



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:27 AM UTC

PDB ID : 4GK7 / pdb_00004gk7
Title : yeast 20S proteasome in complex with the Syringolin-Glidobactin chimera
Authors : Groll, M.; Stein, M.L.; Bachmann, A.
Deposited on : 2012-08-10
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
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

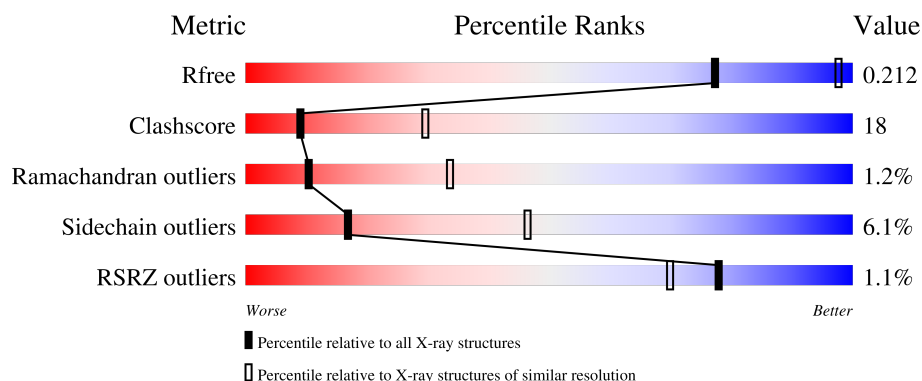
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	250	0.2% 67% 29% •
1	O	250	64% 33% •
2	B	244	3% 62% 32% 6%
2	P	244	3% 62% 32% 6%
3	C	241	2% 57% 40% •

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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	1	4	
15	2	4	

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Mol	Chain	Length	Quality of chain
15	3	4	25% 25% 50%
15	4	4	25% 50% 25%
15	5	4	25% 75%
15	6	4	25% 25% 50%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51109 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 SYRINGOLIN-GLIDOBACTIN CHIMERA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	1	4	Total	C	N	O	0	0	0
			38	29	4	5			
15	2	4	Total	C	N	O	0	0	0
			38	29	4	5			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	3	4	Total	C	N	O	0	0	0
			38	29	4	5			
15	4	4	Total	C	N	O	0	0	0
			38	29	4	5			
15	5	4	Total	C	N	O	0	0	0
			38	29	4	5			
15	6	4	Total	C	N	O	0	0	0
			38	29	4	5			

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	59	Total	O	0	0
			59	59		
16	B	35	Total	O	0	0
			35	35		
16	C	44	Total	O	0	0
			44	44		
16	D	39	Total	O	0	0
			39	39		
16	E	23	Total	O	0	0
			23	23		
16	F	49	Total	O	0	0
			49	49		
16	G	60	Total	O	0	0
			60	60		
16	H	49	Total	O	0	0
			49	49		
16	I	64	Total	O	0	0
			64	64		
16	J	53	Total	O	0	0
			53	53		
16	K	42	Total	O	0	0
			42	42		
16	L	55	Total	O	0	0
			55	55		
16	M	75	Total	O	0	0
			75	75		
16	N	56	Total	O	0	0
			56	56		
16	O	34	Total	O	0	0
			34	34		

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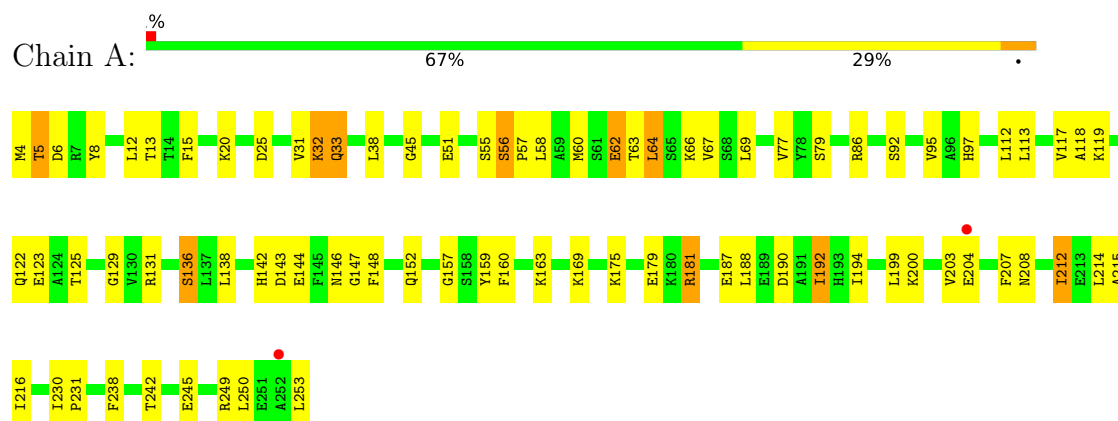
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	P	28	Total 28	O 28	0	0
16	Q	29	Total 29	O 29	0	0
16	R	33	Total 33	O 33	0	0
16	S	21	Total 21	O 21	0	0
16	T	39	Total 39	O 39	0	0
16	U	63	Total 63	O 63	0	0
16	V	47	Total 47	O 47	0	0
16	W	55	Total 55	O 55	0	0
16	X	46	Total 46	O 46	0	0
16	Y	50	Total 50	O 50	0	0
16	Z	51	Total 51	O 51	0	0
16	a	73	Total 73	O 73	0	0
16	b	58	Total 58	O 58	0	0
16	1	1	Total 1	O 1	0	0
16	2	1	Total 1	O 1	0	0
16	3	1	Total 1	O 1	0	0

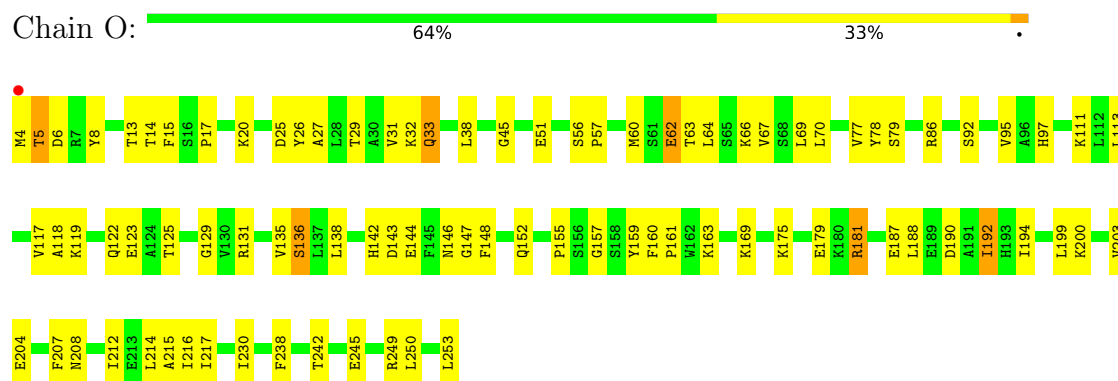
3 Residue-property plots [i](#)

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.

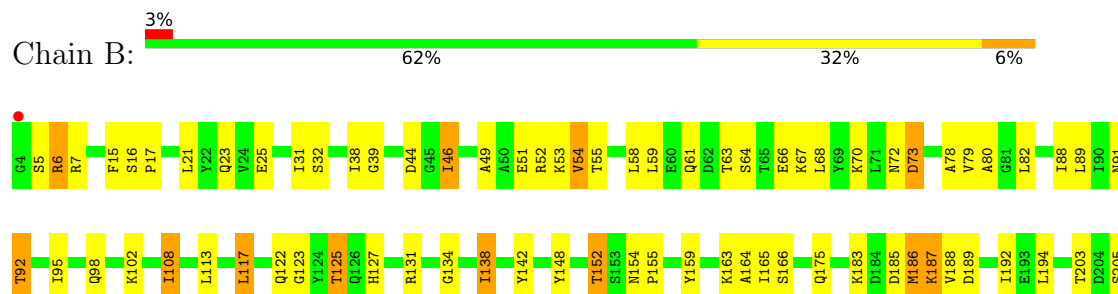
• Molecule 1: Proteasome component Y7



• Molecule 1: Proteasome component Y7

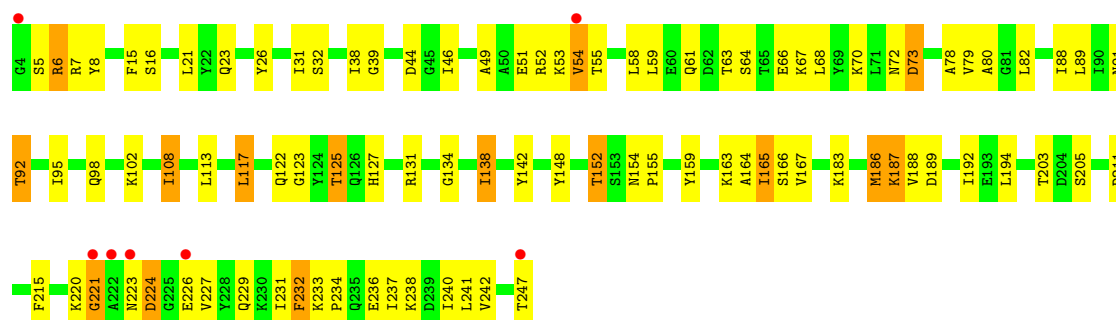


• Molecule 2: Proteasome component Y13

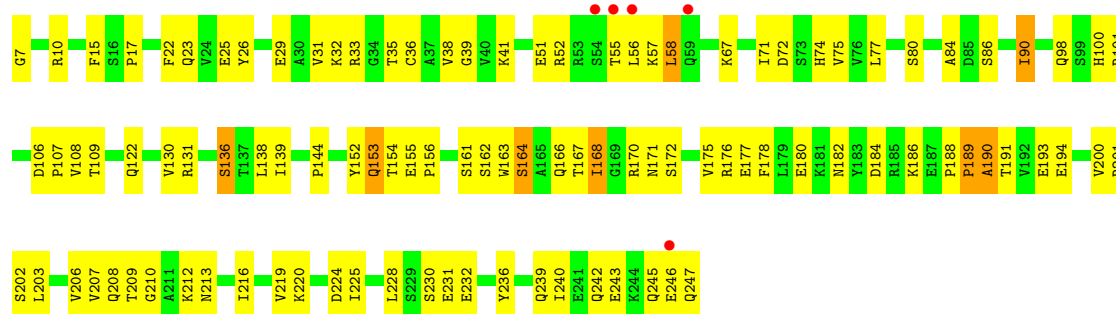




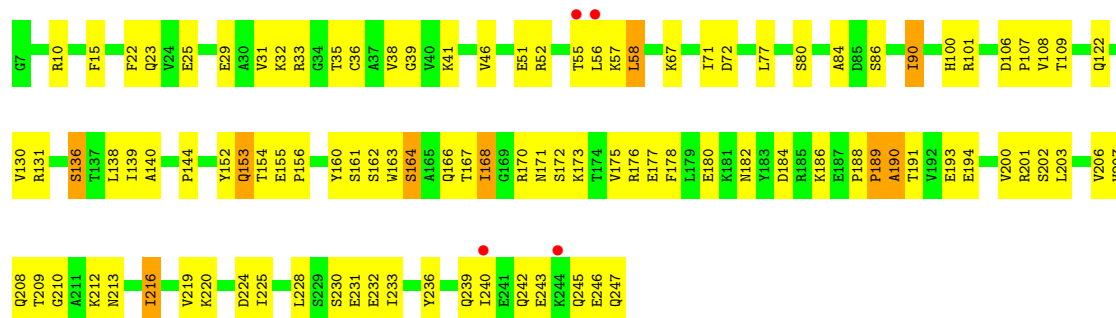
• Molecule 2: Proteasome component Y13



• Molecule 3: Proteasome component PRE6

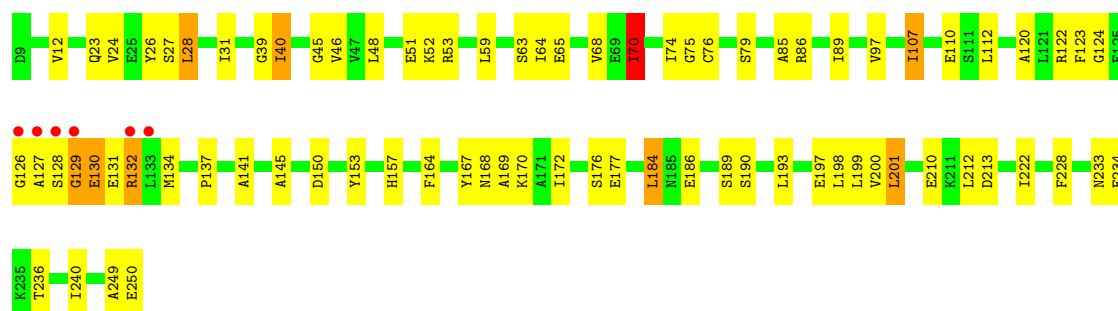


• Molecule 3: Proteasome component PRE6

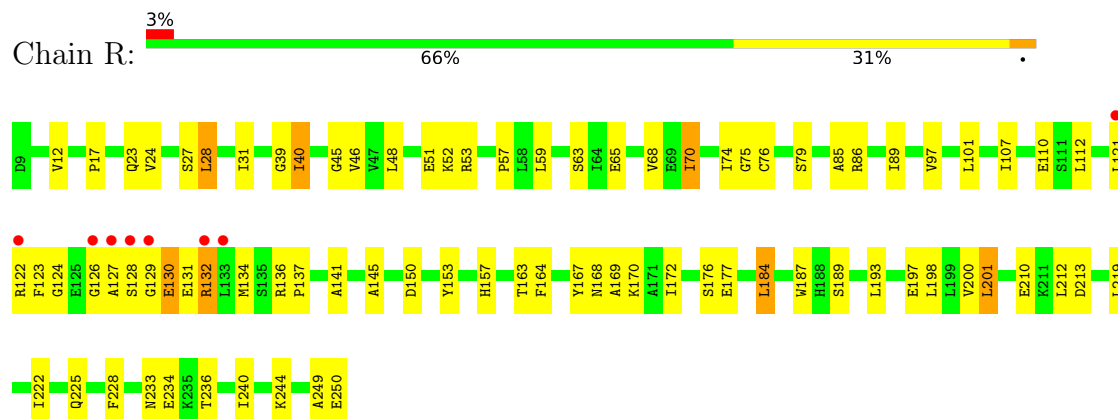


• Molecule 4: Proteasome component PUP2

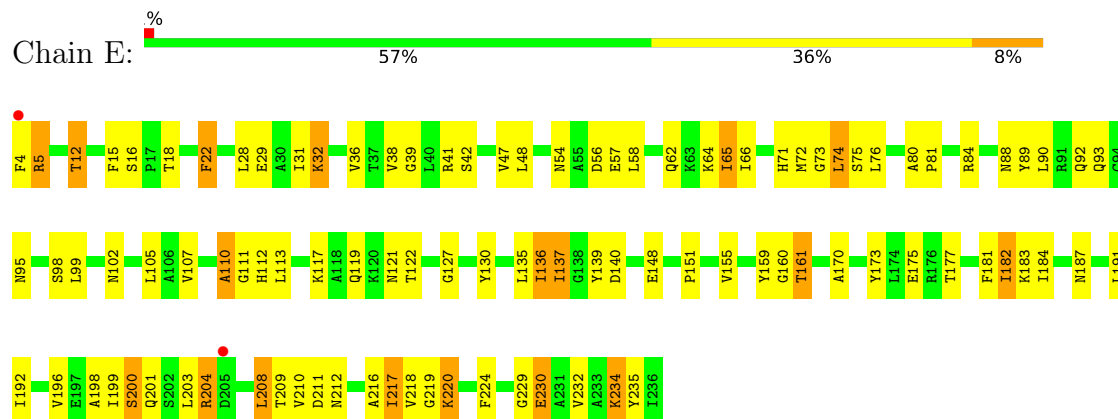




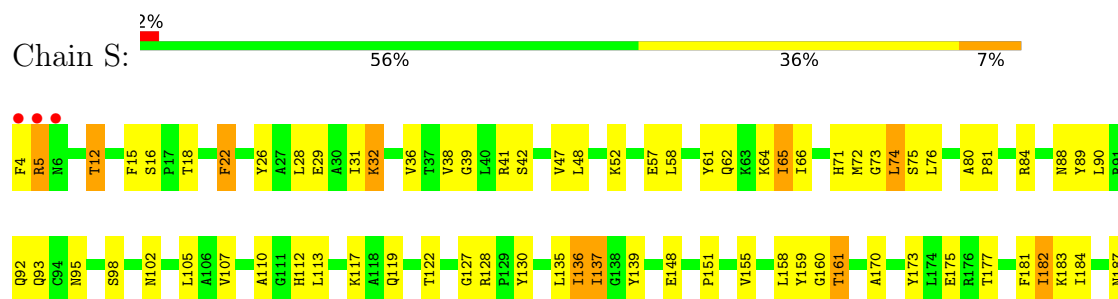
• Molecule 4: Proteasome component PUP2

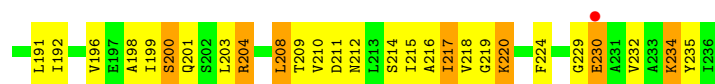


• Molecule 5: Proteasome component PRE5



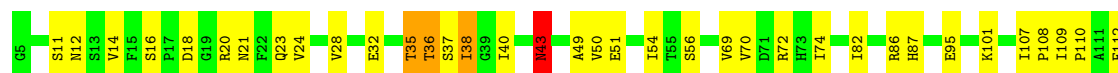
• Molecule 5: Proteasome component PRE5





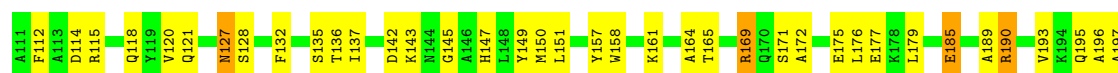
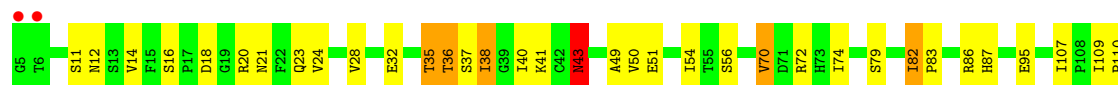
• Molecule 6: Proteasome component C1

Chain F: 62% 32% 5%



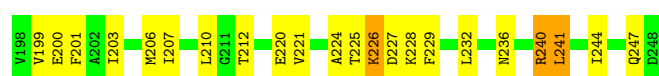
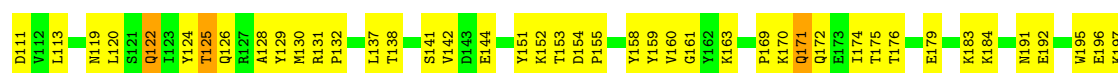
• Molecule 6: Proteasome component C1

Chain T: 61% 32% 6%



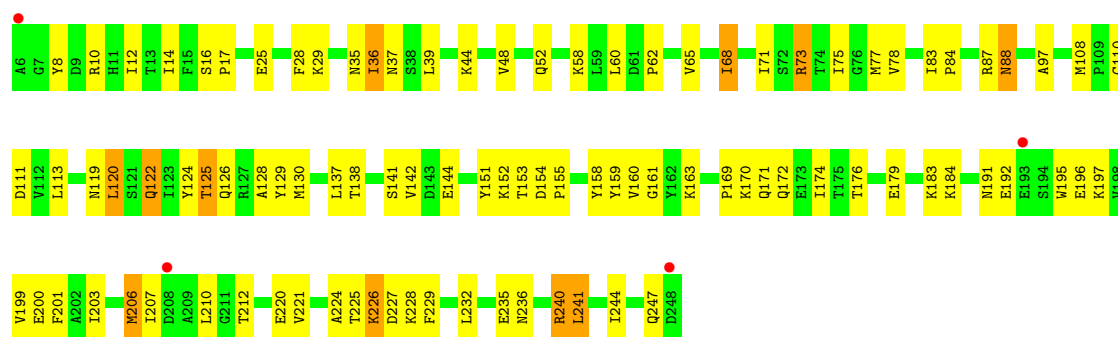
• Molecule 7: Proteasome component C7-alpha

Chain G: 60% 36% 4%



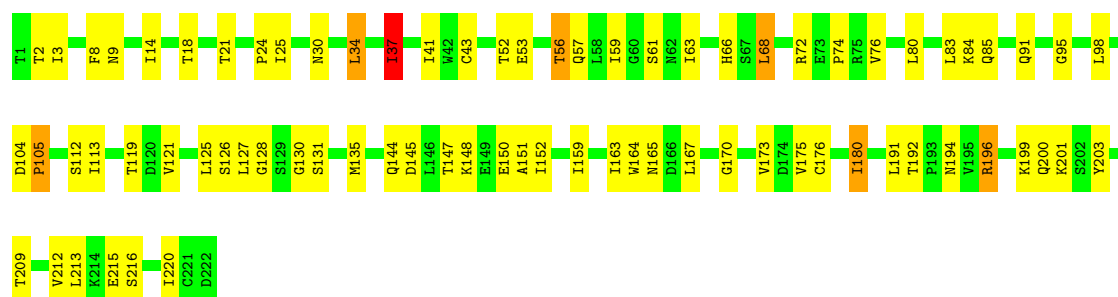
• Molecule 7: Proteasome component C7-alpha

Chain U: 60% 35% 5%



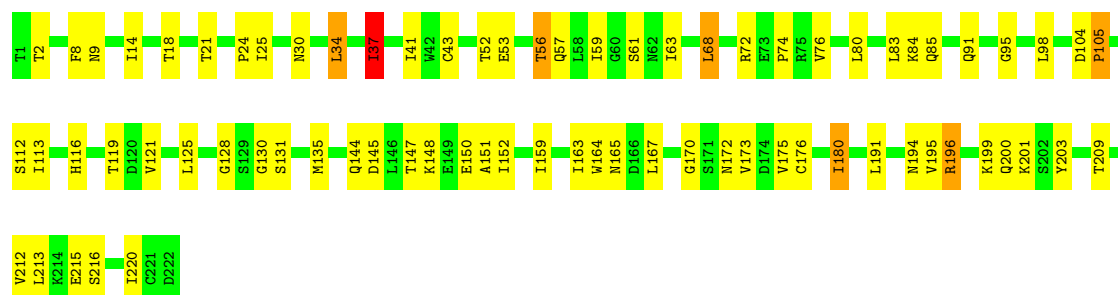
• Molecule 8: Proteasome component PUP1

Chain H: 65% 32% .



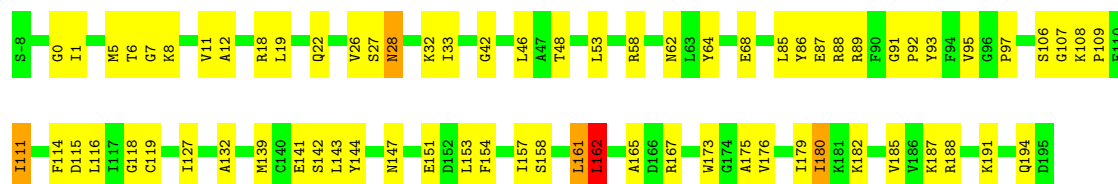
• Molecule 8: Proteasome component PUP1

Chain V: 66% 31% .



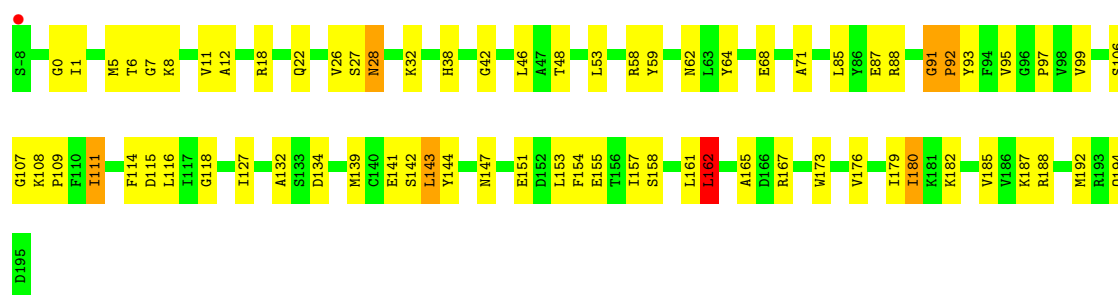
• Molecule 9: Proteasome component PUP3

Chain I: 65% 33% .



