Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2016 – 01:53 PM EDT

PDB ID	:	5E6I
Title	:	Crystal structure of TCR PF8 in complex with flu MP(58-66) epitope presented by HLA-A2
Authors	:	Gao, M.; Mariuzza, R.
Deposited on	:	2015-10-09
Resolution	:	4.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

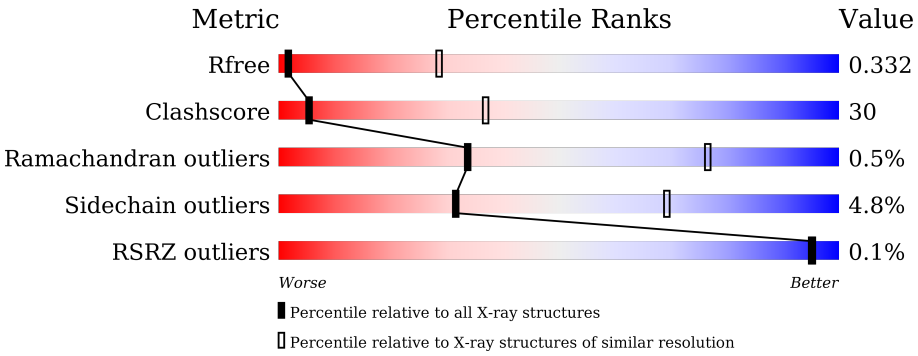
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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

Mol	Chain	Length	Quality of chain
1	A	208	57% 34% • 6%
1	F	208	57% 35% •• 5%
1	G	208	62% 30% 5% •
1	P	208	57% 32% • 8%
2	B	243	60% 36% •••
2	H	243	58% 38% ••

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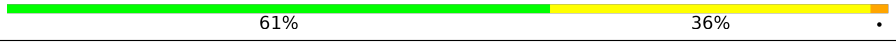
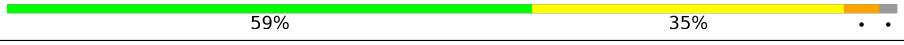
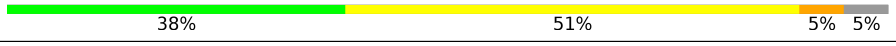
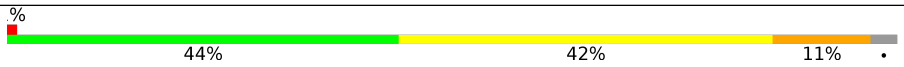
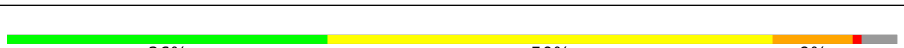
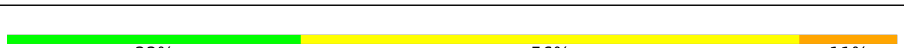
Mol	Chain	Length	Quality of chain
2	L	243	
2	Q	243	
3	C	276	
3	I	276	
3	M	276	
3	R	276	
4	D	100	
4	J	100	
4	N	100	
4	U	100	
5	E	9	
5	K	9	
5	O	9	
5	T	9	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24882 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 TCR alpha chain,Human nkt tcr alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	201	Total	C	N	O	S	0	0	0
			1535	961	252	313	9			
1	A	196	Total	C	N	O	S	0	0	0
			1459	910	241	300	8			
1	F	198	Total	C	N	O	S	0	0	0
			1486	930	243	304	9			
1	P	191	Total	C	N	O	S	0	0	0
			1426	895	232	292	7			

- Molecule 2 is a protein called T-cell receptor beta-2 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	239	Total	C	N	O	S	0	0	0
			1878	1189	320	361	8			
2	B	241	Total	C	N	O	S	0	0	0
			1870	1179	316	367	8			
2	L	242	Total	C	N	O	S	0	0	0
			1891	1199	314	370	8			
2	Q	238	Total	C	N	O	S	0	0	0
			1840	1164	312	356	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	0	MET	LEU	conflict	UNP A0A087WZ08
H	18	GLU	LYS	conflict	UNP A0A087WZ08
H	?	-	SER	deletion	UNP A0A087WZ08
H	96	ILE	THR	conflict	UNP A0A087WZ08
H	97	TYR	VAL	conflict	UNP A0A087WZ08
H	98	PRO	LEU	conflict	UNP A0A087WZ08
H	99	GLY	HIS	conflict	UNP A0A087WZ08
H	100	GLU	SER	conflict	UNP A0A087WZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
H	101	LEU	GLN	conflict	UNP A0A087WZ08
H	102	PHE	TYR	conflict	UNP A0A087WZ08
H	105	GLU	PRO	conflict	UNP A0A087WZ08
H	107	SER	THR	conflict	UNP A0A087WZ08
H	110	THR	LEU	conflict	UNP A0A087WZ08
H	122	GLU	LYS	conflict	UNP A0A087WZ08
H	169	CYS	SER	conflict	UNP A0A087WZ08
H	187	ALA	CYS	conflict	UNP A0A087WZ08
B	0	MET	LEU	conflict	UNP A0A087WZ08
B	18	GLU	LYS	conflict	UNP A0A087WZ08
B	?	-	SER	deletion	UNP A0A087WZ08
B	96	ILE	THR	conflict	UNP A0A087WZ08
B	97	TYR	VAL	conflict	UNP A0A087WZ08
B	98	PRO	LEU	conflict	UNP A0A087WZ08
B	99	GLY	HIS	conflict	UNP A0A087WZ08
B	100	GLU	SER	conflict	UNP A0A087WZ08
B	101	LEU	GLN	conflict	UNP A0A087WZ08
B	102	PHE	TYR	conflict	UNP A0A087WZ08
B	105	GLU	PRO	conflict	UNP A0A087WZ08
B	107	SER	THR	conflict	UNP A0A087WZ08
B	110	THR	LEU	conflict	UNP A0A087WZ08
B	122	GLU	LYS	conflict	UNP A0A087WZ08
B	169	CYS	SER	conflict	UNP A0A087WZ08
B	187	ALA	CYS	conflict	UNP A0A087WZ08
L	0	MET	LEU	conflict	UNP A0A087WZ08
L	18	GLU	LYS	conflict	UNP A0A087WZ08
L	?	-	SER	deletion	UNP A0A087WZ08
L	96	ILE	THR	conflict	UNP A0A087WZ08
L	97	TYR	VAL	conflict	UNP A0A087WZ08
L	98	PRO	LEU	conflict	UNP A0A087WZ08
L	99	GLY	HIS	conflict	UNP A0A087WZ08
L	100	GLU	SER	conflict	UNP A0A087WZ08
L	101	LEU	GLN	conflict	UNP A0A087WZ08
L	102	PHE	TYR	conflict	UNP A0A087WZ08
L	105	GLU	PRO	conflict	UNP A0A087WZ08
L	107	SER	THR	conflict	UNP A0A087WZ08
L	110	THR	LEU	conflict	UNP A0A087WZ08
L	122	GLU	LYS	conflict	UNP A0A087WZ08
L	169	CYS	SER	conflict	UNP A0A087WZ08
L	187	ALA	CYS	conflict	UNP A0A087WZ08
Q	0	MET	LEU	conflict	UNP A0A087WZ08
Q	18	GLU	LYS	conflict	UNP A0A087WZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	?	-	SER	deletion	UNP A0A087WZ08
Q	96	ILE	THR	conflict	UNP A0A087WZ08
Q	97	TYR	VAL	conflict	UNP A0A087WZ08
Q	98	PRO	LEU	conflict	UNP A0A087WZ08
Q	99	GLY	HIS	conflict	UNP A0A087WZ08
Q	100	GLU	SER	conflict	UNP A0A087WZ08
Q	101	LEU	GLN	conflict	UNP A0A087WZ08
Q	102	PHE	TYR	conflict	UNP A0A087WZ08
Q	105	GLU	PRO	conflict	UNP A0A087WZ08
Q	107	SER	THR	conflict	UNP A0A087WZ08
Q	110	THR	LEU	conflict	UNP A0A087WZ08
Q	122	GLU	LYS	conflict	UNP A0A087WZ08
Q	169	CYS	SER	conflict	UNP A0A087WZ08
Q	187	ALA	CYS	conflict	UNP A0A087WZ08

- Molecule 3 is a protein called HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	261	Total	C	N	O	S	0	0	0
			2072	1297	378	388	9			
3	C	258	Total	C	N	O	S	0	0	0
			2034	1273	363	389	9			
3	M	268	Total	C	N	O	S	0	0	0
			2076	1294	375	399	8			
3	R	251	Total	C	N	O	S	0	0	0
			1994	1249	360	376	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	0	MET	-	initiating methionine	UNP P01892
C	0	MET	-	initiating methionine	UNP P01892
M	0	MET	-	initiating methionine	UNP P01892
R	0	MET	-	initiating methionine	UNP P01892

- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	96	Total	C	N	O	S	0	0	0
			772	489	131	149	3			
4	D	97	Total	C	N	O	S	0	0	0
			787	503	131	150	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	92	Total	C	N	O	S	0	0	0
			697	440	123	132	2			
4	U	99	Total	C	N	O	S	0	0	0
			793	504	133	153	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	0	MET	-	initiating methionine	UNP P61769
D	0	MET	-	initiating methionine	UNP P61769
N	0	MET	-	initiating methionine	UNP P61769
U	0	MET	-	initiating methionine	UNP P61769

- Molecule 5 is a protein called Matrix protein 1.

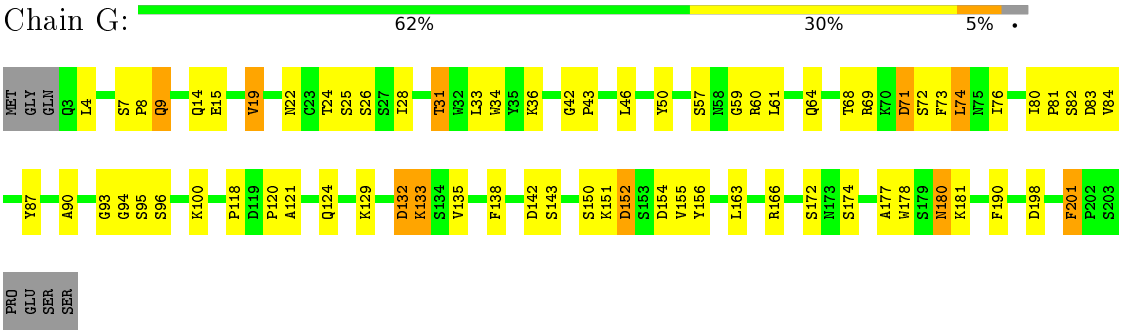
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	9	Total	C	N	O	0	0	0
			68	49	9	10			
5	E	9	Total	C	N	O	0	0	0
			68	49	9	10			
5	O	9	Total	C	N	O	0	0	0
			68	49	9	10			
5	T	9	Total	C	N	O	0	0	0
			68	49	9	10			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

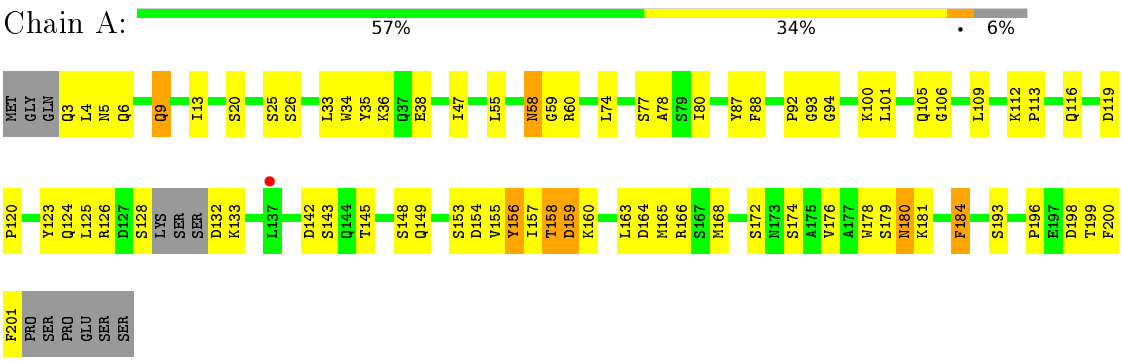
- Molecule 1: TCR alpha chain,Human nkt tcr alpha chain

Chain G:



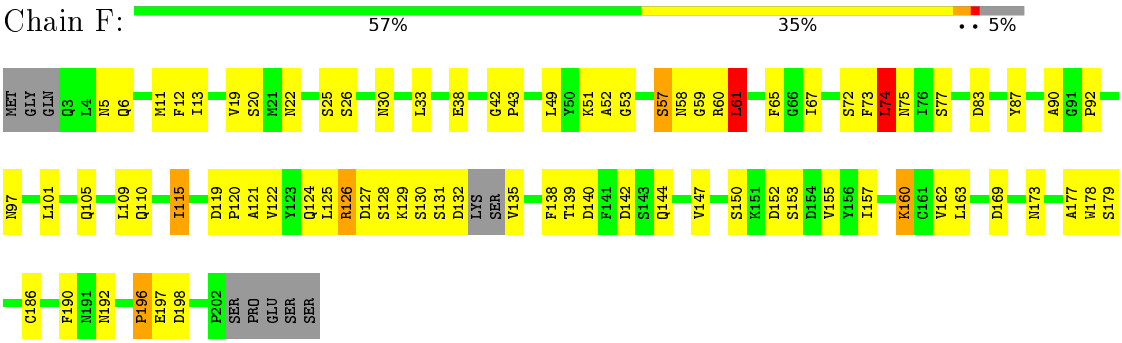
- Molecule 1: TCR alpha chain,Human nkt tcr alpha chain

Chain A:



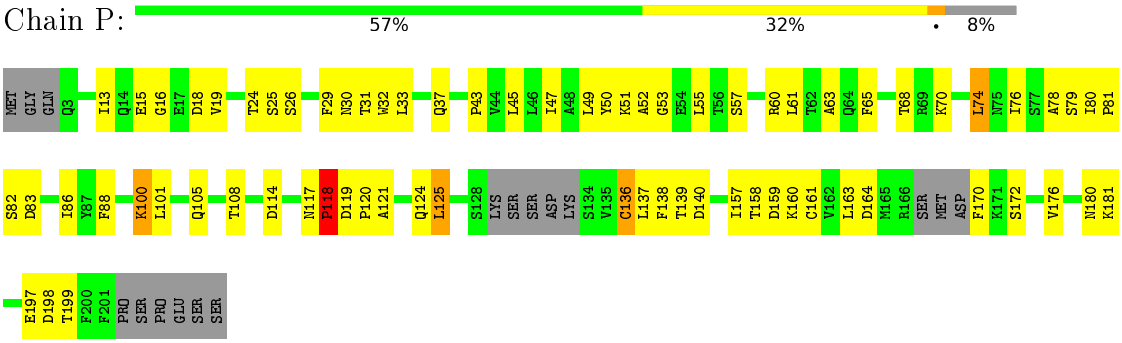
- Molecule 1: TCR alpha chain,Human nkt tcr alpha chain

Chain F:



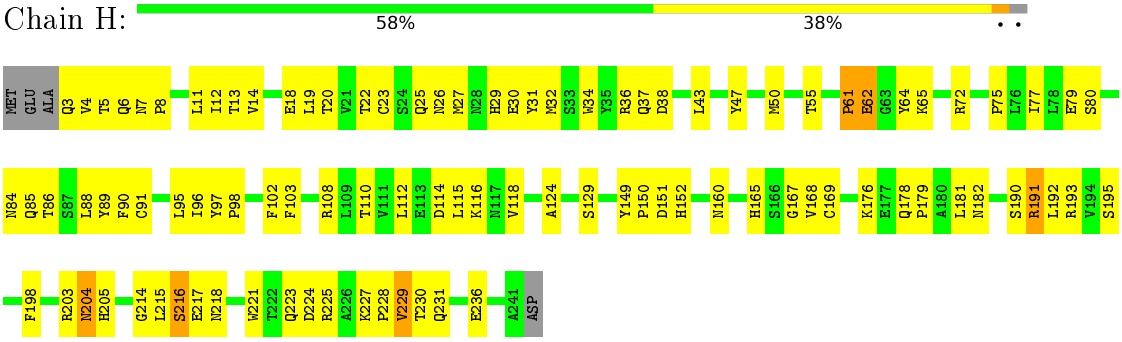
- Molecule 1: TCR alpha chain,Human nkt tcr alpha chain

Chain P:



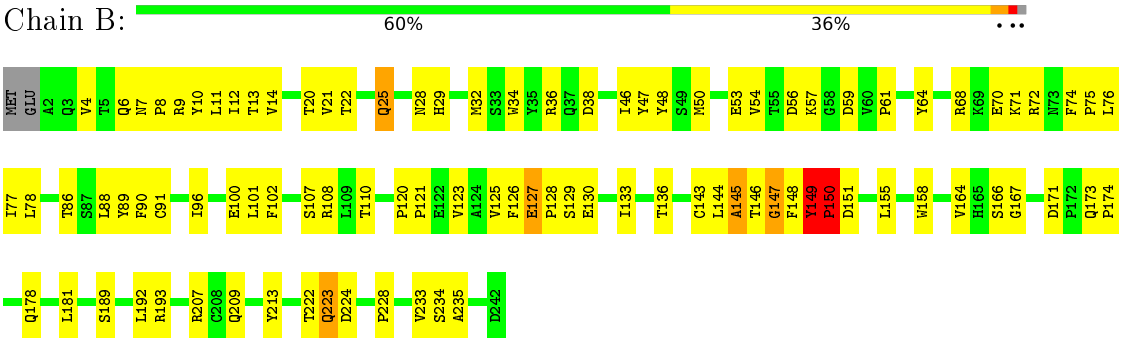
• Molecule 2: T-cell receptor beta-2 chain C region

Chain H:



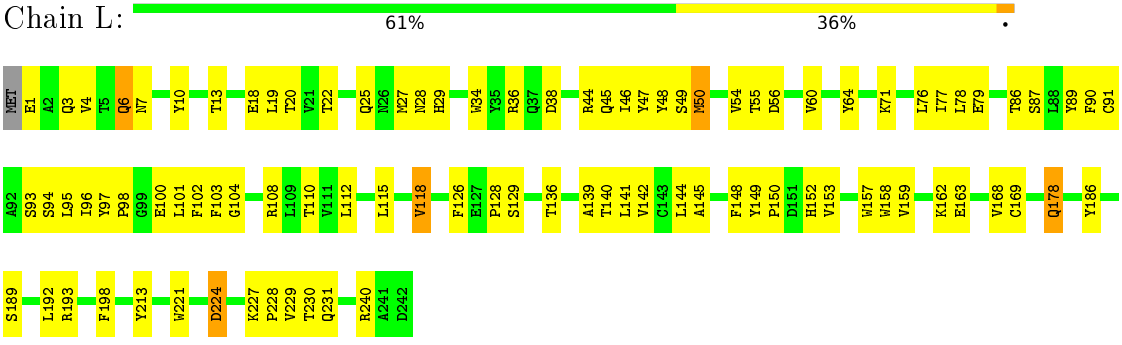
• Molecule 2: T-cell receptor beta-2 chain C region

Chain B:



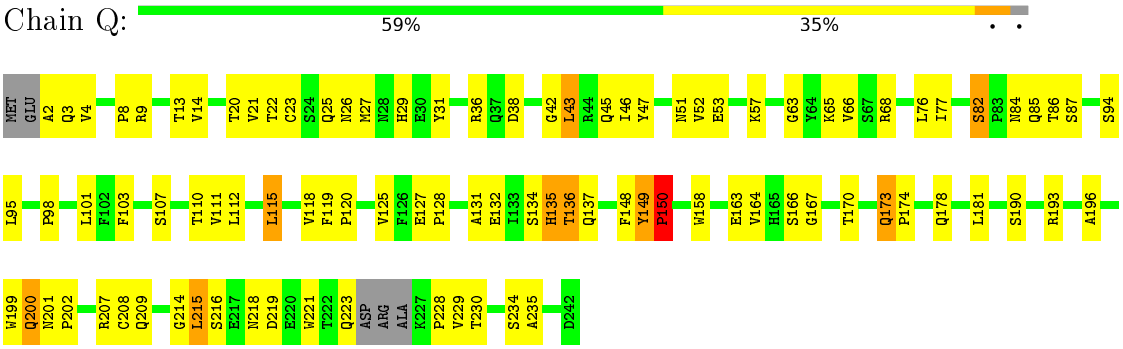
• Molecule 2: T-cell receptor beta-2 chain C region

Chain L:



