205	ALA	2.8
2	E	185	PRO	2.8
2	F	11	SER	2.8
3	k	83	VAL	2.8
2	R	64	THR	2.8
2	I	160	LEU	2.8
3	c	40	LEU	2.8
3	o	40	LEU	2.8
2	R	22	PHE	2.8
2	T	109	PHE	2.8
2	D	273	ARG	2.8
1	7	2	VAL	2.8
2	B	210	PRO	2.8
2	O	95	VAL	2.8
3	o	55	LEU	2.8
2	C	275	GLU	2.8
2	C	213	ILE	2.8
2	G	190	THR	2.8
2	O	257	TYR	2.7
2	Q	7	TYR	2.7
2	O	203	CYS	2.7
2	O	250	PRO	2.7
3	c	6	PRO	2.7
3	a	24	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	8	7	ILE	2.7
1	X	7	ILE	2.7
2	C	36	PHE	2.7
2	C	10	THR	2.7
2	I	227	ASP	2.7
1	w	8	VAL	2.7
2	J	261	VAL	2.7
3	q	2	ILE	2.7
2	G	81	LEU	2.7
3	c	8	ILE	2.7
3	s	93	ILE	2.7
2	M	164	CYS	2.7
2	H	1	GLY	2.7
2	A	244	TRP	2.7
3	c	12	SER	2.7
3	q	96	TRP	2.7
2	Q	192	HIS	2.7
3	d	1	MET	2.7
3	c	16	ALA	2.7
1	u	7	ILE	2.6
3	o	36	ILE	2.6
2	P	22	PHE	2.6
2	M	91	GLY	2.6
3	k	34	SER	2.6
3	o	50	VAL	2.6
2	Q	116	TYR	2.6
3	r	64	TYR	2.6
3	f	35	ASP	2.6
3	k	2	ILE	2.6
2	C	189	MET	2.6
2	H	45	MET	2.6
2	F	177	GLU	2.6
2	R	161	GLU	2.6
2	G	211	ALA	2.6
2	E	74	HIS	2.6
2	R	9	PHE	2.6
3	g	91	PRO	2.6
2	B	265	GLY	2.6
3	c	44	GLY	2.6
2	G	261	VAL	2.6
2	K	51	TRP	2.6
3	a	16	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	K	2	SER	2.6
2	O	13	SER	2.6
2	T	59	TYR	2.6
3	r	8	ILE	2.6
2	E	235	PRO	2.6
1	7	4	ASP	2.6
2	Q	242	GLN	2.6
1	w	3	LEU	2.6
2	R	78	LEU	2.6
2	K	189	MET	2.6
2	A	8	PHE	2.6
3	r	34	SER	2.6
2	P	32	GLN	2.6
2	O	179	LEU	2.6
3	c	24	LEU	2.6
3	g	24	LEU	2.6
2	R	28	VAL	2.6
2	T	149	ALA	2.6
3	o	80	ALA	2.6
3	o	83	VAL	2.6
3	q	50	VAL	2.6
2	B	10	THR	2.6
2	C	258	THR	2.6
2	E	94	THR	2.6
2	F	60	TRP	2.5
2	Q	143	THR	2.6
1	W	7	ILE	2.5
1	7	7	ILE	2.5
3	f	2	ILE	2.5
2	K	8	PHE	2.5
3	f	71	PHE	2.5
2	E	257	TYR	2.5
2	M	7	TYR	2.5
2	M	191	HIS	2.5
3	b	15	PRO	2.5
3	m	29	SER	2.5
2	K	110	LEU	2.5
2	M	160	LEU	2.5
3	l	24	LEU	2.5
2	C	243	LYS	2.5
3	t	94	VAL	2.5
2	C	73	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	64	THR	2.5
3	k	8	ILE	2.5
2	I	118	TYR	2.5
3	c	33	PRO	2.5
2	C	207	SER	2.5
2	R	4	SER	2.5
2	S	224	GLN	2.5
3	a	30	GLY	2.5
2	B	17	ARG	2.5
3	a	38	VAL	2.5
2	H	199	ALA	2.5
2	Q	135	ALA	2.5
2	G	116	TYR	2.5
2	B	2	SER	2.5
2	G	242	GLN	2.5
1	5	9	VAL	2.5
3	f	16	ALA	2.5
2	B	86	ASN	2.5
3	d	93	ILE	2.5
2	P	36	PHE	2.5
2	D	116	TYR	2.5
2	K	269	PRO	2.5
2	L	114	HIS	2.5
2	L	215	LEU	2.5
2	R	116	TYR	2.5
2	Q	221	GLY	2.5
2	L	180	GLN	2.5
3	k	38	VAL	2.5
2	B	150	ALA	2.5
2	N	105	SER	2.5
3	m	80	ALA	2.5
2	E	52	ILE	2.5
3	e	369	GLU	2.5
2	Q	220	ASP	2.5