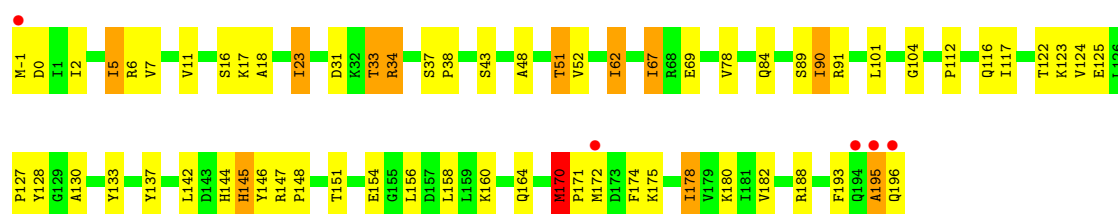
• Molecule 9: Proteasome component PUP3

Chain W:  65% 32%



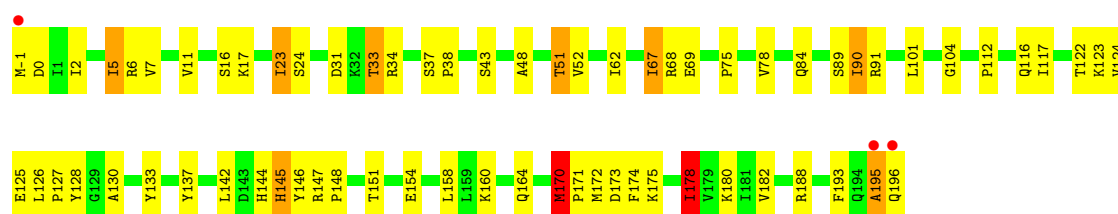
• Molecule 10: Proteasome component C11

Chain J:  3% 67% 27% 6%



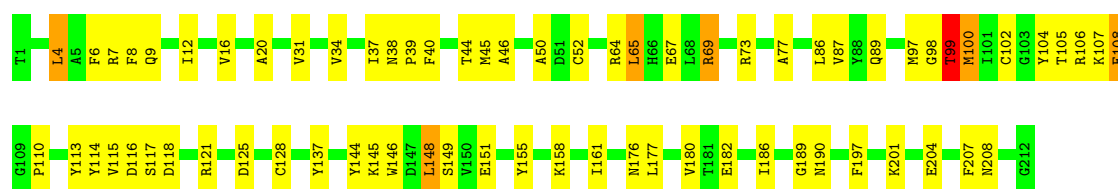
• Molecule 10: Proteasome component C11

Chain X:  2% 65% 30% 2%



• Molecule 11: Proteasome component PRE2

Chain K:  67% 30%



• Molecule 11: Proteasome component PRE2

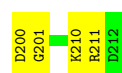
Chain Y:  68% 28%





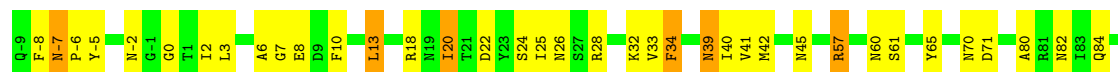
• Molecule 12: Proteasome component C5

Chain L: 64% 30% 5% •



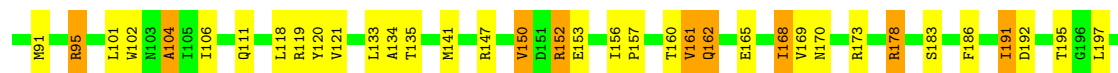
• Molecule 12: Proteasome component C5

Chain Z: 64% 28% 8%



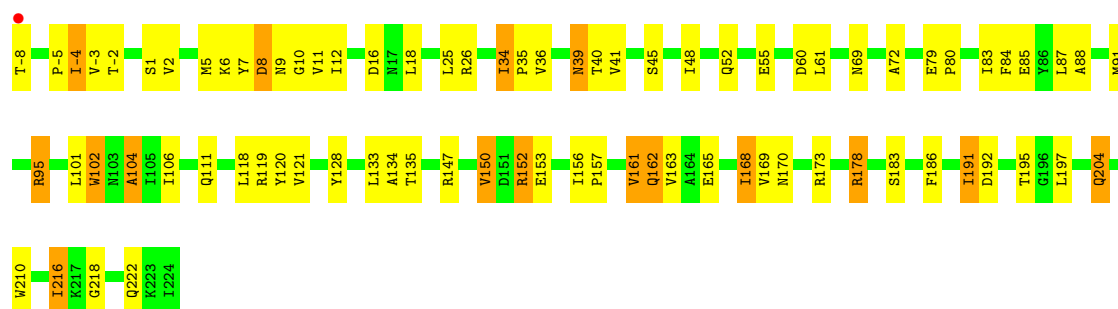
• Molecule 13: Proteasome component PRE4

Chain M: 65% 29% 6%

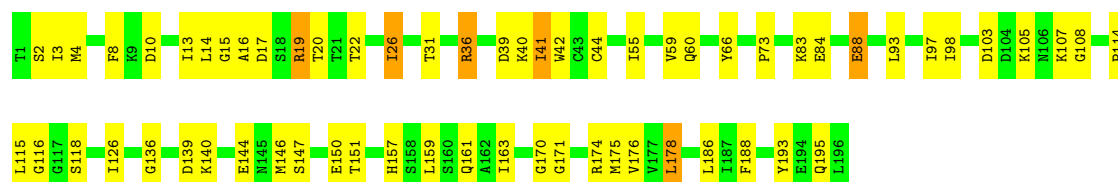


• Molecule 13: Proteasome component PRE4

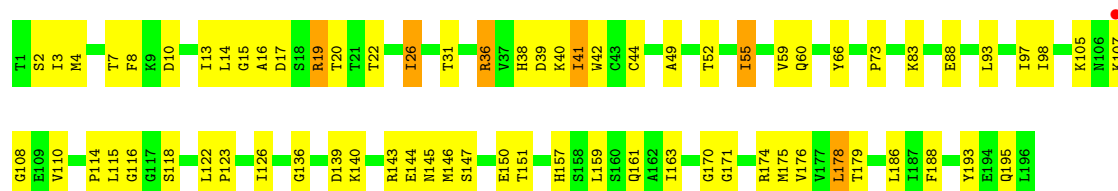
Chain a: 65% 28% 7%



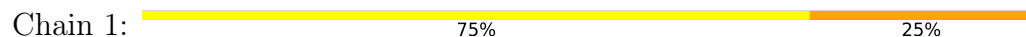
- Molecule 14: Proteasome component PRE3



- Molecule 14: Proteasome component PRE3



- Molecule 15: SYRINGOLIN-GLIDOBACTIN CHIMERA



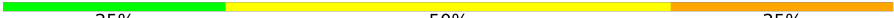
- Molecule 15: SYRINGOLIN-GLIDOBACTIN CHIMERA



- Molecule 15: SYRINGOLIN-GLIDOBACTIN CHIMERA



- Molecule 15: SYRINGOLIN-GLIDOBACTIN CHIMERA

Chain 4:  25% 50% 25%

MR90
T1
LYH2
OJT3

- Molecule 15: SYRINGOLIN-GLIDOBACTIN CHIMERA

Chain 5:  25% 75%

MR90
T1
LYH2
OJT3

- Molecule 15: SYRINGOLIN-GLIDOBACTIN CHIMERA

Chain 6:  25% 25% 50%

MR90
T1
LYH2
OJT3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.85Å 298.45Å 145.25Å 90.00° 112.63° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.00-2.80) 97.3 (15.00-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.241 0.212 , 0.212	Depositor DCC
R_{free} test set	12775 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.648	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	51109	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MH9, LYH, 0JT

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	0.43	0/1952	0.96	6/2642 (0.2%)
1	O	0.44	0/1952	0.96	8/2642 (0.3%)
2	B	0.45	0/1935	0.91	5/2618 (0.2%)
2	P	0.46	0/1935	0.91	5/2618 (0.2%)
3	C	0.43	0/1920	0.92	4/2598 (0.2%)
3	Q	0.44	0/1920	0.92	4/2598 (0.2%)
4	D	0.43	0/1887	0.93	7/2541 (0.3%)
4	R	0.43	0/1887	0.92	7/2541 (0.3%)
5	E	0.42	0/1823	0.95	5/2463 (0.2%)
5	S	0.41	0/1823	0.96	3/2463 (0.1%)
6	F	0.45	0/1937	0.98	11/2614 (0.4%)
6	T	0.45	0/1937	0.99	11/2614 (0.4%)
7	G	0.48	0/1959	0.97	5/2652 (0.2%)
7	U	0.46	0/1959	0.97	6/2652 (0.2%)
8	H	0.47	0/1716	0.96	7/2326 (0.3%)
8	V	0.46	0/1716	0.96	5/2326 (0.2%)
9	I	0.46	0/1611	1.00	10/2174 (0.5%)
9	W	0.45	0/1611	1.00	11/2174 (0.5%)
10	J	0.48	0/1613	0.98	5/2173 (0.2%)
10	X	0.48	0/1613	0.99	6/2173 (0.3%)
11	K	0.45	0/1681	0.94	4/2274 (0.2%)
11	Y	0.45	0/1681	0.94	3/2274 (0.1%)
12	L	0.44	0/1795	1.06	14/2420 (0.6%)
12	Z	0.45	0/1795	1.06	16/2420 (0.7%)
13	M	0.46	0/1855	0.96	7/2514 (0.3%)
13	a	0.46	0/1855	0.97	6/2514 (0.2%)
14	N	0.46	0/1541	0.97	3/2087 (0.1%)
14	b	0.46	0/1541	0.98	6/2087 (0.3%)
15	1	1.63	0/6	1.48	0/7
15	2	1.25	0/6	2.28	0/7
15	3	1.67	0/6	2.00	0/7
15	4	1.72	0/6	1.53	0/7

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	5	1.29	0/6	2.21	0/7
15	6	1.63	0/6	2.03	0/7
All	All	0.45	0/50486	0.97	190/68234 (0.3%)

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 (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	26	ARG	N-CA-C	11.58	123.64	111.14
13	a	26	ARG	N-CA-C	11.46	123.52	111.14
1	O	163	LYS	N-CA-C	-10.38	100.74	113.41
1	A	163	LYS	N-CA-C	-10.06	101.14	113.41
6	F	12	ASN	N-CA-C	8.83	120.52	111.07
6	T	12	ASN	N-CA-C	8.78	120.54	110.97
5	S	57	GLU	N-CA-C	-8.70	102.20	113.17
5	E	57	GLU	N-CA-C	-8.40	102.58	113.17
12	Z	95	TYR	N-CA-C	-8.04	96.94	109.25
8	V	37	ILE	N-CA-C	-7.66	104.32	111.45
12	L	95	TYR	N-CA-C	-7.65	96.80	108.96
11	Y	189	GLY	N-CA-C	7.65	124.85	112.61
8	H	37	ILE	N-CA-C	-7.60	104.38	111.45
2	B	163	LYS	N-CA-C	-7.58	104.16	113.41
11	K	189	GLY	N-CA-C	7.44	124.52	112.61
7	U	16	SER	N-CA-C	-7.42	100.68	110.40
6	T	161	LYS	N-CA-C	-7.39	102.60	111.69
7	G	16	SER	N-CA-C	-7.37	100.75	110.40
12	Z	20	ILE	N-CA-C	7.37	117.81	108.82
2	P	163	LYS	N-CA-C	-7.36	104.44	113.41
12	Z	98	HIS	N-CA-C	-7.34	96.77	108.73
2	P	73	ASP	N-CA-C	-7.31	104.51	113.50
13	M	178	ARG	N-CA-C	7.24	122.29	113.17
7	G	163	LYS	N-CA-C	-7.23	103.12	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	70	ILE	N-CA-C	-7.17	104.78	111.45
3	C	71	ILE	N-CA-C	-7.16	103.20	111.00
3	Q	71	ILE	N-CA-C	-7.14	103.22	111.00
6	F	161	LYS	N-CA-C	-7.08	102.98	111.69
13	a	178	ARG	N-CA-C	7.07	122.08	113.38
2	B	73	ASP	N-CA-C	-7.06	104.81	113.50
5	E	159	TYR	N-CA-C	-7.05	104.81	113.41
12	Z	136	ILE	N-CA-C	6.97	116.98	110.42
7	U	163	LYS	N-CA-C	-6.97	103.45	112.23
12	L	20	ILE	N-CA-C	6.95	117.29	108.82
12	L	136	ILE	N-CA-C	6.93	116.93	110.42
3	C	164	SER	N-CA-C	-6.92	103.52	112.23
5	S	159	TYR	N-CA-C	-6.83	105.07	113.41
9	I	180	ILE	N-CA-C	6.80	117.63	108.11
9	W	180	ILE	N-CA-C	6.71	117.55	107.75
6	T	135	SER	N-CA-C	-6.69	98.50	109.40
3	Q	164	SER	N-CA-C	-6.66	103.83	112.23
4	R	63	SER	N-CA-C	-6.63	104.77	112.92
10	X	170	MET	CA-C-N	6.58	126.36	119.05
10	X	170	MET	C-N-CA	6.58	126.36	119.05
10	J	170	MET	CA-C-N	6.57	126.35	119.05
10	J	170	MET	C-N-CA	6.57	126.35	119.05
6	F	135	SER	N-CA-C	-6.57	98.69	109.40
12	L	119	GLY	N-CA-C	6.55	124.50	115.27
1	O	66	LYS	N-CA-C	-6.52	105.48	113.50
1	A	129	GLY	N-CA-C	6.49	122.96	113.48
3	C	22	PHE	N-CA-C	6.48	119.17	111.33
13	M	8	ASP	N-CA-C	6.43	118.29	111.28
6	F	14	VAL	N-CA-C	6.40	117.92	109.21
12	L	98	HIS	N-CA-C	-6.39	97.28	108.20
1	O	144	GLU	N-CA-C	6.38	119.05	111.33
1	O	129	GLY	N-CA-C	6.38	122.79	113.48
3	Q	22	PHE	N-CA-C	6.37	119.03	111.33
13	a	101	LEU	N-CA-C	-6.37	97.31	108.20
6	T	14	VAL	N-CA-C	6.36	117.86	109.21
4	D	63	SER	N-CA-C	-6.34	105.12	112.92
1	A	66	LYS	N-CA-C	-6.30	105.75	113.50
1	A	187	GLU	N-CA-C	-6.27	101.49	110.59
12	Z	119	GLY	N-CA-C	6.26	124.10	115.27
9	W	93	TYR	N-CA-C	-6.26	100.31	110.20
12	Z	116	ASP	CA-C-N	-6.25	113.25	119.56
12	Z	116	ASP	C-N-CA	-6.25	113.25	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	116	ASP	CA-C-N	-6.25	113.25	119.56
12	L	116	ASP	C-N-CA	-6.25	113.25	119.56
1	A	144	GLU	N-CA-C	6.24	118.88	111.33
13	a	8	ASP	N-CA-C	6.23	118.07	111.28
2	P	16	SER	N-CA-C	-6.21	102.27	110.40
13	M	104	ALA	N-CA-C	-6.20	98.17	108.34
8	H	180	ILE	N-CA-C	6.20	119.72	111.17
5	S	22	PHE	N-CA-C	6.18	118.02	111.28
1	O	187	GLU	N-CA-C	-6.17	101.64	110.59
6	F	171	SER	N-CA-C	-6.15	104.49	111.07
2	B	16	SER	N-CA-C	-6.15	102.35	110.40
11	Y	99	THR	N-CA-C	6.13	119.18	109.50
9	W	144	TYR	N-CA-C	6.10	119.08	110.23
2	B	138	ILE	N-CA-C	-6.10	98.84	107.75
8	V	180	ILE	N-CA-C	6.08	119.56	111.17
5	E	22	PHE	N-CA-C	6.08	117.90	111.28
9	I	93	TYR	N-CA-C	-6.05	100.64	110.20
9	W	91	GLY	CA-C-N	6.04	126.00	120.03
9	W	91	GLY	C-N-CA	6.04	126.00	120.03
10	J	147	ARG	CA-C-N	6.03	125.73	119.82
10	J	147	ARG	C-N-CA	6.03	125.73	119.82
13	a	-2	THR	N-CA-C	6.01	119.35	109.85
9	I	144	TYR	N-CA-C	6.01	118.94	110.23
12	Z	164	TYR	N-CA-C	6.00	119.48	109.95
12	L	164	TYR	N-CA-C	5.98	119.46	109.95
6	F	38	ILE	N-CA-C	5.95	116.73	108.23
12	L	164	TYR	CA-CB-CG	-5.93	103.22	113.90
11	K	118	ASP	N-CA-C	-5.91	105.56	112.89
11	K	99	THR	N-CA-C	5.91	118.83	109.50
11	Y	118	ASP	N-CA-C	-5.91	105.57	112.89
2	P	138	ILE	N-CA-C	-5.90	99.13	107.75
10	X	147	ARG	CA-C-N	5.88	125.58	119.82
10	X	147	ARG	C-N-CA	5.88	125.58	119.82
13	a	104	ALA	N-CA-C	-5.85	98.75	108.34
9	I	91	GLY	CA-C-N	5.84	125.81	120.03
9	I	91	GLY	C-N-CA	5.84	125.81	120.03
9	I	58	ARG	N-CA-C	-5.84	104.83	111.07
12	Z	164	TYR	CA-CB-CG	-5.84	103.39	113.90
6	T	171	SER	N-CA-C	-5.83	104.83	111.07
9	W	118	GLY	N-CA-C	5.82	123.35	115.32
9	I	118	GLY	N-CA-C	5.78	123.29	115.32
4	R	176	SER	N-CA-C	5.78	117.44	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	183	LYS	N-CA-C	-5.76	105.09	111.71
14	b	97	ILE	N-CA-C	5.73	116.73	108.48
13	M	-2	THR	N-CA-C	5.73	118.90	109.85
6	T	38	ILE	N-CA-C	5.72	116.95	108.65
4	D	168	ASN	N-CA-C	-5.71	105.03	112.23
9	W	58	ARG	N-CA-C	-5.71	104.96	111.07
7	G	183	LYS	N-CA-C	-5.71	105.14	111.71
14	N	17	ASP	N-CA-C	-5.71	101.51	110.36
6	T	16	SER	N-CA-C	-5.70	103.58	110.13
8	V	21	THR	N-CA-C	5.69	118.05	109.23
3	Q	109	THR	N-CA-C	-5.68	102.11	110.52
6	F	223	GLU	N-CA-C	5.67	119.37	112.23
14	N	19	ARG	N-CA-C	5.65	117.72	108.52
14	N	97	ILE	N-CA-C	5.65	116.61	108.48
8	H	21	THR	N-CA-C	5.63	117.95	109.23
8	V	98	LEU	N-CA-C	5.59	118.33	109.50
7	G	228	LYS	N-CA-C	5.58	116.89	108.46
4	D	176	SER	N-CA-C	5.57	117.21	111.03
3	C	109	THR	N-CA-C	-5.56	102.30	110.52
4	R	168	ASN	N-CA-C	-5.55	105.24	112.23
7	U	228	LYS	N-CA-C	5.54	116.83	108.46
9	W	162	LEU	N-CA-C	5.54	117.75	111.11
8	H	164	TRP	N-CA-C	5.53	117.39	111.36
14	b	17	ASP	N-CA-C	-5.52	101.80	110.36
9	I	162	LEU	N-CA-C	5.50	117.71	111.11
6	F	16	SER	N-CA-C	-5.50	103.81	110.13
4	R	150	ASP	N-CA-C	5.49	117.35	111.36
6	T	223	GLU	N-CA-C	5.48	119.14	112.23
6	F	247	ILE	N-CA-C	-5.47	106.15	112.98
7	U	128	ALA	N-CA-C	5.46	118.16	111.82
7	G	128	ALA	N-CA-C	5.46	118.15	111.82
9	W	143	LEU	N-CA-C	5.44	117.21	111.28
6	T	247	ILE	N-CA-C	-5.43	106.19	112.98
12	L	93	PHE	CA-C-N	5.41	125.41	119.89
12	L	93	PHE	C-N-CA	5.41	125.41	119.89
12	Z	93	PHE	CA-C-N	5.39	125.39	119.89
12	Z	93	PHE	C-N-CA	5.39	125.39	119.89
4	D	150	ASP	N-CA-C	5.36	117.21	111.36
13	M	101	LEU	N-CA-C	-5.35	97.80	107.75
12	Z	22	ASP	CB-CA-C	-5.33	109.98	117.23
6	T	145	GLY	N-CA-C	5.28	120.64	112.45
14	b	19	ARG	N-CA-C	5.26	117.54	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	122	LEU	CA-C-N	5.26	125.06	119.28
14	b	122	LEU	C-N-CA	5.26	125.06	119.28
9	W	92	PRO	N-CA-C	5.25	119.28	111.41
10	J	145	HIS	N-CA-C	5.25	119.55	113.20
1	O	78	TYR	N-CA-C	5.24	116.24	108.86
4	R	233	ASN	N-CA-C	5.23	117.65	111.33
10	X	145	HIS	N-CA-C	5.22	119.52	113.20
12	L	34	PHE	N-CA-C	5.22	118.09	109.85
2	B	79	VAL	N-CA-C	5.20	116.46	108.71
1	A	12	LEU	N-CA-C	-5.20	106.96	113.72
4	D	233	ASN	N-CA-C	5.19	117.61	111.33
12	Z	201	GLY	N-CA-C	5.18	116.79	111.56
9	W	22	GLN	CB-CA-C	-5.17	110.63	116.63
8	V	164	TRP	N-CA-C	5.15	116.97	111.36
10	X	178	ILE	N-CA-C	-5.15	100.90	108.11
2	P	79	VAL	N-CA-C	5.14	116.37	108.71
9	I	22	GLN	CB-CA-C	-5.13	110.68	116.63
12	L	22	ASP	CB-CA-C	-5.12	110.26	117.23
1	O	217	ILE	N-CA-C	-5.10	99.17	107.28
9	I	92	PRO	N-CA-C	5.09	119.04	111.41
6	T	43	ASN	N-CA-C	5.09	118.59	112.38
8	H	98	LEU	N-CA-C	5.08	117.53	109.50
11	K	102	CYS	N-CA-C	5.08	117.25	109.07
7	U	75	ILE	N-CA-C	5.07	116.27	108.71
8	H	192	THR	CA-C-N	5.07	126.00	120.83
8	H	192	THR	C-N-CA	5.07	126.00	120.83
12	Z	65	TYR	N-CA-C	-5.07	105.75	111.28
5	E	99	LEU	N-CA-C	5.06	116.49	111.07
6	F	43	ASN	N-CA-C	5.06	118.55	112.38
1	O	70	LEU	N-CA-C	-5.06	105.95	112.68
12	Z	34	PHE	N-CA-C	5.05	117.83	109.85
6	F	145	GLY	N-CA-C	5.05	120.28	112.45
12	Z	115	PHE	N-CA-C	5.05	117.83	109.85
13	M	1	SER	N-CA-C	5.03	121.51	110.80
5	E	110	ALA	N-CA-C	-5.03	105.93	111.71
14	b	123	PRO	N-CA-C	-5.02	106.87	113.65
4	D	120	ALA	N-CA-C	5.02	119.59	111.37
12	L	117	PRO	N-CA-C	-5.01	107.59	113.86
4	R	225	GLN	N-CA-C	5.01	117.52	111.40
4	R	187	TRP	N-CA-C	5.01	117.47	109.96

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	164	TYR	Sidechain
12	Z	164	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	67	0
1	O	1915	0	1926	70	0
2	B	1905	0	1901	81	0
2	P	1905	0	1901	87	0
3	C	1891	0	1900	93	0
3	Q	1891	0	1900	92	0
4	D	1862	0	1836	56	0
4	R	1862	0	1836	58	0
5	E	1795	0	1797	100	0
5	S	1795	0	1797	103	0
6	F	1897	0	1886	78	0
6	T	1897	0	1886	81	0
7	G	1921	0	1910	85	0
7	U	1921	0	1910	87	0
8	H	1685	0	1687	61	0
8	V	1685	0	1687	60	0
9	I	1581	0	1574	58	0
9	W	1581	0	1574	58	0
10	J	1585	0	1590	72	0
10	X	1585	0	1590	72	0
11	K	1644	0	1594	58	0
11	Y	1644	0	1594	61	0
12	L	1757	0	1711	68	0
12	Z	1757	0	1711	68	0
13	M	1824	0	1832	67	0
13	a	1824	0	1832	69	0
14	N	1512	0	1480	57	0
14	b	1512	0	1480	57	0
15	1	38	0	34	4	0
15	2	38	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	3	38	0	34	2	0
15	4	38	0	34	4	0
15	5	38	0	34	1	0
15	6	38	0	34	2	0
16	1	1	0	0	0	0
16	2	1	0	0	0	0
16	3	1	0	0	0	0
16	A	59	0	0	1	0
16	B	35	0	0	0	0
16	C	44	0	0	5	0
16	D	39	0	0	4	0
16	E	23	0	0	2	0
16	F	49	0	0	2	0
16	G	60	0	0	6	0
16	H	49	0	0	3	0
16	I	64	0	0	2	0
16	J	53	0	0	2	0
16	K	42	0	0	3	0
16	L	55	0	0	4	0
16	M	75	0	0	3	0
16	N	56	0	0	3	0
16	O	34	0	0	1	0
16	P	28	0	0	1	0
16	Q	29	0	0	2	0
16	R	33	0	0	2	0
16	S	21	0	0	0	0
16	T	39	0	0	2	0
16	U	63	0	0	2	0
16	V	47	0	0	5	0
16	W	55	0	0	2	0
16	X	46	0	0	4	0
16	Y	50	0	0	5	0
16	Z	51	0	0	2	0
16	a	73	0	0	1	0
16	b	58	0	0	7	0
All	All	51109	0	49452	1823	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 18.