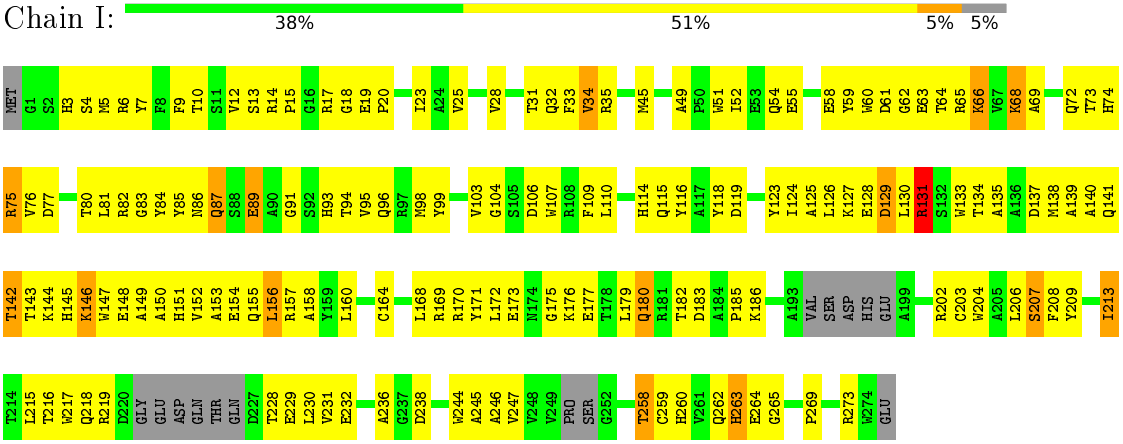
• Molecule 2: T-cell receptor beta-2 chain C region

Chain Q:



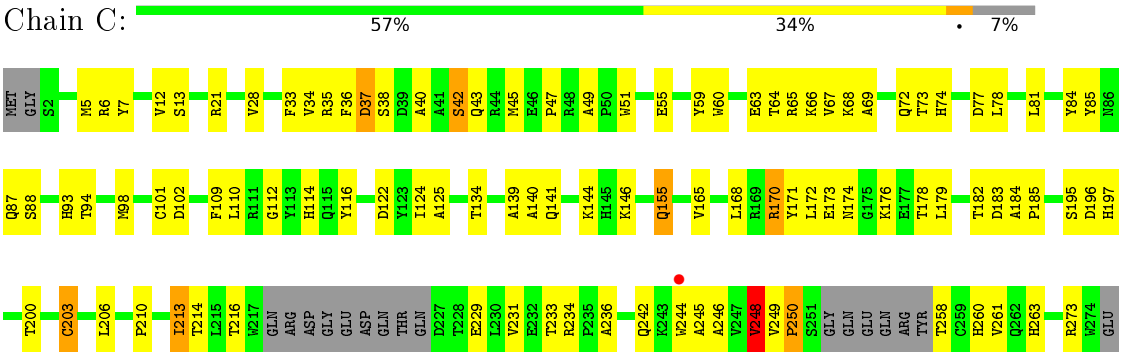
• Molecule 3: HLA class I histocompatibility antigen, A-2 alpha chain

Chain I:



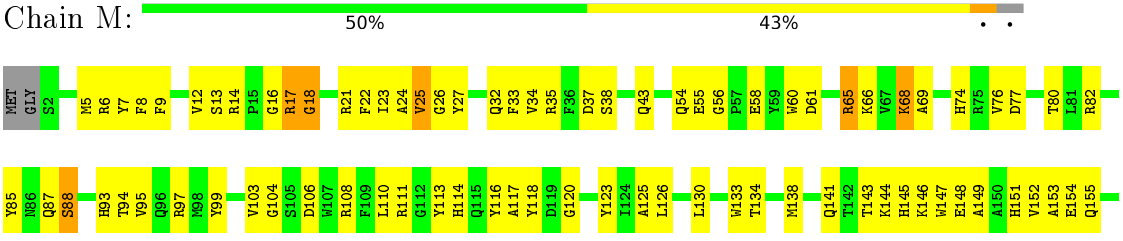
• Molecule 3: HLA class I histocompatibility antigen, A-2 alpha chain

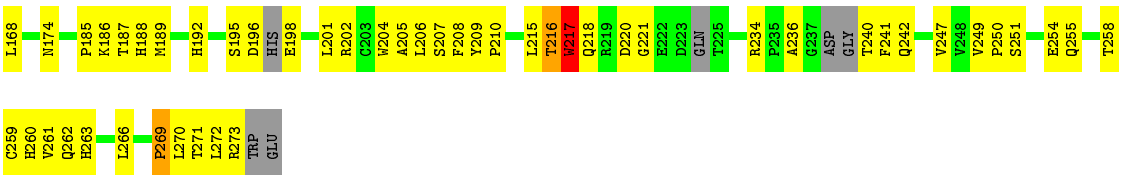
Chain C:



• Molecule 3: HLA class I histocompatibility antigen, A-2 alpha chain

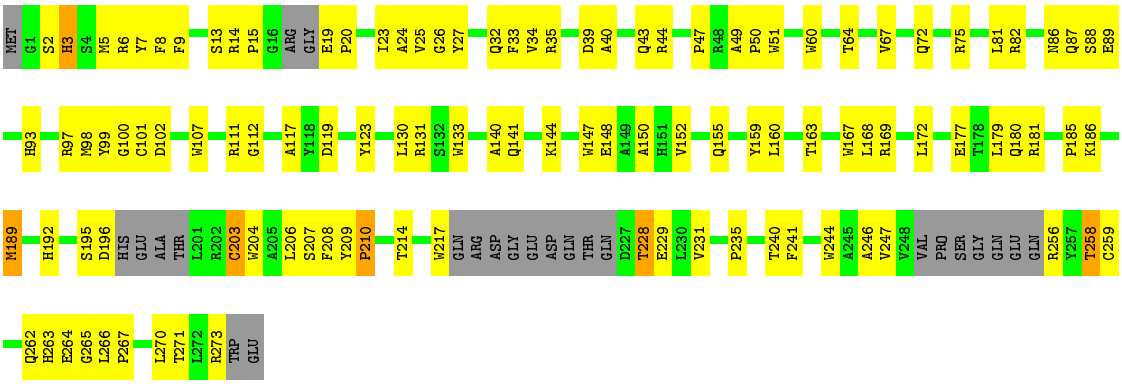
Chain M:





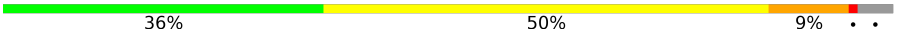
• Molecule 3: HLA class I histocompatibility antigen, A-2 alpha chain

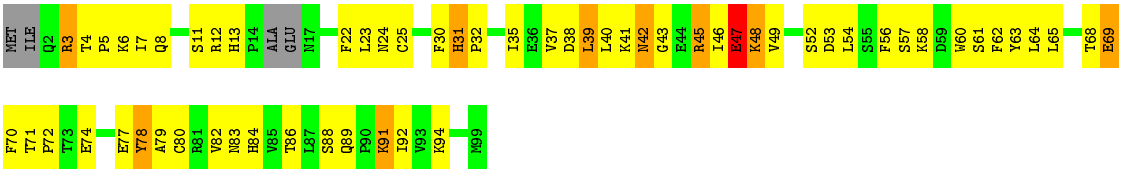
Chain R:



• Molecule 4: Beta-2-microglobulin

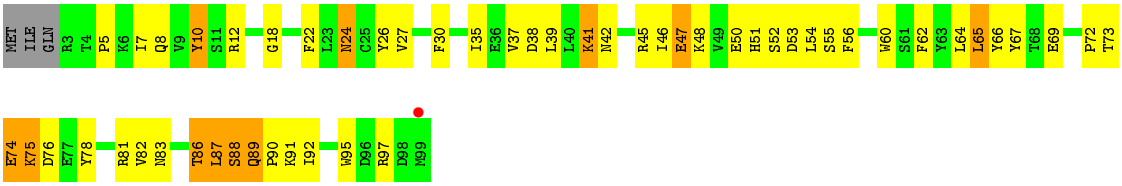
Chain J:





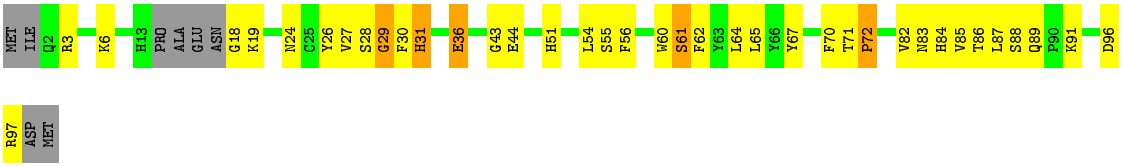
• Molecule 4: Beta-2-microglobulin

Chain D:



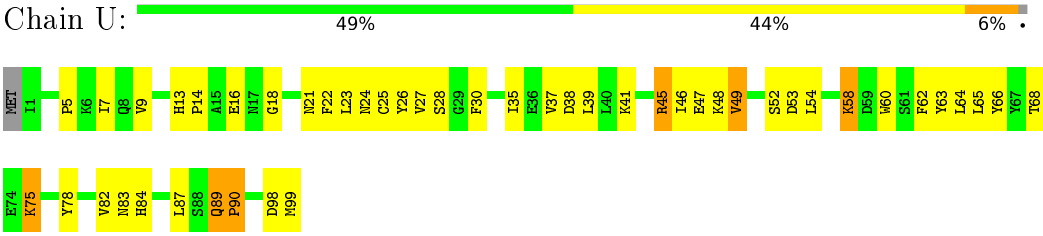
• Molecule 4: Beta-2-microglobulin

Chain N:



• Molecule 4: Beta-2-microglobulin

Chain U:



• Molecule 5: Matrix protein 1

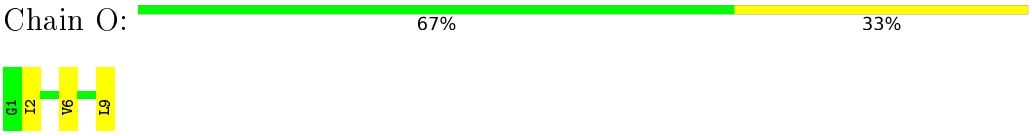
Chain K:

• Molecule 5: Matrix protein 1

Chain E:

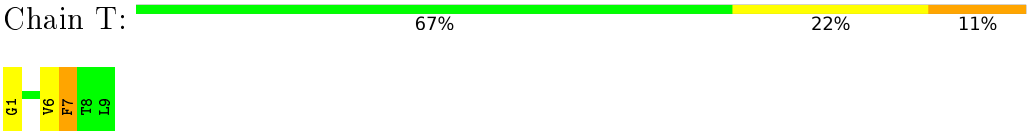
• Molecule 5: Matrix protein 1

Chain O:



• Molecule 5: Matrix protein 1

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.85Å 123.61Å 139.04Å 83.66° 74.87° 73.17°	Depositor
Resolution (Å)	36.56 – 4.00 46.15 – 4.00	Depositor EDS
% Data completeness (in resolution range)	91.0 (36.56-4.00) 79.4 (46.15-4.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 4.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.259 , 0.338 0.258 , 0.332	Depositor DCC
R_{free} test set	1442 reflections (4.80%)	DCC
Wilson B-factor (Å^2)	97.3	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.17 , -11.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.247 for h,h-k,h-l 0.000 for -h,-h+k,-l 0.000 for -h,-k,-h+l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	24882	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.39	0/1486	0.67	1/2013 (0.0%)
1	F	0.40	0/1517	0.70	5/2060 (0.2%)
1	G	0.38	0/1567	0.63	3/2125 (0.1%)
1	P	0.39	0/1454	0.66	4/1977 (0.2%)
2	B	0.39	1/1917 (0.1%)	0.63	2/2616 (0.1%)
2	H	0.35	0/1930	0.63	1/2635 (0.0%)
2	L	0.36	0/1944	0.59	0/2659
2	Q	0.38	0/1891	0.66	2/2583 (0.1%)
3	C	0.42	2/2091 (0.1%)	0.72	3/2841 (0.1%)
3	I	0.48	0/2129	0.77	3/2887 (0.1%)
3	M	0.44	0/2130	0.73	4/2890 (0.1%)
3	R	0.38	0/2048	0.61	0/2777
4	D	0.45	0/809	0.76	2/1098 (0.2%)
4	J	0.38	0/793	0.76	4/1075 (0.4%)
4	N	0.51	0/715	0.85	2/962 (0.2%)
4	U	0.46	1/815 (0.1%)	0.80	2/1104 (0.2%)
5	E	0.31	0/69	0.50	0/92
5	K	0.56	0/69	0.83	1/92 (1.1%)
5	O	0.28	0/69	0.48	0/92
5	T	0.33	0/69	0.52	0/92
All	All	0.41	4/25512 (0.0%)	0.69	39/34670 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
1	P	0	1
2	Q	0	1
3	C	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	I	0	1
3	M	0	2
3	R	0	2
4	D	0	1
4	J	0	2
4	N	0	1
All	All	0	15

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	150	PRO	N-CD	5.22	1.55	1.47
3	C	248	VAL	CB-CG2	-5.20	1.42	1.52
3	C	250	PRO	N-CD	5.10	1.54	1.47
4	U	90	PRO	N-CD	5.04	1.54	1.47

