



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 16, 2026 – 10:23 AM UTC

PDB ID : 1ZGL / pdb_00001zgl
Title : Crystal structure of 3A6 TCR bound to MBP/HLA-DR2a
Authors : Li, Y.; Huang, Y.; Lue, J.; Quandt, J.A.; Martin, R.; Mariuzza, R.A.
Deposited on : 2005-04-21
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

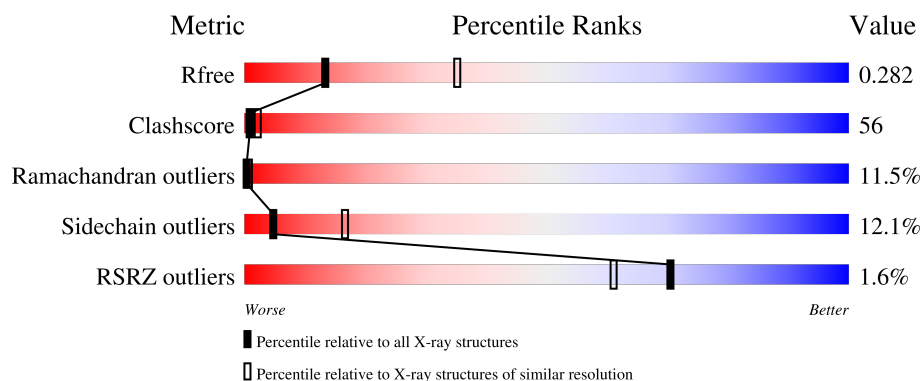
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	181	2% 33% 53% 12%
1	D	181	% 42% 44% 10%
1	G	181	37% 50% 10%
1	J	181	35% 50% 12%
2	B	192	% 36% 43% 9% 9%

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Mol	Chain	Length	Quality of chain
2	E	192	
2	H	192	
2	K	192	
3	C	15	
3	F	15	
3	I	15	
3	L	15	
4	M	209	
4	Q	209	
4	S	209	
4	U	209	
5	P	249	
5	R	249	
5	T	249	
5	V	249	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23456 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HLA class II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1362	887	224	246	5			
1	D	178	Total	C	N	O	S	0	0	0
			1366	889	224	248	5			
1	G	178	Total	C	N	O	S	0	0	0
			1362	887	224	246	5			
1	J	178	Total	C	N	O	S	0	0	0
			1366	889	224	248	5			

- Molecule 2 is a protein called major histocompatibility complex, class II, DR beta 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	8	0	0
			1319	831	234	250	4			
2	E	175	Total	C	N	O	S	0	0	0
			1307	823	230	250	4			
2	H	168	Total	C	N	O	S	0	0	0
			1284	811	226	243	4			
2	K	180	Total	C	N	O	S	5	0	0
			1347	851	235	257	4			

- Molecule 3 is a protein called Myelin basic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	14	Total	C	N	O	0	0	0
			114	76	21	17			
3	F	15	Total	C	N	O	0	0	0
			119	78	22	19			
3	I	13	Total	C	N	O	0	0	0
			107	71	20	16			
3	L	14	Total	C	N	O	0	0	0
			114	76	21	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	14	GLY	-	cloning artifact	UNP Q6AI64
C	15	GLY	-	cloning artifact	UNP Q6AI64
F	14	GLY	-	cloning artifact	UNP Q6AI64
F	15	GLY	-	cloning artifact	UNP Q6AI64
I	14	GLY	-	cloning artifact	UNP Q6AI64
I	15	GLY	-	cloning artifact	UNP Q6AI64
L	14	GLY	-	cloning artifact	UNP Q6AI64
L	15	GLY	-	cloning artifact	UNP Q6AI64

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	178	Total	C	N	O	S	0	0	0
			1268	800	206	258	4			
4	Q	187	Total	C	N	O	S	0	0	0
			1331	835	218	271	7			
4	S	176	Total	C	N	O	S	0	0	0
			1231	770	204	253	4			
4	U	195	Total	C	N	O	S	0	0	0
			1356	850	224	276	6			

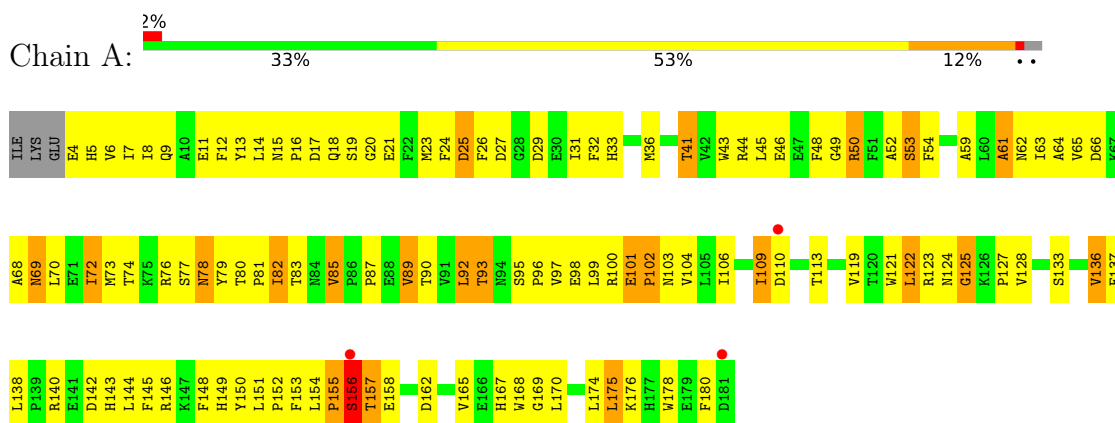
- Molecule 5 is a protein called T cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	242	Total	C	N	O	S	0	0	0
			1813	1135	322	351	5			
5	R	238	Total	C	N	O	S	0	0	0
			1790	1118	321	346	5			
5	T	226	Total	C	N	O	S	0	0	0
			1657	1037	294	321	5			
5	V	242	Total	C	N	O	S	0	0	0
			1843	1156	324	358	5			

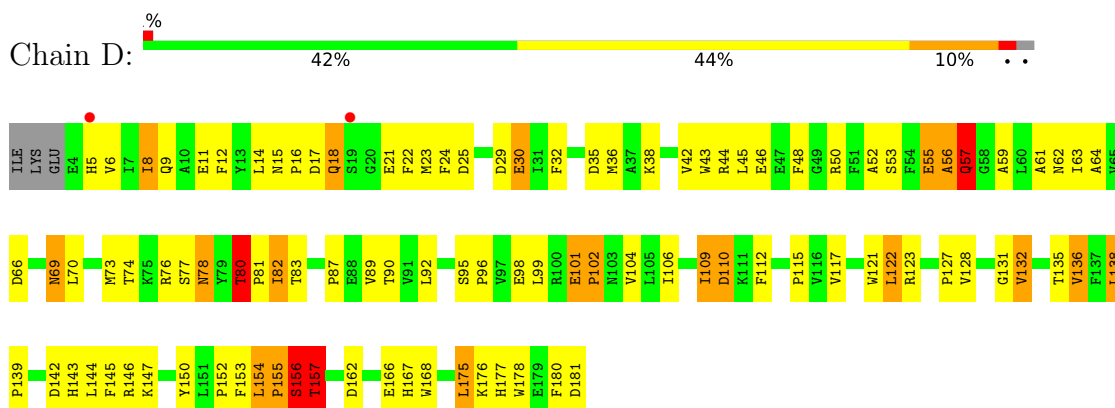
3 Residue-property plots

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

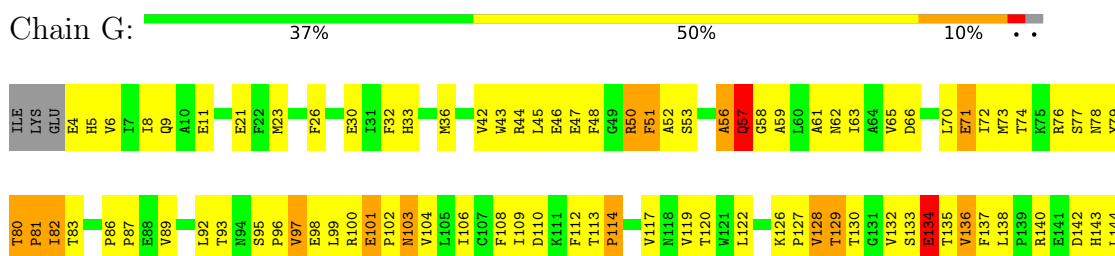
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

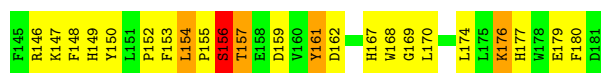


- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



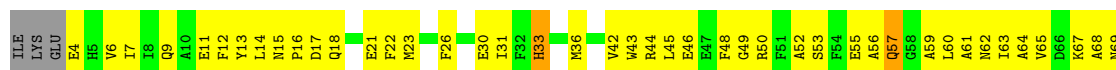
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain





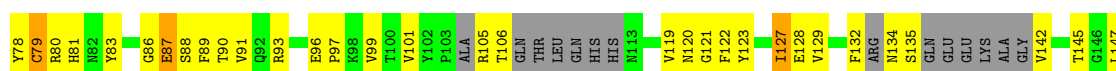
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain J: 35% 50% 12% ..



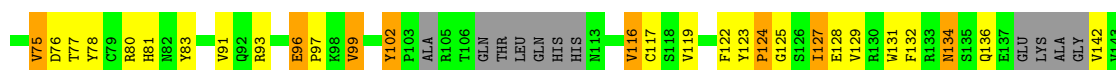
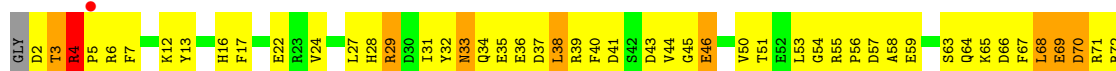
- Molecule 2: major histocompatibility complex, class II, DR beta 5

Chain B: 36% 43% 9% . 9%



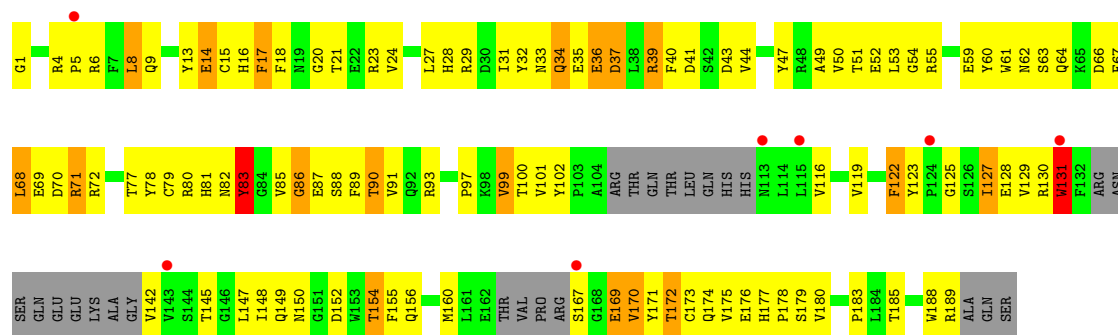
- Molecule 2: major histocompatibility complex, class II, DR beta 5

Chain E: 38% 43% 10% . 9%

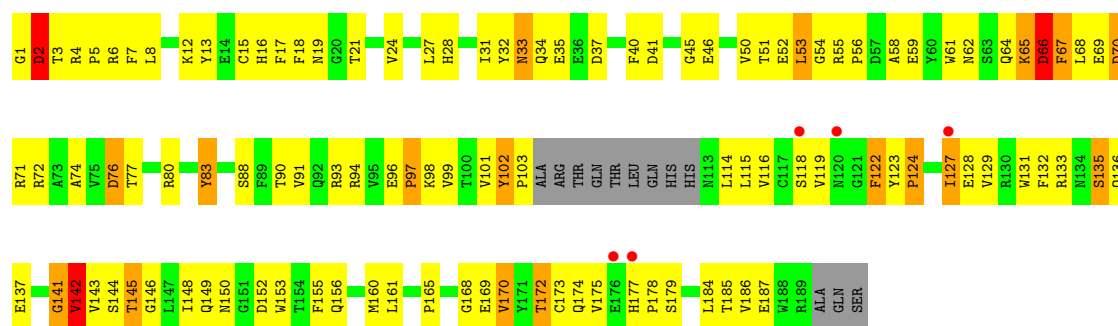


- Molecule 2: major histocompatibility complex, class II, DR beta 5

Chain H: 4% 30% 47% 9% . 12%



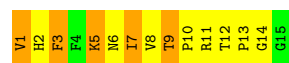
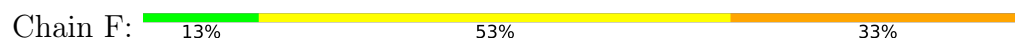
- Molecule 2: major histocompatibility complex, class II, DR beta 5



- Molecule 3: Myelin basic protein



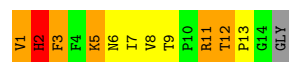
- Molecule 3: Myelin basic protein



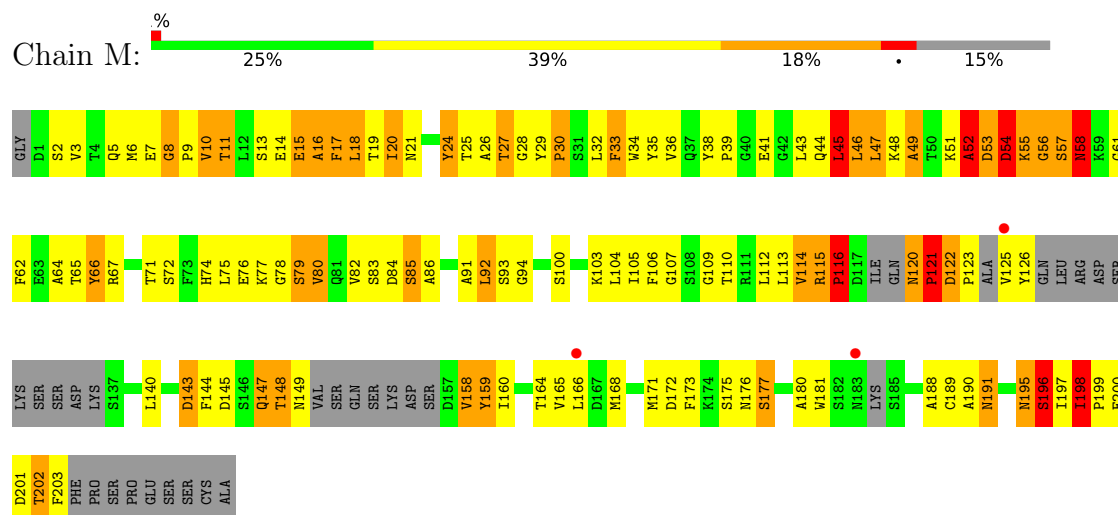
- Molecule 3: Myelin basic protein



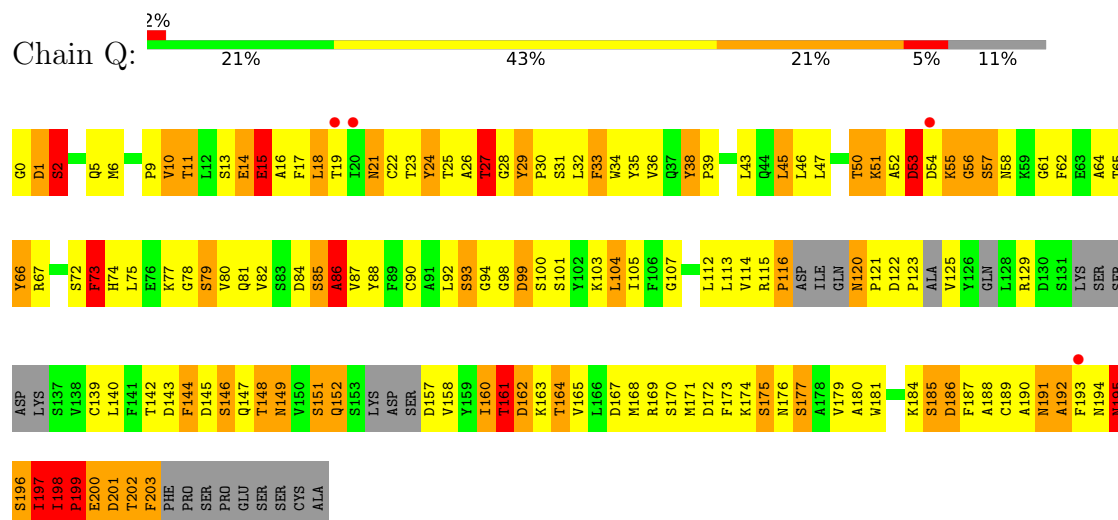
- Molecule 3: Myelin basic protein



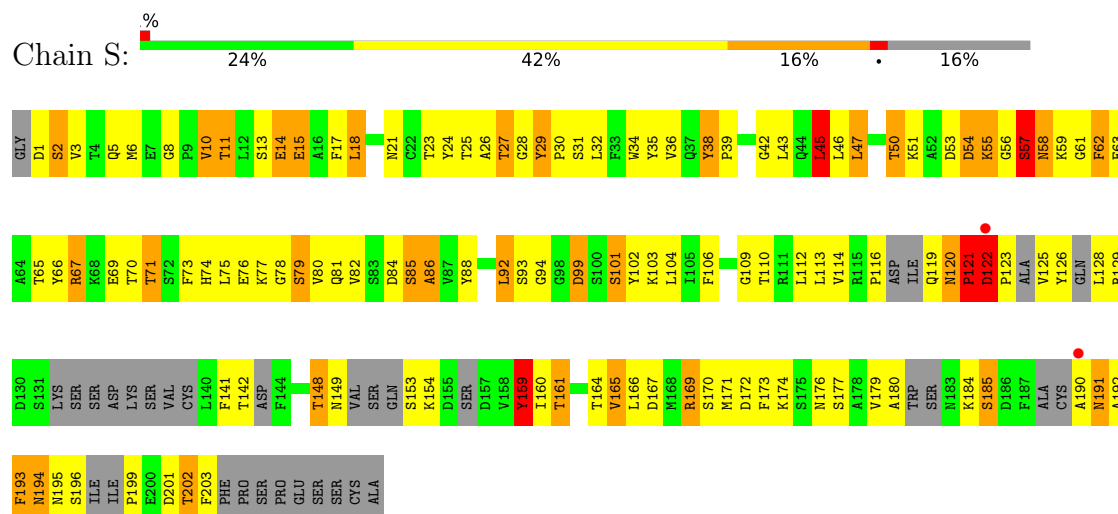
• Molecule 4: T cell receptor alpha chain



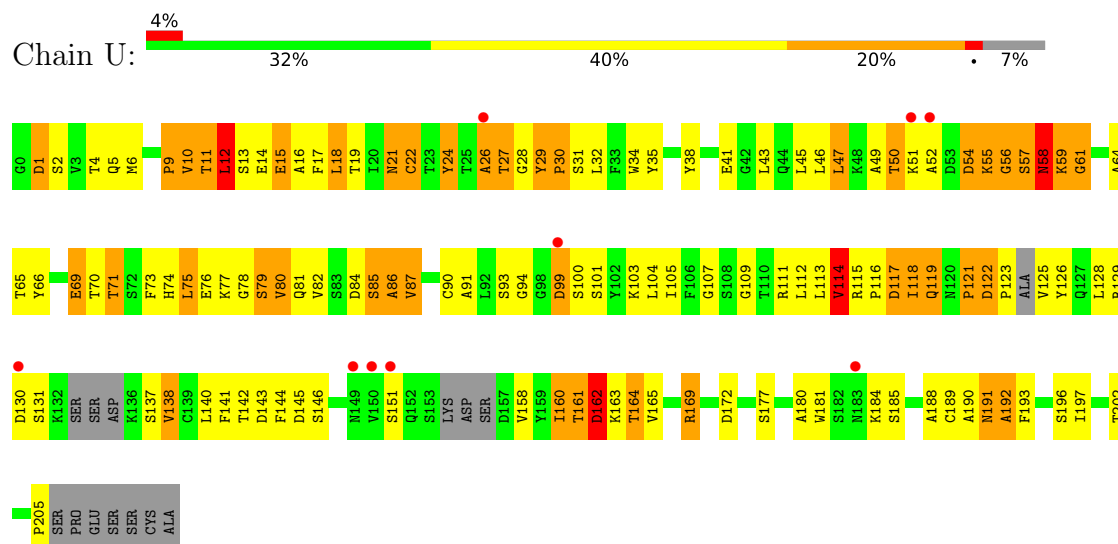
• Molecule 4: T cell receptor alpha chain



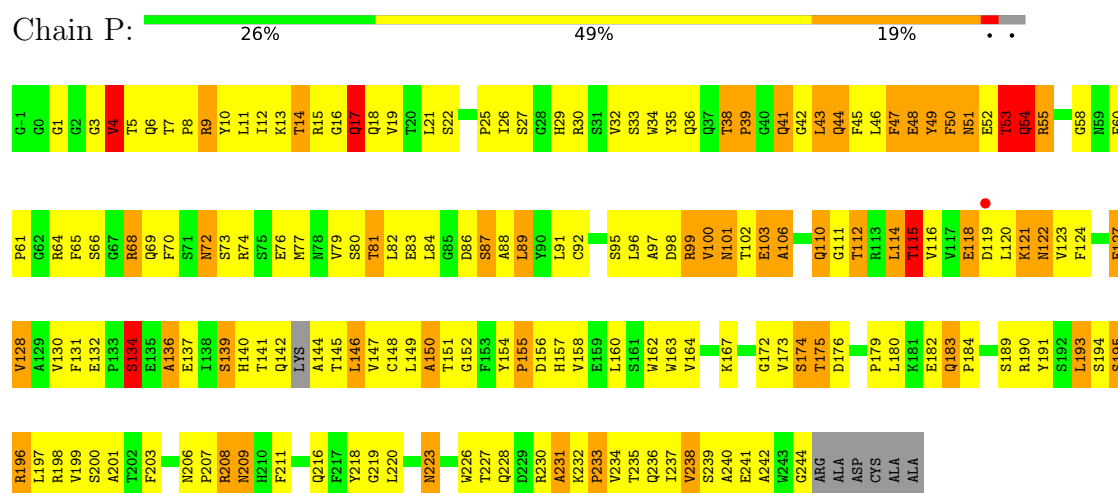
• Molecule 4: T cell receptor alpha chain



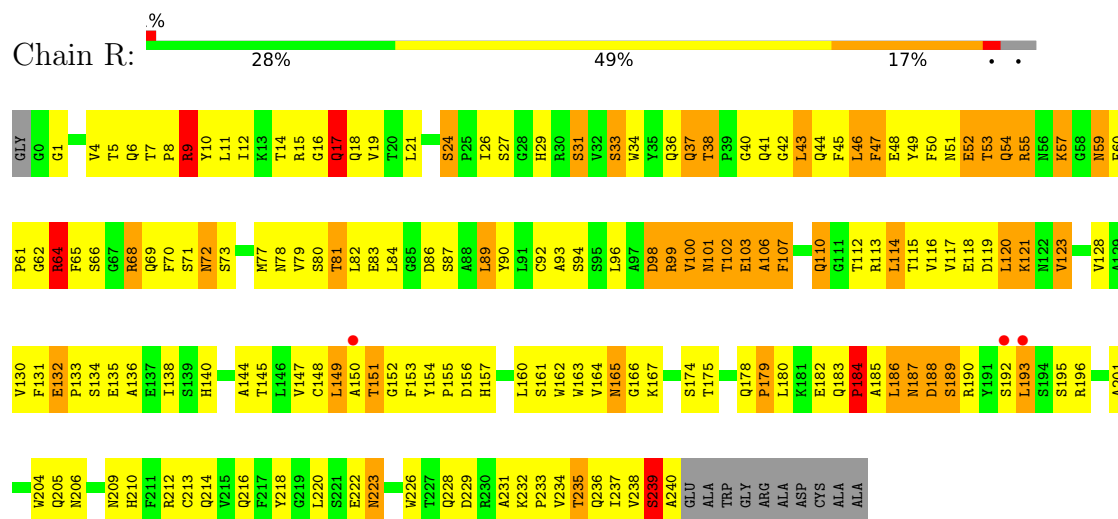
- Molecule 4: T cell receptor alpha chain



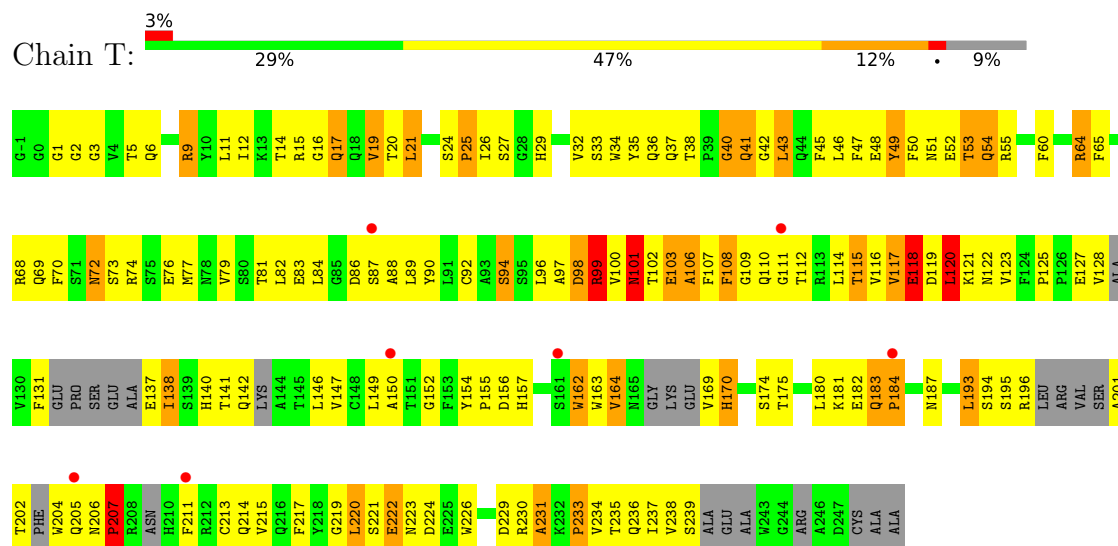
- Molecule 5: T cell receptor beta chain



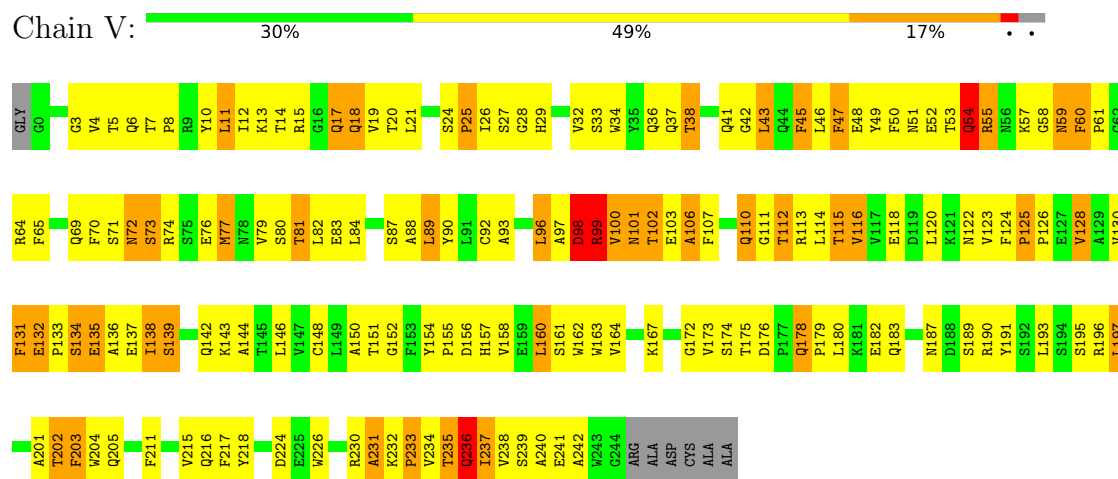
- Molecule 5: T cell receptor beta chain



- Molecule 5: T cell receptor beta chain



- Molecule 5: T cell receptor beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	96.48Å 97.69Å 124.02Å 74.39° 83.19° 61.55°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	86.4 (30.00-2.80) 86.4 (30.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.280 , 0.329 0.287 , 0.282	Depositor DCC
R_{free} test set	5144 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 85.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h-k,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	23456	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.56	0/1406	1.11	12/1930 (0.6%)
1	D	0.54	0/1410	1.14	13/1935 (0.7%)
1	G	0.57	0/1406	1.12	11/1930 (0.6%)
1	J	0.50	0/1410	1.07	8/1935 (0.4%)
2	B	0.59	0/1350	1.13	12/1843 (0.7%)
2	E	0.53	0/1337	1.13	10/1827 (0.5%)
2	H	0.53	0/1316	1.04	12/1796 (0.7%)
2	K	0.51	0/1382	1.10	14/1891 (0.7%)
3	C	0.60	0/118	1.21	1/160 (0.6%)
3	F	0.63	0/123	1.21	1/165 (0.6%)
3	I	0.63	0/111	1.25	0/150
3	L	0.61	0/118	1.16	0/160
4	M	0.55	0/1291	1.09	11/1759 (0.6%)
4	Q	0.62	0/1355	1.20	18/1844 (1.0%)
4	S	0.54	0/1244	1.09	9/1684 (0.5%)
4	U	0.60	0/1380	1.19	15/1885 (0.8%)
5	P	0.59	2/1860 (0.1%)	1.16	25/2538 (1.0%)
5	R	0.59	2/1835 (0.1%)	1.12	18/2505 (0.7%)
5	T	0.60	2/1691 (0.1%)	1.09	7/2297 (0.3%)
5	V	1.72	4/1892 (0.2%)	1.47	28/2580 (1.1%)
All	All	0.73	10/24035 (0.0%)	1.15	225/32814 (0.7%)

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
5	P	0	1
5	T	0	1
5	V	0	1
All	All	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	V	132	GLU	CD-OE2	67.38	2.53	1.25
5	V	132	GLU	CD-OE1	14.91	1.53	1.25
5	V	33	SER	CB-OG	5.82	1.53	1.42
5	T	193	LEU	CB-CG	-5.78	1.41	1.53
5	T	33	SER	CB-OG	5.72	1.53	1.42
5	V	193	LEU	CB-CG	-5.72	1.42	1.53
5	R	33	SER	CB-OG	5.64	1.53	1.42
5	R	193	LEU	CB-CG	-5.60	1.42	1.53
5	P	193	LEU	CB-CG	-5.34	1.42	1.53
5	P	33	SER	CB-OG	5.32	1.52	1.42

