



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:21 PM UTC

PDB ID : 3E47 / pdb_00003e47
Title : Crystal Structure of the Yeast 20S Proteasome in Complex with Homobelactosin C
Authors : Groll, M.; Larionov, O.V.; de Meijere, A.
Deposited on : 2008-08-10
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

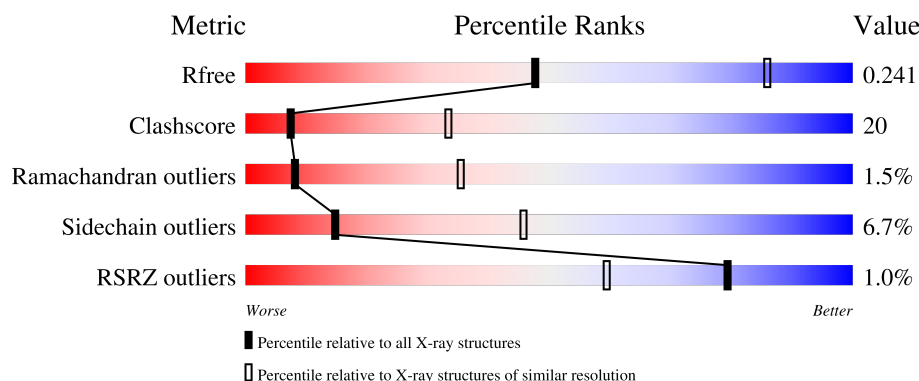
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



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

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

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

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Mol	Chain	Length	Quality of chain
3	Q	241	
4	D	242	
4	R	242	
5	E	233	
5	S	233	
6	F	244	
6	T	244	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	1	233	
13	M	233	
14	2	196	
14	N	196	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50490 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
			1643	1045	280	311	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1643	1045	280	311	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			

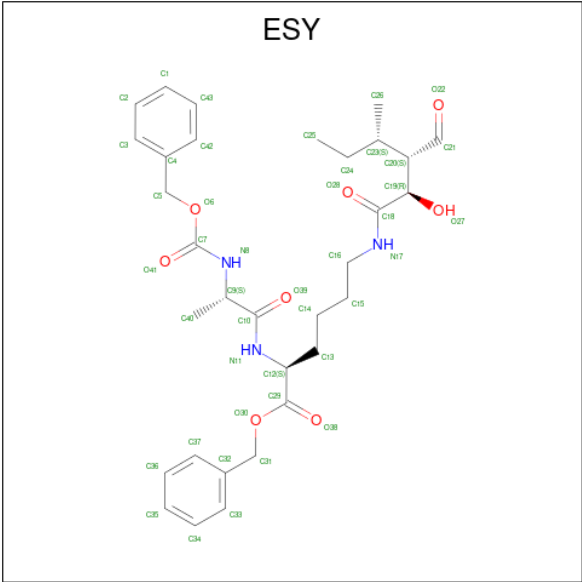
- Molecule 13 is a protein called Proteasome component PRE4.

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 benzyl N-[(benzyloxy)carbonyl]-L-alanyl-N 6 -[(2R,3S,4S)-3-formyl-2-hydroxy-4-methylhexanoyl]-L-lysinate (CCD ID: ESY) (formula: C₃₂H₄₃N₃O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	K	1	Total	C	N	O	0	0
			43	32	3	8		
15	Y	1	Total	C	N	O	0	0
			43	32	3	8		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	38	Total	O	0	0
			38	38		
16	B	31	Total	O	0	0
			31	31		
16	C	24	Total	O	0	0
			24	24		
16	D	25	Total	O	0	0
			25	25		
16	E	15	Total	O	0	0
			15	15		
16	F	27	Total	O	0	0
			27	27		
16	G	41	Total	O	0	0
			41	41		
16	H	28	Total	O	0	0
			28	28		
16	I	42	Total	O	0	0
			42	42		
16	J	32	Total	O	0	0
			32	32		

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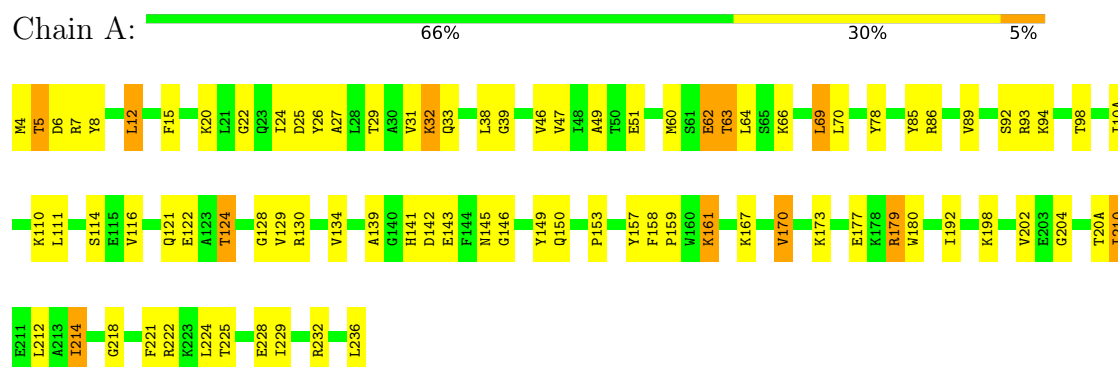
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	K	25	Total 25	O 25	0	0
16	L	35	Total 35	O 35	0	0
16	M	43	Total 43	O 43	0	0
16	N	38	Total 38	O 38	0	0
16	O	18	Total 18	O 18	0	0
16	P	20	Total 20	O 20	0	0
16	Q	17	Total 17	O 17	0	0
16	R	23	Total 23	O 23	0	0
16	S	16	Total 16	O 16	0	0
16	T	26	Total 26	O 26	0	0
16	U	38	Total 38	O 38	0	0
16	V	33	Total 33	O 33	0	0
16	W	39	Total 39	O 39	0	0
16	X	38	Total 38	O 38	0	0
16	Y	24	Total 24	O 24	0	0
16	Z	36	Total 36	O 36	0	0
16	1	45	Total 45	O 45	0	0
16	2	41	Total 41	O 41	0	0

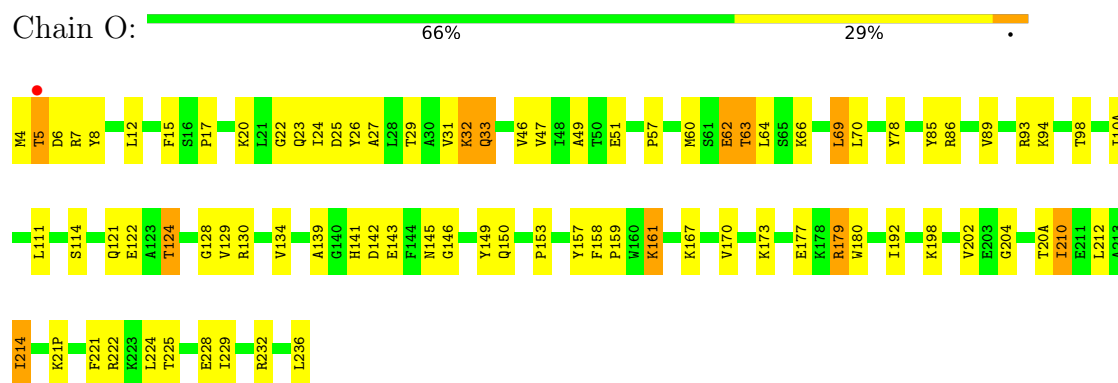
3 Residue-property plots [i](#)

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

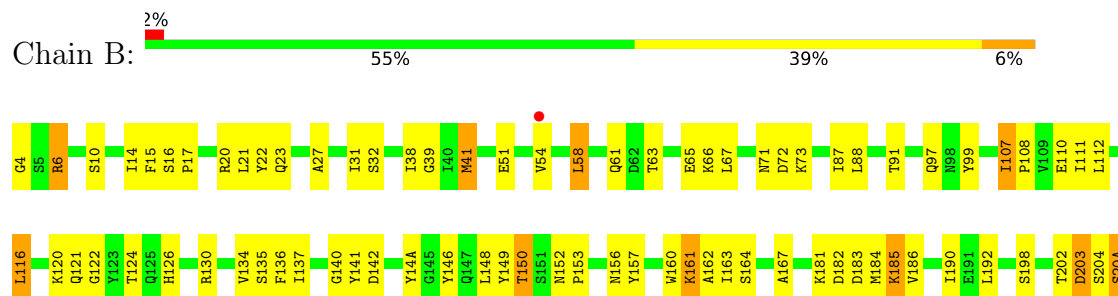
• Molecule 1: Proteasome component Y7



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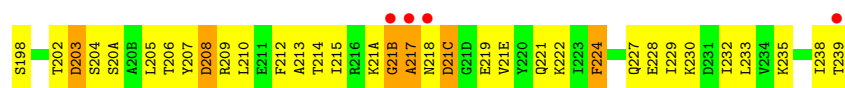
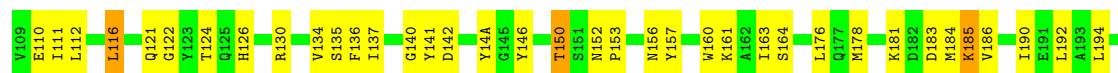


• Molecule 2: Proteasome component Y13





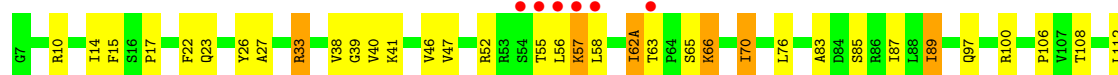
• Molecule 2: Proteasome component Y13



• Molecule 3: Proteasome component PRE6

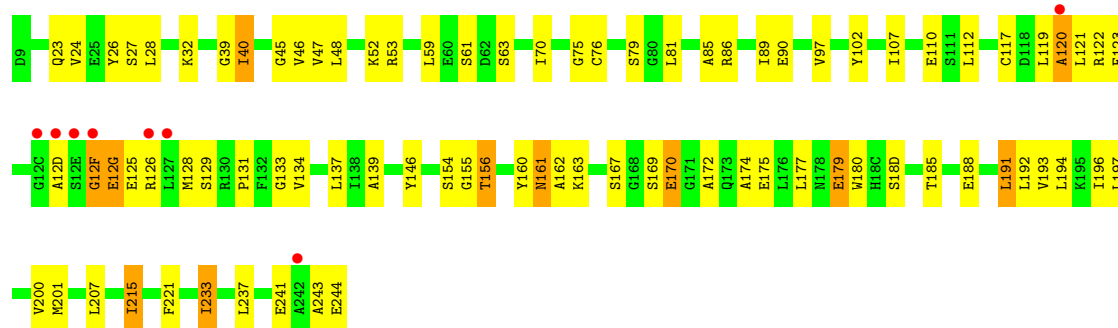


• Molecule 3: Proteasome component PRE6

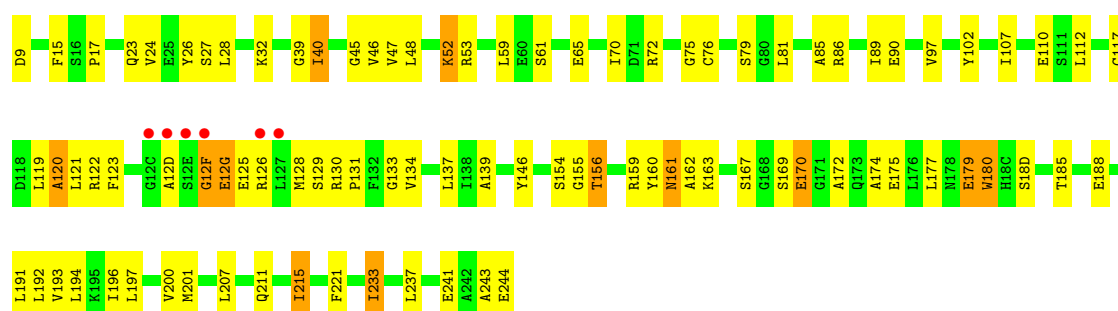


• Molecule 4: Proteasome component PUP2

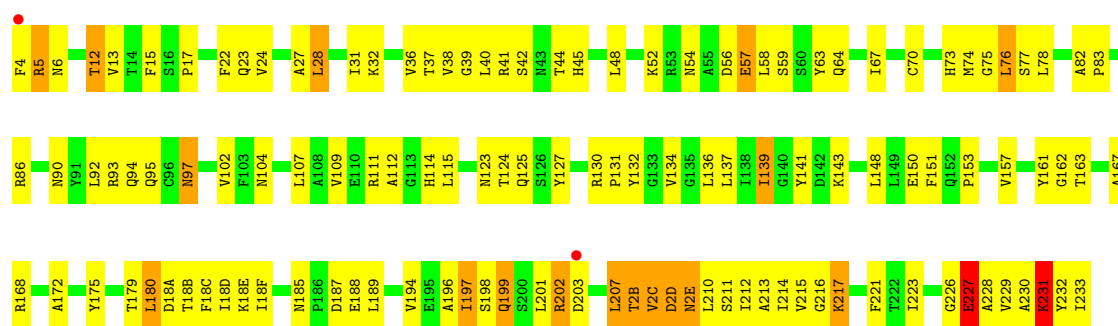




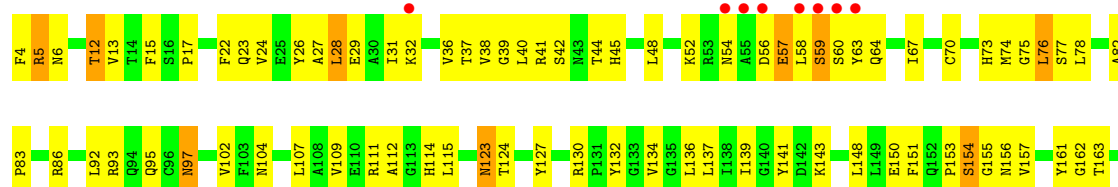
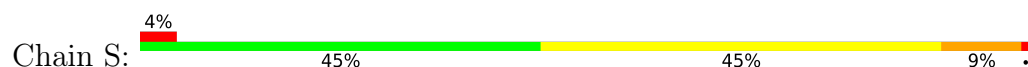
• Molecule 4: Proteasome component PUP2

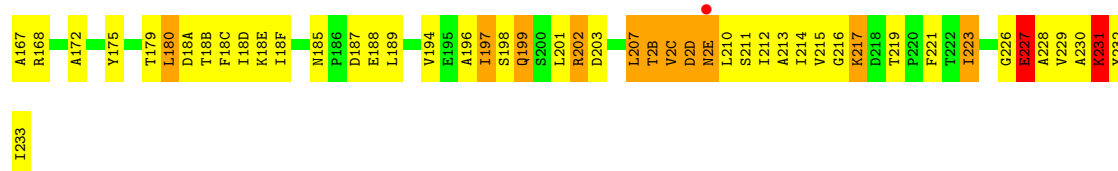


• Molecule 5: Proteasome component PRE5

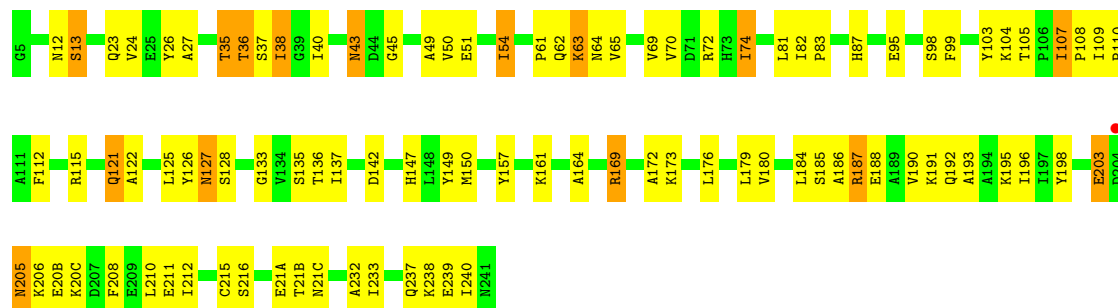


• Molecule 5: Proteasome component PRE5

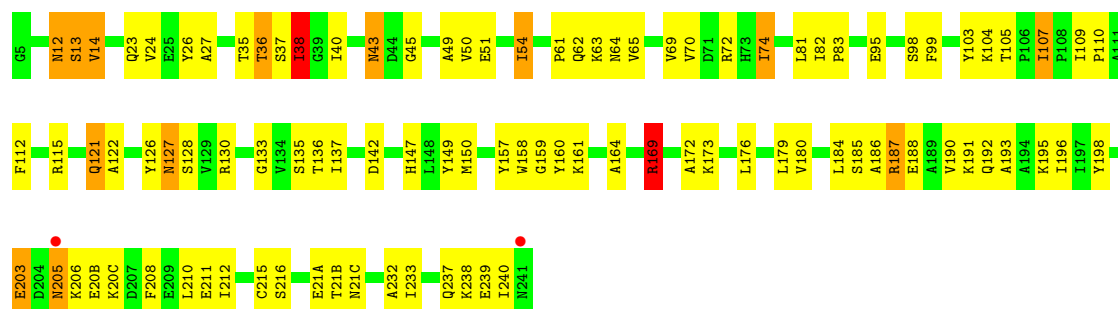




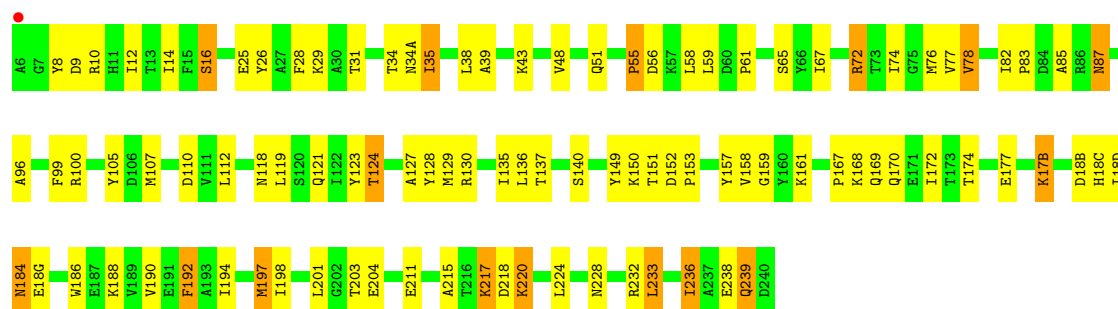
- Molecule 6: Proteasome component C1



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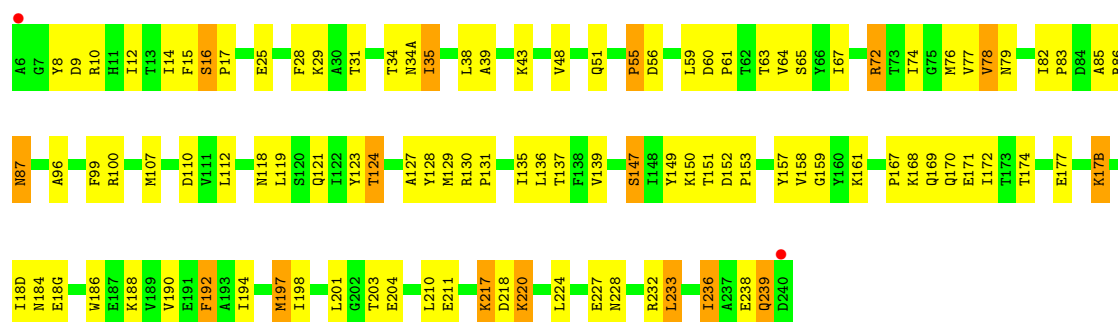


- Molecule 7: Proteasome component C7-alpha



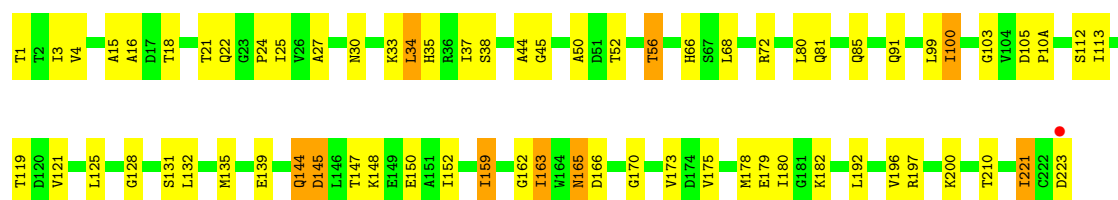
- Molecule 7: Proteasome component C7-alpha





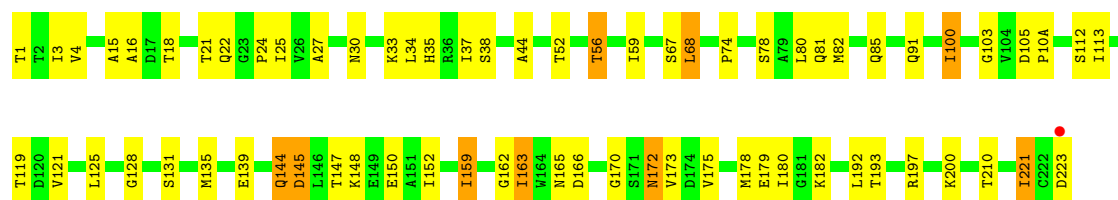
• Molecule 8: Proteasome component PUP1

Chain H: 69% 27%



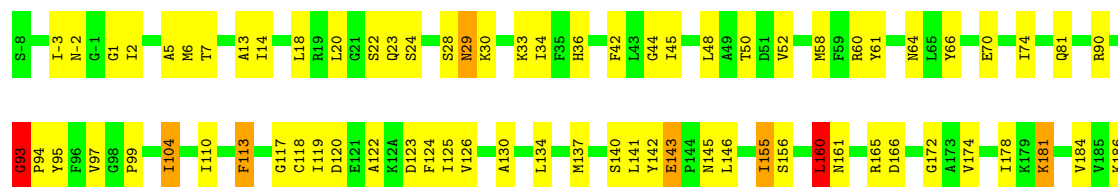
• Molecule 8: Proteasome component PUP1

Chain V: 69% 27%



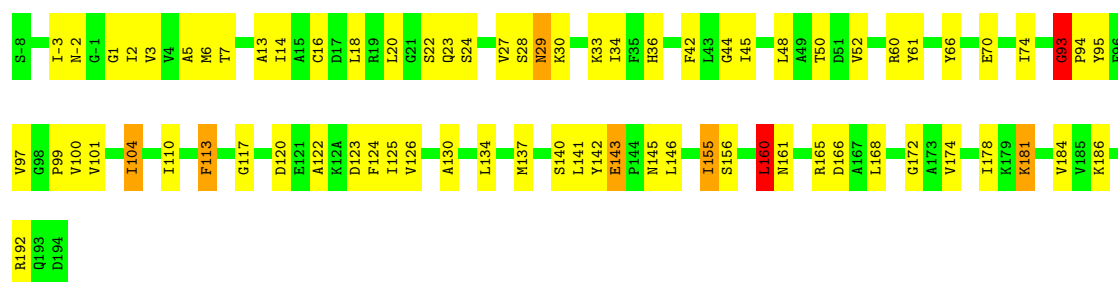
• Molecule 9: Proteasome component PUP3

Chain I: 64% 32%



• Molecule 9: Proteasome component PUP3

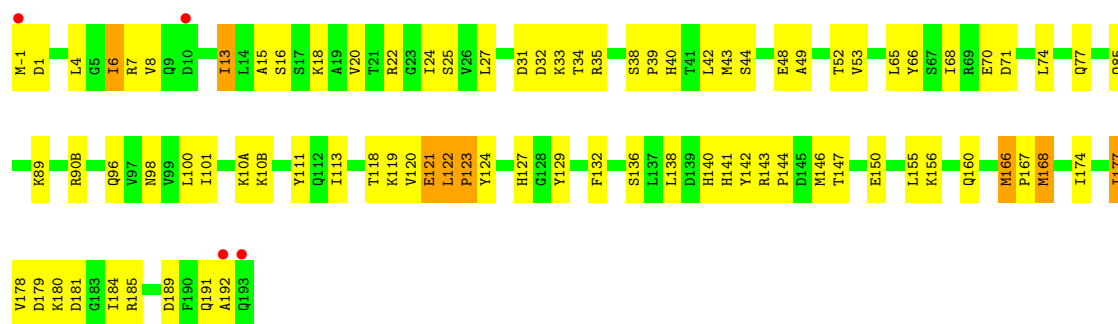
Chain W: 64% 32%



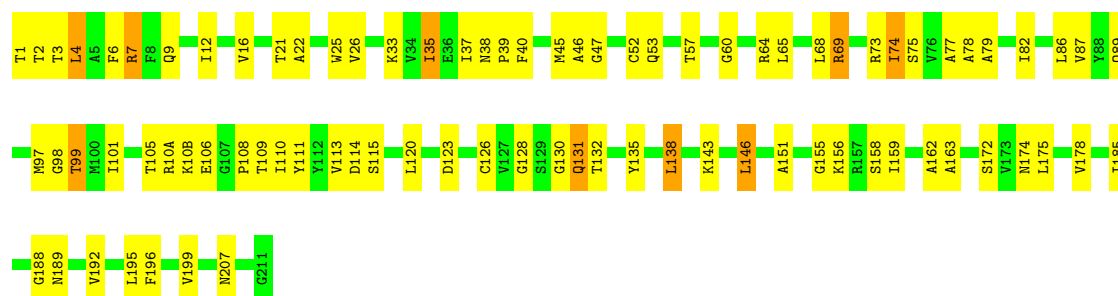
• Molecule 10: Proteasome component C11



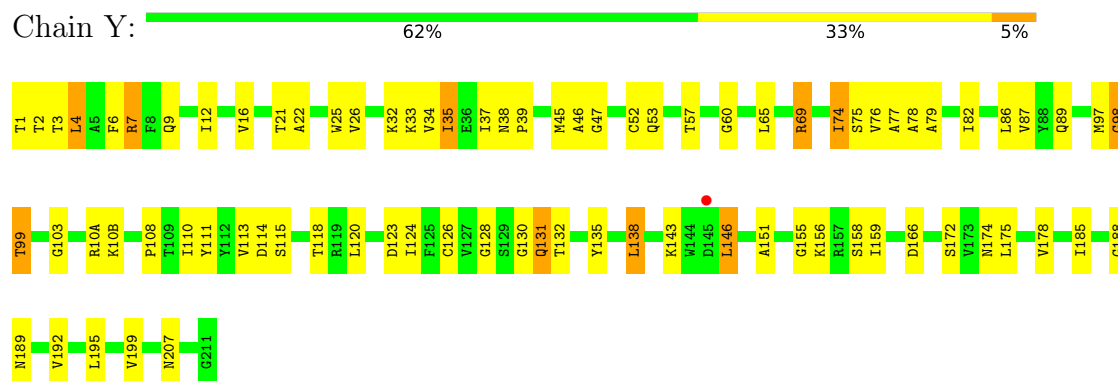
• Molecule 10: Proteasome component C11



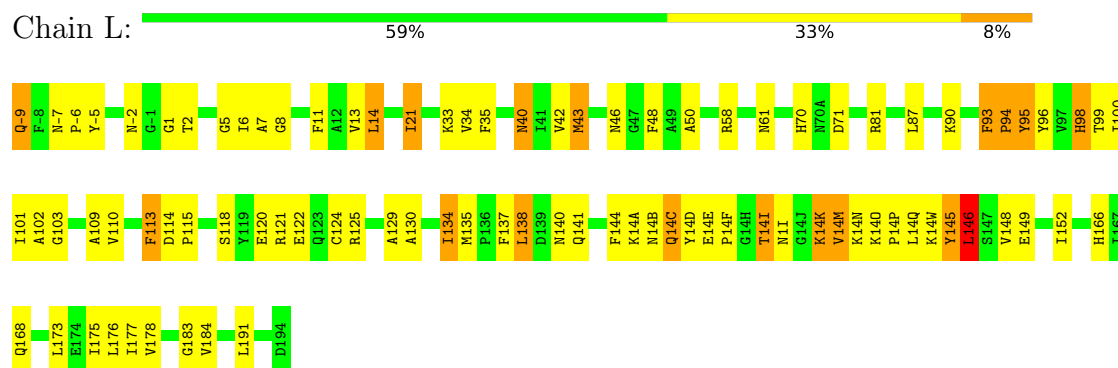
• Molecule 11: Proteasome component PRE2