All (1823) 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)
10:J:172:MET:HE3	10:X:172:MET:HE3	1.24	1.14
2:P:203:THR:HG22	2:P:205:SER:H	1.08	1.13
11:K:107:LYS:H	11:K:107:LYS:HD2	1.03	1.11
11:Y:107:LYS:H	11:Y:107:LYS:HD2	1.04	1.11
2:B:203:THR:HG22	2:B:205:SER:H	1.11	1.06
2:P:72:ASN:ND2	2:P:73:ASP:H	1.56	1.04
2:B:72:ASN:ND2	2:B:73:ASP:H	1.54	1.03
1:A:131:ARG:HH21	7:G:125:THR:HG22	1.23	1.02
1:O:131:ARG:HH21	7:U:125:THR:HG22	1.21	1.02
11:K:208:ASN:HD21	10:X:148:PRO:HG3	1.21	1.01
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.43	1.00
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.24	1.00
10:J:148:PRO:HG3	11:Y:208:ASN:HD21	1.25	1.00
4:R:68:VAL:HG21	4:R:89:ILE:HD12	1.44	0.99
13:a:5:MET:HG2	13:a:168:ILE:HD11	1.46	0.98
13:M:5:MET:HG2	13:M:168:ILE:HD11	1.44	0.98
13:M:170:ASN:HD22	13:M:173:ARG:HH11	1.04	0.98
4:D:68:VAL:HG21	4:D:89:ILE:HD12	1.45	0.98
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.44	0.98
7:U:97:ALA:HA	7:U:108:MET:HE2	1.45	0.97
7:G:97:ALA:HA	7:G:108:MET:HE2	1.47	0.97
9:I:5:MET:HE3	9:I:157:ILE:HG13	1.46	0.97
9:W:5:MET:HE3	9:W:157:ILE:HG13	1.45	0.97
13:a:170:ASN:HD22	13:a:173:ARG:HH11	1.05	0.97
2:B:125:THR:HG22	3:C:131:ARG:HH21	1.30	0.96
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.25	0.95
3:Q:166:GLN:HE21	3:Q:167:THR:H	1.09	0.94
2:B:15:PHE:H	3:C:23:GLN:HE22	1.09	0.94
11:K:45:MET:HG2	11:K:52:CYS:HB3	1.49	0.94
3:C:166:GLN:HE21	3:C:167:THR:H	1.09	0.94
1:A:125:THR:HG22	2:B:131:ARG:HH21	1.30	0.94
1:O:125:THR:HG22	2:P:131:ARG:HH21	1.31	0.94
2:P:125:THR:HG22	3:Q:131:ARG:HH21	1.31	0.94
10:J:-1:MET:HG2	10:J:0:ASP:H	1.33	0.93
10:X:-1:MET:HG2	10:X:0:ASP:H	1.35	0.92
1:O:15:PHE:H	2:P:23:GLN:HE22	1.14	0.91
5:S:203:LEU:HD11	5:S:208:LEU:HD22	1.52	0.91
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.17	0.91
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.36	0.91
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	1.51	0.90
5:E:203:LEU:HD11	5:E:208:LEU:HD22	1.53	0.90
2:B:226:GLU:HG2	2:B:227:VAL:H	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:226:GLU:HG2	2:P:227:VAL:H	1.38	0.88
11:Y:107:LYS:HD2	11:Y:107:LYS:N	1.89	0.88
11:K:107:LYS:HD2	11:K:107:LYS:N	1.88	0.87
2:P:72:ASN:HD22	2:P:73:ASP:H	1.23	0.87
2:B:72:ASN:HD22	2:B:73:ASP:H	1.22	0.86
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.40	0.86
3:C:191:THR:HB	3:C:194:GLU:HG2	1.57	0.85
7:U:71:ILE:HD11	7:U:77:MET:HB3	1.58	0.85
3:Q:191:THR:HB	3:Q:194:GLU:HG2	1.59	0.84
7:G:192:GLU:HG2	7:G:197:LYS:HB2	1.60	0.84
9:W:8:LYS:HD3	9:W:147:ASN:HD22	1.42	0.84
3:Q:201:ARG:HG3	3:Q:240:ILE:HD13	1.58	0.83
3:C:166:GLN:HE22	3:C:176:ARG:HE	1.26	0.83
1:O:33:GLN:HE21	1:O:33:GLN:HA	1.43	0.83
2:B:72:ASN:HD22	2:B:73:ASP:N	1.76	0.83
5:S:209:THR:H	5:S:212:ASN:HD22	1.25	0.83
3:C:101:ARG:NH1	3:C:107:PRO:HB3	1.94	0.83
1:O:86:ARG:HE	7:U:119:ASN:HD21	1.24	0.83
3:Q:236:TYR:O	3:Q:240:ILE:HG13	1.77	0.83
7:U:192:GLU:HG2	7:U:197:LYS:HB2	1.60	0.83
7:G:71:ILE:HD11	7:G:77:MET:HB3	1.61	0.82
8:H:52:THR:O	8:H:56:THR:HB	1.79	0.82
2:B:125:THR:CG2	3:C:131:ARG:HH21	1.92	0.82
9:I:8:LYS:HD3	9:I:147:ASN:HD22	1.45	0.82
12:Z:99:THR:HG23	16:Z:309:HOH:O	1.79	0.82
1:A:15:PHE:H	2:B:23:GLN:HE22	1.26	0.81
5:E:209:THR:H	5:E:212:ASN:HD22	1.26	0.81
2:P:72:ASN:HD22	2:P:73:ASP:N	1.77	0.81
5:S:95:ASN:HD21	12:Z:60:ASN:HD21	1.24	0.81
3:Q:166:GLN:HE22	3:Q:176:ARG:HE	1.25	0.81
3:C:201:ARG:HG3	3:C:240:ILE:HD13	1.61	0.81
3:C:236:TYR:O	3:C:240:ILE:HG13	1.81	0.81
2:P:203:THR:HG22	2:P:205:SER:N	1.92	0.81
3:C:167:THR:HG21	3:C:175:VAL:HG13	1.62	0.80
3:Q:191:THR:HG22	3:Q:193:GLU:H	1.47	0.80
5:E:208:LEU:HD23	5:E:208:LEU:H	1.45	0.80
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.44	0.80
5:S:208:LEU:HD23	5:S:208:LEU:H	1.46	0.80
3:Q:101:ARG:NH1	3:Q:107:PRO:HB3	1.96	0.80
5:E:47:VAL:HG22	5:E:217:ILE:HG13	1.63	0.80
3:C:15:PHE:H	4:D:23:GLN:HE22	1.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:107:LYS:H	11:Y:107:LYS:CD	1.87	0.79
8:V:52:THR:O	8:V:56:THR:HB	1.83	0.79
11:Y:201:LYS:HE2	16:Y:330:HOH:O	1.82	0.79
3:C:166:GLN:NE2	3:C:167:THR:H	1.80	0.79
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.63	0.79
13:a:162:GLN:NE2	13:a:162:GLN:H	1.81	0.79
3:C:191:THR:HG22	3:C:193:GLU:H	1.47	0.79
13:a:152:ARG:HG3	13:a:152:ARG:HH11	1.48	0.79
10:J:172:MET:CE	10:X:172:MET:HE3	2.12	0.79
3:Q:167:THR:HG21	3:Q:175:VAL:HG13	1.62	0.79
13:M:152:ARG:HH11	13:M:152:ARG:HG3	1.49	0.78
3:Q:166:GLN:NE2	3:Q:167:THR:H	1.81	0.78
6:T:35:THR:HG21	6:T:51:GLU:O	1.83	0.78
14:N:136:GLY:HA2	14:b:161:GLN:NE2	1.99	0.78
2:P:72:ASN:ND2	2:P:73:ASP:N	2.32	0.78
4:R:169:ALA:HB3	5:S:58:LEU:HD23	1.66	0.78
8:V:34:LEU:HB2	16:V:315:HOH:O	1.82	0.78
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.65	0.78
5:E:72:MET:HE2	5:E:107:VAL:HA	1.65	0.77
13:M:162:GLN:NE2	13:M:162:GLN:H	1.82	0.77
2:B:72:ASN:ND2	2:B:73:ASP:N	2.30	0.77
5:E:95:ASN:HD21	12:L:60:ASN:HD21	1.27	0.77
11:K:208:ASN:HD21	10:X:148:PRO:CG	1.98	0.77
5:E:181:PHE:HA	5:E:184:ILE:HG12	1.67	0.77
14:N:161:GLN:NE2	14:b:136:GLY:HA2	1.98	0.77
5:E:200:SER:HA	5:E:203:LEU:HG	1.65	0.77
12:L:3:LEU:CD1	12:L:140:LEU:HD21	2.15	0.76
6:F:109:ILE:H	6:F:109:ILE:HD12	1.50	0.76
6:F:35:THR:HG21	6:F:51:GLU:O	1.84	0.76
5:S:72:MET:HE2	5:S:107:VAL:HA	1.67	0.76
13:M:39:ASN:H	13:M:39:ASN:HD22	1.33	0.76
5:S:181:PHE:HA	5:S:184:ILE:HG12	1.66	0.76
5:S:200:SER:HA	5:S:203:LEU:HG	1.66	0.76
7:U:122:GLN:O	7:U:125:THR:HB	1.86	0.76
1:A:86:ARG:HE	7:G:119:ASN:HD21	1.31	0.76
1:O:131:ARG:HH21	7:U:125:THR:CG2	1.98	0.76
13:a:40:THR:OG1	13:a:80:PRO:HG3	1.85	0.76
7:G:122:GLN:O	7:G:125:THR:HB	1.86	0.75
2:B:203:THR:HG22	2:B:205:SER:N	1.95	0.75
2:P:125:THR:CG2	3:Q:131:ARG:HH21	1.98	0.75
12:Z:185:HIS:HD2	12:Z:187:GLN:H	1.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:20:THR:HG23	14:N:31:THR:OG1	1.87	0.74
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.35	0.74
9:I:167:ARG:NH2	12:Z:137:MET:HE2	2.02	0.74
12:Z:3:LEU:CD1	12:Z:140:LEU:HD21	2.18	0.74
10:J:172:MET:HE3	10:X:172:MET:CE	2.11	0.74
1:O:125:THR:CG2	2:P:131:ARG:HH21	2.01	0.74
8:H:34:LEU:HB2	16:H:322:HOH:O	1.87	0.73
3:Q:191:THR:HG22	3:Q:193:GLU:N	2.02	0.73
5:S:47:VAL:HG22	5:S:217:ILE:HG13	1.69	0.73
3:C:191:THR:HG22	3:C:193:GLU:N	2.02	0.73
8:H:24:PRO:HG2	8:H:25:ILE:HD12	1.69	0.73
1:A:125:THR:CG2	2:B:131:ARG:HH21	1.99	0.73
7:G:60:LEU:O	7:G:62:PRO:HD3	1.88	0.73
12:L:137:MET:HE2	9:W:167:ARG:NH2	2.03	0.73
2:B:226:GLU:HG2	2:B:227:VAL:N	2.04	0.73
4:D:45:GLY:HA2	4:D:153:TYR:CE1	2.23	0.73
1:O:181:ARG:HB3	1:O:181:ARG:HH11	1.54	0.72
13:a:39:ASN:H	13:a:39:ASN:HD22	1.33	0.72
14:b:20:THR:HG23	14:b:31:THR:OG1	1.89	0.72
1:A:181:ARG:HB3	1:A:181:ARG:HH11	1.53	0.72
12:Z:13:LEU:HD13	12:Z:33:VAL:HG13	1.71	0.72
10:J:-1:MET:HG2	10:J:0:ASP:N	2.05	0.72
11:K:105:THR:OG1	11:K:108:GLU:HG3	1.89	0.72
11:Y:211:ILE:HG13	16:Y:339:HOH:O	1.90	0.72
6:T:109:ILE:H	6:T:109:ILE:HD12	1.54	0.72
11:Y:105:THR:OG1	11:Y:108:GLU:HG3	1.89	0.72
12:L:185:HIS:HD2	12:L:187:GLN:H	1.36	0.71
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.04	0.71
12:L:13:LEU:HD13	12:L:33:VAL:HG13	1.71	0.71
10:X:137:TYR:CE2	10:X:170:MET:HG3	2.26	0.71
11:K:99:THR:HG22	11:K:115:VAL:HB	1.71	0.71
4:R:45:GLY:HA2	4:R:153:TYR:CE1	2.25	0.71
11:K:107:LYS:H	11:K:107:LYS:CD	1.87	0.71
3:C:166:GLN:HE21	3:C:167:THR:N	1.87	0.71
9:I:139:MET:HE3	9:I:143:LEU:HD11	1.73	0.71
10:J:137:TYR:CE2	10:J:170:MET:HG3	2.26	0.71
11:K:201:LYS:HE2	16:K:332:HOH:O	1.90	0.71
13:M:40:THR:OG1	13:M:80:PRO:HG3	1.90	0.71
1:O:181:ARG:HB3	1:O:181:ARG:NH1	2.06	0.71
5:E:73:GLY:HA3	5:E:224:PHE:CE2	2.27	0.70
11:Y:99:THR:HG22	11:Y:115:VAL:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:236:LEU:O	6:F:240:ILE:HG12	1.91	0.70
2:P:226:GLU:HG2	2:P:227:VAL:N	2.06	0.70
1:A:181:ARG:HB3	1:A:181:ARG:NH1	2.06	0.70
8:V:24:PRO:HG2	8:V:25:ILE:HD12	1.72	0.70
10:J:148:PRO:CG	11:Y:208:ASN:HD21	2.02	0.70
9:W:139:MET:HE3	9:W:143:LEU:HD11	1.74	0.70
5:E:208:LEU:H	5:E:208:LEU:CD2	2.05	0.69
5:S:208:LEU:HA	5:S:212:ASN:ND2	2.06	0.69
7:U:60:LEU:O	7:U:62:PRO:HD3	1.92	0.69
10:X:-1:MET:HG2	10:X:0:ASP:N	2.06	0.69
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.92	0.69
4:D:169:ALA:HB3	5:E:58:LEU:HD23	1.74	0.69
11:Y:99:THR:HG22	11:Y:115:VAL:HB	1.73	0.69
1:O:122:GLN:O	1:O:125:THR:HB	1.92	0.69
2:B:78:ALA:HB3	2:B:138:ILE:HB	1.75	0.69
4:D:45:GLY:HA2	4:D:153:TYR:CD1	2.28	0.69
5:E:139:TYR:CE2	5:E:220:LYS:HA	2.28	0.69
5:E:208:LEU:HA	5:E:212:ASN:ND2	2.08	0.69
11:K:99:THR:HG22	11:K:115:VAL:O	1.91	0.69
5:S:208:LEU:H	5:S:208:LEU:CD2	2.05	0.68
7:U:226:LYS:HA	7:U:226:LYS:HE3	1.75	0.68
9:W:116:LEU:HD21	15:4:0:MH9:H3	1.73	0.68
3:Q:57:LYS:O	3:Q:58:LEU:HB2	1.92	0.68
3:C:57:LYS:O	3:C:58:LEU:HB2	1.92	0.68
3:Q:201:ARG:CG	3:Q:240:ILE:HD13	2.23	0.68
8:V:59:ILE:HG12	8:V:83:LEU:HD23	1.74	0.68
1:A:122:GLN:O	1:A:125:THR:HB	1.93	0.68
1:O:86:ARG:HE	7:U:119:ASN:ND2	1.90	0.68
2:P:78:ALA:HB3	2:P:138:ILE:HB	1.76	0.68
6:T:236:LEU:O	6:T:240:ILE:HG12	1.94	0.68
1:O:33:GLN:HE21	1:O:33:GLN:CA	2.07	0.68
14:N:103:ASP:HB2	16:N:233:HOH:O	1.94	0.67
10:X:62:ILE:HD11	10:X:78:VAL:HG13	1.74	0.67
4:D:24:VAL:O	4:D:27:SER:HB3	1.94	0.67
16:F:341:HOH:O	7:G:131:ARG:HB2	1.95	0.67
8:H:14:ILE:CD1	8:H:34:LEU:HG	2.25	0.67
14:N:107:LYS:HG2	14:N:108:GLY:N	2.09	0.67
2:P:187:LYS:HD3	2:P:188:VAL:N	2.09	0.67
14:b:163:ILE:HG23	14:b:170:GLY:HA2	1.75	0.67
2:B:187:LYS:HD3	2:B:188:VAL:N	2.10	0.67
7:G:241:LEU:O	7:G:244:ILE:HG13	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:20:ILE:HG22	12:L:25:ILE:HA	1.77	0.67
13:M:41:VAL:HG23	13:M:191:ILE:HD11	1.76	0.67
4:R:24:VAL:O	4:R:27:SER:HB3	1.94	0.67
14:b:107:LYS:HG2	14:b:108:GLY:N	2.10	0.67
3:C:201:ARG:CG	3:C:240:ILE:HD13	2.25	0.67
8:H:59:ILE:HG12	8:H:83:LEU:HD23	1.77	0.66
14:b:49:ALA:HA	16:b:219:HOH:O	1.94	0.66
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.94	0.66
3:Q:72:ASP:HA	10:X:67:ILE:HD12	1.77	0.66
10:J:51:THR:HG22	10:J:52:VAL:N	2.10	0.66
8:H:215:GLU:HG3	9:I:188:ARG:HG2	1.77	0.66
9:I:116:LEU:HD21	15:1:0:MH9:H3	1.78	0.66
13:M:39:ASN:HD22	13:M:39:ASN:N	1.93	0.66
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.08	0.66
6:F:95:GLU:HG2	6:F:115:ARG:CB	2.23	0.66
14:b:52:THR:OG1	16:b:219:HOH:O	2.12	0.66
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.77	0.66
2:B:122:GLN:O	2:B:125:THR:HB	1.96	0.66
6:T:190:ARG:HG3	6:T:190:ARG:HH11	1.61	0.66
7:G:226:LYS:HA	7:G:226:LYS:HE3	1.77	0.66
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.77	0.66
3:Q:166:GLN:HE21	3:Q:167:THR:N	1.87	0.66
5:S:139:TYR:CE2	5:S:220:LYS:HA	2.31	0.66
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.61	0.66
1:O:242:THR:OG1	1:O:245:GLU:HG3	1.96	0.65
13:M:178:ARG:NH2	8:V:135:MET:HE3	2.10	0.65
10:J:62:ILE:HD11	10:J:78:VAL:HG13	1.79	0.65
14:N:26:ILE:HG13	13:a:178:ARG:C	2.22	0.65
2:P:21:LEU:HD13	2:P:125:THR:HG23	1.78	0.65
5:S:90:LEU:HD11	5:S:110:ALA:HB1	1.78	0.65
7:U:68:ILE:HG13	7:U:220:GLU:HG2	1.79	0.65
1:A:242:THR:OG1	1:A:245:GLU:HG3	1.97	0.65
8:V:14:ILE:CD1	8:V:34:LEU:HG	2.26	0.65
10:X:51:THR:HG22	10:X:52:VAL:N	2.11	0.65
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.78	0.65
1:A:131:ARG:HH21	7:G:125:THR:CG2	2.03	0.65
12:L:3:LEU:HD11	12:L:140:LEU:HD21	1.79	0.65
5:S:181:PHE:HA	5:S:184:ILE:CG1	2.26	0.65
5:E:90:LEU:HD11	5:E:110:ALA:HB1	1.79	0.65
2:B:21:LEU:HD13	2:B:125:THR:HG23	1.78	0.65
7:U:241:LEU:O	7:U:244:ILE:HG13	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:26:VAL:HG13	16:X:223:HOH:O	1.96	0.65
6:F:136:THR:O	6:F:150:MET:HA	1.98	0.64
5:S:73:GLY:HA3	5:S:224:PHE:CE2	2.32	0.64
8:V:215:GLU:HG3	9:W:188:ARG:HG2	1.79	0.64
13:a:197:LEU:HD23	13:a:197:LEU:C	2.22	0.64
12:Z:20:ILE:HG22	12:Z:25:ILE:HA	1.78	0.64
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.61	0.64
8:H:135:MET:HE3	13:a:178:ARG:NH2	2.12	0.64
2:P:247:THR:OXT	2:P:247:THR:HG22	1.98	0.64
4:R:45:GLY:HA2	4:R:153:TYR:CD1	2.31	0.64
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.80	0.64
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.61	0.64
4:R:212:LEU:HD23	4:R:212:LEU:C	2.21	0.64
11:K:99:THR:CG2	11:K:115:VAL:HB	2.28	0.64
5:S:84:ARG:HH11	5:S:84:ARG:HG3	1.63	0.64
7:U:235:GLU:HG2	16:U:357:HOH:O	1.98	0.64
13:a:39:ASN:HD22	13:a:39:ASN:N	1.94	0.64
4:D:212:LEU:HD23	4:D:212:LEU:C	2.23	0.64
5:E:12:THR:HG21	5:E:122:THR:HA	1.80	0.64
6:T:18:ASP:OD1	6:T:20:ARG:HD3	1.98	0.64
6:F:190:ARG:HH11	6:F:190:ARG:HG3	1.63	0.64
2:P:52:ARG:HH22	2:P:64:SER:HB3	1.62	0.64
14:N:36:ARG:HH21	14:N:60:GLN:HE21	1.44	0.64
5:E:175:GLU:OE1	6:F:56:SER:HB2	1.97	0.64
13:M:170:ASN:HD22	13:M:173:ARG:NH1	1.87	0.64
12:L:116:ASP:HB2	12:L:120:SER:HB3	1.80	0.63
12:L:186:ILE:O	8:V:167:LEU:HD22	1.97	0.63
12:Z:116:ASP:HB2	12:Z:120:SER:HB3	1.80	0.63
5:E:182:ILE:O	5:E:182:ILE:HG12	1.97	0.63
2:P:122:GLN:O	2:P:125:THR:HB	1.98	0.63
5:S:203:LEU:HD11	5:S:208:LEU:CD2	2.28	0.63
14:b:36:ARG:HH21	14:b:60:GLN:HE21	1.46	0.63
2:B:125:THR:HG22	3:C:131:ARG:NH2	2.10	0.63
8:H:167:LEU:HD22	12:Z:186:ILE:O	1.97	0.63
10:J:17:LYS:HG2	10:J:178:ILE:HG13	1.80	0.63
1:O:113:LEU:O	1:O:117:VAL:HG23	1.97	0.63
2:P:61:GLN:OE1	2:P:211:ASP:HA	1.98	0.63
12:Z:3:LEU:HD11	12:Z:140:LEU:HD21	1.80	0.63
3:C:29:GLU:OE2	3:C:32:LYS:HE2	1.98	0.63
5:E:181:PHE:HA	5:E:184:ILE:CG1	2.27	0.63
2:B:52:ARG:HH22	2:B:64:SER:HB3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:182:ILE:O	5:S:182:ILE:HG12	1.97	0.63
5:S:229:GLY:O	5:S:232:VAL:HG22	1.99	0.63
6:T:95:GLU:HG2	6:T:115:ARG:CB	2.25	0.63
1:A:86:ARG:HE	7:G:119:ASN:ND2	1.96	0.63
2:B:247:THR:HG22	2:B:247:THR:OXT	1.98	0.63
4:D:127:ALA:HA	5:E:127:GLY:HA2	1.81	0.62
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.80	0.62
3:Q:29:GLU:OE2	3:Q:32:LYS:HE2	1.97	0.62
6:T:209:GLU:HG3	6:T:210:LYS:HG3	1.80	0.62
1:O:125:THR:HG22	2:P:131:ARG:NH2	2.11	0.62
13:a:41:VAL:HG23	13:a:191:ILE:HD11	1.79	0.62
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.29	0.62
3:Q:245:GLN:C	3:Q:247:GLN:H	2.07	0.62
2:B:61:GLN:OE1	2:B:211:ASP:HA	1.99	0.62
8:V:37:ILE:CD1	8:V:43:CYS:HB2	2.29	0.62
7:G:172:GLN:HE21	7:G:176:THR:HG23	1.64	0.62
5:S:182:ILE:HG23	5:S:183:LYS:HG3	1.81	0.62
3:C:107:PRO:HG2	3:C:144:PRO:HG3	1.81	0.62
5:E:84:ARG:HH11	5:E:84:ARG:HG3	1.64	0.62
2:P:88:ILE:O	2:P:92:THR:HG23	2.00	0.62
11:Y:99:THR:CG2	11:Y:115:VAL:HB	2.30	0.62
12:Z:136:ILE:HD11	12:Z:181:ALA:HB2	1.81	0.62
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.82	0.62
6:F:209:GLU:HG3	6:F:210:LYS:HG3	1.82	0.62
3:Q:107:PRO:HG2	3:Q:144:PRO:HG3	1.82	0.62
12:L:3:LEU:HD13	12:L:140:LEU:HD21	1.82	0.62
14:N:44:CYS:HB2	14:N:98:ILE:HB	1.81	0.62
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.81	0.62
9:W:1:ILE:HG21	9:W:132:ALA:HB3	1.82	0.62
12:Z:-6:PRO:O	13:a:95:ARG:NH1	2.32	0.62
5:S:12:THR:HG21	5:S:122:THR:HA	1.80	0.61
3:C:245:GLN:C	3:C:247:GLN:H	2.07	0.61
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.82	0.61
13:M:118:LEU:HG	13:M:133:LEU:HD12	1.81	0.61
3:Q:163:TRP:CE2	4:R:59:LEU:HD23	2.35	0.61
5:E:203:LEU:HD11	5:E:208:LEU:CD2	2.29	0.61
5:E:208:LEU:HD23	5:E:208:LEU:N	2.14	0.61
5:S:208:LEU:HD23	5:S:208:LEU:N	2.14	0.61
3:C:72:ASP:HA	10:J:67:ILE:HD12	1.83	0.61
4:D:184:LEU:HD22	5:E:58:LEU:HD13	1.83	0.61
4:D:85:ALA:O	4:D:89:ILE:HG12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:229:GLY:O	5:E:232:VAL:HG22	2.00	0.61
6:F:205:GLU:HG3	6:F:208:LYS:NZ	2.15	0.61
6:T:136:THR:O	6:T:150:MET:HA	2.00	0.61
6:F:69:VAL:HG12	16:F:307:HOH:O	1.99	0.61
4:R:85:ALA:O	4:R:89:ILE:HG12	2.01	0.61
6:T:205:GLU:HG3	6:T:208:LYS:NZ	2.16	0.61
13:a:118:LEU:HG	13:a:133:LEU:HD12	1.82	0.61
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.83	0.61
14:b:107:LYS:HG2	14:b:108:GLY:H	1.66	0.61
13:M:18:LEU:HB2	13:M:183:SER:HB2	1.81	0.61
5:S:95:ASN:ND2	12:Z:60:ASN:HD21	1.98	0.61
13:a:18:LEU:HB2	13:a:183:SER:HB2	1.82	0.61
1:A:13:THR:O	2:B:131:ARG:HD3	2.01	0.60
13:M:170:ASN:ND2	13:M:173:ARG:HH11	1.88	0.60
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.31	0.60
8:V:18:THR:HB	8:V:30:ASN:HA	1.82	0.60
10:X:17:LYS:HG2	10:X:178:ILE:HG13	1.83	0.60
8:H:37:ILE:CD1	8:H:43:CYS:HB2	2.30	0.60
14:N:107:LYS:HG2	14:N:108:GLY:H	1.65	0.60
3:Q:77:LEU:HD22	3:Q:90:ILE:HD13	1.83	0.60
2:B:232:PHE:H	2:B:232:PHE:HD2	1.50	0.60
5:E:210:VAL:HG13	5:E:211:ASP:N	2.16	0.60
2:P:102:LYS:HZ1	10:X:84:GLN:NE2	1.99	0.60
13:a:7:TYR:CE2	13:a:161:VAL:HG22	2.37	0.60
14:b:44:CYS:HB2	14:b:98:ILE:HB	1.81	0.60
1:A:113:LEU:O	1:A:117:VAL:HG23	2.00	0.60
5:E:182:ILE:HG23	5:E:183:LYS:HG3	1.82	0.60
6:F:18:ASP:OD1	6:F:20:ARG:HD3	2.01	0.60
10:J:137:TYR:HD1	16:Y:323:HOH:O	1.84	0.60
10:X:62:ILE:CD1	10:X:78:VAL:HG13	2.31	0.60
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.10	0.60
9:I:6:THR:CG2	9:I:111:ILE:HG12	2.31	0.60
1:O:86:ARG:HH21	7:U:119:ASN:HD22	1.49	0.60
11:K:208:ASN:ND2	10:X:148:PRO:HG3	2.06	0.60
5:S:210:VAL:HG13	5:S:211:ASP:N	2.17	0.60
10:J:37:SER:HB2	10:J:38:PRO:HD2	1.84	0.60
2:P:187:LYS:HE2	2:P:189:ASP:OD1	2.01	0.60
3:Q:107:PRO:HG2	3:Q:144:PRO:CG	2.31	0.60
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.66	0.60
3:C:57:LYS:HD2	3:C:58:LEU:N	2.16	0.60
9:W:107:GLY:HA2	9:W:182:LYS:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:LEU:HD23	2:B:113:LEU:C	2.27	0.59
2:P:113:LEU:HD23	2:P:113:LEU:C	2.27	0.59
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.17	0.59
10:X:37:SER:HB2	10:X:38:PRO:HD2	1.84	0.59
14:N:22:THR:HG22	15:3:1:THR:HA	1.82	0.59
7:U:172:GLN:HE21	7:U:176:THR:HG23	1.66	0.59
2:B:187:LYS:HE2	2:B:189:ASP:OD1	2.02	0.59
3:C:163:TRP:CE2	4:D:59:LEU:HD23	2.37	0.59
2:P:232:PHE:HD2	2:P:232:PHE:H	1.49	0.59
4:R:40:ILE:HG13	4:R:200:VAL:CG2	2.32	0.59
1:A:32:LYS:HE2	1:A:32:LYS:HA	1.83	0.59
3:C:107:PRO:HG2	3:C:144:PRO:CG	2.32	0.59
6:F:114:ASP:O	6:F:118:GLN:HG2	2.02	0.59
2:B:88:ILE:O	2:B:92:THR:HG23	2.02	0.59
7:U:12:ILE:HG13	7:U:14:ILE:HG23	1.85	0.59
8:H:18:THR:HB	8:H:30:ASN:HA	1.83	0.59
8:H:173:VAL:HB	8:H:191:LEU:HB2	1.84	0.59
6:T:114:ASP:O	6:T:118:GLN:HG2	2.02	0.59
13:a:170:ASN:ND2	13:a:173:ARG:HH11	1.89	0.59
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.85	0.59
10:J:62:ILE:CD1	10:J:78:VAL:HG13	2.33	0.59
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.38	0.59
12:L:136:ILE:HD11	12:L:181:ALA:HB2	1.85	0.59
13:M:197:LEU:HD23	13:M:197:LEU:C	2.26	0.59
12:Z:7:GLY:HA3	12:Z:10:PHE:CE2	2.37	0.59
3:Q:171:ASN:HB2	3:Q:206:VAL:HG11	1.84	0.59
6:T:195:GLN:O	6:T:199:ILE:HG12	2.03	0.59
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.85	0.59
9:W:6:THR:CG2	9:W:111:ILE:HG12	2.32	0.59
12:Z:20:ILE:HD12	12:Z:20:ILE:C	2.28	0.59
13:a:170:ASN:HD22	13:a:173:ARG:NH1	1.88	0.59
7:G:68:ILE:HG13	7:G:220:GLU:HG2	1.84	0.59
1:O:249:ARG:HH11	1:O:249:ARG:HG3	1.67	0.59
3:Q:231:GLU:H	3:Q:231:GLU:CD	2.11	0.59
5:S:192:ILE:O	5:S:196:VAL:HG23	2.02	0.58
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.84	0.58
12:L:-6:PRO:O	13:M:95:ARG:NH1	2.34	0.58
14:N:175:MET:HB2	14:N:186:LEU:HB2	1.84	0.58
5:S:136:ILE:HD13	5:S:136:ILE:N	2.19	0.58
6:T:158:TRP:CZ3	7:U:65:VAL:HA	2.38	0.58
7:G:207:ILE:HG23	7:G:212:THR:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:80:PRO:HD2	13:M:111:GLN:OE1	2.03	0.58
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.19	0.58
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.85	0.58
8:V:173:VAL:HB	8:V:191:LEU:HB2	1.84	0.58
13:M:7:TYR:CE2	13:M:161:VAL:HG22	2.39	0.58
8:V:195:VAL:HG23	16:V:318:HOH:O	2.03	0.58
1:A:249:ARG:HH11	1:A:249:ARG:HG3	1.69	0.58
7:G:87:ARG:HD2	16:G:317:HOH:O	2.02	0.58
7:U:192:GLU:HG2	7:U:197:LYS:CB	2.33	0.58
5:E:181:PHE:O	5:E:184:ILE:HG12	2.04	0.58
3:Q:173:LYS:HB2	16:Q:316:HOH:O	2.02	0.58
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.39	0.58
14:b:105:LYS:HD3	14:b:105:LYS:C	2.28	0.58
13:M:178:ARG:C	14:b:26:ILE:HG13	2.28	0.58
2:P:154:ASN:HB2	2:P:155:PRO:HD2	1.84	0.58
2:B:183:LYS:O	2:B:186:MET:HG3	2.03	0.58
5:E:130:TYR:O	5:E:151:PRO:HB3	2.04	0.58
6:F:205:GLU:O	6:F:208:LYS:HD2	2.04	0.58
4:R:97:VAL:HG11	11:Y:65:LEU:HD22	1.85	0.58
5:S:181:PHE:O	5:S:184:ILE:HG12	2.03	0.58
14:b:66:TYR:CD2	14:b:73:PRO:HB3	2.38	0.58
9:I:1:ILE:HG21	9:I:132:ALA:HB3	1.84	0.58
11:K:16:VAL:HG21	11:K:34:VAL:HG23	1.84	0.58
6:T:205:GLU:O	6:T:208:LYS:HD2	2.04	0.58
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.86	0.58
7:G:196:GLU:O	7:G:200:GLU:HG3	2.04	0.58
13:M:36:VAL:HG11	13:M:83:ILE:HD13	1.84	0.58
14:N:161:GLN:HE21	14:b:136:GLY:CA	2.08	0.58
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.85	0.58
7:U:207:ILE:HG23	7:U:212:THR:O	2.04	0.58
14:b:22:THR:HG22	15:6:1:THR:HA	1.85	0.58
14:N:105:LYS:C	14:N:105:LYS:HD3	2.29	0.57
5:S:199:ILE:HG23	5:S:200:SER:N	2.19	0.57
6:T:177:GLU:OE2	7:U:58:LYS:HE2	2.03	0.57
13:a:162:GLN:H	13:a:162:GLN:HE21	1.52	0.57
9:I:107:GLY:HA2	9:I:182:LYS:HD3	1.86	0.57
11:K:4:LEU:HD11	11:K:161:ILE:HG12	1.86	0.57
13:a:80:PRO:HD2	13:a:111:GLN:OE1	2.03	0.57
5:E:192:ILE:O	5:E:196:VAL:HG23	2.03	0.57
5:E:199:ILE:HG23	5:E:200:SER:N	2.18	0.57
14:N:66:TYR:CD2	14:N:73:PRO:HB3	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:144:GLN:O	8:V:145:ASP:HB2	2.04	0.57
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	2.01	0.57
3:C:231:GLU:CD	3:C:231:GLU:H	2.13	0.57
10:J:51:THR:HG22	10:J:52:VAL:HG23	1.86	0.57
12:L:111:ALA:HA	16:L:339:HOH:O	2.04	0.57
4:D:40:ILE:HG13	4:D:200:VAL:CG2	2.35	0.57
5:S:160:GLY:O	5:S:161:THR:HB	2.04	0.57
5:S:175:GLU:OE1	6:T:56:SER:HB2	2.04	0.57
9:W:5:MET:HE1	9:W:157:ILE:HA	1.87	0.57
2:B:142:TYR:CD1	2:B:227:VAL:HG21	2.40	0.57
12:L:2:ILE:HD13	12:L:45:ASN:HB2	1.85	0.57
3:Q:175:VAL:HG23	3:Q:202:SER:HB2	1.86	0.57
11:K:176:ASN:HD21	11:K:190:ASN:HD22	1.50	0.57
5:S:130:TYR:O	5:S:151:PRO:HB3	2.03	0.57
1:A:207:PHE:CE1	1:A:212:ILE:HD11	2.39	0.57
6:F:220:SER:HB3	6:F:223:GLU:HB2	1.87	0.57
1:O:13:THR:O	2:P:131:ARG:HD3	2.05	0.57
13:a:36:VAL:HG11	13:a:83:ILE:HD13	1.86	0.57
1:A:86:ARG:HH21	7:G:119:ASN:HD22	1.53	0.57
7:G:12:ILE:HG13	7:G:14:ILE:HG23	1.86	0.57
8:H:144:GLN:O	8:H:145:ASP:HB2	2.04	0.57
12:L:7:GLY:HA3	12:L:10:PHE:CE2	2.39	0.57
3:C:33:ARG:NH1	3:C:33:ARG:HB2	2.20	0.57
5:E:95:ASN:ND2	12:L:60:ASN:HD21	2.01	0.57
9:I:26:VAL:HG13	16:J:240:HOH:O	2.05	0.57
10:J:137:TYR:HE1	16:X:232:HOH:O	1.87	0.57
14:b:55:ILE:HD11	14:b:93:LEU:HD13	1.87	0.57
3:C:41:LYS:HG2	3:C:164:SER:O	2.05	0.56
10:J:151:THR:OG1	10:J:154:GLU:HG3	2.05	0.56
3:Q:176:ARG:O	3:Q:180:GLU:HG3	2.05	0.56
3:C:77:LEU:HD22	3:C:90:ILE:HD13	1.86	0.56
3:C:175:VAL:HG23	3:C:202:SER:HB2	1.87	0.56
13:M:162:GLN:H	13:M:162:GLN:HE21	1.52	0.56
14:N:40:LYS:C	14:N:41:ILE:HD12	2.30	0.56
2:P:154:ASN:HB2	2:P:155:PRO:CD	2.35	0.56
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.86	0.56
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	1.86	0.56
14:b:105:LYS:HD3	14:b:105:LYS:O	2.06	0.56
3:C:201:ARG:HD3	16:C:336:HOH:O	2.05	0.56
6:F:109:ILE:HD12	6:F:109:ILE:N	2.20	0.56
6:F:195:GLN:O	6:F:199:ILE:HG12	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:-7:ASN:ND2	12:L:-5:TYR:H	2.03	0.56
2:P:102:LYS:NZ	10:X:84:GLN:NE2	2.54	0.56
3:Q:203:LEU:O	3:Q:207:VAL:HG23	2.06	0.56
7:U:8:TYR:C	7:U:10:ARG:H	2.13	0.56
8:V:37:ILE:HD11	8:V:43:CYS:HB2	1.87	0.56
3:C:203:LEU:O	3:C:207:VAL:HG23	2.06	0.56
7:G:71:ILE:HD12	7:G:71:ILE:N	2.21	0.56
7:G:80:ASN:HA	16:G:345:HOH:O	2.05	0.56
10:J:51:THR:CG2	10:J:52:VAL:N	2.69	0.56
2:P:91:ASN:O	2:P:95:ILE:HD13	2.05	0.56
4:R:184:LEU:HD22	5:S:58:LEU:HD13	1.87	0.56
6:T:189:ALA:O	6:T:193:VAL:HG23	2.06	0.56
11:Y:4:LEU:HD11	11:Y:161:ILE:HG12	1.86	0.56
4:D:53:ARG:O	4:D:53:ARG:HG2	2.06	0.56
5:E:187:ASN:C	5:E:187:ASN:HD22	2.13	0.56
8:H:37:ILE:HD11	8:H:43:CYS:HB2	1.87	0.56
14:N:136:GLY:CA	14:b:161:GLN:HE21	2.09	0.56
4:R:127:ALA:HB3	4:R:132:ARG:HD3	1.87	0.56
2:B:154:ASN:HB2	2:B:155:PRO:CD	2.36	0.56
2:B:220:LYS:HG3	2:B:226:GLU:O	2.06	0.56
8:V:84:LYS:HG3	8:V:85:GLN:N	2.20	0.56
2:B:175:GLN:HG2	3:C:56:LEU:HD12	1.87	0.56
2:B:238:LYS:O	2:B:242:VAL:HG23	2.05	0.56
8:H:84:LYS:HG3	8:H:85:GLN:N	2.19	0.56
10:J:23:ILE:HG13	10:X:137:TYR:OH	2.05	0.56
14:b:73:PRO:HA	16:b:241:HOH:O	2.05	0.56
2:P:142:TYR:CD1	2:P:227:VAL:HG21	2.41	0.56
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.31	0.56
2:B:15:PHE:N	3:C:23:GLN:HE22	1.92	0.56
7:G:192:GLU:HG2	7:G:197:LYS:CB	2.32	0.56
10:X:151:THR:OG1	10:X:154:GLU:HG3	2.05	0.56
12:Z:3:LEU:HD13	12:Z:140:LEU:HD21	1.85	0.56
11:K:6:PHE:HA	11:K:125:ASP:O	2.06	0.55
14:N:55:ILE:HD11	14:N:93:LEU:HD13	1.88	0.55
7:U:73:ARG:HB2	7:U:73:ARG:NH1	2.20	0.55
7:G:8:TYR:C	7:G:10:ARG:H	2.13	0.55
3:Q:77:LEU:HD22	3:Q:90:ILE:CD1	2.36	0.55
5:S:187:ASN:C	5:S:187:ASN:HD22	2.14	0.55
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.88	0.55
8:H:220:ILE:HD11	9:I:185:VAL:HG21	1.87	0.55
3:Q:41:LYS:HG2	3:Q:164:SER:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:42:MET:HG3	12:Z:101:ILE:HG22	1.88	0.55
12:Z:136:ILE:HG22	12:Z:140:LEU:HD22	1.88	0.55
9:I:5:MET:HE1	9:I:157:ILE:HA	1.87	0.55
12:L:137:MET:CE	9:W:167:ARG:NH2	2.69	0.55
7:G:73:ARG:NH1	7:G:73:ARG:HB2	2.21	0.55
11:K:86:LEU:HD13	11:K:86:LEU:C	2.32	0.55
6:T:220:SER:HB3	6:T:223:GLU:HB2	1.88	0.55
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.21	0.55
14:N:19:ARG:HG3	14:N:26:ILE:HG23	1.89	0.55
5:E:76:LEU:HD12	5:E:76:LEU:C	2.31	0.55
5:E:160:GLY:O	5:E:161:THR:HB	2.05	0.55
5:E:230:GLU:CD	5:E:230:GLU:H	2.13	0.55
8:H:25:ILE:HD12	8:H:25:ILE:N	2.22	0.55
12:Z:13:LEU:HD13	12:Z:33:VAL:CG1	2.37	0.55
14:b:19:ARG:HG3	14:b:26:ILE:HG23	1.89	0.55
1:A:131:ARG:NH2	7:G:125:THR:HG22	2.07	0.55
4:D:97:VAL:HG11	11:K:65:LEU:HD22	1.89	0.55
7:G:39:LEU:C	7:G:39:LEU:HD12	2.31	0.55
11:K:44:THR:OG1	11:K:100:MET:HB2	2.07	0.55
14:N:105:LYS:HD3	14:N:105:LYS:O	2.07	0.55
2:P:38:ILE:HD13	2:P:166:SER:HB3	1.89	0.55
3:Q:171:ASN:O	3:Q:175:VAL:HG12	2.07	0.55
3:Q:232:GLU:O	3:Q:236:TYR:HD1	1.90	0.55
6:T:87:HIS:HD2	6:T:132:PHE:CE2	2.24	0.55
7:U:97:ALA:CA	7:U:108:MET:HE2	2.30	0.55
11:Y:44:THR:OG1	11:Y:100:MET:HB2	2.07	0.55
2:B:154:ASN:HB2	2:B:155:PRO:HD2	1.86	0.54
2:B:220:LYS:O	2:B:221:GLY:C	2.50	0.54
3:C:171:ASN:HB2	3:C:206:VAL:HG11	1.88	0.54
8:H:41:ILE:HD12	8:H:76:VAL:HG22	1.89	0.54
12:L:42:MET:HG3	12:L:101:ILE:HG22	1.88	0.54
2:P:183:LYS:O	2:P:186:MET:HG3	2.06	0.54
4:R:212:LEU:HD23	4:R:213:ASP:N	2.22	0.54
14:b:175:MET:HB2	14:b:186:LEU:HB2	1.89	0.54
1:A:143:ASP:OD1	1:A:146:ASN:HB2	2.08	0.54
13:M:88:ALA:HA	13:M:121:VAL:HG21	1.90	0.54
10:X:33:THR:HG21	10:X:180:LYS:NZ	2.22	0.54
10:X:51:THR:CG2	10:X:52:VAL:N	2.69	0.54
1:A:199:LEU:HD23	1:A:212:ILE:HD13	1.89	0.54
4:D:212:LEU:HD23	4:D:213:ASP:N	2.22	0.54
5:E:209:THR:OG1	5:E:212:ASN:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:172:GLN:NE2	7:G:176:THR:HG23	2.23	0.54
1:O:17:PRO:HA	2:P:26:TYR:CD1	2.42	0.54
1:O:111:LYS:HG2	16:O:310:HOH:O	2.07	0.54
4:R:112:LEU:HD13	4:R:112:LEU:C	2.33	0.54
6:T:109:ILE:HD12	6:T:109:ILE:N	2.23	0.54
3:C:155:GLU:HB2	3:C:156:PRO:HD2	1.89	0.54
6:F:189:ALA:O	6:F:193:VAL:HG23	2.08	0.54
7:U:196:GLU:O	7:U:200:GLU:HG3	2.06	0.54
12:Z:2:ILE:HD13	12:Z:45:ASN:HB2	1.88	0.54
12:Z:90:LYS:HE3	12:Z:93:PHE:O	2.08	0.54
10:J:137:TYR:OH	10:X:23:ILE:HG13	2.08	0.54
2:P:220:LYS:O	2:P:221:GLY:C	2.50	0.54
2:P:232:PHE:CD2	2:P:232:PHE:N	2.76	0.54
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.73	0.54
5:E:136:ILE:N	5:E:136:ILE:CD1	2.70	0.54
6:F:74:ILE:CD1	6:F:109:ILE:HG13	2.38	0.54
13:M:84:PHE:CE1	13:M:119:ARG:HD3	2.43	0.54
3:Q:33:ARG:CB	3:Q:33:ARG:HH11	2.20	0.54
6:T:200:ILE:HG21	6:T:214:LEU:HD13	1.89	0.54
13:a:216:ILE:HD13	13:a:216:ILE:N	2.22	0.54
4:D:130:GLU:HG2	4:D:131:GLU:H	1.71	0.54
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.89	0.54
11:K:158:LYS:HB2	11:K:177:LEU:HD11	1.90	0.54
14:b:15:GLY:HA2	14:b:174:ARG:O	2.08	0.54
5:E:65:ILE:HG21	5:E:216:ALA:HB2	1.90	0.54
2:P:52:ARG:HH22	2:P:64:SER:CB	2.20	0.54
6:T:172:ALA:O	6:T:176:LEU:HD23	2.07	0.54
9:W:5:MET:CE	9:W:157:ILE:HA	2.38	0.54
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.07	0.54
10:J:91:ARG:HG2	10:J:91:ARG:HH11	1.73	0.54