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	V	132	GLU	OE1-CD-OE2	-37.43	33.07	122.90
5	V	100	VAL	N-CA-C	-12.81	93.06	109.58
4	U	161	THR	N-CA-C	12.30	123.94	108.45
5	R	100	VAL	N-CA-C	-12.02	94.27	109.30
5	V	132	GLU	CG-CD-OE2	-11.71	91.46	118.40
2	E	66	ASP	N-CA-C	-11.25	98.22	113.18
2	B	66	ASP	N-CA-C	-10.75	98.88	113.18
5	P	41	GLN	N-CA-C	-9.74	90.05	110.80
5	V	236	GLN	N-CA-C	9.72	116.75	108.78
4	S	54	ASP	N-CA-C	-9.50	101.24	113.12
4	Q	202	THR	N-CA-C	-9.18	95.45	109.96
5	R	135	GLU	N-CA-C	-8.96	102.75	114.31
5	T	183	GLN	CA-C-N	8.79	130.83	119.84
5	T	183	GLN	C-N-CA	8.79	130.83	119.84
1	D	80	THR	CA-C-N	8.56	128.43	120.21
1	D	80	THR	C-N-CA	8.56	128.43	120.21
1	D	157	THR	N-CA-C	-8.41	92.88	110.80
2	B	163	THR	N-CA-C	8.39	128.66	110.80
5	P	98	ASP	N-CA-C	8.08	120.00	111.03
4	Q	24	TYR	N-CA-C	8.04	117.73	108.49
5	R	99	ARG	N-CA-C	8.03	121.59	110.35
4	Q	161	THR	N-CA-C	8.02	127.89	110.80
4	Q	198	ILE	N-CA-C	7.92	125.98	108.88
1	D	154	LEU	CA-C-N	7.72	129.49	119.84
1	D	154	LEU	C-N-CA	7.72	129.49	119.84
2	B	4	ARG	N-CA-C	7.67	126.75	109.81
2	B	165	PRO	N-CA-CB	7.67	111.30	103.25
5	V	24	SER	CA-C-N	7.52	129.24	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	V	24	SER	C-N-CA	7.52	129.24	119.84
5	R	183	GLN	CA-C-N	7.44	129.14	119.84
5	R	183	GLN	C-N-CA	7.44	129.14	119.84
1	G	154	LEU	CA-C-N	7.34	129.02	119.84
1	G	154	LEU	C-N-CA	7.34	129.02	119.84
2	K	66	ASP	N-CA-C	-7.28	95.30	110.80
4	U	116	PRO	N-CA-CB	7.27	109.78	103.31
5	P	118	GLU	N-CA-C	-7.26	102.39	111.11
5	V	128	VAL	N-CA-C	7.25	118.41	108.84
2	B	167	SER	N-CA-C	-7.22	95.42	110.80
1	A	85	VAL	CA-C-N	7.21	127.81	120.38
1	A	85	VAL	C-N-CA	7.21	127.81	120.38
2	H	99	VAL	N-CA-C	7.20	119.48	109.55
1	J	154	LEU	CA-C-N	7.14	128.77	119.84
1	J	154	LEU	C-N-CA	7.14	128.77	119.84
5	V	152	GLY	N-CA-C	7.12	123.88	113.48
4	Q	73	PHE	N-CA-C	-7.07	96.75	108.34
5	P	122	ASN	N-CA-C	-7.01	104.53	113.23
4	Q	23	THR	N-CA-C	-7.01	99.08	109.81
5	P	53	THR	N-CA-C	7.00	120.26	111.24
2	E	179	SER	N-CA-C	-6.92	104.73	113.72
5	R	103	GLU	N-CA-C	-6.90	96.11	110.80
5	V	183	GLN	CA-C-N	6.89	127.18	119.32
5	V	183	GLN	C-N-CA	6.89	127.18	119.32
5	P	158	VAL	N-CA-C	6.81	120.19	108.95
2	K	67	PHE	N-CA-C	-6.78	103.03	112.45
5	P	239	SER	N-CA-C	6.77	116.80	107.73
4	U	205	PRO	N-CA-CB	6.71	110.38	103.00
2	B	67	PHE	N-CA-C	-6.70	103.45	111.69
1	G	179	GLU	N-CA-C	-6.70	99.37	109.96
5	P	14	THR	N-CA-C	6.61	120.83	110.32
3	C	3	PHE	N-CA-C	6.60	119.35	109.25
1	D	101	GLU	CA-C-N	6.58	128.07	119.84
1	D	101	GLU	C-N-CA	6.58	128.07	119.84
4	U	162	ASP	N-CA-C	6.58	124.82	110.80
4	M	24	TYR	N-CA-C	6.58	116.68	108.19
4	M	199	PRO	N-CA-C	-6.57	103.58	114.75
4	Q	29	TYR	CA-C-N	6.57	128.05	119.84
4	Q	29	TYR	C-N-CA	6.57	128.05	119.84
2	E	68	LEU	N-CA-C	-6.56	104.05	111.07
1	D	8	ILE	N-CA-C	6.55	117.27	108.11
1	G	114	PRO	CA-C-N	6.52	127.99	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	114	PRO	C-N-CA	6.52	127.99	119.84
4	U	86	ALA	N-CA-C	6.48	121.25	109.32
5	P	114	LEU	N-CA-C	6.45	121.04	111.04
4	S	45	LEU	N-CA-C	-6.40	102.08	110.53
4	U	24	TYR	N-CA-C	6.38	116.50	108.45
4	U	2	SER	N-CA-C	6.37	119.39	109.52
5	V	132	GLU	CA-C-N	6.35	126.38	119.90
5	V	132	GLU	C-N-CA	6.35	126.38	119.90
5	P	238	VAL	N-CA-C	-6.32	103.16	110.05
1	J	150	TYR	N-CA-C	6.31	118.70	108.41
2	E	116	VAL	N-CA-C	6.30	116.94	108.11
2	E	3	THR	N-CA-C	-6.29	97.40	110.80
2	E	165	PRO	N-CA-CB	6.28	109.91	103.00
4	S	116	PRO	N-CA-CB	6.27	109.90	103.00
4	S	199	PRO	N-CA-CB	6.27	109.90	103.00
2	K	165	PRO	N-CA-CB	6.27	109.83	103.25
5	P	100	VAL	N-CA-C	-6.24	98.56	107.98
5	P	136	ALA	N-CA-C	-6.21	104.51	111.28
4	M	147	GLN	N-CA-C	-6.21	105.86	113.50
2	E	4	ARG	N-CA-C	6.15	123.41	109.81
1	A	122	LEU	N-CA-C	6.15	120.11	107.37
5	V	151	THR	N-CA-C	6.14	119.55	110.46
2	H	72	ARG	N-CA-C	-6.06	104.31	111.03
1	D	110	ASP	CA-CB-CG	6.01	118.61	112.60
1	G	97	VAL	N-CA-C	5.99	116.31	107.15
4	M	116	PRO	N-CA-CB	5.94	109.49	103.25
4	Q	50	THR	N-CA-C	5.93	121.25	113.30
2	K	83	TYR	N-CA-C	-5.92	104.00	111.11
4	M	198	ILE	N-CA-C	5.91	121.65	108.88
4	Q	36	VAL	N-CA-C	5.85	116.58	107.28
1	G	156	SER	N-CA-C	5.82	123.20	110.80
4	U	86	ALA	CB-CA-C	-5.80	108.88	115.79
4	Q	116	PRO	N-CA-CB	5.80	109.38	103.00
4	Q	151	SER	N-CA-C	5.80	118.38	110.55
4	M	58	ASN	N-CA-C	-5.78	98.49	110.80
5	R	151	THR	N-CA-C	5.77	119.12	109.95
4	S	159	TYR	N-CA-C	5.76	118.06	109.59
5	P	99	ARG	N-CA-C	5.76	118.18	110.35
5	P	87	SER	N-CA-C	-5.74	101.15	109.59
1	A	61	ALA	N-CA-C	-5.73	105.11	111.36
2	H	79	CYS	N-CA-C	5.73	117.61	111.36
5	V	98	ASP	N-CA-C	-5.72	98.62	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	179	SER	N-CA-C	-5.71	106.14	113.23
2	K	96	GLU	CA-C-N	5.71	126.98	119.84
2	K	96	GLU	C-N-CA	5.71	126.98	119.84
1	G	101	GLU	CA-C-N	5.71	126.97	119.84
1	G	101	GLU	C-N-CA	5.71	126.97	119.84
4	M	45	LEU	N-CA-C	-5.69	102.06	110.48
4	U	29	TYR	CA-C-N	5.62	126.87	119.84
4	U	29	TYR	C-N-CA	5.62	126.87	119.84
4	Q	200	GLU	N-CA-C	5.62	120.29	113.38
2	K	99	VAL	N-CA-C	5.61	117.27	109.80
2	B	188	TRP	N-CA-C	5.61	117.79	108.20
5	V	187	ASN	N-CA-C	5.60	118.15	111.71
1	D	156	SER	N-CA-C	5.59	122.70	110.80
5	R	132	GLU	N-CA-C	5.58	117.60	109.84
2	H	14	GLU	N-CA-C	5.58	118.58	109.59
2	K	142	VAL	N-CA-C	5.57	120.92	109.34
4	Q	160	ILE	N-CA-C	5.56	120.90	109.34
4	U	151	SER	N-CA-C	5.55	119.54	109.32
5	R	110	GLN	N-CA-C	5.55	119.53	112.87
5	V	136	ALA	N-CA-C	-5.55	105.31	111.36
5	V	57	LYS	N-CA-C	5.54	119.88	113.18
4	M	202	THR	N-CA-C	-5.53	102.28	110.46
5	P	183	GLN	CA-C-N	5.52	126.74	119.84
5	P	183	GLN	C-N-CA	5.52	126.74	119.84
5	T	99	ARG	N-CA-C	5.51	122.54	110.80
2	K	122	PHE	N-CA-C	5.49	118.51	109.72
5	P	132	GLU	N-CA-C	5.49	116.99	110.07
5	V	178	GLN	CA-C-N	5.49	125.95	120.52
5	V	178	GLN	C-N-CA	5.49	125.95	120.52
5	R	24	SER	CA-C-N	5.48	126.25	120.11
5	R	24	SER	C-N-CA	5.48	126.25	120.11
5	P	134	SER	N-CA-C	5.45	122.42	110.80
1	A	89	VAL	N-CA-C	5.45	117.18	108.89
2	E	29	ARG	N-CA-C	5.44	117.28	108.41
3	F	3	PHE	N-CA-C	5.44	118.11	109.96
5	R	102	THR	N-CA-C	5.42	118.09	110.23
1	G	86	PRO	CA-C-N	5.42	125.18	119.76
1	G	86	PRO	C-N-CA	5.42	125.18	119.76
2	H	86	GLY	N-CA-C	5.42	124.39	115.34
1	J	156	SER	N-CA-C	5.41	122.33	110.80
1	J	114	PRO	CA-C-N	5.40	126.59	119.84
1	J	114	PRO	C-N-CA	5.40	126.59	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	V	99	ARG	N-CA-C	5.39	122.29	110.80
5	R	57	LYS	N-CA-C	5.39	118.07	111.82
4	U	138	VAL	N-CA-C	5.38	116.41	108.45
2	H	131	TRP	N-CA-C	5.36	118.43	109.96
2	K	175	VAL	N-CA-C	5.36	115.30	107.37
2	B	29	ARG	N-CA-C	5.35	117.14	108.41
4	M	46	LEU	N-CA-C	-5.35	104.95	112.12
5	P	121	LYS	N-CA-C	-5.35	104.88	113.28
1	A	7	ILE	CB-CA-C	-5.32	104.07	110.99
1	A	31	ILE	CB-CA-C	-5.32	104.88	112.22
4	S	29	TYR	CA-C-N	5.32	126.06	120.11
4	S	29	TYR	C-N-CA	5.32	126.06	120.11
4	M	114	VAL	N-CA-C	5.30	117.72	111.09
2	H	102	TYR	N-CA-C	5.30	112.99	108.22
5	V	45	PHE	N-CA-C	5.30	117.91	110.23
5	P	103	GLU	N-CA-C	-5.29	99.53	110.80
5	R	136	ALA	N-CA-C	-5.29	105.16	111.03
1	A	8	ILE	N-CA-C	5.29	116.19	108.53
5	P	132	GLU	CA-C-N	5.27	126.43	119.84
5	P	132	GLU	C-N-CA	5.27	126.43	119.84
1	D	81	PRO	N-CA-C	5.26	118.58	111.22
2	B	152	ASP	N-CA-C	-5.26	107.40	112.97
4	S	122	ASP	N-CA-C	5.25	121.42	109.81
4	M	52	ALA	N-CA-C	-5.25	99.62	110.80
1	A	156	SER	N-CA-C	5.24	121.97	110.80
4	Q	143	ASP	N-CA-C	5.24	121.96	110.80
2	H	122	PHE	N-CA-C	5.24	118.54	110.42
4	S	23	THR	N-CA-C	-5.24	102.15	109.69
1	A	101	GLU	CA-C-N	5.23	126.38	119.84
1	A	101	GLU	C-N-CA	5.23	126.38	119.84
5	V	125	PRO	CA-C-N	5.23	125.21	120.03
5	V	125	PRO	C-N-CA	5.23	125.21	120.03
5	R	123	VAL	N-CA-C	5.23	116.28	108.54
4	Q	86	ALA	N-CA-C	5.22	121.92	110.80
4	Q	197	ILE	N-CA-C	5.22	120.19	109.34
5	T	125	PRO	CA-C-N	5.21	126.36	119.84
5	T	125	PRO	C-N-CA	5.21	126.36	119.84
2	K	118	SER	N-CA-C	5.21	117.14	108.02
5	R	31	SER	N-CA-C	5.20	117.88	109.40
4	U	131	SER	N-CA-C	-5.20	106.71	113.16
1	J	97	VAL	N-CA-C	5.20	115.83	107.98
5	V	71	SER	N-CA-C	5.20	118.40	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	T	109	GLY	N-CA-C	-5.19	105.65	112.81
4	U	184	LYS	N-CA-C	5.18	117.25	109.23
5	V	102	THR	N-CA-C	5.17	117.16	109.25
2	E	134	ASN	N-CA-C	-5.16	99.80	110.80
2	K	172	THR	N-CA-C	5.15	117.50	109.52
5	R	86	ASP	N-CA-C	-5.14	106.94	114.39
2	K	152	ASP	N-CA-C	-5.14	105.30	112.03
2	H	102	TYR	CA-C-N	5.13	125.53	119.99
2	H	102	TYR	C-N-CA	5.13	125.53	119.99
5	P	50	PHE	N-CA-C	-5.11	100.56	108.42
2	B	161	LEU	CB-CA-C	-5.10	109.72	117.07
5	V	18	GLN	N-CA-C	5.10	118.06	109.95
1	D	122	LEU	N-CA-C	5.09	117.09	108.02
2	B	96	GLU	N-CA-C	5.09	116.08	109.72
2	H	17	PHE	N-CA-C	5.08	117.52	109.24
4	Q	2	SER	N-CA-C	5.07	121.60	110.80
5	P	150	ALA	N-CA-C	-5.07	101.43	109.59
5	T	118	GLU	N-CA-C	-5.07	104.83	111.02
4	U	114	VAL	N-CA-C	5.07	115.06	107.51
5	V	138	ILE	N-CA-C	-5.06	104.76	111.09
5	V	11	LEU	N-CA-C	5.05	116.65	108.26
2	E	96	GLU	N-CA-C	5.04	116.42	110.07
5	R	239	SER	N-CA-C	5.04	115.80	108.14
1	J	122	LEU	N-CA-C	5.04	117.17	107.44
2	K	50	VAL	N-CA-C	-5.03	104.80	111.09
2	H	83	TYR	N-CA-C	-5.03	105.80	111.28
1	D	175	LEU	N-CA-C	5.01	116.69	108.52
5	P	39	PRO	N-CA-C	-5.01	107.69	114.80
1	A	155	PRO	N-CA-C	5.00	122.78	112.47

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	P	49	TYR	Sidechain
5	T	49	TYR	Sidechain
5	V	132	GLU	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1362	0	1227	126	0
1	D	1366	0	1231	105	0
1	G	1362	0	1227	127	0
1	J	1366	0	1231	128	0
2	B	1319	0	1134	145	0
2	E	1307	0	1111	122	0
2	H	1284	0	1119	133	0
2	K	1347	0	1154	138	0
3	C	114	0	119	28	0
3	F	119	0	122	46	0
3	I	107	0	107	28	0
3	L	114	0	119	25	0
4	M	1268	0	1072	182	0
4	Q	1331	0	1116	189	0
4	S	1231	0	1037	171	0
4	U	1356	0	1112	153	0
5	P	1813	0	1629	218	0
5	R	1790	0	1629	221	0
5	T	1657	0	1440	221	0
5	V	1843	0	1674	207	0
All	All	23456	0	20610	2455	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 56.