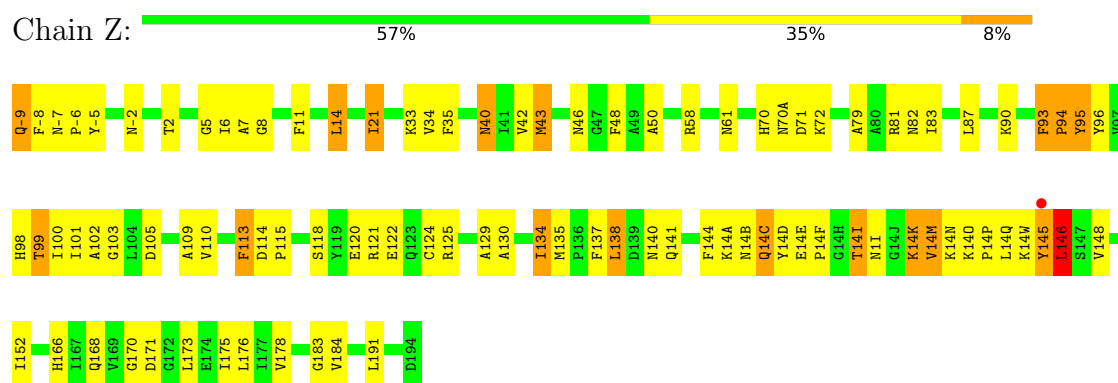
- Molecule 11: Proteasome component PRE2



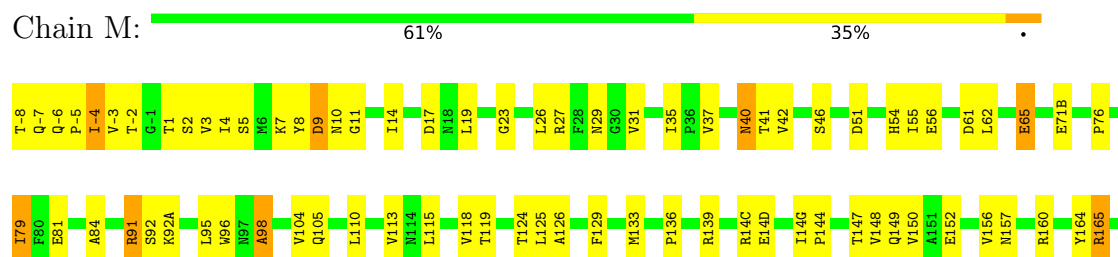
- Molecule 12: Proteasome component C5

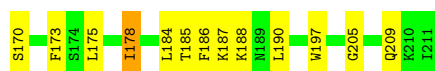


- Molecule 12: Proteasome component C5



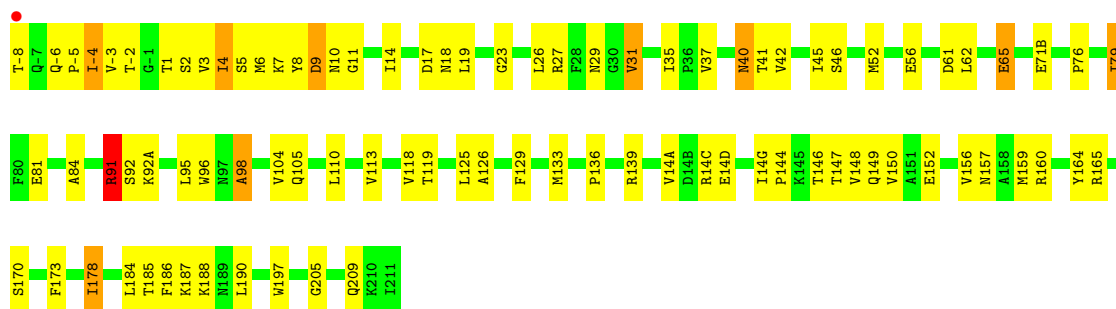
- Molecule 13: Proteasome component PRE4





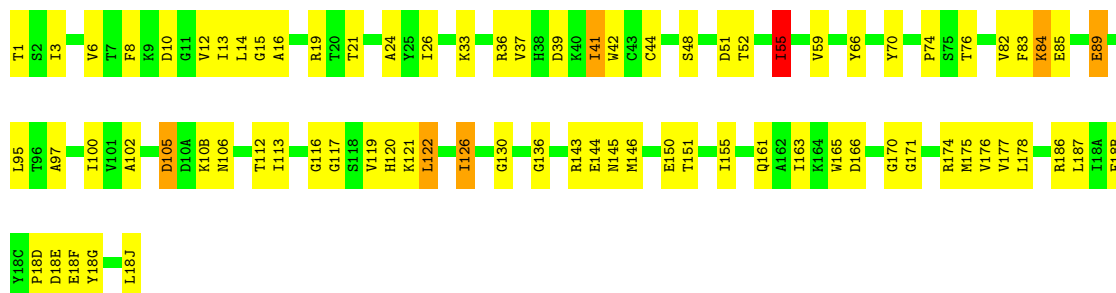
• Molecule 13: Proteasome component PRE4

Chain 1: 61% 34%



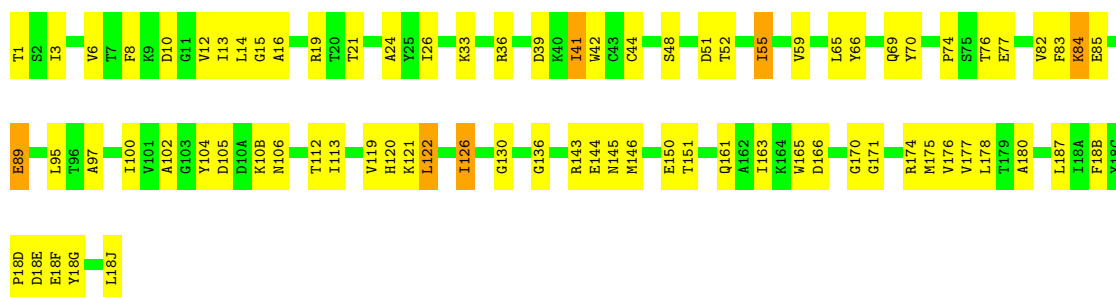
• Molecule 14: Proteasome component PRE3

Chain N: 60% 37%



• Molecule 14: Proteasome component PRE3

Chain 2: 60% 37%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.49Å 301.06Å 144.45Å 90.00° 112.78° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (15.00-3.00) 98.4 (15.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.245 0.217 , 0.241	Depositor DCC
R_{free} test set	10446 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.774	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	50490	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.50	0/1952	0.98	9/2642 (0.3%)
1	O	0.49	0/1952	0.98	6/2642 (0.2%)
2	B	0.48	0/1935	0.93	6/2618 (0.2%)
2	P	0.49	0/1935	0.93	5/2618 (0.2%)
3	C	0.45	0/1920	0.99	10/2598 (0.4%)
3	Q	0.43	0/1920	1.00	10/2598 (0.4%)
4	D	0.45	0/1887	0.94	7/2541 (0.3%)
4	R	0.45	0/1887	0.94	7/2541 (0.3%)
5	E	0.42	0/1823	0.92	3/2463 (0.1%)
5	S	0.43	0/1823	0.92	4/2463 (0.2%)
6	F	0.44	0/1937	0.95	6/2614 (0.2%)
6	T	0.46	0/1937	0.97	8/2614 (0.3%)
7	G	0.49	0/1959	0.99	7/2652 (0.3%)
7	U	0.51	0/1959	0.98	10/2652 (0.4%)
8	H	0.51	0/1716	1.00	7/2326 (0.3%)
8	V	0.50	0/1716	1.00	5/2326 (0.2%)
9	I	0.51	0/1611	1.02	11/2174 (0.5%)
9	W	0.52	0/1611	1.04	10/2174 (0.5%)
10	J	0.51	0/1613	0.99	5/2173 (0.2%)
10	X	0.50	0/1613	1.01	7/2173 (0.3%)
11	K	0.51	0/1680	0.95	4/2274 (0.2%)
11	Y	0.47	0/1680	0.95	5/2274 (0.2%)
12	L	0.48	0/1795	1.09	13/2420 (0.5%)
12	Z	0.47	0/1795	1.08	13/2420 (0.5%)
13	1	0.50	0/1855	0.99	9/2514 (0.4%)
13	M	0.50	0/1855	0.98	9/2514 (0.4%)
14	2	0.51	0/1541	0.97	1/2087 (0.0%)
14	N	0.53	0/1541	0.97	5/2087 (0.2%)
All	All	0.48	0/50448	0.98	202/68192 (0.3%)

There are no bond length outliers.

All (202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	LYS	N-CA-C	-10.25	100.90	113.41
1	O	161	LYS	N-CA-C	-10.14	101.04	113.41
13	M	27	ARG	N-CA-C	9.56	121.39	110.97
13	1	27	ARG	N-CA-C	9.35	121.16	110.97
12	L	93	PHE	CA-C-N	8.80	128.87	119.89
12	L	93	PHE	C-N-CA	8.80	128.87	119.89
12	Z	93	PHE	CA-C-N	8.57	128.63	119.89
12	Z	93	PHE	C-N-CA	8.57	128.63	119.89
4	D	70	ILE	N-CA-C	-8.37	103.66	111.45
10	X	166	MET	CA-C-N	8.28	129.08	119.47
10	X	166	MET	C-N-CA	8.28	129.08	119.47
10	J	166	MET	CA-C-N	8.21	129.00	119.47
10	J	166	MET	C-N-CA	8.21	129.00	119.47
11	K	188	GLY	N-CA-C	8.11	123.19	112.65
9	W	60	ARG	N-CA-C	-8.06	102.19	110.97
6	T	161	LYS	N-CA-C	-7.99	101.35	112.45
3	Q	66	LYS	N-CA-C	7.88	119.50	111.07
3	Q	108	THR	N-CA-C	-7.83	100.43	110.53
11	Y	188	GLY	N-CA-C	7.81	122.80	112.65
3	Q	70	ILE	N-CA-C	-7.77	103.34	111.58
12	L	95	TYR	N-CA-C	-7.75	96.67	108.67
4	R	70	ILE	N-CA-C	-7.71	104.28	111.45
6	F	161	LYS	N-CA-C	-7.68	101.77	112.45
2	B	161	LYS	N-CA-C	-7.63	104.10	113.41
4	R	161	ASN	N-CA-C	-7.59	103.82	113.23
13	M	-2	THR	N-CA-C	7.58	121.27	109.52
4	D	161	ASN	N-CA-C	-7.53	103.89	113.23
3	Q	161	SER	N-CA-C	-7.44	103.16	112.90
13	1	-2	THR	N-CA-C	7.39	120.98	109.52
7	G	127	ALA	N-CA-C	7.37	120.37	111.82
3	C	108	THR	N-CA-C	-7.31	101.10	110.53
7	U	16	SER	N-CA-C	-7.30	100.58	110.36
3	C	66	LYS	N-CA-C	7.29	119.22	111.28
7	U	127	ALA	N-CA-C	7.27	120.26	111.82
13	1	95	LEU	N-CA-C	-7.23	95.83	108.20
1	A	143	GLU	N-CA-C	7.19	119.12	111.28
3	C	70	ILE	N-CA-C	-7.18	103.97	111.58
3	C	161	SER	N-CA-C	-7.04	103.36	112.23
9	I	60	ARG	N-CA-C	-7.04	103.30	110.97
13	M	95	LEU	N-CA-C	-7.03	96.18	108.20
1	A	66	LYS	N-CA-C	-7.01	104.60	113.72
3	C	62(A)	ILE	N-CA-C	7.00	117.61	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	62(A)	ILE	N-CA-C	6.98	117.59	110.82
1	O	143	GLU	N-CA-C	6.94	118.85	111.28
7	G	161	LYS	N-CA-C	-6.94	103.49	112.23
9	I	143	GLU	CA-C-N	6.88	126.86	119.78
9	I	143	GLU	C-N-CA	6.88	126.86	119.78
7	G	16	SER	N-CA-C	-6.84	101.19	110.36
11	Y	57	THR	N-CA-C	-6.82	103.93	111.36
12	Z	95	TYR	N-CA-C	-6.82	98.10	108.67
1	O	66	LYS	N-CA-C	-6.79	104.89	113.72
1	O	128	GLY	N-CA-C	6.70	123.25	113.48
9	W	143	GLU	CA-C-N	6.69	126.67	119.78
9	W	143	GLU	C-N-CA	6.69	126.67	119.78
3	C	186	VAL	N-CA-C	-6.63	103.85	110.62
2	P	161	LYS	N-CA-C	-6.60	104.26	112.90
7	U	161	LYS	N-CA-C	-6.59	103.92	112.23
4	D	169	SER	N-CA-C	6.56	118.12	110.97
8	H	180	ILE	N-CA-C	6.54	118.08	110.62
4	D	179	GLU	N-CA-C	6.48	119.16	111.71
4	R	169	SER	N-CA-C	6.46	118.02	110.97
4	R	179	GLU	N-CA-C	6.46	119.14	111.71
9	W	93	GLY	CA-C-N	6.33	127.20	120.11
9	W	93	GLY	C-N-CA	6.33	127.20	120.11
10	X	122	LEU	CA-C-N	6.33	125.75	118.85
10	X	122	LEU	C-N-CA	6.33	125.75	118.85
3	Q	186	VAL	N-CA-C	-6.32	104.17	110.62
13	M	98	ALA	N-CA-C	-6.31	97.99	108.34
12	Z	115	PRO	N-CA-C	-6.29	106.00	113.86
13	1	98	ALA	N-CA-C	-6.25	98.10	108.34
9	I	93	GLY	CA-C-N	6.23	127.09	120.11
9	I	93	GLY	C-N-CA	6.23	127.09	120.11
8	V	180	ILE	N-CA-C	6.19	117.68	110.62
1	A	128	GLY	N-CA-C	6.08	122.36	113.48
9	I	142	TYR	N-CA-C	6.07	119.46	110.48
4	R	61	SER	N-CA-C	6.04	119.47	111.75
2	B	137	ILE	N-CA-C	-6.00	98.99	107.75
12	L	115	PRO	N-CA-C	-5.98	105.86	114.18
11	K	57	THR	N-CA-C	-5.98	104.85	111.36
13	M	31	VAL	N-CA-C	5.97	116.40	107.51
6	T	135	SER	N-CA-C	-5.96	100.47	109.95
2	B	203	ASP	N-CA-C	-5.93	104.57	112.94
9	W	142	TYR	N-CA-C	5.92	119.24	110.48
13	1	31	VAL	N-CA-C	5.92	116.33	107.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Z	146	LEU	N-CA-C	5.91	118.83	110.50
12	L	146	LEU	N-CA-C	5.86	118.76	110.50
8	H	100	ILE	N-CA-C	-5.84	98.00	107.28
1	O	78	TYR	N-CA-C	5.84	116.80	108.74
8	V	21	THR	N-CA-C	5.83	118.97	109.06
10	X	123	PRO	N-CA-C	-5.83	105.59	113.40
11	K	131	GLN	N-CA-C	5.82	118.10	111.11
13	1	9	ASP	N-CA-C	5.82	119.19	111.75
1	A	10(A)	ILE	CB-CA-C	-5.80	105.89	111.05
13	M	9	ASP	N-CA-C	5.80	119.17	111.75
8	V	100	ILE	N-CA-C	-5.79	98.07	107.28
5	E	102	VAL	N-CA-C	5.78	116.56	110.72
2	P	203	ASP	N-CA-C	-5.76	104.82	112.94
2	P	137	ILE	N-CA-C	-5.76	99.35	107.75
4	D	61	SER	N-CA-C	5.74	119.10	111.75
1	A	78	TYR	N-CA-C	5.69	116.88	108.86
9	I	117	GLY	N-CA-C	5.69	122.31	114.92
8	H	37	ILE	N-CA-C	-5.68	106.28	111.67
9	W	95	TYR	N-CA-C	-5.65	100.08	109.46
12	Z	35	PHE	N-CA-C	5.63	118.73	109.72
8	H	21	THR	N-CA-C	5.62	118.62	109.06
9	W	117	GLY	N-CA-C	5.62	122.23	114.92
6	F	135	SER	N-CA-C	-5.61	100.26	109.40
12	L	35	PHE	N-CA-C	5.60	118.68	109.72
2	B	134	VAL	N-CA-C	5.59	115.72	108.35
3	Q	22	PHE	N-CA-C	5.58	118.89	111.75
5	S	161	TYR	N-CA-C	-5.52	105.28	112.23
3	Q	27	ALA	N-CA-C	-5.51	105.28	111.28
13	1	92(A)	LYS	N-CA-C	-5.50	105.88	112.59
12	Z	184	VAL	N-CA-C	5.50	115.51	107.37
12	Z	70	HIS	N-CA-C	5.49	117.47	110.61
3	C	135	SER	N-CA-C	-5.48	100.74	109.23
5	E	161	TYR	N-CA-C	-5.48	105.33	112.23
2	P	134	VAL	N-CA-C	5.47	115.57	108.35
6	T	107	ILE	CA-C-N	5.47	125.39	119.76
6	T	107	ILE	C-N-CA	5.47	125.39	119.76
7	U	220	LYS	N-CA-C	5.45	116.69	108.46
14	N	117	GLY	N-CA-C	-5.44	107.28	114.95
3	C	22	PHE	N-CA-C	5.43	118.70	111.75
12	L	70	HIS	N-CA-C	5.42	117.39	110.61
3	Q	135	SER	N-CA-C	-5.42	100.83	109.23
1	O	10(A)	ILE	CB-CA-C	-5.41	106.24	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	131	GLN	N-CA-C	5.41	117.62	111.02
8	H	165	ASN	N-CA-C	5.35	119.52	112.89
4	R	129	SER	N-CA-C	5.33	117.84	111.71
12	Z	145	TYR	N-CA-C	5.33	118.17	109.59
5	S	223	ILE	N-CA-C	5.32	115.97	108.36
7	G	17(B)	LYS	N-CA-C	-5.32	105.65	111.82
5	S	102	VAL	N-CA-C	5.32	116.09	110.72
12	L	145	TYR	N-CA-C	5.31	118.15	109.59
13	M	23	GLY	N-CA-C	-5.31	104.97	111.35
4	R	180	TRP	N-CA-C	5.31	118.21	109.76
14	2	122	LEU	N-CA-C	5.31	114.41	108.25
14	N	122	LEU	N-CA-C	5.31	114.41	108.25
12	Z	122	GLU	N-CA-C	5.31	117.25	109.24
2	B	16	SER	N-CA-C	-5.30	103.25	110.36
7	G	78	VAL	N-CA-C	5.29	115.52	108.11
6	T	14	VAL	N-CA-C	5.29	116.20	108.58
12	L	184	VAL	N-CA-C	5.28	115.45	107.80
7	U	17(B)	LYS	N-CA-C	-5.28	105.70	111.82
13	1	91	ARG	N-CA-C	-5.28	105.70	111.82
2	B	210	LEU	N-CA-C	5.27	117.20	109.24
6	F	107	ILE	CA-C-N	5.27	125.18	119.76
6	F	107	ILE	C-N-CA	5.27	125.18	119.76
12	Z	113	PHE	N-CA-C	5.27	118.15	109.72
4	D	129	SER	N-CA-C	5.26	117.76	111.71
13	M	92(A)	LYS	N-CA-C	-5.26	106.17	112.59
13	1	23	GLY	N-CA-C	-5.26	105.04	111.35
2	P	210	LEU	N-CA-C	5.25	117.16	109.24
9	W	145	ASN	N-CA-C	5.24	118.67	111.54
8	V	37	ILE	N-CA-C	-5.24	106.70	111.67
5	E	223	ILE	N-CA-C	5.23	115.84	108.36
9	I	145	ASN	N-CA-C	5.23	118.66	111.54
6	T	38	ILE	N-CA-C	5.23	114.91	108.53
7	G	220	LYS	N-CA-C	5.22	116.34	108.46
10	J	147	THR	N-CA-C	-5.22	103.80	110.53
6	F	240	ILE	N-CA-C	-5.21	105.94	113.07
3	C	27	ALA	N-CA-C	-5.18	105.53	111.07
4	D	63	SER	N-CA-C	-5.17	107.14	112.93
7	U	43	LYS	N-CA-C	-5.17	105.71	112.23
12	L	122	GLU	N-CA-C	5.17	117.04	109.24
10	X	168	MET	N-CA-C	5.15	118.14	109.95
3	C	169	SER	N-CA-C	-5.15	105.79	111.71
12	Z	21	ILE	N-CA-C	5.14	116.30	108.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Z	94	PRO	N-CA-C	5.14	119.28	111.11
1	A	218	GLY	CA-C-N	5.13	125.03	119.85
1	A	218	GLY	C-N-CA	5.13	125.03	119.85
12	L	21	ILE	N-CA-C	5.12	116.28	108.80
9	W	160	LEU	N-CA-C	5.12	117.25	111.11
7	G	43	LYS	N-CA-C	-5.12	105.78	112.23
9	I	119	ILE	N-CA-C	5.12	115.95	108.58
12	L	113	PHE	N-CA-C	5.11	117.90	109.72
12	L	94	PRO	N-CA-C	5.11	119.24	111.11
6	T	240	ILE	N-CA-C	-5.11	106.08	113.07
3	Q	238	GLN	N-CA-C	-5.10	107.18	113.41
5	S	154	SER	N-CA-C	-5.10	106.89	113.01
10	J	168	MET	N-CA-C	5.08	118.03	109.95
11	K	99	THR	N-CA-C	5.08	117.10	109.23
9	I	160	LEU	N-CA-C	5.07	117.20	111.11
7	U	78	VAL	N-CA-C	5.07	115.20	108.11
8	H	99	LEU	N-CA-C	5.06	117.85	109.85
7	U	147	SER	N-CA-C	5.05	117.65	109.06
8	H	45	GLY	N-CA-C	5.05	119.98	111.04
11	Y	99	THR	N-CA-C	5.04	117.05	109.23
7	U	60	ASP	CA-C-N	5.04	126.14	119.84
7	U	60	ASP	C-N-CA	5.04	126.14	119.84
13	M	165	ARG	N-CA-C	5.04	120.27	113.72
10	X	89	LYS	N-CA-C	-5.04	105.44	111.03
6	T	169	ARG	N-CA-C	5.04	117.42	111.33
14	N	105	ASP	N-CA-C	-5.03	102.34	110.14
9	I	95	TYR	N-CA-C	-5.03	101.11	109.46
6	F	63	LYS	N-CA-C	5.03	118.83	111.04
8	V	172	ASN	N-CA-C	5.02	117.52	110.14
14	N	55	ILE	CB-CA-C	-5.02	105.55	111.97
14	N	37	VAL	N-CA-C	-5.02	107.96	113.43
1	A	12	LEU	N-CA-C	-5.01	106.58	113.30
11	Y	98	GLY	N-CA-C	-5.01	101.30	113.18
10	J	141	HIS	N-CA-C	5.00	119.25	113.20

There are no chirality outliers.