1:O:143:ASP:OD1	1:O:146:ASN:HB2	2.08	0.54
2:P:220:LYS:HG3	2:P:226:GLU:O	2.08	0.54
2:P:238:LYS:O	2:P:242:VAL:HG23	2.08	0.54
4:R:121:LEU:HB2	16:R:319:HOH:O	2.07	0.54
5:S:74:LEU:HB2	5:S:136:ILE:HD12	1.89	0.54
11:Y:12:ILE:HB	11:Y:180:VAL:HB	1.90	0.54
2:B:52:ARG:HH22	2:B:64:SER:CB	2.21	0.53
3:C:106:ASP:OD2	3:C:107:PRO:HD2	2.08	0.53
12:L:13:LEU:HD13	12:L:33:VAL:CG1	2.37	0.53
1:O:207:PHE:CE1	1:O:212:ILE:HD11	2.44	0.53
10:X:43:SER:OG	10:X:101:LEU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:6:LYS:HG3	13:a:156:ILE:HD12	1.90	0.53
6:F:87:HIS:HD2	6:F:132:PHE:CE2	2.26	0.53
11:K:145:LYS:HB2	11:K:148:LEU:CD1	2.38	0.53
12:L:136:ILE:HG22	12:L:140:LEU:HD22	1.88	0.53
5:S:65:ILE:HG21	5:S:216:ALA:HB2	1.90	0.53
11:Y:158:LYS:HB2	11:Y:177:LEU:HD11	1.89	0.53
9:I:158:SER:O	9:I:162:LEU:HB2	2.08	0.53
14:b:145:ASN:N	16:b:254:HOH:O	2.41	0.53
1:A:58:LEU:HD12	7:G:175:THR:HG23	1.90	0.53
9:I:167:ARG:NH2	12:Z:137:MET:CE	2.70	0.53
11:Y:65:LEU:HB3	11:Y:69:ARG:NH2	2.24	0.53
3:C:232:GLU:O	3:C:236:TYR:HD1	1.92	0.53
4:D:65:GLU:HA	16:D:311:HOH:O	2.08	0.53
6:F:127:ASN:HD22	6:F:127:ASN:C	2.17	0.53
12:L:20:ILE:C	12:L:20:ILE:HD12	2.33	0.53
12:L:93:PHE:N	12:L:94:PRO:HD3	2.23	0.53
5:S:209:THR:OG1	5:S:212:ASN:HB3	2.09	0.53
6:T:137:ILE:HA	6:T:149:TYR:O	2.09	0.53
3:C:171:ASN:O	3:C:175:VAL:HG12	2.08	0.53
9:I:176:VAL:HG21	9:I:187:LYS:HE3	1.91	0.53
10:J:43:SER:OG	10:J:101:LEU:HB2	2.08	0.53
14:N:139:ASP:HB3	14:b:161:GLN:HE22	1.73	0.53
5:S:230:GLU:CD	5:S:230:GLU:H	2.17	0.53
9:W:115:ASP:OD1	15:4:1:THR:HG23	2.08	0.53
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.22	0.53
3:C:176:ARG:O	3:C:180:GLU:HG3	2.09	0.53
5:E:74:LEU:HB2	5:E:136:ILE:HD12	1.90	0.53
7:G:154:ASP:HB2	7:G:155:PRO:CD	2.39	0.53
9:I:5:MET:CE	9:I:157:ILE:HA	2.39	0.53
14:N:147:SER:OG	14:N:150:GLU:HG3	2.09	0.53
1:O:60:MET:HE3	1:O:63:THR:HG21	1.91	0.53
7:U:71:ILE:HD12	7:U:71:ILE:N	2.24	0.53
9:W:176:VAL:HG21	9:W:187:LYS:CE	2.38	0.53
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.44	0.53
7:G:97:ALA:HA	7:G:108:MET:CE	2.31	0.53
9:I:115:ASP:OD1	15:1:1:THR:HG23	2.09	0.53
7:U:172:GLN:NE2	7:U:176:THR:HG23	2.24	0.53
13:a:88:ALA:HA	13:a:121:VAL:HG21	1.90	0.53
5:E:137:ILE:HG13	5:E:218:VAL:HG12	1.91	0.52
10:J:33:THR:HG21	10:J:180:LYS:NZ	2.24	0.52
12:L:90:LYS:HE3	12:L:93:PHE:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:161:GLN:HE22	14:b:139:ASP:HB3	1.73	0.52
2:B:232:PHE:HD2	2:B:232:PHE:N	2.07	0.52
11:K:12:ILE:HB	11:K:180:VAL:HB	1.89	0.52
11:K:144:TYR:O	11:K:145:LYS:HD2	2.09	0.52
3:Q:242:GLN:O	3:Q:246:GLU:HG3	2.09	0.52
4:R:130:GLU:HG2	4:R:131:GLU:H	1.72	0.52
6:T:214:LEU:HD21	6:T:216:ILE:HD11	1.91	0.52
9:W:5:MET:HB3	9:W:153:LEU:HD11	1.91	0.52
1:A:119:LYS:HE2	1:A:123:GLU:OE1	2.10	0.52
3:C:242:GLN:O	3:C:246:GLU:HG3	2.09	0.52
8:H:167:LEU:HB3	12:Z:186:ILE:HD13	1.92	0.52
8:H:209:THR:CG2	12:Z:149:GLN:HG2	2.39	0.52
11:K:201:LYS:HE3	11:K:207:PHE:O	2.09	0.52
6:T:74:ILE:CD1	6:T:109:ILE:HG13	2.39	0.52
12:Z:185:HIS:CD2	12:Z:187:GLN:H	2.22	0.52
1:A:31:VAL:HG11	1:A:136:SER:HB2	1.91	0.52
2:B:91:ASN:O	2:B:95:ILE:HD13	2.09	0.52
5:E:95:ASN:HD21	12:L:60:ASN:ND2	2.04	0.52
6:F:172:ALA:O	6:F:176:LEU:HD23	2.09	0.52
7:G:73:ARG:HB2	7:G:73:ARG:HH11	1.75	0.52
3:Q:152:TYR:CE1	3:Q:162:SER:HB3	2.44	0.52
5:S:64:LYS:O	5:S:75:SER:HA	2.09	0.52
8:V:53:GLU:O	8:V:57:GLN:HG3	2.10	0.52
10:X:91:ARG:HG2	10:X:91:ARG:HH11	1.74	0.52
11:Y:144:TYR:O	11:Y:145:LYS:HD2	2.10	0.52
5:E:230:GLU:CD	5:E:230:GLU:N	2.68	0.52
8:H:24:PRO:HG2	8:H:25:ILE:CD1	2.40	0.52
4:R:31:ILE:HD13	4:R:141:ALA:HB2	1.90	0.52
5:S:48:LEU:HG	5:S:137:ILE:HD13	1.92	0.52
2:B:232:PHE:N	2:B:232:PHE:CD2	2.77	0.52
7:G:97:ALA:CA	7:G:108:MET:HE2	2.31	0.52
9:I:111:ILE:HD12	9:I:127:ILE:HG12	1.91	0.52
9:I:176:VAL:HG21	9:I:187:LYS:CE	2.39	0.52
2:P:232:PHE:HD2	2:P:232:PHE:N	2.06	0.52
7:U:154:ASP:HB2	7:U:155:PRO:CD	2.39	0.52
8:V:25:ILE:HD12	8:V:25:ILE:N	2.23	0.52
8:V:172:ASN:ND2	16:V:331:HOH:O	2.43	0.52
11:Y:145:LYS:HB2	11:Y:148:LEU:CD1	2.39	0.52
3:C:31:VAL:HG11	3:C:136:SER:HB2	1.92	0.52
5:E:64:LYS:O	5:E:75:SER:HA	2.08	0.52
7:G:236:ASN:HD22	7:G:236:ASN:N	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:31:VAL:HG11	1:O:136:SER:HB2	1.92	0.52
3:Q:231:GLU:OE1	3:Q:231:GLU:N	2.38	0.52
7:U:39:LEU:C	7:U:39:LEU:HD12	2.35	0.52
7:U:97:ALA:HA	7:U:108:MET:CE	2.30	0.52
8:V:41:ILE:HD12	8:V:76:VAL:HG22	1.91	0.52
9:I:28:ASN:HB2	16:I:233:HOH:O	2.09	0.52
13:M:216:ILE:N	13:M:216:ILE:HD13	2.24	0.52
14:N:13:ILE:HD12	14:N:151:THR:CG2	2.40	0.52
1:O:119:LYS:HE2	1:O:123:GLU:OE1	2.09	0.52
4:R:70:ILE:HG13	4:R:74:ILE:HG22	1.91	0.52
5:S:76:LEU:C	5:S:76:LEU:HD12	2.34	0.52
9:W:158:SER:O	9:W:162:LEU:HB2	2.10	0.52
2:B:113:LEU:HD23	2:B:113:LEU:O	2.10	0.52
4:D:167:TYR:CE2	4:D:170:LYS:HD3	2.45	0.52
11:K:105:THR:HG1	11:K:108:GLU:HG3	1.74	0.52
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.45	0.52
13:M:6:LYS:HG3	13:M:156:ILE:HD12	1.92	0.52
7:U:240:ARG:NE	7:U:240:ARG:HA	2.25	0.52
1:A:152:GLN:O	1:A:159:TYR:HA	2.10	0.51
1:A:190:ASP:O	1:A:194:ILE:HG12	2.10	0.51
4:D:24:VAL:O	4:D:28:LEU:HD13	2.11	0.51
1:O:57:PRO:HG3	7:U:179:GLU:CD	2.36	0.51
1:O:200:LYS:HA	1:O:207:PHE:CE1	2.44	0.51
5:S:4:PHE:HZ	5:S:18:THR:HG23	1.75	0.51
5:S:136:ILE:N	5:S:136:ILE:CD1	2.73	0.51
7:U:73:ARG:HB2	7:U:73:ARG:HH11	1.74	0.51
9:W:176:VAL:HG21	9:W:187:LYS:HE3	1.92	0.51
10:X:51:THR:HG22	10:X:52:VAL:HG23	1.92	0.51
1:A:60:MET:HE3	1:A:63:THR:HG21	1.91	0.51
3:C:77:LEU:HD22	3:C:90:ILE:CD1	2.40	0.51
4:D:127:ALA:HB3	4:D:132:ARG:HD3	1.91	0.51
10:J:188:ARG:HG2	10:J:188:ARG:HH11	1.75	0.51
13:M:-5:PRO:C	13:M:-4:ILE:HD12	2.35	0.51
13:M:5:MET:CG	13:M:168:ILE:HD11	2.29	0.51
3:Q:188:PRO:O	3:Q:190:ALA:N	2.43	0.51
4:R:122:ARG:HG2	4:R:122:ARG:HH11	1.75	0.51
5:S:217:ILE:HG12	5:S:218:VAL:N	2.25	0.51
14:b:14:LEU:O	14:b:175:MET:HA	2.10	0.51
3:C:138:LEU:HG	3:C:168:ILE:HD13	1.91	0.51
6:F:185:GLU:H	6:F:185:GLU:CD	2.17	0.51
14:N:15:GLY:HA2	14:N:174:ARG:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:53:ARG:O	4:R:53:ARG:HG2	2.10	0.51
2:B:38:ILE:HD13	2:B:166:SER:HB3	1.92	0.51
4:D:75:GLY:HA3	4:D:228:PHE:CD2	2.45	0.51
4:D:129:GLY:HA3	16:E:315:HOH:O	2.10	0.51
5:E:36:VAL:HG13	5:E:199:ILE:HD11	1.91	0.51
9:I:5:MET:HB3	9:I:153:LEU:HD11	1.93	0.51
9:I:154:PHE:HB2	9:I:179:ILE:HD11	1.92	0.51
4:R:167:TYR:CE2	4:R:170:LYS:HD3	2.45	0.51
6:T:87:HIS:HD2	6:T:132:PHE:HE2	1.58	0.51
6:T:127:ASN:HD22	6:T:127:ASN:C	2.18	0.51
8:V:2:THR:OG1	8:V:130:GLY:HA3	2.10	0.51
2:B:192:ILE:HG23	2:B:215:PHE:CE2	2.46	0.51
5:E:111:GLY:HA3	16:E:317:HOH:O	2.10	0.51
6:F:244:GLN:O	6:F:247:ILE:HG22	2.11	0.51
7:G:83:ILE:N	7:G:84:PRO:HD2	2.25	0.51
2:P:63:THR:O	2:P:63:THR:HG22	2.11	0.51
13:a:152:ARG:HH11	13:a:152:ARG:CG	2.22	0.51
1:A:208:ASN:HA	1:A:250:LEU:CD1	2.41	0.51
1:A:208:ASN:O	1:A:212:ILE:HG13	2.11	0.51
2:B:63:THR:O	2:B:63:THR:HG22	2.11	0.51
4:D:70:ILE:HG13	4:D:74:ILE:HG22	1.93	0.51
4:D:210:GLU:HA	4:D:210:GLU:OE2	2.11	0.51
5:E:48:LEU:HD13	5:E:75:SER:HB3	1.92	0.51
7:G:240:ARG:HA	7:G:240:ARG:NE	2.26	0.51
10:J:127:PRO:HB2	10:J:128:TYR:CD1	2.45	0.51
3:Q:155:GLU:HB2	3:Q:156:PRO:HD2	1.91	0.51
4:R:210:GLU:HA	4:R:210:GLU:OE2	2.11	0.51
10:X:101:LEU:CD2	10:X:116:GLN:HG3	2.40	0.51
3:C:239:GLN:O	3:C:243:GLU:HG2	2.11	0.51
8:H:2:THR:OG1	8:H:130:GLY:HA3	2.11	0.51
12:L:198:THR:C	12:L:200:ASP:H	2.19	0.51
2:P:102:LYS:HZ1	10:X:84:GLN:HE22	1.59	0.51
5:S:137:ILE:HG13	5:S:218:VAL:HG12	1.92	0.51
6:T:209:GLU:HG3	6:T:210:LYS:N	2.26	0.51
7:U:83:ILE:N	7:U:84:PRO:HD2	2.25	0.51
12:Z:198:THR:C	12:Z:200:ASP:H	2.19	0.51
4:D:112:LEU:C	4:D:112:LEU:HD13	2.36	0.51
2:P:192:ILE:HG23	2:P:215:PHE:CE2	2.46	0.51
5:S:74:LEU:CB	5:S:136:ILE:HD12	2.40	0.51
6:T:120:VAL:HG21	6:T:151:LEU:HD21	1.93	0.51
6:T:185:GLU:H	6:T:185:GLU:CD	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:111:ILE:HD12	9:W:127:ILE:HG12	1.92	0.51
5:E:4:PHE:HZ	5:E:18:THR:HG23	1.75	0.51
7:G:203:ILE:O	7:G:207:ILE:HG13	2.11	0.51
3:Q:239:GLN:O	3:Q:243:GLU:HG2	2.10	0.51
6:T:244:GLN:O	6:T:247:ILE:HG22	2.10	0.51
12:Z:-7:ASN:C	12:Z:-7:ASN:HD22	2.18	0.51
5:E:136:ILE:N	5:E:136:ILE:HD13	2.26	0.50
10:J:160:LYS:O	10:J:164:GLN:HG3	2.12	0.50
13:M:218:GLY:HA3	13:M:222:GLN:HB3	1.93	0.50
10:X:51:THR:HG22	10:X:52:VAL:H	1.77	0.50
11:Y:176:ASN:HD21	11:Y:190:ASN:HD22	1.56	0.50
1:A:200:LYS:HA	1:A:207:PHE:CE1	2.47	0.50
10:J:128:TYR:CD2	10:J:142:LEU:HD13	2.47	0.50
12:L:6:ALA:HB2	12:L:112:VAL:HG23	1.93	0.50
12:Z:116:ASP:CB	12:Z:120:SER:H	2.23	0.50
13:a:18:LEU:HD21	13:a:25:LEU:HD22	1.93	0.50
13:a:152:ARG:HG3	13:a:152:ARG:NH1	2.23	0.50
3:C:231:GLU:OE1	3:C:231:GLU:N	2.38	0.50
6:F:120:VAL:HG21	6:F:151:LEU:HD21	1.93	0.50
6:F:137:ILE:HA	6:F:149:TYR:O	2.11	0.50
8:H:159:ILE:O	8:H:163:ILE:HG12	2.11	0.50
14:N:114:PRO:HD2	14:N:118:SER:O	2.12	0.50
2:P:236:GLU:O	2:P:240:ILE:HG22	2.11	0.50
6:T:35:THR:CG2	6:T:36:THR:N	2.74	0.50
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.92	0.50
8:V:220:ILE:HD11	9:W:185:VAL:HG21	1.92	0.50
13:a:218:GLY:HA3	13:a:222:GLN:HB3	1.93	0.50
2:B:70:LYS:HE2	2:B:231:ILE:HD11	1.94	0.50
5:E:72:MET:CE	5:E:107:VAL:HA	2.37	0.50
7:G:21:LEU:HA	16:G:304:HOH:O	2.11	0.50
12:L:0:GLY:HA3	12:L:32:LYS:NZ	2.27	0.50
7:U:153:THR:HG22	7:U:159:TYR:HB2	1.94	0.50
14:b:147:SER:OG	14:b:150:GLU:HG3	2.11	0.50
1:A:51:GLU:OE1	1:A:203:VAL:HG22	2.11	0.50
3:C:100:HIS:CG	3:C:108:VAL:HG12	2.47	0.50
7:G:44:LYS:HZ2	7:G:191:ASN:ND2	2.10	0.50
7:G:78:VAL:HG12	7:G:138:THR:HB	1.94	0.50
7:G:153:THR:HG22	7:G:159:TYR:HB2	1.94	0.50
4:R:24:VAL:O	4:R:28:LEU:HD13	2.12	0.50
5:S:62:GLN:NE2	5:S:80:ALA:HB2	2.27	0.50
7:U:88:ASN:C	7:U:88:ASN:HD22	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:18:ARG:HB2	9:W:173:TRP:HB2	1.94	0.50
5:E:71:HIS:HE1	5:E:105:LEU:O	1.95	0.50
7:G:108:MET:HE3	7:G:113:LEU:HD13	1.94	0.50
9:W:154:PHE:HB2	9:W:179:ILE:HD11	1.94	0.50
13:a:84:PHE:CE1	13:a:119:ARG:HD3	2.47	0.50
6:F:158:TRP:CZ3	7:G:65:VAL:HA	2.47	0.50
6:F:214:LEU:HD21	6:F:216:ILE:HD11	1.93	0.50
13:M:-4:ILE:HG22	13:M:-3:VAL:N	2.26	0.50
7:U:78:VAL:HG12	7:U:138:THR:HB	1.92	0.50
7:G:195:TRP:O	7:G:199:VAL:HG23	2.12	0.50
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.93	0.50
8:H:196:ARG:NH2	9:I:141:GLU:O	2.45	0.50
9:I:33:ILE:HB	16:I:258:HOH:O	2.11	0.50
6:T:247:ILE:O	6:T:247:ILE:HG12	2.10	0.50
10:X:127:PRO:HB2	10:X:128:TYR:CD1	2.47	0.50
5:E:181:PHE:CA	5:E:184:ILE:HG12	2.40	0.50
7:G:225:THR:HB	16:G:323:HOH:O	2.11	0.50
14:N:26:ILE:HG13	13:a:178:ARG:HA	1.93	0.50
3:Q:31:VAL:HG11	3:Q:136:SER:HB2	1.94	0.50
5:S:71:HIS:HE1	5:S:105:LEU:O	1.95	0.50
6:T:200:ILE:HG21	6:T:214:LEU:CD1	2.42	0.50
11:Y:4:LEU:CD1	11:Y:161:ILE:HG12	2.41	0.50
10:J:2:ILE:HG22	10:J:101:LEU:CD1	2.42	0.49
11:K:65:LEU:HB3	11:K:69:ARG:NH2	2.28	0.49
3:Q:106:ASP:OD2	3:Q:107:PRO:HD2	2.12	0.49
5:S:203:LEU:O	5:S:204:ARG:HB2	2.12	0.49
7:U:35:ASN:HD22	7:U:169:PRO:HG2	1.77	0.49
4:D:31:ILE:HD13	4:D:141:ALA:HB2	1.94	0.49
12:L:-2:ASN:HA	12:L:20:ILE:O	2.11	0.49
12:L:186:ILE:HD13	8:V:167:LEU:HB3	1.94	0.49
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.94	0.49
3:Q:212:LYS:HD2	3:Q:212:LYS:O	2.12	0.49
10:X:2:ILE:HG22	10:X:101:LEU:CD1	2.41	0.49
2:B:98:GLN:HE22	9:I:62:ASN:HD22	1.59	0.49
1:O:152:GLN:O	1:O:159:TYR:HA	2.11	0.49
2:P:125:THR:HG22	3:Q:131:ARG:NH2	2.12	0.49
3:Q:138:LEU:HG	3:Q:168:ILE:HD13	1.93	0.49
5:S:36:VAL:HG13	5:S:199:ILE:HD11	1.93	0.49
5:S:72:MET:CE	5:S:107:VAL:HA	2.39	0.49
6:T:206:ASP:OD1	6:T:206:ASP:N	2.45	0.49
7:U:170:LYS:O	7:U:174:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:160:LYS:O	10:X:164:GLN:HG3	2.12	0.49
2:B:236:GLU:O	2:B:240:ILE:HG22	2.12	0.49
3:C:35:THR:HB	3:C:51:GLU:HG3	1.93	0.49
8:H:199:LYS:HE3	9:I:142:SER:O	2.12	0.49
11:K:106:ARG:HG2	11:K:106:ARG:HH11	1.77	0.49
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.76	0.49
12:L:176:ASP:OD1	8:V:203:TYR:OH	2.27	0.49
13:M:45:SER:OG	13:M:104:ALA:HB3	2.12	0.49
13:M:152:ARG:HH11	13:M:152:ARG:CG	2.23	0.49
14:N:4:MET:HE3	14:N:126:ILE:HG22	1.94	0.49
14:N:14:LEU:O	14:N:175:MET:HA	2.12	0.49
3:Q:100:HIS:CG	3:Q:108:VAL:HG12	2.46	0.49
4:R:75:GLY:HA3	4:R:228:PHE:CD2	2.47	0.49
5:S:177:THR:O	5:S:177:THR:HG22	2.12	0.49
7:U:88:ASN:C	7:U:88:ASN:ND2	2.70	0.49
9:W:87:GLU:HG2	9:W:88:ARG:HH12	1.77	0.49
11:Y:151:GLU:HB2	16:Y:336:HOH:O	2.13	0.49
5:E:203:LEU:O	5:E:204:ARG:HB2	2.12	0.49
7:G:36:ILE:HG22	7:G:37:ASN:N	2.27	0.49
7:G:88:ASN:C	7:G:88:ASN:HD22	2.21	0.49
7:U:36:ILE:HG22	7:U:37:ASN:N	2.27	0.49
9:W:46:LEU:HG	9:W:48:THR:HG22	1.95	0.49
10:X:117:ILE:HG12	10:X:123:LYS:HG3	1.95	0.49
5:E:210:VAL:CG1	5:E:211:ASP:N	2.75	0.49
6:F:40:ILE:HD12	6:F:196:ALA:HB2	1.95	0.49
7:G:78:VAL:CG1	7:G:138:THR:HB	2.43	0.49
12:L:97:VAL:HG23	12:L:99:THR:HG22	1.93	0.49
3:Q:180:GLU:OE2	4:R:57:PRO:HD2	2.11	0.49
6:T:189:ALA:HB3	6:T:223:GLU:HG3	1.94	0.49
3:C:188:PRO:O	3:C:190:ALA:N	2.45	0.49
5:E:62:GLN:NE2	5:E:80:ALA:HB2	2.27	0.49
7:G:201:PHE:C	7:G:201:PHE:CD1	2.90	0.49
10:J:84:GLN:HB3	16:J:208:HOH:O	2.13	0.49
1:O:190:ASP:O	1:O:194:ILE:HG12	2.11	0.49
2:P:66:GLU:HG3	2:P:67:LYS:HG3	1.94	0.49
12:Z:142:ASN:O	12:Z:146:PHE:HA	2.12	0.49
5:E:234:LYS:H	5:E:234:LYS:HD2	1.78	0.49
6:F:200:ILE:HG21	6:F:214:LEU:HD13	1.93	0.49
7:G:170:LYS:O	7:G:174:ILE:HG12	2.13	0.49
10:J:51:THR:HG22	10:J:52:VAL:H	1.75	0.49
11:K:77:ALA:HA	11:K:113:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:116:ASP:CB	12:L:120:SER:H	2.26	0.49
12:L:185:HIS:CD2	12:L:187:GLN:H	2.23	0.49
1:O:208:ASN:HA	1:O:250:LEU:CD1	2.41	0.49
3:Q:36:CYS:H	3:Q:51:GLU:HG2	1.78	0.49
5:S:210:VAL:CG1	5:S:211:ASP:N	2.76	0.49
7:U:44:LYS:NZ	7:U:191:ASN:HD21	2.10	0.49
10:X:5:ILE:HD11	10:X:146:TYR:CD1	2.48	0.49
3:C:212:LYS:O	3:C:212:LYS:HD2	2.13	0.49
1:O:51:GLU:OE1	1:O:203:VAL:HG22	2.13	0.49
2:P:113:LEU:HD23	2:P:113:LEU:O	2.12	0.49
7:G:88:ASN:C	7:G:88:ASN:ND2	2.70	0.49
2:P:167:VAL:HA	16:P:315:HOH:O	2.12	0.49
10:X:188:ARG:HG2	10:X:188:ARG:HH11	1.78	0.49
11:Y:77:ALA:HA	11:Y:113:TYR:CE2	2.48	0.49
3:C:152:TYR:CE1	3:C:162:SER:HB3	2.48	0.48
4:D:123:PHE:CZ	4:D:137:PRO:HG3	2.48	0.48
6:F:87:HIS:HD2	6:F:132:PHE:HE2	1.60	0.48
7:G:44:LYS:HB2	7:G:192:GLU:O	2.13	0.48
2:P:223:ASN:O	2:P:224:ASP:HB2	2.13	0.48
6:T:40:ILE:HD12	6:T:196:ALA:HB2	1.95	0.48
2:B:223:ASN:O	2:B:224:ASP:HB2	2.13	0.48
3:C:184:ASP:OD1	3:C:186:LYS:HB2	2.12	0.48
6:F:189:ALA:HB3	6:F:223:GLU:HG3	1.94	0.48
13:M:178:ARG:HA	14:b:26:ILE:HG13	1.94	0.48
3:Q:163:TRP:CZ2	4:R:59:LEU:HD23	2.48	0.48
3:Q:171:ASN:CB	3:Q:206:VAL:HG11	2.42	0.48
8:V:18:THR:HG21	8:V:30:ASN:ND2	2.28	0.48
6:F:35:THR:CG2	6:F:36:THR:N	2.74	0.48
7:G:35:ASN:HD22	7:G:169:PRO:HG2	1.77	0.48
8:H:148:LYS:O	8:H:152:ILE:HG13	2.13	0.48
9:I:32:LYS:O	9:I:42:GLY:HA2	2.13	0.48
2:P:52:ARG:NH2	2:P:64:SER:HB3	2.28	0.48
5:S:80:ALA:HB3	5:S:81:PRO:HD3	1.94	0.48
7:U:78:VAL:CG1	7:U:138:THR:HB	2.43	0.48
5:E:217:ILE:HG12	5:E:218:VAL:N	2.29	0.48
6:F:157:TYR:CD1	6:F:157:TYR:C	2.91	0.48
9:I:6:THR:HG23	9:I:111:ILE:HG12	1.95	0.48
11:K:4:LEU:CD1	11:K:161:ILE:HG12	2.42	0.48
13:M:39:ASN:N	13:M:39:ASN:ND2	2.61	0.48
3:Q:77:LEU:HD12	3:Q:139:ILE:HG12	1.94	0.48
11:Y:201:LYS:HE3	11:Y:207:PHE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:179:THR:HB	16:b:243:HOH:O	2.14	0.48
8:H:147:THR:OG1	8:H:150:GLU:HG3	2.13	0.48
10:J:23:ILE:HD11	10:X:133:TYR:HB3	1.95	0.48
10:J:34:ARG:HD3	10:J:34:ARG:HA	1.61	0.48
5:S:181:PHE:CA	5:S:184:ILE:HG12	2.39	0.48
9:W:180:ILE:HG23	9:W:185:VAL:HG22	1.95	0.48
10:X:128:TYR:CD2	10:X:142:LEU:HD13	2.49	0.48
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.78	0.48
5:E:89:TYR:CD1	5:E:117:LYS:HD2	2.48	0.48
6:F:109:ILE:HG21	6:F:147:HIS:HB2	1.95	0.48
9:I:46:LEU:HG	9:I:48:THR:HG22	1.94	0.48
2:P:70:LYS:HE2	2:P:231:ILE:HD11	1.95	0.48
4:R:123:PHE:CZ	4:R:137:PRO:HG3	2.48	0.48
12:Z:-2:ASN:HA	12:Z:20:ILE:O	2.13	0.48
5:E:80:ALA:HB3	5:E:81:PRO:HD3	1.95	0.48
9:I:0:GLY:HA3	9:I:32:LYS:HE2	1.96	0.48
5:S:230:GLU:CD	5:S:230:GLU:N	2.70	0.48
5:S:234:LYS:HG2	5:S:235:TYR:CD1	2.49	0.48
7:U:201:PHE:CD1	7:U:201:PHE:C	2.90	0.48
8:V:147:THR:OG1	8:V:150:GLU:HG3	2.14	0.48
12:Z:18:ARG:NE	12:Z:190:ASP:OD2	2.46	0.48
6:F:209:GLU:HG3	6:F:210:LYS:N	2.28	0.48
10:J:101:LEU:CD2	10:J:116:GLN:HG3	2.43	0.48
10:J:133:TYR:HB3	10:X:23:ILE:HD11	1.96	0.48
4:R:127:ALA:HA	5:S:127:GLY:HA2	1.96	0.48
5:S:208:LEU:HA	5:S:212:ASN:HD22	1.78	0.48
7:U:44:LYS:HZ2	7:U:191:ASN:ND2	2.10	0.48
9:W:0:GLY:HA3	9:W:32:LYS:HE2	1.96	0.48
9:W:71:ALA:HB1	16:W:209:HOH:O	2.14	0.48
9:W:85:LEU:HD11	9:W:97:PRO:HG2	1.95	0.48
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.96	0.48
9:I:87:GLU:HG2	9:I:88:ARG:HH12	1.78	0.48
13:M:165:GLU:O	13:M:169:VAL:HG23	2.14	0.48
13:a:8:ASP:OD1	13:a:9:ASN:N	2.47	0.48
2:B:70:LYS:HG3	2:B:229:GLN:OE1	2.14	0.48
5:E:66:ILE:HB	5:E:74:LEU:CD2	2.44	0.48
8:H:200:GLN:O	8:H:201:LYS:HB2	2.13	0.48
9:I:11:VAL:CG1	9:I:109:PRO:HB3	2.44	0.48
11:K:208:ASN:ND2	10:X:148:PRO:CG	2.73	0.48
12:L:8:GLU:O	12:L:109:LYS:HA	2.13	0.48
14:N:3:ILE:HB	14:N:44:CYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:131:ARG:HG3	3:Q:131:ARG:HH11	1.79	0.48
8:V:196:ARG:NH2	9:W:141:GLU:O	2.47	0.48
14:b:13:ILE:HD12	14:b:151:THR:CG2	2.43	0.48
8:H:148:LYS:HD2	16:H:341:HOH:O	2.13	0.47
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.27	0.47
5:S:89:TYR:CD1	5:S:117:LYS:HD2	2.49	0.47
6:T:175:GLU:HB3	6:T:199:ILE:HD12	1.95	0.47
7:U:195:TRP:O	7:U:199:VAL:HG23	2.14	0.47
7:U:236:ASN:HD22	7:U:236:ASN:N	2.12	0.47
10:X:11:VAL:HG23	10:X:112:PRO:HB2	1.97	0.47
8:H:18:THR:HG21	8:H:30:ASN:ND2	2.29	0.47
11:K:64:ARG:HD2	16:K:328:HOH:O	2.13	0.47
13:M:-3:VAL:HG12	13:M:48:ILE:HG13	1.96	0.47
6:T:197:ALA:O	6:T:201:TYR:HD1	1.98	0.47
11:Y:116:ASP:C	11:Y:116:ASP:OD1	2.57	0.47
2:B:44:ASP:OD2	2:B:188:VAL:HG23	2.13	0.47
2:B:66:GLU:HG3	2:B:67:LYS:HG3	1.97	0.47
3:C:38:VAL:HG22	3:C:39:GLY:N	2.29	0.47
3:C:170:ARG:O	3:C:171:ASN:HB2	2.14	0.47
5:E:234:LYS:HG2	5:E:235:TYR:CD1	2.49	0.47
9:I:18:ARG:HB2	9:I:173:TRP:HB2	1.95	0.47
11:K:104:TYR:CE2	11:K:110:PRO:HG3	2.49	0.47
12:L:-7:ASN:HD22	12:L:-7:ASN:C	2.21	0.47
14:N:175:MET:HE3	14:N:188:PHE:CE2	2.49	0.47
2:P:39:GLY:O	2:P:164:ALA:HA	2.14	0.47
2:P:44:ASP:OD2	2:P:188:VAL:HG23	2.15	0.47
5:S:5:ARG:HG3	5:S:22:PHE:CE1	2.49	0.47
5:S:209:THR:N	5:S:212:ASN:HD22	2.04	0.47
9:W:12:ALA:HB3	9:W:157:ILE:HD12	1.96	0.47
9:W:134:ASP:HB2	16:W:251:HOH:O	2.14	0.47
10:X:90:ILE:HG23	10:X:91:ARG:HG3	1.96	0.47
7:G:44:LYS:NZ	7:G:191:ASN:HD21	2.13	0.47
7:G:160:VAL:HG22	7:G:161:GLY:N	2.29	0.47
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.97	0.47
1:O:97:HIS:HD2	8:V:61:SER:OG	1.97	0.47
5:S:48:LEU:HG	5:S:137:ILE:CD1	2.43	0.47
5:S:48:LEU:HD13	5:S:75:SER:HB3	1.94	0.47
9:W:6:THR:HG23	9:W:111:ILE:HG12	1.96	0.47
13:a:-4:ILE:HG22	13:a:-3:VAL:N	2.30	0.47
14:b:3:ILE:HB	14:b:44:CYS:HB3	1.96	0.47
3:C:171:ASN:CB	3:C:206:VAL:HG11	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:71:ILE:CD1	7:G:77:MET:HB3	2.40	0.47
9:I:28:ASN:HB3	9:I:173:TRP:CE3	2.49	0.47
9:I:85:LEU:HD11	9:I:97:PRO:HG2	1.95	0.47
14:N:116:GLY:N	16:N:206:HOH:O	2.47	0.47
6:T:43:ASN:HD22	6:T:43:ASN:N	2.12	0.47
11:Y:104:TYR:CE2	11:Y:110:PRO:HG3	2.50	0.47
12:Z:8:GLU:O	12:Z:109:LYS:HA	2.14	0.47
1:A:45:GLY:HA2	1:A:148:PHE:CE2	2.49	0.47
2:B:52:ARG:NH2	2:B:64:SER:HB3	2.28	0.47
6:F:179:LEU:HD11	6:F:195:GLN:HG3	1.97	0.47
12:L:84:GLN:HG3	12:L:119:GLY:O	2.14	0.47
1:O:45:GLY:HA2	1:O:148:PHE:CE2	2.49	0.47
1:O:62:GLU:CD	1:O:62:GLU:H	2.22	0.47
3:Q:38:VAL:HG22	3:Q:39:GLY:N	2.29	0.47
3:Q:172:SER:HA	3:Q:175:VAL:CG1	2.45	0.47
5:S:66:ILE:HB	5:S:74:LEU:CD2	2.44	0.47
7:U:184:LYS:HB2	7:U:184:LYS:HE3	1.59	0.47
12:Z:6:ALA:HB2	12:Z:112:VAL:HG23	1.96	0.47
12:Z:97:VAL:HG23	12:Z:99:THR:HG22	1.96	0.47
13:a:165:GLU:O	13:a:169:VAL:HG23	2.15	0.47
1:A:86:ARG:HD3	16:A:316:HOH:O	2.15	0.47
1:A:188:LEU:HD21	1:A:216:ILE:HD12	1.97	0.47
2:B:142:TYR:CD1	2:B:142:TYR:C	2.93	0.47
3:C:80:SER:HA	16:C:322:HOH:O	2.13	0.47
4:D:75:GLY:HA3	4:D:228:PHE:CE2	2.50	0.47
4:D:234:GLU:OE2	4:D:234:GLU:N	2.43	0.47
6:F:109:ILE:HB	6:F:110:PRO:HD3	1.97	0.47
6:F:206:ASP:N	6:F:206:ASP:OD1	2.47	0.47
9:I:194:GLN:HG3	11:Y:197:PHE:CE1	2.49	0.47
11:K:104:TYR:CE1	11:K:182:GLU:HB2	2.50	0.47
12:L:104:LEU:HB2	16:L:336:HOH:O	2.15	0.47
2:P:70:LYS:HG3	2:P:229:GLN:OE1	2.14	0.47
5:S:234:LYS:H	5:S:234:LYS:HD2	1.79	0.47
6:T:109:ILE:HG21	6:T:147:HIS:HB2	1.96	0.47
7:U:44:LYS:NZ	7:U:191:ASN:ND2	2.62	0.47
7:U:129:TYR:CE2	7:U:130:MET:HG2	2.49	0.47
9:W:11:VAL:CG1	9:W:109:PRO:HB3	2.45	0.47
10:X:116:GLN:NE2	10:X:130:ALA:H	2.11	0.47
11:Y:4:LEU:O	11:Y:4:LEU:HD22	2.15	0.47
11:Y:106:ARG:HG2	11:Y:106:ARG:HH11	1.78	0.47
12:Z:82:ASN:HD22	12:Z:82:ASN:C	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:116:ASP:CG	15:5:1:THR:HG22	2.40	0.47
5:E:48:LEU:HG	5:E:137:ILE:CD1	2.45	0.47
14:N:140:LYS:NZ	14:b:157:HIS:HD2	2.12	0.47
4:R:40:ILE:HG13	4:R:200:VAL:HG23	1.96	0.47
1:A:69:LEU:HD23	1:A:69:LEU:C	2.40	0.47
3:C:57:LYS:O	3:C:58:LEU:CB	2.62	0.47
6:F:43:ASN:N	6:F:43:ASN:HD22	2.11	0.47
9:I:53:LEU:CD1	9:I:95:VAL:HG21	2.45	0.47
10:J:117:ILE:HG12	10:J:123:LYS:HG3	1.97	0.47
12:L:18:ARG:NE	12:L:190:ASP:OD2	2.47	0.47
12:L:82:ASN:C	12:L:82:ASN:HD22	2.22	0.47
12:L:142:ASN:O	12:L:146:PHE:HA	2.15	0.47
13:M:222:GLN:HB2	16:M:355:HOH:O	2.14	0.47
9:W:32:LYS:O	9:W:42:GLY:HA2	2.14	0.47
11:Y:104:TYR:CE1	11:Y:182:GLU:HB2	2.49	0.47
13:a:45:SER:OG	13:a:104:ALA:HB3	2.15	0.47
14:b:116:GLY:CA	16:b:204:HOH:O	2.63	0.47
1:A:62:GLU:CD	1:A:62:GLU:H	2.23	0.47
1:A:214:LEU:HD23	1:A:214:LEU:C	2.40	0.47
2:B:82:LEU:HD23	2:B:134:GLY:HA3	1.97	0.47
9:I:27:SER:CB	10:J:124:VAL:HG21	2.45	0.47
11:Y:114:TYR:O	11:Y:121:ARG:HA	2.15	0.47
3:C:36:CYS:H	3:C:51:GLU:HG2	1.79	0.46
5:E:31:ILE:HD11	5:E:151:PRO:CD	2.45	0.46
8:H:53:GLU:O	8:H:57:GLN:HG3	2.13	0.46
8:H:165:ASN:HD21	13:a:147:ARG:HD2	1.80	0.46
11:K:4:LEU:O	11:K:4:LEU:HD22	2.15	0.46
14:N:40:LYS:O	14:N:41:ILE:HD12	2.15	0.46
14:N:157:HIS:HD2	14:b:140:LYS:NZ	2.13	0.46
2:P:237:ILE:O	2:P:241:LEU:HB2	2.15	0.46
5:S:95:ASN:HD21	12:Z:60:ASN:ND2	2.01	0.46
6:T:18:ASP:OD2	6:T:18:ASP:N	2.37	0.46
6:T:79:SER:HA	16:T:333:HOH:O	2.15	0.46
6:T:109:ILE:HB	6:T:110:PRO:HD3	1.96	0.46
7:U:71:ILE:CD1	7:U:77:MET:HB3	2.38	0.46
13:a:39:ASN:N	13:a:39:ASN:ND2	2.63	0.46
14:b:114:PRO:HD2	14:b:118:SER:O	2.15	0.46
5:E:177:THR:HG22	5:E:177:THR:O	2.14	0.46
11:K:114:TYR:O	11:K:121:ARG:HA	2.16	0.46
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.13	0.46
13:M:6:LYS:HB3	13:M:11:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:28:VAL:O	6:T:32:GLU:HG3	2.15	0.46
6:T:82:ILE:HD13	6:T:82:ILE:N	2.29	0.46
14:b:40:LYS:C	14:b:41:ILE:HD12	2.41	0.46
2:B:39:GLY:O	2:B:164:ALA:HA	2.16	0.46
3:C:77:LEU:HD12	3:C:139:ILE:HG12	1.96	0.46
3:C:161:SER:HB2	4:D:59:LEU:HD21	1.96	0.46
3:C:163:TRP:CZ2	4:D:59:LEU:HD23	2.51	0.46
6:F:175:GLU:HB3	6:F:199:ILE:HD12	1.98	0.46
7:G:153:THR:HG22	7:G:159:TYR:CB	2.45	0.46
9:I:7:GLY:HA3	9:I:153:LEU:HD22	1.96	0.46
14:N:146:MET:CE	14:N:150:GLU:HB3	2.45	0.46
5:S:12:THR:CG2	5:S:122:THR:HA	2.45	0.46
5:S:38:VAL:HG12	5:S:39:GLY:N	2.29	0.46
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.98	0.46
7:U:87:ARG:HD2	16:U:309:HOH:O	2.14	0.46
9:W:53:LEU:CD1	9:W:95:VAL:HG21	2.44	0.46
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.97	0.46
6:F:21:ASN:ND2	6:F:24:VAL:HG23	2.31	0.46
6:F:28:VAL:O	6:F:32:GLU:HG3	2.15	0.46
10:J:196:GLN:OXT	10:J:196:GLN:HG2	2.15	0.46
13:M:18:LEU:HD21	13:M:25:LEU:HD22	1.98	0.46
13:M:120:TYR:HE1	13:M:135:THR:HG22	1.80	0.46
6:T:127:ASN:C	6:T:127:ASN:ND2	2.73	0.46
7:U:124:TYR:CE1	7:U:130:MET:HE2	2.50	0.46
7:U:203:ILE:O	7:U:207:ILE:HG13	2.14	0.46
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.45	0.46
9:W:28:ASN:HB3	9:W:173:TRP:CE3	2.50	0.46
10:X:17:LYS:HD3	10:X:178:ILE:HG12	1.98	0.46
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.72	0.46
14:b:55:ILE:O	14:b:59:VAL:HG23	2.16	0.46
3:C:220:LYS:HB2	3:C:224:ASP:HB3	1.98	0.46
5:E:199:ILE:CG2	5:E:200:SER:N	2.78	0.46
11:K:197:PHE:CE1	9:W:194:GLN:HG3	2.50	0.46
14:N:107:LYS:CG	14:N:108:GLY:H	2.26	0.46
1:O:253:LEU:HD13	1:O:253:LEU:C	2.40	0.46
4:R:234:GLU:OE2	4:R:234:GLU:N	2.45	0.46
8:V:159:ILE:O	8:V:163:ILE:HG12	2.15	0.46
9:W:7:GLY:HA3	9:W:153:LEU:HD22	1.97	0.46
12:Z:0:GLY:HA3	12:Z:32:LYS:NZ	2.30	0.46
6:F:200:ILE:HG21	6:F:214:LEU:CD1	2.45	0.46
1:O:31:VAL:HG13	1:O:79:SER:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:131:ARG:NH2	7:U:125:THR:HG22	2.06	0.46
1:O:214:LEU:HD23	1:O:214:LEU:C	2.40	0.46
4:R:75:GLY:HA3	4:R:228:PHE:CE2	2.51	0.46
4:R:193:LEU:O	4:R:197:GLU:HG3	2.16	0.46
5:S:199:ILE:CG2	5:S:200:SER:N	2.79	0.46
14:b:116:GLY:HA3	16:b:204:HOH:O	2.15	0.46
1:A:57:PRO:HG3	7:G:179:GLU:CD	2.40	0.46
2:B:237:ILE:O	2:B:241:LEU:HB2	2.15	0.46
3:C:33:ARG:NH1	3:C:33:ARG:CB	2.79	0.46
6:F:197:ALA:O	6:F:201:TYR:HD1	1.98	0.46
7:G:8:TYR:C	7:G:10:ARG:N	2.73	0.46
10:J:16:SER:HB2	10:J:174:PHE:HB2	1.98	0.46
2:P:53:LYS:HG2	2:P:54:VAL:HG23	1.98	0.46
6:T:36:THR:CG2	6:T:51:GLU:OE2	2.64	0.46
8:V:53:GLU:O	8:V:56:THR:HG22	2.15	0.46
10:X:31:ASP:OD2	10:X:33:THR:HG22	2.15	0.46
13:a:5:MET:CG	13:a:168:ILE:HD11	2.31	0.46
1:A:204:GLU:OE2	1:A:204:GLU:N	2.49	0.46
10:J:148:PRO:HG3	11:Y:208:ASN:ND2	2.10	0.46
11:K:116:ASP:C	11:K:116:ASP:OD1	2.59	0.46
1:O:204:GLU:N	1:O:204:GLU:OE2	2.47	0.46
3:Q:184:ASP:OD1	3:Q:186:LYS:HB2	2.15	0.46
3:Q:219:VAL:HG23	3:Q:225:ILE:HG12	1.97	0.46
9:W:151:GLU:H	9:W:151:GLU:CD	2.23	0.46
12:Z:-7:ASN:HD22	12:Z:-6:PRO:N	2.13	0.46
12:Z:116:ASP:HB3	12:Z:120:SER:H	1.80	0.46
13:a:69:ASN:ND2	13:a:72:ALA:HA	2.30	0.46
1:A:118:ALA:HB1	1:A:157:GLY:O	2.16	0.46
2:P:8:TYR:CD2	7:U:12:ILE:HD13	2.51	0.46
7:U:44:LYS:HB2	7:U:192:GLU:O	2.16	0.46
10:X:101:LEU:HD21	10:X:116:GLN:HG3	1.98	0.46
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.28	0.46
5:E:140:ASP:HB2	16:M:353:HOH:O	2.15	0.46
12:L:149:GLN:HG2	8:V:209:THR:CG2	2.45	0.46
2:P:31:ILE:HD12	2:P:80:ALA:O	2.16	0.46
3:Q:162:SER:HB2	16:Q:324:HOH:O	2.15	0.46
8:V:200:GLN:O	8:V:201:LYS:HB2	2.14	0.46
5:E:38:VAL:HG12	5:E:39:GLY:N	2.31	0.45
8:H:72:ARG:HG3	8:H:72:ARG:NH1	2.28	0.45
10:J:11:VAL:HG23	10:J:112:PRO:HB2	1.99	0.45
10:J:31:ASP:OD2	10:J:33:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:69:LEU:C	1:O:69:LEU:HD23	2.41	0.45
4:R:46:VAL:HG11	4:R:145:ALA:HB1	1.99	0.45
10:X:196:GLN:OXT	10:X:196:GLN:HG2	2.16	0.45
13:a:-5:PRO:C	13:a:-4:ILE:HD12	2.41	0.45
1:A:31:VAL:HG13	1:A:79:SER:O	2.17	0.45
1:A:253:LEU:HD13	1:A:253:LEU:C	2.42	0.45
7:G:153:THR:HA	7:G:158:TYR:O	2.16	0.45
10:J:116:GLN:NE2	10:J:130:ALA:H	2.14	0.45
2:P:122:GLN:CG	3:Q:84:ALA:HB1	2.46	0.45
2:P:142:TYR:CD1	2:P:142:TYR:C	2.94	0.45
5:S:148:GLU:O	5:S:155:VAL:HA	2.16	0.45
7:U:71:ILE:HD11	7:U:77:MET:CB	2.40	0.45
7:U:153:THR:HA	7:U:158:TYR:O	2.16	0.45
8:V:24:PRO:HG2	8:V:25:ILE:CD1	2.42	0.45
13:a:120:TYR:HE1	13:a:135:THR:HG22	1.81	0.45
2:B:53:LYS:HG2	2:B:54:VAL:HG23	1.98	0.45
2:B:203:THR:CG2	2:B:205:SER:HB2	2.47	0.45
3:C:245:GLN:C	3:C:247:GLN:N	2.74	0.45
8:H:194:ASN:HB3	12:Z:210:LYS:HE3	1.97	0.45
9:I:115:ASP:HB3	15:1:1:THR:HG23	1.97	0.45
14:N:20:THR:CG2	14:N:31:THR:OG1	2.60	0.45
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.51	0.45
4:R:212:LEU:C	4:R:212:LEU:CD2	2.89	0.45
5:S:119:GLN:NE2	5:S:119:GLN:C	2.74	0.45
7:U:8:TYR:C	7:U:10:ARG:N	2.74	0.45
10:X:5:ILE:HD11	10:X:146:TYR:HD1	1.80	0.45
11:Y:105:THR:HG1	11:Y:108:GLU:HG3	1.78	0.45
1:A:125:THR:HG22	2:B:131:ARG:NH2	2.13	0.45
7:G:224:ALA:HB2	7:G:229:PHE:HD2	1.81	0.45
11:K:7:ARG:HG2	11:K:110:PRO:HB2	1.99	0.45
4:R:236:THR:O	4:R:240:ILE:HG13	2.17	0.45
7:U:224:ALA:HB2	7:U:229:PHE:HD2	1.81	0.45
14:b:4:MET:HE3	14:b:126:ILE:HG22	1.98	0.45
14:b:175:MET:HE3	14:b:188:PHE:CE2	2.51	0.45
4:D:79:SER:HB3	4:D:172:ILE:HD12	1.98	0.45
6:F:36:THR:HG23	6:F:51:GLU:OE2	2.17	0.45
6:F:247:ILE:O	6:F:247:ILE:HG12	2.16	0.45
13:M:16:ASP:HA	13:M:186:PHE:CB	2.46	0.45
2:P:82:LEU:HD23	2:P:134:GLY:HA3	1.98	0.45
7:U:108:MET:HE3	7:U:113:LEU:HD13	1.97	0.45
8:V:199:LYS:HE3	9:W:142:SER:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:7:ARG:HG2	11:Y:110:PRO:HB2	1.98	0.45
