



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:29 AM UTC

PDB ID : 3GPJ / pdb_00003gpj
Title : Crystal structure of the yeast 20S proteasome in complex with syringolin B
Authors : Groll, M.; Huber, R.; Kaiser, M.
Deposited on : 2009-03-23
Resolution : 2.70 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

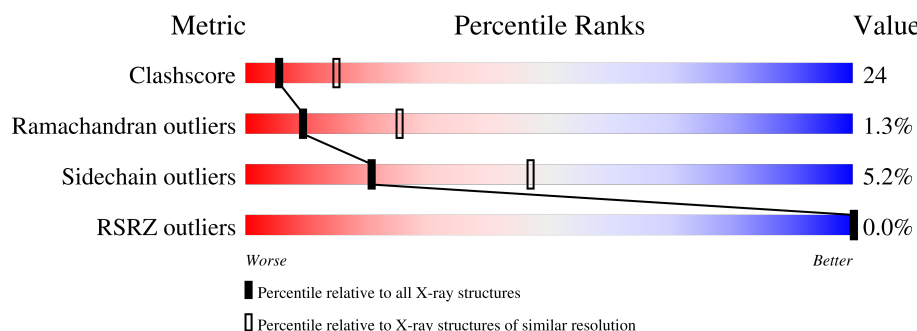
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



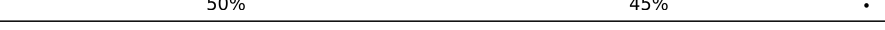
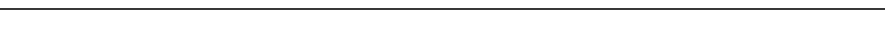
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	250	
1	O	250	
2	B	244	
2	P	244	
3	C	241	
3	Q	241	

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Mol	Chain	Length	Quality of chain
4	D	242	 61% 33% 5%
4	R	242	 62% 32% 5%
5	E	233	 59% 36% 5%
5	S	233	 58% 38% 5%
6	F	244	 57% 39% 5%
6	T	244	 54% 42% 5%
7	G	243	 60% 36% 5%
7	U	243	 58% 38% 5%
8	H	222	 60% 37% 5%
8	V	222	 61% 36% 5%
9	I	204	 58% 38% 5%
9	W	204	 55% 41% 5%
10	J	198	 48% 46% 5%
10	X	198	 50% 45% 5%
11	K	212	 59% 38% 5%
11	Y	212	 57% 40% 5%
12	L	222	 54% 37% 8%
12	Z	222	 54% 36% 9%
13	1	233	 60% 37% 5%
13	M	233	 61% 35% 5%
14	2	196	 64% 33% 5%
14	N	196	 62% 35% 5%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51023 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			

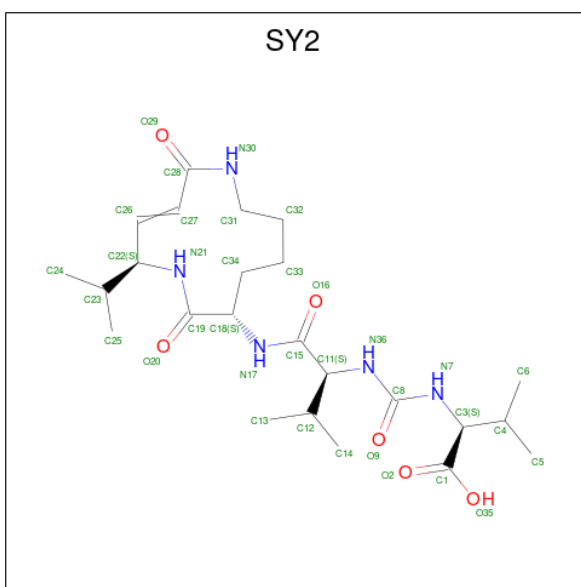
- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	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	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is N-{[(1S)-2-methyl-1-{[(5S,8S)-5-(1-methylethyl)-2,7-dioxo-1,6-diazacyclododec-3-en-8-yl]carbamoyl}propyl]carbamoyl}-L-valine (CCD ID: SY2) (formula: C₂₄H₄₁N₅O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			35	24	5	6		
15	K	1	Total	C	N	O	0	0
			35	24	5	6		
15	V	1	Total	C	N	O	0	0
			35	24	5	6		
15	Y	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	58	Total	O	0	0
			58	58		
16	B	39	Total	O	0	0
			39	39		
16	C	44	Total	O	0	0
			44	44		
16	D	42	Total	O	0	0
			42	42		
16	E	24	Total	O	0	0
			24	24		
16	F	49	Total	O	0	0
			49	49		
16	G	61	Total	O	0	0
			61	61		
16	H	48	Total	O	0	0
			48	48		

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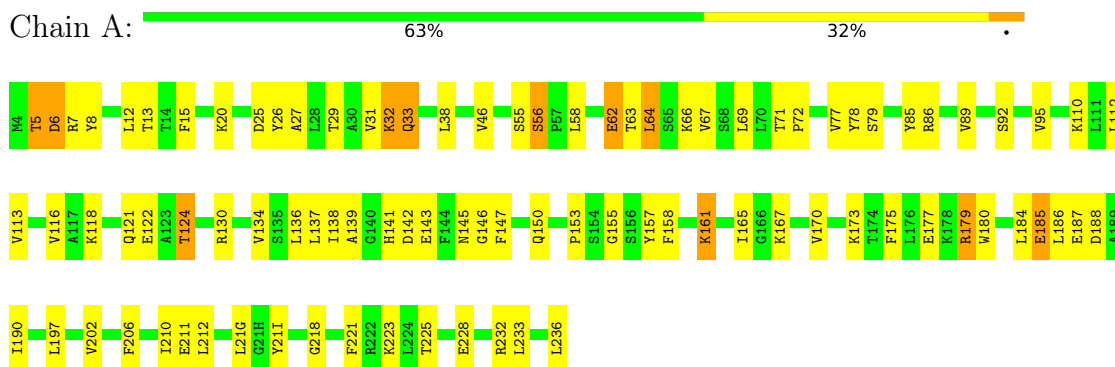
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	I	65	Total 65	O 65	0	0
16	J	49	Total 49	O 49	0	0
16	K	43	Total 43	O 43	0	0
16	L	58	Total 58	O 58	0	0
16	M	70	Total 70	O 70	0	0
16	N	55	Total 55	O 55	0	0
16	O	33	Total 33	O 33	0	0
16	P	30	Total 30	O 30	0	0
16	Q	27	Total 27	O 27	0	0
16	R	30	Total 30	O 30	0	0
16	S	23	Total 23	O 23	0	0
16	T	42	Total 42	O 42	0	0
16	U	60	Total 60	O 60	0	0
16	V	43	Total 43	O 43	0	0
16	W	62	Total 62	O 62	0	0
16	X	45	Total 45	O 45	0	0
16	Y	50	Total 50	O 50	0	0
16	Z	52	Total 52	O 52	0	0
16	1	71	Total 71	O 71	0	0
16	2	62	Total 62	O 62	0	0

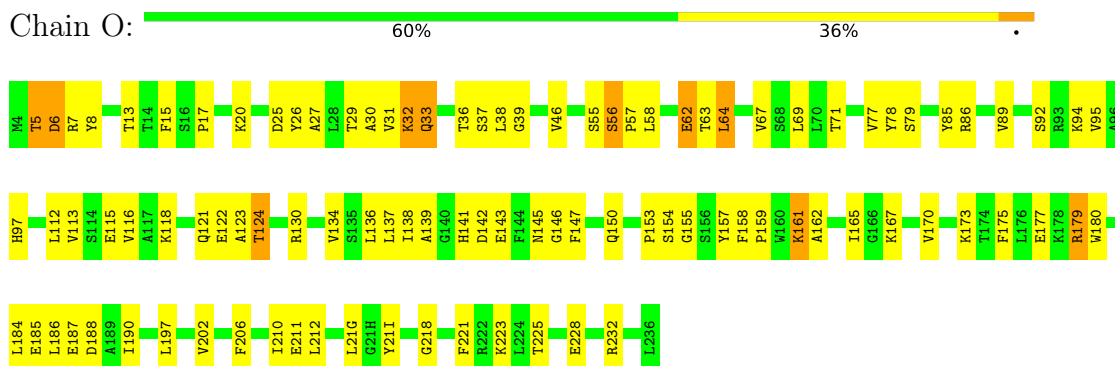
3 Residue-property plots

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

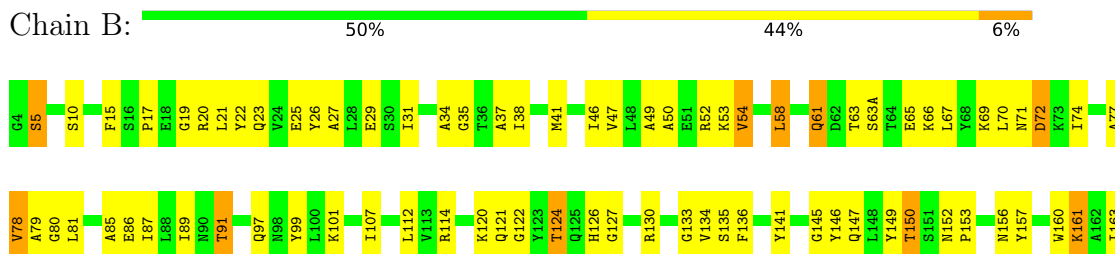
• Molecule 1: Proteasome component Y7

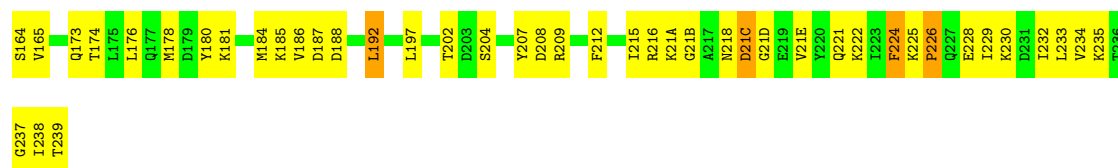


• Molecule 1: Proteasome component Y7



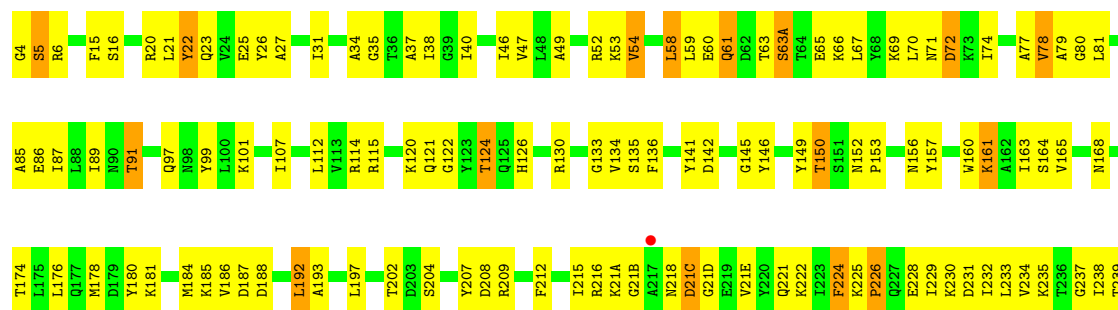
• Molecule 2: Proteasome component Y13





• Molecule 2: Proteasome component Y13

Chain P: 49% 44% 7%



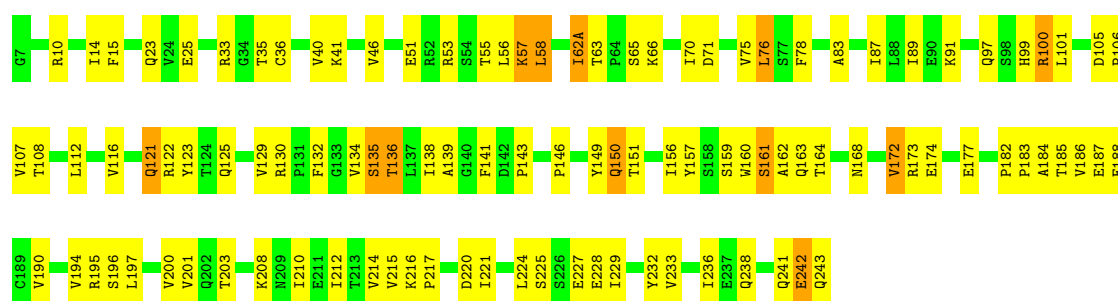
• Molecule 3: Proteasome component PRE6

Chain C: 54% 41% 5%



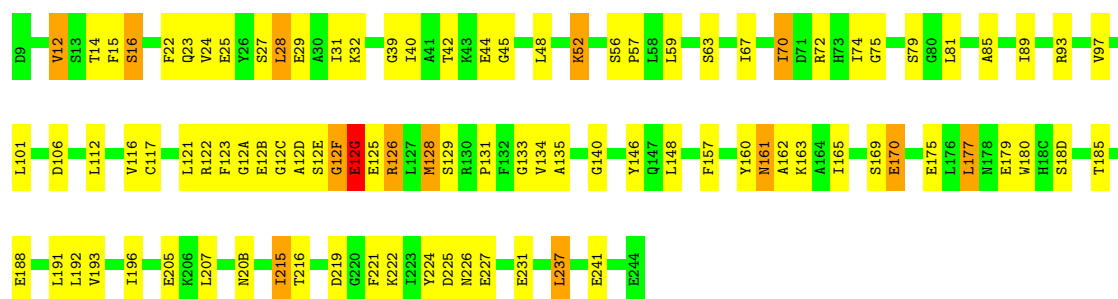
• Molecule 3: Proteasome component PRE6

Chain Q: 56% 39% 5%



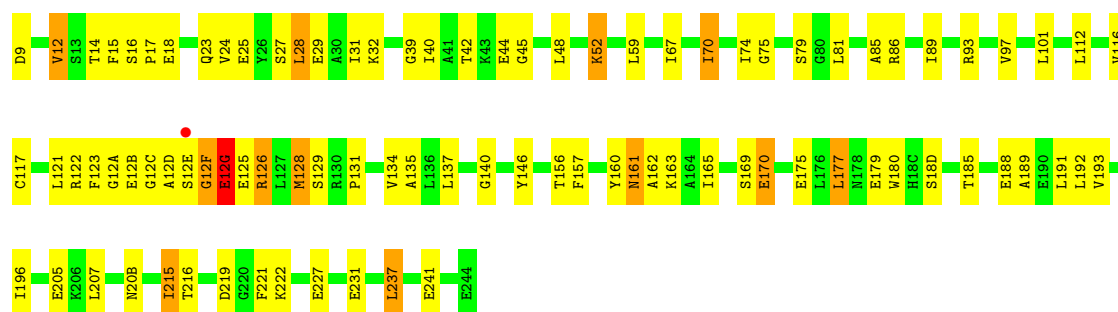
• Molecule 4: Proteasome component PUP2

Chain D: 61% 33% 5%



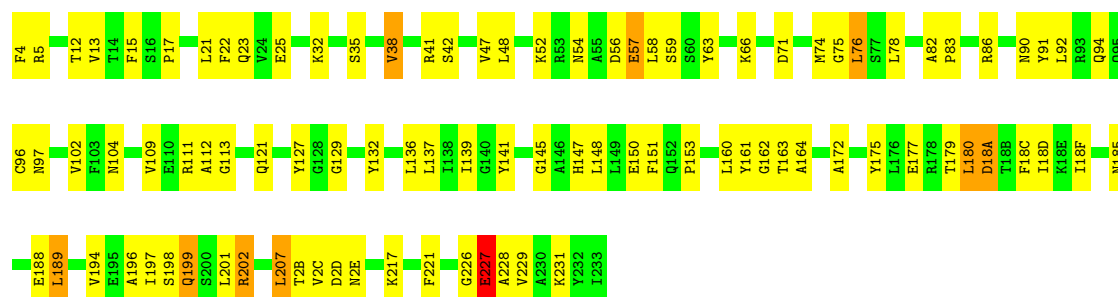
• Molecule 4: Proteasome component PUP2

Chain R: 62% 32% 5%



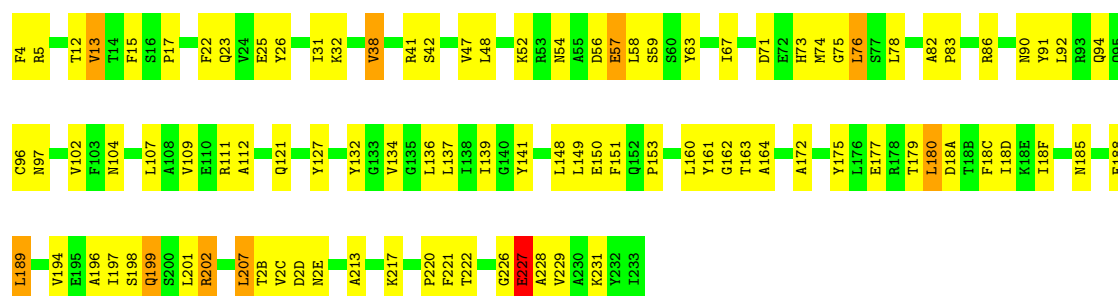
• Molecule 5: Proteasome component PRE5

Chain E: 59% 36% 5%

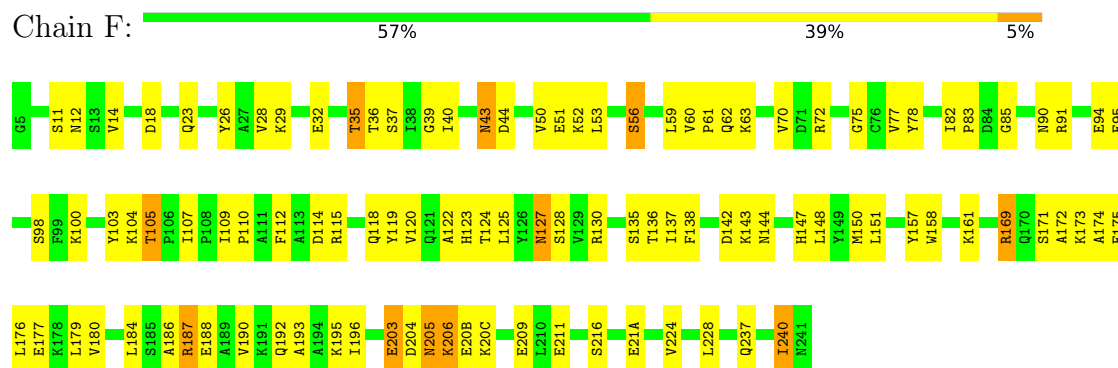


• Molecule 5: Proteasome component PRE5

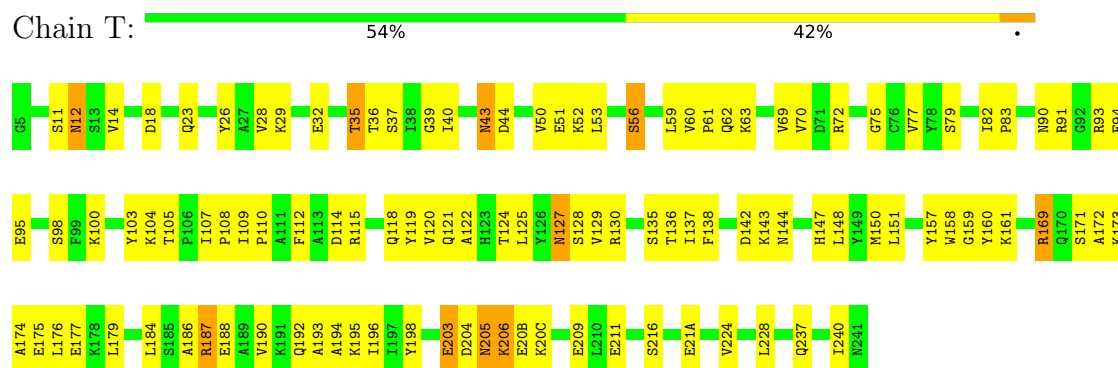
Chain S: 58% 38% 4%



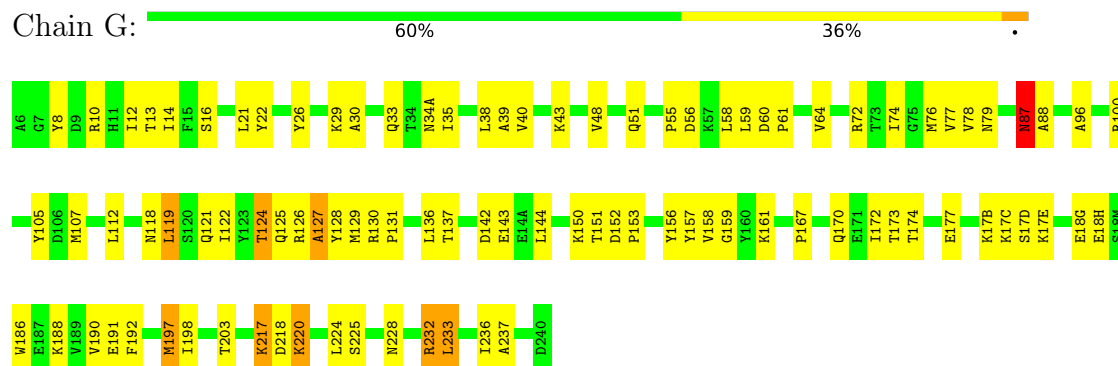
- Molecule 6: Proteasome component C1



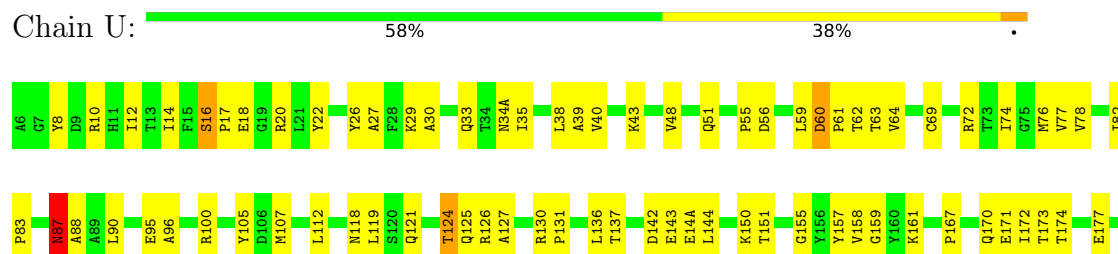
- Molecule 6: Proteasome component C1



- Molecule 7: Proteasome component C7-alpha

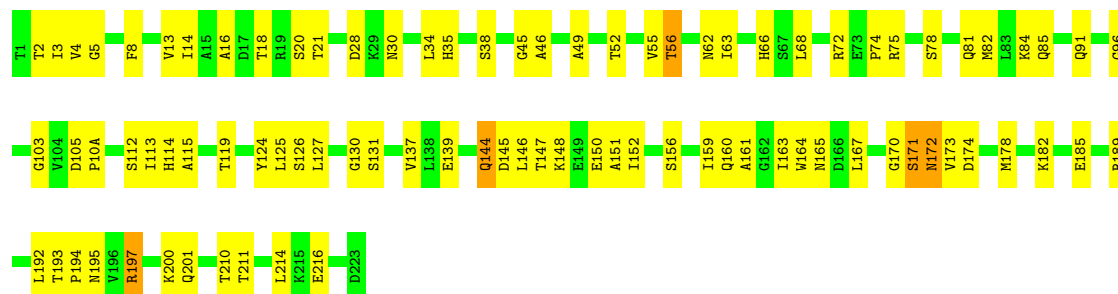


- Molecule 7: Proteasome component C7-alpha

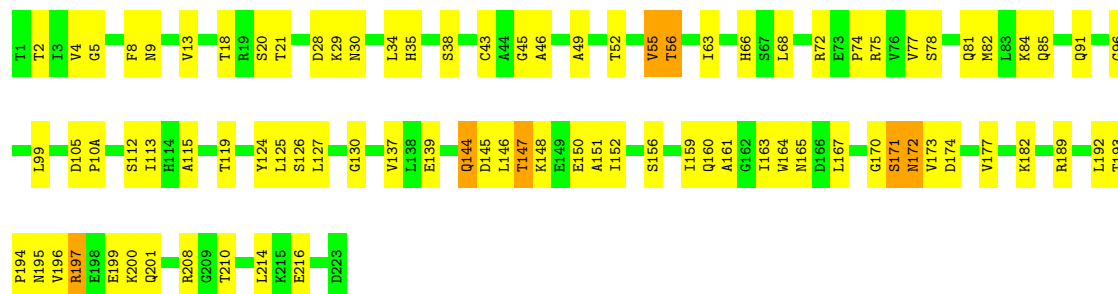




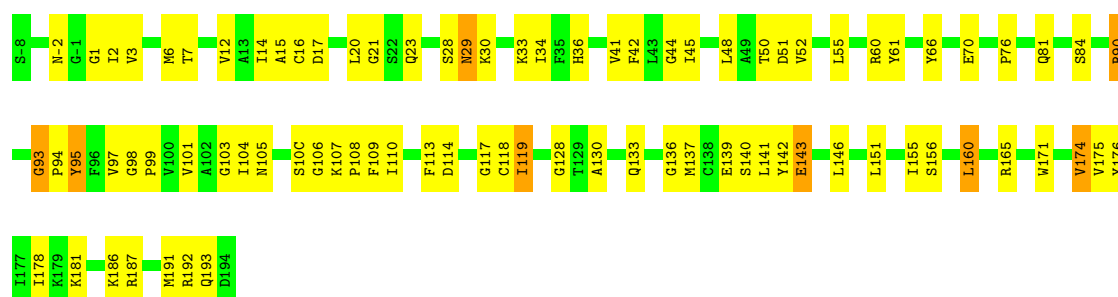
• Molecule 8: Proteasome component PUP1



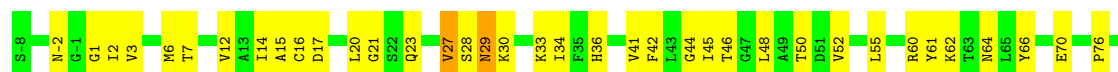
• Molecule 8: Proteasome component PUP1

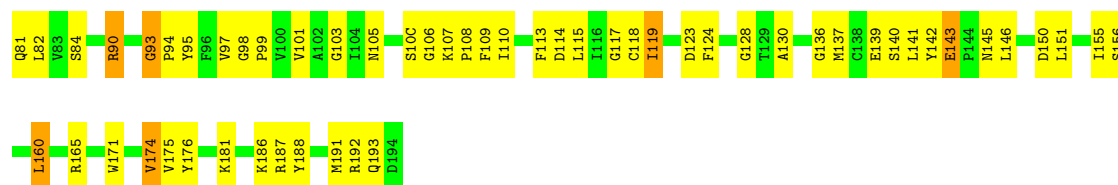


• Molecule 9: Proteasome component PUP3



• Molecule 9: Proteasome component PUP3

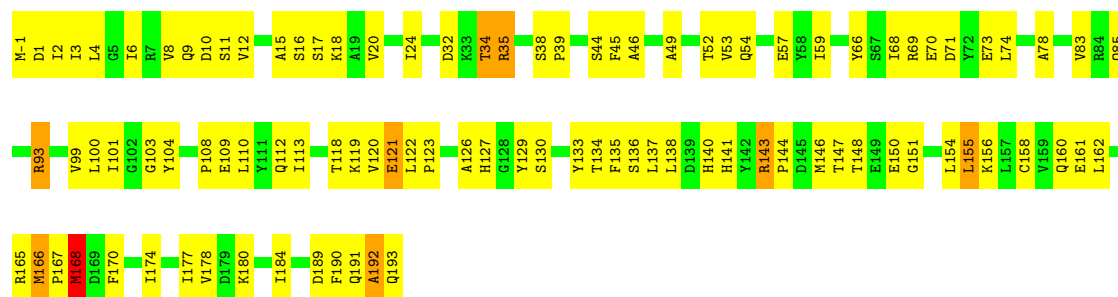




- Molecule 10: Proteasome component C11



- Molecule 10: Proteasome component C11

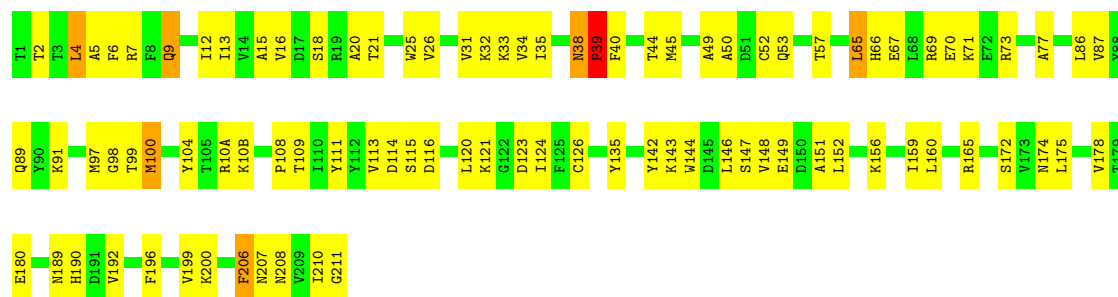


- Molecule 11: Proteasome component PRE2



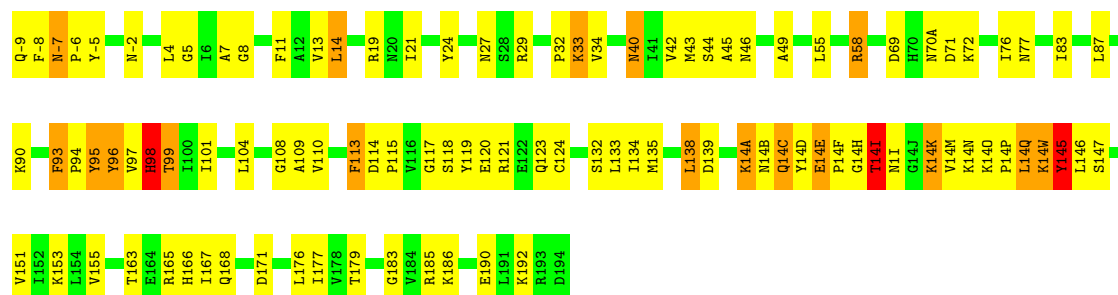
- Molecule 11: Proteasome component PRE2





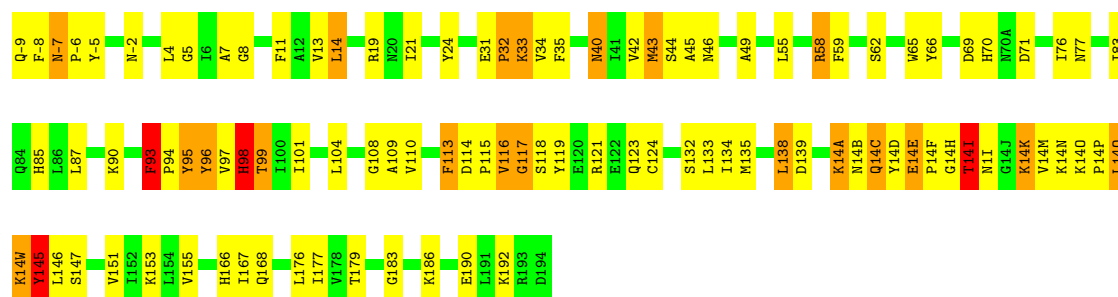
• Molecule 12: Proteasome component C5

Chain L: 54% 37% 8% .



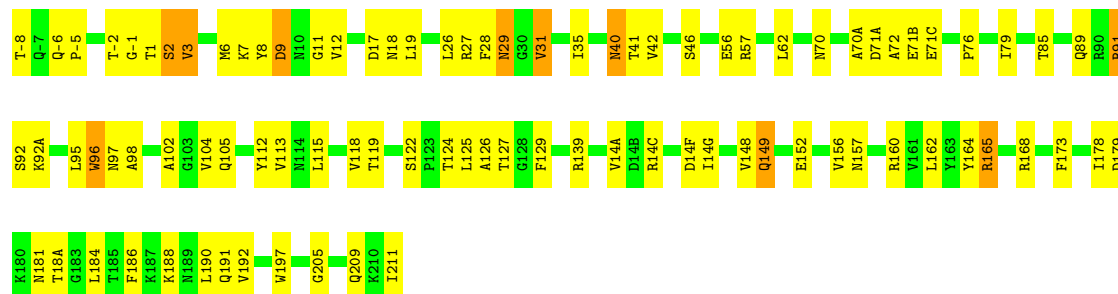
• Molecule 12: Proteasome component C5

Chain Z: 54% 36% 9% .



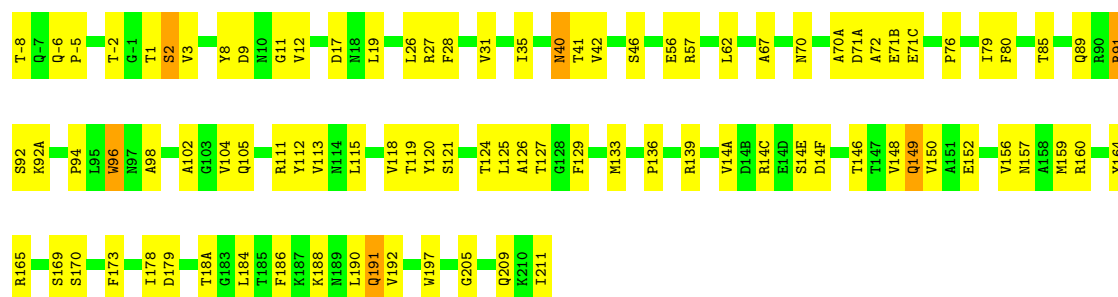
• Molecule 13: Proteasome component PRE4

Chain M: 61% 35% .



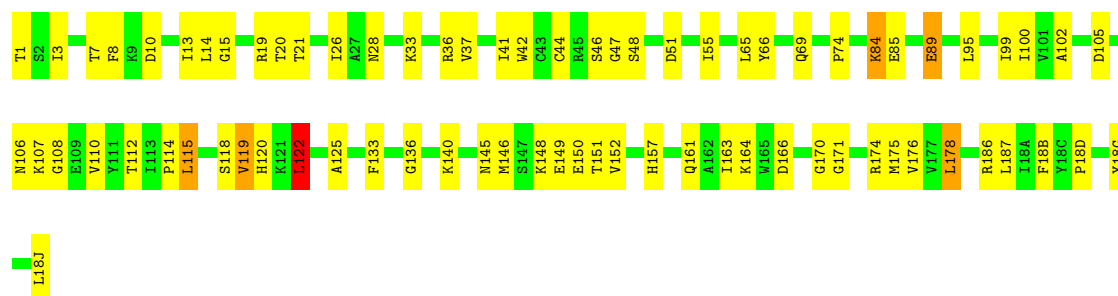
• Molecule 13: Proteasome component PRE4

Chain 1:  60% 37% .



