



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:33 PM UTC

PDB ID : 4FZG / pdb_00004fzg
Title : 20S yeast proteasome in complex with glidobactin
Authors : Stein, M.; Beck, P.; Kaiser, M.; Dudler, R.; Becker, C.F.W.; Groll, M.
Deposited on : 2012-07-06
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

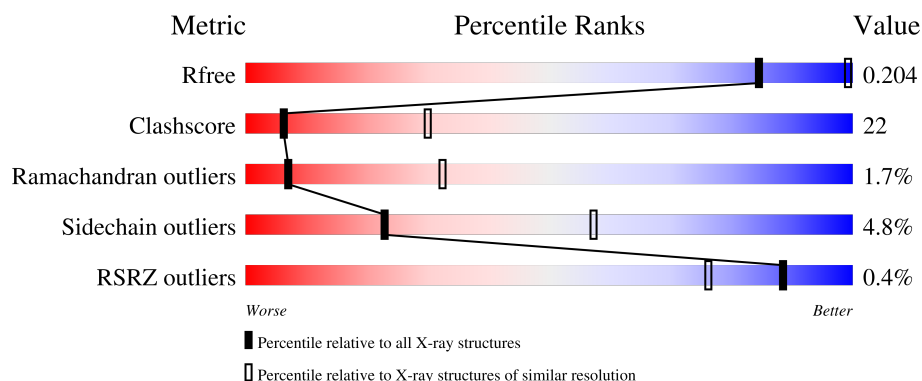
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



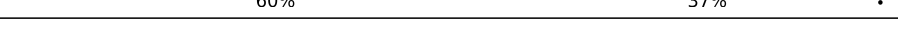
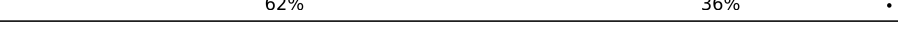
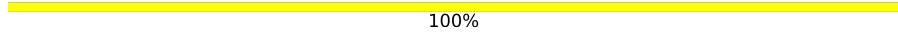
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	250	
1	O	250	
2	B	244	
2	P	244	
3	C	241	

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Mol	Chain	Length	Quality of chain
3	Q	241	
4	D	242	
4	R	242	
5	E	233	
5	S	233	
6	F	244	
6	T	244	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	233	
13	a	233	
14	N	196	
14	b	196	
15	c	4	
15	d	4	

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Mol	Chain	Length	Quality of chain
15	e	4	 25%75%
15	f	4	 50%50%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50986 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 Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			
2	P	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			
4	R	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			
6	T	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
8	V	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 9 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called Proteasome component C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is a protein called Glidobactin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	4	Total	C	N	O	0	0	0
			37	27	4	6			
15	d	4	Total	C	N	O	0	0	0
			37	27	4	6			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	e	4	Total	C	N	O	0	0	0
			37	27	4	6			
15	f	4	Total	C	N	O	0	0	0
			37	27	4	6			

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	56	Total	O	0	0
			56	56		
16	B	35	Total	O	0	0
			35	35		
16	C	41	Total	O	0	0
			41	41		
16	D	39	Total	O	0	0
			39	39		
16	E	25	Total	O	0	0
			25	25		
16	F	45	Total	O	0	0
			45	45		
16	G	59	Total	O	0	0
			59	59		
16	H	52	Total	O	0	0
			52	52		
16	I	61	Total	O	0	0
			61	61		
16	J	55	Total	O	0	0
			55	55		
16	K	41	Total	O	0	0
			41	41		
16	L	57	Total	O	0	0
			57	57		
16	M	63	Total	O	0	0
			63	63		
16	N	61	Total	O	0	0
			61	61		
16	O	34	Total	O	0	0
			34	34		
16	P	27	Total	O	0	0
			27	27		
16	Q	29	Total	O	0	0
			29	29		

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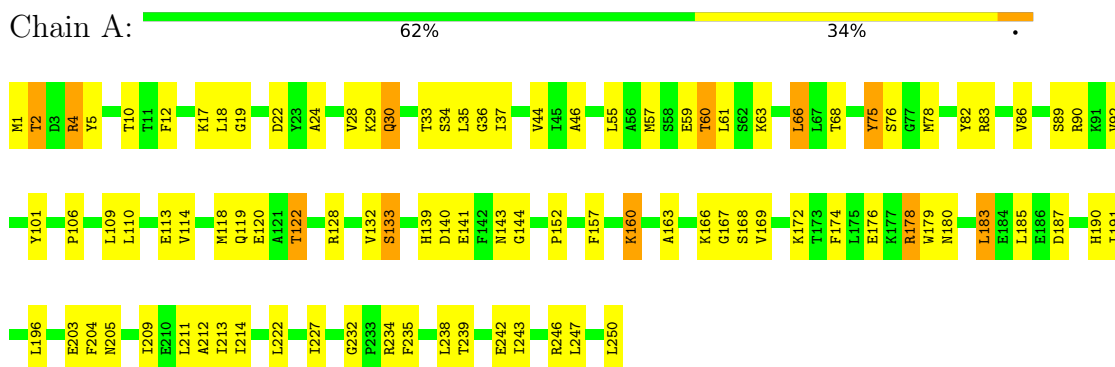
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	R	31	Total 31	O 31	0	0
16	S	21	Total 21	O 21	0	0
16	T	36	Total 36	O 36	0	0
16	U	63	Total 63	O 63	0	0
16	V	46	Total 46	O 46	0	0
16	W	47	Total 47	O 47	0	0
16	X	47	Total 47	O 47	0	0
16	Y	44	Total 44	O 44	0	0
16	Z	49	Total 49	O 49	0	0
16	a	72	Total 72	O 72	0	0
16	b	54	Total 54	O 54	0	0

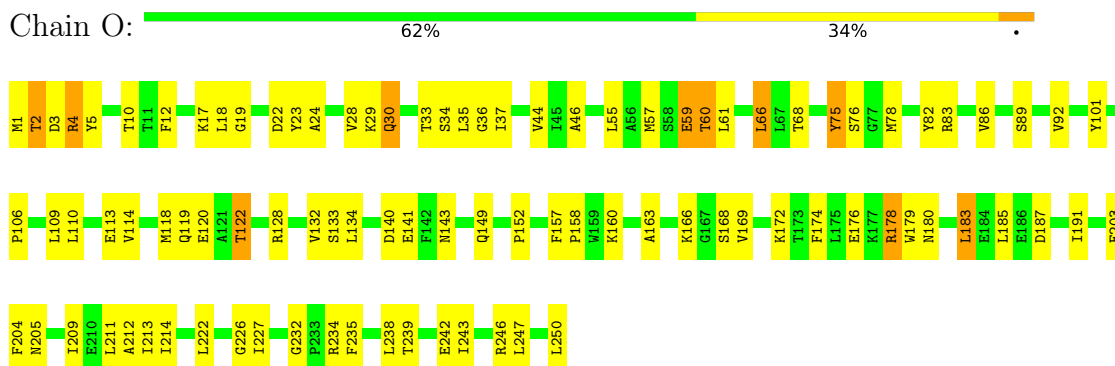
3 Residue-property plots [i](#)

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

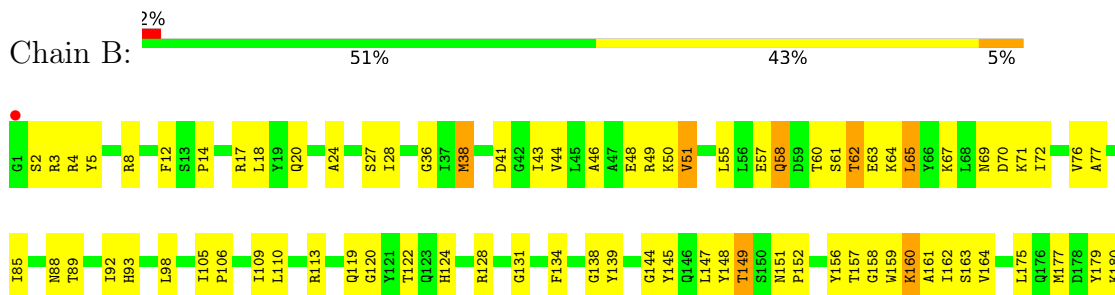
• Molecule 1: Proteasome component Y7

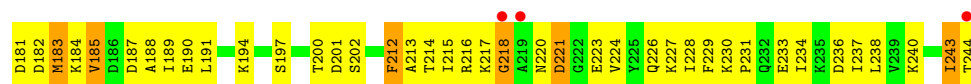


• Molecule 1: Proteasome component Y7



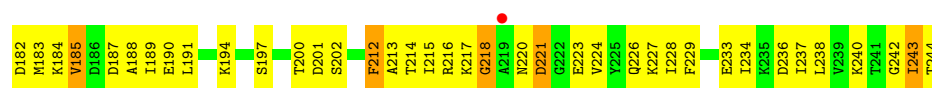
• Molecule 2: Proteasome component Y13





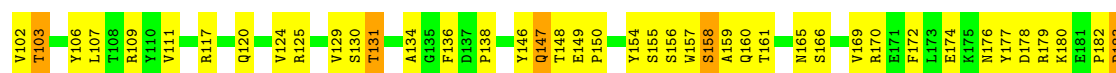
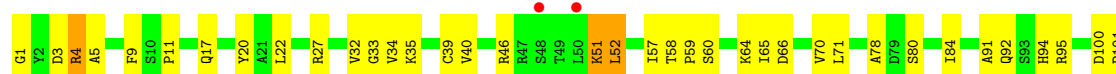
• Molecule 2: Proteasome component Y13

Chain P: 52% 43% 5%



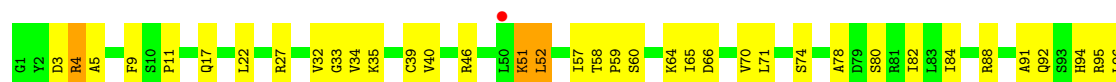
• Molecule 3: Proteasome component PRE6

Chain C: 54% 41% .



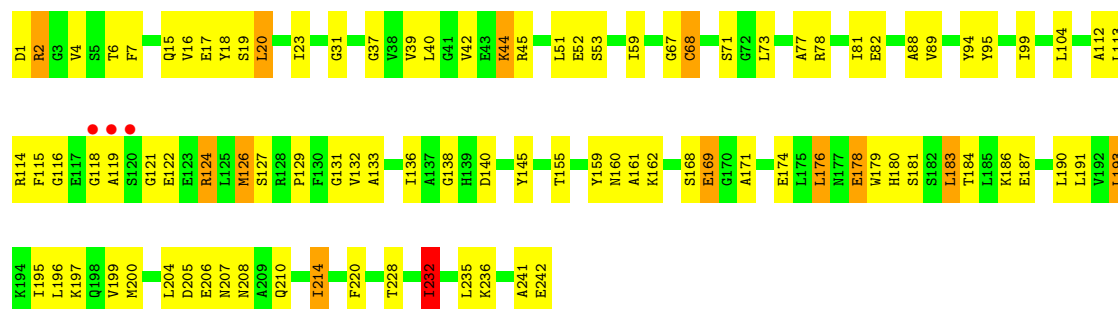
• Molecule 3: Proteasome component PRE6

Chain Q: 53% 43% .

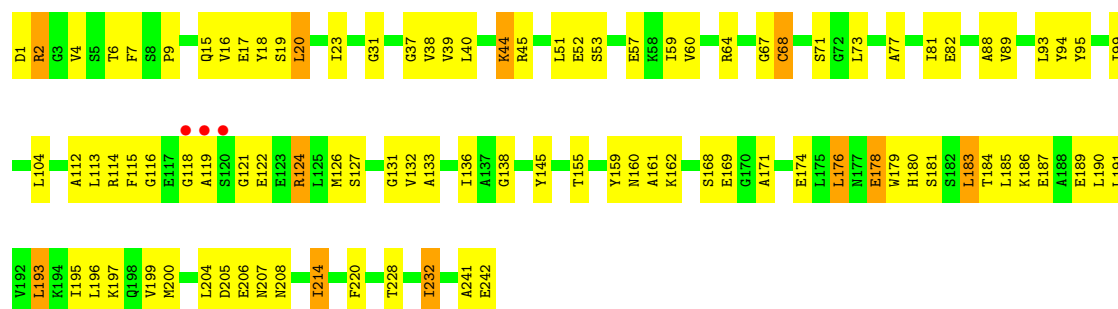


• Molecule 4: Proteasome component PUP2

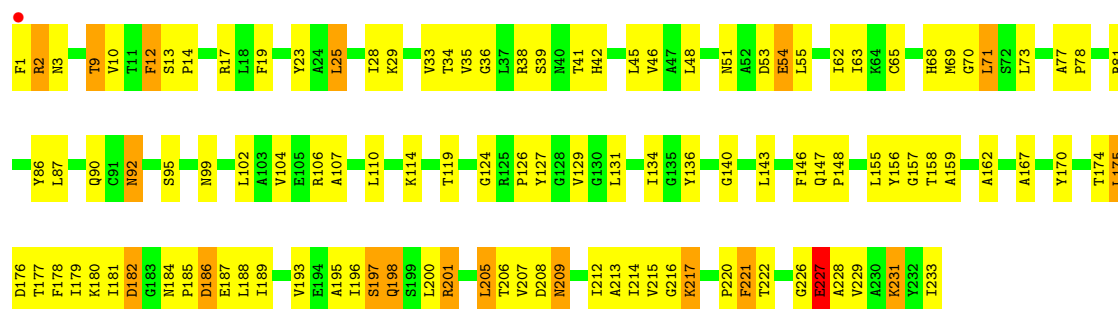
Chain D: 60% 35% 5%



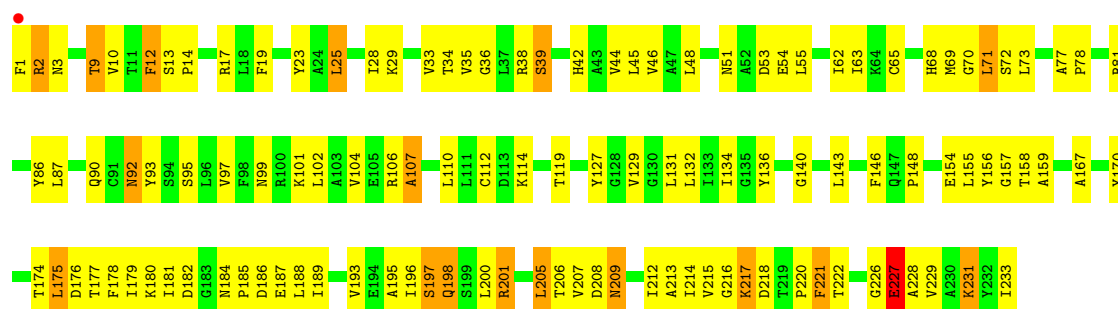
• Molecule 4: Proteasome component PUP2



• Molecule 5: Proteasome component PRE5

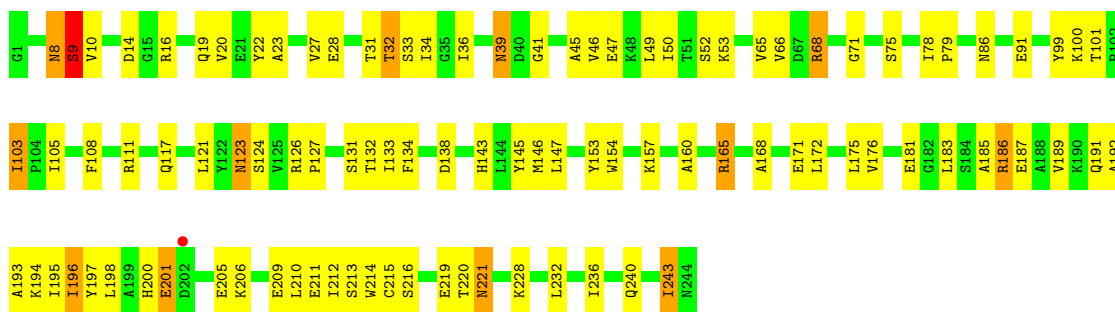


• Molecule 5: Proteasome component PRE5



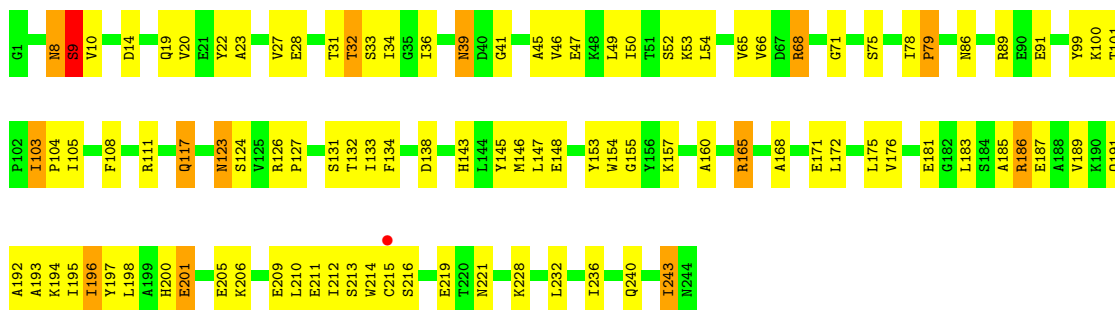
- Molecule 6: Proteasome component C1

Chain F: 



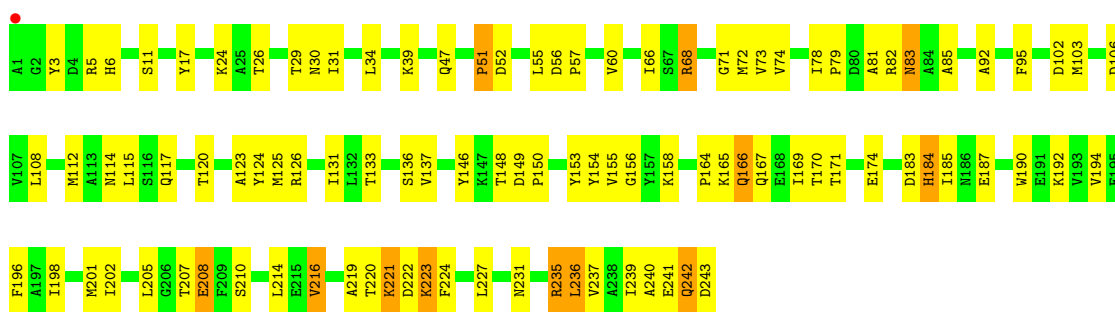
- Molecule 6: Proteasome component C1

Chain T: 



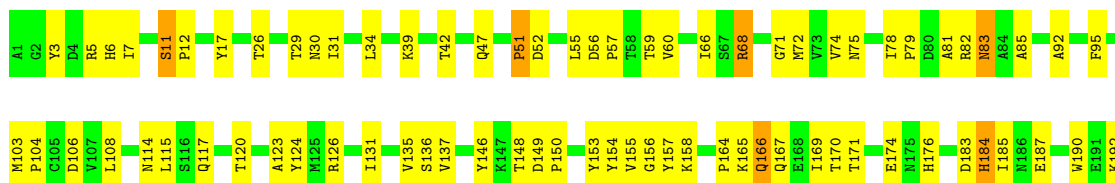
- Molecule 7: Proteasome component C7-alpha

Chain G: 



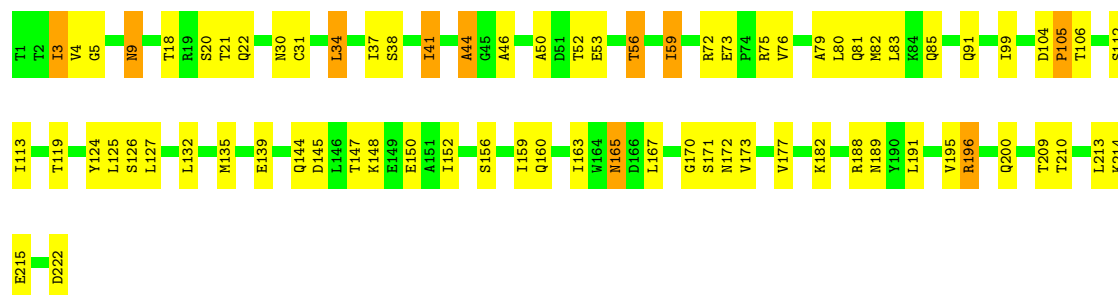
- Molecule 7: Proteasome component C7-alpha

Chain U: 

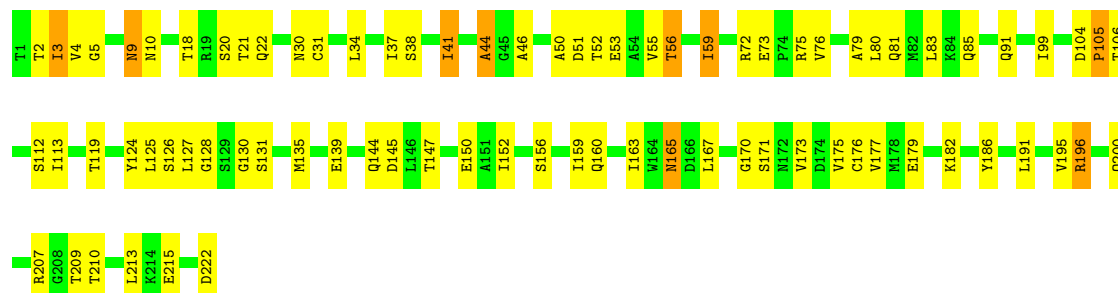




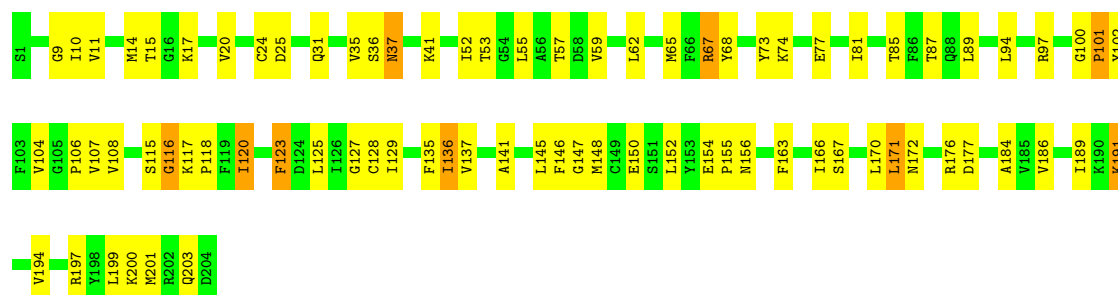
• Molecule 8: Proteasome component PUP1



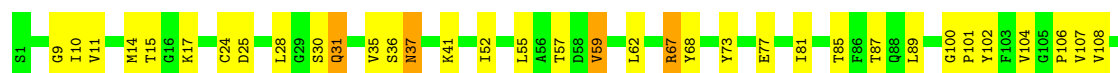
• Molecule 8: Proteasome component PUP1

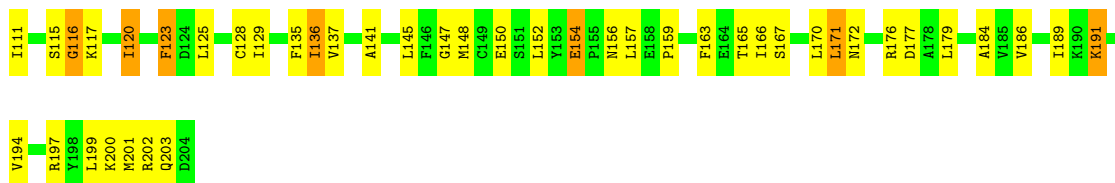


• Molecule 9: Proteasome component PUP3

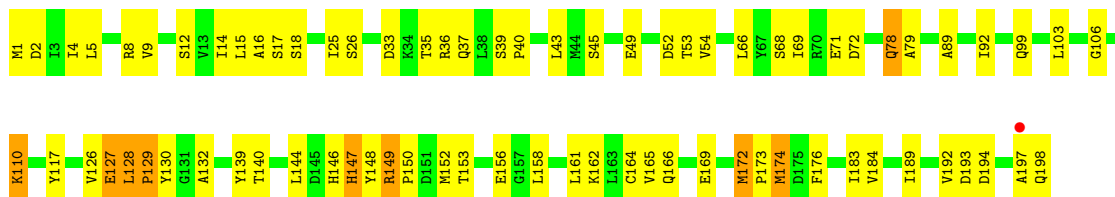


• Molecule 9: Proteasome component PUP3

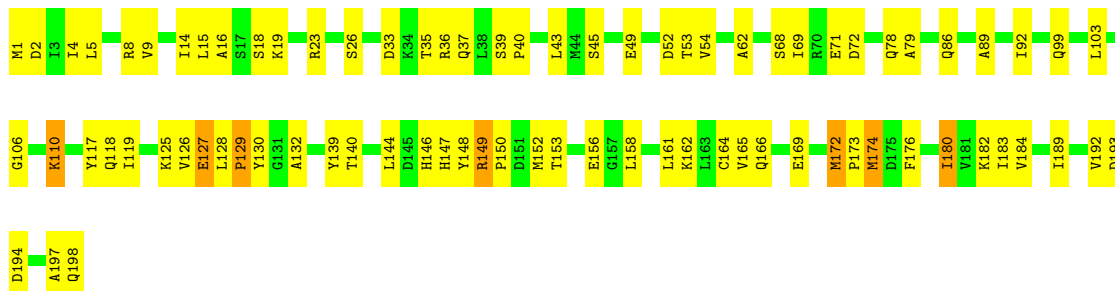




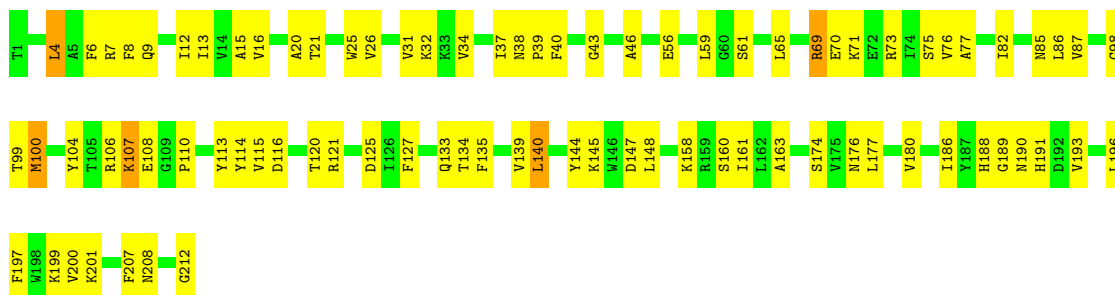
• Molecule 10: Proteasome component C11



• Molecule 10: Proteasome component C11

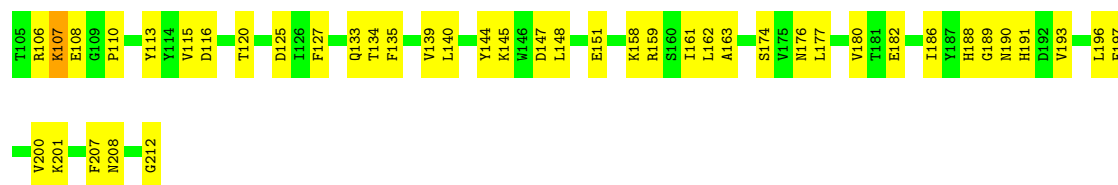


• Molecule 11: Proteasome component PRE2



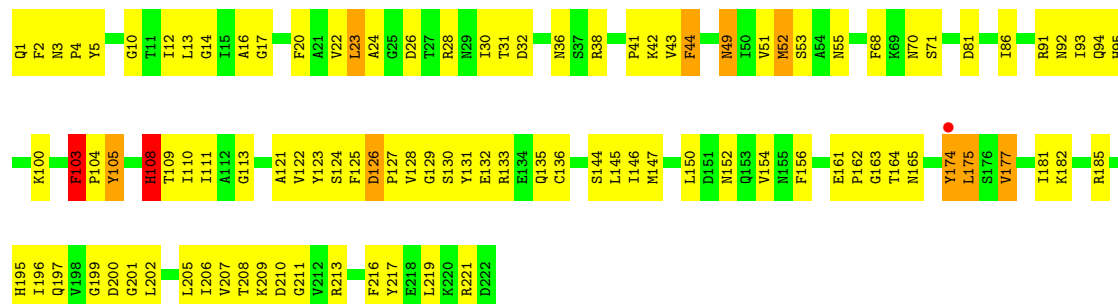
• Molecule 11: Proteasome component PRE2





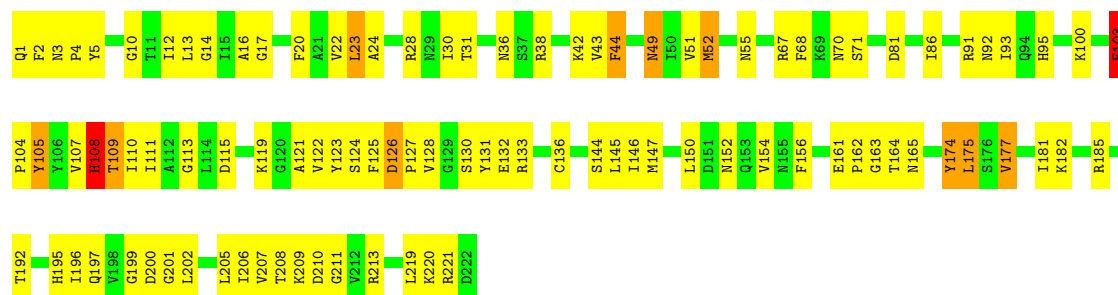
• Molecule 12: Proteasome component C5

Chain L: 54% 41% . .



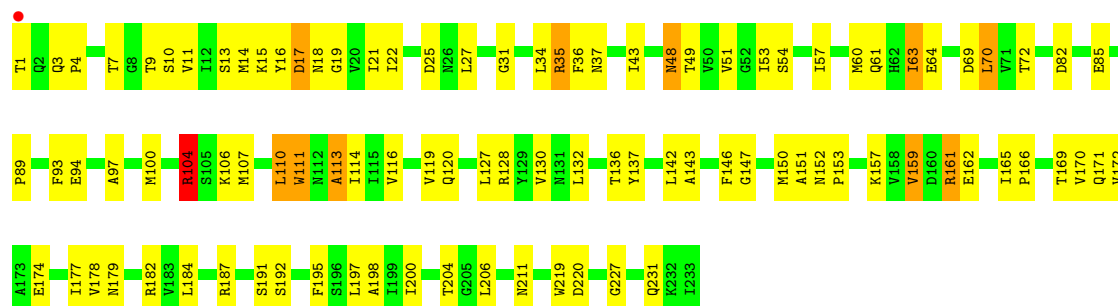
• Molecule 12: Proteasome component C5

Chain Z: 55% 40% 5% .



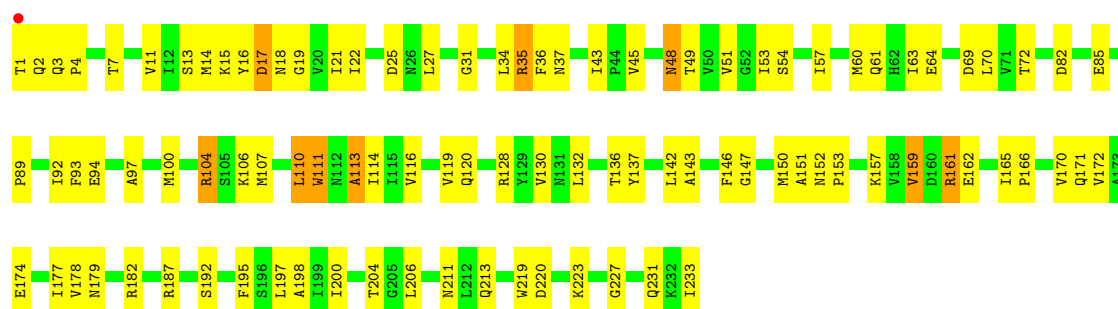
• Molecule 13: Proteasome component PRE4

Chain M: 58% 37% .