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	179	LEU	CA-CB-CG	9.22	136.52	115.30
2	H	231	GLN	N-CA-CB	9.00	126.79	110.60
4	N	19	LYS	N-CA-C	-8.43	88.24	111.00
3	I	203	CYS	CA-CB-SG	8.22	128.80	114.00
1	F	196	PRO	CA-N-CD	-8.14	100.10	111.50
2	B	147	GLY	N-CA-C	8.04	133.20	113.10
4	U	58	LYS	CD-CE-NZ	-6.48	96.79	111.70
3	I	129	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	F	126	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	F	74	LEU	CA-CB-CG	6.02	129.15	115.30
4	U	89	GLN	C-N-CD	5.99	140.98	128.40
3	M	192	HIS	N-CA-C	5.95	127.08	111.00
3	C	249	VAL	C-N-CD	5.92	140.83	128.40
4	D	89	GLN	C-N-CD	5.92	140.82	128.40
2	Q	150	PRO	CA-N-CD	-5.92	103.22	111.50
3	M	207	SER	N-CA-C	5.89	126.91	111.00
1	G	201	PHE	C-N-CD	5.81	140.59	128.40
1	P	55	LEU	CB-CA-C	5.75	121.13	110.20
1	P	117	ASN	C-N-CD	5.74	140.45	128.40
3	M	269	PRO	N-CA-C	-5.65	97.41	112.10
4	D	65	LEU	CA-CB-CG	5.65	128.29	115.30
1	F	61	LEU	CA-CB-CG	5.64	128.27	115.30
4	N	29	GLY	N-CA-C	5.63	127.19	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	149	TYR	C-N-CD	5.62	140.19	128.40
4	J	48	LYS	N-CA-C	5.61	126.14	111.00
1	P	53	GLY	N-CA-C	-5.52	99.30	113.10
1	P	118	PRO	CA-N-CD	-5.48	103.83	111.50
4	J	47	GLU	N-CA-C	5.46	125.73	111.00
3	M	68	LYS	CD-CE-NZ	5.38	124.08	111.70
1	G	132	ASP	CB-CG-OD2	5.24	123.02	118.30
3	C	37	ASP	CB-CG-OD2	5.23	123.00	118.30
4	J	53	ASP	CB-CG-OD2	5.21	122.99	118.30
1	G	152	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	159	ASP	CB-CG-OD2	5.17	122.95	118.30
5	K	2	ILE	CG1-CB-CG2	-5.15	100.07	111.40
4	J	42	ASN	N-CA-C	-5.15	97.11	111.00
3	I	131	ARG	CG-CD-NE	-5.14	101.00	111.80
2	B	149	TYR	C-N-CD	5.12	139.14	128.40
1	F	126	ARG	NE-CZ-NH2	-5.05	117.77	120.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	THR	Peptide
3	C	178	THR	Peptide
3	C	233	THR	Peptide
4	D	86	THR	Peptide
1	F	57	SER	Peptide
3	I	131	ARG	Peptide
4	J	47	GLU	Peptide
4	J	68	THR	Peptide
3	M	217	TRP	Peptide
3	M	88	SER	Peptide
4	N	83	ASN	Peptide
1	P	197	GLU	Peptide
2	Q	135	HIS	Peptide
3	R	258	THR	Peptide
3	R	43	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1459	0	1369	65	0
1	F	1486	0	1377	72	0
1	G	1535	0	1459	86	0
1	P	1426	0	1324	72	0
2	B	1870	0	1737	107	0
2	H	1878	0	1760	101	0
2	L	1891	0	1754	109	0
2	Q	1840	0	1701	88	0
3	C	2034	0	1862	109	0
3	I	2072	0	1914	210	0
3	M	2076	0	1865	138	0
3	R	1994	0	1836	116	0
4	D	787	0	736	79	0
4	J	772	0	706	80	0
4	N	697	0	612	51	0
4	U	793	0	732	68	0
5	E	68	0	75	6	0
5	K	68	0	75	17	0
5	O	68	0	75	6	0
5	T	68	0	75	4	0
All	All	24882	0	23044	1434	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (1434) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133:LYS:CB	1:G:180:ASN:HD21	1.15	1.51
1:P:47:ILE:CD1	1:P:57:SER:HB2	1.37	1.50
1:G:59:GLY:CA	1:G:61:LEU:H	1.24	1.50
1:G:59:GLY:HA3	1:G:61:LEU:N	1.32	1.44
1:G:133:LYS:CB	1:G:180:ASN:ND2	1.89	1.33
1:G:133:LYS:HB3	1:G:180:ASN:ND2	1.43	1.28
2:H:97:TYR:O	3:I:152:VAL:HG12	1.23	1.25
4:D:73:THR:HB	4:D:76:ASP:OD2	1.27	1.24
2:Q:136:THR:OG1	2:Q:137:GLN:HA	1.37	1.21
2:B:145:ALA:HB1	2:B:148:PHE:CZ	1.76	1.20
2:B:121:PRO:CB	2:B:148:PHE:HE1	1.54	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:96:ILE:CD1	3:M:146:LYS:HE2	1.73	1.18
4:N:18:GLY:HA2	4:N:72:PRO:O	1.38	1.18
2:L:96:ILE:HD12	3:M:146:LYS:CE	1.74	1.17
2:B:222:THR:HB	2:B:223:GLN:CG	1.74	1.16
4:J:4:THR:HB	4:J:86:THR:CG2	1.75	1.16
1:P:47:ILE:HD12	1:P:57:SER:CB	1.75	1.15
2:H:97:TYR:O	3:I:152:VAL:CG1	1.95	1.13
1:G:133:LYS:CA	1:G:180:ASN:HD21	1.62	1.12
1:P:47:ILE:CD1	1:P:57:SER:CB	2.27	1.11
4:N:84:HIS:CD2	4:N:86:THR:H	1.69	1.11
4:U:58:LYS:HA	4:U:60:TRP:H	1.13	1.10
2:H:97:TYR:C	3:I:152:VAL:HG12	1.72	1.10
3:I:63:GLU:HA	3:I:66:LYS:HZ2	1.14	1.09
1:P:47:ILE:CG1	1:P:57:SER:HB2	1.83	1.08
2:B:145:ALA:HB1	2:B:148:PHE:HZ	1.05	1.07
1:G:133:LYS:CG	1:G:180:ASN:HD21	1.68	1.06
2:B:222:THR:HB	2:B:223:GLN:HG3	1.12	1.06
2:B:96:ILE:HD12	3:C:146:LYS:HE2	1.32	1.06
3:C:49:ALA:HB1	3:C:51:TRP:CZ3	1.90	1.06
4:J:45:ARG:H	4:J:45:ARG:HD2	1.22	1.05
4:U:83:ASN:HB2	4:U:90:PRO:HB3	1.11	1.05
2:L:96:ILE:HD11	3:M:146:LYS:NZ	1.73	1.04
2:H:96:ILE:HG22	3:I:152:VAL:HG11	1.39	1.04
2:B:149:TYR:CE2	2:B:150:PRO:HB3	1.94	1.03
1:G:57:SER:O	1:G:59:GLY:N	1.89	1.03
4:D:76:ASP:HB3	4:D:78:TYR:HE2	1.23	1.03
2:Q:119:PHE:HB2	2:Q:120:PRO:HD2	1.38	1.03
2:L:96:ILE:CD1	3:M:146:LYS:CE	2.34	1.02
3:I:218:GLN:HG3	3:I:219:ARG:H	1.25	1.01
1:G:132:ASP:O	1:G:180:ASN:OD1	1.78	1.01
4:N:84:HIS:HD2	4:N:86:THR:HG22	1.22	1.00
2:Q:132:GLU:O	2:Q:136:THR:HA	1.59	1.00
4:N:84:HIS:CD2	4:N:86:THR:HB	1.98	0.99
4:J:4:THR:HB	4:J:86:THR:HG21	1.02	0.99
4:N:84:HIS:HD2	4:N:86:THR:CG2	1.74	0.99
4:D:76:ASP:HB3	4:D:78:TYR:CE2	1.99	0.98
2:B:121:PRO:CB	2:B:148:PHE:CE1	2.47	0.98
1:G:133:LYS:HA	1:G:180:ASN:ND2	1.77	0.98
3:I:155:GLN:O	3:I:157:ARG:N	1.97	0.98
3:M:55:GLU:HB3	3:M:58:GLU:HG3	1.44	0.97
3:C:173:GLU:HG3	3:C:174:ASN:N	1.76	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:60:ARG:NH2	1:G:83:ASP:OD2	1.97	0.96
2:L:227:LYS:O	2:L:229:VAL:HG23	1.65	0.96
4:N:84:HIS:NE2	4:N:86:THR:HB	1.80	0.96
2:B:222:THR:CB	2:B:223:GLN:HG3	1.95	0.95
2:Q:134:SER:O	2:Q:136:THR:HB	1.67	0.95
1:G:133:LYS:CA	1:G:180:ASN:ND2	2.24	0.95
4:D:74:GLU:N	4:D:74:GLU:OE2	2.00	0.94
3:M:65:ARG:O	3:M:68:LYS:CD	2.16	0.94
4:J:46:ILE:CD1	4:J:70:PHE:HZ	1.80	0.94
2:B:121:PRO:HA	2:B:148:PHE:CE1	2.02	0.94
3:M:126:LEU:HD21	3:M:130:LEU:HA	1.49	0.94
4:J:4:THR:CB	4:J:86:THR:HG21	1.97	0.93
4:U:58:LYS:HA	4:U:60:TRP:N	1.83	0.93
3:M:32:GLN:OE1	3:M:34:VAL:N	2.02	0.93
3:M:17:ARG:HG2	3:M:17:ARG:HH11	1.34	0.92
4:N:84:HIS:CD2	4:N:86:THR:CB	2.52	0.92
3:I:218:GLN:HG3	3:I:219:ARG:N	1.84	0.91
4:D:73:THR:CB	4:D:76:ASP:OD2	2.19	0.91
4:N:18:GLY:CA	4:N:72:PRO:O	2.19	0.90
3:M:6:ARG:HH12	3:M:113:TYR:HD2	1.17	0.90
2:L:96:ILE:HD11	3:M:146:LYS:HZ3	1.36	0.90
2:Q:149:TYR:CE1	2:Q:150:PRO:HB3	2.07	0.90
2:B:96:ILE:HD12	3:C:146:LYS:CE	2.02	0.90
1:G:133:LYS:HB3	1:G:180:ASN:HD22	1.36	0.89
4:J:46:ILE:HD13	4:J:70:PHE:CZ	2.07	0.89
1:G:59:GLY:CA	1:G:61:LEU:N	2.07	0.89
3:M:65:ARG:HG3	3:M:65:ARG:HH11	1.35	0.89
1:P:47:ILE:CG1	1:P:57:SER:CB	2.50	0.89
4:U:28:SER:HB3	4:U:63:TYR:HA	1.54	0.89
3:C:66:LYS:HD2	5:E:4:GLY:HA2	1.51	0.89
2:H:228:PRO:O	2:H:229:VAL:HG22	1.72	0.89
1:P:52:ALA:HA	1:P:65:PHE:HB3	1.52	0.89
2:Q:136:THR:OG1	2:Q:137:GLN:CA	2.21	0.89
4:D:75:LYS:O	4:D:76:ASP:OD1	1.91	0.89
1:F:115:ILE:HD13	1:F:142:ASP:HA	1.53	0.89
3:C:146:LYS:NZ	5:E:9:LEU:O	2.04	0.88
3:R:263:HIS:ND1	3:R:265:GLY:N	2.22	0.88
3:M:65:ARG:O	3:M:68:LYS:HD3	1.73	0.88
2:L:96:ILE:HD12	3:M:146:LYS:HE2	0.89	0.87
4:D:76:ASP:CB	4:D:78:TYR:HE2	1.87	0.87
2:B:121:PRO:CA	2:B:148:PHE:CE1	2.58	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:5:PRO:HB3	4:D:30:PHE:HB3	1.56	0.87
3:R:207:SER:HA	3:R:240:THR:HB	1.55	0.87
2:L:95:LEU:HD12	2:L:96:ILE:N	1.90	0.86
1:P:47:ILE:HG13	1:P:57:SER:CB	2.05	0.86
2:Q:134:SER:C	2:Q:136:THR:HB	1.94	0.86
4:J:46:ILE:CD1	4:J:70:PHE:CZ	2.58	0.86
3:I:218:GLN:CG	3:I:219:ARG:H	1.88	0.86
3:M:215:LEU:HB3	3:M:261:VAL:HG12	1.57	0.86
4:J:89:GLN:HB2	4:J:91:LYS:HG2	1.58	0.86
3:R:185:PRO:HD3	3:R:263:HIS:CD2	2.10	0.86
2:H:47:TYR:HE1	2:H:61:PRO:HA	1.39	0.86
3:I:145:HIS:O	3:I:148:GLU:N	2.08	0.85
4:J:3:ARG:O	4:J:30:PHE:HA	1.76	0.85
2:Q:149:TYR:CD1	2:Q:150:PRO:HB3	2.10	0.85
3:I:183:ASP:OD2	3:I:207:SER:O	1.95	0.85
4:J:46:ILE:HD13	4:J:70:PHE:HZ	1.38	0.85
3:C:173:GLU:HG3	3:C:174:ASN:H	1.37	0.85
2:B:7:ASN:ND2	2:B:22:THR:OG1	2.08	0.85
1:P:47:ILE:HD12	1:P:57:SER:HB2	0.87	0.85
4:N:88:SER:OG	4:N:89:GLN:N	2.10	0.85
2:B:53:GLU:O	3:C:68:LYS:HE2	1.76	0.84
1:F:129:LYS:HG3	1:F:131:SER:H	1.43	0.84
4:D:83:ASN:HB2	4:D:90:PRO:HB3	1.60	0.84
3:I:263:HIS:CE1	3:I:265:GLY:H	1.94	0.84
1:A:158:THR:HG22	1:A:159:ASP:H	1.42	0.84
4:N:84:HIS:CD2	4:N:86:THR:N	2.46	0.83
1:P:37:GLN:HB3	1:P:86:ILE:HD11	1.59	0.83
2:Q:214:GLY:H	2:Q:230:THR:HB	1.42	0.83
4:J:41:LYS:HG3	4:J:78:TYR:HD1	1.43	0.83
2:L:96:ILE:CD1	3:M:146:LYS:NZ	2.41	0.83
3:I:202:ARG:HG2	3:I:246:ALA:HA	1.59	0.83
2:L:20:THR:HA	2:L:77:ILE:HG22	1.59	0.83
3:M:65:ARG:O	3:M:68:LYS:CE	2.27	0.83
4:D:46:ILE:HG12	4:D:47:GLU:H	1.43	0.82
4:N:24:ASN:HB3	4:N:67:TYR:HB3	1.61	0.82
1:G:60:ARG:HH12	1:G:83:ASP:CG	1.81	0.82
3:I:6:ARG:NH1	3:I:99:TYR:O	2.11	0.82
3:I:93:HIS:ND1	3:I:118:TYR:OH	2.12	0.82
2:H:25:GLN:HE22	2:H:29:HIS:CD2	1.96	0.82
2:L:36:ARG:HB2	2:L:46:ILE:HD11	1.61	0.82
3:R:35:ARG:NH1	4:U:53:ASP:HB3	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:234:ARG:HD2	4:D:8:GLN:HE22	1.43	0.82
1:G:150:SER:HA	1:G:151:LYS:HB2	1.60	0.82
3:M:220:ASP:CB	3:M:221:GLY:HA3	2.09	0.82
4:J:45:ARG:HD2	4:J:45:ARG:N	1.94	0.82
3:M:26:GLY:O	3:M:32:GLN:NE2	2.11	0.82
3:M:259:CYS:HB3	3:M:272:LEU:HB2	1.61	0.82
3:I:155:GLN:O	3:I:158:ALA:N	2.12	0.81
3:M:65:ARG:O	3:M:68:LYS:HE2	1.79	0.81
1:F:127:ASP:OD1	1:F:128:SER:N	2.12	0.81
3:I:150:ALA:O	3:I:151:HIS:HB2	1.80	0.81
3:C:49:ALA:CB	3:C:51:TRP:CZ3	2.63	0.81
3:M:215:LEU:HD12	3:M:215:LEU:O	1.81	0.80
1:P:198:ASP:OD1	1:P:199:THR:N	2.13	0.80
2:B:121:PRO:CA	2:B:148:PHE:HE1	1.92	0.80
2:L:148:PHE:HB2	2:L:186:TYR:HB2	1.62	0.80
4:N:18:GLY:HA2	4:N:72:PRO:C	2.01	0.80
3:I:133:TRP:CZ2	3:I:153:ALA:HB1	2.17	0.80
2:L:27:MET:HB3	2:L:29:HIS:CD2	2.16	0.80
3:C:64:THR:HA	3:C:67:VAL:HG12	1.62	0.80
4:N:84:HIS:CD2	4:N:86:THR:CG2	2.63	0.80
1:F:57:SER:O	1:F:61:LEU:O	2.00	0.80
3:I:213:ILE:HD12	3:I:263:HIS:CD2	2.17	0.79
3:I:144:LYS:HD3	3:I:148:GLU:OE2	1.81	0.79
2:H:96:ILE:CG2	3:I:152:VAL:HG11	2.12	0.79
3:I:133:TRP:HZ2	3:I:153:ALA:CB	1.95	0.79
4:N:84:HIS:CD2	4:N:86:THR:HG22	2.14	0.79
2:B:108:ARG:NH2	2:B:150:PRO:HG2	1.98	0.79
1:A:158:THR:CG2	1:A:159:ASP:H	1.95	0.79
1:G:133:LYS:CG	1:G:180:ASN:ND2	2.36	0.79
2:B:9:ARG:NH1	2:B:213:TYR:OH	2.16	0.79
2:B:149:TYR:CD2	2:B:150:PRO:HB3	2.18	0.78
3:C:37:ASP:OD1	3:C:38:SER:N	2.16	0.78
1:A:156:TYR:HB3	1:A:178:TRP:O	1.84	0.78
1:F:129:LYS:HE2	1:F:132:ASP:HA	1.64	0.78
3:I:147:TRP:CZ2	5:K:7:PHE:CE1	2.71	0.78
4:J:41:LYS:HD2	4:J:46:ILE:HD11	1.66	0.78
3:R:263:HIS:CE1	3:R:265:GLY:H	2.01	0.78
1:G:133:LYS:HG2	1:G:180:ASN:ND2	1.99	0.78
2:B:22:THR:HA	2:B:75:PRO:HA	1.67	0.77
1:G:135:VAL:HG12	1:G:178:TRP:HB3	1.67	0.77
3:I:85:TYR:HB3	3:I:87:GLN:HG2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:ARG:HH22	2:B:150:PRO:HG2	1.47	0.77
2:L:38:ASP:OD2	2:L:44:ARG:NH2	2.17	0.77
3:R:35:ARG:HH12	4:U:53:ASP:HB3	1.50	0.77
3:I:99:TYR:HB3	3:I:114:HIS:HD2	1.49	0.77
1:F:57:SER:O	1:F:61:LEU:HB2	1.85	0.77
2:Q:119:PHE:HB2	2:Q:120:PRO:CD	2.14	0.77
3:M:7:TYR:HA	3:M:26:GLY:HA2	1.66	0.77
2:Q:215:LEU:HD13	2:Q:219:ASP:HB2	1.67	0.77
3:C:203:CYS:N	3:C:245:ALA:O	2.18	0.76
4:D:18:GLY:H	4:D:72:PRO:HG2	1.50	0.76
3:M:186:LYS:O	3:M:206:LEU:N	2.19	0.76
4:N:27:VAL:O	4:N:28:SER:OG	2.03	0.76
3:C:55:GLU:OE2	3:C:170:ARG:NH2	2.19	0.76
2:H:88:LEU:HD12	2:H:108:ARG:HB3	1.68	0.76
3:C:85:TYR:HD2	3:C:87:GLN:HB2	1.51	0.76
3:I:72:GLN:OE1	3:I:75:ARG:NH1	2.16	0.76
3:M:138:MET:HA	3:M:141:GLN:HG2	1.66	0.75
3:C:5:MET:HB2	3:C:168:LEU:HD13	1.66	0.75
3:C:66:LYS:CD	5:E:4:GLY:HA2	2.16	0.75
4:U:24:ASN:OD1	4:U:65:LEU:HD11	1.85	0.75
3:M:217:TRP:NE1	3:M:258:THR:O	2.19	0.75
2:L:112:LEU:HD11	2:L:149:TYR:HE2	1.52	0.75
3:M:85:TYR:HD2	3:M:87:GLN:HE22	1.35	0.75
2:Q:132:GLU:O	2:Q:136:THR:CA	2.35	0.75
3:R:163:THR:O	3:R:167:TRP:HD1	1.70	0.75
2:Q:125:VAL:HG23	2:Q:235:ALA:HB3	1.69	0.75
1:A:142:ASP:OD1	1:A:143:SER:N	2.20	0.75
1:G:121:ALA:HA	1:G:198:ASP:HB3	1.68	0.75
3:I:133:TRP:CZ2	3:I:153:ALA:CB	2.70	0.75
2:H:178:GLN:CD	2:H:178:GLN:H	1.90	0.74
3:I:5:MET:HB2	3:I:168:LEU:HD13	1.69	0.74
3:R:25:VAL:HG11	4:U:54:LEU:O	1.88	0.74
1:F:127:ASP:HB3	1:F:129:LYS:HG2	1.68	0.74
2:H:37:GLN:HB2	2:H:43:LEU:HD12	1.70	0.74
3:M:38:SER:O	3:M:43:GLN:NE2	2.21	0.74
4:D:89:GLN:HB2	4:D:90:PRO:HD2	1.70	0.73
1:G:60:ARG:NH2	1:G:80:ILE:HB	2.02	0.73
3:R:185:PRO:HD3	3:R:263:HIS:HD2	1.51	0.73
3:M:82:ARG:NH1	3:M:118:TYR:OH	2.21	0.73
2:H:61:PRO:O	2:H:64:TYR:HD2	1.71	0.73
3:I:99:TYR:HB3	3:I:114:HIS:CD2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:17:ARG:HG2	3:M:17:ARG:NH1	2.02	0.73
3:C:35:ARG:HG2	3:C:35:ARG:HH11	1.54	0.73
1:F:126:ARG:NH1	1:F:127:ASP:H	1.86	0.73
4:J:40:LEU:HD11	4:J:45:ARG:HE	1.53	0.73
4:D:73:THR:CG2	4:D:74:GLU:OE2	2.37	0.73
2:H:229:VAL:HG23	2:H:230:THR:N	2.03	0.73
2:H:25:GLN:HE22	2:H:29:HIS:HD2	1.33	0.73
1:P:118:PRO:O	1:P:119:ASP:OD1	2.06	0.73
1:G:50:TYR:CZ	3:I:151:HIS:NE2	2.57	0.72
3:C:36:PHE:HB2	3:C:45:MET:HB3	1.71	0.72
3:I:137:ASP:O	3:I:141:GLN:HB2	1.89	0.72
3:I:169:ARG:NH2	3:I:173:GLU:OE1	2.23	0.72
2:L:27:MET:CB	2:L:29:HIS:CD2	2.72	0.72
1:F:160:LYS:HD3	1:F:160:LYS:N	2.05	0.72
1:A:163:LEU:HD23	1:A:172:SER:HB2	1.70	0.72
3:I:145:HIS:O	3:I:149:ALA:N	2.21	0.72
1:A:13:ILE:HG12	1:A:109:LEU:HD11	1.70	0.72
2:B:28:ASN:OD1	2:B:71:LYS:NZ	2.22	0.72
2:L:25:GLN:NE2	2:L:27:MET:SD	2.63	0.72
1:A:5:ASN:OD1	1:A:6:GLN:N	2.21	0.72
3:I:104:GLY:H	3:I:110:LEU:HD13	1.54	0.72
4:J:57:SER:HB3	4:J:61:SER:H	1.53	0.72
3:M:6:ARG:O	3:M:27:TYR:N	2.22	0.71
2:B:164:VAL:HG22	2:B:166:SER:H	1.55	0.71
1:G:42:GLY:HA2	2:H:90:PHE:HE2	1.54	0.71
1:A:158:THR:HG22	1:A:159:ASP:N	2.03	0.71
3:R:34:VAL:HG12	3:R:47:PRO:HA	1.72	0.71
4:D:52:SER:HB3	4:D:65:LEU:HB3	1.72	0.71
1:F:20:SER:HA	1:F:75:ASN:HA	1.72	0.71
2:L:144:LEU:HD22	2:L:189:SER:OG	1.91	0.71
3:I:175:GLY:O	3:I:179:LEU:HB2	1.91	0.71
4:D:73:THR:HG23	4:D:74:GLU:OE2	1.91	0.70
4:D:88:SER:CB	4:D:89:GLN:HA	2.20	0.70
3:M:215:LEU:HD12	3:M:215:LEU:C	2.12	0.70
3:R:263:HIS:CE1	3:R:265:GLY:N	2.60	0.70
1:G:60:ARG:NH1	1:G:83:ASP:OD2	2.24	0.70
2:Q:163:GLU:N	2:Q:163:GLU:OE1	2.24	0.70
3:M:201:LEU:HD13	3:M:217:TRP:HZ3	1.56	0.70
3:M:263:HIS:H	3:M:266:LEU:HB2	1.56	0.70
3:I:62:GLY:O	3:I:66:LYS:HD3	1.91	0.70
3:R:180:GLN:OE1	3:R:180:GLN:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HD13	1:A:35:TYR:HE1	1.56	0.70
2:H:228:PRO:C	2:H:229:VAL:HG22	2.11	0.70
1:G:59:GLY:HA2	1:G:60:ARG:HB3	1.74	0.69
1:G:59:GLY:HA3	1:G:61:LEU:CA	2.22	0.69
2:Q:115:LEU:HD12	2:Q:115:LEU:H	1.57	0.69
1:A:36:LYS:HE3	1:A:87:TYR:CE2	2.28	0.69
1:P:86:ILE:HG22	1:P:108:THR:HG22	1.73	0.69
2:L:144:LEU:CD2	2:L:189:SER:OG	2.40	0.69
3:M:120:GLY:HA2	4:N:60:TRP:HD1	1.57	0.69
3:R:6:ARG:HD3	3:R:100:GLY:HA3	1.73	0.69
4:J:41:LYS:HG2	4:J:42:ASN:N	2.07	0.69
1:F:30:ASN:ND2	3:M:154:GLU:HB3	2.08	0.69
1:G:9:GLN:HB3	2:L:198:PHE:HZ	1.58	0.69
2:L:87:SER:HB3	2:L:89:TYR:HE1	1.57	0.69
4:N:29:GLY:HA2	4:N:61:SER:OG	1.93	0.69
2:H:221:TRP:NE1	2:H:223:GLN:O	2.26	0.68
3:C:81:LEU:HA	3:C:84:TYR:HD2	1.59	0.68
4:D:41:LYS:O	4:D:41:LYS:HG2	1.91	0.68
3:C:37:ASP:OD2	3:C:40:ALA:HB2	1.94	0.68
2:H:215:LEU:O	2:H:229:VAL:HA	1.94	0.68
1:F:126:ARG:HH11	1:F:127:ASP:H	1.39	0.68
3:I:51:TRP:CE2	3:I:179:LEU:HD11	2.28	0.68
4:J:35:ILE:HB	4:J:84:HIS:HD2	1.59	0.68
2:Q:221:TRP:CH2	2:Q:223:GLN:C	2.67	0.68
4:D:88:SER:HB3	4:D:89:GLN:HA	1.74	0.68
4:N:27:VAL:N	4:N:64:LEU:O	2.27	0.68
4:N:84:HIS:HD2	4:N:86:THR:CB	1.97	0.68
2:B:36:ARG:HB2	2:B:46:ILE:HD11	1.74	0.68
4:D:87:LEU:O	4:D:87:LEU:HD12	1.94	0.68
1:G:133:LYS:HA	1:G:180:ASN:CG	2.15	0.67
2:H:98:PRO:HD2	3:I:152:VAL:HA	1.75	0.67
3:M:187:THR:HG22	3:M:205:ALA:HA	1.76	0.67
1:P:47:ILE:HG13	1:P:57:SER:OG	1.94	0.67
2:H:221:TRP:CG	2:H:227:LYS:HG2	2.30	0.67
2:Q:137:GLN:O	2:Q:196:ALA:HB2	1.95	0.67
3:R:228:THR:OG1	3:R:247:VAL:HB	1.94	0.67
4:U:58:LYS:CA	4:U:60:TRP:H	2.01	0.67
2:B:100:GLU:HB3	2:B:102:PHE:CE1	2.29	0.67
2:B:88:LEU:HD22	2:B:108:ARG:HA	1.77	0.67
4:J:41:LYS:HG3	4:J:78:TYR:CD1	2.27	0.67
2:L:25:GLN:CD	2:L:27:MET:HG2	2.14	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:177:GLU:HA	3:R:180:GLN:HB2	1.77	0.67
2:B:86:THR:HG23	2:B:110:THR:HA	1.76	0.67
2:H:214:GLY:CA	2:H:229:VAL:O	2.43	0.67
4:U:38:ASP:OD2	4:U:45:ARG:NH2	2.28	0.67
2:B:145:ALA:CB	2:B:148:PHE:CZ	2.67	0.66
2:H:195:SER:HB2	2:H:198:PHE:HB2	1.78	0.66
3:M:120:GLY:HA3	4:N:31:HIS:NE2	2.10	0.66
1:F:177:ALA:HB3	1:F:190:PHE:CE1	2.31	0.66
2:Q:164:VAL:HG12	2:Q:166:SER:H	1.61	0.66
3:R:8:PHE:HB2	3:R:25:VAL:HG22	1.77	0.66
3:C:234:ARG:HD2	4:D:8:GLN:NE2	2.11	0.66
3:I:145:HIS:C	3:I:148:GLU:H	1.98	0.66
4:J:39:LEU:HD23	4:J:49:VAL:HG11	1.77	0.66
4:D:46:ILE:HG12	4:D:47:GLU:N	2.10	0.66
1:A:60:ARG:HB2	1:A:77:SER:OG	1.96	0.66
4:D:7:ILE:HD13	4:D:27:VAL:HG22	1.77	0.66
4:D:83:ASN:ND2	4:D:90:PRO:HD3	2.10	0.66
3:I:127:LYS:HD2	3:I:128:GLU:H	1.61	0.66
2:L:229:VAL:O	2:L:231:GLN:HB2	1.95	0.66
1:P:47:ILE:HG21	1:P:57:SER:HB3	1.77	0.66
4:D:83:ASN:CB	4:D:90:PRO:HB3	2.24	0.66
1:F:177:ALA:HB3	1:F:190:PHE:HE1	1.60	0.66
1:G:60:ARG:CZ	1:G:83:ASP:OD2	2.44	0.66
3:R:98:MET:HG3	4:U:58:LYS:HZ1	1.60	0.66
4:J:4:THR:OG1	4:J:5:PRO:HD2	1.96	0.66
3:R:107:TRP:O	3:R:169:ARG:NH1	2.29	0.66
4:D:81:ARG:HA	4:D:92:ILE:HG22	1.77	0.65
2:H:214:GLY:HA3	2:H:229:VAL:O	1.96	0.65
3:M:148:GLU:HA	3:M:151:HIS:H	1.59	0.65
3:M:215:LEU:CB	3:M:261:VAL:HG12	2.25	0.65
3:R:263:HIS:ND1	3:R:264:GLU:N	2.44	0.65
3:I:151:HIS:O	3:I:154:GLU:N	2.30	0.65
3:I:7:TYR:CD2	5:K:2:ILE:HD12	2.31	0.65
3:R:189:MET:SD	3:R:273:ARG:HD2	2.37	0.65
3:M:188:HIS:CG	3:M:189:MET:H	2.15	0.65
2:L:157:TRP:O	2:L:163:GLU:HB2	1.97	0.65
2:L:94:SER:HB2	2:L:100:GLU:O	1.96	0.65
3:M:254:GLU:HG3	3:M:255:GLN:HG3	1.79	0.65
2:B:145:ALA:HB1	2:B:148:PHE:CE2	2.29	0.65
2:L:25:GLN:NE2	2:L:27:MET:CG	2.60	0.65
3:R:217:TRP:HD1	3:R:258:THR:HA	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:TYR:CE1	3:I:151:HIS:CD2	2.85	0.65
3:I:6:ARG:NH1	3:I:7:TYR:H	1.95	0.65
3:C:258:THR:HG22	3:C:273:ARG:HD2	1.78	0.64
3:C:236:ALA:HB1	4:D:12:ARG:HG2	1.78	0.64
3:M:262:GLN:HB2	3:M:269:PRO:HB3	1.78	0.64
2:H:227:LYS:O	2:H:229:VAL:HG13	1.97	0.64
3:I:169:ARG:CZ	3:I:173:GLU:HA	2.28	0.64
3:I:63:GLU:CA	3:I:66:LYS:HZ2	2.02	0.64
1:P:158:THR:HG21	1:P:176:VAL:H	1.62	0.64
1:F:163:LEU:HB3	2:L:169:CYS:HB2	1.79	0.64
2:Q:120:PRO:HD3	2:Q:228:PRO:HB3	1.78	0.64
3:I:213:ILE:CD1	3:I:263:HIS:CD2	2.80	0.64
2:L:96:ILE:HD11	3:M:146:LYS:CE	2.17	0.64
3:M:185:PRO:HB3	3:M:208:PHE:HB3	1.79	0.64
4:N:88:SER:HG	4:N:89:GLN:H	1.43	0.64
3:C:33:PHE:CD2	3:C:51:TRP:HZ2	2.16	0.64
2:Q:158:TRP:HB2	2:Q:207:ARG:HB3	1.80	0.64
2:B:222:THR:HB	2:B:223:GLN:CB	2.28	0.64
1:G:163:LEU:HB3	2:H:169:CYS:HB3	1.79	0.64
2:H:204:ASN:N	2:H:204:ASN:OD1	2.31	0.64
3:I:186:LYS:HB2	3:I:206:LEU:HD22	1.78	0.64
3:R:163:THR:HG22	3:R:167:TRP:NE1	2.13	0.64
1:A:158:THR:CG2	1:A:159:ASP:N	2.59	0.63
2:L:1:GLU:N	2:L:1:GLU:OE1	2.28	0.63
1:P:51:LYS:HE2	3:R:131:ARG:HE	1.63	0.63
1:A:9:GLN:HE21	1:A:105:GLN:HE22	1.45	0.63
3:R:72:GLN:N	3:R:72:GLN:OE1	2.30	0.63
3:R:159:TYR:OH	5:T:1:GLY:O	2.17	0.63
3:I:155:GLN:C	3:I:157:ARG:N	2.46	0.63
3:M:198:GLU:O	3:M:251:SER:HB3	1.99	0.63
3:M:14:ARG:HD3	3:M:21:ARG:HH12	1.63	0.63
1:G:59:GLY:HA3	1:G:61:LEU:H	0.49	0.63
1:G:80:ILE:HG22	1:G:82:SER:H	1.63	0.63
4:J:88:SER:OG	4:J:89:GLN:NE2	2.31	0.63
3:M:155:GLN:HA	3:M:155:GLN:HE21	1.64	0.63
4:N:30:PHE:CE2	4:N:84:HIS:CE1	2.86	0.63
4:D:86:THR:HG22	4:D:87:LEU:H	1.64	0.63
3:M:32:GLN:HG2	3:M:35:ARG:HH11	1.63	0.63
2:L:36:ARG:NH1	2:L:38:ASP:OD2	2.31	0.63
3:C:236:ALA:O	4:D:12:ARG:NE	2.32	0.63
1:F:60:ARG:HB2	1:F:77:SER:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:155:GLN:C	3:I:157:ARG:H	2.03	0.63
2:L:221:TRP:CG	2:L:227:LYS:HG2	2.34	0.63
3:M:77:ASP:HB3	5:O:9:LEU:HD12	1.81	0.62
1:F:162:VAL:HG12	1:F:173:ASN:HA	1.80	0.62
2:H:86:THR:HG23	2:H:110:THR:HA	1.80	0.62
4:J:46:ILE:HD12	4:J:70:PHE:HZ	1.61	0.62
1:P:158:THR:OG1	1:P:159:ASP:N	2.30	0.62
2:Q:13:THR:HB	2:Q:111:VAL:HG12	1.81	0.62
1:A:100:LYS:NZ	2:B:59:ASP:OD1	2.27	0.62
1:P:158:THR:CG2	1:P:176:VAL:H	2.11	0.62
2:Q:207:ARG:NH2	2:Q:209:GLN:OE1	2.31	0.62
4:U:83:ASN:CB	4:U:90:PRO:HB3	2.07	0.62
1:F:52:ALA:HB1	1:F:67:ILE:HG22	1.81	0.62
3:R:93:HIS:ND1	3:R:119:ASP:OD1	2.23	0.62
1:A:60:ARG:NE	1:A:78:ALA:O	2.31	0.62
2:H:228:PRO:O	2:H:229:VAL:CG2	2.47	0.62
2:H:20:THR:HG22	2:H:77:ILE:HG12	1.80	0.62
3:M:54:GLN:NE2	3:M:174:ASN:OD1	2.33	0.62
1:A:36:LYS:HD2	1:A:87:TYR:CE1	2.33	0.62
2:Q:51:ASN:O	2:Q:68:ARG:NH1	2.28	0.62
2:H:96:ILE:HG22	3:I:152:VAL:CG1	2.24	0.62
1:A:47:ILE:HG23	1:A:55:LEU:HD11	1.81	0.62
4:D:54:LEU:HD11	4:D:62:PHE:HD1	1.65	0.62
2:L:27:MET:HB3	2:L:29:HIS:NE2	2.14	0.62
4:N:70:PHE:CE2	4:N:71:THR:O	2.53	0.62
4:N:86:THR:HG23	4:N:87:LEU:N	2.14	0.62
2:B:100:GLU:HB3	2:B:102:PHE:HE1	1.64	0.62
1:F:147:VAL:O	1:F:160:LYS:NZ	2.32	0.62
4:J:41:LYS:O	4:J:42:ASN:C	2.35	0.62
4:J:6:LYS:HD2	4:J:7:ILE:H	1.64	0.62
1:P:47:ILE:CG2	1:P:57:SER:HB3	2.30	0.62
1:A:198:ASP:OD1	1:A:199:THR:N	2.33	0.61
1:F:6:GLN:O	1:F:105:GLN:NE2	2.33	0.61
1:F:33:LEU:N	1:F:90:ALA:O	2.32	0.61
3:M:65:ARG:HG3	3:M:65:ARG:NH1	2.09	0.61
4:U:28:SER:HA	4:U:30:PHE:HD1	1.63	0.61
4:D:35:ILE:HD13	4:D:64:LEU:HD12	1.81	0.61
1:G:71:ASP:N	1:G:71:ASP:OD1	2.33	0.61
2:Q:46:ILE:HG22	2:Q:47:TYR:HD1	1.65	0.61
3:R:163:THR:HG22	3:R:167:TRP:CD1	2.35	0.61
3:C:242:GLN:OE1	4:D:10:TYR:HE1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:137:GLN:O	2:Q:196:ALA:CB	2.48	0.61
2:Q:3:GLN:HG2	2:Q:4:VAL:H	1.64	0.61
3:C:35:ARG:HG2	3:C:35:ARG:NH1	2.15	0.61
1:F:43:PRO:HD2	2:L:103:PHE:CG	2.36	0.61
3:I:68:LYS:HG3	3:I:69:ALA:N	2.15	0.61
2:L:229:VAL:O	2:L:230:THR:C	2.38	0.61
3:R:47:PRO:HB3	3:R:60:TRP:CH2	2.36	0.61
4:U:23:LEU:HD21	4:U:39:LEU:HD22	1.82	0.61
3:I:129:ASP:OD1	3:I:131:ARG:HG2	2.00	0.61
2:L:168:VAL:HG12	2:L:192:LEU:HD13	1.81	0.61
2:Q:52:VAL:HG12	2:Q:53:GLU:HG2	1.83	0.61
2:B:22:THR:HG22	2:B:75:PRO:HB3	1.83	0.61
2:Q:170:THR:HG22	2:Q:190:SER:HB2	1.83	0.61
2:B:158:TRP:HB2	2:B:207:ARG:HB3	1.83	0.61
3:I:229:GLU:HB2	3:I:246:ALA:HB3	1.83	0.61
3:I:49:ALA:O	3:I:52:ILE:HG22	2.01	0.61
1:P:33:LEU:HD23	1:P:45:LEU:HD13	1.82	0.61
4:U:23:LEU:HD22	4:U:41:LYS:NZ	2.15	0.61
1:F:101:LEU:HD22	2:L:101:LEU:HD11	1.81	0.61
3:I:45:MET:HB3	3:I:60:TRP:HE3	1.66	0.61
4:J:46:ILE:HG22	4:J:47:GLU:N	2.16	0.61