3	a	57	PHE	2.5
2	D	147	TRP	2.5
2	E	51	TRP	2.5
2	R	240	THR	2.5
3	m	5	THR	2.5
2	P	160	LEU	2.5
3	g	40	LEU	2.5
3	g	65	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	O	116	TYR	2.5
3	a	52	HIS	2.5
2	S	16	GLY	2.5
2	K	1	GLY	2.5
1	X	8	VAL	2.5
3	e	10	VAL	2.5
2	I	136	ALA	2.4
2	E	2	SER	2.4
2	P	23	ILE	2.4
2	A	177	GLU	2.4
2	A	254	GLU	2.4
2	C	45	MET	2.4
2	D	256	ARG	2.4
2	B	73	THR	2.4
2	C	178	THR	2.4
2	E	73	THR	2.4
2	J	223	ASP	2.4
3	c	5	THR	2.4
2	O	269	PRO	2.4
2	G	26	GLY	2.4
2	J	224	GLN	2.4
2	G	124	ILE	2.4
3	l	2	ILE	2.4
2	C	101	CYS	2.4
3	a	65	LEU	2.4
2	B	258	THR	2.4
2	F	10	THR	2.4
2	M	50	PRO	2.4
2	J	249	VAL	2.4
2	O	123	TYR	2.4
2	Q	237	GLY	2.4
2	T	16	GLY	2.4
3	h	94	VAL	2.4
3	q	94	VAL	2.4
2	B	236	ALA	2.4
2	G	43	GLN	2.4
2	K	23	ILE	2.4
2	N	140	ALA	2.4
2	J	111	ARG	2.4
3	q	95	LYS	2.4
2	C	168	LEU	2.4
2	E	179	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	K	179	LEU	2.4
3	h	55	LEU	2.4
2	N	274	TRP	2.4
2	D	1	GLY	2.4
2	R	112	GLY	2.4
2	G	52	ILE	2.4
3	a	80	ALA	2.4
2	N	273	ARG	2.4
2	N	275	GLU	2.4
2	O	164	CYS	2.4
1	3	8	VAL	2.4
2	C	50	PRO	2.4
2	L	134	THR	2.4
2	M	196	ASP	2.4
2	O	43	GLN	2.4
2	Q	9	PHE	2.4
2	F	160	LEU	2.4
2	G	172	LEU	2.4
2	A	11	SER	2.4
2	O	71	SER	2.4
3	a	34	SER	2.4
1	W	8	VAL	2.4
2	C	51	TRP	2.4
2	C	67	VAL	2.4
3	g	69	THR	2.3
3	e	380	CYS	2.4
2	D	26	GLY	2.3
1	x	7	ILE	2.3
3	c	25	ASN	2.3
2	B	196	ASP	2.3
2	C	7	TYR	2.3
3	f	99	ASP	2.3
2	B	172	LEU	2.3
2	C	156	LEU	2.3
3	c	9	GLN	2.3
2	P	58	GLU	2.3
3	e	382	VAL	2.3
2	H	51	TRP	2.3
2	H	273	ARG	2.3
2	R	94	THR	2.3
3	q	85	HIS	2.3
2	S	255	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	I	224	GLN	2.3
2	N	67	VAL	2.3
3	q	91	PRO	2.3
1	1	7	ILE	2.3
2	B	217	TRP	2.3
2	C	41	ALA	2.3
2	G	216	THR	2.3
2	S	251	SER	2.3
2	T	251	SER	2.3
3	a	47	ILE	2.3
3	k	96	TRP	2.3
2	G	74	HIS	2.3
2	Q	113	TYR	2.3
3	m	88	LEU	2.3
2	I	109	PHE	2.3
2	B	63	GLU	2.3
3	j	37	GLU	2.3
2	A	25	VAL	2.3
2	F	152	VAL	2.3
2	G	95	VAL	2.3
2	G	249	VAL	2.3
2	A	47	PRO	2.3
2	R	250	PRO	2.3
2	A	18	GLY	2.3
2	K	274	TRP	2.3
2	P	73	THR	2.3
3	f	62	SER	2.3
3	r	40	LEU	2.3
2	H	171	TYR	2.3
2	I	180	GLN	2.3
3	o	99	ASP	2.3
2	E	103	VAL	2.3
2	N	95	VAL	2.3
2	C	235	PRO	2.3
2	R	69	ALA	2.3
3	i	1	MET	2.3
2	R	156	LEU	2.3
3	l	65	LEU	2.3
2	F	114	HIS	2.3
2	P	11	SER	2.3
2	B	116	TYR	2.3
2	S	63	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	K	63	GLU	2.2
3	f	66	LEU	2.2
3	n	61	TRP	2.2