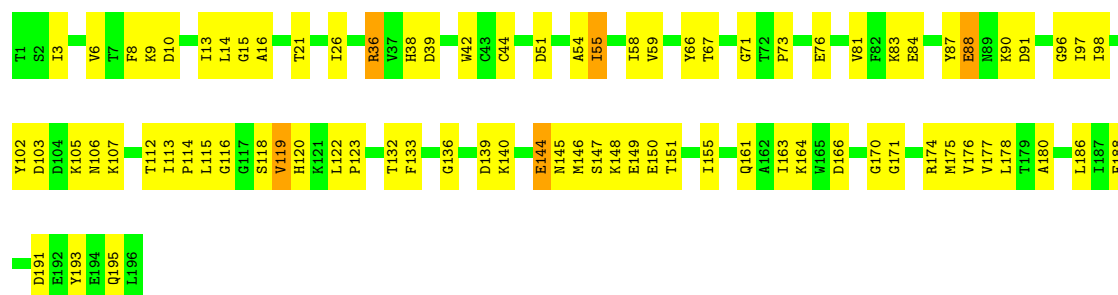


• Molecule 13: Proteasome component PRE4

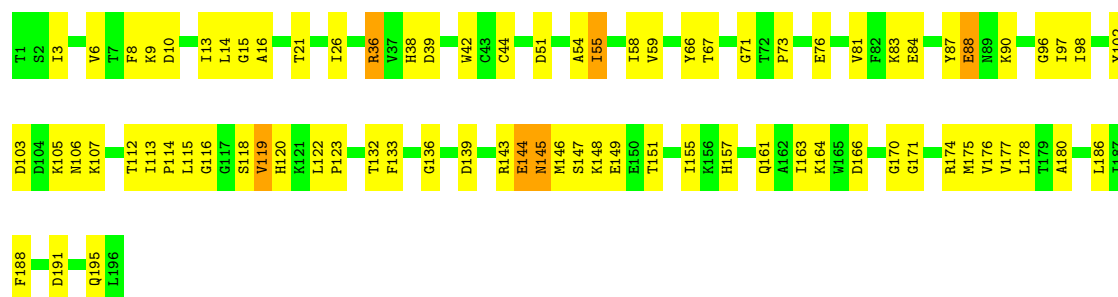
Chain a: 58% 38% .



• Molecule 14: Proteasome component PRE3



• Molecule 14: Proteasome component PRE3



• Molecule 15: Glidobactin



• Molecule 15: Glidobactin



• Molecule 15: Glidobactin

Chain e:  25% 75%

HH91
T2
K3
OM64

● Molecule 15: Glidobactin

Chain f:  50% 50%

HH91
T2
K3
OM64

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.77Å 300.35Å 144.49Å 90.00° 112.67° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (15.00-3.00) 98.8 (15.00-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.99Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.197 , 0.226 0.204 , 0.204	Depositor DCC
R_{free} test set	10479 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.875	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	50986	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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

Bond lengths and bond angles in the following residue types are not validated in this section: LYO, OW6, MH9

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	0.46	0/1952	0.95	5/2642 (0.2%)
1	O	0.44	0/1952	0.95	4/2642 (0.2%)
2	B	0.46	0/1935	0.92	3/2618 (0.1%)
2	P	0.46	0/1935	0.92	3/2618 (0.1%)
3	C	0.44	0/1920	0.91	5/2598 (0.2%)
3	Q	0.42	0/1920	0.91	5/2598 (0.2%)
4	D	0.43	0/1887	0.93	8/2541 (0.3%)
4	R	0.43	0/1887	0.94	7/2541 (0.3%)
5	E	0.42	0/1823	0.89	2/2463 (0.1%)
5	S	0.42	0/1823	0.91	4/2463 (0.2%)
6	F	0.46	0/1937	0.95	6/2614 (0.2%)
6	T	0.45	0/1937	0.96	6/2614 (0.2%)
7	G	0.46	0/1959	0.96	7/2652 (0.3%)
7	U	0.45	0/1959	0.95	7/2652 (0.3%)
8	H	0.48	0/1716	0.94	5/2326 (0.2%)
8	V	0.47	0/1716	0.93	5/2326 (0.2%)
9	I	0.46	0/1611	0.99	8/2174 (0.4%)
9	W	0.47	0/1611	1.00	9/2174 (0.4%)
10	J	0.50	0/1613	1.00	9/2173 (0.4%)
10	X	0.48	0/1613	1.00	7/2173 (0.3%)
11	K	0.47	0/1681	0.92	1/2274 (0.0%)
11	Y	0.47	0/1681	0.92	1/2274 (0.0%)
12	L	0.47	0/1795	1.02	11/2420 (0.5%)
12	Z	0.46	0/1795	1.01	10/2420 (0.4%)
13	M	0.48	0/1855	0.98	13/2514 (0.5%)
13	a	0.48	0/1855	0.98	10/2514 (0.4%)
14	N	0.50	0/1541	0.96	3/2087 (0.1%)
14	b	0.49	0/1541	0.95	3/2087 (0.1%)
15	c	1.05	0/6	0.75	0/7
15	d	1.02	0/6	1.05	0/7
15	e	1.09	0/6	0.74	0/7
15	f	0.75	0/6	1.05	0/7

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.46	0/50474	0.95	167/68220 (0.2%)

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
12	L	0	1
12	Z	0	1
All	All	0	2

There are no bond length outliers.

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	189	GLY	N-CA-C	9.69	125.24	112.65
11	K	189	GLY	N-CA-C	9.45	124.93	112.65
13	a	35	ARG	N-CA-C	9.26	122.22	111.11
13	M	35	ARG	N-CA-C	9.22	122.18	111.11
10	J	172	MET	CA-C-N	8.98	129.56	119.32
10	J	172	MET	C-N-CA	8.98	129.56	119.32
10	X	172	MET	CA-C-N	8.82	129.38	119.32
10	X	172	MET	C-N-CA	8.82	129.38	119.32
1	O	160	LYS	N-CA-C	-8.15	101.12	112.45
1	A	160	LYS	N-CA-C	-7.96	101.38	112.45
2	B	160	LYS	N-CA-C	-7.87	103.80	113.41
6	T	157	LYS	N-CA-C	-7.66	102.27	111.69
12	L	103	PHE	CA-C-N	7.57	129.31	119.84
12	L	103	PHE	C-N-CA	7.57	129.31	119.84
7	G	158	LYS	N-CA-C	-7.45	103.14	112.90
13	a	110	LEU	N-CA-C	-7.42	94.85	107.99
2	P	160	LYS	N-CA-C	-7.41	103.86	113.12
3	C	158	SER	N-CA-C	-7.32	103.33	111.82
13	M	110	LEU	N-CA-C	-7.07	95.47	107.99
13	M	211	ASN	N-CA-C	7.07	121.15	111.54
13	a	113	ALA	N-CA-C	-7.06	96.83	108.76
3	Q	240	GLU	N-CA-C	-7.05	105.50	112.97
7	U	158	LYS	N-CA-C	-7.04	103.68	112.90
12	Z	103	PHE	CA-C-N	7.02	128.61	119.84
12	Z	103	PHE	C-N-CA	7.02	128.61	119.84
12	L	126	ASP	CA-C-N	-7.00	112.59	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	126	ASP	C-N-CA	-7.00	112.59	119.87
9	I	67	ARG	N-CA-C	-6.97	103.37	110.97
4	R	160	ASN	N-CA-C	-6.96	104.61	113.23
3	Q	158	SER	N-CA-C	-6.92	103.51	112.23
6	F	157	LYS	N-CA-C	-6.91	102.84	112.45
13	a	106	LYS	N-CA-C	-6.88	104.19	112.59
13	a	211	ASN	N-CA-C	6.87	120.88	111.54
7	G	123	ALA	N-CA-C	6.84	120.84	112.23
3	C	240	GLU	N-CA-C	-6.75	105.81	112.97
13	M	106	LYS	N-CA-C	-6.74	104.37	112.59
9	W	67	ARG	N-CA-C	-6.71	103.66	110.97
13	M	113	ALA	N-CA-C	-6.70	97.44	108.76
3	Q	131	THR	N-CA-C	6.58	119.73	109.52
5	E	156	TYR	N-CA-C	-6.58	105.38	113.41
3	C	131	THR	N-CA-C	6.55	119.67	109.52
12	Z	126	ASP	CA-C-N	-6.48	113.13	119.87
12	Z	126	ASP	C-N-CA	-6.48	113.13	119.87
7	U	123	ALA	N-CA-C	6.46	120.37	112.23
13	a	17	ASP	N-CA-C	6.45	118.31	111.28
10	J	129	PRO	N-CA-C	-6.44	104.78	113.40
8	H	44	ALA	N-CA-C	-6.42	98.74	109.07
1	A	75	TYR	N-CA-C	6.37	116.68	108.34
6	T	103	ILE	CA-C-N	6.37	126.32	119.76
6	T	103	ILE	C-N-CA	6.37	126.32	119.76
4	R	95	TYR	N-CA-C	6.35	121.81	113.30
8	V	21	THR	N-CA-C	6.34	119.05	109.41
9	W	154	GLU	CA-C-N	6.33	127.75	119.84
9	W	154	GLU	C-N-CA	6.33	127.75	119.84
4	D	160	ASN	N-CA-C	-6.32	104.62	112.90
8	H	37	ILE	N-CA-C	-6.32	104.69	110.82
1	O	75	TYR	N-CA-C	6.31	116.61	108.34
12	Z	105	TYR	N-CA-C	-6.30	98.27	108.41
5	S	156	TYR	N-CA-C	-6.26	105.77	113.41
13	M	7	THR	N-CA-C	6.25	119.38	109.50
12	L	105	TYR	N-CA-C	-6.25	98.35	108.41
13	a	7	THR	N-CA-C	6.24	119.35	109.50
9	I	100	GLY	CA-C-N	6.23	126.58	119.92
9	I	100	GLY	C-N-CA	6.23	126.58	119.92
9	W	100	GLY	CA-C-N	6.23	126.58	119.92
9	W	100	GLY	C-N-CA	6.23	126.58	119.92
8	V	44	ALA	N-CA-C	-6.20	99.08	109.07
6	F	103	ILE	CA-C-N	6.20	126.14	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	103	ILE	C-N-CA	6.20	126.14	119.76
4	D	95	TYR	N-CA-C	6.20	121.60	113.30
8	H	21	THR	N-CA-C	6.11	118.69	109.41
13	a	31	GLY	N-CA-C	-6.05	104.09	111.35
7	G	223	LYS	N-CA-C	6.04	117.59	108.46
8	V	37	ILE	N-CA-C	-6.03	104.97	110.82
6	F	9	SER	N-CA-C	6.03	123.63	110.80
5	S	54	GLU	N-CA-C	-6.03	105.58	113.17
6	T	9	SER	N-CA-C	5.99	123.56	110.80
9	W	102	TYR	N-CA-C	-5.98	99.92	109.96
9	I	154	GLU	CA-C-N	5.97	127.31	119.84
9	I	154	GLU	C-N-CA	5.97	127.31	119.84
6	F	131	SER	N-CA-C	-5.96	99.68	109.40
7	U	223	LYS	N-CA-C	5.96	117.45	108.46
7	G	11	SER	N-CA-C	-5.95	103.17	110.31
10	X	129	PRO	N-CA-C	-5.95	105.43	113.40
14	b	122	LEU	N-CA-C	5.93	114.96	108.14
7	U	11	SER	N-CA-C	-5.92	103.20	110.31
9	W	31	GLN	CB-CA-C	-5.92	109.76	116.63
13	M	157	LYS	N-CA-C	-5.86	105.62	112.89
4	D	178	GLU	N-CA-C	5.86	119.24	111.75
5	E	54	GLU	N-CA-C	-5.84	105.82	113.17
4	R	168	SER	N-CA-C	5.83	117.44	111.14
8	V	171	SER	CB-CA-C	-5.78	109.36	117.23
4	R	178	GLU	N-CA-C	5.74	119.10	111.75
4	R	232	ILE	N-CA-C	-5.71	105.16	110.53
14	N	122	LEU	N-CA-C	5.70	114.70	108.14
1	A	4	ARG	N-CA-C	-5.70	106.29	113.18
4	R	127	SER	N-CA-C	5.69	119.84	113.01
4	D	127	SER	N-CA-C	5.66	119.80	113.01
7	U	39	LYS	N-CA-C	-5.65	105.11	112.23
4	R	179	TRP	N-CA-C	5.64	118.72	109.76
12	L	146	ILE	N-CA-C	5.63	117.14	111.00
13	a	157	LYS	N-CA-C	-5.63	105.91	112.89
7	G	39	LYS	N-CA-C	-5.62	105.15	112.23
8	H	171	SER	CB-CA-C	-5.61	109.59	117.23
1	O	4	ARG	N-CA-C	-5.59	106.41	113.18
4	D	232	ILE	N-CA-C	-5.59	105.28	110.53
9	I	31	GLN	CB-CA-C	-5.57	110.17	116.63
2	P	135	ILE	N-CA-C	-5.56	99.63	107.75
6	T	243	ILE	N-CA-C	-5.54	105.53	113.07
4	D	179	TRP	N-CA-C	5.53	118.55	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	210	SER	N-CA-C	-5.50	102.03	109.95
4	D	168	SER	N-CA-C	5.48	117.06	111.14
7	G	216	VAL	N-CA-C	5.46	115.99	108.12
13	M	31	GLY	N-CA-C	-5.46	104.80	111.35
8	H	165	ASN	N-CA-C	5.45	119.93	113.28
9	I	102	TYR	N-CA-C	-5.44	101.11	109.76
6	T	131	SER	N-CA-C	-5.43	100.55	109.40
14	N	55	ILE	CB-CA-C	-5.42	105.03	111.97
1	A	141	GLU	N-CA-C	5.42	118.69	111.75
6	F	243	ILE	N-CA-C	-5.42	105.71	113.07
12	L	175	LEU	N-CA-C	5.40	117.66	110.53
7	U	216	VAL	N-CA-C	5.39	115.88	108.12
3	Q	103	THR	N-CA-C	-5.38	101.77	110.32
7	G	210	SER	N-CA-C	-5.37	102.21	109.95
2	B	187	ASP	N-CA-C	-5.37	105.34	111.14
2	P	187	ASP	N-CA-C	-5.37	105.34	111.14
10	J	147	HIS	N-CA-C	5.36	119.69	113.20
12	Z	146	ILE	N-CA-C	5.35	116.83	111.00
3	C	65	ILE	N-CA-C	-5.34	104.82	112.35
14	b	55	ILE	CB-CA-C	-5.34	105.13	111.97
10	J	148	TYR	N-CA-C	5.34	118.25	109.76
9	W	59	VAL	N-CA-C	-5.33	105.31	110.42
1	O	141	GLU	N-CA-C	5.32	118.56	111.75
13	M	17	ASP	N-CA-C	5.31	118.55	111.75
13	M	220	ASP	N-CA-C	5.30	116.74	111.07
13	a	220	ASP	N-CA-C	5.28	116.72	111.07
12	L	32	ASP	CB-CA-C	-5.28	110.06	117.23
12	Z	175	LEU	N-CA-C	5.27	117.48	110.53
3	C	103	THR	N-CA-C	-5.26	101.95	110.32
12	L	108	HIS	N-CA-C	-5.24	100.19	108.73
10	X	180	ILE	N-CA-C	-5.23	100.84	108.17
10	X	148	TYR	N-CA-C	5.23	118.07	109.76
5	S	107	ALA	N-CA-C	-5.22	105.77	111.82
13	M	70	LEU	N-CA-C	-5.21	105.72	111.71
3	Q	65	ILE	N-CA-C	-5.18	105.04	112.35
12	L	127	PRO	N-CA-C	-5.17	107.67	114.03
13	M	104	ARG	N-CA-C	-5.13	106.28	112.54
14	N	123	PRO	N-CA-C	-5.13	106.53	113.40
2	B	181	ASP	N-CA-C	5.13	119.00	112.34
12	Z	127	PRO	N-CA-C	-5.12	107.73	114.03
9	I	101	PRO	N-CA-C	5.10	119.25	111.34
4	D	126	MET	N-CA-C	-5.10	99.93	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	140	THR	N-CA-C	5.10	118.66	112.23
5	S	39	SER	N-CA-C	-5.10	104.60	108.78
12	Z	44	PHE	N-CA-C	5.09	117.41	109.52
10	J	128	LEU	N-CA-C	5.08	116.48	108.55
1	A	63	LYS	N-CA-C	-5.06	107.16	113.38
12	L	44	PHE	N-CA-C	5.04	117.34	109.52
14	b	123	PRO	N-CA-C	-5.04	106.52	113.53
10	J	149	ARG	CA-C-N	5.04	126.14	119.84
10	J	149	ARG	C-N-CA	5.04	126.14	119.84
9	W	101	PRO	N-CA-C	5.04	119.15	111.34
8	V	165	ASN	N-CA-C	5.03	119.41	113.28
12	Z	108	HIS	N-CA-C	-5.02	100.55	108.73
10	X	149	ARG	CA-C-N	5.01	126.10	119.84
10	X	149	ARG	C-N-CA	5.01	126.10	119.84
13	M	63	ILE	CB-CA-C	-5.01	105.38	112.14

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	174	TYR	Sidechain
12	Z	174	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	86	0
1	O	1915	0	1929	85	0
2	B	1905	0	1904	114	0
2	P	1905	0	1904	115	0
3	C	1891	0	1903	99	0
3	Q	1891	0	1903	98	0
4	D	1862	0	1839	71	0
4	R	1862	0	1839	74	0
5	E	1795	0	1800	128	0
5	S	1795	0	1800	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1897	0	1889	78	0
6	T	1897	0	1889	85	0
7	G	1921	0	1913	90	0
7	U	1921	0	1913	99	0
8	H	1685	0	1687	62	0
8	V	1685	0	1687	63	0
9	I	1581	0	1574	74	0
9	W	1581	0	1574	77	0
10	J	1585	0	1590	71	0
10	X	1585	0	1590	79	0
11	K	1644	0	1594	76	0
11	Y	1644	0	1594	74	0
12	L	1757	0	1711	89	0
12	Z	1757	0	1711	90	0
13	M	1824	0	1832	83	0
13	a	1824	0	1832	85	0
14	N	1512	0	1481	68	0
14	b	1512	0	1481	64	0
15	c	37	0	35	4	0
15	d	37	0	35	1	0
15	e	37	0	35	4	0
15	f	37	0	35	1	0
16	A	56	0	0	2	0
16	B	35	0	0	1	0
16	C	41	0	0	5	0
16	D	39	0	0	3	0
16	E	25	0	0	3	0
16	F	45	0	0	4	0
16	G	59	0	0	7	0
16	H	52	0	0	5	0
16	I	61	0	0	4	0
16	J	55	0	0	3	0
16	K	41	0	0	4	0
16	L	57	0	0	3	0
16	M	63	0	0	7	0
16	N	61	0	0	5	0
16	O	34	0	0	0	0
16	P	27	0	0	6	0
16	Q	29	0	0	8	0
16	R	31	0	0	4	0
16	S	21	0	0	3	0
16	T	36	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	U	63	0	0	6	0
16	V	46	0	0	3	0
16	W	47	0	0	8	0
16	X	47	0	0	4	0
16	Y	44	0	0	4	0
16	Z	49	0	0	6	0
16	a	72	0	0	8	0
16	b	54	0	0	2	0
All	All	50986	0	49432	2205	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 22.