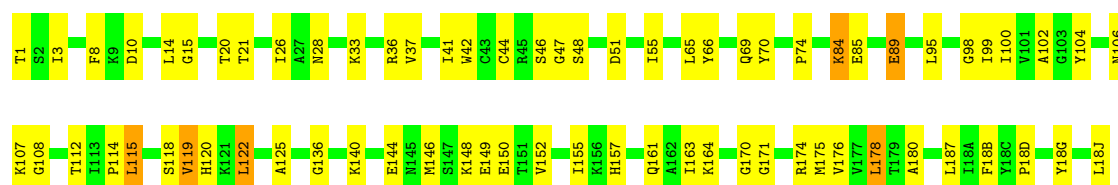
• Molecule 14: Proteasome component PRE3

Chain N:  62% 35% . .



• Molecule 14: Proteasome component PRE3

Chain 2:  64% 33% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	133.51Å 301.59Å 143.37Å 90.00° 112.59° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (15.00-2.70) 99.0 (15.00-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.264 0.260 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.911	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	51023	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SY2

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	0.49	0/1952	0.96	5/2642 (0.2%)
1	O	0.47	0/1952	0.95	5/2642 (0.2%)
2	B	0.46	0/1935	0.93	3/2618 (0.1%)
2	P	0.47	0/1935	0.93	5/2618 (0.2%)
3	C	0.44	0/1920	0.90	4/2598 (0.2%)
3	Q	0.44	0/1920	0.90	5/2598 (0.2%)
4	D	0.45	0/1887	0.92	6/2541 (0.2%)
4	R	0.44	0/1887	0.92	6/2541 (0.2%)
5	E	0.46	0/1823	0.96	4/2463 (0.2%)
5	S	0.46	0/1823	0.96	4/2463 (0.2%)
6	F	0.46	0/1937	0.97	8/2614 (0.3%)
6	T	0.49	0/1937	0.98	7/2614 (0.3%)
7	G	0.50	0/1959	0.99	7/2652 (0.3%)
7	U	0.50	0/1959	1.00	8/2652 (0.3%)
8	H	0.50	0/1716	0.97	6/2326 (0.3%)
8	V	0.48	0/1716	0.97	6/2326 (0.3%)
9	I	0.47	0/1611	1.03	11/2174 (0.5%)
9	W	0.50	0/1611	1.05	12/2174 (0.6%)
10	J	0.53	1/1613 (0.1%)	1.03	11/2173 (0.5%)
10	X	0.52	1/1613 (0.1%)	1.03	10/2173 (0.5%)
11	K	0.47	0/1681	0.92	5/2274 (0.2%)
11	Y	0.46	0/1681	0.93	4/2274 (0.2%)
12	L	0.49	0/1795	1.04	11/2420 (0.5%)
12	Z	0.48	0/1795	1.05	14/2420 (0.6%)
13	1	0.51	0/1855	0.97	5/2514 (0.2%)
13	M	0.48	0/1855	0.97	8/2514 (0.3%)
14	2	0.50	0/1541	0.96	4/2087 (0.2%)
14	N	0.52	0/1541	0.98	5/2087 (0.2%)
All	All	0.48	2/50450 (0.0%)	0.97	189/68192 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	X	166	MET	SD-CE	5.78	1.94	1.79
10	J	166	MET	SD-CE	5.58	1.93	1.79

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	27	ARG	N-CA-C	9.77	121.69	111.14
13	1	27	ARG	N-CA-C	9.47	121.37	111.14
6	T	12	ASN	N-CA-C	8.21	120.31	111.36
12	Z	117	GLY	N-CA-C	8.21	122.36	113.58
2	B	161	LYS	N-CA-C	-8.19	102.88	113.12
12	L	117	GLY	N-CA-C	8.11	123.28	113.79
12	Z	93	PHE	CA-C-N	8.06	129.91	119.84
12	Z	93	PHE	C-N-CA	8.06	129.91	119.84
12	L	93	PHE	CA-C-N	7.92	129.75	119.84
12	L	93	PHE	C-N-CA	7.92	129.75	119.84
6	T	161	LYS	N-CA-C	-7.80	102.69	112.90
6	F	12	ASN	N-CA-C	7.79	119.86	111.36
6	T	14	VAL	N-CA-C	7.60	118.92	108.89
6	F	161	LYS	N-CA-C	-7.59	102.96	112.90
9	W	60	ARG	N-CA-C	-7.58	102.71	110.97
1	A	161	LYS	N-CA-C	-7.57	102.98	112.90
4	R	161	ASN	N-CA-C	-7.38	102.93	112.23
10	J	166	MET	CA-C-N	7.37	126.90	119.24
10	J	166	MET	C-N-CA	7.37	126.90	119.24
5	S	57	GLU	N-CA-C	-7.35	103.45	113.30
7	G	161	LYS	N-CA-C	-7.27	103.07	112.23
1	O	161	LYS	N-CA-C	-7.23	103.43	112.90
5	E	57	GLU	N-CA-C	-7.21	103.64	113.30
10	X	166	MET	CA-C-N	7.19	126.71	119.24
10	X	166	MET	C-N-CA	7.19	126.71	119.24
4	D	161	ASN	N-CA-C	-7.14	103.23	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	-2	THR	N-CA-C	7.13	120.01	109.24
7	G	127	ALA	N-CA-C	7.05	118.96	111.28
7	U	127	ALA	N-CA-C	6.95	118.86	111.28
6	F	14	VAL	N-CA-C	6.95	118.66	109.21
13	M	98	ALA	N-CA-C	-6.88	97.68	108.90
2	P	161	LYS	N-CA-C	-6.87	102.90	112.45
13	M	-2	THR	N-CA-C	6.87	120.16	109.52
12	Z	-7	ASN	CA-C-N	6.86	126.49	119.56
12	Z	-7	ASN	C-N-CA	6.86	126.49	119.56
13	1	98	ALA	N-CA-C	-6.86	97.72	108.90
7	U	161	LYS	N-CA-C	-6.86	103.59	112.23
10	X	143	ARG	CA-C-N	6.85	126.81	119.28
10	X	143	ARG	C-N-CA	6.85	126.81	119.28
9	I	60	ARG	N-CA-C	-6.83	103.53	110.97
9	W	95	TYR	N-CA-C	-6.78	98.58	109.96
12	L	-7	ASN	CA-C-N	6.77	126.40	119.56
12	L	-7	ASN	C-N-CA	6.77	126.40	119.56
10	J	143	ARG	CA-C-N	6.74	126.69	119.28
10	J	143	ARG	C-N-CA	6.74	126.69	119.28
6	T	135	SER	N-CA-C	-6.69	98.81	109.59
10	X	93	ARG	CA-C-N	6.51	126.46	119.76
10	X	93	ARG	C-N-CA	6.51	126.46	119.76
1	O	185	GLU	N-CA-C	-6.45	101.24	110.59
9	I	142	TYR	N-CA-C	6.42	119.30	110.24
5	E	102	VAL	N-CA-C	6.42	118.38	111.58
6	F	135	SER	N-CA-C	-6.37	99.02	109.40
7	G	60	ASP	CA-C-N	6.29	127.71	119.84
7	G	60	ASP	C-N-CA	6.29	127.71	119.84
9	W	142	TYR	N-CA-C	6.28	119.09	110.24
5	S	102	VAL	N-CA-C	6.27	118.23	111.58
7	G	16	SER	N-CA-C	-6.24	101.01	110.50
10	J	123	PRO	N-CA-C	-6.24	105.04	113.40
3	Q	70	ILE	N-CA-C	-6.23	104.98	111.58
7	U	60	ASP	CA-C-N	6.21	127.60	119.84
7	U	60	ASP	C-N-CA	6.21	127.60	119.84
3	Q	161	SER	N-CA-C	-6.20	104.42	112.23
6	T	63	LYS	N-CA-C	6.18	120.95	112.04
6	F	63	LYS	N-CA-C	6.12	120.86	112.04
9	I	95	TYR	N-CA-C	-6.11	99.70	109.96
9	W	23	GLN	CB-CA-C	-6.09	109.56	116.63
1	A	185	GLU	N-CA-C	-6.08	101.52	110.52
10	J	93	ARG	CA-C-N	6.06	126.03	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	93	ARG	C-N-CA	6.06	126.03	119.78
2	B	72	ASP	N-CA-C	-6.06	106.05	113.50
3	C	70	ILE	N-CA-C	-6.05	105.16	111.58
4	D	16	SER	N-CA-C	-6.01	102.30	110.36
9	W	98	GLY	CA-C-N	5.97	126.44	119.99
9	W	98	GLY	C-N-CA	5.97	126.44	119.99
4	D	70	ILE	N-CA-C	-5.96	105.91	111.45
11	K	98	GLY	N-CA-C	-5.94	99.09	113.18
9	W	143	GLU	CA-C-N	5.93	126.26	119.92
9	W	143	GLU	C-N-CA	5.93	126.26	119.92
11	Y	98	GLY	N-CA-C	-5.92	99.16	113.18
3	C	161	SER	N-CA-C	-5.89	104.81	112.23
8	V	182	LYS	N-CA-C	5.86	119.22	109.96
14	N	115	LEU	N-CA-C	5.86	118.42	111.33
5	E	104	ASN	N-CA-C	-5.86	103.31	111.39
5	S	104	ASN	N-CA-C	-5.85	103.31	111.39
7	U	16	SER	N-CA-C	-5.85	101.61	110.50
13	M	165	ARG	N-CA-C	5.83	121.30	113.72
2	P	72	ASP	N-CA-C	-5.81	106.35	113.50
9	I	98	GLY	CA-C-N	5.81	126.26	119.99
9	I	98	GLY	C-N-CA	5.81	126.26	119.99
10	X	165	ARG	N-CA-C	5.80	120.36	113.28
9	I	23	GLN	CB-CA-C	-5.79	109.91	116.63
9	I	114	ASP	N-CA-C	-5.79	102.37	110.35
8	H	21	THR	N-CA-C	5.77	118.17	109.23
9	W	119	ILE	N-CA-C	5.76	116.88	108.58
4	R	128	MET	N-CA-C	-5.74	98.58	110.80
12	L	69	ASP	N-CA-C	5.70	118.23	111.33
13	1	165	ARG	N-CA-C	5.70	121.13	113.72
13	M	3	VAL	N-CA-C	-5.70	99.30	107.78
4	D	128	MET	N-CA-C	-5.67	98.73	110.80
8	V	164	TRP	N-CA-C	5.66	117.12	111.07
4	R	70	ILE	N-CA-C	-5.65	106.20	111.45
10	X	123	PRO	N-CA-C	-5.64	105.84	113.40
8	V	172	ASN	N-CA-C	5.64	118.68	110.17
14	N	99	ILE	N-CA-C	5.62	116.58	108.48
8	H	182	LYS	N-CA-C	5.61	118.83	109.96
2	P	61	GLN	N-CA-C	5.60	118.31	111.82
10	J	165	ARG	N-CA-C	5.58	120.08	113.16
14	N	47	GLY	N-CA-C	-5.58	104.87	112.52
6	F	124	THR	N-CA-C	-5.58	105.07	112.94
11	K	206	PHE	N-CA-C	-5.57	105.11	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	129	SER	N-CA-C	5.57	118.11	111.71
13	1	31	VAL	N-CA-C	5.57	116.19	108.84
12	L	134	ILE	N-CA-C	5.56	117.47	111.58
9	I	119	ILE	N-CA-C	5.54	116.55	108.58
2	B	61	GLN	N-CA-C	5.53	118.24	111.82
4	R	16	SER	N-CA-C	-5.53	102.94	110.36
12	L	95	TYR	N-CA-C	-5.53	99.51	108.41
9	I	178	ILE	N-CA-C	5.52	116.26	108.36
9	I	143	GLU	CA-C-N	5.52	125.83	119.92
9	I	143	GLU	C-N-CA	5.52	125.83	119.92
8	V	21	THR	N-CA-C	5.52	117.78	109.23
14	N	122	LEU	CA-C-N	5.50	125.02	119.19
14	N	122	LEU	C-N-CA	5.50	125.02	119.19
9	W	27	VAL	N-CA-C	5.49	115.96	111.62
14	2	99	ILE	N-CA-C	5.49	116.38	108.48
12	Z	134	ILE	N-CA-C	5.48	117.38	111.58
7	U	87	ASN	N-CA-C	-5.47	105.22	111.07
4	R	179	GLU	N-CA-C	5.45	116.90	111.07
8	V	45	GLY	N-CA-C	5.45	120.99	111.46
11	Y	38	ASN	CA-C-N	5.44	126.64	119.84
11	Y	38	ASN	C-N-CA	5.44	126.64	119.84
8	H	172	ASN	N-CA-C	5.43	118.38	110.17
12	Z	116	VAL	CA-C-N	-5.43	117.54	123.30
12	Z	116	VAL	C-N-CA	-5.43	117.54	123.30
8	H	164	TRP	N-CA-C	5.43	116.88	111.07
8	V	38	SER	N-CA-C	-5.43	103.33	108.22
12	L	113	PHE	N-CA-C	5.42	117.92	109.52
11	Y	206	PHE	N-CA-C	-5.42	105.31	112.24
11	K	131	GLN	N-CA-C	5.41	117.61	111.11
5	E	38	VAL	N-CA-C	5.41	116.27	108.48
7	U	27	ALA	N-CA-C	-5.38	105.33	111.14
3	C	136	THR	N-CA-C	5.37	118.34	109.85
12	L	98	HIS	N-CA-C	-5.37	99.78	108.52
8	H	45	GLY	N-CA-C	5.36	120.85	111.46
12	Z	69	ASP	N-CA-C	5.36	117.81	111.33
1	A	143	GLU	N-CA-C	5.35	117.53	111.11
6	T	124	THR	N-CA-C	-5.35	105.39	112.94
4	R	129	SER	N-CA-C	5.29	117.80	111.71
9	W	114	ASP	N-CA-C	-5.29	103.05	110.35
6	T	204	ASP	N-CA-C	-5.28	107.37	112.97
10	X	134	THR	N-CA-C	5.28	119.81	112.90
7	G	87	ASN	N-CA-C	-5.26	105.44	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Z	113	PHE	N-CA-C	5.26	117.68	109.52
1	A	66	LYS	N-CA-C	-5.24	106.73	113.23
8	H	38	SER	N-CA-C	-5.24	103.50	108.22
11	K	38	ASN	CA-C-N	5.23	126.38	119.84
11	K	38	ASN	C-N-CA	5.23	126.38	119.84
14	2	47	GLY	N-CA-C	-5.23	105.36	112.52
12	Z	145	TYR	N-CA-C	5.22	118.00	109.59
2	P	16	SER	N-CA-C	-5.22	103.37	110.36
4	D	179	GLU	N-CA-C	5.22	116.65	111.07
3	Q	62(A)	ILE	N-CA-C	5.20	115.87	110.82
12	Z	98	HIS	N-CA-C	-5.20	100.04	108.52
1	O	143	GLU	N-CA-C	5.20	117.34	111.11
2	P	63(A)	SER	N-CA-C	5.19	118.46	110.42
7	U	155	GLY	N-CA-C	-5.18	106.58	115.08
10	J	134	THR	N-CA-C	5.18	119.69	112.90
6	F	240	ILE	N-CA-C	-5.17	106.85	112.80
5	S	38	VAL	N-CA-C	5.16	115.91	108.48
12	Z	95	TYR	N-CA-C	-5.16	100.11	108.41
10	X	168	MET	N-CA-C	5.16	118.11	110.48
3	C	62(A)	ILE	N-CA-C	5.15	115.82	110.82
3	Q	136	THR	N-CA-C	5.14	117.97	109.85
12	Z	35	PHE	N-CA-C	5.14	117.94	109.72
1	A	155	GLY	N-CA-C	-5.13	107.98	115.63
12	L	145	TYR	N-CA-C	5.12	117.84	109.59
3	Q	78	PHE	N-CA-C	5.12	116.58	108.96
1	O	154	SER	N-CA-C	-5.11	106.55	112.89
14	2	115	LEU	N-CA-C	5.11	117.51	111.33
14	2	98	GLY	N-CA-C	-5.11	101.08	113.18
10	J	168	MET	N-CA-C	5.10	118.03	110.48
1	O	155	GLY	N-CA-C	-5.09	108.20	115.64
13	M	31	VAL	N-CA-C	5.09	115.56	108.84
9	W	145	ASN	N-CA-C	5.08	118.21	111.30
13	M	29	ASN	N-CA-C	5.08	120.10	113.30
7	G	13	THR	N-CA-C	5.06	117.44	109.39
6	F	204	ASP	N-CA-C	-5.06	107.61	112.97
10	J	89	LYS	N-CA-C	-5.03	105.71	111.14
13	M	9	ASP	N-CA-C	5.01	116.74	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	145	TYR	Sidechain
12	Z	145	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	84	0
1	O	1915	0	1926	93	0
2	B	1905	0	1901	128	0
2	P	1905	0	1901	135	0
3	C	1891	0	1900	121	0
3	Q	1891	0	1900	114	0
4	D	1862	0	1836	77	0
4	R	1862	0	1836	82	0
5	E	1795	0	1797	91	0
5	S	1795	0	1797	106	0
6	F	1897	0	1886	99	0
6	T	1897	0	1886	109	0
7	G	1921	0	1910	87	0
7	U	1921	0	1910	95	0
8	H	1685	0	1687	67	0
8	V	1685	0	1687	67	0
9	I	1581	0	1574	73	0
9	W	1581	0	1574	82	0
10	J	1585	0	1590	107	0
10	X	1585	0	1590	101	0
11	K	1644	0	1594	99	0
11	Y	1644	0	1594	107	0
12	L	1757	0	1711	90	0
12	Z	1757	0	1711	92	0
13	1	1824	0	1832	89	0
13	M	1824	0	1832	86	0
14	2	1512	0	1481	57	0
14	N	1512	0	1481	62	0
15	H	35	0	39	2	0
15	K	35	0	40	0	0
15	V	35	0	39	2	0
15	Y	35	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	1	71	0	0	16	0
16	2	62	0	0	4	0
16	A	58	0	0	2	0
16	B	39	0	0	5	0
16	C	44	0	0	5	0
16	D	42	0	0	6	0
16	E	24	0	0	3	0
16	F	49	0	0	5	0
16	G	61	0	0	7	0
16	H	48	0	0	6	0
16	I	65	0	0	2	0
16	J	49	0	0	6	0
16	K	43	0	0	3	0
16	L	58	0	0	4	0
16	M	70	0	0	11	0
16	N	55	0	0	6	0
16	O	33	0	0	2	0
16	P	30	0	0	5	0
16	Q	27	0	0	3	0
16	R	30	0	0	4	0
16	S	23	0	0	1	0
16	T	42	0	0	7	0
16	U	60	0	0	9	0
16	V	43	0	0	6	0
16	W	62	0	0	6	0
16	X	45	0	0	9	0
16	Y	50	0	0	13	0
16	Z	52	0	0	7	0
All	All	51023	0	49407	2347	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 24.