1:A:38:LEU:C	1:A:38:LEU:HD12	2.42	0.45
3:C:172:SER:HA	3:C:175:VAL:CG1	2.46	0.45
3:C:219:VAL:HG23	3:C:225:ILE:HG12	1.98	0.45
6:F:127:ASN:HD22	6:F:128:SER:N	2.15	0.45
6:F:127:ASN:C	6:F:127:ASN:ND2	2.72	0.45
11:K:67:GLU:HB2	16:K:328:HOH:O	2.15	0.45
13:M:87:LEU:O	13:M:91:MET:HG2	2.17	0.45
7:U:48:VAL:HG11	7:U:199:VAL:HA	1.99	0.45
2:B:31:ILE:HD12	2:B:80:ALA:O	2.16	0.45
12:L:151:GLU:O	12:L:152:PRO:C	2.60	0.45
3:Q:228:LEU:HD12	3:Q:228:LEU:N	2.31	0.45
3:Q:230:SER:HB2	3:Q:231:GLU:OE1	2.17	0.45
5:S:84:ARG:HG3	5:S:84:ARG:NH1	2.31	0.45
9:W:27:SER:CB	10:X:124:VAL:HG21	2.47	0.45
2:B:152:THR:O	2:B:159:TYR:HA	2.17	0.45
3:C:98:GLN:NE2	16:C:301:HOH:O	2.47	0.45
3:C:101:ARG:HH11	3:C:107:PRO:HB3	1.77	0.45
5:E:187:ASN:C	5:E:187:ASN:ND2	2.74	0.45
6:F:36:THR:CG2	6:F:51:GLU:OE2	2.64	0.45
9:I:64:TYR:CZ	9:I:68:GLU:HG3	2.52	0.45
10:J:104:GLY:HA2	10:J:182:VAL:HG11	1.98	0.45
13:M:192:ASP:HB3	13:M:195:THR:OG1	2.17	0.45
1:O:32:LYS:HA	1:O:32:LYS:CE	2.46	0.45
1:O:118:ALA:HB1	1:O:157:GLY:O	2.16	0.45
5:S:219:GLY:O	5:S:220:LYS:C	2.59	0.45
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.51	0.45
3:C:178:PHE:O	3:C:182:ASN:HB2	2.17	0.45
5:E:29:GLU:HA	5:E:32:LYS:HE3	1.99	0.45
8:H:41:ILE:CD1	8:H:76:VAL:HG22	2.46	0.45
10:J:5:ILE:HD11	10:J:146:TYR:HD1	1.82	0.45
12:L:-8:PHE:CB	13:M:-8:THR:HG23	2.47	0.45
16:L:306:HOH:O	9:W:192:MET:HB2	2.16	0.45
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.77	0.45
6:T:41:LYS:HD2	16:T:320:HOH:O	2.16	0.45
8:V:148:LYS:O	8:V:152:ILE:HG13	2.17	0.45
1:A:131:ARG:HG2	7:G:126:GLN:HG3	1.98	0.45
3:C:17:PRO:HA	4:D:26:TYR:CD1	2.52	0.45
12:L:39:ASN:HD21	12:L:201:GLY:HA2	1.82	0.45
13:M:8:ASP:OD1	13:M:9:ASN:N	2.50	0.45
14:N:159:LEU:O	14:N:163:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:249:ARG:HG3	1:O:249:ARG:NH1	2.31	0.45
3:Q:72:ASP:HA	10:X:67:ILE:CD1	2.45	0.45
3:Q:161:SER:HB2	4:R:59:LEU:HD21	1.99	0.45
5:S:181:PHE:C	5:S:184:ILE:HG12	2.42	0.45
6:T:206:ASP:O	6:T:207:ASN:HB2	2.17	0.45
12:Z:26:ASN:HB3	13:a:128:TYR:CE1	2.52	0.45
3:C:189:PRO:C	3:C:191:THR:H	2.25	0.44
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.47	0.44
9:I:151:GLU:H	9:I:151:GLU:CD	2.23	0.44
11:K:86:LEU:O	11:K:89:GLN:HB2	2.17	0.44
1:O:86:ARG:HH21	7:U:119:ASN:ND2	2.14	0.44
5:S:187:ASN:C	5:S:187:ASN:ND2	2.75	0.44
7:U:25:GLU:O	7:U:28:PHE:HB2	2.17	0.44
14:b:8:PHE:CE1	14:b:10:ASP:HB2	2.52	0.44
5:E:84:ARG:HG3	5:E:84:ARG:NH1	2.32	0.44
5:E:148:GLU:O	5:E:155:VAL:HA	2.17	0.44
5:E:181:PHE:C	5:E:181:PHE:CD1	2.95	0.44
7:G:44:LYS:NZ	7:G:191:ASN:ND2	2.65	0.44
7:G:142:VAL:HG21	7:G:225:THR:HA	1.99	0.44
2:P:49:ALA:HB2	2:P:215:PHE:CE1	2.51	0.44
8:V:212:VAL:HG12	8:V:213:LEU:N	2.32	0.44
8:V:220:ILE:HG21	9:W:38:HIS:HB3	1.98	0.44
14:b:146:MET:CE	14:b:150:GLU:HB3	2.47	0.44
14:b:159:LEU:O	14:b:163:ILE:HG13	2.16	0.44
4:D:193:LEU:O	4:D:197:GLU:HG3	2.17	0.44
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.53	0.44
14:N:116:GLY:CA	16:N:206:HOH:O	2.65	0.44
14:N:171:GLY:HA2	13:a:210:TRP:CH2	2.52	0.44
5:S:29:GLU:HA	5:S:32:LYS:HE3	1.99	0.44
5:S:31:ILE:HD11	5:S:151:PRO:CD	2.47	0.44
6:T:179:LEU:HD11	6:T:195:GLN:HG3	1.99	0.44
10:X:104:GLY:HA2	10:X:182:VAL:HG11	1.99	0.44
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.61	0.44
2:B:89:LEU:HB3	2:B:117:LEU:HD21	1.99	0.44
5:E:181:PHE:C	5:E:184:ILE:HG12	2.43	0.44
5:E:208:LEU:HA	5:E:212:ASN:HD22	1.79	0.44
7:G:124:TYR:CE1	7:G:130:MET:HE2	2.52	0.44
8:H:194:ASN:HB3	12:Z:210:LYS:CE	2.47	0.44
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.53	0.44
12:L:116:ASP:HB3	12:L:120:SER:H	1.82	0.44
2:P:203:THR:CG2	2:P:205:SER:HB2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:57:LYS:O	3:Q:58:LEU:CB	2.62	0.44
7:U:144:GLU:HA	7:U:226:LYS:NZ	2.33	0.44
12:Z:39:ASN:HD21	12:Z:201:GLY:HA2	1.81	0.44
3:C:230:SER:HB2	3:C:231:GLU:OE1	2.18	0.44
7:G:221:VAL:HB	7:G:232:LEU:HD12	1.99	0.44
14:N:20:THR:HA	15:3:2:LYH:O	2.18	0.44
2:P:123:GLY:C	2:P:125:THR:H	2.26	0.44
6:T:36:THR:HG23	6:T:51:GLU:OE2	2.17	0.44
7:U:44:LYS:HZ3	7:U:191:ASN:HD21	1.63	0.44
9:W:115:ASP:HB3	15:4:1:THR:HG23	2.00	0.44
1:A:175:LYS:O	1:A:179:GLU:HG3	2.18	0.44
4:D:123:PHE:HB3	4:D:134:MET:HE2	2.00	0.44
9:I:115:ASP:HB3	15:1:1:THR:CG2	2.47	0.44
11:K:208:ASN:ND2	10:X:148:PRO:HD3	2.32	0.44
1:O:175:LYS:O	1:O:179:GLU:HG3	2.18	0.44
5:S:112:HIS:HB3	6:T:86:ARG:NH2	2.32	0.44
6:T:127:ASN:HD22	6:T:128:SER:N	2.16	0.44
7:U:142:VAL:HG21	7:U:225:THR:HA	1.99	0.44
7:U:174:ILE:HD11	7:U:210:LEU:HD21	2.00	0.44
13:a:48:ILE:O	13:a:52:GLN:HG3	2.18	0.44
13:a:192:ASP:HB3	13:a:195:THR:OG1	2.17	0.44
4:D:122:ARG:C	4:D:132:ARG:HB2	2.43	0.44
4:D:177:GLU:OE1	4:D:177:GLU:N	2.49	0.44
5:E:93:GLN:HG3	5:E:113:LEU:HD13	1.98	0.44
5:E:170:ALA:HB2	5:E:198:ALA:O	2.18	0.44
7:G:83:ILE:HG22	7:G:84:PRO:HD3	1.98	0.44
7:G:110:CYS:HB2	7:G:141:SER:OG	2.18	0.44
7:G:129:TYR:CE2	7:G:130:MET:HG2	2.53	0.44
10:J:145:HIS:HB2	10:J:158:LEU:CD1	2.48	0.44
12:L:162:LEU:O	12:L:163:LYS:C	2.59	0.44
13:M:48:ILE:O	13:M:52:GLN:HG3	2.17	0.44
13:M:69:ASN:ND2	13:M:72:ALA:HA	2.33	0.44
3:Q:86:SER:O	3:Q:90:ILE:HG12	2.17	0.44
3:Q:170:ARG:O	3:Q:171:ASN:HB2	2.17	0.44
4:R:249:ALA:O	4:R:250:GLU:CB	2.65	0.44
5:S:181:PHE:C	5:S:181:PHE:CD1	2.95	0.44
8:V:175:VAL:HG12	8:V:176:CYS:N	2.32	0.44
11:Y:38:ASN:ND2	16:Y:349:HOH:O	2.48	0.44
13:a:16:ASP:HA	13:a:186:PHE:CB	2.46	0.44
14:b:193:TYR:CD1	14:b:193:TYR:C	2.96	0.44
5:E:102:ASN:HB2	13:M:85:GLU:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:74:ILE:HD11	6:F:109:ILE:HG13	1.99	0.44
7:G:174:ILE:HD11	7:G:210:LEU:HD21	2.00	0.44
8:H:68:LEU:HD12	8:H:68:LEU:HA	1.89	0.44
11:K:155:TYR:OH	11:K:204:GLU:OE1	2.34	0.44
1:O:161:PRO:O	2:P:59:LEU:HD12	2.18	0.44
4:R:39:GLY:O	4:R:169:ALA:HA	2.17	0.44
6:T:175:GLU:HB3	6:T:199:ILE:CD1	2.47	0.44
7:U:226:LYS:O	7:U:227:ASP:HB2	2.16	0.44
11:Y:50:ALA:CB	12:Z:118:VAL:HG23	2.48	0.44
12:Z:197:VAL:HG22	12:Z:202:VAL:HG22	1.99	0.44
1:A:188:LEU:O	1:A:192:ILE:HG13	2.17	0.44
6:F:109:ILE:H	6:F:109:ILE:CD1	2.25	0.44
6:F:201:TYR:HE2	6:F:244:GLN:HE21	1.66	0.44
7:G:48:VAL:HG11	7:G:199:VAL:HA	2.00	0.44
7:G:70:CYS:HB3	16:G:342:HOH:O	2.18	0.44
10:J:145:HIS:HB2	10:J:158:LEU:HD11	1.99	0.44
11:K:106:ARG:HG2	11:K:106:ARG:NH1	2.33	0.44
1:O:125:THR:CG2	2:P:131:ARG:NH2	2.78	0.44
4:R:79:SER:HB3	4:R:172:ILE:HD12	1.99	0.44
10:X:193:PHE:C	10:X:195:ALA:H	2.26	0.44
14:b:107:LYS:CG	14:b:108:GLY:H	2.27	0.44
2:B:49:ALA:HB2	2:B:215:PHE:CE1	2.53	0.43
2:B:123:GLY:C	2:B:125:THR:H	2.24	0.43
3:C:131:ARG:HH11	3:C:131:ARG:HG3	1.82	0.43
4:D:46:VAL:HG11	4:D:145:ALA:HB1	1.99	0.43
5:E:12:THR:CG2	5:E:122:THR:HA	2.45	0.43
7:G:25:GLU:O	7:G:28:PHE:HB2	2.18	0.43
10:J:90:ILE:HG23	10:J:91:ARG:HG3	2.00	0.43
10:J:188:ARG:HG2	10:J:188:ARG:NH1	2.33	0.43
12:L:164:TYR:CD1	12:L:165:LEU:N	2.86	0.43
13:M:5:MET:HE3	13:M:150:VAL:HG21	2.00	0.43
14:N:193:TYR:CD1	14:N:193:TYR:C	2.96	0.43
1:O:17:PRO:HA	2:P:26:TYR:CE1	2.53	0.43
2:P:108:ILE:HG12	2:P:113:LEU:HB2	2.00	0.43
4:R:65:GLU:HA	16:R:313:HOH:O	2.17	0.43
6:T:137:ILE:CD1	6:T:165:THR:HG22	2.48	0.43
7:U:153:THR:HG22	7:U:159:TYR:CB	2.48	0.43
8:V:215:GLU:O	8:V:216:SER:HB3	2.18	0.43
11:K:38:ASN:OD1	11:K:38:ASN:C	2.61	0.43
13:M:10:GLY:HA3	13:M:191:ILE:O	2.18	0.43
3:Q:178:PHE:O	3:Q:182:ASN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:12:VAL:CG2	4:R:124:GLY:HA2	2.47	0.43
6:T:195:GLN:NE2	6:T:198:LYS:HE3	2.33	0.43
8:V:116:HIS:HB2	16:V:345:HOH:O	2.16	0.43
10:X:170:MET:HA	10:X:171:PRO:HD3	1.76	0.43
13:a:87:LEU:O	13:a:91:MET:HG2	2.18	0.43
14:b:176:VAL:HG12	14:b:178:LEU:HD13	2.00	0.43
3:C:155:GLU:HB2	3:C:156:PRO:CD	2.46	0.43
7:G:108:MET:HE3	7:G:113:LEU:HB2	2.00	0.43
7:G:226:LYS:O	7:G:227:ASP:HB2	2.18	0.43
8:H:203:TYR:OH	12:Z:176:ASP:OD1	2.28	0.43
10:J:5:ILE:HD11	10:J:146:TYR:CD1	2.52	0.43
12:L:116:ASP:CG	15:2:1:THR:HG22	2.44	0.43
1:O:14:THR:HB	2:P:23:GLN:NE2	2.32	0.43
1:O:188:LEU:HD21	1:O:216:ILE:HD12	2.00	0.43
7:U:36:ILE:HG23	7:U:52:GLN:HB2	2.00	0.43
7:U:160:VAL:HG22	7:U:161:GLY:N	2.33	0.43
8:V:72:ARG:HG3	8:V:72:ARG:NH1	2.32	0.43
13:a:-3:VAL:HG12	13:a:48:ILE:HG13	2.00	0.43
14:b:40:LYS:O	14:b:41:ILE:HD12	2.18	0.43
1:A:97:HIS:HD2	8:H:61:SER:OG	2.02	0.43
2:B:15:PHE:H	3:C:23:GLN:NE2	1.93	0.43
5:E:112:HIS:HB3	6:F:86:ARG:NH2	2.34	0.43
7:G:144:GLU:HA	7:G:226:LYS:NZ	2.32	0.43
9:I:12:ALA:HB3	9:I:157:ILE:HD12	1.99	0.43
10:J:101:LEU:HD21	10:J:116:GLN:HG3	2.01	0.43
12:L:28:ARG:NH1	12:L:211:ARG:HB3	2.32	0.43
12:L:210:LYS:HE3	8:V:194:ASN:HB3	2.00	0.43
2:P:98:GLN:HB3	9:W:59:TYR:CD2	2.54	0.43
3:Q:220:LYS:HB2	3:Q:224:ASP:HB3	2.00	0.43
5:S:170:ALA:HB2	5:S:198:ALA:O	2.18	0.43
6:T:157:TYR:CD1	6:T:157:TYR:C	2.95	0.43
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.75	0.43
13:M:-5:PRO:O	13:M:-4:ILE:HD12	2.18	0.43
13:M:12:ILE:HB	13:M:168:ILE:HD13	2.01	0.43
10:X:170:MET:HE2	10:X:170:MET:HB3	1.96	0.43
12:Z:34:PHE:O	12:Z:41:VAL:HA	2.18	0.43
3:C:200:VAL:HG22	3:C:216:ILE:HD11	2.00	0.43
4:D:212:LEU:C	4:D:212:LEU:CD2	2.90	0.43
5:E:137:ILE:O	5:E:137:ILE:HG12	2.18	0.43
8:H:128:GLY:O	8:H:131:SER:HB2	2.18	0.43
10:J:17:LYS:HD3	10:J:178:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:163:ILE:CG2	14:N:170:GLY:HA2	2.47	0.43
10:X:145:HIS:HB2	10:X:158:LEU:HD11	2.00	0.43
12:Z:82:ASN:C	12:Z:82:ASN:ND2	2.77	0.43
14:b:20:THR:HA	15:6:2:LYH:O	2.18	0.43
1:A:67:VAL:HG11	1:A:215:ALA:HB3	2.01	0.43
4:D:40:ILE:HG13	4:D:200:VAL:HG23	2.00	0.43
7:G:132:PRO:HB3	16:G:303:HOH:O	2.17	0.43
8:H:220:ILE:HD11	9:I:185:VAL:CG2	2.48	0.43
10:J:5:ILE:HG13	10:J:6:ARG:N	2.33	0.43
12:L:82:ASN:C	12:L:82:ASN:ND2	2.76	0.43
14:N:55:ILE:O	14:N:59:VAL:HG23	2.18	0.43
1:O:199:LEU:HD23	1:O:212:ILE:HD13	2.01	0.43
3:Q:155:GLU:HB2	3:Q:156:PRO:CD	2.48	0.43
5:S:196:VAL:C	5:S:199:ILE:HG22	2.43	0.43
8:V:41:ILE:CD1	8:V:76:VAL:HG22	2.48	0.43
2:B:148:TYR:OH	2:B:220:LYS:HB2	2.18	0.43
3:C:228:LEU:N	3:C:228:LEU:HD12	2.33	0.43
4:D:39:GLY:O	4:D:169:ALA:HA	2.19	0.43
4:D:201:LEU:HD12	4:D:201:LEU:HA	1.88	0.43
4:D:236:THR:O	4:D:240:ILE:HG13	2.18	0.43
5:E:47:VAL:HG12	5:E:48:LEU:N	2.33	0.43
7:G:111:ASP:HB3	7:G:151:TYR:CZ	2.54	0.43
7:G:184:LYS:HE3	7:G:184:LYS:HB2	1.60	0.43
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.00	0.43
9:I:108:LYS:HA	9:I:109:PRO:HD3	1.92	0.43
10:J:156:LEU:HD13	10:J:196:GLN:HE22	1.83	0.43
12:L:98:HIS:HD2	16:L:305:HOH:O	2.01	0.43
1:O:4:MET:CG	1:O:5:THR:H	2.32	0.43
2:P:165:ILE:HG12	2:P:166:SER:H	1.83	0.43
5:S:137:ILE:HG13	5:S:218:VAL:CG1	2.49	0.43
8:V:8:PHE:HB3	8:V:151:ALA:HB2	2.01	0.43
9:W:115:ASP:HB3	15:4:1:THR:CG2	2.49	0.43
10:X:90:ILE:HD12	10:X:90:ILE:HA	1.79	0.43
12:Z:151:GLU:O	12:Z:152:PRO:C	2.61	0.43
12:Z:162:LEU:O	12:Z:163:LYS:C	2.59	0.43
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.53	0.43
1:A:67:VAL:HG11	1:A:215:ALA:CB	2.49	0.43
3:C:153:GLN:HG2	3:C:154:THR:N	2.34	0.43
4:D:12:VAL:CG2	4:D:124:GLY:HA2	2.48	0.43
5:E:219:GLY:O	5:E:220:LYS:C	2.61	0.43
9:I:97:PRO:HD2	9:I:114:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:144:HIS:HD2	10:J:145:HIS:CE1	2.37	0.43
13:M:204:GLN:HE21	13:M:204:GLN:HB3	1.62	0.43
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.01	0.43
1:O:97:HIS:CD2	8:V:61:SER:OG	2.72	0.43
2:P:5:SER:O	2:P:7:ARG:N	2.52	0.43
2:P:98:GLN:HE22	9:W:62:ASN:HD22	1.67	0.43
2:P:152:THR:O	2:P:159:TYR:HA	2.18	0.43
4:R:17:PRO:HA	5:S:26:TYR:CD1	2.53	0.43
4:R:122:ARG:C	4:R:132:ARG:HB2	2.43	0.43
6:T:21:ASN:ND2	6:T:24:VAL:HG23	2.34	0.43
7:U:174:ILE:HD12	7:U:206:MET:CE	2.49	0.43
10:X:16:SER:HB2	10:X:174:PHE:HB2	2.01	0.43
13:a:197:LEU:C	13:a:197:LEU:CD2	2.91	0.43
1:A:92:SER:O	1:A:95:VAL:HG12	2.19	0.43
8:H:212:VAL:HG12	8:H:213:LEU:N	2.33	0.43
11:K:38:ASN:O	11:K:40:PHE:N	2.52	0.43
13:M:41:VAL:CG2	13:M:191:ILE:HD11	2.46	0.43
6:T:190:ARG:HH11	6:T:190:ARG:CG	2.30	0.43
11:Y:76:VAL:N	11:Y:108:GLU:OE2	2.51	0.43
13:a:34:ILE:HA	13:a:35:PRO:HD3	1.91	0.43
13:a:162:GLN:NE2	13:a:162:GLN:N	2.59	0.43
5:E:196:VAL:C	5:E:199:ILE:HG22	2.43	0.42
6:F:205:GLU:HG3	6:F:208:LYS:HZ1	1.84	0.42
9:I:106:SER:C	9:I:108:LYS:H	2.27	0.42
13:M:156:ILE:HB	13:M:157:PRO:CD	2.49	0.42
1:O:188:LEU:O	1:O:192:ILE:HG13	2.19	0.42
5:S:93:GLN:HG3	5:S:113:LEU:HD13	2.00	0.42
6:T:109:ILE:CD1	6:T:142:ASP:HB3	2.49	0.42
10:X:145:HIS:HB2	10:X:158:LEU:CD1	2.49	0.42
12:Z:164:TYR:CD1	12:Z:165:LEU:N	2.87	0.42
13:a:204:GLN:HE21	13:a:204:GLN:HB3	1.61	0.42
1:A:207:PHE:CD1	1:A:212:ILE:HD11	2.55	0.42
10:J:148:PRO:HD3	11:Y:208:ASN:ND2	2.35	0.42
11:K:149:SER:C	11:K:151:GLU:N	2.76	0.42
3:Q:41:LYS:HD3	3:Q:163:TRP:O	2.20	0.42
5:S:88:ASN:O	5:S:92:GLN:HG3	2.18	0.42
6:T:137:ILE:HD11	6:T:165:THR:HG22	2.01	0.42
13:a:156:ILE:HB	13:a:157:PRO:HD3	2.01	0.42
2:B:17:PRO:HA	3:C:26:TYR:CE1	2.53	0.42
3:C:52:ARG:HB2	3:C:213:ASN:HA	2.01	0.42
5:E:73:GLY:HA3	5:E:224:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:18:ASP:OD2	6:F:18:ASP:N	2.39	0.42
9:I:86:TYR:CE1	9:I:89:ARG:HD3	2.54	0.42
14:N:107:LYS:CG	14:N:108:GLY:N	2.77	0.42
1:O:77:VAL:HG12	1:O:138:LEU:HB2	2.00	0.42
10:X:5:ILE:HG13	10:X:6:ARG:N	2.32	0.42
10:X:173:ASP:OD1	10:X:175:LYS:HD3	2.19	0.42
12:Z:26:ASN:HB3	13:a:128:TYR:CZ	2.54	0.42
13:a:163:VAL:HG21	16:a:322:HOH:O	2.19	0.42
3:C:86:SER:O	3:C:90:ILE:HG12	2.19	0.42
4:D:59:LEU:HD13	4:D:59:LEU:C	2.44	0.42
7:G:29:LYS:HD2	7:G:29:LYS:HA	1.87	0.42
8:H:201:LYS:HE3	12:Z:169:GLU:OE2	2.19	0.42
1:O:142:HIS:HA	1:O:147:GLY:O	2.20	0.42
2:P:127:HIS:HB3	3:Q:130:VAL:HG12	2.00	0.42
13:a:152:ARG:CG	13:a:152:ARG:NH1	2.82	0.42
14:b:20:THR:CG2	14:b:31:THR:OG1	2.64	0.42
1:A:238:PHE:CD2	1:A:238:PHE:C	2.98	0.42
3:C:161:SER:CB	4:D:59:LEU:HD21	2.50	0.42
5:E:5:ARG:HG3	5:E:22:PHE:CE1	2.54	0.42
5:E:119:GLN:NE2	5:E:119:GLN:C	2.77	0.42
6:F:206:ASP:O	6:F:207:ASN:HB2	2.19	0.42
8:H:175:VAL:HG12	8:H:176:CYS:N	2.33	0.42
13:M:147:ARG:HD2	8:V:165:ASN:HD21	1.84	0.42
2:P:233:LYS:O	2:P:234:PRO:C	2.62	0.42
3:Q:52:ARG:HB2	3:Q:213:ASN:HA	2.00	0.42
12:Z:-8:PHE:CB	13:a:-8:THR:HG23	2.50	0.42
12:Z:28:ARG:NH1	12:Z:211:ARG:HB3	2.35	0.42
13:a:156:ILE:HB	13:a:157:PRO:CD	2.49	0.42
1:A:230:ILE:HD12	1:A:230:ILE:N	2.34	0.42
5:E:121:ASN:HD22	5:E:121:ASN:N	2.18	0.42
8:H:148:LYS:CD	16:H:341:HOH:O	2.67	0.42
8:H:165:ASN:ND2	13:a:147:ARG:HD2	2.35	0.42
8:H:215:GLU:O	8:H:216:SER:HB3	2.20	0.42
9:I:1:ILE:HD11	9:I:165:ALA:HB2	2.02	0.42
10:J:170:MET:HA	10:J:171:PRO:HD3	1.77	0.42
11:K:8:PHE:HA	11:K:146:TRP:CE3	2.54	0.42
12:L:-8:PHE:HB2	13:M:-8:THR:HG23	2.02	0.42
12:L:210:LYS:CE	8:V:194:ASN:HB3	2.50	0.42
13:M:79:GLU:O	13:M:83:ILE:HG13	2.20	0.42
1:O:38:LEU:C	1:O:38:LEU:HD12	2.44	0.42
1:O:92:SER:O	1:O:95:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:50:VAL:HG22	6:T:51:GLU:N	2.34	0.42
6:T:109:ILE:HD12	6:T:142:ASP:HB3	2.01	0.42
9:W:11:VAL:HG13	9:W:109:PRO:HB3	2.01	0.42
1:A:4:MET:CG	1:A:5:THR:H	2.33	0.42
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.87	0.42
1:A:142:HIS:HA	1:A:147:GLY:O	2.20	0.42
2:B:5:SER:O	2:B:7:ARG:N	2.52	0.42
2:B:17:PRO:HA	3:C:26:TYR:CD1	2.54	0.42
4:D:51:GLU:HG2	4:D:53:ARG:HB2	2.01	0.42
4:D:186:GLU:HG3	4:D:199:LEU:HD11	2.01	0.42
6:F:175:GLU:HB3	6:F:199:ILE:CD1	2.49	0.42
8:H:213:LEU:HG	9:I:191:LYS:HB2	2.02	0.42
14:N:84:GLU:O	14:N:88:GLU:HB2	2.19	0.42
6:T:49:ALA:HA	6:T:215:GLU:O	2.19	0.42
7:U:29:LYS:HA	7:U:29:LYS:HD2	1.84	0.42
1:A:77:VAL:HG12	1:A:138:LEU:HB2	2.00	0.42
3:C:74:HIS:CE1	3:C:75:VAL:HG23	2.54	0.42
5:E:74:LEU:CB	5:E:136:ILE:HD12	2.49	0.42
5:E:196:VAL:O	5:E:199:ILE:HG22	2.20	0.42
8:H:18:THR:HB	8:H:30:ASN:HD22	1.84	0.42
8:H:53:GLU:O	8:H:56:THR:HG22	2.20	0.42
10:J:23:ILE:O	10:X:137:TYR:OH	2.30	0.42
2:P:89:LEU:HB3	2:P:117:LEU:HD21	2.01	0.42
2:P:148:TYR:OH	2:P:220:LYS:HB2	2.19	0.42
5:S:47:VAL:HG12	5:S:48:LEU:N	2.34	0.42
7:U:221:VAL:HB	7:U:232:LEU:HD12	2.01	0.42
10:X:91:ARG:HG2	10:X:91:ARG:NH1	2.34	0.42
13:a:34:ILE:HG12	13:a:55:GLU:HG3	2.00	0.42
2:B:21:LEU:O	2:B:25:GLU:HG2	2.19	0.42
2:B:51:GLU:OE2	2:B:203:THR:HG23	2.20	0.42
4:D:107:ILE:HG22	16:D:322:HOH:O	2.19	0.42
6:F:50:VAL:HG22	6:F:51:GLU:N	2.35	0.42
7:G:106:TYR:OH	8:H:66:HIS:HE1	2.03	0.42
5:S:5:ARG:HG3	5:S:22:PHE:CD1	2.54	0.42
5:S:181:PHE:CD1	5:S:182:ILE:N	2.88	0.42
1:A:181:ARG:HH11	1:A:181:ARG:CB	2.29	0.42
5:E:181:PHE:CD1	5:E:182:ILE:N	2.88	0.42
10:J:117:ILE:HA	10:J:122:THR:O	2.20	0.42
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.19	0.42
3:Q:216:ILE:HG13	3:Q:233:ILE:HD13	2.01	0.42
6:T:74:ILE:HD11	6:T:109:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:120:LEU:HD12	7:U:120:LEU:HA	1.86	0.42
10:X:144:HIS:HD2	10:X:145:HIS:CE1	2.37	0.42
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.19	0.41
1:A:32:LYS:HA	1:A:32:LYS:CE	2.49	0.41
2:B:44:ASP:CG	2:B:188:VAL:HG23	2.45	0.41
2:B:108:ILE:HG12	2:B:113:LEU:HB2	2.02	0.41
4:D:249:ALA:O	4:D:250:GLU:CB	2.67	0.41
5:E:173:TYR:CD2	5:E:198:ALA:HA	2.55	0.41
2:P:203:THR:HG21	2:P:205:SER:HB2	2.02	0.41
5:S:158:LEU:HD13	5:S:161:THR:HB	2.02	0.41
8:V:63:ILE:HG23	8:V:74:PRO:HB3	2.01	0.41
10:X:75:PRO:HD2	16:X:212:HOH:O	2.20	0.41
11:Y:106:ARG:HG2	11:Y:106:ARG:NH1	2.34	0.41
2:B:127:HIS:HA	16:C:326:HOH:O	2.19	0.41
5:E:98:SER:O	5:E:102:ASN:HA	2.20	0.41
7:G:171:GLN:HE21	7:G:171:GLN:HB3	1.64	0.41
12:L:34:PHE:O	12:L:41:VAL:HA	2.21	0.41
1:O:26:TYR:CD1	7:U:17:PRO:HA	2.54	0.41
3:Q:210:GLY:HA3	3:Q:213:ASN:HB2	2.02	0.41
5:S:52:LYS:HB3	5:S:61:TYR:HB3	2.02	0.41
9:W:97:PRO:HD2	9:W:114:PHE:HB2	2.01	0.41
11:Y:38:ASN:O	11:Y:40:PHE:N	2.53	0.41
12:Z:57:ARG:NH2	16:Z:349:HOH:O	2.53	0.41
14:b:2:SER:O	14:b:16:ALA:HA	2.20	0.41
10:J:62:ILE:HD13	10:J:78:VAL:HG22	2.02	0.41
13:M:160:THR:HG23	16:M:362:HOH:O	2.19	0.41
4:R:244:LYS:HE2	4:R:244:LYS:HB3	1.89	0.41
6:T:82:ILE:HB	6:T:83:PRO:HD3	2.02	0.41
7:U:108:MET:HE3	7:U:113:LEU:HB2	2.03	0.41
11:Y:174:SER:HA	11:Y:193:VAL:HG23	2.03	0.41
12:Z:84:GLN:HG3	12:Z:119:GLY:O	2.20	0.41
13:a:153:GLU:O	13:a:156:ILE:HG12	2.20	0.41
14:b:38:HIS:O	14:b:39:ASP:C	2.64	0.41
2:B:102:LYS:NZ	10:J:84:GLN:NE2	2.68	0.41
6:F:179:LEU:HD21	6:F:195:GLN:CD	2.46	0.41
2:P:5:SER:C	2:P:7:ARG:N	2.79	0.41
2:P:7:ARG:HG2	7:U:8:TYR:CE2	2.56	0.41
2:P:44:ASP:OD2	2:P:44:ASP:N	2.51	0.41
2:P:51:GLU:OE2	2:P:203:THR:HG23	2.20	0.41
3:Q:77:LEU:C	3:Q:77:LEU:HD23	2.46	0.41
3:Q:245:GLN:C	3:Q:247:GLN:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:134:MET:HE3	4:R:136:ARG:O	2.20	0.41
5:S:41:ARG:NH1	5:S:42:SER:O	2.53	0.41
5:S:102:ASN:HB2	13:a:85:GLU:HG2	2.02	0.41
5:S:173:TYR:CD2	5:S:198:ALA:HA	2.56	0.41
9:W:99:VAL:O	9:W:111:ILE:HA	2.21	0.41
11:Y:149:SER:C	11:Y:151:GLU:N	2.76	0.41
14:b:7:THR:HG23	14:b:110:VAL:HG23	2.01	0.41
14:b:143:ARG:NH2	14:b:146:MET:HE3	2.35	0.41
1:A:249:ARG:HG3	1:A:249:ARG:NH1	2.32	0.41
2:B:203:THR:HG21	2:B:205:SER:HB2	2.02	0.41
5:E:15:PHE:H	6:F:23:GLN:HE22	1.66	0.41
5:E:88:ASN:O	5:E:92:GLN:HG3	2.21	0.41
7:G:137:LEU:O	7:G:152:LYS:HA	2.19	0.41
7:G:236:ASN:N	7:G:236:ASN:ND2	2.67	0.41
11:K:40:PHE:CD1	11:K:73:ARG:NH1	2.89	0.41
11:K:145:LYS:CB	11:K:148:LEU:HD13	2.50	0.41
13:M:2:VAL:O	13:M:134:ALA:HA	2.20	0.41
13:M:156:ILE:HB	13:M:157:PRO:HD3	2.02	0.41
1:O:27:ALA:O	1:O:31:VAL:HG23	2.21	0.41
4:R:163:THR:HG22	5:S:81:PRO:HD3	2.03	0.41
5:S:214:SER:C	5:S:215:ILE:HG13	2.45	0.41
9:W:64:TYR:CZ	9:W:68:GLU:HG3	2.55	0.41
11:Y:100:MET:HB2	11:Y:100:MET:HE2	1.84	0.41
13:a:16:ASP:C	13:a:16:ASP:OD2	2.63	0.41
13:a:79:GLU:O	13:a:83:ILE:HG13	2.21	0.41
3:C:206:VAL:O	3:C:206:VAL:HG12	2.20	0.41
9:I:11:VAL:HG13	9:I:109:PRO:HB3	2.02	0.41
10:J:2:ILE:O	10:J:130:ALA:HA	2.20	0.41
10:J:193:PHE:C	10:J:195:ALA:N	2.79	0.41
3:Q:131:ARG:HG3	3:Q:131:ARG:NH1	2.36	0.41
3:Q:189:PRO:C	3:Q:191:THR:H	2.27	0.41
3:Q:206:VAL:O	3:Q:206:VAL:HG12	2.20	0.41
4:R:101:LEU:CD1	11:Y:57:THR:HG22	2.51	0.41
6:T:175:GLU:OE1	6:T:202:LEU:HD23	2.20	0.41
7:U:110:CYS:HB2	7:U:141:SER:OG	2.20	0.41
7:U:111:ASP:HB3	7:U:151:TYR:CZ	2.55	0.41
7:U:137:LEU:O	7:U:152:LYS:HA	2.20	0.41
3:C:122:GLN:NE2	3:C:122:GLN:C	2.79	0.41
5:E:41:ARG:NH1	5:E:42:SER:O	2.53	0.41
6:F:137:ILE:CD1	6:F:165:THR:HG22	2.50	0.41
9:I:11:VAL:HG23	9:I:180:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:18:ALA:HB2	10:J:175:LYS:HG2	2.02	0.41
10:J:193:PHE:C	10:J:195:ALA:H	2.28	0.41
11:K:100:MET:HB2	11:K:100:MET:HE2	1.84	0.41
5:S:98:SER:O	5:S:102:ASN:HA	2.21	0.41
6:T:107:ILE:HG23	6:T:107:ILE:O	2.20	0.41
7:U:152:LYS:O	7:U:159:TYR:HA	2.21	0.41
11:Y:149:SER:O	11:Y:150:VAL:C	2.63	0.41
12:Z:167:VAL:O	12:Z:171:ILE:HG13	2.20	0.41
2:B:122:GLN:CG	3:C:84:ALA:HB1	2.51	0.41
6:F:54:ILE:HG13	6:F:212:PHE:HA	2.03	0.41
8:H:8:PHE:HB3	8:H:151:ALA:HB2	2.01	0.41
12:L:80:ALA:HA	12:L:115:PHE:HZ	1.86	0.41
12:L:169:GLU:OE2	8:V:201:LYS:HE3	2.21	0.41
1:O:238:PHE:CD2	1:O:238:PHE:C	2.98	0.41
3:Q:153:GLN:HG2	3:Q:154:THR:N	2.35	0.41
4:R:157:HIS:O	4:R:164:PHE:HA	2.20	0.41
5:S:196:VAL:O	5:S:196:VAL:HG12	2.21	0.41
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.35	0.41
9:W:106:SER:C	9:W:108:LYS:H	2.28	0.41
10:X:33:THR:CG2	10:X:180:LYS:NZ	2.83	0.41
13:a:10:GLY:HA3	13:a:191:ILE:O	2.21	0.41
2:B:46:ILE:HD11	2:B:148:TYR:HB3	2.03	0.41
2:B:185:ASP:O	2:B:186:MET:C	2.63	0.41
4:D:89:ILE:HB	16:D:323:HOH:O	2.20	0.41
4:D:190:SER:HA	16:D:335:HOH:O	2.21	0.41
6:F:70:VAL:HB	6:F:74:ILE:HB	2.03	0.41
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.93	0.41
6:F:109:ILE:CD1	6:F:142:ASP:HB3	2.50	0.41
6:F:193:VAL:HG13	6:F:216:ILE:HG21	2.02	0.41
9:I:53:LEU:HD12	9:I:95:VAL:HG21	2.02	0.41
9:I:114:PHE:HA	9:I:119:CYS:O	2.21	0.41
9:I:154:PHE:HB2	9:I:179:ILE:CD1	2.51	0.41
10:J:91:ARG:HG2	10:J:91:ARG:NH1	2.34	0.41
13:M:79:GLU:HB2	13:M:82:TYR:CD2	2.56	0.41
13:M:141:MET:HE1	13:M:178:ARG:HG3	2.03	0.41
2:P:55:THR:HG22	2:P:59:LEU:HD23	2.03	0.41
2:P:188:VAL:O	2:P:192:ILE:HG13	2.21	0.41
3:Q:161:SER:CB	4:R:59:LEU:HD21	2.51	0.41
4:R:86:ARG:HA	4:R:86:ARG:HD3	1.82	0.41
5:S:15:PHE:H	6:T:23:GLN:HE22	1.66	0.41
5:S:74:LEU:HA	5:S:135:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:54:ILE:HG13	6:T:212:PHE:HA	2.02	0.41
8:V:128:GLY:O	8:V:131:SER:HB2	2.21	0.41
9:W:11:VAL:HG23	9:W:180:ILE:HB	2.03	0.41
9:W:99:VAL:HG23	9:W:114:PHE:HE2	1.86	0.41
10:X:188:ARG:HG2	10:X:188:ARG:NH1	2.35	0.41
11:Y:86:LEU:O	11:Y:89:GLN:HB2	2.21	0.41
11:Y:176:ASN:ND2	11:Y:190:ASN:HD22	2.19	0.41
12:Z:136:ILE:HD12	12:Z:177:SER:HB3	2.03	0.41
2:B:98:GLN:NE2	9:I:62:ASN:HD22	2.18	0.41
5:E:54:ASN:ND2	5:E:56:ASP:O	2.53	0.41
5:E:74:LEU:HA	5:E:135:LEU:O	2.21	0.41
6:F:70:VAL:HG11	6:F:112:PHE:CE1	2.56	0.41
9:I:161:LEU:HD21	9:I:175:ALA:HB1	2.03	0.41
13:M:0:THR:O	13:M:32:ARG:NH1	2.54	0.41
13:M:152:ARG:HG3	13:M:152:ARG:NH1	2.24	0.41
1:O:29:THR:O	1:O:33:GLN:HG2	2.21	0.41
1:O:67:VAL:HG11	1:O:215:ALA:CB	2.51	0.41
1:O:131:ARG:HG2	7:U:126:GLN:HG3	2.02	0.41
3:Q:200:VAL:HG22	3:Q:216:ILE:HD11	2.02	0.41
4:R:59:LEU:HD13	4:R:59:LEU:C	2.46	0.41
7:U:83:ILE:HG22	7:U:84:PRO:HD3	2.02	0.41
8:V:68:LEU:HD12	8:V:68:LEU:HA	1.91	0.41
9:W:87:GLU:HG2	9:W:88:ARG:NH1	2.36	0.41
11:Y:40:PHE:CD1	11:Y:73:ARG:NH1	2.89	0.41
13:a:-5:PRO:O	13:a:-4:ILE:HD12	2.20	0.41
1:A:55:SER:O	1:A:56:SER:HB2	2.21	0.40
1:A:62:GLU:C	1:A:64:LEU:H	2.29	0.40
4:D:157:HIS:O	4:D:164:PHE:HA	2.20	0.40
5:E:66:ILE:HB	5:E:74:LEU:HD21	2.03	0.40
5:E:217:ILE:HG12	5:E:218:VAL:H	1.85	0.40
6:F:101:LYS:NZ	14:N:84:GLU:OE1	2.44	0.40
8:H:126:SER:O	8:H:127:LEU:HD23	2.21	0.40
10:J:33:THR:HG21	10:J:180:LYS:HZ2	1.84	0.40
10:J:172:MET:HE1	10:X:171:PRO:CB	2.51	0.40
10:J:172:MET:HE2	10:X:171:PRO:O	2.21	0.40
11:K:50:ALA:CB	12:L:118:VAL:HG23	2.51	0.40
14:N:13:ILE:HD12	14:N:151:THR:HG22	2.04	0.40
1:O:135:VAL:O	1:O:155:PRO:HG3	2.21	0.40
4:R:51:GLU:HG2	4:R:53:ARG:HB2	2.03	0.40
4:R:249:ALA:O	4:R:250:GLU:HB2	2.20	0.40
6:T:70:VAL:HG11	6:T:112:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:179:LEU:HD21	6:T:195:GLN:CD	2.47	0.40
7:U:37:ASN:HB2	7:U:52:GLN:OE1	2.21	0.40
9:W:1:ILE:HD11	9:W:165:ALA:HB2	2.03	0.40
10:X:68:ARG:HD2	16:X:219:HOH:O	2.21	0.40
10:X:126:LEU:HB3	10:X:127:PRO:CD	2.52	0.40
11:Y:145:LYS:CB	11:Y:148:LEU:HD13	2.51	0.40
12:Z:80:ALA:HA	12:Z:115:PHE:HZ	1.86	0.40
13:a:12:ILE:HB	13:a:168:ILE:HD13	2.02	0.40
1:A:86:ARG:HH21	7:G:119:ASN:ND2	2.17	0.40
3:C:7:GLY:N	16:C:332:HOH:O	2.54	0.40
3:C:166:GLN:HG3	3:C:167:THR:N	2.36	0.40
4:D:86:ARG:HA	4:D:86:ARG:HD3	1.82	0.40
10:J:6:ARG:HH11	10:J:6:ARG:HG2	1.87	0.40
10:J:23:ILE:HG13	10:J:23:ILE:O	2.20	0.40
12:L:21:THR:O	12:L:22:ASP:HB2	2.20	0.40
12:L:167:VAL:O	12:L:171:ILE:HG13	2.21	0.40
13:M:152:ARG:CG	13:M:152:ARG:NH1	2.83	0.40
13:M:153:GLU:O	13:M:156:ILE:HG12	2.22	0.40
1:O:67:VAL:HG11	1:O:215:ALA:HB3	2.02	0.40
3:Q:46:VAL:HG11	3:Q:140:ALA:HB1	2.02	0.40
3:Q:80:SER:HB2	3:Q:168:ILE:HG13	2.03	0.40
4:R:201:LEU:HD22	4:R:219:LEU:HD11	2.02	0.40
16:V:339:HOH:O	9:W:155:GLU:HG3	2.21	0.40
10:X:117:ILE:HA	10:X:122:THR:O	2.20	0.40
13:a:2:VAL:O	13:a:134:ALA:HA	2.22	0.40
13:a:5:MET:HE3	13:a:150:VAL:HG21	2.03	0.40
13:a:6:LYS:HB3	13:a:11:VAL:HG12	2.02	0.40
6:F:49:ALA:HA	6:F:215:GLU:O	2.20	0.40
8:H:3:ILE:O	8:H:126:SER:HA	2.21	0.40
10:J:33:THR:CG2	10:J:180:LYS:NZ	2.85	0.40
11:K:46:ALA:HB3	11:K:98:GLY:O	2.21	0.40
13:M:210:TRP:CH2	14:b:171:GLY:HA2	2.56	0.40
4:R:177:GLU:OE1	4:R:177:GLU:N	2.50	0.40
3:C:210:GLY:HA3	3:C:213:ASN:HB2	2.02	0.40
11:K:97:MET:HG2	11:K:117:SER:HB3	2.03	0.40
14:N:2:SER:O	14:N:16:ALA:HA	2.20	0.40
14:N:41:ILE:N	14:N:41:ILE:CD1	2.84	0.40
1:O:230:ILE:HD12	1:O:230:ILE:N	2.36	0.40
3:Q:36:CYS:N	3:Q:51:GLU:HG2	2.36	0.40
3:Q:122:GLN:C	3:Q:122:GLN:NE2	2.79	0.40
5:S:73:GLY:HA3	5:S:224:PHE:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:241:LEU:HD12	7:U:241:LEU:HA	1.90	0.40
8:V:18:THR:HB	8:V:30:ASN:HD22	1.87	0.40
9:W:91:GLY:N	9:W:92:PRO:CD	2.83	0.40
10:X:24:SER:OG	11:Y:133:GLN:NE2	2.54	0.40
13:a:-5:PRO:HD3	13:a:102:TRP:CE2	2.57	0.40
2:B:55:THR:HG22	2:B:59:LEU:HD23	2.04	0.40
3:C:41:LYS:HD3	3:C:163:TRP:O	2.21	0.40
6:F:43:ASN:N	6:F:43:ASN:ND2	2.70	0.40
7:G:73:ARG:NH2	14:N:39:ASP:OD2	2.55	0.40
11:K:176:ASN:ND2	11:K:190:ASN:HD22	2.15	0.40
12:L:198:THR:C	12:L:200:ASP:N	2.80	0.40
13:M:178:ARG:CZ	8:V:135:MET:HE3	2.52	0.40
3:Q:153:GLN:O	3:Q:160:TYR:HA	2.22	0.40
4:R:121:LEU:HD13	5:S:128:ARG:HH21	1.86	0.40
8:V:84:LYS:HE2	8:V:119:THR:HG23	2.03	0.40
10:X:193:PHE:C	10:X:195:ALA:N	2.78	0.40
11:Y:4:LEU:HD13	11:Y:161:ILE:HD11	2.03	0.40
11:Y:155:TYR:OH	11:Y:204:GLU:OE1	2.36	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%)	235 (95%)	10 (4%)	3 (1%)	10	34
1	O	248/250 (99%)	236 (95%)	9 (4%)	3 (1%)	10	34
2	B	242/244 (99%)	214 (88%)	22 (9%)	6 (2%)	4	16
2	P	242/244 (99%)	215 (89%)	21 (9%)	6 (2%)	4	16
3	C	239/241 (99%)	220 (92%)	14 (6%)	5 (2%)	5	20
3	Q	239/241 (99%)	221 (92%)	13 (5%)	5 (2%)	5	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	240/242 (99%)	219 (91%)	16 (7%)	5 (2%)	5	20
4	R	240/242 (99%)	221 (92%)	14 (6%)	5 (2%)	5	20
5	E	231/233 (99%)	207 (90%)	20 (9%)	4 (2%)	7	25
5	S	231/233 (99%)	207 (90%)	20 (9%)	4 (2%)	7	25
6	F	242/244 (99%)	226 (93%)	13 (5%)	3 (1%)	10	34
6	T	242/244 (99%)	226 (93%)	13 (5%)	3 (1%)	10	34
7	G	241/243 (99%)	228 (95%)	12 (5%)	1 (0%)	30	60
7	U	241/243 (99%)	228 (95%)	12 (5%)	1 (0%)	30	60
8	H	220/222 (99%)	206 (94%)	10 (4%)	4 (2%)	6	23
8	V	220/222 (99%)	207 (94%)	9 (4%)	4 (2%)	6	23
9	I	202/204 (99%)	195 (96%)	7 (4%)	0	100	100
9	W	202/204 (99%)	195 (96%)	7 (4%)	0	100	100
10	J	196/198 (99%)	184 (94%)	9 (5%)	3 (2%)	8	28
10	X	196/198 (99%)	184 (94%)	9 (5%)	3 (2%)	8	28
11	K	210/212 (99%)	199 (95%)	10 (5%)	1 (0%)	24	55
11	Y	210/212 (99%)	199 (95%)	10 (5%)	1 (0%)	24	55
12	L	220/222 (99%)	206 (94%)	13 (6%)	1 (0%)	24	55
12	Z	220/222 (99%)	208 (94%)	10 (4%)	2 (1%)	14	41
13	M	231/233 (99%)	215 (93%)	14 (6%)	2 (1%)	14	41
13	a	231/233 (99%)	215 (93%)	14 (6%)	2 (1%)	14	41
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
15	1	1/4 (25%)	0	1 (100%)	0	100	100
15	2	1/4 (25%)	1 (100%)	0	0	100	100
15	3	1/4 (25%)	1 (100%)	0	0	100	100
15	4	1/4 (25%)	0	1 (100%)	0	100	100
15	5	1/4 (25%)	1 (100%)	0	0	100	100
15	6	1/4 (25%)	1 (100%)	0	0	100	100
All	All	6318/6392 (99%)	5894 (93%)	347 (6%)	77 (1%)	10	34