All (2455) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:82:VAL:HA	4:M:114:VAL:HG11	1.24	1.20
4:M:26:ALA:HB1	4:M:30:PRO:HG2	1.18	1.17
4:S:26:ALA:HB1	4:S:30:PRO:HG2	1.21	1.16
2:B:71:ARG:HH12	3:C:9:THR:HB	1.12	1.14
4:Q:120:ASN:HB3	4:Q:121:PRO:HD2	1.25	1.14
4:S:120:ASN:H	4:S:121:PRO:HD3	0.97	1.13
5:R:160:LEU:HD23	5:R:161:SER:H	1.16	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:46:LEU:HD12	4:U:58:ASN:ND2	1.66	1.09
4:M:120:ASN:HB3	4:M:121:PRO:HD2	1.28	1.08
4:S:120:ASN:H	4:S:121:PRO:CD	1.65	1.08
4:M:77:LYS:HE3	4:M:80:VAL:HB	1.34	1.08
4:Q:26:ALA:HB1	4:Q:30:PRO:HG2	1.36	1.06
4:M:120:ASN:HB3	4:M:121:PRO:CD	1.86	1.05
4:U:46:LEU:HD12	4:U:58:ASN:HD22	0.91	1.05
2:H:129:VAL:HG22	2:H:175:VAL:HG22	1.39	1.03
1:A:110:ASP:HB2	1:A:146:ARG:HG2	1.39	1.03
5:T:89:LEU:HD21	5:T:111:GLY:HA3	1.38	1.03
4:U:26:ALA:HB1	4:U:30:PRO:HG2	1.40	1.03
3:C:1:VAL:HG12	4:M:27:THR:HG23	1.41	1.02
4:M:164:THR:HG22	4:M:165:VAL:H	1.25	1.01
4:M:123:PRO:HB2	4:M:198:ILE:CD1	1.89	1.00
4:U:12:LEU:HD11	4:U:80:VAL:HG11	1.01	1.00
2:K:71:ARG:HH12	3:L:9:THR:HB	1.19	1.00
5:P:87:SER:HB3	5:P:115:THR:HA	1.42	0.99
4:S:62:PHE:HD1	4:S:75:LEU:HD21	1.21	0.99
4:S:65:THR:HG21	4:S:67:ARG:NH2	1.78	0.98
2:E:127:ILE:HD13	2:E:128:GLU:N	1.78	0.98
4:U:12:LEU:CD1	4:U:80:VAL:HG11	1.94	0.97
2:B:81:HIS:ND1	4:M:28:GLY:HA3	1.78	0.97
5:R:121:LYS:HZ1	5:R:228:GLN:NE2	1.62	0.97
2:H:71:ARG:HH12	3:I:9:THR:HB	1.29	0.97
2:E:24:VAL:HG12	2:E:75:VAL:HG12	1.45	0.96
4:S:43:LEU:HD11	5:T:43:LEU:HD21	1.44	0.96
4:M:123:PRO:HB2	4:M:198:ILE:HD13	0.99	0.96
4:U:12:LEU:HD11	4:U:80:VAL:CG1	1.96	0.96
1:G:176:LYS:HE3	1:G:176:LYS:HA	1.49	0.95
2:H:1:GLY:HA3	2:H:4:ARG:HH21	1.30	0.95
2:K:127:ILE:HG12	2:K:177:HIS:HB2	1.47	0.95
4:U:118:ILE:HD12	4:U:145:ASP:HA	1.49	0.94
4:M:10:VAL:HG12	4:M:112:LEU:HA	1.47	0.94
4:Q:28:GLY:C	4:Q:30:PRO:HD3	1.91	0.94
2:B:174:GLN:HA	2:B:185:THR:HG22	1.49	0.94
5:T:1:GLY:H	5:T:5:THR:HG21	1.26	0.94
4:M:10:VAL:HG13	4:M:11:THR:H	1.31	0.93
5:R:72:ASN:HD22	5:R:72:ASN:H	1.09	0.93
4:U:10:VAL:HG11	4:U:112:LEU:HA	1.49	0.93
4:M:26:ALA:CB	4:M:30:PRO:HG2	1.97	0.93
1:A:96:PRO:HD3	2:B:120:ASN:ND2	1.83	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:55:LYS:CB	4:Q:64:ALA:H	1.81	0.92
5:V:113:ARG:HB3	5:V:157:HIS:CE1	2.04	0.92
5:R:102:THR:HG22	5:R:103:GLU:O	1.69	0.92
4:U:26:ALA:CB	4:U:30:PRO:HG2	1.99	0.92
5:T:14:THR:HG21	5:T:120:LEU:HD12	1.52	0.91
5:P:6:GLN:HE22	5:P:111:GLY:HA2	1.36	0.91
1:J:15:ASN:HB2	1:J:70:LEU:HD21	1.53	0.91
5:V:113:ARG:HB3	5:V:157:HIS:HE1	1.34	0.91
4:S:120:ASN:N	4:S:121:PRO:HD3	1.83	0.90
4:Q:191:ASN:H	4:Q:191:ASN:HD22	1.09	0.90
4:U:46:LEU:CD1	4:U:58:ASN:HD22	1.82	0.90
4:Q:120:ASN:HB3	4:Q:121:PRO:CD	2.02	0.90
5:T:163:TRP:HA	5:T:169:VAL:CB	2.02	0.90
5:P:6:GLN:NE2	5:P:111:GLY:HA2	1.86	0.90
1:A:89:VAL:HG22	1:A:109:ILE:HG23	1.53	0.90
4:S:26:ALA:CB	4:S:30:PRO:HG2	2.01	0.90
5:T:14:THR:H	5:T:17:GLN:NE2	1.69	0.90
5:T:1:GLY:N	5:T:5:THR:HG21	1.87	0.89
5:R:147:VAL:HG22	5:R:196:ARG:HG2	1.54	0.89
1:D:45:LEU:HD12	1:D:48:PHE:CZ	2.08	0.89
5:R:160:LEU:HD23	5:R:161:SER:N	1.88	0.89
4:U:1:ASP:HB2	4:U:99:ASP:OD1	1.72	0.89
4:M:11:THR:HA	4:M:113:LEU:O	1.72	0.89
4:M:10:VAL:CG1	4:M:11:THR:H	1.85	0.89
5:T:214:GLN:HA	5:T:239:SER:HB3	1.52	0.89
4:S:62:PHE:CD1	4:S:75:LEU:HD21	2.06	0.89
5:R:130:VAL:HG23	5:R:240:ALA:HB3	1.53	0.88
4:Q:202:THR:HG22	4:Q:203:PHE:H	1.37	0.88
1:G:154:LEU:HD12	1:G:155:PRO:HD2	1.54	0.88
5:V:118:GLU:HB2	5:V:122:ASN:HD21	1.36	0.88
2:B:127:ILE:HD11	2:B:175:VAL:HG13	1.53	0.88
1:D:29:ASP:HB3	2:E:153:TRP:NE1	1.89	0.88
5:R:12:ILE:HD11	5:R:155:PRO:HG3	1.55	0.88
4:M:82:VAL:HA	4:M:114:VAL:CG1	2.02	0.87
4:M:62:PHE:HB3	4:M:75:LEU:HD11	1.56	0.87
4:U:118:ILE:HD11	4:U:121:PRO:HB3	1.56	0.87
4:M:10:VAL:HG13	4:M:11:THR:N	1.88	0.87
5:P:21:LEU:HD22	5:P:77:MET:HE1	1.56	0.87
5:R:19:VAL:HG23	5:R:82:LEU:HD11	1.55	0.87
5:V:175:THR:HG23	5:V:195:SER:HB2	1.57	0.87
1:J:23:MET:HE2	1:J:30:GLU:HG3	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:232:LYS:O	5:V:234:VAL:HG13	1.74	0.86
1:D:14:LEU:HD12	2:E:7:PHE:O	1.73	0.86
5:T:9:ARG:HD3	5:T:9:ARG:H	1.39	0.86
2:B:4:ARG:HB2	2:B:5:PRO:HD3	1.57	0.86
2:B:164:VAL:HG22	2:B:165:PRO:N	1.89	0.86
5:V:100:VAL:O	5:V:101:ASN:HB2	1.75	0.86
5:T:49:TYR:CE2	5:T:54:GLN:HB2	2.11	0.85
5:R:9:ARG:HD3	5:R:10:TYR:H	1.37	0.85
4:M:14:GLU:O	4:M:15:GLU:HG2	1.76	0.85
4:S:119:GLN:HB2	4:S:121:PRO:HD3	1.58	0.85
4:S:121:PRO:C	4:S:123:PRO:HD3	2.01	0.85
2:E:177:HIS:CD2	2:E:178:PRO:HD2	2.12	0.85
5:T:68:ARG:NE	5:T:70:PHE:HE1	1.75	0.85
2:K:127:ILE:HD13	2:K:128:GLU:N	1.92	0.85
4:M:82:VAL:CA	4:M:114:VAL:HG11	2.07	0.85
2:H:174:GLN:HA	2:H:185:THR:HG22	1.56	0.84
4:U:43:LEU:HD11	5:V:43:LEU:HD21	1.57	0.84
2:H:97:PRO:HD3	2:H:179:SER:OG	1.77	0.84
5:T:154:TYR:CD1	5:T:155:PRO:HA	2.13	0.84
5:R:72:ASN:HD22	5:R:72:ASN:N	1.76	0.84
4:U:14:GLU:O	4:U:15:GLU:HB2	1.78	0.83
1:D:101:GLU:H	1:D:155:PRO:HG2	1.40	0.83
1:J:110:ASP:HB2	1:J:140:ARG:NH1	1.93	0.83
2:B:122:PHE:HE2	2:B:156:GLN:HA	1.43	0.83
4:U:11:THR:O	4:U:12:LEU:HB3	1.77	0.83
5:R:132:GLU:HG3	5:R:133:PRO:HD2	1.60	0.83
5:T:121:LYS:HD2	5:T:230:ARG:HH21	1.43	0.83
4:U:18:LEU:HD13	4:U:18:LEU:O	1.79	0.83
5:R:99:ARG:H	5:R:99:ARG:HD2	1.41	0.83
2:K:67:PHE:HA	5:V:99:ARG:HH21	1.43	0.83
1:J:101:GLU:H	1:J:155:PRO:CG	1.92	0.83
5:P:175:THR:HG23	5:P:195:SER:HB2	1.59	0.83
1:D:53:SER:O	3:F:3:PHE:HA	1.79	0.82
4:S:18:LEU:HD13	4:S:77:LYS:HB3	1.61	0.82
2:B:122:PHE:CE2	2:B:156:GLN:HA	2.14	0.82
4:M:123:PRO:CB	4:M:198:ILE:HD13	1.96	0.82
5:V:64:ARG:NH1	5:V:65:PHE:HE1	1.78	0.82
5:P:49:TYR:CZ	5:P:54:GLN:HG3	2.14	0.82
5:R:48:GLU:OE1	5:R:55:ARG:HD3	1.79	0.82
4:U:21:ASN:HA	4:U:74:HIS:CD2	2.13	0.82
1:A:96:PRO:HD3	2:B:120:ASN:HD21	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1:VAL:HG11	4:U:99:ASP:CG	2.04	0.82
4:M:35:TYR:HD1	4:M:45:LEU:HA	1.45	0.82
4:U:28:GLY:C	4:U:30:PRO:HD3	2.05	0.81
5:V:11:LEU:O	5:V:114:LEU:O	1.97	0.81
4:Q:198:ILE:HA	4:Q:201:ASP:OD2	1.81	0.81
1:G:5:HIS:NE2	2:H:91:VAL:HG13	1.96	0.81
4:S:54:ASP:HA	4:S:65:THR:HA	1.62	0.81
4:Q:123:PRO:O	4:Q:201:ASP:HA	1.81	0.81
1:A:41:THR:HG21	1:A:54:PHE:HB3	1.61	0.80
4:S:159:TYR:H	4:S:159:TYR:HD2	1.26	0.80
5:T:120:LEU:HD12	5:T:120:LEU:H	1.46	0.80
5:T:72:ASN:ND2	5:T:72:ASN:H	1.80	0.80
4:M:14:GLU:HB2	4:M:116:PRO:HA	1.62	0.80
2:E:13:TYR:OH	3:F:9:THR:HG22	1.82	0.80
5:V:49:TYR:CE2	5:V:54:GLN:HB2	2.15	0.80
4:M:28:GLY:C	4:M:30:PRO:HD3	2.07	0.80
5:P:19:VAL:HG23	5:P:82:LEU:HD11	1.62	0.80
4:Q:198:ILE:HG23	4:Q:199:PRO:HD3	1.64	0.80
4:S:94:GLY:HA2	5:T:101:ASN:CG	2.06	0.80
2:K:114:LEU:HA	2:K:161:LEU:O	1.81	0.80
2:B:134:ASN:O	2:B:135:SER:HB3	1.82	0.80
4:S:34:TRP:O	4:S:46:LEU:HB3	1.81	0.80
4:M:21:ASN:HA	4:M:74:HIS:HD2	1.46	0.79
2:B:71:ARG:NH1	3:C:9:THR:HB	1.95	0.79
3:I:7:ILE:HD13	3:I:7:ILE:H	1.47	0.79
4:U:34:TRP:CD2	4:U:75:LEU:HG	2.17	0.79
1:A:77:SER:O	1:A:78:ASN:HB2	1.82	0.79
2:H:127:ILE:HG12	2:H:177:HIS:CD2	2.17	0.79
5:T:72:ASN:H	5:T:72:ASN:HD22	1.30	0.79
4:S:62:PHE:CE2	4:S:77:LYS:HD2	2.18	0.79
4:M:18:LEU:HD23	4:M:77:LYS:HG2	1.65	0.79
2:H:1:GLY:CA	2:H:4:ARG:HH21	1.95	0.79
2:B:142:VAL:HA	2:B:160:MET:O	1.82	0.78
5:R:121:LYS:HZ1	5:R:228:GLN:HE21	1.30	0.78
4:U:12:LEU:HD13	4:U:16:ALA:HB3	1.64	0.78
5:P:207:PRO:HA	5:P:244:GLY:O	1.82	0.78
2:H:1:GLY:N	2:H:4:ARG:HE	1.81	0.78
2:B:165:PRO:O	2:B:166:ARG:HG3	1.84	0.78
5:V:19:VAL:HG23	5:V:82:LEU:HD11	1.66	0.78
2:H:130:ARG:HH11	2:H:130:ARG:HB2	1.47	0.78
4:M:200:GLU:O	4:M:200:GLU:HG2	1.80	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:67:PHE:HA	5:V:99:ARG:NH2	1.99	0.78
2:K:71:ARG:NH1	3:L:9:THR:HB	1.97	0.78
2:B:64:GLN:O	2:B:66:ASP:N	2.17	0.78
4:Q:93:SER:HB3	4:Q:104:LEU:HD22	1.66	0.78
5:T:72:ASN:HD22	5:T:72:ASN:N	1.79	0.78
4:U:117:ASP:O	4:U:118:ILE:HB	1.84	0.78
4:Q:202:THR:HG22	4:Q:203:PHE:N	1.99	0.77
5:R:21:LEU:HD22	5:R:77:MET:HE3	1.66	0.77
5:T:21:LEU:HD12	5:T:21:LEU:N	2.00	0.77
4:U:82:VAL:HA	4:U:114:VAL:HG13	1.66	0.77
1:G:136:VAL:HG23	1:G:137:PHE:N	1.99	0.77
1:J:154:LEU:HD12	1:J:155:PRO:HD2	1.65	0.77
1:A:140:ARG:HB3	1:A:142:ASP:OD1	1.83	0.77
4:M:55:LYS:O	4:M:57:SER:N	2.14	0.77
2:H:130:ARG:HB2	2:H:130:ARG:NH1	2.00	0.77
5:V:59:ASN:O	5:V:60:PHE:HB2	1.84	0.77
4:M:26:ALA:HB1	4:M:30:PRO:CG	2.08	0.77
1:A:93:THR:HG22	1:A:103:ASN:OD1	1.85	0.77
5:T:121:LYS:HE2	5:T:230:ARG:HE	1.47	0.77
4:U:12:LEU:C	4:U:12:LEU:HD12	2.10	0.77
4:U:160:ILE:CB	4:U:180:ALA:HA	2.14	0.77
2:E:127:ILE:HD13	2:E:128:GLU:H	1.46	0.77
5:R:121:LYS:NZ	5:R:228:GLN:NE2	2.33	0.77
2:K:1:GLY:HA3	2:K:4:ARG:HH12	1.49	0.77
5:R:180:LEU:O	5:R:180:LEU:HD12	1.84	0.76
4:U:17:PHE:O	4:U:77:LYS:O	2.03	0.76
5:R:103:GLU:O	5:R:106:ALA:HB2	1.84	0.76
5:R:206:ASN:HB3	5:R:209:ASN:HD22	1.49	0.76
5:P:16:GLY:O	5:P:81:THR:HA	1.85	0.76
4:M:164:THR:HG22	4:M:165:VAL:N	2.00	0.76
5:V:217:PHE:HD1	5:V:218:TYR:H	1.34	0.76
4:Q:98:GLY:O	4:Q:99:ASP:HB2	1.85	0.76
4:U:5:GLN:HE21	4:U:107:GLY:HA3	1.48	0.76
4:Q:179:VAL:HG23	5:R:196:ARG:HH11	1.49	0.76
4:Q:191:ASN:H	4:Q:191:ASN:ND2	1.80	0.76
4:U:191:ASN:H	4:U:191:ASN:ND2	1.82	0.76
2:B:127:ILE:HD13	2:B:128:GLU:N	2.00	0.76
4:U:28:GLY:O	4:U:30:PRO:HD3	1.85	0.76
4:M:158:VAL:HG12	4:M:159:TYR:H	1.50	0.75
4:Q:164:THR:HG22	4:Q:165:VAL:H	1.50	0.75
5:T:83:GLU:O	5:T:116:VAL:HG11	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:PHE:N	1:G:51:PHE:HD2	1.85	0.75
4:U:26:ALA:HB1	4:U:30:PRO:CG	2.14	0.75
5:R:31:SER:OG	5:R:48:GLU:OE2	2.04	0.75
4:Q:55:LYS:O	4:Q:56:GLY:O	2.04	0.75
4:S:46:LEU:HD12	4:S:58:ASN:ND2	2.01	0.75
5:V:72:ASN:H	5:V:72:ASN:HD22	1.34	0.75
5:R:72:ASN:H	5:R:72:ASN:ND2	1.80	0.75
5:T:48:GLU:O	5:T:54:GLN:HA	1.87	0.75
2:K:123:TYR:HA	2:K:124:PRO:O	1.85	0.75
5:P:163:TRP:HA	5:P:167:LYS:O	1.85	0.75
1:J:33:HIS:ND1	1:J:136:VAL:HG11	2.02	0.75
2:K:93:ARG:HD3	2:K:123:TYR:CD1	2.22	0.75
5:V:226:TRP:HB2	5:V:232:LYS:HZ3	1.50	0.75
2:B:13:TYR:OH	3:C:9:THR:HG22	1.86	0.75
5:V:72:ASN:H	5:V:72:ASN:ND2	1.84	0.75
5:P:160:LEU:HD23	5:P:160:LEU:O	1.87	0.74
4:U:14:GLU:HG2	4:U:15:GLU:OE1	1.87	0.74
1:J:4:GLU:OE2	2:K:19:ASN:HA	1.87	0.74
1:J:101:GLU:H	1:J:155:PRO:HG3	1.53	0.74
4:M:14:GLU:C	4:M:15:GLU:HG2	2.11	0.74
5:T:138:ILE:C	5:T:140:HIS:H	1.95	0.74
4:M:35:TYR:CD1	4:M:45:LEU:HA	2.21	0.74
4:U:10:VAL:CG1	4:U:112:LEU:HA	2.18	0.74
4:U:118:ILE:HG12	4:U:119:GLN:H	1.49	0.74
5:R:148:CYS:HB2	5:R:162:TRP:CZ2	2.23	0.74
1:J:144:LEU:N	1:J:144:LEU:HD23	2.03	0.74
2:K:142:VAL:HB	2:K:160:MET:O	1.87	0.74
5:P:220:LEU:HD12	5:P:233:PRO:HD2	1.68	0.74
4:U:24:TYR:HH	4:U:66:TYR:HE2	1.35	0.74
5:V:217:PHE:CD1	5:V:218:TYR:N	2.55	0.74
5:P:120:LEU:O	5:P:121:LYS:HB3	1.87	0.74
4:S:195:ASN:HD22	4:S:196:SER:H	1.33	0.74
1:A:45:LEU:HD12	1:A:48:PHE:CZ	2.23	0.73
5:T:14:THR:HG21	5:T:120:LEU:CD1	2.19	0.73
5:T:49:TYR:HE2	5:T:54:GLN:HB2	1.51	0.73
4:Q:189:CYS:HA	4:Q:192:ALA:HB2	1.70	0.73
1:D:61:ALA:HA	5:R:53:THR:HG21	1.71	0.73
4:Q:38:TYR:HA	4:Q:86:ALA:HB2	1.69	0.73
4:S:92:LEU:C	4:S:92:LEU:HD12	2.12	0.73
4:Q:43:LEU:HD11	5:R:43:LEU:HD21	1.71	0.73
4:Q:103:LYS:C	4:Q:104:LEU:HD23	2.14	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:77:THR:O	3:L:5:LYS:NZ	2.22	0.73
4:M:2:SER:H	4:M:25:THR:HB	1.54	0.73
1:J:113:THR:HG21	2:K:34:GLN:NE2	2.03	0.73
5:T:35:TYR:CE1	5:T:45:PHE:HD2	2.06	0.73
4:U:123:PRO:HG3	4:U:144:PHE:HB3	1.71	0.73
2:B:40:PHE:HB2	2:B:47:TYR:CE2	2.24	0.73
3:F:14:GLY:HA2	5:T:27:SER:HB2	1.71	0.73
1:G:101:GLU:H	1:G:155:PRO:HG3	1.53	0.73
4:U:164:THR:HG22	4:U:165:VAL:H	1.54	0.73
4:Q:14:GLU:O	4:Q:15:GLU:HB2	1.89	0.72
1:G:51:PHE:N	1:G:51:PHE:CD2	2.55	0.72
5:R:68:ARG:HD2	5:R:70:PHE:CE1	2.24	0.72
5:R:113:ARG:HG3	5:R:157:HIS:HE1	1.54	0.72
1:J:77:SER:O	1:J:78:ASN:HB2	1.90	0.72
5:V:72:ASN:HD22	5:V:72:ASN:N	1.86	0.72
5:P:10:TYR:HB3	5:P:157:HIS:HD2	1.53	0.72
5:P:103:GLU:O	5:P:106:ALA:CB	2.36	0.72
5:P:220:LEU:O	5:P:234:VAL:HG12	1.89	0.72
2:B:2:ASP:O	2:B:3:THR:CG2	2.38	0.72
4:Q:62:PHE:HD1	4:Q:75:LEU:HD11	1.53	0.72
1:G:52:ALA:HA	3:I:2:HIS:HB3	1.70	0.72
5:T:6:GLN:HE21	5:T:112:THR:HG23	1.53	0.72
4:U:56:GLY:O	4:U:57:SER:HB2	1.89	0.72
1:G:134:GLU:HB2	1:G:147:LYS:HZ1	1.54	0.72
4:S:31:SER:C	4:S:32:LEU:HD12	2.14	0.72
5:T:87:SER:HB3	5:T:115:THR:HA	1.72	0.72
5:P:180:LEU:HD12	5:P:180:LEU:O	1.90	0.72
2:K:1:GLY:CA	2:K:4:ARG:HH12	2.02	0.72
5:V:126:PRO:HD3	5:V:217:PHE:CD2	2.24	0.72
3:C:1:VAL:HG12	4:M:27:THR:CG2	2.19	0.72
1:D:82:ILE:HD13	1:D:83:THR:H	1.54	0.72
1:G:110:ASP:HB2	1:G:146:ARG:HG2	1.71	0.72
4:Q:120:ASN:CB	4:Q:121:PRO:HD2	2.13	0.71
1:A:16:PRO:HD2	2:B:6:ARG:HG2	1.72	0.71
5:R:84:LEU:H	5:R:84:LEU:HD12	1.56	0.71
1:G:45:LEU:HD12	1:G:48:PHE:CZ	2.24	0.71
2:B:1:GLY:O	2:B:3:THR:N	2.24	0.71
4:M:18:LEU:HD22	4:M:77:LYS:HE2	1.73	0.71
5:P:157:HIS:HB3	5:P:218:TYR:HB2	1.72	0.71
4:Q:34:TRP:CZ2	4:Q:90:CYS:HB2	2.26	0.71
5:T:89:LEU:HD23	5:T:90:TYR:N	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:237:ILE:HD12	2:K:2:ASP:HB2	1.72	0.71
2:K:172:THR:HG22	2:K:173:CYS:N	2.06	0.71
2:B:55:ARG:HH11	2:B:55:ARG:HG3	1.56	0.71
4:M:173:PHE:HE2	4:M:175:SER:HB3	1.56	0.71
5:R:119:ASP:OD2	5:R:121:LYS:HG3	1.91	0.71
2:H:129:VAL:CG2	2:H:175:VAL:HG22	2.19	0.71
1:A:6:VAL:HG13	2:B:16:HIS:HD2	1.55	0.71
1:A:170:LEU:HD13	1:A:174:LEU:HB2	1.72	0.71
1:G:159:ASP:HB3	1:G:161:TYR:HE1	1.56	0.71
5:T:237:ILE:HD12	2:K:2:ASP:H	1.56	0.71
1:D:23:MET:HE1	1:D:25:ASP:HB2	1.71	0.70
3:F:1:VAL:HB	4:Q:27:THR:HG23	1.72	0.70
5:T:34:TRP:O	5:T:46:LEU:HB2	1.91	0.70
2:B:97:PRO:HG3	2:B:122:PHE:HB3	1.73	0.70
2:E:78:TYR:CE2	3:F:7:ILE:HD11	2.26	0.70
2:H:41:ASP:OD1	2:H:43:ASP:HB2	1.91	0.70
5:T:46:LEU:HD13	5:T:60:PHE:CD1	2.25	0.70
1:J:15:ASN:HB2	1:J:70:LEU:CD2	2.20	0.70
2:K:64:GLN:O	2:K:65:LYS:C	2.34	0.70
3:F:6:ASN:ND2	3:F:7:ILE:N	2.39	0.70
2:E:76:ASP:OD2	2:E:80:ARG:HD2	1.91	0.70
5:T:49:TYR:HB3	5:T:69:GLN:HE21	1.55	0.70
2:K:101:VAL:HA	2:K:116:VAL:O	1.91	0.70
1:A:122:LEU:HB2	1:A:162:ASP:HB2	1.74	0.70
5:P:103:GLU:O	5:P:106:ALA:HB3	1.90	0.70
5:P:154:TYR:HA	5:P:155:PRO:O	1.92	0.70
5:T:38:THR:HG22	5:T:88:ALA:CB	2.22	0.70
4:M:21:ASN:HA	4:M:74:HIS:CD2	2.26	0.70
2:K:141:GLY:O	2:K:142:VAL:HB	1.92	0.70
4:U:24:TYR:CE1	4:U:32:LEU:HD21	2.27	0.70
5:T:127:GLU:O	5:T:150:ALA:HA	1.92	0.70
5:P:46:LEU:HB3	5:P:47:PHE:CE1	2.26	0.70
1:D:17:ASP:O	1:D:18:GLN:HB2	1.92	0.70
2:E:99:VAL:HG21	2:E:175:VAL:HG21	1.73	0.70
1:G:45:LEU:HD12	1:G:48:PHE:CE2	2.27	0.70
1:G:82:ILE:HB	2:H:33:ASN:OD1	1.91	0.70
5:T:84:LEU:HA	5:T:116:VAL:CG1	2.22	0.70
5:T:181:LYS:CB	5:T:184:PRO:HG3	2.22	0.70
5:V:124:PHE:CE1	5:V:230:ARG:CZ	2.74	0.70
5:V:160:LEU:HD23	5:V:161:SER:N	2.06	0.70
2:H:167:SER:C	2:H:169:GLU:H	1.97	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:118:ILE:HD12	4:U:145:ASP:CA	2.21	0.70
4:M:46:LEU:HD12	4:M:58:ASN:HD22	1.57	0.69
4:Q:29:TYR:N	4:Q:30:PRO:HD3	2.06	0.69
5:P:100:VAL:O	5:P:101:ASN:HB2	1.91	0.69
2:H:78:TYR:CE1	2:H:82:ASN:ND2	2.60	0.69
4:M:77:LYS:HE3	4:M:80:VAL:CB	2.18	0.69
3:F:1:VAL:HB	4:Q:27:THR:CG2	2.22	0.69
4:Q:144:PHE:HB2	4:Q:148:THR:OG1	1.93	0.69
5:T:89:LEU:HD21	5:T:111:GLY:CA	2.18	0.69
1:A:17:ASP:OD1	2:B:6:ARG:NE	2.25	0.69
5:P:21:LEU:HB2	5:P:77:MET:HE2	1.74	0.69
5:P:146:LEU:HD12	5:P:146:LEU:N	2.06	0.69
2:E:71:ARG:NH1	3:F:9:THR:HB	2.07	0.69
2:E:93:ARG:HH11	2:E:93:ARG:HG3	1.57	0.69
1:A:53:SER:HB2	3:C:3:PHE:CE2	2.26	0.69
5:R:12:ILE:HD11	5:R:155:PRO:CG	2.21	0.69
4:U:21:ASN:HA	4:U:74:HIS:HD2	1.55	0.69
5:V:13:LYS:HD2	5:V:17:GLN:NE2	2.08	0.69
1:D:82:ILE:HD13	1:D:83:THR:N	2.07	0.69
2:K:149:GLN:HG2	2:K:155:PHE:CE2	2.28	0.69
4:U:103:LYS:O	4:U:104:LEU:HD23	1.93	0.69
4:Q:34:TRP:O	4:Q:46:LEU:HB3	1.92	0.69
3:F:1:VAL:HG23	3:F:1:VAL:O	1.92	0.69
3:F:1:VAL:HG12	4:Q:27:THR:OG1	1.91	0.69
4:Q:10:VAL:HG23	4:Q:113:LEU:H	1.56	0.69
4:Q:139:CYS:SG	4:Q:187:PHE:HE1	2.15	0.69
4:Q:164:THR:HG21	5:R:196:ARG:HH21	1.58	0.69
4:Q:62:PHE:HB3	4:Q:75:LEU:HD11	1.73	0.69
4:Q:164:THR:HG22	4:Q:165:VAL:N	2.07	0.69
5:R:206:ASN:HD22	5:R:209:ASN:ND2	1.90	0.69
2:H:67:PHE:CE1	2:H:71:ARG:NH2	2.61	0.69
5:T:50:PHE:HB3	5:T:55:ARG:HD2	1.74	0.69
5:V:64:ARG:NH2	5:V:83:GLU:HG3	2.07	0.68
5:R:49:TYR:CE2	5:R:54:GLN:HB2	2.27	0.68
4:Q:6:MET:HE1	4:Q:19:THR:O	1.93	0.68
5:V:236:GLN:O	5:V:237:ILE:HG13	1.93	0.68
5:V:128:VAL:HB	5:V:238:VAL:HG12	1.74	0.68
4:M:16:ALA:HB3	4:M:80:VAL:CG1	2.23	0.68
5:R:84:LEU:HA	5:R:116:VAL:HG13	1.75	0.68
2:H:64:GLN:HB3	2:H:67:PHE:HB3	1.75	0.68
2:E:81:HIS:ND1	3:F:5:LYS:NZ	2.34	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:52:GLU:HA	5:R:69:GLN:HB3	1.75	0.68
5:R:62:GLY:O	5:R:65:PHE:N	2.27	0.68
5:V:201:ALA:O	5:V:205:GLN:HG3	1.94	0.68
1:D:162:ASP:HB3	1:D:175:LEU:HD22	1.75	0.68
5:T:12:ILE:HD12	5:T:219:GLY:HA2	1.74	0.68
1:D:77:SER:O	1:D:78:ASN:HB2	1.92	0.68
5:R:186:LEU:O	5:R:188:ASP:N	2.27	0.68
1:A:26:PHE:CE2	2:B:90:THR:HB	2.29	0.68
1:A:53:SER:HB2	3:C:3:PHE:CD2	2.29	0.68
2:B:93:ARG:HH11	2:B:93:ARG:HG3	1.57	0.67
5:R:49:TYR:CE2	5:R:54:GLN:HG3	2.29	0.67
5:R:201:ALA:O	5:R:205:GLN:HG3	1.94	0.67
2:H:89:PHE:O	2:H:93:ARG:HB2	1.95	0.67
5:P:49:TYR:CE2	5:P:54:GLN:HG3	2.29	0.67
1:D:6:VAL:HG13	2:E:16:HIS:HD2	1.58	0.67
2:E:4:ARG:HH21	2:E:4:ARG:HG3	1.57	0.67
4:Q:38:TYR:HA	4:Q:86:ALA:CB	2.24	0.67
1:A:14:LEU:HD13	2:B:8:LEU:HD13	1.76	0.67
1:A:29:ASP:HB3	2:B:153:TRP:NE1	2.10	0.67
2:B:55:ARG:CZ	5:V:110:GLN:HE22	2.08	0.67
4:Q:62:PHE:CD1	4:Q:75:LEU:HD11	2.29	0.67
4:Q:179:VAL:HG23	5:R:196:ARG:NH1	2.10	0.67
2:H:77:THR:HA	4:S:29:TYR:HB2	1.76	0.67
2:K:102:TYR:CE2	2:K:116:VAL:HB	2.29	0.67
4:U:6:MET:HE3	4:U:21:ASN:ND2	2.09	0.67
4:M:164:THR:CG2	4:M:165:VAL:H	2.06	0.67
5:T:35:TYR:HA	5:T:46:LEU:HD23	1.77	0.67
5:V:237:ILE:O	5:V:237:ILE:HG22	1.95	0.67
2:B:55:ARG:HB3	2:B:56:PRO:HD3	1.77	0.67
2:B:77:THR:O	3:C:5:LYS:HE3	1.95	0.67
1:D:144:LEU:HD21	2:E:34:GLN:OE1	1.94	0.67
2:E:24:VAL:CG1	2:E:75:VAL:HG12	2.22	0.67
2:B:97:PRO:HG3	2:B:122:PHE:CB	2.25	0.67
4:M:148:THR:O	4:M:149:ASN:HB2	1.94	0.67
4:Q:35:TYR:HD1	4:Q:45:LEU:HA	1.60	0.67
4:S:179:VAL:CG2	5:T:196:ARG:HD3	2.25	0.67
4:M:198:ILE:HG13	4:M:198:ILE:O	1.94	0.66
4:S:38:TYR:HB3	4:S:39:PRO:CD	2.25	0.66
2:K:62:ASN:HA	2:K:68:LEU:HD22	1.77	0.66
5:V:18:GLN:HB3	5:V:80:SER:HA	1.77	0.66
3:C:14:GLY:HA3	5:V:27:SER:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:84:LEU:HA	5:P:116:VAL:HG13	1.77	0.66
5:R:87:SER:HB3	5:R:115:THR:HA	1.77	0.66
4:S:125:VAL:N	4:S:201:ASP:HB3	2.10	0.66
4:U:10:VAL:HG13	4:U:11:THR:N	2.10	0.66
4:M:17:PHE:H	4:M:17:PHE:HD1	1.43	0.66
1:G:53:SER:HB2	3:I:3:PHE:CD1	2.30	0.66
4:S:26:ALA:HB1	4:S:30:PRO:CG	2.12	0.66
1:A:53:SER:O	3:C:3:PHE:HA	1.96	0.66
4:Q:10:VAL:CG2	4:Q:112:LEU:HA	2.24	0.66
1:J:92:LEU:HD23	1:J:106:ILE:O	1.94	0.66
5:V:26:ILE:HB	5:V:29:HIS:ND1	2.11	0.66
5:P:50:PHE:O	5:P:52:GLU:N	2.28	0.66
4:Q:58:ASN:C	4:Q:61:GLY:H	2.02	0.66
4:Q:191:ASN:HD22	4:Q:191:ASN:N	1.79	0.66
5:R:134:SER:O	5:R:138:ILE:HG12	1.95	0.66
5:R:220:LEU:HD12	5:R:233:PRO:HD2	1.78	0.66
2:H:99:VAL:HG22	2:H:119:VAL:HG22	1.76	0.66
1:J:52:ALA:HA	3:L:2:HIS:HB3	1.76	0.66
5:V:77:MET:HE1	5:V:90:TYR:CD1	2.31	0.66
5:P:172:GLY:O	5:P:197:LEU:HA	1.96	0.66
2:E:64:GLN:HB3	2:E:67:PHE:HB3	1.78	0.66
5:R:21:LEU:HD22	5:R:77:MET:CE	2.24	0.66
2:K:27:LEU:HD12	2:K:41:ASP:HA	1.76	0.66
1:A:92:LEU:HD23	1:A:106:ILE:O	1.96	0.66
5:P:110:GLN:HE22	2:K:55:ARG:NE	1.93	0.66
4:Q:26:ALA:CB	4:Q:30:PRO:HG2	2.22	0.66
4:Q:55:LYS:CB	4:Q:64:ALA:N	2.58	0.66
2:B:40:PHE:HB2	2:B:47:TYR:CD2	2.31	0.66
5:P:53:THR:O	5:P:54:GLN:CB	2.43	0.66
3:L:9:THR:HG23	3:L:9:THR:O	1.94	0.66
4:Q:5:GLN:HE21	4:Q:107:GLY:HA3	1.61	0.66
5:T:19:VAL:CG2	5:T:82:LEU:HD11	2.25	0.66
5:R:46:LEU:HD13	5:R:60:PHE:CD1	2.31	0.65
4:S:1:ASP:O	4:S:2:SER:HB2	1.94	0.65
5:V:32:VAL:HG13	5:V:92:CYS:SG	2.36	0.65
5:V:74:ARG:HH22	5:V:76:GLU:CD	2.03	0.65
4:M:18:LEU:CD2	4:M:77:LYS:HG2	2.25	0.65
4:M:85:SER:OG	4:M:114:VAL:HG12	1.95	0.65
3:F:1:VAL:O	3:F:1:VAL:CG2	2.44	0.65
2:K:174:GLN:HA	2:K:185:THR:HG22	1.79	0.65
2:B:2:ASP:HA	5:R:237:ILE:HB	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:154:TYR:CG	5:P:155:PRO:HA	2.31	0.65
5:P:122:ASN:O	5:P:154:TYR:HB3	1.97	0.65
2:E:13:TYR:CD2	3:F:7:ILE:HD12	2.32	0.65
4:Q:82:VAL:HA	4:Q:114:VAL:CG1	2.27	0.65
1:A:32:PHE:HD2	1:A:41:THR:HG22	1.60	0.65
4:M:48:LYS:O	4:M:49:ALA:HB2	1.97	0.65
4:Q:181:TRP:CE3	5:R:149:LEU:HD21	2.31	0.65
1:G:5:HIS:CE1	2:H:91:VAL:HG13	2.32	0.65
1:G:113:THR:CG2	1:G:144:LEU:HD22	2.27	0.65
4:S:179:VAL:HG23	5:T:196:ARG:NH1	2.11	0.65
5:V:190:ARG:C	5:V:191:TYR:HD1	2.04	0.65
5:R:120:LEU:HD11	5:R:220:LEU:HD22	1.79	0.65
1:G:156:SER:OG	1:G:157:THR:N	2.24	0.65
2:H:29:ARG:HB3	2:H:31:ILE:HD11	1.77	0.65
2:K:71:ARG:HH12	3:L:9:THR:CB	2.03	0.65
3:L:8:VAL:O	3:L:9:THR:HG22	1.95	0.65
4:S:78:GLY:O	4:S:79:SER:CB	2.45	0.65
4:S:190:ALA:O	4:S:191:ASN:HB3	1.96	0.65
2:E:55:ARG:O	2:E:59:GLU:HG3	1.97	0.65
5:R:16:GLY:O	5:R:81:THR:HA	1.96	0.65
5:R:34:TRP:O	5:R:46:LEU:HB2	1.97	0.65
4:S:36:VAL:HB	4:S:46:LEU:HD22	1.79	0.65
4:M:77:LYS:NZ	4:M:84:ASP:HB2	2.12	0.65
5:P:10:TYR:HB3	5:P:157:HIS:CD2	2.32	0.65
2:E:81:HIS:CE1	3:F:5:LYS:HZ3	2.13	0.65
4:Q:198:ILE:HG23	4:Q:199:PRO:CD	2.26	0.65
5:R:19:VAL:CG2	5:R:82:LEU:HD11	2.26	0.65
2:H:78:TYR:HE1	2:H:82:ASN:HD21	1.45	0.65
5:V:48:GLU:O	5:V:54:GLN:HA	1.96	0.65
1:A:59:ALA:O	1:A:62:ASN:HB2	1.97	0.65
1:D:156:SER:HB2	1:D:180:PHE:HB2	1.77	0.65
4:Q:34:TRP:CH2	4:Q:90:CYS:HB2	2.32	0.65
2:H:18:PHE:HB2	2:H:23:ARG:HB3	1.78	0.65
3:F:3:PHE:HD2	4:Q:99:ASP:O	1.80	0.64
2:H:31:ILE:HG23	2:H:35:GLU:C	2.22	0.64
4:M:198:ILE:HD12	4:M:201:ASP:CB	2.27	0.64
2:B:71:ARG:HH12	3:C:9:THR:CB	2.01	0.64
3:L:11:ARG:HG2	3:L:12:THR:N	2.12	0.64
2:B:38:LEU:HD11	2:B:47:TYR:HB3	1.80	0.64
4:U:19:THR:HA	4:U:76:GLU:HG2	1.80	0.64
5:P:147:VAL:HG22	5:P:196:ARG:CG	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:GLU:HB2	1:G:147:LYS:NZ	2.12	0.64
5:P:128:VAL:HG23	5:P:238:VAL:CG1	2.27	0.64
4:Q:164:THR:CG2	5:R:174:SER:HB2	2.27	0.64
5:R:26:ILE:HB	5:R:29:HIS:CD2	2.33	0.64
4:U:138:VAL:HG23	5:V:131:PHE:CE2	2.32	0.64
5:P:147:VAL:HG22	5:P:196:ARG:HG2	1.77	0.64
1:D:112:PHE:O	1:D:144:LEU:HB3	1.98	0.64
1:D:156:SER:OG	1:D:157:THR:N	2.24	0.64
1:G:45:LEU:HB2	1:G:48:PHE:CE2	2.33	0.64
2:H:1:GLY:H1	2:H:4:ARG:HE	1.44	0.64
3:L:1:VAL:HG13	3:L:2:HIS:O	1.98	0.64
1:A:154:LEU:HD12	1:A:155:PRO:HD2	1.80	0.64
5:R:9:ARG:HD3	5:R:10:TYR:N	2.11	0.64
5:R:46:LEU:O	5:R:57:LYS:O	2.16	0.64
2:K:13:TYR:OH	3:L:9:THR:HG22	1.96	0.64
1:D:73:MET:SD	1:D:76:ARG:NH1	2.71	0.64
5:R:84:LEU:HA	5:R:116:VAL:CG1	2.28	0.64
3:I:2:HIS:O	3:I:3:PHE:HB2	1.97	0.64
4:U:35:TYR:CE1	4:U:45:LEU:HG	2.33	0.64
4:S:29:TYR:N	4:S:30:PRO:HD3	2.12	0.63
5:T:183:GLN:N	5:T:184:PRO:HD3	2.12	0.63
5:P:87:SER:CB	5:P:115:THR:HA	2.24	0.63
2:E:127:ILE:HD12	2:E:129:VAL:HG23	1.81	0.63
1:A:156:SER:OG	1:A:157:THR:N	2.30	0.63
5:P:8:PRO:O	5:P:112:THR:HB	1.98	0.63
1:D:82:ILE:HG12	2:E:33:ASN:HB3	1.80	0.63
4:Q:93:SER:CB	4:Q:104:LEU:HD22	2.28	0.63
5:R:48:GLU:O	5:R:54:GLN:HA	1.97	0.63
5:T:155:PRO:HG2	5:T:157:HIS:CD2	2.33	0.63
5:P:42:GLY:O	5:P:43:LEU:C	2.42	0.63
1:G:176:LYS:HA	1:G:176:LYS:CE	2.24	0.63
2:H:127:ILE:HG12	2:H:177:HIS:HD2	1.62	0.63
5:T:96:LEU:HD22	5:T:96:LEU:N	2.14	0.63
4:U:34:TRP:HB2	4:U:47:LEU:CD1	2.28	0.63
4:U:94:GLY:HA3	5:V:101:ASN:ND2	2.14	0.63
2:B:2:ASP:O	2:B:3:THR:HG23	1.98	0.63
5:R:212:ARG:HH12	5:R:214:GLN:NE2	1.96	0.63
1:G:26:PHE:CE2	2:H:90:THR:HB	2.33	0.63
4:S:93:SER:HB3	4:S:104:LEU:HD22	1.80	0.63
1:J:59:ALA:O	1:J:62:ASN:HB2	1.98	0.63
4:U:32:LEU:HD22	4:U:73:PHE:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ARG:HG3	1:A:50:ARG:HH21	1.63	0.63
5:P:197:LEU:HD12	5:P:198:ARG:N	2.14	0.63
1:D:57:GLN:HB3	5:R:55:ARG:O	1.99	0.63
4:Q:77:LYS:HD3	4:Q:80:VAL:HA	1.80	0.63
2:H:62:ASN:HA	2:H:68:LEU:CD2	2.28	0.63
4:S:28:GLY:C	4:S:30:PRO:HD3	2.24	0.63
4:S:128:LEU:HB2	5:T:131:PHE:HB3	1.80	0.63
5:T:14:THR:HG22	5:T:117:VAL:HG12	1.80	0.63
1:A:24:PHE:HB2	1:A:32:PHE:CE1	2.34	0.63
5:R:83:GLU:O	5:R:116:VAL:HG11	1.98	0.63
4:S:195:ASN:HD22	4:S:196:SER:N	1.96	0.63
4:S:54:ASP:O	4:S:55:LYS:C	2.41	0.63
4:S:202:THR:HG22	4:S:202:THR:O	1.99	0.63
5:T:89:LEU:CD2	5:T:111:GLY:HA3	2.22	0.63
1:G:159:ASP:CB	1:G:161:TYR:HE1	2.11	0.63
4:S:82:VAL:HA	4:S:114:VAL:CG1	2.28	0.63
2:B:55:ARG:CZ	5:V:110:GLN:NE2	2.63	0.62
3:F:12:THR:HG22	5:T:2:GLY:HA3	1.81	0.62
5:T:164:VAL:HA	5:T:211:PHE:HA	1.81	0.62
1:J:82:ILE:HD13	1:J:83:THR:N	2.14	0.62
5:V:8:PRO:HG2	5:V:11:LEU:HG	1.81	0.62
5:P:11:LEU:O	5:P:114:LEU:O	2.17	0.62
2:K:133:ARG:C	2:K:135:SER:H	2.07	0.62
2:K:172:THR:HG23	2:K:186:VAL:O	1.98	0.62
4:M:58:ASN:C	4:M:61:GLY:H	2.06	0.62
4:Q:179:VAL:CG2	5:R:196:ARG:HH11	2.11	0.62
4:S:112:LEU:HD23	4:S:113:LEU:N	2.14	0.62
4:U:93:SER:HB3	4:U:104:LEU:HD22	1.81	0.62
2:B:27:LEU:HD21	2:B:29:ARG:NH2	2.15	0.62
2:B:28:HIS:CE1	3:C:9:THR:HG21	2.33	0.62
5:P:12:ILE:O	5:P:13:LYS:HD3	1.99	0.62
5:P:89:LEU:HD22	5:P:91:LEU:HG	1.80	0.62
5:P:232:LYS:O	5:P:234:VAL:HG22	1.99	0.62
2:B:13:TYR:OH	3:C:9:THR:CG2	2.47	0.62
2:B:81:HIS:CE1	4:M:28:GLY:HA3	2.35	0.62
5:P:83:GLU:O	5:P:116:VAL:HG11	2.00	0.62
5:P:99:ARG:N	5:P:99:ARG:HD2	2.14	0.62
5:R:93:ALA:HA	5:R:107:PHE:O	1.99	0.62
4:U:158:VAL:O	4:U:158:VAL:HG12	1.98	0.62
4:S:82:VAL:HA	4:S:114:VAL:HG13	1.81	0.62
4:M:77:LYS:HG3	4:M:77:LYS:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:234:VAL:O	5:R:236:GLN:HG2	1.99	0.62
1:D:6:VAL:HG13	2:E:16:HIS:CD2	2.35	0.62
1:G:73:MET:HE1	2:H:53:LEU:HG	1.79	0.62
5:T:38:THR:HG22	5:T:88:ALA:HB2	1.82	0.62
5:T:162:TRP:HZ3	5:T:195:SER:HG	1.45	0.62
1:J:11:GLU:HB3	1:J:22:PHE:HD2	1.65	0.62
2:K:102:TYR:CD2	2:K:116:VAL:HB	2.35	0.62
5:V:130:VAL:HG23	5:V:240:ALA:HB3	1.82	0.62
1:D:115:PRO:HD3	1:D:145:PHE:CE1	2.34	0.62
4:Q:22:CYS:HB3	4:Q:73:PHE:O	2.00	0.62
5:T:120:LEU:H	5:T:120:LEU:CD1	2.13	0.62
5:T:204:TRP:O	5:T:206:ASN:N	2.24	0.62
5:V:155:PRO:HG2	5:V:157:HIS:HD2	1.65	0.62
2:B:155:PHE:O	2:B:156:GLN:HB3	2.00	0.61
4:M:82:VAL:HG23	4:M:114:VAL:HG13	1.82	0.61
5:P:48:GLU:OE1	5:P:55:ARG:HD3	2.00	0.61
1:G:100:ARG:H	1:G:155:PRO:HG2	1.65	0.61
5:T:9:ARG:HD3	5:T:9:ARG:N	2.11	0.61
4:U:118:ILE:CD1	4:U:121:PRO:HB3	2.27	0.61
2:E:4:ARG:CB	2:E:5:PRO:HD3	2.30	0.61
4:Q:198:ILE:O	4:Q:200:GLU:N	2.32	0.61
2:K:123:TYR:CD1	2:K:124:PRO:HA	2.35	0.61
4:U:38:TYR:CD1	4:U:86:ALA:HB2	2.34	0.61
1:A:9:GLN:HG3	1:A:24:PHE:CE1	2.34	0.61
1:G:170:LEU:HD13	1:G:174:LEU:HB2	1.81	0.61
5:V:226:TRP:HB2	5:V:232:LYS:NZ	2.15	0.61
4:M:67:ARG:HG2	4:M:67:ARG:HH11	1.64	0.61
4:M:120:ASN:CB	4:M:121:PRO:CD	2.69	0.61
2:E:72:ARG:O	2:E:75:VAL:HG22	2.01	0.61
5:T:50:PHE:HB2	5:T:55:ARG:HH11	1.64	0.61
1:A:61:ALA:O	1:A:64:ALA:HB3	2.00	0.61
2:B:164:VAL:O	2:B:165:PRO:CB	2.47	0.61
1:G:101:GLU:H	1:G:155:PRO:CG	2.14	0.61
4:S:179:VAL:HG23	5:T:196:ARG:HH11	1.66	0.61
5:V:160:LEU:HD23	5:V:160:LEU:C	2.25	0.61
2:B:148:ILE:HB	2:B:156:GLN:O	2.00	0.61
5:R:212:ARG:HH12	5:R:214:GLN:HE22	1.48	0.61
4:S:103:LYS:C	4:S:104:LEU:HD23	2.26	0.61
5:T:36:GLN:HG2	5:T:38:THR:HG23	1.81	0.61
1:D:156:SER:CB	1:D:180:PHE:HB2	2.30	0.61
4:Q:21:ASN:N	4:Q:21:ASN:HD22	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:196:SER:O	4:Q:197:ILE:CB	2.47	0.61
1:G:140:ARG:HD2	1:G:146:ARG:HG3	1.81	0.61
4:U:47:LEU:HD11	4:U:75:LEU:HD21	1.82	0.61
4:M:78:GLY:O	4:M:79:SER:CB	2.49	0.61
4:Q:35:TYR:CD1	4:Q:45:LEU:HA	2.36	0.61
4:S:161:THR:HG21	4:S:179:VAL:C	2.26	0.61
5:T:110:GLN:HG3	5:T:110:GLN:O	1.99	0.61
5:V:19:VAL:CG2	5:V:82:LEU:HD11	2.31	0.61
5:V:148:CYS:HB2	5:V:162:TRP:CZ2	2.36	0.61
4:M:65:THR:HG21	4:M:67:ARG:NH1	2.16	0.61
2:E:4:ARG:HB3	2:E:5:PRO:HD3	1.82	0.61
5:R:128:VAL:HB	5:R:238:VAL:HG12	1.81	0.61
5:P:21:LEU:N	5:P:21:LEU:HD12	2.16	0.61
5:P:160:LEU:HD23	5:P:160:LEU:C	2.25	0.61
5:R:128:VAL:HG11	5:R:239:SER:HA	1.83	0.61
5:T:84:LEU:HA	5:T:116:VAL:HG11	1.83	0.61
4:U:34:TRP:HB2	4:U:47:LEU:HD12	1.81	0.61
2:E:2:ASP:O	2:E:2:ASP:OD2	2.18	0.60
4:Q:120:ASN:CB	4:Q:121:PRO:CD	2.77	0.60
5:R:212:ARG:NH1	5:R:214:GLN:NE2	2.48	0.60
4:M:24:TYR:HE2	4:M:26:ALA:HB2	1.66	0.60
5:P:35:TYR:HA	5:P:46:LEU:HD23	1.84	0.60
1:D:45:LEU:HD12	1:D:48:PHE:CE2	2.35	0.60
4:Q:10:VAL:CG2	4:Q:113:LEU:H	2.14	0.60
3:I:7:ILE:HD13	3:I:7:ILE:N	2.15	0.60
5:T:6:GLN:NE2	5:T:112:THR:HG23	2.16	0.60
1:J:53:SER:O	3:L:3:PHE:HA	2.01	0.60
2:B:17:PHE:CZ	2:B:83:TYR:HB2	2.37	0.60
5:P:48:GLU:HG2	5:P:49:TYR:N	2.16	0.60
5:R:186:LEU:C	5:R:188:ASP:H	2.08	0.60
1:G:51:PHE:CD1	2:H:89:PHE:HB3	2.37	0.60
3:I:3:PHE:HB2	4:S:99:ASP:HB3	1.84	0.60
4:M:58:ASN:C	4:M:61:GLY:N	2.58	0.60
5:P:26:ILE:HB	5:P:29:HIS:ND1	2.17	0.60
4:Q:6:MET:HE3	4:Q:21:ASN:H	1.66	0.60
4:S:148:THR:HG22	4:S:149:ASN:N	2.17	0.60
2:K:70:ASP:OD2	5:V:99:ARG:HG3	2.01	0.60
2:B:28:HIS:HB3	2:B:40:PHE:HB3	1.83	0.60
5:T:6:GLN:OE1	5:T:92:CYS:HB3	2.00	0.60
5:V:59:ASN:O	5:V:60:PHE:CB	2.49	0.60
2:B:164:VAL:CG2	2:B:165:PRO:N	2.61	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:ILE:HA	1:G:66:ASP:OD2	2.02	0.60
4:U:99:ASP:OD2	4:U:99:ASP:N	2.34	0.60
1:D:155:PRO:O	1:D:156:SER:O	2.20	0.60
5:R:151:THR:HG22	5:R:192:SER:HB3	1.84	0.60
5:R:182:GLU:O	5:R:184:PRO:HD3	2.01	0.60
5:T:50:PHE:HB2	5:T:55:ARG:NH1	2.17	0.60
4:U:47:LEU:HD23	4:U:57:SER:HB2	1.83	0.60
1:A:101:GLU:H	1:A:155:PRO:CG	2.14	0.60
2:E:177:HIS:CG	2:E:178:PRO:HD2	2.36	0.60
1:G:59:ALA:O	1:G:62:ASN:HB2	2.02	0.60
5:T:99:ARG:HD3	5:T:99:ARG:H	1.66	0.60
5:V:51:ASN:C	5:V:52:GLU:HG2	2.25	0.60
4:S:26:ALA:O	4:S:27:THR:OG1	2.13	0.60
1:J:45:LEU:HB2	1:J:48:PHE:CE2	2.37	0.60
5:V:34:TRP:CE3	5:V:77:MET:SD	2.94	0.60
2:E:63:SER:HA	5:T:107:PHE:CE1	2.37	0.60
4:S:43:LEU:CD1	5:T:43:LEU:HD21	2.26	0.60
4:S:112:LEU:HD23	4:S:112:LEU:C	2.27	0.60
1:J:45:LEU:HD12	1:J:48:PHE:CZ	2.37	0.60
1:D:16:PRO:HG3	2:E:3:THR:HB	1.84	0.59
4:U:189:CYS:O	4:U:190:ALA:C	2.43	0.59
5:V:173:VAL:HA	5:V:196:ARG:O	2.02	0.59
1:A:63:ILE:O	1:A:66:ASP:HB2	2.02	0.59
5:P:234:VAL:O	5:P:236:GLN:HG2	2.02	0.59
1:D:104:VAL:HG22	1:D:152:PRO:HB3	1.84	0.59
4:Q:202:THR:CG2	4:Q:203:PHE:H	2.11	0.59
5:R:103:GLU:O	5:R:106:ALA:CB	2.46	0.59
5:T:77:MET:HE1	5:T:90:TYR:CD1	2.37	0.59
1:J:142:ASP:O	1:J:143:HIS:HB2	2.01	0.59
5:V:138:ILE:O	5:V:142:GLN:HA	2.02	0.59
1:A:29:ASP:HB3	2:B:153:TRP:CD1	2.36	0.59
1:A:82:ILE:HD13	1:A:83:THR:N	2.17	0.59
1:D:153:PHE:HE2	1:D:155:PRO:HA	1.67	0.59
5:R:212:ARG:HH22	5:R:214:GLN:CD	2.10	0.59
4:S:159:TYR:HD2	4:S:159:TYR:N	1.97	0.59
5:T:74:ARG:NH2	5:T:76:GLU:OE2	2.32	0.59
1:J:113:THR:HG21	2:K:34:GLN:HE21	1.66	0.59
1:A:11:GLU:HA	1:A:21:GLU:O	2.03	0.59
5:P:79:VAL:O	5:P:79:VAL:HG23	2.03	0.59
1:D:121:TRP:O	1:D:122:LEU:HD23	2.02	0.59
2:E:2:ASP:C	2:E:3:THR:O	2.39	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:THR:O	1:G:147:LYS:HE2	2.03	0.59
3:I:2:HIS:O	4:S:99:ASP:HB3	2.03	0.59
2:E:144:SER:OG	2:E:145:THR:N	2.35	0.59
5:T:70:PHE:CE2	5:T:74:ARG:NH2	2.70	0.59
4:U:78:GLY:O	4:U:79:SER:CB	2.50	0.59
5:V:103:GLU:O	5:V:106:ALA:HB3	2.02	0.59
2:B:64:GLN:C	2:B:66:ASP:H	2.10	0.59
2:B:132:PHE:O	2:B:172:THR:N	2.36	0.59
4:M:120:ASN:O	4:M:121:PRO:O	2.21	0.59
5:R:1:GLY:CA	5:R:5:THR:HG21	2.33	0.59
2:H:78:TYR:CE2	3:I:7:ILE:HD12	2.37	0.59
4:S:24:TYR:HH	4:S:66:TYR:HE2	1.49	0.59
2:B:4:ARG:HB2	2:B:5:PRO:CD	2.32	0.59
3:C:5:LYS:NZ	4:M:94:GLY:O	2.35	0.59
4:Q:176:ASN:O	4:Q:177:SER:HB3	2.01	0.59
4:S:65:THR:CG2	4:S:67:ARG:NH2	2.60	0.59
4:S:120:ASN:N	4:S:121:PRO:CD	2.45	0.59
5:T:87:SER:CB	5:T:115:THR:HA	2.33	0.59
5:T:99:ARG:H	5:T:99:ARG:CD	2.15	0.59
2:K:64:GLN:HB3	2:K:67:PHE:HB3	1.85	0.59
2:B:1:GLY:N	2:B:4:ARG:NE	2.51	0.59
1:D:30:GLU:HB2	1:D:138:LEU:HD21	1.85	0.59
3:F:13:PRO:O	5:T:2:GLY:HA2	2.02	0.59
4:Q:188:ALA:O	4:Q:191:ASN:ND2	2.36	0.59
4:S:38:TYR:HD1	4:S:86:ALA:HB2	1.68	0.59
5:P:110:GLN:NE2	2:K:55:ARG:NE	2.51	0.59
5:R:15:ARG:HD3	5:R:84:LEU:HD11	1.85	0.59
4:S:15:GLU:OE2	4:S:79:SER:HA	2.03	0.59
4:S:179:VAL:O	4:S:180:ALA:HB3	2.03	0.59
3:L:1:VAL:HG13	3:L:2:HIS:N	2.17	0.59
4:M:93:SER:HB3	4:M:104:LEU:HD22	1.85	0.58
5:P:48:GLU:O	5:P:54:GLN:HA	2.03	0.58
1:D:6:VAL:HG22	2:E:16:HIS:CD2	2.38	0.58
4:S:34:TRP:CE2	4:S:75:LEU:HB2	2.38	0.58
5:V:3:GLY:HA2	5:V:26:ILE:HD13	1.85	0.58
5:V:4:VAL:HG23	5:V:26:ILE:HD11	1.84	0.58
2:B:27:LEU:HD11	2:B:39:ARG:HD3	1.84	0.58
5:P:223:ASN:O	5:P:223:ASN:CG	2.46	0.58
2:E:2:ASP:HA	2:E:6:ARG:HH12	1.68	0.58
3:F:1:VAL:CG1	4:Q:27:THR:OG1	2.51	0.58
2:E:71:ARG:HH12	3:F:9:THR:HB	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:102:TYR:N	2:E:102:TYR:CD1	2.70	0.58
2:H:64:GLN:O	2:H:66:ASP:N	2.35	0.58
4:U:24:TYR:OH	4:U:66:TYR:HE2	1.85	0.58
5:V:125:PRO:HA	5:V:217:PHE:CD2	2.38	0.58
4:Q:0:GLY:N	4:Q:98:GLY:O	2.36	0.58
1:J:33:HIS:C	1:J:33:HIS:CD2	2.81	0.58
4:M:43:LEU:HD11	5:P:43:LEU:HD21	1.84	0.58
1:D:45:LEU:HD11	2:E:153:TRP:HB2	1.86	0.58
2:E:93:ARG:HG3	2:E:93:ARG:NH1	2.18	0.58
5:T:14:THR:H	5:T:17:GLN:HE21	1.50	0.58
1:J:112:PHE:O	1:J:144:LEU:HB3	2.02	0.58
2:K:93:ARG:HH11	2:K:93:ARG:HG3	1.68	0.58
4:U:69:GLU:CD	4:U:69:GLU:H	2.10	0.58
1:A:123:ARG:CB	1:A:128:VAL:HG11	2.34	0.58
4:Q:10:VAL:HG22	4:Q:112:LEU:HA	1.83	0.58
1:G:112:PHE:O	1:G:144:LEU:HB3	2.03	0.58
5:T:9:ARG:H	5:T:9:ARG:CD	2.00	0.58
5:T:15:ARG:HG2	5:T:15:ARG:HH11	1.67	0.58
2:K:64:GLN:CB	2:K:67:PHE:HB3	2.34	0.58
4:U:34:TRP:CH2	4:U:90:CYS:HB2	2.39	0.58
1:A:167:HIS:CD2	1:A:169:GLY:H	2.22	0.58
4:M:188:ALA:H	4:M:191:ASN:HD21	1.52	0.58
5:P:156:ASP:HB2	5:P:191:TYR:CE2	2.39	0.58
1:J:104:VAL:HG22	1:J:152:PRO:HB3	1.85	0.58
5:V:230:ARG:O	5:V:231:ALA:O	2.21	0.58
1:G:53:SER:HB2	3:I:3:PHE:CE1	2.39	0.58
1:G:147:LYS:NZ	1:G:149:HIS:CE1	2.72	0.58
4:S:153:SER:HA	4:S:160:ILE:CB	2.33	0.58
4:U:191:ASN:H	4:U:191:ASN:HD22	1.50	0.58
3:C:1:VAL:HG23	3:C:1:VAL:O	2.04	0.58
5:P:100:VAL:O	5:P:101:ASN:CB	2.52	0.58
5:P:152:GLY:C	5:P:190:ARG:HD2	2.29	0.58
3:F:14:GLY:CA	5:T:27:SER:HB2	2.34	0.58
4:Q:65:THR:HG21	4:Q:67:ARG:CZ	2.34	0.58
4:S:14:GLU:O	4:S:15:GLU:CB	2.51	0.58
4:S:51:LYS:HD3	4:S:53:ASP:OD2	2.03	0.58
5:T:118:GLU:H	5:T:118:GLU:CD	2.05	0.58
5:T:221:SER:O	5:T:223:ASN:N	2.37	0.58
1:J:156:SER:CB	1:J:180:PHE:HB3	2.33	0.58
4:M:176:ASN:O	4:M:177:SER:HB3	2.03	0.58
5:P:116:VAL:HG13	5:P:116:VAL:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:35:TYR:CE1	4:Q:45:LEU:HD23	2.39	0.58
4:Q:38:TYR:HB3	4:Q:39:PRO:CD	2.34	0.58
4:Q:122:ASP:O	4:Q:122:ASP:OD2	2.22	0.58
1:G:4:GLU:N	2:H:17:PHE:O	2.37	0.58
1:J:134:GLU:HB3	1:J:149:HIS:CD2	2.39	0.58
4:U:49:ALA:HB2	4:U:73:PHE:CZ	2.39	0.58
5:P:13:LYS:O	5:P:116:VAL:HA	2.04	0.57
5:R:107:PHE:CD2	5:R:107:PHE:N	2.72	0.57
1:G:159:ASP:HB3	1:G:161:TYR:CE1	2.38	0.57
4:S:179:VAL:HG21	5:T:196:ARG:HD3	1.85	0.57
1:J:16:PRO:O	1:J:18:GLN:HG2	2.03	0.57
2:K:97:PRO:HB3	2:K:119:VAL:HG13	1.85	0.57
4:U:55:LYS:O	4:U:56:GLY:C	2.47	0.57
5:V:133:PRO:HB2	5:V:138:ILE:HD11	1.86	0.57
5:V:224:ASP:O	5:V:232:LYS:NZ	2.32	0.57
5:P:130:VAL:HG23	5:P:240:ALA:HB3	1.85	0.57
2:E:119:VAL:HG12	2:E:122:PHE:CD2	2.39	0.57
2:H:67:PHE:HE1	2:H:71:ARG:NH2	2.03	0.57
5:P:38:THR:HG22	5:P:39:PRO:HD2	1.86	0.57
5:P:197:LEU:HD12	5:P:198:ARG:H	1.69	0.57
4:Q:58:ASN:C	4:Q:61:GLY:N	2.58	0.57
5:T:204:TRP:C	5:T:206:ASN:H	2.12	0.57
2:K:127:ILE:HD13	2:K:128:GLU:H	1.67	0.57
1:A:82:ILE:HG12	2:B:33:ASN:HB3	1.86	0.57
1:G:44:ARG:HG3	1:G:44:ARG:O	2.03	0.57
1:J:17:ASP:OD1	2:K:6:ARG:NE	2.37	0.57
2:B:172:THR:HA	2:B:186:VAL:O	2.05	0.57
3:F:6:ASN:HD22	3:F:7:ILE:N	2.01	0.57
5:R:160:LEU:HD13	5:R:195:SER:HB2	1.86	0.57
4:S:2:SER:HB3	4:S:25:THR:HB	1.85	0.57
2:K:142:VAL:CG1	2:K:143:VAL:N	2.67	0.57
3:C:5:LYS:HD3	5:P:101:ASN:ND2	2.20	0.57
5:P:154:TYR:CD1	5:P:155:PRO:HA	2.39	0.57