All (2347) 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:168:MET:HE3	10:X:168:MET:HE3	1.08	1.07
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.38	1.05
7:G:96:ALA:HA	7:G:107:MET:HE2	1.42	1.01
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.23	1.01
11:Y:4:LEU:HD12	11:Y:159:ILE:HD11	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:10(B):LYS:H	11:Y:10(B):LYS:HD2	1.26	1.00
7:U:96:ALA:HA	7:U:107:MET:HE2	1.42	1.00
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.20	1.00
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.21	1.00
2:B:15:PHE:H	3:C:23:GLN:HE22	1.05	0.99
2:B:202:THR:HG22	2:B:204:SER:H	1.27	0.99
2:P:202:THR:HG22	2:P:204:SER:H	1.23	0.98
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.05	0.97
9:I:6:MET:HE1	9:I:155:ILE:HA	1.46	0.96
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.27	0.96
9:W:6:MET:HE1	9:W:155:ILE:HA	1.46	0.96
2:P:71:ASN:ND2	2:P:72:ASP:H	1.64	0.95
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	1.81	0.95
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.48	0.94
2:B:71:ASN:ND2	2:B:72:ASP:H	1.64	0.94
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.49	0.94
3:C:100:ARG:NH1	3:C:106:PRO:HB3	1.83	0.93
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.31	0.93
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.05	0.92
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.49	0.92
10:J:2:ILE:HD13	10:J:162:LEU:HD13	1.51	0.90
10:X:2:ILE:HD13	10:X:162:LEU:HD13	1.53	0.90
10:J:-1:MET:HG2	10:J:1:ASP:H	1.36	0.89
10:X:-1:MET:HG2	10:X:1:ASP:H	1.38	0.89
3:C:15:PHE:H	4:D:23:GLN:HE22	1.21	0.88
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.21	0.87
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.17	0.87
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.39	0.87
10:J:133:TYR:HD1	16:Y:593:HOH:O	1.56	0.86
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.55	0.86
10:J:168:MET:CE	10:X:168:MET:HE3	2.02	0.86
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.39	0.86
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.56	0.86
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.59	0.85
3:C:185:THR:HG22	3:C:187:GLU:H	1.41	0.85
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.58	0.85
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.41	0.85
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.56	0.84
14:N:161:GLN:NE2	14:2:136:GLY:HA2	1.92	0.84
10:J:168:MET:HE3	10:X:168:MET:CE	2.02	0.84
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:ARG:HH11	3:C:106:PRO:HB3	1.43	0.84
11:Y:143:LYS:O	11:Y:146:LEU:HD13	1.74	0.84
11:K:143:LYS:O	11:K:146:LEU:HD13	1.77	0.84
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.42	0.84
14:N:136:GLY:HA2	14:2:161:GLN:NE2	1.92	0.83
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.43	0.83
3:C:185:THR:HB	3:C:188:GLU:HG2	1.60	0.83
7:G:87:ASN:C	7:G:87:ASN:HD22	1.87	0.82
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.26	0.81
3:C:163:GLN:HE21	3:C:164:THR:H	1.27	0.81
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.43	0.81
2:P:202:THR:HG22	2:P:204:SER:N	1.96	0.81
10:J:133:TYR:HE1	16:X:876:HOH:O	1.63	0.81
9:I:165:ARG:NH2	12:Z:135:MET:HE3	1.96	0.80
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.92	0.80
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.79	0.80
12:L:135:MET:HE3	9:W:165:ARG:NH2	1.97	0.80
2:P:224:PHE:H	2:P:224:PHE:HD2	1.30	0.80
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.79	0.80
7:U:87:ASN:C	7:U:87:ASN:HD22	1.88	0.80
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	1.97	0.79
12:Z:33:LYS:HD2	12:Z:46:ASN:HD22	1.48	0.79
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.29	0.79
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.42	0.79
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.83	0.79
2:B:224:PHE:H	2:B:224:PHE:HD2	1.29	0.79
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	1.97	0.79
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.65	0.79
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.94	0.79
1:O:15:PHE:H	2:P:23:GLN:HE22	1.31	0.79
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.31	0.79
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.17	0.78
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.80	0.78
13:1:40:ASN:H	13:1:40:ASN:HD22	1.32	0.78
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.64	0.78
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.65	0.78
11:K:142:TYR:O	11:K:143:LYS:HD2	1.84	0.77
1:O:124:THR:CG2	2:P:130:ARG:HH21	1.97	0.77
11:Y:35:ILE:HD11	11:Y:45:MET:CE	2.14	0.77
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.32	0.77
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:185:THR:HG22	3:Q:187:GLU:N	1.98	0.77
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.65	0.77
6:T:79:SER:HA	16:T:1238:HOH:O	1.84	0.77
7:G:96:ALA:HA	7:G:107:MET:CE	2.14	0.77
2:B:202:THR:HG22	2:B:204:SER:N	1.99	0.77
8:V:81:GLN:O	8:V:85:GLN:HG3	1.84	0.77
1:O:33:GLN:HE21	1:O:33:GLN:HA	1.49	0.76
9:W:137:MET:HE3	9:W:141:LEU:HD11	1.66	0.76
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.66	0.76
3:C:185:THR:HG22	3:C:187:GLU:N	1.98	0.76
13:M:40:ASN:HD22	13:M:40:ASN:H	1.32	0.76
10:J:20:VAL:HG11	11:K:120:LEU:HD11	1.66	0.76
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.67	0.76
7:U:96:ALA:HA	7:U:107:MET:CE	2.14	0.76
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.51	0.76
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.21	0.76
1:A:21(G):LEU:HD13	1:A:218:GLY:HA2	1.67	0.75
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	1.68	0.75
12:L:33:LYS:HD2	12:L:46:ASN:HD22	1.51	0.75
13:M:149:GLN:NE2	13:M:149:GLN:H	1.84	0.75
9:W:29:ASN:ND2	9:W:29:ASN:H	1.83	0.75
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.68	0.75
11:K:35:ILE:HD11	11:K:45:MET:CE	2.16	0.75
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.68	0.75
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.69	0.75
7:U:217:LYS:HA	7:U:217:LYS:HE3	1.69	0.75
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.69	0.74
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.68	0.74
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.22	0.74
7:U:236:ILE:HD12	7:U:237:ALA:N	2.02	0.74
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.84	0.74
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.51	0.74
13:M:41:THR:HG21	13:M:79:ILE:HD12	1.70	0.74
9:I:29:ASN:ND2	9:I:29:ASN:H	1.83	0.74
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.22	0.74
3:C:71:ASP:HA	10:J:68:ILE:CD1	2.18	0.74
10:J:133:TYR:OH	10:X:24:ILE:HG12	1.87	0.74
12:L:123:GLN:HG3	12:L:145:TYR:OH	1.87	0.74
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.70	0.74
2:B:15:PHE:N	3:C:23:GLN:HE22	1.85	0.74
2:B:186:VAL:HG21	2:B:216:ARG:HD3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:207:LEU:HD23	5:E:207:LEU:H	1.53	0.74
8:H:81:GLN:O	8:H:85:GLN:HG3	1.88	0.74
10:J:12:VAL:HG23	10:J:108:PRO:HB2	1.69	0.74
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.03	0.74
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.50	0.73
7:U:121:GLN:O	7:U:124:THR:HB	1.88	0.73
1:A:67:VAL:HB	1:A:223:LYS:HZ1	1.52	0.73
13:1:76:PRO:HD2	13:1:105:GLN:OE1	1.88	0.73
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.34	0.73
7:G:198:ILE:HG23	7:G:203:THR:O	1.88	0.73
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.70	0.73
2:P:186:VAL:HG21	2:P:216:ARG:HD3	1.69	0.73
5:S:207:LEU:HD23	5:S:207:LEU:H	1.54	0.73
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.23	0.73
10:X:46:ALA:HA	16:X:891:HOH:O	1.89	0.73
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.69	0.73
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.24	0.73
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.54	0.72
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.54	0.72
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.02	0.72
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.01	0.72
12:Z:123:GLN:HG3	12:Z:145:TYR:OH	1.89	0.72
13:1:149:GLN:NE2	13:1:149:GLN:H	1.88	0.72
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.71	0.72
2:P:71:ASN:ND2	2:P:72:ASP:N	2.37	0.72
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.19	0.72
3:Q:33:ARG:CB	3:Q:33:ARG:HH11	2.02	0.72
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.72	0.72
2:B:71:ASN:ND2	2:B:72:ASP:N	2.37	0.72
13:M:76:PRO:HD2	13:M:105:GLN:OE1	1.90	0.72
5:E:132:TYR:O	5:E:153:PRO:HB3	1.90	0.72
9:I:29:ASN:H	9:I:29:ASN:HD22	1.38	0.72
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:N	2.03	0.72
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.84	0.71
1:O:67:VAL:HB	1:O:223:LYS:HZ2	1.55	0.71
5:S:198:SER:HA	5:S:201:LEU:HG	1.72	0.71
10:X:12:VAL:HG23	10:X:108:PRO:HB2	1.72	0.71
6:F:179:LEU:HD21	6:F:192:GLN:HG2	1.71	0.71
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.38	0.71
11:K:207:ASN:HD21	10:X:144:PRO:CG	2.04	0.71
3:C:33:ARG:NH1	3:C:33:ARG:HB2	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.73	0.71
8:V:18:THR:HB	8:V:30:ASN:HD22	1.56	0.71
6:T:179:LEU:HD21	6:T:192:GLN:HG2	1.72	0.71
11:Y:45:MET:HG3	11:Y:52:CYS:CB	2.21	0.71
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.71	0.71
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.26	0.71
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.54	0.71
10:X:44:SER:OG	10:X:100:LEU:HB2	1.90	0.71
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.04	0.70
9:W:6:MET:CE	9:W:155:ILE:HA	2.21	0.70
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.21	0.70
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.21	0.70
8:V:84:LYS:HG3	8:V:85:GLN:N	2.07	0.70
10:J:69:ARG:HD2	16:J:514:HOH:O	1.91	0.70
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.72	0.70
1:O:179:ARG:HB3	1:O:179:ARG:HH11	1.56	0.70
1:O:21(G):LEU:HD13	1:O:218:GLY:HA2	1.72	0.70
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.04	0.70
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.74	0.70
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.73	0.70
13:1:8:TYR:CE2	13:1:148:VAL:HG22	2.26	0.70
5:E:198:SER:HA	5:E:201:LEU:HG	1.72	0.70
11:K:44:THR:HG21	11:K:100:MET:HE2	1.73	0.70
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.73	0.70
10:J:52:THR:HG23	10:J:53:VAL:N	2.06	0.70
11:K:10(B):LYS:HD2	11:K:10(B):LYS:N	2.03	0.70
10:X:103:GLY:HA2	10:X:178:VAL:HG11	1.73	0.70
2:B:15:PHE:H	3:C:23:GLN:NE2	1.86	0.69
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.74	0.69
7:U:87:ASN:C	7:U:87:ASN:ND2	2.50	0.69
1:O:67:VAL:HB	1:O:223:LYS:NZ	2.07	0.69
12:L:135:MET:CE	9:W:165:ARG:NH2	2.55	0.69
2:B:185:LYS:HD3	2:B:186:VAL:N	2.07	0.69
7:G:236:ILE:HD12	7:G:237:ALA:N	2.07	0.69
12:Z:21:ILE:C	12:Z:21:ILE:HD12	2.18	0.69
4:D:175:GLU:HG2	4:D:196:ILE:HG12	1.74	0.69
13:M:35:ILE:HG12	13:M:56:GLU:HG3	1.73	0.69
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.75	0.69
7:G:121:GLN:O	7:G:124:THR:HB	1.92	0.69
5:S:17:PRO:HA	6:T:26:TYR:CD1	2.27	0.69
10:X:52:THR:HG23	10:X:53:VAL:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:GLN:O	2:B:124:THR:HB	1.92	0.69
8:H:18:THR:HB	8:H:30:ASN:HD22	1.58	0.69
13:1:40:ASN:HD22	13:1:40:ASN:N	1.89	0.69
11:K:45:MET:HG3	11:K:52:CYS:CB	2.22	0.68
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.74	0.68
13:M:40:ASN:HD22	13:M:40:ASN:N	1.89	0.68
3:Q:173:ARG:O	3:Q:177:GLU:HG3	1.93	0.68
12:Z:109:ALA:HA	16:Z:375:HOH:O	1.91	0.68
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.75	0.68
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.29	0.68
7:U:198:ILE:HG23	7:U:203:THR:O	1.94	0.68
1:A:15:PHE:H	2:B:23:GLN:HE22	1.40	0.68
2:B:156:ASN:HD22	2:B:157:TYR:H	1.42	0.68
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.76	0.68
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.75	0.68
10:J:44:SER:OG	10:J:100:LEU:HB2	1.93	0.68
10:J:52:THR:HG23	10:J:53:VAL:H	1.58	0.68
12:L:21:ILE:C	12:L:21:ILE:HD12	2.18	0.68
9:W:29:ASN:H	9:W:29:ASN:HD22	1.40	0.68
10:X:52:THR:HG23	10:X:53:VAL:H	1.58	0.68
2:P:185:LYS:HD3	2:P:186:VAL:N	2.09	0.68
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.58	0.68
2:P:156:ASN:HD22	2:P:157:TYR:H	1.42	0.68
3:C:41:LYS:HG2	3:C:161:SER:O	1.94	0.67
11:K:38:ASN:O	11:K:40:PHE:N	2.27	0.67
5:E:207:LEU:H	5:E:207:LEU:CD2	2.07	0.67
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.75	0.67
9:I:6:MET:CE	9:I:155:ILE:HA	2.22	0.67
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.57	0.67
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.77	0.67
13:1:35:ILE:HG12	13:1:56:GLU:HG3	1.76	0.67
13:1:152:GLU:O	13:1:156:VAL:HG23	1.94	0.67
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.58	0.67
9:I:48:LEU:HG	9:I:50:THR:HG22	1.77	0.67
4:R:70:ILE:HB	4:R:74:ILE:HG22	1.77	0.67
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.42	0.67
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.58	0.67
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.29	0.67
12:L:166:HIS:HD2	12:L:168:GLN:H	1.40	0.67
9:W:-2:ASN:HA	9:W:21:GLY:O	1.94	0.67
8:V:172:ASN:HD22	8:V:193:THR:HA	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:ARG:O	3:C:177:GLU:HG3	1.94	0.67
5:E:175:TYR:CD2	5:E:196:ALA:HA	2.30	0.67
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.77	0.67
4:R:185:THR:HG23	4:R:188:GLU:OE1	1.95	0.67
5:S:132:TYR:O	5:S:153:PRO:HB3	1.94	0.67
1:A:67:VAL:HB	1:A:223:LYS:NZ	2.09	0.67
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.10	0.67
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.77	0.67
9:W:20:LEU:HA	16:W:240:HOH:O	1.93	0.67
14:2:144:GLU:HG2	16:2:1115:HOH:O	1.93	0.67
4:R:175:GLU:HG2	4:R:196:ILE:HG12	1.77	0.67
7:U:12:ILE:HG13	7:U:14:ILE:HG23	1.74	0.67
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.25	0.67
13:M:149:GLN:H	13:M:149:GLN:HE21	1.43	0.67
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.77	0.67
4:D:185:THR:HG23	4:D:188:GLU:OE1	1.94	0.66
12:L:109:ALA:HA	16:L:975:HOH:O	1.94	0.66
11:K:12:ILE:HB	11:K:178:VAL:HB	1.76	0.66
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.76	0.66
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.76	0.66
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.95	0.66
2:P:101:LYS:NZ	10:X:85:GLN:HE22	1.93	0.66
2:P:121:GLN:O	2:P:124:THR:HB	1.96	0.66
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.77	0.66
7:G:87:ASN:C	7:G:87:ASN:ND2	2.50	0.66
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.31	0.66
9:W:48:LEU:HG	9:W:50:THR:HG22	1.77	0.66
7:G:12:ILE:HG13	7:G:14:ILE:HG23	1.77	0.66
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.76	0.66
1:O:232:ARG:HH11	1:O:232:ARG:HG3	1.59	0.66
5:S:175:TYR:CD2	5:S:196:ALA:HA	2.30	0.66
5:S:207:LEU:H	5:S:207:LEU:CD2	2.08	0.66
7:U:35:ILE:HG23	7:U:51:GLN:HB2	1.78	0.66
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.10	0.66
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.30	0.66
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.96	0.66
7:U:172:ILE:HD13	7:U:197:MET:HE1	1.78	0.66
1:O:179:ARG:HB3	1:O:179:ARG:NH1	2.10	0.65
9:I:-2:ASN:HA	9:I:21:GLY:O	1.97	0.65
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.11	0.65
14:N:21:THR:HG22	14:N:26:ILE:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.44	0.65
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.79	0.65
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.79	0.65
14:2:21:THR:HG22	14:2:26:ILE:HA	1.77	0.65
4:D:70:ILE:HB	4:D:74:ILE:HG22	1.79	0.65
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.78	0.65
8:H:84:LYS:HG3	8:H:85:GLN:N	2.10	0.65
4:R:40:ILE:HD12	4:R:193:VAL:HG23	1.78	0.65
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.78	0.65
8:V:34:LEU:HB2	16:V:578:HOH:O	1.96	0.65
11:Y:38:ASN:O	11:Y:40:PHE:N	2.29	0.65
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.79	0.65
7:G:77:VAL:HG12	7:G:137:THR:HB	1.78	0.65
7:G:218:ASP:O	7:G:220:LYS:HB2	1.96	0.65
11:K:209:VAL:HG13	16:W:348:HOH:O	1.97	0.65
11:Y:71:LYS:HA	16:Y:912:HOH:O	1.97	0.65
3:C:121:GLN:NE2	3:C:121:GLN:C	2.55	0.64
7:G:172:ILE:HD13	7:G:197:MET:HE1	1.78	0.64
11:K:142:TYR:C	11:K:143:LYS:HD2	2.22	0.64
11:Y:4:LEU:HD12	11:Y:159:ILE:CD1	2.23	0.64
2:B:149:TYR:OH	3:C:62(A):ILE:HB	1.97	0.64
6:F:35:THR:HG21	6:F:51:GLU:O	1.97	0.64
6:F:119:TYR:O	6:F:122:ALA:HB3	1.97	0.64
7:U:218:ASP:O	7:U:220:LYS:HB2	1.96	0.64
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.12	0.64
3:Q:121:GLN:NE2	3:Q:121:GLN:C	2.55	0.64
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.62	0.64
10:J:103:GLY:HA2	10:J:178:VAL:HG11	1.78	0.64
16:P:462:HOH:O	3:Q:87:ILE:HD11	1.95	0.64
9:W:6:MET:HE3	9:W:155:ILE:HG13	1.77	0.64
5:E:47:VAL:HG23	5:E:189:LEU:HD13	1.78	0.64
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.33	0.64
11:Y:40:PHE:HB3	11:Y:73:ARG:NH2	2.11	0.64
4:D:177:LEU:HD13	5:E:58:LEU:HD11	1.79	0.64
6:F:28:VAL:O	6:F:32:GLU:HG3	1.98	0.64
1:O:57:PRO:HG3	7:U:177:GLU:CD	2.22	0.64
6:T:184:LEU:HD11	6:T:188:GLU:HB3	1.80	0.64
4:D:12(F):GLY:HA3	16:D:965:HOH:O	1.97	0.64
11:K:67:GLU:CD	11:K:73:ARG:HA	2.22	0.64
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.28	0.64
8:V:78:SER:O	8:V:82:MET:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:160:LEU:HD11	9:W:191:MET:HB3	1.79	0.64
11:Y:44:THR:HG21	11:Y:100:MET:HE2	1.78	0.64
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.78	0.64
3:C:201:VAL:HG21	3:C:210:ILE:HD11	1.79	0.64
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.11	0.64
10:J:18:LYS:HG2	10:J:174:ILE:HG13	1.80	0.64
12:Z:-2:ASN:HD21	13:1:118:VAL:HG11	1.63	0.64
7:G:35:ILE:HG23	7:G:51:GLN:HB2	1.80	0.64
9:I:105:ASN:HB3	9:I:10(C):SER:OG	1.98	0.64
10:J:147:THR:HG23	10:J:150:GLU:OE2	1.98	0.64
12:L:43:MET:HE3	12:L:83:ILE:HD13	1.79	0.64
10:X:147:THR:HG23	10:X:150:GLU:OE2	1.98	0.64
3:C:35:THR:HB	3:C:51:GLU:HG3	1.80	0.64
12:L:93:PHE:N	12:L:94:PRO:HD3	2.12	0.64
13:M:152:GLU:O	13:M:156:VAL:HG23	1.97	0.64
2:P:239:THR:HG22	2:P:239:THR:OXT	1.98	0.64
13:1:41:THR:HG21	13:1:79:ILE:HD12	1.79	0.64
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.80	0.63
8:H:172:ASN:HD22	8:H:193:THR:HA	1.63	0.63
11:Y:210:ILE:HB	16:Y:1150:HOH:O	1.97	0.63
13:1:-6:GLN:O	13:1:-6:GLN:HG3	1.98	0.63
4:D:112:LEU:C	4:D:112:LEU:HD13	2.23	0.63
9:I:1:GLY:HA2	9:I:17:ASP:OD1	1.98	0.63
12:L:13:VAL:HG12	12:L:177:ILE:HG13	1.80	0.63
5:S:78:LEU:HD12	5:S:78:LEU:C	2.23	0.63
9:W:156:SER:O	9:W:160:LEU:HB2	1.97	0.63
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.34	0.63
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.45	0.63
10:J:144:PRO:CG	11:Y:207:ASN:HD21	2.12	0.63
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.81	0.63
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.62	0.63
13:M:3:VAL:HG23	13:M:46:SER:HB3	1.81	0.63
3:Q:33:ARG:HB2	3:Q:33:ARG:HH11	1.62	0.63
11:Y:67:GLU:CD	11:Y:73:ARG:HA	2.24	0.63
10:J:15:ALA:HB2	10:J:155:LEU:HD11	1.80	0.63
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.62	0.63
6:T:119:TYR:O	6:T:122:ALA:HB3	1.99	0.63
5:E:226:GLY:O	5:E:229:VAL:HG22	1.98	0.63
9:I:55:LEU:CD1	9:I:97:VAL:HG21	2.29	0.63
11:K:207:ASN:ND2	10:X:144:PRO:HG3	2.13	0.63
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:10(B):LYS:H	11:Y:10(B):LYS:CD	2.07	0.63
6:F:120:VAL:HG21	6:F:151:LEU:HD21	1.80	0.63
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.12	0.63
8:V:4:VAL:HG22	8:V:159:ILE:HD11	1.81	0.63
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.14	0.63
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.99	0.62
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.10	0.62
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.34	0.62
3:C:71:ASP:HA	10:J:68:ILE:HD11	1.81	0.62
3:C:241:GLN:C	3:C:243:GLN:H	2.08	0.62
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.34	0.62
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.98	0.62
13:M:122:SER:HA	16:M:1128:HOH:O	1.98	0.62
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.80	0.62
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.46	0.62
1:A:69:LEU:HD23	1:A:69:LEU:C	2.25	0.62
6:F:127:ASN:HD22	6:F:128:SER:N	1.97	0.62
4:R:29:GLU:OE2	4:R:32:LYS:HD2	1.99	0.62
8:V:172:ASN:ND2	8:V:193:THR:HA	2.15	0.62
10:X:18:LYS:HG2	10:X:174:ILE:HG13	1.80	0.62
5:S:47:VAL:HG23	5:S:189:LEU:HD13	1.80	0.62
10:X:156:LYS:O	10:X:160:GLN:HG3	2.00	0.62
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.30	0.62
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.81	0.62
10:X:178:VAL:HG22	10:X:184:ILE:HG12	1.81	0.62
5:E:78:LEU:C	5:E:78:LEU:HD12	2.25	0.62
1:O:33:GLN:HE21	1:O:33:GLN:CA	2.11	0.62
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.30	0.62
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.30	0.62
5:S:207:LEU:HD23	5:S:207:LEU:N	2.15	0.62
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.23	0.62
13:1:148:VAL:HG23	16:1:182:HOH:O	2.00	0.62
13:1:149:GLN:H	13:1:149:GLN:HE21	1.47	0.62
2:B:156:ASN:HB2	16:C:1179:HOH:O	2.00	0.62
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.80	0.62
5:E:17:PRO:HA	6:F:26:TYR:CD1	2.35	0.62
6:F:184:LEU:HD11	6:F:188:GLU:HB3	1.82	0.62
10:X:113:ILE:HA	10:X:118:THR:O	2.00	0.62
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.34	0.62
2:P:234:VAL:HA	2:P:239:THR:HA	1.82	0.62
3:Q:241:GLN:C	3:Q:243:GLN:H	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:105:ASN:HB3	9:W:10(C):SER:OG	2.00	0.62
13:1:41:THR:OG1	13:1:76:PRO:HG3	2.00	0.62
3:Q:71:ASP:HA	10:X:68:ILE:CD1	2.31	0.61
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.82	0.61
5:E:207:LEU:HD23	5:E:207:LEU:N	2.15	0.61
10:J:-1:MET:HG2	10:J:1:ASP:N	2.12	0.61
10:J:162:LEU:O	10:J:166:MET:HB2	1.99	0.61
9:W:14:ILE:HG23	9:W:34:ILE:HD13	1.80	0.61
2:B:160:TRP:HA	3:C:59:GLN:HA	1.82	0.61
9:I:160:LEU:HD11	9:I:191:MET:HB3	1.81	0.61
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.83	0.61
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.14	0.61
10:X:162:LEU:O	10:X:166:MET:HB2	2.00	0.61
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.34	0.61
12:L:-2:ASN:HA	12:L:21:ILE:O	2.00	0.61
16:L:200:HOH:O	9:W:192:ARG:HG3	1.99	0.61
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.82	0.61
9:W:101:VAL:O	9:W:110:ILE:HA	2.00	0.61
12:Z:58:ARG:NH2	16:Z:1275:HOH:O	2.33	0.61
7:G:136:LEU:O	7:G:150:LYS:HA	2.00	0.61
6:T:127:ASN:HD22	6:T:128:SER:N	1.99	0.61
11:Y:180:GLU:N	16:Y:812:HOH:O	2.32	0.61
3:C:215:VAL:HG23	3:C:221:ILE:HG12	1.82	0.61
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.35	0.61
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.25	0.61
7:U:77:VAL:HG12	7:U:137:THR:HB	1.82	0.61
7:U:95:GLU:HB3	16:U:925:HOH:O	1.99	0.61
8:V:35:HIS:CB	8:V:56:THR:HG21	2.27	0.61
1:O:69:LEU:C	1:O:69:LEU:HD23	2.25	0.61
4:R:122:ARG:HG2	4:R:122:ARG:HH11	1.66	0.61
8:V:18:THR:CB	8:V:30:ASN:HD22	2.13	0.61
10:X:15:ALA:HB2	10:X:155:LEU:HD11	1.82	0.61
10:J:24:ILE:HG12	10:X:133:TYR:OH	2.01	0.61
10:J:156:LYS:O	10:J:160:GLN:HG3	1.99	0.61
10:J:178:VAL:HG22	10:J:184:ILE:HG12	1.83	0.61
11:K:200:LYS:HE3	11:K:206:PHE:O	2.00	0.61
13:M:-6:GLN:HG3	13:M:-6:GLN:O	1.99	0.61
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.82	0.61
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.01	0.61
3:Q:215:VAL:HG23	3:Q:221:ILE:HG12	1.83	0.61
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.65	0.61
8:H:34:LEU:HB2	16:H:540:HOH:O	2.01	0.61
9:I:90:ARG:HA	9:I:90:ARG:HH11	1.66	0.61
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.81	0.61
9:W:174:VAL:HG21	9:W:186:LYS:HE3	1.83	0.61
2:B:239:THR:HG22	2:B:239:THR:OXT	2.01	0.60
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.31	0.60
11:K:86:LEU:HD13	11:K:86:LEU:C	2.26	0.60
11:K:208:ASN:HB3	16:X:776:HOH:O	2.01	0.60
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.83	0.60
9:W:27:VAL:HG13	16:X:622:HOH:O	2.01	0.60
10:X:-1:MET:CG	10:X:1:ASP:H	2.13	0.60
12:Z:13:VAL:HG12	12:Z:177:ILE:HG13	1.83	0.60
1:A:20:LYS:HE3	1:A:25:ASP:OD1	2.02	0.60
4:D:25:GLU:HA	4:D:28:LEU:HD22	1.83	0.60
9:W:113:PHE:HA	9:W:118:CYS:O	2.00	0.60
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.36	0.60
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.46	0.60
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.65	0.60
7:U:100:ARG:HH11	7:U:100:ARG:HG3	1.67	0.60
9:W:46:THR:HA	16:W:608:HOH:O	2.01	0.60
10:X:49:ALA:HB2	16:X:1094:HOH:O	2.01	0.60
6:F:192:GLN:O	6:F:196:ILE:HG13	2.02	0.60
2:P:112:LEU:HD23	2:P:112:LEU:C	2.26	0.60
2:P:146:TYR:HE1	2:P:215:ILE:HG22	1.67	0.60
2:P:21(A):LYS:HE2	2:P:21(D):GLY:O	2.01	0.60
11:Y:45:MET:HG3	11:Y:52:CYS:HB2	1.81	0.60
2:B:21(A):LYS:HE2	2:B:21(D):GLY:O	2.01	0.60
12:L:-2:ASN:HD21	13:M:118:VAL:HG11	1.66	0.60
4:R:25:GLU:HA	4:R:28:LEU:HD22	1.84	0.60
9:W:7:THR:HG23	9:W:110:ILE:HD13	1.84	0.60
14:2:65:LEU:HG	14:2:69:GLN:HE21	1.66	0.60
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.49	0.60
3:C:186:VAL:O	3:C:190:VAL:HG23	2.01	0.60
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.02	0.60
4:R:177:LEU:HD13	5:S:58:LEU:HD11	1.83	0.60
6:T:173:LYS:O	6:T:177:GLU:HG3	2.01	0.60
7:U:186:TRP:O	7:U:190:VAL:HG23	2.01	0.60
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.32	0.60
9:W:90:ARG:HA	9:W:90:ARG:HH11	1.66	0.60
12:Z:4:LEU:CD1	12:Z:138:LEU:HD21	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:18:THR:CB	8:H:30:ASN:HD22	2.15	0.60
2:P:71:ASN:HD22	2:P:72:ASP:N	1.98	0.60
7:U:8:TYR:C	7:U:10:ARG:H	2.10	0.60
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.84	0.60
2:B:71:ASN:HD22	2:B:72:ASP:N	1.99	0.60
3:C:156:ILE:HA	16:C:1013:HOH:O	2.01	0.60
4:R:205:GLU:HA	4:R:205:GLU:OE2	2.01	0.60
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.01	0.60
8:H:172:ASN:ND2	8:H:193:THR:HA	2.17	0.59
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.34	0.59
2:B:41:MET:HE1	3:C:60:ASP:OD1	2.02	0.59
9:I:156:SER:O	9:I:160:LEU:HB2	2.01	0.59
11:K:207:ASN:HD21	10:X:144:PRO:HG3	1.67	0.59
13:M:29:ASN:N	16:M:802:HOH:O	2.33	0.59
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.37	0.59
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.31	0.59
13:1:3:VAL:HG23	13:1:46:SER:HB3	1.84	0.59
10:J:143:ARG:HB2	10:J:146:MET:HG3	1.83	0.59
5:S:175:TYR:HB2	5:S:199:GLN:HG2	1.83	0.59
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.02	0.59
2:B:234:VAL:HA	2:B:239:THR:HA	1.82	0.59
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.65	0.59
6:T:120:VAL:HG21	6:T:151:LEU:HD21	1.82	0.59
7:U:136:LEU:O	7:U:150:LYS:HA	2.02	0.59
9:W:1:GLY:HA2	9:W:17:ASP:OD1	2.01	0.59
10:X:143:ARG:HB2	10:X:146:MET:HG3	1.84	0.59
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.32	0.59
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.85	0.59
10:J:24:ILE:O	10:X:133:TYR:OH	2.21	0.59
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	2.08	0.59
5:S:226:GLY:O	5:S:229:VAL:HG22	2.02	0.59
6:T:28:VAL:O	6:T:32:GLU:HG3	2.01	0.59
6:T:35:THR:HG21	6:T:51:GLU:O	2.01	0.59
2:B:10:SER:HB2	16:B:248:HOH:O	2.02	0.59
6:F:32:GLU:HB3	6:F:169:ARG:NH2	2.17	0.59
9:I:137:MET:HE3	9:I:141:LEU:CD1	2.33	0.59
10:J:113:ILE:HA	10:J:118:THR:O	2.01	0.59
1:O:161:LYS:HD3	1:O:180:TRP:CH2	2.37	0.59
2:P:181:LYS:HG3	2:P:184:MET:HG3	1.85	0.59
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.84	0.59
3:C:163:GLN:NE2	3:C:164:THR:H	1.99	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:7:THR:HG23	9:I:110:ILE:HD13	1.85	0.59
11:K:156:LYS:HE2	11:K:190:HIS:CD2	2.38	0.59
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.02	0.59
9:I:113:PHE:HA	9:I:118:CYS:O	2.03	0.59
9:I:137:MET:CE	9:I:141:LEU:HD11	2.32	0.59
7:U:38:LEU:HD23	7:U:197:MET:HE3	1.84	0.59
1:O:134:VAL:O	1:O:153:PRO:HG3	2.02	0.59
10:X:-1:MET:HG2	10:X:1:ASP:N	2.14	0.59
1:A:150:GLN:O	1:A:157:TYR:HA	2.03	0.59
4:D:205:GLU:HA	4:D:205:GLU:OE2	2.01	0.59
6:F:90:ASN:O	6:F:94:GLU:HG3	2.02	0.59
9:I:174:VAL:HG21	9:I:186:LYS:HE3	1.84	0.59
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.15	0.59
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.33	0.59
11:Y:174:ASN:HD21	11:Y:189:ASN:ND2	1.98	0.59
2:B:163:ILE:HG13	2:B:164:SER:N	2.18	0.58
11:K:13:ILE:HD12	11:K:152:LEU:HD23	1.85	0.58
11:K:45:MET:HG3	11:K:52:CYS:HB2	1.83	0.58
2:B:112:LEU:HD23	2:B:112:LEU:C	2.28	0.58
9:W:29:ASN:HD22	9:W:29:ASN:N	2.00	0.58
2:B:156:ASN:ND2	2:B:157:TYR:H	2.01	0.58
6:F:109:ILE:HB	6:F:110:PRO:HD3	1.85	0.58
1:O:7:ARG:HD3	5:S:127:TYR:HD2	1.68	0.58
1:O:20:LYS:HE3	1:O:25:ASP:OD1	2.03	0.58
2:P:121:GLN:HG2	3:Q:83:ALA:HB1	1.85	0.58
1:A:161:LYS:HD3	1:A:180:TRP:CH2	2.39	0.58
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.14	0.58
9:I:101:VAL:O	9:I:110:ILE:HA	2.04	0.58
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.86	0.58
4:D:29:GLU:OE2	4:D:32:LYS:HD2	2.03	0.58
6:F:136:THR:HB	16:F:1005:HOH:O	2.04	0.58
1:A:79:SER:HB2	1:A:165:ILE:HD12	1.86	0.58
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.19	0.58
2:B:181:LYS:HG3	2:B:184:MET:HG3	1.85	0.58
3:C:227:GLU:OE1	3:C:227:GLU:N	2.36	0.58
2:P:156:ASN:ND2	2:P:157:TYR:H	2.02	0.58
8:V:200:LYS:HE3	9:W:140:SER:O	2.03	0.58
13:1:91:ARG:HG3	13:1:92:SER:N	2.18	0.58
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.39	0.58
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.34	0.58
6:T:237:GLN:O	6:T:240:ILE:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:6:ILE:HD11	10:X:154:LEU:HD23	1.86	0.58
12:Z:151:VAL:O	12:Z:155:VAL:HG23	2.04	0.58
11:K:211:GLY:HA2	8:V:214:LEU:HD22	1.83	0.58
13:M:57:ARG:NE	16:M:621:HOH:O	2.37	0.58
1:O:112:LEU:O	1:O:116:VAL:HG23	2.03	0.58
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.39	0.58
4:R:85:ALA:O	4:R:89:ILE:HG12	2.03	0.58
6:T:172:ALA:C	6:T:176:LEU:HD23	2.29	0.58
8:V:208:ARG:HG3	16:V:1135:HOH:O	2.03	0.58
10:X:6:ILE:CD1	10:X:154:LEU:HD23	2.34	0.58
3:C:101:LEU:HD11	10:J:57:GLU:HB3	1.86	0.58
6:F:173:LYS:O	6:F:177:GLU:HG3	2.04	0.58
9:I:14:ILE:HG23	9:I:34:ILE:HD13	1.84	0.58
10:J:6:ILE:CD1	10:J:154:LEU:HD23	2.34	0.58
5:S:41:ARG:NH1	5:S:42:SER:O	2.37	0.58
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.37	0.58
2:P:15:PHE:N	3:Q:23:GLN:HE22	1.97	0.58
3:Q:101:LEU:HD11	10:X:57:GLU:HB3	1.84	0.58
3:Q:190:VAL:HG13	3:Q:212:ILE:HG21	1.86	0.58
4:R:40:ILE:HD13	4:R:192:LEU:HD23	1.86	0.58
9:W:137:MET:CE	9:W:141:LEU:HD11	2.34	0.58
11:Y:200:LYS:HE3	11:Y:206:PHE:O	2.03	0.58
2:B:121:GLN:HG2	3:C:83:ALA:HB1	1.86	0.57
3:C:232:TYR:O	3:C:236:ILE:HG13	2.04	0.57
14:N:157:HIS:HD2	14:2:140:LYS:NZ	2.02	0.57
1:O:202:VAL:HG21	1:O:206:PHE:CD1	2.39	0.57
3:Q:232:TYR:O	3:Q:236:ILE:HG13	2.04	0.57
5:S:136:LEU:HB2	5:S:151:PHE:HB3	1.86	0.57
13:1:159:MET:HE3	16:1:450:HOH:O	2.03	0.57
2:B:238:ILE:O	2:B:239:THR:O	2.21	0.57
10:J:133:TYR:OH	10:X:24:ILE:O	2.21	0.57
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.34	0.57
14:N:140:LYS:NZ	14:2:157:HIS:HD2	2.02	0.57
4:R:15:PHE:HB2	5:S:23:GLN:OE1	2.04	0.57
2:B:146:TYR:HE1	2:B:215:ILE:HG22	1.68	0.57
14:N:120:HIS:HA	16:N:1107:HOH:O	2.04	0.57
6:T:90:ASN:O	6:T:94:GLU:HG3	2.04	0.57
10:X:127:HIS:O	16:X:1164:HOH:O	2.17	0.57
1:A:142:ASP:OD1	1:A:145:ASN:HB2	2.04	0.57
2:B:185:LYS:HE2	2:B:187:ASP:OD1	2.04	0.57
7:G:8:TYR:C	7:G:10:ARG:H	2.10	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:139:ASP:O	12:L:14(A):LYS:HG2	2.04	0.57
1:O:212:LEU:HD23	1:O:212:LEU:C	2.30	0.57
7:U:100:ARG:HG3	7:U:100:ARG:NH1	2.19	0.57
1:A:202:VAL:HG21	1:A:206:PHE:CD1	2.39	0.57
1:A:212:LEU:HD23	1:A:212:LEU:C	2.29	0.57
3:C:151:THR:HG22	3:C:157:TYR:HB3	1.84	0.57
5:E:136:LEU:HB2	5:E:151:PHE:HB3	1.87	0.57
11:K:6:PHE:HA	11:K:123:ASP:O	2.04	0.57
2:P:38:ILE:HD12	2:P:197:LEU:HG	1.86	0.57
4:R:112:LEU:HD13	4:R:112:LEU:C	2.30	0.57
11:Y:45:MET:HG3	11:Y:52:CYS:HB3	1.86	0.57
11:Y:111:TYR:OH	16:Y:471:HOH:O	2.16	0.57
3:C:33:ARG:HB2	3:C:33:ARG:HH11	1.64	0.57
7:G:38:LEU:HD23	7:G:197:MET:HE3	1.85	0.57
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.68	0.57
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.39	0.57
1:O:79:SER:HB2	1:O:165:ILE:HD12	1.86	0.57
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.85	0.57
13:1:112:TYR:HE1	13:1:127:THR:HG22	1.70	0.57
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.87	0.57
6:F:20(B):GLU:HG3	6:F:20(C):LYS:H	1.68	0.57
11:K:35:ILE:HD11	11:K:45:MET:HE3	1.86	0.57
1:O:150:GLN:O	1:O:157:TYR:HA	2.03	0.57
2:P:163:ILE:HG13	2:P:164:SER:N	2.19	0.57
3:Q:227:GLU:OE1	3:Q:227:GLU:N	2.37	0.57
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.68	0.57
11:Y:13:ILE:HD12	11:Y:152:LEU:HD23	1.86	0.57
2:P:87:ILE:O	2:P:91:THR:HG23	2.04	0.57
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.17	0.57
2:B:173:GLN:HG2	3:C:56:LEU:HD12	1.87	0.57
4:D:93:ARG:HD2	16:D:248:HOH:O	2.04	0.57
14:N:106:ASN:O	14:N:107:LYS:HB3	2.03	0.57
2:P:101:LYS:HZ2	10:X:85:GLN:HE22	1.52	0.57
13:1:12:VAL:HG21	13:1:102:ALA:HB1	1.86	0.57
1:O:57:PRO:HG2	7:U:177:GLU:HG2	1.86	0.57
3:Q:57:LYS:HG2	3:Q:208:LYS:NZ	2.20	0.57
5:S:86:ARG:O	5:S:90:ASN:HB2	2.04	0.57
13:1:42:VAL:CG2	13:1:178:ILE:HD11	2.35	0.57
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.87	0.56
2:B:225:LYS:HG3	2:B:228:GLU:OE1	2.04	0.56
5:E:86:ARG:O	5:E:90:ASN:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:192:ARG:HD2	16:W:1258:HOH:O	2.03	0.56
14:2:106:ASN:O	14:2:107:LYS:HB3	2.04	0.56
1:A:112:LEU:O	1:A:116:VAL:HG23	2.04	0.56
5:E:145:GLY:HA3	16:E:1070:HOH:O	2.03	0.56
7:G:77:VAL:CG1	7:G:137:THR:HB	2.35	0.56
10:J:144:PRO:HG3	11:Y:207:ASN:ND2	2.20	0.56
11:K:45:MET:HG3	11:K:52:CYS:HB3	1.87	0.56
3:Q:121:GLN:HE21	3:Q:122:ARG:N	2.03	0.56
8:H:84:LYS:HD3	16:H:237:HOH:O	2.05	0.56
10:J:6:ILE:HD11	10:J:154:LEU:HD23	1.86	0.56
11:K:210:ILE:HD13	9:W:30:LYS:HE3	1.87	0.56
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.05	0.56
4:R:101:LEU:CD1	11:Y:57:THR:HG22	2.35	0.56
5:S:194:VAL:O	5:S:197:ILE:HG22	2.05	0.56
1:A:38:LEU:C	1:A:38:LEU:HD12	2.29	0.56
2:B:19:GLY:O	16:B:565:HOH:O	2.17	0.56
13:M:12:VAL:HG21	13:M:102:ALA:HB1	1.86	0.56
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.19	0.56
4:R:12(G):GLU:HG2	4:R:125:GLU:H	1.69	0.56
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.40	0.56
8:H:35:HIS:CB	8:H:56:THR:HG21	2.28	0.56
2:P:202:THR:CG2	2:P:204:SER:H	2.08	0.56
9:W:12:VAL:CG1	9:W:108:PRO:HB3	2.35	0.56
11:Y:38:ASN:C	11:Y:38:ASN:OD1	2.48	0.56
3:C:163:GLN:HG3	3:C:164:THR:N	2.21	0.56
4:D:24:VAL:O	4:D:27:SER:HB3	2.06	0.56
8:H:200:LYS:HE3	9:I:140:SER:O	2.06	0.56
1:O:38:LEU:C	1:O:38:LEU:HD12	2.29	0.56
2:B:141:TYR:CD1	2:B:141:TYR:C	2.84	0.56
2:B:228:GLU:O	2:B:232:ILE:HG22	2.05	0.56
4:D:12(G):GLU:HG2	4:D:125:GLU:H	1.70	0.56
5:E:175:TYR:HB2	5:E:199:GLN:HG2	1.85	0.56
6:F:179:LEU:HD11	6:F:192:GLN:CG	2.36	0.56
11:K:99:THR:HG22	11:K:113:VAL:O	2.05	0.56
12:L:14(C):GLN:HG2	8:V:210:THR:CG2	2.35	0.56
2:P:225:LYS:HG3	2:P:228:GLU:OE1	2.05	0.56
7:U:10:ARG:HG2	7:U:22:TYR:CD2	2.40	0.56
7:U:17(D):SER:O	7:U:17(E):LYS:HB2	2.05	0.56
10:X:136:SER:HA	16:X:559:HOH:O	2.06	0.56
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.05	0.56
1:A:72:PRO:HD3	16:H:1303:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:O	1:A:190:ILE:HG13	2.05	0.56
12:L:14(H):GLY:C	12:L:1(I):ASN:H	2.13	0.56
13:M:112:TYR:HE1	13:M:127:THR:HG22	1.71	0.56
2:P:228:GLU:O	2:P:232:ILE:HG22	2.06	0.56
3:C:15:PHE:N	4:D:23:GLN:HE22	1.99	0.56
5:E:194:VAL:O	5:E:197:ILE:HG22	2.06	0.56
6:F:171:SER:O	6:F:174:ALA:HB3	2.05	0.56
8:H:210:THR:CG2	12:Z:14(C):GLN:HG2	2.36	0.56
14:N:14:LEU:O	14:N:175:MET:HA	2.04	0.56
2:P:185:LYS:HE2	2:P:187:ASP:OD1	2.06	0.56
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.88	0.56
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.88	0.56
6:T:171:SER:O	6:T:174:ALA:HB3	2.05	0.56
14:2:28:ASN:HA	16:2:199:HOH:O	2.06	0.56
3:Q:76:LEU:HD12	3:Q:138:ILE:HG12	1.88	0.56
3:Q:112:LEU:O	3:Q:116:VAL:HG23	2.06	0.56
4:R:207:LEU:HD23	4:R:207:LEU:C	2.30	0.56
8:V:8:PHE:HB2	8:V:146:LEU:O	2.05	0.56
9:I:12:VAL:CG1	9:I:108:PRO:HB3	2.35	0.55
11:K:38:ASN:C	11:K:38:ASN:OD1	2.49	0.55
6:T:179:LEU:HD21	6:T:192:GLN:CG	2.36	0.55
11:Y:66:HIS:HA	16:Y:1210:HOH:O	2.06	0.55
8:H:147:THR:HG23	8:H:150:GLU:OE1	2.05	0.55
8:H:165:ASN:ND2	13:1:139:ARG:HH11	2.01	0.55
13:M:40:ASN:N	13:M:40:ASN:ND2	2.55	0.55
1:A:29:THR:O	1:A:33:GLN:HG2	2.06	0.55
6:T:20(B):GLU:HG3	6:T:20(C):LYS:H	1.69	0.55
9:W:137:MET:HE3	9:W:141:LEU:CD1	2.35	0.55
12:Z:11:PHE:O	12:Z:108:GLY:HA3	2.06	0.55
14:2:14:LEU:O	14:2:175:MET:HA	2.05	0.55
3:C:76:LEU:HD22	3:C:89:ILE:HG12	1.89	0.55
4:D:207:LEU:C	4:D:207:LEU:HD23	2.31	0.55
9:I:6:MET:HB3	9:I:151:LEU:HD11	1.87	0.55
13:M:211:ILE:HG12	16:M:544:HOH:O	2.06	0.55
3:Q:224:LEU:HD12	3:Q:224:LEU:N	2.22	0.55
6:T:147:HIS:HD2	16:T:242:HOH:O	1.88	0.55
10:X:4:LEU:HD23	10:X:126:ALA:HB2	1.88	0.55
11:Y:18:SER:HA	11:Y:33:LYS:HE3	1.88	0.55
12:L:185:ARG:HA	16:L:1212:HOH:O	2.04	0.55
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.42	0.55
10:J:-1:MET:CG	10:J:1:ASP:H	2.12	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:71:ASN:CG	2:P:72:ASP:H	2.15	0.55
7:U:87:ASN:HD22	7:U:88:ALA:N	2.04	0.55