There are no planarity outliers.

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	64	0
1	O	1915	0	1926	70	0
2	B	1905	0	1901	94	0
2	P	1905	0	1901	96	0
3	C	1891	0	1900	104	0
3	Q	1891	0	1900	101	0
4	D	1862	0	1836	66	0
4	R	1862	0	1836	81	0
5	E	1795	0	1797	122	0
5	S	1795	0	1797	129	0
6	F	1897	0	1886	85	0
6	T	1897	0	1886	91	0
7	G	1921	0	1910	92	0
7	U	1921	0	1910	99	0
8	H	1685	0	1688	46	0
8	V	1685	0	1688	45	0
9	I	1581	0	1574	61	0
9	W	1581	0	1574	61	0
10	J	1585	0	1590	71	0
10	X	1585	0	1590	78	0
11	K	1643	0	1594	71	0
11	Y	1643	0	1594	72	0
12	L	1757	0	1711	69	0
12	Z	1757	0	1711	71	0
13	1	1824	0	1832	73	0
13	M	1824	0	1832	69	0
14	2	1512	0	1481	65	0
14	N	1512	0	1481	62	0
15	K	43	0	42	5	0
15	Y	43	0	42	5	0
16	1	45	0	0	7	0
16	2	41	0	0	2	0
16	A	38	0	0	2	0
16	B	31	0	0	4	0
16	C	24	0	0	2	0
16	D	25	0	0	0	0
16	E	15	0	0	3	0
16	F	27	0	0	1	0
16	G	41	0	0	1	0
16	H	28	0	0	3	0
16	I	42	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	J	32	0	0	0	0
16	K	25	0	0	3	0
16	L	35	0	0	4	0
16	M	43	0	0	4	0
16	N	38	0	0	2	0
16	O	18	0	0	3	0
16	P	20	0	0	1	0
16	Q	17	0	0	2	0
16	R	23	0	0	3	0
16	S	16	0	0	1	0
16	T	26	0	0	2	0
16	U	38	0	0	4	0
16	V	33	0	0	2	0
16	W	39	0	0	2	0
16	X	38	0	0	3	0
16	Y	24	0	0	2	0
16	Z	36	0	0	3	0
All	All	50490	0	49336	2017	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 20.

All (2017) 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)
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.07	1.11
11:Y:10(B):LYS:H	11:Y:10(B):LYS:HD2	1.07	1.11
2:P:202:THR:HG22	2:P:204:SER:H	1.16	1.05
2:B:202:THR:HG22	2:B:204:SER:H	1.16	1.03
3:C:185:THR:HB	3:C:188:GLU:HG2	1.42	1.01
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.59	1.00
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.41	1.00
3:C:163:GLN:NE2	3:C:164:THR:H	1.60	0.99
7:G:96:ALA:HA	7:G:107:MET:HE2	1.44	0.99
2:B:15:PHE:H	3:C:23:GLN:HE22	0.99	0.99
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.28	0.98
3:C:163:GLN:HE21	3:C:164:THR:N	1.62	0.98
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.62	0.98
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.27	0.97
7:U:96:ALA:HA	7:U:107:MET:HE2	1.43	0.97
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.51	0.92
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.52	0.90
11:Y:35:ILE:HD11	11:Y:45:MET:HE3	1.56	0.88
2:B:71:ASN:ND2	2:B:72:ASP:H	1.71	0.87
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.57	0.87
11:Y:35:ILE:HD11	11:Y:45:MET:CE	2.04	0.86
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:N	1.90	0.86
2:P:71:ASN:ND2	2:P:72:ASP:H	1.74	0.85
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.42	0.85
11:K:10(B):LYS:HD2	11:K:10(B):LYS:N	1.90	0.85
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.40	0.85
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.08	0.84
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	1.91	0.84
11:K:35:ILE:HD11	11:K:45:MET:CE	2.08	0.84
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.60	0.83
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.58	0.83
6:T:35:THR:HG21	6:T:51:GLU:O	1.80	0.82
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.25	0.82
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.09	0.82
6:F:35:THR:HG21	6:F:51:GLU:O	1.78	0.81
11:K:35:ILE:HD11	11:K:45:MET:HE3	1.63	0.81
2:B:124:THR:CG2	3:C:130:ARG:HH21	1.94	0.81
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.79	0.81
3:C:185:THR:HG22	3:C:187:GLU:H	1.44	0.81
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.63	0.80
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.44	0.80
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.63	0.80
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.29	0.80
3:C:15:PHE:H	4:D:23:GLN:HE22	1.29	0.80
7:G:67:ILE:HG13	7:G:211:GLU:HG2	1.64	0.80
14:N:136:GLY:HA2	14:2:161:GLN:NE2	1.97	0.79
11:K:21:THR:HG22	11:K:26:VAL:HA	1.65	0.79
2:B:20:ARG:NE	3:C:33:ARG:HH21	1.81	0.79
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.62	0.79
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.64	0.79
11:Y:21:THR:HG22	11:Y:26:VAL:HA	1.66	0.78
5:S:2(C):VAL:HG13	5:S:2(D):ASP:H	1.49	0.78
7:U:121:GLN:O	7:U:124:THR:HB	1.83	0.78
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.65	0.78
14:N:161:GLN:NE2	14:2:136:GLY:HA2	1.98	0.78
5:S:52:LYS:HB3	5:S:63:TYR:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:2(C):VAL:HG13	5:E:2(D):ASP:H	1.48	0.78
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.66	0.78
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.31	0.78
7:U:67:ILE:HG13	7:U:211:GLU:HG2	1.64	0.78
5:E:48:LEU:HG	5:E:139:ILE:HD13	1.67	0.77
5:E:198:SER:HA	5:E:201:LEU:HG	1.66	0.77
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.65	0.77
2:P:160:TRP:CE2	2:P:163:ILE:HD12	2.20	0.77
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.82	0.76
13:1:76:PRO:HD2	13:1:105:GLN:OE1	1.85	0.76
14:2:48:SER:HB3	14:2:51:ASP:HB2	1.66	0.76
5:S:198:SER:HA	5:S:201:LEU:HG	1.66	0.76
13:1:152:GLU:O	13:1:156:VAL:HG23	1.86	0.76
3:Q:159:SER:HB2	16:Q:256:HOH:O	1.86	0.76
3:Q:33:ARG:HB2	3:Q:33:ARG:HH11	1.50	0.75
9:W:137:MET:HE3	9:W:141:LEU:HD11	1.67	0.75
2:B:181:LYS:O	2:B:184:MET:HG3	1.87	0.75
8:H:128:GLY:O	8:H:131:SER:HB2	1.87	0.75
3:C:33:ARG:HB2	3:C:33:ARG:HH11	1.50	0.75
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.67	0.75
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.52	0.75
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.50	0.75
7:G:121:GLN:O	7:G:124:THR:HB	1.86	0.75
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.49	0.75
13:M:152:GLU:O	13:M:156:VAL:HG23	1.87	0.75
7:U:59:LEU:O	7:U:61:PRO:HD3	1.87	0.75
10:X:143:ARG:O	10:X:146:MET:HG3	1.86	0.75
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.53	0.74
2:B:202:THR:HG22	2:B:204:SER:N	1.99	0.74
2:P:202:THR:HG22	2:P:204:SER:N	1.99	0.74
8:V:128:GLY:O	8:V:131:SER:HB2	1.87	0.74
13:1:37:VAL:HG11	13:1:79:ILE:HD13	1.69	0.74
1:O:121:GLN:O	1:O:124:THR:HB	1.87	0.74
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.36	0.74
5:E:52:LYS:HB3	5:E:63:TYR:O	1.88	0.74
10:J:143:ARG:O	10:J:146:MET:HG3	1.88	0.74
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.34	0.74
7:U:96:ALA:CA	7:U:107:MET:HE2	2.17	0.73
2:B:160:TRP:CE2	2:B:163:ILE:HD12	2.22	0.73
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.35	0.73
6:T:40:ILE:HD12	6:T:193:ALA:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:132:TYR:O	5:S:153:PRO:HB3	1.88	0.73
9:W:192:ARG:HG3	16:W:200:HOH:O	1.88	0.73
5:E:132:TYR:O	5:E:153:PRO:HB3	1.88	0.73
13:M:40:ASN:HD22	13:M:40:ASN:H	1.35	0.73
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.69	0.73
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.71	0.73
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.24	0.73
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.23	0.73
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.89	0.73
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.71	0.73
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.88	0.73
9:W:29:ASN:HD22	9:W:29:ASN:H	1.37	0.73
12:L:166:HIS:HD2	12:L:168:GLN:H	1.36	0.72
6:F:69:VAL:HG12	16:F:248:HOH:O	1.88	0.72
7:G:198:ILE:HG23	7:G:203:THR:O	1.89	0.72
2:P:181:LYS:O	2:P:184:MET:HG3	1.88	0.72
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.71	0.72
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.71	0.72
11:Y:131:GLN:HG3	11:Y:132:THR:N	2.04	0.72
14:2:175:MET:HE3	14:2:18(B):PHE:CE2	2.23	0.72
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.72	0.72
6:F:40:ILE:HD12	6:F:193:ALA:HB2	1.72	0.72
7:G:96:ALA:CA	7:G:107:MET:HE2	2.17	0.72
14:2:10(B):LYS:HD3	14:2:10(B):LYS:C	2.15	0.72
7:U:198:ILE:HG23	7:U:203:THR:O	1.90	0.71
10:X:156:LYS:O	10:X:160:GLN:HG3	1.89	0.71
3:C:33:ARG:HH11	3:C:33:ARG:CB	2.03	0.71
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.37	0.71
3:Q:33:ARG:HH11	3:Q:33:ARG:CB	2.03	0.71
3:C:33:ARG:HB2	3:C:33:ARG:NH1	2.05	0.71
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.38	0.71
11:K:131:GLN:HG3	11:K:132:THR:N	2.04	0.71
10:X:52:THR:HG23	10:X:53:VAL:N	2.05	0.71
2:B:15:PHE:N	3:C:23:GLN:HE22	1.83	0.71
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.73	0.71
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.73	0.71
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.04	0.71
7:G:59:LEU:O	7:G:61:PRO:HD3	1.91	0.70
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.39	0.70
10:J:156:LYS:O	10:J:160:GLN:HG3	1.91	0.70
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:LYS:HG2	3:C:161:SER:O	1.90	0.70
5:E:2(C):VAL:HG13	5:E:2(D):ASP:N	2.06	0.70
1:O:130:ARG:HH21	7:U:124:THR:CG2	2.04	0.70
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.73	0.70
9:W:29:ASN:H	9:W:29:ASN:ND2	1.89	0.70
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.92	0.70
7:U:87:ASN:C	7:U:87:ASN:HD22	1.99	0.70
1:A:170:VAL:HG23	16:A:250:HOH:O	1.90	0.70
10:J:-1:MET:HG2	10:J:1:ASP:H	1.56	0.70
10:J:25:SER:HB2	11:K:131:GLN:HE22	1.56	0.70
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.73	0.70
14:N:10(B):LYS:C	14:N:10(B):LYS:HD3	2.16	0.70
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.92	0.70
10:X:32:ASP:OD2	10:X:34:THR:HG22	1.90	0.70
10:X:-1:MET:HG2	10:X:1:ASP:H	1.56	0.70
13:1:40:ASN:H	13:1:40:ASN:HD22	1.36	0.70
1:A:121:GLN:O	1:A:124:THR:HB	1.92	0.70
5:E:227:GLU:N	5:E:227:GLU:CD	2.49	0.70
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.74	0.69
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.05	0.69
11:Y:7:ARG:HG2	11:Y:108:PRO:HB2	1.74	0.69
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.91	0.69
14:N:175:MET:HE3	14:N:18(B):PHE:CE2	2.27	0.69
8:V:52:THR:O	8:V:56:THR:HB	1.92	0.69
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.73	0.69
10:J:52:THR:HG23	10:J:53:VAL:N	2.06	0.69
5:S:175:TYR:HB2	5:S:199:GLN:HG2	1.74	0.69
5:E:17:PRO:HA	6:F:26:TYR:CD2	2.28	0.69
5:S:2(C):VAL:HG13	5:S:2(D):ASP:N	2.08	0.69
2:B:51:GLU:OE2	2:B:202:THR:HG23	1.93	0.69
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.75	0.69
9:I:29:ASN:ND2	9:I:29:ASN:H	1.91	0.69
1:O:60:MET:HE3	1:O:63:THR:HG21	1.75	0.69
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.40	0.69
9:I:29:ASN:H	9:I:29:ASN:HD22	1.39	0.69
11:K:33:LYS:HE2	15:K:2000:ESY:H23	1.75	0.69
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.72	0.69
13:M:76:PRO:HD2	13:M:105:GLN:OE1	1.93	0.69
8:V:3:ILE:HG22	8:V:16:ALA:HB2	1.75	0.69
5:E:175:TYR:HB2	5:E:199:GLN:HG2	1.74	0.69
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:12:ILE:HG13	7:G:14:ILE:HG23	1.75	0.68
8:H:52:THR:O	8:H:56:THR:HB	1.93	0.68
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.73	0.68
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.74	0.68
10:J:32:ASP:OD2	10:J:34:THR:HG22	1.92	0.68
9:W:137:MET:HE2	9:W:161:ASN:HB2	1.74	0.68
13:M:37:VAL:HG11	13:M:79:ILE:HD13	1.75	0.68
11:Y:33:LYS:HE2	15:Y:2000:ESY:H23	1.75	0.68
5:E:12:THR:HG21	5:E:124:THR:HA	1.75	0.68
7:G:87:ASN:C	7:G:87:ASN:HD22	2.01	0.68
11:Y:35:ILE:CD1	11:Y:45:MET:HE3	2.24	0.68
5:E:48:LEU:HD13	5:E:77:SER:HB3	1.75	0.68
5:E:167:ALA:HB3	16:E:246:HOH:O	1.93	0.68
13:M:42:VAL:HG23	13:M:178:ILE:HD11	1.75	0.68
5:S:227:GLU:CD	5:S:227:GLU:N	2.48	0.68
13:1:42:VAL:HG23	13:1:178:ILE:HD11	1.76	0.68
10:X:25:SER:HB2	11:Y:131:GLN:HE22	1.59	0.68
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	1.76	0.68
4:D:40:ILE:HG13	4:D:193:VAL:HG23	1.76	0.67
2:P:51:GLU:OE2	2:P:202:THR:HG23	1.93	0.67
4:D:177:LEU:HD13	5:E:58:LEU:HD11	1.76	0.67
11:K:7:ARG:HG2	11:K:108:PRO:HB2	1.75	0.67
1:O:15:PHE:H	2:P:23:GLN:HE22	1.40	0.67
3:Q:65:SER:HB2	16:Q:247:HOH:O	1.92	0.67
6:T:210:LEU:HD12	6:T:211:GLU:H	1.59	0.67
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.76	0.67
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.76	0.67
5:S:111:ARG:HG3	16:S:243:HOH:O	1.93	0.67
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.76	0.67
3:Q:241:GLN:C	3:Q:243:GLN:H	2.03	0.67
5:S:48:LEU:HD13	5:S:77:SER:HB3	1.75	0.67
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.09	0.67
7:G:107:MET:HE3	7:G:112:LEU:HD13	1.76	0.67
4:R:40:ILE:HG13	4:R:193:VAL:HG23	1.75	0.67
7:U:12:ILE:HG13	7:U:14:ILE:HG23	1.76	0.67
9:W:6:MET:HE3	9:W:155:ILE:HG13	1.75	0.67
11:Y:174:ASN:HD21	11:Y:189:ASN:HB2	1.60	0.67
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.76	0.67
13:M:14(D):GLU:O	13:M:14(G):ILE:HG13	1.95	0.67
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.40	0.67
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.78	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:14(D):GLU:O	13:1:14(G):ILE:HG13	1.95	0.67
5:S:12:THR:HG21	5:S:124:THR:HA	1.74	0.66
9:I:137:MET:HE2	9:I:161:ASN:HB2	1.76	0.66
5:S:18(D):ILE:O	5:S:18(D):ILE:HG12	1.94	0.66
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.77	0.66
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.30	0.66
3:Q:163:GLN:HE21	3:Q:164:THR:H	0.78	0.66
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.09	0.66
2:B:163:ILE:HG12	2:B:164:SER:H	1.60	0.66
3:C:241:GLN:C	3:C:243:GLN:H	2.04	0.66
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.59	0.66
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.78	0.66
4:R:102:TYR:O	12:Z:81:ARG:HG3	1.95	0.66
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	1.95	0.66
1:A:60:MET:HE3	1:A:63:THR:HG21	1.76	0.65
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.77	0.65
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	1.78	0.65
3:Q:85:SER:O	3:Q:89:ILE:HG13	1.97	0.65
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.61	0.65
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.09	0.65
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.43	0.65
9:I:137:MET:HE3	9:I:141:LEU:CD1	2.25	0.65
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.44	0.65
5:E:18(D):ILE:HG12	5:E:18(D):ILE:O	1.96	0.65
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.11	0.65
2:B:121:GLN:O	2:B:124:THR:HB	1.97	0.65
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	1.96	0.65
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.78	0.65
7:U:107:MET:HE3	7:U:112:LEU:HD13	1.78	0.65
2:B:15:PHE:H	3:C:23:GLN:NE2	1.83	0.65
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.27	0.65
6:T:186:ALA:O	6:T:190:VAL:HG23	1.96	0.65
12:Z:114:ASP:HB2	12:Z:118:SER:HB3	1.79	0.65
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.76	0.65
13:1:14(C):ARG:HH11	13:1:14(C):ARG:HG3	1.61	0.65
14:2:18(G):TYR:HA	14:2:18(J):LEU:HG	1.79	0.65
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.78	0.65
6:T:176:LEU:HD22	6:T:196:ILE:HD13	1.77	0.65
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.61	0.64
13:M:40:ASN:HD22	13:M:40:ASN:N	1.94	0.64
8:V:3:ILE:HG22	8:V:16:ALA:CB	2.27	0.64