All (2205) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLU:HG2	2:B:55:LEU:HD21	1.30	1.10
2:B:43:ILE:HD11	2:B:145:TYR:HB3	1.36	1.06
2:P:43:ILE:HD11	2:P:145:TYR:HB3	1.37	1.04
1:A:128:ARG:HH21	7:G:120:THR:HG22	1.25	1.01
10:J:174:MET:HE3	10:X:174:MET:HE3	1.39	1.01
11:Y:107:LYS:H	11:Y:107:LYS:HD2	1.25	1.01
1:A:176:GLU:HG2	2:B:55:LEU:CD2	1.91	0.99
11:K:107:LYS:H	11:K:107:LYS:HD2	1.24	0.98
1:O:12:PHE:H	2:P:20:GLN:HE22	1.11	0.97
2:B:223:GLU:HG2	2:B:224:VAL:H	1.27	0.97
1:O:128:ARG:HH21	7:U:120:THR:HG22	1.25	0.97
2:P:200:THR:HG22	2:P:202:SER:H	1.27	0.97
2:P:223:GLU:HG2	2:P:224:VAL:H	1.29	0.97
9:W:14:MET:HE3	9:W:166:ILE:HG13	1.49	0.94
10:X:162:LYS:O	10:X:166:GLN:HG3	1.68	0.94
6:T:91:GLU:HG2	6:T:111:ARG:HB3	1.48	0.94
2:B:200:THR:HG22	2:B:202:SER:H	1.29	0.93
9:I:14:MET:HE3	9:I:166:ILE:HG13	1.46	0.93
6:F:91:GLU:HG2	6:F:111:ARG:HB3	1.49	0.92
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.50	0.92
3:Q:160:GLN:NE2	3:Q:161:THR:H	1.67	0.92
2:B:122:THR:HG22	3:C:125:ARG:HH21	1.35	0.91
2:P:122:THR:HG22	3:Q:125:ARG:HH21	1.33	0.91
1:A:211:LEU:HD22	1:A:238:LEU:HD12	1.51	0.91
10:J:162:LYS:O	10:J:166:GLN:HG3	1.68	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:ASN:ND2	2:B:70:ASP:H	1.69	0.90
3:C:160:GLN:NE2	3:C:161:THR:H	1.67	0.90
1:O:211:LEU:HD22	1:O:238:LEU:HD12	1.53	0.90
13:a:161:ARG:HH11	13:a:161:ARG:HG3	1.37	0.89
3:Q:60:SER:HB2	16:Q:303:HOH:O	1.72	0.89
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.52	0.89
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.38	0.88
6:T:34:ILE:HG22	6:T:160:ALA:HB2	1.55	0.88
5:E:12:PHE:HB2	6:F:19:GLN:HE22	1.37	0.88
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.36	0.88
7:U:103:MET:HE3	7:U:108:LEU:HB2	1.55	0.87
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.37	0.87
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.39	0.87
9:W:148:MET:HE2	9:W:172:ASN:HB2	1.56	0.87
3:C:160:GLN:HE21	3:C:161:THR:N	1.72	0.87
2:P:69:ASN:ND2	2:P:70:ASP:H	1.72	0.87
7:G:103:MET:HE3	7:G:108:LEU:HB2	1.55	0.86
1:A:12:PHE:H	2:B:20:GLN:HE22	1.18	0.86
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.18	0.86
3:Q:160:GLN:HE21	3:Q:161:THR:N	1.71	0.86
1:A:46:ALA:HB2	1:A:211:LEU:HG	1.56	0.85
2:B:12:PHE:H	3:C:17:GLN:HE22	1.20	0.85
1:O:46:ALA:HB2	1:O:211:LEU:HG	1.55	0.85
11:K:135:PHE:HA	16:X:212:HOH:O	1.74	0.85
6:F:34:ILE:HG22	6:F:160:ALA:HB2	1.58	0.85
1:O:128:ARG:HH21	7:U:120:THR:CG2	1.89	0.85
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.41	0.84
9:I:148:MET:HE2	9:I:172:ASN:HB2	1.57	0.84
3:Q:160:GLN:HE21	3:Q:161:THR:H	0.85	0.84
13:M:161:ARG:HG3	13:M:161:ARG:HH11	1.41	0.83
3:C:185:THR:HG22	3:C:187:GLU:H	1.42	0.83
5:E:205:LEU:HD23	5:E:205:LEU:H	1.44	0.82
9:W:202:ARG:HG3	16:W:307:HOH:O	1.78	0.82
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.22	0.82
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.61	0.81
10:J:1:MET:HG2	10:J:2:ASP:H	1.45	0.81
1:A:30:GLN:HE21	1:A:30:GLN:HA	1.45	0.81
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.61	0.81
5:S:205:LEU:H	5:S:205:LEU:HD23	1.44	0.81
5:S:12:PHE:HB2	6:T:19:GLN:HE22	1.46	0.81
6:T:65:VAL:HG12	16:T:322:HOH:O	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:160:GLN:HE21	3:C:161:THR:H	0.86	0.80
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	1.79	0.80
1:A:128:ARG:HH21	7:G:120:THR:CG2	1.94	0.79
12:L:52:MET:HB2	12:L:111:ILE:HG22	1.65	0.79
5:E:200:LEU:HD11	5:E:205:LEU:HD22	1.65	0.79
1:O:30:GLN:HA	1:O:30:GLN:HE21	1.46	0.79
4:R:155:THR:HG22	5:S:77:ALA:HB3	1.66	0.78
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.65	0.78
4:D:241:ALA:O	4:D:242:GLU:HB2	1.83	0.78
11:K:107:LYS:H	11:K:107:LYS:CD	1.95	0.78
4:R:241:ALA:O	4:R:242:GLU:HB2	1.82	0.78
9:W:35:VAL:HG13	16:X:227:HOH:O	1.82	0.78
14:b:112:THR:HG22	14:b:120:HIS:HB2	1.66	0.78
5:S:200:LEU:HD11	5:S:205:LEU:HD22	1.65	0.78
10:X:1:MET:HG2	10:X:2:ASP:H	1.47	0.77
8:H:81:GLN:O	8:H:85:GLN:HG3	1.84	0.77
5:S:197:SER:HA	5:S:200:LEU:HG	1.65	0.77
3:Q:80:SER:O	3:Q:84:ILE:HG12	1.84	0.77
5:S:189:ILE:HG23	5:S:212:ILE:HD13	1.66	0.77
13:M:130:VAL:HG23	13:M:136:THR:HG22	1.67	0.77
7:G:68:ARG:HB3	16:G:352:HOH:O	1.85	0.77
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.67	0.77
3:C:66:ASP:HA	10:J:69:ILE:HD13	1.67	0.76
6:F:65:VAL:HG12	16:F:308:HOH:O	1.85	0.76
6:T:34:ILE:HG22	6:T:160:ALA:CB	2.14	0.76
5:E:69:MET:HE2	5:E:104:VAL:HG22	1.67	0.76
5:E:197:SER:HA	5:E:200:LEU:HG	1.66	0.76
8:V:81:GLN:O	8:V:85:GLN:HG3	1.86	0.76
5:E:92:ASN:HD21	12:L:70:ASN:ND2	1.83	0.76
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.67	0.76
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.66	0.76
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.67	0.76
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.68	0.76
2:B:223:GLU:HG2	2:B:224:VAL:N	2.00	0.76
7:U:55:LEU:O	7:U:57:PRO:HD3	1.85	0.76
3:C:80:SER:O	3:C:84:ILE:HG12	1.85	0.76
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.67	0.75
11:Y:107:LYS:H	11:Y:107:LYS:CD	1.95	0.75
12:Z:52:MET:HB2	12:Z:111:ILE:HG22	1.66	0.75
14:N:139:ASP:HB3	14:b:161:GLN:HE22	1.50	0.75
2:B:122:THR:CG2	3:C:125:ARG:HH21	1.99	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:189:ILE:HG23	5:E:212:ILE:HD13	1.68	0.75
14:N:161:GLN:HE22	14:b:139:ASP:HB3	1.51	0.75
7:G:92:ALA:HA	7:G:103:MET:HE2	1.69	0.75
12:L:17:GLY:HA3	12:L:20:PHE:CE2	2.22	0.75
3:Q:213:VAL:HG23	3:Q:219:ILE:HG12	1.68	0.75
12:Z:17:GLY:HA3	12:Z:20:PHE:CE2	2.20	0.75
13:a:130:VAL:HG23	13:a:136:THR:HG22	1.69	0.75
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.69	0.74
7:G:55:LEU:O	7:G:57:PRO:HD3	1.87	0.74
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.33	0.74
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	1.68	0.74
7:U:92:ALA:HA	7:U:103:MET:HE2	1.69	0.74
6:T:31:THR:HG21	6:T:47:GLU:O	1.88	0.74
8:V:4:VAL:HG22	8:V:159:ILE:HD11	1.67	0.74
3:C:9:PHE:H	4:D:15:GLN:HE22	1.33	0.74
3:C:161:THR:HG21	3:C:169:VAL:HG13	1.68	0.74
6:F:34:ILE:HG22	6:F:160:ALA:CB	2.16	0.74
2:P:223:GLU:HG2	2:P:224:VAL:N	2.02	0.74
7:U:221:LYS:HE3	7:U:221:LYS:HA	1.70	0.73
1:O:178:ARG:HB3	1:O:178:ARG:HH11	1.52	0.73
8:H:165:ASN:OD1	13:a:153:PRO:HA	1.88	0.72
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.36	0.72
3:Q:156:SER:HB2	16:Q:323:HOH:O	1.89	0.72
3:C:35:LYS:HG2	3:C:158:SER:O	1.88	0.72
5:E:81:ARG:HH11	5:E:81:ARG:HG3	1.54	0.72
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.69	0.72
13:a:51:VAL:HG22	13:a:116:VAL:HG22	1.71	0.72
1:A:204:PHE:CE1	1:A:209:ILE:HD11	2.23	0.72
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.02	0.72
5:S:81:ARG:HH11	5:S:81:ARG:HG3	1.53	0.72
11:K:208:ASN:HD21	10:X:150:PRO:HG3	1.54	0.72
14:N:51:ASP:O	14:N:55:ILE:HG12	1.90	0.72
6:F:31:THR:HG21	6:F:47:GLU:O	1.90	0.72
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	1.87	0.72
5:E:87:LEU:HD11	5:E:107:ALA:HB1	1.72	0.72
8:H:3:ILE:CD1	8:H:127:LEU:HB2	2.20	0.72
6:T:33:SER:HB3	6:T:46:VAL:HG23	1.71	0.72
7:U:11:SER:HA	16:U:326:HOH:O	1.90	0.72
5:E:12:PHE:HB2	6:F:19:GLN:NE2	2.05	0.71
1:O:119:GLN:O	1:O:122:THR:HB	1.91	0.71
6:T:31:THR:HG22	6:T:32:THR:N	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:221:LYS:HA	7:G:221:LYS:HE3	1.71	0.71
10:X:33:ASP:OD2	10:X:35:THR:HG22	1.89	0.71
1:A:178:ARG:HB3	1:A:178:ARG:HH11	1.54	0.71
3:C:64:LYS:HE3	3:C:219:ILE:HD12	1.71	0.71
2:B:119:GLN:O	2:B:122:THR:HB	1.90	0.71
3:C:213:VAL:HG23	3:C:219:ILE:HG12	1.72	0.71
7:G:30:ASN:HD22	7:G:164:PRO:HG2	1.56	0.71
10:J:139:TYR:HD1	16:Y:319:HOH:O	1.74	0.71
2:P:119:GLN:O	2:P:122:THR:HB	1.90	0.71
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.02	0.71
6:F:33:SER:HB3	6:F:46:VAL:HG23	1.73	0.71
6:F:196:ILE:HG21	6:F:210:LEU:HD13	1.72	0.71
8:V:3:ILE:CD1	8:V:127:LEU:HB2	2.19	0.71
4:D:159:TYR:CE2	4:D:162:LYS:HD3	2.26	0.71
12:L:22:VAL:HG12	12:L:206:ILE:HG13	1.73	0.71
8:V:52:THR:O	8:V:56:THR:HB	1.91	0.71
4:D:186:LYS:O	4:D:190:LEU:HD23	1.91	0.70
8:V:53:GLU:O	8:V:56:THR:HG22	1.91	0.70
10:J:33:ASP:OD2	10:J:35:THR:HG22	1.90	0.70
1:O:204:PHE:CE1	1:O:209:ILE:HD11	2.27	0.70
4:R:186:LYS:O	4:R:190:LEU:HD23	1.91	0.70
5:S:205:LEU:HA	5:S:209:ASN:ND2	2.06	0.70
14:b:51:ASP:O	14:b:55:ILE:HG12	1.90	0.70
13:a:174:GLU:O	13:a:178:VAL:HG23	1.90	0.70
11:K:107:LYS:HD2	11:K:107:LYS:N	2.05	0.70
4:R:161:ALA:HB3	5:S:55:LEU:HD23	1.72	0.70
6:T:196:ILE:HG21	6:T:210:LEU:HD13	1.72	0.70
1:A:119:GLN:O	1:A:122:THR:HB	1.90	0.70
2:P:122:THR:CG2	3:Q:125:ARG:HH21	2.02	0.70
4:R:159:TYR:CE2	4:R:162:LYS:HD3	2.26	0.70
13:M:48:ASN:H	13:M:48:ASN:HD22	1.38	0.70
7:U:30:ASN:HD22	7:U:164:PRO:HG2	1.56	0.70
13:a:48:ASN:HD22	13:a:48:ASN:H	1.39	0.70
12:Z:22:VAL:HG12	12:Z:206:ILE:HG13	1.73	0.70
13:M:51:VAL:HG22	13:M:116:VAL:HG22	1.74	0.69
7:U:117:GLN:O	7:U:120:THR:HB	1.92	0.69
8:H:52:THR:O	8:H:56:THR:HB	1.92	0.69
3:Q:64:LYS:HE3	3:Q:219:ILE:HD12	1.73	0.69
3:C:204:GLY:HA3	3:C:207:ASN:HB2	1.75	0.69
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.91	0.69
5:S:70:GLY:HA3	5:S:221:PHE:CE2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:89:PRO:HD2	13:a:120:GLN:OE1	1.93	0.69
9:W:52:ILE:HB	9:W:59:VAL:HG13	1.74	0.69
10:X:14:ILE:HD13	10:X:158:LEU:HD23	1.74	0.69
11:K:208:ASN:HD21	10:X:150:PRO:CG	2.06	0.69
1:O:57:MET:HE3	1:O:60:THR:HG21	1.74	0.69
5:E:70:GLY:HA3	5:E:221:PHE:CE2	2.27	0.69
14:N:105:LYS:O	14:N:105:LYS:HD3	1.93	0.69
14:N:161:GLN:NE2	14:b:136:GLY:HA2	2.06	0.69
3:Q:35:LYS:HG2	3:Q:158:SER:O	1.92	0.69
3:C:51:LYS:O	3:C:52:LEU:HB2	1.93	0.69
7:G:117:GLN:O	7:G:120:THR:HB	1.91	0.69
9:W:17:LYS:HD3	9:W:156:ASN:HD22	1.57	0.69
14:b:105:LYS:O	14:b:105:LYS:HD3	1.92	0.69
13:M:174:GLU:O	13:M:178:VAL:HG23	1.93	0.69
12:Z:202:LEU:HB2	12:Z:219:LEU:HD11	1.75	0.68
5:E:92:ASN:ND2	12:L:70:ASN:HD21	1.90	0.68
13:M:172:VAL:HG21	16:M:350:HOH:O	1.94	0.68
6:F:31:THR:HG22	6:F:32:THR:N	2.07	0.68
14:N:136:GLY:HA2	14:b:161:GLN:NE2	2.08	0.68
9:I:17:LYS:HD3	9:I:156:ASN:HD22	1.58	0.68
12:Z:126:ASP:HB2	12:Z:130:SER:H	1.57	0.68
13:a:179:ASN:HB3	16:a:337:HOH:O	1.93	0.68
5:E:205:LEU:HA	5:E:209:ASN:ND2	2.08	0.68
12:L:126:ASP:HB2	12:L:130:SER:H	1.57	0.68
5:S:77:ALA:HB3	5:S:78:PRO:HD3	1.75	0.68
6:T:78:ILE:HB	6:T:79:PRO:HD3	1.76	0.68
5:E:178:PHE:HA	5:E:181:ILE:HG13	1.76	0.68
10:J:174:MET:HE3	10:X:174:MET:CE	2.20	0.68
3:Q:204:GLY:HA3	3:Q:207:ASN:HB2	1.75	0.68
1:A:57:MET:HE3	1:A:60:THR:HG21	1.75	0.67
1:O:176:GLU:HG2	2:P:55:LEU:HD21	1.76	0.67
5:S:69:MET:HE2	5:S:104:VAL:HG22	1.75	0.67
10:J:149:ARG:O	10:J:152:MET:HG3	1.95	0.67
14:b:21:THR:HG22	14:b:26:ILE:HA	1.77	0.67
5:S:127:TYR:O	5:S:148:PRO:HB3	1.94	0.67
5:S:178:PHE:HA	5:S:181:ILE:HG13	1.75	0.67
12:L:202:LEU:HB2	12:L:219:LEU:HD11	1.75	0.67
5:S:206:THR:H	5:S:209:ASN:HD22	1.41	0.67
13:a:119:VAL:HG23	13:a:200:ILE:HG22	1.74	0.67
2:B:43:ILE:CD1	2:B:145:TYR:HB3	2.22	0.67
5:E:167:ALA:HB2	5:E:195:ALA:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:21:THR:HG22	14:N:26:ILE:HA	1.77	0.67
4:R:180:HIS:O	4:R:183:LEU:HD12	1.95	0.67
13:a:161:ARG:HH11	13:a:161:ARG:CG	2.07	0.67
5:S:136:TYR:CE2	5:S:217:LYS:HA	2.29	0.66
8:H:135:MET:HE3	13:a:187:ARG:NH2	2.09	0.66
1:A:172:LYS:O	1:A:176:GLU:HG3	1.95	0.66
1:O:178:ARG:HB3	1:O:178:ARG:NH1	2.10	0.66
4:D:180:HIS:O	4:D:183:LEU:HD12	1.95	0.66
5:E:77:ALA:HB3	5:E:78:PRO:HD3	1.76	0.66
5:S:12:PHE:HB2	6:T:19:GLN:NE2	2.10	0.66
11:Y:40:PHE:HB3	11:Y:73:ARG:NH2	2.11	0.66
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.31	0.66
10:J:14:ILE:HD13	10:J:158:LEU:HD23	1.78	0.66
5:E:136:TYR:CE2	5:E:217:LYS:HA	2.31	0.66
6:F:147:LEU:HB3	16:F:333:HOH:O	1.96	0.66
10:J:174:MET:CE	10:X:174:MET:HE3	2.21	0.66
3:Q:51:LYS:HD2	3:Q:52:LEU:N	2.11	0.66
5:S:167:ALA:HB2	5:S:195:ALA:O	1.96	0.66
6:F:78:ILE:HB	6:F:79:PRO:HD3	1.77	0.65
6:T:143:HIS:HD2	16:T:301:HOH:O	1.78	0.65
3:C:60:SER:HB2	16:C:309:HOH:O	1.96	0.65
5:E:207:VAL:HA	5:E:233:ILE:HD11	1.79	0.65
12:L:28:ARG:NE	12:L:200:ASP:OD2	2.30	0.65
12:L:195:HIS:HD2	12:L:197:GLN:H	1.44	0.65
1:O:176:GLU:HG2	2:P:55:LEU:CD2	2.26	0.65
2:P:85:ILE:O	2:P:89:THR:HG23	1.96	0.65
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.77	0.65
1:A:178:ARG:HB3	1:A:178:ARG:NH1	2.11	0.65
6:F:191:GLN:O	6:F:195:ILE:HG12	1.97	0.65
13:M:16:TYR:CE2	13:M:170:VAL:HG22	2.30	0.65
13:a:16:TYR:CE2	13:a:170:VAL:HG22	2.32	0.65
5:E:207:VAL:HG13	5:E:208:ASP:N	2.09	0.65
2:P:48:GLU:OE2	2:P:200:THR:HG23	1.96	0.65
3:Q:66:ASP:HA	10:X:69:ILE:HD13	1.78	0.65
10:X:149:ARG:O	10:X:152:MET:HG3	1.97	0.65
7:G:187:GLU:HG2	7:G:192:LYS:CB	2.25	0.65
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.10	0.65
10:J:150:PRO:HG3	11:Y:208:ASN:HD21	1.60	0.65
2:P:119:GLN:HG3	3:Q:78:ALA:HB1	1.79	0.65
5:S:207:VAL:HG13	5:S:208:ASP:N	2.10	0.65
5:E:193:VAL:O	5:E:196:ILE:HG22	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:39:SER:HB2	10:J:40:PRO:HD2	1.79	0.65
12:L:38:ARG:NH1	12:L:221:ARG:HB3	2.12	0.65
7:U:202:ILE:HG23	7:U:207:THR:O	1.96	0.65
12:Z:181:ILE:O	12:Z:185:ARG:HG3	1.96	0.65
13:M:153:PRO:HA	8:V:165:ASN:OD1	1.97	0.65
3:C:27:ARG:HD2	16:C:319:HOH:O	1.96	0.65
5:S:9:THR:HG21	5:S:119:THR:HA	1.78	0.65
12:Z:38:ARG:NH1	12:Z:221:ARG:HB3	2.11	0.65
13:a:35:ARG:HG2	16:a:318:HOH:O	1.97	0.65
1:A:66:LEU:C	1:A:66:LEU:HD23	2.22	0.64
2:B:48:GLU:OE2	2:B:200:THR:HG23	1.97	0.64
5:S:207:VAL:HA	5:S:233:ILE:HD11	1.79	0.64
3:C:51:LYS:HD2	3:C:52:LEU:N	2.12	0.64
5:E:9:THR:HG21	5:E:119:THR:HA	1.79	0.64
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.79	0.64
13:M:89:PRO:HD2	13:M:120:GLN:OE1	1.97	0.64
10:X:127:GLU:O	10:X:128:LEU:HD23	1.97	0.64
2:B:69:ASN:ND2	2:B:70:ASP:N	2.44	0.64
7:G:72:MET:HE3	7:G:74:VAL:CG2	2.28	0.64
1:O:83:ARG:HE	7:U:114:ASN:HD21	1.45	0.64
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.79	0.64
12:Z:28:ARG:NE	12:Z:200:ASP:OD2	2.30	0.64
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.61	0.64
5:S:193:VAL:O	5:S:196:ILE:HG22	1.98	0.64
1:A:83:ARG:HE	7:G:114:ASN:HD21	1.45	0.64
7:G:148:THR:HG22	7:G:154:TYR:HB2	1.80	0.64
10:J:53:THR:HG23	10:J:54:VAL:N	2.13	0.64
2:P:217:LYS:HG3	2:P:223:GLU:O	1.97	0.64
8:H:3:ILE:HG12	8:H:99:ILE:HD12	1.78	0.64
4:R:94:TYR:O	12:Z:91:ARG:HG3	1.98	0.64
6:T:147:LEU:HD13	6:T:153:TYR:HB3	1.79	0.64
2:B:217:LYS:HG3	2:B:223:GLU:O	1.98	0.64
3:C:27:ARG:NH1	3:C:27:ARG:HB2	2.12	0.64
10:J:127:GLU:O	10:J:128:LEU:HD23	1.97	0.64
2:P:158:GLY:HA3	3:Q:57:ILE:CD1	2.28	0.64
1:O:66:LEU:HD23	1:O:66:LEU:C	2.23	0.64
5:S:90:GLN:HG3	5:S:110:LEU:HD13	1.78	0.64
1:A:246:ARG:HH11	1:A:246:ARG:HG3	1.63	0.64
7:G:202:ILE:HG23	7:G:207:THR:O	1.97	0.64
13:M:49:THR:OG1	13:M:89:PRO:HG3	1.98	0.64
13:M:150:MET:C	13:M:153:PRO:HD2	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:120:ILE:HD12	9:W:136:ILE:HD13	1.79	0.64
11:Y:145:LYS:O	11:Y:148:LEU:HD13	1.98	0.64
12:Z:13:LEU:HD11	12:Z:150:LEU:CD2	2.28	0.64
6:F:36:ILE:HD12	6:F:192:ALA:HB2	1.80	0.63
8:H:53:GLU:O	8:H:56:THR:HG22	1.98	0.63
13:M:161:ARG:HH11	13:M:161:ARG:CG	2.10	0.63
7:U:187:GLU:HG2	7:U:192:LYS:CB	2.28	0.63
12:Z:13:LEU:HD12	12:Z:14:GLY:H	1.63	0.63
3:C:157:TRP:CE2	4:D:51:LEU:HD23	2.33	0.63
1:O:246:ARG:HG3	1:O:246:ARG:HH11	1.61	0.63
3:Q:27:ARG:NH1	3:Q:27:ARG:HB2	2.13	0.63
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.64	0.63
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.44	0.63
13:a:150:MET:C	13:a:153:PRO:HD2	2.22	0.63
5:E:90:GLN:HG3	5:E:110:LEU:HD13	1.80	0.63
5:E:206:THR:H	5:E:209:ASN:HD22	1.44	0.63
10:J:150:PRO:CG	11:Y:208:ASN:HD21	2.10	0.63
10:X:39:SER:HB2	10:X:40:PRO:HD2	1.79	0.63
2:B:220:ASN:O	2:B:221:ASP:HB2	1.99	0.63
13:M:114:ILE:HB	13:M:130:VAL:HG12	1.80	0.63
4:R:9:PRO:HA	5:S:23:TYR:CD2	2.34	0.63
7:U:148:THR:HG22	7:U:154:TYR:HB2	1.81	0.63
4:D:155:THR:HG22	5:E:77:ALA:HB3	1.80	0.63
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.34	0.63
7:U:239:ILE:C	7:U:239:ILE:HD12	2.23	0.63
11:K:21:THR:HG22	11:K:26:VAL:HA	1.81	0.63
6:T:31:THR:CG2	6:T:32:THR:N	2.62	0.63
1:O:30:GLN:HE21	1:O:30:GLN:CA	2.12	0.63
9:I:120:ILE:HD12	9:I:136:ILE:HD13	1.79	0.63
3:Q:190:VAL:O	3:Q:194:VAL:HG23	1.99	0.63
6:T:185:ALA:O	6:T:189:VAL:HG23	1.99	0.63
11:Y:21:THR:HG22	11:Y:26:VAL:HA	1.81	0.63
2:P:139:TYR:CD1	2:P:224:VAL:HG21	2.34	0.62
3:C:101:PRO:HG2	3:C:138:PRO:CG	2.29	0.62
9:I:52:ILE:HB	9:I:59:VAL:HG13	1.80	0.62
6:T:191:GLN:O	6:T:195:ILE:HG12	1.99	0.62
5:E:127:TYR:O	5:E:148:PRO:HB3	1.99	0.62
1:O:28:VAL:HG13	1:O:76:SER:O	1.99	0.62
8:V:195:VAL:HG23	16:V:316:HOH:O	1.99	0.62
2:B:158:GLY:HA3	3:C:57:ILE:CD1	2.29	0.62
4:D:94:TYR:O	12:L:91:ARG:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:207:VAL:HG13	5:E:208:ASP:H	1.64	0.62
6:F:147:LEU:HD13	6:F:153:TYR:HB3	1.81	0.62
13:M:119:VAL:HG23	13:M:200:ILE:HG22	1.79	0.62
1:O:172:LYS:O	1:O:176:GLU:HG3	1.99	0.62
4:R:193:LEU:HD21	4:R:232:ILE:HD12	1.82	0.62
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.79	0.62
10:X:53:THR:HG23	10:X:54:VAL:N	2.14	0.62
12:L:181:ILE:O	12:L:185:ARG:HG3	2.00	0.62
11:Y:7:ARG:HG2	11:Y:110:PRO:HB2	1.80	0.62
8:H:132:LEU:HB2	16:H:315:HOH:O	1.99	0.62
11:K:208:ASN:ND2	10:X:150:PRO:HD3	2.14	0.62
2:P:69:ASN:ND2	2:P:70:ASP:N	2.46	0.62
7:U:201:MET:HA	7:U:201:MET:HE3	1.81	0.62
2:B:85:ILE:O	2:B:89:THR:HG23	2.00	0.62
12:Z:3:ASN:HD22	12:Z:3:ASN:C	2.06	0.62
3:C:190:VAL:O	3:C:194:VAL:HG23	2.00	0.62
11:K:7:ARG:HG2	11:K:110:PRO:HB2	1.82	0.62
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.63	0.62
12:L:13:LEU:HD11	12:L:150:LEU:CD2	2.29	0.62
12:L:13:LEU:HD12	12:L:14:GLY:H	1.63	0.61
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.82	0.61
7:G:239:ILE:HD12	7:G:239:ILE:C	2.25	0.61
3:Q:91:ALA:O	3:Q:95:ARG:HG3	2.00	0.61
3:Q:157:TRP:CE2	4:R:51:LEU:HD23	2.35	0.61
9:W:9:GLY:HA2	9:W:25:ASP:OD1	2.00	0.61
12:Z:3:ASN:ND2	12:Z:5:TYR:H	1.97	0.61
7:G:51:PRO:HG2	7:G:52:ASP:H	1.65	0.61
10:J:45:SER:OG	10:J:103:LEU:HB2	2.00	0.61
13:M:179:ASN:ND2	13:M:182:ARG:HH11	1.98	0.61
10:X:45:SER:OG	10:X:103:LEU:HB2	2.00	0.61
6:F:31:THR:CG2	6:F:32:THR:N	2.63	0.61
14:N:6:VAL:CG2	14:N:155:ILE:HD11	2.31	0.61
7:U:198:ILE:HG23	7:U:214:LEU:HD11	1.83	0.61
2:B:89:THR:HG22	16:B:335:HOH:O	2.00	0.61
3:C:91:ALA:O	3:C:95:ARG:HG3	2.00	0.61
2:B:180:LYS:O	2:B:183:MET:HG3	2.01	0.61
4:D:197:LYS:HG3	16:D:310:HOH:O	2.00	0.61
5:E:45:LEU:HG	5:E:134:ILE:HD13	1.81	0.61
12:L:3:ASN:HD22	12:L:3:ASN:C	2.08	0.61
13:a:179:ASN:ND2	13:a:182:ARG:HH11	1.99	0.61
7:G:155:VAL:HG22	7:G:156:GLY:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:220:ASN:O	2:P:221:ASP:HB2	1.99	0.61
5:S:207:VAL:HG13	5:S:208:ASP:H	1.65	0.61
6:T:186:ARG:HH11	6:T:186:ARG:HG3	1.66	0.61
7:U:72:MET:HE3	7:U:74:VAL:CG2	2.30	0.61
10:J:150:PRO:HD3	11:Y:208:ASN:ND2	2.16	0.61
8:V:3:ILE:HG12	8:V:99:ILE:HD12	1.83	0.61
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.83	0.61
5:E:162:ALA:HB3	16:E:321:HOH:O	2.00	0.60
1:A:128:ARG:NH2	7:G:120:THR:HG22	2.08	0.60
4:D:193:LEU:HD21	4:D:232:ILE:HD12	1.83	0.60
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.83	0.60
12:Z:103:PHE:N	12:Z:104:PRO:HD3	2.16	0.60
1:A:160:LYS:HE3	2:B:57:GLU:OE1	2.00	0.60
7:G:3:TYR:C	7:G:5:ARG:H	2.09	0.60
9:I:14:MET:CE	9:I:166:ILE:HA	2.32	0.60
3:C:101:PRO:HG2	3:C:138:PRO:HG3	1.82	0.60
12:L:3:ASN:ND2	12:L:5:TYR:H	1.98	0.60
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.83	0.60
14:N:8:PHE:HE2	14:N:13:ILE:HG13	1.67	0.60
3:Q:101:PRO:HG2	3:Q:138:PRO:CG	2.31	0.60
4:R:45:ARG:O	4:R:45:ARG:HG2	2.00	0.60
7:U:5:ARG:HD3	7:U:17:TYR:CD2	2.36	0.60
11:Y:107:LYS:HD2	11:Y:107:LYS:N	2.05	0.60
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.82	0.60
13:a:114:ILE:HB	13:a:130:VAL:HG12	1.81	0.60
2:B:18:LEU:HD13	2:B:122:THR:HG23	1.82	0.60
2:P:18:LEU:HD13	2:P:122:THR:HG23	1.82	0.60
3:Q:167:LYS:HB2	16:Q:316:HOH:O	2.01	0.60
6:F:185:ALA:O	6:F:189:VAL:HG23	2.01	0.60
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.82	0.60
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.66	0.60
2:B:233:GLU:O	2:B:237:ILE:HG22	2.02	0.60
4:D:104:LEU:C	4:D:104:LEU:HD13	2.27	0.60
5:E:14:PRO:HA	6:F:22:TYR:CD2	2.36	0.60
7:G:194:VAL:O	7:G:198:ILE:HG13	2.02	0.60
4:R:60:VAL:HA	16:R:324:HOH:O	2.02	0.60
4:R:119:ALA:HB3	4:R:124:ARG:HD3	1.83	0.60
5:S:45:LEU:HG	5:S:134:ILE:HD13	1.83	0.60
13:a:21:ILE:HG23	13:a:197:LEU:HD21	1.84	0.60
1:A:17:LYS:HE3	1:A:22:ASP:OD1	2.01	0.60
12:L:206:ILE:HD12	12:L:206:ILE:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:139:ASP:HB3	14:b:161:GLN:NE2	2.17	0.60
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.82	0.60
2:P:99:LYS:HZ3	10:X:86:GLN:NE2	1.99	0.59
6:T:8:ASN:HB3	6:T:123:ASN:HA	1.84	0.59
11:K:106:ARG:HG2	11:K:106:ARG:HH11	1.67	0.59
2:P:180:LYS:O	2:P:183:MET:HG3	2.02	0.59
11:Y:106:ARG:HG2	11:Y:106:ARG:HH11	1.67	0.59
14:N:14:LEU:O	14:N:175:MET:HA	2.01	0.59
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.84	0.59
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.84	0.59
11:K:61:SER:O	11:K:65:LEU:HD23	2.01	0.59
13:M:179:ASN:HD22	13:M:182:ARG:NH1	2.00	0.59
1:O:128:ARG:NH2	7:U:120:THR:HG22	2.06	0.59
5:S:73:LEU:HD12	5:S:73:LEU:O	2.03	0.59
6:T:36:ILE:HD12	6:T:192:ALA:HB2	1.84	0.59
10:J:53:THR:HG23	10:J:54:VAL:HG23	1.83	0.59
14:N:161:GLN:HE21	14:b:136:GLY:CA	2.13	0.59
7:U:51:PRO:HG2	7:U:52:ASP:H	1.68	0.59
9:W:171:LEU:CD2	9:W:199:LEU:HD13	2.33	0.59
14:b:14:LEU:O	14:b:175:MET:HA	2.03	0.59
6:F:186:ARG:HG3	6:F:186:ARG:HH11	1.66	0.59
7:G:185:ILE:HD12	7:G:185:ILE:N	2.18	0.59
5:S:69:MET:HE2	5:S:104:VAL:HA	1.84	0.59
6:F:8:ASN:HB3	6:F:123:ASN:HA	1.85	0.59
7:G:198:ILE:HG23	7:G:214:LEU:HD11	1.85	0.59
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.68	0.59
3:Q:101:PRO:HG2	3:Q:138:PRO:HG3	1.84	0.59
5:S:200:LEU:O	5:S:201:ARG:HB2	2.03	0.59
7:G:201:MET:HA	7:G:201:MET:HE3	1.83	0.59
5:E:35:VAL:HG22	5:E:159:ALA:HB2	1.85	0.59
4:R:104:LEU:C	4:R:104:LEU:HD13	2.28	0.59
5:S:181:ILE:HG21	5:S:187:GLU:HB2	1.85	0.59
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.68	0.59
13:a:179:ASN:HD22	13:a:182:ARG:NH1	2.00	0.59
11:K:145:LYS:O	11:K:148:LEU:HD13	2.03	0.58
14:N:175:MET:HE3	14:N:188:PHE:CE2	2.37	0.58
4:R:1:ASP:O	4:R:2:ARG:HB2	2.03	0.58
5:S:95:SER:O	5:S:99:ASN:HA	2.03	0.58
6:T:183:LEU:HD11	6:T:187:GLU:HB3	1.85	0.58
11:Y:61:SER:O	11:Y:65:LEU:HD23	2.03	0.58
13:a:49:THR:OG1	13:a:89:PRO:HG3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:73:LEU:HD12	5:E:73:LEU:O	2.03	0.58
5:E:95:SER:O	5:E:99:ASN:HA	2.04	0.58
3:Q:92:GLN:HG2	16:Q:302:HOH:O	2.02	0.58
9:W:137:VAL:HG11	9:W:145:LEU:HB3	1.85	0.58
10:X:26:SER:HB2	11:Y:133:GLN:HE22	1.69	0.58
12:Z:14:GLY:O	12:Z:136:CYS:HA	2.03	0.58
14:b:8:PHE:HE2	14:b:13:ILE:HG13	1.68	0.58
6:T:8:ASN:O	6:T:10:VAL:N	2.33	0.58
12:Z:206:ILE:N	12:Z:206:ILE:HD12	2.17	0.58
1:A:222:LEU:HD13	1:A:232:GLY:HA2	1.85	0.58
1:O:17:LYS:HE3	1:O:22:ASP:OD1	2.04	0.58
1:O:29:LYS:HE2	1:O:29:LYS:HA	1.85	0.58
4:R:197:LYS:HA	16:R:304:HOH:O	2.03	0.58
7:U:92:ALA:CA	7:U:103:MET:HE2	2.34	0.58
5:E:51:ASN:ND2	5:E:53:ASP:O	2.36	0.58
2:P:95:GLN:HG2	16:P:306:HOH:O	2.02	0.58
7:U:155:VAL:HG22	7:U:156:GLY:N	2.18	0.58
13:a:197:LEU:HD23	13:a:198:ALA:N	2.19	0.58
10:J:129:PRO:HB2	10:J:130:TYR:CD1	2.39	0.58
1:O:211:LEU:HD22	1:O:238:LEU:CD1	2.30	0.58
6:T:105:ILE:HG21	6:T:143:HIS:HB2	1.86	0.58
7:U:185:ILE:N	7:U:185:ILE:HD12	2.19	0.58
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.85	0.58
8:V:156:SER:O	8:V:160:GLN:HG3	2.03	0.58
12:Z:4:PRO:O	13:a:104:ARG:NH1	2.35	0.58
14:b:105:LYS:HD3	14:b:105:LYS:C	2.28	0.58
2:B:215:ILE:HG12	2:B:226:GLN:HG2	1.86	0.58
4:D:45:ARG:O	4:D:45:ARG:HG2	2.02	0.58
4:D:119:ALA:HB3	4:D:124:ARG:HD3	1.84	0.58
2:P:233:GLU:O	2:P:237:ILE:HG22	2.03	0.58
11:Y:145:LYS:HB2	11:Y:148:LEU:CD1	2.34	0.58
14:b:175:MET:HE3	14:b:188:PHE:CE2	2.38	0.58
12:L:103:PHE:N	12:L:104:PRO:HD3	2.17	0.58
1:A:29:LYS:HE2	1:A:29:LYS:HA	1.85	0.58
6:F:132:THR:O	6:F:146:MET:HA	2.04	0.58
6:T:132:THR:O	6:T:146:MET:HA	2.04	0.58
5:E:55:LEU:N	5:E:55:LEU:HD12	2.19	0.58
5:E:69:MET:HE2	5:E:104:VAL:HA	1.86	0.58
8:H:156:SER:O	8:H:160:GLN:HG3	2.04	0.58
12:L:52:MET:CB	12:L:111:ILE:HG22	2.33	0.58
5:S:42:HIS:HD2	5:S:214:ILE:HD11	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:31:ILE:HG23	7:U:47:GLN:HB2	1.86	0.58
6:F:183:LEU:HD11	6:F:187:GLU:HB3	1.84	0.57
9:I:170:LEU:HD21	9:I:184:ALA:HB1	1.86	0.57
12:L:14:GLY:O	12:L:136:CYS:HA	2.04	0.57
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.85	0.57
3:Q:230:TYR:O	3:Q:234:ILE:HG13	2.04	0.57
4:R:89:VAL:HG21	11:Y:65:LEU:HD22	1.86	0.57
7:U:3:TYR:C	7:U:5:ARG:H	2.11	0.57
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.34	0.57
14:N:83:LYS:HG3	14:N:119:VAL:HG22	1.85	0.57
2:P:200:THR:HG22	2:P:202:SER:N	2.09	0.57
7:U:68:ARG:HH11	7:U:68:ARG:HB2	1.69	0.57
9:W:148:MET:HE3	9:W:152:LEU:HD11	1.86	0.57
12:Z:109:THR:HG23	16:Z:309:HOH:O	2.03	0.57
1:A:28:VAL:HG13	1:A:76:SER:O	2.04	0.57
5:E:42:HIS:HD2	5:E:214:ILE:HD11	1.69	0.57
11:K:75:SER:HB2	11:K:108:GLU:OE2	2.04	0.57
14:N:136:GLY:CA	14:b:161:GLN:HE21	2.14	0.57
2:P:43:ILE:CD1	2:P:145:TYR:HB3	2.23	0.57
2:P:145:TYR:OH	2:P:217:LYS:HB2	2.04	0.57
14:b:83:LYS:HG3	14:b:119:VAL:HG22	1.85	0.57
5:E:134:ILE:HG22	5:E:143:LEU:HD13	1.87	0.57
5:E:200:LEU:O	5:E:201:ARG:HB2	2.03	0.57
11:K:197:PHE:CE1	9:W:203:GLN:HG3	2.39	0.57
1:O:180:ASN:H	1:O:183:LEU:HD12	1.69	0.57
5:S:35:VAL:HG22	5:S:159:ALA:HB2	1.86	0.57
13:M:21:ILE:HG23	13:M:197:LEU:HD21	1.85	0.57
10:X:53:THR:HG23	10:X:54:VAL:HG23	1.86	0.57
12:Z:100:LYS:HE3	12:Z:103:PHE:O	2.04	0.57
1:A:37:ILE:HD12	1:A:37:ILE:N	2.19	0.57
2:B:145:TYR:OH	2:B:217:LYS:HB2	2.03	0.57
6:F:8:ASN:O	6:F:10:VAL:N	2.33	0.57
6:F:175:LEU:HD11	6:F:191:GLN:HG3	1.86	0.57
9:I:148:MET:HE3	9:I:152:LEU:HD11	1.87	0.57
12:Z:3:ASN:HD22	12:Z:4:PRO:CD	2.18	0.57
1:A:180:ASN:H	1:A:183:LEU:HD12	1.70	0.57
6:T:75:SER:HA	16:T:330:HOH:O	2.05	0.57
9:W:31:GLN:HB3	16:W:334:HOH:O	2.04	0.57
3:C:66:ASP:OD1	3:C:95:ARG:NH1	2.36	0.57
4:D:176:LEU:HD13	5:E:55:LEU:HD11	1.87	0.57
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:68:ARG:HB2	7:U:68:ARG:NH1	2.19	0.57
7:U:103:MET:HE3	7:U:108:LEU:CB	2.33	0.57
9:W:55:LEU:HG	9:W:57:THR:HG22	1.86	0.57
9:W:170:LEU:HD21	9:W:184:ALA:HB1	1.87	0.57
6:F:32:THR:HG23	6:F:47:GLU:OE2	2.05	0.57
8:H:34:LEU:HB2	16:H:326:HOH:O	2.03	0.57
9:I:55:LEU:HG	9:I:57:THR:HG22	1.87	0.57
7:U:216:VAL:HB	7:U:227:LEU:HD12	1.87	0.57
9:W:165:THR:HG23	16:W:318:HOH:O	2.05	0.57
7:G:92:ALA:CA	7:G:103:MET:HE2	2.34	0.56
6:T:32:THR:HG23	6:T:47:GLU:OE2	2.05	0.56
1:A:211:LEU:HD23	1:A:212:ALA:N	2.20	0.56
7:G:5:ARG:HD3	7:G:17:TYR:CD2	2.40	0.56
7:G:68:ARG:HH11	7:G:68:ARG:HB2	1.70	0.56
13:M:179:ASN:HB3	16:M:318:HOH:O	2.04	0.56
14:N:59:VAL:HG22	14:N:81:VAL:HG12	1.88	0.56
14:N:105:LYS:HD3	14:N:105:LYS:C	2.29	0.56
1:O:78:MET:H	1:O:132:VAL:HG12	1.70	0.56
1:A:110:LEU:O	1:A:114:VAL:HG23	2.06	0.56
2:B:119:GLN:HG3	3:C:78:ALA:HB1	1.87	0.56
5:E:181:ILE:HG21	5:E:187:GLU:HB2	1.86	0.56
13:M:18:ASN:HB2	16:M:359:HOH:O	2.05	0.56
1:O:37:ILE:HD12	1:O:37:ILE:N	2.20	0.56
1:O:211:LEU:HD23	1:O:212:ALA:N	2.21	0.56
2:P:119:GLN:CG	3:Q:78:ALA:HB1	2.35	0.56
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.35	0.56
3:Q:107:LEU:O	3:Q:111:VAL:HG23	2.04	0.56
1:A:176:GLU:CG	2:B:55:LEU:HD21	2.21	0.56
4:D:89:VAL:HG21	11:K:65:LEU:HD22	1.87	0.56
8:H:73:GLU:OE1	8:H:73:GLU:HA	2.03	0.56
4:R:82:GLU:OE2	11:Y:69:ARG:NH1	2.38	0.56
7:U:194:VAL:O	7:U:198:ILE:HG13	2.04	0.56
3:C:11:PRO:HA	4:D:18:TYR:CD1	2.41	0.56
10:J:174:MET:CE	10:X:174:MET:HG2	2.36	0.56
1:O:110:LEU:O	1:O:114:VAL:HG23	2.05	0.56
2:P:38:MET:HG3	2:P:43:ILE:CD1	2.36	0.56
1:A:113:GLU:HA	1:A:113:GLU:OE1	2.06	0.56
7:G:68:ARG:HB2	7:G:68:ARG:NH1	2.20	0.56
2:P:106:PRO:HD2	2:P:109:ILE:HD12	1.87	0.56
9:W:14:MET:CE	9:W:166:ILE:HA	2.35	0.56
14:b:175:MET:HB2	14:b:186:LEU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:68:PHE:O	12:L:71:SER:HB3	2.06	0.56
13:M:197:LEU:HD23	13:M:198:ALA:N	2.21	0.56
5:S:134:ILE:HG22	5:S:143:LEU:HD13	1.86	0.56
6:T:175:LEU:HD11	6:T:191:GLN:HG3	1.87	0.56
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.87	0.56
5:E:231:LYS:H	5:E:231:LYS:HD2	1.70	0.56
9:I:9:GLY:HA2	9:I:25:ASP:OD1	2.05	0.56
5:S:227:GLU:H	5:S:227:GLU:CD	2.14	0.56
1:A:35:LEU:HB3	1:A:163:ALA:HB2	1.88	0.56
9:I:171:LEU:CD2	9:I:199:LEU:HD13	2.35	0.56
11:K:145:LYS:HB2	11:K:148:LEU:CD1	2.35	0.56
13:M:179:ASN:ND2	13:M:182:ARG:NH1	2.54	0.56
14:N:175:MET:HB2	14:N:186:LEU:HB2	1.88	0.56
5:S:184:ASN:OD1	5:S:187:GLU:HG2	2.06	0.56
14:b:13:ILE:HD12	14:b:151:THR:HG22	1.88	0.56
1:A:90:ARG:NH1	16:A:309:HOH:O	2.35	0.56
3:C:230:TYR:O	3:C:234:ILE:HG13	2.04	0.56
4:D:1:ASP:O	4:D:2:ARG:HB2	2.05	0.56
5:S:51:ASN:ND2	5:S:53:ASP:O	2.39	0.56
5:S:181:ILE:CG2	5:S:187:GLU:HB2	2.35	0.56
13:a:170:VAL:HG23	16:a:315:HOH:O	2.06	0.56
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.88	0.55
1:O:83:ARG:HE	7:U:114:ASN:ND2	2.04	0.55
5:E:205:LEU:H	5:E:205:LEU:CD2	2.17	0.55
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.88	0.55
2:B:49:ARG:NH2	2:B:58:GLN:HE21	2.04	0.55
3:C:107:LEU:O	3:C:111:VAL:HG23	2.06	0.55
7:G:216:VAL:HB	7:G:227:LEU:HD12	1.87	0.55
14:N:84:GLU:HA	14:N:84:GLU:OE2	2.06	0.55
14:N:161:GLN:NE2	14:b:139:ASP:HB3	2.19	0.55
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.41	0.55
9:W:37:ASN:H	9:W:37:ASN:ND2	2.04	0.55
6:F:105:ILE:HG21	6:F:143:HIS:HB2	1.87	0.55
6:F:205:GLU:HG3	6:F:206:LYS:HG3	1.88	0.55
2:P:215:ILE:HG12	2:P:226:GLN:HG2	1.87	0.55
3:C:185:THR:HB	3:C:188:GLU:HG2	1.87	0.55
14:N:13:ILE:HD12	14:N:151:THR:HG22	1.89	0.55
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.89	0.55
6:T:205:GLU:HG3	6:T:206:LYS:HG3	1.89	0.55
7:U:103:MET:CE	7:U:108:LEU:HD13	2.37	0.55
13:a:18:ASN:HB2	16:a:342:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:49:ARG:NH2	2:P:58:GLN:HE21	2.04	0.55
5:S:65:CYS:SG	5:S:87:LEU:HD23	2.47	0.55
9:W:17:LYS:HD3	9:W:156:ASN:HB3	1.89	0.55
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.41	0.55
7:G:183:ASP:O	7:G:184:HIS:HB3	2.07	0.55
9:I:14:MET:HE1	9:I:166:ILE:HA	1.89	0.55
10:J:174:MET:HG2	10:X:174:MET:CE	2.37	0.55
1:O:158:PRO:O	2:P:56:LEU:HD12	2.07	0.55
2:P:99:LYS:NZ	10:X:86:GLN:NE2	2.54	0.55
5:S:55:LEU:N	5:S:55:LEU:HD12	2.21	0.55
12:Z:68:PHE:O	12:Z:71:SER:HB3	2.07	0.55
9:I:203:GLN:HG3	11:Y:197:PHE:CE1	2.42	0.55
10:J:26:SER:HB2	11:K:133:GLN:HE22	1.71	0.55
13:M:25:ASP:HA	13:M:195:PHE:CB	2.36	0.55
7:U:169:ILE:HD12	7:U:201:MET:CE	2.36	0.55
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.71	0.55
9:I:97:ARG:HD2	16:I:357:HOH:O	2.06	0.55
1:O:59:GLU:C	1:O:61:LEU:H	2.14	0.55
1:O:239:THR:OG1	1:O:242:GLU:HG3	2.07	0.55
3:Q:165:ASN:HB2	3:Q:200:VAL:HG11	1.88	0.55
14:b:163:ILE:HG23	14:b:170:GLY:HA2	1.89	0.55
2:B:159:TRP:CE3	2:B:162:ILE:HD13	2.41	0.55
5:E:184:ASN:OD1	5:E:187:GLU:HG2	2.05	0.55
10:J:53:THR:CG2	10:J:54:VAL:N	2.70	0.55
2:P:228:ILE:HD12	2:P:228:ILE:N	2.22	0.55
2:P:244:THR:OXT	2:P:244:THR:HG22	2.07	0.55
5:S:1:PHE:O	5:S:3:ASN:N	2.40	0.55
5:S:35:VAL:HG12	5:S:36:GLY:N	2.22	0.55
5:S:189:ILE:N	5:S:189:ILE:HD12	2.22	0.55
10:X:146:HIS:HD2	10:X:147:HIS:CE1	2.25	0.55
5:E:181:ILE:CG2	5:E:187:GLU:HB2	2.36	0.54
12:L:3:ASN:HD22	12:L:4:PRO:N	2.05	0.54
6:T:193:ALA:O	6:T:197:TYR:HD1	1.89	0.54
7:U:230:GLU:HG2	16:U:357:HOH:O	2.07	0.54
8:V:73:GLU:OE1	8:V:73:GLU:HA	2.05	0.54
10:X:149:ARG:HG2	10:X:149:ARG:HH11	1.72	0.54
1:A:55:LEU:HD12	7:G:170:THR:HG23	1.89	0.54
1:A:118:MET:HE2	1:A:152:PRO:HA	1.89	0.54
1:A:211:LEU:HD22	1:A:238:LEU:CD1	2.29	0.54
13:M:187:ARG:NH2	8:V:135:MET:HE3	2.21	0.54
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:142:LEU:HA	16:a:305:HOH:O	2.06	0.54
14:b:59:VAL:HG22	14:b:81:VAL:HG12	1.89	0.54
7:G:235:ARG:HA	7:G:235:ARG:HE	1.72	0.54
12:L:92:ASN:C	12:L:92:ASN:HD22	2.16	0.54
12:L:121:ALA:HB2	12:L:133:ARG:NH2	2.22	0.54
13:M:14:MET:HE3	13:M:159:VAL:HG21	1.89	0.54
1:A:78:MET:H	1:A:132:VAL:HG12	1.73	0.54
1:A:83:ARG:HE	7:G:114:ASN:ND2	2.05	0.54
2:P:162:ILE:HG13	2:P:163:SER:N	2.23	0.54
2:P:190:GLU:O	2:P:194:LYS:HG2	2.07	0.54
9:W:141:ALA:HB2	9:W:177:ASP:HB2	1.89	0.54
14:b:6:VAL:CG2	14:b:155:ILE:HD11	2.38	0.54
5:E:227:GLU:H	5:E:227:GLU:CD	2.14	0.54
6:F:66:VAL:HG11	6:F:108:PHE:CE1	2.42	0.54
7:G:169:ILE:HD12	7:G:201:MET:CE	2.37	0.54
9:I:37:ASN:ND2	9:I:37:ASN:H	2.05	0.54
5:S:12:PHE:H	6:T:19:GLN:HE22	1.54	0.54
5:S:185:PRO:HG2	5:S:186:ASP:H	1.72	0.54
6:T:147:LEU:CD1	6:T:153:TYR:HB3	2.37	0.54
11:Y:75:SER:HB2	11:Y:108:GLU:OE2	2.07	0.54
12:Z:52:MET:CB	12:Z:111:ILE:HG22	2.34	0.54
12:Z:121:ALA:HB2	12:Z:133:ARG:NH2	2.22	0.54
2:B:24:ALA:O	2:B:28:ILE:HG12	2.08	0.54
5:E:86:TYR:CD1	5:E:114:LYS:HD2	2.42	0.54
5:E:99:ASN:HB2	13:M:94:GLU:HG2	1.88	0.54
1:O:89:SER:O	1:O:92:VAL:HG12	2.08	0.54
7:U:183:ASP:O	7:U:184:HIS:HB3	2.06	0.54
1:A:4:ARG:HB2	2:B:2:SER:OG	2.08	0.54
9:I:137:VAL:HG11	9:I:145:LEU:HB3	1.88	0.54
9:I:141:ALA:HB2	9:I:177:ASP:HB2	1.88	0.54
1:O:12:PHE:N	2:P:20:GLN:HE22	1.94	0.54
1:O:239:THR:O	1:O:243:ILE:HG12	2.08	0.54
2:P:119:GLN:NE2	16:P:310:HOH:O	2.41	0.54
2:P:180:LYS:HE2	2:P:182:ASP:OD1	2.08	0.54
5:S:73:LEU:HD12	5:S:73:LEU:C	2.33	0.54
9:W:137:VAL:CG1	9:W:145:LEU:HB3	2.37	0.54
10:X:139:TYR:CE2	10:X:172:MET:HG3	2.43	0.54
5:E:13:SER:HB3	5:E:17:ARG:H	1.73	0.54
7:G:103:MET:HB3	16:G:306:HOH:O	2.07	0.54
10:J:78:GLN:NE2	10:J:78:GLN:C	2.65	0.54
12:L:108:HIS:HE1	12:L:124:SER:HB2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:159:TRP:CE3	2:P:162:ILE:HD13	2.42	0.54
5:S:205:LEU:H	5:S:205:LEU:CD2	2.17	0.54
7:U:78:ILE:N	7:U:79:PRO:HD2	2.23	0.54
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.33	0.54
2:B:69:ASN:HD22	2:B:70:ASP:H	1.52	0.54
2:B:190:GLU:O	2:B:194:LYS:HG2	2.08	0.54
12:L:3:ASN:HD22	12:L:4:PRO:CD	2.20	0.54
13:M:21:ILE:CG2	13:M:197:LEU:HD21	2.38	0.54