2	E	240	THR	2.2
2	L	258	THR	2.2
1	7	1	TYR	2.2
2	C	116	TYR	2.2
2	G	257	TYR	2.2
3	f	34	SER	2.2
3	g	11	TYR	2.2
3	s	62	SER	2.2
2	J	37	ASP	2.2
3	k	77	ASP	2.2
2	F	239	GLY	2.2
2	Q	20	PRO	2.2
2	N	179	LEU	2.2
2	R	215	LEU	2.2
2	F	274	TRP	2.2
2	R	178	THR	2.2
2	F	84	TYR	2.2
2	R	99	TYR	2.2
2	I	59	TYR	2.2
3	e	367	TYR	2.2
1	6	9	VAL	2.2
2	E	247	VAL	2.2
2	M	226	GLN	2.2
2	T	255	GLN	2.2
3	e	321	ASN	2.2
2	A	213	ILE	2.2
3	q	36	ILE	2.2
2	H	156	LEU	2.2
2	M	119	ASP	2.2
2	P	172	LEU	2.2
3	f	54	ASP	2.2
3	g	99	ASP	2.2
3	q	65	LEU	2.2
3	r	16	ALA	2.2
2	A	33	PHE	2.2
2	E	274	TRP	2.2
2	G	217	TRP	2.2
2	E	200	THR	2.2
2	M	31	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	195	SER	2.2
1	Y	3	LEU	2.2
2	E	168	LEU	2.2
2	G	128	GLU	2.2
2	O	81	LEU	2.2
2	E	16	GLY	2.2
2	E	41	ALA	2.2
2	S	211	ALA	2.2
2	Q	269	PRO	2.2
3	o	91	PRO	2.2
2	I	122	ASP	2.2
2	E	273	ARG	2.2
2	A	217	TRP	2.2
2	F	94	THR	2.2
2	S	73	THR	2.2
2	S	80	THR	2.2
3	p	5	THR	2.2
2	D	152	VAL	2.2
2	E	231	VAL	2.2
2	F	25	VAL	2.2
2	H	113	TYR	2.2
3	a	86	VAL	2.2
2	B	124	ILE	2.2
2	R	23	ILE	2.2
3	h	34	SER	2.2
3	e	352	SER	2.2
1	8	3	LEU	2.2
3	a	40	LEU	2.2
2	E	174	ASN	2.2
2	S	264	GLU	2.2
2	I	135	ALA	2.2
3	q	22	ASN	2.2
2	E	237	GLY	2.2
2	K	57	PRO	2.2
2	M	18	GLY	2.2
2	D	164	CYS	2.2
3	k	13	ARG	2.2
2	L	133	TRP	2.2
2	A	200	THR	2.1
2	C	25	VAL	2.1
2	H	216	THR	2.1
2	M	247	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	O	231	VAL	2.1
3	g	83	VAL	2.1
3	q	5	THR	2.1
2	F	7	TYR	2.1
2	G	113	TYR	2.1
2	K	113	TYR	2.1
2	N	85	TYR	2.1
1	z	7	ILE	2.1
2	B	226	GLN	2.1
2	R	179	LEU	2.1
2	K	42	SER	2.1
2	R	189	MET	2.1
3	c	92	LYS	2.1
3	f	42	LYS	2.1
3	o	1	MET	2.1
2	A	15	PRO	2.1
2	J	104	GLY	2.1
2	Q	120	GLY	2.1
2	M	174	ASN	2.1
3	k	33	PRO	2.1
3	q	15	PRO	2.1
2	F	77	ASP	2.1
2	G	203	CYS	2.1
2	H	101	CYS	2.1
2	S	227	ASP	2.1
2	A	167	TRP	2.1
2	D	249	VAL	2.1
2	S	249	VAL	2.1
2	Q	147	TRP	2.1
2	I	145	HIS	2.1
3	q	83	VAL	2.1
2	A	216	THR	2.1
2	P	94	THR	2.1
3	b	5	THR	2.1
2	A	171	TYR	2.1
2	G	209	TYR	2.1
2	S	171	TYR	2.1
3	q	67	TYR	2.1
2	Q	272	LEU	2.1
3	f	40	LEU	2.1
3	k	55	LEU	2.1
3	q	40	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	J	255	GLN	2.1
2	L	155	GLN	2.1
2	D	245	ALA	2.1
2	G	41	ALA	2.1
2	G	199	ALA	2.1
3	h	16	ALA	2.1
3	s	80	ALA	2.1
2	K	252	GLY	2.1
2	L	91	GLY	2.1
2	N	210	PRO	2.1
2	O	22	PHE	2.1
2	Q	109	PHE	2.1
2	A	247	VAL	2.1
2	G	25	VAL	2.1
2	H	77	ASP	2.1
3	o	35	ASP	2.1