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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	1.91	0.64
4:D:102:TYR:O	12:L:81:ARG:HG3	1.97	0.64
6:F:186:ALA:O	6:F:190:VAL:HG23	1.97	0.64
6:T:43:ASN:HD22	6:T:43:ASN:N	1.95	0.64
2:B:6:ARG:HB2	5:E:127:TYR:OH	1.98	0.64
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.27	0.64
11:K:174:ASN:HD21	11:K:189:ASN:HB2	1.63	0.64
2:P:163:ILE:HG12	2:P:164:SER:H	1.60	0.64
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.96	0.64
6:F:210:LEU:HD12	6:F:211:GLU:H	1.63	0.64
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.79	0.64
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.61	0.64
14:2:14:LEU:O	14:2:175:MET:HA	1.97	0.64
6:F:43:ASN:N	6:F:43:ASN:HD22	1.96	0.64
2:B:163:ILE:HG12	2:B:164:SER:N	2.13	0.64
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.33	0.64
7:U:18(G):GLU:HG2	7:U:188:LYS:HB3	1.79	0.64
9:I:29:ASN:ND2	9:I:30:LYS:HG3	2.13	0.64
2:P:202:THR:HG22	2:P:203:ASP:N	2.12	0.64
6:T:121:GLN:C	6:T:121:GLN:HE21	2.05	0.64
2:B:202:THR:HG22	2:B:203:ASP:N	2.14	0.63
13:1:8:TYR:CE2	13:1:148:VAL:HG22	2.33	0.63
2:B:71:ASN:ND2	2:B:72:ASP:N	2.45	0.63
8:V:148:LYS:O	8:V:152:ILE:HG12	1.97	0.63
14:N:143:ARG:NH2	14:N:146:MET:HE3	2.14	0.63
7:U:168:LYS:HD2	7:U:201:LEU:HD22	1.81	0.63
9:W:137:MET:HE3	9:W:141:LEU:CD1	2.27	0.63
6:F:176:LEU:HD22	6:F:196:ILE:HD13	1.78	0.63
12:L:114:ASP:HB2	12:L:118:SER:HB3	1.80	0.63
9:W:27:VAL:HG13	16:X:215:HOH:O	1.98	0.63
10:J:24:ILE:HG22	15:K:2000:ESY:O41	1.99	0.63
5:S:77:SER:OG	5:S:137:LEU:HB2	1.98	0.63
1:A:173:LYS:O	1:A:177:GLU:HG3	1.99	0.63
9:I:165:ARG:NH2	12:Z:135:MET:HE3	2.13	0.63
11:K:195:LEU:O	11:K:199:VAL:HG23	1.98	0.63
14:N:126:ILE:HD13	14:N:126:ILE:H	1.64	0.63
2:P:163:ILE:HG12	2:P:164:SER:N	2.14	0.63
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.33	0.63
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.12	0.63
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.79	0.63
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:232:TYR:O	3:C:236:ILE:HG13	1.99	0.63
6:F:43:ASN:H	6:F:43:ASN:ND2	1.97	0.62
6:F:109:ILE:HD12	6:F:109:ILE:N	2.13	0.62
1:O:173:LYS:O	1:O:177:GLU:HG3	1.99	0.62
2:P:219:GLU:HG2	2:P:21(E):VAL:H	1.64	0.62
6:T:109:ILE:HD12	6:T:109:ILE:N	2.14	0.62
6:T:136:THR:O	6:T:150:MET:HA	1.99	0.62
1:A:130:ARG:HH21	7:G:124:THR:CG2	2.11	0.62
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.34	0.62
14:2:112:THR:CG2	14:2:120:HIS:HB2	2.28	0.62
14:2:126:ILE:H	14:2:126:ILE:HD13	1.64	0.62
14:N:14:LEU:O	14:N:175:MET:HA	1.98	0.62
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.47	0.62
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.79	0.62
4:D:185:THR:OG1	4:D:188:GLU:HG3	1.99	0.62
3:Q:185:THR:CB	3:Q:188:GLU:HG2	2.24	0.62
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.79	0.62
8:H:148:LYS:O	8:H:152:ILE:HG12	2.00	0.62
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.34	0.62
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.82	0.62
2:P:121:GLN:O	2:P:124:THR:HB	1.98	0.62
7:U:158:VAL:HG22	7:U:159:GLY:N	2.14	0.62
9:W:156:SER:O	9:W:160:LEU:HB2	2.00	0.62
2:B:219:GLU:HG2	2:B:21(E):VAL:H	1.64	0.62
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.30	0.62
9:I:113:PHE:CD2	9:I:113:PHE:N	2.68	0.62
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.82	0.62
9:W:29:ASN:HD22	9:W:29:ASN:N	1.97	0.62
10:X:52:THR:HG23	10:X:53:VAL:H	1.64	0.62
3:C:206:GLY:HA3	3:C:209:ASN:HB2	1.82	0.61
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.82	0.61
6:T:43:ASN:ND2	6:T:43:ASN:H	1.96	0.61
8:H:144:GLN:O	8:H:145:ASP:HB2	2.00	0.61
6:T:121:GLN:C	6:T:121:GLN:NE2	2.59	0.61
12:Z:109:ALA:HB2	12:Z:121:ARG:NH2	2.16	0.61
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.97	0.61
2:P:71:ASN:ND2	2:P:72:ASP:N	2.47	0.61
10:X:48:GLU:HB2	10:X:96:GLN:HB2	1.81	0.61
13:1:113:VAL:HG23	13:1:119:THR:HG22	1.83	0.61
3:C:85:SER:O	3:C:89:ILE:HG13	2.00	0.61
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.49	0.61
8:H:196:VAL:HG23	16:H:239:HOH:O	2.01	0.61
4:R:185:THR:OG1	4:R:188:GLU:HG3	2.00	0.61
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.65	0.61
5:S:18(C):PHE:C	5:S:18(E):LYS:H	2.08	0.61
11:Y:35:ILE:HD11	11:Y:45:MET:HE2	1.82	0.61
3:C:41:LYS:HD3	3:C:161:SER:HA	1.82	0.61
5:E:194:VAL:HA	5:E:197:ILE:HG22	1.83	0.61
10:J:48:GLU:HB2	10:J:96:GLN:HB2	1.81	0.61
13:M:14(G):ILE:N	13:M:144:PRO:HD2	2.16	0.61
3:Q:206:GLY:HA3	3:Q:209:ASN:HB2	1.83	0.61
5:S:73:HIS:HE1	5:S:107:LEU:O	1.83	0.61
7:G:158:VAL:HG22	7:G:159:GLY:N	2.16	0.60
10:J:147:THR:HG23	10:J:150:GLU:OE2	2.01	0.60
13:M:148:VAL:HG23	16:M:236:HOH:O	2.01	0.60
2:B:124:THR:HG22	3:C:130:ARG:NH2	2.13	0.60
8:H:3:ILE:HG22	8:H:16:ALA:HB2	1.83	0.60
3:Q:55:THR:O	3:Q:56:LEU:HD13	2.01	0.60
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.36	0.60
7:U:192:PHE:C	7:U:192:PHE:CD1	2.78	0.60
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.82	0.60
10:J:168:MET:HG2	10:X:168:MET:CE	2.31	0.60
9:W:113:PHE:CD2	9:W:113:PHE:N	2.69	0.60
11:Y:86:LEU:O	11:Y:89:GLN:HB2	2.01	0.60
7:G:168:LYS:HD2	7:G:201:LEU:HD22	1.83	0.60
1:A:15:PHE:H	2:B:23:GLN:HE22	1.48	0.60
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.81	0.60
12:L:109:ALA:HB2	12:L:121:ARG:NH2	2.16	0.60
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.83	0.60
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.84	0.60
10:X:147:THR:HG23	10:X:150:GLU:OE2	2.00	0.60
13:1:41:THR:OG1	13:1:76:PRO:HG3	2.02	0.60
6:F:121:GLN:HE21	6:F:121:GLN:C	2.10	0.60
1:O:26:TYR:CD1	7:U:17:PRO:HA	2.36	0.60
13:1:37:VAL:HG11	13:1:79:ILE:CD1	2.31	0.60
13:1:14(G):ILE:N	13:1:144:PRO:HD2	2.15	0.60
1:O:27:ALA:O	1:O:31:VAL:HG23	2.01	0.60
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.84	0.60
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.17	0.59
1:O:69:LEU:C	1:O:69:LEU:HD23	2.27	0.59
16:O:241:HOH:O	2:P:81:LEU:HD12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ALA:O	1:A:31:VAL:HG23	2.02	0.59
3:C:46:VAL:O	3:C:215:VAL:HG12	2.02	0.59
6:T:187:ARG:HH11	6:T:187:ARG:HG3	1.67	0.59
10:X:24:ILE:HG22	15:Y:2000:ESY:O41	2.02	0.59
10:X:44:SER:OG	10:X:100:LEU:HB2	2.01	0.59
10:X:140:HIS:HD2	10:X:141:HIS:CE1	2.20	0.59
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.14	0.59
5:E:77:SER:OG	5:E:137:LEU:HB2	2.01	0.59
7:G:192:PHE:C	7:G:192:PHE:CD1	2.79	0.59
10:J:18:LYS:HG2	10:J:174:ILE:HG13	1.84	0.59
5:S:74:MET:HE2	5:S:109:VAL:HA	1.84	0.59
6:T:54:ILE:HG13	6:T:208:PHE:HA	1.84	0.59
6:T:126:TYR:HE1	7:U:129:MET:SD	2.25	0.59
8:V:144:GLN:O	8:V:145:ASP:HB2	2.02	0.59
10:X:52:THR:CG2	10:X:53:VAL:H	2.15	0.59
11:K:10(A):ARG:HG2	11:K:10(A):ARG:HH11	1.67	0.59
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.15	0.59
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.84	0.59
6:T:172:ALA:C	6:T:176:LEU:HD23	2.28	0.59
6:T:172:ALA:O	6:T:176:LEU:HD23	2.03	0.59
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.17	0.59
1:A:51:GLU:OE1	1:A:202:VAL:HG22	2.02	0.59
6:F:54:ILE:HG13	6:F:208:PHE:HA	1.85	0.59
3:Q:106:PRO:HG2	3:Q:143:PRO:HG2	1.85	0.59
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.83	0.59
9:I:156:SER:O	9:I:160:LEU:HB2	2.02	0.59
11:K:35:ILE:CD1	11:K:45:MET:HE3	2.31	0.59
11:K:35:ILE:HD11	11:K:45:MET:HE2	1.82	0.59
4:R:196:ILE:H	4:R:196:ILE:HD12	1.67	0.59
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.68	0.59
10:X:52:THR:CG2	10:X:53:VAL:N	2.66	0.59
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:HH11	1.66	0.59
5:E:18(C):PHE:HA	5:E:18(F):ILE:CG1	2.33	0.58
13:M:14(C):ARG:HG3	13:M:14(C):ARG:HH11	1.68	0.58
2:P:239:THR:HG22	2:P:239:THR:OXT	2.02	0.58
13:M:17:ASP:HA	13:M:173:PHE:CB	2.33	0.58
2:B:97:GLN:NE2	16:B:246:HOH:O	2.35	0.58
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.68	0.58
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.86	0.58
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.85	0.58
3:C:106:PRO:HG2	3:C:143:PRO:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:135:MET:HE3	13:1:165:ARG:NH2	2.19	0.58
11:K:12:ILE:HB	11:K:178:VAL:HB	1.84	0.58
1:O:86:ARG:HH21	7:U:118:ASN:ND2	1.99	0.58
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.03	0.58
5:S:70:CYS:SG	5:S:92:LEU:HD23	2.43	0.58
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.03	0.58
5:S:201:LEU:O	5:S:202:ARG:HB2	2.04	0.58
1:O:86:ARG:HE	7:U:118:ASN:ND2	2.00	0.58
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	2.00	0.58
14:2:3:ILE:HG22	14:2:16:ALA:CB	2.33	0.58
2:B:71:ASN:HD22	2:B:72:ASP:H	1.47	0.58
5:E:73:HIS:HE1	5:E:107:LEU:O	1.85	0.58
5:E:18(C):PHE:C	5:E:18(E):LYS:H	2.11	0.58
10:J:52:THR:HG23	10:J:53:VAL:H	1.68	0.58
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.39	0.58
3:Q:232:TYR:O	3:Q:236:ILE:HG13	2.03	0.58
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.85	0.58
1:A:69:LEU:HD23	1:A:69:LEU:C	2.28	0.58
3:C:185:THR:HG22	3:C:187:GLU:N	2.15	0.58
5:S:194:VAL:HA	5:S:197:ILE:HG22	1.85	0.58
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.39	0.58
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.85	0.58
1:O:51:GLU:OE1	1:O:202:VAL:HG22	2.02	0.58
4:R:207:LEU:HD23	4:R:207:LEU:C	2.29	0.58
7:U:217:LYS:HA	7:U:217:LYS:HE3	1.86	0.58
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.86	0.58
3:C:163:GLN:HE21	3:C:164:THR:H	0.78	0.58
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.69	0.58
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.85	0.58
4:R:40:ILE:HG13	4:R:193:VAL:CG2	2.34	0.58
12:Z:99:THR:CG2	16:Z:202:HOH:O	2.52	0.58
12:Z:14(I):THR:O	12:Z:14(K):LYS:HB2	2.04	0.58
13:1:40:ASN:HD22	13:1:40:ASN:N	1.94	0.58
4:D:112:LEU:C	4:D:112:LEU:HD13	2.29	0.57
9:I:29:ASN:HD22	9:I:29:ASN:N	1.98	0.57
16:K:2016:HOH:O	10:X:136:SER:HA	2.04	0.57
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.13	0.57
4:D:24:VAL:O	4:D:27:SER:HB3	2.03	0.57
6:F:121:GLN:C	6:F:121:GLN:NE2	2.62	0.57
6:F:136:THR:O	6:F:150:MET:HA	2.04	0.57
8:H:3:ILE:HG22	8:H:16:ALA:CB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.04	0.57
5:S:18(C):PHE:HA	5:S:18(F):ILE:CG1	2.33	0.57
4:D:170:GLU:CD	4:D:170:GLU:H	2.13	0.57
12:L:33:LYS:HD2	12:L:46:ASN:HD22	1.69	0.57
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.85	0.57
3:Q:190:VAL:HG13	3:Q:212:ILE:HG21	1.85	0.57
9:W:178:ILE:HG13	9:W:184:VAL:HG22	1.86	0.57
10:X:18:LYS:HG2	10:X:174:ILE:HG13	1.86	0.57
14:2:143:ARG:NH2	14:2:146:MET:HE3	2.18	0.57
12:L:93:PHE:N	12:L:94:PRO:HD3	2.18	0.57
12:L:14(I):THR:O	12:L:1(I):ASN:HB3	2.04	0.57
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.70	0.57
10:J:52:THR:CG2	10:J:53:VAL:N	2.67	0.57
10:J:168:MET:HE3	10:X:168:MET:HE3	1.86	0.57
1:O:62:GLU:C	1:O:64:LEU:H	2.13	0.57
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.35	0.57
12:Z:14(I):THR:O	12:Z:1(I):ASN:HB3	2.03	0.57
14:2:21:THR:HG22	14:2:26:ILE:HA	1.85	0.57
3:C:17:PRO:HA	4:D:26:TYR:CD1	2.39	0.57
5:E:95:GLN:HG3	5:E:115:LEU:HD13	1.86	0.57
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.87	0.57
9:W:29:ASN:ND2	9:W:30:LYS:HG3	2.19	0.57
15:K:2000:ESY:H1	9:W:24:SER:OG	2.05	0.57
14:N:3:ILE:HG22	14:N:16:ALA:CB	2.35	0.57
4:R:81:LEU:HB3	16:R:599:HOH:O	2.04	0.57
4:D:40:ILE:HG13	4:D:193:VAL:CG2	2.34	0.57
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.87	0.57
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.86	0.57
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.87	0.57
3:C:190:VAL:HG13	3:C:212:ILE:HG21	1.86	0.57
7:G:77:VAL:CG1	7:G:137:THR:HB	2.35	0.57
7:G:190:VAL:O	7:G:194:ILE:HG13	2.05	0.57
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.86	0.57
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.86	0.57
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.86	0.57
5:S:210:LEU:HD21	5:S:212:ILE:HD11	1.87	0.57
2:B:20:ARG:HE	3:C:33:ARG:HH21	1.52	0.57
10:J:-1:MET:HG2	10:J:1:ASP:N	2.19	0.57
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	2.20	0.57
13:1:35:ILE:HD12	13:1:56:GLU:HG3	1.87	0.57
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:52:THR:CG2	10:J:53:VAL:H	2.18	0.56
12:L:98:HIS:HB2	16:L:200:HOH:O	2.05	0.56
12:L:14(I):THR:O	12:L:14(K):LYS:HB2	2.04	0.56
1:O:212:LEU:HD22	1:O:224:LEU:HD12	1.87	0.56
4:R:24:VAL:O	4:R:27:SER:HB3	2.05	0.56
5:S:185:ASN:HD21	5:S:187:ASP:HB2	1.70	0.56
5:S:207:LEU:HD23	5:S:207:LEU:N	2.20	0.56
3:C:55:THR:O	3:C:56:LEU:HD13	2.05	0.56
10:J:168:MET:CE	10:X:168:MET:HG2	2.35	0.56
4:R:81:LEU:HD12	4:R:133:GLY:HA3	1.86	0.56
7:U:31:THR:HG21	7:U:135:ILE:HG13	1.87	0.56
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.70	0.56
13:1:11:GLY:HA3	13:1:178:ILE:O	2.05	0.56
1:A:212:LEU:HD22	1:A:224:LEU:HD12	1.86	0.56
3:C:185:THR:CB	3:C:188:GLU:HG2	2.24	0.56
5:E:74:MET:HE2	5:E:109:VAL:HA	1.87	0.56
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.35	0.56
13:M:-6:GLN:HG3	13:M:-6:GLN:O	2.05	0.56
13:M:113:VAL:HG23	13:M:119:THR:HG22	1.87	0.56
1:O:122:GLU:C	1:O:124:THR:H	2.13	0.56
10:X:-1:MET:HG2	10:X:1:ASP:N	2.19	0.56
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.40	0.56
11:Y:131:GLN:HG3	11:Y:132:THR:H	1.69	0.56
3:C:46:VAL:HB	3:C:215:VAL:CG1	2.35	0.56
4:D:196:ILE:HD12	4:D:196:ILE:H	1.70	0.56
4:D:207:LEU:C	4:D:207:LEU:HD23	2.31	0.56
11:K:86:LEU:O	11:K:89:GLN:HB2	2.04	0.56
12:Z:99:THR:HG22	16:Z:202:HOH:O	2.04	0.56
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.87	0.56
7:G:72:ARG:NH2	14:N:39:ASP:OD2	2.38	0.56
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.87	0.56
3:C:52:ARG:HD2	3:C:208:LYS:O	2.06	0.56
3:C:159:SER:O	4:D:59:LEU:HD22	2.06	0.56
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.88	0.56
10:J:140:HIS:HD2	10:J:141:HIS:CE1	2.23	0.56
2:B:161:LYS:HG3	3:C:59:GLN:O	2.06	0.56
4:D:172:ALA:HB1	4:D:196:ILE:HG21	1.88	0.56
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.88	0.56
9:I:178:ILE:HG13	9:I:184:VAL:HG22	1.87	0.56
10:J:111:TYR:CE1	10:J:121:GLU:HG3	2.40	0.56
11:K:156:LYS:HB2	11:K:175:LEU:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:20(A):THR:C	1:O:210:ILE:HD13	2.31	0.56
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.88	0.56
6:T:127:ASN:HD22	6:T:128:SER:N	2.03	0.56
10:X:111:TYR:CE1	10:X:121:GLU:HG3	2.41	0.56
6:F:127:ASN:HD22	6:F:128:SER:N	2.03	0.56
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.71	0.56
1:A:86:ARG:HH21	7:G:118:ASN:ND2	2.03	0.56
1:A:214:ILE:CD1	1:A:214:ILE:C	2.79	0.56
13:M:11:GLY:HA3	13:M:178:ILE:O	2.06	0.56
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	2.03	0.56
2:P:185:LYS:HD3	2:P:186:VAL:N	2.20	0.56
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.36	0.56
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.04	0.56
2:B:239:THR:HG22	2:B:239:THR:OXT	2.06	0.56
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.54	0.56
5:E:231:LYS:H	5:E:231:LYS:HD2	1.71	0.56
12:L:129:ALA:HB1	12:L:166:HIS:CE1	2.41	0.56
12:L:14(C):GLN:HG2	8:V:210:THR:CG2	2.36	0.56
10:X:43:MET:HG3	10:X:101:ILE:HG13	1.88	0.56
11:Y:4:LEU:HD11	11:Y:159:ILE:HG12	1.88	0.56
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.86	0.55
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	2.04	0.55
6:T:43:ASN:HD22	6:T:43:ASN:H	1.53	0.55
8:V:179:GLU:OE2	8:V:182:LYS:HE2	2.06	0.55
7:G:172:ILE:HD11	7:G:201:LEU:HD21	1.87	0.55
10:J:43:MET:HG3	10:J:101:ILE:HG13	1.89	0.55
1:O:214:ILE:C	1:O:214:ILE:CD1	2.78	0.55
7:U:8:TYR:C	7:U:10:ARG:H	2.13	0.55
7:G:35:ILE:HG23	7:G:51:GLN:HB2	1.88	0.55
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.87	0.55
14:N:186:ARG:HD3	16:N:218:HOH:O	2.06	0.55
6:T:203:GLU:C	6:T:205:ASN:H	2.13	0.55
1:A:20(A):THR:C	1:A:210:ILE:HD13	2.31	0.55
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.88	0.55
7:G:72:ARG:HB2	7:G:72:ARG:HH11	1.71	0.55
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.03	0.55
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.41	0.55
4:R:170:GLU:CD	4:R:170:GLU:H	2.15	0.55
7:U:35:ILE:HG23	7:U:51:GLN:HB2	1.87	0.55
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.52	0.55