4:J:45:ARG:H	4:J:45:ARG:CD	2.06	0.60
3:I:182:THR:HB	3:I:265:GLY:HA2	1.82	0.60
4:D:76:ASP:CB	4:D:78:TYR:CE2	2.72	0.60
3:I:66:LYS:HE2	5:K:2:ILE:HG22	1.83	0.60
2:B:47:TYR:HE1	2:B:61:PRO:HA	1.66	0.60
2:L:20:THR:HA	2:L:77:ILE:CG2	2.29	0.60
1:P:124:GLN:HA	1:P:136:CYS:HB3	1.84	0.60
3:I:176:LYS:HG3	3:I:177:GLU:HG2	1.84	0.60
4:U:46:ILE:HD11	4:U:49:VAL:HG13	1.83	0.60
3:I:244:TRP:HZ3	3:I:246:ALA:HB2	1.65	0.60
3:R:263:HIS:CG	3:R:265:GLY:H	2.16	0.60
2:H:221:TRP:HB2	2:H:227:LYS:HD3	1.83	0.60
4:U:41:LYS:HD2	4:U:78:TYR:HD1	1.67	0.60
3:I:218:GLN:CG	3:I:219:ARG:N	2.51	0.60
3:I:263:HIS:ND1	3:I:264:GLU:N	2.49	0.60
2:L:152:HIS:HB3	2:L:213:TYR:HB2	1.82	0.60
3:M:236:ALA:O	3:M:240:THR:OG1	2.12	0.60
3:M:217:TRP:HE1	3:M:259:CYS:HA	1.65	0.60
3:R:163:THR:O	3:R:167:TRP:CD1	2.53	0.60
3:C:28:VAL:HB	3:C:33:PHE:HE1	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:ALA:O	3:C:73:THR:N	2.28	0.59
2:B:149:TYR:CD2	2:B:150:PRO:CA	2.85	0.59
2:B:96:ILE:CD1	3:C:146:LYS:HE2	2.20	0.59
3:C:206:LEU:HB2	3:C:242:GLN:HG2	1.83	0.59
1:G:68:THR:HG22	1:A:20:SER:HB2	1.85	0.59
1:G:60:ARG:HH22	1:G:80:ILE:HB	1.68	0.59
1:F:196:PRO:O	1:F:198:ASP:OD1	2.20	0.59
3:I:82:ARG:HA	3:I:85:TYR:HB2	1.84	0.59
4:J:54:LEU:HD12	4:J:64:LEU:HD21	1.83	0.59
3:R:159:TYR:HD2	3:R:160:LEU:HD12	1.68	0.59
4:U:75:LYS:HB2	4:U:75:LYS:NZ	2.17	0.59
1:F:122:VAL:HG22	1:F:138:PHE:HB2	1.84	0.59
2:H:64:TYR:HH	2:H:89:TYR:HH	1.50	0.59
3:I:172:LEU:HD23	3:I:179:LEU:HD23	1.85	0.59
1:G:42:GLY:HA2	2:H:90:PHE:CE2	2.37	0.59
2:L:112:LEU:HD11	2:L:149:TYR:CE2	2.37	0.59
3:I:141:GLN:NE2	3:I:144:LYS:HE3	2.17	0.59
3:M:206:LEU:CA	3:M:242:GLN:HE22	2.16	0.59
3:I:142:THR:O	3:I:143:THR:C	2.40	0.59
4:J:52:SER:HB3	4:J:65:LEU:H	1.68	0.59
3:C:69:ALA:O	3:C:72:GLN:N	2.36	0.58
1:F:125:LEU:HD22	2:L:128:PRO:HA	1.84	0.58
4:J:57:SER:OG	4:J:58:LYS:N	2.36	0.58
1:P:125:LEU:HD21	2:Q:128:PRO:HA	1.84	0.58
4:U:52:SER:HB3	4:U:65:LEU:H	1.68	0.58
2:B:149:TYR:CD2	2:B:150:PRO:CB	2.85	0.58
2:B:7:ASN:HD22	2:B:22:THR:HG1	1.44	0.58
1:G:50:TYR:CZ	3:I:151:HIS:CE1	2.91	0.58
3:M:23:ILE:HD12	4:N:54:LEU:HD22	1.84	0.58
4:D:87:LEU:HD12	4:D:87:LEU:C	2.23	0.58
1:F:121:ALA:HA	1:F:198:ASP:HB3	1.84	0.58
3:I:61:ASP:O	3:I:65:ARG:HG3	2.03	0.58
4:J:54:LEU:HA	4:J:64:LEU:HD21	1.84	0.58
3:M:5:MET:HB2	3:M:168:LEU:HD13	1.84	0.58
3:C:173:GLU:CG	3:C:174:ASN:N	2.61	0.58
3:M:74:HIS:HA	3:M:77:ASP:HB2	1.85	0.58
1:P:60:ARG:NH1	1:P:78:ALA:O	2.31	0.58
4:U:23:LEU:N	4:U:68:THR:O	2.30	0.58
2:L:25:GLN:HG2	2:L:27:MET:HG2	1.85	0.58
1:P:31:THR:HG22	1:P:50:TYR:HD1	1.69	0.58
4:J:39:LEU:CD2	4:J:49:VAL:HG11	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:SER:C	1:G:59:GLY:N	2.52	0.58
2:L:71:LYS:HD3	2:L:71:LYS:N	2.19	0.58
3:M:259:CYS:CB	3:M:272:LEU:HB2	2.33	0.58
4:U:7:ILE:HD12	4:U:27:VAL:HG12	1.85	0.58
3:C:173:GLU:CG	3:C:174:ASN:H	2.14	0.57
1:G:28:ILE:HD11	1:G:69:ARG:CZ	2.35	0.57
1:G:33:LEU:O	1:G:90:ALA:N	2.35	0.57
2:H:98:PRO:N	3:I:152:VAL:HG12	2.17	0.57
3:I:85:TYR:HB3	3:I:87:GLN:CG	2.35	0.57
4:J:78:TYR:CD2	4:J:78:TYR:N	2.73	0.57
4:U:7:ILE:HG13	4:U:82:VAL:HG21	1.86	0.57
2:B:149:TYR:HD2	2:B:150:PRO:N	2.00	0.57
3:I:133:TRP:HZ2	3:I:153:ALA:HB1	1.59	0.57
2:L:145:ALA:HB1	2:L:148:PHE:CE2	2.39	0.57
2:L:27:MET:O	2:L:28:ASN:HB2	2.03	0.57
3:R:102:ASP:N	3:R:111:ARG:O	2.29	0.57
3:R:266:LEU:HD12	3:R:267:PRO:HD2	1.86	0.57
3:C:59:TYR:O	3:C:63:GLU:N	2.35	0.57
4:D:46:ILE:HG23	4:D:47:GLU:O	2.04	0.57
1:F:30:ASN:HD22	3:M:154:GLU:HB3	1.67	0.57
2:L:178:GLN:HA	2:L:178:GLN:OE1	2.05	0.57
4:N:85:VAL:O	4:N:85:VAL:HG12	2.04	0.57
1:A:9:GLN:NE2	1:A:105:GLN:HE22	2.03	0.57
3:I:171:TYR:OH	5:K:1:GLY:N	2.32	0.57
2:L:150:PRO:HD2	2:L:152:HIS:HD2	1.69	0.57
3:R:27:TYR:CE1	3:R:32:GLN:HG2	2.39	0.57
4:J:37:VAL:HG13	4:J:82:VAL:HG22	1.87	0.57
4:U:21:ASN:OD1	4:U:22:PHE:N	2.37	0.57
2:H:47:TYR:HE1	2:H:61:PRO:CA	2.14	0.56
3:I:137:ASP:OD1	3:I:137:ASP:N	2.38	0.56
3:R:32:GLN:OE1	3:R:35:ARG:NH2	2.38	0.56
2:B:149:TYR:CD2	2:B:150:PRO:N	2.73	0.56
3:I:17:ARG:HB3	3:I:18:GLY:HA2	1.87	0.56
1:F:135:VAL:HG11	2:L:126:PHE:CD1	2.40	0.56
3:M:144:LYS:O	3:M:147:TRP:N	2.38	0.56
2:B:10:TYR:CD1	2:B:108:ARG:HB2	2.41	0.56
3:I:28:VAL:O	3:I:31:THR:OG1	2.21	0.56
2:L:86:THR:HG23	2:L:110:THR:HA	1.87	0.56
2:L:50:MET:HE1	5:O:6:VAL:H	1.69	0.56
4:D:24:ASN:N	4:D:24:ASN:OD1	2.39	0.56
2:H:151:ASP:O	2:H:152:HIS:ND1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:58:GLU:N	3:I:58:GLU:OE1	2.32	0.56
4:J:24:ASN:HB3	4:J:65:LEU:HD11	1.86	0.56
1:A:184:PHE:N	1:A:184:PHE:CD1	2.72	0.56
3:C:60:TRP:O	3:C:64:THR:HG23	2.05	0.56
3:I:25:VAL:HG11	3:I:32:GLN:HE21	1.71	0.56
2:B:57:LYS:HE2	2:B:61:PRO:HB2	1.87	0.56
4:D:38:ASP:OD2	4:D:45:ARG:NH1	2.39	0.56
1:F:74:LEU:O	1:F:74:LEU:HD13	2.04	0.56
1:G:59:GLY:HA2	1:G:60:ARG:CB	2.33	0.56
3:I:169:ARG:NH2	3:I:173:GLU:HA	2.21	0.56
2:L:38:ASP:OD1	2:L:87:SER:OG	2.12	0.56
3:M:56:GLY:N	3:M:58:GLU:HG2	2.20	0.56
1:G:25:SER:OG	1:G:26:SER:N	2.38	0.56
1:P:47:ILE:CG2	1:P:57:SER:CB	2.83	0.56
4:U:13:HIS:HB3	4:U:14:PRO:HD2	1.86	0.56
2:H:176:LYS:HE2	2:H:182:ASN:H	1.71	0.56
4:U:65:LEU:HD12	4:U:66:TYR:N	2.21	0.56
1:A:148:SER:H	1:A:193:SER:HB3	1.69	0.56
2:B:89:TYR:O	2:B:107:SER:OG	2.24	0.56
1:G:19:VAL:HG13	1:G:76:ILE:HB	1.88	0.56
3:I:81:LEU:HB3	3:I:85:TYR:HE2	1.71	0.56
2:L:140:THR:HG23	2:L:193:ARG:HB2	1.88	0.56
4:N:70:PHE:CZ	4:N:71:THR:O	2.57	0.56
4:U:23:LEU:HD22	4:U:41:LYS:HZ3	1.71	0.56
1:A:88:PHE:HA	1:A:106:GLY:HA2	1.87	0.55
2:B:145:ALA:CB	2:B:148:PHE:CE2	2.89	0.55
2:B:125:VAL:HG23	2:B:235:ALA:HB3	1.88	0.55
2:B:88:LEU:HD22	2:B:108:ARG:HG3	1.89	0.55
3:C:170:ARG:HG2	3:C:173:GLU:CD	2.26	0.55
3:I:106:ASP:O	3:I:107:TRP:HB2	2.05	0.55
2:H:221:TRP:NE1	2:H:225:ARG:O	2.38	0.55
1:G:31:THR:OG1	3:I:155:GLN:NE2	2.38	0.55
4:N:61:SER:O	4:N:61:SER:OG	2.22	0.55
2:Q:136:THR:OG1	2:Q:137:GLN:OE1	2.24	0.55
3:M:234:ARG:N	3:M:242:GLN:O	2.38	0.55
3:R:163:THR:HG22	3:R:167:TRP:HE1	1.70	0.55
3:I:217:TRP:NE1	3:I:259:CYS:HB3	2.22	0.55
3:M:117:ALA:HA	3:M:123:TYR:HB3	1.86	0.55
4:D:73:THR:HG22	4:D:74:GLU:OE2	2.07	0.55
1:G:163:LEU:HD11	2:H:193:ARG:HD3	1.89	0.55
3:I:15:PRO:HG2	3:I:91:GLY:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:160:LEU:O	3:I:164:CYS:HB3	2.07	0.55
2:L:27:MET:O	2:L:29:HIS:HD2	1.90	0.55
2:L:44:ARG:HD2	2:L:60:VAL:HG21	1.88	0.55
3:C:213:ILE:HD11	3:C:261:VAL:HG13	1.88	0.55
3:I:213:ILE:HD12	3:I:263:HIS:HD2	1.66	0.55
1:A:166:ARG:HG3	1:A:168:MET:O	2.07	0.55
2:H:160:ASN:HA	2:H:205:HIS:HB2	1.88	0.55
3:I:73:THR:HG23	5:K:8:THR:HG22	1.89	0.55
2:L:64:TYR:HB3	2:L:76:LEU:HD11	1.89	0.55
3:M:188:HIS:CG	3:M:189:MET:N	2.75	0.54
2:B:46:ILE:HG22	2:B:47:TYR:N	2.22	0.54
3:I:125:ALA:HB3	3:I:134:THR:HB	1.89	0.54
3:R:270:LEU:HD22	3:R:271:THR:H	1.73	0.54
4:J:22:PHE:CD1	4:J:69:GLU:HA	2.42	0.54
1:F:92:PRO:HG2	3:M:155:GLN:OE1	2.07	0.54
1:A:38:GLU:OE1	1:A:38:GLU:N	2.40	0.54
3:I:155:GLN:O	3:I:156:LEU:C	2.46	0.54
2:L:25:GLN:CG	2:L:27:MET:HG2	2.37	0.54
4:N:24:ASN:N	4:N:24:ASN:OD1	2.40	0.54
2:Q:170:THR:HA	2:Q:190:SER:HA	1.88	0.54
1:P:88:PHE:CZ	2:Q:43:LEU:HD12	2.42	0.54
3:C:12:VAL:HG12	3:C:94:THR:HG23	1.89	0.54
3:I:14:ARG:CB	3:I:19:GLU:H	2.19	0.54
3:R:186:LYS:N	3:R:206:LEU:O	2.36	0.54
3:R:206:LEU:HD12	3:R:207:SER:H	1.73	0.54
4:U:28:SER:HA	4:U:30:PHE:CD1	2.41	0.54
1:P:105:GLN:HA	2:Q:42:GLY:HA3	1.89	0.54
3:C:74:HIS:HA	3:C:77:ASP:HB2	1.88	0.54
1:F:11:MET:HG3	1:F:109:LEU:HD12	1.88	0.54
1:G:83:ASP:O	1:G:87:TYR:OH	2.21	0.54
4:J:5:PRO:HB3	4:J:30:PHE:CD2	2.43	0.54
3:R:82:ARG:HH21	3:R:88:SER:HA	1.73	0.54
1:F:126:ARG:NH1	1:F:127:ASP:N	2.56	0.54
1:P:51:LYS:HE2	3:R:131:ARG:NE	2.23	0.54
1:F:129:LYS:HG3	1:F:131:SER:N	2.18	0.54
3:I:73:THR:OG1	5:K:6:VAL:HG11	2.08	0.54
4:U:45:ARG:HG3	4:U:46:ILE:N	2.21	0.54
3:C:116:TYR:HB2	3:C:124:ILE:HG22	1.89	0.53
1:P:139:THR:OG1	1:P:140:ASP:OD1	2.23	0.53
2:Q:118:VAL:HG23	2:Q:118:VAL:O	2.07	0.53
3:I:151:HIS:O	3:I:154:GLU:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:2:ILE:HG13	5:K:3:LEU:H	1.72	0.53
2:L:126:PHE:CE2	2:L:144:LEU:HD12	2.42	0.53
2:L:18:GLU:HG3	2:L:79:GLU:HA	1.90	0.53
1:G:34:TRP:CE2	1:G:74:LEU:HB2	2.44	0.53
4:D:10:TYR:HB2	4:D:24:ASN:O	2.08	0.53
3:R:144:LYS:NZ	3:R:148:GLU:OE2	2.41	0.53
2:B:21:VAL:O	2:B:76:LEU:N	2.40	0.53
3:C:33:PHE:HZ	3:C:171:TYR:HB3	1.74	0.53
3:C:49:ALA:CB	3:C:51:TRP:CH2	2.91	0.53
3:I:141:GLN:HE22	3:I:144:LYS:HE3	1.73	0.53
1:P:49:LEU:HD21	1:P:63:ALA:HB3	1.91	0.53
4:D:56:PHE:CZ	4:D:60:TRP:HA	2.42	0.53
2:L:45:GLN:OE1	2:L:48:TYR:HB3	2.08	0.53
3:M:65:ARG:CG	3:M:65:ARG:HH11	2.13	0.53
2:B:10:TYR:CD1	2:B:108:ARG:CB	2.92	0.53
3:C:234:ARG:O	4:D:10:TYR:OH	2.27	0.53
2:H:97:TYR:C	3:I:152:VAL:CG1	2.61	0.53
3:I:231:VAL:HG22	3:I:232:GLU:O	2.09	0.53
3:I:81:LEU:O	3:I:84:TYR:N	2.42	0.53
3:M:120:GLY:HA2	4:N:60:TRP:CD1	2.41	0.53
2:Q:36:ARG:NH2	2:Q:84:ASN:O	2.23	0.53
3:C:42:SER:O	3:C:43:GLN:HB3	2.08	0.53
1:G:36:LYS:HG2	1:G:46:LEU:HG	1.90	0.53
1:G:9:GLN:HB3	2:L:198:PHE:CZ	2.42	0.53
3:I:202:ARG:HB2	3:I:204:TRP:CZ3	2.43	0.53
4:J:56:PHE:HA	4:J:62:PHE:CD1	2.44	0.53
1:P:51:LYS:HE2	3:R:131:ARG:HH21	1.74	0.53
3:R:23:ILE:HD11	4:U:54:LEU:HD22	1.91	0.53
3:R:117:ALA:HB2	4:U:60:TRP:CH2	2.44	0.53
4:U:54:LEU:HD21	4:U:62:PHE:CE1	2.44	0.53
1:A:148:SER:HB2	1:A:193:SER:HB3	1.91	0.53
1:F:83:ASP:O	1:F:87:TYR:OH	2.22	0.53
3:R:5:MET:HB2	3:R:168:LEU:HD13	1.90	0.53
4:U:65:LEU:HD12	4:U:66:TYR:H	1.74	0.53
1:F:49:LEU:HD13	1:F:65:PHE:HB2	1.92	0.52
2:H:190:SER:OG	2:H:191:ARG:N	2.42	0.52
2:Q:131:ALA:O	2:Q:134:SER:OG	2.19	0.52
4:U:46:ILE:CD1	4:U:49:VAL:HG13	2.39	0.52
4:D:26:TYR:HA	4:D:64:LEU:O	2.09	0.52
1:F:177:ALA:HA	1:F:178:TRP:CE3	2.44	0.52
3:M:262:GLN:CB	3:M:269:PRO:HB3	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:31:THR:HG23	3:I:209:TYR:OH	2.09	0.52
2:Q:95:LEU:HD12	2:Q:95:LEU:H	1.73	0.52
3:I:32:GLN:O	3:I:49:ALA:HB2	2.09	0.52
3:I:81:LEU:HB3	3:I:85:TYR:CE2	2.44	0.52
4:J:41:LYS:HA	4:J:78:TYR:HB3	1.91	0.52
1:A:180:ASN:HD22	1:A:180:ASN:C	2.11	0.52
1:A:133:LYS:HB2	2:B:126:PHE:HE1	1.74	0.52
2:L:145:ALA:HB1	2:L:148:PHE:CZ	2.45	0.52
2:L:29:HIS:HA	2:L:95:LEU:HA	1.91	0.52
2:B:10:TYR:HD1	2:B:108:ARG:CB	2.23	0.52
1:P:60:ARG:NH1	1:P:83:ASP:OD2	2.43	0.52
3:R:214:THR:H	3:R:262:GLN:HB2	1.75	0.52
1:F:22:ASN:HB3	1:F:73:PHE:CD2	2.45	0.52
3:I:139:ALA:O	3:I:142:THR:CG2	2.57	0.52
4:N:30:PHE:CG	4:N:31:HIS:N	2.77	0.52
2:Q:47:TYR:HA	2:Q:57:LYS:CB	2.39	0.52
3:R:217:TRP:CD1	3:R:258:THR:HA	2.44	0.52
4:U:37:VAL:HG22	4:U:82:VAL:HA	1.91	0.52
3:R:98:MET:HG3	4:U:58:LYS:NZ	2.24	0.52
1:G:14:GLN:HG2	1:G:15:GLU:N	2.25	0.52
2:B:20:THR:HA	2:B:77:ILE:HG22	1.90	0.52
2:H:34:TRP:CH2	2:H:91:CYS:HB2	2.45	0.52
3:I:123:TYR:CZ	3:I:140:ALA:HA	2.44	0.52
4:J:12:ARG:HG3	4:J:13:HIS:CE1	2.45	0.52
3:M:104:GLY:C	3:M:106:ASP:H	2.13	0.52
2:B:96:ILE:CD1	3:C:146:LYS:CE	2.81	0.52
3:C:87:GLN:HG2	3:C:93:HIS:CE1	2.45	0.52
3:I:213:ILE:HG23	3:I:263:HIS:HB3	1.91	0.52
2:L:34:TRP:CD1	2:L:76:LEU:HB2	2.45	0.51
5:O:2:ILE:H	5:O:2:ILE:HD12	1.76	0.51
3:R:256:ARG:HD3	3:R:256:ARG:N	2.24	0.51
4:U:9:VAL:HG13	4:U:24:ASN:O	2.09	0.51
3:C:33:PHE:CG	3:C:51:TRP:HZ2	2.29	0.51
2:L:148:PHE:HE1	2:L:153:VAL:HG11	1.74	0.51
4:U:75:LYS:HZ3	4:U:75:LYS:HB2	1.75	0.51
1:F:152:ASP:OD1	1:F:153:SER:N	2.44	0.51
2:H:169:CYS:SG	2:H:191:ARG:NE	2.75	0.51
3:M:133:TRP:HE1	3:M:153:ALA:HB2	1.76	0.51
1:A:36:LYS:HG3	1:A:87:TYR:HA	1.93	0.51
1:G:24:THR:HA	1:G:71:ASP:HB3	1.93	0.51
1:G:50:TYR:OH	3:I:151:HIS:CE1	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:229:VAL:HG23	2:H:230:THR:O	2.10	0.51
3:I:12:VAL:O	3:I:20:PRO:HA	2.10	0.51
2:L:27:MET:HB2	2:L:29:HIS:CD2	2.46	0.51
3:M:7:TYR:CD1	3:M:26:GLY:HA3	2.45	0.51
3:M:76:VAL:O	3:M:80:THR:N	2.44	0.51
2:Q:137:GLN:HG3	2:Q:137:GLN:O	2.10	0.51
2:Q:173:GLN:OE1	2:Q:174:PRO:HD2	2.10	0.51
3:R:9:PHE:HB2	3:R:97:ARG:HB3	1.91	0.51
3:I:263:HIS:CE1	3:I:265:GLY:N	2.72	0.51
1:P:80:ILE:HG22	1:P:82:SER:H	1.75	0.51
2:Q:20:THR:HG23	2:Q:77:ILE:HG22	1.91	0.51
1:F:196:PRO:HD2	1:F:196:PRO:O	2.09	0.51
3:I:145:HIS:O	3:I:148:GLU:CA	2.59	0.51
1:P:13:ILE:HD13	1:P:19:VAL:HG21	1.93	0.51
4:U:24:ASN:OD1	4:U:25:CYS:N	2.44	0.51
3:C:183:ASP:OD1	3:C:184:ALA:N	2.44	0.51
3:I:230:LEU:HD12	3:I:231:VAL:N	2.25	0.51
3:M:263:HIS:HB3	3:M:266:LEU:HG	1.93	0.51
2:Q:14:VAL:HA	2:Q:112:LEU:O	2.11	0.51
2:Q:25:GLN:NE2	2:Q:29:HIS:O	2.38	0.51
4:J:40:LEU:CD1	4:J:45:ARG:HE	2.22	0.51
4:J:4:THR:HB	4:J:86:THR:CB	2.40	0.51
4:J:5:PRO:HB3	4:J:30:PHE:HB3	1.93	0.51
2:L:7:ASN:H	2:L:22:THR:HB	1.74	0.51
3:M:202:ARG:HG3	3:M:204:TRP:HE1	1.76	0.51
2:Q:119:PHE:O	2:Q:148:PHE:HA	2.11	0.51
3:I:116:TYR:HB2	3:I:124:ILE:HG22	1.93	0.51
3:M:68:LYS:HG2	3:M:69:ALA:N	2.26	0.51
4:U:28:SER:HB3	4:U:63:TYR:CA	2.36	0.51
2:B:108:ARG:HH22	2:B:150:PRO:CG	2.22	0.51
3:C:122:ASP:OD1	4:D:60:TRP:NE1	2.43	0.51
1:F:5:ASN:OD1	1:F:6:GLN:N	2.44	0.51
3:I:6:ARG:NH2	3:I:98:MET:HG2	2.26	0.51
2:L:224:ASP:OD1	2:L:224:ASP:N	2.35	0.51
4:U:47:GLU:HG2	4:U:48:LYS:H	1.76	0.51
3:R:235:PRO:HG2	4:U:65:LEU:HD22	1.92	0.51
2:B:178:GLN:OE1	2:B:178:GLN:N	2.43	0.50
3:C:45:MET:HG2	3:C:64:THR:HG22	1.93	0.50
2:H:38:ASP:N	2:H:38:ASP:OD1	2.44	0.50
2:L:144:LEU:HD23	2:L:189:SER:OG	2.11	0.50
2:Q:196:ALA:O	2:Q:200:GLN:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:63:GLY:O	2:Q:85:GLN:NE2	2.44	0.50
3:I:66:LYS:O	3:I:69:ALA:N	2.43	0.50
4:J:37:VAL:HG22	4:J:82:VAL:HG13	1.93	0.50
4:J:39:LEU:HD12	4:J:80:CYS:HB3	1.94	0.50
3:I:66:LYS:CE	5:K:2:ILE:HG22	2.41	0.50
1:P:29:PHE:HB2	1:P:32:TRP:NE1	2.26	0.50
2:Q:221:TRP:CZ2	2:Q:223:GLN:C	2.84	0.50
2:B:10:TYR:HD1	2:B:108:ARG:HB3	1.77	0.50
2:B:151:ASP:O	2:B:151:ASP:OD1	2.29	0.50
3:I:263:HIS:ND1	3:I:263:HIS:C	2.64	0.50
4:J:56:PHE:HA	4:J:62:PHE:CE1	2.47	0.50
4:D:55:SER:OG	4:D:56:PHE:N	2.45	0.50
2:H:181:LEU:HD22	1:F:169:ASP:HB2	1.93	0.50
3:I:104:GLY:C	3:I:106:ASP:H	2.14	0.50
1:P:47:ILE:HD12	1:P:57:SER:CA	2.38	0.50
2:Q:51:ASN:O	2:Q:68:ARG:HD3	2.12	0.50
3:R:51:TRP:CH2	3:R:179:LEU:HD11	2.47	0.50
4:U:75:LYS:NZ	4:U:75:LYS:CB	2.73	0.50
3:I:126:LEU:HB2	3:I:133:TRP:CZ3	2.46	0.50
3:I:133:TRP:CE2	3:I:153:ALA:HB1	2.46	0.50
3:M:99:TYR:HB3	3:M:114:HIS:HA	1.94	0.50
4:U:23:LEU:CD2	4:U:39:LEU:HD22	2.42	0.50
1:G:154:ASP:CG	1:G:181:LYS:O	2.50	0.50
4:J:40:LEU:HA	4:J:45:ARG:HA	1.93	0.50
2:L:25:GLN:NE2	2:L:27:MET:HG2	2.26	0.50
3:M:148:GLU:HA	3:M:151:HIS:N	2.26	0.50
1:G:9:GLN:HE21	2:L:198:PHE:HE2	1.57	0.50
3:R:72:GLN:HA	3:R:75:ARG:HB2	1.94	0.50
1:G:43:PRO:HD2	2:H:103:PHE:CD1	2.47	0.50
3:I:217:TRP:HA	3:I:258:THR:O	2.12	0.50
2:H:229:VAL:HG23	2:H:230:THR:H	1.76	0.49
3:M:99:TYR:HB3	3:M:114:HIS:ND1	2.26	0.49
4:N:24:ASN:HD22	4:N:65:LEU:HD13	1.77	0.49
4:U:60:TRP:HA	4:U:60:TRP:CE3	2.46	0.49
2:H:61:PRO:O	2:H:64:TYR:CD2	2.58	0.49
4:J:35:ILE:HG13	4:J:83:ASN:O	2.12	0.49
3:M:262:GLN:NE2	3:M:266:LEU:O	2.44	0.49
2:Q:98:PRO:HG3	3:R:155:GLN:HG2	1.94	0.49
3:I:17:ARG:CB	3:I:18:GLY:HA2	2.42	0.49
3:I:60:TRP:O	3:I:64:THR:HG23	2.12	0.49
3:M:117:ALA:HB3	4:N:60:TRP:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:15:GLU:OE2	1:P:81:PRO:HG3	2.13	0.49
3:C:234:ARG:NH1	3:C:244:TRP:CD1	2.80	0.49
3:C:81:LEU:HD23	3:C:84:TYR:HB2	1.95	0.49
4:D:95:TRP:CZ2	4:D:97:ARG:HB2	2.47	0.49
3:I:142:THR:O	3:I:144:LYS:N	2.45	0.49
3:I:133:TRP:HE1	3:I:153:ALA:CB	2.25	0.49
2:L:95:LEU:HD12	2:L:96:ILE:CB	2.43	0.49
3:M:103:VAL:HG23	3:M:108:ARG:O	2.12	0.49
1:A:87:TYR:HE2	1:A:109:LEU:HB3	1.78	0.49
1:A:3:GLN:O	1:A:4:LEU:HD23	2.13	0.49
3:I:144:LYS:CD	3:I:148:GLU:OE2	2.55	0.49
2:L:110:THR:OG1	2:L:152:HIS:NE2	2.41	0.49
4:N:54:LEU:HD21	4:N:62:PHE:CE2	2.47	0.49
3:R:98:MET:CG	4:U:58:LYS:HZ1	2.23	0.49
1:A:58:ASN:HD22	1:A:58:ASN:C	2.14	0.49
2:B:123:VAL:HG13	2:B:144:LEU:O	2.12	0.49
3:C:197:HIS:NE2	3:C:250:PRO:CB	2.76	0.49
4:D:91:LYS:O	4:D:92:ILE:HG23	2.11	0.49
1:G:9:GLN:NE2	2:L:198:PHE:HE2	2.10	0.49
3:C:155:GLN:OE1	3:C:155:GLN:HA	2.12	0.49
4:D:37:VAL:HB	4:D:66:TYR:CE1	2.47	0.49
3:I:169:ARG:HD2	3:I:172:LEU:HB2	1.95	0.49
2:L:48:TYR:O	2:L:49:SER:OG	2.27	0.49
3:M:201:LEU:HD11	3:M:247:VAL:HB	1.94	0.49
3:M:22:PHE:CE2	3:M:24:ALA:HB2	2.48	0.49
3:R:133:TRP:HB2	3:R:144:LYS:NZ	2.27	0.49
4:U:16:GLU:O	4:U:18:GLY:HA2	2.13	0.49
2:B:25:GLN:NE2	2:B:72:ARG:HA	2.28	0.49
3:C:229:GLU:HG2	3:C:244:TRP:CZ3	2.48	0.49
4:D:83:ASN:ND2	4:D:90:PRO:HB3	2.28	0.49
2:H:221:TRP:CB	2:H:227:LYS:HD3	2.43	0.49
3:I:15:PRO:HB3	3:I:89:GLU:O	2.11	0.49
3:M:133:TRP:NE1	3:M:153:ALA:HB2	2.27	0.49
3:I:147:TRP:CZ2	5:K:7:PHE:CD1	3.01	0.49
3:R:7:TYR:HD2	3:R:99:TYR:CE1	2.31	0.49
3:C:64:THR:CA	3:C:67:VAL:HG12	2.37	0.49
1:G:34:TRP:CZ2	1:G:74:LEU:HB2	2.48	0.49
4:J:32:PRO:O	4:J:84:HIS:NE2	2.44	0.49
4:J:40:LEU:HD11	4:J:45:ARG:NE	2.26	0.49
3:M:6:ARG:HG2	3:M:8:PHE:CE1	2.48	0.49
2:H:112:LEU:HD23	2:H:115:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:5:THR:O	2:H:23:CYS:HA	2.13	0.48
1:G:150:SER:HB3	1:G:152:ASP:N	2.28	0.48
1:G:155:VAL:HG12	1:G:156:TYR:N	2.28	0.48
2:H:216:SER:O	2:H:218:ASN:N	2.43	0.48
3:I:139:ALA:O	3:I:142:THR:HG22	2.13	0.48
3:I:145:HIS:HA	3:I:148:GLU:HB2	1.95	0.48
4:J:4:THR:CB	4:J:86:THR:CG2	2.69	0.48
3:M:117:ALA:HB3	4:N:60:TRP:CZ2	2.48	0.48
1:F:51:LYS:HE2	1:F:53:GLY:HA3	1.96	0.48
2:H:36:ARG:NH1	2:H:84:ASN:O	2.46	0.48
1:P:137:LEU:HD23	1:P:138:PHE:N	2.27	0.48
1:P:16:GLY:N	1:P:79:SER:OG	2.39	0.48
1:A:126:ARG:O	2:B:127:GLU:N	2.36	0.48
3:I:229:GLU:O	3:I:246:ALA:N	2.46	0.48
3:I:96:GLN:HG2	4:J:62:PHE:CZ	2.48	0.48
4:J:40:LEU:CD1	4:J:45:ARG:HG3	2.43	0.48
4:J:83:ASN:OD1	4:J:84:HIS:N	2.47	0.48
3:M:65:ARG:O	3:M:68:LYS:CG	2.61	0.48
3:R:82:ARG:O	3:R:86:ASN:N	2.44	0.48
2:B:146:THR:HG22	2:B:147:GLY:N	2.28	0.48
3:I:54:GLN:O	3:I:55:GLU:C	2.50	0.48
3:I:9:PHE:HZ	5:K:2:ILE:HD11	1.78	0.48
3:I:115:GLN:HG2	4:J:60:TRP:HZ2	1.78	0.48
2:L:77:ILE:HA	2:L:78:LEU:HD12	1.94	0.48
1:A:160:LYS:HA	1:A:174:SER:O	2.13	0.48
2:L:95:LEU:HD13	3:M:146:LYS:CE	2.44	0.48
4:N:30:PHE:CZ	4:N:84:HIS:CE1	3.01	0.48
1:A:36:LYS:HE3	1:A:87:TYR:CD2	2.48	0.48
2:B:48:TYR:CZ	2:B:56:ASP:HB2	2.48	0.48
4:D:50:GLU:O	4:D:67:TYR:N	2.33	0.48
2:H:165:HIS:O	2:H:168:VAL:HG12	2.12	0.48
2:H:221:TRP:HB2	2:H:227:LYS:CD	2.43	0.48
4:J:11:SER:OG	4:J:13:HIS:O	2.27	0.48
3:M:65:ARG:CG	3:M:65:ARG:NH1	2.73	0.48
3:C:229:GLU:HB3	3:C:246:ALA:O	2.14	0.48
3:C:234:ARG:HG2	4:D:10:TYR:CE2	2.48	0.48
4:J:63:TYR:O	4:J:64:LEU:HD23	2.14	0.48
2:L:91:CYS:O	2:L:104:GLY:N	2.45	0.48
3:R:133:TRP:HB2	3:R:144:LYS:HZ1	1.78	0.48
1:F:119:ASP:O	1:F:140:ASP:HB2	2.14	0.48
1:F:139:THR:HG23	1:F:140:ASP:OD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:PRO:O	1:G:120:PRO:HD3	2.14	0.48
1:G:43:PRO:HB2	2:H:103:PHE:CE2	2.49	0.48
2:L:110:THR:HG1	2:L:152:HIS:CE1	2.32	0.48
4:U:46:ILE:HD11	4:U:49:VAL:HG22	1.95	0.48
3:I:176:LYS:HG3	3:I:177:GLU:N	2.29	0.48
5:K:7:PHE:CD1	5:K:7:PHE:O	2.67	0.48
1:P:114:ASP:OD1	1:P:114:ASP:N	2.42	0.48
3:C:125:ALA:HB3	3:C:134:THR:HB	1.95	0.47
3:C:34:VAL:HG12	3:C:35:ARG:H	1.79	0.47
3:C:7:TYR:CE1	5:E:2:ILE:HB	2.49	0.47
1:F:19:VAL:O	1:F:75:ASN:HB2	2.14	0.47
3:I:150:ALA:O	3:I:151:HIS:CB	2.51	0.47
3:I:202:ARG:HD2	3:I:204:TRP:CH2	2.49	0.47
3:I:186:LYS:O	3:I:206:LEU:HD13	2.13	0.47
3:I:52:ILE:HG12	3:I:60:TRP:CZ2	2.49	0.47
3:M:270:LEU:HA	3:M:270:LEU:HD12	1.70	0.47
1:A:123:TYR:HB3	2:B:129:SER:HB2	1.96	0.47
4:D:89:GLN:HG3	4:D:90:PRO:O	2.15	0.47
4:J:40:LEU:HD12	4:J:45:ARG:HG3	1.95	0.47
2:L:3:GLN:HA	2:L:25:GLN:NE2	2.28	0.47
2:Q:216:SER:O	2:Q:218:ASN:N	2.47	0.47
3:I:93:HIS:HB3	3:I:118:TYR:CE1	2.49	0.47
3:I:81:LEU:O	3:I:83:GLY:N	2.47	0.47
4:N:86:THR:CG2	4:N:87:LEU:N	2.77	0.47
3:C:185:PRO:HG3	3:C:263:HIS:ND1	2.29	0.47
4:D:41:LYS:O	4:D:42:ASN:HB2	2.15	0.47
1:F:58:ASN:H	1:F:61:LEU:HD22	1.80	0.47
3:I:218:GLN:HG3	3:I:219:ARG:HG2	1.96	0.47
4:J:46:ILE:CG2	4:J:47:GLU:N	2.77	0.47
4:J:38:ASP:O	4:J:80:CYS:HB2	2.15	0.47
3:R:23:ILE:HD13	4:U:54:LEU:HB3	1.96	0.47
1:G:142:ASP:OD1	1:G:143:SER:N	2.48	0.47
2:H:6:GLN:HE22	2:H:90:PHE:HA	1.79	0.47
4:J:3:ARG:O	4:J:31:HIS:N	2.47	0.47
5:K:7:PHE:CD1	5:K:7:PHE:C	2.88	0.47
2:L:95:LEU:HD12	2:L:96:ILE:HG13	1.96	0.47
3:M:271:THR:OG1	3:M:272:LEU:N	2.46	0.47
4:D:78:TYR:O	4:D:95:TRP:HB3	2.15	0.47
2:L:95:LEU:C	2:L:95:LEU:HD12	2.35	0.47
3:M:138:MET:SD	3:M:141:GLN:NE2	2.87	0.47
3:R:172:LEU:O	3:R:180:GLN:NE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:235:PRO:HG2	4:U:65:LEU:CD2	2.44	0.47
2:B:32:MET:SD	2:B:68:ARG:NH1	2.86	0.47
1:F:57:SER:C	1:F:61:LEU:HB2	2.33	0.47
2:H:55:THR:OG1	3:I:65:ARG:NH2	2.47	0.47
4:J:79:ALA:HB2	4:J:94:LYS:HA	1.97	0.47
2:L:150:PRO:HD2	2:L:152:HIS:CD2	2.49	0.47
1:P:51:LYS:HE2	3:R:131:ARG:NH2	2.29	0.47
3:R:163:THR:CG2	3:R:167:TRP:HE1	2.27	0.47
3:R:9:PHE:CD1	3:R:97:ARG:HG2	2.50	0.47
4:U:48:LYS:HZ3	4:U:69:GLU:HB2	1.80	0.47
1:A:156:TYR:C	1:A:156:TYR:CD1	2.86	0.47
3:C:170:ARG:O	3:C:173:GLU:HG2	2.14	0.47
2:L:152:HIS:O	2:L:213:TYR:HD2	1.97	0.47
3:C:33:PHE:CZ	3:C:171:TYR:HB3	2.50	0.47
4:D:8:GLN:O	4:D:8:GLN:HG3	2.14	0.47
3:I:129:ASP:OD1	3:I:130:LEU:N	2.48	0.47
3:I:59:TYR:O	3:I:63:GLU:HG2	2.14	0.47
1:P:170:PHE:CE1	1:P:172:SER:HB2	2.50	0.47
4:U:23:LEU:HB2	4:U:70:PHE:CD2	2.50	0.47
1:F:160:LYS:N	1:F:160:LYS:CD	2.77	0.47
3:I:245:ALA:O	3:I:247:VAL:HG23	2.15	0.47
4:N:84:HIS:CG	4:N:85:VAL:N	2.83	0.47
2:H:80:SER:OG	3:R:270:LEU:HG	2.15	0.47
2:B:6:GLN:HE21	2:B:91:CYS:H	1.62	0.47
3:C:13:SER:HB3	3:C:78:LEU:HD22	1.96	0.47
3:C:81:LEU:HA	3:C:84:TYR:CD2	2.44	0.47
2:L:49:SER:HB3	2:L:54:VAL:O	2.14	0.47
3:M:56:GLY:C	3:M:58:GLU:HG2	2.35	0.47
3:M:147:TRP:CZ2	5:O:9:LEU:HD23	2.49	0.47
2:Q:98:PRO:O	3:R:150:ALA:HB1	2.15	0.47
4:D:37:VAL:HB	4:D:66:TYR:CZ	2.50	0.46
4:D:74:GLU:CD	4:D:74:GLU:H	1.92	0.46
1:G:124:GLN:O	2:H:129:SER:HB2	2.14	0.46
2:H:110:THR:HG21	2:H:150:PRO:HG2	1.96	0.46
2:H:114:ASP:OD1	2:H:116:LYS:HG3	2.15	0.46
2:H:150:PRO:HD2	2:H:152:HIS:CD2	2.50	0.46
3:I:84:TYR:HD2	3:I:85:TYR:CE2	2.33	0.46
4:J:3:ARG:O	4:J:30:PHE:CA	2.58	0.46
3:M:262:GLN:CG	3:M:269:PRO:HB3	2.45	0.46