1:D:62:ASN:OD1	3:F:8:VAL:HG12	2.05	0.57
4:Q:85:SER:HA	4:Q:112:LEU:HD22	1.86	0.57
4:S:17:PHE:CG	4:S:18:LEU:N	2.72	0.57
5:T:96:LEU:HD22	5:T:96:LEU:H	1.68	0.57
1:J:6:VAL:HG13	2:K:16:HIS:CD2	2.39	0.57
1:J:156:SER:HB2	1:J:180:PHE:HB3	1.87	0.57
4:U:18:LEU:HD12	4:U:77:LYS:HB3	1.87	0.57
4:U:34:TRP:CG	4:U:75:LEU:HG	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:SER:HA	2:B:120:ASN:ND2	2.20	0.57
5:P:152:GLY:O	5:P:190:ARG:HD2	2.04	0.57
1:D:43:TRP:HZ2	1:D:53:SER:HA	1.69	0.57
2:E:27:LEU:CD1	2:E:41:ASP:HA	2.35	0.57
2:H:1:GLY:N	2:H:4:ARG:HB2	2.19	0.57
2:B:127:ILE:HD12	2:B:129:VAL:HG23	1.85	0.57
4:M:72:SER:HB2	4:M:74:HIS:CE1	2.40	0.57
5:P:130:VAL:C	5:P:131:PHE:HD1	2.12	0.57
1:G:100:ARG:N	1:G:155:PRO:HG2	2.19	0.57
4:S:43:LEU:HD12	5:T:108:PHE:CE2	2.40	0.57
1:J:92:LEU:HD23	1:J:92:LEU:N	2.20	0.57
1:J:107:CYS:HB2	1:J:121:TRP:CH2	2.40	0.57
4:U:29:TYR:N	4:U:29:TYR:CD1	2.71	0.57
4:U:103:LYS:C	4:U:104:LEU:HD23	2.29	0.57
5:V:29:HIS:CD2	5:V:96:LEU:HD22	2.40	0.57
4:Q:14:GLU:O	4:Q:15:GLU:CB	2.52	0.57
5:T:118:GLU:OE1	5:T:118:GLU:N	2.36	0.57
4:U:87:VAL:HG22	4:U:111:ARG:HA	1.87	0.57
5:P:72:ASN:ND2	5:P:74:ARG:H	2.03	0.57
1:J:135:THR:O	1:J:147:LYS:HG3	2.05	0.57
5:V:64:ARG:CZ	5:V:83:GLU:OE2	2.52	0.57
2:E:155:PHE:CD1	2:E:155:PHE:N	2.73	0.56
3:I:7:ILE:HG22	5:T:100:VAL:HG22	1.87	0.56
5:T:156:ASP:OD1	5:T:156:ASP:O	2.23	0.56
4:U:128:LEU:O	4:U:137:SER:CB	2.53	0.56
2:E:172:THR:HG23	2:E:186:VAL:O	2.05	0.56
2:H:61:TRP:HA	2:H:61:TRP:CE3	2.40	0.56
4:S:94:GLY:N	5:T:101:ASN:ND2	2.52	0.56
2:B:64:GLN:HB3	2:B:67:PHE:HB3	1.86	0.56
4:M:16:ALA:O	4:M:78:GLY:HA2	2.05	0.56
4:Q:32:LEU:HD23	4:Q:92:LEU:HB3	1.87	0.56
5:R:46:LEU:HD13	5:R:60:PHE:CE1	2.39	0.56
4:S:46:LEU:HD12	4:S:58:ASN:HD21	1.69	0.56
5:T:19:VAL:HG23	5:T:82:LEU:HD11	1.86	0.56
1:J:33:HIS:CD2	1:J:42:VAL:HB	2.40	0.56
2:K:70:ASP:OD1	2:K:70:ASP:O	2.24	0.56
2:K:115:LEU:O	2:K:160:MET:HA	2.04	0.56
2:K:123:TYR:HA	2:K:124:PRO:C	2.31	0.56
2:K:172:THR:CG2	2:K:173:CYS:N	2.68	0.56
5:V:45:PHE:HD1	5:V:58:GLY:HA3	1.70	0.56
5:P:227:THR:O	5:P:228:GLN:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:31:ILE:HG23	2:H:36:GLU:N	2.21	0.56
5:V:72:ASN:ND2	5:V:72:ASN:N	2.47	0.56
5:V:155:PRO:CG	5:V:157:HIS:HD2	2.19	0.56
4:M:94:GLY:HA3	5:P:101:ASN:OD1	2.06	0.56
2:E:81:HIS:CE1	3:F:5:LYS:NZ	2.73	0.56
5:R:1:GLY:HA2	5:R:5:THR:HG21	1.86	0.56
1:J:12:PHE:CE2	1:J:21:GLU:HB3	2.39	0.56
1:J:138:LEU:HB3	1:J:146:ARG:HH21	1.69	0.56
5:P:50:PHE:C	5:P:52:GLU:H	2.14	0.56
4:Q:10:VAL:HG23	4:Q:11:THR:H	1.71	0.56
5:T:182:GLU:C	5:T:184:PRO:HD3	2.30	0.56
4:U:21:ASN:HD22	4:U:21:ASN:N	2.04	0.56
5:P:130:VAL:HG12	5:P:131:PHE:N	2.21	0.56
1:D:153:PHE:CE2	1:D:155:PRO:HA	2.41	0.56
2:H:31:ILE:HD12	2:H:31:ILE:N	2.21	0.56
4:S:128:LEU:CB	5:T:131:PHE:HB3	2.35	0.56
4:U:47:LEU:CD1	4:U:75:LEU:HD21	2.36	0.56
5:P:79:VAL:HG23	5:P:82:LEU:HD21	1.88	0.56
4:Q:171:MET:C	4:Q:173:PHE:H	2.13	0.56
2:H:64:GLN:CB	2:H:67:PHE:HB3	2.36	0.56
5:T:149:LEU:HD23	5:T:193:LEU:O	2.05	0.56
1:J:44:ARG:O	1:J:44:ARG:HG3	2.05	0.56
5:V:238:VAL:HG12	5:V:239:SER:H	1.71	0.56
2:E:155:PHE:N	2:E:155:PHE:HD1	2.03	0.56
4:Q:198:ILE:HG13	4:Q:199:PRO:N	2.20	0.56
1:G:70:LEU:HD12	1:G:70:LEU:O	2.06	0.56
1:G:77:SER:O	1:G:78:ASN:HB2	2.06	0.56
1:G:138:LEU:HD12	1:G:148:PHE:HE1	1.71	0.56
2:H:34:GLN:HG2	2:H:34:GLN:O	2.06	0.56
5:V:79:VAL:HG23	5:V:82:LEU:HD21	1.88	0.56
2:B:166:ARG:O	2:B:167:SER:CB	2.53	0.56
4:M:14:GLU:HB2	4:M:116:PRO:CA	2.33	0.56
4:M:32:LEU:N	4:M:32:LEU:HD12	2.21	0.56
1:D:117:VAL:HG23	1:D:166:GLU:O	2.06	0.56
1:D:162:ASP:HB3	1:D:175:LEU:CD2	2.36	0.56
4:Q:115:ARG:O	4:Q:116:PRO:C	2.48	0.56
5:R:113:ARG:CG	5:R:157:HIS:HE1	2.19	0.56
2:H:1:GLY:H3	2:H:4:ARG:HE	1.54	0.56
4:S:57:SER:O	4:S:58:ASN:O	2.22	0.56
1:J:162:ASP:OD1	1:J:177:HIS:HB3	2.06	0.56
4:U:45:LEU:HD23	4:U:46:LEU:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:117:ASP:O	4:U:118:ILE:CB	2.52	0.56
5:V:232:LYS:O	5:V:234:VAL:N	2.38	0.56
1:D:62:ASN:ND2	3:F:8:VAL:HG12	2.21	0.55
1:G:162:ASP:HA	1:G:176:LYS:O	2.06	0.55
2:B:44:VAL:O	2:B:44:VAL:HG12	2.06	0.55
4:Q:123:PRO:CB	4:Q:201:ASP:OD1	2.54	0.55
5:R:226:TRP:CD1	5:R:232:LYS:HA	2.41	0.55
4:S:24:TYR:CE1	4:S:32:LEU:HD21	2.41	0.55
4:S:191:ASN:O	4:S:194:ASN:ND2	2.39	0.55
5:T:11:LEU:O	5:T:114:LEU:HD12	2.06	0.55
2:K:94:ARG:HA	2:K:124:PRO:HD3	1.88	0.55
5:V:133:PRO:HD3	5:V:146:LEU:CD1	2.36	0.55
2:B:147:LEU:HG	2:B:155:PHE:HD2	1.70	0.55
5:P:99:ARG:HG2	5:P:99:ARG:HH11	1.72	0.55
5:R:42:GLY:O	5:R:43:LEU:C	2.49	0.55
5:R:130:VAL:HG23	5:R:240:ALA:CB	2.33	0.55
5:R:206:ASN:HB3	5:R:209:ASN:ND2	2.19	0.55
4:S:161:THR:HG23	4:S:180:ALA:O	2.07	0.55
5:T:121:LYS:O	5:T:230:ARG:NH2	2.39	0.55
4:U:118:ILE:HG23	4:U:119:GLN:N	2.21	0.55
2:B:28:HIS:HE1	3:C:9:THR:HG21	1.71	0.55
2:E:102:TYR:N	2:E:102:TYR:HD1	2.03	0.55
4:Q:151:SER:O	4:Q:152:GLN:O	2.25	0.55
4:S:27:THR:HG22	4:S:27:THR:O	2.05	0.55
5:T:70:PHE:HE2	5:T:74:ARG:NH2	2.04	0.55
5:V:64:ARG:NH1	5:V:65:PHE:CE1	2.66	0.55
5:V:138:ILE:HD12	5:V:144:ALA:HB2	1.88	0.55
2:B:2:ASP:O	2:B:3:THR:HG22	2.06	0.55
2:B:6:ARG:HH21	2:B:6:ARG:HG3	1.72	0.55
2:E:166:ARG:O	2:E:167:SER:CB	2.54	0.55
5:R:114:LEU:O	5:R:115:THR:CB	2.55	0.55
5:R:150:ALA:O	5:R:192:SER:HA	2.06	0.55
4:S:169:ARG:C	4:S:171:MET:H	2.15	0.55
5:T:84:LEU:HA	5:T:116:VAL:HG13	1.88	0.55
5:V:10:TYR:HD2	5:V:157:HIS:ND1	2.04	0.55
5:T:11:LEU:O	5:T:114:LEU:O	2.25	0.55
5:T:38:THR:O	5:T:40:GLY:N	2.40	0.55
5:V:6:GLN:O	5:V:7:THR:HG23	2.07	0.55
4:Q:47:LEU:HD22	4:Q:55:LYS:O	2.06	0.55
5:T:114:LEU:HD12	5:T:114:LEU:C	2.30	0.55
1:A:162:ASP:HB3	1:A:175:LEU:CD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:GLN:C	2:B:66:ASP:N	2.64	0.55
4:Q:82:VAL:HA	4:Q:114:VAL:HG11	1.89	0.55
4:Q:145:ASP:O	4:Q:147:GLN:N	2.40	0.55
5:R:115:THR:HG21	5:R:155:PRO:HB3	1.88	0.55
1:G:61:ALA:O	1:G:65:VAL:HG23	2.07	0.55
3:I:3:PHE:HB2	4:S:99:ASP:CB	2.37	0.55
1:J:26:PHE:CE2	2:K:90:THR:HB	2.42	0.55
2:K:156:GLN:HG3	2:K:156:GLN:O	2.07	0.55
1:A:6:VAL:CG1	2:B:16:HIS:HD2	2.20	0.55
5:P:48:GLU:HG2	5:P:49:TYR:H	1.71	0.55
5:T:26:ILE:HD12	5:T:29:HIS:CE1	2.41	0.55
5:T:51:ASN:O	5:T:51:ASN:CG	2.48	0.55
3:L:8:VAL:O	3:L:9:THR:CG2	2.55	0.55
5:V:8:PRO:O	5:V:112:THR:HB	2.07	0.55
1:A:81:PRO:HB3	2:B:7:PHE:CZ	2.42	0.55
2:B:86:GLY:O	2:B:90:THR:HG23	2.07	0.55
4:Q:81:GLN:O	4:Q:114:VAL:HG21	2.07	0.55
5:R:49:TYR:CZ	5:R:54:GLN:HG3	2.42	0.55
5:R:206:ASN:HD22	5:R:209:ASN:HD21	1.55	0.55
3:I:5:LYS:HE3	5:T:101:ASN:OD1	2.06	0.55
4:S:179:VAL:HG11	5:T:147:VAL:HG11	1.89	0.55
1:A:140:ARG:HD3	1:A:144:LEU:HB2	1.89	0.54
5:P:175:THR:HG23	5:P:195:SER:CB	2.36	0.54
5:P:237:ILE:HB	2:E:2:ASP:HB3	1.89	0.54
1:G:6:VAL:HG13	2:H:16:HIS:HD2	1.72	0.54
2:H:62:ASN:HA	2:H:68:LEU:HD22	1.88	0.54
4:M:16:ALA:O	4:M:79:SER:N	2.39	0.54
5:P:19:VAL:CG2	5:P:82:LEU:HD11	2.36	0.54
2:H:8:LEU:HD12	2:H:9:GLN:N	2.22	0.54
4:S:161:THR:CG2	4:S:179:VAL:O	2.55	0.54
5:T:35:TYR:CE1	5:T:45:PHE:CD2	2.92	0.54
5:T:221:SER:N	5:T:224:ASP:OD2	2.27	0.54
1:J:36:MET:HE1	1:J:63:ILE:HG13	1.90	0.54
1:J:110:ASP:HB2	1:J:140:ARG:HH12	1.72	0.54
4:U:180:ALA:HB3	4:U:193:PHE:CE1	2.43	0.54
1:A:19:SER:HA	5:R:222:GLU:OE1	2.07	0.54
4:M:46:LEU:HG	4:M:47:LEU:HG	1.90	0.54
4:M:202:THR:HG22	4:M:203:PHE:N	2.22	0.54
5:P:1:GLY:HA3	5:P:5:THR:HG21	1.89	0.54
2:E:63:SER:HA	5:T:107:PHE:HE1	1.72	0.54
5:R:120:LEU:HD11	5:R:220:LEU:CD2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:ILE:HD13	1:G:83:THR:O	2.07	0.54
4:S:34:TRP:O	4:S:46:LEU:CB	2.53	0.54
4:U:41:GLU:HG2	5:V:110:GLN:NE2	2.22	0.54
4:M:57:SER:HA	4:M:62:PHE:O	2.06	0.54
1:J:156:SER:OG	1:J:180:PHE:HB3	2.08	0.54
1:A:153:PHE:C	1:A:153:PHE:CD2	2.85	0.54
2:B:78:TYR:CD2	3:C:7:ILE:HD11	2.42	0.54
5:P:84:LEU:HD23	5:P:116:VAL:O	2.08	0.54
4:Q:1:ASP:O	4:Q:2:SER:HB3	2.07	0.54
1:G:56:ALA:O	1:G:58:GLY:N	2.40	0.54
2:H:37:ASP:OD1	2:H:54:GLY:CA	2.56	0.54
2:H:170:VAL:HG23	2:H:171:TYR:N	2.23	0.54
1:A:17:ASP:O	1:A:18:GLN:HB2	2.08	0.54
2:B:38:LEU:HD12	2:B:48:ARG:O	2.07	0.54
1:D:29:ASP:HB3	2:E:153:TRP:CD1	2.42	0.54
2:E:147:LEU:HG	2:E:155:PHE:HD2	1.73	0.54
4:Q:51:LYS:HZ2	4:Q:53:ASP:CG	2.16	0.54
2:K:69:GLU:O	2:K:72:ARG:N	2.41	0.54
1:D:87:PRO:HD3	1:D:167:HIS:CD2	2.43	0.54
5:R:160:LEU:HD21	5:R:213:CYS:SG	2.48	0.54
5:T:226:TRP:CZ2	5:T:233:PRO:HD3	2.43	0.54
1:A:144:LEU:HD23	1:A:144:LEU:N	2.22	0.54
2:H:86:GLY:O	2:H:90:THR:HG23	2.08	0.54
4:U:121:PRO:O	4:U:122:ASP:HB3	2.07	0.54
5:V:131:PHE:N	5:V:131:PHE:CD1	2.75	0.54
2:B:64:GLN:CB	2:B:67:PHE:HB3	2.38	0.54
2:B:129:VAL:HG22	2:B:175:VAL:HG22	1.88	0.54
4:M:158:VAL:O	4:M:159:TYR:CB	2.54	0.54
5:R:134:SER:O	5:R:138:ILE:CG1	2.56	0.54
5:R:226:TRP:HB2	5:R:232:LYS:HE2	1.89	0.54
4:S:24:TYR:OH	4:S:66:TYR:HE2	1.90	0.54
4:S:142:THR:HA	4:S:177:SER:HB3	1.90	0.54
5:T:29:HIS:HA	5:T:96:LEU:HD13	1.88	0.54
2:K:141:GLY:O	2:K:142:VAL:CB	2.54	0.54
2:K:168:GLY:O	2:K:170:VAL:N	2.41	0.54
5:V:137:GLU:O	5:V:137:GLU:HG2	2.07	0.54
5:V:138:ILE:HD13	5:V:143:LYS:O	2.07	0.54
4:M:10:VAL:CG1	4:M:112:LEU:HA	2.31	0.54
4:M:62:PHE:CZ	4:M:77:LYS:HD3	2.42	0.54
2:E:78:TYR:CZ	3:F:7:ILE:HD11	2.42	0.54
4:Q:64:ALA:O	4:Q:73:PHE:CE2	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:85:SER:O	4:Q:86:ALA:O	2.25	0.54
4:U:188:ALA:O	4:U:191:ASN:ND2	2.41	0.54
1:A:85:VAL:HG21	2:B:34:GLN:HE22	1.73	0.53
1:A:97:VAL:HG21	1:A:178:TRP:HZ2	1.72	0.53
3:C:8:VAL:HG21	5:P:55:ARG:HH21	1.73	0.53
5:T:89:LEU:HD23	5:T:89:LEU:C	2.33	0.53
5:T:121:LYS:CD	5:T:230:ARG:HH21	2.17	0.53
2:K:69:GLU:O	2:K:71:ARG:N	2.41	0.53
2:K:142:VAL:HG12	2:K:143:VAL:N	2.22	0.53
1:A:104:VAL:HA	1:A:152:PRO:HA	1.90	0.53
2:B:70:ASP:CG	5:P:99:ARG:HG3	2.33	0.53
1:D:56:ALA:O	1:D:59:ALA:N	2.28	0.53
4:Q:10:VAL:O	4:Q:11:THR:CB	2.56	0.53
4:S:14:GLU:O	4:S:15:GLU:HB3	2.07	0.53
1:J:77:SER:OG	1:J:80:THR:HG23	2.07	0.53
2:K:31:ILE:HG23	2:K:35:GLU:C	2.33	0.53
5:V:123:VAL:HG12	5:V:233:PRO:HB3	1.88	0.53
1:A:69:ASN:O	1:A:73:MET:HG2	2.09	0.53
4:M:51:LYS:HD3	4:M:53:ASP:OD2	2.07	0.53
4:M:188:ALA:O	4:M:191:ASN:ND2	2.42	0.53
2:E:45:GLY:O	2:E:46:GLU:HB3	2.09	0.53
4:Q:46:LEU:HD12	4:Q:58:ASN:ND2	2.22	0.53
2:H:148:ILE:HB	2:H:156:GLN:O	2.08	0.53
5:T:50:PHE:CB	5:T:55:ARG:HH11	2.20	0.53
4:U:5:GLN:HE22	4:U:90:CYS:H	1.57	0.53
4:U:160:ILE:CB	4:U:180:ALA:CA	2.86	0.53
5:V:84:LEU:HA	5:V:116:VAL:HG13	1.90	0.53
1:A:26:PHE:O	1:A:27:ASP:C	2.51	0.53
1:A:82:ILE:HD13	1:A:83:THR:H	1.72	0.53
1:A:119:VAL:HB	1:A:149:HIS:CE1	2.43	0.53
4:M:29:TYR:N	4:M:30:PRO:HD3	2.22	0.53
4:M:48:LYS:O	4:M:49:ALA:CB	2.56	0.53
4:M:62:PHE:CD1	4:M:75:LEU:HD21	2.43	0.53
5:P:38:THR:HG23	5:P:88:ALA:HB2	1.89	0.53
5:P:220:LEU:CD1	5:P:233:PRO:HD2	2.39	0.53
1:D:62:ASN:CG	3:F:8:VAL:HG12	2.34	0.53
1:D:109:ILE:HG12	1:D:147:LYS:O	2.08	0.53
2:E:93:ARG:HD3	2:E:123:TYR:CE1	2.44	0.53
4:Q:174:LYS:O	4:Q:175:SER:HB3	2.08	0.53
4:S:167:ASP:HA	4:S:174:LYS:CB	2.38	0.53
1:J:11:GLU:HA	1:J:21:GLU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:3:GLY:C	5:V:26:ILE:HD13	2.33	0.53
5:V:133:PRO:HD3	5:V:146:LEU:HD12	1.91	0.53
5:V:234:VAL:O	5:V:236:GLN:HG2	2.09	0.53
1:A:32:PHE:CD2	1:A:41:THR:HG22	2.42	0.53
4:M:165:VAL:HG12	4:M:166:LEU:O	2.09	0.53
2:H:101:VAL:HG13	2:H:116:VAL:O	2.09	0.53
2:H:177:HIS:ND1	2:H:178:PRO:HD2	2.24	0.53
4:S:10:VAL:CB	4:S:112:LEU:HA	2.38	0.53
5:T:237:ILE:HG22	5:T:238:VAL:N	2.23	0.53
5:V:113:ARG:HG2	5:V:113:ARG:HH11	1.72	0.53
4:M:24:TYR:CE2	4:M:26:ALA:HB2	2.42	0.53
1:G:77:SER:O	1:G:80:THR:CG2	2.57	0.53
4:S:193:PHE:O	4:S:195:ASN:N	2.41	0.53
5:T:29:HIS:ND1	5:T:94:SER:OG	2.40	0.53
1:J:77:SER:CB	1:J:80:THR:HG23	2.38	0.53
4:U:54:ASP:HB2	4:U:65:THR:OG1	2.08	0.53
5:V:13:LYS:HD2	5:V:17:GLN:HE22	1.74	0.53
5:V:128:VAL:H	5:V:238:VAL:HG11	1.73	0.53
3:C:5:LYS:HD3	5:P:101:ASN:HD21	1.73	0.53
5:R:131:PHE:CE1	5:R:149:LEU:HD13	2.43	0.53
5:R:186:LEU:C	5:R:188:ASP:N	2.67	0.53
4:S:192:ALA:C	4:S:194:ASN:H	2.17	0.53
5:T:237:ILE:HD12	2:K:2:ASP:N	2.22	0.53
5:V:116:VAL:HG22	5:V:116:VAL:O	2.08	0.53
5:V:238:VAL:HG12	5:V:239:SER:N	2.24	0.53
1:A:13:TYR:HE1	1:A:15:ASN:OD1	1.91	0.53
2:B:93:ARG:HD3	2:B:123:TYR:CD1	2.44	0.53
2:E:50:VAL:HG12	2:E:51:THR:HG23	1.91	0.53
1:G:122:LEU:O	1:G:161:TYR:HA	2.09	0.53
5:T:221:SER:O	5:T:222:GLU:C	2.52	0.53
1:J:98:GLU:O	1:J:99:LEU:C	2.51	0.53
2:H:62:ASN:HA	2:H:68:LEU:HD21	1.90	0.53
5:T:48:GLU:OE1	5:T:55:ARG:HD3	2.09	0.53
5:T:64:ARG:NH2	5:T:86:ASP:OD2	2.42	0.53
5:V:84:LEU:HD23	5:V:116:VAL:O	2.09	0.53
4:M:198:ILE:CD1	4:M:201:ASP:CB	2.87	0.53
4:Q:139:CYS:SG	4:Q:187:PHE:CE1	2.99	0.53
5:R:15:ARG:HG2	5:R:15:ARG:HH11	1.73	0.53
5:R:212:ARG:NH1	5:R:214:GLN:HE22	2.06	0.53
2:H:81:HIS:HB2	4:S:29:TYR:HD1	1.73	0.53
1:J:73:MET:HE1	2:K:53:LEU:HG	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:77:SER:HB2	1:J:80:THR:HG23	1.91	0.53
4:U:82:VAL:HA	4:U:114:VAL:CG1	2.38	0.53
2:E:28:HIS:CE1	3:F:9:THR:HG21	2.44	0.52
2:E:38:LEU:HD13	2:E:57:ASP:HB2	1.91	0.52
5:R:12:ILE:HD11	5:R:155:PRO:CD	2.40	0.52
1:G:113:THR:HG22	1:G:144:LEU:HD22	1.90	0.52
2:H:8:LEU:HD12	2:H:9:GLN:H	1.74	0.52
3:I:2:HIS:N	3:I:2:HIS:ND1	2.57	0.52
4:S:159:TYR:N	4:S:159:TYR:CD2	2.69	0.52
5:T:103:GLU:O	5:T:106:ALA:HB3	2.09	0.52
1:J:26:PHE:HB2	1:J:31:ILE:HD11	1.90	0.52
5:V:128:VAL:HG21	5:V:215:VAL:HB	1.90	0.52
1:A:68:ALA:O	1:A:72:ILE:HG13	2.08	0.52
4:M:15:GLU:O	4:M:16:ALA:HB2	2.09	0.52
5:P:6:GLN:NE2	5:P:111:GLY:CA	2.67	0.52
4:Q:38:TYR:HD1	4:Q:86:ALA:HB2	1.73	0.52
4:Q:56:GLY:O	4:Q:57:SER:O	2.28	0.52
4:S:201:ASP:O	4:S:203:PHE:N	2.39	0.52
5:T:162:TRP:HZ3	5:T:195:SER:OG	1.92	0.52
1:A:162:ASP:HB3	1:A:175:LEU:HD23	1.91	0.52
5:P:124:PHE:CE1	5:P:230:ARG:CZ	2.92	0.52
5:R:100:VAL:O	5:R:101:ASN:HB2	2.09	0.52
1:G:142:ASP:O	1:G:143:HIS:HB2	2.10	0.52
4:S:70:THR:O	4:S:71:THR:C	2.53	0.52
5:T:46:LEU:HD13	5:T:60:PHE:CE1	2.44	0.52
2:B:55:ARG:HG3	2:B:55:ARG:NH1	2.19	0.52
2:B:165:PRO:O	2:B:166:ARG:CG	2.57	0.52
5:P:157:HIS:O	5:P:218:TYR:HD1	1.92	0.52
5:T:50:PHE:N	5:T:69:GLN:HE22	2.07	0.52
2:B:174:GLN:CA	2:B:185:THR:HG22	2.30	0.52
4:M:38:TYR:HB3	4:M:39:PRO:CD	2.39	0.52
4:M:58:ASN:O	4:M:61:GLY:N	2.43	0.52
4:M:62:PHE:HD1	4:M:75:LEU:HD21	1.74	0.52
1:D:82:ILE:HG12	2:E:33:ASN:CB	2.39	0.52
4:Q:15:GLU:OE2	4:Q:15:GLU:C	2.52	0.52
4:Q:17:PHE:O	4:Q:18:LEU:O	2.28	0.52
5:R:11:LEU:O	5:R:114:LEU:O	2.27	0.52
5:R:119:ASP:OD2	5:R:119:ASP:C	2.52	0.52
1:G:89:VAL:HG22	1:G:109:ILE:HD12	1.90	0.52
4:S:92:LEU:C	4:S:92:LEU:CD1	2.82	0.52
1:J:55:GLU:O	1:J:56:ALA:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:104:VAL:HA	1:J:152:PRO:HA	1.92	0.52
5:R:5:THR:OG1	5:R:24:SER:HB3	2.09	0.52
5:T:42:GLY:O	5:T:43:LEU:C	2.52	0.52
5:T:146:LEU:O	5:T:196:ARG:HA	2.09	0.52
1:J:44:ARG:O	1:J:45:LEU:HG	2.10	0.52
2:K:142:VAL:HG12	2:K:143:VAL:O	2.09	0.52
4:U:10:VAL:HG13	4:U:11:THR:H	1.75	0.52
5:V:80:SER:O	5:V:81:THR:C	2.51	0.52
2:E:142:VAL:HA	2:E:160:MET:O	2.10	0.52
4:Q:57:SER:O	4:Q:58:ASN:HB3	2.10	0.52
5:R:152:GLY:C	5:R:190:ARG:HD2	2.35	0.52
2:H:167:SER:C	2:H:169:GLU:N	2.64	0.52
4:S:5:GLN:NE2	4:S:109:GLY:H	2.07	0.52
4:S:85:SER:HA	4:S:112:LEU:HD22	1.92	0.52
5:T:219:GLY:O	5:T:220:LEU:C	2.53	0.52
4:U:34:TRP:CZ3	4:U:90:CYS:HB2	2.45	0.52
5:V:52:GLU:HA	5:V:69:GLN:HB3	1.92	0.52
5:P:6:GLN:CD	5:P:111:GLY:HA2	2.35	0.52
1:D:122:LEU:HD23	1:D:127:PRO:HA	1.92	0.52
1:D:135:THR:O	1:D:136:VAL:O	2.26	0.52
4:Q:65:THR:HG21	4:Q:67:ARG:NE	2.24	0.52
4:Q:78:GLY:O	4:Q:79:SER:CB	2.58	0.52
5:R:114:LEU:C	5:R:114:LEU:HD12	2.34	0.52
1:G:87:PRO:HD2	1:G:170:LEU:HD21	1.91	0.52
5:T:138:ILE:C	5:T:140:HIS:N	2.65	0.52
5:T:230:ARG:HG3	5:T:230:ARG:NH1	2.24	0.52
1:J:101:GLU:N	1:J:155:PRO:HG3	2.23	0.52
3:L:1:VAL:CG1	4:U:99:ASP:CG	2.80	0.52
5:V:124:PHE:HE1	5:V:230:ARG:CZ	2.19	0.52
4:M:18:LEU:HD11	4:M:20:ILE:HD11	1.91	0.52
4:M:35:TYR:HE1	4:M:45:LEU:HG	1.74	0.52
4:M:122:ASP:N	4:M:123:PRO:CD	2.73	0.52
5:P:32:VAL:HG13	5:P:92:CYS:SG	2.50	0.52
1:D:59:ALA:O	1:D:62:ASN:HB2	2.09	0.52
2:E:27:LEU:HD12	2:E:41:ASP:HA	1.91	0.52
5:R:10:TYR:HD2	5:R:157:HIS:ND1	2.08	0.52
5:R:138:ILE:CD1	5:R:144:ALA:HA	2.40	0.52
5:T:21:LEU:N	5:T:21:LEU:CD1	2.72	0.52
1:J:62:ASN:OD1	3:L:8:VAL:HG12	2.09	0.52
1:A:70:LEU:HD13	2:B:9:GLN:HB2	1.91	0.52
2:B:145:THR:HG23	2:B:158:LEU:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:145:ASP:C	4:M:147:GLN:H	2.16	0.52
5:P:175:THR:O	5:P:176:ASP:C	2.53	0.52
1:J:36:MET:CE	1:J:63:ILE:HG13	2.40	0.52
2:B:13:TYR:HE2	2:B:28:HIS:CD2	2.27	0.51
5:P:148:CYS:O	5:P:149:LEU:HD23	2.10	0.51
1:D:11:GLU:HA	1:D:21:GLU:O	2.10	0.51
2:E:41:ASP:OD1	2:E:43:ASP:HB2	2.10	0.51
5:R:50:PHE:HB2	5:R:55:ARG:NH1	2.25	0.51
5:R:114:LEU:O	5:R:115:THR:HB	2.09	0.51
1:G:140:ARG:HD2	1:G:146:ARG:CG	2.40	0.51
1:J:82:ILE:HG12	2:K:33:ASN:HB3	1.91	0.51
2:K:24:VAL:CG2	2:K:80:ARG:HE	2.23	0.51
2:K:69:GLU:O	2:K:70:ASP:C	2.53	0.51
2:K:133:ARG:C	2:K:135:SER:N	2.68	0.51
5:P:26:ILE:O	5:P:27:SER:C	2.53	0.51
5:P:35:TYR:CA	5:P:46:LEU:HD23	2.40	0.51
5:R:185:ALA:O	5:R:186:LEU:C	2.53	0.51
4:S:66:TYR:C	4:S:66:TYR:CD2	2.88	0.51
5:T:36:GLN:HG2	5:T:38:THR:CG2	2.41	0.51
2:K:32:TYR:O	2:K:33:ASN:HB2	2.10	0.51
2:K:102:TYR:CE2	2:K:116:VAL:CB	2.93	0.51
4:M:126:TYR:CZ	5:P:137:GLU:HA	2.45	0.51
2:E:77:THR:O	3:F:5:LYS:CE	2.58	0.51
5:T:96:LEU:O	5:T:97:ALA:HB3	2.10	0.51
5:P:84:LEU:HA	5:P:116:VAL:CG1	2.40	0.51
1:D:104:VAL:HA	1:D:152:PRO:HA	1.92	0.51
5:R:152:GLY:O	5:R:190:ARG:HD2	2.11	0.51
4:S:43:LEU:HD12	5:T:108:PHE:CZ	2.45	0.51
1:J:168:TRP:CH2	2:K:6:ARG:NE	2.79	0.51
2:K:53:LEU:HG	2:K:53:LEU:O	2.10	0.51
5:V:26:ILE:O	5:V:27:SER:C	2.52	0.51
4:Q:123:PRO:HB2	4:Q:201:ASP:OD1	2.10	0.51
5:R:52:GLU:OE2	5:R:71:SER:HA	2.10	0.51
5:R:162:TRP:HA	5:R:212:ARG:O	2.11	0.51
2:H:15:CYS:HB3	2:H:17:PHE:CZ	2.45	0.51
5:T:147:VAL:HA	5:T:195:SER:O	2.11	0.51
3:L:1:VAL:HG22	3:L:2:HIS:H	1.76	0.51
2:B:134:ASN:O	2:B:135:SER:CB	2.57	0.51
4:M:33:PHE:N	4:M:33:PHE:CD1	2.78	0.51
5:P:79:VAL:CG2	5:P:82:LEU:HD21	2.40	0.51
4:Q:31:SER:OG	4:Q:50:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:94:GLY:HA2	5:T:101:ASN:ND2	2.26	0.51
4:U:114:VAL:O	4:U:114:VAL:HG22	2.10	0.51
1:A:142:ASP:O	1:A:143:HIS:HB2	2.11	0.51
4:M:115:ARG:O	4:M:116:PRO:O	2.28	0.51
5:P:130:VAL:O	5:P:131:PHE:CD1	2.64	0.51
1:D:11:GLU:HG3	1:D:66:ASP:OD2	2.11	0.51
1:D:12:PHE:CD1	1:D:12:PHE:C	2.89	0.51
4:Q:62:PHE:CD1	4:Q:75:LEU:HD21	2.46	0.51
1:G:156:SER:HB2	1:G:180:PHE:HB2	1.93	0.51
2:K:24:VAL:HG21	2:K:80:ARG:HE	1.76	0.51
5:V:77:MET:HE2	5:V:79:VAL:HG13	1.92	0.51
4:M:82:VAL:HG23	4:M:114:VAL:CG1	2.40	0.51
5:P:51:ASN:O	5:P:52:GLU:HB2	2.10	0.51
5:P:87:SER:OG	5:P:116:VAL:HG12	2.10	0.51
4:Q:94:GLY:HA2	5:R:101:ASN:OD1	2.11	0.51
1:G:56:ALA:O	1:G:57:GLN:C	2.52	0.51
4:S:161:THR:HG23	4:S:180:ALA:C	2.35	0.51
4:S:190:ALA:O	4:S:191:ASN:CB	2.58	0.51
1:J:31:ILE:HG22	1:J:43:TRP:HZ3	1.76	0.51
1:A:144:LEU:C	1:A:145:PHE:CD1	2.89	0.51
4:M:82:VAL:HB	4:M:116:PRO:CB	2.41	0.51
5:R:14:THR:O	5:R:15:ARG:C	2.54	0.51
5:R:37:GLN:HB3	5:R:89:LEU:HB3	1.92	0.51
1:G:53:SER:O	3:I:3:PHE:HA	2.11	0.51
1:G:104:VAL:HA	1:G:152:PRO:HA	1.93	0.51
1:J:33:HIS:CE1	1:J:136:VAL:HG11	2.44	0.51
5:P:52:GLU:N	5:P:69:GLN:OE1	2.44	0.51
5:P:68:ARG:HD2	5:P:70:PHE:CE1	2.46	0.51
5:P:128:VAL:HG23	5:P:238:VAL:HG12	1.92	0.51
5:P:146:LEU:HD12	5:P:146:LEU:H	1.76	0.51
1:D:106:ILE:HG12	1:D:150:TYR:CD1	2.46	0.51
2:E:13:TYR:OH	3:F:9:THR:CG2	2.55	0.51
2:H:67:PHE:CZ	2:H:71:ARG:NH2	2.79	0.51
5:T:35:TYR:CA	5:T:46:LEU:HD23	2.40	0.51
5:T:219:GLY:O	5:T:220:LEU:O	2.28	0.51
1:J:13:TYR:CD1	1:J:67:LYS:HA	2.46	0.51
4:U:79:SER:O	4:U:80:VAL:C	2.54	0.51
1:A:41:THR:CG2	1:A:54:PHE:HB3	2.36	0.50
2:B:39:ARG:HG2	2:B:40:PHE:N	2.26	0.50
5:T:79:VAL:HG21	5:T:82:LEU:HD21	1.93	0.50
2:B:55:ARG:NE	5:V:110:GLN:NE2	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:142:VAL:HG22	2:E:161:LEU:CB	2.41	0.50
1:G:128:VAL:O	1:G:129:THR:HG23	2.10	0.50
5:T:74:ARG:HH22	5:T:76:GLU:CD	2.19	0.50
5:T:79:VAL:CG2	5:T:82:LEU:HD21	2.41	0.50
1:D:168:TRP:CH2	2:E:6:ARG:NE	2.79	0.50
4:Q:148:THR:O	4:Q:149:ASN:HB2	2.11	0.50
5:R:50:PHE:O	5:R:53:THR:OG1	2.29	0.50
1:G:136:VAL:HG23	1:G:137:PHE:H	1.76	0.50
4:S:84:ASP:O	4:S:88:TYR:OH	2.23	0.50
4:S:94:GLY:H	5:T:101:ASN:ND2	2.08	0.50
1:J:174:LEU:HD12	1:J:175:LEU:H	1.76	0.50
4:U:38:TYR:HD1	4:U:86:ALA:HB2	1.77	0.50
1:A:180:PHE:HD2	1:A:180:PHE:O	1.95	0.50
2:B:93:ARG:HG3	2:B:93:ARG:NH1	2.26	0.50
2:B:171:TYR:O	2:B:187:GLU:HA	2.11	0.50
4:M:3:VAL:HG12	4:M:105:ILE:HG22	1.93	0.50
5:P:21:LEU:N	5:P:21:LEU:CD1	2.74	0.50
4:Q:191:ASN:ND2	4:Q:191:ASN:N	2.48	0.50
5:R:156:ASP:OD2	5:R:179:PRO:HG2	2.11	0.50
2:H:90:THR:OG1	2:H:91:VAL:N	2.44	0.50
5:R:121:LYS:HA	5:R:226:TRP:HH2	1.76	0.50
1:G:73:MET:O	1:G:74:THR:C	2.52	0.50
5:T:128:VAL:HG11	5:T:239:SER:HA	1.93	0.50
1:J:61:ALA:O	1:J:65:VAL:HG23	2.11	0.50
4:M:17:PHE:CG	4:M:18:LEU:N	2.78	0.50
1:D:45:LEU:O	1:D:46:GLU:C	2.54	0.50
4:Q:179:VAL:HG12	4:Q:180:ALA:N	2.25	0.50
5:R:50:PHE:CA	5:R:69:GLN:HE22	2.25	0.50
5:R:116:VAL:HG13	5:R:116:VAL:O	2.10	0.50
4:S:34:TRP:CG	4:S:75:LEU:HD12	2.46	0.50
1:J:97:VAL:HG21	1:J:178:TRP:CZ2	2.47	0.50
2:K:122:PHE:O	2:K:155:PHE:N	2.43	0.50
5:P:47:PHE:N	5:P:47:PHE:CD1	2.80	0.50
5:P:145:THR:HA	5:P:197:LEU:O	2.12	0.50
5:R:164:VAL:HG12	5:R:165:ASN:CG	2.36	0.50
5:R:223:ASN:OD1	5:R:223:ASN:O	2.30	0.50
1:G:45:LEU:HB2	1:G:48:PHE:CD2	2.46	0.50
2:H:127:ILE:HD13	2:H:128:GLU:H	1.77	0.50
2:H:188:TRP:O	2:H:189:ARG:C	2.54	0.50
4:S:161:THR:HG21	4:S:179:VAL:O	2.11	0.50
5:T:50:PHE:CA	5:T:69:GLN:HE22	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:36:VAL:HG12	4:M:44:GLN:HB2	1.94	0.50
2:E:99:VAL:CG2	2:E:175:VAL:HG21	2.41	0.50
3:F:6:ASN:ND2	3:F:7:ILE:O	2.45	0.50
4:Q:125:VAL:HA	4:Q:140:LEU:O	2.12	0.50
4:S:81:GLN:O	4:S:114:VAL:HG11	2.12	0.50
4:U:34:TRP:CE2	4:U:75:LEU:HG	2.47	0.50
4:U:46:LEU:HB3	4:U:47:LEU:HD12	1.93	0.50
5:P:3:GLY:O	5:P:4:VAL:C	2.54	0.50
1:D:122:LEU:HB2	1:D:162:ASP:HB2	1.94	0.50
2:E:69:GLU:O	2:E:72:ARG:N	2.44	0.50
2:E:69:GLU:O	2:E:70:ASP:C	2.55	0.50
1:G:140:ARG:O	1:G:143:HIS:N	2.38	0.50
3:I:8:VAL:O	3:I:9:THR:CG2	2.60	0.50
1:J:33:HIS:ND1	1:J:136:VAL:CG1	2.74	0.50
2:K:132:PHE:O	2:K:172:THR:N	2.34	0.50
1:A:89:VAL:HG21	1:A:165:VAL:HG21	1.94	0.49
2:B:172:THR:HG23	2:B:186:VAL:O	2.12	0.49
4:M:91:ALA:HB2	4:M:106:PHE:CD1	2.47	0.49
4:M:140:LEU:O	4:M:140:LEU:HG	2.12	0.49
4:M:202:THR:OG1	5:P:140:HIS:HE1	1.95	0.49
3:F:12:THR:CG2	5:T:2:GLY:HA3	2.40	0.49
4:Q:62:PHE:CE2	4:Q:77:LYS:HD2	2.47	0.49
4:Q:87:VAL:HG12	4:Q:88:TYR:N	2.26	0.49
1:G:136:VAL:CG2	1:G:137:PHE:N	2.70	0.49
1:J:101:GLU:H	1:J:155:PRO:HG2	1.73	0.49
2:K:65:LYS:HD3	2:K:68:LEU:HD23	1.94	0.49
4:U:9:PRO:O	4:U:10:VAL:HB	2.11	0.49
4:M:17:PHE:CD1	4:M:18:LEU:N	2.79	0.49
5:P:130:VAL:C	5:P:131:PHE:CD1	2.90	0.49
5:R:14:THR:O	5:R:17:GLN:HG3	2.12	0.49
5:R:87:SER:CB	5:R:115:THR:HA	2.41	0.49
5:R:175:THR:HA	5:R:195:SER:HA	1.95	0.49
5:T:21:LEU:HD23	5:T:112:THR:OG1	2.12	0.49
2:K:62:ASN:HA	2:K:68:LEU:CD2	2.42	0.49
1:A:73:MET:HE1	1:A:76:ARG:NH1	2.27	0.49
2:B:99:VAL:HG22	2:B:119:VAL:HG13	1.93	0.49
5:P:45:PHE:C	5:P:46:LEU:HD22	2.38	0.49
5:P:150:ALA:HB3	5:P:193:LEU:HB3	1.94	0.49
5:P:226:TRP:CZ2	5:P:228:GLN:HB2	2.47	0.49
3:F:8:VAL:O	3:F:9:THR:O	2.30	0.49
4:Q:21:ASN:N	4:Q:21:ASN:ND2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:154:TYR:CZ	5:R:188:ASP:OD2	2.65	0.49
1:G:82:ILE:HD12	1:G:114:PRO:HD3	1.94	0.49
1:G:87:PRO:HB3	1:G:112:PHE:HB3	1.94	0.49
5:T:46:LEU:HD13	5:T:60:PHE:HD1	1.74	0.49
5:T:140:HIS:O	5:T:140:HIS:HD2	1.95	0.49
2:K:52:GLU:O	2:K:54:GLY:N	2.45	0.49
4:U:18:LEU:CD1	4:U:77:LYS:H	2.25	0.49
4:M:34:TRP:O	4:M:46:LEU:HB3	2.13	0.49
4:M:46:LEU:C	4:M:47:LEU:HG	2.36	0.49
4:M:120:ASN:O	4:M:121:PRO:C	2.54	0.49
4:Q:164:THR:CG2	4:Q:165:VAL:H	2.22	0.49
4:S:32:LEU:CD2	4:S:73:PHE:HB2	2.42	0.49
5:T:50:PHE:CB	5:T:55:ARG:NH1	2.74	0.49
5:T:116:VAL:HG13	5:T:116:VAL:O	2.11	0.49
1:A:50:ARG:HG3	1:A:50:ARG:NH2	2.27	0.49
1:A:136:VAL:HG23	1:A:137:PHE:N	2.26	0.49
4:Q:29:TYR:N	4:Q:29:TYR:CD1	2.80	0.49
4:Q:194:ASN:O	4:Q:195:ASN:HB2	2.12	0.49
5:R:80:SER:O	5:R:81:THR:C	2.55	0.49
1:G:32:PHE:HB3	1:G:43:TRP:CE3	2.48	0.49
1:G:50:ARG:C	1:G:51:PHE:HD2	2.20	0.49
1:G:135:THR:O	1:G:147:LYS:CE	2.60	0.49
4:S:11:THR:HA	4:S:113:LEU:O	2.13	0.49
1:J:48:PHE:O	1:J:50:ARG:N	2.46	0.49
2:K:77:THR:HA	4:U:29:TYR:HB2	1.94	0.49
4:U:18:LEU:C	4:U:18:LEU:HD22	2.37	0.49
2:B:28:HIS:CD2	2:B:28:HIS:C	2.89	0.49
5:P:46:LEU:C	5:P:47:PHE:CG	2.90	0.49
5:R:94:SER:O	5:R:107:PHE:HD2	1.95	0.49
4:U:31:SER:OG	4:U:50:THR:HB	2.13	0.49
5:V:14:THR:HG22	5:V:15:ARG:N	2.27	0.49
2:B:1:GLY:N	2:B:4:ARG:CD	2.76	0.49
5:P:127:GLU:HB3	5:P:151:THR:OG1	2.13	0.49
3:F:3:PHE:N	3:F:3:PHE:CD1	2.79	0.49
5:R:49:TYR:CE2	5:R:54:GLN:CB	2.95	0.49
5:R:119:ASP:CG	5:R:121:LYS:HG3	2.37	0.49
2:H:71:ARG:HH21	2:H:71:ARG:HG2	1.77	0.49
2:H:129:VAL:HG22	2:H:175:VAL:CG2	2.28	0.49
4:S:85:SER:O	4:S:88:TYR:HE1	1.94	0.49
5:V:48:GLU:OE2	5:V:55:ARG:NH1	2.43	0.49
5:P:148:CYS:HB2	5:P:162:TRP:CH2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:LEU:N	1:D:92:LEU:HD23	2.28	0.49
5:R:51:ASN:O	5:R:52:GLU:HG2	2.13	0.49
2:H:66:ASP:OD2	5:T:99:ARG:NH2	2.45	0.49
4:S:85:SER:OG	4:S:114:VAL:HG12	2.13	0.49
5:T:70:PHE:HE2	5:T:74:ARG:HH21	1.54	0.49
5:T:234:VAL:O	5:T:236:GLN:HG2	2.13	0.49
1:J:144:LEU:N	1:J:144:LEU:CD2	2.73	0.49
5:V:72:ASN:O	5:V:73:SER:CB	2.60	0.49
5:V:241:GLU:HG3	5:V:242:ALA:N	2.27	0.49
4:M:202:THR:O	4:M:203:PHE:CG	2.66	0.49
5:P:26:ILE:HB	5:P:29:HIS:CE1	2.48	0.49
1:D:62:ASN:HD21	3:F:8:VAL:HG12	1.77	0.49
4:Q:164:THR:HG21	5:R:174:SER:HB2	1.95	0.49
1:J:4:GLU:OE2	2:K:19:ASN:CA	2.57	0.49
2:K:61:TRP:O	2:K:64:GLN:HG2	2.13	0.49
4:U:10:VAL:O	4:U:11:THR:O	2.30	0.49
5:V:38:THR:HG23	5:V:88:ALA:HB2	1.95	0.49
2:B:4:ARG:O	2:B:5:PRO:C	2.55	0.49
5:P:207:PRO:O	5:P:208:ARG:O	2.30	0.49
1:D:110:ASP:HB2	1:D:146:ARG:HG2	1.95	0.49
5:R:45:PHE:CZ	5:R:47:PHE:HA	2.47	0.49
1:G:82:ILE:HD13	1:G:82:ILE:C	2.38	0.49
4:S:32:LEU:HD12	4:S:32:LEU:N	2.28	0.49
1:J:174:LEU:HD12	1:J:175:LEU:N	2.28	0.49
4:Q:33:PHE:N	4:Q:33:PHE:CD1	2.81	0.48
4:Q:92:LEU:O	4:Q:93:SER:HB3	2.12	0.48
1:G:47:GLU:O	1:G:50:ARG:HB2	2.13	0.48
5:T:37:GLN:O	5:T:88:ALA:HB1	2.13	0.48
5:V:19:VAL:HG12	5:V:20:THR:N	2.28	0.48
1:A:36:MET:HE2	5:R:222:GLU:OE2	2.13	0.48
2:B:29:ARG:HG2	2:B:36:GLU:OE2	2.13	0.48
4:M:6:MET:HE1	4:M:19:THR:O	2.13	0.48
4:Q:112:LEU:HD23	4:Q:112:LEU:C	2.38	0.48
1:G:6:VAL:HG13	2:H:16:HIS:CD2	2.48	0.48
4:S:13:SER:O	4:S:15:GLU:N	2.45	0.48
4:S:62:PHE:CZ	4:S:77:LYS:HD2	2.47	0.48
2:K:31:ILE:HD12	2:K:31:ILE:N	2.27	0.48
5:V:12:ILE:HG22	5:V:13:LYS:N	2.28	0.48
5:V:45:PHE:CD1	5:V:58:GLY:HA3	2.47	0.48
5:V:100:VAL:O	5:V:101:ASN:CB	2.48	0.48
4:M:160:ILE:CB	4:M:180:ALA:HA	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:51:LYS:HB2	4:Q:53:ASP:OD2	2.13	0.48
5:R:19:VAL:HG12	5:R:21:LEU:CD1	2.43	0.48
5:R:115:THR:HG21	5:R:155:PRO:CB	2.43	0.48
5:T:3:GLY:HA2	5:T:26:ILE:HG23	1.95	0.48
2:K:93:ARG:HD3	2:K:123:TYR:CE1	2.48	0.48
5:V:203:PHE:CD2	5:V:203:PHE:O	2.66	0.48
1:A:25:ASP:C	1:A:25:ASP:OD1	2.56	0.48
1:A:44:ARG:O	1:A:45:LEU:HD23	2.14	0.48
2:H:127:ILE:HD13	2:H:176:GLU:O	2.12	0.48
5:T:201:ALA:O	5:T:202:THR:CB	2.61	0.48
1:A:32:PHE:HE2	1:A:54:PHE:CD2	2.31	0.48
2:B:65:LYS:HA	2:B:68:LEU:HB2	1.95	0.48
2:B:164:VAL:HG22	2:B:166:ARG:H	1.79	0.48
1:D:89:VAL:O	1:D:176:LYS:HE2	2.13	0.48
3:F:6:ASN:ND2	3:F:7:ILE:H	2.11	0.48
4:Q:28:GLY:O	4:Q:30:PRO:HD3	2.11	0.48
5:R:123:VAL:O	5:R:233:PRO:HG2	2.13	0.48
5:R:149:LEU:HA	5:R:193:LEU:O	2.13	0.48
4:S:18:LEU:C	4:S:18:LEU:HD23	2.38	0.48
4:S:166:LEU:O	4:S:167:ASP:HB3	2.14	0.48
1:A:33:HIS:C	1:A:33:HIS:CD2	2.91	0.48
1:A:33:HIS:ND1	1:A:136:VAL:HG11	2.29	0.48
2:B:41:ASP:O	2:B:42:SER:C	2.56	0.48
1:D:73:MET:O	1:D:74:THR:C	2.57	0.48
4:Q:10:VAL:HG23	4:Q:11:THR:N	2.29	0.48
4:Q:164:THR:CG2	4:Q:165:VAL:N	2.77	0.48
5:R:161:SER:OG	5:R:214:GLN:HB3	2.13	0.48
1:G:9:GLN:HB3	2:H:13:TYR:HB2	1.95	0.48
5:T:128:VAL:HG23	5:T:238:VAL:HG12	1.96	0.48
5:V:11:LEU:HD13	5:V:19:VAL:HG11	1.95	0.48
5:V:124:PHE:O	5:V:217:PHE:CE2	2.67	0.48
5:P:64:ARG:NH2	5:P:83:GLU:HG3	2.29	0.48
5:P:141:THR:O	5:P:142:GLN:HB3	2.14	0.48
4:Q:103:LYS:HD3	5:R:45:PHE:CG	2.48	0.48
5:R:121:LYS:HZ1	5:R:228:GLN:CD	2.18	0.48
4:S:201:ASP:C	4:S:203:PHE:H	2.19	0.48
2:K:40:PHE:HE2	2:K:45:GLY:O	1.96	0.48
4:U:138:VAL:HG22	4:U:181:TRP:HB3	1.95	0.48
1:A:12:PHE:CD1	1:A:12:PHE:C	2.91	0.48
1:A:167:HIS:HD2	1:A:169:GLY:H	1.60	0.48
4:Q:43:LEU:HD11	5:R:43:LEU:CD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:125:VAL:HG11	4:Q:189:CYS:HB3	1.95	0.48
2:H:87:GLU:O	2:H:88:SER:C	2.57	0.48
4:S:164:THR:HG22	4:S:165:VAL:N	2.29	0.48
5:T:16:GLY:O	5:T:81:THR:HA	2.14	0.48
5:T:141:THR:O	5:T:142:GLN:C	2.56	0.48
2:K:1:GLY:O	2:K:2:ASP:O	2.32	0.48
2:K:142:VAL:CG2	2:K:161:LEU:HA	2.43	0.48
3:L:8:VAL:C	3:L:9:THR:HG22	2.38	0.48
5:P:46:LEU:HB3	5:P:47:PHE:CD1	2.48	0.48
2:E:37:ASP:HB2	2:E:53:LEU:O	2.14	0.48
2:E:58:ALA:O	2:E:59:GLU:C	2.57	0.48
2:E:132:PHE:O	2:E:171:TYR:HA	2.13	0.48
4:Q:51:LYS:HB2	4:Q:51:LYS:NZ	2.28	0.48
5:T:237:ILE:CD1	2:K:2:ASP:HB2	2.43	0.48
2:K:40:PHE:CD1	2:K:40:PHE:O	2.66	0.48
2:K:127:ILE:HD12	2:K:129:VAL:HG23	1.95	0.48
4:U:81:GLN:O	4:U:114:VAL:HG11	2.14	0.48
5:V:50:PHE:CA	5:V:69:GLN:HE22	2.25	0.48
2:B:59:GLU:OE1	5:V:3:GLY:HA3	2.13	0.48
4:M:6:MET:HE3	4:M:21:ASN:H	1.79	0.48
5:P:44:GLN:OE1	5:P:44:GLN:HA	2.11	0.48
2:E:4:ARG:CB	2:E:5:PRO:CD	2.92	0.48
5:R:12:ILE:HD11	5:R:155:PRO:HD3	1.96	0.48
2:H:1:GLY:HA3	2:H:4:ARG:NH2	2.13	0.48
5:V:37:GLN:O	5:V:88:ALA:HB1	2.13	0.48
5:V:50:PHE:O	5:V:51:ASN:C	2.56	0.48
2:B:55:ARG:NH2	5:V:110:GLN:HE22	2.12	0.47
4:M:5:GLN:HE21	4:M:107:GLY:HA3	1.78	0.47
5:P:49:TYR:OH	5:P:54:GLN:HG3	2.13	0.47
5:P:130:VAL:CG1	5:P:131:PHE:N	2.77	0.47
3:F:3:PHE:CD2	4:Q:99:ASP:O	2.66	0.47
5:R:53:THR:O	5:R:54:GLN:CB	2.62	0.47
5:R:62:GLY:O	5:R:64:ARG:C	2.57	0.47
5:R:140:HIS:C	5:R:140:HIS:CD2	2.92	0.47
2:H:152:ASP:O	2:H:154:THR:HG23	2.13	0.47
4:S:169:ARG:O	4:S:171:MET:N	2.47	0.47
2:B:4:ARG:HG3	2:B:4:ARG:NH1	2.28	0.47
2:B:32:TYR:O	2:B:33:ASN:HB2	2.14	0.47
2:B:87:GLU:O	2:B:88:SER:C	2.57	0.47
5:P:148:CYS:HB2	5:P:162:TRP:CZ2	2.50	0.47
5:P:189:SER:OG	5:P:190:ARG:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:31:ILE:HG23	2:E:35:GLU:C	2.39	0.47
2:E:93:ARG:HD3	2:E:123:TYR:CD1	2.49	0.47
4:Q:0:GLY:CA	4:Q:98:GLY:O	2.62	0.47
1:G:8:ILE:HG23	2:H:14:GLU:HG2	1.96	0.47
4:S:77:LYS:NZ	4:S:84:ASP:OD2	2.45	0.47
5:T:115:THR:HG21	5:T:155:PRO:HB3	1.95	0.47
5:T:206:ASN:O	5:T:207:PRO:C	2.56	0.47
1:J:45:LEU:O	1:J:46:GLU:C	2.57	0.47
4:M:41:GLU:OE1	2:K:55:ARG:NH2	2.47	0.47
4:M:56:GLY:O	4:M:57:SER:CB	2.61	0.47
5:P:182:GLU:HG3	5:P:190:ARG:O	2.14	0.47
2:E:2:ASP:HA	2:E:6:ARG:NH1	2.28	0.47
2:H:61:TRP:HA	2:H:61:TRP:HE3	1.79	0.47
4:S:159:TYR:CE1	4:S:180:ALA:HB1	2.49	0.47
5:T:68:ARG:HE	5:T:70:PHE:HE1	1.57	0.47
2:K:177:HIS:O	2:K:179:SER:N	2.47	0.47
5:V:79:VAL:HG23	5:V:79:VAL:O	2.14	0.47
4:M:24:TYR:CE1	4:M:71:THR:HB	2.49	0.47
4:M:56:GLY:O	4:M:57:SER:HB3	2.14	0.47
2:E:122:PHE:CE1	2:E:155:PHE:HB2	2.49	0.47
5:R:38:THR:C	5:R:40:GLY:H	2.22	0.47
5:R:52:GLU:H	5:R:69:GLN:NE2	2.12	0.47
2:H:13:TYR:OH	3:I:9:THR:CG2	2.61	0.47
1:J:155:PRO:O	1:J:156:SER:O	2.32	0.47
4:U:99:ASP:HB2	4:U:100:SER:H	1.49	0.47
4:M:14:GLU:O	4:M:15:GLU:CG	2.56	0.47
5:P:200:SER:O	5:P:201:ALA:C	2.57	0.47
1:D:9:GLN:HB3	2:E:13:TYR:HB2	1.97	0.47
1:D:52:ALA:HA	3:F:2:HIS:HB3	1.95	0.47
1:D:131:GLY:O	1:D:132:VAL:O	2.33	0.47
4:S:31:SER:OG	4:S:50:THR:HA	2.15	0.47
5:T:26:ILE:O	5:T:27:SER:C	2.57	0.47
2:K:41:ASP:C	2:K:41:ASP:OD1	2.58	0.47
2:K:52:GLU:C	2:K:54:GLY:H	2.23	0.47
2:B:40:PHE:C	2:B:40:PHE:CD1	2.92	0.47
4:M:16:ALA:HB3	4:M:80:VAL:HG11	1.95	0.47
5:R:113:ARG:CG	5:R:157:HIS:CE1	2.97	0.47
1:G:51:PHE:CE1	2:H:89:PHE:HB3	2.49	0.47
5:V:191:TYR:N	5:V:191:TYR:CD1	2.83	0.47
1:A:73:MET:HE1	1:A:76:ARG:HH11	1.79	0.47
4:M:5:GLN:NE2	4:M:109:GLY:H	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:114:LEU:O	5:P:115:THR:O	2.33	0.47
5:P:219:GLY:O	5:P:220:LEU:C	2.57	0.47
1:D:77:SER:O	1:D:80:THR:CG2	2.63	0.47
4:Q:114:VAL:HG13	4:Q:114:VAL:O	2.14	0.47
5:R:18:GLN:HB3	5:R:80:SER:HA	1.96	0.47
5:R:90:TYR:CE2	5:R:114:LEU:HD23	2.50	0.47
5:R:98:ASP:HB2	5:R:99:ARG:HD2	1.96	0.47
1:G:119:VAL:HG21	1:G:149:HIS:CE1	2.50	0.47
1:G:148:PHE:HE2	2:H:149:GLN:O	1.97	0.47
2:H:55:ARG:O	2:H:59:GLU:HG3	2.15	0.47
2:H:78:TYR:CZ	3:I:7:ILE:HD12	2.50	0.47
4:S:32:LEU:HD22	4:S:73:PHE:HB2	1.96	0.47
1:J:57:GLN:OE1	1:J:57:GLN:HA	2.14	0.47
1:J:137:PHE:HB3	1:J:145:PHE:HD2	1.80	0.47
2:K:51:THR:O	2:K:52:GLU:C	2.58	0.47
2:K:93:ARG:O	2:K:124:PRO:HD3	2.15	0.47
3:L:5:LYS:CE	5:V:100:VAL:HG12	2.45	0.47
2:B:75:VAL:O	2:B:79:CYS:HB2	2.15	0.47
2:B:122:PHE:CE2	2:B:156:GLN:CA	2.93	0.47
4:M:43:LEU:HD11	5:P:43:LEU:CD2	2.45	0.47
4:M:198:ILE:HD12	4:M:201:ASP:CA	2.45	0.47
5:P:45:PHE:HD1	5:P:58:GLY:HA3	1.79	0.47
5:P:208:ARG:O	5:P:209:ASN:C	2.58	0.47
2:E:77:THR:O	3:F:5:LYS:HE3	2.15	0.47
4:Q:33:PHE:HA	4:Q:47:LEU:O	2.15	0.47
5:R:238:VAL:HG12	5:R:239:SER:N	2.29	0.47
2:H:68:LEU:HD12	2:H:68:LEU:HA	1.78	0.47
4:S:195:ASN:ND2	4:S:196:SER:H	2.08	0.47
2:K:28:HIS:C	2:K:28:HIS:CD2	2.93	0.47
5:V:123:VAL:HA	5:V:154:TYR:O	2.15	0.47
5:V:124:PHE:CE1	5:V:230:ARG:NH2	2.82	0.47
4:M:188:ALA:C	4:M:190:ALA:H	2.22	0.47
5:P:4:VAL:HG22	5:P:26:ILE:HG13	1.97	0.47
5:P:196:ARG:HE	5:P:196:ARG:N	2.13	0.47
1:D:53:SER:HB2	3:F:3:PHE:CD1	2.50	0.47
2:K:131:TRP:O	2:K:137:GLU:HA	2.15	0.47
4:U:70:THR:O	4:U:71:THR:C	2.58	0.47
4:U:163:LYS:HA	4:U:177:SER:O	2.15	0.47
5:V:87:SER:HB3	5:V:115:THR:HA	1.97	0.47
5:V:131:PHE:N	5:V:131:PHE:HD1	2.11	0.47
1:A:5:HIS:CE1	2:B:91:VAL:HG22	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:55:LYS:CB	4:M:64:ALA:O	2.62	0.47
5:P:100:VAL:HG12	5:P:101:ASN:ND2	2.29	0.47
5:P:120:LEU:C	5:P:122:ASN:H	2.21	0.47
5:P:128:VAL:HA	5:P:149:LEU:O	2.15	0.47
5:R:226:TRP:CE3	5:R:226:TRP:HA	2.50	0.47
4:S:24:TYR:CE2	4:S:71:THR:HB	2.50	0.47
5:T:14:THR:O	5:T:15:ARG:C	2.58	0.47
5:V:32:VAL:CG1	5:V:92:CYS:SG	3.03	0.47
5:V:202:THR:O	5:V:205:GLN:N	2.37	0.47
5:P:19:VAL:HG12	5:P:21:LEU:CD1	2.44	0.46
2:E:125:GLY:CA	2:E:147:LEU:HD21	2.45	0.46
4:Q:164:THR:CB	5:R:196:ARG:NH2	2.78	0.46
1:G:44:ARG:O	1:G:44:ARG:NH1	2.48	0.46
1:G:103:ASN:HB3	1:G:153:PHE:CE1	2.49	0.46
1:G:113:THR:HG21	1:G:144:LEU:HD22	1.97	0.46
5:T:49:TYR:HB3	5:T:69:GLN:NE2	2.27	0.46
5:T:169:VAL:O	5:T:170:HIS:CB	2.62	0.46
1:J:82:ILE:HD13	1:J:83:THR:H	1.80	0.46
4:U:64:ALA:HA	4:U:74:HIS:O	2.14	0.46
1:A:17:ASP:OD1	1:A:17:ASP:N	2.47	0.46
5:P:176:ASP:OD2	5:P:194:SER:OG	2.30	0.46
1:D:29:ASP:HB3	2:E:153:TRP:CE2	2.50	0.46
1:D:123:ARG:CB	1:D:128:VAL:HG11	2.45	0.46
2:E:102:TYR:O	2:E:116:VAL:HB	2.14	0.46
4:Q:21:ASN:HA	4:Q:74:HIS:ND1	2.30	0.46
4:Q:53:ASP:OD2	4:Q:53:ASP:N	2.48	0.46
4:Q:94:GLY:CA	5:R:101:ASN:OD1	2.63	0.46
5:R:160:LEU:CD2	5:R:161:SER:N	2.69	0.46
3:I:11:ARG:HE	3:I:11:ARG:HB3	1.58	0.46
4:U:58:ASN:O	4:U:59:LYS:C	2.58	0.46
4:U:115:ARG:HB3	4:U:146:SER:OG	2.15	0.46
5:V:64:ARG:NH1	5:V:83:GLU:OE2	2.48	0.46
5:V:150:ALA:HB2	5:V:215:VAL:HG21	1.96	0.46
2:B:83:TYR:C	2:B:83:TYR:CD1	2.94	0.46
5:P:29:HIS:CD2	5:P:96:LEU:HD22	2.50	0.46
1:D:22:PHE:CZ	3:F:6:ASN:OD1	2.69	0.46
4:Q:171:MET:O	4:Q:172:ASP:HB2	2.16	0.46
2:H:99:VAL:HG13	2:H:119:VAL:HG22	1.97	0.46
4:S:38:TYR:HA	4:S:86:ALA:CB	2.46	0.46
5:T:49:TYR:CD2	5:T:54:GLN:HB2	2.51	0.46
1:J:73:MET:HE2	2:K:37:ASP:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:28:HIS:HB3	2:K:40:PHE:HB3	1.97	0.46