12:Z:43:MET:HE3	12:Z:83:ILE:HD13	1.88	0.55
12:Z:139:ASP:O	12:Z:14(A):LYS:HG2	2.06	0.55
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.89	0.55
3:C:57:LYS:HG2	3:C:208:LYS:NZ	2.22	0.55
5:E:41:ARG:NH1	5:E:42:SER:O	2.39	0.55
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.37	0.55
1:O:62:GLU:C	1:O:64:LEU:H	2.14	0.55
1:A:130:ARG:HG2	7:G:125:GLN:HG3	1.89	0.55
5:E:227:GLU:N	5:E:227:GLU:CD	2.65	0.55
11:K:7:ARG:HG3	11:K:12:ILE:HG12	1.89	0.55
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.41	0.55
11:Y:156:LYS:HE2	11:Y:190:HIS:CD2	2.42	0.55
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.89	0.55
1:A:173:LYS:O	1:A:177:GLU:HG3	2.07	0.55
6:F:179:LEU:HD21	6:F:192:GLN:CG	2.35	0.55
7:G:76:MET:HE3	7:G:78:VAL:CG2	2.36	0.55
4:D:85:ALA:O	4:D:89:ILE:HG12	2.07	0.55
13:M:17:ASP:HA	13:M:173:PHE:HA	1.89	0.55
1:O:142:ASP:OD1	1:O:145:ASN:HB2	2.07	0.55
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.89	0.55
7:U:76:MET:HE3	7:U:78:VAL:CG2	2.37	0.55
10:X:32:ASP:OD2	10:X:34:THR:HG22	2.07	0.55
11:Y:174:ASN:ND2	11:Y:189:ASN:HD22	2.01	0.55
2:B:87:ILE:O	2:B:91:THR:HG23	2.06	0.54
3:C:190:VAL:HG13	3:C:212:ILE:HG21	1.89	0.54
4:D:219:ASP:O	4:D:222:LYS:HE2	2.06	0.54
5:E:21:LEU:HA	16:E:346:HOH:O	2.06	0.54
7:G:17(D):SER:O	7:G:17(E):LYS:HB2	2.07	0.54
10:J:66:TYR:CE2	10:J:74:LEU:HG	2.43	0.54
11:K:73:ARG:NH2	11:K:104:TYR:O	2.40	0.54
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.40	0.54
9:W:28:SER:HB2	10:X:120:VAL:HG21	1.89	0.54
14:2:36:ARG:HG3	14:2:42:TRP:CZ2	2.41	0.54
14:2:84:LYS:HG3	14:2:119:VAL:CG2	2.37	0.54
3:C:121:GLN:HE21	3:C:122:ARG:N	2.05	0.54
11:K:38:ASN:C	11:K:40:PHE:H	2.15	0.54
12:L:192:LYS:HE3	8:V:195:ASN:HB3	1.89	0.54
14:N:65:LEU:HG	14:N:69:GLN:HE21	1.70	0.54
7:U:228:ASN:HB3	16:U:242:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:236:ILE:HD12	7:U:236:ILE:C	2.32	0.54
11:Y:7:ARG:HG3	11:Y:12:ILE:HG12	1.88	0.54
1:O:173:LYS:O	1:O:177:GLU:HG3	2.07	0.54
1:O:186:LEU:O	1:O:190:ILE:HG13	2.07	0.54
11:Y:12:ILE:HG13	11:Y:108:PRO:HB3	1.89	0.54
5:E:74:MET:HE2	5:E:109:VAL:HA	1.89	0.54
6:F:172:ALA:C	6:F:176:LEU:HD23	2.33	0.54
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.08	0.54
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.90	0.54
14:2:48:SER:HB3	14:2:51:ASP:HB2	1.90	0.54
9:I:29:ASN:HD22	9:I:29:ASN:N	1.99	0.54
12:L:151:VAL:O	12:L:155:VAL:HG23	2.07	0.54
1:O:225:THR:OG1	1:O:228:GLU:HG3	2.07	0.54
2:P:136:PHE:O	2:P:150:THR:HA	2.08	0.54
3:Q:14:ILE:HB	4:R:23:GLN:NE2	2.23	0.54
6:T:192:GLN:O	6:T:196:ILE:HG13	2.07	0.54
3:C:57:LYS:O	3:C:58:LEU:HB2	2.08	0.54
3:C:224:LEU:HD12	3:C:224:LEU:N	2.23	0.54
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.89	0.54
1:O:29:THR:O	1:O:33:GLN:HG2	2.07	0.54
7:U:59:LEU:O	7:U:61:PRO:HD3	2.06	0.54
11:Y:35:ILE:HD11	11:Y:45:MET:HE3	1.86	0.54
2:B:74:ILE:C	2:B:221:GLN:HE22	2.16	0.54
8:H:167:LEU:HD22	12:Z:167:ILE:O	2.07	0.54
6:T:205:ASN:C	6:T:20(B):GLU:H	2.15	0.54
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.89	0.54
3:C:182:PRO:O	3:C:184:ALA:N	2.41	0.54
6:F:127:ASN:HD22	6:F:127:ASN:C	2.15	0.54
13:M:91:ARG:HG3	13:M:92:SER:N	2.22	0.54
13:M:184:LEU:HD23	13:M:184:LEU:C	2.33	0.54
2:P:141:TYR:CD1	2:P:141:TYR:C	2.84	0.54
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG13	1.90	0.54
12:Z:-5:TYR:CD2	12:Z:96:TYR:HB2	2.43	0.54
12:Z:14(H):GLY:C	12:Z:1(I):ASN:H	2.15	0.54
3:C:14:ILE:HB	4:D:23:GLN:NE2	2.23	0.54
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.90	0.54
4:D:112:LEU:O	4:D:116:VAL:HG23	2.08	0.54
7:G:87:ASN:HD22	7:G:88:ALA:N	2.05	0.54
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.90	0.54
11:K:12:ILE:HG13	11:K:108:PRO:HB3	1.89	0.54
2:P:122:GLY:C	2:P:124:THR:H	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:59:LEU:HD13	4:R:59:LEU:C	2.33	0.54
5:S:74:MET:HE2	5:S:109:VAL:HA	1.90	0.54
5:S:185:ASN:OD1	5:S:188:GLU:HG2	2.08	0.54
7:U:16:SER:HA	16:U:584:HOH:O	2.07	0.54
9:W:81:GLN:HA	9:W:81:GLN:NE2	2.22	0.54
11:Y:38:ASN:C	11:Y:40:PHE:H	2.16	0.54
13:1:40:ASN:N	13:1:40:ASN:ND2	2.55	0.54
1:A:7:ARG:HB2	2:B:5:SER:OG	2.08	0.54
6:F:40:ILE:HD12	6:F:193:ALA:HB2	1.90	0.54
6:F:205:ASN:C	6:F:20(B):GLU:H	2.15	0.54
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.88	0.54
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.38	0.54
14:N:136:GLY:CA	14:2:161:GLN:HE21	2.08	0.54
2:P:238:ILE:O	2:P:239:THR:O	2.26	0.54
8:V:148:LYS:O	8:V:152:ILE:HG13	2.08	0.54
9:W:20:LEU:C	9:W:20:LEU:HD13	2.32	0.54
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	1.89	0.54
12:L:11:PHE:O	12:L:108:GLY:HA3	2.07	0.53
13:M:17:ASP:HA	13:M:173:PHE:CB	2.38	0.53
2:P:224:PHE:N	2:P:224:PHE:CD2	2.74	0.53
3:Q:57:LYS:HG2	3:Q:208:LYS:HZ3	1.72	0.53
5:S:227:GLU:CD	5:S:227:GLU:N	2.66	0.53
6:T:53:LEU:HD11	6:T:205:ASN:OD1	2.08	0.53
10:X:133:TYR:CE2	10:X:166:MET:CG	2.92	0.53
3:C:121:GLN:C	3:C:121:GLN:HE21	2.16	0.53
6:F:187:ARG:HB2	16:F:698:HOH:O	2.07	0.53
7:G:186:TRP:O	7:G:190:VAL:HG23	2.08	0.53
8:H:78:SER:O	8:H:82:MET:HG3	2.07	0.53
10:J:74:LEU:HD22	10:J:78:ALA:CB	2.39	0.53
11:K:208:ASN:ND2	9:W:29:ASN:HD21	2.06	0.53
2:P:229:ILE:O	2:P:233:LEU:HB2	2.07	0.53
3:Q:71:ASP:HA	10:X:68:ILE:HD11	1.90	0.53
6:T:179:LEU:HD11	6:T:192:GLN:CG	2.37	0.53
7:U:77:VAL:CG1	7:U:137:THR:HB	2.38	0.53
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG13	1.90	0.53
5:E:185:ASN:OD1	5:E:188:GLU:HG2	2.08	0.53
9:I:20:LEU:HD13	9:I:20:LEU:C	2.33	0.53
3:Q:76:LEU:HD22	3:Q:89:ILE:HG12	1.91	0.53
3:Q:228:GLU:O	3:Q:232:TYR:HD1	1.91	0.53
5:S:47:VAL:HG12	5:S:48:LEU:N	2.23	0.53
6:T:95:GLU:CD	6:T:115:ARG:HD2	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:14(C):ARG:HH11	13:1:14(C):ARG:HG3	1.72	0.53
1:A:62:GLU:C	1:A:64:LEU:H	2.16	0.53
1:A:85:TYR:O	1:A:89:VAL:HG23	2.09	0.53
3:C:76:LEU:HD12	3:C:138:ILE:HG12	1.91	0.53
4:D:79:SER:HB3	4:D:165:ILE:HD12	1.91	0.53
5:E:47:VAL:HG12	5:E:48:LEU:N	2.22	0.53
4:R:156:THR:HG22	5:S:83:PRO:HD3	1.90	0.53
5:S:71:ASP:OD1	5:S:96:CYS:HB3	2.09	0.53
6:T:35:THR:CG2	6:T:36:THR:N	2.70	0.53
3:C:112:LEU:O	3:C:116:VAL:HG23	2.09	0.53
8:H:174:ASP:OD2	8:H:189:ARG:NH1	2.37	0.53
9:I:30:LYS:HE3	11:Y:210:ILE:HD13	1.90	0.53
10:J:167:PRO:O	10:X:168:MET:HE2	2.08	0.53
11:K:208:ASN:HD21	9:W:29:ASN:HD21	1.55	0.53
12:L:1(I):ASN:O	12:L:14(K):LYS:HG2	2.09	0.53
3:Q:15:PHE:N	4:R:23:GLN:HE22	1.98	0.53
8:V:147:THR:HG23	8:V:150:GLU:OE1	2.08	0.53
9:W:6:MET:HB3	9:W:151:LEU:HD11	1.89	0.53
13:1:112:TYR:CE1	13:1:127:THR:HG22	2.44	0.53
1:A:15:PHE:HB2	2:B:23:GLN:NE2	2.24	0.53
6:F:20(B):GLU:CD	6:F:20(C):LYS:HE3	2.34	0.53
8:H:211:THR:HA	16:Z:781:HOH:O	2.07	0.53
16:T:515:HOH:O	7:U:130:ARG:HB2	2.06	0.53
8:H:195:ASN:HB3	12:Z:192:LYS:HE3	1.91	0.53
10:J:52:THR:CG2	10:J:53:VAL:H	2.22	0.53
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.44	0.53
6:T:95:GLU:OE1	6:T:115:ARG:HD2	2.09	0.53
6:T:127:ASN:HD22	6:T:127:ASN:C	2.16	0.53
7:U:225:SER:H	7:U:228:ASN:HB2	1.74	0.53
3:C:15:PHE:H	4:D:23:GLN:NE2	2.00	0.53
6:F:115:ARG:HG2	16:F:382:HOH:O	2.09	0.53
10:J:141:HIS:HB2	10:J:154:LEU:HD11	1.91	0.53
11:Y:210:ILE:N	16:Y:1226:HOH:O	2.34	0.53
12:Z:147:SER:O	12:Z:151:VAL:HG23	2.08	0.53
2:B:71:ASN:CG	2:B:72:ASP:H	2.16	0.53
2:B:229:ILE:O	2:B:233:LEU:HB2	2.08	0.53
9:I:81:GLN:HA	9:I:81:GLN:NE2	2.23	0.53
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.91	0.53
2:P:63:THR:O	2:P:63:THR:HG22	2.09	0.53
3:Q:46:VAL:HG11	3:Q:139:ALA:HB1	1.91	0.53
12:Z:1(I):ASN:O	12:Z:14(K):LYS:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:177:ILE:HD12	12:Z:177:ILE:N	2.23	0.53
2:B:63:THR:O	2:B:63:THR:HG22	2.09	0.53
3:C:46:VAL:HG11	3:C:139:ALA:HB1	1.91	0.53
7:G:100:ARG:HG3	7:G:100:ARG:HH11	1.74	0.53
10:J:17:SER:HB2	10:J:170:PHE:HB2	1.91	0.53
12:L:43:MET:HG2	12:L:44:SER:N	2.24	0.53
2:P:156:ASN:HD22	2:P:157:TYR:N	2.07	0.53
10:X:74:LEU:HD22	10:X:78:ALA:CB	2.38	0.53
12:Z:95:TYR:O	12:Z:97:VAL:N	2.41	0.53
2:B:156:ASN:HD22	2:B:157:TYR:N	2.07	0.52
8:H:5:GLY:O	8:H:124:TYR:HA	2.09	0.52
1:O:113:VAL:HG22	1:O:138:ILE:HD12	1.90	0.52
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	2.09	0.52
1:A:46:VAL:HG11	1:A:139:ALA:HB1	1.90	0.52
8:H:126:SER:O	8:H:127:LEU:HD23	2.09	0.52
8:V:196:VAL:HG23	16:V:652:HOH:O	2.09	0.52
1:A:110:LYS:HG2	16:A:285:HOH:O	2.08	0.52
2:B:97:GLN:HA	2:B:97:GLN:NE2	2.24	0.52
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.89	0.52
9:I:176:TYR:CE1	9:I:186:LYS:HD2	2.44	0.52
4:R:24:VAL:O	4:R:27:SER:HB3	2.09	0.52
10:X:52:THR:CG2	10:X:53:VAL:H	2.20	0.52
10:X:190:PHE:C	10:X:192:ALA:H	2.18	0.52
6:F:237:GLN:O	6:F:240:ILE:HG22	2.09	0.52
9:I:143:GLU:HG3	9:I:146:LEU:HD21	1.90	0.52
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.91	0.52
14:N:146:MET:HE2	14:N:150:GLU:HB3	1.92	0.52
3:Q:125:GLN:NE2	16:Q:872:HOH:O	2.41	0.52
3:Q:182:PRO:O	3:Q:184:ALA:N	2.42	0.52
4:R:160:TYR:CG	4:R:163:LYS:HB2	2.44	0.52
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.92	0.52
7:G:142:ASP:OD2	7:G:144:LEU:N	2.42	0.52
10:J:4:LEU:HD23	10:J:126:ALA:HB2	1.91	0.52
11:K:174:ASN:HD21	11:K:189:ASN:ND2	2.03	0.52
1:O:46:VAL:HG11	1:O:139:ALA:HB1	1.90	0.52
4:R:79:SER:HB3	4:R:165:ILE:HD12	1.92	0.52
4:R:219:ASP:O	4:R:222:LYS:HE2	2.09	0.52
6:T:20(B):GLU:CD	6:T:20(C):LYS:HE3	2.34	0.52
13:1:105:GLN:HG3	16:1:769:HOH:O	2.09	0.52
6:F:53:LEU:HD11	6:F:205:ASN:OD1	2.10	0.52
7:G:228:ASN:HB3	16:G:255:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.67	0.52
6:T:35:THR:HG23	6:T:36:THR:N	2.23	0.52
9:W:41:VAL:HG22	9:W:76:PRO:HG3	1.90	0.52
12:Z:43:MET:HG2	12:Z:44:SER:N	2.24	0.52
1:A:6:ASP:OD1	7:G:126:ARG:NH2	2.40	0.52
4:D:123:PHE:CZ	4:D:131:PRO:HG3	2.44	0.52
11:K:25:TRP:CH2	12:L:132:SER:HA	2.45	0.52
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.10	0.52
4:D:59:LEU:HD13	4:D:59:LEU:C	2.34	0.52
9:I:29:ASN:HD21	11:Y:208:ASN:HD21	1.56	0.52
11:K:18:SER:HA	11:K:33:LYS:HE3	1.91	0.52
11:K:174:ASN:ND2	11:K:189:ASN:HD22	2.05	0.52
13:M:112:TYR:CE1	13:M:127:THR:HG22	2.45	0.52
14:N:36:ARG:HG3	14:N:42:TRP:CZ2	2.44	0.52
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.92	0.52
2:P:222:LYS:NZ	2:P:228:GLU:OE2	2.43	0.52
3:Q:151:THR:HG22	3:Q:157:TYR:HB3	1.90	0.52
13:1:169:SER:HB2	16:1:295:HOH:O	2.10	0.52
3:C:105:ASP:OD2	3:C:106:PRO:HD2	2.10	0.52
9:I:15:ALA:CB	9:I:175:VAL:HG22	2.39	0.52
13:1:113:VAL:HA	13:1:118:VAL:O	2.10	0.52
2:B:163:ILE:HG13	2:B:164:SER:H	1.74	0.52
6:F:109:ILE:HG21	6:F:147:HIS:HB2	1.92	0.52
9:I:2:ILE:HG22	9:I:128:GLY:HA3	1.91	0.52
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.92	0.52
5:S:111:ARG:HG2	5:S:111:ARG:HH11	1.75	0.52
5:S:185:ASN:C	5:S:185:ASN:HD22	2.17	0.52
9:W:12:VAL:HG13	9:W:108:PRO:HB3	1.92	0.52
10:X:141:HIS:HB2	10:X:154:LEU:HD11	1.92	0.52
12:Z:114:ASP:HB2	12:Z:118:SER:HB3	1.92	0.52
4:D:160:TYR:CG	4:D:163:LYS:HB2	2.45	0.51
1:O:121:GLN:O	1:O:124:THR:HB	2.10	0.51
4:R:52:LYS:HB2	4:R:20(B):ASN:HA	1.91	0.51
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.45	0.51
8:V:20:SER:HB3	8:V:28:ASP:HB3	1.92	0.51
9:W:93:GLY:C	16:W:266:HOH:O	2.53	0.51
2:B:122:GLY:C	2:B:124:THR:H	2.17	0.51
7:G:151:THR:HG22	7:G:157:TYR:CB	2.40	0.51
10:J:52:THR:CG2	10:J:53:VAL:N	2.73	0.51
4:R:86:ARG:HB2	16:R:1021:HOH:O	2.09	0.51
6:T:40:ILE:HD12	6:T:193:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:158:VAL:HG22	7:U:159:GLY:N	2.25	0.51
10:X:52:THR:CG2	10:X:53:VAL:N	2.73	0.51
11:Y:5:ALA:CB	11:Y:100:MET:HE3	2.40	0.51
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:HH11	1.75	0.51
2:B:224:PHE:N	2:B:224:PHE:CD2	2.74	0.51
5:E:185:ASN:C	5:E:185:ASN:HD22	2.16	0.51
12:L:147:SER:O	12:L:151:VAL:HG23	2.10	0.51
2:P:97:GLN:HA	2:P:97:GLN:NE2	2.24	0.51
3:Q:163:GLN:NE2	3:Q:164:THR:H	2.06	0.51
4:R:123:PHE:CZ	4:R:131:PRO:HG3	2.45	0.51
7:U:233:LEU:O	7:U:236:ILE:HG13	2.10	0.51
3:C:75:VAL:HG13	3:C:221:ILE:HD13	1.92	0.51
6:F:95:GLU:CD	6:F:115:ARG:HD2	2.36	0.51
9:I:29:ASN:HD21	11:Y:208:ASN:ND2	2.07	0.51
9:I:41:VAL:HG22	9:I:76:PRO:HG3	1.93	0.51
12:L:-8:PHE:CB	13:M:-8:THR:HG23	2.41	0.51
12:L:123:GLN:CG	12:L:145:TYR:OH	2.57	0.51
13:M:35:ILE:N	13:M:35:ILE:HD12	2.25	0.51
2:P:163:ILE:HG13	2:P:164:SER:H	1.76	0.51
12:Z:49:ALA:HB3	13:1:118:VAL:HG13	1.93	0.51
13:1:17:ASP:HA	13:1:173:PHE:HA	1.91	0.51
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.92	0.51
4:D:40:ILE:HD13	4:D:192:LEU:HD23	1.91	0.51
9:I:12:VAL:HG13	9:I:108:PRO:HB3	1.93	0.51
9:I:104:ILE:HB	16:I:202:HOH:O	2.10	0.51
8:V:63:ILE:HG23	8:V:74:PRO:HB3	1.92	0.51
11:Y:99:THR:HG22	11:Y:113:VAL:O	2.10	0.51
13:M:125:LEU:HA	16:M:224:HOH:O	2.09	0.51
5:S:136:LEU:HD12	5:S:151:PHE:CD2	2.46	0.51
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.43	0.51
12:Z:123:GLN:CG	12:Z:145:TYR:OH	2.58	0.51
11:K:7:ARG:HD2	11:K:108:PRO:O	2.11	0.51
12:L:14(H):GLY:O	12:L:1(I):ASN:N	2.43	0.51
3:Q:87:ILE:HD12	3:Q:87:ILE:N	2.26	0.51
1:A:32:LYS:HE2	1:A:32:LYS:HA	1.93	0.51
6:F:187:ARG:HH12	6:F:228:LEU:HD13	1.76	0.51
14:N:161:GLN:O	14:N:164:LYS:HB3	2.11	0.51
1:O:62:GLU:CD	1:O:62:GLU:H	2.19	0.51
2:P:74:ILE:C	2:P:221:GLN:HE22	2.18	0.51
4:R:81:LEU:HB3	16:R:599:HOH:O	2.10	0.51
10:X:39:PRO:HG2	10:X:73:GLU:OE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:18(H):GLU:CD	7:U:18(H):GLU:N	2.69	0.51
9:W:2:ILE:HG22	9:W:128:GLY:HA3	1.93	0.51
9:W:45:ILE:HB	9:W:52:VAL:HG13	1.93	0.51
10:X:2:ILE:O	10:X:16:SER:HA	2.11	0.51
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.92	0.51
14:2:8:PHE:CE1	14:2:10:ASP:HB2	2.46	0.51
11:K:44:THR:OG1	11:K:100:MET:HB2	2.11	0.51
2:P:78:VAL:HG11	2:P:85:ALA:HB2	1.91	0.51
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.10	0.51
3:Q:121:GLN:C	3:Q:121:GLN:HE21	2.18	0.51
3:Q:163:GLN:HG3	3:Q:164:THR:N	2.25	0.51
3:Q:201:VAL:HG21	3:Q:210:ILE:CD1	2.41	0.51
5:S:15:PHE:H	6:T:23:GLN:HE22	1.59	0.51
14:2:37:VAL:CG2	14:2:41:ILE:HG22	2.41	0.51
14:2:146:MET:HE2	14:2:150:GLU:HB3	1.92	0.51
2:B:136:PHE:O	2:B:150:THR:HA	2.10	0.50
6:F:35:THR:CG2	6:F:36:THR:N	2.74	0.50
8:H:214:LEU:HD22	11:Y:211:GLY:HA2	1.93	0.50
10:X:66:TYR:CE2	10:X:74:LEU:HG	2.46	0.50
7:G:55:PRO:HG2	7:G:56:ASP:H	1.76	0.50
7:G:236:ILE:HD12	7:G:236:ILE:C	2.36	0.50
10:J:39:PRO:HG2	10:J:73:GLU:OE2	2.11	0.50
5:S:162:GLY:O	5:S:163:THR:HB	2.10	0.50
10:X:70:GLU:O	10:X:71:ASP:C	2.54	0.50
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.46	0.50
7:G:233:LEU:O	7:G:236:ILE:HG13	2.12	0.50
8:H:148:LYS:O	8:H:152:ILE:HG13	2.11	0.50
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.10	0.50
14:N:37:VAL:CG2	14:N:41:ILE:HG22	2.41	0.50
14:N:145:ASN:N	16:N:601:HOH:O	2.43	0.50
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.93	0.50
6:T:93:ARG:NH1	16:T:378:HOH:O	2.42	0.50
7:U:55:PRO:HG2	7:U:56:ASP:H	1.77	0.50
12:Z:-5:TYR:CE2	12:Z:96:TYR:HB2	2.47	0.50
13:1:170:SER:HA	16:1:1294:HOH:O	2.10	0.50
2:B:78:VAL:HG11	2:B:85:ALA:HB2	1.92	0.50
6:F:35:THR:HG23	6:F:36:THR:N	2.25	0.50
6:F:203:GLU:O	6:F:206:LYS:HD2	2.11	0.50
2:P:134:VAL:O	2:P:153:PRO:HD3	2.12	0.50
10:X:138:LEU:HD21	10:X:158:CYS:SG	2.51	0.50
14:2:1:THR:HG23	14:2:33:LYS:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:TYR:N	1:A:26:TYR:CD1	2.79	0.50
2:B:101:LYS:NZ	10:J:85:GLN:HE22	2.08	0.50
2:B:222:LYS:NZ	2:B:228:GLU:OE2	2.44	0.50
4:D:42:THR:C	4:D:44:GLU:H	2.18	0.50
6:T:127:ASN:C	6:T:127:ASN:ND2	2.69	0.50
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.46	0.50
16:T:1339:HOH:O	13:1:67:ALA:HB3	2.12	0.50
2:B:17:PRO:HA	3:C:26:TYR:CE1	2.45	0.50
5:E:162:GLY:O	5:E:163:THR:HB	2.12	0.50
12:L:-5:TYR:CD2	12:L:96:TYR:HB2	2.47	0.50
13:M:164:TYR:O	14:2:26:ILE:HD12	2.12	0.50
1:O:58:LEU:HD12	7:U:173:THR:HG23	1.93	0.50
3:Q:241:GLN:O	3:Q:243:GLN:N	2.40	0.50
4:R:12:VAL:CG2	4:R:12(A):GLY:HA2	2.42	0.50
5:S:177:GLU:OE1	6:T:56:SER:HB2	2.12	0.50
6:T:130:ARG:HG2	6:T:130:ARG:HH11	1.76	0.50
14:2:1:THR:HG23	14:2:33:LYS:NZ	2.27	0.50
2:B:156:ASN:ND2	2:B:157:TYR:N	2.60	0.50
3:C:228:GLU:O	3:C:232:TYR:HD1	1.94	0.50
4:D:101:LEU:CD1	11:K:57:THR:HG22	2.42	0.50
6:F:122:ALA:HA	6:F:125:LEU:HD12	1.94	0.50
6:F:127:ASN:C	6:F:127:ASN:ND2	2.69	0.50
7:G:191:GLU:HG3	7:G:232:ARG:HG3	1.93	0.50
12:L:109:ALA:HB2	12:L:121:ARG:NH2	2.27	0.50
13:M:1:THR:OG1	13:M:2:SER:N	2.44	0.50
13:M:14(C):ARG:HG3	13:M:14(C):ARG:HH11	1.76	0.50
14:N:1:THR:HG23	14:N:33:LYS:HD3	1.94	0.50
1:O:187:GLU:HA	1:O:190:ILE:HD12	1.94	0.50
5:S:132:TYR:HD1	16:S:1059:HOH:O	1.94	0.50
6:T:122:ALA:HA	6:T:125:LEU:HD12	1.93	0.50
13:1:17:ASP:HA	13:1:173:PHE:CB	2.41	0.50
3:C:136:THR:O	3:C:150:GLN:HA	2.11	0.50
5:E:177:GLU:OE1	6:F:56:SER:HB2	2.11	0.50
7:G:100:ARG:HG3	7:G:100:ARG:NH1	2.25	0.50
8:H:20:SER:HB3	8:H:28:ASP:HB3	1.93	0.50
10:J:144:PRO:HG3	11:Y:207:ASN:HD21	1.74	0.50
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.76	0.50
5:S:52:LYS:HB3	5:S:63:TYR:HB3	1.94	0.50
6:T:100:LYS:O	6:T:104:LYS:N	2.43	0.50
6:T:203:GLU:O	6:T:206:LYS:HD2	2.11	0.50
8:V:5:GLY:O	8:V:124:TYR:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:126:SER:O	8:V:127:LEU:HD23	2.12	0.50
14:2:122:LEU:HD12	14:2:125:ALA:HB2	1.94	0.50
3:C:141:PHE:CE1	3:C:217:PRO:HG3	2.47	0.50
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.46	0.50
7:G:177:GLU:O	7:G:17(B):LYS:HG3	2.11	0.50
11:K:4:LEU:HD11	11:K:15:ALA:HB3	1.94	0.50
1:O:159:PRO:HB2	2:P:60:GLU:HB3	1.94	0.50
2:P:15:PHE:H	3:Q:23:GLN:NE2	1.98	0.50
4:R:160:TYR:HB3	4:R:162:ALA:O	2.12	0.50
1:A:187:GLU:HA	1:A:190:ILE:HD12	1.94	0.49
1:O:122:GLU:C	1:O:124:THR:H	2.20	0.49
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.77	0.49
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.94	0.49
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.77	0.49
6:F:179:LEU:CD2	6:F:192:GLN:HG2	2.42	0.49
7:G:10:ARG:HG2	7:G:22:TYR:CD2	2.46	0.49
7:G:21:LEU:HA	16:G:246:HOH:O	2.12	0.49
12:L:34:VAL:HG12	12:L:176:LEU:HD22	1.94	0.49
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.94	0.49
2:P:27:ALA:O	2:P:31:ILE:HG13	2.12	0.49
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.75	0.49
7:U:72:ARG:O	7:U:220:LYS:HA	2.11	0.49
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.94	0.49
12:Z:-9:GLN:HE21	13:1:-8:THR:HG21	1.77	0.49
1:A:134:VAL:O	1:A:153:PRO:HG3	2.11	0.49
2:B:20:ARG:NH1	2:B:20:ARG:HG2	2.27	0.49
2:B:230:LYS:O	2:B:234:VAL:HG23	2.13	0.49
11:K:5:ALA:CB	11:K:100:MET:HE3	2.42	0.49
2:P:78:VAL:HG11	2:P:85:ALA:CB	2.42	0.49
4:R:29:GLU:OE2	4:R:29:GLU:HA	2.12	0.49
4:R:12(D):ALA:HB3	4:R:126:ARG:HG3	1.94	0.49
8:V:84:LYS:HE2	8:V:119:THR:HG23	1.94	0.49
1:A:62:GLU:CD	1:A:62:GLU:H	2.20	0.49
4:D:52:LYS:HB2	4:D:20(B):ASN:HA	1.93	0.49
8:H:46:ALA:HA	15:H:7710:SY2:H24A	1.93	0.49
9:I:3:VAL:HG22	9:I:16:CYS:HB3	1.93	0.49
2:P:186:VAL:HG21	2:P:216:ARG:CD	2.39	0.49
4:R:42:THR:C	4:R:44:GLU:H	2.21	0.49
6:T:103:TYR:O	6:T:104:LYS:HB3	2.12	0.49
2:B:27:ALA:O	2:B:31:ILE:HG13	2.12	0.49
2:B:186:VAL:HG21	2:B:216:ARG:CD	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:114:ASP:HB2	12:L:118:SER:HB3	1.93	0.49
3:Q:15:PHE:H	4:R:23:GLN:NE2	2.00	0.49
5:S:111:ARG:HG2	5:S:111:ARG:NH1	2.28	0.49
5:S:226:GLY:O	5:S:228:ALA:N	2.46	0.49
7:U:18(H):GLU:CD	7:U:18(H):GLU:H	2.20	0.49
9:W:176:TYR:CE1	9:W:186:LYS:HD2	2.48	0.49
2:B:120:LYS:HZ1	2:B:136:PHE:HD1	1.60	0.49
2:B:202:THR:CG2	2:B:204:SER:H	2.11	0.49
11:K:207:ASN:HD21	10:X:144:PRO:HG2	1.76	0.49
2:P:20:ARG:NH1	2:P:20:ARG:HG2	2.28	0.49
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.48	0.49
5:S:148:LEU:HD23	5:S:162:GLY:HA2	1.94	0.49
7:U:173:THR:HG22	7:U:177:GLU:OE2	2.13	0.49
13:1:1:THR:OG1	13:1:2:SER:N	2.44	0.49
1:A:113:VAL:HG22	1:A:138:ILE:HD12	1.94	0.49
7:G:76:MET:HE3	7:G:78:VAL:HG23	1.93	0.49
8:H:156:SER:O	8:H:160:GLN:HG3	2.13	0.49
10:J:133:TYR:CE2	10:J:166:MET:CG	2.96	0.49
11:K:196:PHE:CE1	9:W:193:GLN:HG3	2.48	0.49
12:L:176:LEU:CD1	12:L:186:LYS:HG2	2.43	0.49
12:L:177:ILE:HD12	12:L:177:ILE:N	2.27	0.49
1:O:7:ARG:HD3	5:S:127:TYR:CD2	2.47	0.49
1:O:15:PHE:HB2	2:P:23:GLN:NE2	2.27	0.49
2:P:156:ASN:ND2	2:P:157:TYR:N	2.61	0.49
4:R:112:LEU:O	4:R:116:VAL:HG23	2.13	0.49
9:W:84:SER:HB2	9:W:119:ILE:HD11	1.95	0.49
11:Y:21:THR:HG22	11:Y:26:VAL:HA	1.94	0.49
3:C:151:THR:HG22	3:C:157:TYR:CB	2.43	0.49
3:C:214:VAL:HG23	3:C:224:LEU:HD11	1.95	0.49
4:D:12:VAL:CG2	4:D:12(A):GLY:HA2	2.43	0.49
7:G:72:ARG:O	7:G:220:LYS:HA	2.12	0.49
7:G:18(H):GLU:CD	7:G:18(H):GLU:N	2.71	0.49
8:H:8:PHE:HB2	8:H:146:LEU:O	2.12	0.49
9:I:117:GLY:O	9:I:118:CYS:C	2.54	0.49
10:J:190:PHE:C	10:J:192:ALA:H	2.18	0.49
12:L:95:TYR:O	12:L:97:VAL:N	2.42	0.49
13:M:211:ILE:HD11	14:2:36:ARG:CD	2.42	0.49
14:N:107:LYS:HG2	14:N:108:GLY:N	2.27	0.49
14:N:148:LYS:O	14:N:152:VAL:HG23	2.13	0.49
3:Q:136:THR:O	3:Q:150:GLN:HA	2.11	0.49
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:25:TRP:CH2	12:Z:132:SER:HA	2.47	0.49
13:1:104:VAL:CG2	13:1:178:ILE:HG22	2.40	0.49
4:D:12(D):ALA:HB3	4:D:126:ARG:HG3	1.95	0.49
11:K:172:SER:HA	11:K:192:VAL:HG23	1.95	0.49
1:O:161:LYS:HG3	2:P:58:LEU:O	2.12	0.49
2:P:101:LYS:HA	16:W:530:HOH:O	2.11	0.49
2:P:150:THR:CG2	2:P:160:TRP:HE1	2.25	0.49
3:Q:75:VAL:HG13	3:Q:221:ILE:HD13	1.95	0.49
4:R:79:SER:O	4:R:134:VAL:HG23	2.12	0.49
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.95	0.49
14:2:161:GLN:O	14:2:164:LYS:HB3	2.13	0.49
4:D:39:GLY:O	4:D:162:ALA:HA	2.13	0.49
5:E:22:PHE:O	5:E:25:GLU:N	2.46	0.49
7:G:225:SER:H	7:G:228:ASN:HB2	1.77	0.49
9:I:193:GLN:HG3	11:Y:196:PHE:CE1	2.47	0.49
11:K:10(A):ARG:HG2	11:K:10(A):ARG:HH11	1.78	0.49
12:L:167:ILE:O	8:V:167:LEU:HD22	2.13	0.49
13:M:57:ARG:HH11	13:M:57:ARG:HG2	1.77	0.49
14:N:157:HIS:HD2	14:2:140:LYS:HZ1	1.58	0.49
3:Q:33:ARG:HH11	3:Q:33:ARG:HB3	1.78	0.49
6:T:136:THR:O	6:T:150:MET:HA	2.12	0.49
14:2:114:PRO:HD2	14:2:118:SER:O	2.13	0.49
11:K:195:LEU:O	11:K:199:VAL:HG23	2.13	0.48
14:N:140:LYS:HZ1	14:2:157:HIS:HD2	1.61	0.48
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.94	0.48
6:T:109:ILE:HB	6:T:110:PRO:HD3	1.94	0.48
6:T:186:ALA:O	6:T:190:VAL:HG23	2.13	0.48
9:W:15:ALA:CB	9:W:175:VAL:HG22	2.43	0.48
12:Z:-8:PHE:CB	13:1:-8:THR:HG23	2.43	0.48
5:E:227:GLU:CD	5:E:227:GLU:H	2.22	0.48
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.95	0.48
8:H:147:THR:HG23	8:H:150:GLU:CD	2.38	0.48
4:R:121:LEU:HA	4:R:123:PHE:CE1	2.48	0.48
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.47	0.48
13:1:157:ASN:HB3	16:1:558:HOH:O	2.13	0.48
3:C:201:VAL:HG21	3:C:210:ILE:CD1	2.42	0.48
8:H:63:ILE:HG23	8:H:74:PRO:HB3	1.95	0.48
10:J:135:PHE:HB3	11:Y:165:ARG:NE	2.28	0.48
11:K:200:LYS:HG3	11:K:206:PHE:HB2	1.95	0.48
12:L:163:THR:HG21	16:L:1193:HOH:O	2.13	0.48
2:P:66:LYS:O	2:P:77:ALA:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:174:ASP:OD2	8:V:189:ARG:NH1	2.40	0.48
11:Y:172:SER:HA	11:Y:192:VAL:HG23	1.95	0.48
14:2:44:CYS:HB2	14:2:100:ILE:HB	1.94	0.48
2:B:127:GLY:N	16:B:710:HOH:O	2.45	0.48
4:D:79:SER:O	4:D:134:VAL:HG23	2.14	0.48
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.78	0.48
1:O:85:TYR:O	1:O:89:VAL:HG23	2.12	0.48
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.60	0.48
6:T:187:ARG:HH12	6:T:228:LEU:HD13	1.77	0.48
7:U:17:PRO:HD3	16:U:584:HOH:O	2.14	0.48
11:Y:44:THR:OG1	11:Y:100:MET:HB2	2.13	0.48
1:A:7:ARG:HD3	5:E:127:TYR:HD2	1.76	0.48
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.79	0.48
7:G:122:ILE:HG12	16:G:642:HOH:O	2.12	0.48
8:H:114:HIS:HB2	16:H:324:HOH:O	2.14	0.48
12:L:113:PHE:CD2	12:L:119:TYR:HB3	2.49	0.48
3:Q:141:PHE:CE1	3:Q:217:PRO:HG3	2.49	0.48
6:T:18:ASP:OD2	6:T:18:ASP:N	2.37	0.48
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.43	0.48
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.48	0.48
11:Y:149:GLU:N	16:Y:973:HOH:O	2.46	0.48
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.95	0.48
13:1:160:ARG:HG3	13:1:192:VAL:CG1	2.44	0.48
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.13	0.48
1:A:175:PHE:O	1:A:179:ARG:HG2	2.12	0.48
5:E:48:LEU:HG	5:E:139:ILE:HD13	1.95	0.48
6:F:187:ARG:NH1	6:F:228:LEU:HD13	2.29	0.48
7:G:173:THR:HG22	7:G:177:GLU:OE2	2.12	0.48
10:J:70:GLU:O	10:J:71:ASP:C	2.56	0.48
12:L:145:TYR:CD1	12:L:146:LEU:N	2.82	0.48
13:M:85:THR:O	13:M:89:GLN:HG3	2.14	0.48
2:P:121:GLN:NE2	2:P:121:GLN:C	2.72	0.48
6:T:77:VAL:CG1	6:T:137:ILE:HB	2.43	0.48
14:2:107:LYS:HG2	14:2:108:GLY:N	2.27	0.48
2:B:97:GLN:NE2	16:B:246:HOH:O	2.43	0.48
2:B:150:THR:CG2	2:B:160:TRP:HE1	2.27	0.48
6:F:43:ASN:N	6:F:43:ASN:HD22	2.11	0.48
6:F:172:ALA:O	6:F:173:LYS:C	2.56	0.48
8:H:160:GLN:O	8:H:161:ALA:C	2.56	0.48
11:K:147:SER:C	11:K:149:GLU:N	2.71	0.48
12:L:21:ILE:C	12:L:21:ILE:CD1	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:149:TYR:OH	3:Q:62(A):ILE:HB	2.14	0.48
3:Q:65:SER:HB2	16:Q:303:HOH:O	2.14	0.48
6:T:44:ASP:OD2	6:T:44:ASP:C	2.57	0.48
11:Y:35:ILE:HD11	11:Y:45:MET:HE2	1.94	0.48
1:A:13:THR:O	2:B:130:ARG:HD3	2.14	0.48
3:C:33:ARG:NH1	3:C:33:ARG:CB	2.69	0.48
11:K:165:ARG:NE	10:X:135:PHE:HB3	2.28	0.48
3:Q:55:THR:O	3:Q:56:LEU:HD22	2.13	0.48
6:T:50:VAL:HG22	6:T:51:GLU:N	2.28	0.48
7:U:48:VAL:HG23	7:U:48:VAL:O	2.14	0.48
7:U:192:PHE:C	7:U:192:PHE:CD1	2.92	0.48
8:V:147:THR:HG23	8:V:150:GLU:CD	2.39	0.48
9:W:117:GLY:O	9:W:118:CYS:C	2.57	0.48
12:Z:45:ALA:HA	12:Z:99:THR:HB	1.96	0.48
14:2:15:GLY:HA2	14:2:174:ARG:O	2.13	0.48
2:B:78:VAL:HG11	2:B:85:ALA:CB	2.43	0.48
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	1.95	0.48
5:E:52:LYS:HB3	5:E:63:TYR:HB3	1.94	0.48
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.95	0.48
8:H:201:GLN:HG3	12:Z:153:LYS:HG2	1.96	0.48
11:K:38:ASN:OD1	11:K:40:PHE:N	2.46	0.48
14:N:15:GLY:HA2	14:N:174:ARG:O	2.13	0.48
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.95	0.48
1:O:26:TYR:N	1:O:26:TYR:CD1	2.80	0.48
1:O:130:ARG:HG2	7:U:125:GLN:HG3	1.95	0.48
1:O:175:PHE:O	1:O:179:ARG:HG2	2.14	0.48
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.96	0.48
10:X:53:VAL:HB	16:Y:726:HOH:O	2.12	0.48
13:1:184:LEU:C	13:1:184:LEU:HD23	2.39	0.48
3:C:168:ASN:CB	3:C:200:VAL:HG11	2.43	0.48
6:F:91:ARG:O	6:F:95:GLU:HB2	2.14	0.48
7:G:8:TYR:C	7:G:10:ARG:N	2.72	0.48
7:G:192:PHE:C	7:G:192:PHE:CD1	2.91	0.48
13:M:164:TYR:HA	16:M:639:HOH:O	2.14	0.48
16:R:886:HOH:O	12:Z:70:HIS:HE1	1.96	0.48
13:1:150:VAL:HG21	16:1:323:HOH:O	2.13	0.48
2:B:70:LEU:CD2	2:B:89:ILE:HG23	2.43	0.47
3:C:87:ILE:HD12	3:C:87:ILE:N	2.28	0.47
1:O:17:PRO:HA	2:P:26:TYR:CD1	2.49	0.47
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.96	0.47
8:V:46:ALA:HA	15:V:7710:SY2:H24A	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.14	0.47
13:1:85:THR:O	13:1:89:GLN:HG3	2.14	0.47
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.96	0.47
6:F:52:LYS:HB2	6:F:209:GLU:O	2.13	0.47
6:F:114:ASP:O	6:F:118:GLN:HG2	2.14	0.47
6:F:136:THR:O	6:F:150:MET:HA	2.14	0.47
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.76	0.47
12:L:123:GLN:HG3	12:L:145:TYR:HH	1.77	0.47
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.49	0.47
2:P:184:MET:CE	2:P:188:ASP:HB3	2.44	0.47
7:U:76:MET:HE3	7:U:78:VAL:HG23	1.96	0.47
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.95	0.47
13:1:35:ILE:HD12	13:1:35:ILE:N	2.30	0.47
6:F:95:GLU:OE1	6:F:115:ARG:HD2	2.14	0.47
11:K:95:LEU:HB2	16:K:511:HOH:O	2.15	0.47
12:L:5:GLY:O	12:L:124:CYS:HA	2.14	0.47
14:N:105:ASP:HB2	16:N:775:HOH:O	2.13	0.47
3:Q:35:THR:OG1	3:Q:66:LYS:NZ	2.47	0.47
8:V:160:GLN:O	8:V:161:ALA:C	2.57	0.47
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.83	0.47
14:2:146:MET:CE	14:2:150:GLU:HB3	2.44	0.47
2:B:20:ARG:HG2	2:B:20:ARG:HH11	1.79	0.47
2:B:122:GLY:C	2:B:124:THR:N	2.73	0.47
2:B:160:TRP:CE3	2:B:163:ILE:HD13	2.49	0.47
12:L:-5:TYR:CE2	12:L:96:TYR:HB2	2.49	0.47
5:S:17:PRO:HA	6:T:26:TYR:CG	2.49	0.47
7:U:172:ILE:CD1	7:U:197:MET:HE1	2.44	0.47
9:W:61:TYR:CD1	9:W:61:TYR:C	2.93	0.47
11:Y:200:LYS:HG3	11:Y:206:PHE:HB2	1.96	0.47
12:Z:14(H):GLY:O	12:Z:1(I):ASN:N	2.47	0.47
1:A:15:PHE:HB2	2:B:23:GLN:HE22	1.79	0.47
5:E:71:ASP:OD1	5:E:96:CYS:HB3	2.13	0.47
6:F:50:VAL:HG22	6:F:51:GLU:N	2.29	0.47
13:M:115:LEU:HD23	13:M:115:LEU:N	2.29	0.47
6:T:43:ASN:HD22	6:T:43:ASN:N	2.13	0.47
10:X:4:LEU:HD23	10:X:126:ALA:CB	2.44	0.47
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	2.13	0.47
2:B:114:ARG:NH1	10:J:70:GLU:OE2	2.38	0.47
3:C:100:ARG:HD2	16:C:244:HOH:O	2.14	0.47
4:D:140:GLY:HA2	4:D:215:ILE:HG12	1.96	0.47
7:G:130:ARG:HG3	7:G:131:PRO:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.44	0.47
10:J:189:ASP:O	10:J:193:GLN:HB2	2.15	0.47
12:L:19:ARG:HG2	12:L:21:ILE:HG23	1.97	0.47
12:L:153:LYS:HG2	8:V:201:GLN:HG3	1.96	0.47
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.05	0.47
6:T:159:GLY:HA3	7:U:63:THR:HG21	1.97	0.47
7:U:151:THR:HG22	7:U:157:TYR:CB	2.44	0.47
11:Y:4:LEU:HD11	11:Y:15:ALA:HB3	1.96	0.47
13:1:164:TYR:HA	16:1:284:HOH:O	2.14	0.47
14:2:18(D):PRO:HA	14:2:18(G):TYR:CE2	2.50	0.47
7:G:43:LYS:HB2	7:G:18(G):GLU:O	2.14	0.47
12:L:21:ILE:HD11	12:L:168:GLN:NE2	2.30	0.47
14:N:19:ARG:HB2	16:N:194:HOH:O	2.15	0.47
2:P:107:ILE:HG22	16:P:410:HOH:O	2.14	0.47
2:P:150:THR:HG22	2:P:160:TRP:HE1	1.79	0.47
5:S:38:VAL:HG22	5:S:164:ALA:HB2	1.96	0.47
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.50	0.47
13:1:3:VAL:O	13:1:126:ALA:HA	2.15	0.47
13:1:190:LEU:N	13:1:190:LEU:CD1	2.77	0.47
6:F:123:HIS:HB2	16:F:243:HOH:O	2.14	0.47
11:K:200:LYS:HE2	16:K:1088:HOH:O	2.14	0.47
12:L:45:ALA:HA	12:L:99:THR:HB	1.96	0.47
12:L:14(Q):LEU:O	12:L:14(W):LYS:C	2.57	0.47
7:U:72:ARG:HG2	16:U:696:HOH:O	2.14	0.47
9:W:84:SER:CB	9:W:119:ILE:HD11	2.45	0.47
12:Z:-9:GLN:NE2	12:Z:-8:PHE:H	2.13	0.47
13:1:91:ARG:NH2	16:1:213:HOH:O	2.48	0.47
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.15	0.47
3:C:241:GLN:C	3:C:243:GLN:N	2.70	0.47
7:G:172:ILE:CD1	7:G:197:MET:HE1	2.45	0.47
10:J:166:MET:HA	10:J:167:PRO:HD3	1.75	0.47
14:N:37:VAL:HG22	14:N:41:ILE:O	2.15	0.47
6:T:187:ARG:NH1	6:T:228:LEU:HD13	2.30	0.47
7:U:18(G):GLU:CG	7:U:188:LYS:HB2	2.45	0.47
10:X:11:SER:HB2	10:X:178:VAL:O	2.14	0.47
10:X:104:TYR:CD1	10:X:180:LYS:HA	2.50	0.47
2:B:184:MET:CE	2:B:188:ASP:HB3	2.45	0.47
16:B:242:HOH:O	10:J:85:GLN:HB2	2.15	0.47
5:E:113:GLY:HA3	16:E:1004:HOH:O	2.14	0.47
7:G:59:LEU:O	7:G:61:PRO:HD3	2.14	0.47
1:O:184:LEU:HD22	1:O:188:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:168:ASN:HA	16:P:943:HOH:O	2.13	0.47
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.15	0.47
14:2:65:LEU:HG	14:2:69:GLN:NE2	2.30	0.47
2:B:121:GLN:NE2	2:B:121:GLN:C	2.74	0.46
5:E:38:VAL:HG22	5:E:164:ALA:HB2	1.96	0.46
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.98	0.46
8:H:84:LYS:HE2	8:H:119:THR:HG23	1.97	0.46
2:P:160:TRP:CE3	2:P:163:ILE:HD13	2.50	0.46
2:P:230:LYS:O	2:P:234:VAL:HG23	2.15	0.46
8:V:216:GLU:HG3	9:W:187:ARG:HG2	1.97	0.46
5:E:76:LEU:HD23	5:E:76:LEU:O	2.15	0.46
6:F:130:ARG:HG2	6:F:130:ARG:HH11	1.79	0.46
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.79	0.46
11:K:40:PHE:CG	11:K:73:ARG:CZ	2.98	0.46
12:L:104:LEU:HD11	12:L:179:THR:C	2.40	0.46
14:N:114:PRO:HD2	14:N:118:SER:O	2.14	0.46
1:O:221:PHE:CD2	1:O:221:PHE:C	2.93	0.46
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.96	0.46
2:B:66:LYS:O	2:B:77:ALA:HA	2.15	0.46
4:D:160:TYR:CE2	5:E:59:SER:HB3	2.51	0.46
5:E:15:PHE:H	6:F:23:GLN:HE22	1.61	0.46
7:G:158:VAL:HG22	7:G:159:GLY:N	2.31	0.46
9:I:55:LEU:HD12	9:I:97:VAL:HG21	1.96	0.46
10:J:146:MET:HE3	10:J:150:GLU:HB3	1.98	0.46
10:J:168:MET:HE2	10:X:167:PRO:O	2.15	0.46
13:M:3:VAL:O	13:M:126:ALA:HA	2.15	0.46
14:N:13:ILE:HD12	14:N:151:THR:HG22	1.96	0.46
4:R:237:LEU:O	4:R:241:GLU:HG3	2.15	0.46
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.16	0.46
11:Y:147:SER:C	11:Y:149:GLU:N	2.71	0.46
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.96	0.46
6:F:77:VAL:CG1	6:F:137:ILE:HB	2.46	0.46
7:G:48:VAL:HG23	7:G:48:VAL:O	2.15	0.46
7:G:18(H):GLU:CD	7:G:18(H):GLU:H	2.23	0.46
12:L:33:LYS:HB3	12:L:33:LYS:HE2	1.75	0.46
12:L:49:ALA:HB3	13:M:118:VAL:HG13	1.96	0.46
13:M:127:THR:HB	16:M:918:HOH:O	2.16	0.46
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.15	0.46
4:R:237:LEU:HD22	4:R:241:GLU:HG3	1.97	0.46
6:T:172:ALA:O	6:T:176:LEU:HD23	2.16	0.46
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:62:LYS:HD3	9:W:82:LEU:HD11	1.97	0.46
11:Y:65:LEU:HD12	11:Y:65:LEU:HA	1.82	0.46
13:1:57:ARG:HG2	13:1:57:ARG:HH11	1.80	0.46
13:1:14(E):SER:C	16:1:1126:HOH:O	2.59	0.46
13:1:186:PHE:CE1	13:1:188:LYS:HG3	2.51	0.46
1:A:136:LEU:O	1:A:150:GLN:HA	2.16	0.46
5:E:226:GLY:O	5:E:228:ALA:N	2.48	0.46
14:N:8:PHE:HE1	14:N:10:ASP:HB2	1.80	0.46
1:O:141:HIS:HA	1:O:146:GLY:O	2.16	0.46
9:W:99:PRO:HB2	9:W:113:PHE:HD2	1.81	0.46
5:E:185:ASN:C	5:E:185:ASN:ND2	2.72	0.46
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.31	0.46
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.97	0.46
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.50	0.46
2:P:122:GLY:C	2:P:124:THR:N	2.72	0.46
3:Q:214:VAL:HG23	3:Q:224:LEU:HD11	1.97	0.46
4:R:227:GLU:O	4:R:231:GLU:HG3	2.16	0.46
6:T:91:ARG:O	6:T:95:GLU:HB2	2.15	0.46
6:T:130:ARG:HG2	6:T:130:ARG:NH1	2.31	0.46
6:T:172:ALA:O	6:T:173:LYS:C	2.58	0.46
9:W:29:ASN:ND2	9:W:29:ASN:N	2.51	0.46
9:W:186:LYS:HE2	9:W:188:TYR:CE1	2.50	0.46
13:1:17:ASP:C	13:1:17:ASP:OD2	2.59	0.46
1:A:38:LEU:HD12	1:A:38:LEU:O	2.16	0.46
1:A:221:PHE:C	1:A:221:PHE:CD2	2.93	0.46
2:B:37:ALA:HB3	2:B:165:VAL:CG2	2.46	0.46
2:B:49:ALA:HB2	2:B:212:PHE:HE1	1.78	0.46
2:B:99:TYR:CD2	2:B:107:ILE:HA	2.51	0.46
2:B:160:TRP:CD2	2:B:163:ILE:HD13	2.51	0.46
6:F:186:ALA:O	6:F:190:VAL:HG23	2.15	0.46
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.98	0.46
10:J:2:ILE:O	10:J:16:SER:HA	2.16	0.46
12:L:14(Q):LEU:C	12:L:14(W):LYS:O	2.58	0.46
13:M:8:TYR:HD2	13:M:9:ASP:OD1	1.97	0.46
1:O:13:THR:O	2:P:130:ARG:HD3	2.15	0.46
2:P:186:VAL:CG2	2:P:216:ARG:HD3	2.43	0.46
5:S:185:ASN:C	5:S:185:ASN:ND2	2.74	0.46
7:U:29:LYS:HA	7:U:29:LYS:HD2	1.74	0.46
11:Y:143:LYS:HB2	11:Y:146:LEU:HD11	1.98	0.46
13:1:104:VAL:HG23	13:1:178:ILE:CG2	2.43	0.46
3:C:197:LEU:O	3:C:201:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:121:LEU:HA	4:D:123:PHE:CE1	2.51	0.46
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.98	0.46
4:D:237:LEU:HD22	4:D:241:GLU:HG3	1.97	0.46
7:G:30:ALA:O	7:G:33:GLN:HB2	2.15	0.46
10:J:15:ALA:HB2	10:J:155:LEU:CD1	2.44	0.46
10:J:131:GLY:HA3	16:J:594:HOH:O	2.16	0.46
13:M:113:VAL:HA	13:M:118:VAL:O	2.15	0.46
2:P:46:ILE:HG22	2:P:47:VAL:N	2.31	0.46
2:P:107:ILE:O	2:P:107:ILE:HG23	2.15	0.46
3:Q:87:ILE:N	3:Q:87:ILE:CD1	2.79	0.46
10:X:110:LEU:O	10:X:121:GLU:HG2	2.16	0.46
13:1:11:GLY:HA3	13:1:178:ILE:O	2.16	0.46
1:A:121:GLN:O	1:A:124:THR:HB	2.15	0.46
3:C:190:VAL:O	3:C:194:VAL:HG23	2.16	0.46
4:D:237:LEU:O	4:D:241:GLU:HG3	2.16	0.46
5:E:136:LEU:HD12	5:E:151:PHE:CD2	2.51	0.46
6:F:107:ILE:HG23	6:F:107:ILE:O	2.15	0.46
14:N:8:PHE:HB2	14:N:146:MET:O	2.16	0.46
1:O:57:PRO:CG	7:U:177:GLU:HG2	2.46	0.46
5:S:172:ALA:CB	5:S:196:ALA:O	2.64	0.46
10:X:15:ALA:HB2	10:X:155:LEU:CD1	2.46	0.46
5:E:148:LEU:HD23	5:E:162:GLY:HA2	1.98	0.46
6:F:39:GLY:C	6:F:148:LEU:HD21	2.41	0.46
10:J:129:TYR:O	10:J:130:SER:C	2.58	0.46
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.31	0.46
7:U:30:ALA:O	7:U:33:GLN:HB2	2.16	0.46
10:X:189:ASP:O	10:X:193:GLN:HB2	2.16	0.46
11:Y:114:ASP:C	11:Y:116:ASP:H	2.24	0.46
12:Z:58:ARG:HG2	12:Z:58:ARG:NH1	2.30	0.46
1:A:5:THR:O	1:A:7:ARG:HG2	2.16	0.45
1:A:58:LEU:HD12	7:G:173:THR:HG23	1.99	0.45
4:D:106:ASP:HA	16:D:1036:HOH:O	2.15	0.45
8:H:14:ILE:O	8:H:14:ILE:HG13	2.15	0.45
8:H:197:ARG:NH2	9:I:139:GLU:HG3	2.31	0.45
1:O:136:LEU:O	1:O:150:GLN:HA	2.17	0.45
2:P:161:LYS:HB3	2:P:180:TYR:CE2	2.51	0.45
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.41	0.45
6:T:109:ILE:HG21	6:T:147:HIS:HB2	1.97	0.45
14:2:84:LYS:HG3	14:2:119:VAL:HG22	1.97	0.45
1:A:141:HIS:HA	1:A:146:GLY:O	2.16	0.45
4:D:170:GLU:N	4:D:170:GLU:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:148:THR:HG21	10:J:177:ILE:HD13	1.99	0.45
11:K:21:THR:HG22	11:K:26:VAL:HA	1.97	0.45
13:M:11:GLY:HA3	13:M:178:ILE:O	2.16	0.45
10:X:12:VAL:HG21	10:X:109:GLU:O	2.16	0.45
12:Z:14(Q):LEU:O	12:Z:14(W):LYS:C	2.59	0.45
7:G:18(G):GLU:CG	7:G:188:LYS:HB2	2.46	0.45
9:I:33:LYS:O	9:I:44:GLY:HA2	2.15	0.45
12:L:-8:PHE:HB2	13:M:-8:THR:HG23	1.98	0.45
12:L:58:ARG:HG2	12:L:58:ARG:NH1	2.29	0.45
1:O:7:ARG:HB2	2:P:5:SER:OG	2.16	0.45
3:Q:241:GLN:C	3:Q:243:GLN:N	2.71	0.45
5:S:13:VAL:HG13	5:S:13:VAL:O	2.16	0.45
5:S:161:TYR:CE2	6:T:60:VAL:HA	2.52	0.45
6:T:114:ASP:O	6:T:118:GLN:HG2	2.15	0.45
7:U:8:TYR:C	7:U:10:ARG:N	2.73	0.45
12:Z:59:PHE:O	12:Z:62:SER:HB3	2.17	0.45
12:Z:14(E):GLU:HB2	12:Z:14(I):THR:HG21	1.99	0.45
13:1:8:TYR:HD2	13:1:9:ASP:OD1	1.98	0.45
2:B:149:TYR:CZ	3:C:62(A):ILE:HB	2.51	0.45
3:C:35:THR:OG1	3:C:66:LYS:NZ	2.49	0.45
3:C:87:ILE:O	3:C:91:LYS:HG3	2.16	0.45
5:E:111:ARG:HG2	5:E:111:ARG:NH1	2.31	0.45
6:F:179:LEU:HD11	6:F:192:GLN:HG2	1.98	0.45
8:H:52:THR:O	8:H:56:THR:HB	2.17	0.45
12:L:55:LEU:CD2	12:L:87:LEU:HD21	2.47	0.45
13:M:14(C):ARG:O	13:M:14(F):ASP:HB2	2.17	0.45
4:R:17:PRO:HA	5:S:26:TYR:CG	2.51	0.45
5:S:17:PRO:HA	6:T:26:TYR:CE1	2.51	0.45
5:S:180:LEU:O	5:S:18(D):ILE:HG22	2.16	0.45
6:T:169:ARG:O	6:T:173:LYS:HG3	2.17	0.45
8:V:197:ARG:NH2	9:W:139:GLU:HG3	2.32	0.45
11:Y:15:ALA:HB2	11:Y:175:LEU:HD23	1.97	0.45