5:E:207:LEU:N	5:E:207:LEU:HD23	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:210:LEU:HD21	5:E:212:ILE:HD11	1.89	0.55
6:F:172:ALA:C	6:F:176:LEU:HD23	2.31	0.55
7:G:8:TYR:C	7:G:10:ARG:H	2.13	0.55
7:G:31:THR:HG21	7:G:135:ILE:HG13	1.88	0.55
1:O:214:ILE:C	1:O:214:ILE:HD13	2.31	0.55
12:Z:129:ALA:HB1	12:Z:166:HIS:CE1	2.41	0.55
14:2:44:CYS:HB2	14:2:100:ILE:HB	1.87	0.55
5:E:201:LEU:O	5:E:202:ARG:HB2	2.06	0.55
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.37	0.55
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.88	0.55
7:U:172:ILE:HD11	7:U:201:LEU:HD21	1.89	0.55
13:1:17:ASP:HA	13:1:173:PHE:CB	2.37	0.55
13:1:113:VAL:HA	13:1:118:VAL:O	2.06	0.55
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.88	0.55
1:A:179:ARG:NH1	1:A:179:ARG:HB3	2.22	0.55
11:K:7:ARG:HD2	11:K:108:PRO:O	2.07	0.55
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.41	0.55
9:W:122:ALA:HB3	9:W:125:ILE:CD1	2.36	0.55
10:X:10(B):LYS:HB2	10:X:10(B):LYS:NZ	2.22	0.55
11:Y:174:ASN:ND2	11:Y:189:ASN:HB2	2.21	0.55
12:L:-7:ASN:ND2	12:L:-5:TYR:H	2.04	0.55
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.07	0.55
5:S:17:PRO:HA	6:T:26:TYR:CD2	2.41	0.55
5:S:95:GLN:HG3	5:S:115:LEU:HD13	1.88	0.55
6:T:127:ASN:HD22	6:T:127:ASN:C	2.14	0.55
7:U:123:TYR:CE1	7:U:129:MET:HE3	2.42	0.55
10:X:10(B):LYS:HB2	10:X:10(B):LYS:HZ2	1.71	0.55
11:Y:143:LYS:HB2	11:Y:146:LEU:HD12	1.89	0.55
12:Z:33:LYS:HD2	12:Z:46:ASN:HD22	1.72	0.55
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.88	0.55
2:B:185:LYS:HD3	2:B:186:VAL:N	2.22	0.55
3:C:227:GLU:OE1	3:C:227:GLU:N	2.39	0.55
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.07	0.55
7:U:9:ASP:OD2	7:U:16:SER:HA	2.06	0.55
9:W:45:ILE:HB	9:W:52:VAL:HG13	1.89	0.55
6:F:127:ASN:HD22	6:F:127:ASN:C	2.13	0.55
13:M:113:VAL:HA	13:M:118:VAL:O	2.07	0.55
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.37	0.55
6:T:147:HIS:HD2	16:T:242:HOH:O	1.89	0.55
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.88	0.55
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:203:GLU:C	6:F:205:ASN:H	2.13	0.54
6:F:21(B):THR:O	6:F:21(C):ASN:HB2	2.07	0.54
7:G:9:ASP:OD2	7:G:16:SER:HA	2.07	0.54
8:H:139:GLU:HA	8:H:139:GLU:OE2	2.07	0.54
8:H:179:GLU:OE2	8:H:182:LYS:HE2	2.07	0.54
7:U:77:VAL:CG1	7:U:137:THR:HB	2.37	0.54
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:NH1	2.23	0.54
1:A:62:GLU:C	1:A:64:LEU:H	2.14	0.54
2:B:224:PHE:N	2:B:224:PHE:CD2	2.75	0.54
3:C:15:PHE:N	4:D:23:GLN:HE22	2.02	0.54
6:F:63:LYS:O	6:F:65:VAL:N	2.40	0.54
10:J:13:ILE:HD13	10:J:177:ILE:HD13	1.89	0.54
2:P:202:THR:HG22	2:P:203:ASP:H	1.72	0.54
5:S:212:ILE:HD12	5:S:229:VAL:CG1	2.37	0.54
2:B:224:PHE:N	2:B:224:PHE:HD2	2.05	0.54
11:K:4:LEU:HD11	11:K:159:ILE:HG12	1.88	0.54
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.07	0.54
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.42	0.54
9:I:81:GLN:HG2	16:I:214:HOH:O	2.08	0.54
10:J:168:MET:HG2	10:X:168:MET:HE3	1.90	0.54
10:X:77:GLN:C	10:X:77:GLN:NE2	2.66	0.54
2:B:71:ASN:HD22	2:B:72:ASP:N	2.03	0.54
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.89	0.54
11:K:138:LEU:HD13	11:K:158:SER:OG	2.07	0.54
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.43	0.54
6:T:63:LYS:O	6:T:65:VAL:N	2.40	0.54
7:U:34:THR:HB	7:U:35:ILE:HG13	1.88	0.54
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.08	0.54
11:Y:156:LYS:HB2	11:Y:175:LEU:HD11	1.89	0.54
14:2:143:ARG:O	14:2:146:MET:HG3	2.07	0.54
6:F:126:TYR:HE1	7:G:129:MET:SD	2.31	0.54
9:I:124:PHE:O	9:I:125:ILE:HD12	2.07	0.54
13:M:35:ILE:HD12	13:M:56:GLU:HG3	1.89	0.54
2:P:110:GLU:O	2:P:110:GLU:HG2	2.08	0.54
9:W:97:VAL:HG23	9:W:99:PRO:HD3	1.88	0.54
1:A:49:ALA:HB2	1:A:212:LEU:HG	1.90	0.54
1:A:111:LEU:O	1:A:114:SER:HB3	2.07	0.54
5:E:226:GLY:O	5:E:229:VAL:HG22	2.07	0.54
1:O:49:ALA:HB2	1:O:212:LEU:HG	1.89	0.54
2:P:121:GLN:NE2	16:P:249:HOH:O	2.39	0.54
2:P:228:GLU:O	2:P:232:ILE:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:69:VAL:HG12	16:1:249:HOH:O	2.07	0.54
12:Z:-5:TYR:CE2	12:Z:96:TYR:HB2	2.43	0.54
5:E:70:CYS:SG	5:E:92:LEU:HD23	2.48	0.54
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.89	0.54
7:G:76:MET:HE3	7:G:78:VAL:CG2	2.38	0.54
2:P:71:ASN:HD22	2:P:72:ASP:N	2.05	0.54
2:P:224:PHE:N	2:P:224:PHE:CD2	2.76	0.54
3:Q:76:LEU:HD12	3:Q:138:ILE:HG12	1.90	0.54
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.90	0.54
2:B:99:TYR:CG	2:B:107:ILE:HG12	2.43	0.54
2:B:202:THR:HG22	2:B:203:ASP:H	1.73	0.54
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.73	0.54
9:I:97:VAL:HG23	9:I:99:PRO:HD3	1.89	0.54
9:I:122:ALA:HB3	9:I:125:ILE:CD1	2.37	0.54
11:K:174:ASN:ND2	11:K:189:ASN:HB2	2.22	0.54
13:M:165:ARG:NH2	8:V:135:MET:HE3	2.23	0.54
14:N:3:ILE:HD12	14:N:44:CYS:HB3	1.90	0.54
1:O:179:ARG:NH1	1:O:179:ARG:HB3	2.23	0.54
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.08	0.54
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.08	0.54
9:W:130:ALA:HB2	9:W:166:ASP:HB2	1.89	0.54
11:Y:138:LEU:HD13	11:Y:158:SER:OG	2.08	0.54
2:P:229:ILE:O	2:P:233:LEU:HB2	2.08	0.53
3:Q:15:PHE:N	4:R:23:GLN:HE22	2.03	0.53
10:X:13:ILE:HD13	10:X:177:ILE:HD13	1.90	0.53
13:M:184:LEU:HD23	13:M:184:LEU:C	2.33	0.53
6:T:109:ILE:HG21	6:T:147:HIS:HB2	1.90	0.53
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.43	0.53
4:D:81:LEU:HD12	4:D:133:GLY:HA3	1.90	0.53
2:P:87:ILE:O	2:P:91:THR:HG23	2.08	0.53
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.56	0.53
7:U:82:ILE:N	7:U:83:PRO:HD2	2.24	0.53
13:1:-6:GLN:O	13:1:-6:GLN:HG3	2.08	0.53
5:E:212:ILE:HD12	5:E:229:VAL:CG1	2.38	0.53
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.73	0.53
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.44	0.53
4:R:172:ALA:HB1	4:R:196:ILE:HG21	1.91	0.53
2:B:229:ILE:O	2:B:233:LEU:HB2	2.08	0.53
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.90	0.53
10:J:10(B):LYS:NZ	10:J:10(B):LYS:HB2	2.23	0.53
1:O:232:ARG:HH11	1:O:232:ARG:HG3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:53:ARG:O	4:R:53:ARG:HG2	2.09	0.53
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.38	0.53
4:D:170:GLU:N	4:D:170:GLU:OE1	2.41	0.53
9:I:7:THR:HG23	9:I:110:ILE:HD13	1.90	0.53
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.23	0.53
14:N:21:THR:HG22	14:N:26:ILE:HA	1.90	0.53
14:N:44:CYS:HB2	14:N:100:ILE:HB	1.91	0.53
4:R:85:ALA:O	4:R:89:ILE:HG12	2.08	0.53
5:S:226:GLY:O	5:S:229:VAL:HG22	2.09	0.53
7:U:131:PRO:HB3	16:U:256:HOH:O	2.08	0.53
9:W:18:LEU:HD12	9:W:172:GLY:HA3	1.90	0.53
2:B:121:GLN:HG3	3:C:83:ALA:HB1	1.90	0.53
10:J:44:SER:OG	10:J:100:LEU:HB2	2.09	0.53
11:K:131:GLN:HG3	11:K:132:THR:H	1.71	0.53
2:P:224:PHE:N	2:P:224:PHE:HD2	2.06	0.53
8:V:1:THR:HG23	8:V:33:LYS:HD3	1.90	0.53
9:W:124:PHE:O	9:W:125:ILE:HD12	2.09	0.53
1:A:4:MET:SD	1:A:5:THR:N	2.72	0.53
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.44	0.53
11:K:146:LEU:HD23	11:K:151:ALA:HA	1.91	0.53
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.43	0.53
4:R:120:ALA:CB	4:R:155:GLY:HA2	2.38	0.53
13:1:184:LEU:C	13:1:184:LEU:HD23	2.33	0.53
13:M:147:THR:OG1	13:M:150:VAL:HG23	2.09	0.53
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.44	0.53
11:Y:172:SER:HA	11:Y:192:VAL:HG23	1.91	0.53
7:G:87:ASN:C	7:G:87:ASN:ND2	2.66	0.53
9:I:48:LEU:HG	9:I:50:THR:HG22	1.91	0.53
9:I:130:ALA:HB2	9:I:166:ASP:HB2	1.92	0.53
2:P:99:TYR:CG	2:P:107:ILE:HG12	2.43	0.53
4:D:179:GLU:HB3	4:D:192:LEU:HD21	1.91	0.52
5:E:198:SER:HA	5:E:201:LEU:CG	2.39	0.52
10:J:77:GLN:NE2	10:J:77:GLN:C	2.66	0.52
11:K:126:CYS:HB2	11:K:135:TYR:CZ	2.44	0.52
13:M:37:VAL:HG11	13:M:79:ILE:CD1	2.37	0.52
2:P:198:SER:HA	2:P:205:LEU:HD22	1.91	0.52
5:S:207:LEU:N	5:S:207:LEU:CD2	2.72	0.52
7:U:224:LEU:HB3	7:U:228:ASN:HB2	1.91	0.52
2:B:228:GLU:O	2:B:232:ILE:HG22	2.09	0.52
7:G:123:TYR:CE1	7:G:129:MET:HE3	2.45	0.52
8:H:24:PRO:HG2	8:H:25:ILE:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.92	0.52
14:N:143:ARG:O	14:N:146:MET:HG3	2.08	0.52
4:R:154:SER:OG	4:R:156:THR:HG23	2.09	0.52
9:W:6:MET:HE3	9:W:155:ILE:CG1	2.38	0.52
13:1:5:SER:HB3	13:1:14:ILE:HG13	1.92	0.52
4:D:85:ALA:O	4:D:89:ILE:HG12	2.09	0.52
10:J:48:GLU:CB	10:J:96:GLN:HB2	2.39	0.52
16:T:244:HOH:O	7:U:86:ARG:HD2	2.09	0.52
7:U:87:ASN:C	7:U:87:ASN:ND2	2.64	0.52
6:F:172:ALA:O	6:F:176:LEU:HD23	2.09	0.52
9:I:24:SER:OG	15:Y:2000:ESY:H1	2.09	0.52
10:J:20:VAL:HG11	11:K:120:LEU:HD11	1.91	0.52
4:R:170:GLU:OE1	4:R:170:GLU:N	2.42	0.52
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.74	0.52
7:U:190:VAL:O	7:U:194:ILE:HG13	2.10	0.52
5:E:185:ASN:HD21	5:E:187:ASP:HB2	1.74	0.52
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.74	0.52
3:Q:134:VAL:HG12	3:Q:135:SER:N	2.25	0.52
6:T:21(B):THR:O	6:T:21(C):ASN:HB2	2.08	0.52
7:U:136:LEU:O	7:U:150:LYS:HA	2.08	0.52
9:W:45:ILE:HG22	9:W:52:VAL:HG22	1.91	0.52
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.17	0.52
1:A:85:TYR:O	1:A:89:VAL:HG23	2.08	0.52
7:G:136:LEU:O	7:G:150:LYS:HA	2.09	0.52
8:H:210:THR:CG2	12:Z:14(C):GLN:HG2	2.39	0.52
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.90	0.52
5:S:231:LYS:H	5:S:231:LYS:HD2	1.74	0.52
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.45	0.52
8:V:139:GLU:HA	8:V:139:GLU:OE2	2.08	0.52
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.92	0.52
13:1:113:VAL:HG23	13:1:119:THR:CG2	2.39	0.52
13:1:146:THR:HA	16:1:231:HOH:O	2.09	0.52
2:B:107:ILE:CD1	2:B:111:ILE:HB	2.40	0.52
1:O:159:PRO:O	2:P:59:LEU:HD12	2.10	0.52
6:F:109:ILE:HG21	6:F:147:HIS:HB2	1.92	0.52
15:K:2000:ESY:H43	10:X:132:PHE:CE1	2.45	0.52
10:X:22:ARG:HG3	10:X:27:LEU:HD12	1.92	0.52
10:X:48:GLU:CB	10:X:96:GLN:HB2	2.39	0.52
14:2:85:GLU:O	14:2:89:GLU:HB2	2.10	0.52
6:F:70:VAL:HG11	6:F:112:PHE:CE1	2.44	0.52
6:F:109:ILE:HD12	6:F:109:ILE:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:127:ASN:C	6:F:127:ASN:ND2	2.67	0.52
11:K:99:THR:HG22	11:K:113:VAL:O	2.10	0.52
11:K:143:LYS:HB2	11:K:146:LEU:HD12	1.92	0.52
12:L:1:GLY:N	16:L:214:HOH:O	2.43	0.52
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.92	0.52
3:C:134:VAL:HG12	3:C:135:SER:N	2.24	0.52
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.45	0.52
10:J:185:ARG:HG2	10:J:185:ARG:HH11	1.74	0.52
2:P:71:ASN:HD22	2:P:72:ASP:H	1.51	0.52
4:R:156:THR:HG22	5:S:83:PRO:HD3	1.92	0.52
5:S:172:ALA:HB2	5:S:196:ALA:O	2.09	0.52
8:V:162:GLY:O	8:V:166:ASP:HB3	2.09	0.52
9:W:48:LEU:HG	9:W:50:THR:HG22	1.92	0.52
14:2:84:LYS:HD3	14:2:85:GLU:N	2.25	0.52
14:2:146:MET:HE2	14:2:150:GLU:HB3	1.91	0.52
2:B:63:THR:O	2:B:63:THR:HG22	2.09	0.51
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.45	0.51
3:C:173:ARG:O	3:C:177:GLU:HG3	2.10	0.51
8:H:44:ALA:HB3	8:H:100:ILE:HB	1.92	0.51
9:I:6:MET:HE3	9:I:155:ILE:CG1	2.40	0.51
14:N:146:MET:HE2	14:N:150:GLU:HB3	1.90	0.51
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.10	0.51
3:Q:227:GLU:OE1	3:Q:227:GLU:N	2.41	0.51
6:T:70:VAL:HG11	6:T:112:PHE:CE1	2.45	0.51
7:U:186:TRP:O	7:U:190:VAL:HG23	2.10	0.51
12:Z:166:HIS:CD2	12:Z:168:GLN:H	2.23	0.51
14:2:3:ILE:HG22	14:2:16:ALA:HB2	1.92	0.51
14:2:10(B):LYS:HD3	14:2:10(B):LYS:O	2.10	0.51
3:C:194:VAL:HG22	3:C:212:ILE:HD11	1.92	0.51
12:L:14(C):GLN:HG2	8:V:210:THR:HG21	1.92	0.51
5:S:78:LEU:HD12	5:S:78:LEU:C	2.35	0.51
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.45	0.51
1:A:122:GLU:C	1:A:124:THR:H	2.16	0.51
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.59	0.51
5:E:86:ARG:HG3	5:E:86:ARG:NH1	2.25	0.51
7:G:38:LEU:C	7:G:38:LEU:HD12	2.36	0.51
13:M:5:SER:HB3	13:M:14:ILE:HG13	1.92	0.51
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.92	0.51
4:R:179:GLU:HB3	4:R:192:LEU:HD21	1.92	0.51
7:U:72:ARG:HB2	7:U:72:ARG:HH11	1.75	0.51
5:E:18(C):PHE:C	5:E:18(E):LYS:N	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:207:LEU:N	5:E:207:LEU:CD2	2.73	0.51
7:G:82:ILE:N	7:G:83:PRO:HD2	2.25	0.51
6:T:169:ARG:HG3	6:T:173:LYS:HE3	1.91	0.51
2:B:20:ARG:NE	3:C:33:ARG:NH2	2.56	0.51
2:B:235:LYS:HD3	2:B:235:LYS:N	2.26	0.51
5:E:78:LEU:C	5:E:78:LEU:HD12	2.36	0.51
13:M:164:TYR:HE2	16:M:254:HOH:O	1.94	0.51
4:R:215:ILE:HD13	4:R:215:ILE:C	2.35	0.51
5:S:18(C):PHE:C	5:S:18(E):LYS:N	2.67	0.51
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG12	1.92	0.51
5:S:2(C):VAL:CG1	5:S:2(D):ASP:H	2.22	0.51
8:V:24:PRO:HG2	8:V:25:ILE:HD12	1.92	0.51
11:Y:146:LEU:HD23	11:Y:151:ALA:HA	1.90	0.51
13:1:147:THR:OG1	13:1:150:VAL:HG23	2.10	0.51
14:2:3:ILE:HD12	14:2:44:CYS:HB3	1.92	0.51
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.91	0.51
12:L:42:VAL:HG23	12:L:102:ALA:HB3	1.92	0.51
3:C:76:LEU:HD12	3:C:138:ILE:HG12	1.93	0.51
8:H:1:THR:HG23	8:H:33:LYS:HD3	1.91	0.51
11:K:77:ALA:HA	11:K:111:TYR:CE2	2.45	0.51
11:K:172:SER:HA	11:K:192:VAL:HG23	1.92	0.51
13:M:129:PHE:HE2	14:2:24:ALA:HB3	1.75	0.51
2:P:63:THR:O	2:P:63:THR:HG22	2.11	0.51
5:S:227:GLU:CD	5:S:227:GLU:H	2.17	0.51
9:W:28:SER:HB2	10:X:120:VAL:HG21	1.93	0.51
1:A:8:TYR:HD2	7:G:128:TYR:HB3	1.76	0.51
7:G:34:THR:HB	7:G:35:ILE:HG13	1.92	0.51
8:H:165:ASN:ND2	13:1:139:ARG:HH11	2.07	0.51
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.39	0.51
12:L:48:PHE:CZ	12:L:50:ALA:HB3	2.46	0.51
1:O:93:ARG:HD3	8:V:68:LEU:HD23	1.92	0.51
9:W:137:MET:CE	9:W:141:LEU:HD11	2.40	0.51
3:C:100:ARG:NH1	3:C:106:PRO:HB3	2.24	0.51
5:E:227:GLU:CD	5:E:227:GLU:H	2.17	0.51
14:N:41:ILE:CD1	14:N:76:THR:HA	2.41	0.51
5:S:207:LEU:CD2	5:S:207:LEU:H	2.23	0.51
11:Y:77:ALA:HA	11:Y:111:TYR:CE2	2.46	0.51
1:A:93:ARG:HD3	8:H:68:LEU:HD23	1.93	0.51
11:K:10(A):ARG:HG2	11:K:10(A):ARG:NH1	2.24	0.51
14:N:24:ALA:HB3	13:1:129:PHE:HE2	1.75	0.51
6:T:210:LEU:HD12	6:T:211:GLU:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:-9:GLN:HE21	13:1:-8:THR:HG21	1.77	0.51
14:2:66:TYR:CD2	14:2:74:PRO:HB3	2.46	0.51
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.75	0.50
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.12	0.50
7:G:186:TRP:O	7:G:190:VAL:HG23	2.10	0.50
12:L:145:TYR:CD1	12:L:146:LEU:N	2.78	0.50
2:P:160:TRP:CD2	2:P:163:ILE:HD12	2.46	0.50
4:R:112:LEU:HD13	4:R:112:LEU:C	2.37	0.50
7:U:55:PRO:HG2	7:U:56:ASP:H	1.76	0.50
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	1.92	0.50
2:B:27:ALA:O	2:B:31:ILE:HG12	2.11	0.50
3:C:186:VAL:O	3:C:190:VAL:HG23	2.11	0.50
7:G:48:VAL:HG23	7:G:48:VAL:O	2.11	0.50
2:P:107:ILE:CD1	2:P:111:ILE:HB	2.41	0.50
3:Q:52:ARG:HH21	3:Q:211:GLU:HB3	1.75	0.50
6:T:127:ASN:C	6:T:127:ASN:ND2	2.68	0.50
7:U:172:ILE:HD12	7:U:197:MET:CE	2.42	0.50
7:U:197:MET:HE2	7:U:201:LEU:HG	1.94	0.50
9:W:7:THR:HG23	9:W:110:ILE:HD13	1.93	0.50
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.92	0.50
1:A:198:LYS:HE3	1:A:236:LEU:HD11	1.93	0.50
4:D:175:GLU:HG2	4:D:196:ILE:HG13	1.94	0.50
5:E:18(C):PHE:C	5:E:18(C):PHE:CD1	2.89	0.50
2:P:146:TYR:OH	2:P:21(A):LYS:HB2	2.11	0.50
2:P:235:LYS:HD3	2:P:235:LYS:N	2.25	0.50
4:R:72:ARG:HG3	16:R:1302:HOH:O	2.11	0.50
5:S:18(C):PHE:C	5:S:18(C):PHE:CD1	2.90	0.50
8:H:221:ILE:HD11	9:I:184:VAL:HG21	1.93	0.50
14:N:10(B):LYS:HD3	14:N:10(B):LYS:O	2.10	0.50
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.42	0.50
4:R:79:SER:O	4:R:134:VAL:HG23	2.11	0.50
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.79	0.50
13:1:133:MET:O	13:1:136:PRO:HD2	2.10	0.50
3:C:52:ARG:HH21	3:C:211:GLU:HB3	1.76	0.50
6:F:169:ARG:HG3	6:F:173:LYS:HE3	1.93	0.50
10:J:7:ARG:HG2	10:J:7:ARG:HH11	1.77	0.50
10:J:132:PHE:CE1	15:Y:2000:ESY:H43	2.47	0.50
11:K:46:ALA:HB3	11:K:98:GLY:O	2.10	0.50
12:L:-7:ASN:HD22	12:L:-7:ASN:C	2.19	0.50
4:R:162:ALA:HB3	5:S:58:LEU:CD2	2.41	0.50
5:S:104:ASN:HB2	13:1:81:GLU:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.47	0.50
12:Z:42:VAL:HG23	12:Z:102:ALA:HB3	1.94	0.50
2:B:198:SER:HA	2:B:205:LEU:HD22	1.92	0.50
4:D:53:ARG:O	4:D:53:ARG:HG2	2.11	0.50
5:E:172:ALA:HB2	5:E:196:ALA:O	2.11	0.50
1:O:221:PHE:CD2	1:O:221:PHE:C	2.90	0.50
12:Z:6:ILE:HG12	12:Z:124:CYS:HB2	1.94	0.50
1:A:32:LYS:HE2	1:A:32:LYS:HA	1.94	0.50
4:D:120:ALA:CB	4:D:155:GLY:HA2	2.41	0.50
6:F:203:GLU:OE1	6:F:203:GLU:HA	2.11	0.50