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	169	LYS
2	B	186	MET
2	B	224	ASP
3	C	58	LEU
4	D	130	GLU
4	D	189	SER
6	F	207	ASN
12	L	71	ASP
13	M	1	SER
1	O	5	THR
1	O	169	LYS
2	P	186	MET
2	P	224	ASP
3	Q	58	LEU
4	R	130	GLU
6	T	207	ASN
2	B	6	ARG
2	B	54	VAL
2	B	221	GLY
3	C	189	PRO
3	C	209	THR
4	D	126	GLY
5	E	204	ARG
5	E	220	LYS
8	H	91	GLN
10	J	195	ALA
2	P	6	ARG
2	P	54	VAL
2	P	221	GLY
3	Q	209	THR
4	R	126	GLY
4	R	189	SER
5	S	5	ARG
5	S	204	ARG
5	S	220	LYS
8	V	9	ASN
8	V	91	GLN
10	X	195	ALA
12	Z	71	ASP
13	a	1	SER
3	C	208	GLN
4	D	129	GLY

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Mol	Chain	Res	Type
5	E	5	ARG
6	F	208	LYS
8	H	9	ASN
8	H	95	GLY
10	J	48	ALA
11	K	39	PRO
13	M	102	TRP
3	Q	189	PRO
4	R	129	GLY
6	T	208	LYS
10	X	48	ALA
11	Y	39	PRO
2	B	32	SER
4	D	128	SER
6	F	143	LYS
7	G	247	GLN
2	P	32	SER
3	Q	208	GLN
4	R	128	SER
5	S	161	THR
6	T	143	LYS
7	U	247	GLN
13	a	102	TRP
3	C	190	ALA
5	E	161	THR
3	Q	190	ALA
8	V	95	GLY
12	Z	163	LYS
1	A	56	SER
1	O	56	SER
8	H	105	PRO
8	V	105	PRO
10	J	7	VAL
10	X	7	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%)	199 (95%)	10 (5%)	23	56
1	O	209/209 (100%)	202 (97%)	7 (3%)	33	69
2	B	203/203 (100%)	190 (94%)	13 (6%)	16	44
2	P	203/203 (100%)	190 (94%)	13 (6%)	16	44
3	C	213/213 (100%)	204 (96%)	9 (4%)	26	61
3	Q	213/213 (100%)	204 (96%)	9 (4%)	26	61
4	D	198/198 (100%)	184 (93%)	14 (7%)	13	39
4	R	198/198 (100%)	185 (93%)	13 (7%)	15	43
5	E	192/192 (100%)	176 (92%)	16 (8%)	10	32
5	S	192/192 (100%)	176 (92%)	16 (8%)	10	32
6	F	201/201 (100%)	184 (92%)	17 (8%)	10	31
6	T	201/201 (100%)	183 (91%)	18 (9%)	9	28
7	G	207/207 (100%)	195 (94%)	12 (6%)	18	49
7	U	207/207 (100%)	195 (94%)	12 (6%)	18	49
8	H	181/181 (100%)	174 (96%)	7 (4%)	28	64
8	V	181/181 (100%)	174 (96%)	7 (4%)	28	64
9	I	172/172 (100%)	167 (97%)	5 (3%)	37	73
9	W	172/172 (100%)	168 (98%)	4 (2%)	44	78
10	J	175/175 (100%)	162 (93%)	13 (7%)	13	37
10	X	175/175 (100%)	163 (93%)	12 (7%)	14	41
11	K	169/169 (100%)	158 (94%)	11 (6%)	15	43
11	Y	169/169 (100%)	157 (93%)	12 (7%)	13	39
12	L	185/185 (100%)	174 (94%)	11 (6%)	18	48
12	Z	185/185 (100%)	173 (94%)	12 (6%)	15	43
13	M	199/199 (100%)	184 (92%)	15 (8%)	12	37
13	a	199/199 (100%)	184 (92%)	15 (8%)	12	37
14	N	162/162 (100%)	153 (94%)	9 (6%)	19	50
14	b	162/162 (100%)	152 (94%)	10 (6%)	16	45
15	1	1/1 (100%)	0	1 (100%)	0	0
15	2	1/1 (100%)	1 (100%)	0	100	100
15	3	1/1 (100%)	0	1 (100%)	0	0
15	4	1/1 (100%)	0	1 (100%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	5	1/1 (100%)	1 (100%)	0	100	100
15	6	1/1 (100%)	0	1 (100%)	0	0
All	All	5338/5338 (100%)	5012 (94%)	326 (6%)	17	46