11:Y:40:PHE:CG	11:Y:73:ARG:CZ	2.99	0.45
12:Z:98:HIS:C	12:Z:98:HIS:ND1	2.74	0.45
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.98	0.45
2:B:161:LYS:HB3	2:B:180:TYR:CE2	2.52	0.45
3:C:8:TYR:HB3	16:C:1062:HOH:O	2.17	0.45
6:F:100:LYS:O	6:F:104:LYS:N	2.46	0.45
6:F:180:VAL:HG21	7:G:58:LEU:HD23	1.97	0.45
7:G:74:ILE:HG21	7:G:112:LEU:HD23	1.99	0.45
10:J:85:GLN:HG2	16:J:202:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.99	0.45
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.98	0.45
14:N:18(D):PRO:HA	14:N:18(G):TYR:CE2	2.51	0.45
7:U:69:CYS:HB3	16:U:1186:HOH:O	2.16	0.45
8:V:77:VAL:HG13	16:V:351:HOH:O	2.15	0.45
9:W:3:VAL:HG22	9:W:16:CYS:HB3	1.98	0.45
9:W:7:THR:HG23	9:W:110:ILE:CD1	2.46	0.45
9:W:36:HIS:HB3	9:W:42:PHE:CD2	2.52	0.45
2:B:134:VAL:HG12	2:B:135:SER:N	2.31	0.45
6:F:43:ASN:H	6:F:43:ASN:ND2	2.14	0.45
8:H:55:VAL:CG1	8:H:56:THR:N	2.79	0.45
9:I:93:GLY:N	9:I:94:PRO:CD	2.80	0.45
10:J:148:THR:CG2	10:J:177:ILE:HD13	2.47	0.45
13:M:41:THR:HG21	13:M:79:ILE:CD1	2.45	0.45
2:P:120:LYS:HZ1	2:P:136:PHE:HD1	1.62	0.45
3:Q:99:HIS:CG	3:Q:107:VAL:HG12	2.52	0.45
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.52	0.45
3:Q:151:THR:HG22	3:Q:157:TYR:CB	2.46	0.45
6:T:52:LYS:HB2	6:T:209:GLU:O	2.17	0.45
6:T:91:ARG:HG2	6:T:119:TYR:CD2	2.52	0.45
7:U:191:GLU:HG3	7:U:232:ARG:HG3	1.98	0.45
8:V:18:THR:HB	8:V:30:ASN:HA	1.99	0.45
11:Y:9:GLN:CD	11:Y:9:GLN:C	2.84	0.45
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.16	0.45
4:D:29:GLU:OE2	4:D:29:GLU:HA	2.17	0.45
4:D:227:GLU:O	4:D:231:GLU:HG3	2.16	0.45
5:E:160:LEU:CD2	6:F:59:LEU:HD12	2.47	0.45
11:K:67:GLU:OE1	11:K:73:ARG:HA	2.16	0.45
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.47	0.45
5:S:201:LEU:O	5:S:202:ARG:HB2	2.16	0.45
12:Z:113:PHE:CD2	12:Z:119:TYR:HB3	2.51	0.45
13:1:70:ASN:ND2	13:1:70(A):ALA:HA	2.31	0.45
2:B:150:THR:HG22	2:B:160:TRP:HE1	1.81	0.45
3:C:33:ARG:HH11	3:C:33:ARG:HB3	1.79	0.45
7:G:79:ASN:HA	16:G:926:HOH:O	2.16	0.45
6:T:107:ILE:HG23	6:T:107:ILE:O	2.17	0.45
10:X:146:MET:HE3	10:X:150:GLU:HB3	1.98	0.45
11:Y:6:PHE:HB2	11:Y:124:ILE:HG12	1.98	0.45
14:2:37:VAL:HG22	14:2:41:ILE:O	2.16	0.45
2:B:225:LYS:O	2:B:226:PRO:C	2.59	0.45
6:F:43:ASN:N	6:F:43:ASN:ND2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:137:VAL:HG21	8:H:161:ALA:HB2	1.98	0.45
9:I:45:ILE:HB	9:I:52:VAL:HG13	1.99	0.45
9:I:61:TYR:CD1	9:I:61:TYR:C	2.95	0.45
11:K:143:LYS:HB2	11:K:146:LEU:HD11	1.99	0.45
12:L:33:LYS:CD	12:L:46:ASN:HD22	2.26	0.45
13:M:160:ARG:HG3	13:M:192:VAL:CG1	2.46	0.45
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.52	0.45
2:P:99:TYR:CD2	2:P:107:ILE:HA	2.52	0.45
6:T:121:GLN:NE2	16:T:385:HOH:O	2.50	0.45
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.80	0.45
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.99	0.45
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.99	0.45
11:Y:148:VAL:HB	16:Y:973:HOH:O	2.16	0.45
3:C:24:VAL:O	3:C:27:ALA:HB3	2.17	0.45
4:D:160:TYR:HB3	4:D:162:ALA:O	2.17	0.45
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.52	0.45
7:G:129:MET:HE3	16:G:561:HOH:O	2.16	0.45
11:K:9:GLN:C	11:K:9:GLN:CD	2.85	0.45
13:M:19:LEU:HD12	13:M:28:PHE:O	2.17	0.45
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.99	0.45
2:P:52:ARG:HH22	2:P:63(A):SER:HB3	1.82	0.45
2:P:186:VAL:HG21	2:P:216:ARG:HG2	1.99	0.45
7:U:74:ILE:HG21	7:U:112:LEU:HD23	1.98	0.45
7:U:142:ASP:OD2	7:U:144:LEU:N	2.44	0.45
12:Z:166:HIS:CD2	12:Z:168:GLN:H	2.29	0.45
14:2:148:LYS:O	14:2:152:VAL:HG23	2.17	0.45
2:B:17:PRO:HA	3:C:26:TYR:CD1	2.52	0.44
5:E:86:ARG:HG3	5:E:86:ARG:NH1	2.32	0.44
5:E:18(A):ASP:OD2	5:E:18(A):ASP:N	2.49	0.44
9:I:84:SER:CB	9:I:119:ILE:HD11	2.47	0.44
13:M:17:ASP:OD2	13:M:17:ASP:C	2.60	0.44
13:M:165:ARG:NH1	8:V:139:GLU:OE1	2.46	0.44
14:N:146:MET:CE	14:N:150:GLU:HB3	2.46	0.44
7:U:130:ARG:HG3	7:U:131:PRO:O	2.17	0.44
9:W:115:LEU:HD23	9:W:115:LEU:H	1.83	0.44
12:Z:19:ARG:HG2	12:Z:21:ILE:HG23	1.99	0.44
14:2:85:GLU:O	14:2:89:GLU:HB2	2.17	0.44
3:C:99:HIS:CG	3:C:107:VAL:HG12	2.52	0.44
5:E:2(B):THR:OG1	5:E:2(E):ASN:HB3	2.17	0.44
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.99	0.44
1:O:69:LEU:HG	1:O:71:THR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:184:LEU:HB2	16:O:486:HOH:O	2.17	0.44
6:T:95:GLU:CG	6:T:115:ARG:HD2	2.48	0.44
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.82	0.44
8:V:139:GLU:HA	8:V:139:GLU:OE2	2.18	0.44
9:W:106:GLY:HA2	9:W:181:LYS:HD3	1.99	0.44
10:X:129:TYR:O	10:X:130:SER:C	2.59	0.44
2:B:46:ILE:HG22	2:B:47:VAL:N	2.32	0.44
6:F:158:TRP:CZ3	7:G:64:VAL:HA	2.52	0.44
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.27	0.44
12:L:98:HIS:C	12:L:98:HIS:ND1	2.75	0.44
12:L:166:HIS:CD2	12:L:168:GLN:HB2	2.53	0.44
12:L:166:HIS:CD2	12:L:168:GLN:H	2.27	0.44
1:O:123:ALA:HB3	16:O:237:HOH:O	2.17	0.44
2:P:20:ARG:HG2	2:P:20:ARG:HH11	1.81	0.44
3:Q:46:VAL:HG22	3:Q:146:PRO:HB2	1.99	0.44
4:R:93:ARG:HD2	16:R:733:HOH:O	2.17	0.44
4:R:122:ARG:HG2	4:R:122:ARG:NH1	2.31	0.44
6:T:37:SER:HB3	6:T:50:VAL:HG23	2.00	0.44
6:T:39:GLY:C	6:T:148:LEU:HD21	2.43	0.44
14:2:112:THR:CG2	14:2:120:HIS:HB2	2.47	0.44
1:A:122:GLU:C	1:A:124:THR:H	2.24	0.44
5:E:76:LEU:HD23	5:E:76:LEU:C	2.43	0.44
6:F:44:ASP:OD2	6:F:44:ASP:C	2.59	0.44
6:F:136:THR:CB	16:F:1005:HOH:O	2.63	0.44
7:G:96:ALA:HB3	16:G:623:HOH:O	2.17	0.44
9:I:7:THR:HG23	9:I:110:ILE:CD1	2.47	0.44
10:J:74:LEU:HD22	10:J:78:ALA:HB1	2.00	0.44
14:N:161:GLN:HE21	14:2:136:GLY:CA	2.09	0.44
1:O:27:ALA:O	1:O:31:VAL:HG23	2.18	0.44
3:Q:168:ASN:CB	3:Q:200:VAL:HG11	2.44	0.44
4:R:18:GLU:N	4:R:18:GLU:OE2	2.50	0.44
5:S:134:VAL:O	5:S:153:PRO:HG3	2.17	0.44
5:S:227:GLU:CD	5:S:227:GLU:H	2.23	0.44
6:T:12:ASN:OD1	6:T:12:ASN:O	2.35	0.44
10:X:138:LEU:C	10:X:140:HIS:N	2.74	0.44
13:1:115:LEU:N	13:1:115:LEU:HD23	2.33	0.44
4:D:123:PHE:CE2	4:D:131:PRO:HG3	2.52	0.44
6:F:50:VAL:HG12	6:F:211:GLU:HB3	2.00	0.44
13:M:186:PHE:CE1	13:M:188:LYS:HG3	2.51	0.44
2:P:160:TRP:CD2	2:P:163:ILE:HD13	2.52	0.44
3:Q:58:LEU:HD12	3:Q:58:LEU:HA	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:177:LEU:HD13	5:S:58:LEU:CD1	2.47	0.44
9:W:33:LYS:O	9:W:44:GLY:HA2	2.17	0.44
10:X:35:ARG:HD3	10:X:35:ARG:HA	1.85	0.44
2:B:26:TYR:O	2:B:29:GLU:HB3	2.17	0.44
2:B:235:LYS:C	2:B:237:GLY:H	2.25	0.44
5:E:54:ASN:ND2	5:E:56:ASP:O	2.51	0.44
5:E:91:TYR:CD1	5:E:91:TYR:C	2.95	0.44
5:E:2(B):THR:N	5:E:2(E):ASN:HD22	2.15	0.44
7:G:151:THR:HA	7:G:156:TYR:O	2.18	0.44
9:I:84:SER:HB2	9:I:119:ILE:HD11	1.98	0.44
11:K:114:ASP:C	11:K:116:ASP:H	2.26	0.44
2:P:209:ARG:HB3	2:P:209:ARG:CZ	2.48	0.44
7:U:105:TYR:OH	8:V:66:HIS:HE1	2.00	0.44
8:V:156:SER:O	8:V:160:GLN:HG3	2.18	0.44
8:V:170:GLY:O	8:V:171:SER:HB2	2.18	0.44
10:X:148:THR:CG2	10:X:177:ILE:HD13	2.48	0.44
12:Z:176:LEU:CD1	12:Z:186:LYS:HG2	2.47	0.44
13:1:209:GLN:N	16:1:367:HOH:O	2.51	0.44
1:A:184:LEU:HD22	1:A:188:ASP:HB3	1.98	0.44
2:B:17:PRO:HA	3:C:26:TYR:CZ	2.52	0.44
3:C:55:THR:O	3:C:56:LEU:HD22	2.18	0.44
11:K:77:ALA:HA	11:K:111:TYR:CE2	2.53	0.44
3:Q:76:LEU:HD12	3:Q:138:ILE:CG1	2.48	0.44
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.42	0.44
11:Y:38:ASN:OD1	11:Y:40:PHE:N	2.47	0.44
11:Y:67:GLU:OE1	11:Y:73:ARG:HA	2.17	0.44
1:A:69:LEU:HG	1:A:71:THR:O	2.17	0.44
16:A:658:HOH:O	8:H:185:GLU:HB2	2.17	0.44
2:B:52:ARG:HH22	2:B:63(A):SER:HB3	1.82	0.44
4:D:56:SER:OG	4:D:57:PRO:HD2	2.18	0.44
8:H:144:GLN:O	8:H:145:ASP:HB2	2.18	0.44
8:H:170:GLY:O	8:H:171:SER:HB2	2.18	0.44
14:N:1:THR:HG23	14:N:33:LYS:NZ	2.32	0.44
14:N:85:GLU:O	14:N:89:GLU:HB2	2.17	0.44
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.47	0.44
14:N:186:ARG:HD3	16:N:933:HOH:O	2.18	0.44
1:O:27:ALA:O	1:O:30:ALA:HB3	2.17	0.44
2:P:97:GLN:OE1	9:W:64:ASN:HB3	2.18	0.44
2:P:176:LEU:HD23	2:P:192:LEU:HD22	2.00	0.44
5:S:220:PRO:O	5:S:222:THR:HG23	2.18	0.44
6:T:205:ASN:O	6:T:20(B):GLU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:160:ARG:HG3	13:1:192:VAL:HG11	1.99	0.44
1:A:21(G):LEU:HG	1:A:21(I):TYR:CE1	2.53	0.44
5:E:226:GLY:HA3	5:E:227:GLU:OE2	2.18	0.44
6:F:91:ARG:HG2	6:F:119:TYR:CD2	2.52	0.44
6:F:142:ASP:C	6:F:142:ASP:OD2	2.61	0.44
9:I:90:ARG:HG3	9:I:95:TYR:CE1	2.53	0.44
11:K:65:LEU:HD12	11:K:65:LEU:HA	1.85	0.44
3:Q:87:ILE:O	3:Q:91:LYS:HG3	2.18	0.44
3:Q:224:LEU:HD12	3:Q:224:LEU:H	1.82	0.44
5:S:91:TYR:CD1	5:S:91:TYR:C	2.96	0.44
8:V:55:VAL:CG1	8:V:56:THR:N	2.80	0.44
9:W:55:LEU:HD12	9:W:97:VAL:HG21	1.99	0.44
10:X:93:ARG:HG2	10:X:93:ARG:HH11	1.83	0.44
11:Y:5:ALA:HB3	11:Y:100:MET:HE3	2.00	0.44
11:Y:49:ALA:O	11:Y:50:ALA:C	2.61	0.44
13:1:146:THR:HA	16:1:323:HOH:O	2.18	0.44
5:E:201:LEU:O	5:E:202:ARG:HB2	2.17	0.43
8:H:3:ILE:HG22	8:H:16:ALA:CB	2.48	0.43
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.53	0.43
11:K:160:LEU:HD22	11:K:199:VAL:HG21	1.99	0.43
14:N:122:LEU:HD12	14:N:125:ALA:HB2	2.00	0.43
3:Q:108:THR:HG23	16:Q:1056:HOH:O	2.18	0.43
3:Q:123:TYR:CD1	3:Q:132:PHE:HE1	2.35	0.43
4:R:123:PHE:CE2	4:R:131:PRO:HG3	2.53	0.43
4:R:160:TYR:CZ	4:R:163:LYS:HD3	2.53	0.43
5:S:54:ASN:ND2	5:S:56:ASP:O	2.51	0.43
7:U:177:GLU:O	7:U:17(B):LYS:HG3	2.17	0.43
11:Y:144:TRP:HB2	16:Y:1321:HOH:O	2.17	0.43
12:Z:85:HIS:HE1	16:Z:196:HOH:O	2.00	0.43
1:A:12:LEU:HD11	7:G:127:ALA:HB2	2.00	0.43
3:C:229:ILE:O	3:C:233:VAL:HG23	2.18	0.43
6:F:172:ALA:O	6:F:175:GLU:N	2.51	0.43
9:I:187:ARG:HH11	9:I:187:ARG:HG3	1.83	0.43
11:K:4:LEU:HD22	11:K:4:LEU:C	2.43	0.43
13:M:17:ASP:HA	13:M:173:PHE:CA	2.48	0.43
1:O:92:SER:HA	1:O:95:VAL:HG12	1.99	0.43
2:P:25:GLU:HA	2:P:25:GLU:OE2	2.18	0.43
2:P:141:TYR:CE2	2:P:145:GLY:HA2	2.53	0.43
2:P:186:VAL:HG11	2:P:216:ARG:HD3	2.00	0.43
2:P:235:LYS:C	2:P:237:GLY:H	2.25	0.43
5:S:18(A):ASP:OD2	5:S:18(A):ASP:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:205:ASN:C	6:T:20(B):GLU:N	2.76	0.43
9:W:93:GLY:N	9:W:94:PRO:CD	2.81	0.43
11:Y:45:MET:HE2	11:Y:53:GLN:CA	2.48	0.43
14:2:114:PRO:HG2	16:2:191:HOH:O	2.16	0.43
2:B:53:LYS:HG2	2:B:54:VAL:HG23	2.00	0.43
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.18	0.43
5:E:199:GLN:CA	5:E:199:GLN:HE21	2.31	0.43
8:H:62:ASN:ND2	16:H:227:HOH:O	2.30	0.43
9:I:55:LEU:HD23	9:I:55:LEU:HA	1.84	0.43
9:I:106:GLY:HA2	9:I:181:LYS:HD3	1.98	0.43
11:K:156:LYS:HB2	11:K:175:LEU:HD11	2.01	0.43
1:O:6:ASP:OD1	7:U:126:ARG:NH2	2.44	0.43
3:Q:159:SER:O	4:R:59:LEU:HD22	2.18	0.43
4:R:39:GLY:O	4:R:162:ALA:HA	2.18	0.43
6:T:43:ASN:ND2	6:T:43:ASN:H	2.16	0.43
6:T:179:LEU:CD2	6:T:192:GLN:HG2	2.43	0.43
6:T:224:VAL:HG13	6:T:228:LEU:HD23	2.01	0.43
7:U:158:VAL:HG22	7:U:159:GLY:H	1.82	0.43
9:W:66:TYR:CZ	9:W:70:GLU:HG3	2.54	0.43
12:Z:21:ILE:HD11	12:Z:168:GLN:NE2	2.32	0.43
13:1:19:LEU:HB3	16:1:212:HOH:O	2.17	0.43
1:A:92:SER:HA	1:A:95:VAL:HG12	2.00	0.43
3:C:241:GLN:O	3:C:243:GLN:N	2.39	0.43
4:D:79:SER:HA	16:D:250:HOH:O	2.18	0.43
4:D:121:LEU:HA	4:D:123:PHE:HE1	1.84	0.43
5:E:180:LEU:O	5:E:18(D):ILE:HG22	2.19	0.43
6:F:78:TYR:CE1	6:F:85:GLY:HA3	2.54	0.43
10:J:4:LEU:HD23	10:J:126:ALA:CB	2.47	0.43
11:K:35:ILE:HD11	11:K:45:MET:HE2	1.95	0.43
11:K:126:CYS:HB2	11:K:135:TYR:CZ	2.52	0.43
13:M:14(A):VAL:HG23	13:M:14(A):VAL:O	2.18	0.43
2:P:207:TYR:CG	2:P:208:ASP:N	2.86	0.43
4:R:14:THR:HG22	4:R:15:PHE:N	2.34	0.43
6:T:118:GLN:HE21	7:U:90:LEU:HD22	1.84	0.43
7:U:17(C):LYS:HB2	7:U:17(C):LYS:HE3	1.78	0.43
9:W:107:LYS:HA	9:W:108:PRO:HD3	1.80	0.43
12:Z:21:ILE:C	12:Z:21:ILE:CD1	2.86	0.43
13:1:112:TYR:O	13:1:119:THR:HA	2.17	0.43
1:A:27:ALA:O	1:A:31:VAL:HG23	2.18	0.43
3:C:159:SER:OG	4:D:63:SER:HB3	2.18	0.43
4:D:122:ARG:HG2	4:D:122:ARG:NH1	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:199:GLN:HE21	5:E:199:GLN:N	2.17	0.43
5:E:201:LEU:HD11	5:E:207:LEU:CD2	2.40	0.43
6:F:205:ASN:C	6:F:20(B):GLU:N	2.76	0.43
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	2.01	0.43
10:J:142:TYR:O	10:J:143:ARG:HD3	2.18	0.43
11:K:13:ILE:HG13	11:K:151:ALA:HB1	2.01	0.43
11:K:97:MET:O	11:K:114:ASP:HA	2.18	0.43
14:N:44:CYS:HB2	14:N:100:ILE:HB	2.00	0.43
4:R:31:ILE:HD13	4:R:135:ALA:HB2	2.01	0.43
5:S:160:LEU:CD2	6:T:59:LEU:HD12	2.48	0.43
5:S:2(B):THR:OG1	5:S:2(E):ASN:HB3	2.18	0.43
6:T:43:ASN:N	6:T:43:ASN:ND2	2.66	0.43
6:T:118:GLN:NE2	7:U:90:LEU:HD22	2.33	0.43
7:U:100:ARG:HG3	16:U:937:HOH:O	2.18	0.43
10:X:45:PHE:HB3	10:X:99:VAL:HG12	2.01	0.43
5:E:2(C):VAL:CG1	5:E:2(D):ASP:N	2.81	0.43
6:F:203:GLU:OE1	6:F:203:GLU:HA	2.18	0.43
7:G:29:LYS:HD2	7:G:29:LYS:HA	1.79	0.43
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.99	0.43
11:K:111:TYR:CE1	11:K:121:LYS:HB2	2.53	0.43
1:O:55:SER:O	1:O:56:SER:HB2	2.19	0.43
4:R:215:ILE:HD12	4:R:216:THR:N	2.34	0.43
6:T:143:LYS:O	6:T:143:LYS:HG2	2.18	0.43
6:T:157:TYR:CD1	6:T:157:TYR:C	2.97	0.43
8:V:49:ALA:HB3	15:V:7710:SY2:H13A	2.01	0.43
10:X:74:LEU:HD22	10:X:78:ALA:HB1	1.99	0.43
11:Y:12:ILE:HD11	11:Y:109:THR:N	2.33	0.43
1:A:8:TYR:HD2	7:G:128:TYR:HB3	1.83	0.43
2:B:238:ILE:C	2:B:239:THR:O	2.62	0.43
11:K:35:ILE:CD1	11:K:45:MET:HE3	2.49	0.43
14:N:66:TYR:CD2	14:N:74:PRO:HB3	2.54	0.43
1:O:5:THR:O	1:O:7:ARG:HG2	2.18	0.43
8:V:52:THR:O	8:V:56:THR:HB	2.18	0.43
12:Z:-8:PHE:HB2	13:1:-8:THR:HG23	2.01	0.43
12:Z:76:ILE:HG23	12:Z:77:ASN:N	2.33	0.43
13:1:125:LEU:HA	16:1:218:HOH:O	2.17	0.43
1:A:78:TYR:HB3	1:A:85:TYR:CD1	2.54	0.43
3:C:46:VAL:HB	3:C:215:VAL:CG1	2.48	0.43
3:C:57:LYS:HD2	3:C:57:LYS:C	2.44	0.43
3:C:58:LEU:HA	3:C:58:LEU:HD12	1.82	0.43
4:D:40:ILE:CD1	4:D:193:VAL:HG23	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:35:SER:HB3	5:E:66:LYS:NZ	2.34	0.43
6:F:130:ARG:HG2	6:F:130:ARG:NH1	2.34	0.43
10:J:11:SER:HB2	10:J:178:VAL:O	2.19	0.43
10:J:112:GLN:NE2	16:J:898:HOH:O	2.41	0.43
11:K:15:ALA:HB2	11:K:175:LEU:HD23	2.00	0.43
13:M:104:VAL:CG2	13:M:178:ILE:HG22	2.46	0.43
14:N:3:ILE:HD13	14:N:46:SER:HB3	2.00	0.43
4:R:17:PRO:HG3	5:S:26:TYR:CZ	2.54	0.43
5:S:58:LEU:N	5:S:58:LEU:HD12	2.34	0.43
6:T:179:LEU:HD11	6:T:192:GLN:HG2	2.00	0.43
8:V:199:GLU:N	16:V:1207:HOH:O	2.31	0.43
11:Y:32:LYS:N	11:Y:32:LYS:HD2	2.33	0.43
12:Z:33:LYS:CD	12:Z:46:ASN:HD22	2.26	0.43
1:A:6:ASP:HB2	7:G:128:TYR:CE2	2.54	0.43
2:B:80:GLY:HA3	2:B:133:GLY:O	2.19	0.43
3:C:36:CYS:H	3:C:51:GLU:HG2	1.84	0.43
3:C:87:ILE:N	3:C:87:ILE:CD1	2.82	0.43
3:C:156:ILE:HD11	16:D:246:HOH:O	2.18	0.43
4:D:14:THR:HG22	4:D:15:PHE:N	2.33	0.43
6:F:205:ASN:O	6:F:20(B):GLU:N	2.52	0.43
8:H:81:GLN:NE2	16:H:747:HOH:O	2.51	0.43
10:J:32:ASP:OD2	10:J:34:THR:HG22	2.18	0.43
10:J:104:TYR:CD1	10:J:180:LYS:HA	2.54	0.43
11:K:32:LYS:N	11:K:32:LYS:HD2	2.34	0.43
11:K:45:MET:HE2	11:K:53:GLN:CA	2.48	0.43
1:O:159:PRO:O	2:P:59:LEU:HD12	2.18	0.43
3:Q:76:LEU:O	3:Q:76:LEU:HD23	2.18	0.43
3:Q:229:ILE:O	3:Q:233:VAL:HG23	2.18	0.43
4:R:17:PRO:HA	5:S:26:TYR:CD1	2.54	0.43
2:B:25:GLU:HA	2:B:25:GLU:OE2	2.19	0.43
5:E:4:PHE:CG	5:E:5:ARG:N	2.87	0.43
6:F:103:TYR:O	6:F:104:LYS:HB3	2.19	0.43
8:H:49:ALA:HB3	15:H:7710:SY2:H13A	2.00	0.43
10:J:138:LEU:C	10:J:140:HIS:N	2.75	0.43
12:L:21:ILE:C	12:L:27:ASN:ND2	2.77	0.43
12:L:29:ARG:NH1	12:L:171:ASP:OD1	2.49	0.43
13:M:-5:PRO:HD3	13:M:96:TRP:CE2	2.53	0.43
13:M:112:TYR:CD2	13:M:112:TYR:C	2.97	0.43
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.17	0.43
3:Q:224:LEU:H	3:Q:224:LEU:CD1	2.32	0.43
3:Q:225:SER:O	3:Q:229:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:121:LEU:HA	4:R:123:PHE:HE1	1.82	0.43
5:S:47:VAL:CG1	5:S:48:LEU:N	2.82	0.43
5:S:18(C):PHE:HA	5:S:18(F):ILE:CD1	2.49	0.43
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.83	0.43
10:X:39:PRO:HG2	10:X:73:GLU:CD	2.44	0.43
10:X:59:ILE:HA	10:X:59:ILE:HD13	1.86	0.43
11:Y:2:THR:HG22	11:Y:159:ILE:CD1	2.49	0.43
11:Y:126:CYS:HB2	11:Y:135:TYR:CZ	2.53	0.43
14:2:66:TYR:CD2	14:2:74:PRO:HB3	2.53	0.43
2:B:209:ARG:HB3	2:B:209:ARG:CZ	2.48	0.42
4:D:81:LEU:HD12	4:D:133:GLY:HA3	2.00	0.42
7:G:150:LYS:O	7:G:157:TYR:HA	2.19	0.42
8:H:18:THR:HB	8:H:30:ASN:HA	2.01	0.42
9:I:107:LYS:HA	9:I:108:PRO:HD3	1.80	0.42
10:J:3:ILE:HG22	10:J:100:LEU:CD1	2.49	0.42
10:J:45:PHE:HB3	10:J:99:VAL:HG12	2.01	0.42
11:K:45:MET:HE2	11:K:53:GLN:HA	2.01	0.42
12:L:-9:GLN:NE2	12:L:-8:PHE:H	2.16	0.42
12:L:14(E):GLU:HB2	12:L:14(I):THR:HG21	2.01	0.42
13:M:89:GLN:O	13:M:92(A):LYS:HG3	2.19	0.42
2:P:184:MET:HE2	2:P:188:ASP:CB	2.49	0.42
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.49	0.42
5:S:2(C):VAL:CG1	5:S:2(D):ASP:N	2.81	0.42
5:S:226:GLY:O	5:S:227:GLU:C	2.61	0.42
5:S:226:GLY:HA3	5:S:227:GLU:OE2	2.19	0.42
6:T:69:VAL:HG12	16:T:811:HOH:O	2.18	0.42
6:T:142:ASP:OD2	6:T:142:ASP:C	2.62	0.42
9:W:143:GLU:CG	9:W:146:LEU:HD21	2.49	0.42
10:X:8:VAL:HG11	10:X:151:GLY:HA3	2.02	0.42
10:X:53:VAL:O	10:X:54:GLN:C	2.62	0.42
11:Y:160:LEU:HD22	11:Y:199:VAL:HG21	2.00	0.42
13:1:124:THR:O	13:1:125:LEU:HD23	2.19	0.42
1:A:7:ARG:HD3	5:E:127:TYR:CD2	2.53	0.42
1:A:77:VAL:HG12	1:A:137:LEU:HB2	2.01	0.42
2:B:141:TYR:CE2	2:B:145:GLY:HA2	2.54	0.42
3:C:225:SER:O	3:C:229:ILE:HG13	2.18	0.42
5:E:47:VAL:CG1	5:E:48:LEU:N	2.82	0.42
6:F:103:TYR:O	6:F:105:THR:HG22	2.19	0.42
7:G:217:LYS:HA	7:G:217:LYS:CE	2.46	0.42
8:H:124:TYR:O	8:H:125:LEU:HD23	2.20	0.42
12:L:76:ILE:HG23	12:L:77:ASN:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:21:LEU:O	2:P:22:TYR:C	2.63	0.42
2:P:235:LYS:N	2:P:235:LYS:HD3	2.34	0.42
3:Q:156:ILE:HG22	3:Q:157:TYR:N	2.32	0.42
4:R:170:GLU:OE1	4:R:170:GLU:N	2.51	0.42
5:S:137:LEU:CD2	5:S:150:GLU:HG3	2.49	0.42
5:S:160:LEU:HD13	5:S:163:THR:HB	2.01	0.42
5:S:18(C):PHE:C	5:S:18(C):PHE:CD1	2.98	0.42
5:S:2(B):THR:N	5:S:2(E):ASN:HD22	2.16	0.42
7:U:60:ASP:OD2	7:U:62:THR:OG1	2.36	0.42
10:X:137:LEU:CD1	10:X:158:CYS:HA	2.49	0.42
12:Z:109:ALA:HB2	12:Z:121:ARG:NH2	2.34	0.42
13:1:157:ASN:ND2	16:1:905:HOH:O	2.51	0.42
2:B:184:MET:HE2	2:B:188:ASP:CB	2.50	0.42
3:C:76:LEU:O	3:C:76:LEU:HD23	2.19	0.42
3:C:123:TYR:CD1	3:C:132:PHE:HE1	2.37	0.42
4:D:225:ASP:O	4:D:226:ASN:C	2.62	0.42
6:F:224:VAL:HG13	6:F:228:LEU:HD23	2.00	0.42
10:J:147:THR:OG1	10:J:150:GLU:HG3	2.20	0.42
13:M:160:ARG:HG3	13:M:192:VAL:HG11	2.01	0.42
13:M:168:ARG:HD2	16:M:464:HOH:O	2.18	0.42
2:P:34:ALA:O	2:P:35:GLY:C	2.62	0.42
2:P:37:ALA:HB3	2:P:165:VAL:CG2	2.48	0.42
3:Q:62(A):ILE:HG13	3:Q:63:THR:N	2.34	0.42
3:Q:97:GLN:NE2	3:Q:97:GLN:HA	2.35	0.42
5:S:199:GLN:CA	5:S:199:GLN:HE21	2.32	0.42
6:T:75:GLY:O	6:T:138:PHE:HA	2.19	0.42
6:T:203:GLU:HA	6:T:203:GLU:OE1	2.19	0.42
7:U:14(A):GLU:HB2	16:U:915:HOH:O	2.19	0.42
7:U:217:LYS:HA	7:U:217:LYS:CE	2.45	0.42
10:X:3:ILE:HD13	10:X:3:ILE:HA	1.83	0.42
10:X:52:THR:HG23	10:X:53:VAL:HG23	2.01	0.42
10:X:148:THR:HG21	10:X:177:ILE:HD13	2.01	0.42
12:Z:31:GLU:OE1	13:1:120:TYR:HA	2.20	0.42
12:Z:55:LEU:CD2	12:Z:87:LEU:HD21	2.50	0.42
12:Z:93:PHE:N	12:Z:94:PRO:CD	2.80	0.42
13:1:14(C):ARG:O	13:1:14(F):ASP:HB2	2.18	0.42
14:2:18(G):TYR:HA	14:2:18(J):LEU:HG	2.01	0.42
3:C:39:GLY:O	3:C:162:ALA:HA	2.20	0.42
3:C:156:ILE:HG22	3:C:157:TYR:N	2.35	0.42
3:C:238:GLN:O	3:C:242:GLU:HG3	2.19	0.42
4:D:12(D):ALA:HB3	4:D:126:ARG:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:22:PHE:O	5:E:23:GLN:C	2.60	0.42
9:I:15:ALA:HB2	9:I:175:VAL:HG22	2.00	0.42
10:J:155:LEU:HD23	10:J:155:LEU:HA	1.89	0.42
11:K:49:ALA:O	11:K:50:ALA:C	2.61	0.42
12:L:14(H):GLY:C	12:L:1(I):ASN:N	2.77	0.42
2:P:114:ARG:NH1	10:X:70:GLU:OE2	2.43	0.42
7:U:224:LEU:HB3	7:U:228:ASN:HB2	2.00	0.42
10:X:112:GLN:NE2	10:X:126:ALA:H	2.16	0.42
11:Y:25:TRP:CZ3	12:Z:132:SER:HA	2.54	0.42
3:C:57:LYS:HD2	3:C:58:LEU:N	2.34	0.42
5:E:137:LEU:CD2	5:E:150:GLU:HG3	2.49	0.42
5:E:18(C):PHE:CD1	5:E:18(C):PHE:C	2.98	0.42
6:F:37:SER:HB3	6:F:50:VAL:HG23	2.02	0.42
6:F:157:TYR:CD1	6:F:157:TYR:C	2.96	0.42
10:J:112:GLN:NE2	10:J:126:ALA:H	2.17	0.42
2:P:31:ILE:HG23	2:P:79:ALA:O	2.19	0.42
2:P:70:LEU:CD2	2:P:89:ILE:HG23	2.50	0.42
2:P:142:ASP:C	2:P:142:ASP:OD1	2.63	0.42
2:P:202:THR:CG2	2:P:204:SER:HB2	2.49	0.42
2:P:225:LYS:O	2:P:226:PRO:C	2.61	0.42
4:R:12(D):ALA:HB3	4:R:126:ARG:CG	2.49	0.42
6:T:50:VAL:HG12	6:T:211:GLU:HB3	2.01	0.42
6:T:179:LEU:HD11	6:T:192:GLN:HG3	2.01	0.42
7:U:18:GLU:HB2	7:U:20:ARG:HD3	2.01	0.42
8:V:197:ARG:NH2	9:W:139:GLU:O	2.52	0.42
11:Y:97:MET:HG2	11:Y:115:SER:HB3	2.02	0.42
13:1:19:LEU:HD12	13:1:28:PHE:O	2.20	0.42
13:1:42:VAL:HG23	13:1:178:ILE:HD11	2.00	0.42
13:1:14(A):VAL:HG23	13:1:14(A):VAL:O	2.20	0.42
1:A:77:VAL:CG1	1:A:137:LEU:HB2	2.50	0.42
2:B:69:LYS:HE2	2:B:221:GLN:OE1	2.20	0.42
5:E:199:GLN:CA	5:E:199:GLN:NE2	2.82	0.42
6:F:169:ARG:HE	6:F:169:ARG:HB3	1.59	0.42
10:J:161:GLU:HA	10:J:161:GLU:OE2	2.19	0.42
13:M:112:TYR:O	13:M:119:THR:HA	2.19	0.42
13:M:190:LEU:N	13:M:190:LEU:CD1	2.82	0.42
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.55	0.42
5:S:78:LEU:HD12	5:S:78:LEU:O	2.19	0.42
6:T:203:GLU:C	6:T:205:ASN:H	2.27	0.42
11:Y:9:GLN:HE21	11:Y:9:GLN:HB3	1.72	0.42
11:Y:156:LYS:HB2	11:Y:175:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:166:HIS:CD2	12:Z:168:GLN:HB2	2.53	0.42
13:1:191:GLN:HE21	13:1:191:GLN:HB3	1.60	0.42
1:A:55:SER:O	1:A:56:SER:HB2	2.20	0.42
2:B:186:VAL:HG21	2:B:216:ARG:HG2	2.01	0.42
10:J:93:ARG:HG2	10:J:93:ARG:HH11	1.84	0.42
11:K:99:THR:HG23	11:K:113:VAL:HB	2.02	0.42
12:L:4:LEU:HD12	12:L:5:GLY:N	2.35	0.42
12:L:42:VAL:HG12	12:L:176:LEU:HD23	2.02	0.42
1:O:121:GLN:C	1:O:121:GLN:CD	2.88	0.42
2:P:115:ARG:HG2	16:P:249:HOH:O	2.18	0.42
3:Q:100:ARG:HG3	3:Q:106:PRO:HA	2.01	0.42
3:Q:121:GLN:NE2	3:Q:122:ARG:N	2.66	0.42
4:R:86:ARG:HA	4:R:86:ARG:HD3	1.87	0.42
4:R:117:CYS:SG	4:R:157:PHE:HB3	2.60	0.42
5:S:188:GLU:OE1	5:S:188:GLU:HA	2.20	0.42
8:V:137:VAL:HG21	8:V:161:ALA:HB2	2.00	0.42
11:Y:86:LEU:C	11:Y:86:LEU:CD1	2.93	0.42
11:Y:200:LYS:HG2	16:Y:772:HOH:O	2.19	0.42
12:Z:65:TRP:O	12:Z:66:TYR:C	2.62	0.42
13:1:133:MET:O	13:1:136:PRO:HD2	2.19	0.42
3:C:46:VAL:HG22	3:C:146:PRO:HB2	2.01	0.42
6:F:169:ARG:O	6:F:173:LYS:HG3	2.20	0.42
9:I:51:ASP:OD1	10:J:90(B):ARG:NH2	2.53	0.42
9:I:192:ARG:HD3	16:I:1187:HOH:O	2.19	0.42
11:K:146:LEU:HD23	11:K:151:ALA:HA	2.01	0.42
12:L:133:LEU:O	9:W:136:GLY:HA3	2.19	0.42
13:M:6:MET:HA	13:M:124:THR:HA	2.01	0.42
14:N:36:ARG:CD	13:1:211:ILE:HD11	2.49	0.42
14:N:175:MET:HE3	14:N:18(B):PHE:CE2	2.54	0.42
1:O:124:THR:CG2	1:O:124:THR:O	2.67	0.42
2:P:186:VAL:HG11	2:P:216:ARG:CD	2.49	0.42
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	2.20	0.42
13:1:133:MET:HE2	13:1:133:MET:HB3	1.93	0.42
14:2:155:ILE:HG22	14:2:175:MET:HE2	2.02	0.42
3:C:159:SER:O	4:D:59:LEU:HD22	2.20	0.42
10:J:83:VAL:HG21	10:J:101:ILE:HD11	2.02	0.42
1:O:38:LEU:HD12	1:O:38:LEU:O	2.19	0.42
3:Q:14:ILE:HB	4:R:23:GLN:HE22	1.84	0.42
5:S:201:LEU:HD11	5:S:207:LEU:CD2	2.39	0.42
7:U:43:LYS:HB2	7:U:18(G):GLU:O	2.19	0.42
10:X:3:ILE:O	10:X:126:ALA:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:-5:PRO:HD3	13:1:96:TRP:CD2	2.54	0.42
14:2:3:ILE:HD13	14:2:46:SER:HB3	2.01	0.42
1:A:8:TYR:CD2	7:G:128:TYR:HB3	2.55	0.42
3:C:195:ARG:HG3	3:C:236:ILE:HD13	2.01	0.42
5:E:188:GLU:OE1	5:E:188:GLU:HA	2.20	0.42
6:F:18:ASP:OD2	6:F:18:ASP:N	2.38	0.42
9:I:103:GLY:O	9:I:109:PHE:N	2.52	0.42
9:I:143:GLU:CG	9:I:146:LEU:HD21	2.49	0.42
13:M:157:ASN:ND2	16:M:1332:HOH:O	2.52	0.42
14:N:7:THR:HG22	14:N:110:VAL:HG23	2.02	0.42
2:P:233:LEU:HD12	2:P:233:LEU:HA	1.93	0.42
7:U:191:GLU:CG	7:U:232:ARG:HG3	2.50	0.42
10:X:133:TYR:C	16:X:203:HOH:O	2.63	0.42
11:Y:45:MET:HE2	11:Y:53:GLN:HA	2.02	0.42
12:Z:32:PRO:HD2	16:Z:1177:HOH:O	2.19	0.42
12:Z:58:ARG:HG2	12:Z:58:ARG:HH11	1.85	0.42
12:Z:104:LEU:HD11	12:Z:179:THR:C	2.44	0.42
13:1:94:PRO:HA	16:1:220:HOH:O	2.19	0.42
2:B:34:ALA:O	2:B:35:GLY:C	2.60	0.41
3:C:62(A):ILE:HG13	3:C:63:THR:N	2.35	0.41
3:C:175:PHE:O	3:C:179:ASN:HB2	2.20	0.41
5:E:139:ILE:HA	5:E:147:HIS:O	2.20	0.41
6:F:26:TYR:O	6:F:29:LYS:HB2	2.20	0.41
12:L:24:TYR:HA	8:V:167:LEU:HD12	2.02	0.41
12:L:153:LYS:HG2	8:V:201:GLN:CG	2.50	0.41
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	2.00	0.41
1:O:36:THR:HG22	1:O:37:SER:N	2.34	0.41
1:O:202:VAL:HG21	1:O:206:PHE:HD1	1.84	0.41
5:S:90:ASN:O	5:S:94:GLN:HG3	2.20	0.41
9:W:55:LEU:HD11	9:W:97:VAL:HG21	2.01	0.41
3:C:55:THR:C	3:C:56:LEU:HD22	2.45	0.41
8:H:167:LEU:HD12	12:Z:24:TYR:HA	2.00	0.41
13:M:18:ASN:HA	13:M:31:VAL:O	2.19	0.41
1:O:197:LEU:CD2	1:O:210:ILE:HD12	2.49	0.41
2:P:86:GLU:O	2:P:87:ILE:C	2.63	0.41
2:P:126:HIS:CB	3:Q:129:VAL:HG12	2.47	0.41
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.54	0.41
5:S:179:THR:HG22	5:S:179:THR:O	2.20	0.41
5:S:199:GLN:CA	5:S:199:GLN:NE2	2.82	0.41
7:U:26:TYR:N	7:U:26:TYR:CD1	2.86	0.41
7:U:171:GLU:OE1	7:U:171:GLU:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:146:MET:HE1	10:X:154:LEU:HD22	2.02	0.41
11:Y:15:ALA:HA	11:Y:174:ASN:O	2.20	0.41
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	2.02	0.41
1:A:141:HIS:HB2	1:A:147:PHE:CD2	2.55	0.41
1:A:197:LEU:CD2	1:A:210:ILE:HD12	2.51	0.41
2:B:31:ILE:HG23	2:B:79:ALA:O	2.20	0.41
2:B:176:LEU:HD23	2:B:192:LEU:HD22	2.01	0.41
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	2.02	0.41
5:E:90:ASN:O	5:E:94:GLN:HG3	2.19	0.41
5:E:18(C):PHE:HA	5:E:18(F):ILE:CD1	2.50	0.41
6:F:143:LYS:O	6:F:143:LYS:HG2	2.20	0.41
10:J:113:ILE:HG12	10:J:119:LYS:HG3	2.02	0.41
12:L:58:ARG:HG2	12:L:58:ARG:HH11	1.85	0.41
14:N:65:LEU:HG	14:N:69:GLN:NE2	2.34	0.41
9:W:187:ARG:HH11	9:W:187:ARG:HG3	1.85	0.41
10:X:166:MET:HA	10:X:167:PRO:HD3	1.74	0.41
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	2.19	0.41
5:E:172:ALA:CB	5:E:196:ALA:O	2.68	0.41
5:E:179:THR:HG22	5:E:179:THR:O	2.21	0.41
9:I:136:GLY:HA3	12:Z:133:LEU:O	2.20	0.41
11:K:70:GLU:O	11:K:71:LYS:C	2.63	0.41
13:M:205:GLY:HA2	16:2:194:HOH:O	2.19	0.41
14:N:105:ASP:HB2	16:N:980:HOH:O	2.20	0.41
4:R:137:LEU:HD23	4:R:137:LEU:HA	1.95	0.41
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.49	0.41
5:S:4:PHE:CG	5:S:5:ARG:N	2.87	0.41
8:V:43:CYS:SG	8:V:99:LEU:HB3	2.61	0.41
16:Z:383:HOH:O	13:1:121:SER:HB2	2.19	0.41
1:A:121:GLN:CD	1:A:121:GLN:C	2.88	0.41
4:D:117:CYS:SG	4:D:157:PHE:HB3	2.60	0.41
6:F:61:PRO:O	6:F:62:GLN:HB2	2.20	0.41
6:F:95:GLU:CG	6:F:115:ARG:HD2	2.51	0.41
8:H:201:GLN:CG	12:Z:153:LYS:HG2	2.49	0.41
9:I:55:LEU:HD11	9:I:97:VAL:HG21	2.01	0.41
10:J:52:THR:HG23	10:J:53:VAL:HG23	2.03	0.41
11:K:119:ARG:NH2	16:K:1295:HOH:O	2.48	0.41
12:L:-7:ASN:ND2	12:L:-5:TYR:H	2.18	0.41
13:M:3:VAL:CG2	13:M:46:SER:HB3	2.49	0.41
13:M:42:VAL:HG23	13:M:178:ILE:HD11	2.03	0.41
13:M:162:LEU:HB3	16:M:225:HOH:O	2.20	0.41
2:P:6:ARG:HD2	4:R:9:ASP:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:100:ARG:HH12	3:Q:106:PRO:HB3	1.78	0.41
4:R:185:THR:OG1	4:R:188:GLU:HG3	2.20	0.41
16:U:509:HOH:O	8:V:72:ARG:HA	2.21	0.41
11:Y:35:ILE:CD1	11:Y:45:MET:HE3	2.48	0.41
11:Y:70:GLU:O	11:Y:71:LYS:C	2.62	0.41
11:Y:146:LEU:HD23	11:Y:151:ALA:HA	2.01	0.41
2:B:37:ALA:HB3	2:B:165:VAL:HG22	2.03	0.41
5:E:78:LEU:HD12	5:E:78:LEU:O	2.20	0.41
7:G:26:TYR:N	7:G:26:TYR:CD1	2.87	0.41
8:H:2:THR:O	8:H:16:ALA:HA	2.21	0.41
9:I:28:SER:CB	10:J:120:VAL:HG21	2.50	0.41
10:J:53:VAL:O	10:J:54:GLN:C	2.63	0.41
11:K:174:ASN:HD22	11:K:174:ASN:HA	1.65	0.41
12:L:14(C):GLN:HG2	8:V:210:THR:HG21	2.02	0.41
13:M:70:ASN:ND2	13:M:70(A):ALA:HA	2.36	0.41
14:N:8:PHE:CE2	14:N:13:ILE:HG13	2.55	0.41
6:T:184:LEU:CD1	6:T:188:GLU:HB3	2.49	0.41
7:U:225:SER:O	7:U:226:ALA:C	2.63	0.41
9:W:28:SER:CB	10:X:120:VAL:HG21	2.49	0.41
10:X:69:ARG:HD2	16:X:553:HOH:O	2.21	0.41
11:Y:86:LEU:O	11:Y:89:GLN:HB2	2.21	0.41
12:Z:33:LYS:HB3	12:Z:33:LYS:HE2	1.78	0.41
1:A:21(G):LEU:HA	1:A:21(G):LEU:HD12	1.85	0.41
2:B:86:GLU:O	2:B:87:ILE:C	2.64	0.41
2:B:134:VAL:O	2:B:153:PRO:HD3	2.21	0.41
2:B:207:TYR:CG	2:B:208:ASP:N	2.88	0.41
7:G:39:ALA:HB2	7:G:48:VAL:HG12	2.03	0.41
8:H:139:GLU:HA	8:H:139:GLU:OE2	2.20	0.41
11:K:6:PHE:HB2	11:K:124:ILE:HG12	2.03	0.41
12:L:55:LEU:HD22	12:L:87:LEU:HD21	2.02	0.41
13:M:-1:GLY:HA2	16:M:213:HOH:O	2.21	0.41
13:M:179:ASP:C	13:M:181:ASN:H	2.29	0.41
2:P:80:GLY:HA3	2:P:133:GLY:O	2.21	0.41
5:S:13:VAL:HG22	6:T:129:VAL:C	2.46	0.41
6:T:70:VAL:HG11	6:T:112:PHE:CE1	2.56	0.41
10:X:83:VAL:HG21	10:X:101:ILE:HD11	2.02	0.41
11:Y:39:PRO:HG3	16:Y:1267:HOH:O	2.21	0.41
11:Y:174:ASN:HD22	11:Y:174:ASN:HA	1.67	0.41
13:1:89:GLN:O	13:1:92(A):LYS:HG3	2.21	0.41
1:A:233:LEU:O	1:A:236:LEU:HB2	2.21	0.41
2:B:174:THR:O	2:B:178:MET:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:ALA:O	3:C:30:ALA:HB3	2.21	0.41
4:D:31:ILE:HD13	4:D:135:ALA:HB2	2.03	0.41
5:E:58:LEU:HD12	5:E:58:LEU:N	2.35	0.41
7:G:143:GLU:CD	8:H:75:ARG:HH22	2.28	0.41
10:J:85:GLN:HG2	10:J:89:LYS:HE3	2.03	0.41
10:J:88:ALA:O	10:J:90(A):ILE:HG22	2.20	0.41
10:J:90(A):ILE:HD12	10:J:90(A):ILE:HA	1.89	0.41
10:J:138:LEU:HD21	10:J:158:CYS:SG	2.61	0.41
11:K:86:LEU:C	11:K:86:LEU:CD1	2.93	0.41
1:O:78:TYR:HB3	1:O:85:TYR:CD1	2.55	0.41
1:O:137:LEU:HD23	1:O:137:LEU:HA	1.91	0.41
2:P:69:LYS:HE2	2:P:221:GLN:OE1	2.20	0.41
3:Q:134:VAL:HG12	3:Q:135:SER:N	2.36	0.41
4:R:189:ALA:O	4:R:193:VAL:HG23	2.21	0.41
10:X:191:GLN:O	10:X:192:ALA:HB2	2.20	0.41
12:Z:4:LEU:HD12	12:Z:5:GLY:N	2.36	0.41
12:Z:42:VAL:HG12	12:Z:176:LEU:HD23	2.02	0.41
1:A:67:VAL:HG23	1:A:211:GLU:HG2	2.02	0.41
2:B:186:VAL:HG11	2:B:216:ARG:CD	2.51	0.41
3:C:157:TYR:N	16:C:1013:HOH:O	2.42	0.41
4:D:72:ARG:HG3	16:D:662:HOH:O	2.21	0.41
4:D:112:LEU:C	4:D:112:LEU:CD1	2.93	0.41
4:D:148:LEU:HB3	4:D:160:TYR:O	2.20	0.41
5:E:161:TYR:CE2	6:F:60:VAL:HA	2.55	0.41
6:F:75:GLY:O	6:F:138:PHE:HA	2.21	0.41
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.46	0.41
7:G:78:VAL:HG22	7:G:136:LEU:CD2	2.50	0.41
7:G:17(C):LYS:HE3	7:G:17(C):LYS:HB2	1.77	0.41
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.56	0.41
10:J:190:PHE:C	10:J:192:ALA:N	2.79	0.41
10:J:191:GLN:O	10:J:192:ALA:HB2	2.21	0.41
11:K:4:LEU:CD1	11:K:15:ALA:HB3	2.51	0.41
1:O:67:VAL:CG2	1:O:211:GLU:HG2	2.51	0.41
3:Q:57:LYS:HD2	3:Q:57:LYS:C	2.46	0.41
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.36	0.41
5:S:22:PHE:O	5:S:25:GLU:N	2.54	0.41
5:S:76:LEU:C	5:S:76:LEU:HD23	2.46	0.41
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	2.01	0.41
9:W:15:ALA:HB2	9:W:175:VAL:HG22	2.03	0.41
9:W:81:GLN:NE2	9:W:81:GLN:CA	2.83	0.41
9:W:103:GLY:O	9:W:109:PHE:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:9:GLN:HG3	10:X:10:ASP:CG	2.46	0.41
12:Z:32:PRO:N	16:Z:1177:HOH:O	2.53	0.41
13:1:190:LEU:N	13:1:190:LEU:HD12	2.36	0.41
1:A:185:GLU:OE1	1:A:187:GLU:HB2	2.21	0.41
5:E:148:LEU:HB3	5:E:160:LEU:O	2.22	0.41
7:G:55:PRO:HG2	7:G:56:ASP:N	2.36	0.41
7:G:119:LEU:HD12	7:G:119:LEU:HA	1.91	0.41
8:H:63:ILE:HD13	8:H:63:ILE:HA	1.98	0.41
8:H:130:GLY:O	8:H:131:SER:C	2.64	0.41
9:I:15:ALA:HB1	9:I:175:VAL:HG22	2.02	0.41
9:I:66:TYR:CZ	9:I:70:GLU:HG3	2.55	0.41
10:J:64:GLN:O	10:J:67:SER:HB2	2.20	0.41
11:K:5:ALA:HB3	11:K:100:MET:HE3	2.02	0.41
1:O:77:VAL:CG1	1:O:137:LEU:HB2	2.51	0.41
1:O:112:LEU:O	1:O:115:GLU:HB2	2.21	0.41
2:P:40:ILE:HD12	2:P:193:ALA:HB2	2.02	0.41
3:Q:238:GLN:O	3:Q:242:GLU:HG3	2.21	0.41
4:R:177:LEU:HA	5:S:58:LEU:HD11	2.02	0.41
5:S:148:LEU:O	5:S:149:LEU:HD12	2.21	0.41
6:T:148:LEU:HB3	6:T:160:TYR:O	2.21	0.41
6:T:194:ALA:O	6:T:198:TYR:HD1	2.04	0.41
7:U:82:ILE:N	7:U:83:PRO:HD2	2.36	0.41
11:Y:13:ILE:HG13	11:Y:151:ALA:HB1	2.02	0.41
11:Y:50:ALA:CB	12:Z:116:VAL:HG23	2.51	0.41
11:Y:97:MET:O	11:Y:114:ASP:HA	2.21	0.41
14:2:175:MET:HE3	14:2:18(B):PHE:CE2	2.56	0.41
1:A:62:GLU:O	1:A:64:LEU:N	2.52	0.40
6:F:203:GLU:C	6:F:205:ASN:H	2.28	0.40
9:I:133:GLN:OE1	9:I:133:GLN:N	2.44	0.40
10:J:3:ILE:O	10:J:126:ALA:HA	2.20	0.40
10:J:9:GLN:HG3	10:J:10:ASP:CG	2.45	0.40
11:K:25:TRP:CZ3	12:L:132:SER:HA	2.56	0.40
13:M:7:LYS:HD2	13:M:14(G):ILE:HD13	2.02	0.40
1:O:15:PHE:HB2	2:P:23:GLN:HE22	1.86	0.40
1:O:31:VAL:HG13	1:O:79:SER:O	2.21	0.40
1:O:197:LEU:HD23	1:O:210:ILE:HD12	2.03	0.40
2:P:53:LYS:HG2	2:P:54:VAL:HG23	2.03	0.40
4:R:24:VAL:O	4:R:28:LEU:HD13	2.20	0.40
4:R:140:GLY:HA2	4:R:215:ILE:HG12	2.01	0.40
6:T:151:LEU:HD12	6:T:157:TYR:HB3	2.02	0.40
6:T:172:ALA:O	6:T:175:GLU:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:55:PRO:HG2	7:U:56:ASP:N	2.36	0.40
12:Z:55:LEU:HD22	12:Z:87:LEU:HD21	2.02	0.40
12:Z:117:GLY:O	12:Z:118:SER:C	2.64	0.40
13:1:80:PHE:CE1	13:1:111:ARG:HD3	2.56	0.40
4:D:215:ILE:HD12	4:D:216:THR:N	2.36	0.40
10:J:8:VAL:HG11	10:J:151:GLY:HA3	2.03	0.40
10:J:22:ARG:HD3	10:J:22:ARG:HA	1.96	0.40
10:J:77:GLN:NE2	10:J:77:GLN:C	2.79	0.40
10:J:85:GLN:HB3	16:J:202:HOH:O	2.21	0.40
11:K:102:CYS:SG	11:K:110:ILE:HG23	2.61	0.40
1:O:39:GLY:O	1:O:162:ALA:HA	2.21	0.40
1:O:62:GLU:O	1:O:64:LEU:N	2.49	0.40
1:O:67:VAL:HG23	1:O:211:GLU:HG2	2.03	0.40
1:O:94:LYS:O	1:O:97:HIS:N	2.54	0.40
1:O:141:HIS:HB2	1:O:147:PHE:CD2	2.55	0.40
2:P:121:GLN:NE2	16:P:462:HOH:O	2.54	0.40
2:P:134:VAL:HG12	2:P:135:SER:N	2.36	0.40
2:P:239:THR:OXT	2:P:239:THR:CG2	2.68	0.40
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	2.02	0.40
6:T:26:TYR:O	6:T:29:LYS:HB2	2.21	0.40
6:T:172:ALA:C	6:T:174:ALA:N	2.78	0.40
7:U:143:GLU:CD	8:V:75:ARG:HH22	2.29	0.40
8:V:84:LYS:HE2	8:V:119:THR:CG2	2.52	0.40
9:W:123:ASP:OD1	9:W:124:PHE:N	2.45	0.40
1:A:38:LEU:C	1:A:38:LEU:CD1	2.94	0.40
2:B:74:ILE:C	2:B:221:GLN:NE2	2.80	0.40
2:B:235:LYS:N	2:B:235:LYS:HD3	2.36	0.40
2:B:238:ILE:O	2:B:239:THR:C	2.63	0.40
3:C:100:ARG:HG3	3:C:106:PRO:HA	2.03	0.40
3:C:224:LEU:H	3:C:224:LEU:CD1	2.35	0.40
3:C:227:GLU:H	3:C:227:GLU:CD	2.30	0.40
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.57	0.40
8:H:103:GLY:HA2	8:H:178:MET:SD	2.61	0.40
13:M:95:LEU:O	13:M:97:ASN:N	2.54	0.40
13:M:211:ILE:HD11	14:2:36:ARG:HD3	2.03	0.40
1:O:77:VAL:HG12	1:O:137:LEU:HB2	2.02	0.40
2:P:218:ASN:C	2:P:218:ASN:HD22	2.29	0.40
3:Q:201:VAL:HG21	3:Q:210:ILE:CG1	2.52	0.40
6:T:61:PRO:O	6:T:62:GLN:HB2	2.21	0.40
10:X:120:VAL:HG13	10:X:122:LEU:HG	2.03	0.40
11:Y:77:ALA:HA	11:Y:111:TYR:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:14(H):GLY:C	12:Z:1(I):ASN:N	2.78	0.40
12:Z:14(Q):LEU:C	12:Z:14(W):LYS:O	2.62	0.40
14:2:104:TYR:OH	14:2:180:ALA:HB2	2.21	0.40
3:C:163:GLN:HE21	3:C:164:THR:N	2.05	0.40
4:D:224:TYR:N	4:D:224:TYR:CD2	2.90	0.40
6:F:70:VAL:HG11	6:F:112:PHE:CE1	2.56	0.40
7:G:143:GLU:HG2	16:G:532:HOH:O	2.20	0.40
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.51	0.40
10:J:85:GLN:CG	16:J:202:HOH:O	2.70	0.40
10:J:137:LEU:CD1	10:J:158:CYS:HA	2.51	0.40
10:J:193:GLN:OXT	10:J:193:GLN:HG2	2.21	0.40
12:L:70(A):ASN:O	12:L:72:LYS:N	2.55	0.40
2:P:174:THR:O	2:P:178:MET:HB2	2.21	0.40
2:P:231:ASP:O	2:P:235:LYS:HG2	2.21	0.40
3:Q:224:LEU:N	3:Q:224:LEU:CD1	2.84	0.40
5:S:67:ILE:HD13	5:S:213:ALA:HB2	2.03	0.40
5:S:172:ALA:HB2	5:S:196:ALA:O	2.21	0.40
5:S:199:GLN:HE21	5:S:199:GLN:N	2.19	0.40
7:U:39:ALA:HB2	7:U:48:VAL:HG12	2.03	0.40
8:V:2:THR:OG1	8:V:130:GLY:HA3	2.22	0.40
8:V:148:LYS:HE3	8:V:177:VAL:HG11	2.03	0.40
16:V:1181:HOH:O	9:W:150:ASP:HA	2.21	0.40
10:X:93:ARG:NH2	11:Y:91:LYS:HD3	2.37	0.40
2:B:50:ALA:HB1	2:B:66:LYS:HD3	2.03	0.40
3:C:14:ILE:HB	4:D:23:GLN:HE22	1.86	0.40
3:C:57:LYS:HG2	3:C:208:LYS:HZ3	1.86	0.40
3:C:57:LYS:C	3:C:57:LYS:CD	2.95	0.40
4:D:16:SER:HA	4:D:22:PHE:CZ	2.56	0.40
4:D:24:VAL:O	4:D:28:LEU:HD13	2.22	0.40
10:J:110:LEU:O	10:J:121:GLU:HG2	2.21	0.40
10:J:120:VAL:HG13	10:J:122:LEU:HG	2.02	0.40
10:J:143:ARG:HA	10:J:144:PRO:HD3	1.81	0.40
11:K:15:ALA:HA	11:K:174:ASN:O	2.22	0.40
12:L:114:ASP:CB	12:L:118:SER:HB3	2.51	0.40
14:N:133:PHE:CE2	14:N:166:ASP:HB2	2.57	0.40
1:O:21(G):LEU:HG	1:O:21(I):TYR:CE1	2.55	0.40
2:P:184:MET:HE2	2:P:188:ASP:HB3	2.03	0.40
2:P:186:VAL:HG21	2:P:216:ARG:CG	2.51	0.40
3:Q:36:CYS:H	3:Q:51:GLU:HG2	1.87	0.40
4:R:17:PRO:HG3	5:S:26:TYR:CE2	2.55	0.40
5:S:73:HIS:HE1	5:S:107:LEU:O	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:38:LEU:HD23	7:U:197:MET:CE	2.49	0.40
7:U:78:VAL:HG22	7:U:136:LEU:CD2	2.52	0.40
7:U:222:PHE:CD2	7:U:222:PHE:N	2.89	0.40
8:V:144:GLN:O	8:V:145:ASP:HB2	2.20	0.40
11:Y:111:TYR:CE1	11:Y:121:LYS:HB2	2.57	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%)	220 (89%)	23 (9%)	5 (2%)	6	16
1	O	248/250 (99%)	222 (90%)	21 (8%)	5 (2%)	6	16
2	B	242/244 (99%)	215 (89%)	23 (10%)	4 (2%)	7	19
2	P	242/244 (99%)	215 (89%)	23 (10%)	4 (2%)	7	19
3	C	239/241 (99%)	220 (92%)	14 (6%)	5 (2%)	5	15
3	Q	239/241 (99%)	220 (92%)	14 (6%)	5 (2%)	5	15
4	D	240/242 (99%)	217 (90%)	17 (7%)	6 (2%)	4	11
4	R	240/242 (99%)	216 (90%)	18 (8%)	6 (2%)	4	11
5	E	231/233 (99%)	204 (88%)	23 (10%)	4 (2%)	7	19
5	S	231/233 (99%)	205 (89%)	23 (10%)	3 (1%)	9	25
6	F	242/244 (99%)	229 (95%)	11 (4%)	2 (1%)	16	37
6	T	242/244 (99%)	229 (95%)	11 (4%)	2 (1%)	16	37
7	G	241/243 (99%)	223 (92%)	17 (7%)	1 (0%)	30	54
7	U	241/243 (99%)	221 (92%)	19 (8%)	1 (0%)	30	54
8	H	220/222 (99%)	197 (90%)	19 (9%)	4 (2%)	6	18
8	V	220/222 (99%)	197 (90%)	18 (8%)	5 (2%)	5	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	202/204 (99%)	191 (95%)	10 (5%)	1 (0%)	24	48
9	W	202/204 (99%)	190 (94%)	11 (5%)	1 (0%)	24	48
10	J	196/198 (99%)	180 (92%)	15 (8%)	1 (0%)	24	48
10	X	196/198 (99%)	180 (92%)	15 (8%)	1 (0%)	24	48
11	K	210/212 (99%)	191 (91%)	18 (9%)	1 (0%)	24	48
11	Y	210/212 (99%)	192 (91%)	17 (8%)	1 (0%)	24	48
12	L	220/222 (99%)	201 (91%)	16 (7%)	3 (1%)	9	23
12	Z	220/222 (99%)	202 (92%)	13 (6%)	5 (2%)	5	13
13	1	231/233 (99%)	208 (90%)	20 (9%)	3 (1%)	9	25
13	M	231/233 (99%)	208 (90%)	20 (9%)	3 (1%)	9	25
14	2	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6312/6368 (99%)	5769 (91%)	461 (7%)	82 (1%)	9	25