2:Q:208:CYS:O	2:Q:234:SER:HB3	2.15	0.46
2:H:31:TYR:HD1	2:H:50:MET:HA	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:PRO:HG2	2:H:62:GLU:N	2.30	0.46
1:P:159:ASP:OD1	1:P:160:LYS:N	2.48	0.46
4:D:5:PRO:CB	4:D:30:PHE:HB3	2.39	0.46
3:I:228:THR:HG23	3:I:247:VAL:HG22	1.98	0.46
3:M:16:GLY:HA2	3:M:18:GLY:HA2	1.98	0.46
1:P:157:ILE:HG22	1:P:158:THR:H	1.79	0.46
3:R:19:GLU:OE1	3:R:19:GLU:N	2.49	0.46
1:A:157:ILE:HA	1:A:176:VAL:O	2.16	0.46
4:D:54:LEU:HA	4:D:64:LEU:HD21	1.96	0.46
2:H:13:THR:OG1	2:H:14:VAL:N	2.48	0.46
3:I:125:ALA:O	3:I:134:THR:N	2.47	0.46
3:I:81:LEU:O	3:I:82:ARG:C	2.54	0.46
3:M:110:LEU:HG	3:M:111:ARG:HG3	1.98	0.46
2:B:146:THR:O	2:B:148:PHE:CE2	2.68	0.46
3:C:140:ALA:O	3:C:144:LYS:N	2.44	0.46
3:C:65:ARG:O	3:C:65:ARG:HG2	2.15	0.46
3:I:63:GLU:HA	3:I:66:LYS:NZ	2.03	0.46
3:I:82:ARG:NH1	3:I:89:GLU:HB3	2.30	0.46
3:I:96:GLN:HG2	4:J:62:PHE:HZ	1.81	0.46
4:J:31:HIS:HE1	4:J:62:PHE:CD2	2.33	0.46
3:M:249:VAL:HG22	3:M:250:PRO:N	2.30	0.46
1:P:121:ALA:HA	1:P:198:ASP:OD1	2.16	0.46
4:U:46:ILE:HD12	4:U:48:LYS:N	2.29	0.46
1:A:154:ASP:CG	1:A:181:LYS:HD3	2.35	0.46
1:A:25:SER:OG	1:A:26:SER:N	2.49	0.46
2:B:70:GLU:OE1	2:B:70:GLU:N	2.48	0.46
3:C:7:TYR:HE1	5:E:2:ILE:HB	1.80	0.46
3:I:135:ALA:CB	3:I:141:GLN:OE1	2.64	0.46
3:I:144:LYS:O	3:I:148:GLU:N	2.49	0.46
3:I:3:HIS:NE2	3:I:180:GLN:HB2	2.29	0.46
3:I:64:THR:O	3:I:68:LYS:HB3	2.16	0.46
1:A:116:GLN:OE1	1:A:116:GLN:N	2.49	0.46
4:D:12:ARG:NH1	4:D:22:PHE:HD2	2.14	0.46
1:F:190:PHE:C	1:F:192:ASN:H	2.19	0.46
3:I:7:TYR:OH	5:K:1:GLY:N	2.39	0.46
3:M:61:ASP:O	3:M:65:ARG:N	2.41	0.46
1:P:125:LEU:HD11	2:Q:128:PRO:C	2.36	0.46
2:Q:136:THR:HG23	2:Q:137:GLN:N	2.30	0.46
2:Q:149:TYR:HA	2:Q:150:PRO:HA	1.58	0.46
1:A:128:SER:HB3	1:A:133:LYS:HE2	1.98	0.46
2:B:149:TYR:C	2:B:149:TYR:CD2	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:ASP:OD1	2:B:38:ASP:N	2.48	0.46
3:C:67:VAL:HG22	3:C:67:VAL:O	2.15	0.46
1:F:126:ARG:HD2	1:F:126:ARG:HA	1.84	0.46
3:M:254:GLU:CG	3:M:255:GLN:HG3	2.45	0.46
4:N:43:GLY:HA2	4:N:44:GLU:HA	1.48	0.46
4:N:55:SER:OG	4:N:56:PHE:N	2.49	0.46
2:Q:82:SER:O	2:Q:111:VAL:HG21	2.16	0.46
1:F:124:GLN:HG2	1:F:186:CYS:SG	2.56	0.46
3:I:124:ILE:HD13	3:I:147:TRP:CZ3	2.50	0.46
2:L:25:GLN:CD	2:L:27:MET:CG	2.82	0.46
3:C:234:ARG:NH1	3:C:244:TRP:HD1	2.14	0.46
1:G:150:SER:HA	1:G:151:LYS:CB	2.41	0.46
3:I:103:VAL:HG22	3:I:109:PHE:HA	1.97	0.46
2:L:4:VAL:HG13	2:L:104:GLY:HA2	1.98	0.46
2:Q:82:SER:OG	2:Q:84:ASN:HB3	2.16	0.46
1:G:138:PHE:CB	1:G:190:PHE:HE2	2.29	0.45
2:H:167:GLY:O	2:H:192:LEU:HD12	2.16	0.45
3:I:10:THR:HB	3:I:23:ILE:HD11	1.97	0.45
4:N:30:PHE:CD2	4:N:30:PHE:C	2.89	0.45
2:B:222:THR:HB	2:B:223:GLN:CA	2.46	0.45
4:D:88:SER:CB	4:D:89:GLN:CA	2.93	0.45
1:F:25:SER:OG	1:F:26:SER:N	2.49	0.45
1:G:64:GLN:O	1:G:72:SER:HB2	2.16	0.45
2:H:203:ARG:C	2:H:204:ASN:OD1	2.53	0.45
2:Q:31:TYR:HB3	2:Q:94:SER:HB3	1.97	0.45
3:R:192:HIS:NE2	4:U:98:ASP:HB2	2.31	0.45
1:A:132:ASP:O	1:A:133:LYS:HD3	2.16	0.45
1:A:145:THR:HG21	1:A:196:PRO:HD3	1.98	0.45
3:C:197:HIS:NE2	3:C:250:PRO:HB3	2.31	0.45
4:D:89:GLN:HB2	4:D:90:PRO:CD	2.43	0.45
2:H:18:GLU:HG2	2:H:79:GLU:HA	1.97	0.45
3:I:141:GLN:HE22	3:I:144:LYS:CE	2.29	0.45
3:I:236:ALA:O	4:J:12:ARG:NE	2.50	0.45
4:J:22:PHE:CD1	4:J:22:PHE:N	2.82	0.45
3:R:101:CYS:HA	3:R:112:GLY:HA2	1.99	0.45
1:A:93:GLY:HA2	1:A:94:GLY:HA3	1.74	0.45
3:C:231:VAL:HG21	3:C:244:TRP:CE2	2.52	0.45
4:D:88:SER:HB3	4:D:89:GLN:CA	2.44	0.45
1:F:38:GLU:OE1	1:F:38:GLU:N	2.50	0.45
1:G:174:SER:OG	2:H:191:ARG:HD2	2.17	0.45
2:H:118:VAL:O	2:H:228:PRO:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:76:VAL:O	3:I:80:THR:OG1	2.29	0.45
2:L:47:TYR:OH	2:L:55:THR:HB	2.17	0.45
2:B:4:VAL:O	2:B:4:VAL:HG23	2.16	0.45
1:G:19:VAL:CG1	1:G:76:ILE:HB	2.46	0.45
1:G:7:SER:OG	1:G:8:PRO:HA	2.17	0.45
3:I:207:SER:O	3:I:207:SER:OG	2.27	0.45
2:L:56:ASP:OD1	3:M:68:LYS:NZ	2.50	0.45
1:P:86:ILE:HD13	1:P:88:PHE:CE2	2.52	0.45
2:L:158:TRP:HA	2:L:163:GLU:HA	1.99	0.45
1:P:101:LEU:HD23	2:Q:101:LEU:HD11	1.98	0.45
1:P:118:PRO:O	1:P:118:PRO:HD2	2.17	0.45
2:Q:119:PHE:CB	2:Q:120:PRO:CD	2.82	0.45
3:R:231:VAL:HG21	3:R:244:TRP:CE3	2.51	0.45
3:R:3:HIS:N	3:R:3:HIS:ND1	2.65	0.45
3:R:97:ARG:NH2	5:T:7:PHE:HZ	2.15	0.45
4:D:91:LYS:O	4:D:92:ILE:CG2	2.65	0.45
3:I:45:MET:HB3	3:I:60:TRP:CE3	2.48	0.45
3:M:220:ASP:CB	3:M:221:GLY:CA	2.91	0.45
2:Q:2:ALA:HA	2:Q:26:ASN:HD21	1.80	0.45
3:R:195:SER:HA	3:R:196:ASP:HA	1.65	0.45
3:R:25:VAL:HG12	3:R:35:ARG:NH1	2.32	0.45
3:C:114:HIS:CE1	5:E:7:PHE:HZ	2.35	0.45
3:C:182:THR:HG22	3:C:210:PRO:HD3	1.98	0.45
2:H:114:ASP:OD1	2:H:115:LEU:N	2.50	0.45
2:L:148:PHE:CB	2:L:186:TYR:HB2	2.42	0.45
4:N:31:HIS:HB2	4:N:62:PHE:CE1	2.52	0.45
1:P:25:SER:OG	1:P:26:SER:N	2.49	0.45
1:P:31:THR:HG22	1:P:50:TYR:CD1	2.50	0.45
4:U:26:TYR:HA	4:U:65:LEU:HD13	1.97	0.45
4:U:64:LEU:HD12	4:U:64:LEU:HA	1.59	0.45
1:A:163:LEU:HB3	1:A:172:SER:O	2.17	0.45
3:C:200:THR:OG1	3:C:248:VAL:HG21	2.17	0.45
2:H:30:GLU:N	2:H:32:MET:HE1	2.32	0.45
3:I:107:TRP:CH2	3:I:169:ARG:CZ	3.00	0.45
3:I:115:GLN:HG3	3:I:124:ILE:O	2.17	0.45
2:L:34:TRP:CH2	2:L:91:CYS:HB2	2.52	0.45
3:M:32:GLN:OE1	3:M:33:PHE:N	2.49	0.45
3:R:14:ARG:HE	3:R:14:ARG:HB3	1.53	0.45
4:U:54:LEU:HA	4:U:64:LEU:HD13	1.99	0.45
3:C:141:GLN:N	3:C:141:GLN:OE1	2.50	0.45
2:H:13:THR:HG21	2:H:19:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:115:LEU:O	2:L:118:VAL:HG22	2.16	0.45
2:L:6:GLN:NE2	2:L:34:TRP:CH2	2.84	0.45
2:L:87:SER:HB3	2:L:89:TYR:CE1	2.46	0.45
3:M:117:ALA:HA	3:M:123:TYR:CB	2.47	0.45
3:M:85:TYR:HB3	3:M:87:GLN:NE2	2.32	0.45
3:R:270:LEU:CD2	3:R:271:THR:H	2.30	0.45
1:A:155:VAL:HA	1:A:179:SER:HB2	1.98	0.44
1:A:165:MET:CE	1:A:166:ARG:H	2.30	0.44
1:A:199:THR:OG1	1:A:199:THR:O	2.29	0.44
2:B:53:GLU:OE1	3:C:72:GLN:NE2	2.50	0.44
4:J:54:LEU:HA	4:J:64:LEU:CD2	2.46	0.44
3:M:123:TYR:HE2	3:M:143:THR:HG21	1.81	0.44
3:M:215:LEU:HB2	3:M:260:HIS:O	2.17	0.44
3:M:216:THR:O	3:M:217:TRP:CD1	2.70	0.44
3:R:15:PRO:HB3	3:R:89:GLU:O	2.17	0.44
3:R:263:HIS:CE1	3:R:265:GLY:CA	3.00	0.44
1:A:78:ALA:O	1:A:80:ILE:N	2.47	0.44
1:A:163:LEU:HD21	2:B:193:ARG:HD2	1.99	0.44
1:F:155:VAL:HG12	1:F:179:SER:HB2	1.99	0.44
3:I:85:TYR:CZ	3:I:118:TYR:CE2	3.05	0.44
2:L:10:TYR:CD1	2:L:108:ARG:HB2	2.52	0.44
2:L:159:VAL:N	2:L:162:LYS:O	2.48	0.44
3:M:216:THR:O	3:M:217:TRP:HD1	2.01	0.44
3:M:9:PHE:HB2	3:M:97:ARG:CB	2.47	0.44
2:Q:216:SER:HA	2:Q:229:VAL:CG1	2.47	0.44
2:B:209:GLN:HG3	2:B:234:SER:OG	2.17	0.44
1:G:46:LEU:HA	1:G:46:LEU:HD23	1.73	0.44
4:J:46:ILE:HD12	4:J:70:PHE:CZ	2.43	0.44
2:L:128:PRO:HG3	2:L:141:LEU:HG	2.00	0.44
3:R:7:TYR:HD2	3:R:99:TYR:HE1	1.65	0.44
4:U:13:HIS:HB2	4:U:21:ASN:ND2	2.32	0.44
1:A:58:ASN:HA	1:A:59:GLY:HA2	1.44	0.44
3:C:109:PHE:CD1	3:C:165:VAL:HG21	2.52	0.44
3:C:234:ARG:HB3	3:C:242:GLN:O	2.17	0.44
4:D:56:PHE:CZ	4:D:60:TRP:HE3	2.35	0.44
1:F:157:ILE:HA	1:F:177:ALA:HB2	1.99	0.44
2:H:26:ASN:HA	2:H:27:MET:HA	1.49	0.44
2:H:3:GLN:OE1	2:H:4:VAL:N	2.50	0.44
2:H:61:PRO:CG	2:H:62:GLU:N	2.80	0.44
4:J:25:CYS:O	4:J:65:LEU:HD12	2.17	0.44
2:Q:29:HIS:NE2	2:Q:95:LEU:HG	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:47:TYR:OH	2:H:61:PRO:HB2	2.18	0.44
2:H:25:GLN:HB3	2:H:72:ARG:O	2.18	0.44
3:I:146:LYS:HD2	3:I:146:LYS:HA	1.67	0.44
1:A:124:GLN:O	1:A:125:LEU:HD23	2.17	0.44
3:C:170:ARG:HG2	3:C:173:GLU:OE2	2.17	0.44
3:I:28:VAL:HG23	3:I:33:PHE:CE1	2.52	0.44
3:I:82:ARG:O	3:I:86:ASN:N	2.46	0.44
3:M:56:GLY:O	3:M:60:TRP:HD1	2.01	0.44
4:N:3:ARG:H	4:N:30:PHE:HE1	1.64	0.44
3:R:263:HIS:CE1	3:R:265:GLY:HA3	2.52	0.44
3:I:89:GLU:OE1	3:I:89:GLU:N	2.51	0.44
4:J:41:LYS:O	4:J:43:GLY:N	2.51	0.44
2:Q:22:THR:OG1	2:Q:23:CYS:N	2.50	0.44
1:A:34:TRP:CE3	1:A:74:LEU:HD22	2.53	0.44
3:C:172:LEU:O	3:C:176:LYS:HG3	2.18	0.44
3:I:52:ILE:CD1	3:I:60:TRP:CH2	3.01	0.44
3:M:217:TRP:NE1	3:M:259:CYS:HA	2.32	0.44
1:P:125:LEU:HG	2:Q:127:GLU:O	2.17	0.44
1:P:47:ILE:CG2	1:P:57:SER:HB2	2.48	0.44
1:A:148:SER:CB	1:A:193:SER:HB3	2.47	0.44
3:C:47:PRO:HD3	3:C:60:TRP:CH2	2.53	0.44
4:D:87:LEU:CD1	4:D:87:LEU:C	2.85	0.44
4:D:56:PHE:CE2	4:D:60:TRP:CE3	3.06	0.43
3:I:93:HIS:CG	3:I:118:TYR:HH	2.36	0.43
2:Q:201:ASN:HA	2:Q:202:PRO:HD3	1.85	0.43
4:U:27:VAL:HG11	4:U:37:VAL:HG21	2.00	0.43
1:A:165:MET:HG3	2:B:166:SER:OG	2.18	0.43
3:I:217:TRP:HE1	3:I:259:CYS:HB3	1.82	0.43
3:I:61:ASP:C	3:I:63:GLU:N	2.71	0.43
1:P:24:THR:OG1	1:P:25:SER:N	2.50	0.43
2:B:130:GLU:CD	2:B:130:GLU:H	2.21	0.43
1:P:13:ILE:HD13	1:P:19:VAL:CG2	2.47	0.43
1:P:74:LEU:HD22	1:P:74:LEU:HA	1.88	0.43
3:R:3:HIS:HD2	3:R:172:LEU:HD21	1.84	0.43
2:B:173:GLN:HA	2:B:174:PRO:HD3	1.74	0.43
2:B:121:PRO:O	2:B:233:VAL:HG21	2.19	0.43
3:I:133:TRP:CZ2	3:I:153:ALA:HB2	2.51	0.43
3:I:66:LYS:HE2	5:K:2:ILE:CG2	2.46	0.43
4:J:31:HIS:CE1	4:J:62:PHE:CD2	3.06	0.43
2:L:102:PHE:CD1	2:L:102:PHE:N	2.85	0.43
2:L:13:THR:HG21	2:L:19:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:201:LEU:HD13	3:M:217:TRP:CZ3	2.45	0.43
3:M:13:SER:OG	3:M:82:ARG:NH2	2.51	0.43
2:Q:8:PRO:HD2	2:Q:21:VAL:HG22	2.00	0.43
4:U:41:LYS:HB3	4:U:78:TYR:CE1	2.54	0.43
3:C:200:THR:HA	3:C:248:VAL:HG23	2.00	0.43
3:C:33:PHE:CE2	3:C:51:TRP:CZ2	3.07	0.43
3:C:85:TYR:HE2	3:C:87:GLN:NE2	2.16	0.43
3:I:138:MET:HA	3:I:141:GLN:HB3	2.01	0.43
2:L:136:THR:HG21	2:L:193:ARG:NH2	2.34	0.43
2:Q:66:VAL:HG12	2:Q:76:LEU:HA	2.00	0.43
3:R:51:TRP:CD1	3:R:51:TRP:N	2.87	0.43
3:C:102:ASP:O	3:C:110:LEU:HB3	2.17	0.43
3:C:84:TYR:HB3	3:C:139:ALA:HB1	2.00	0.43
4:D:81:ARG:CA	4:D:92:ILE:HG22	2.45	0.43
1:F:139:THR:OG1	1:F:140:ASP:N	2.51	0.43
4:J:42:ASN:HB3	4:J:43:GLY:H	1.64	0.43
1:P:100:LYS:HG2	2:Q:45:GLN:OE1	2.18	0.43
1:P:60:ARG:HH12	1:P:80:ILE:H	1.66	0.43
3:R:228:THR:HB	3:R:229:GLU:H	1.52	0.43
1:A:101:LEU:HD22	2:B:101:LEU:HD11	2.00	0.43
2:B:143:CYS:SG	2:B:155:LEU:HD11	2.59	0.43
3:C:195:SER:HA	3:C:196:ASP:HA	1.70	0.43
3:C:234:ARG:HG2	4:D:10:TYR:CZ	2.54	0.43
4:D:64:LEU:HD23	4:D:64:LEU:HA	1.75	0.43
1:G:81:PRO:O	1:G:84:VAL:HG23	2.17	0.43
3:I:127:LYS:CD	3:I:128:GLU:H	2.29	0.43
3:M:209:TYR:CD1	3:M:210:PRO:HA	2.53	0.43
1:P:124:GLN:O	1:P:125:LEU:HD13	2.19	0.43
2:Q:221:TRP:CH2	2:Q:223:GLN:O	2.72	0.43
1:A:156:TYR:CG	1:A:156:TYR:O	2.70	0.43
1:G:177:ALA:HB3	1:G:190:PHE:HE1	1.83	0.43
1:G:129:LYS:HE2	2:H:124:ALA:HB2	2.01	0.43
3:I:126:LEU:HD11	3:I:130:LEU:HA	1.99	0.43
2:L:126:PHE:HD2	2:L:142:VAL:O	2.02	0.43
2:Q:136:THR:CB	2:Q:137:GLN:HA	2.38	0.43
2:Q:150:PRO:O	2:Q:150:PRO:HD2	2.19	0.43
3:R:81:LEU:HD23	3:R:81:LEU:HA	1.77	0.43
4:U:5:PRO:HB2	4:U:7:ILE:HD11	2.00	0.43
2:B:10:TYR:CD1	2:B:108:ARG:HB3	2.54	0.43
2:B:167:GLY:O	2:B:192:LEU:HA	2.18	0.43
3:I:141:GLN:HE22	3:I:144:LYS:NZ	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3:HIS:O	3:I:4:SER:OG	2.32	0.43
3:I:95:VAL:HG22	3:I:118:TYR:HD1	1.83	0.43
4:N:36:GLU:O	4:N:82:VAL:HG13	2.19	0.43
1:P:61:LEU:HD23	1:P:76:ILE:HG12	2.01	0.43
2:B:12:ILE:HD11	2:B:108:ARG:HH21	1.83	0.43
2:B:13:THR:OG1	2:B:14:VAL:N	2.52	0.43
2:B:149:TYR:HA	2:B:150:PRO:HA	1.75	0.43
3:C:197:HIS:NE2	3:C:250:PRO:HB2	2.34	0.43
3:I:180:GLN:O	3:I:180:GLN:HG3	2.19	0.43
3:I:7:TYR:HE2	5:K:1:GLY:O	2.01	0.43
4:N:91:LYS:HB3	4:N:91:LYS:HE2	1.76	0.43
1:P:163:LEU:HD11	1:P:172:SER:HB3	2.01	0.43
3:R:168:LEU:O	3:R:172:LEU:N	2.52	0.43
4:D:39:LEU:HB2	4:D:46:ILE:HG21	2.01	0.42
1:G:172:SER:OG	2:H:193:ARG:NH1	2.52	0.42
1:G:22:ASN:HB3	1:G:73:PHE:CD2	2.53	0.42
2:H:64:TYR:O	2:H:65:LYS:HG3	2.18	0.42
3:I:34:VAL:HG12	3:I:35:ARG:H	1.84	0.42
2:L:139:ALA:O	2:L:193:ARG:HA	2.18	0.42
3:M:126:LEU:HD21	3:M:130:LEU:HD23	2.00	0.42
3:M:99:TYR:CB	3:M:114:HIS:HA	2.49	0.42
1:P:100:LYS:HB3	1:P:100:LYS:HE3	1.87	0.42
3:C:6:ARG:HD2	3:C:98:MET:CE	2.49	0.42
1:G:93:GLY:HA2	1:G:94:GLY:HA3	1.62	0.42
3:I:55:GLU:OE1	3:I:170:ARG:NH2	2.52	0.42
2:Q:8:PRO:HD2	2:Q:21:VAL:HG13	2.01	0.42
3:R:33:PHE:CD1	3:R:34:VAL:HG22	2.54	0.42
3:R:204:TRP:HH2	4:U:99:MET:HA	1.84	0.42
4:J:4:THR:OG1	4:J:5:PRO:CD	2.65	0.42
3:M:146:LYS:HA	3:M:149:ALA:HB3	2.01	0.42
4:N:30:PHE:O	4:N:62:PHE:HB2	2.20	0.42
2:B:64:TYR:CD1	2:B:78:LEU:HG	2.54	0.42
2:B:8:PRO:HG3	2:B:11:LEU:HD12	2.00	0.42
1:F:129:LYS:HZ3	1:F:132:ASP:N	2.17	0.42
1:F:135:VAL:HA	1:F:178:TRP:HB3	2.00	0.42
2:H:8:PRO:HG3	2:H:11:LEU:HD12	2.02	0.42
3:M:262:GLN:NE2	3:M:263:HIS:O	2.52	0.42
1:P:164:ASP:O	2:Q:167:GLY:N	2.44	0.42
2:Q:128:PRO:HD2	2:Q:199:TRP:CZ2	2.54	0.42
2:Q:215:LEU:O	2:Q:229:VAL:HG13	2.19	0.42
1:F:120:PRO:HG3	1:F:196:PRO:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:95:VAL:HG22	3:M:118:TYR:HD1	1.84	0.42
4:N:30:PHE:CD2	4:N:31:HIS:N	2.88	0.42
2:B:88:LEU:HD22	2:B:108:ARG:CA	2.48	0.42
1:F:126:ARG:NH1	1:F:129:LYS:HZ2	2.18	0.42
3:I:12:VAL:HG22	3:I:94:THR:HG23	2.01	0.42
2:Q:86:THR:HG23	2:Q:110:THR:HA	2.01	0.42
5:T:6:VAL:HB	5:T:7:PHE:H	1.68	0.42
1:A:119:ASP:HA	1:A:120:PRO:HD2	1.87	0.42
2:B:34:TRP:CG	2:B:76:LEU:HD22	2.55	0.42
3:C:37:ASP:HB3	3:C:40:ALA:HB3	2.02	0.42
3:I:33:PHE:O	3:I:52:ILE:CD1	2.68	0.42
3:R:144:LYS:O	3:R:148:GLU:N	2.51	0.42
3:R:39:ASP:OD1	3:R:40:ALA:N	2.52	0.42
4:U:23:LEU:HB3	4:U:68:THR:HG23	2.01	0.42
1:A:92:PRO:HG2	3:C:155:GLN:NE2	2.34	0.42
2:B:7:ASN:HA	2:B:8:PRO:HA	1.73	0.42
4:D:51:HIS:HB3	4:D:66:TYR:CD1	2.54	0.42
2:H:160:ASN:CA	2:H:205:HIS:HB2	2.50	0.42
2:H:30:GLU:H	2:H:95:LEU:HA	1.84	0.42
3:I:139:ALA:O	3:I:142:THR:HG23	2.20	0.42
3:I:180:GLN:O	3:I:180:GLN:CG	2.68	0.42
3:I:215:LEU:HA	3:I:260:HIS:O	2.20	0.42
2:L:50:MET:H	2:L:50:MET:HG3	1.50	0.42
1:P:157:ILE:HG22	1:P:158:THR:N	2.35	0.42
2:Q:29:HIS:HB3	2:Q:94:SER:O	2.19	0.42
3:R:49:ALA:HA	3:R:50:PRO:HD3	1.88	0.42
1:A:153:SER:OG	1:A:153:SER:O	2.34	0.42
1:F:147:VAL:HB	1:F:160:LYS:HZ2	1.84	0.42
4:J:80:CYS:C	4:J:92:ILE:HG23	2.39	0.42
3:M:148:GLU:CA	3:M:151:HIS:H	2.30	0.42
3:M:241:PHE:CD1	3:M:241:PHE:N	2.86	0.42
3:R:35:ARG:HD3	3:R:35:ARG:HA	1.76	0.42
2:B:8:PRO:HG2	2:B:11:LEU:HB2	2.02	0.42
2:H:149:TYR:HA	2:H:150:PRO:HA	1.90	0.42
3:R:177:GLU:O	3:R:181:ARG:N	2.53	0.42
3:R:64:THR:O	3:R:67:VAL:HG12	2.20	0.42
2:B:149:TYR:C	2:B:149:TYR:HD2	2.24	0.41
2:B:171:ASP:OD1	2:B:189:SER:HB3	2.20	0.41
3:C:21:ARG:NH1	3:C:21:ARG:HG2	2.35	0.41
2:H:84:ASN:OD1	2:H:85:GLN:HG3	2.19	0.41
2:L:228:PRO:C	2:L:229:VAL:HG23	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:116:TYR:CD2	5:O:9:LEU:HD21	2.54	0.41
3:M:125:ALA:HB3	3:M:134:THR:OG1	2.19	0.41
3:M:143:THR:OG1	3:M:144:LYS:N	2.54	0.41
2:Q:135:HIS:O	2:Q:135:HIS:ND1	2.53	0.41
3:R:123:TYR:CZ	3:R:140:ALA:HA	2.55	0.41
2:H:79:GLU:O	3:R:270:LEU:HD21	2.20	0.41
3:R:27:TYR:HE1	3:R:32:GLN:HG2	1.84	0.41
3:C:250:PRO:HG2	3:C:250:PRO:O	2.20	0.41
3:C:59:TYR:CZ	3:C:63:GLU:HG3	2.55	0.41
3:C:87:GLN:OE1	3:C:88:SER:N	2.37	0.41
1:G:60:ARG:NH1	1:G:83:ASP:CG	2.60	0.41
2:H:12:ILE:HD13	2:H:214:GLY:HA2	2.01	0.41
2:H:7:ASN:HB2	2:H:22:THR:HG23	2.01	0.41
3:I:126:LEU:HD21	3:I:130:LEU:HD22	2.01	0.41
3:I:231:VAL:HG21	4:J:8:GLN:HE22	1.85	0.41
1:P:139:THR:OG1	1:P:140:ASP:N	2.53	0.41
1:P:26:SER:C	1:P:70:LYS:HD2	2.40	0.41
2:Q:9:ARG:HA	2:Q:107:SER:HB2	2.00	0.41
4:D:76:ASP:HB3	4:D:78:TYR:CD2	2.53	0.41
3:I:129:ASP:CG	3:I:131:ARG:HG2	2.41	0.41
3:I:51:TRP:NE1	3:I:179:LEU:HD11	2.35	0.41
3:I:208:PHE:CE1	3:I:213:ILE:HG13	2.56	0.41
3:I:7:TYR:CG	5:K:2:ILE:HD12	2.55	0.41
3:C:109:PHE:HD1	3:C:165:VAL:HG21	1.86	0.41
3:C:33:PHE:CD2	3:C:51:TRP:CZ2	3.02	0.41
4:D:83:ASN:CG	4:D:90:PRO:HB3	2.40	0.41
1:F:97:ASN:O	3:M:66:LYS:NZ	2.49	0.41
4:J:3:ARG:HD2	4:J:3:ARG:HA	1.81	0.41
2:L:95:LEU:HD12	2:L:96:ILE:CG1	2.50	0.41
2:Q:137:GLN:O	2:Q:196:ALA:HB3	2.21	0.41
3:R:209:TYR:CD1	3:R:210:PRO:HA	2.55	0.41
3:R:185:PRO:CD	3:R:263:HIS:HD2	2.25	0.41
3:R:98:MET:CE	4:U:58:LYS:HZ1	2.34	0.41
2:B:10:TYR:HA	2:B:108:ARG:HB3	2.03	0.41
3:C:33:PHE:CE2	3:C:51:TRP:HZ2	2.38	0.41
3:C:5:MET:C	3:C:6:ARG:HG2	2.41	0.41
1:F:126:ARG:NH1	1:F:129:LYS:NZ	2.69	0.41
1:G:59:GLY:CA	1:G:60:ARG:CB	2.98	0.41
2:H:178:GLN:H	2:H:178:GLN:NE2	2.18	0.41
2:H:27:MET:SD	2:H:27:MET:O	2.79	0.41
2:H:25:GLN:NE2	2:H:29:HIS:CD2	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:186:LYS:O	3:I:206:LEU:HB2	2.19	0.41
3:I:84:TYR:CD2	3:I:139:ALA:HB2	2.55	0.41
1:F:42:GLY:HA2	2:L:90:PHE:CE1	2.56	0.41
4:N:64:LEU:HD23	4:N:64:LEU:HA	1.75	0.41
2:Q:215:LEU:O	2:Q:215:LEU:HD12	2.21	0.41
3:R:7:TYR:HD1	3:R:26:GLY:HA2	1.85	0.41
1:A:163:LEU:HD12	1:A:164:ASP:H	1.84	0.41
3:C:101:CYS:HA	3:C:112:GLY:HA2	2.01	0.41
1:F:147:VAL:HB	1:F:160:LYS:NZ	2.35	0.41
1:G:59:GLY:HA3	1:G:61:LEU:CB	2.50	0.41
3:I:74:HIS:HA	3:I:77:ASP:HB2	2.01	0.41
3:M:147:TRP:O	3:M:152:VAL:HB	2.20	0.41
3:M:23:ILE:HA	3:M:37:ASP:HB3	2.02	0.41
2:Q:27:MET:HB3	2:Q:29:HIS:CD2	2.56	0.41
3:R:3:HIS:CD2	3:R:172:LEU:HD11	2.56	0.41
3:R:203:CYS:HB2	3:R:217:TRP:CZ2	2.56	0.41
1:A:125:LEU:HD22	2:B:128:PRO:HA	2.03	0.41
3:C:35:ARG:HD3	4:D:53:ASP:CG	2.41	0.41
4:D:47:GLU:HG2	4:D:47:GLU:H	1.57	0.41
2:H:190:SER:O	2:H:191:ARG:HG3	2.21	0.41
3:I:175:GLY:HA3	3:I:179:LEU:HD22	2.03	0.41
3:I:52:ILE:HD13	3:I:60:TRP:CH2	2.56	0.41
2:L:97:TYR:HA	2:L:98:PRO:HA	1.84	0.41
3:M:12:VAL:HG12	3:M:94:THR:HG23	2.01	0.41
2:Q:178:GLN:HB2	2:Q:181:LEU:HD13	2.02	0.41
3:R:208:PHE:O	3:R:241:PHE:N	2.50	0.41
3:C:6:ARG:HD2	3:C:98:MET:HE1	2.01	0.41
4:D:22:PHE:CD1	4:D:69:GLU:HA	2.56	0.41
4:J:5:PRO:HB3	4:J:30:PHE:HD2	1.83	0.41
3:M:17:ARG:CG	3:M:17:ARG:NH1	2.73	0.41
3:M:201:LEU:HD23	3:M:249:VAL:HG11	2.01	0.41
3:R:141:GLN:HA	3:R:144:LYS:HB3	2.03	0.41
1:F:13:ILE:HD13	1:F:19:VAL:HG22	2.02	0.41
4:N:18:GLY:N	4:N:72:PRO:O	2.52	0.41
3:R:44:ARG:HA	3:R:64:THR:HG21	2.03	0.41
3:R:97:ARG:CZ	5:T:7:PHE:HZ	2.34	0.41
4:U:23:LEU:HD12	4:U:24:ASN:H	1.86	0.41
4:U:35:ILE:HG22	4:U:84:HIS:CG	2.54	0.41
3:R:117:ALA:CB	4:U:60:TRP:CZ3	3.04	0.41
4:U:73:THR:HG22	4:U:75:LYS:H	1.85	0.41
4:D:37:VAL:HG22	4:D:82:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:166:ARG:H	1:G:166:ARG:HG2	1.69	0.41
2:H:29:HIS:HE1	2:H:102:PHE:CE2	2.39	0.41
1:G:50:TYR:CE1	3:I:151:HIS:NE2	2.89	0.41
3:R:147:TRP:CD1	3:R:152:VAL:HG21	2.56	0.41
4:U:75:LYS:HZ3	4:U:75:LYS:CB	2.33	0.41
2:B:6:GLN:HE22	2:B:90:PHE:HA	1.86	0.41
4:D:10:TYR:HB3	4:D:24:ASN:OD1	2.21	0.41
1:F:197:GLU:C	1:F:198:ASP:OD1	2.59	0.41
2:H:205:HIS:HD2	2:H:236:GLU:OE2	2.03	0.41
2:H:34:TRP:CZ3	2:H:91:CYS:HB2	2.55	0.41
3:I:133:TRP:NE1	3:I:153:ALA:CB	2.84	0.41
3:I:185:PRO:HB3	3:I:208:PHE:HB3	2.02	0.41
3:I:229:GLU:CB	3:I:246:ALA:HB3	2.50	0.41
4:J:71:THR:HA	4:J:72:PRO:HD3	1.92	0.41
3:R:82:ARG:NE	3:R:87:GLN:O	2.53	0.41
2:B:121:PRO:HA	2:B:148:PHE:CD1	2.52	0.40
2:B:129:SER:O	2:B:133:ILE:HG13	2.21	0.40
2:B:46:ILE:C	2:B:47:TYR:HD1	2.25	0.40
2:B:6:GLN:NE2	2:B:90:PHE:HA	2.36	0.40
4:D:37:VAL:HG13	4:D:82:VAL:HG22	2.02	0.40
1:F:12:PHE:HD1	1:F:110:GLN:H	1.69	0.40
1:G:24:THR:HG22	1:G:71:ASP:HB3	2.03	0.40
1:G:36:LYS:HB2	1:G:36:LYS:HE3	1.92	0.40
2:H:150:PRO:HG2	2:H:152:HIS:NE2	2.36	0.40
2:L:6:GLN:HE21	2:L:34:TRP:HH2	1.69	0.40
2:Q:115:LEU:H	2:Q:115:LEU:CD1	2.19	0.40
3:R:217:TRP:HD1	3:R:258:THR:CA	2.33	0.40
3:R:24:ALA:O	3:R:35:ARG:HD3	2.21	0.40
2:B:173:GLN:CD	2:B:173:GLN:H	2.23	0.40
2:B:50:MET:O	2:B:54:VAL:HB	2.21	0.40
1:F:129:LYS:HG3	1:F:130:SER:N	2.35	0.40
4:J:41:LYS:CG	4:J:78:TYR:HD1	2.23	0.40
1:A:112:LYS:HA	1:A:113:PRO:HD3	1.97	0.40
2:B:88:LEU:CD2	2:B:108:ARG:HG3	2.49	0.40
2:B:7:ASN:O	2:B:21:VAL:HG13	2.22	0.40
2:B:222:THR:HA	2:B:223:GLN:HA	1.69	0.40
2:B:68:ARG:HD2	2:B:74:PHE:CD1	2.56	0.40
3:C:49:ALA:HB3	3:C:51:TRP:CH2	2.56	0.40
1:G:100:LYS:HB2	1:G:100:LYS:HE2	1.78	0.40
3:M:16:GLY:HA2	3:M:17:ARG:HA	1.50	0.40
3:M:85:TYR:HB3	3:M:87:GLN:HE22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:96:ASP:OD1	4:N:97:ARG:N	2.53	0.40
3:M:116:TYR:HD2	5:O:9:LEU:HD21	1.85	0.40
1:P:180:ASN:O	1:P:181:LYS:HB3	2.21	0.40
1:P:43:PRO:HD2	2:Q:103:PHE:CG	2.56	0.40
3:R:244:TRP:HE1	3:R:246:ALA:HB2	1.86	0.40
1:A:200:PHE:CG	1:A:201:PHE:N	2.89	0.40
2:B:120:PRO:HD3	2:B:228:PRO:HB3	2.03	0.40
3:C:216:THR:O	3:C:260:HIS:CE1	2.74	0.40
1:F:20:SER:HB2	1:P:68:THR:HG22	2.04	0.40
2:H:221:TRP:CD2	2:H:227:LYS:HG2	2.57	0.40
3:I:116:TYR:OH	5:K:7:PHE:CE1	2.73	0.40
1:F:124:GLN:O	2:L:129:SER:HB2	2.21	0.40
3:M:8:PHE:N	3:M:25:VAL:O	2.55	0.40
1:P:47:ILE:HG23	1:P:57:SER:CB	2.51	0.40
2:Q:38:ASP:OD1	2:Q:87:SER:OG	2.23	0.40
3:R:13:SER:HA	3:R:20:PRO:HB3	2.03	0.40
1:G:4:LEU:HD13	1:G:25:SER:HB2	2.02	0.40
3:I:216:THR:C	3:I:217:TRP:HD1	2.24	0.40
3:I:262:GLN:HB3	3:I:269:PRO:HB3	2.03	0.40
3:I:87:GLN:NE2	3:I:87:GLN:HA	2.36	0.40
4:J:23:LEU:HG	4:J:70:PHE:HD2	1.85	0.40
2:L:229:VAL:HG12	2:L:230:THR:N	2.36	0.40
3:M:14:ARG:HD3	3:M:21:ARG:NH1	2.32	0.40
3:M:195:SER:O	3:M:196:ASP:HB2	2.22	0.40
4:N:54:LEU:HD21	4:N:62:PHE:HE2	1.86	0.40
1:P:30:ASN:HA	1:P:65:PHE:HZ	1.87	0.40
1:P:37:GLN:O	1:P:86:ILE:HG13	2.22	0.40
2:Q:65:LYS:HE3	2:Q:65:LYS:HB2	1.85	0.40
3:R:130:LEU:O	3:R:131:ARG:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	192/208 (92%)	161 (84%)	31 (16%)	0	100	100
1	F	194/208 (93%)	173 (89%)	20 (10%)	1 (0%)	34	76
1	G	199/208 (96%)	176 (88%)	23 (12%)	0	100	100
1	P	185/208 (89%)	151 (82%)	32 (17%)	2 (1%)	17	64
2	B	239/243 (98%)	212 (89%)	26 (11%)	1 (0%)	39	79
2	H	237/243 (98%)	201 (85%)	32 (14%)	4 (2%)	11	56
2	L	240/243 (99%)	213 (89%)	27 (11%)	0	100	100
2	Q	234/243 (96%)	211 (90%)	21 (9%)	2 (1%)	21	66
3	C	252/276 (91%)	223 (88%)	29 (12%)	0	100	100
3	I	253/276 (92%)	218 (86%)	34 (13%)	1 (0%)	39	79
3	M	260/276 (94%)	225 (86%)	33 (13%)	2 (1%)	24	69
3	R	241/276 (87%)	210 (87%)	31 (13%)	0	100	100
4	D	95/100 (95%)	82 (86%)	13 (14%)	0	100	100
4	J	92/100 (92%)	86 (94%)	6 (6%)	0	100	100
4	N	88/100 (88%)	76 (86%)	10 (11%)	2 (2%)	8	51
4	U	97/100 (97%)	82 (84%)	14 (14%)	1 (1%)	19	65
5	E	7/9 (78%)	7 (100%)	0	0	100	100
5	K	7/9 (78%)	7 (100%)	0	0	100	100
5	O	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
5	T	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
All	All	3126/3344 (94%)	2724 (87%)	386 (12%)	16 (0%)	34	76