14:N:9:LYS:O	14:N:107:LYS:HD3	2.07	0.54
10:X:130:TYR:CD2	10:X:144:LEU:HD13	2.43	0.54
1:A:59:GLU:C	1:A:61:LEU:H	2.16	0.54
2:B:106:PRO:HD2	2:B:109:ILE:HD12	1.89	0.54
2:B:244:THR:OXT	2:B:244:THR:HG22	2.08	0.54
7:G:190:TRP:O	7:G:194:VAL:HG23	2.08	0.54
7:U:190:TRP:O	7:U:194:VAL:HG23	2.08	0.54
9:W:171:LEU:HD21	9:W:199:LEU:HD13	1.89	0.54
11:Y:151:GLU:HB2	16:Y:332:HOH:O	2.07	0.54
12:Z:3:ASN:HD22	12:Z:4:PRO:N	2.05	0.54
13:a:21:ILE:CG2	13:a:197:LEU:HD21	2.38	0.54
5:E:35:VAL:HG22	5:E:159:ALA:CB	2.37	0.53
8:H:3:ILE:HB	8:H:44:ALA:HB1	1.90	0.53
8:H:22:GLN:HG2	15:c:2:THR:HG22	1.91	0.53
13:M:48:ASN:HD22	13:M:48:ASN:N	2.01	0.53
5:S:35:VAL:HG22	5:S:159:ALA:CB	2.38	0.53
5:S:214:ILE:HG12	5:S:215:VAL:N	2.23	0.53
7:U:137:VAL:HG21	7:U:220:THR:HA	1.90	0.53
11:Y:176:ASN:HD22	11:Y:190:ASN:HA	1.73	0.53
13:a:179:ASN:ND2	13:a:182:ARG:NH1	2.55	0.53
6:F:52:SER:OG	6:F:53:LYS:N	2.41	0.53
7:G:235:ARG:HA	7:G:235:ARG:NE	2.23	0.53
5:S:231:LYS:H	5:S:231:LYS:HD2	1.73	0.53
6:T:66:VAL:HG11	6:T:108:PHE:CE1	2.43	0.53
4:D:184:THR:HG23	4:D:187:GLU:OE1	2.09	0.53
9:I:17:LYS:HD3	9:I:156:ASN:HB3	1.91	0.53
9:I:137:VAL:CG1	9:I:145:LEU:HB3	2.39	0.53
10:J:149:ARG:HG2	10:J:149:ARG:HH11	1.73	0.53
11:K:38:ASN:HB3	16:K:335:HOH:O	2.09	0.53
10:X:78:GLN:NE2	10:X:78:GLN:C	2.66	0.53
5:E:1:PHE:O	5:E:3:ASN:N	2.42	0.53
5:E:35:VAL:HG12	5:E:36:GLY:N	2.22	0.53
5:E:185:PRO:HG2	5:E:186:ASP:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:189:ILE:HD12	5:E:189:ILE:N	2.23	0.53
7:U:235:ARG:HA	7:U:235:ARG:HE	1.73	0.53
2:B:180:LYS:HE2	2:B:182:ASP:OD1	2.09	0.53
10:J:146:HIS:HD2	10:J:147:HIS:CE1	2.26	0.53
4:R:9:PRO:HG3	5:S:23:TYR:CE2	2.43	0.53
4:D:82:GLU:OE2	11:K:69:ARG:NH1	2.42	0.53
7:G:31:ILE:HG23	7:G:47:GLN:HB2	1.90	0.53
8:H:59:ILE:HG12	8:H:83:LEU:HD23	1.91	0.53
12:L:100:LYS:HE3	12:L:103:PHE:O	2.08	0.53
5:S:99:ASN:HB2	13:a:94:GLU:HG2	1.89	0.53
13:a:54:SER:OG	13:a:113:ALA:HB3	2.09	0.53
13:a:227:GLY:HA3	16:a:326:HOH:O	2.08	0.53
2:B:105:ILE:HD11	2:B:109:ILE:CG2	2.38	0.53
10:J:153:THR:OG1	10:J:156:GLU:HG3	2.08	0.53
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.91	0.53
5:S:226:GLY:O	5:S:229:VAL:HG22	2.09	0.53
14:b:84:GLU:HA	14:b:84:GLU:OE2	2.07	0.53
2:B:38:MET:HG3	2:B:43:ILE:CD1	2.39	0.53
4:D:44:LYS:HB2	4:D:208:ASN:C	2.34	0.53
5:E:227:GLU:CD	5:E:227:GLU:N	2.67	0.53
6:F:39:ASN:HD22	6:F:39:ASN:N	2.07	0.53
11:K:176:ASN:HD22	11:K:190:ASN:HA	1.73	0.53
1:O:4:ARG:HB2	2:P:2:SER:OG	2.09	0.53
2:P:24:ALA:O	2:P:28:ILE:HG12	2.08	0.53
2:P:99:LYS:NZ	10:X:86:GLN:HE22	2.07	0.53
3:Q:40:VAL:HG11	3:Q:134:ALA:HB1	1.89	0.53
7:U:235:ARG:HA	7:U:235:ARG:NE	2.23	0.53
1:A:140:ASP:OD1	1:A:143:ASN:HB2	2.09	0.53
3:C:165:ASN:HB2	3:C:200:VAL:HG11	1.89	0.53
10:J:130:TYR:CD2	10:J:144:LEU:HD13	2.43	0.53
2:P:69:ASN:HD22	2:P:70:ASP:H	1.53	0.53
8:V:22:GLN:CG	15:e:2:THR:HG22	2.39	0.53
8:V:59:ILE:HG12	8:V:83:LEU:HD23	1.90	0.53
3:C:117:ARG:NH2	16:C:326:HOH:O	2.41	0.53
6:F:193:ALA:O	6:F:197:TYR:HD1	1.92	0.53
9:I:74:LYS:HD3	16:I:325:HOH:O	2.08	0.53
9:I:116:GLY:HA2	9:I:191:LYS:HD3	1.90	0.53
3:Q:165:ASN:O	3:Q:169:VAL:HG12	2.09	0.53
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.08	0.53
10:X:53:THR:CG2	10:X:54:VAL:N	2.72	0.53
1:A:89:SER:O	1:A:92:VAL:HG12	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:THR:OG1	1:A:242:GLU:HG3	2.09	0.52
5:E:63:ILE:HB	5:E:71:LEU:CD2	2.39	0.52
5:E:73:LEU:HD12	5:E:73:LEU:C	2.33	0.52
12:L:201:GLY:C	12:L:219:LEU:HD12	2.33	0.52
14:N:67:THR:HA	14:N:71:GLY:O	2.09	0.52
1:O:140:ASP:OD1	1:O:143:ASN:HB2	2.09	0.52
3:Q:233:GLN:O	3:Q:237:GLU:HG2	2.09	0.52
9:W:17:LYS:CD	9:W:156:ASN:HD22	2.22	0.52
12:Z:123:TYR:CE1	12:Z:133:ARG:HB2	2.44	0.52
13:a:4:PRO:HD3	13:a:111:TRP:CE2	2.44	0.52
13:a:25:ASP:HA	13:a:195:PHE:CB	2.38	0.52
1:A:239:THR:O	1:A:243:ILE:HG12	2.09	0.52
2:B:228:ILE:N	2:B:228:ILE:HD12	2.24	0.52
3:C:170:ARG:O	3:C:174:GLU:HG3	2.10	0.52
4:D:16:VAL:O	4:D:19:SER:HB3	2.09	0.52
4:D:89:VAL:HG11	11:K:65:LEU:CD2	2.40	0.52
5:E:226:GLY:O	5:E:229:VAL:HG22	2.10	0.52
1:O:35:LEU:HB3	1:O:163:ALA:HB2	1.90	0.52
1:O:44:VAL:HG23	1:O:211:LEU:HD21	1.92	0.52
1:O:113:GLU:OE1	1:O:113:GLU:HA	2.08	0.52
1:A:5:TYR:HD2	7:G:124:TYR:HB3	1.74	0.52
1:A:120:GLU:C	1:A:122:THR:H	2.18	0.52
5:E:214:ILE:HG12	5:E:215:VAL:N	2.24	0.52
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.90	0.52
7:G:137:VAL:HG21	7:G:220:THR:HA	1.91	0.52
12:L:123:TYR:CE1	12:L:133:ARG:HB2	2.44	0.52
4:R:204:LEU:HD23	4:R:204:LEU:C	2.34	0.52
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	1.89	0.52
12:Z:3:ASN:C	12:Z:3:ASN:ND2	2.67	0.52
16:J:205:HOH:O	11:Y:135:PHE:HA	2.09	0.52
7:U:165:LYS:O	7:U:169:ILE:HG12	2.10	0.52
10:X:129:PRO:HB2	10:X:130:TYR:CD1	2.44	0.52
12:Z:208:THR:C	12:Z:210:ASP:H	2.16	0.52
13:a:63:ILE:HD11	13:a:110:LEU:HD13	1.92	0.52
14:b:9:LYS:O	14:b:107:LYS:HD3	2.09	0.52
5:E:147:GLN:HG3	16:E:314:HOH:O	2.08	0.52
8:H:22:GLN:CG	15:c:2:THR:HG22	2.39	0.52
10:J:5:LEU:HD23	10:J:132:ALA:HB2	1.91	0.52
1:O:28:VAL:HG11	1:O:133:SER:HB2	1.92	0.52
9:W:28:LEU:HA	16:W:315:HOH:O	2.09	0.52
2:B:162:ILE:HG13	2:B:163:SER:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:78:ILE:N	7:G:79:PRO:HD2	2.24	0.52
9:I:171:LEU:HD21	9:I:199:LEU:HD13	1.91	0.52
2:P:200:THR:HG22	2:P:201:ASP:N	2.23	0.52
3:Q:170:ARG:O	3:Q:174:GLU:HG3	2.10	0.52
9:W:81:ILE:HD11	9:W:85:THR:HG22	1.91	0.52
13:a:162:GLU:O	13:a:165:ILE:HG12	2.10	0.52
4:D:204:LEU:HD23	4:D:204:LEU:C	2.34	0.52
9:I:14:MET:HE3	9:I:166:ILE:CG1	2.31	0.52
12:L:208:THR:C	12:L:210:ASP:H	2.15	0.52
10:X:153:THR:OG1	10:X:156:GLU:HG3	2.10	0.52
12:Z:92:ASN:HD22	12:Z:92:ASN:C	2.16	0.52
13:a:150:MET:O	13:a:153:PRO:HD2	2.10	0.52
1:A:10:THR:HG22	1:A:18:LEU:HD22	1.92	0.52
1:A:101:TYR:CE1	9:I:89:LEU:HD13	2.45	0.52
5:E:81:ARG:HG3	5:E:81:ARG:NH1	2.21	0.52
11:K:4:LEU:HD11	11:K:15:ALA:HB3	1.92	0.52
13:M:54:SER:OG	13:M:113:ALA:HB3	2.10	0.52
5:S:63:ILE:HB	5:S:71:LEU:CD2	2.40	0.52
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.43	0.52
14:b:66:TYR:CD2	14:b:73:PRO:HB3	2.45	0.52
3:C:40:VAL:HG11	3:C:134:ALA:HB1	1.92	0.52
3:C:233:GLN:O	3:C:237:GLU:HG2	2.10	0.52
5:E:197:SER:HA	5:E:200:LEU:CG	2.40	0.52
9:I:166:ILE:CG2	9:I:167:SER:N	2.72	0.52
1:O:82:TYR:O	1:O:86:VAL:HG23	2.10	0.52
4:R:57:GLU:HA	16:R:312:HOH:O	2.09	0.52
5:S:178:PHE:CD1	5:S:179:ILE:N	2.78	0.52
1:A:30:GLN:HE21	1:A:30:GLN:CA	2.12	0.52
5:E:38:ARG:NH1	5:E:39:SER:O	2.43	0.52
5:E:178:PHE:CD1	5:E:179:ILE:N	2.78	0.52
1:O:106:PRO:HD2	1:O:109:LEU:HD12	1.92	0.52
2:P:105:ILE:HD11	2:P:109:ILE:CG2	2.40	0.52
3:Q:66:ASP:OD1	3:Q:95:ARG:NH1	2.38	0.52
5:S:81:ARG:HG3	5:S:81:ARG:NH1	2.20	0.52
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.40	0.52
10:X:36:ARG:O	10:X:43:LEU:HD12	2.10	0.52
12:Z:195:HIS:CD2	12:Z:197:GLN:H	2.27	0.52
1:O:118:MET:HE2	1:O:152:PRO:HA	1.92	0.51
6:T:45:ALA:HA	6:T:211:GLU:O	2.10	0.51
8:V:3:ILE:HB	8:V:44:ALA:HB1	1.92	0.51
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:VAL:HG22	3:C:33:GLY:N	2.24	0.51
8:H:50:ALA:HB2	9:I:128:CYS:HB2	1.92	0.51
8:H:144:GLN:O	8:H:145:ASP:HB2	2.10	0.51
10:J:8:ARG:HG2	10:J:8:ARG:HH11	1.76	0.51
13:M:53:ILE:HG21	13:M:60:MET:HG3	1.92	0.51
8:V:22:GLN:HG2	15:e:2:THR:HG22	1.91	0.51
1:A:179:TRP:HA	1:A:183:LEU:HD11	1.92	0.51
2:B:119:GLN:CG	3:C:78:ALA:HB1	2.40	0.51
10:J:139:TYR:CE2	10:J:172:MET:HG3	2.45	0.51
11:K:86:LEU:HD13	11:K:86:LEU:C	2.36	0.51
4:R:184:THR:HG23	4:R:187:GLU:OE1	2.10	0.51
3:C:27:ARG:CB	3:C:27:ARG:HH11	2.23	0.51
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.92	0.51
13:M:227:GLY:HA3	13:M:231:GLN:HB3	1.92	0.51
9:W:135:PHE:O	9:W:136:ILE:HD12	2.10	0.51
9:W:163:PHE:CE1	9:W:197:ARG:HD2	2.45	0.51
2:B:200:THR:HG22	2:B:201:ASP:N	2.26	0.51
12:L:16:ALA:HB2	12:L:122:VAL:HG23	1.91	0.51
13:M:150:MET:O	13:M:153:PRO:HD2	2.11	0.51
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.92	0.51
4:R:159:TYR:HA	5:S:55:LEU:O	2.10	0.51
5:S:106:ARG:HG2	5:S:106:ARG:HH11	1.76	0.51
6:T:52:SER:OG	6:T:53:LYS:N	2.42	0.51
9:W:116:GLY:HA2	9:W:191:LYS:HD3	1.91	0.51
9:I:17:LYS:CD	9:I:156:ASN:HD22	2.24	0.51
10:J:15:LEU:HD12	10:J:43:LEU:HD23	1.91	0.51
13:M:27:LEU:HB2	13:M:192:SER:HB2	1.93	0.51
5:S:14:PRO:HA	6:T:22:TYR:CD2	2.45	0.51
7:U:201:MET:HE2	7:U:205:LEU:HG	1.93	0.51
13:a:48:ASN:HD22	13:a:48:ASN:N	2.01	0.51
1:A:183:LEU:HD21	1:A:191:ILE:HD11	1.92	0.51
1:A:227:ILE:HD12	1:A:227:ILE:N	2.26	0.51
8:H:18:THR:HB	8:H:30:ASN:HD22	1.76	0.51
3:Q:96:LEU:HD13	16:X:237:HOH:O	2.10	0.51
5:S:38:ARG:NH1	5:S:39:SER:O	2.43	0.51
5:S:86:TYR:CD1	5:S:114:LYS:HD2	2.46	0.51
6:T:39:ASN:HD22	6:T:39:ASN:N	2.07	0.51
7:U:196:PHE:CD1	7:U:196:PHE:C	2.89	0.51
14:b:76:GLU:HB2	16:b:212:HOH:O	2.09	0.51
14:b:113:ILE:HG12	14:b:119:VAL:HG13	1.92	0.51
1:A:82:TYR:O	1:A:86:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:165:ASN:O	3:C:169:VAL:HG12	2.11	0.51
7:G:106:ASP:HB3	7:G:146:TYR:CZ	2.46	0.51
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.40	0.51
7:U:34:LEU:C	7:U:34:LEU:HD12	2.36	0.51
11:Y:106:ARG:HG2	11:Y:106:ARG:NH1	2.26	0.51
9:I:73:TYR:CZ	9:I:77:GLU:HG3	2.46	0.51
9:I:135:PHE:O	9:I:136:ILE:HD12	2.10	0.51
11:K:73:ARG:NH2	11:K:104:TYR:O	2.44	0.51
13:M:4:PRO:HD3	13:M:111:TRP:CE2	2.46	0.51
14:N:8:PHE:HE1	14:N:10:ASP:HB2	1.76	0.51
1:O:179:TRP:HA	1:O:183:LEU:HD11	1.92	0.51
1:O:183:LEU:HD21	1:O:191:ILE:HD11	1.93	0.51
3:Q:160:GLN:HG3	3:Q:161:THR:N	2.25	0.51
4:R:176:LEU:HD13	5:S:55:LEU:HD11	1.92	0.51
12:Z:44:PHE:O	12:Z:51:VAL:HA	2.09	0.51
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.91	0.51
2:B:217:LYS:O	2:B:218:GLY:C	2.53	0.51
3:C:27:ARG:NH1	3:C:27:ARG:CB	2.74	0.51
4:D:114:ARG:HH11	4:D:114:ARG:HG2	1.76	0.51
11:K:12:ILE:HB	11:K:180:VAL:HB	1.93	0.51
11:K:196:LEU:O	11:K:196:LEU:HD12	2.11	0.51
10:X:14:ILE:HD13	10:X:158:LEU:CD2	2.39	0.51
12:Z:201:GLY:C	12:Z:219:LEU:HD12	2.36	0.51
2:B:148:TYR:CE1	3:C:57:ILE:HD13	2.46	0.50
3:C:5:ALA:HB3	4:D:4:VAL:HG11	1.92	0.50
3:C:94:HIS:CD2	3:C:102:VAL:HG12	2.46	0.50
7:G:103:MET:CE	7:G:108:LEU:HD13	2.41	0.50
7:G:167:GLN:NE2	7:G:171:THR:HG23	2.25	0.50
12:L:3:ASN:C	12:L:3:ASN:ND2	2.69	0.50
12:L:126:ASP:HB2	12:L:130:SER:N	2.26	0.50
3:Q:32:VAL:HG22	3:Q:33:GLY:N	2.26	0.50
5:S:227:GLU:CD	5:S:227:GLU:N	2.68	0.50
11:Y:8:PHE:CE2	11:Y:13:ILE:HG12	2.47	0.50
13:a:14:MET:HE3	13:a:159:VAL:HG21	1.93	0.50
5:E:65:CYS:SG	5:E:87:LEU:HD23	2.51	0.50
6:F:45:ALA:HA	6:F:211:GLU:O	2.10	0.50
7:G:103:MET:HE3	7:G:108:LEU:CB	2.33	0.50
9:I:35:VAL:HG13	16:J:242:HOH:O	2.11	0.50
12:L:213:ARG:NH1	12:L:213:ARG:HB3	2.25	0.50
9:W:73:TYR:CZ	9:W:77:GLU:HG3	2.46	0.50
10:X:5:LEU:HD23	10:X:132:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:119:VAL:HG23	13:a:200:ILE:CG2	2.41	0.50
3:C:131:THR:O	3:C:147:GLN:HA	2.11	0.50
11:K:16:VAL:HG21	11:K:34:VAL:HG23	1.93	0.50
12:L:195:HIS:CD2	12:L:197:GLN:H	2.27	0.50
13:M:57:ILE:O	13:M:61:GLN:HG3	2.11	0.50
3:Q:27:ARG:CB	3:Q:27:ARG:HH11	2.24	0.50
4:R:89:VAL:HG11	11:Y:65:LEU:CD2	2.41	0.50
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.93	0.50
7:U:106:ASP:HB3	7:U:146:TYR:CZ	2.46	0.50
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.94	0.50
9:W:179:LEU:HD22	16:W:311:HOH:O	2.10	0.50
11:Y:12:ILE:HB	11:Y:180:VAL:HB	1.93	0.50
3:C:160:GLN:HG3	3:C:161:THR:N	2.26	0.50
11:K:8:PHE:CE2	11:K:13:ILE:HG12	2.46	0.50
12:L:13:LEU:HD12	12:L:14:GLY:N	2.25	0.50
13:M:43:ILE:HD12	13:M:64:GLU:HG3	1.94	0.50
3:Q:100:ASP:OD2	3:Q:101:PRO:HD2	2.11	0.50
4:R:44:LYS:HB2	4:R:208:ASN:C	2.37	0.50
6:T:9:SER:HB2	7:U:126:ARG:HD3	1.93	0.50
11:Y:176:ASN:ND2	11:Y:190:ASN:HA	2.26	0.50
13:a:27:LEU:HB2	13:a:192:SER:HB2	1.93	0.50
14:b:8:PHE:HE1	14:b:10:ASP:HB2	1.76	0.50
14:b:144:GLU:O	14:b:145:ASN:HB2	2.11	0.50
3:C:100:ASP:OD2	3:C:101:PRO:HD2	2.12	0.50
14:N:144:GLU:O	14:N:145:ASN:HB2	2.12	0.50
3:Q:27:ARG:NH1	3:Q:27:ARG:CB	2.74	0.50
3:Q:126:PRO:HB3	16:Q:307:HOH:O	2.10	0.50
4:R:114:ARG:HG2	4:R:114:ARG:HH11	1.76	0.50
10:X:15:LEU:HD12	10:X:43:LEU:HD23	1.93	0.50
13:a:165:ILE:N	13:a:166:PRO:HD2	2.26	0.50
3:C:197:LEU:O	3:C:201:VAL:HG23	2.12	0.50
7:G:112:MET:HE3	16:G:331:HOH:O	2.11	0.50
7:G:201:MET:HE2	7:G:205:LEU:HG	1.93	0.50
14:N:66:TYR:CD2	14:N:73:PRO:HB3	2.47	0.50
13:a:57:ILE:O	13:a:61:GLN:HG3	2.12	0.50
4:D:31:GLY:O	4:D:161:ALA:HA	2.11	0.50
5:E:214:ILE:O	5:E:221:PHE:HA	2.11	0.50
6:F:196:ILE:HG21	6:F:210:LEU:CD1	2.42	0.50
11:K:4:LEU:HD22	11:K:4:LEU:C	2.37	0.50
11:K:25:TRP:CH2	12:L:144:SER:HA	2.47	0.50
13:M:165:ILE:N	13:M:166:PRO:HD2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:120:GLU:C	1:O:122:THR:H	2.19	0.50
5:S:63:ILE:HB	5:S:71:LEU:HD21	1.94	0.50
8:V:18:THR:HB	8:V:30:ASN:HD22	1.77	0.50
9:W:107:VAL:HG13	9:W:136:ILE:HG21	1.94	0.50
7:G:34:LEU:C	7:G:34:LEU:HD12	2.37	0.50
12:L:113:GLY:HA2	12:L:207:VAL:HG11	1.94	0.50
13:M:162:GLU:O	13:M:165:ILE:HG12	2.12	0.50
2:P:69:ASN:HD22	2:P:70:ASP:N	2.09	0.50
4:R:31:GLY:HA2	4:R:39:VAL:O	2.11	0.50
6:T:41:GLY:HA3	6:T:215:CYS:O	2.12	0.50
7:U:136:SER:HA	7:U:219:ALA:HB1	1.94	0.50
7:U:167:GLN:NE2	7:U:171:THR:HG23	2.27	0.50
7:U:207:THR:HG22	7:U:208:GLU:N	2.27	0.50
9:W:189:ILE:HD12	9:W:189:ILE:N	2.27	0.50
11:Y:4:LEU:HD11	11:Y:15:ALA:HB3	1.93	0.50
13:a:147:GLY:O	13:a:151:ALA:HB3	2.12	0.50
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.59	0.50
4:D:31:GLY:HA2	4:D:39:VAL:O	2.11	0.50
5:E:63:ILE:HB	5:E:71:LEU:HD21	1.94	0.50
9:I:189:ILE:HD12	9:I:189:ILE:N	2.27	0.50
14:N:116:GLY:HA3	16:N:209:HOH:O	2.12	0.50
1:O:246:ARG:HG3	1:O:246:ARG:NH1	2.27	0.50
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.12	0.50
4:R:241:ALA:O	4:R:242:GLU:CB	2.56	0.50
14:b:13:ILE:HD12	14:b:151:THR:CG2	2.41	0.50
1:A:174:PHE:O	1:A:178:ARG:HG2	2.12	0.49
6:F:147:LEU:CD1	6:F:153:TYR:HB3	2.42	0.49
10:J:18:SER:HB2	10:J:176:PHE:HB2	1.94	0.49
10:J:161:LEU:O	10:J:164:CYS:N	2.45	0.49
11:K:176:ASN:ND2	11:K:190:ASN:HA	2.26	0.49
12:Z:152:ASN:O	12:Z:156:PHE:HA	2.12	0.49
5:E:12:PHE:H	6:F:19:GLN:HE22	1.59	0.49
6:F:41:GLY:HA3	6:F:215:CYS:O	2.11	0.49
6:F:154:TRP:CZ3	7:G:60:VAL:HA	2.47	0.49
10:J:194:ASP:O	10:J:198:GLN:HB2	2.12	0.49
5:S:101:LYS:HA	16:S:313:HOH:O	2.11	0.49
9:W:189:ILE:HA	9:W:194:VAL:HG22	1.95	0.49
12:Z:220:LYS:HG3	16:Z:331:HOH:O	2.10	0.49
2:B:69:ASN:HD22	2:B:70:ASP:N	2.07	0.49
3:C:3:ASP:O	3:C:4:ARG:C	2.55	0.49
7:G:74:VAL:HG11	7:G:81:ALA:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:36:ARG:O	10:J:43:LEU:HD12	2.12	0.49
11:K:85:ASN:ND2	16:K:320:HOH:O	2.44	0.49
11:K:199:LYS:HB2	16:K:336:HOH:O	2.12	0.49
13:M:14:MET:HE3	13:M:159:VAL:CG2	2.42	0.49
6:T:20:VAL:O	6:T:23:ALA:HB3	2.13	0.49
7:U:74:VAL:HG11	7:U:81:ALA:CB	2.42	0.49
8:V:144:GLN:O	8:V:145:ASP:HB2	2.12	0.49
1:A:106:PRO:HD2	1:A:109:LEU:HD12	1.94	0.49
6:F:198:LEU:H	6:F:198:LEU:HD12	1.78	0.49
9:I:123:PHE:CD2	9:I:123:PHE:N	2.80	0.49
5:S:13:SER:HB3	5:S:17:ARG:H	1.77	0.49
5:S:189:ILE:HD12	5:S:189:ILE:H	1.76	0.49
5:S:189:ILE:CG2	5:S:212:ILE:HD13	2.41	0.49
7:U:231:ASN:HB3	16:U:302:HOH:O	2.12	0.49
3:C:148:THR:HG22	3:C:154:TYR:HB3	1.94	0.49
4:D:68:CYS:HB2	4:D:136:ILE:HA	1.94	0.49
5:E:69:MET:CE	5:E:104:VAL:HA	2.41	0.49
6:F:20:VAL:O	6:F:23:ALA:HB3	2.13	0.49
1:O:36:GLY:HA2	1:O:44:VAL:O	2.12	0.49
8:V:4:VAL:HG12	8:V:126:SER:CB	2.42	0.49
10:X:8:ARG:HG2	10:X:8:ARG:HH11	1.78	0.49
1:A:36:GLY:HA2	1:A:44:VAL:O	2.12	0.49
7:G:136:SER:HA	7:G:219:ALA:HB1	1.94	0.49
9:I:163:PHE:CE1	9:I:197:ARG:HD2	2.47	0.49
1:O:5:TYR:HD2	7:U:124:TYR:HB3	1.77	0.49
2:P:98:LEU:HG	9:W:67:ARG:HH21	1.78	0.49
2:P:162:ILE:HG13	2:P:163:SER:H	1.78	0.49
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.58	0.49
4:R:204:LEU:HD23	4:R:205:ASP:N	2.28	0.49
3:C:51:LYS:O	3:C:52:LEU:CB	2.61	0.49
5:E:179:ILE:HG12	5:E:179:ILE:O	2.12	0.49
14:N:133:PHE:HE2	14:N:166:ASP:HB2	1.77	0.49
2:P:94:ALA:HB3	16:P:306:HOH:O	2.11	0.49
16:P:305:HOH:O	3:Q:57:ILE:HD11	2.12	0.49
3:Q:103:THR:HG23	16:Q:314:HOH:O	2.12	0.49
3:Q:131:THR:O	3:Q:147:GLN:HA	2.12	0.49
3:Q:148:THR:HG22	3:Q:154:TYR:HB3	1.94	0.49
5:S:214:ILE:O	5:S:221:PHE:HA	2.13	0.49
6:T:198:LEU:H	6:T:198:LEU:HD12	1.77	0.49
8:V:104:ASP:O	8:V:106:THR:N	2.45	0.49
9:W:14:MET:HE1	9:W:166:ILE:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:32:LYS:N	11:Y:32:LYS:HD2	2.27	0.49
11:Y:56:GLU:O	11:Y:59:LEU:HB3	2.13	0.49
11:Y:196:LEU:HD12	11:Y:196:LEU:O	2.12	0.49
3:C:186:VAL:O	3:C:190:VAL:HG23	2.13	0.49
5:E:189:ILE:HD12	5:E:189:ILE:H	1.78	0.49
6:F:232:LEU:O	6:F:236:ILE:HD13	2.12	0.49
7:G:170:THR:O	7:G:174:GLU:HB2	2.13	0.49
12:L:4:PRO:O	13:M:104:ARG:NH1	2.38	0.49
14:N:103:ASP:HB3	14:N:106:ASN:HB2	1.93	0.49
1:O:23:TYR:CE1	7:U:12:PRO:HA	2.48	0.49
2:P:217:LYS:O	2:P:218:GLY:C	2.54	0.49
6:T:31:THR:CG2	6:T:32:THR:H	2.24	0.49
6:T:123:ASN:C	6:T:123:ASN:HD22	2.21	0.49
6:T:240:GLN:O	6:T:243:ILE:HG22	2.12	0.49
10:X:18:SER:HB2	10:X:176:PHE:HB2	1.95	0.49
12:Z:126:ASP:CB	12:Z:130:SER:H	2.25	0.49
2:B:55:LEU:N	2:B:55:LEU:HD22	2.28	0.49
2:B:200:THR:HG22	2:B:202:SER:N	2.12	0.49
5:E:207:VAL:CG1	5:E:208:ASP:N	2.76	0.49
11:K:106:ARG:HG2	11:K:106:ARG:NH1	2.28	0.49
3:Q:3:ASP:O	3:Q:4:ARG:C	2.54	0.49
6:T:172:LEU:O	6:T:176:VAL:HG23	2.12	0.49
9:W:166:ILE:CG2	9:W:167:SER:N	2.76	0.49
13:a:14:MET:HE3	13:a:159:VAL:CG2	2.43	0.49
4:D:113:LEU:HD23	4:D:115:PHE:HE1	1.77	0.48
4:D:119:ALA:HA	5:E:124:GLY:HA2	1.93	0.48
9:I:36:SER:HB2	10:J:126:VAL:HG21	1.94	0.48
10:J:17:SER:HB2	16:J:215:HOH:O	2.13	0.48
1:O:33:THR:HG22	1:O:34:SER:N	2.27	0.48
1:O:227:ILE:N	1:O:227:ILE:HD12	2.27	0.48
5:S:69:MET:CE	5:S:104:VAL:HA	2.43	0.48
7:U:72:MET:HE1	7:U:85:ALA:HB2	1.95	0.48
9:W:87:THR:HG22	9:W:129:ILE:HD13	1.93	0.48
7:U:75:ASN:HA	16:U:308:HOH:O	2.13	0.48
12:L:126:ASP:HB2	12:L:130:SER:HB3	1.94	0.48
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.48	0.48
3:Q:96:LEU:HD22	10:X:62:ALA:HB2	1.94	0.48
4:R:68:CYS:HB2	4:R:136:ILE:HA	1.95	0.48
5:S:197:SER:HA	5:S:200:LEU:CG	2.39	0.48
10:X:53:THR:CG2	10:X:54:VAL:H	2.27	0.48
14:b:103:ASP:HB3	14:b:106:ASN:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:116:GLY:HA3	16:b:203:HOH:O	2.11	0.48
7:G:72:MET:HE1	7:G:85:ALA:HB2	1.95	0.48
7:G:196:PHE:CD1	7:G:196:PHE:C	2.91	0.48
8:H:167:LEU:HD22	12:Z:196:ILE:O	2.13	0.48
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.49	0.48
14:N:114:PRO:HD2	14:N:118:SER:O	2.14	0.48
1:O:10:THR:HG22	1:O:18:LEU:HD22	1.95	0.48
2:P:44:VAL:HG22	2:P:214:THR:HG22	1.95	0.48
2:P:105:ILE:HG12	2:P:110:LEU:HB2	1.95	0.48
3:Q:166:SER:HA	3:Q:169:VAL:CG1	2.43	0.48
5:S:200:LEU:HD11	5:S:205:LEU:CD2	2.40	0.48
9:W:36:SER:HB2	10:X:126:VAL:HG21	1.96	0.48
11:Y:133:GLN:HG3	11:Y:134:THR:N	2.27	0.48
12:Z:13:LEU:HD12	12:Z:14:GLY:N	2.26	0.48
13:a:227:GLY:HA3	13:a:231:GLN:HB3	1.94	0.48
2:B:28:ILE:HD11	2:B:131:GLY:C	2.38	0.48
9:I:81:ILE:HD11	9:I:85:THR:HG22	1.94	0.48
12:L:44:PHE:O	12:L:51:VAL:HA	2.13	0.48
14:N:13:ILE:HD12	14:N:151:THR:CG2	2.42	0.48
6:T:14:ASP:OD2	6:T:14:ASP:N	2.44	0.48
6:T:28:GLU:HB3	6:T:165:ARG:NH2	2.28	0.48
8:V:20:SER:HB2	8:V:31:CYS:SG	2.54	0.48
9:W:37:ASN:HD22	9:W:37:ASN:C	2.21	0.48
12:Z:126:ASP:OD2	15:f:2:THR:HG23	2.13	0.48
14:b:67:THR:HA	14:b:71:GLY:O	2.13	0.48
3:C:58:THR:HG23	3:C:59:PRO:HD2	1.95	0.48
8:H:148:LYS:HD3	16:H:344:HOH:O	2.12	0.48
10:J:4:ILE:O	10:J:132:ALA:HA	2.14	0.48
12:L:152:ASN:O	12:L:156:PHE:HA	2.12	0.48
14:N:14:LEU:N	14:N:14:LEU:HD12	2.29	0.48
2:P:28:ILE:HD11	2:P:131:GLY:C	2.38	0.48
2:P:36:GLY:O	2:P:161:ALA:HA	2.14	0.48
2:P:159:TRP:CD2	2:P:162:ILE:HD13	2.49	0.48
3:Q:5:ALA:HB3	4:R:4:VAL:HG11	1.94	0.48
3:Q:34:VAL:HG12	3:Q:159:ALA:HB1	1.95	0.48
9:W:123:PHE:N	9:W:123:PHE:CD2	2.81	0.48
12:Z:42:LYS:HD2	12:Z:55:ASN:ND2	2.28	0.48
12:Z:126:ASP:HB2	12:Z:130:SER:HB3	1.95	0.48
2:B:44:VAL:HG22	2:B:214:THR:HG22	1.96	0.48
8:H:104:ASP:O	8:H:106:THR:N	2.46	0.48
12:L:208:THR:C	12:L:210:ASP:N	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:3:ILE:HG22	14:N:16:ALA:CB	2.43	0.48
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.49	0.48
1:O:174:PHE:O	1:O:178:ARG:HG2	2.13	0.48
4:R:113:LEU:HD23	4:R:115:PHE:HE1	1.78	0.48
5:S:174:THR:HG22	5:S:177:THR:HB	1.96	0.48
5:S:179:ILE:O	5:S:179:ILE:HG12	2.13	0.48
5:S:181:ILE:HG21	5:S:187:GLU:CB	2.44	0.48
10:X:161:LEU:O	10:X:164:CYS:N	2.46	0.48
10:X:194:ASP:O	10:X:198:GLN:HB2	2.13	0.48
13:a:48:ASN:H	13:a:48:ASN:ND2	2.10	0.48
13:a:161:ARG:CG	13:a:161:ARG:NH1	2.72	0.48
2:B:159:TRP:CD2	2:B:162:ILE:HD13	2.49	0.48
3:Q:51:LYS:O	3:Q:52:LEU:CB	2.60	0.48
7:U:237:VAL:O	7:U:240:ALA:HB3	2.14	0.48
10:X:4:ILE:O	10:X:132:ALA:HA	2.14	0.48
11:Y:99:THR:HG22	11:Y:115:VAL:O	2.13	0.48
10:J:53:THR:CG2	10:J:54:VAL:H	2.26	0.48
12:L:196:ILE:O	8:V:167:LEU:HD22	2.14	0.48
4:R:31:GLY:O	4:R:161:ALA:HA	2.13	0.48
8:V:4:VAL:HG12	8:V:126:SER:HB3	1.95	0.48
2:B:120:GLY:C	2:B:122:THR:H	2.21	0.48
3:C:34:VAL:HG12	3:C:159:ALA:HB1	1.96	0.48
6:F:27:VAL:HG13	6:F:75:SER:O	2.14	0.48
6:F:41:GLY:CA	6:F:215:CYS:O	2.62	0.48
16:F:305:HOH:O	7:G:82:ARG:HD2	2.14	0.48
7:G:102:ASP:HA	16:G:315:HOH:O	2.14	0.48
8:H:72:ARG:HG3	8:H:72:ARG:NH1	2.27	0.48
9:I:37:ASN:C	9:I:37:ASN:HD22	2.22	0.48
14:N:91:ASP:HB2	16:N:212:HOH:O	2.13	0.48
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.95	0.48
6:T:168:ALA:O	6:T:172:LEU:HD23	2.14	0.48
1:A:28:VAL:HG11	1:A:133:SER:HB2	1.95	0.47
2:B:49:ARG:HH21	2:B:58:GLN:HE21	1.62	0.47
7:G:207:THR:HG22	7:G:208:GLU:N	2.29	0.47
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.96	0.47
11:K:99:THR:HG22	11:K:115:VAL:O	2.14	0.47
12:L:52:MET:HE3	12:L:93:ILE:HD13	1.95	0.47
3:Q:120:GLN:HG3	3:Q:120:GLN:O	2.13	0.47
3:Q:179:ARG:HH22	4:R:52:GLU:HA	1.79	0.47
5:S:220:PRO:O	5:S:221:PHE:C	2.57	0.47
10:X:110:LYS:HB2	10:X:110:LYS:NZ	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:15:LYS:HG3	13:a:165:ILE:HD12	1.96	0.47
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.48	0.47
5:E:106:ARG:HG2	5:E:106:ARG:HH11	1.79	0.47
13:M:169:THR:HA	16:M:323:HOH:O	2.14	0.47
2:P:139:TYR:HA	2:P:144:GLY:O	2.14	0.47
5:S:68:HIS:HE1	5:S:102:LEU:O	1.97	0.47
6:T:123:ASN:C	6:T:123:ASN:ND2	2.72	0.47
7:U:236:LEU:O	7:U:239:ILE:HG13	2.14	0.47
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.39	0.47
12:Z:126:ASP:HB2	12:Z:130:SER:N	2.26	0.47
4:D:37:GLY:HA2	4:D:145:TYR:CD1	2.50	0.47
11:K:32:LYS:N	11:K:32:LYS:HD2	2.29	0.47
13:M:15:LYS:HG3	13:M:165:ILE:HD12	1.96	0.47
2:P:120:GLY:C	2:P:122:THR:H	2.22	0.47
6:T:198:LEU:HD12	6:T:198:LEU:N	2.30	0.47
7:U:170:THR:O	7:U:174:GLU:HB2	2.14	0.47
12:Z:52:MET:HE3	12:Z:93:ILE:HD13	1.94	0.47
2:B:76:VAL:HG22	2:B:134:PHE:CE2	2.49	0.47
4:D:140:ASP:HA	16:D:337:HOH:O	2.14	0.47
4:D:204:LEU:HD23	4:D:205:ASP:N	2.29	0.47
6:F:191:GLN:NE2	6:F:194:LYS:CE	2.77	0.47
8:H:4:VAL:HG12	8:H:126:SER:CB	2.43	0.47
11:K:4:LEU:HD22	11:K:4:LEU:O	2.14	0.47
12:L:86:ILE:HG23	12:L:123:TYR:HE2	1.79	0.47
13:M:119:VAL:HG23	13:M:200:ILE:CG2	2.45	0.47
14:N:13:ILE:HG12	14:N:177:VAL:HG13	1.97	0.47
6:T:212:ILE:HG22	6:T:213:SER:N	2.28	0.47
13:a:43:ILE:HD12	13:a:64:GLU:HG3	1.96	0.47
13:a:172:VAL:HG21	16:a:322:HOH:O	2.14	0.47
14:b:133:PHE:HE2	14:b:166:ASP:HB2	1.79	0.47
6:F:31:THR:CG2	6:F:32:THR:H	2.27	0.47
6:F:103:ILE:HG22	16:F:327:HOH:O	2.13	0.47
6:F:212:ILE:HG22	6:F:213:SER:N	2.29	0.47
7:G:165:LYS:O	7:G:169:ILE:HG12	2.15	0.47
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.44	0.47
10:J:14:ILE:HD13	10:J:158:LEU:CD2	2.44	0.47
11:K:196:LEU:HD12	11:K:200:VAL:HG23	1.96	0.47
13:M:63:ILE:HD11	13:M:110:LEU:HD13	1.95	0.47
3:Q:74:SER:OG	3:Q:162:ILE:HG13	2.15	0.47
3:Q:94:HIS:CD2	3:Q:102:VAL:HG12	2.48	0.47
12:Z:192:THR:HG21	16:Z:331:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:213:ARG:NH1	12:Z:213:ARG:HB3	2.28	0.47
13:a:35:ARG:HD3	13:a:36:PHE:CZ	2.50	0.47
14:b:88:GLU:HA	14:b:88:GLU:OE1	2.14	0.47
4:D:67:GLY:HA3	4:D:220:PHE:CD2	2.49	0.47
8:H:20:SER:HB2	8:H:31:CYS:SG	2.55	0.47
9:I:107:VAL:HG13	9:I:136:ILE:HG21	1.96	0.47
10:J:89:ALA:O	10:J:92:ILE:HG22	2.15	0.47
3:Q:223:SER:O	3:Q:224:SER:C	2.57	0.47
4:R:113:LEU:HB2	16:R:318:HOH:O	2.14	0.47
14:b:14:LEU:HD12	14:b:14:LEU:N	2.28	0.47
1:A:33:THR:HG22	1:A:34:SER:N	2.29	0.47
3:C:71:LEU:HD22	3:C:84:ILE:CD1	2.45	0.47
5:E:42:HIS:CD2	5:E:214:ILE:HD11	2.48	0.47
5:E:174:THR:HG22	5:E:177:THR:HB	1.95	0.47
5:E:181:ILE:HG21	5:E:187:GLU:CB	2.45	0.47
13:M:100:MET:HE3	13:M:132:LEU:HA	1.95	0.47
13:M:147:GLY:O	13:M:151:ALA:HB3	2.14	0.47
14:N:175:MET:HE3	14:N:188:PHE:CD2	2.49	0.47
4:R:16:VAL:O	4:R:19:SER:HB3	2.14	0.47
5:S:102:LEU:HA	16:S:321:HOH:O	2.15	0.47
5:S:207:VAL:CG1	5:S:208:ASP:N	2.78	0.47
6:T:89:ARG:HD2	16:T:307:HOH:O	2.14	0.47
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.44	0.47
11:Y:139:VAL:HG21	11:Y:163:ALA:HB2	1.96	0.47
13:a:100:MET:HE3	13:a:132:LEU:HA	1.97	0.47
2:B:36:GLY:O	2:B:161:ALA:HA	2.14	0.47
3:C:66:ASP:HA	10:J:69:ILE:CD1	2.41	0.47
6:F:50:ILE:HD11	6:F:209:GLU:HB2	1.96	0.47
7:G:26:THR:HG21	7:G:131:ILE:HG13	1.96	0.47
13:M:16:TYR:CZ	13:M:170:VAL:HG22	2.50	0.47
2:P:49:ARG:HH21	2:P:58:GLN:HE21	1.63	0.47
5:S:2:ARG:HG3	5:S:19:PHE:CE1	2.50	0.47
5:S:154:GLU:HG3	16:S:306:HOH:O	2.14	0.47
8:V:99:ILE:HG13	8:V:127:LEU:HD12	1.97	0.47
12:Z:95:HIS:HE1	16:Z:303:HOH:O	1.98	0.47
14:b:8:PHE:CE1	14:b:10:ASP:HB2	2.50	0.47
3:Q:71:LEU:HD22	3:Q:84:ILE:CD1	2.44	0.47
5:S:42:HIS:CD2	5:S:214:ILE:HD11	2.48	0.47
5:S:178:PHE:HA	5:S:181:ILE:CG1	2.44	0.47
13:a:21:ILE:HB	13:a:177:ILE:HD12	1.97	0.47
13:a:223:LYS:HA	16:a:346:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:LYS:O	2:B:51:VAL:O	2.33	0.47
5:E:68:HIS:HE1	5:E:102:LEU:O	1.98	0.47
13:M:35:ARG:HD3	13:M:36:PHE:CZ	2.50	0.47
14:N:102:TYR:OH	14:N:180:ALA:HB2	2.15	0.47
8:V:50:ALA:HB2	9:W:128:CYS:HB2	1.97	0.47
1:A:176:GLU:HG2	2:B:55:LEU:HD23	1.90	0.46
1:A:185:LEU:HD21	1:A:213:ILE:HD12	1.97	0.46
2:B:189:ILE:HG23	2:B:212:PHE:CE2	2.50	0.46
8:H:4:VAL:HG12	8:H:126:SER:HB3	1.97	0.46
9:I:176:ARG:NH2	12:Z:147:MET:CE	2.79	0.46
13:M:184:LEU:HD13	16:M:314:HOH:O	2.16	0.46
9:W:14:MET:HG2	9:W:135:PHE:HB3	1.96	0.46
11:Y:25:TRP:CH2	12:Z:144:SER:HA	2.49	0.46
12:Z:113:GLY:HA2	12:Z:207:VAL:HG11	1.96	0.46
2:B:110:LEU:HD23	2:B:110:LEU:C	2.40	0.46
2:B:139:TYR:HA	2:B:144:GLY:O	2.15	0.46
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.95	0.46
4:D:241:ALA:O	4:D:242:GLU:CB	2.57	0.46
14:N:44:CYS:HB2	14:N:98:ILE:HB	1.97	0.46
5:S:193:VAL:HG22	5:S:212:ILE:HD11	1.97	0.46
7:U:3:TYR:C	7:U:5:ARG:N	2.72	0.46
8:V:22:GLN:CD	15:e:2:THR:HG22	2.40	0.46
9:W:15:THR:CG2	9:W:120:ILE:HG12	2.45	0.46
9:W:15:THR:HG23	9:W:120:ILE:HG12	1.96	0.46
12:Z:17:GLY:HA3	12:Z:20:PHE:CZ	2.49	0.46
2:B:98:LEU:HG	9:I:67:ARG:HH21	1.80	0.46
5:E:205:LEU:HD23	5:E:205:LEU:N	2.22	0.46
14:N:15:GLY:HA2	14:N:174:ARG:O	2.14	0.46
2:P:148:TYR:CE1	3:Q:57:ILE:HD13	2.50	0.46
6:T:41:GLY:CA	6:T:215:CYS:O	2.63	0.46
6:T:126:ARG:HG2	6:T:126:ARG:HH11	1.80	0.46
8:V:38:SER:OG	8:V:41:ILE:HG13	2.15	0.46
12:Z:36:ASN:HB3	13:a:137:TYR:CZ	2.51	0.46
12:Z:67:ARG:NH2	16:Z:347:HOH:O	2.39	0.46
12:Z:108:HIS:HE1	12:Z:124:SER:HB2	1.80	0.46
13:a:13:SER:HB3	13:a:22:ILE:HG13	1.97	0.46
14:b:3:ILE:HG22	14:b:16:ALA:CB	2.45	0.46
14:b:13:ILE:HG12	14:b:177:VAL:HG13	1.97	0.46
5:E:14:PRO:HA	6:F:22:TYR:CE2	2.50	0.46
5:E:143:LEU:CD2	5:E:157:GLY:HA2	2.45	0.46
8:H:213:LEU:HD22	11:Y:212:GLY:HA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:101:PRO:HA	16:I:310:HOH:O	2.15	0.46
10:J:78:GLN:HE21	10:J:79:ALA:N	2.14	0.46
1:O:24:ALA:O	1:O:28:VAL:HG23	2.16	0.46
2:P:110:LEU:C	2:P:110:LEU:HD23	2.41	0.46
5:S:25:LEU:O	5:S:28:ILE:HB	2.15	0.46
5:S:143:LEU:CD2	5:S:157:GLY:HA2	2.45	0.46
5:S:205:LEU:HD23	5:S:205:LEU:N	2.21	0.46
6:T:123:ASN:HD22	6:T:124:SER:N	2.13	0.46
7:U:227:LEU:HB3	7:U:231:ASN:HB2	1.97	0.46
10:X:78:GLN:HE21	10:X:79:ALA:N	2.14	0.46
10:X:192:VAL:C	10:X:194:ASP:H	2.23	0.46
3:C:120:GLN:HG3	3:C:120:GLN:O	2.15	0.46
3:C:166:SER:HA	3:C:169:VAL:CG1	2.45	0.46
3:C:222:LEU:HD12	3:C:222:LEU:N	2.31	0.46
5:E:220:PRO:O	5:E:221:PHE:C	2.57	0.46
6:F:123:ASN:HD22	6:F:123:ASN:N	2.12	0.46
7:G:71:GLY:HA3	7:G:224:PHE:CE2	2.51	0.46
9:I:87:THR:HG22	9:I:129:ILE:HD13	1.97	0.46
12:L:145:LEU:O	9:W:147:GLY:HA3	2.15	0.46
2:P:189:ILE:HG23	2:P:212:PHE:CE2	2.51	0.46
5:S:129:VAL:O	5:S:148:PRO:HG3	2.15	0.46
6:T:50:ILE:HD11	6:T:209:GLU:HB2	1.98	0.46
7:U:95:PHE:CD1	7:U:95:PHE:C	2.94	0.46
12:Z:92:ASN:C	12:Z:92:ASN:ND2	2.73	0.46
12:Z:150:LEU:O	12:Z:154:VAL:HB	2.16	0.46
14:b:15:GLY:HA2	14:b:174:ARG:O	2.16	0.46
6:F:240:GLN:O	6:F:243:ILE:HG22	2.15	0.46
8:H:147:THR:OG1	8:H:150:GLU:HG3	2.14	0.46
14:N:3:ILE:HD12	14:N:44:CYS:HB3	1.96	0.46
14:N:113:ILE:HG12	14:N:119:VAL:HG13	1.96	0.46
4:R:93:LEU:CD1	11:Y:57:THR:HG22	2.45	0.46
6:T:168:ALA:C	6:T:172:LEU:HD23	2.41	0.46
7:U:103:MET:HE1	7:U:108:LEU:HD13	1.97	0.46
11:Y:4:LEU:HD13	11:Y:161:ILE:HD11	1.97	0.46
11:Y:196:LEU:HD12	11:Y:200:VAL:HG23	1.96	0.46
2:B:43:ILE:HD11	2:B:145:TYR:CB	2.26	0.46
2:B:61:SER:O	2:B:62:THR:OG1	2.30	0.46
5:E:207:VAL:HG22	5:E:226:GLY:HA2	1.98	0.46
6:F:168:ALA:C	6:F:172:LEU:HD23	2.41	0.46
9:I:167:SER:O	9:I:171:LEU:HD23	2.16	0.46
10:J:192:VAL:C	10:J:194:ASP:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:48:ASN:N	13:M:48:ASN:ND2	2.64	0.46
13:M:94:GLU:HA	13:M:94:GLU:OE2	2.16	0.46
13:M:130:VAL:HG23	13:M:136:THR:CG2	2.42	0.46
5:S:207:VAL:HG22	5:S:226:GLY:HA2	1.97	0.46
7:U:7:ILE:HA	16:U:335:HOH:O	2.14	0.46
7:U:26:THR:HG21	7:U:131:ILE:HG13	1.97	0.46
8:V:152:ILE:HD11	8:V:177:VAL:HG21	1.97	0.46
8:V:173:VAL:HB	8:V:191:LEU:HB2	1.98	0.46
9:W:148:MET:CE	9:W:172:ASN:HB2	2.39	0.46
1:A:205:ASN:HA	1:A:247:LEU:CD1	2.46	0.46
6:F:99:TYR:O	6:F:100:LYS:HB3	2.16	0.46
8:H:200:GLN:HG2	12:Z:182:LYS:HA	1.98	0.46
9:I:106:PRO:HB2	9:I:123:PHE:CD2	2.50	0.46
11:K:4:LEU:CD1	11:K:161:ILE:HD11	2.46	0.46
12:L:51:VAL:HG12	12:L:205:LEU:HD23	1.98	0.46
2:P:167:ASN:HA	16:P:319:HOH:O	2.16	0.46
2:P:236:ASP:O	2:P:240:LYS:HG2	2.16	0.46
4:R:37:GLY:HA2	4:R:145:TYR:CD1	2.50	0.46
9:W:73:TYR:CE1	9:W:77:GLU:HG3	2.51	0.46
12:Z:86:ILE:HG23	12:Z:123:TYR:HE2	1.81	0.46
12:Z:208:THR:C	12:Z:210:ASP:N	2.73	0.46
13:a:119:VAL:CG2	13:a:200:ILE:HG22	2.45	0.46
2:B:77:ALA:HB2	2:B:164:VAL:HG23	1.97	0.46
2:B:162:ILE:HG13	2:B:163:SER:H	1.80	0.46
5:E:62:ILE:HG21	5:E:213:ALA:HB2	1.98	0.46
12:L:177:VAL:O	12:L:181:ILE:HG13	2.16	0.46
14:N:88:GLU:OE1	14:N:88:GLU:HA	2.15	0.46
3:Q:58:THR:HG23	3:Q:59:PRO:HD2	1.97	0.46
3:Q:161:THR:HG23	3:Q:166:SER:HB2	1.98	0.46
4:R:67:GLY:HA3	4:R:220:PHE:CD2	2.50	0.46
9:W:201:MET:HB2	16:W:307:HOH:O	2.15	0.46
2:B:158:GLY:HA3	3:C:57:ILE:HD12	1.97	0.46
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.98	0.46
6:F:126:ARG:HG2	6:F:126:ARG:HH11	1.81	0.46
6:F:172:LEU:O	6:F:176:VAL:HG23	2.16	0.46
11:K:4:LEU:HD13	11:K:161:ILE:HD11	1.97	0.46
6:T:191:GLN:NE2	6:T:194:LYS:CE	2.79	0.46
8:V:104:ASP:C	8:V:106:THR:H	2.24	0.46
12:Z:208:THR:O	12:Z:210:ASP:N	2.49	0.46
4:D:161:ALA:HB3	5:E:55:LEU:HD23	1.99	0.45
5:E:200:LEU:HD11	5:E:205:LEU:CD2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:198:LEU:HD12	6:F:198:LEU:N	2.31	0.45
8:H:196:ARG:NH2	9:I:150:GLU:O	2.50	0.45
11:K:208:ASN:ND2	10:X:150:PRO:CG	2.75	0.45
12:L:42:LYS:HD2	12:L:55:ASN:ND2	2.30	0.45
7:U:166:GLN:NE2	7:U:167:GLN:N	2.64	0.45
8:V:179:GLU:N	16:V:326:HOH:O	2.48	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.97	0.45
12:Z:51:VAL:HG12	12:Z:205:LEU:HD23	1.98	0.45
14:b:87:TYR:O	14:b:90:LYS:HG2	2.16	0.45
1:A:29:LYS:NZ	1:A:168:SER:OG	2.47	0.45
6:F:123:ASN:HD22	6:F:123:ASN:C	2.24	0.45
8:H:38:SER:OG	8:H:41:ILE:HG13	2.16	0.45
12:L:17:GLY:HA3	12:L:20:PHE:CZ	2.51	0.45
12:L:125:PHE:N	12:L:125:PHE:CD1	2.83	0.45
13:M:11:VAL:O	13:M:143:ALA:HA	2.17	0.45
13:M:85:GLU:HA	13:M:85:GLU:OE2	2.16	0.45
2:P:77:ALA:HB2	2:P:164:VAL:HG23	1.97	0.45
14:b:38:HIS:O	14:b:39:ASP:C	2.59	0.45
5:E:2:ARG:HG3	5:E:19:PHE:CE1	2.50	0.45
5:E:25:LEU:O	5:E:28:ILE:HB	2.15	0.45
6:F:8:ASN:ND2	6:F:127:PRO:HD3	2.31	0.45
9:I:73:TYR:CE1	9:I:77:GLU:HG3	2.51	0.45
9:I:189:ILE:HA	9:I:194:VAL:HG22	1.98	0.45
6:T:71:GLY:O	6:T:134:PHE:HA	2.16	0.45
6:T:138:ASP:C	6:T:138:ASP:OD2	2.60	0.45
10:X:53:THR:HG23	10:X:54:VAL:H	1.82	0.45
1:A:44:VAL:HG23	1:A:211:LEU:HD21	1.97	0.45
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.31	0.45
2:B:105:ILE:HG12	2:B:110:LEU:HB2	1.98	0.45
2:B:236:ASP:O	2:B:240:LYS:HG2	2.15	0.45
4:D:71:SER:O	4:D:132:VAL:HG23	2.17	0.45
6:F:133:ILE:HA	6:F:145:TYR:O	2.16	0.45
6:F:201:GLU:HA	6:F:201:GLU:OE1	2.17	0.45
8:H:195:VAL:HA	16:H:346:HOH:O	2.17	0.45
8:H:213:LEU:HG	9:I:200:LYS:HB2	1.98	0.45
11:K:196:LEU:O	11:K:200:VAL:HG23	2.17	0.45
2:P:50:LYS:O	2:P:51:VAL:O	2.33	0.45
2:P:55:LEU:HD22	2:P:55:LEU:N	2.31	0.45
3:Q:129:VAL:HG12	3:Q:130:SER:N	2.32	0.45
4:R:71:SER:O	4:R:132:VAL:HG23	2.15	0.45
5:S:1:PHE:O	5:S:2:ARG:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:8:ASN:ND2	6:T:127:PRO:HD3	2.31	0.45
10:X:89:ALA:O	10:X:92:ILE:HG22	2.16	0.45
13:a:11:VAL:O	13:a:143:ALA:HA	2.16	0.45
14:b:175:MET:HE3	14:b:188:PHE:CD2	2.51	0.45
1:A:246:ARG:HG3	1:A:246:ARG:NH1	2.28	0.45
2:B:43:ILE:CG2	2:B:147:LEU:HD13	2.46	0.45
8:H:79:ALA:O	8:H:83:LEU:HG	2.16	0.45
9:I:14:MET:HG2	9:I:135:PHE:HB3	1.98	0.45
2:P:76:VAL:HG22	2:P:134:PHE:CE2	2.51	0.45
3:Q:46:ARG:HD2	3:Q:206:LYS:O	2.17	0.45
4:R:6:THR:HG22	4:R:7:PHE:N	2.31	0.45
5:S:62:ILE:HG21	5:S:213:ALA:HB2	1.99	0.45
6:T:232:LEU:O	6:T:236:ILE:HD13	2.16	0.45
12:Z:125:PHE:N	12:Z:125:PHE:CD1	2.84	0.45
13:a:16:TYR:CZ	13:a:170:VAL:HG22	2.50	0.45
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.51	0.45
6:F:71:GLY:O	6:F:134:PHE:HA	2.15	0.45
8:H:152:ILE:HD11	8:H:177:VAL:HG21	1.99	0.45
12:L:12:ILE:HG13	12:L:110:ILE:HD12	1.99	0.45
12:L:126:ASP:CB	12:L:130:SER:H	2.26	0.45
12:L:150:LEU:O	12:L:154:VAL:HB	2.15	0.45
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.52	0.45
1:O:250:LEU:C	1:O:250:LEU:HD13	2.42	0.45