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	167	LYS
3	C	58	LEU
3	C	203	THR
4	D	12(G)	GLU
7	G	220	LYS
10	J	192	ALA
11	K	39	PRO
12	L	71	ASP
12	L	14(I)	THR
13	M	96	TRP
1	O	167	LYS
3	Q	58	LEU
3	Q	203	THR
4	R	12(G)	GLU
7	U	220	LYS
10	X	192	ALA
11	Y	39	PRO
12	Z	71	ASP
12	Z	14(I)	THR
1	A	56	SER

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Mol	Chain	Res	Type
2	B	54	VAL
2	B	21(B)	GLY
2	B	21(C)	ASP
3	C	183	PRO
4	D	18(D)	SER
5	E	202	ARG
5	E	227	GLU
6	F	205	ASN
6	F	206	LYS
8	H	91	GLN
8	H	96	GLY
1	O	5	THR
1	O	56	SER
2	P	54	VAL
2	P	21(B)	GLY
2	P	21(C)	ASP
3	Q	183	PRO
4	R	18(D)	SER
5	S	202	ARG
5	S	227	GLU
6	T	205	ASN
6	T	206	LYS
8	V	91	GLN
8	V	96	GLY
13	1	96	TRP
1	A	6	ASP
1	A	63	THR
4	D	12(F)	GLY
4	D	128	MET
5	E	180	LEU
13	M	2	SER
1	O	6	ASP
1	O	63	THR
4	R	12(F)	GLY
4	R	128	MET
5	S	180	LEU
13	1	2	SER
2	B	22	TYR
3	C	53	ARG
3	C	242	GLU
4	D	169	SER
8	H	115	ALA