2:K:83:TYR:CD1	2:K:83:TYR:C	2.93	0.46
5:V:99:ARG:HB3	5:V:101:ASN:O	2.15	0.46
5:V:163:TRP:HA	5:V:167:LYS:O	2.15	0.46
1:D:162:ASP:HA	1:D:176:LYS:O	2.15	0.46
2:E:2:ASP:O	2:E:3:THR:C	2.55	0.46
4:Q:13:SER:O	4:Q:14:GLU:C	2.59	0.46
4:Q:145:ASP:C	4:Q:147:GLN:H	2.23	0.46
5:R:187:ASN:OD1	5:R:187:ASN:O	2.34	0.46
1:G:92:LEU:HD23	1:G:106:ILE:HB	1.96	0.46
5:P:7:THR:OG1	5:P:22:SER:HB3	2.16	0.46
5:P:223:ASN:O	5:P:223:ASN:OD1	2.33	0.46
4:Q:85:SER:OG	4:Q:114:VAL:HG12	2.16	0.46
4:Q:104:LEU:HD23	4:Q:104:LEU:N	2.28	0.46
2:H:99:VAL:HG22	2:H:119:VAL:CG2	2.44	0.46
4:S:80:VAL:HG13	4:S:80:VAL:O	2.15	0.46
4:S:119:GLN:CB	4:S:121:PRO:HD3	2.37	0.46
5:T:51:ASN:C	5:T:52:GLU:HG2	2.41	0.46
2:K:145:THR:OG1	2:K:146:GLY:N	2.49	0.46
4:M:123:PRO:HA	4:M:143:ASP:O	2.16	0.46
5:P:124:PHE:CD2	5:P:190:ARG:HD3	2.50	0.46
3:F:9:THR:O	3:F:9:THR:HG23	2.16	0.46
5:R:160:LEU:O	5:R:161:SER:HB3	2.15	0.46
2:H:60:TYR:CE2	3:I:13:PRO:HD2	2.51	0.46
2:H:131:TRP:HE3	2:H:131:TRP:O	1.99	0.46
2:H:172:THR:CG2	2:H:173:CYS:N	2.78	0.46
1:J:45:LEU:HB2	1:J:48:PHE:CD2	2.50	0.46
2:K:46:GLU:HB2	2:K:62:ASN:OD1	2.16	0.46
5:V:49:TYR:HB3	5:V:69:GLN:HE21	1.80	0.46
5:V:125:PRO:HA	5:V:217:PHE:CE2	2.50	0.46
1:A:92:LEU:HD21	1:A:106:ILE:HG22	1.98	0.46
4:M:82:VAL:HA	4:M:114:VAL:HG21	1.97	0.46
3:F:11:ARG:HG2	3:F:12:THR:N	2.30	0.46
4:Q:5:GLN:HE22	4:Q:90:CYS:H	1.63	0.46
5:R:148:CYS:O	5:R:149:LEU:HD12	2.15	0.46
1:G:161:TYR:CD1	1:G:161:TYR:N	2.84	0.46
2:H:99:VAL:O	2:H:100:THR:HG23	2.15	0.46
5:T:221:SER:C	5:T:223:ASN:N	2.73	0.46
5:T:230:ARG:HG3	5:T:230:ARG:HH11	1.79	0.46
4:U:129:ARG:HA	4:U:137:SER:CB	2.45	0.46
1:A:101:GLU:H	1:A:155:PRO:HG2	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:42:GLY:O	5:P:43:LEU:O	2.33	0.46
5:P:72:ASN:HD22	5:P:72:ASN:C	2.24	0.46
4:Q:62:PHE:HB3	4:Q:75:LEU:CD1	2.44	0.46
5:R:4:VAL:HG12	5:R:4:VAL:O	2.15	0.46
5:R:26:ILE:HB	5:R:29:HIS:NE2	2.31	0.46
1:G:62:ASN:OD1	3:I:8:VAL:HG12	2.16	0.46
1:G:167:HIS:C	1:G:169:GLY:H	2.24	0.46
4:S:164:THR:CG2	5:T:174:SER:HB2	2.45	0.46
2:K:186:VAL:HG12	2:K:187:GLU:N	2.30	0.46
5:V:42:GLY:O	5:V:43:LEU:C	2.59	0.46
1:A:26:PHE:CD2	2:B:90:THR:HB	2.51	0.46
2:B:156:GLN:O	2:B:156:GLN:HG3	2.15	0.46
4:M:93:SER:HB3	4:M:104:LEU:CD2	2.46	0.46
4:M:173:PHE:CE2	4:M:175:SER:HB3	2.45	0.46
5:P:64:ARG:NH1	5:P:65:PHE:HE1	2.14	0.46
5:P:227:THR:C	5:P:228:GLN:HG2	2.40	0.46
4:Q:103:LYS:O	4:Q:104:LEU:HD23	2.16	0.46
1:G:147:LYS:HZ2	1:G:149:HIS:CE1	2.32	0.46
4:S:10:VAL:O	4:S:11:THR:HG23	2.15	0.46
5:V:25:PRO:HG3	5:V:73:SER:OG	2.16	0.46
1:A:23:MET:SD	1:A:23:MET:C	2.99	0.46
1:A:48:PHE:N	1:A:48:PHE:CD1	2.84	0.46
1:A:77:SER:O	1:A:80:THR:HG23	2.16	0.46
2:E:69:GLU:O	2:E:71:ARG:N	2.49	0.46
5:R:8:PRO:O	5:R:112:THR:HB	2.16	0.46
5:R:121:LYS:NZ	5:R:228:GLN:CD	2.74	0.46
5:R:216:GLN:NE2	5:R:237:ILE:HD11	2.31	0.46
4:S:82:VAL:HG23	4:S:114:VAL:O	2.16	0.46
4:S:101:SER:HB2	4:S:102:TYR:CD2	2.51	0.46
4:S:172:ASP:O	4:S:173:PHE:HB2	2.16	0.46
4:S:195:ASN:ND2	4:S:196:SER:N	2.62	0.46
5:T:15:ARG:HG2	5:T:15:ARG:NH1	2.31	0.46
1:J:61:ALA:O	1:J:64:ALA:HB3	2.16	0.46
4:U:104:LEU:HD11	5:V:103:GLU:O	2.15	0.46
5:V:3:GLY:CA	5:V:26:ILE:HD13	2.46	0.46
5:V:155:PRO:HG2	5:V:157:HIS:CD2	2.48	0.46
5:P:53:THR:O	5:P:54:GLN:HB2	2.16	0.45
5:P:162:TRP:NE1	5:P:195:SER:OG	2.42	0.45
4:Q:26:ALA:O	4:Q:27:THR:OG1	2.31	0.45
5:T:163:TRP:CA	5:T:169:VAL:CB	2.85	0.45
2:K:141:GLY:O	2:K:161:LEU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:46:LEU:HA	4:U:58:ASN:ND2	2.31	0.45
4:M:84:ASP:O	4:M:85:SER:C	2.59	0.45
1:D:56:ALA:O	1:D:57:GLN:C	2.59	0.45
4:Q:168:MET:O	4:Q:170:SER:N	2.49	0.45
1:G:89:VAL:HG22	1:G:109:ILE:HG23	1.98	0.45
1:G:101:GLU:N	1:G:155:PRO:HG3	2.27	0.45
4:S:164:THR:O	4:S:176:ASN:HA	2.16	0.45
5:T:21:LEU:HD12	5:T:21:LEU:H	1.76	0.45
1:J:167:HIS:O	1:J:169:GLY:N	2.49	0.45
4:U:160:ILE:C	4:U:161:THR:HG23	2.41	0.45
1:A:79:TYR:CD1	1:G:79:TYR:HD1	2.34	0.45
1:A:167:HIS:O	1:A:169:GLY:N	2.50	0.45
5:P:35:TYR:CD1	5:P:45:PHE:HA	2.51	0.45
5:P:101:ASN:N	5:P:101:ASN:HD22	2.12	0.45
5:P:164:VAL:O	5:P:167:LYS:N	2.50	0.45
1:D:30:GLU:O	1:D:30:GLU:HG2	2.16	0.45
4:Q:87:VAL:CG1	4:Q:88:TYR:N	2.78	0.45
4:Q:92:LEU:HD12	4:Q:92:LEU:C	2.41	0.45
4:Q:123:PRO:HB3	4:Q:201:ASP:OD1	2.16	0.45
2:H:20:GLY:O	2:H:83:TYR:HE2	1.99	0.45
1:J:87:PRO:HB2	1:J:109:ILE:HG22	1.97	0.45
1:J:98:GLU:O	1:J:99:LEU:O	2.34	0.45
1:J:121:TRP:O	1:J:122:LEU:HD23	2.16	0.45
4:U:17:PHE:O	4:U:18:LEU:HB3	2.16	0.45
2:B:41:ASP:O	2:B:43:ASP:N	2.49	0.45
5:P:9:ARG:HG3	5:P:10:TYR:CD1	2.52	0.45
2:E:32:TYR:O	2:E:33:ASN:HB2	2.16	0.45
2:E:127:ILE:CD1	2:E:128:GLU:N	2.67	0.45
4:Q:184:LYS:O	4:Q:186:ASP:N	2.49	0.45
5:R:120:LEU:O	5:R:123:VAL:HG23	2.17	0.45
5:T:115:THR:HG21	5:T:155:PRO:CB	2.46	0.45
3:L:1:VAL:HG11	4:U:99:ASP:CB	2.45	0.45
2:E:75:VAL:O	2:E:80:ARG:HG3	2.17	0.45
5:R:38:THR:O	5:R:42:GLY:N	2.50	0.45
4:S:18:LEU:O	4:S:76:GLU:HA	2.17	0.45
5:T:175:THR:HG23	5:T:195:SER:HB2	1.98	0.45
4:U:18:LEU:HD13	4:U:77:LYS:H	1.80	0.45
5:V:6:GLN:HE21	5:V:112:THR:CG2	2.29	0.45
5:V:172:GLY:O	5:V:197:LEU:HA	2.16	0.45
1:A:23:MET:SD	1:A:23:MET:O	2.75	0.45
1:A:98:GLU:O	1:A:99:LEU:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:14:GLU:C	4:M:15:GLU:CG	2.82	0.45
5:P:146:LEU:N	5:P:146:LEU:CD1	2.77	0.45
2:H:142:VAL:HA	2:H:160:MET:O	2.17	0.45
4:S:34:TRP:CD1	4:S:75:LEU:HD12	2.52	0.45
5:T:60:PHE:N	5:T:60:PHE:CD2	2.82	0.45
5:T:230:ARG:O	5:T:231:ALA:C	2.60	0.45
1:J:12:PHE:CD1	1:J:12:PHE:C	2.95	0.45
1:J:14:LEU:HD13	2:K:8:LEU:HD13	1.99	0.45
4:U:41:GLU:HG2	5:V:110:GLN:CD	2.41	0.45
4:U:43:LEU:HD11	5:V:43:LEU:CD2	2.39	0.45
4:U:56:GLY:O	4:U:57:SER:CB	2.62	0.45
4:U:57:SER:O	4:U:58:ASN:O	2.34	0.45
5:V:232:LYS:O	5:V:233:PRO:C	2.58	0.45
5:P:70:PHE:HE2	5:P:76:GLU:HG3	1.82	0.45
5:P:140:HIS:HD2	5:P:140:HIS:O	1.99	0.45
1:D:53:SER:HB2	3:F:3:PHE:CE1	2.51	0.45
2:E:4:ARG:HB3	2:E:5:PRO:CD	2.43	0.45
5:R:195:SER:O	5:R:196:ARG:HG3	2.17	0.45
2:K:55:ARG:N	2:K:56:PRO:CD	2.80	0.45
5:V:52:GLU:H	5:V:69:GLN:CD	2.25	0.45
5:V:59:ASN:O	5:V:60:PHE:HD1	2.00	0.45
1:A:52:ALA:HB1	3:C:4:PHE:HE1	1.81	0.45
3:C:8:VAL:O	3:C:9:THR:HG22	2.16	0.45
5:P:3:GLY:O	5:P:5:THR:HG23	2.17	0.45
2:E:145:THR:HG23	2:E:158:LEU:O	2.17	0.45
2:E:148:ILE:HB	2:E:156:GLN:HG2	1.99	0.45
4:S:38:TYR:HA	4:S:86:ALA:HB2	1.98	0.45
4:S:122:ASP:N	4:S:123:PRO:HD3	2.31	0.45
1:J:103:ASN:HB3	1:J:153:PHE:CE1	2.52	0.45
1:J:138:LEU:HB2	1:J:146:ARG:HE	1.81	0.45
5:V:13:LYS:HG3	5:V:19:VAL:HG22	1.99	0.45
5:V:138:ILE:CD1	5:V:144:ALA:HB2	2.46	0.45
4:M:66:TYR:C	4:M:66:TYR:CD2	2.95	0.45
4:M:171:MET:O	4:M:173:PHE:N	2.50	0.45
2:E:17:PHE:CD2	2:E:24:VAL:HG22	2.52	0.45
2:E:125:GLY:HA3	2:E:147:LEU:HD21	1.99	0.45
5:R:36:GLN:OE1	5:R:60:PHE:HE2	1.99	0.45
5:R:132:GLU:HG3	5:R:204:TRP:CH2	2.52	0.45
3:I:8:VAL:C	3:I:9:THR:HG22	2.42	0.45
4:S:1:ASP:O	4:S:2:SER:CB	2.62	0.45
1:J:167:HIS:CD2	1:J:169:GLY:H	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:101:SER:C	4:U:103:LYS:H	2.25	0.45
5:V:38:THR:HG23	5:V:88:ALA:CB	2.47	0.45
1:A:79:TYR:CD1	1:G:79:TYR:CD1	3.05	0.45
2:B:90:THR:OG1	2:B:91:VAL:N	2.46	0.45
2:B:119:VAL:O	2:B:156:GLN:HA	2.17	0.45
5:P:64:ARG:O	5:P:79:VAL:HA	2.17	0.45
2:E:154:THR:C	2:E:155:PHE:HD1	2.25	0.45
5:R:237:ILE:O	5:R:237:ILE:HG22	2.15	0.45
1:G:82:ILE:HG23	1:G:82:ILE:O	2.17	0.45
2:H:51:THR:O	2:H:53:LEU:N	2.50	0.45
5:T:118:GLU:CD	5:T:118:GLU:N	2.74	0.45
5:T:162:TRP:CE2	5:T:213:CYS:HB2	2.52	0.45
5:V:36:GLN:HB2	5:V:46:LEU:HD21	1.99	0.45
5:V:133:PRO:CG	5:V:204:TRP:CE2	3.00	0.45
5:V:204:TRP:O	5:V:204:TRP:CG	2.67	0.45
1:A:16:PRO:HG3	2:B:3:THR:HG23	1.99	0.44
4:M:55:LYS:CB	4:M:64:ALA:H	2.30	0.44
4:M:100:SER:HB2	4:M:103:LYS:HZ3	1.81	0.44
2:H:50:VAL:C	2:H:51:THR:HG23	2.42	0.44
4:S:17:PHE:H	4:S:17:PHE:HD1	1.64	0.44
4:S:80:VAL:HG23	4:S:84:ASP:OD1	2.17	0.44
1:J:71:GLU:O	1:J:72:ILE:C	2.60	0.44
2:K:172:THR:CG2	2:K:173:CYS:H	2.30	0.44
4:U:10:VAL:CG1	4:U:11:THR:N	2.79	0.44
5:V:135:GLU:O	5:V:139:SER:HB3	2.17	0.44
5:V:142:GLN:HA	5:V:142:GLN:NE2	2.33	0.44
4:M:3:VAL:CG1	4:M:105:ILE:HG22	2.48	0.44
5:P:64:ARG:NH2	5:P:86:ASP:OD2	2.49	0.44
2:E:68:LEU:HD12	2:E:68:LEU:HA	1.74	0.44
2:E:96:GLU:HA	2:E:97:PRO:HD3	1.78	0.44
4:Q:181:TRP:CZ3	5:R:149:LEU:HD21	2.52	0.44
5:R:164:VAL:O	5:R:165:ASN:C	2.59	0.44
1:G:144:LEU:HD21	2:H:34:GLN:NE2	2.33	0.44
2:H:125:GLY:O	2:H:147:LEU:HD21	2.17	0.44
4:S:184:LYS:O	4:S:185:SER:C	2.60	0.44
5:T:96:LEU:H	5:T:96:LEU:CD2	2.29	0.44
1:J:162:ASP:HB3	1:J:175:LEU:HD22	1.99	0.44
2:K:64:GLN:HG3	2:K:67:PHE:CD2	2.53	0.44
4:U:35:TYR:CD1	4:U:45:LEU:HA	2.52	0.44
4:U:126:TYR:CZ	5:V:137:GLU:HB2	2.52	0.44
5:V:160:LEU:C	5:V:160:LEU:CD2	2.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:234:VAL:O	5:V:236:GLN:N	2.50	0.44
3:C:14:GLY:HA3	5:V:27:SER:CB	2.45	0.44
4:M:29:TYR:N	4:M:29:TYR:CD1	2.84	0.44
4:M:125:VAL:HG12	4:M:126:TYR:N	2.32	0.44
4:M:149:ASN:OD1	4:M:195:ASN:OD1	2.35	0.44
1:D:139:PRO:HB2	2:E:12:LYS:NZ	2.32	0.44
5:R:132:GLU:CG	5:R:133:PRO:HD2	2.41	0.44
4:S:59:LYS:CB	4:S:62:PHE:HD2	2.30	0.44
4:S:125:VAL:O	4:S:126:TYR:C	2.60	0.44
5:T:51:ASN:O	5:T:52:GLU:HG2	2.18	0.44
5:T:99:ARG:HA	5:T:99:ARG:HD2	1.87	0.44
2:K:58:ALA:O	2:K:59:GLU:C	2.59	0.44
4:U:46:LEU:C	4:U:58:ASN:HD21	2.25	0.44
4:U:142:THR:O	4:U:143:ASP:HB2	2.17	0.44
1:A:20:GLY:N	5:R:222:GLU:OE1	2.50	0.44
2:B:75:VAL:HG23	2:B:76:ASP:N	2.32	0.44
4:M:32:LEU:HA	4:M:92:LEU:HA	2.00	0.44
5:P:53:THR:O	5:P:54:GLN:HB3	2.16	0.44
5:P:81:THR:O	5:P:81:THR:OG1	2.32	0.44
5:R:49:TYR:CE2	5:R:54:GLN:CG	2.98	0.44
5:R:49:TYR:HB3	5:R:69:GLN:HB2	1.99	0.44
5:R:77:MET:HE1	5:R:90:TYR:HB3	1.99	0.44
2:H:81:HIS:CE1	3:I:5:LYS:HG3	2.53	0.44
4:S:123:PRO:C	4:S:201:ASP:HA	2.42	0.44
5:T:32:VAL:HG13	5:T:92:CYS:SG	2.57	0.44
5:T:140:HIS:CD2	5:T:140:HIS:C	2.95	0.44
2:K:97:PRO:HB3	2:K:119:VAL:CG1	2.48	0.44
5:V:38:THR:CG2	5:V:88:ALA:HB2	2.48	0.44
5:V:134:SER:OG	5:V:135:GLU:N	2.48	0.44
1:A:87:PRO:HB2	1:A:109:ILE:HG22	2.00	0.44
2:B:180:VAL:O	2:B:180:VAL:HG23	2.18	0.44
5:P:15:ARG:HD2	5:P:118:GLU:HA	1.99	0.44
4:Q:62:PHE:CD2	4:Q:62:PHE:N	2.86	0.44
5:R:53:THR:O	5:R:54:GLN:HB3	2.17	0.44
1:G:23:MET:CE	1:G:138:LEU:HD23	2.48	0.44
1:G:114:PRO:O	1:G:167:HIS:HE1	2.01	0.44
5:T:128:VAL:HG12	5:T:128:VAL:O	2.16	0.44
2:K:4:ARG:HG2	2:K:4:ARG:HH11	1.83	0.44
4:U:11:THR:HA	4:U:113:LEU:O	2.18	0.44
4:U:22:CYS:HB3	4:U:73:PHE:O	2.17	0.44
5:V:19:VAL:HG12	5:V:20:THR:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:241:GLU:HG3	5:V:242:ALA:H	1.82	0.44
1:A:61:ALA:HA	5:P:53:THR:HG21	2.00	0.44
2:B:153:TRP:O	2:B:154:THR:HG22	2.17	0.44
4:M:34:TRP:HB2	4:M:47:LEU:HD12	1.99	0.44
4:M:168:MET:HE3	5:P:198:ARG:O	2.17	0.44
5:P:96:LEU:O	5:P:97:ALA:HB3	2.17	0.44
1:D:142:ASP:O	1:D:143:HIS:HB2	2.18	0.44
5:R:163:TRP:HA	5:R:167:LYS:O	2.17	0.44
1:G:11:GLU:HA	1:G:21:GLU:O	2.18	0.44
1:G:122:LEU:HA	1:G:126:LYS:O	2.17	0.44
1:G:156:SER:O	1:G:157:THR:CB	2.65	0.44
2:H:177:HIS:CG	2:H:179:SER:HG	2.34	0.44
4:S:38:TYR:HB3	4:S:39:PRO:HD3	1.97	0.44
4:S:121:PRO:O	4:S:123:PRO:HD3	2.14	0.44
4:S:179:VAL:O	4:S:180:ALA:CB	2.66	0.44
4:U:126:TYR:CE1	5:V:137:GLU:HB2	2.51	0.44
5:V:59:ASN:O	5:V:60:PHE:CD1	2.70	0.44
4:M:125:VAL:O	4:M:126:TYR:CG	2.71	0.44
4:M:145:ASP:C	4:M:147:GLN:N	2.75	0.44
4:M:171:MET:C	4:M:173:PHE:N	2.75	0.44
1:D:89:VAL:HG12	1:D:90:THR:N	2.32	0.44
4:Q:26:ALA:O	4:Q:27:THR:CB	2.65	0.44
4:Q:195:ASN:O	4:Q:196:SER:O	2.36	0.44
1:G:92:LEU:HD23	1:G:92:LEU:N	2.32	0.44
2:H:32:TYR:CZ	2:H:33:ASN:ND2	2.85	0.44
4:U:32:LEU:N	4:U:49:ALA:O	2.46	0.44
4:M:32:LEU:C	4:M:33:PHE:CD1	2.96	0.44
5:P:34:TRP:CE3	5:P:77:MET:SD	3.10	0.44
5:P:110:GLN:HE22	2:K:55:ARG:HE	1.61	0.44
5:P:149:LEU:HD23	5:P:194:SER:HA	2.00	0.44
5:P:226:TRP:CZ2	5:P:228:GLN:HG3	2.52	0.44
1:D:22:PHE:CD1	1:D:22:PHE:C	2.95	0.44
4:Q:92:LEU:CD1	4:Q:105:ILE:HB	2.48	0.44
4:Q:174:LYS:O	4:Q:175:SER:CB	2.66	0.44
5:R:1:GLY:HA3	5:R:5:THR:HG21	2.00	0.44
2:H:129:VAL:HA	2:H:174:GLN:O	2.18	0.44
4:S:18:LEU:C	4:S:18:LEU:CD2	2.91	0.44
4:S:61:GLY:O	4:S:62:PHE:O	2.36	0.44
1:J:60:LEU:HD23	1:J:60:LEU:HA	1.70	0.44
1:J:122:LEU:HB2	1:J:162:ASP:HB2	1.99	0.44
4:U:5:GLN:NE2	4:U:90:CYS:H	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:10:TYR:CD2	5:V:157:HIS:HB3	2.53	0.44
1:A:61:ALA:O	1:A:65:VAL:HG23	2.18	0.44
1:A:92:LEU:HD23	1:A:92:LEU:N	2.33	0.44
5:P:232:LYS:HA	5:P:233:PRO:HD3	1.88	0.44
1:D:17:ASP:O	1:D:18:GLN:CB	2.63	0.44
2:H:61:TRP:HE3	2:H:64:GLN:HG3	1.82	0.44
4:S:88:TYR:CD1	4:S:88:TYR:N	2.86	0.44
5:T:40:GLY:O	5:T:41:GLN:CB	2.65	0.44
4:U:164:THR:HG22	4:U:165:VAL:N	2.28	0.44
5:V:6:GLN:HE21	5:V:6:GLN:HB3	1.52	0.44
5:V:125:PRO:HA	5:V:126:PRO:HD3	1.83	0.44
2:B:61:TRP:HH2	3:C:10:PRO:HG2	1.83	0.43
5:P:96:LEU:HD22	5:P:96:LEU:N	2.33	0.43
5:P:241:GLU:O	5:P:242:ALA:HB2	2.17	0.43
5:R:93:ALA:CA	5:R:107:PHE:O	2.66	0.43
5:R:150:ALA:O	5:R:153:PHE:HE1	2.01	0.43
1:G:122:LEU:HD23	1:G:127:PRO:HA	2.00	0.43
1:G:161:TYR:N	1:G:161:TYR:HD1	2.15	0.43
2:H:13:TYR:OH	3:I:9:THR:HG22	2.18	0.43
2:H:40:PHE:HB2	2:H:47:TYR:CE2	2.52	0.43
2:H:142:VAL:O	2:H:142:VAL:HG12	2.18	0.43
4:S:35:TYR:HD2	4:S:106:PHE:HE1	1.66	0.43
5:T:68:ARG:NE	5:T:70:PHE:CE1	2.67	0.43
1:J:145:PHE:N	1:J:145:PHE:CD1	2.86	0.43
5:V:87:SER:CB	5:V:115:THR:HA	2.47	0.43
1:A:154:LEU:HD12	1:A:154:LEU:HA	1.77	0.43
2:B:65:LYS:HA	2:B:68:LEU:CB	2.48	0.43
2:B:165:PRO:O	2:B:188:TRP:CZ3	2.71	0.43
5:P:226:TRP:CH2	5:P:228:GLN:HG3	2.54	0.43
1:D:92:LEU:N	1:D:92:LEU:CD2	2.81	0.43
4:S:61:GLY:O	4:S:62:PHE:C	2.61	0.43
1:J:7:ILE:HD13	1:J:26:PHE:HD1	1.83	0.43
1:J:31:ILE:HG22	1:J:43:TRP:CZ3	2.52	0.43
1:J:70:LEU:HD11	2:K:7:PHE:HB3	2.00	0.43
2:K:90:THR:OG1	2:K:91:VAL:N	2.50	0.43
2:K:102:TYR:CD2	2:K:102:TYR:C	2.96	0.43
5:V:3:GLY:HA2	5:V:26:ILE:CD1	2.47	0.43
5:V:103:GLU:O	5:V:106:ALA:CB	2.64	0.43
5:V:114:LEU:O	5:V:115:THR:HB	2.18	0.43
2:B:58:ALA:O	2:B:59:GLU:C	2.60	0.43
1:D:5:HIS:NE2	2:E:91:VAL:HG13	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:14:GLY:HA2	5:T:27:SER:CB	2.45	0.43
4:Q:17:PHE:CG	4:Q:18:LEU:N	2.86	0.43
1:G:45:LEU:O	1:G:46:GLU:C	2.61	0.43
1:G:92:LEU:CD2	1:G:106:ILE:HB	2.48	0.43
2:H:99:VAL:HG12	2:H:100:THR:N	2.34	0.43
4:S:45:LEU:HD23	4:S:46:LEU:H	1.83	0.43
1:J:122:LEU:HD23	1:J:127:PRO:HA	1.99	0.43
4:U:138:VAL:HG22	4:U:181:TRP:CB	2.49	0.43
4:U:191:ASN:HD22	4:U:191:ASN:N	2.13	0.43
5:V:133:PRO:HG2	5:V:204:TRP:CE2	2.53	0.43
5:V:216:GLN:OE1	5:V:217:PHE:O	2.37	0.43
5:P:89:LEU:HD21	5:P:111:GLY:HA3	2.01	0.43
5:P:128:VAL:HG23	5:P:238:VAL:HB	2.00	0.43
3:F:10:PRO:HB3	5:R:50:PHE:HZ	1.83	0.43
4:Q:82:VAL:HA	4:Q:114:VAL:HG13	2.00	0.43
1:G:154:LEU:HA	1:G:155:PRO:HD2	1.74	0.43
2:H:40:PHE:HB2	2:H:47:TYR:CD2	2.53	0.43
2:K:15:CYS:HB3	2:K:17:PHE:CE1	2.52	0.43
4:U:104:LEU:HD21	5:V:102:THR:O	2.18	0.43
5:V:77:MET:HE1	5:V:90:TYR:CE1	2.53	0.43
1:A:176:LYS:HD2	1:A:176:LYS:HA	1.85	0.43
3:C:10:PRO:HG3	5:P:30:ARG:NE	2.32	0.43
4:M:77:LYS:HZ3	4:M:84:ASP:CB	2.31	0.43
5:P:203:PHE:O	5:P:206:ASN:HB3	2.18	0.43
1:D:15:ASN:ND2	1:D:70:LEU:HD23	2.33	0.43
1:D:21:GLU:OE1	1:D:136:VAL:HB	2.17	0.43
2:E:4:ARG:HD3	2:E:4:ARG:HA	1.78	0.43
2:E:17:PHE:CE1	2:E:83:TYR:HD2	2.36	0.43
4:Q:148:THR:HG22	4:Q:149:ASN:N	2.33	0.43
5:R:206:ASN:ND2	5:R:209:ASN:ND2	2.62	0.43
2:H:49:ALA:C	2:H:51:THR:N	2.77	0.43
2:H:128:GLU:O	2:H:176:GLU:N	2.39	0.43
4:S:27:THR:O	4:S:27:THR:CG2	2.67	0.43
5:T:162:TRP:O	5:T:169:VAL:CB	2.67	0.43
5:T:220:LEU:O	5:T:234:VAL:HA	2.19	0.43
1:J:67:LYS:O	1:J:68:ALA:C	2.60	0.43
2:K:18:PHE:CD1	2:K:18:PHE:N	2.86	0.43
4:U:12:LEU:O	4:U:114:VAL:HA	2.18	0.43
4:U:140:LEU:HD12	4:U:141:PHE:H	1.83	0.43
1:A:4:GLU:O	1:A:5:HIS:CG	2.71	0.43
1:A:6:VAL:CG1	2:B:16:HIS:CD2	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:PHE:CD1	2:B:89:PHE:N	2.87	0.43
4:M:44:GLN:HE21	4:M:44:GLN:HB3	1.62	0.43
4:M:100:SER:HB2	4:M:103:LYS:NZ	2.33	0.43
5:P:34:TRP:O	5:P:46:LEU:HB2	2.19	0.43
2:E:2:ASP:O	2:E:2:ASP:CG	2.60	0.43
2:E:4:ARG:O	2:E:6:ARG:NH2	2.51	0.43
2:E:117:CYS:HB2	2:E:131:TRP:CZ2	2.54	0.43
4:Q:115:ARG:HD2	4:Q:146:SER:O	2.17	0.43
5:R:79:VAL:CG2	5:R:82:LEU:HD21	2.48	0.43
5:R:138:ILE:CG2	5:R:201:ALA:HB1	2.49	0.43
5:R:182:GLU:C	5:R:184:PRO:HD3	2.44	0.43
2:H:1:GLY:HA2	2:H:6:ARG:HH12	1.83	0.43
1:J:33:HIS:C	1:J:33:HIS:HD2	2.25	0.43
4:U:12:LEU:HD12	4:U:13:SER:O	2.19	0.43
4:U:15:GLU:HA	4:U:79:SER:HA	2.00	0.43
1:A:64:ALA:O	1:A:65:VAL:C	2.62	0.43
2:E:17:PHE:CZ	2:E:83:TYR:HB2	2.53	0.43
4:Q:194:ASN:O	4:Q:195:ASN:CB	2.65	0.43
5:R:79:VAL:HG23	5:R:82:LEU:HD21	2.00	0.43
4:S:10:VAL:O	4:S:11:THR:OG1	2.28	0.43
4:S:56:GLY:HA3	4:S:63:GLU:HA	2.00	0.43
5:T:46:LEU:CD1	5:T:60:PHE:CE1	3.02	0.43
4:U:24:TYR:C	4:U:24:TYR:CD2	2.97	0.43
5:V:6:GLN:NE2	5:V:111:GLY:HA2	2.34	0.43
5:V:236:GLN:HG2	5:V:236:GLN:H	1.65	0.43
1:A:44:ARG:HH22	1:A:150:TYR:HE2	1.65	0.43
1:A:52:ALA:CB	3:C:4:PHE:HE1	2.32	0.43
1:A:106:ILE:HG12	1:A:150:TYR:CD1	2.54	0.43
1:D:12:PHE:C	1:D:12:PHE:HD1	2.27	0.43
1:D:17:ASP:OD1	2:E:6:ARG:NE	2.52	0.43
1:D:106:ILE:HG12	1:D:150:TYR:HD1	1.82	0.43
5:R:164:VAL:HA	5:R:210:HIS:O	2.19	0.43
1:G:108:PHE:O	1:G:109:ILE:HD13	2.19	0.43
2:H:14:GLU:HB2	2:H:27:LEU:HB3	2.01	0.43
4:S:59:LYS:CB	4:S:62:PHE:CD2	3.02	0.43
4:S:101:SER:C	4:S:103:LYS:H	2.26	0.43
5:V:49:TYR:CD2	5:V:54:GLN:HB2	2.53	0.43
5:V:97:ALA:C	5:V:98:ASP:O	2.61	0.43
4:M:188:ALA:C	4:M:190:ALA:N	2.74	0.43
5:P:46:LEU:HD22	5:P:46:LEU:N	2.33	0.43
5:P:51:ASN:O	5:P:52:GLU:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:LEU:HD23	1:D:92:LEU:H	1.84	0.43
2:E:5:PRO:HG2	1:J:81:PRO:HD3	2.01	0.43
4:Q:31:SER:CB	4:Q:50:THR:HG22	2.49	0.43
4:Q:38:TYR:CD1	4:Q:86:ALA:HB2	2.53	0.43
2:H:173:CYS:O	2:H:185:THR:HB	2.18	0.43
5:T:180:LEU:HD12	5:T:180:LEU:O	2.19	0.43
1:J:156:SER:OG	1:J:157:THR:N	2.51	0.43
1:A:79:TYR:HD1	1:G:79:TYR:CD1	2.37	0.43
2:B:27:LEU:HD21	2:B:29:ARG:CZ	2.48	0.43
2:B:32:TYR:CE2	2:B:33:ASN:ND2	2.87	0.43
2:B:97:PRO:HB3	2:B:119:VAL:CG1	2.49	0.43
5:P:232:LYS:O	5:P:234:VAL:N	2.52	0.43
1:D:36:MET:CE	1:D:63:ILE:HG13	2.48	0.43
4:Q:142:THR:HA	4:Q:177:SER:HB3	2.00	0.43
4:Q:202:THR:O	4:Q:203:PHE:CG	2.71	0.43
1:G:93:THR:HG21	1:G:97:VAL:HG22	2.01	0.43
1:G:133:SER:OG	1:G:150:TYR:HB2	2.18	0.43
2:H:97:PRO:HG3	2:H:122:PHE:HB3	2.01	0.43
4:S:6:MET:O	4:S:110:THR:OG1	2.34	0.43
4:S:94:GLY:CA	5:T:101:ASN:ND2	2.82	0.43
5:T:149:LEU:HD23	5:T:149:LEU:HA	1.80	0.43
1:J:95:SER:O	1:J:96:PRO:C	2.61	0.43
4:U:10:VAL:C	4:U:11:THR:O	2.61	0.43
1:A:83:THR:O	1:A:83:THR:HG22	2.19	0.42
4:M:80:VAL:CG2	4:M:114:VAL:HG23	2.49	0.42
5:P:175:THR:CG2	5:P:195:SER:HB2	2.40	0.42
2:E:161:LEU:O	2:E:162:GLU:CB	2.67	0.42
5:R:6:GLN:CD	5:R:92:CYS:HB3	2.44	0.42
5:R:201:ALA:O	5:R:205:GLN:CG	2.66	0.42
1:G:30:GLU:HB2	1:G:138:LEU:HD21	2.01	0.42
1:G:43:TRP:HZ2	1:G:53:SER:HA	1.83	0.42
2:H:80:ARG:HH11	2:H:80:ARG:HG3	1.84	0.42
2:H:83:TYR:HD1	2:H:83:TYR:O	2.02	0.42
4:S:99:ASP:OD2	4:S:99:ASP:N	2.51	0.42
4:S:165:VAL:O	5:T:174:SER:CB	2.66	0.42
1:J:77:SER:O	1:J:78:ASN:CB	2.63	0.42
1:J:167:HIS:O	1:J:168:TRP:C	2.62	0.42
2:K:65:LYS:HA	2:K:65:LYS:HD2	1.90	0.42
2:K:127:ILE:HG12	2:K:177:HIS:CB	2.34	0.42
5:V:8:PRO:HG3	5:V:11:LEU:HD21	2.01	0.42
5:V:12:ILE:HD12	5:V:12:ILE:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:164:VAL:HG11	5:V:203:PHE:HZ	1.83	0.42
1:A:121:TRP:CE2	1:A:151:LEU:CB	3.02	0.42
4:M:77:LYS:HZ3	4:M:84:ASP:HB2	1.82	0.42
4:M:181:TRP:CZ3	5:P:194:SER:HB3	2.53	0.42
5:P:72:ASN:ND2	5:P:72:ASN:C	2.77	0.42
5:P:99:ARG:HD2	5:P:99:ARG:H	1.84	0.42
5:P:235:THR:O	5:P:235:THR:HG22	2.18	0.42
2:E:36:GLU:OE1	2:E:50:VAL:HG21	2.19	0.42
2:E:55:ARG:N	2:E:56:PRO:CD	2.82	0.42
4:Q:32:LEU:HD12	4:Q:66:TYR:CD1	2.54	0.42
4:Q:85:SER:HA	4:Q:112:LEU:CD2	2.49	0.42
5:R:15:ARG:HG2	5:R:15:ARG:NH1	2.34	0.42
5:R:26:ILE:HD12	5:R:29:HIS:CE1	2.54	0.42
5:R:214:GLN:HE21	5:R:214:GLN:HB2	1.63	0.42
4:S:47:LEU:CD2	4:S:56:GLY:O	2.67	0.42
5:T:229:ASP:OD2	5:T:229:ASP:N	2.51	0.42
1:J:100:ARG:N	1:J:155:PRO:HG2	2.34	0.42
2:K:142:VAL:CB	2:K:160:MET:O	2.63	0.42
4:U:191:ASN:ND2	4:U:192:ALA:H	2.17	0.42
2:B:165:PRO:O	2:B:166:ARG:CB	2.67	0.42
4:M:7:GLU:O	4:M:8:GLY:O	2.35	0.42
4:M:52:ALA:HA	4:M:66:TYR:O	2.18	0.42
4:M:57:SER:O	4:M:58:ASN:HB2	2.19	0.42
1:D:23:MET:CE	1:D:138:LEU:HD23	2.49	0.42
4:Q:24:TYR:HB2	4:Q:25:THR:H	1.66	0.42
5:R:119:ASP:OD2	5:R:120:LEU:N	2.52	0.42
1:G:51:PHE:HD1	2:H:89:PHE:HB3	1.84	0.42
5:T:96:LEU:N	5:T:96:LEU:CD2	2.82	0.42
1:J:114:PRO:O	1:J:167:HIS:HE1	2.00	0.42
1:J:153:PHE:CE2	1:J:155:PRO:HA	2.53	0.42
2:K:93:ARG:HG3	2:K:93:ARG:NH1	2.33	0.42
2:K:143:VAL:HG12	2:K:144:SER:N	2.34	0.42
3:L:2:HIS:N	3:L:2:HIS:ND1	2.64	0.42
3:L:5:LYS:HE3	5:V:100:VAL:HG12	2.01	0.42
4:U:12:LEU:CD1	4:U:12:LEU:C	2.84	0.42
4:M:8:GLY:O	4:M:9:PRO:C	2.61	0.42
4:M:75:LEU:HD12	4:M:76:GLU:H	1.85	0.42
5:P:144:ALA:HB3	5:P:199:VAL:HG23	2.01	0.42
3:F:1:VAL:HA	4:Q:99:ASP:OD1	2.20	0.42
4:Q:193:PHE:CD1	4:Q:193:PHE:N	2.87	0.42
1:J:101:GLU:O	1:J:155:PRO:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:53:LEU:O	2:K:53:LEU:CG	2.67	0.42
4:U:21:ASN:O	4:U:22:CYS:HB2	2.20	0.42
5:V:128:VAL:CG2	5:V:238:VAL:HB	2.50	0.42
2:B:1:GLY:H3	2:B:4:ARG:NE	2.17	0.42
4:M:18:LEU:CB	4:M:77:LYS:HG2	2.49	0.42
4:M:82:VAL:CG1	4:M:83:SER:N	2.83	0.42
5:P:21:LEU:HD22	5:P:77:MET:CE	2.39	0.42
5:P:147:VAL:HG22	5:P:196:ARG:HG3	1.98	0.42
4:Q:62:PHE:HD1	4:Q:75:LEU:HD21	1.83	0.42
5:R:120:LEU:HD22	5:R:120:LEU:HA	1.88	0.42
1:G:6:VAL:CG1	2:H:16:HIS:HD2	2.32	0.42
5:T:53:THR:O	5:T:54:GLN:HB3	2.19	0.42
5:T:98:ASP:HB3	5:T:99:ARG:HD3	2.02	0.42
4:U:34:TRP:HB2	4:U:47:LEU:HD13	2.00	0.42
5:V:49:TYR:CB	5:V:69:GLN:HE21	2.33	0.42
5:V:70:PHE:CE2	5:V:74:ARG:NH2	2.87	0.42
5:V:120:LEU:O	5:V:123:VAL:HG23	2.19	0.42
1:A:32:PHE:HB3	1:A:43:TRP:CE3	2.55	0.42
1:A:122:LEU:HD23	1:A:127:PRO:HA	2.00	0.42
3:C:8:VAL:O	3:C:9:THR:CG2	2.68	0.42
4:M:79:SER:O	4:M:80:VAL:C	2.62	0.42
5:P:64:ARG:NH1	5:P:83:GLU:OE2	2.53	0.42
4:Q:161:THR:HB	4:Q:162:ASP:H	1.66	0.42
4:Q:179:VAL:CG1	4:Q:180:ALA:N	2.82	0.42
2:H:64:GLN:C	2:H:66:ASP:N	2.77	0.42
5:T:149:LEU:HD23	5:T:194:SER:HA	2.02	0.42
1:J:9:GLN:NE2	3:L:6:ASN:OD1	2.50	0.42
4:U:84:ASP:O	4:U:85:SER:C	2.63	0.42
1:A:16:PRO:CG	2:B:3:THR:HG23	2.49	0.42
1:A:100:ARG:N	1:A:155:PRO:HG2	2.34	0.42
5:P:45:PHE:CD1	5:P:58:GLY:HA3	2.55	0.42
1:D:35:ASP:OD1	1:D:38:LYS:N	2.50	0.42
1:D:59:ALA:O	1:D:62:ASN:N	2.52	0.42
1:D:69:ASN:O	1:D:70:LEU:C	2.61	0.42
2:E:185:THR:C	2:E:186:VAL:HG23	2.45	0.42
4:Q:10:VAL:HG21	4:Q:112:LEU:HA	2.00	0.42
1:G:48:PHE:C	1:G:50:ARG:H	2.28	0.42
2:H:37:ASP:OD1	2:H:54:GLY:HA2	2.19	0.42
2:H:128:GLU:O	2:H:175:VAL:HA	2.19	0.42
5:T:68:ARG:CG	5:T:69:GLN:N	2.83	0.42
5:T:119:ASP:OD2	5:T:119:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:234:VAL:O	5:T:235:THR:C	2.63	0.42
2:K:123:TYR:CA	2:K:124:PRO:O	2.63	0.42
4:U:59:LYS:O	4:U:61:GLY:C	2.62	0.42
5:V:173:VAL:HG12	5:V:174:SER:N	2.35	0.42
1:A:25:ASP:OD1	1:A:25:ASP:O	2.37	0.42
2:B:165:PRO:O	2:B:188:TRP:HZ3	2.02	0.42
4:M:84:ASP:O	4:M:85:SER:O	2.38	0.42
4:M:202:THR:CG2	4:M:203:PHE:N	2.83	0.42
5:P:173:VAL:HG12	5:P:174:SER:N	2.35	0.42
5:T:68:ARG:HG3	5:T:69:GLN:N	2.35	0.42
1:J:123:ARG:CB	1:J:128:VAL:HG11	2.50	0.42
1:A:156:SER:HB2	1:A:180:PHE:HB2	2.02	0.42
1:D:30:GLU:O	1:D:44:ARG:HB2	2.20	0.42
1:G:112:PHE:O	1:G:113:THR:HB	2.19	0.42
2:H:24:VAL:HB	2:H:80:ARG:NH2	2.34	0.42
2:H:71:ARG:HH21	2:H:71:ARG:CG	2.33	0.42
5:T:98:ASP:HB3	5:T:99:ARG:H	1.45	0.42
1:J:7:ILE:CD1	1:J:26:PHE:HD1	2.33	0.42
1:J:106:ILE:HG12	1:J:150:TYR:HD1	1.85	0.42
4:U:46:LEU:O	4:U:58:ASN:ND2	2.44	0.42
1:A:85:VAL:HB	1:A:113:THR:HG22	2.02	0.42
2:B:173:CYS:O	2:B:185:THR:HA	2.19	0.42
4:M:33:PHE:HA	4:M:47:LEU:O	2.20	0.42
4:M:103:LYS:HB3	5:P:45:PHE:CE2	2.55	0.42
1:D:61:ALA:O	1:D:64:ALA:HB3	2.20	0.42
2:E:123:TYR:HA	2:E:124:PRO:O	2.20	0.42
4:Q:184:LYS:O	4:Q:185:SER:C	2.63	0.42
5:R:113:ARG:HG2	5:R:113:ARG:HH11	1.85	0.42
1:G:59:ALA:O	1:G:62:ASN:N	2.46	0.42
4:S:35:TYR:CD1	4:S:45:LEU:HA	2.55	0.42
5:T:6:GLN:HE21	5:T:6:GLN:HB3	1.57	0.42
5:T:162:TRP:HB3	5:T:169:VAL:N	2.35	0.42
2:K:127:ILE:HB	2:K:177:HIS:HD2	1.85	0.42
4:U:47:LEU:HD23	4:U:57:SER:CB	2.49	0.42
1:A:24:PHE:CG	1:A:32:PHE:HE1	2.38	0.41
2:B:2:ASP:C	2:B:3:THR:CG2	2.93	0.41
2:B:155:PHE:N	2:B:155:PHE:CD1	2.88	0.41
2:H:69:GLU:O	2:H:70:ASP:C	2.63	0.41
4:S:193:PHE:HD1	4:S:193:PHE:H	1.68	0.41
1:J:162:ASP:HA	1:J:176:LYS:O	2.20	0.41
3:L:8:VAL:HG23	3:L:9:THR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:ARG:HH11	2:B:4:ARG:CG	2.33	0.41
2:B:105:ARG:O	2:B:106:THR:CB	2.68	0.41
2:B:152:ASP:O	2:B:153:TRP:HB2	2.19	0.41
4:M:181:TRP:CD1	4:M:181:TRP:C	2.97	0.41
1:D:32:PHE:HB2	1:D:42:VAL:O	2.20	0.41
2:E:53:LEU:O	2:E:53:LEU:HG	2.20	0.41
1:G:95:SER:O	1:G:96:PRO:C	2.63	0.41
3:I:8:VAL:HG23	3:I:9:THR:N	2.35	0.41
4:S:71:THR:O	4:S:71:THR:OG1	2.36	0.41
5:T:14:THR:HA	5:T:117:VAL:O	2.19	0.41
5:V:156:ASP:HB2	5:V:191:TYR:CE2	2.55	0.41
1:A:89:VAL:HG12	1:A:90:THR:N	2.34	0.41
4:M:54:ASP:HB2	4:M:56:GLY:H	1.86	0.41
1:D:128:VAL:O	1:D:128:VAL:HG23	2.19	0.41
5:R:61:PRO:HG2	5:R:64:ARG:HG3	2.01	0.41
5:R:178:GLN:HA	5:R:179:PRO:HD3	1.86	0.41
2:H:155:PHE:O	2:H:156:GLN:HB3	2.20	0.41
2:H:177:HIS:ND1	2:H:178:PRO:CD	2.83	0.41
4:S:21:ASN:HD22	4:S:21:ASN:N	2.18	0.41
5:T:65:PHE:CD2	5:T:79:VAL:HG12	2.56	0.41
1:J:180:PHE:O	1:J:181:ASP:OXT	2.39	0.41
2:K:55:ARG:HH11	2:K:55:ARG:HG3	1.85	0.41
2:K:64:GLN:O	2:K:66:ASP:HB2	2.21	0.41
2:K:131:TRP:CE3	2:K:172:THR:O	2.74	0.41
5:V:231:ALA:O	5:V:233:PRO:HD3	2.20	0.41
5:P:64:ARG:H	5:P:64:ARG:HG2	1.67	0.41
5:P:80:SER:O	5:P:81:THR:C	2.62	0.41
5:P:226:TRP:CE2	5:P:228:GLN:HB2	2.55	0.41
5:P:231:ALA:O	5:P:233:PRO:HD3	2.20	0.41
1:D:30:GLU:CB	1:D:138:LEU:HD21	2.49	0.41
1:D:153:PHE:HB2	1:D:154:LEU:H	1.70	0.41
2:E:35:GLU:O	2:E:35:GLU:HG3	2.20	0.41
5:R:46:LEU:HD13	5:R:46:LEU:HA	1.90	0.41
1:G:71:GLU:O	1:G:72:ILE:C	2.63	0.41
4:S:38:TYR:CD1	4:S:86:ALA:HB2	2.51	0.41
1:J:93:THR:HG21	1:J:97:VAL:CG2	2.50	0.41
1:J:140:ARG:HD2	1:J:146:ARG:CG	2.50	0.41
2:K:17:PHE:CD2	2:K:24:VAL:HG22	2.55	0.41
2:K:68:LEU:HD12	2:K:68:LEU:HA	1.66	0.41
2:K:77:THR:HG22	4:U:29:TYR:O	2.21	0.41
2:K:102:TYR:HB2	2:K:103:PRO:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:91:ALA:HB1	4:U:105:ILE:O	2.20	0.41
5:V:48:GLU:OE1	5:V:55:ARG:CD	2.68	0.41
5:V:178:GLN:HA	5:V:179:PRO:HD3	1.75	0.41
4:M:18:LEU:O	4:M:76:GLU:HA	2.20	0.41
4:M:55:LYS:C	4:M:57:SER:N	2.77	0.41
5:P:49:TYR:CE2	5:P:54:GLN:HB2	2.56	0.41
1:D:6:VAL:CG1	2:E:16:HIS:CD2	3.02	0.41
1:D:180:PHE:O	1:D:181:ASP:CB	2.67	0.41
5:R:148:CYS:HB2	5:R:162:TRP:CH2	2.55	0.41
1:G:161:TYR:O	1:G:177:HIS:HD2	2.04	0.41
2:H:28:HIS:HB3	2:H:40:PHE:HB3	2.02	0.41
2:H:123:TYR:CD2	2:H:155:PHE:HE1	2.39	0.41
5:T:35:TYR:CD1	5:T:45:PHE:HA	2.55	0.41
1:J:48:PHE:C	1:J:50:ARG:N	2.79	0.41
1:J:56:ALA:O	1:J:59:ALA:HB3	2.21	0.41
4:U:123:PRO:O	4:U:125:VAL:N	2.54	0.41
5:V:158:VAL:O	5:V:158:VAL:HG23	2.21	0.41
1:A:74:THR:HA	2:B:32:TYR:OH	2.21	0.41
4:M:54:ASP:HB2	4:M:55:LYS:H	1.52	0.41
4:M:67:ARG:HG2	4:M:67:ARG:NH1	2.34	0.41
5:P:134:SER:C	5:P:136:ALA:H	2.28	0.41
5:P:216:GLN:HG3	5:P:218:TYR:CZ	2.55	0.41
5:R:7:THR:HB	5:R:8:PRO:HA	2.02	0.41
1:G:81:PRO:HB3	2:H:5:PRO:HB3	2.02	0.41
1:J:33:HIS:CE1	1:J:136:VAL:CG1	3.03	0.41
1:J:134:GLU:OE1	1:J:149:HIS:NE2	2.53	0.41
2:K:55:ARG:HG3	2:K:55:ARG:NH1	2.36	0.41
5:V:130:VAL:C	5:V:131:PHE:CD1	2.99	0.41
1:A:17:ASP:O	1:A:18:GLN:CB	2.66	0.41
1:A:148:PHE:HB3	1:A:150:TYR:CE1	2.55	0.41
1:D:98:GLU:O	1:D:99:LEU:C	2.63	0.41
2:E:28:HIS:HB3	2:E:40:PHE:HB3	2.02	0.41
1:G:140:ARG:HB3	1:G:142:ASP:OD1	2.21	0.41
2:H:61:TRP:C	2:H:63:SER:H	2.29	0.41
2:H:131:TRP:HE3	2:H:131:TRP:C	2.28	0.41
1:J:60:LEU:O	1:J:61:ALA:C	2.63	0.41
1:J:109:ILE:HG12	1:J:147:LYS:O	2.20	0.41
2:K:172:THR:HG22	2:K:173:CYS:H	1.82	0.41
5:V:79:VAL:CG2	5:V:82:LEU:HD21	2.50	0.41
1:A:43:TRP:NE1	1:A:49:GLY:HA2	2.36	0.41
1:A:119:VAL:HG21	1:A:149:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:LEU:O	2:B:53:LEU:HG	2.21	0.41
4:M:165:VAL:HG12	4:M:166:LEU:N	2.34	0.41
5:P:156:ASP:HB2	5:P:191:TYR:CD2	2.55	0.41
5:P:156:ASP:OD2	5:P:179:PRO:HG2	2.20	0.41
5:P:211:PHE:O	5:P:241:GLU:HA	2.20	0.41
1:D:89:VAL:HG22	1:D:109:ILE:HG23	2.02	0.41
1:D:101:GLU:O	1:D:155:PRO:HG3	2.21	0.41
4:Q:1:ASP:O	4:Q:2:SER:CB	2.68	0.41
4:Q:79:SER:O	4:Q:80:VAL:C	2.63	0.41
4:Q:104:LEU:HD21	5:R:102:THR:HB	2.03	0.41
5:R:189:SER:OG	5:R:190:ARG:N	2.54	0.41
1:G:36:MET:HE3	1:G:36:MET:HB3	1.94	0.41
4:S:193:PHE:N	4:S:193:PHE:CD1	2.89	0.41
2:K:102:TYR:C	2:K:102:TYR:HD2	2.28	0.41
5:V:12:ILE:O	5:V:13:LYS:HG2	2.19	0.41
5:V:182:GLU:HG3	5:V:190:ARG:O	2.20	0.41
2:B:1:GLY:O	2:B:2:ASP:C	2.64	0.41
2:B:151:GLY:C	2:B:153:TRP:H	2.28	0.41
4:M:114:VAL:O	4:M:116:PRO:N	2.53	0.41
4:M:191:ASN:ND2	4:M:191:ASN:C	2.79	0.41
5:P:17:GLN:HB2	5:P:18:GLN:H	1.70	0.41
5:P:36:GLN:HB2	5:P:46:LEU:HD21	2.02	0.41
1:D:55:GLU:O	1:D:56:ALA:HB3	2.21	0.41
1:D:110:ASP:CB	1:D:146:ARG:HG2	2.50	0.41
2:E:122:PHE:CE2	2:E:157:THR:HG22	2.56	0.41
4:Q:0:GLY:H3	4:Q:98:GLY:C	2.25	0.41
4:Q:72:SER:HB2	4:Q:74:HIS:NE2	2.36	0.41
4:Q:104:LEU:CD2	5:R:102:THR:HB	2.51	0.41
4:Q:173:PHE:CE2	4:Q:175:SER:HB3	2.56	0.41
4:Q:189:CYS:O	4:Q:190:ALA:C	2.64	0.41
5:R:17:GLN:HG3	5:R:17:GLN:H	1.52	0.41
5:R:117:VAL:O	5:R:118:GLU:C	2.64	0.41
5:R:218:TYR:HA	5:R:235:THR:HG23	2.03	0.41
1:G:110:ASP:CG	1:G:140:ARG:NH1	2.79	0.41
1:G:119:VAL:HG11	1:G:149:HIS:CG	2.56	0.41
1:G:147:LYS:HZ1	1:G:149:HIS:CE1	2.38	0.41
2:H:51:THR:C	2:H:53:LEU:N	2.79	0.41
2:H:150:ASN:ND2	2:H:154:THR:O	2.54	0.41
3:I:8:VAL:O	3:I:9:THR:HG23	2.21	0.41
4:S:21:ASN:HA	4:S:74:HIS:HD2	1.85	0.41
5:T:38:THR:HG22	5:T:88:ALA:HB1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:121:LYS:O	5:T:123:VAL:N	2.54	0.41
5:T:231:ALA:O	5:T:233:PRO:HD3	2.21	0.41
1:J:93:THR:HG21	1:J:97:VAL:HG22	2.02	0.41
1:J:142:ASP:O	1:J:143:HIS:CB	2.63	0.41
1:A:121:TRP:O	1:A:122:LEU:HD23	2.21	0.41
1:A:124:ASN:O	1:A:125:GLY:C	2.62	0.41
1:A:138:LEU:HB3	1:A:146:ARG:NH2	2.36	0.41
2:B:2:ASP:C	2:B:3:THR:HG22	2.46	0.41
2:B:128:GLU:O	2:B:175:VAL:HA	2.21	0.41
1:D:95:SER:HB2	1:D:96:PRO:HD2	2.03	0.41
4:Q:51:LYS:HZ2	4:Q:51:LYS:HB2	1.85	0.41
4:Q:84:ASP:O	4:Q:88:TYR:OH	2.38	0.41
4:Q:157:ASP:C	4:Q:158:VAL:HG23	2.46	0.41
1:G:99:LEU:O	1:G:100:ARG:CB	2.69	0.41
3:I:8:VAL:C	3:I:9:THR:CG2	2.94	0.41
4:S:103:LYS:O	4:S:104:LEU:HD23	2.21	0.41
5:T:24:SER:O	5:T:25:PRO:O	2.39	0.41
4:U:12:LEU:HD12	4:U:12:LEU:O	2.18	0.41
5:V:84:LEU:CD2	5:V:116:VAL:O	2.69	0.41
5:V:93:ALA:HA	5:V:107:PHE:O	2.20	0.41
1:A:140:ARG:CB	1:A:142:ASP:OD1	2.62	0.40
2:B:89:PHE:O	2:B:93:ARG:HB2	2.21	0.40
4:M:10:VAL:O	4:M:11:THR:CB	2.69	0.40
4:M:176:ASN:O	4:M:177:SER:CB	2.69	0.40
5:P:29:HIS:HB3	5:P:95:SER:O	2.21	0.40
5:P:123:VAL:O	5:P:230:ARG:NH2	2.43	0.40
5:P:139:SER:OG	5:P:140:HIS:N	2.49	0.40
2:E:4:ARG:HG3	2:E:4:ARG:NH2	2.29	0.40
2:E:4:ARG:O	2:E:5:PRO:C	2.63	0.40
1:G:45:LEU:CD1	1:G:48:PHE:CZ	3.00	0.40
2:H:28:HIS:CE1	3:I:9:THR:HG21	2.56	0.40
2:H:86:GLY:O	2:H:90:THR:CG2	2.69	0.40
2:H:150:ASN:HB2	2:H:152:ASP:OD1	2.20	0.40
4:S:29:TYR:N	4:S:30:PRO:CD	2.81	0.40
5:T:36:GLN:HB2	5:T:46:LEU:HD21	2.03	0.40
1:J:26:PHE:HD2	2:K:153:TRP:CH2	2.39	0.40
4:U:26:ALA:O	4:U:27:THR:OG1	2.29	0.40
5:V:176:ASP:C	5:V:178:GLN:H	2.29	0.40
5:V:202:THR:O	5:V:204:TRP:N	2.54	0.40
1:A:16:PRO:O	1:A:18:GLN:HG2	2.22	0.40
1:A:119:VAL:HB	1:A:149:HIS:NE2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:GLY:H2	2:B:4:ARG:CD	2.34	0.40
3:C:13:PRO:HB2	3:C:14:GLY:H	1.70	0.40
4:M:188:ALA:O	4:M:190:ALA:N	2.55	0.40
5:P:89:LEU:CD2	5:P:111:GLY:HA3	2.50	0.40
2:E:34:GLN:HG2	2:E:34:GLN:O	2.21	0.40
4:Q:202:THR:O	4:Q:203:PHE:CD2	2.74	0.40
5:R:48:GLU:OE2	5:R:55:ARG:NH1	2.55	0.40
5:R:49:TYR:HE2	5:R:54:GLN:HB2	1.82	0.40
5:R:107:PHE:HE1	2:H:63:SER:HA	1.87	0.40
5:R:239:SER:OG	5:R:240:ALA:N	2.54	0.40
2:H:44:VAL:HG12	2:H:44:VAL:O	2.21	0.40
4:S:42:GLY:N	5:T:110:GLN:OE1	2.53	0.40
1:J:9:GLN:O	2:K:12:LYS:HA	2.22	0.40
5:V:89:LEU:CD2	5:V:111:GLY:HA3	2.52	0.40
5:V:202:THR:C	5:V:204:TRP:H	2.29	0.40
5:V:235:THR:O	5:V:235:THR:HG22	2.21	0.40
2:B:76:ASP:OD2	2:B:80:ARG:HD2	2.21	0.40
4:M:195:ASN:O	4:M:196:SER:O	2.40	0.40
5:P:227:THR:O	5:P:228:GLN:NE2	2.53	0.40
2:E:29:ARG:HD3	2:E:36:GLU:OE2	2.22	0.40
2:E:44:VAL:HG12	2:E:46:GLU:HG2	2.02	0.40
2:E:51:THR:C	2:E:53:LEU:H	2.29	0.40
2:E:173:CYS:O	2:E:185:THR:HA	2.21	0.40
4:Q:140:LEU:HD21	5:R:145:THR:HG21	2.02	0.40
1:G:33:HIS:CE1	1:G:42:VAL:HB	2.57	0.40
1:G:98:GLU:O	1:G:155:PRO:HG3	2.21	0.40
2:H:28:HIS:O	2:H:39:ARG:HA	2.22	0.40
2:H:78:TYR:HE1	2:H:82:ASN:ND2	2.04	0.40
1:J:150:TYR:OH	2:K:150:ASN:O	2.35	0.40
2:K:76:ASP:OD2	2:K:80:ARG:HD2	2.21	0.40
3:L:7:ILE:HG22	3:L:8:VAL:N	2.37	0.40
5:V:11:LEU:HD13	5:V:19:VAL:CG1	2.51	0.40
4:M:13:SER:O	4:M:14:GLU:C	2.63	0.40
4:M:18:LEU:HB3	4:M:77:LYS:HG2	2.02	0.40
4:M:123:PRO:HB3	4:M:144:PHE:HB3	2.02	0.40
5:P:50:PHE:CA	5:P:69:GLN:HE22	2.35	0.40
5:P:72:ASN:O	5:P:73:SER:OG	2.36	0.40
5:P:155:PRO:HG2	5:P:157:HIS:ND1	2.36	0.40
1:D:178:TRP:C	1:D:178:TRP:CE3	3.00	0.40
2:E:17:PHE:CZ	2:E:83:TYR:HD2	2.40	0.40
5:R:78:ASN:OD1	5:R:78:ASN:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:100:VAL:O	5:R:101:ASN:CB	2.70	0.40
1:J:126:LYS:HA	1:J:127:PRO:HD3	1.96	0.40
1:J:156:SER:HB2	1:J:180:PHE:CB	2.50	0.40
2:K:148:ILE:HB	2:K:156:GLN:O	2.21	0.40
4:U:193:PHE:HD1	4:U:193:PHE:H	1.69	0.40
2:B:44:VAL:O	2:B:44:VAL:CG1	2.68	0.40
4:M:24:TYR:CD1	4:M:24:TYR:N	2.89	0.40
5:P:46:LEU:HD13	5:P:60:PHE:CD1	2.56	0.40
5:R:59:ASN:O	5:R:60:PHE:HB2	2.21	0.40
5:R:99:ARG:HD2	5:R:99:ARG:N	2.22	0.40
5:R:120:LEU:HD21	5:R:220:LEU:HD21	2.04	0.40
5:R:164:VAL:O	5:R:166:GLY:N	2.54	0.40
1:G:153:PHE:N	1:G:153:PHE:CD1	2.89	0.40
2:H:17:PHE:CE2	2:H:83:TYR:HD2	2.40	0.40
4:S:165:VAL:O	5:T:174:SER:HB2	2.20	0.40
5:T:25:PRO:HB3	5:T:94:SER:HB2	2.03	0.40
5:T:64:ARG:NH1	5:T:65:PHE:CE1	2.89	0.40
5:T:204:TRP:C	5:T:204:TRP:CD2	2.99	0.40
5:T:217:PHE:HB3	5:T:236:GLN:O	2.21	0.40
2:K:72:ARG:C	2:K:74:ALA:H	2.30	0.40
2:K:184:LEU:O	2:K:185:THR:HG23	2.22	0.40
4:U:26:ALA:HB2	4:U:30:PRO:HG2	1.97	0.40
5:V:15:ARG:H	5:V:15:ARG:HG2	1.42	0.40
5:V:28:GLY:O	5:V:96:LEU:HD13	2.21	0.40
5:V:46:LEU:C	5:V:47:PHE:CG	2.99	0.40
5:V:99:ARG:HG2	5:V:103:GLU:HG2	2.04	0.40
5:V:114:LEU:HA	5:V:114:LEU:HD12	1.87	0.40
5:V:162:TRP:CE3	5:V:197:LEU:HD23	2.56	0.40
5:V:203:PHE:CE2	5:V:211:PHE:CZ	3.09	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	176/181 (97%)	143 (81%)	24 (14%)	9 (5%)	1	5
1	D	176/181 (97%)	148 (84%)	18 (10%)	10 (6%)	1	4
1	G	176/181 (97%)	141 (80%)	24 (14%)	11 (6%)	1	3
1	J	176/181 (97%)	141 (80%)	23 (13%)	12 (7%)	1	2
2	B	165/192 (86%)	120 (73%)	29 (18%)	16 (10%)	0	1
2	E	165/192 (86%)	121 (73%)	31 (19%)	13 (8%)	1	1
2	H	160/192 (83%)	122 (76%)	30 (19%)	8 (5%)	1	5
2	K	176/192 (92%)	133 (76%)	23 (13%)	20 (11%)	0	1
3	C	12/15 (80%)	7 (58%)	1 (8%)	4 (33%)	0	0
3	F	13/15 (87%)	7 (54%)	5 (38%)	1 (8%)	1	2
3	I	11/15 (73%)	5 (46%)	2 (18%)	4 (36%)	0	0
3	L	12/15 (80%)	7 (58%)	2 (17%)	3 (25%)	0	0
4	M	166/209 (79%)	99 (60%)	37 (22%)	30 (18%)	0	0
4	Q	175/209 (84%)	97 (55%)	32 (18%)	46 (26%)	0	0
4	S	154/209 (74%)	92 (60%)	31 (20%)	31 (20%)	0	0
4	U	185/209 (88%)	112 (60%)	35 (19%)	38 (20%)	0	0
5	P	238/249 (96%)	176 (74%)	42 (18%)	20 (8%)	0	1
5	R	236/249 (95%)	161 (68%)	56 (24%)	19 (8%)	1	1
5	T	206/249 (83%)	140 (68%)	37 (18%)	29 (14%)	0	0
5	V	240/249 (96%)	185 (77%)	33 (14%)	22 (9%)	0	1
All	All	3018/3384 (89%)	2157 (72%)	515 (17%)	346 (12%)	0	1