2:P:139:TYR:CE2	2:P:144:GLY:HA2	2.51	0.45
2:P:185:VAL:HG21	2:P:216:ARG:HG3	1.99	0.45
6:T:123:ASN:HD22	6:T:123:ASN:N	2.14	0.45
6:T:148:GLU:HG2	16:T:326:HOH:O	2.16	0.45
7:U:83:ASN:C	7:U:83:ASN:ND2	2.74	0.45
8:V:147:THR:OG1	8:V:150:GLU:HG3	2.17	0.45
9:W:106:PRO:HB2	9:W:123:PHE:CD2	2.51	0.45
11:Y:4:LEU:CD1	11:Y:161:ILE:HD11	2.46	0.45
4:D:159:TYR:HA	5:E:55:LEU:O	2.17	0.45
7:G:3:TYR:C	7:G:5:ARG:N	2.70	0.45
9:I:170:LEU:CD2	9:I:184:ALA:HB1	2.47	0.45
3:Q:146:TYR:CE1	3:Q:156:SER:HB3	2.52	0.45
6:T:99:TYR:O	6:T:100:LYS:HB3	2.15	0.45
6:T:133:ILE:HA	6:T:145:TYR:O	2.17	0.45
6:T:196:ILE:HG21	6:T:210:LEU:CD1	2.43	0.45
10:X:106:GLY:HA2	10:X:184:VAL:HG11	1.98	0.45
11:Y:191:HIS:CD2	11:Y:191:HIS:N	2.85	0.45
13:a:53:ILE:HG21	13:a:60:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:PHE:O	3:C:176:ASN:HB2	2.16	0.45
7:G:185:ILE:N	7:G:185:ILE:CD1	2.79	0.45
8:H:173:VAL:HB	8:H:191:LEU:HB2	1.99	0.45
9:I:15:THR:CG2	9:I:120:ILE:HG12	2.47	0.45
12:L:135:GLN:NE2	12:L:174:TYR:OH	2.50	0.45
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.52	0.45
2:P:67:LYS:CE	2:P:228:ILE:HD11	2.47	0.45
2:P:149:THR:O	2:P:156:TYR:HA	2.17	0.45
3:Q:222:LEU:N	3:Q:222:LEU:HD12	2.32	0.45
5:S:207:VAL:CG1	5:S:208:ASP:H	2.29	0.45
16:T:303:HOH:O	7:U:82:ARG:HD2	2.17	0.45
8:V:3:ILE:HD12	8:V:46:ALA:HB2	1.99	0.45
1:A:204:PHE:CD1	1:A:209:ILE:HD11	2.52	0.45
7:G:72:MET:HE3	7:G:74:VAL:HG23	1.98	0.45
7:G:95:PHE:C	7:G:95:PHE:CD1	2.95	0.45
8:H:3:ILE:HD12	8:H:46:ALA:HB2	1.98	0.45
10:J:161:LEU:O	10:J:162:LYS:C	2.60	0.45
11:K:46:ALA:HB3	11:K:98:GLY:O	2.17	0.45
11:K:174:SER:HA	11:K:193:VAL:HG23	1.99	0.45
2:P:17:ARG:HG2	2:P:17:ARG:HH11	1.81	0.45
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.99	0.45
4:R:180:HIS:H	4:R:183:LEU:CD1	2.30	0.45
5:S:36:GLY:O	5:S:157:GLY:HA2	2.17	0.45
6:T:47:GLU:OE1	6:T:49:LEU:HD21	2.17	0.45
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.17	0.45
12:Z:52:MET:HE3	12:Z:93:ILE:CD1	2.47	0.45
5:E:136:TYR:CE1	5:E:140:GLY:HA2	2.52	0.45
5:E:207:VAL:CG1	5:E:208:ASP:H	2.28	0.45
8:H:22:GLN:CD	15:c:2:THR:HG22	2.41	0.45
10:J:165:VAL:O	10:J:169:GLU:HG3	2.17	0.45
11:K:4:LEU:CD1	11:K:15:ALA:HB3	2.46	0.45
11:K:186:ILE:O	11:K:188:HIS:HD2	2.00	0.45
12:L:95:HIS:HE1	16:L:304:HOH:O	2.00	0.45
13:M:21:ILE:HB	13:M:177:ILE:HD12	1.98	0.45
13:M:187:ARG:HA	14:b:26:ILE:HB	1.97	0.45
14:N:132:THR:O	14:b:133:PHE:HA	2.17	0.45
1:O:180:ASN:H	1:O:183:LEU:CD1	2.30	0.45
2:P:71:LYS:O	2:P:138:GLY:HA2	2.17	0.45
4:R:180:HIS:H	4:R:183:LEU:HD11	1.82	0.45
7:U:103:MET:HE3	7:U:108:LEU:HD13	1.98	0.45
9:W:111:ILE:N	16:W:306:HOH:O	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:103:LEU:HD23	10:X:103:LEU:HA	1.74	0.45
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.99	0.45
4:D:17:GLU:O	4:D:20:LEU:HB2	2.18	0.44
4:D:178:GLU:HB3	4:D:191:LEU:HD21	2.00	0.44
5:E:129:VAL:O	5:E:148:PRO:HG3	2.17	0.44
5:E:221:PHE:C	5:E:221:PHE:CD1	2.96	0.44
11:K:139:VAL:HG21	11:K:163:ALA:HB2	2.00	0.44
2:P:175:LEU:C	2:P:177:MET:H	2.24	0.44
3:Q:209:GLU:C	3:Q:210:ILE:HD12	2.42	0.44
7:U:241:GLU:O	7:U:242:GLN:HB2	2.17	0.44
12:Z:161:GLU:O	12:Z:162:PRO:C	2.59	0.44
14:b:102:TYR:OH	14:b:180:ALA:HB2	2.18	0.44
1:A:1:MET:CG	1:A:2:THR:H	2.30	0.44
2:B:139:TYR:CE2	2:B:144:GLY:HA2	2.52	0.44
3:C:223:SER:O	3:C:224:SER:C	2.59	0.44
11:K:133:GLN:HG3	11:K:134:THR:N	2.32	0.44
11:K:158:LYS:HB2	11:K:177:LEU:HD11	1.99	0.44
11:K:201:LYS:HE3	11:K:207:PHE:O	2.17	0.44
13:M:19:GLY:HA3	13:M:200:ILE:O	2.17	0.44
14:N:6:VAL:HG21	14:N:155:ILE:HD11	1.99	0.44
2:P:236:ASP:C	2:P:238:LEU:H	2.24	0.44
3:Q:51:LYS:HD2	3:Q:52:LEU:H	1.82	0.44
3:Q:107:LEU:O	3:Q:107:LEU:HD13	2.17	0.44
5:S:155:LEU:HD12	5:S:158:THR:HG21	1.99	0.44
8:V:72:ARG:HG3	8:V:72:ARG:NH1	2.30	0.44
14:b:96:GLY:C	14:b:97:ILE:HD12	2.43	0.44
7:G:237:VAL:O	7:G:240:ALA:HB3	2.16	0.44
11:K:4:LEU:C	11:K:4:LEU:CD2	2.90	0.44
12:L:174:TYR:CD1	12:L:175:LEU:N	2.86	0.44
13:M:161:ARG:CG	13:M:161:ARG:NH1	2.74	0.44
13:M:191:SER:HB2	16:M:322:HOH:O	2.17	0.44
14:N:26:ILE:HB	13:a:187:ARG:HA	1.98	0.44
2:P:141:ASP:OD2	10:X:110:LYS:HE2	2.17	0.44
2:P:229:PHE:N	2:P:229:PHE:CD2	2.85	0.44
4:R:196:LEU:O	4:R:200:MET:HG3	2.16	0.44
5:S:28:ILE:HD11	5:S:148:PRO:CD	2.48	0.44
9:W:108:VAL:O	9:W:120:ILE:HA	2.18	0.44
9:W:167:SER:O	9:W:171:LEU:HD23	2.17	0.44
11:Y:196:LEU:O	11:Y:200:VAL:HG23	2.17	0.44
3:C:209:GLU:C	3:C:210:ILE:HD12	2.43	0.44
4:D:6:THR:HG22	4:D:7:PHE:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:175:LEU:O	5:E:177:THR:N	2.51	0.44
6:F:68:ARG:NH1	13:M:72:THR:OG1	2.51	0.44
7:G:236:LEU:O	7:G:239:ILE:HG13	2.18	0.44
8:H:104:ASP:C	8:H:106:THR:H	2.25	0.44
2:P:60:THR:HG22	2:P:60:THR:O	2.18	0.44
4:R:59:ILE:HG22	4:R:220:PHE:HZ	1.82	0.44
4:R:205:ASP:C	4:R:207:ASN:H	2.26	0.44
5:S:136:TYR:CE1	5:S:140:GLY:HA2	2.52	0.44
7:U:185:ILE:N	7:U:185:ILE:CD1	2.80	0.44
10:X:117:TYR:CE1	10:X:127:GLU:HG3	2.52	0.44
13:a:130:VAL:HG23	13:a:136:THR:CG2	2.44	0.44
14:b:114:PRO:HD2	14:b:118:SER:O	2.17	0.44
1:A:24:ALA:O	1:A:28:VAL:HG23	2.17	0.44
2:B:67:LYS:CE	2:B:228:ILE:HD11	2.48	0.44
2:B:105:ILE:HD11	2:B:109:ILE:HG22	1.99	0.44
3:C:129:VAL:HG12	3:C:130:SER:N	2.32	0.44
4:D:205:ASP:C	4:D:207:ASN:H	2.26	0.44
6:F:47:GLU:OE1	6:F:49:LEU:HD21	2.16	0.44
7:G:227:LEU:HB3	7:G:231:ASN:HB2	1.98	0.44
9:I:11:VAL:HG22	9:I:24:CYS:HB3	1.99	0.44
10:J:150:PRO:CG	11:Y:208:ASN:ND2	2.81	0.44
11:K:56:GLU:O	11:K:59:LEU:HB3	2.17	0.44
12:L:92:ASN:C	12:L:92:ASN:ND2	2.73	0.44
12:L:161:GLU:O	12:L:162:PRO:C	2.59	0.44
2:P:158:GLY:HA3	3:Q:57:ILE:HD11	2.00	0.44
14:b:44:CYS:HB2	14:b:98:ILE:HB	1.99	0.44
4:D:171:ALA:O	4:D:174:GLU:HB3	2.17	0.44
5:E:28:ILE:HD11	5:E:148:PRO:CD	2.47	0.44
6:F:28:GLU:HB3	6:F:165:ARG:NH2	2.33	0.44
10:J:117:TYR:CE1	10:J:127:GLU:HG3	2.52	0.44
12:L:213:ARG:CB	12:L:213:ARG:HH11	2.30	0.44
2:P:243:ILE:O	2:P:243:ILE:HG22	2.17	0.44
7:U:71:GLY:HA3	7:U:224:PHE:CE2	2.52	0.44
9:W:157:LEU:HG	16:W:327:HOH:O	2.17	0.44
10:X:5:LEU:HB2	10:X:16:ALA:HB3	2.00	0.44
11:Y:158:LYS:HB2	11:Y:177:LEU:HD11	1.98	0.44
6:F:123:ASN:HD22	6:F:124:SER:N	2.16	0.44
6:F:138:ASP:OD2	6:F:138:ASP:C	2.61	0.44
7:G:92:ALA:HA	7:G:103:MET:CE	2.45	0.44
8:H:41:ILE:HD13	8:H:76:VAL:HA	1.98	0.44
10:J:172:MET:HA	10:J:173:PRO:HD3	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:24:ALA:HB1	12:L:202:LEU:HD11	2.00	0.44
12:L:182:LYS:HA	8:V:200:GLN:HG2	1.99	0.44
12:L:208:THR:O	12:L:210:ASP:N	2.51	0.44
5:S:157:GLY:O	5:S:158:THR:HB	2.17	0.44
12:Z:154:VAL:O	12:Z:154:VAL:HG12	2.18	0.44
2:B:60:THR:HG22	2:B:60:THR:O	2.18	0.44
2:B:237:ILE:O	2:B:237:ILE:HG13	2.18	0.44
5:E:216:GLY:O	5:E:217:LYS:C	2.61	0.44
9:I:125:LEU:HD21	15:c:1:MH9:H3	2.00	0.44
11:K:4:LEU:HA	11:K:127:PHE:O	2.18	0.44
14:N:87:TYR:O	14:N:90:LYS:HG2	2.18	0.44
1:O:1:MET:CG	1:O:2:THR:H	2.30	0.44
8:V:9:ASN:HD21	8:V:147:THR:HA	1.82	0.44
3:C:182:PRO:O	3:C:183:PRO:C	2.59	0.44
7:G:155:VAL:CG2	7:G:156:GLY:N	2.80	0.44
9:I:15:THR:HG23	9:I:120:ILE:HG12	2.00	0.44
12:L:41:PRO:HA	16:L:344:HOH:O	2.16	0.44
1:O:185:LEU:HD21	1:O:213:ILE:HD12	1.99	0.44
2:P:105:ILE:HD11	2:P:109:ILE:HG22	2.00	0.44
4:R:73:LEU:N	4:R:131:GLY:O	2.47	0.44
14:b:54:ALA:O	14:b:58:ILE:HG12	2.18	0.44
2:B:234:ILE:O	2:B:238:LEU:HB2	2.18	0.43
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.00	0.43
9:I:53:THR:HA	16:I:305:HOH:O	2.18	0.43
13:M:165:ILE:HB	13:M:166:PRO:CD	2.49	0.43
2:P:236:ASP:C	2:P:238:LEU:N	2.75	0.43
4:R:82:GLU:CD	11:Y:69:ARG:HH11	2.26	0.43
13:a:165:ILE:HB	13:a:166:PRO:CD	2.48	0.43
2:B:149:THR:O	2:B:156:TYR:HA	2.18	0.43
5:E:48:LEU:HD12	5:E:209:ASN:OD1	2.18	0.43
5:E:193:VAL:HG22	5:E:212:ILE:HD11	2.00	0.43
9:I:108:VAL:O	9:I:120:ILE:HA	2.18	0.43
10:J:68:SER:O	10:J:72:ASP:N	2.51	0.43
4:R:89:VAL:HG21	11:Y:65:LEU:CD2	2.48	0.43
5:S:48:LEU:HD12	5:S:209:ASN:OD1	2.17	0.43
8:V:51:ASP:O	8:V:55:VAL:HG12	2.18	0.43
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.18	0.43
7:G:241:GLU:O	7:G:242:GLN:HB2	2.18	0.43
8:H:5:GLY:O	8:H:124:TYR:HA	2.18	0.43
9:I:104:VAL:HG23	9:I:106:PRO:HD3	2.00	0.43
13:M:53:ILE:CD1	13:M:60:MET:HG3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:54:ALA:O	14:N:58:ILE:HG12	2.18	0.43
14:N:161:GLN:O	14:N:164:LYS:HB3	2.18	0.43
1:O:203:GLU:OE2	1:O:203:GLU:HA	2.19	0.43
5:S:1:PHE:CG	5:S:2:ARG:N	2.86	0.43
5:S:170:TYR:HB2	5:S:198:GLN:HG2	2.00	0.43
5:S:205:LEU:HA	5:S:209:ASN:HD22	1.81	0.43
7:U:56:ASP:C	7:U:56:ASP:OD2	2.60	0.43
7:U:222:ASP:O	7:U:223:LYS:HB2	2.18	0.43
11:Y:43:GLY:HA2	11:Y:100:MET:O	2.19	0.43
11:Y:116:ASP:C	11:Y:116:ASP:OD1	2.62	0.43
14:b:161:GLN:O	14:b:164:LYS:HB3	2.18	0.43
1:A:35:LEU:C	1:A:35:LEU:HD12	2.43	0.43
1:A:214:ILE:HD11	1:A:235:PHE:HD1	1.84	0.43
2:B:71:LYS:O	2:B:138:GLY:HA2	2.18	0.43
2:B:236:ASP:C	2:B:238:LEU:N	2.76	0.43
4:D:89:VAL:HG21	11:K:65:LEU:CD2	2.48	0.43
10:J:37:GLN:HG3	10:J:189:ILE:HG13	2.01	0.43
2:P:194:LYS:O	2:P:197:SER:HB3	2.18	0.43
2:P:237:ILE:O	2:P:237:ILE:HG13	2.18	0.43
3:Q:172:PHE:O	3:Q:176:ASN:HB2	2.18	0.43
5:S:70:GLY:HA3	5:S:221:PHE:CZ	2.52	0.43
6:T:201:GLU:OE1	6:T:201:GLU:HA	2.19	0.43
7:U:149:ASP:HB2	7:U:150:PRO:HD2	2.00	0.43
10:X:68:SER:O	10:X:72:ASP:N	2.52	0.43
11:Y:186:ILE:O	11:Y:188:HIS:HD2	2.00	0.43
12:Z:12:ILE:HG13	12:Z:110:ILE:HD12	2.00	0.43
2:B:120:GLY:C	2:B:122:THR:N	2.77	0.43
6:F:123:ASN:C	6:F:123:ASN:ND2	2.75	0.43
6:F:168:ALA:O	6:F:172:LEU:HD23	2.17	0.43
13:M:13:SER:HB3	13:M:22:ILE:HG13	2.00	0.43
14:N:38:HIS:O	14:N:39:ASP:C	2.61	0.43
1:O:226:GLY:HA3	8:V:186:TYR:HB3	2.00	0.43
2:P:2:SER:O	2:P:4:ARG:N	2.52	0.43
3:Q:11:PRO:HA	4:R:18:TYR:CE1	2.53	0.43
8:V:213:LEU:HG	9:W:200:LYS:HB2	1.99	0.43
9:W:11:VAL:HG22	9:W:24:CYS:HB3	2.00	0.43
12:Z:30:ILE:HD11	12:Z:197:GLN:NE2	2.34	0.43
2:B:122:THR:HG22	3:C:125:ARG:NH2	2.18	0.43
3:C:46:ARG:HD2	3:C:206:LYS:O	2.18	0.43
3:C:161:THR:HG23	3:C:166:SER:HB2	2.00	0.43
4:D:115:PHE:CZ	4:D:129:PRO:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:9:ASN:HD21	8:H:147:THR:HA	1.82	0.43
10:J:106:GLY:HA2	10:J:184:VAL:HG11	1.99	0.43
11:K:76:VAL:N	11:K:108:GLU:OE2	2.51	0.43
12:L:30:ILE:HD11	12:L:197:GLN:NE2	2.33	0.43
13:M:3:GLN:O	13:M:3:GLN:HG3	2.18	0.43
13:M:53:ILE:HD12	13:M:60:MET:HG3	2.00	0.43
5:S:221:PHE:C	5:S:221:PHE:CD1	2.97	0.43
8:V:2:THR:OG1	8:V:130:GLY:HA3	2.19	0.43
8:V:207:ARG:HG3	16:V:335:HOH:O	2.19	0.43
8:V:210:THR:CG2	9:W:199:LEU:HD22	2.49	0.43
14:b:3:ILE:HD12	14:b:44:CYS:HB3	2.00	0.43
14:b:112:THR:CG2	14:b:120:HIS:HB2	2.42	0.43
1:A:211:LEU:HD23	1:A:211:LEU:C	2.43	0.43
2:B:185:VAL:HG21	2:B:216:ARG:HG3	2.00	0.43
2:B:194:LYS:O	2:B:197:SER:HB3	2.18	0.43
2:B:236:ASP:C	2:B:238:LEU:H	2.25	0.43
4:D:180:HIS:H	4:D:183:LEU:HD11	1.83	0.43
5:E:70:GLY:HA3	5:E:221:PHE:CZ	2.54	0.43
10:J:172:MET:HG2	10:J:173:PRO:HD2	2.01	0.43
4:R:77:ALA:O	4:R:81:ILE:HG12	2.18	0.43
10:X:172:MET:HG2	10:X:173:PRO:HD2	2.01	0.43
13:a:48:ASN:N	13:a:48:ASN:ND2	2.65	0.43
14:b:176:VAL:HG12	14:b:178:LEU:HD13	2.01	0.43
4:D:4:VAL:HG23	4:D:116:GLY:HA2	2.01	0.43
5:E:157:GLY:O	5:E:158:THR:HB	2.19	0.43
8:H:210:THR:CG2	9:I:199:LEU:HD22	2.48	0.43
11:K:6:PHE:HA	11:K:125:ASP:O	2.18	0.43
11:K:208:ASN:ND2	10:X:150:PRO:CD	2.80	0.43
11:K:212:GLY:HA2	8:V:213:LEU:HD22	2.01	0.43
13:M:93:PHE:CE1	13:M:128:ARG:HD3	2.54	0.43
14:N:8:PHE:CE2	14:N:13:ILE:HG13	2.51	0.43
14:N:133:PHE:CE2	14:N:166:ASP:HB2	2.53	0.43
5:S:175:LEU:O	5:S:177:THR:N	2.51	0.43
5:S:178:PHE:C	5:S:180:LYS:N	2.77	0.43
7:U:155:VAL:CG2	7:U:156:GLY:N	2.82	0.43
8:V:5:GLY:O	8:V:124:TYR:HA	2.19	0.43
11:Y:144:TYR:CD1	11:Y:144:TYR:C	2.97	0.43
12:Z:126:ASP:C	12:Z:128:VAL:N	2.75	0.43
3:C:109:ARG:HD3	3:C:154:TYR:OH	2.19	0.43
5:E:1:PHE:O	5:E:2:ARG:C	2.61	0.43
1:O:205:ASN:HA	1:O:247:LEU:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:42:GLY:HA2	2:P:145:TYR:CE1	2.53	0.43
3:Q:147:GLN:HE21	3:Q:147:GLN:HB3	1.49	0.43
7:U:68:ARG:HH11	7:U:68:ARG:CB	2.32	0.43
8:V:79:ALA:O	8:V:83:LEU:HG	2.19	0.43
10:X:149:ARG:HG2	10:X:149:ARG:NH1	2.34	0.43
12:Z:199:GLY:O	12:Z:200:ASP:HB2	2.18	0.43
13:a:151:ALA:O	13:a:152:ASN:C	2.62	0.43
14:b:8:PHE:CE2	14:b:13:ILE:HG13	2.52	0.43
2:B:175:LEU:C	2:B:177:MET:H	2.26	0.43
10:J:198:GLN:OXT	10:J:198:GLN:HG2	2.18	0.43
11:K:40:PHE:HB3	11:K:73:ARG:HH21	1.83	0.43
12:L:147:MET:CE	9:W:176:ARG:NH2	2.81	0.43
7:U:74:VAL:HG11	7:U:81:ALA:HB2	2.01	0.43
7:U:83:ASN:C	7:U:83:ASN:HD22	2.27	0.43
8:V:4:VAL:HG22	8:V:159:ILE:CD1	2.42	0.43
10:X:149:ARG:HA	10:X:150:PRO:HD3	1.89	0.43
11:Y:4:LEU:CD1	11:Y:15:ALA:HB3	2.48	0.43
11:Y:76:VAL:N	11:Y:108:GLU:OE2	2.52	0.43
12:Z:10:GLY:HA3	12:Z:42:LYS:NZ	2.34	0.43
1:A:66:LEU:C	1:A:66:LEU:CD2	2.91	0.42
2:B:148:TYR:OH	3:C:57:ILE:HB	2.19	0.42
2:B:213:ALA:HA	2:B:227:LYS:O	2.19	0.42
2:B:229:PHE:N	2:B:229:PHE:CD2	2.86	0.42
2:B:243:ILE:O	2:B:243:ILE:HG22	2.17	0.42
4:D:77:ALA:O	4:D:81:ILE:HG12	2.19	0.42
11:K:191:HIS:N	11:K:191:HIS:CD2	2.86	0.42
13:M:17:ASP:OD1	13:M:18:ASN:N	2.52	0.42
14:N:96:GLY:C	14:N:97:ILE:HD12	2.44	0.42
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.00	0.42
4:R:23:ILE:HD13	4:R:133:ALA:HB2	2.01	0.42
5:S:181:ILE:O	5:S:181:ILE:HG22	2.19	0.42
13:a:17:ASP:OD1	13:a:18:ASN:N	2.52	0.42
13:a:25:ASP:C	13:a:25:ASP:OD2	2.62	0.42
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.52	0.42
2:B:41:ASP:CG	2:B:185:VAL:HG23	2.44	0.42
8:H:139:GLU:OE1	13:a:187:ARG:NH1	2.52	0.42
13:M:25:ASP:HA	13:M:195:PHE:HA	2.00	0.42
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.54	0.42
1:O:29:LYS:NZ	1:O:168:SER:OG	2.51	0.42
1:O:66:LEU:C	1:O:66:LEU:CD2	2.92	0.42
1:O:183:LEU:HD23	1:O:187:ASP:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:214:ILE:HD11	1:O:235:PHE:HD1	1.84	0.42
3:Q:182:PRO:O	3:Q:183:PRO:C	2.60	0.42
6:T:214:TRP:CH2	6:T:219:GLU:HB3	2.54	0.42
12:Z:109:THR:CG2	16:Z:309:HOH:O	2.62	0.42
1:A:203:GLU:HA	1:A:203:GLU:OE2	2.18	0.42
5:E:1:PHE:CG	5:E:2:ARG:N	2.87	0.42
5:E:178:PHE:HA	5:E:181:ILE:CG1	2.46	0.42
8:H:172:ASN:ND2	8:H:172:ASN:N	2.66	0.42
9:I:94:LEU:HD12	9:I:127:GLY:HA2	2.01	0.42
9:I:186:VAL:HG21	9:I:199:LEU:HD11	2.01	0.42
11:K:43:GLY:HA2	11:K:100:MET:O	2.19	0.42
12:L:126:ASP:C	12:L:128:VAL:N	2.76	0.42
1:O:234:ARG:HG2	1:O:234:ARG:HH11	1.84	0.42
4:R:155:THR:CG2	5:S:78:PRO:HD3	2.49	0.42
6:T:171:GLU:HB3	6:T:195:ILE:CD1	2.49	0.42
12:Z:174:TYR:CD1	12:Z:175:LEU:N	2.86	0.42
5:E:170:TYR:CE2	5:E:195:ALA:HB2	2.54	0.42
6:F:9:SER:HB2	7:G:126:ARG:HD3	2.01	0.42
7:G:56:ASP:OD2	7:G:56:ASP:C	2.62	0.42
7:G:74:VAL:HG11	7:G:81:ALA:HB2	2.02	0.42
8:H:215:GLU:HG3	9:I:197:ARG:HG2	2.01	0.42
9:I:147:GLY:HA3	12:Z:145:LEU:O	2.19	0.42
10:J:49:GLU:HB2	10:J:99:GLN:HB2	2.01	0.42
12:L:199:GLY:O	12:L:200:ASP:HB2	2.19	0.42
13:M:9:THR:OG1	13:M:10:SER:N	2.52	0.42
2:P:41:ASP:CG	2:P:185:VAL:HG23	2.44	0.42
2:P:139:TYR:CD1	2:P:139:TYR:C	2.96	0.42
3:Q:39:CYS:HA	3:Q:136:PHE:HZ	1.84	0.42
3:Q:158:SER:HB3	3:Q:177:TYR:CE1	2.55	0.42
4:R:4:VAL:HG23	4:R:116:GLY:HA2	2.01	0.42
7:U:106:ASP:OD2	7:U:106:ASP:N	2.52	0.42
10:X:35:THR:HG21	10:X:182:LYS:NZ	2.35	0.42
11:Y:115:VAL:HA	11:Y:120:THR:O	2.19	0.42
12:Z:105:TYR:O	12:Z:107:VAL:N	2.51	0.42
1:A:128:ARG:HH11	1:A:128:ARG:HG3	1.84	0.42
1:A:180:ASN:H	1:A:183:LEU:CD1	2.31	0.42
2:B:4:ARG:HD2	2:B:5:TYR:CZ	2.55	0.42
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.55	0.42
4:D:196:LEU:O	4:D:200:MET:HG3	2.19	0.42
6:F:214:TRP:N	6:F:214:TRP:CD1	2.88	0.42
7:G:29:THR:O	7:G:31:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:75:ARG:HG3	16:H:318:HOH:O	2.19	0.42
10:J:110:LYS:HB2	10:J:110:LYS:NZ	2.33	0.42
13:M:151:ALA:O	13:M:152:ASN:C	2.63	0.42
14:N:133:PHE:HA	14:b:132:THR:O	2.19	0.42
2:P:234:ILE:O	2:P:238:LEU:HB2	2.19	0.42
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.02	0.42
7:U:12:PRO:HD3	16:U:326:HOH:O	2.18	0.42
12:Z:177:VAL:O	12:Z:181:ILE:HG13	2.20	0.42
14:b:133:PHE:CE2	14:b:166:ASP:HB2	2.54	0.42
1:A:30:GLN:CA	1:A:30:GLN:NE2	2.81	0.42
1:A:204:PHE:CZ	1:A:209:ILE:HD11	2.55	0.42
4:D:180:HIS:H	4:D:183:LEU:CD1	2.32	0.42
5:E:36:GLY:O	5:E:157:GLY:HA2	2.19	0.42
5:E:41:THR:HG23	5:E:182:ASP:HB3	2.01	0.42
5:E:170:TYR:HB2	5:E:198:GLN:HG2	2.00	0.42
6:F:171:GLU:HB3	6:F:195:ILE:CD1	2.50	0.42
9:I:117:LYS:HA	9:I:118:PRO:HD3	1.88	0.42
10:J:5:LEU:HB2	10:J:16:ALA:HB3	2.02	0.42
1:O:134:LEU:O	1:O:149:GLN:HA	2.20	0.42
1:O:211:LEU:HD23	1:O:211:LEU:C	2.45	0.42
4:R:6:THR:CG2	4:R:7:PHE:N	2.83	0.42
4:R:9:PRO:HG3	5:S:23:TYR:HE2	1.82	0.42
5:S:39:SER:HB3	5:S:188:LEU:HD11	2.02	0.42
6:T:39:ASN:N	6:T:39:ASN:ND2	2.68	0.42
6:T:103:ILE:HA	6:T:104:PRO:HD3	1.84	0.42
7:U:29:THR:O	7:U:31:ILE:HG13	2.20	0.42
10:X:49:GLU:HB2	10:X:99:GLN:HB2	2.01	0.42
10:X:184:VAL:HG22	10:X:189:ILE:HD12	2.01	0.42
11:Y:174:SER:HA	11:Y:193:VAL:HG23	2.01	0.42
11:Y:201:LYS:HE3	11:Y:207:PHE:O	2.20	0.42
2:B:17:ARG:HG2	2:B:17:ARG:HH11	1.84	0.42
3:C:107:LEU:O	3:C:107:LEU:HD13	2.19	0.42
3:C:146:TYR:CE1	3:C:156:SER:HB3	2.54	0.42
4:D:23:ILE:HD13	4:D:133:ALA:HB2	2.02	0.42
4:D:59:ILE:HG22	4:D:220:PHE:HZ	1.85	0.42
4:D:195:ILE:O	4:D:199:VAL:HG22	2.20	0.42
7:G:66:ILE:HG21	7:G:108:LEU:HD21	2.01	0.42
7:G:103:MET:HE3	7:G:108:LEU:HD13	2.01	0.42
12:L:52:MET:HE3	12:L:93:ILE:CD1	2.50	0.42
1:O:44:VAL:CG2	1:O:211:LEU:HD21	2.50	0.42
3:Q:106:TYR:CD2	3:Q:106:TYR:C	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:178:GLU:HB3	4:R:191:LEU:HD21	2.02	0.42
7:U:6:HIS:N	7:U:6:HIS:CD2	2.88	0.42
8:V:215:GLU:HG3	9:W:197:ARG:HG2	2.00	0.42
9:W:145:LEU:HD23	9:W:145:LEU:HA	1.88	0.42
10:X:198:GLN:OXT	10:X:198:GLN:HG2	2.20	0.42
11:Y:4:LEU:HD22	11:Y:4:LEU:O	2.19	0.42
14:b:147:SER:O	14:b:148:LYS:C	2.62	0.42
5:E:131:LEU:HB2	5:E:146:PHE:HB3	2.01	0.42
5:E:178:PHE:C	5:E:180:LYS:H	2.28	0.42
9:I:65:MET:O	9:I:68:TYR:HB3	2.20	0.42
9:I:115:SER:C	9:I:117:LYS:H	2.28	0.42
11:K:116:ASP:OD1	11:K:116:ASP:C	2.60	0.42
12:L:23:LEU:HD13	12:L:43:VAL:HG13	2.01	0.42
12:L:163:GLY:C	12:L:165:ASN:H	2.28	0.42
14:N:76:GLU:HB2	16:N:211:HOH:O	2.19	0.42
1:O:57:MET:HE3	1:O:60:THR:CG2	2.48	0.42
2:P:4:ARG:HD2	2:P:5:TYR:CZ	2.55	0.42
2:P:61:SER:O	2:P:62:THR:OG1	2.29	0.42
2:P:228:ILE:HD12	2:P:228:ILE:H	1.83	0.42
4:R:171:ALA:O	4:R:174:GLU:HB3	2.20	0.42
5:S:35:VAL:HG23	5:S:196:ILE:CD1	2.49	0.42
5:S:36:GLY:O	5:S:158:THR:N	2.48	0.42
8:V:175:VAL:HG12	8:V:176:CYS:N	2.35	0.42
10:X:165:VAL:O	10:X:169:GLU:HG3	2.20	0.42
10:X:172:MET:HA	10:X:173:PRO:HD3	1.70	0.42
12:Z:28:ARG:HB2	12:Z:200:ASP:HB2	2.01	0.42
12:Z:163:GLY:C	12:Z:165:ASN:H	2.27	0.42
13:a:19:GLY:HA3	13:a:200:ILE:O	2.20	0.42
13:a:45:VAL:HG11	13:a:92:ILE:CD1	2.49	0.42
13:a:213:GLN:HE21	13:a:213:GLN:HB3	1.59	0.42
14:b:143:ARG:O	14:b:146:MET:HG3	2.19	0.42
5:E:155:LEU:HD12	5:E:158:THR:HG21	2.02	0.42
10:J:150:PRO:CD	11:Y:208:ASN:ND2	2.83	0.42
11:K:82:ILE:HG13	16:K:334:HOH:O	2.20	0.42
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.44	0.42
16:N:228:HOH:O	13:a:233:ILE:CD1	2.68	0.42
3:Q:213:VAL:HG13	3:Q:213:VAL:O	2.20	0.42
3:Q:239:GLN:C	3:Q:241:GLN:H	2.28	0.42
4:R:9:PRO:HA	5:S:23:TYR:CE2	2.54	0.42
4:R:195:ILE:O	4:R:199:VAL:HG22	2.20	0.42
5:S:157:GLY:O	6:T:54:LEU:HD13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:170:TYR:CE2	5:S:195:ALA:HB2	2.54	0.42
5:S:189:ILE:O	5:S:193:VAL:HG23	2.20	0.42
5:S:216:GLY:O	5:S:217:LYS:C	2.62	0.42
7:U:135:VAL:O	7:U:136:SER:HB3	2.19	0.42
9:W:115:SER:C	9:W:117:LYS:H	2.27	0.42
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.93	0.42
2:B:183:MET:HE1	2:B:188:ALA:HA	2.02	0.42
3:C:225:GLU:OE1	3:C:225:GLU:N	2.52	0.42
5:E:39:SER:HB3	5:E:188:LEU:HD11	2.01	0.42
7:G:125:MET:HE3	16:G:332:HOH:O	2.19	0.42
8:H:124:TYR:O	8:H:125:LEU:HD23	2.20	0.42
8:H:214:LYS:CG	8:H:215:GLU:N	2.83	0.42
1:O:101:TYR:CE1	9:W:89:LEU:HD13	2.55	0.42
5:S:33:VAL:HG22	5:S:34:THR:N	2.34	0.42
5:S:35:VAL:HG13	5:S:159:ALA:HB2	2.02	0.42
7:U:66:ILE:HG21	7:U:108:LEU:HD21	2.02	0.42
9:W:170:LEU:CD2	9:W:184:ALA:HB1	2.48	0.42
2:B:139:TYR:CD1	2:B:139:TYR:C	2.98	0.41
5:E:23:TYR:N	5:E:23:TYR:CD1	2.88	0.41
9:I:171:LEU:HD11	9:I:201:MET:HB3	2.02	0.41
14:N:140:LYS:NZ	14:b:157:HIS:HD2	2.18	0.41
1:O:55:LEU:HD12	7:U:170:THR:HG23	2.02	0.41
1:O:187:ASP:O	1:O:191:ILE:HG13	2.20	0.41
2:P:8:ARG:HD2	3:Q:4:ARG:NH2	2.35	0.41
2:P:43:ILE:CG2	2:P:147:LEU:HD13	2.50	0.41
4:R:159:TYR:CD2	4:R:162:LYS:HB2	2.55	0.41
9:W:189:ILE:HG13	9:W:194:VAL:HG22	2.01	0.41
11:Y:7:ARG:HD2	11:Y:110:PRO:O	2.20	0.41
1:A:187:ASP:O	1:A:191:ILE:HG13	2.20	0.41
2:B:160:LYS:HB3	2:B:179:TYR:CZ	2.56	0.41
3:C:179:ARG:HH22	4:D:52:GLU:HA	1.85	0.41
4:D:42:VAL:HG22	4:D:59:ILE:HD11	2.03	0.41
5:E:46:VAL:HG13	5:E:212:ILE:HG12	2.03	0.41
5:E:178:PHE:O	5:E:181:ILE:HG13	2.20	0.41
7:G:83:ASN:ND2	7:G:83:ASN:C	2.78	0.41
7:G:222:ASP:O	7:G:223:LYS:HB2	2.18	0.41
9:I:189:ILE:HG13	9:I:194:VAL:HG22	2.01	0.41
10:J:12:SER:HB2	10:J:184:VAL:O	2.20	0.41
12:L:28:ARG:HB2	12:L:200:ASP:HB2	2.02	0.41
13:M:48:ASN:H	13:M:48:ASN:ND2	2.09	0.41
2:P:17:ARG:HG2	2:P:17:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:185:LEU:O	4:R:189:GLU:HG3	2.20	0.41
5:S:167:ALA:CB	5:S:195:ALA:O	2.67	0.41
7:U:72:MET:HE3	7:U:74:VAL:HG23	2.01	0.41
8:V:41:ILE:HD13	8:V:76:VAL:HA	2.00	0.41
8:V:196:ARG:NH2	9:W:150:GLU:O	2.53	0.41
9:W:62:LEU:HD23	9:W:62:LEU:HA	1.87	0.41
10:X:23:ARG:HA	10:X:23:ARG:HD3	1.86	0.41
11:Y:3:THR:HG21	16:Y:333:HOH:O	2.20	0.41
11:Y:4:LEU:HA	11:Y:127:PHE:O	2.20	0.41
12:Z:24:ALA:HB1	12:Z:202:LEU:HD11	2.00	0.41
12:Z:51:VAL:CG1	12:Z:205:LEU:HD23	2.50	0.41
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.55	0.41
13:a:3:GLN:O	13:a:3:GLN:HG3	2.19	0.41
13:a:93:PHE:CE1	13:a:128:ARG:HD3	2.54	0.41
1:A:187:ASP:O	1:A:190:HIS:HB3	2.20	0.41
8:H:188:ARG:O	8:H:189:ASN:HB2	2.20	0.41
9:I:62:LEU:CD1	9:I:104:VAL:HG21	2.51	0.41
10:J:149:ARG:HG2	10:J:149:ARG:NH1	2.35	0.41
11:K:37:ILE:HD13	11:K:59:LEU:HD23	2.01	0.41
11:K:115:VAL:HA	11:K:120:THR:O	2.20	0.41
1:O:59:GLU:H	1:O:59:GLU:CD	2.27	0.41
2:P:160:LYS:HB3	2:P:179:TYR:CZ	2.55	0.41
4:R:64:ARG:O	4:R:64:ARG:HG2	2.20	0.41
5:S:131:LEU:HD12	5:S:146:PHE:CD2	2.56	0.41
9:W:14:MET:HE3	9:W:166:ILE:CG1	2.34	0.41
10:X:119:ILE:HG12	10:X:125:LYS:HG3	2.02	0.41
1:A:250:LEU:HD13	1:A:250:LEU:C	2.45	0.41
3:C:70:VAL:HG13	3:C:219:ILE:HD13	2.03	0.41
3:C:157:TRP:CZ2	4:D:51:LEU:HD23	2.55	0.41
3:C:160:GLN:CG	3:C:161:THR:N	2.83	0.41
5:E:167:ALA:CB	5:E:195:ALA:O	2.67	0.41
6:F:214:TRP:CH2	6:F:219:GLU:HB3	2.55	0.41
7:G:153:TYR:CD1	7:G:153:TYR:C	2.99	0.41
7:G:166:GLN:NE2	7:G:167:GLN:N	2.68	0.41
10:J:174:MET:HE3	10:X:174:MET:HG2	2.00	0.41
2:P:183:MET:HE1	2:P:188:ALA:HA	2.01	0.41
2:P:240:LYS:C	2:P:242:GLY:H	2.29	0.41
3:Q:88:ARG:NH1	16:Q:304:HOH:O	2.40	0.41
3:Q:109:ARG:HD3	3:Q:154:TYR:OH	2.20	0.41
3:Q:178:ASP:OD1	3:Q:180:LYS:HB2	2.21	0.41
6:T:148:GLU:HB3	16:T:336:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:42:THR:HG21	7:U:135:VAL:HB	2.02	0.41
8:V:3:ILE:O	8:V:126:SER:HA	2.20	0.41
11:Y:4:LEU:HD11	11:Y:161:ILE:HG12	2.02	0.41
13:a:85:GLU:HA	13:a:85:GLU:OE2	2.19	0.41
1:A:57:MET:HE3	1:A:60:THR:CG2	2.49	0.41
2:B:24:ALA:O	2:B:27:SER:HB3	2.21	0.41
3:C:11:PRO:HA	4:D:18:TYR:CE1	2.54	0.41
3:C:178:ASP:OD1	3:C:180:LYS:HB2	2.21	0.41
5:E:174:THR:HG22	5:E:174:THR:O	2.20	0.41
5:E:189:ILE:CG2	5:E:212:ILE:HD13	2.44	0.41
6:F:200:HIS:O	6:F:200:HIS:CG	2.74	0.41
7:G:68:ARG:HH11	7:G:68:ARG:CB	2.32	0.41
7:G:103:MET:HE1	7:G:108:LEU:HD13	2.02	0.41
4:R:73:LEU:HD12	4:R:131:GLY:HA3	2.03	0.41
4:R:205:ASP:O	4:R:207:ASN:N	2.54	0.41
6:T:68:ARG:NH1	13:a:72:THR:OG1	2.54	0.41
6:T:126:ARG:HG2	6:T:126:ARG:NH1	2.35	0.41
6:T:191:GLN:O	6:T:194:LYS:HB3	2.20	0.41
9:W:171:LEU:HD11	9:W:201:MET:HB3	2.02	0.41
1:A:183:LEU:HD23	1:A:187:ASP:HB3	2.01	0.41
3:C:1:GLY:N	16:C:329:HOH:O	2.48	0.41
4:D:73:LEU:HD12	4:D:131:GLY:HA3	2.03	0.41
4:D:205:ASP:O	4:D:207:ASN:N	2.54	0.41
4:D:228:THR:HG22	4:D:232:ILE:HD13	2.02	0.41
4:D:236:LYS:HE2	4:D:236:LYS:HB3	1.91	0.41
7:G:24:LYS:HD2	7:G:24:LYS:HA	1.80	0.41
10:J:8:ARG:HG2	10:J:8:ARG:NH1	2.34	0.41
10:J:158:LEU:HD21	10:J:183:ILE:HD11	2.03	0.41
12:L:216:PHE:C	12:L:217:TYR:CD1	2.99	0.41
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.02	0.41
3:Q:70:VAL:HG13	3:Q:219:ILE:HD13	2.02	0.41
5:S:23:TYR:N	5:S:23:TYR:CD1	2.88	0.41
5:S:178:PHE:C	5:S:180:LYS:H	2.28	0.41
7:U:224:PHE:CD1	7:U:224:PHE:C	2.98	0.41
11:Y:77:ALA:HA	11:Y:113:TYR:CE2	2.55	0.41
13:a:1:THR:N	13:a:107:MET:O	2.46	0.41
2:B:46:ALA:HB2	2:B:212:PHE:CE1	2.55	0.41
3:C:106:TYR:CD2	3:C:106:TYR:C	2.98	0.41
5:E:178:PHE:C	5:E:180:LYS:N	2.77	0.41
16:G:308:HOH:O	8:H:82:MET:HA	2.19	0.41
10:J:184:VAL:HG22	10:J:189:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:154:VAL:O	12:L:154:VAL:HG12	2.20	0.41
13:M:159:VAL:HG11	13:M:165:ILE:HD13	2.03	0.41
2:P:65:LEU:HD23	2:P:213:ALA:HB2	2.02	0.41
2:P:120:GLY:C	2:P:122:THR:N	2.77	0.41
5:S:72:SER:OG	5:S:132:LEU:HB2	2.21	0.41
5:S:174:THR:HG22	5:S:174:THR:O	2.21	0.41
7:U:103:MET:HA	7:U:104:PRO:HD3	1.94	0.41
10:X:37:GLN:HG3	10:X:189:ILE:HG13	2.03	0.41
11:Y:159:ARG:O	11:Y:162:LEU:HB3	2.21	0.41
12:Z:115:ASP:OD2	12:Z:119:LYS:HB2	2.20	0.41
13:a:1:THR:HG22	13:a:2:GLN:N	2.36	0.41
1:A:139:HIS:HA	1:A:144:GLY:O	2.21	0.41
2:B:63:GLU:HG3	2:B:64:LYS:HG3	2.02	0.41
2:B:134:PHE:O	2:B:149:THR:HA	2.21	0.41
3:C:239:GLN:C	3:C:241:GLN:H	2.28	0.41
4:D:235:LEU:C	4:D:235:LEU:HD13	2.45	0.41
5:E:35:VAL:HG13	5:E:159:ALA:HB2	2.03	0.41
5:E:226:GLY:C	5:E:228:ALA:N	2.76	0.41
6:F:86:ASN:HD22	6:F:86:ASN:HA	1.65	0.41
9:I:14:MET:HE3	9:I:166:ILE:HA	2.01	0.41
9:I:148:MET:CE	9:I:172:ASN:HB2	2.40	0.41
10:J:172:MET:CE	10:J:174:MET:HB2	2.51	0.41
13:M:1:THR:N	13:M:107:MET:O	2.49	0.41
2:B:65:LEU:HD23	2:B:213:ALA:HB2	2.03	0.41
3:C:51:LYS:HD2	3:C:52:LEU:H	1.82	0.41
3:C:92:GLN:HG3	10:J:66:LEU:HB2	2.03	0.41
3:C:158:SER:HB3	3:C:177:TYR:CE1	2.56	0.41
4:D:6:THR:CG2	4:D:7:PHE:N	2.83	0.41
4:D:193:LEU:HD12	4:D:193:LEU:HA	1.82	0.41
5:E:35:VAL:HG23	5:E:196:ILE:CD1	2.51	0.41
5:E:126:PRO:HA	16:E:303:HOH:O	2.20	0.41
5:E:181:ILE:HG22	5:E:181:ILE:O	2.21	0.41
5:E:189:ILE:O	5:E:193:VAL:HG23	2.20	0.41
7:G:6:HIS:CD2	7:G:6:HIS:N	2.87	0.41
7:G:73:VAL:CG1	7:G:133:THR:HB	2.51	0.41
10:J:25:ILE:O	10:X:139:TYR:OH	2.39	0.41
11:K:144:TYR:CD1	11:K:144:TYR:C	2.98	0.41
13:M:54:SER:HG	13:M:113:ALA:HB3	1.85	0.41
13:M:170:VAL:HG23	16:M:323:HOH:O	2.21	0.41
14:N:146:MET:HE2	14:N:150:GLU:HB3	2.03	0.41
14:N:193:TYR:CD1	14:N:193:TYR:C	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:176:GLN:HG2	2:P:176:GLN:O	2.21	0.41
4:R:38:VAL:HB	4:R:214:ILE:CG2	2.51	0.41
5:S:93:TYR:CE1	5:S:97:VAL:HG21	2.56	0.41
5:S:226:GLY:C	5:S:228:ALA:N	2.77	0.41
7:U:239:ILE:C	7:U:239:ILE:CD1	2.92	0.41
8:V:128:GLY:O	8:V:131:SER:HB2	2.20	0.41
9:W:104:VAL:HG23	9:W:106:PRO:HD3	2.02	0.41
9:W:186:VAL:HG21	9:W:199:LEU:HD11	2.03	0.41
10:X:26:SER:HB2	11:Y:133:GLN:NE2	2.34	0.41
11:Y:37:ILE:HD13	11:Y:59:LEU:HD23	2.02	0.41
11:Y:106:ARG:HD3	11:Y:182:GLU:OE1	2.21	0.41
12:Z:2:PHE:CB	13:a:1:THR:HG23	2.51	0.41
12:Z:213:ARG:HH11	12:Z:213:ARG:CB	2.33	0.41
2:B:2:SER:O	2:B:4:ARG:N	2.54	0.41
2:B:93:HIS:CE1	2:B:113:ARG:HD3	2.56	0.41
3:C:103:THR:N	16:C:306:HOH:O	2.48	0.41
7:G:167:GLN:HB3	16:G:339:HOH:O	2.21	0.41
8:H:3:ILE:O	8:H:126:SER:HA	2.20	0.41
12:L:10:GLY:N	16:L:330:HOH:O	2.54	0.41
12:L:36:ASN:HB3	13:M:137:TYR:CZ	2.56	0.41
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.56	0.41
12:L:126:ASP:OD2	15:d:2:THR:HG23	2.20	0.41
12:L:195:HIS:CD2	12:L:197:GLN:HB2	2.56	0.41
1:O:3:ASP:OD2	1:O:5:TYR:HB2	2.21	0.41
4:R:17:GLU:O	4:R:20:LEU:HB2	2.21	0.41
5:S:12:PHE:N	6:T:19:GLN:HE22	2.18	0.41
6:T:27:VAL:HG13	6:T:75:SER:O	2.21	0.41
6:T:91:GLU:HG2	6:T:111:ARG:CB	2.35	0.41
9:W:163:PHE:CD2	9:W:163:PHE:C	2.99	0.41
10:X:33:ASP:CG	10:X:35:THR:HG22	2.46	0.41
10:X:103:LEU:HD21	10:X:118:GLN:HG3	2.02	0.41
10:X:140:THR:HG22	10:X:164:CYS:HB3	2.03	0.41
3:C:155:SER:HB2	4:D:51:LEU:HD21	2.03	0.40
3:C:210:ILE:CG2	3:C:211:THR:N	2.84	0.40
4:D:78:ARG:HD3	4:D:78:ARG:HA	1.92	0.40
5:E:33:VAL:HG22	5:E:34:THR:N	2.36	0.40
8:H:147:THR:HG23	8:H:150:GLU:OE1	2.21	0.40
10:J:103:LEU:HD23	10:J:103:LEU:HA	1.77	0.40
11:K:77:ALA:HA	11:K:113:TYR:CE2	2.56	0.40
12:L:2:PHE:CB	13:M:1:THR:HG23	2.51	0.40
12:L:10:GLY:HA3	12:L:42:LYS:NZ	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:52:MET:HG2	12:L:53:SER:N	2.36	0.40
2:P:24:ALA:O	2:P:27:SER:HB3	2.21	0.40
2:P:46:ALA:HB2	2:P:212:PHE:CE1	2.56	0.40
2:P:95:GLN:NE2	16:P:307:HOH:O	2.53	0.40
2:P:213:ALA:HA	2:P:227:LYS:O	2.20	0.40
3:Q:105:GLU:HB3	16:Q:305:HOH:O	2.21	0.40
3:Q:160:GLN:CG	3:Q:161:THR:N	2.83	0.40
4:R:228:THR:HG22	4:R:232:ILE:HD13	2.03	0.40
6:T:86:ASN:HD22	6:T:86:ASN:HA	1.67	0.40
6:T:200:HIS:O	6:T:200:HIS:CG	2.74	0.40
8:V:10:ASN:HD22	8:V:179:GLU:HG2	1.86	0.40
9:W:30:SER:O	9:W:31:GLN:HB2	2.22	0.40
11:Y:201:LYS:HG2	16:Y:326:HOH:O	2.21	0.40
13:a:45:VAL:HG11	13:a:92:ILE:HD13	2.04	0.40
1:A:167:GLY:HA2	16:A:317:HOH:O	2.22	0.40
1:A:196:LEU:HD12	1:A:196:LEU:HA	1.88	0.40
2:B:228:ILE:HD12	2:B:228:ILE:H	1.84	0.40
5:E:188:LEU:HD23	5:E:188:LEU:HA	1.90	0.40
8:H:3:ILE:HD13	8:H:127:LEU:O	2.21	0.40
9:I:145:LEU:HD23	9:I:145:LEU:HA	1.88	0.40
10:J:4:ILE:HG22	10:J:103:LEU:CD1	2.51	0.40
11:K:38:ASN:HB2	11:K:39:PRO:HD2	2.02	0.40
11:K:65:LEU:O	11:K:69:ARG:HB2	2.22	0.40
11:K:114:TYR:O	11:K:121:ARG:HA	2.21	0.40
11:K:140:LEU:HD13	11:K:160:SER:OG	2.21	0.40
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.56	0.40
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.04	0.40
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.55	0.40
5:S:184:ASN:HA	5:S:185:PRO:HD2	1.96	0.40
5:S:216:GLY:O	5:S:218:ASP:N	2.54	0.40
6:T:117:GLN:NE2	6:T:117:GLN:C	2.80	0.40
9:W:14:MET:HE3	9:W:166:ILE:HA	2.04	0.40
10:X:110:LYS:HB2	10:X:110:LYS:HZ3	1.87	0.40
10:X:161:LEU:O	10:X:162:LYS:C	2.62	0.40
13:a:132:LEU:HD23	13:a:132:LEU:N	2.36	0.40
3:C:39:CYS:HA	3:C:136:PHE:HZ	1.87	0.40
3:C:213:VAL:O	3:C:213:VAL:HG13	2.20	0.40
4:D:169:GLU:N	4:D:169:GLU:OE1	2.55	0.40
6:F:191:GLN:NE2	6:F:194:LYS:HE2	2.37	0.40
7:G:149:ASP:HB2	7:G:150:PRO:HD2	2.02	0.40
9:I:146:PHE:O	9:I:150:GLU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:53:THR:HG23	10:J:54:VAL:H	1.83	0.40
11:K:20:ALA:CB	11:K:31:VAL:HG21	2.49	0.40
11:K:70:GLU:O	11:K:71:LYS:C	2.63	0.40
14:N:147:SER:O	14:N:148:LYS:C	2.62	0.40
2:P:134:PHE:O	2:P:149:THR:HA	2.21	0.40
5:S:23:TYR:N	5:S:23:TYR:HD1	2.19	0.40
5:S:178:PHE:O	5:S:181:ILE:HG13	2.21	0.40
7:U:153:TYR:CD1	7:U:153:TYR:C	2.99	0.40
8:V:3:ILE:HD13	8:V:127:LEU:O	2.21	0.40
8:V:75:ARG:HA	8:V:104:ASP:OD1	2.21	0.40
9:W:154:GLU:CG	9:W:157:LEU:HD21	2.51	0.40
10:X:23:ARG:NE	16:X:222:HOH:O	2.42	0.40
13:a:53:ILE:HD12	13:a:60:MET:HG3	2.03	0.40
13:a:94:GLU:OE2	13:a:94:GLU:HA	2.21	0.40
1:A:234:ARG:HG2	1:A:234:ARG:HH11	1.87	0.40
2:B:72:ILE:C	2:B:226:GLN:HE22	2.29	0.40
2:B:88:ASN:O	2:B:92:ILE:HG12	2.22	0.40
2:B:230:LYS:O	2:B:231:PRO:C	2.64	0.40
4:D:210:GLN:HA	16:D:318:HOH:O	2.21	0.40
5:E:193:VAL:C	5:E:196:ILE:HG22	2.46	0.40
6:F:9:SER:HB3	6:F:121:LEU:C	2.46	0.40
6:F:14:ASP:OD1	6:F:16:ARG:HD3	2.21	0.40
9:I:20:VAL:CG2	9:I:189:ILE:HB	2.52	0.40
11:K:7:ARG:HD2	11:K:110:PRO:O	2.22	0.40
14:N:114:PRO:HA	16:N:220:HOH:O	2.21	0.40
1:O:35:LEU:HD12	1:O:35:LEU:C	2.46	0.40
1:O:204:PHE:CD1	1:O:209:ILE:HD11	2.55	0.40
3:Q:225:GLU:N	3:Q:225:GLU:OE1	2.54	0.40
5:S:44:VAL:HG12	5:S:45:LEU:N	2.36	0.40
5:S:46:VAL:HG13	5:S:212:ILE:HG12	2.02	0.40
7:U:155:VAL:HG13	7:U:157:TYR:CE1	2.57	0.40
7:U:176:HIS:ND1	7:U:176:HIS:C	2.79	0.40
9:W:68:TYR:CD1	9:W:68:TYR:C	3.00	0.40
9:W:125:LEU:HD21	15:e:1:MH9:H3	2.03	0.40
10:X:19:LYS:HG2	10:X:180:ILE:HG13	2.04	0.40
12:Z:103:PHE:N	12:Z:104:PRO:CD	2.82	0.40
3:C:224:SER:HB2	3:C:225:GLU:OE1	2.22	0.40
5:E:131:LEU:HD12	5:E:146:PHE:CD2	2.56	0.40
6:F:220:THR:O	6:F:221:ASN:CB	2.69	0.40
12:L:94:GLN:HG3	12:L:129:GLY:O	2.21	0.40
13:M:27:LEU:HD11	13:M:34:LEU:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:59:GLU:C	1:O:61:LEU:N	2.79	0.40
3:Q:82:ILE:N	3:Q:82:ILE:CD1	2.85	0.40
5:S:106:ARG:HG2	5:S:106:ARG:NH1	2.35	0.40
5:S:131:LEU:HB2	5:S:146:PHE:HB3	2.02	0.40
5:S:205:LEU:HA	5:S:209:ASN:HD21	1.83	0.40
10:X:158:LEU:HD21	10:X:183:ILE:HD11	2.02	0.40
13:a:165:ILE:HB	13:a:166:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	226 (91%)	18 (7%)	4 (2%)	7	34
1	O	248/250 (99%)	224 (90%)	20 (8%)	4 (2%)	7	34
2	B	242/244 (99%)	213 (88%)	21 (9%)	8 (3%)	3	17
2	P	242/244 (99%)	212 (88%)	23 (10%)	7 (3%)	3	20
3	C	239/241 (99%)	214 (90%)	20 (8%)	5 (2%)	5	27
3	Q	239/241 (99%)	215 (90%)	19 (8%)	5 (2%)	5	27
4	D	240/242 (99%)	212 (88%)	19 (8%)	9 (4%)	2	15
4	R	240/242 (99%)	212 (88%)	19 (8%)	9 (4%)	2	15
5	E	231/233 (99%)	202 (87%)	21 (9%)	8 (4%)	3	16
5	S	231/233 (99%)	202 (87%)	22 (10%)	7 (3%)	3	19
6	F	242/244 (99%)	224 (93%)	16 (7%)	2 (1%)	16	50
6	T	242/244 (99%)	223 (92%)	17 (7%)	2 (1%)	16	50
7	G	241/243 (99%)	219 (91%)	19 (8%)	3 (1%)	10	40
7	U	241/243 (99%)	218 (90%)	20 (8%)	3 (1%)	10	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	220/222 (99%)	197 (90%)	20 (9%)	3 (1%)	9	36
8	V	220/222 (99%)	195 (89%)	22 (10%)	3 (1%)	9	36
9	I	202/204 (99%)	185 (92%)	14 (7%)	3 (2%)	8	35
9	W	202/204 (99%)	185 (92%)	15 (7%)	2 (1%)	12	45
10	J	196/198 (99%)	183 (93%)	10 (5%)	3 (2%)	8	35
10	X	196/198 (99%)	182 (93%)	11 (6%)	3 (2%)	8	35
11	K	210/212 (99%)	199 (95%)	11 (5%)	0	100	100
11	Y	210/212 (99%)	199 (95%)	11 (5%)	0	100	100
12	L	220/222 (99%)	199 (90%)	16 (7%)	5 (2%)	5	25
12	Z	220/222 (99%)	202 (92%)	14 (6%)	4 (2%)	6	31
13	M	231/233 (99%)	206 (89%)	24 (10%)	1 (0%)	30	65
13	a	231/233 (99%)	206 (89%)	24 (10%)	1 (0%)	30	65
14	N	194/196 (99%)	183 (94%)	10 (5%)	1 (0%)	24	60
14	b	194/196 (99%)	183 (94%)	9 (5%)	2 (1%)	12	45
15	c	1/4 (25%)	1 (100%)	0	0	100	100
15	d	1/4 (25%)	1 (100%)	0	0	100	100
15	e	1/4 (25%)	1 (100%)	0	0	100	100
15	f	1/4 (25%)	1 (100%)	0	0	100	100
All	All	6316/6384 (99%)	5724 (91%)	485 (8%)	107 (2%)	7	32