All (326) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	33	GLN
1	A	62	GLU
1	A	64	LEU
1	A	136	SER
1	A	160	PHE
1	A	181	ARG
1	A	192	ILE
1	A	212	ILE
1	A	231	PRO
2	B	6	ARG
2	B	46	ILE
2	B	58	LEU
2	B	68	LEU
2	B	92	THR
2	B	108	ILE
2	B	117	LEU
2	B	125	THR
2	B	152	THR
2	B	165	ILE
2	B	187	LYS
2	B	194	LEU
2	B	232	PHE
3	C	10	ARG
3	C	25	GLU
3	C	67	LYS
3	C	90	ILE
3	C	130	VAL
3	C	136	SER
3	C	153	GLN
3	C	168	ILE
3	C	177	GLU
4	D	28	LEU
4	D	40	ILE

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Mol	Chain	Res	Type
4	D	48	LEU
4	D	52	LYS
4	D	64	ILE
4	D	70	ILE
4	D	76	CYS
4	D	107	ILE
4	D	110	GLU
4	D	132	ARG
4	D	184	LEU
4	D	198	LEU
4	D	201	LEU
4	D	222	ILE
5	E	12	THR
5	E	16	SER
5	E	28	LEU
5	E	32	LYS
5	E	65	ILE
5	E	74	LEU
5	E	136	ILE
5	E	137	ILE
5	E	182	ILE
5	E	191	LEU
5	E	200	SER
5	E	201	GLN
5	E	208	LEU
5	E	217	ILE
5	E	230	GLU
5	E	234	LYS
6	F	11	SER
6	F	35	THR
6	F	36	THR
6	F	43	ASN
6	F	72	ARG
6	F	82	ILE
6	F	121	GLN
6	F	127	ASN
6	F	169	ARG
6	F	185	GLU
6	F	190	ARG
6	F	205	GLU
6	F	206	ASP
6	F	216	ILE