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.92	0.50
5:S:198:SER:HA	5:S:201:LEU:CG	2.39	0.50
11:Y:45:MET:HE2	11:Y:53:GLN:HB2	1.92	0.50
1:A:86:ARG:HE	7:G:118:ASN:ND2	2.06	0.50
5:E:2(C):VAL:CG1	5:E:2(D):ASP:H	2.21	0.50
5:E:226:GLY:O	5:E:228:ALA:N	2.45	0.50
6:F:210:LEU:HD21	6:F:212:ILE:HD11	1.94	0.50
7:G:55:PRO:HG2	7:G:56:ASP:H	1.76	0.50
8:H:15:ALA:HB2	8:H:175:VAL:HG22	1.93	0.50
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.93	0.50
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.11	0.50
4:R:161:ASN:N	5:S:58:LEU:O	2.45	0.50
12:Z:114:ASP:CB	12:Z:118:SER:H	2.24	0.50
5:E:216:GLY:O	5:E:217:LYS:C	2.55	0.50
9:I:137:MET:CE	9:I:141:LEU:HD11	2.37	0.50
4:R:160:TYR:HA	5:S:59:SER:HA	1.94	0.50
5:S:86:ARG:HG3	5:S:86:ARG:NH1	2.27	0.50
5:S:216:GLY:O	5:S:217:LYS:C	2.53	0.50
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.93	0.50
11:Y:166:ASP:O	16:Y:2010:HOH:O	2.20	0.50
1:A:62:GLU:CD	1:A:62:GLU:H	2.20	0.49
16:B:257:HOH:O	3:C:33:ARG:HD2	2.10	0.49
5:E:97:ASN:HD21	12:L:61:ASN:ND2	2.09	0.49
5:E:207:LEU:CD2	5:E:207:LEU:H	2.24	0.49
6:F:49:ALA:HA	6:F:211:GLU:O	2.12	0.49
7:G:172:ILE:HD12	7:G:197:MET:CE	2.41	0.49
8:H:210:THR:HG21	12:Z:14(C):GLN:HG2	1.93	0.49
3:Q:121:GLN:NE2	3:Q:121:GLN:C	2.70	0.49
8:V:78:SER:O	8:V:82:MET:HG3	2.12	0.49
10:X:7:ARG:HG2	10:X:7:ARG:HH11	1.77	0.49
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:36:VAL:HG22	5:E:37:THR:N	2.26	0.49
7:G:72:ARG:HB2	7:G:72:ARG:NH1	2.26	0.49
5:S:15:PHE:H	6:T:23:GLN:HE22	1.60	0.49
5:S:52:LYS:HB2	5:S:63:TYR:HB3	1.93	0.49
10:J:168:MET:HE2	10:X:168:MET:HG2	1.94	0.49
1:O:94:LYS:O	1:O:98:THR:HG23	2.12	0.49
1:O:198:LYS:HE3	1:O:236:LEU:HD11	1.94	0.49
5:S:179:THR:HG22	5:S:179:THR:O	2.13	0.49
6:T:184:LEU:HD11	6:T:188:GLU:HB3	1.94	0.49
6:T:203:GLU:OE1	6:T:203:GLU:HA	2.12	0.49
14:2:15:GLY:HA2	14:2:174:ARG:O	2.13	0.49
1:A:214:ILE:C	1:A:214:ILE:HD13	2.38	0.49
2:B:146:TYR:OH	2:B:21(A):LYS:HB2	2.13	0.49
6:F:238:LYS:HZ2	6:F:239:GLU:HG3	1.77	0.49
10:J:35:ARG:O	10:J:42:LEU:HD12	2.12	0.49
2:P:227:GLN:OE1	2:P:230:LYS:HD3	2.12	0.49
10:X:185:ARG:HG2	10:X:185:ARG:HH11	1.77	0.49
14:2:175:MET:HE3	14:2:18(B):PHE:HE2	1.76	0.49
3:C:226:SER:O	3:C:230:ASN:HB2	2.13	0.49
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.42	0.49
5:E:40:LEU:N	5:E:40:LEU:HD23	2.27	0.49
8:H:147:THR:HG23	8:H:150:GLU:OE1	2.12	0.49
11:K:86:LEU:HD13	11:K:86:LEU:C	2.38	0.49
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.94	0.49
14:N:6:VAL:O	14:N:12:VAL:HG23	2.13	0.49
14:N:84:LYS:HD3	14:N:85:GLU:N	2.27	0.49
1:O:62:GLU:CD	1:O:62:GLU:H	2.19	0.49
1:O:111:LEU:O	1:O:114:SER:HB3	2.12	0.49
2:B:148:LEU:N	16:B:240:HOH:O	2.43	0.49
3:C:216:LYS:HD2	3:C:220:ASP:OD1	2.13	0.49
6:F:184:LEU:HD11	6:F:188:GLU:HB3	1.94	0.49
1:O:17:PRO:HA	2:P:26:TYR:CD1	2.48	0.49
2:P:6:ARG:HD2	4:R:9:ASP:HB3	1.95	0.49
2:P:122:GLY:C	2:P:124:THR:H	2.20	0.49
11:Y:22:ALA:HB3	11:Y:25:TRP:HD1	1.78	0.49
6:F:176:LEU:O	6:F:180:VAL:HG23	2.13	0.49
8:H:22:GLN:HG3	8:H:27:ALA:HB2	1.95	0.49
10:J:184:ILE:N	10:J:184:ILE:HD12	2.28	0.49
13:M:-7:GLN:NE2	16:M:230:HOH:O	2.38	0.49
1:O:161:LYS:HD3	1:O:180:TRP:CH2	2.48	0.49
10:X:184:ILE:N	10:X:184:ILE:HD12	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:97:GLN:HG3	10:J:65:LEU:HB2	1.94	0.49
5:E:58:LEU:HD12	5:E:58:LEU:N	2.28	0.49
6:F:180:VAL:HG21	7:G:58:LEU:HD23	1.95	0.49
9:I:126:VAL:HG11	9:I:134:LEU:HB3	1.95	0.49
12:L:6:ILE:HG12	12:L:124:CYS:HB2	1.95	0.49
14:N:13:ILE:HD12	14:N:151:THR:CG2	2.42	0.49
3:Q:237:GLU:O	3:Q:241:GLN:HG3	2.12	0.49
6:T:210:LEU:HD21	6:T:212:ILE:HD11	1.94	0.49
7:U:168:LYS:O	7:U:172:ILE:HG12	2.13	0.49
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.37	0.49
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.78	0.49
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG12	1.94	0.49
14:N:3:ILE:HG22	14:N:16:ALA:HB2	1.94	0.49
4:R:160:TYR:HA	5:S:58:LEU:O	2.12	0.49
5:S:136:LEU:HD12	5:S:151:PHE:CD2	2.48	0.49
13:1:187:LYS:HB3	13:1:190:LEU:HD11	1.95	0.49
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.93	0.49
1:A:94:LYS:O	1:A:98:THR:HG23	2.13	0.49
5:E:52:LYS:HB2	5:E:63:TYR:HB3	1.94	0.49
10:J:147:THR:OG1	10:J:150:GLU:HG3	2.12	0.49
1:O:85:TYR:O	1:O:89:VAL:HG23	2.13	0.49
3:Q:194:VAL:HG22	3:Q:212:ILE:HD11	1.94	0.49
4:R:90:GLU:OE2	11:Y:69:ARG:NH1	2.43	0.49
5:S:36:VAL:HG22	5:S:37:THR:N	2.27	0.49
7:U:48:VAL:HG23	7:U:48:VAL:O	2.12	0.49
8:V:4:VAL:HG22	8:V:159:ILE:HD11	1.95	0.49
11:Y:126:CYS:HB2	11:Y:135:TYR:CZ	2.48	0.49
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.26	0.49
4:D:39:GLY:HA2	4:D:47:VAL:O	2.13	0.48
4:D:154:SER:OG	4:D:156:THR:HG23	2.12	0.48
5:E:2(C):VAL:CG1	5:E:2(D):ASP:N	2.76	0.48
6:F:43:ASN:ND2	6:F:185:SER:HA	2.28	0.48
6:F:109:ILE:H	6:F:109:ILE:CD1	2.25	0.48
12:L:-5:TYR:CE2	12:L:96:TYR:HB2	2.48	0.48
12:L:166:HIS:CD2	12:L:168:GLN:H	2.23	0.48
13:M:113:VAL:HG23	13:M:119:THR:CG2	2.43	0.48
12:Z:-5:TYR:CD2	12:Z:96:TYR:HB2	2.48	0.48
3:C:237:GLU:O	3:C:241:GLN:HG3	2.13	0.48
12:L:-2:ASN:HA	12:L:21:ILE:O	2.12	0.48
13:M:149:GLN:NE2	13:M:149:GLN:H	2.11	0.48
13:M:187:LYS:HB3	13:M:190:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:40:LEU:N	5:S:40:LEU:HD23	2.27	0.48
5:S:214:ILE:HG12	5:S:215:VAL:N	2.27	0.48
9:W:174:VAL:HG21	9:W:186:LYS:HE3	1.95	0.48
12:Z:-7:ASN:HD22	12:Z:-6:PRO:N	2.10	0.48
2:B:110:GLU:O	2:B:110:GLU:HG2	2.11	0.48
3:C:65:SER:HB2	16:C:252:HOH:O	2.13	0.48
12:L:42:VAL:CG2	12:L:102:ALA:HB3	2.44	0.48
2:P:27:ALA:O	2:P:31:ILE:HG12	2.13	0.48
5:S:226:GLY:O	5:S:228:ALA:N	2.45	0.48
9:W:126:VAL:HG11	9:W:134:LEU:HB3	1.95	0.48
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.48	0.48
5:E:162:GLY:O	5:E:163:THR:HB	2.12	0.48
5:E:214:ILE:HG12	5:E:215:VAL:N	2.28	0.48
9:I:18:LEU:HD12	9:I:172:GLY:HA3	1.94	0.48
4:R:159:ARG:O	5:S:60:SER:N	2.45	0.48
9:W:100:VAL:HG13	9:W:125:ILE:HG21	1.96	0.48
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.95	0.48
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.48	0.48
13:M:40:ASN:N	13:M:40:ASN:ND2	2.61	0.48
14:N:66:TYR:CD2	14:N:74:PRO:HB3	2.48	0.48
14:N:85:GLU:O	14:N:89:GLU:HB2	2.13	0.48
11:Y:99:THR:HG22	11:Y:113:VAL:O	2.13	0.48
1:A:221:PHE:C	1:A:221:PHE:CD2	2.91	0.48
5:E:104:ASN:HB2	13:M:81:GLU:HG2	1.94	0.48
3:Q:226:SER:O	3:Q:230:ASN:HB2	2.13	0.48
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.41	0.48
6:T:35:THR:CG2	6:T:36:THR:N	2.76	0.48
7:U:76:MET:HE3	7:U:78:VAL:CG2	2.44	0.48
14:2:13:ILE:HD12	14:2:151:THR:CG2	2.43	0.48
2:B:227:GLN:OE1	2:B:230:LYS:HD3	2.14	0.48
4:D:215:ILE:C	4:D:215:ILE:HD13	2.39	0.48
7:G:238:GLU:O	7:G:239:GLN:HB2	2.13	0.48
3:Q:159:SER:O	4:R:59:LEU:HD22	2.14	0.48
14:2:41:ILE:CD1	14:2:76:THR:HA	2.44	0.48
4:D:233:ILE:O	4:D:237:LEU:HB3	2.13	0.48
6:T:109:ILE:HD12	6:T:109:ILE:H	1.77	0.48
6:T:109:ILE:N	6:T:109:ILE:CD1	2.77	0.48
11:Y:2:THR:HG22	11:Y:159:ILE:HD13	1.95	0.48
6:T:49:ALA:HA	6:T:211:GLU:O	2.14	0.48
7:U:158:VAL:CG2	7:U:159:GLY:N	2.77	0.48
8:V:221:ILE:HD11	9:W:184:VAL:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.78	0.48
3:C:190:VAL:O	3:C:194:VAL:HG23	2.13	0.48
9:I:174:VAL:HG21	9:I:186:LYS:HE3	1.96	0.48
14:N:116:GLY:HA3	16:N:193:HOH:O	2.14	0.48
2:P:150:THR:O	2:P:157:TYR:HA	2.13	0.48
5:S:162:GLY:O	5:S:163:THR:HB	2.14	0.48
8:V:44:ALA:HB3	8:V:100:ILE:HB	1.96	0.48
5:E:131:PRO:HA	16:E:236:HOH:O	2.14	0.47
5:E:180:LEU:O	5:E:18(B):THR:N	2.47	0.47
9:I:45:ILE:HB	9:I:52:VAL:HG13	1.96	0.47
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.95	0.47
2:P:101:LYS:HZ2	10:X:85:GLN:HE21	1.61	0.47
5:S:28:LEU:O	5:S:31:ILE:HB	2.14	0.47
5:S:185:ASN:C	5:S:185:ASN:HD22	2.22	0.47
10:X:25:SER:HB2	11:Y:131:GLN:NE2	2.29	0.47
10:X:35:ARG:O	10:X:42:LEU:HD12	2.13	0.47
2:B:160:TRP:CD2	2:B:163:ILE:HD12	2.48	0.47
5:E:199:GLN:CA	5:E:199:GLN:HE21	2.26	0.47
8:H:34:LEU:HB2	16:H:240:HOH:O	2.13	0.47
11:K:97:MET:O	11:K:114:ASP:HA	2.14	0.47
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.79	0.47
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.45	0.47
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.48	0.47
6:T:176:LEU:O	6:T:180:VAL:HG23	2.13	0.47
4:D:170:GLU:CD	4:D:170:GLU:N	2.73	0.47
5:E:28:LEU:O	5:E:31:ILE:HB	2.15	0.47
6:F:109:ILE:N	6:F:109:ILE:CD1	2.77	0.47
7:G:28:PHE:CZ	7:G:152:ASP:HB2	2.49	0.47
11:Y:143:LYS:H	11:Y:146:LEU:HD13	1.80	0.47
3:C:235:GLN:O	3:C:239:GLU:HG2	2.14	0.47
4:D:90:GLU:OE2	11:K:69:ARG:NH1	2.47	0.47
5:E:4:PHE:O	5:E:6:ASN:N	2.47	0.47
5:E:44:THR:C	5:E:45:HIS:ND1	2.72	0.47
10:J:168:MET:HG2	10:X:168:MET:HE2	1.95	0.47
11:K:45:MET:HE2	11:K:53:GLN:HB2	1.97	0.47
12:L:140:ASN:O	12:L:144:PHE:HA	2.14	0.47
7:U:28:PHE:CZ	7:U:152:ASP:HB2	2.49	0.47
1:A:110:LYS:HG2	16:A:246:HOH:O	2.13	0.47
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.44	0.47
14:N:19:ARG:HG3	14:N:26:ILE:HG23	1.96	0.47
1:O:17:PRO:HG3	2:P:26:TYR:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:109:ILE:H	6:T:109:ILE:CD1	2.27	0.47
13:1:149:GLN:NE2	13:1:149:GLN:H	2.13	0.47
14:2:59:VAL:HG22	14:2:82:VAL:HG12	1.96	0.47
3:C:241:GLN:C	3:C:243:GLN:N	2.71	0.47
5:E:4:PHE:CG	5:E:5:ARG:N	2.83	0.47
6:F:45:GLY:HA3	6:F:215:CYS:O	2.15	0.47
6:F:210:LEU:HD12	6:F:211:GLU:N	2.27	0.47
7:G:151:THR:HG22	7:G:157:TYR:CB	2.43	0.47
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.97	0.47
10:J:185:ARG:HG2	10:J:185:ARG:NH1	2.30	0.47
11:K:3:THR:HG22	11:K:16:VAL:HG12	1.96	0.47
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.13	0.47
4:R:46:VAL:HG11	4:R:139:ALA:HB1	1.96	0.47
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.95	0.47
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.96	0.47
11:Y:3:THR:HG22	11:Y:16:VAL:HG12	1.96	0.47
12:Z:173:LEU:HB2	12:Z:191:LEU:HD11	1.96	0.47
14:2:175:MET:HE3	14:2:18(B):PHE:CD2	2.49	0.47
2:B:87:ILE:O	2:B:91:THR:HG23	2.14	0.47
2:B:150:THR:O	2:B:157:TYR:HA	2.15	0.47
5:E:185:ASN:C	5:E:185:ASN:HD22	2.23	0.47
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.96	0.47
9:I:123:ASP:HB2	9:I:124:PHE:CD2	2.49	0.47
11:K:22:ALA:HB3	11:K:25:TRP:HD1	1.78	0.47
11:K:74:ILE:HD12	11:K:79:ALA:HB2	1.97	0.47
13:M:133:MET:O	13:M:136:PRO:HD2	2.13	0.47
13:M:165:ARG:NH1	8:V:139:GLU:OE1	2.45	0.47
4:R:39:GLY:HA2	4:R:47:VAL:O	2.15	0.47
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.15	0.47
11:Y:155:GLY:O	11:Y:156:LYS:C	2.58	0.47
12:Z:2:THR:HG21	12:Z:130:ALA:HB3	1.97	0.47
13:1:40:ASN:N	13:1:40:ASN:ND2	2.62	0.47
6:F:54:ILE:HG13	6:F:208:PHE:CA	2.45	0.47
9:I:6:MET:HG2	9:I:124:PHE:HB3	1.97	0.47
12:L:148:VAL:O	12:L:152:ILE:HG13	2.15	0.47
2:P:185:LYS:HD3	2:P:186:VAL:H	1.80	0.47
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.96	0.47
2:B:108:PRO:HD2	2:B:111:ILE:HD12	1.97	0.47
5:E:179:THR:HG22	5:E:179:THR:O	2.14	0.47
6:F:121:GLN:HE21	6:F:122:ALA:N	2.13	0.47
11:K:155:GLY:O	11:K:156:LYS:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:44:THR:C	5:S:45:HIS:ND1	2.72	0.47
5:S:2(C):VAL:CG1	5:S:2(D):ASP:N	2.77	0.47
7:U:238:GLU:O	7:U:239:GLN:HB2	2.15	0.47
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.15	0.47
3:C:18(B):ARG:O	3:C:182:PRO:HD3	2.15	0.47
5:E:57:GLU:C	5:E:58:LEU:HD12	2.41	0.47
7:G:135:ILE:CG2	7:G:150:LYS:HD2	2.45	0.47
8:H:162:GLY:O	8:H:166:ASP:HB3	2.14	0.47
12:L:173:LEU:HB2	12:L:191:LEU:HD11	1.96	0.47
5:S:24:VAL:O	5:S:27:ALA:HB3	2.15	0.47
7:U:38:LEU:C	7:U:38:LEU:HD12	2.40	0.47
6:F:35:THR:CG2	6:F:36:THR:N	2.78	0.46
9:I:90:ARG:NE	16:I:235:HOH:O	2.48	0.46
10:J:25:SER:OG	11:K:131:GLN:NE2	2.48	0.46
12:L:100:ILE:HD11	12:L:125:ARG:HG3	1.96	0.46
13:M:3:VAL:O	13:M:126:ALA:HA	2.15	0.46
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.79	0.46
5:S:199:GLN:HE21	5:S:199:GLN:CA	2.27	0.46
6:T:81:LEU:HD12	6:T:133:GLY:HA3	1.96	0.46
9:W:61:TYR:CD1	9:W:61:TYR:C	2.93	0.46
10:X:90(B):ARG:NH1	16:X:205:HOH:O	2.48	0.46
11:Y:114:ASP:C	11:Y:114:ASP:OD1	2.57	0.46
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.15	0.46
12:Z:42:VAL:CG2	12:Z:102:ALA:HB3	2.45	0.46
14:2:6:VAL:O	14:2:12:VAL:HG23	2.15	0.46
6:F:192:GLN:O	6:F:196:ILE:HG13	2.15	0.46
10:J:40:HIS:CD2	10:J:10(A):LYS:HD3	2.51	0.46
12:L:1:GLY:CA	16:L:214:HOH:O	2.64	0.46
1:O:4:MET:SD	1:O:5:THR:N	2.73	0.46
3:Q:224:LEU:HD12	3:Q:224:LEU:N	2.31	0.46
5:S:4:PHE:CG	5:S:5:ARG:N	2.83	0.46
9:W:6:MET:HG2	9:W:124:PHE:HB3	1.98	0.46
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.97	0.46
10:X:124:TYR:CD2	10:X:138:LEU:HD13	2.51	0.46
13:1:125:LEU:HA	16:1:217:HOH:O	2.15	0.46
4:D:46:VAL:HG11	4:D:139:ALA:HB1	1.97	0.46
6:F:238:LYS:NZ	6:F:239:GLU:HG3	2.30	0.46
10:J:22:ARG:HG3	10:J:27:LEU:HD12	1.96	0.46
10:J:66:TYR:CE2	10:J:74:LEU:HG	2.51	0.46
13:M:7:LYS:HG3	13:M:14(G):ILE:HD13	1.98	0.46
3:Q:227:GLU:HA	3:Q:230:ASN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	2.12	0.46
8:V:81:GLN:O	8:V:85:GLN:HG3	2.15	0.46
12:Z:-8:PHE:CB	13:1:-8:THR:HG23	2.45	0.46
1:A:161:LYS:HD3	1:A:180:TRP:CH2	2.49	0.46
3:C:224:LEU:HD12	3:C:224:LEU:N	2.30	0.46
5:E:24:VAL:O	5:E:27:ALA:HB3	2.15	0.46
5:E:130:ARG:HH11	5:E:130:ARG:HG3	1.80	0.46
7:G:197:MET:HE2	7:G:201:LEU:HG	1.96	0.46
7:G:203:THR:HG22	7:G:204:GLU:N	2.30	0.46
14:N:15:GLY:HA2	14:N:174:ARG:O	2.15	0.46
12:Z:103:GLY:HA2	12:Z:178:VAL:HG11	1.97	0.46
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.97	0.46
5:E:70:CYS:HA	5:E:93:ARG:HG2	1.98	0.46
13:M:133:MET:C	13:M:136:PRO:HD2	2.40	0.46
3:Q:46:VAL:HG11	3:Q:139:ALA:HB1	1.97	0.46
4:R:175:GLU:HG2	4:R:196:ILE:HG13	1.96	0.46
4:R:196:ILE:HD12	4:R:196:ILE:N	2.29	0.46
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.45	0.46
5:S:230:ALA:C	5:S:232:TYR:H	2.24	0.46
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.98	0.46
13:1:190:LEU:N	13:1:190:LEU:HD12	2.30	0.46
5:E:150:GLU:O	5:E:157:VAL:HA	2.16	0.46
12:L:114:ASP:CB	12:L:118:SER:H	2.28	0.46
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.96	0.46
3:Q:216:LYS:HD2	3:Q:220:ASP:OD1	2.15	0.46
5:S:134:VAL:O	5:S:153:PRO:HG3	2.15	0.46
6:T:43:ASN:ND2	6:T:185:SER:HA	2.31	0.46
12:Z:113:PHE:N	12:Z:113:PHE:CD1	2.84	0.46
12:Z:114:ASP:HB2	12:Z:118:SER:H	1.79	0.46
13:1:3:VAL:O	13:1:126:ALA:HA	2.16	0.46
1:A:141:HIS:HA	1:A:146:GLY:O	2.15	0.46
3:C:46:VAL:HG11	3:C:139:ALA:HB1	1.98	0.46
3:C:121:GLN:NE2	3:C:121:GLN:C	2.73	0.46
4:D:79:SER:O	4:D:134:VAL:HG23	2.16	0.46
7:G:197:MET:HE2	7:G:201:LEU:CD1	2.46	0.46
1:O:7:ARG:HH11	5:S:127:TYR:HD2	1.64	0.46
1:O:8:TYR:HD2	7:U:128:TYR:HB3	1.81	0.46
3:Q:62(A):ILE:HG13	3:Q:63:THR:N	2.30	0.46
4:R:15:PHE:HB2	5:S:23:GLN:OE1	2.15	0.46
5:S:4:PHE:O	5:S:6:ASN:N	2.48	0.46
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:178:VAL:HG22	10:X:184:ILE:HG13	1.98	0.46
12:Z:48:PHE:CZ	12:Z:50:ALA:HB3	2.50	0.46
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.81	0.46
3:C:15:PHE:H	4:D:23:GLN:NE2	2.05	0.46
4:D:76:CYS:HB2	4:D:137:LEU:O	2.16	0.46
8:H:81:GLN:O	8:H:85:GLN:HG3	2.15	0.46
10:J:124:TYR:CD2	10:J:138:LEU:HD13	2.51	0.46
13:M:61:ASP:O	13:M:65:GLU:HB2	2.16	0.46
3:Q:15:PHE:H	4:R:23:GLN:NE2	2.06	0.46
3:Q:39:GLY:HA2	3:Q:47:VAL:O	2.16	0.46
6:T:45:GLY:HA3	6:T:215:CYS:O	2.15	0.46
7:U:203:THR:HG22	7:U:204:GLU:N	2.31	0.46
12:Z:114:ASP:HB2	12:Z:118:SER:N	2.31	0.46
1:A:149:TYR:CE1	1:A:159:PRO:HB3	2.50	0.46
3:C:136:THR:O	3:C:150:GLN:HA	2.16	0.46
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.46	0.46
5:E:230:ALA:C	5:E:232:TYR:H	2.23	0.46
4:R:122:ARG:HG2	4:R:122:ARG:HH11	1.81	0.46
6:T:54:ILE:HG13	6:T:208:PHE:CA	2.45	0.46
6:T:121:GLN:HE21	6:T:122:ALA:N	2.13	0.46
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.31	0.46
7:U:227:GLU:HG2	16:U:277:HOH:O	2.16	0.46
9:W:130:ALA:HB2	9:W:166:ASP:CB	2.46	0.46
10:X:113:ILE:HA	10:X:118:THR:O	2.16	0.46
12:Z:43:MET:CB	12:Z:101:ILE:HG22	2.43	0.46
13:1:133:MET:C	13:1:136:PRO:HD2	2.40	0.46
2:B:238:ILE:O	2:B:239:THR:O	2.34	0.46
5:E:38:VAL:HG23	5:E:197:ILE:HD12	1.97	0.46
5:E:52:LYS:HD3	5:E:211:SER:HB2	1.98	0.46
7:G:74:ILE:HD13	16:G:247:HOH:O	2.16	0.46
10:J:142:TYR:O	10:J:143:ARG:HD3	2.15	0.46
14:N:14:LEU:N	14:N:14:LEU:HD12	2.31	0.46
4:R:233:ILE:O	4:R:237:LEU:HB3	2.15	0.46