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	62	THR
2	B	221	ASP
3	C	52	LEU
4	D	122	GLU
5	E	2	ARG
5	E	201	ARG
5	E	217	LYS
6	F	8	ASN
6	F	9	SER
7	G	242	GLN
12	L	81	ASP
2	P	51	VAL

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Mol	Chain	Res	Type
2	P	62	THR
2	P	221	ASP
3	Q	52	LEU
4	R	122	GLU
5	S	2	ARG
5	S	201	ARG
5	S	217	LYS
6	T	8	ASN
6	T	9	SER
7	U	242	GLN
12	Z	81	ASP
2	B	3	ARG
2	B	218	GLY
3	C	203	THR
4	D	53	SER
4	D	126	MET
4	D	181	SER
4	D	206	GLU
5	E	175	LEU
5	E	176	ASP
9	I	191	LYS
10	J	193	ASP
10	J	197	ALA
12	L	164	THR
2	P	3	ARG
2	P	218	GLY
3	Q	203	THR
4	R	53	SER
4	R	126	MET
4	R	181	SER
4	R	206	GLU
5	S	175	LEU
5	S	176	ASP
8	V	9	ASN
8	V	91	GLN
9	W	191	LYS
10	X	193	ASP
10	X	197	ALA
12	Z	164	THR
14	b	191	ASP
1	A	60	THR
3	C	202	GLN