All (346) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	PRO
1	A	156	SER
1	A	158	GLU
2	B	2	ASP
2	B	65	LYS
2	B	163	THR
2	B	164	VAL
2	B	165	PRO
2	B	166	ARG
2	B	167	SER
2	B	169	GLU

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Mol	Chain	Res	Type
4	M	8	GLY
4	M	49	ALA
4	M	52	ALA
4	M	53	ASP
4	M	54	ASP
4	M	55	LYS
4	M	56	GLY
4	M	57	SER
4	M	79	SER
4	M	85	SER
4	M	86	ALA
4	M	115	ARG
4	M	116	PRO
4	M	121	PRO
4	M	143	ASP
4	M	148	THR
4	M	159	TYR
4	M	172	ASP
4	M	196	SER
4	M	198	ILE
5	P	4	VAL
5	P	17	GLN
5	P	25	PRO
5	P	41	GLN
5	P	43	LEU
5	P	51	ASN
5	P	54	GLN
5	P	106	ALA
5	P	134	SER
5	P	208	ARG
5	P	209	ASN
1	D	102	PRO
1	D	132	VAL
1	D	136	VAL
1	D	155	PRO
1	D	156	SER
1	D	157	THR
2	E	4	ARG
2	E	124	PRO
2	E	134	ASN
2	E	167	SER
4	Q	1	ASP