5:S:41:ARG:NH1	5:S:42:SER:O	2.49	0.46
7:U:74:ILE:HG21	7:U:112:LEU:HD23	1.98	0.46
9:W:5:ALA:HB2	9:W:14:ILE:CD1	2.46	0.46
9:W:123:ASP:HB2	9:W:124:PHE:CD2	2.51	0.46
5:E:17:PRO:HA	6:F:26:TYR:CE2	2.50	0.45
12:L:11:PHE:CE1	12:L:148:VAL:HA	2.52	0.45
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.51	0.45
3:C:227:GLU:HA	3:C:230:ASN:HB2	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:243:ALA:O	4:D:244:GLU:CB	2.64	0.45
13:M:-4:ILE:HG22	13:M:-3:VAL:N	2.31	0.45
3:Q:70:ILE:HG21	3:Q:112:LEU:HD21	1.97	0.45
3:Q:18(B):ARG:O	3:Q:182:PRO:HD3	2.16	0.45
4:R:90:GLU:OE1	11:Y:69:ARG:HD2	2.16	0.45
5:S:58:LEU:N	5:S:58:LEU:HD12	2.31	0.45
5:S:130:ARG:HH11	5:S:130:ARG:HG3	1.80	0.45
7:U:18(D):ILE:HD12	7:U:18(D):ILE:N	2.32	0.45
9:W:36:HIS:HB3	9:W:42:PHE:CD2	2.51	0.45
11:Y:97:MET:O	11:Y:114:ASP:HA	2.17	0.45
3:C:195:ARG:HG3	3:C:236:ILE:HD13	1.98	0.45
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.98	0.45
7:G:18(D):ILE:HD12	7:G:18(D):ILE:N	2.31	0.45
7:G:186:TRP:CZ3	7:G:224:LEU:HD21	2.52	0.45
1:O:12:LEU:HD12	1:O:129:VAL:N	2.32	0.45
3:Q:225:SER:O	3:Q:226:SER:C	2.60	0.45
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.51	0.45
9:W:14:ILE:HG13	9:W:34:ILE:HD12	1.97	0.45
10:X:185:ARG:HG2	10:X:185:ARG:NH1	2.32	0.45
14:2:104:TYR:OH	14:2:180:ALA:HB2	2.16	0.45
6:F:63:LYS:O	6:F:65:VAL:HG23	2.16	0.45
12:L:113:PHE:N	12:L:113:PHE:CD1	2.83	0.45
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.97	0.45
5:S:180:LEU:O	5:S:18(B):THR:N	2.48	0.45
10:X:40:HIS:CD2	10:X:10(A):LYS:HD3	2.52	0.45
1:A:7:ARG:NH1	5:E:127:TYR:HD2	2.15	0.45
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.98	0.45
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.98	0.45
7:U:218:ASP:O	7:U:220:LYS:HB2	2.16	0.45
9:W:14:ILE:CG1	9:W:34:ILE:HD12	2.46	0.45
10:X:66:TYR:CE2	10:X:74:LEU:HG	2.52	0.45
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.52	0.45
6:F:103:TYR:O	6:F:104:LYS:HB3	2.17	0.45
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.97	0.45
5:S:45:HIS:HB2	5:S:189:LEU:HD12	1.99	0.45
6:T:192:GLN:NE2	6:T:195:LYS:HE2	2.31	0.45
10:X:18:LYS:HD3	10:X:174:ILE:HG13	1.99	0.45
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.16	0.45
3:C:161:SER:HB3	3:C:180:TYR:CE1	2.51	0.45
6:F:81:LEU:HD12	6:F:133:GLY:HA3	1.98	0.45
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:191:LYS:HA	6:T:232:ALA:HB1	1.98	0.45
8:V:147:THR:HG23	8:V:150:GLU:OE1	2.17	0.45
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.99	0.45
2:B:209:ARG:HG2	2:B:209:ARG:HH11	1.82	0.45
2:B:21(A):LYS:O	2:B:21(B):GLY:C	2.59	0.45
4:D:121:LEU:HD23	4:D:123:PHE:HE1	1.82	0.45
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.84	0.45
7:G:177:GLU:O	7:G:17(B):LYS:HG3	2.16	0.45
11:K:6:PHE:HA	11:K:123:ASP:O	2.17	0.45
2:P:108:PRO:HD2	2:P:111:ILE:HD12	1.99	0.45
2:P:121:GLN:NE2	2:P:121:GLN:C	2.75	0.45
4:R:243:ALA:O	4:R:244:GLU:CB	2.64	0.45
5:S:70:CYS:HA	5:S:93:ARG:HG2	1.98	0.45
5:S:226:GLY:HA3	5:S:227:GLU:OE2	2.17	0.45
6:T:192:GLN:O	6:T:196:ILE:HG13	2.17	0.45
7:U:78:VAL:HG11	7:U:85:ALA:CB	2.47	0.45
12:Z:134:ILE:HG22	12:Z:138:LEU:HD22	1.99	0.45
5:E:67:ILE:HG21	5:E:213:ALA:HB2	1.98	0.45
9:I:61:TYR:CD1	9:I:61:TYR:C	2.95	0.45
13:M:184:LEU:HD23	13:M:185:THR:N	2.31	0.45
4:R:17:PRO:HG3	5:S:26:TYR:CE2	2.52	0.45
8:V:67:SER:HB2	8:V:74:PRO:HG3	1.99	0.45
10:X:142:TYR:O	10:X:143:ARG:HD3	2.17	0.45
12:Z:11:PHE:CE1	12:Z:148:VAL:HA	2.52	0.45
13:1:150:VAL:HG21	16:1:231:HOH:O	2.17	0.45
4:D:196:ILE:HD12	4:D:196:ILE:N	2.32	0.45
5:E:136:LEU:HD12	5:E:151:PHE:CD2	2.51	0.45
7:G:158:VAL:CG2	7:G:159:GLY:N	2.79	0.45
10:J:189:ASP:HA	10:J:191:GLN:OE1	2.17	0.45
12:L:-5:TYR:CD2	12:L:96:TYR:HB2	2.52	0.45
3:Q:136:THR:O	3:Q:150:GLN:HA	2.16	0.45
4:R:172:ALA:HB2	4:R:200:VAL:HG11	2.00	0.45
5:S:38:VAL:HG23	5:S:197:ILE:HD12	1.99	0.45
5:S:67:ILE:HG21	5:S:213:ALA:HB2	1.98	0.45
13:1:148:VAL:HG23	16:1:224:HOH:O	2.17	0.45
14:2:83:PHE:HB3	14:2:113:ILE:HD13	1.99	0.45
2:B:41:MET:HE3	16:B:240:HOH:O	2.16	0.44
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.99	0.44
10:J:10(B):LYS:HB2	10:J:10(B):LYS:HZ2	1.81	0.44
12:L:109:ALA:HA	16:L:220:HOH:O	2.17	0.44
13:M:190:LEU:HD12	13:M:190:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:207:TYR:CG	2:P:208:ASP:N	2.85	0.44
4:R:121:LEU:HD23	4:R:123:PHE:HE1	1.81	0.44
6:T:107:ILE:O	6:T:107:ILE:HG23	2.16	0.44
7:U:72:ARG:NH2	14:2:39:ASP:OD2	2.50	0.44
8:V:15:ALA:HB2	8:V:175:VAL:HG22	1.98	0.44
8:V:59:ILE:HD12	16:V:247:HOH:O	2.17	0.44
12:Z:137:PHE:CE1	12:Z:141:GLN:HG3	2.52	0.44
1:A:142:ASP:OD1	1:A:145:ASN:HB2	2.18	0.44
2:B:88:LEU:HB3	2:B:116:LEU:HD21	1.98	0.44
2:B:207:TYR:CG	2:B:208:ASP:N	2.85	0.44
3:C:62(A):ILE:O	3:C:63:THR:C	2.60	0.44
5:E:226:GLY:HA3	5:E:227:GLU:OE2	2.17	0.44
2:P:198:SER:CA	2:P:205:LEU:HD22	2.47	0.44
5:S:57:GLU:C	5:S:58:LEU:HD12	2.42	0.44
6:T:109:ILE:HD13	6:T:142:ASP:HB3	2.00	0.44
7:U:197:MET:HE2	7:U:201:LEU:CD1	2.47	0.44
9:W:20:LEU:C	9:W:20:LEU:HD13	2.41	0.44
13:1:7:LYS:HG3	13:1:14(G):ILE:HD13	1.99	0.44
14:2:84:LYS:HD2	16:2:220:HOH:O	2.17	0.44
4:D:172:ALA:O	4:D:175:GLU:HB3	2.18	0.44
4:D:174:ALA:O	4:D:177:LEU:HB2	2.17	0.44
9:I:5:ALA:HB2	9:I:14:ILE:CD1	2.48	0.44
9:I:14:ILE:HG13	9:I:34:ILE:HD12	2.00	0.44
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.52	0.44
12:L:114:ASP:HB2	12:L:118:SER:N	2.33	0.44
7:U:18(G):GLU:CG	7:U:188:LYS:HB2	2.42	0.44
10:X:140:HIS:CD2	10:X:141:HIS:CE1	3.04	0.44
2:B:122:GLY:C	2:B:124:THR:H	2.25	0.44
6:F:13:SER:HB2	7:G:130:ARG:HB3	2.00	0.44
8:H:135:MET:HE3	13:1:165:ARG:CZ	2.48	0.44
9:I:20:LEU:HD13	9:I:20:LEU:C	2.42	0.44
13:M:91:ARG:HG3	13:M:92:SER:N	2.32	0.44
1:O:150:GLN:O	1:O:157:TYR:HA	2.17	0.44
2:P:21:LEU:O	2:P:22:TYR:C	2.60	0.44
2:P:21(A):LYS:O	2:P:21(B):GLY:C	2.60	0.44
3:Q:38:VAL:HG22	3:Q:39:GLY:N	2.32	0.44
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.53	0.44
5:S:97:ASN:HD22	5:S:97:ASN:HA	1.66	0.44
6:T:238:LYS:HZ2	6:T:239:GLU:HG3	1.81	0.44
8:V:200:LYS:HE3	9:W:140:SER:O	2.17	0.44
11:Y:87:VAL:HG11	11:Y:115:SER:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:140:ASN:O	12:Z:144:PHE:HA	2.17	0.44
2:B:41:MET:HE2	2:B:146:TYR:O	2.18	0.44
2:B:213:ALA:HA	2:B:222:LYS:O	2.18	0.44
3:C:225:SER:O	3:C:226:SER:C	2.61	0.44
5:E:41:ARG:NH1	5:E:42:SER:O	2.50	0.44
6:F:61:PRO:O	6:F:62:GLN:HB2	2.17	0.44
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.82	0.44
9:I:-2:ASN:HB3	9:I:20:LEU:HD22	1.99	0.44
11:K:143:LYS:H	11:K:146:LEU:HD13	1.83	0.44
13:M:-5:PRO:HD3	13:M:96:TRP:CE2	2.52	0.44
14:N:163:ILE:CG2	14:N:170:GLY:HA2	2.47	0.44
1:O:122:GLU:C	1:O:124:THR:N	2.76	0.44
6:T:238:LYS:NZ	6:T:239:GLU:HG3	2.32	0.44
7:U:79:ASN:HA	16:U:250:HOH:O	2.17	0.44
7:U:177:GLU:O	7:U:17(B):LYS:HG3	2.17	0.44
7:U:186:TRP:CZ3	7:U:224:LEU:HD21	2.53	0.44
10:X:25:SER:OG	11:Y:131:GLN:NE2	2.51	0.44
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.46	0.44
12:Z:175:ILE:C	12:Z:176:LEU:HD12	2.42	0.44
14:2:13:ILE:HD12	14:2:151:THR:HG22	1.99	0.44
1:A:69:LEU:HD23	1:A:70:LEU:N	2.32	0.44
2:B:185:LYS:HD3	2:B:186:VAL:H	1.82	0.44
3:C:62(A):ILE:HG13	3:C:63:THR:N	2.32	0.44
4:D:160:TYR:HB3	4:D:162:ALA:O	2.17	0.44
6:F:192:GLN:NE2	6:F:195:LYS:HE2	2.33	0.44
10:J:168:MET:HE3	10:X:168:MET:HG2	1.98	0.44
10:J:178:VAL:HG22	10:J:184:ILE:HG13	1.99	0.44
14:N:13:ILE:HD12	14:N:151:THR:HG22	1.98	0.44
14:N:83:PHE:HB3	14:N:113:ILE:HD13	1.98	0.44
14:N:146:MET:CE	14:N:150:GLU:HB3	2.47	0.44
1:O:15:PHE:HB2	2:P:23:GLN:NE2	2.33	0.44
1:O:22:GLY:O	1:O:25:ASP:HB2	2.17	0.44
2:P:136:PHE:O	2:P:150:THR:HA	2.18	0.44
8:V:59:ILE:CD1	16:V:247:HOH:O	2.64	0.44
12:Z:129:ALA:HB1	12:Z:166:HIS:NE2	2.33	0.44
12:Z:134:ILE:O	12:Z:137:PHE:HB3	2.17	0.44
3:C:39:GLY:HA2	3:C:47:VAL:O	2.18	0.44
5:E:143:LYS:HD3	13:M:71(B):GLU:O	2.18	0.44
7:G:65:SER:HA	7:G:211:GLU:OE2	2.18	0.44
7:G:168:LYS:O	7:G:172:ILE:HG12	2.17	0.44
8:H:200:LYS:HE3	9:I:140:SER:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:6:MET:CE	9:I:155:ILE:HA	2.47	0.44
11:K:40:PHE:CD1	11:K:73:ARG:NH1	2.86	0.44
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.17	0.44
1:O:141:HIS:HA	1:O:146:GLY:O	2.18	0.44
2:P:202:THR:CG2	2:P:203:ASP:N	2.80	0.44
5:S:123:ASN:HD22	5:S:123:ASN:N	2.16	0.44
6:T:24:VAL:O	6:T:27:ALA:HB3	2.17	0.44
9:W:5:ALA:HA	9:W:13:ALA:O	2.18	0.44
9:W:6:MET:CE	9:W:155:ILE:HA	2.48	0.44
12:Z:170:GLY:O	12:Z:171:ASP:HB2	2.18	0.44
13:1:91:ARG:HG3	13:1:92:SER:N	2.32	0.44
3:C:26:TYR:N	3:C:26:TYR:CD1	2.86	0.44
3:C:163:GLN:HG3	3:C:164:THR:N	2.33	0.44
7:G:18(D):ILE:N	7:G:18(D):ILE:CD1	2.81	0.44
10:J:98:ASN:HB3	10:J:127:HIS:CD2	2.53	0.44
14:N:144:GLU:O	14:N:145:ASN:HB2	2.18	0.44
4:R:86:ARG:HA	4:R:86:ARG:HD3	1.85	0.44
6:T:103:TYR:O	6:T:104:LYS:HB3	2.16	0.44
7:U:121:GLN:NE2	7:U:121:GLN:C	2.76	0.44
1:A:225:THR:O	1:A:229:ILE:HG12	2.18	0.44
3:C:70:ILE:HG21	3:C:112:LEU:HD21	1.99	0.44
4:D:86:ARG:HD3	4:D:86:ARG:HA	1.86	0.44
11:K:1:THR:O	11:K:128:GLY:HA3	2.18	0.44
14:N:12:VAL:HG22	14:N:13:ILE:N	2.33	0.44
1:O:179:ARG:HB3	1:O:179:ARG:HH11	1.82	0.44
2:P:122:GLY:C	2:P:124:THR:N	2.75	0.44
7:U:151:THR:HG22	7:U:157:TYR:CB	2.47	0.44
8:V:159:ILE:HD13	8:V:159:ILE:N	2.33	0.44
10:X:189:ASP:HA	10:X:191:GLN:OE1	2.18	0.44
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	2.00	0.44
11:Y:89:GLN:HG3	16:Y:2014:HOH:O	2.18	0.44
12:Z:90:LYS:HE3	12:Z:93:PHE:O	2.18	0.44
14:2:144:GLU:O	14:2:145:ASN:HB2	2.18	0.44
2:B:21:LEU:HD13	2:B:124:THR:HG23	2.00	0.43
2:B:198:SER:CA	2:B:205:LEU:HD22	2.48	0.43
4:D:59:LEU:HD13	4:D:59:LEU:C	2.43	0.43
5:E:180:LEU:C	5:E:18(B):THR:N	2.76	0.43
6:F:43:ASN:HD21	6:F:185:SER:HA	1.82	0.43
7:G:228:ASN:N	7:G:228:ASN:HD22	2.16	0.43
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.99	0.43
9:I:33:LYS:O	9:I:44:GLY:HA2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:140:HIS:CD2	10:J:141:HIS:CE1	3.05	0.43
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.48	0.43
12:L:103:GLY:HA2	12:L:178:VAL:HG11	2.00	0.43
3:Q:57:LYS:HD2	3:Q:57:LYS:C	2.43	0.43
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.18	0.43
9:I:66:TYR:CE1	9:I:70:GLU:HG3	2.53	0.43
12:L:129:ALA:HB1	12:L:166:HIS:NE2	2.32	0.43
4:R:174:ALA:O	4:R:177:LEU:HB2	2.18	0.43
6:T:38:ILE:HG22	6:T:164:ALA:HB1	2.00	0.43
6:T:179:LEU:CD1	6:T:196:ILE:HD11	2.48	0.43
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.99	0.43
9:W:66:TYR:CE1	9:W:70:GLU:HG3	2.53	0.43
13:1:45:ILE:HG21	13:1:52:MET:HG3	1.99	0.43
6:F:43:ASN:HD22	6:F:43:ASN:H	1.54	0.43
7:G:110:ASP:HB3	7:G:149:TYR:CE2	2.53	0.43
10:J:25:SER:HB2	11:K:131:GLN:NE2	2.29	0.43
13:M:115:LEU:HD23	13:M:115:LEU:N	2.33	0.43
14:N:175:MET:HE3	14:N:18(B):PHE:CD2	2.53	0.43
14:2:84:LYS:HD3	14:2:84:LYS:C	2.43	0.43
3:C:57:LYS:HD2	3:C:57:LYS:C	2.43	0.43
3:C:156:ILE:HG23	16:C:264:HOH:O	2.18	0.43
4:D:119:LEU:O	4:D:120:ALA:C	2.62	0.43
5:E:22:PHE:O	5:E:23:GLN:C	2.61	0.43
5:E:38:VAL:HG12	5:E:39:GLY:N	2.34	0.43
7:G:121:GLN:NE2	7:G:121:GLN:C	2.76	0.43
11:K:47:GLY:CA	15:K:2000:ESY:H31	2.48	0.43
12:L:5:GLY:O	12:L:124:CYS:HA	2.18	0.43
1:O:225:THR:OG1	1:O:228:GLU:HG3	2.18	0.43
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.17	0.43
4:R:119:LEU:O	4:R:120:ALA:C	2.61	0.43
4:R:170:GLU:CD	4:R:170:GLU:N	2.75	0.43
6:T:63:LYS:O	6:T:65:VAL:HG23	2.18	0.43
7:U:8:TYR:C	7:U:10:ARG:N	2.75	0.43
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.48	0.43
12:Z:14(I):THR:HG21	12:Z:14(M):VAL:HB	2.01	0.43
14:2:14:LEU:HD12	14:2:14:LEU:N	2.33	0.43
1:A:38:LEU:C	1:A:38:LEU:HD12	2.43	0.43
3:C:150:GLN:HG2	3:C:151:THR:N	2.33	0.43
4:D:117:CYS:HB3	4:D:155:GLY:O	2.18	0.43
5:E:48:LEU:HD23	5:E:48:LEU:HA	1.87	0.43
10:J:18:LYS:HD3	10:J:174:ILE:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:113:ILE:HA	10:J:118:THR:O	2.19	0.43
1:O:142:ASP:OD1	1:O:145:ASN:HB2	2.18	0.43
3:Q:187:GLU:HG3	3:Q:232:TYR:OH	2.17	0.43
7:U:39:ALA:CB	7:U:48:VAL:HG12	2.47	0.43
8:V:18:THR:HB	8:V:30:ASN:HD22	1.84	0.43
11:Y:74:ILE:HD11	11:Y:78:ALA:HB3	2.00	0.43
1:A:12:LEU:HD12	1:A:129:VAL:N	2.33	0.43
5:E:226:GLY:O	5:E:227:GLU:C	2.61	0.43
7:G:74:ILE:HD11	7:G:107:MET:O	2.19	0.43
10:J:25:SER:CB	11:K:131:GLN:NE2	2.82	0.43
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.81	0.43
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.54	0.43
3:Q:112:LEU:O	3:Q:112:LEU:HD13	2.18	0.43
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.53	0.43
4:R:172:ALA:O	4:R:175:GLU:HB3	2.19	0.43
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.49	0.43
5:S:111:ARG:HA	5:S:114:HIS:HD2	1.84	0.43
5:S:155:GLY:O	6:T:83:PRO:HG3	2.19	0.43
5:S:180:LEU:C	5:S:18(B):THR:N	2.77	0.43
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.74	0.43
14:2:1:THR:HA	14:2:33:LYS:NZ	2.33	0.43
14:2:161:GLN:NE2	14:2:165:TRP:HE1	2.16	0.43
1:A:46:VAL:HG11	1:A:139:ALA:HB1	1.99	0.43
2:B:136:PHE:O	2:B:150:THR:HA	2.19	0.43
2:B:20(A):SER:HB2	2:B:20(B):ALA:H	1.68	0.43
3:C:40:VAL:HG12	3:C:162:ALA:CB	2.43	0.43
5:E:15:PHE:H	6:F:23:GLN:HE22	1.66	0.43
7:G:82:ILE:HG22	7:G:83:PRO:HD3	2.01	0.43
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.76	0.43
13:M:110:LEU:HG	13:M:125:LEU:HD12	2.01	0.43
14:N:1:THR:HA	14:N:33:LYS:NZ	2.34	0.43
1:O:142:ASP:HB2	16:O:254:HOH:O	2.17	0.43
2:P:21:LEU:HD13	2:P:124:THR:HG23	2.00	0.43
2:P:213:ALA:HA	2:P:222:LYS:O	2.18	0.43
3:Q:40:VAL:HG12	3:Q:162:ALA:CB	2.45	0.43
5:S:76:LEU:HA	5:S:137:LEU:O	2.19	0.43
7:U:29:LYS:HA	7:U:29:LYS:HD2	1.75	0.43
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.99	0.43
10:X:143:ARG:HG2	10:X:143:ARG:HH11	1.84	0.43
11:Y:47:GLY:CA	15:Y:2000:ESY:H31	2.48	0.43
14:2:13:ILE:HG12	14:2:177:VAL:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:93:GLY:N	9:I:94:PRO:CD	2.82	0.43
12:L:114:ASP:HB2	12:L:118:SER:H	1.82	0.43
14:N:105:ASP:HB3	14:N:106:ASN:HB2	2.01	0.43
1:O:46:VAL:HG11	1:O:139:ALA:HB1	2.00	0.43
2:P:107:ILE:HG21	2:P:112:LEU:HD12	2.00	0.43
3:Q:26:TYR:N	3:Q:26:TYR:CD1	2.86	0.43
3:Q:150:GLN:HG2	3:Q:151:THR:N	2.33	0.43
3:Q:195:ARG:HG3	3:Q:236:ILE:CD1	2.48	0.43
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.54	0.43
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.82	0.43
7:U:139:VAL:HA	7:U:147:SER:O	2.19	0.43
7:U:171:GLU:OE1	7:U:171:GLU:N	2.50	0.43
10:X:6:ILE:CG2	10:X:13:ILE:HB	2.49	0.43
11:Y:113:VAL:HA	11:Y:118:THR:O	2.18	0.43
13:1:61:ASP:O	13:1:65:GLU:HB2	2.18	0.43
1:A:92:SER:OG	1:A:116:VAL:HG22	2.19	0.43
3:C:38:VAL:HG22	3:C:39:GLY:N	2.34	0.43
3:C:57:LYS:O	3:C:57:LYS:HE3	2.19	0.43
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.54	0.43
4:D:172:ALA:HB2	4:D:200:VAL:HG11	2.00	0.43
5:E:45:HIS:HB2	5:E:189:LEU:HD12	2.00	0.43
9:I:104:ILE:HG21	9:I:181:LYS:HG2	1.99	0.43
9:I:130:ALA:HB2	9:I:166:ASP:CB	2.49	0.43
10:J:18:LYS:CG	10:J:174:ILE:HG13	2.49	0.43
11:K:2:THR:OG1	11:K:130:GLY:HA3	2.18	0.43
11:K:196:PHE:HB3	16:K:2005:HOH:O	2.18	0.43
14:N:59:VAL:HG22	14:N:82:VAL:HG12	2.00	0.43
5:S:52:LYS:HD3	5:S:211:SER:HB2	2.01	0.43
7:U:25:GLU:O	7:U:28:PHE:HB2	2.19	0.43
10:X:4:LEU:HB2	10:X:15:ALA:HB3	2.01	0.43
11:Y:1:THR:O	11:Y:128:GLY:HA3	2.19	0.43
11:Y:2:THR:OG1	11:Y:130:GLY:HA3	2.19	0.43
12:Z:100:ILE:HD11	12:Z:125:ARG:HG3	2.01	0.43
4:D:179:GLU:HG3	4:D:192:LEU:HD11	2.01	0.43
6:F:191:LYS:HA	6:F:232:ALA:HB1	2.00	0.43
9:I:5:ALA:HA	9:I:13:ALA:O	2.18	0.43
14:N:52:THR:HG22	14:N:97:ALA:HB1	2.00	0.43
3:Q:57:LYS:O	3:Q:57:LYS:HE3	2.18	0.43
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.49	0.43
4:R:241:GLU:C	4:R:243:ALA:H	2.27	0.43
10:X:98:ASN:HB3	10:X:127:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:129:TYR:O	10:X:132:PHE:HB2	2.19	0.43
13:1:1:THR:OG1	13:1:2:SER:N	2.52	0.43
13:1:4:ILE:CD1	13:1:159:MET:SD	3.07	0.43
14:2:52:THR:HG22	14:2:97:ALA:HB1	2.00	0.43
14:2:77:GLU:HB2	16:2:197:HOH:O	2.18	0.43
2:B:73:LYS:O	2:B:140:GLY:HA2	2.19	0.42
3:C:57:LYS:C	3:C:57:LYS:CD	2.93	0.42
3:C:195:ARG:HG3	3:C:236:ILE:CD1	2.49	0.42
5:E:17:PRO:HG3	6:F:26:TYR:CE2	2.53	0.42
10:J:113:ILE:HG12	10:J:119:LYS:HG3	2.01	0.42
13:M:1:THR:HG22	16:M:212:HOH:O	2.19	0.42
1:O:214:ILE:HD12	1:O:222:ARG:O	2.19	0.42
3:Q:97:GLN:HG3	10:X:65:LEU:HB2	2.01	0.42