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	156	LEU
4	N	26	TYR
4	N	72	PRO
2	Q	136	THR
2	H	61	PRO
3	M	218	GLN
1	P	118	PRO
4	U	87	LEU
2	H	229	VAL
2	B	145	ALA
3	M	18	GLY

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Mol	Chain	Res	Type
2	Q	150	PRO
1	F	59	GLY
2	H	75	PRO
1	P	120	PRO
2	H	179	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	A	162/183 (88%)	156 (96%)	6 (4%)	41 75
1	F	165/183 (90%)	158 (96%)	7 (4%)	36 72
1	G	175/183 (96%)	165 (94%)	10 (6%)	25 65
1	P	157/183 (86%)	151 (96%)	6 (4%)	40 74
2	B	201/217 (93%)	192 (96%)	9 (4%)	34 71
2	H	204/217 (94%)	198 (97%)	6 (3%)	50 79
2	L	205/217 (94%)	198 (97%)	7 (3%)	44 77
2	Q	198/217 (91%)	191 (96%)	7 (4%)	43 76
3	C	205/232 (88%)	198 (97%)	7 (3%)	44 77
3	I	206/232 (89%)	189 (92%)	17 (8%)	14 51
3	M	203/232 (88%)	194 (96%)	9 (4%)	35 71
3	R	201/232 (87%)	194 (96%)	7 (4%)	43 76
4	D	87/95 (92%)	78 (90%)	9 (10%)	9 40
4	J	85/95 (90%)	75 (88%)	10 (12%)	6 35
4	N	70/95 (74%)	65 (93%)	5 (7%)	18 58
4	U	87/95 (92%)	83 (95%)	4 (5%)	33 70
5	E	7/7 (100%)	7 (100%)	0	100 100
5	K	7/7 (100%)	7 (100%)	0	100 100
5	O	7/7 (100%)	7 (100%)	0	100 100
5	T	7/7 (100%)	6 (86%)	1 (14%)	4 28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2639/2936 (90%)	2512 (95%)	127 (5%)	31 69