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Mol	Chain	Res	Type
8	H	171	SER
9	I	93	GLY
2	P	22	TYR
3	Q	53	ARG
3	Q	242	GLU
4	R	169	SER
8	V	171	SER
9	W	93	GLY
12	Z	96	TYR
13	1	72	ALA
4	D	12(C)	GLY
5	E	18(A)	ASP
12	L	96	TYR
13	M	72	ALA
4	R	12(C)	GLY
8	V	115	ALA
8	V	9	ASN
12	Z	32	PRO
12	Z	93	PHE

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%)	201 (96%)	8 (4%)	29	58
1	O	209/209 (100%)	201 (96%)	8 (4%)	29	58
2	B	203/203 (100%)	193 (95%)	10 (5%)	22	49
2	P	203/203 (100%)	193 (95%)	10 (5%)	22	49
3	C	213/213 (100%)	203 (95%)	10 (5%)	23	51
3	Q	213/213 (100%)	203 (95%)	10 (5%)	23	51
4	D	198/198 (100%)	185 (93%)	13 (7%)	15	36
4	R	198/198 (100%)	185 (93%)	13 (7%)	15	36
5	E	192/192 (100%)	180 (94%)	12 (6%)	16	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	192/192 (100%)	180 (94%)	12 (6%)	16	39
6	F	201/201 (100%)	189 (94%)	12 (6%)	17	41
6	T	201/201 (100%)	189 (94%)	12 (6%)	17	41
7	G	207/207 (100%)	199 (96%)	8 (4%)	28	57
7	U	207/207 (100%)	199 (96%)	8 (4%)	28	57
8	H	181/181 (100%)	175 (97%)	6 (3%)	33	63
8	V	181/181 (100%)	173 (96%)	8 (4%)	25	53
9	I	172/172 (100%)	167 (97%)	5 (3%)	37	67
9	W	172/172 (100%)	167 (97%)	5 (3%)	37	67
10	J	175/175 (100%)	170 (97%)	5 (3%)	37	67
10	X	175/175 (100%)	170 (97%)	5 (3%)	37	67
11	K	169/169 (100%)	162 (96%)	7 (4%)	27	56
11	Y	169/169 (100%)	162 (96%)	7 (4%)	27	56
12	L	185/185 (100%)	160 (86%)	25 (14%)	4	9
12	Z	185/185 (100%)	161 (87%)	24 (13%)	4	10
13	1	199/199 (100%)	190 (96%)	9 (4%)	24	52
13	M	199/199 (100%)	190 (96%)	9 (4%)	24	52
14	2	162/162 (100%)	154 (95%)	8 (5%)	22	49
14	N	162/162 (100%)	155 (96%)	7 (4%)	26	54
All	All	5332/5332 (100%)	5056 (95%)	276 (5%)	21	47

All (276) 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	124	THR
1	A	158	PHE
1	A	170	VAL
1	A	179	ARG
2	B	5	SER
2	B	58	LEU
2	B	67	LEU

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Mol	Chain	Res	Type
2	B	78	VAL
2	B	91	THR
2	B	124	THR
2	B	150	THR
2	B	192	LEU
2	B	224	PHE
2	B	226	PRO
3	C	10	ARG
3	C	25	GLU
3	C	57	LYS
3	C	76	LEU
3	C	100	ARG
3	C	121	GLN
3	C	135	SER
3	C	150	GLN
3	C	172	VAL
3	C	174	GLU
4	D	12	VAL
4	D	28	LEU
4	D	48	LEU
4	D	52	LYS
4	D	12(B)	GLU
4	D	12(E)	SER
4	D	12(G)	GLU
4	D	126	ARG
4	D	170	GLU
4	D	177	LEU
4	D	191	LEU
4	D	215	ILE
4	D	237	LEU
5	E	12	THR
5	E	13	VAL
5	E	32	LYS
5	E	57	GLU
5	E	76	LEU
5	E	97	ASN
5	E	121	GLN
5	E	189	LEU
5	E	199	GLN
5	E	207	LEU
5	E	227	GLU
5	E	231	LYS

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Mol	Chain	Res	Type
6	F	11	SER
6	F	35	THR
6	F	43	ASN
6	F	56	SER
6	F	72	ARG
6	F	98	SER
6	F	105	THR
6	F	127	ASN
6	F	144	ASN
6	F	169	ARG
6	F	187	ARG
6	F	203	GLU
7	G	40	VAL
7	G	87	ASN
7	G	119	LEU
7	G	124	THR
7	G	197	MET
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	13	VAL
8	H	56	THR
8	H	68	LEU
8	H	144	GLN
8	H	194	PRO
8	H	197	ARG
9	I	29	ASN
9	I	90	ARG
9	I	160	LEU
9	I	171	TRP
9	I	174	VAL
10	J	34	THR
10	J	68	ILE
10	J	121	GLU
10	J	155	LEU
10	J	168	MET
11	K	4	LEU
11	K	9	GLN
11	K	39	PRO
11	K	65	LEU
11	K	69	ARG
11	K	87	VAL

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Mol	Chain	Res	Type
11	K	100	MET
12	L	14	LEU
12	L	32	PRO
12	L	33	LYS
12	L	40	ASN
12	L	58	ARG
12	L	98	HIS
12	L	99	THR
12	L	115	PRO
12	L	120	GLU
12	L	138	LEU
12	L	14(A)	LYS
12	L	14(B)	ASN
12	L	14(C)	GLN
12	L	14(D)	TYR
12	L	14(E)	GLU
12	L	14(F)	PRO
12	L	14(I)	THR
12	L	14(K)	LYS
12	L	14(M)	VAL
12	L	14(N)	LYS
12	L	14(O)	LYS
12	L	14(P)	PRO
12	L	14(Q)	LEU
12	L	14(W)	LYS
12	L	190	GLU
13	M	40	ASN
13	M	62	LEU
13	M	71(A)	ASP
13	M	71(B)	GLU
13	M	71(C)	GLU
13	M	91	ARG
13	M	129	PHE
13	M	149	GLN
13	M	191	GLN
14	N	84	LYS
14	N	89	GLU
14	N	115	LEU
14	N	119	VAL
14	N	122	LEU
14	N	149	GLU
14	N	178	LEU

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Mol	Chain	Res	Type
1	O	32	LYS
1	O	33	GLN
1	O	62	GLU
1	O	64	LEU
1	O	124	THR
1	O	158	PHE
1	O	170	VAL
1	O	179	ARG
2	P	5	SER
2	P	58	LEU
2	P	67	LEU
2	P	78	VAL
2	P	91	THR
2	P	124	THR
2	P	150	THR
2	P	192	LEU
2	P	224	PHE
2	P	226	PRO
3	Q	10	ARG
3	Q	25	GLU
3	Q	57	LYS
3	Q	76	LEU
3	Q	100	ARG
3	Q	121	GLN
3	Q	135	SER
3	Q	150	GLN
3	Q	172	VAL
3	Q	174	GLU
4	R	12	VAL
4	R	28	LEU
4	R	48	LEU
4	R	52	LYS
4	R	12(B)	GLU
4	R	12(E)	SER
4	R	12(G)	GLU
4	R	126	ARG
4	R	170	GLU
4	R	177	LEU
4	R	191	LEU
4	R	215	ILE
4	R	237	LEU
5	S	12	THR

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Mol	Chain	Res	Type
5	S	13	VAL
5	S	32	LYS
5	S	57	GLU
5	S	76	LEU
5	S	97	ASN
5	S	121	GLN
5	S	189	LEU
5	S	199	GLN
5	S	207	LEU
5	S	227	GLU
5	S	231	LYS
6	T	11	SER
6	T	35	THR
6	T	43	ASN
6	T	56	SER
6	T	72	ARG
6	T	98	SER
6	T	105	THR
6	T	127	ASN
6	T	144	ASN
6	T	169	ARG
6	T	187	ARG
6	T	203	GLU
7	U	40	VAL
7	U	87	ASN
7	U	119	LEU
7	U	124	THR
7	U	197	MET
7	U	217	LYS
7	U	232	ARG
7	U	233	LEU
8	V	13	VAL
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	144	GLN
8	V	147	THR
8	V	194	PRO
8	V	197	ARG
9	W	29	ASN
9	W	90	ARG
9	W	160	LEU