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Mol	Chain	Res	Type
4	Q	11	THR
4	Q	14	GLU
4	Q	15	GLU
4	Q	27	THR
4	Q	52	ALA
4	Q	54	ASP
4	Q	55	LYS
4	Q	56	GLY
4	Q	57	SER
4	Q	79	SER
4	Q	86	ALA
4	Q	129	ARG
4	Q	146	SER
4	Q	148	THR
4	Q	149	ASN
4	Q	152	GLN
4	Q	160	ILE
4	Q	163	LYS
4	Q	185	SER
4	Q	186	ASP
4	Q	196	SER
4	Q	197	ILE
4	Q	199	PRO
4	Q	201	ASP
5	R	41	GLN
5	R	64	ARG
5	R	106	ALA
5	R	184	PRO
5	R	187	ASN
5	R	231	ALA
1	G	57	GLN
1	G	136	VAL
1	G	156	SER
1	G	157	THR
2	H	170	VAL
4	S	11	THR
4	S	14	GLU
4	S	15	GLU
4	S	27	THR
4	S	38	TYR
4	S	58	ASN
4	S	62	PHE

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Mol	Chain	Res	Type
4	S	79	SER
4	S	85	SER
4	S	120	ASN
4	S	121	PRO
4	S	122	ASP
4	S	148	THR
4	S	154	LYS
4	S	161	THR
4	S	169	ARG
4	S	170	SER
4	S	191	ASN
4	S	194	ASN
5	T	25	PRO
5	T	41	GLN
5	T	98	ASP
5	T	99	ARG
5	T	102	THR
5	T	108	PHE
5	T	120	LEU
5	T	205	GLN
5	T	207	PRO
5	T	220	LEU
1	J	78	ASN
1	J	136	VAL
1	J	156	SER
1	J	157	THR
2	K	2	ASP
2	K	3	THR
2	K	97	PRO
2	K	136	GLN
2	K	142	VAL
4	U	10	VAL
4	U	12	LEU
4	U	52	ALA
4	U	58	ASN
4	U	79	SER
4	U	85	SER
4	U	118	ILE
4	U	122	ASP
4	U	162	ASP
4	U	197	ILE
5	V	25	PRO