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	9	GLN
1	G	19	VAL
1	G	31	THR
1	G	71	ASP
1	G	74	LEU
1	G	95	SER
1	G	96	SER
1	G	133	LYS
1	G	180	ASN
1	G	201	PHE
2	H	62	GLU
2	H	191	ARG
2	H	204	ASN
2	H	216	SER
2	H	217	GLU
2	H	224	ASP
3	I	13	SER
3	I	34	VAL
3	I	66	LYS
3	I	68	LYS
3	I	75	ARG
3	I	87	GLN
3	I	89	GLU
3	I	119	ASP
3	I	142	THR
3	I	146	LYS
3	I	180	GLN
3	I	207	SER
3	I	213	ILE
3	I	238	ASP
3	I	258	THR
3	I	263	HIS
3	I	273	ARG
4	J	3	ARG
4	J	31	HIS
4	J	39	LEU
4	J	45	ARG

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Mol	Chain	Res	Type
4	J	48	LYS
4	J	69	GLU
4	J	74	GLU
4	J	77	GLU
4	J	78	TYR
4	J	91	LYS
1	A	9	GLN
1	A	58	ASN
1	A	149	GLN
1	A	156	TYR
1	A	180	ASN
1	A	184	PHE
2	B	25	GLN
2	B	29	HIS
2	B	127	GLU
2	B	136	THR
2	B	149	TYR
2	B	150	PRO
2	B	181	LEU
2	B	223	GLN
2	B	224	ASP
3	C	42	SER
3	C	155	GLN
3	C	170	ARG
3	C	203	CYS
3	C	213	ILE
3	C	214	THR
3	C	248	VAL
4	D	10	TYR
4	D	24	ASN
4	D	41	LYS
4	D	47	GLU
4	D	48	LYS
4	D	74	GLU
4	D	75	LYS
4	D	87	LEU
4	D	88	SER
1	F	61	LEU
1	F	72	SER
1	F	74	LEU
1	F	115	ILE
1	F	144	GLN