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Mol	Chain	Res	Type
3	C	224	SER
4	D	2	ARG
5	E	227	GLU
8	H	9	ASN
8	H	91	GLN
8	H	105	PRO
12	L	103	PHE
14	N	191	ASP
1	O	2	THR
1	O	60	THR
3	Q	202	GLN
4	R	2	ARG
8	V	105	PRO
12	Z	209	LYS
1	A	2	THR
2	B	183	MET
5	E	221	PHE
10	J	9	VAL
12	L	209	LYS
3	Q	224	SER
5	S	221	PHE
10	X	9	VAL
12	Z	103	PHE
13	a	111	TRP
1	A	166	LYS
2	B	243	ILE
4	D	112	ALA
4	D	118	GLY
7	G	51	PRO
7	G	184	HIS
9	I	116	GLY
12	L	26	ASP
13	M	111	TRP
1	O	19	GLY
1	O	166	LYS
2	P	243	ILE
4	R	112	ALA
4	R	118	GLY
5	S	227	GLU
7	U	51	PRO
7	U	184	HIS
9	W	116	GLY

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Mol	Chain	Res	Type
1	A	19	GLY
4	D	121	GLY
5	E	186	ASP
4	R	121	GLY
14	b	145	ASN
3	C	183	PRO
3	Q	183	PRO
9	I	155	PRO
2	B	185	VAL
2	P	185	VAL