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Mol	Chain	Res	Type
9	W	171	TRP
9	W	174	VAL
10	X	34	THR
10	X	35	ARG
10	X	121	GLU
10	X	155	LEU
10	X	168	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	39	PRO
11	Y	65	LEU
11	Y	69	ARG
11	Y	87	VAL
11	Y	100	MET
12	Z	14	LEU
12	Z	33	LYS
12	Z	40	ASN
12	Z	43	MET
12	Z	58	ARG
12	Z	98	HIS
12	Z	99	THR
12	Z	115	PRO
12	Z	138	LEU
12	Z	14(A)	LYS
12	Z	14(B)	ASN
12	Z	14(C)	GLN
12	Z	14(D)	TYR
12	Z	14(E)	GLU
12	Z	14(F)	PRO
12	Z	14(I)	THR
12	Z	14(K)	LYS
12	Z	14(M)	VAL
12	Z	14(N)	LYS
12	Z	14(O)	LYS
12	Z	14(P)	PRO
12	Z	14(Q)	LEU
12	Z	14(W)	LYS
12	Z	190	GLU
13	1	40	ASN
13	1	62	LEU
13	1	71(A)	ASP
13	1	71(B)	GLU

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Mol	Chain	Res	Type
13	1	71(C)	GLU
13	1	91	ARG
13	1	129	PHE
13	1	149	GLN
13	1	191	GLN
14	2	70	TYR
14	2	84	LYS
14	2	89	GLU
14	2	115	LEU
14	2	119	VAL
14	2	122	LEU
14	2	149	GLU
14	2	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (243) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
1	A	145	ASN
1	A	191	HIS
1	A	227	GLN
2	B	23	GLN
2	B	71	ASN
2	B	90	ASN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	173	GLN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	82	ASN
3	C	97	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	209	ASN
3	C	243	GLN
4	D	23	GLN

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Mol	Chain	Res	Type
4	D	108	ASN
4	D	147	GLN
4	D	161	ASN
4	D	199	GLN
4	D	211	GLN
4	D	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	73	HIS
5	E	95	GLN
5	E	97	ASN
5	E	104	ASN
5	E	114	HIS
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	156	ASN
5	E	199	GLN
5	E	2(E)	ASN
6	F	12	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	192	GLN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	184	ASN
7	G	228	ASN
8	H	30	ASN
8	H	66	HIS
8	H	91	GLN
8	H	141	HIS
8	H	144	GLN

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Mol	Chain	Res	Type
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
8	H	220	ASN
9	I	29	ASN
9	I	81	GLN
9	I	157	GLN
10	J	36	GLN
10	J	62	ASN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	140	HIS
10	J	186	GLN
10	J	193	GLN
11	K	9	GLN
11	K	24	ASN
11	K	53	GLN
11	K	85	ASN
11	K	174	ASN
11	K	189	ASN
11	K	190	HIS
11	K	207	ASN
11	K	208	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	-2	ASN
12	L	27	ASN
12	L	40	ASN
12	L	46	ASN
12	L	61	ASN
12	L	67	HIS
12	L	70	HIS
12	L	70(A)	ASN
12	L	82	ASN
12	L	14(C)	GLN
12	L	1(I)	ASN
12	L	166	HIS
12	L	168	GLN
13	M	-7	GLN
13	M	10	ASN
13	M	40	ASN

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Mol	Chain	Res	Type
13	M	54	HIS
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
13	M	191	GLN
14	N	69	GLN
14	N	141	ASN
14	N	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	145	ASN
1	O	150	GLN
1	O	191	HIS
1	O	227	GLN
2	P	23	GLN
2	P	71	ASN
2	P	90	ASN
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	173	GLN
2	P	177	GLN
2	P	218	ASN
3	Q	23	GLN
3	Q	82	ASN
3	Q	97	GLN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	147	GLN
4	R	161	ASN
4	R	199	GLN
4	R	211	GLN
4	R	226	ASN
5	S	7	ASN

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Mol	Chain	Res	Type
5	S	33	GLN
5	S	64	GLN
5	S	73	HIS
5	S	95	GLN
5	S	97	ASN
5	S	104	ASN
5	S	114	HIS
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	156	ASN
5	S	199	GLN
5	S	2(E)	ASN
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	147	HIS
6	T	192	GLN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN
7	U	170	GLN
7	U	178	ASN
7	U	184	ASN
7	U	228	ASN
8	V	30	ASN
8	V	66	HIS
8	V	85	GLN
8	V	141	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
8	V	201	GLN
8	V	220	ASN
9	W	29	ASN

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Mol	Chain	Res	Type
9	W	81	GLN
10	X	36	GLN
10	X	54	GLN
10	X	62	ASN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	141	HIS
10	X	186	GLN
10	X	193	GLN
11	Y	9	GLN
11	Y	24	ASN
11	Y	53	GLN
11	Y	85	ASN
11	Y	174	ASN
11	Y	189	ASN
11	Y	190	HIS
11	Y	207	ASN
11	Y	208	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	-2	ASN
12	Z	27	ASN
12	Z	40	ASN
12	Z	46	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70	HIS
12	Z	70(A)	ASN
12	Z	82	ASN
12	Z	85	HIS
12	Z	14(C)	GLN
12	Z	1(I)	ASN
12	Z	166	HIS
12	Z	168	GLN
13	1	-7	GLN
13	1	10	ASN
13	1	40	ASN
13	1	54	HIS
13	1	89	GLN
13	1	93	ASN
13	1	132	HIS

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Mol	Chain	Res	Type
13	1	149	GLN
13	1	157	ASN
13	1	191	GLN
14	2	69	GLN
14	2	141	ASN
14	2	145	ASN
14	2	157	HIS
14	2	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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	SY2	Y	7710	11	35,35,35	2.18	4 (11%)	47,47,47	1.97	8 (17%)
15	SY2	H	7710	8	35,35,35	2.27	5 (14%)	47,47,47	1.90	7 (14%)
15	SY2	V	7710	8	35,35,35	2.32	5 (14%)	47,47,47	1.94	6 (12%)
15	SY2	K	7710	11	35,35,35	2.31	3 (8%)	47,47,47	1.96	8 (17%)

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	SY2	Y	7710	11	-	17/53/53/53	0/0/1/1
15	SY2	H	7710	8	-	18/53/53/53	0/0/1/1
15	SY2	V	7710	8	-	19/53/53/53	0/0/1/1
15	SY2	K	7710	11	-	13/53/53/53	0/0/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	7710	SY2	C27-C26	10.95	1.56	1.32
15	H	7710	SY2	C27-C26	10.88	1.56	1.32
15	K	7710	SY2	C27-C26	10.58	1.56	1.32
15	Y	7710	SY2	C27-C26	10.49	1.55	1.32
15	K	7710	SY2	C23-C22	3.96	1.60	1.54
15	V	7710	SY2	C23-C22	3.79	1.60	1.54
15	K	7710	SY2	C11-N36	2.58	1.51	1.45
15	H	7710	SY2	C27-C28	2.54	1.53	1.48
15	Y	7710	SY2	C23-C22	2.52	1.58	1.54
15	H	7710	SY2	C22-C26	2.44	1.56	1.49
15	H	7710	SY2	C23-C22	2.25	1.58	1.54
15	V	7710	SY2	C27-C28	2.18	1.52	1.48
15	Y	7710	SY2	C11-N36	2.18	1.50	1.45
15	V	7710	SY2	C22-C26	2.09	1.55	1.49
15	V	7710	SY2	C28-N30	2.07	1.38	1.34
15	Y	7710	SY2	C15-N17	2.04	1.38	1.34
15	H	7710	SY2	C24-C23	2.02	1.59	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	7710	SY2	C22-C26-C27	-8.91	110.72	126.78
15	Y	7710	SY2	C22-C26-C27	-8.86	110.81	126.78
15	K	7710	SY2	C22-C26-C27	-8.60	111.28	126.78
15	V	7710	SY2	C22-C26-C27	-8.39	111.67	126.78
15	V	7710	SY2	C27-C28-N30	5.09	126.23	115.07
15	Y	7710	SY2	C27-C28-N30	4.78	125.55	115.07
15	H	7710	SY2	C27-C28-N30	4.76	125.50	115.07
15	K	7710	SY2	C27-C28-N30	4.69	125.34	115.07
15	K	7710	SY2	C26-C27-C28	-4.63	111.80	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Y	7710	SY2	C26-C27-C28	-4.54	112.00	122.67
15	V	7710	SY2	C26-C27-C28	-4.31	112.53	122.67
15	H	7710	SY2	C26-C27-C28	-3.81	113.71	122.67
15	V	7710	SY2	O29-C28-C27	-3.11	115.77	122.95
15	H	7710	SY2	O29-C28-C27	-2.92	116.22	122.95
15	K	7710	SY2	C18-N17-C15	-2.87	115.49	121.65
15	Y	7710	SY2	O29-C28-C27	-2.87	116.34	122.95
15	Y	7710	SY2	C18-N17-C15	-2.79	115.65	121.65
15	K	7710	SY2	O29-C28-N30	-2.77	117.94	122.29
15	V	7710	SY2	O29-C28-N30	-2.74	118.00	122.29
15	Y	7710	SY2	C31-N30-C28	2.74	126.40	122.46
15	Y	7710	SY2	C11-N36-C8	2.71	126.50	121.99
15	K	7710	SY2	O29-C28-C27	-2.70	116.72	122.95
15	Y	7710	SY2	O29-C28-N30	-2.67	118.10	122.29
15	K	7710	SY2	C11-N36-C8	2.59	126.30	121.99
15	V	7710	SY2	C31-N30-C28	2.56	126.15	122.46
15	H	7710	SY2	O29-C28-N30	-2.55	118.28	122.29
15	K	7710	SY2	C31-N30-C28	2.49	126.04	122.46
15	H	7710	SY2	C31-N30-C28	2.43	125.97	122.46
15	H	7710	SY2	O9-C8-N7	-2.02	118.35	122.67

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	H	7710	SY2	O29-C28-N30-C31
15	H	7710	SY2	C27-C28-N30-C31
15	H	7710	SY2	C22-C26-C27-C28
15	H	7710	SY2	C23-C22-C26-C27
15	H	7710	SY2	N21-C22-C26-C27
15	K	7710	SY2	O29-C28-N30-C31
15	K	7710	SY2	C27-C28-N30-C31
15	K	7710	SY2	C22-C26-C27-C28
15	K	7710	SY2	C23-C22-C26-C27
15	K	7710	SY2	N21-C22-C26-C27
15	V	7710	SY2	O29-C28-N30-C31
15	V	7710	SY2	C27-C28-N30-C31
15	V	7710	SY2	C22-C26-C27-C28
15	V	7710	SY2	C23-C22-C26-C27
15	V	7710	SY2	N21-C22-C26-C27
15	V	7710	SY2	C26-C22-C23-C24
15	V	7710	SY2	N21-C22-C23-C25

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Mol	Chain	Res	Type	Atoms
15	Y	7710	SY2	O29-C28-N30-C31
15	Y	7710	SY2	C27-C28-N30-C31
15	Y	7710	SY2	C22-C26-C27-C28
15	Y	7710	SY2	C23-C22-C26-C27
15	Y	7710	SY2	N21-C22-C26-C27
15	Y	7710	SY2	N30-C31-C32-C33
15	K	7710	SY2	N30-C31-C32-C33
15	V	7710	SY2	C26-C27-C28-O29
15	V	7710	SY2	C26-C27-C28-N30
15	H	7710	SY2	C26-C27-C28-O29
15	H	7710	SY2	C26-C27-C28-N30
15	K	7710	SY2	C31-C32-C33-C34
15	Y	7710	SY2	C31-C32-C33-C34
15	K	7710	SY2	C26-C27-C28-N30
15	K	7710	SY2	C26-C27-C28-O29
15	V	7710	SY2	N30-C31-C32-C33
15	H	7710	SY2	N30-C31-C32-C33
15	V	7710	SY2	N17-C18-C19-O20
15	H	7710	SY2	N17-C18-C19-O20
15	K	7710	SY2	N17-C18-C19-O20
15	Y	7710	SY2	N17-C18-C19-O20
15	V	7710	SY2	N17-C18-C19-N21
15	H	7710	SY2	C12-C11-N36-C8
15	K	7710	SY2	C12-C11-N36-C8
15	V	7710	SY2	C12-C11-N36-C8
15	Y	7710	SY2	C12-C11-N36-C8
15	H	7710	SY2	N17-C18-C19-N21
15	H	7710	SY2	C26-C22-C23-C25
15	V	7710	SY2	C26-C22-C23-C25
15	Y	7710	SY2	C26-C22-C23-C24
15	Y	7710	SY2	C26-C27-C28-O29
15	H	7710	SY2	N21-C22-C23-C25
15	V	7710	SY2	N21-C22-C23-C24
15	Y	7710	SY2	N21-C22-C23-C25
15	K	7710	SY2	N17-C18-C19-N21
15	Y	7710	SY2	C26-C27-C28-N30
15	Y	7710	SY2	N17-C18-C19-N21
15	V	7710	SY2	N17-C18-C34-C33
15	H	7710	SY2	N17-C18-C34-C33
15	K	7710	SY2	C34-C18-C19-O20
15	Y	7710	SY2	C34-C18-C19-O20
15	V	7710	SY2	C34-C18-C19-O20

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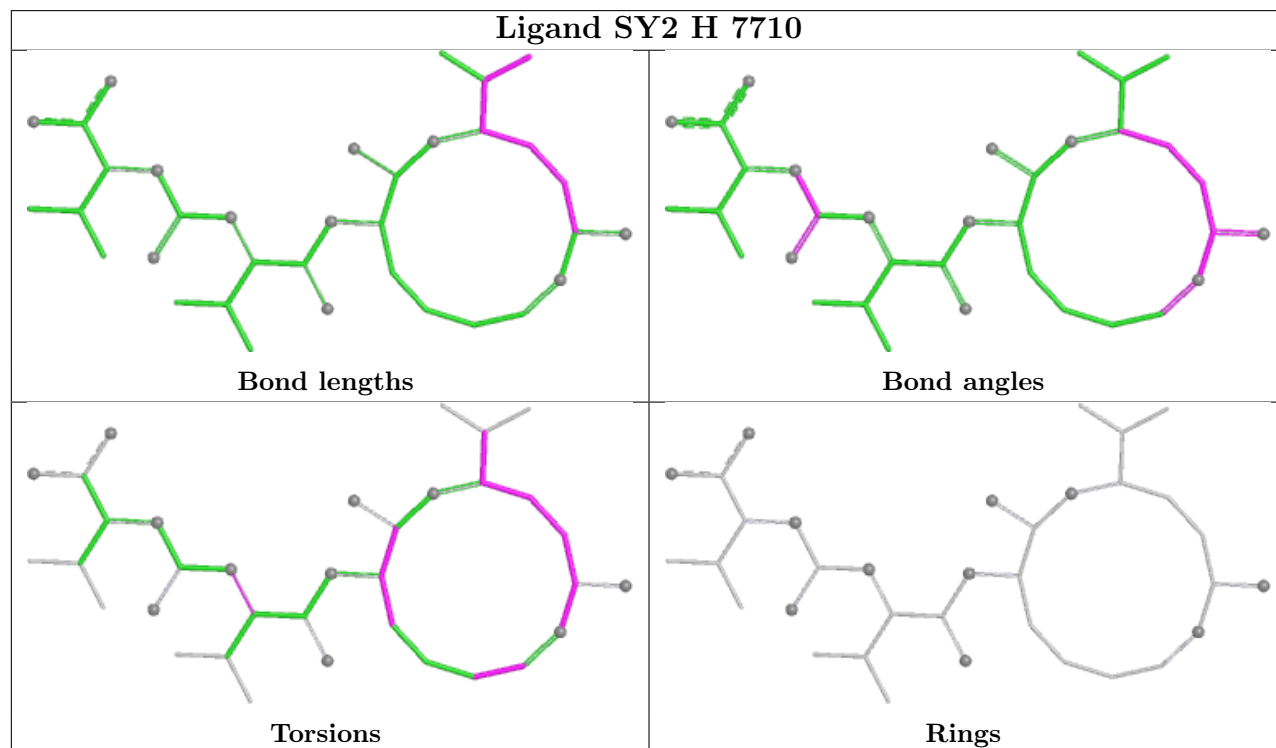
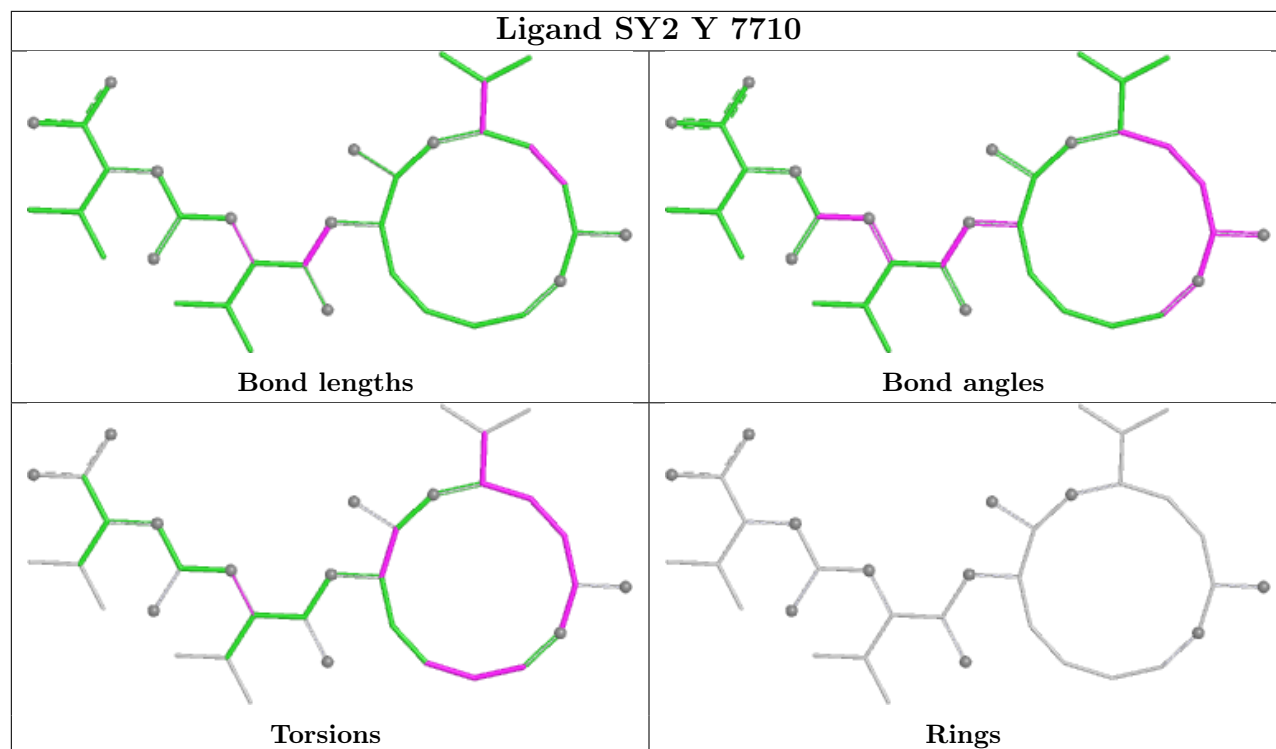
Mol	Chain	Res	Type	Atoms
15	H	7710	SY2	C34-C18-C19-O20
15	V	7710	SY2	C19-C18-C34-C33
15	H	7710	SY2	C19-C18-C34-C33
15	H	7710	SY2	C26-C22-C23-C24
15	Y	7710	SY2	C26-C22-C23-C25
15	H	7710	SY2	N21-C22-C23-C24
15	Y	7710	SY2	N21-C22-C23-C24
15	V	7710	SY2	C34-C18-C19-N21

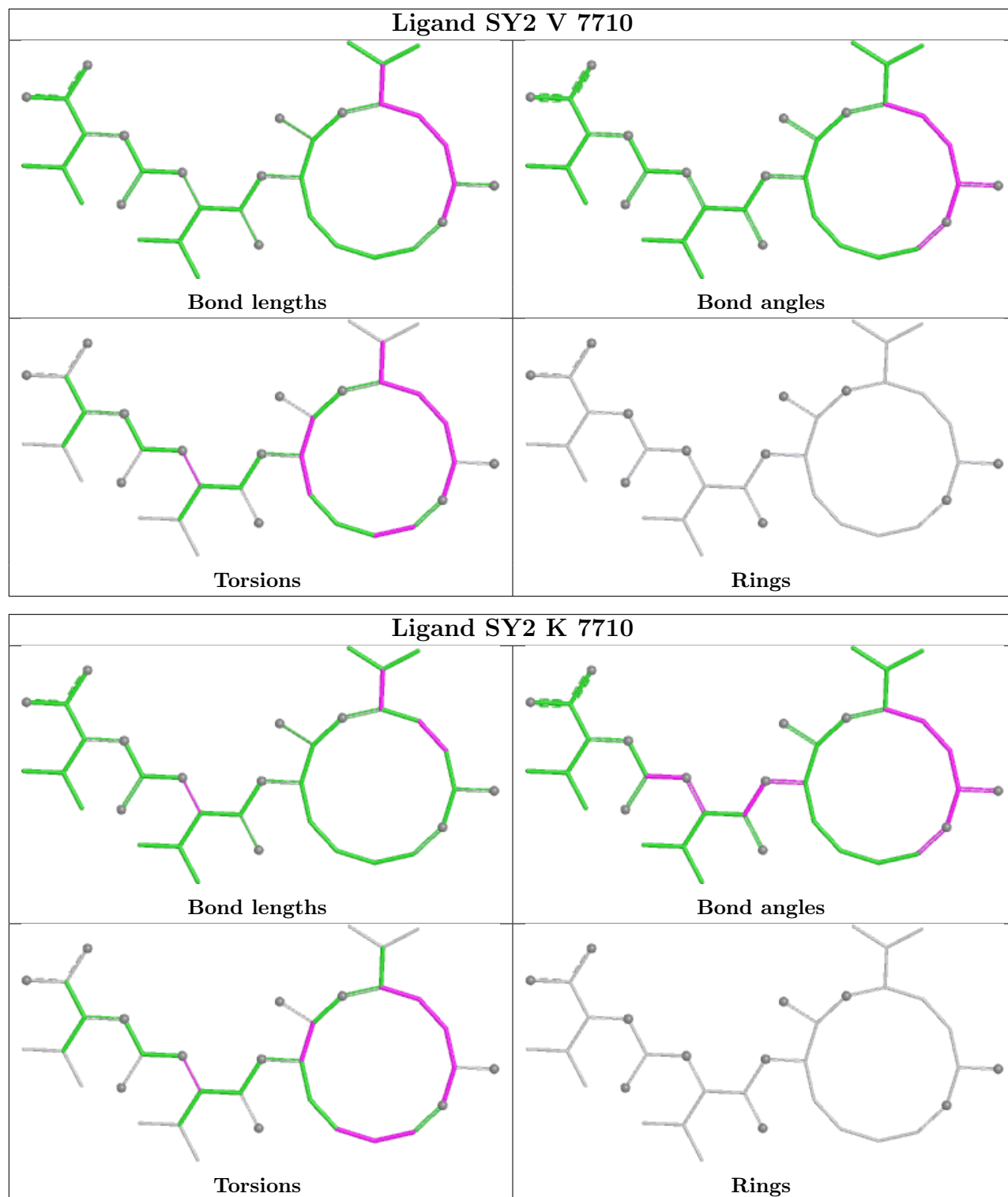
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	H	7710	SY2	2	0
15	V	7710	SY2	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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%)	-1.79	0 100 100	17, 35, 65, 90	0
1	O	250/250 (100%)	-1.78	0 100 100	16, 36, 66, 89	0
2	B	244/244 (100%)	-1.69	0 100 100	19, 40, 71, 96	0
2	P	244/244 (100%)	-1.67	1 (0%) 88 87	20, 40, 70, 96	0
3	C	241/241 (100%)	-1.63	0 100 100	24, 46, 90, 112	0
3	Q	241/241 (100%)	-1.56	0 100 100	25, 47, 90, 111	0
4	D	242/242 (100%)	-1.67	0 100 100	23, 43, 74, 105	0
4	R	242/242 (100%)	-1.66	1 (0%) 88 87	23, 44, 76, 105	0
5	E	233/233 (100%)	-1.73	0 100 100	23, 40, 66, 86	0
5	S	233/233 (100%)	-1.73	0 100 100	24, 40, 66, 86	0
6	F	244/244 (100%)	-1.80	0 100 100	16, 34, 69, 90	0
6	T	244/244 (100%)	-1.81	0 100 100	16, 34, 69, 90	0
7	G	243/243 (100%)	-1.80	0 100 100	15, 32, 59, 96	0
7	U	243/243 (100%)	-1.82	0 100 100	17, 32, 59, 96	0
8	H	222/222 (100%)	-1.84	0 100 100	14, 28, 46, 92	0
8	V	222/222 (100%)	-1.86	0 100 100	14, 28, 47, 92	0
9	I	204/204 (100%)	-1.85	0 100 100	16, 32, 48, 64	0
9	W	204/204 (100%)	-1.87	0 100 100	17, 31, 48, 63	0
10	J	198/198 (100%)	-1.79	1 (0%) 87 86	21, 35, 52, 108	0
10	X	198/198 (100%)	-1.80	0 100 100	21, 35, 52, 109	0
11	K	212/212 (100%)	-1.78	0 100 100	16, 35, 61, 71	0
11	Y	212/212 (100%)	-1.80	0 100 100	17, 36, 61, 70	0
12	L	222/222 (100%)	-1.79	0 100 100	19, 32, 56, 71	0
12	Z	222/222 (100%)	-1.85	0 100 100	21, 32, 56, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9	
13	1	233/233 (100%)	-1.89	0	100	100	14, 28, 42, 50	0
13	M	233/233 (100%)	-1.91	0	100	100	15, 28, 43, 50	0
14	2	196/196 (100%)	-1.90	0	100	100	18, 26, 47, 68	0
14	N	196/196 (100%)	-1.88	0	100	100	17, 26, 47, 68	0
All	All	6368/6368 (100%)	-1.78	3 (0%)	100	100	14, 35, 67, 112	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	217	ALA	2.4
4	R	12(E)	SER	2.3
10	J	192	ALA	2.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

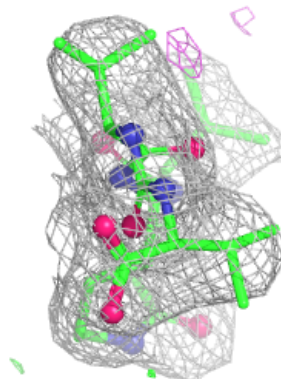
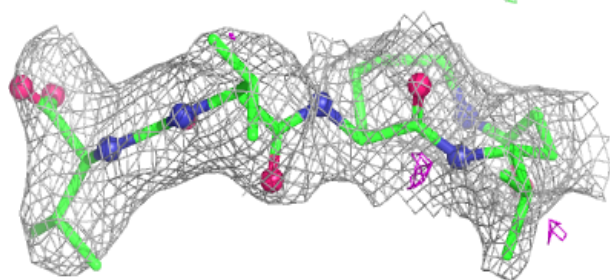
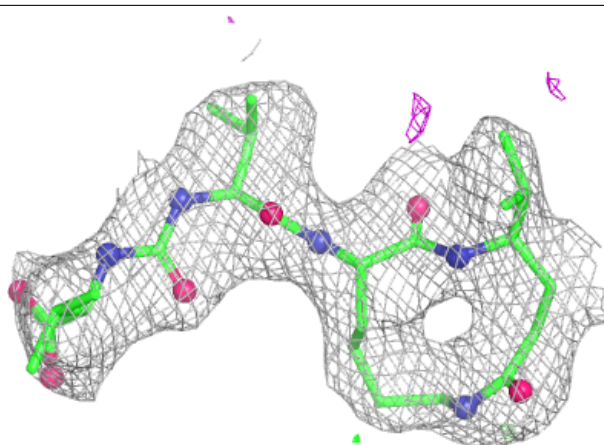
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SY2	H	7710	35/35	1.00	0.02	32,37,50,51	0
15	SY2	K	7710	35/35	1.00	0.02	23,33,51,54	0
15	SY2	V	7710	35/35	1.00	0.03	30,37,49,51	0
15	SY2	Y	7710	35/35	1.00	0.02	24,34,52,54	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

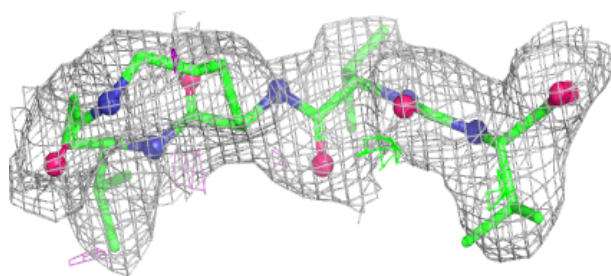
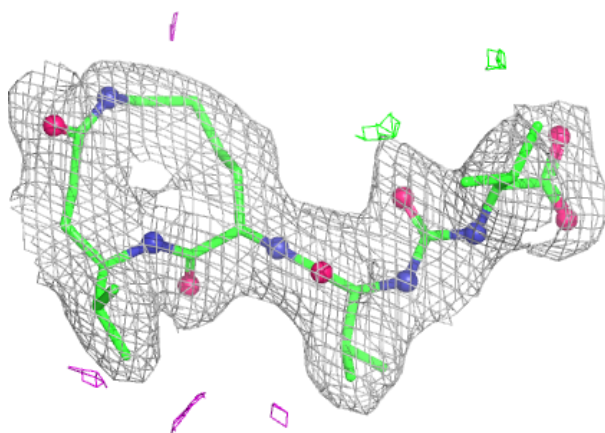
Electron density around SY2 H 7710:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

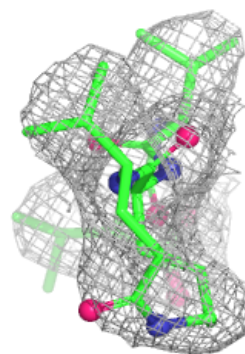
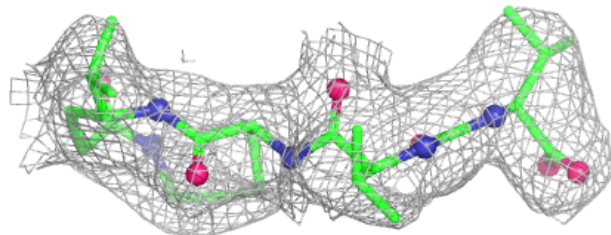
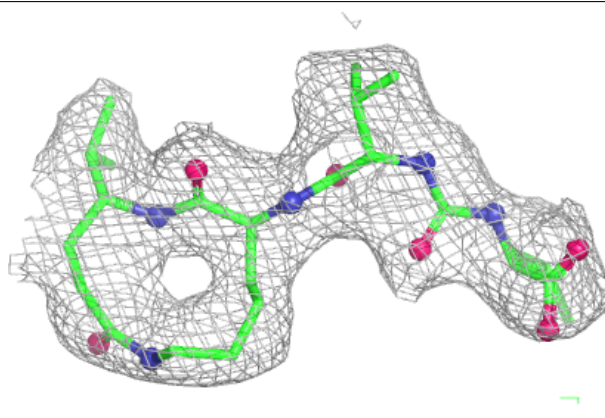


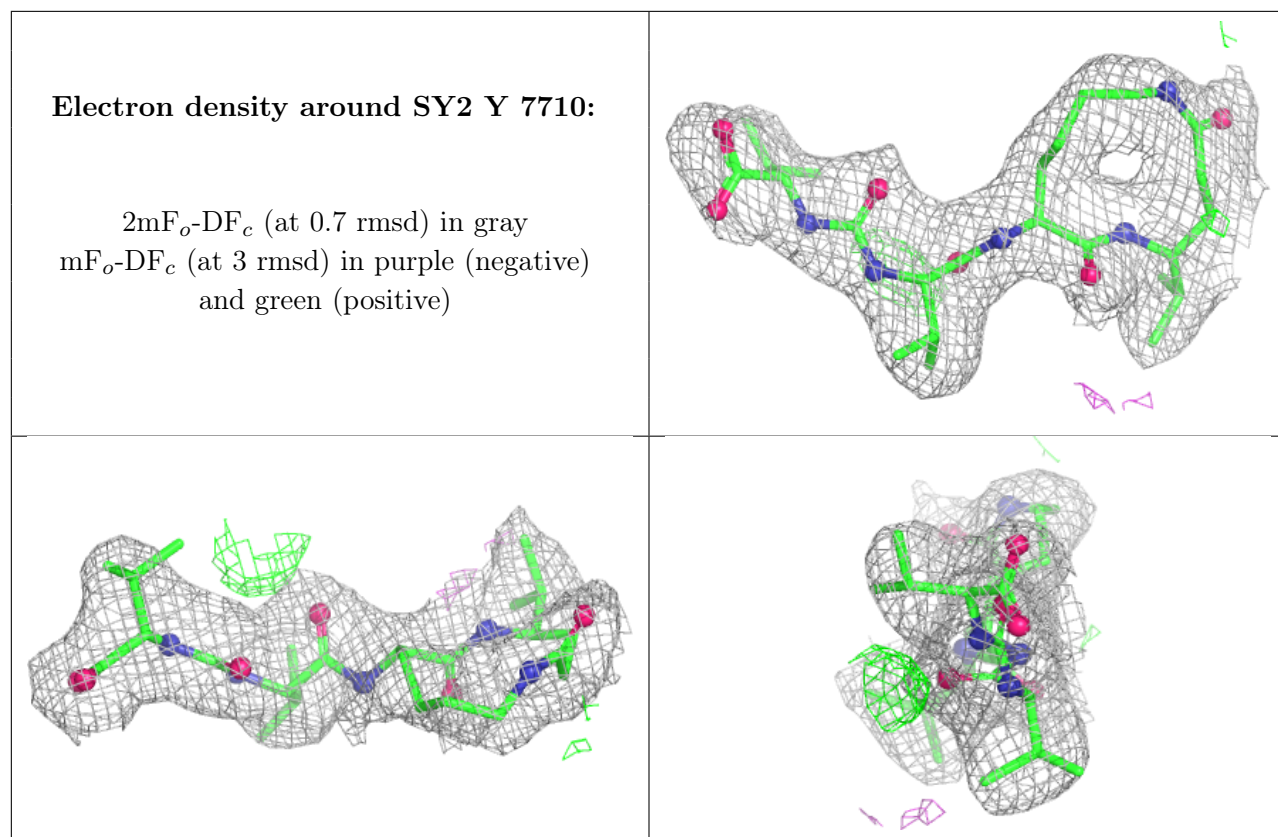
Electron density around SY2 K 7710:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around SY2 V 7710:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.