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Mol	Chain	Res	Type
1	F	150	SER
1	F	160	LYS
2	L	6	GLN
2	L	50	MET
2	L	93	SER
2	L	118	VAL
2	L	178	GLN
2	L	224	ASP
2	L	240	ARG
3	M	17	ARG
3	M	25	VAL
3	M	65	ARG
3	M	88	SER
3	M	93	HIS
3	M	145	HIS
3	M	216	THR
3	M	217	TRP
3	M	273	ARG
4	N	6	LYS
4	N	31	HIS
4	N	36	GLU
4	N	51	HIS
4	N	61	SER
1	P	18	ASP
1	P	74	LEU
1	P	100	LYS
1	P	125	LEU
1	P	136	CYS
1	P	161	CYS
2	Q	43	LEU
2	Q	82	SER
2	Q	115	LEU
2	Q	173	GLN
2	Q	193	ARG
2	Q	200	GLN
2	Q	215	LEU
3	R	2	SER
3	R	3	HIS
3	R	189	MET
3	R	203	CYS
3	R	210	PRO
3	R	228	THR

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Mol	Chain	Res	Type
3	R	259	CYS
4	U	45	ARG
4	U	49	VAL
4	U	75	LYS
4	U	89	GLN
5	T	7	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	180	ASN
2	H	29	HIS
2	H	182	ASN
3	I	114	HIS
3	I	141	GLN
3	I	151	HIS
3	I	155	GLN
4	J	89	GLN
1	A	9	GLN
1	A	149	GLN
2	B	7	ASN
3	C	192	HIS
3	C	260	HIS
2	L	25	GLN
2	L	29	HIS
4	N	42	ASN
4	N	84	HIS
1	P	6	GLN
2	Q	152	HIS
2	Q	165	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	196/208 (94%)	-0.62	1 (0%) 91 88	57, 111, 150, 165	0
1	F	198/208 (95%)	-0.76	0 100 100	57, 94, 135, 145	0
1	G	201/208 (96%)	-0.79	0 100 100	50, 92, 133, 156	0
1	P	191/208 (91%)	-0.65	0 100 100	60, 101, 146, 158	0
2	B	241/243 (99%)	-0.77	0 100 100	61, 99, 139, 160	0
2	H	239/243 (98%)	-0.72	0 100 100	65, 92, 132, 144	0
2	L	242/243 (99%)	-0.76	0 100 100	70, 91, 131, 165	0
2	Q	238/243 (97%)	-0.69	0 100 100	77, 102, 130, 151	0
3	C	258/276 (93%)	-0.66	1 (0%) 93 90	74, 110, 154, 176	0
3	I	261/276 (94%)	-0.69	0 100 100	91, 119, 150, 182	0
3	M	268/276 (97%)	-0.67	0 100 100	83, 122, 159, 176	0
3	R	251/276 (90%)	-0.68	0 100 100	72, 106, 145, 152	0
4	D	97/100 (97%)	-0.59	1 (1%) 84 77	84, 127, 157, 167	0
4	J	96/100 (96%)	-0.74	0 100 100	106, 135, 164, 170	0
4	N	92/100 (92%)	-0.68	0 100 100	100, 136, 168, 174	0
4	U	99/100 (99%)	-0.78	0 100 100	79, 130, 151, 174	0
5	E	9/9 (100%)	-0.71	0 100 100	80, 83, 89, 92	0
5	K	9/9 (100%)	-0.57	0 100 100	91, 97, 103, 106	0
5	O	9/9 (100%)	-0.42	0 100 100	87, 104, 113, 114	0
5	T	9/9 (100%)	-0.52	0 100 100	78, 83, 90, 91	0
All	All	3204/3344 (95%)	-0.70	3 (0%) 95 95	50, 107, 149, 182	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	244	TRP	2.2
4	D	99	MET	2.2
1	A	137	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.