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Mol	Chain	Res	Type
6	F	225	ASN
6	F	232	LYS
6	F	247	ILE
7	G	36	ILE
7	G	68	ILE
7	G	73	ARG
7	G	88	ASN
7	G	120	LEU
7	G	122	GLN
7	G	125	THR
7	G	171	GLN
7	G	206	MET
7	G	226	LYS
7	G	240	ARG
7	G	241	LEU
8	H	34	LEU
8	H	37	ILE
8	H	56	THR
8	H	68	LEU
8	H	121	VAL
8	H	180	ILE
8	H	196	ARG
9	I	19	LEU
9	I	28	ASN
9	I	111	ILE
9	I	161	LEU
9	I	162	LEU
10	J	5	ILE
10	J	23	ILE
10	J	33	THR
10	J	34	ARG
10	J	51	THR
10	J	62	ILE
10	J	67	ILE
10	J	69	GLU
10	J	89	SER
10	J	90	ILE
10	J	125	GLU
10	J	170	MET
10	J	178	ILE
11	K	4	LEU
11	K	9	GLN

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Mol	Chain	Res	Type
11	K	37	ILE
11	K	65	LEU
11	K	69	ARG
11	K	87	VAL
11	K	99	THR
11	K	100	MET
11	K	108	GLU
11	K	148	LEU
11	K	186	ILE
12	L	-9	GLN
12	L	13	LEU
12	L	24	SER
12	L	39	ASN
12	L	40	ILE
12	L	57	ARG
12	L	61	SER
12	L	70	ASN
12	L	98	HIS
12	L	99	THR
12	L	140	LEU
13	M	-4	ILE
13	M	34	ILE
13	M	39	ASN
13	M	60	ASP
13	M	61	LEU
13	M	95	ARG
13	M	106	ILE
13	M	150	VAL
13	M	152	ARG
13	M	161	VAL
13	M	162	GLN
13	M	168	ILE
13	M	191	ILE
13	M	204	GLN
13	M	216	ILE
14	N	26	ILE
14	N	36	ARG
14	N	41	ILE
14	N	83	LYS
14	N	88	GLU
14	N	115	LEU
14	N	144	GLU

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Mol	Chain	Res	Type
14	N	178	LEU
14	N	195	GLN
1	O	33	GLN
1	O	62	GLU
1	O	64	LEU
1	O	136	SER
1	O	160	PHE
1	O	181	ARG
1	O	192	ILE
2	P	6	ARG
2	P	46	ILE
2	P	58	LEU
2	P	68	LEU
2	P	92	THR
2	P	108	ILE
2	P	117	LEU
2	P	125	THR
2	P	152	THR
2	P	165	ILE
2	P	187	LYS
2	P	194	LEU
2	P	232	PHE
3	Q	10	ARG
3	Q	25	GLU
3	Q	67	LYS
3	Q	90	ILE
3	Q	136	SER
3	Q	153	GLN
3	Q	168	ILE
3	Q	177	GLU
3	Q	216	ILE
4	R	28	LEU
4	R	40	ILE
4	R	48	LEU
4	R	52	LYS
4	R	70	ILE
4	R	76	CYS
4	R	107	ILE
4	R	110	GLU
4	R	132	ARG
4	R	184	LEU
4	R	198	LEU

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Mol	Chain	Res	Type
4	R	201	LEU
4	R	222	ILE
5	S	12	THR
5	S	16	SER
5	S	28	LEU
5	S	32	LYS
5	S	65	ILE
5	S	74	LEU
5	S	136	ILE
5	S	137	ILE
5	S	182	ILE
5	S	191	LEU
5	S	200	SER
5	S	201	GLN
5	S	208	LEU
5	S	217	ILE
5	S	230	GLU
5	S	234	LYS
6	T	11	SER
6	T	35	THR
6	T	36	THR
6	T	43	ASN
6	T	70	VAL
6	T	72	ARG
6	T	82	ILE
6	T	121	GLN
6	T	127	ASN
6	T	169	ARG
6	T	185	GLU
6	T	190	ARG
6	T	205	GLU
6	T	206	ASP
6	T	216	ILE
6	T	225	ASN
6	T	232	LYS
6	T	247	ILE
7	U	36	ILE
7	U	68	ILE
7	U	73	ARG
7	U	88	ASN
7	U	120	LEU
7	U	122	GLN

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Mol	Chain	Res	Type
7	U	125	THR
7	U	171	GLN
7	U	206	MET
7	U	226	LYS
7	U	240	ARG
7	U	241	LEU
8	V	34	LEU
8	V	37	ILE
8	V	56	THR
8	V	68	LEU
8	V	121	VAL
8	V	180	ILE
8	V	196	ARG
9	W	28	ASN
9	W	111	ILE
9	W	161	LEU
9	W	162	LEU
10	X	5	ILE
10	X	23	ILE
10	X	33	THR
10	X	34	ARG
10	X	51	THR
10	X	67	ILE
10	X	69	GLU
10	X	89	SER
10	X	90	ILE
10	X	125	GLU
10	X	170	MET
10	X	178	ILE
11	Y	4	LEU
11	Y	9	GLN
11	Y	37	ILE
11	Y	39	PRO
11	Y	65	LEU
11	Y	69	ARG
11	Y	87	VAL
11	Y	99	THR
11	Y	100	MET
11	Y	108	GLU
11	Y	148	LEU
11	Y	186	ILE
12	Z	-7	ASN

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Mol	Chain	Res	Type
12	Z	13	LEU
12	Z	24	SER
12	Z	39	ASN
12	Z	40	ILE
12	Z	57	ARG
12	Z	61	SER
12	Z	70	ASN
12	Z	98	HIS
12	Z	99	THR
12	Z	140	LEU
12	Z	167	VAL
13	a	-4	ILE
13	a	34	ILE
13	a	39	ASN
13	a	60	ASP
13	a	61	LEU
13	a	95	ARG
13	a	106	ILE
13	a	150	VAL
13	a	152	ARG
13	a	161	VAL
13	a	162	GLN
13	a	168	ILE
13	a	191	ILE
13	a	204	GLN
13	a	216	ILE
14	b	26	ILE
14	b	36	ARG
14	b	41	ILE
14	b	55	ILE
14	b	83	LYS
14	b	88	GLU
14	b	115	LEU
14	b	144	GLU
14	b	178	LEU
14	b	195	GLN
15	1	1	THR
15	3	1	THR
15	4	1	THR
15	6	1	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (250) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
1	A	146	ASN
1	A	152	GLN
2	B	23	GLN
2	B	72	ASN
2	B	96	HIS
2	B	98	GLN
2	B	122	GLN
2	B	126	GLN
2	B	158	ASN
2	B	179	GLN
2	B	223	ASN
3	C	23	GLN
3	C	83	ASN
3	C	122	GLN
3	C	126	GLN
3	C	153	GLN
3	C	166	GLN
3	C	213	ASN
3	C	239	GLN
3	C	242	GLN
3	C	247	GLN
4	D	23	GLN
4	D	108	ASN
4	D	154	GLN
4	D	168	ASN
4	D	215	ASN
4	D	233	ASN
5	E	7	ASN
5	E	33	GLN
5	E	62	GLN
5	E	71	HIS
5	E	92	GLN
5	E	93	GLN
5	E	102	ASN
5	E	119	GLN
5	E	121	ASN
5	E	123	GLN
5	E	150	GLN
5	E	154	ASN
5	E	187	ASN
5	E	201	GLN

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Mol	Chain	Res	Type
5	E	212	ASN
6	F	23	GLN
6	F	43	ASN
6	F	87	HIS
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	195	GLN
6	F	244	GLN
7	G	35	ASN
7	G	88	ASN
7	G	119	ASN
7	G	122	GLN
7	G	126	GLN
7	G	171	GLN
7	G	172	GLN
7	G	180	ASN
7	G	191	ASN
7	G	236	ASN
8	H	30	ASN
8	H	66	HIS
8	H	81	GLN
8	H	86	HIS
8	H	141	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	28	ASN
9	I	35	HIS
9	I	54	ASN
9	I	147	ASN
9	I	159	GLN
10	J	8	GLN
10	J	35	GLN
10	J	53	GLN
10	J	61	ASN
10	J	76	GLN
10	J	84	GLN
10	J	116	GLN
10	J	145	HIS
10	J	164	GLN

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Mol	Chain	Res	Type
10	J	189	GLN
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	176	ASN
11	K	188	HIS
11	K	191	HIS
11	K	208	ASN
11	K	209	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	19	ASN
12	L	26	ASN
12	L	39	ASN
12	L	45	ASN
12	L	60	ASN
12	L	70	ASN
12	L	142	ASN
12	L	143	GLN
12	L	148	ASN
12	L	155	ASN
12	L	185	HIS
12	L	187	GLN
13	M	-7	GLN
13	M	9	ASN
13	M	17	ASN
13	M	39	ASN
13	M	53	HIS
13	M	93	GLN
13	M	99	ASN
13	M	162	GLN
13	M	170	ASN
13	M	202	ASN
13	M	204	GLN
14	N	60	GLN
14	N	106	ASN
14	N	141	ASN
14	N	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
1	O	146	ASN

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Mol	Chain	Res	Type
1	O	152	GLN
2	P	23	GLN
2	P	72	ASN
2	P	91	ASN
2	P	96	HIS
2	P	98	GLN
2	P	122	GLN
2	P	126	GLN
2	P	158	ASN
2	P	179	GLN
2	P	223	ASN
3	Q	23	GLN
3	Q	83	ASN
3	Q	122	GLN
3	Q	126	GLN
3	Q	153	GLN
3	Q	166	GLN
3	Q	213	ASN
3	Q	239	GLN
3	Q	242	GLN
3	Q	247	GLN
4	R	23	GLN
4	R	99	HIS
4	R	108	ASN
4	R	157	HIS
4	R	168	ASN
4	R	215	ASN
4	R	218	GLN
4	R	225	GLN
4	R	233	ASN
5	S	7	ASN
5	S	33	GLN
5	S	62	GLN
5	S	71	HIS
5	S	92	GLN
5	S	93	GLN
5	S	102	ASN
5	S	119	GLN
5	S	121	ASN
5	S	123	GLN
5	S	150	GLN
5	S	154	ASN

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Mol	Chain	Res	Type
5	S	187	ASN
5	S	201	GLN
6	T	23	GLN
6	T	43	ASN
6	T	87	HIS
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	195	GLN
6	T	244	GLN
6	T	248	ASN
7	U	35	ASN
7	U	88	ASN
7	U	119	ASN
7	U	122	GLN
7	U	126	GLN
7	U	171	GLN
7	U	172	GLN
7	U	180	ASN
7	U	191	ASN
7	U	236	ASN
8	V	30	ASN
8	V	66	HIS
8	V	86	HIS
8	V	116	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	28	ASN
9	W	35	HIS
9	W	79	GLN
9	W	147	ASN
9	W	159	GLN
10	X	8	GLN
10	X	35	GLN
10	X	53	GLN
10	X	61	ASN
10	X	84	GLN
10	X	116	GLN
10	X	145	HIS
10	X	164	GLN

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Mol	Chain	Res	Type
10	X	189	GLN
11	Y	9	GLN
11	Y	62	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	176	ASN
11	Y	188	HIS
11	Y	191	HIS
11	Y	208	ASN
11	Y	209	ASN
12	Z	-7	ASN
12	Z	39	ASN
12	Z	45	ASN
12	Z	60	ASN
12	Z	70	ASN
12	Z	142	ASN
12	Z	143	GLN
12	Z	148	ASN
12	Z	155	ASN
12	Z	185	HIS
12	Z	187	GLN
13	a	-7	GLN
13	a	9	ASN
13	a	17	ASN
13	a	39	ASN
13	a	53	HIS
13	a	93	GLN
13	a	99	ASN
13	a	162	GLN
13	a	170	ASN
13	a	202	ASN
13	a	204	GLN
14	b	60	GLN
14	b	69	GLN
14	b	106	ASN
14	b	141	ASN
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 ⓘ

12 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	OJT	5	3	15,11	7,8,9	1.45	2 (28%)	7,9,11	1.12	1 (14%)
15	LYH	3	2	15	7,8,9	1.76	1 (14%)	4,8,10	1.38	1 (25%)
15	LYH	5	2	15	7,8,9	1.75	1 (14%)	4,8,10	1.34	1 (25%)
15	OJT	3	3	14,15	7,8,9	1.41	2 (28%)	7,9,11	1.00	0
15	OJT	1	3	15,8	7,8,9	1.26	1 (14%)	7,9,11	0.97	0
15	OJT	4	3	15,8	7,8,9	1.19	0	7,9,11	0.94	0
15	LYH	2	2	15	7,8,9	1.65	1 (14%)	4,8,10	1.30	1 (25%)
15	OJT	6	3	14,15	7,8,9	1.50	2 (28%)	7,9,11	0.93	0
15	LYH	4	2	15	7,8,9	1.81	1 (14%)	4,8,10	0.98	0
15	LYH	1	2	15	7,8,9	1.73	1 (14%)	4,8,10	0.92	0
15	LYH	6	2	15	7,8,9	1.56	1 (14%)	4,8,10	1.39	1 (25%)
15	OJT	2	3	15,11	7,8,9	1.32	1 (14%)	7,9,11	1.09	1 (14%)

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	OJT	5	3	15,11	-	2/8/8/9	-
15	LYH	3	2	15	-	1/3/7/9	-
15	LYH	5	2	15	-	1/3/7/9	-
15	OJT	3	3	14,15	-	2/8/8/9	-
15	OJT	1	3	15,8	-	5/8/8/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	OJT	4	3	15,8	-	5/8/8/9	-
15	LYH	2	2	15	-	1/3/7/9	-
15	OJT	6	3	14,15	-	2/8/8/9	-
15	LYH	4	2	15	-	1/3/7/9	-
15	LYH	1	2	15	-	1/3/7/9	-
15	LYH	6	2	15	-	1/3/7/9	-
15	OJT	2	3	15,11	-	2/8/8/9	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	2	LYH	CA-CB	4.15	1.55	1.51
15	5	2	LYH	CA-CB	3.99	1.55	1.51
15	3	2	LYH	CA-CB	3.91	1.55	1.51
15	1	2	LYH	CA-CB	3.86	1.55	1.51
15	2	2	LYH	CA-CB	3.55	1.55	1.51
15	6	2	LYH	CA-CB	3.31	1.54	1.51
15	6	3	OJT	C19-CA	2.53	1.58	1.53
15	5	3	OJT	C19-CA	2.47	1.58	1.53
15	6	3	OJT	C17-CA	2.39	1.56	1.53
15	3	3	OJT	C19-CA	2.35	1.58	1.53
15	2	3	OJT	C19-CA	2.29	1.58	1.53
15	5	3	OJT	C17-CA	2.28	1.56	1.53
15	3	3	OJT	C17-CA	2.25	1.56	1.53
15	1	3	OJT	C17-CA	2.15	1.56	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	5	2	LYH	CE-CD-CG	-2.16	107.75	112.91
15	6	2	LYH	CE-CD-CG	-2.15	107.77	112.91
15	3	2	LYH	CE-CD-CG	-2.12	107.85	112.91
15	5	3	OJT	C17-C16-C	2.05	118.02	112.27
15	2	3	OJT	C17-C16-C	2.03	117.96	112.27
15	2	2	LYH	CE-CD-CG	-2.03	108.06	112.91

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	2	2	LYH	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
15	3	2	LYH	CG-CD-CE-NZ
15	5	2	LYH	CG-CD-CE-NZ
15	6	2	LYH	CG-CD-CE-NZ
15	1	3	0JT	C-C16-C17-CA
15	4	3	0JT	C-C16-C17-CA
15	2	3	0JT	C-C16-C17-CA
15	3	3	0JT	C-C16-C17-CA
15	5	3	0JT	C-C16-C17-CA
15	6	3	0JT	C-C16-C17-CA
15	1	2	LYH	CG-CD-CE-NZ
15	4	2	LYH	CG-CD-CE-NZ
15	1	3	0JT	C21-C19-CA-C17
15	4	3	0JT	C21-C19-CA-C17
15	1	3	0JT	C20-C19-CA-C17
15	4	3	0JT	C20-C19-CA-C17
15	1	3	0JT	C16-C17-CA-N
15	3	3	0JT	C16-C17-CA-N
15	4	3	0JT	C16-C17-CA-N
15	6	3	0JT	C16-C17-CA-N
15	1	3	0JT	C21-C19-CA-N
15	4	3	0JT	C21-C19-CA-N
15	2	3	0JT	C16-C17-CA-N
15	5	3	0JT	C16-C17-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	3	2	LYH	1	0
15	6	2	LYH	1	0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.39	2 (0%) 82 75	35, 55, 84, 105	0
1	O	250/250 (100%)	-0.41	1 (0%) 88 84	36, 55, 84, 105	0
2	B	244/244 (100%)	-0.18	7 (2%) 53 43	39, 56, 94, 118	0
2	P	244/244 (100%)	-0.19	7 (2%) 53 43	39, 57, 95, 118	0
3	C	241/241 (100%)	-0.14	5 (2%) 63 54	40, 59, 110, 129	0
3	Q	241/241 (100%)	-0.15	4 (1%) 69 60	42, 61, 110, 129	0
4	D	242/242 (100%)	-0.11	6 (2%) 58 48	39, 60, 92, 125	0
4	R	242/242 (100%)	-0.08	8 (3%) 49 39	41, 61, 93, 126	0
5	E	233/233 (100%)	-0.16	2 (0%) 81 74	42, 62, 87, 111	0
5	S	233/233 (100%)	-0.12	4 (1%) 69 60	42, 62, 87, 111	0
6	F	244/244 (100%)	-0.26	1 (0%) 88 84	39, 56, 92, 106	0
6	T	244/244 (100%)	-0.22	3 (1%) 76 68	39, 56, 93, 105	0
7	G	243/243 (100%)	-0.35	1 (0%) 88 84	37, 53, 80, 112	0
7	U	243/243 (100%)	-0.42	4 (1%) 70 61	36, 53, 79, 112	0
8	H	222/222 (100%)	-0.55	0 100 100	31, 48, 68, 98	0
8	V	222/222 (100%)	-0.54	0 100 100	33, 48, 67, 98	0
9	I	204/204 (100%)	-0.63	0 100 100	35, 50, 67, 84	0
9	W	204/204 (100%)	-0.57	1 (0%) 87 82	37, 50, 68, 84	0
10	J	198/198 (100%)	-0.45	5 (2%) 58 48	37, 51, 68, 124	0
10	X	198/198 (100%)	-0.48	3 (1%) 72 63	38, 51, 70, 124	0
11	K	212/212 (100%)	-0.49	0 100 100	34, 51, 75, 82	0
11	Y	212/212 (100%)	-0.44	0 100 100	35, 51, 74, 82	0
12	L	222/222 (100%)	-0.50	1 (0%) 87 82	33, 50, 71, 96	0
12	Z	222/222 (100%)	-0.48	1 (0%) 87 82	33, 50, 71, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/233 (100%)	-0.54	1 (0%) 88 84	35, 49, 64, 69	0
13	a	233/233 (100%)	-0.55	1 (0%) 88 84	34, 48, 64, 69	0
14	N	196/196 (100%)	-0.60	0 100 100	33, 45, 67, 77	0
14	b	196/196 (100%)	-0.56	1 (0%) 87 82	33, 46, 68, 77	0
15	1	1/4 (25%)	0.77	0 100 100	50, 50, 50, 50	0
15	2	1/4 (25%)	1.01	0 100 100	52, 52, 52, 52	0
15	3	1/4 (25%)	0.84	0 100 100	57, 57, 57, 57	0
15	4	1/4 (25%)	0.64	0 100 100	51, 51, 51, 51	0
15	5	1/4 (25%)	0.79	0 100 100	51, 51, 51, 51	0
15	6	1/4 (25%)	0.89	0 100 100	57, 57, 57, 57	0
All	All	6374/6392 (99%)	-0.37	69 (1%) 78 70	31, 53, 84, 129	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	126	GLY	7.3
4	D	128	SER	6.4
12	L	164	TYR	5.3
4	R	128	SER	5.0
2	B	221	GLY	4.8
4	D	127	ALA	4.8
5	S	4	PHE	4.8
7	U	248	ASP	4.8
4	R	127	ALA	4.5
10	X	196	GLN	4.5
12	Z	164	TYR	4.5
7	U	6	ALA	4.4
4	R	126	GLY	4.2
3	C	55	THR	3.9
4	R	132	ARG	3.7
6	F	206	ASP	3.5
5	E	4	PHE	3.5
3	C	56	LEU	3.4
2	B	222	ALA	3.4
2	P	222	ALA	3.4
3	Q	56	LEU	3.3
4	R	133	LEU	3.3
10	J	196	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
3	C	54	SER	3.3
9	W	-8	SER	3.3
10	J	-1	MET	3.2
5	S	5	ARG	3.2
4	D	132	ARG	2.9
10	J	195	ALA	2.9
3	C	59	GLN	2.8
7	G	6	ALA	2.8
2	P	247	THR	2.8
4	R	129	GLY	2.8
7	U	193	GLU	2.8
13	a	-8	THR	2.7
1	A	252	ALA	2.7
2	B	223	ASN	2.7
2	P	221	GLY	2.6
2	P	54	VAL	2.6
3	Q	244	LYS	2.6
2	B	247	THR	2.6
3	Q	55	THR	2.6
13	M	-8	THR	2.4
6	T	247	ILE	2.4
3	C	246	GLU	2.3
14	b	107	LYS	2.3
3	Q	240	ILE	2.3
1	O	4	MET	2.3
2	P	223	ASN	2.2
5	S	6	ASN	2.2
10	J	194	GLN	2.2
10	J	172	MET	2.2
10	X	195	ALA	2.2
2	B	220	LYS	2.2
6	T	5	GLY	2.1
6	T	6	THR	2.1
4	R	121	LEU	2.1
2	B	4	GLY	2.1
2	B	225	GLY	2.1
4	D	129	GLY	2.1
5	S	230	GLU	2.1
2	P	4	GLY	2.1
5	E	205	ASP	2.1
10	X	-1	MET	2.1
4	R	122	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	204	GLU	2.1
7	U	208	ASP	2.0
4	D	133	LEU	2.0
2	P	226	GLU	2.0

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(Å ²)	Q<0.9
15	LYH	3	2	9/10	0.80	0.17	46,50,52,52	0
15	LYH	6	2	9/10	0.80	0.17	46,48,50,50	0
15	LYH	1	2	9/10	0.82	0.13	47,48,50,50	0
15	LYH	5	2	9/10	0.85	0.12	46,47,49,49	0
15	LYH	2	2	9/10	0.87	0.12	45,46,47,47	0
15	LYH	4	2	9/10	0.88	0.14	47,48,50,50	0
15	OJT	3	3	9/10	0.93	0.09	39,45,50,52	0
15	OJT	4	3	9/10	0.93	0.11	40,43,48,49	0
15	OJT	6	3	9/10	0.93	0.09	38,44,47,50	0
15	OJT	2	3	9/10	0.94	0.10	39,43,46,46	0
15	OJT	1	3	9/10	0.94	0.10	40,45,48,49	0
15	OJT	5	3	9/10	0.96	0.08	42,44,47,47	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.