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	209/209 (100%)	200 (96%)	9 (4%)	26	60
1	O	209/209 (100%)	200 (96%)	9 (4%)	26	60
2	B	203/203 (100%)	195 (96%)	8 (4%)	28	62
2	P	203/203 (100%)	195 (96%)	8 (4%)	28	62
3	C	213/213 (100%)	208 (98%)	5 (2%)	44	74
3	Q	213/213 (100%)	208 (98%)	5 (2%)	44	74
4	D	198/198 (100%)	187 (94%)	11 (6%)	19	52
4	R	198/198 (100%)	188 (95%)	10 (5%)	21	55
5	E	192/192 (100%)	176 (92%)	16 (8%)	10	37
5	S	192/192 (100%)	176 (92%)	16 (8%)	10	37
6	F	201/201 (100%)	188 (94%)	13 (6%)	15	47
6	T	201/201 (100%)	187 (93%)	14 (7%)	14	44
7	G	207/207 (100%)	198 (96%)	9 (4%)	26	60
7	U	207/207 (100%)	198 (96%)	9 (4%)	26	60
8	H	181/181 (100%)	172 (95%)	9 (5%)	22	56
8	V	181/181 (100%)	172 (95%)	9 (5%)	22	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	172/172 (100%)	167 (97%)	5 (3%)	37	70
9	W	172/172 (100%)	166 (96%)	6 (4%)	32	65
10	J	175/175 (100%)	169 (97%)	6 (3%)	32	66
10	X	175/175 (100%)	170 (97%)	5 (3%)	37	70
11	K	169/169 (100%)	161 (95%)	8 (5%)	23	58
11	Y	169/169 (100%)	161 (95%)	8 (5%)	23	58
12	L	185/185 (100%)	176 (95%)	9 (5%)	22	56
12	Z	185/185 (100%)	176 (95%)	9 (5%)	22	56
13	M	199/199 (100%)	187 (94%)	12 (6%)	17	50
13	a	199/199 (100%)	187 (94%)	12 (6%)	17	50
14	N	162/162 (100%)	155 (96%)	7 (4%)	26	60
14	b	162/162 (100%)	155 (96%)	7 (4%)	26	60
15	c	1/1 (100%)	1 (100%)	0	100	100
15	d	1/1 (100%)	1 (100%)	0	100	100
15	e	1/1 (100%)	1 (100%)	0	100	100
15	f	1/1 (100%)	1 (100%)	0	100	100
All	All	5336/5336 (100%)	5082 (95%)	254 (5%)	23	57

All (254) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	66	LEU
1	A	68	THR
1	A	122	THR
1	A	133	SER
1	A	157	PHE
1	A	169	VAL
1	A	178	ARG
1	A	183	LEU
2	B	38	MET
2	B	58	GLN
2	B	65	LEU
2	B	149	THR
2	B	157	THR
2	B	184	LYS

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Mol	Chain	Res	Type
2	B	191	LEU
2	B	212	PHE
3	C	4	ARG
3	C	22	LEU
3	C	51	LYS
3	C	147	GLN
3	C	225	GLU
4	D	20	LEU
4	D	40	LEU
4	D	44	LYS
4	D	68	CYS
4	D	124	ARG
4	D	169	GLU
4	D	176	LEU
4	D	183	LEU
4	D	193	LEU
4	D	214	ILE
4	D	232	ILE
5	E	9	THR
5	E	10	VAL
5	E	12	PHE
5	E	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	92	ASN
5	E	182	ASP
5	E	197	SER
5	E	198	GLN
5	E	205	LEU
5	E	209	ASN
5	E	222	THR
5	E	227	GLU
5	E	231	LYS
6	F	32	THR
6	F	39	ASN
6	F	68	ARG
6	F	101	THR
6	F	117	GLN
6	F	123	ASN
6	F	165	ARG
6	F	181	GLU

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Mol	Chain	Res	Type
6	F	186	ARG
6	F	196	ILE
6	F	201	GLU
6	F	221	ASN
6	F	228	LYS
7	G	68	ARG
7	G	83	ASN
7	G	115	LEU
7	G	166	GLN
7	G	208	GLU
7	G	221	LYS
7	G	235	ARG
7	G	236	LEU
7	G	243	ASP
8	H	3	ILE
8	H	34	LEU
8	H	41	ILE
8	H	56	THR
8	H	59	ILE
8	H	182	LYS
8	H	196	ARG
8	H	209	THR
8	H	222	ASP
9	I	37	ASN
9	I	120	ILE
9	I	123	PHE
9	I	136	ILE
9	I	171	LEU
10	J	52	ASP
10	J	71	GLU
10	J	78	GLN
10	J	110	LYS
10	J	127	GLU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	69	ARG
11	K	87	VAL
11	K	100	MET
11	K	107	LYS
11	K	140	LEU
11	K	147	ASP

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Mol	Chain	Res	Type
12	L	1	GLN
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	52	MET
12	L	108	HIS
12	L	109	THR
12	L	132	GLU
12	L	177	VAL
13	M	37	ASN
13	M	48	ASN
13	M	69	ASP
13	M	70	LEU
13	M	82	ASP
13	M	104	ARG
13	M	146	PHE
13	M	159	VAL
13	M	161	ARG
13	M	171	GLN
13	M	204	THR
13	M	206	LEU
14	N	36	ARG
14	N	88	GLU
14	N	115	LEU
14	N	119	VAL
14	N	144	GLU
14	N	149	GLU
14	N	195	GLN
1	O	30	GLN
1	O	59	GLU
1	O	66	LEU
1	O	68	THR
1	O	122	THR
1	O	157	PHE
1	O	169	VAL
1	O	178	ARG
1	O	183	LEU
2	P	38	MET
2	P	58	GLN
2	P	65	LEU
2	P	149	THR
2	P	157	THR

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Mol	Chain	Res	Type
2	P	184	LYS
2	P	191	LEU
2	P	212	PHE
3	Q	4	ARG
3	Q	22	LEU
3	Q	51	LYS
3	Q	147	GLN
3	Q	225	GLU
4	R	20	LEU
4	R	40	LEU
4	R	44	LYS
4	R	68	CYS
4	R	124	ARG
4	R	169	GLU
4	R	176	LEU
4	R	183	LEU
4	R	193	LEU
4	R	214	ILE
5	S	9	THR
5	S	10	VAL
5	S	12	PHE
5	S	25	LEU
5	S	29	LYS
5	S	71	LEU
5	S	92	ASN
5	S	112	CYS
5	S	182	ASP
5	S	197	SER
5	S	198	GLN
5	S	205	LEU
5	S	209	ASN
5	S	222	THR
5	S	227	GLU
5	S	231	LYS
6	T	32	THR
6	T	39	ASN
6	T	68	ARG
6	T	79	PRO
6	T	101	THR
6	T	117	GLN
6	T	123	ASN
6	T	165	ARG

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Mol	Chain	Res	Type
6	T	181	GLU
6	T	186	ARG
6	T	196	ILE
6	T	201	GLU
6	T	221	ASN
6	T	228	LYS
7	U	68	ARG
7	U	83	ASN
7	U	115	LEU
7	U	166	GLN
7	U	208	GLU
7	U	221	LYS
7	U	235	ARG
7	U	236	LEU
7	U	243	ASP
8	V	3	ILE
8	V	34	LEU
8	V	41	ILE
8	V	56	THR
8	V	59	ILE
8	V	182	LYS
8	V	196	ARG
8	V	209	THR
8	V	222	ASP
9	W	37	ASN
9	W	120	ILE
9	W	123	PHE
9	W	136	ILE
9	W	159	PRO
9	W	171	LEU
10	X	52	ASP
10	X	71	GLU
10	X	110	LYS
10	X	127	GLU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	69	ARG
11	Y	87	VAL
11	Y	100	MET
11	Y	107	LYS
11	Y	140	LEU

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Mol	Chain	Res	Type
11	Y	147	ASP
12	Z	1	GLN
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	52	MET
12	Z	108	HIS
12	Z	109	THR
12	Z	132	GLU
12	Z	177	VAL
13	a	37	ASN
13	a	48	ASN
13	a	69	ASP
13	a	70	LEU
13	a	82	ASP
13	a	104	ARG
13	a	146	PHE
13	a	159	VAL
13	a	161	ARG
13	a	171	GLN
13	a	204	THR
13	a	206	LEU
14	b	36	ARG
14	b	88	GLU
14	b	115	LEU
14	b	119	VAL
14	b	144	GLU
14	b	149	GLU
14	b	195	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (217) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
1	A	190	HIS
2	B	20	GLN
2	B	58	GLN
2	B	69	ASN
2	B	93	HIS
2	B	95	GLN
2	B	119	GLN

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Mol	Chain	Res	Type
2	B	123	GLN
2	B	155	ASN
2	B	172	GLN
2	B	176	GLN
2	B	220	ASN
2	B	226	GLN
3	C	17	GLN
3	C	92	GLN
3	C	115	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	165	ASN
3	C	207	ASN
3	C	241	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	139	HIS
4	D	146	GLN
4	D	160	ASN
4	D	198	GLN
4	D	225	ASN
5	E	4	ASN
5	E	30	GLN
5	E	59	GLN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	147	GLN
5	E	151	ASN
5	E	198	GLN
6	F	19	GLN
6	F	39	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	224	HIS
7	G	30	ASN

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Mol	Chain	Res	Type
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
7	G	186	ASN
7	G	231	ASN
8	H	10	ASN
8	H	30	ASN
8	H	66	HIS
8	H	144	GLN
8	H	172	ASN
9	I	37	ASN
9	I	71	ASN
9	I	88	GLN
9	I	156	ASN
9	I	203	GLN
10	J	55	GLN
10	J	78	GLN
10	J	86	GLN
10	J	118	GLN
10	J	146	HIS
10	J	191	GLN
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	176	ASN
11	K	188	HIS
11	K	208	ASN
11	K	209	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	92	ASN
12	L	135	GLN
12	L	165	ASN
12	L	195	HIS
12	L	197	GLN
13	M	2	GLN

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Mol	Chain	Res	Type
13	M	18	ASN
13	M	37	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	152	ASN
13	M	171	GLN
13	M	179	ASN
13	M	211	ASN
13	M	213	GLN
14	N	60	GLN
14	N	69	GLN
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS
1	O	190	HIS
2	P	20	GLN
2	P	58	GLN
2	P	69	ASN
2	P	88	ASN
2	P	93	HIS
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
2	P	220	ASN
3	Q	17	GLN
3	Q	77	ASN
3	Q	92	GLN
3	Q	115	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	165	ASN
3	Q	207	ASN
3	Q	241	GLN
4	R	15	GLN
4	R	91	HIS

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Mol	Chain	Res	Type
4	R	100	ASN
4	R	139	HIS
4	R	146	GLN
4	R	160	ASN
4	R	198	GLN
4	R	225	ASN
5	S	4	ASN
5	S	30	GLN
5	S	59	GLN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	147	GLN
5	S	151	ASN
5	S	198	GLN
6	T	19	GLN
6	T	39	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	224	HIS
7	U	6	HIS
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
7	U	186	ASN
7	U	231	ASN
8	V	10	ASN
8	V	30	ASN
8	V	66	HIS
8	V	144	GLN
8	V	172	ASN
9	W	37	ASN
9	W	71	ASN
9	W	88	GLN

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Mol	Chain	Res	Type
9	W	156	ASN
9	W	203	GLN
10	X	55	GLN
10	X	63	ASN
10	X	78	GLN
10	X	86	GLN
10	X	118	GLN
10	X	146	HIS
10	X	191	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	176	ASN
11	Y	188	HIS
11	Y	208	ASN
11	Y	209	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	92	ASN
12	Z	135	GLN
12	Z	165	ASN
12	Z	195	HIS
12	Z	197	GLN
13	a	2	GLN
13	a	18	ASN
13	a	37	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	171	GLN
13	a	179	ASN
13	a	211	ASN
13	a	213	GLN
14	b	60	GLN
14	b	69	GLN
14	b	145	ASN
14	b	157	HIS
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	LYO	f	3	15	7,9,10	1.03	0	7,10,12	1.26	1 (14%)
15	OW6	e	4	15,8	5,6,7	1.17	0	5,6,8	0.84	0
15	OW6	f	4	15,11	5,6,7	1.19	0	5,6,8	0.52	0
15	OW6	d	4	15,11	5,6,7	1.17	0	5,6,8	0.55	0
15	LYO	d	3	15	7,9,10	0.95	0	7,10,12	1.35	1 (14%)
15	LYO	e	3	15	7,9,10	1.01	0	7,10,12	1.18	1 (14%)
15	LYO	c	3	15	7,9,10	1.06	0	7,10,12	1.18	1 (14%)
15	OW6	c	4	15,8	5,6,7	1.57	1 (20%)	5,6,8	0.79	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	LYO	f	3	15	-	3/8/9/11	-
15	OW6	e	4	15,8	-	2/4/4/5	-
15	OW6	f	4	15,11	-	1/4/4/5	-
15	OW6	d	4	15,11	-	1/4/4/5	-
15	LYO	d	3	15	-	3/8/9/11	-
15	LYO	e	3	15	-	4/8/9/11	-
15	LYO	c	3	15	-	4/8/9/11	-
15	OW6	c	4	15,8	-	2/4/4/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	4	0W6	C17-CA	3.00	1.57	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	d	3	LYO	CB-CA-C	-3.32	105.88	110.99
15	f	3	LYO	CB-CA-C	-3.08	106.25	110.99
15	e	3	LYO	CB-CA-C	-2.92	106.50	110.99
15	c	3	LYO	CB-CA-C	-2.79	106.70	110.99

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	c	3	LYO	N-CA-CB-CG
15	c	3	LYO	C-CA-CB-CG
15	c	3	LYO	CG-CD-CE-NZ
15	d	3	LYO	N-CA-CB-CG
15	d	3	LYO	C-CA-CB-CG
15	d	3	LYO	CG-CD-CE-NZ
15	e	3	LYO	N-CA-CB-CG
15	e	3	LYO	C-CA-CB-CG
15	e	3	LYO	CG-CD-CE-NZ
15	f	3	LYO	N-CA-CB-CG
15	f	3	LYO	C-CA-CB-CG
15	f	3	LYO	CG-CD-CE-NZ
15	c	4	0W6	O-C-C18-C17
15	e	4	0W6	O-C-C18-C17
15	e	4	0W6	CA-C17-C18-C
15	c	4	0W6	CA-C17-C18-C
15	d	4	0W6	CA-C17-C18-C
15	f	4	0W6	CA-C17-C18-C
15	c	3	LYO	CE-CD-CG-OG
15	e	3	LYO	CE-CD-CG-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.45	0 100 100	61, 83, 116, 141	0
1	O	250/250 (100%)	-0.51	0 100 100	61, 83, 117, 141	0
2	B	244/244 (100%)	-0.30	4 (1%) 70 47	61, 83, 131, 151	0
2	P	244/244 (100%)	-0.35	1 (0%) 88 76	61, 83, 131, 151	0
3	C	241/241 (100%)	-0.33	2 (0%) 82 64	63, 89, 135, 162	0
3	Q	241/241 (100%)	-0.34	1 (0%) 88 76	65, 91, 136, 162	0
4	D	242/242 (100%)	-0.29	3 (1%) 76 55	61, 90, 125, 155	0
4	R	242/242 (100%)	-0.29	3 (1%) 76 55	63, 91, 126, 155	0
5	E	233/233 (100%)	-0.18	1 (0%) 88 76	67, 95, 125, 145	0
5	S	233/233 (100%)	-0.18	1 (0%) 88 76	68, 95, 125, 145	0
6	F	244/244 (100%)	-0.27	1 (0%) 88 76	64, 87, 124, 141	0
6	T	244/244 (100%)	-0.31	1 (0%) 88 76	65, 87, 125, 140	0
7	G	243/243 (100%)	-0.38	1 (0%) 88 76	62, 84, 116, 152	0
7	U	243/243 (100%)	-0.45	1 (0%) 88 76	63, 83, 115, 153	0
8	H	222/222 (100%)	-0.56	0 100 100	59, 75, 98, 140	0
8	V	222/222 (100%)	-0.58	0 100 100	61, 74, 98, 142	0
9	I	204/204 (100%)	-0.63	0 100 100	57, 75, 99, 117	0
9	W	204/204 (100%)	-0.59	0 100 100	58, 75, 99, 116	0
10	J	198/198 (100%)	-0.53	1 (0%) 87 72	56, 76, 99, 161	0
10	X	198/198 (100%)	-0.59	0 100 100	57, 77, 98, 162	0
11	K	212/212 (100%)	-0.62	0 100 100	55, 75, 99, 115	0
11	Y	212/212 (100%)	-0.61	0 100 100	56, 75, 101, 117	0
12	L	222/222 (100%)	-0.54	1 (0%) 87 72	59, 77, 105, 129	0
12	Z	222/222 (100%)	-0.55	0 100 100	59, 77, 104, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/233 (100%)	-0.53	1 (0%) 88 76	59, 77, 99, 110	0
13	a	233/233 (100%)	-0.56	1 (0%) 88 76	58, 77, 99, 110	0
14	N	196/196 (100%)	-0.55	0 100 100	58, 74, 100, 115	0
14	b	196/196 (100%)	-0.58	0 100 100	58, 74, 101, 114	0
15	c	1/4 (25%)	0.01	0 100 100	75, 75, 75, 75	0
15	d	1/4 (25%)	-0.75	0 100 100	63, 63, 63, 63	0
15	e	1/4 (25%)	0.63	0 100 100	75, 75, 75, 75	0
15	f	1/4 (25%)	-1.06	0 100 100	66, 66, 66, 66	0
All	All	6372/6384 (99%)	-0.44	24 (0%) 88 76	55, 81, 120, 162	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	119	ALA	4.1
7	U	243	ASP	3.9
4	R	119	ALA	3.9
2	P	219	ALA	3.8
3	Q	50	LEU	3.8
4	D	118	GLY	3.4
2	B	218	GLY	3.2
6	F	202	ASP	3.0
2	B	219	ALA	2.7
7	G	1	ALA	2.5
10	J	197	ALA	2.5
12	L	174	TYR	2.5
13	M	1	THR	2.5
4	D	120	SER	2.4
5	E	1	PHE	2.4
5	S	1	PHE	2.3
3	C	50	LEU	2.3
4	R	120	SER	2.2
13	a	1	THR	2.1
2	B	1	GLY	2.1
3	C	48	SER	2.1
6	T	215	CYS	2.1
2	B	244	THR	2.1
4	R	118	GLY	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	LYO	e	3	10/11	0.91	0.11	73,75,78,79	0
15	LYO	c	3	10/11	0.92	0.10	72,74,78,78	0
15	LYO	d	3	10/11	0.93	0.09	64,68,71,71	0
15	LYO	f	3	10/11	0.93	0.08	64,67,71,72	0
15	OW6	e	4	7/8	0.93	0.12	71,73,77,77	0
15	OW6	d	4	7/8	0.95	0.09	67,67,72,72	0
15	OW6	f	4	7/8	0.96	0.08	67,68,72,73	0
15	OW6	c	4	7/8	0.97	0.08	70,72,76,77	0

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.