3	e	351	HIS	2.1
1	v	7	ILE	2.1
2	M	225	THR	2.1
2	A	209	TYR	2.1
2	O	78	LEU	2.1
2	F	6	ARG	2.1
3	r	1	MET	2.1
2	C	91	GLY	2.1
2	F	58	GLU	2.1
3	c	91	PRO	2.1
3	r	70	GLU	2.1
2	G	207	SER	2.1
2	H	22	PHE	2.1
2	O	33	PHE	2.1
3	f	58	SER	2.1
2	C	174	ASN	2.1
2	L	152	VAL	2.1
2	M	103	VAL	2.1
3	d	94	VAL	2.1
3	r	50	VAL	2.1
1	3	4	ASP	2.1
2	A	23	ILE	2.1
2	R	126	LEU	2.1
3	c	2	ILE	2.1
3	m	24	LEU	2.1
2	C	271	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	75	ARG	2.1
2	A	189	MET	2.1
2	J	59	TYR	2.1
2	P	159	TYR	2.1
2	T	123	TYR	2.1
2	D	149	ALA	2.1
2	I	255	GLN	2.1
2	O	91	GLY	2.1
2	P	252	GLY	2.1
2	G	185	PRO	2.1
2	L	241	PHE	2.1
2	O	185	PRO	2.1
2	Q	250	PRO	2.1
2	I	33	PHE	2.1
3	q	6	PRO	2.1
2	F	71	SER	2.1
3	l	62	SER	2.1
3	m	56	SER	2.1
2	O	67	VAL	2.1
3	o	10	VAL	2.1
2	P	66	LYS	2.1
2	A	179	LEU	2.1
2	C	215	LEU	2.1
2	C	270	LEU	2.1
2	F	23	ILE	2.1
2	G	147	TRP	2.1
2	K	167	TRP	2.1
2	M	156	LEU	2.1
1	Y	4	ASP	2.1
2	F	98	MET	2.1
2	O	220	ASP	2.1
3	t	35	ASP	2.1
2	G	99	TYR	2.1
2	Q	259	CYS	2.1
2	R	73	THR	2.1
3	m	79	TYR	2.1
2	C	117	ALA	2.1
2	B	262	GLN	2.1
2	C	120	GLY	2.1
2	E	242	GLN	2.1
2	S	100	GLY	2.1
2	C	208	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	232	GLU	2.1
2	M	185	PRO	2.1
2	B	103	VAL	2.0
2	B	152	VAL	2.0
2	H	95	VAL	2.0
2	P	67	VAL	2.0
2	L	132	SER	2.0
3	l	21	SER	2.0
2	H	23	ILE	2.0
2	H	124	ILE	2.0
2	M	179	LEU	2.0
3	e	365	LEU	2.0
2	A	188	HIS	2.0
2	A	27	TYR	2.0
2	B	223	ASP	2.0
2	C	190	THR	2.0
2	E	113	TYR	2.0
2	E	143	THR	2.0
2	S	216	THR	2.0
2	R	220	ASP	2.0
3	p	35	ASP	2.0
2	L	96	GLN	2.0
2	C	185	PRO	2.0
2	H	20	PRO	2.0
2	M	210	PRO	2.0
2	J	63	GLU	2.0
2	A	231	VAL	2.0
2	B	67	VAL	2.0
2	J	12	VAL	2.0
2	O	34	VAL	2.0
3	c	83	VAL	2.0
1	V	6	LEU	2.0
2	H	126	LEU	2.0
2	J	23	ILE	2.0
2	M	23	ILE	2.0
2	M	92	SER	2.0
2	O	207	SER	2.0
3	a	21	SER	2.0
3	j	56	SER	2.0
2	A	74	HIS	2.0
2	Q	98	MET	2.0
2	T	244	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
2	A	134	THR	2.0
2	A	139	ALA	2.0
2	A	211	ALA	2.0
2	B	199	ALA	2.0
2	J	199	ALA	2.0
2	Q	140	ALA	2.0
2	T	24	ALA	2.0
3	o	11	TYR	2.0
3	e	5	THR	2.0
2	N	223	ASP	2.0
2	P	223	ASP	2.0
2	Q	29	ASP	2.0
2	C	1	GLY	2.0
2	S	109	PHE	2.0
2	S	120	GLY	2.0
2	G	269	PRO	2.0
2	J	121	LYS	2.0
3	m	15	PRO	2.0
1	1	8	VAL	2.0
2	C	19	GLU	2.0
2	N	76	VAL	2.0
3	c	28	VAL	2.0
3	g	50	VAL	2.0
3	g	86	VAL	2.0
3	r	65	LEU	2.0
3	r	66	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.