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Mol	Chain	Res	Type
5	V	99	ARG
5	V	134	SER
5	V	231	ALA
5	V	233	PRO
5	V	237	ILE
1	A	136	VAL
1	A	157	THR
1	A	168	TRP
2	B	156	GLN
4	M	27	THR
4	M	30	PRO
4	M	58	ASN
4	M	197	ILE
5	P	102	THR
5	P	115	THR
5	P	139	SER
1	D	55	GLU
2	E	136	GLN
3	F	9	THR
4	Q	10	VAL
4	Q	38	TYR
4	Q	162	ASP
4	Q	169	ARG
4	Q	177	SER
5	R	43	LEU
5	R	235	THR
2	H	52	GLU
3	I	10	PRO
4	S	8	GLY
4	S	10	VAL
4	S	55	LYS
4	S	71	THR
4	S	185	SER
5	T	17	GLN
5	T	43	LEU
5	T	138	ILE
5	T	152	GLY
5	T	184	PRO
5	T	187	ASN
5	T	222	GLU
1	J	99	LEU
1	J	168	TRP

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Mol	Chain	Res	Type
2	K	53	LEU
2	K	66	ASP
2	K	70	ASP
2	K	88	SER
2	K	98	LYS
2	K	135	SER
2	K	141	GLY
2	K	170	VAL
2	K	178	PRO
4	U	1	ASP
4	U	11	THR
4	U	27	THR
4	U	55	LYS
4	U	56	GLY
4	U	59	LYS
4	U	109	GLY
4	U	185	SER
5	V	43	LEU
5	V	54	GLN
5	V	135	GLU
5	V	202	THR
5	V	203	PHE
5	V	235	THR
2	B	4	ARG
2	B	42	SER
2	B	162	GLU
3	C	13	PRO
4	M	16	ALA
4	M	18	LEU
4	M	177	SER
5	P	101	ASN
5	P	231	ALA
1	D	57	GLN
1	D	78	ASN
4	Q	2	SER
4	Q	18	LEU
4	Q	85	SER
4	Q	93	SER
4	Q	99	ASP
4	Q	144	PHE
4	Q	161	THR
4	Q	164	THR

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Mol	Chain	Res	Type
4	Q	175	SER
4	Q	192	ALA
4	Q	198	ILE
5	R	9	ARG
5	R	81	THR
5	R	188	ASP
1	G	102	PRO
1	G	132	VAL
1	G	168	TRP
2	H	90	THR
2	H	169	GLU
4	S	86	ALA
4	S	202	THR
5	T	40	GLY
5	T	101	ASN
5	T	122	ASN
5	T	170	HIS
5	T	231	ALA
1	J	49	GLY
1	J	102	PRO
2	K	145	THR
4	U	9	PRO
4	U	15	GLU
4	U	22	CYS
4	U	26	ALA
4	U	80	VAL
4	U	117	ASP
4	U	119	GLN
4	U	169	ARG
4	U	172	ASP
4	U	192	ALA
4	U	202	THR
5	V	98	ASP
5	V	115	THR
1	A	46	GLU
1	A	78	ASN
4	M	11	THR
1	D	56	ALA
2	E	22	GLU
2	E	33	ASN
2	E	54	GLY
2	E	69	GLU

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Mol	Chain	Res	Type
2	E	99	VAL
4	Q	9	PRO
4	Q	16	ALA
5	R	27	SER
2	H	34	GLN
3	I	3	PHE
4	S	193	PHE
1	J	132	VAL
2	K	5	PRO
2	K	33	ASN
2	K	169	GLU
3	L	13	PRO
4	U	30	PRO
4	U	71	THR
4	U	130	ASP
4	U	196	SER
5	V	41	GLN
5	V	73	SER
5	V	106	ALA
5	V	189	SER
2	B	79	CYS
3	C	2	HIS
3	C	9	THR
5	P	61	PRO
5	P	233	PRO
2	E	46	GLU
2	E	70	ASP
2	E	161	LEU
4	Q	53	ASP
4	Q	167	ASP
4	Q	195	ASN
5	R	98	ASP
5	R	101	ASN
5	R	165	ASN
5	R	179	PRO
5	R	186	LEU
1	G	56	ALA
1	G	76	ARG
1	G	134	GLU
2	H	145	THR
4	S	2	SER
4	S	57	SER

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Mol	Chain	Res	Type
4	S	69	GLU
4	S	141	PHE
5	T	54	GLN
5	T	64	ARG
3	L	2	HIS
3	L	3	PHE
4	U	57	SER
5	V	60	PHE
5	V	81	THR
2	B	3	THR
2	B	44	VAL
4	M	189	CYS
5	R	17	GLN
5	R	73	SER
2	H	85	VAL
3	I	9	THR
5	T	106	ALA
5	T	115	THR
2	K	65	LYS
4	U	51	LYS
5	V	101	ASN
1	A	125	GLY
2	B	121	GLY
5	T	164	VAL
4	U	121	PRO
4	M	122	ASP
1	J	81	PRO
1	J	155	PRO
4	U	160	ILE
5	V	61	PRO
5	T	233	PRO
4	U	61	GLY
1	G	81	PRO
2	H	183	PRO
5	T	215	VAL
1	J	96	PRO
3	C	10	PRO
5	P	184	PRO
3	I	13	PRO
5	P	155	PRO
2	K	124	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	136/166 (82%)	123 (90%)	13 (10%)	8	26
1	D	137/166 (82%)	124 (90%)	13 (10%)	8	26
1	G	136/166 (82%)	121 (89%)	15 (11%)	6	20
1	J	137/166 (82%)	122 (89%)	15 (11%)	6	21
2	B	126/173 (73%)	113 (90%)	13 (10%)	7	23
2	E	124/173 (72%)	116 (94%)	8 (6%)	15	43
2	H	125/173 (72%)	112 (90%)	13 (10%)	7	22
2	K	128/173 (74%)	123 (96%)	5 (4%)	28	64
3	C	13/13 (100%)	11 (85%)	2 (15%)	2	10
3	F	13/13 (100%)	10 (77%)	3 (23%)	1	3
3	I	12/13 (92%)	7 (58%)	5 (42%)	0	0
3	L	13/13 (100%)	8 (62%)	5 (38%)	0	0
4	M	117/183 (64%)	99 (85%)	18 (15%)	2	10
4	Q	124/183 (68%)	107 (86%)	17 (14%)	3	13
4	S	112/183 (61%)	98 (88%)	14 (12%)	4	15
4	U	120/183 (66%)	103 (86%)	17 (14%)	3	12
5	P	183/213 (86%)	154 (84%)	29 (16%)	2	9
5	R	184/213 (86%)	154 (84%)	30 (16%)	2	8
5	T	160/213 (75%)	142 (89%)	18 (11%)	5	19
5	V	190/213 (89%)	167 (88%)	23 (12%)	5	16
All	All	2290/2992 (76%)	2014 (88%)	276 (12%)	5	16

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASP
1	A	41	THR
1	A	50	ARG

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Mol	Chain	Res	Type
1	A	53	SER
1	A	69	ASN
1	A	72	ILE
1	A	82	ILE
1	A	92	LEU
1	A	93	THR
1	A	102	PRO
1	A	109	ILE
1	A	133	SER
1	A	175	LEU
2	B	3	THR
2	B	4	ARG
2	B	8	LEU
2	B	21	THR
2	B	68	LEU
2	B	77	THR
2	B	87	GLU
2	B	101	VAL
2	B	127	ILE
2	B	157	THR
2	B	163	THR
2	B	164	VAL
2	B	186	VAL
3	C	8	VAL
3	C	11	ARG
4	M	10	VAL
4	M	15	GLU
4	M	17	PHE
4	M	20	ILE
4	M	33	PHE
4	M	45	LEU
4	M	47	LEU
4	M	54	ASP
4	M	66	TYR
4	M	80	VAL
4	M	92	LEU
4	M	110	THR
4	M	120	ASN
4	M	121	PRO
4	M	158	VAL
4	M	191	ASN
4	M	195	ASN

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Mol	Chain	Res	Type
4	M	196	SER
5	P	4	VAL
5	P	9	ARG
5	P	14	THR
5	P	17	GLN
5	P	38	THR
5	P	44	GLN
5	P	47	PHE
5	P	48	GLU
5	P	53	THR
5	P	54	GLN
5	P	55	ARG
5	P	66	SER
5	P	68	ARG
5	P	72	ASN
5	P	81	THR
5	P	89	LEU
5	P	110	GLN
5	P	112	THR
5	P	115	THR
5	P	119	ASP
5	P	127	GLU
5	P	128	VAL
5	P	146	LEU
5	P	174	SER
5	P	175	THR
5	P	183	GLN
5	P	195	SER
5	P	196	ARG
5	P	223	ASN
1	D	8	ILE
1	D	18	GLN
1	D	24	PHE
1	D	30	GLU
1	D	50	ARG
1	D	57	GLN
1	D	69	ASN
1	D	80	THR
1	D	82	ILE
1	D	102	PRO
1	D	109	ILE
1	D	138	LEU

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Mol	Chain	Res	Type
1	D	177	HIS
2	E	4	ARG
2	E	38	LEU
2	E	39	ARG
2	E	65	LYS
2	E	75	VAL
2	E	102	TYR
2	E	127	ILE
2	E	155	PHE
3	F	1	VAL
3	F	5	LYS
3	F	7	ILE
4	Q	15	GLU
4	Q	21	ASN
4	Q	27	THR
4	Q	33	PHE
4	Q	45	LEU
4	Q	51	LYS
4	Q	53	ASP
4	Q	66	TYR
4	Q	73	PHE
4	Q	100	SER
4	Q	101	SER
4	Q	104	LEU
4	Q	120	ASN
4	Q	191	ASN
4	Q	195	ASN
4	Q	199	PRO
4	Q	203	PHE
5	R	9	ARG
5	R	17	GLN
5	R	33	SER
5	R	37	GLN
5	R	38	THR
5	R	44	GLN
5	R	46	LEU
5	R	47	PHE
5	R	52	GLU
5	R	53	THR
5	R	54	GLN
5	R	55	ARG
5	R	59	ASN

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Mol	Chain	Res	Type
5	R	64	ARG
5	R	66	SER
5	R	68	ARG
5	R	72	ASN
5	R	89	LEU
5	R	96	LEU
5	R	107	PHE
5	R	110	GLN
5	R	114	LEU
5	R	120	LEU
5	R	121	LYS
5	R	149	LEU
5	R	184	PRO
5	R	189	SER
5	R	223	ASN
5	R	229	ASP
5	R	239	SER
1	G	50	ARG
1	G	51	PHE
1	G	57	GLN
1	G	71	GLU
1	G	80	THR
1	G	82	ILE
1	G	103	ASN
1	G	117	VAL
1	G	120	THR
1	G	128	VAL
1	G	129	THR
1	G	130	THR
1	G	134	GLU
1	G	161	TYR
1	G	176	LYS
2	H	8	LEU
2	H	21	THR
2	H	36	GLU
2	H	37	ASP
2	H	39	ARG
2	H	68	LEU
2	H	71	ARG
2	H	83	TYR
2	H	127	ILE
2	H	131	TRP

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Mol	Chain	Res	Type
2	H	154	THR
2	H	172	THR
2	H	180	VAL
3	I	2	HIS
3	I	5	LYS
3	I	7	ILE
3	I	11	ARG
3	I	13	PRO
4	S	3	VAL
4	S	18	LEU
4	S	45	LEU
4	S	47	LEU
4	S	50	THR
4	S	57	SER
4	S	67	ARG
4	S	92	LEU
4	S	99	ASP
4	S	101	SER
4	S	121	PRO
4	S	129	ARG
4	S	159	TYR
4	S	165	VAL
5	T	9	ARG
5	T	19	VAL
5	T	20	THR
5	T	21	LEU
5	T	47	PHE
5	T	53	THR
5	T	72	ASN
5	T	73	SER
5	T	94	SER
5	T	99	ARG
5	T	101	ASN
5	T	103	GLU
5	T	117	VAL
5	T	118	GLU
5	T	120	LEU
5	T	137	GLU
5	T	162	TRP
5	T	207	PRO
1	J	33	HIS
1	J	57	GLN

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Mol	Chain	Res	Type
1	J	69	ASN
1	J	80	THR
1	J	82	ILE
1	J	89	VAL
1	J	92	LEU
1	J	93	THR
1	J	96	PRO
1	J	102	PRO
1	J	109	ILE
1	J	120	THR
1	J	144	LEU
1	J	171	ASP
1	J	180	PHE
2	K	2	ASP
2	K	21	THR
2	K	76	ASP
2	K	102	TYR
2	K	127	ILE
3	L	1	VAL
3	L	2	HIS
3	L	5	LYS
3	L	11	ARG
3	L	12	THR
4	U	4	THR
4	U	12	LEU
4	U	18	LEU
4	U	21	ASN
4	U	47	LEU
4	U	50	THR
4	U	54	ASP
4	U	58	ASN
4	U	69	GLU
4	U	75	LEU
4	U	87	VAL
4	U	99	ASP
4	U	114	VAL
4	U	162	ASP
4	U	164	THR
4	U	169	ARG
4	U	191	ASN
5	V	5	THR
5	V	17	GLN

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Mol	Chain	Res	Type
5	V	21	LEU
5	V	38	THR
5	V	47	PHE
5	V	53	THR
5	V	54	GLN
5	V	55	ARG
5	V	59	ASN
5	V	72	ASN
5	V	77	MET
5	V	89	LEU
5	V	96	LEU
5	V	99	ARG
5	V	110	GLN
5	V	112	THR
5	V	116	VAL
5	V	131	PHE
5	V	139	SER
5	V	160	LEU
5	V	180	LEU
5	V	197	LEU
5	V	236	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	18	GLN
1	A	84	ASN
1	A	167	HIS
2	B	16	HIS
2	B	34	GLN
4	M	5	GLN
4	M	21	ASN
4	M	58	ASN
4	M	74	HIS
4	M	81	GLN
4	M	191	ASN
5	P	6	GLN
5	P	37	GLN
5	P	54	GLN
5	P	72	ASN
5	P	101	ASN

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Mol	Chain	Res	Type
5	P	110	GLN
5	P	140	HIS
5	P	157	HIS
5	P	170	HIS
5	P	209	ASN
1	D	18	GLN
1	D	33	HIS
1	D	57	GLN
1	D	84	ASN
1	D	94	ASN
1	D	149	HIS
1	D	167	HIS
2	E	16	HIS
2	E	64	GLN
2	E	149	GLN
2	E	156	GLN
2	E	177	HIS
3	F	6	ASN
4	Q	5	GLN
4	Q	21	ASN
4	Q	44	GLN
4	Q	58	ASN
4	Q	81	GLN
4	Q	147	GLN
4	Q	191	ASN
5	R	44	GLN
5	R	56	ASN
5	R	69	GLN
5	R	72	ASN
5	R	140	HIS
5	R	187	ASN
5	R	209	ASN
5	R	214	GLN
5	R	216	GLN
5	R	228	GLN
1	G	9	GLN
1	G	15	ASN
1	G	18	GLN
1	G	33	HIS
1	G	149	HIS
1	G	167	HIS
2	H	16	HIS

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Mol	Chain	Res	Type
2	H	64	GLN
2	H	149	GLN
4	S	5	GLN
4	S	21	ASN
4	S	44	GLN
4	S	74	HIS
4	S	119	GLN
4	S	149	ASN
4	S	195	ASN
5	T	17	GLN
5	T	18	GLN
5	T	44	GLN
5	T	56	ASN
5	T	69	GLN
5	T	72	ASN
5	T	78	ASN
5	T	140	HIS
5	T	157	HIS
5	T	236	GLN
1	J	9	GLN
1	J	18	GLN
1	J	167	HIS
2	K	16	HIS
2	K	33	ASN
2	K	34	GLN
2	K	149	GLN
4	U	5	GLN
4	U	21	ASN
4	U	44	GLN
4	U	58	ASN
4	U	74	HIS
4	U	81	GLN
4	U	191	ASN
5	V	6	GLN
5	V	69	GLN
5	V	72	ASN
5	V	78	ASN
5	V	101	ASN
5	V	110	GLN
5	V	122	ASN
5	V	142	GLN
5	V	187	ASN

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Mol	Chain	Res	Type
5	V	205	GLN
5	V	223	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	U	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	149:ASN	C	150:VAL	N	6.07

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	178/181 (98%)	0.04	3 (1%) 69 60	32, 54, 80, 90	1 (0%)
1	D	178/181 (98%)	0.07	2 (1%) 78 70	35, 56, 79, 87	1 (0%)
1	G	178/181 (98%)	0.20	0 100 100	14, 56, 70, 80	1 (0%)
1	J	178/181 (98%)	0.15	0 100 100	30, 61, 87, 94	1 (0%)
2	B	175/192 (91%)	0.16	1 (0%) 85 80	14, 59, 88, 96	2 (1%)
2	E	175/192 (91%)	0.06	2 (1%) 78 70	30, 58, 87, 92	0
2	H	168/192 (87%)	0.39	7 (4%) 40 32	35, 60, 102, 106	0
2	K	179/192 (93%)	0.31	5 (2%) 55 45	37, 63, 91, 97	0
3	C	14/15 (93%)	0.12	0 100 100	31, 54, 59, 59	0
3	F	15/15 (100%)	0.03	0 100 100	32, 46, 55, 56	0
3	I	13/15 (86%)	-0.03	0 100 100	41, 48, 53, 53	0
3	L	14/15 (93%)	0.13	0 100 100	46, 53, 58, 60	0
4	M	178/209 (85%)	0.31	3 (1%) 69 60	39, 63, 89, 103	0
4	Q	187/209 (89%)	0.31	4 (2%) 63 54	16, 60, 96, 99	0
4	S	176/209 (84%)	0.31	2 (1%) 78 70	35, 64, 99, 103	0
4	U	195/209 (93%)	0.29	9 (4%) 37 29	14, 59, 83, 90	0
5	P	242/249 (97%)	0.08	1 (0%) 88 84	9, 63, 82, 97	0
5	R	238/249 (95%)	0.15	3 (1%) 75 66	26, 59, 86, 91	0
5	T	226/249 (90%)	0.35	7 (3%) 51 41	20, 63, 98, 102	0
5	V	242/249 (97%)	-0.04	0 100 100	23, 50, 68, 80	0
All	All	3149/3384 (93%)	0.19	49 (1%) 70 61	9, 59, 90, 106	6 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	T	87	SER	3.9
4	U	52	ALA	3.8
2	H	5	PRO	3.4
2	H	131	TRP	3.1
5	T	150	ALA	3.1
5	T	205	GLN	3.1
2	K	176	GLU	3.1
1	D	5	HIS	3.0
2	K	177	HIS	3.0
4	Q	19	THR	2.9
4	M	166	LEU	2.9
1	A	110	ASP	2.8
5	R	192	SER	2.8
4	Q	20	ILE	2.8
5	R	193	LEU	2.8
2	H	115	LEU	2.6
4	S	190	ALA	2.6
2	H	143	VAL	2.5
4	U	150	VAL	2.5
2	K	120	ASN	2.5
1	D	19	SER	2.4
2	K	127	ILE	2.3
5	T	184	PRO	2.3
5	P	119	ASP	2.3
4	U	26	ALA	2.3
4	U	151	SER	2.3
4	U	183	ASN	2.2
4	M	125	VAL	2.2
4	S	122	ASP	2.2
2	B	3	THR	2.2
2	K	118	SER	2.2
5	T	211	PHE	2.1
5	R	150	ALA	2.1
2	H	113	ASN	2.1
2	E	171	TYR	2.1
1	A	156	SER	2.1
2	H	167	SER	2.1
4	M	183	ASN	2.1
4	U	51	LYS	2.1
5	T	161	SER	2.1
2	E	5	PRO	2.1
4	U	130	ASP	2.1
2	H	124	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
4	U	149	ASN	2.0
5	T	111	GLY	2.0
1	A	181	ASP	2.0
4	Q	193	PHE	2.0
4	Q	54	ASP	2.0
4	U	99	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.