3:Q:125:GLN:HB2	4:R:130:ARG:HG2	2.00	0.42
3:Q:161:SER:HB3	3:Q:180:TYR:CE1	2.54	0.42
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.49	0.42
6:T:203:GLU:C	6:T:205:ASN:N	2.77	0.42
9:W:-2:ASN:HB3	9:W:20:LEU:HD22	2.00	0.42
13:1:190:LEU:N	13:1:190:LEU:CD1	2.82	0.42
14:2:19:ARG:HG3	14:2:26:ILE:HG23	2.01	0.42
2:B:141:TYR:CD1	2:B:141:TYR:C	2.98	0.42
4:D:123:PHE:CZ	4:D:131:PRO:HG3	2.53	0.42
5:E:134:VAL:O	5:E:153:PRO:HG3	2.19	0.42
7:G:74:ILE:HG21	7:G:112:LEU:HD23	2.00	0.42
7:G:18(B):ASP:O	7:G:18(C):HIS:HB3	2.19	0.42
8:H:1:THR:HA	8:H:33:LYS:NZ	2.34	0.42
8:H:18:THR:HB	8:H:30:ASN:HD22	1.84	0.42
9:I:6:MET:HE1	9:I:155:ILE:HA	2.00	0.42
10:J:175:VAL:HG12	10:J:176:LYS:N	2.34	0.42
2:P:5:SER:O	2:P:7:ARG:N	2.52	0.42
3:Q:57:LYS:HG2	3:Q:208:LYS:HZ3	1.84	0.42
4:R:160:TYR:HB3	4:R:162:ALA:O	2.19	0.42
13:1:37:VAL:CG1	13:1:79:ILE:CD1	2.97	0.42
3:C:18(D):GLU:N	3:C:182:PRO:HD3	2.34	0.42
5:E:74:MET:HE2	5:E:109:VAL:HG22	2.00	0.42
5:E:111:ARG:O	5:E:115:LEU:HG	2.20	0.42
6:F:179:LEU:CD1	6:F:196:ILE:HD11	2.49	0.42
7:G:39:ALA:CB	7:G:48:VAL:HG12	2.49	0.42
7:G:105:TYR:OH	8:H:66:HIS:HE1	2.02	0.42
7:G:233:LEU:O	7:G:236:ILE:HG13	2.19	0.42
11:K:45:MET:HG2	11:K:52:CYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:69:LEU:C	1:O:69:LEU:CD2	2.93	0.42
2:P:209:ARG:HH11	2:P:209:ARG:HG2	1.83	0.42
5:S:18(D):ILE:HG23	5:S:18(E):LYS:HG3	2.02	0.42
6:T:157:TYR:CD1	6:T:157:TYR:C	2.97	0.42
7:U:233:LEU:O	7:U:236:ILE:HG13	2.19	0.42
10:X:16:SER:HB2	16:X:226:HOH:O	2.19	0.42
13:1:184:LEU:HD23	13:1:185:THR:N	2.34	0.42
14:2:89:GLU:OE1	14:2:89:GLU:HA	2.18	0.42
5:E:54:ASN:ND2	5:E:56:ASP:O	2.45	0.42
7:G:77:VAL:HG12	7:G:137:THR:HB	2.01	0.42
9:I:45:ILE:HG22	9:I:52:VAL:HG22	2.01	0.42
10:J:6:ILE:CG2	10:J:13:ILE:HB	2.50	0.42
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.49	0.42
12:L:13:VAL:HG12	12:L:177:ILE:HG12	2.02	0.42
1:O:47:VAL:HG23	1:O:214:ILE:HG22	2.00	0.42
2:P:176:LEU:C	2:P:178:MET:H	2.27	0.42
3:Q:18(D):GLU:N	3:Q:182:PRO:HD3	2.34	0.42
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.19	0.42
5:S:38:VAL:HG12	5:S:39:GLY:N	2.34	0.42
6:T:43:ASN:HD21	6:T:185:SER:HA	1.84	0.42
6:T:70:VAL:HB	6:T:74:ILE:HB	2.01	0.42
7:U:65:SER:HA	7:U:211:GLU:OE2	2.19	0.42
7:U:74:ILE:HD11	7:U:107:MET:O	2.20	0.42
9:W:104:ILE:HG21	9:W:181:LYS:HG2	2.00	0.42
13:1:164:TYR:C	13:1:165:ARG:HD2	2.45	0.42
14:2:146:MET:CE	14:2:150:GLU:HB3	2.48	0.42
1:A:150:GLN:O	1:A:157:TYR:HA	2.19	0.42
5:E:4:PHE:O	5:E:5:ARG:C	2.62	0.42
5:E:90:ASN:O	5:E:94:GLN:HG3	2.20	0.42
6:F:137:ILE:HA	6:F:149:TYR:O	2.20	0.42
7:G:172:ILE:HD12	7:G:197:MET:HE3	2.01	0.42
10:J:7:ARG:HG2	10:J:7:ARG:NH1	2.35	0.42
12:L:14(I):THR:O	12:L:1(I):ASN:CB	2.68	0.42
3:Q:163:GLN:HG3	3:Q:164:THR:N	2.33	0.42
5:S:4:PHE:O	5:S:5:ARG:C	2.62	0.42
5:S:154:SER:OG	5:S:156:ASN:ND2	2.49	0.42
8:V:172:ASN:ND2	8:V:193:THR:HA	2.34	0.42
9:W:168:LEU:HD22	16:W:206:HOH:O	2.19	0.42
10:X:52:THR:HG23	10:X:53:VAL:HG23	2.01	0.42
11:Y:7:ARG:CG	11:Y:108:PRO:HB2	2.48	0.42
12:Z:83:ILE:HB	12:Z:113:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:87:LEU:HD23	12:Z:95:TYR:HD1	1.85	0.42
2:B:215:ILE:HG13	2:B:221:GLN:HG2	2.02	0.42
3:C:100:ARG:HH11	3:C:106:PRO:HB3	1.84	0.42
4:D:177:LEU:CD1	5:E:58:LEU:HD11	2.47	0.42
4:D:241:GLU:C	4:D:243:ALA:H	2.27	0.42
5:E:44:THR:C	5:E:45:HIS:HD1	2.27	0.42
5:E:97:ASN:HD22	5:E:97:ASN:HA	1.67	0.42
9:I:120:ASP:OD2	9:I:120:ASP:C	2.62	0.42
11:K:2:THR:HG22	11:K:159:ILE:HD13	2.01	0.42
11:K:25:TRP:HH2	12:L:135:MET:HB2	1.83	0.42
3:Q:62(A):ILE:O	3:Q:63:THR:C	2.61	0.42
7:U:110:ASP:HB3	7:U:149:TYR:CE2	2.54	0.42
9:W:3:VAL:HG22	9:W:16:CYS:HB3	2.00	0.42
1:A:214:ILE:HD12	1:A:222:ARG:O	2.20	0.42
3:C:224:LEU:N	3:C:224:LEU:CD1	2.83	0.42
6:F:109:ILE:HD13	6:F:142:ASP:HB3	2.01	0.42
9:I:14:ILE:CG1	9:I:34:ILE:HD12	2.50	0.42
11:K:114:ASP:C	11:K:114:ASP:OD1	2.60	0.42
14:N:18(D):PRO:C	14:N:18(F):GLU:N	2.78	0.42
2:P:66:LYS:O	2:P:77:ALA:HA	2.20	0.42
4:R:32:LYS:O	4:R:167:SER:HA	2.19	0.42
5:S:44:THR:C	5:S:45:HIS:HD1	2.28	0.42
5:S:150:GLU:O	5:S:157:VAL:HA	2.19	0.42
9:W:66:TYR:CZ	9:W:74:ILE:HD12	2.55	0.42
6:F:198:TYR:HE2	6:F:237:GLN:NE2	2.17	0.42
11:K:64:ARG:NH2	11:K:68:LEU:HD21	2.35	0.42
14:N:41:ILE:HD13	14:N:76:THR:HA	2.01	0.42
1:O:21(P):LYS:N	16:O:248:HOH:O	2.38	0.42
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	2.02	0.42
6:T:192:GLN:HE21	6:T:195:LYS:CE	2.31	0.42
9:W:120:ASP:OD2	9:W:120:ASP:C	2.62	0.42
10:X:121:GLU:O	10:X:122:LEU:HD23	2.20	0.42
11:Y:76:VAL:HG22	11:Y:103:GLY:HA3	2.00	0.42
13:1:-4:ILE:HG22	13:1:-3:VAL:N	2.34	0.42
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.18	0.42
5:E:76:LEU:HA	5:E:137:LEU:O	2.19	0.42
8:H:159:ILE:HD13	8:H:159:ILE:N	2.33	0.42
12:L:90:LYS:HE3	12:L:93:PHE:O	2.19	0.42
13:M:124:THR:O	13:M:125:LEU:HD23	2.20	0.42
1:O:69:LEU:HD23	1:O:70:LEU:N	2.35	0.42
2:P:73:LYS:O	2:P:140:GLY:HA2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:229:ILE:HA	2:P:232:ILE:HG22	2.02	0.42
5:S:167:ALA:O	5:S:168:ARG:HB2	2.19	0.42
5:S:18(C):PHE:CD1	5:S:18(D):ILE:N	2.88	0.42
5:S:185:ASN:OD1	5:S:188:GLU:HG2	2.20	0.42
5:S:201:LEU:O	5:S:202:ARG:CB	2.67	0.42
5:S:212:ILE:HD12	5:S:229:VAL:HG11	2.01	0.42
8:V:25:ILE:HD12	8:V:25:ILE:N	2.35	0.42
11:Y:45:MET:HG2	11:Y:52:CYS:HB2	2.02	0.42
11:Y:172:SER:CA	11:Y:192:VAL:HG23	2.50	0.42
13:1:17:ASP:OD2	13:1:17:ASP:C	2.63	0.42
14:2:121:LYS:O	14:2:122:LEU:HD23	2.20	0.42
2:B:17:PRO:HA	3:C:26:TYR:CE2	2.55	0.42
2:B:122:GLY:C	2:B:124:THR:N	2.78	0.42
5:E:18(C):PHE:CD1	5:E:18(D):ILE:N	2.88	0.42
6:F:179:LEU:HD11	6:F:196:ILE:HD11	2.02	0.42
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.55	0.42
2:P:194:LEU:HD21	2:P:212:PHE:CE1	2.55	0.42
2:P:214:THR:C	2:P:215:ILE:HD12	2.44	0.42
3:Q:150:GLN:HE21	3:Q:150:GLN:HB3	1.61	0.42
3:Q:158:SER:HB2	4:R:59:LEU:HD21	2.02	0.42
8:V:103:GLY:HA2	8:V:178:MET:SD	2.60	0.42
9:W:22:SER:O	9:W:23:GLN:HB2	2.20	0.42
9:W:33:LYS:O	9:W:44:GLY:HA2	2.20	0.42
10:X:25:SER:CB	11:Y:131:GLN:NE2	2.83	0.42
10:X:31:ASP:HB3	10:X:33:LYS:NZ	2.35	0.42
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.20	0.41
3:C:169:SER:HA	3:C:172:VAL:CG1	2.50	0.41
5:E:214:ILE:O	5:E:221:PHE:HA	2.20	0.41
7:G:107:MET:CE	7:G:112:LEU:HD13	2.48	0.41
9:I:58:MET:O	9:I:61:TYR:HB3	2.20	0.41
10:J:129:TYR:O	10:J:132:PHE:HB2	2.20	0.41
11:K:74:ILE:HD13	11:K:75:SER:O	2.20	0.41
14:N:130:GLY:HA2	14:N:166:ASP:HB2	2.02	0.41
2:P:88:LEU:HB3	2:P:116:LEU:HD21	2.01	0.41
2:P:89:ILE:O	2:P:92:ALA:HB3	2.19	0.41
3:Q:125:GLN:HG3	3:Q:125:GLN:O	2.20	0.41
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.54	0.41
6:T:137:ILE:HA	6:T:149:TYR:O	2.20	0.41
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.85	0.41
10:X:18:LYS:HD3	10:X:174:ILE:CG1	2.50	0.41
11:Y:74:ILE:HD12	11:Y:79:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:126:ILE:HD13	14:2:126:ILE:N	2.33	0.41
14:2:130:GLY:HA2	14:2:166:ASP:HB2	2.01	0.41
5:E:125:GLN:HB3	16:E:248:HOH:O	2.19	0.41
7:G:184:ASN:HD22	7:G:184:ASN:HA	1.69	0.41
14:N:84:LYS:HD3	14:N:84:LYS:C	2.45	0.41
12:Z:70(A):ASN:O	12:Z:72:LYS:N	2.53	0.41
3:C:175:PHE:O	3:C:179:ASN:HB2	2.21	0.41
5:E:167:ALA:O	5:E:168:ARG:HB2	2.20	0.41
5:E:199:GLN:NE2	5:E:199:GLN:HA	2.36	0.41
5:E:212:ILE:HD12	5:E:229:VAL:HG11	2.02	0.41
6:F:107:ILE:O	6:F:107:ILE:HG23	2.20	0.41
7:G:25:GLU:O	7:G:28:PHE:HB2	2.21	0.41
10:J:31:ASP:HB3	10:J:33:LYS:NZ	2.35	0.41
10:J:93:ARG:HH11	10:J:93:ARG:HG2	1.85	0.41
11:K:109:THR:HA	16:K:2004:HOH:O	2.19	0.41
11:K:131:GLN:CG	11:K:132:THR:N	2.81	0.41
12:L:14(I):THR:HG21	12:L:14(M):VAL:HB	2.02	0.41
4:R:17:PRO:HA	5:S:26:TYR:CD2	2.55	0.41
4:R:120:ALA:HB3	4:R:155:GLY:HA2	2.03	0.41
4:R:243:ALA:O	4:R:244:GLU:HG2	2.19	0.41
6:T:130:ARG:HG2	6:T:130:ARG:HH11	1.85	0.41
7:U:135:ILE:CG2	7:U:150:LYS:HD2	2.49	0.41
7:U:18(D):ILE:N	7:U:18(D):ILE:CD1	2.83	0.41
10:X:166:MET:HA	10:X:167:PRO:HD3	1.77	0.41
14:2:8:PHE:CE1	14:2:10:ASP:HB2	2.55	0.41
14:2:65:LEU:HG	14:2:69:GLN:HE21	1.86	0.41
1:A:62:GLU:O	1:A:64:LEU:N	2.53	0.41
4:D:32:LYS:O	4:D:167:SER:HA	2.20	0.41
5:E:123:ASN:N	5:E:123:ASN:HD22	2.18	0.41
6:F:24:VAL:O	6:F:27:ALA:HB3	2.20	0.41
7:G:218:ASP:O	7:G:220:LYS:HB2	2.19	0.41
8:H:18:THR:HB	8:H:30:ASN:HA	2.01	0.41
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.84	0.41
11:K:87:VAL:HG11	11:K:115:SER:HA	2.02	0.41
14:N:13:ILE:HG12	14:N:177:VAL:HG13	2.02	0.41
3:Q:112:LEU:HD13	3:Q:112:LEU:C	2.45	0.41
5:S:54:ASN:ND2	5:S:56:ASP:O	2.46	0.41
5:S:226:GLY:O	5:S:227:GLU:C	2.62	0.41
6:T:61:PRO:O	6:T:62:GLN:HB2	2.20	0.41
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.68	0.41
8:V:18:THR:HB	8:V:30:ASN:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:93:GLY:N	9:W:94:PRO:CD	2.82	0.41
14:2:105:ASP:HB3	14:2:106:ASN:HB2	2.03	0.41
14:2:10(B):LYS:C	14:2:10(B):LYS:CD	2.91	0.41
1:A:39:GLY:HA2	1:A:47:VAL:O	2.21	0.41
5:E:185:ASN:OD1	5:E:188:GLU:HG2	2.19	0.41
6:F:192:GLN:HE21	6:F:195:LYS:CE	2.34	0.41
7:G:78:VAL:HG11	7:G:85:ALA:CB	2.50	0.41
13:M:46:SER:HG	13:M:98:ALA:HB3	1.85	0.41
13:M:164:TYR:O	14:2:26:ILE:HD12	2.20	0.41
3:Q:57:LYS:C	3:Q:57:LYS:CD	2.93	0.41
4:R:59:LEU:HD13	4:R:59:LEU:C	2.46	0.41
4:R:117:CYS:HB3	4:R:155:GLY:O	2.20	0.41
4:R:123:PHE:CZ	4:R:131:PRO:HG3	2.56	0.41
5:S:189:LEU:HD23	5:S:189:LEU:HA	1.91	0.41
5:S:226:GLY:C	5:S:228:ALA:N	2.78	0.41
9:W:101:VAL:O	9:W:110:ILE:HA	2.21	0.41
13:1:19:LEU:HB3	16:1:212:HOH:O	2.20	0.41
2:B:229:ILE:HA	2:B:232:ILE:HG22	2.02	0.41
3:C:87:ILE:HD13	3:C:87:ILE:N	2.35	0.41
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.54	0.41
6:F:99:PHE:CD1	6:F:99:PHE:C	2.99	0.41
8:H:103:GLY:HA2	8:H:178:MET:SD	2.60	0.41
9:I:22:SER:O	9:I:23:GLN:HB2	2.20	0.41
10:J:18:LYS:HD3	10:J:174:ILE:HG13	2.02	0.41
12:L:134:ILE:HG22	12:L:138:LEU:HD22	2.02	0.41
1:O:23:GLN:OE1	7:U:15:PHE:HB2	2.21	0.41
1:O:212:LEU:HD23	1:O:212:LEU:C	2.46	0.41
2:P:11:ARG:O	2:P:14:ILE:HD13	2.21	0.41
2:P:126:HIS:CB	3:Q:129:VAL:HG12	2.48	0.41
3:Q:121:GLN:NE2	3:Q:122:ARG:N	2.69	0.41
4:R:52:LYS:HE3	4:R:211:GLN:HB2	2.03	0.41
6:T:99:PHE:CD1	6:T:99:PHE:C	2.98	0.41
7:U:82:ILE:HG22	7:U:83:PRO:HD3	2.02	0.41
14:2:18(D):PRO:C	14:2:18(F):GLU:N	2.78	0.41
2:B:4:GLY:HA3	5:E:127:TYR:CE1	2.56	0.41
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.50	0.41
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.84	0.41
10:J:168:MET:CG	10:X:168:MET:HE3	2.50	0.41
11:K:172:SER:CA	11:K:192:VAL:HG23	2.50	0.41
1:O:15:PHE:HD2	2:P:23:GLN:NE2	2.19	0.41
1:O:26:TYR:O	1:O:29:THR:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:29:THR:O	1:O:33:GLN:HG2	2.21	0.41
1:O:225:THR:O	1:O:229:ILE:HG12	2.19	0.41
3:Q:224:LEU:N	3:Q:224:LEU:CD1	2.83	0.41
4:R:12(G):GLU:HG2	4:R:125:GLU:H	1.85	0.41
4:R:197:LEU:O	4:R:201:MET:HG3	2.19	0.41
6:T:109:ILE:N	6:T:110:PRO:CD	2.84	0.41
10:X:7:ARG:HG2	10:X:7:ARG:NH1	2.36	0.41
12:Z:99:THR:HG23	16:Z:202:HOH:O	2.19	0.41
1:A:47:VAL:HG23	1:A:214:ILE:HG22	2.03	0.41
3:C:152:GLU:HB2	3:C:153:PRO:HD2	2.03	0.41
3:C:187:GLU:HG3	3:C:232:TYR:OH	2.20	0.41
7:G:29:LYS:HA	7:G:29:LYS:HD2	1.78	0.41
8:H:25:ILE:HD12	8:H:25:ILE:N	2.35	0.41
11:K:37:ILE:H	11:K:37:ILE:HD12	1.86	0.41
12:L:148:VAL:HG13	12:L:149:GLU:N	2.36	0.41
12:L:175:ILE:C	12:L:176:LEU:HD12	2.45	0.41
4:R:119:LEU:O	4:R:122:ARG:HB2	2.21	0.41
5:S:22:PHE:O	5:S:23:GLN:C	2.63	0.41
6:T:12:ASN:O	6:T:14:VAL:N	2.54	0.41
6:T:159:GLY:C	6:T:160:TYR:CD1	2.98	0.41
7:U:107:MET:CE	7:U:112:LEU:HD13	2.48	0.41
11:Y:74:ILE:HD13	11:Y:75:SER:O	2.21	0.41
13:1:46:SER:OG	13:1:98:ALA:HB3	2.21	0.41
14:2:12:VAL:HG22	14:2:13:ILE:N	2.36	0.41
1:A:22:GLY:O	1:A:25:ASP:HB2	2.21	0.41
1:A:62:GLU:C	1:A:64:LEU:N	2.79	0.41
2:B:32:SER:O	2:B:167:ALA:HA	2.21	0.41
4:D:12(G):GLU:HG2	4:D:125:GLU:H	1.85	0.41
4:D:243:ALA:O	4:D:244:GLU:HG2	2.21	0.41
6:F:13:SER:HB3	6:F:125:LEU:C	2.46	0.41
6:F:87:HIS:CD2	6:F:87:HIS:C	2.98	0.41
8:H:132:LEU:HB2	16:H:233:HOH:O	2.20	0.41
9:I:5:ALA:HB2	9:I:14:ILE:HD13	2.03	0.41
10:J:25:SER:CB	11:K:131:GLN:HE22	2.29	0.41
11:K:105:THR:OG1	11:K:106:GLU:HG3	2.21	0.41
11:K:162:ALA:O	11:K:163:ALA:C	2.63	0.41
12:L:2:THR:HG21	12:L:130:ALA:HB3	2.02	0.41
13:M:175:LEU:C	13:M:175:LEU:HD23	2.45	0.41
1:O:62:GLU:O	1:O:64:LEU:N	2.52	0.41
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.34	0.41
2:P:142:ASP:OD1	2:P:142:ASP:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:186:VAL:O	2:P:190:ILE:HG13	2.21	0.41
2:P:215:ILE:HG13	2:P:221:GLN:HG2	2.01	0.41
5:S:29:GLU:C	5:S:31:ILE:N	2.79	0.41
5:S:67:ILE:HG22	5:S:223:ILE:HD11	2.03	0.41
6:T:13:SER:HB2	7:U:130:ARG:HB3	2.03	0.41
6:T:198:TYR:HE2	6:T:237:GLN:NE2	2.19	0.41
7:U:77:VAL:HG12	7:U:137:THR:HB	2.02	0.41
7:U:158:VAL:HG22	7:U:159:GLY:H	1.85	0.41
10:X:18:LYS:CG	10:X:174:ILE:HG13	2.50	0.41
10:X:179:ASP:O	10:X:181:ASP:N	2.54	0.41
13:1:205:GLY:HA3	16:1:234:HOH:O	2.20	0.41
1:A:210:ILE:HD13	1:A:210:ILE:N	2.36	0.41
2:B:186:VAL:O	2:B:190:ILE:HG13	2.20	0.41
2:B:214:THR:C	2:B:215:ILE:HD12	2.45	0.41
5:E:97:ASN:ND2	12:L:61:ASN:HD21	2.17	0.41
1:O:149:TYR:CE1	1:O:159:PRO:HB3	2.56	0.41
2:P:233:LEU:HD12	2:P:233:LEU:HA	1.94	0.41
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	2.01	0.41
4:R:76:CYS:HB2	4:R:137:LEU:O	2.21	0.41
4:R:192:LEU:O	4:R:196:ILE:CD1	2.69	0.41
5:S:214:ILE:O	5:S:221:PHE:HA	2.20	0.41
6:T:179:LEU:HD11	6:T:196:ILE:HD11	2.01	0.41
7:U:99:PHE:CD1	7:U:99:PHE:C	2.99	0.41
7:U:194:ILE:HG23	7:U:210:LEU:HD11	2.01	0.41
9:W:6:MET:HE1	9:W:155:ILE:HA	2.03	0.41
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.63	0.41
12:Z:148:VAL:O	12:Z:152:ILE:HG13	2.20	0.41
1:A:26:TYR:O	1:A:29:THR:HB	2.21	0.40
2:B:142:ASP:OD1	2:B:142:ASP:C	2.63	0.40
4:D:119:LEU:O	4:D:122:ARG:HB2	2.20	0.40
4:D:191:LEU:HD12	4:D:191:LEU:HA	1.96	0.40
5:E:198:SER:HA	5:E:201:LEU:CD1	2.50	0.40
7:G:8:TYR:C	7:G:10:ARG:N	2.75	0.40
8:H:50:ALA:HB2	9:I:118:CYS:HB2	2.03	0.40
9:I:143:GLU:HG3	9:I:146:LEU:HD21	2.03	0.40
10:J:6:ILE:HG23	10:J:13:ILE:HG13	2.02	0.40
11:K:74:ILE:HD11	11:K:78:ALA:HB3	2.03	0.40
4:R:65:GLU:HA	16:R:750:HOH:O	2.21	0.40
11:Y:32:LYS:HD2	11:Y:32:LYS:N	2.36	0.40
11:Y:45:MET:HE2	11:Y:53:GLN:CB	2.50	0.40
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:93:PHE:N	12:Z:94:PRO:CD	2.83	0.40
12:Z:105:ASP:OD1	12:Z:105:ASP:C	2.64	0.40
13:1:186:PHE:HE1	13:1:188:LYS:HG3	1.86	0.40
1:A:134:VAL:O	1:A:153:PRO:HG3	2.21	0.40
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.56	0.40
4:D:197:LEU:O	4:D:201:MET:HG3	2.21	0.40
5:E:111:ARG:HA	5:E:114:HIS:HD2	1.86	0.40
6:F:157:TYR:CD1	6:F:157:TYR:C	2.98	0.40
6:F:192:GLN:HE21	6:F:195:LYS:HE3	1.87	0.40
7:G:26:TYR:N	7:G:26:TYR:CD1	2.88	0.40
9:I:124:PHE:C	9:I:125:ILE:HD12	2.46	0.40
10:J:155:LEU:HD23	10:J:155:LEU:HA	1.93	0.40
12:L:134:ILE:O	12:L:137:PHE:HB3	2.20	0.40
13:M:9:ASP:OD1	13:M:10:ASN:N	2.54	0.40
14:N:6:VAL:HG23	14:N:155:ILE:HD11	2.03	0.40
1:O:57:PRO:HG2	7:U:177:GLU:HG2	2.01	0.40
2:P:21(B):GLY:O	2:P:217:ALA:C	2.64	0.40
3:Q:134:VAL:CG1	3:Q:135:SER:N	2.85	0.40
8:V:147:THR:OG1	8:V:150:GLU:HG3	2.21	0.40
10:X:70:GLU:O	10:X:71:ASP:C	2.64	0.40
1:A:212:LEU:HD23	1:A:212:LEU:C	2.46	0.40
2:B:39:GLY:O	2:B:162:ALA:HA	2.22	0.40
2:B:182:ASP:C	2:B:184:MET:H	2.30	0.40
2:B:21(B):GLY:O	2:B:217:ALA:C	2.64	0.40
6:F:70:VAL:HB	6:F:74:ILE:HB	2.03	0.40
7:G:56:ASP:HB3	7:G:59:LEU:HG	2.04	0.40
7:G:99:PHE:CD1	7:G:99:PHE:C	2.99	0.40
7:G:140:SER:HA	7:G:215:ALA:HB1	2.03	0.40
9:I:66:TYR:CZ	9:I:74:ILE:HD12	2.56	0.40
12:L:87:LEU:HD23	12:L:95:TYR:HD1	1.87	0.40
12:L:140:ASN:ND2	9:W:161:ASN:HD21	2.19	0.40
13:M:1:THR:OG1	13:M:2:SER:N	2.53	0.40
13:M:17:ASP:C	13:M:17:ASP:OD2	2.64	0.40
14:N:1:THR:HG23	14:N:33:LYS:HD3	2.03	0.40
1:O:62:GLU:C	1:O:64:LEU:N	2.78	0.40
2:P:7:ARG:HG2	7:U:8:TYR:CZ	2.56	0.40
2:P:238:ILE:O	2:P:239:THR:O	2.38	0.40
3:Q:175:PHE:O	3:Q:179:ASN:HB2	2.21	0.40
6:T:187:ARG:HG3	6:T:187:ARG:NH1	2.35	0.40
7:U:17:PRO:HD3	16:U:259:HOH:O	2.22	0.40
7:U:56:ASP:HB3	7:U:59:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:100:ARG:HH11	7:U:100:ARG:HG3	1.85	0.40
9:W:29:ASN:ND2	9:W:29:ASN:N	2.55	0.40
12:Z:79:ALA:O	12:Z:82:ASN:HB3	2.22	0.40
12:Z:82:ASN:C	12:Z:82:ASN:HD22	2.28	0.40
13:1:9:ASP:OD1	13:1:10:ASN:N	2.54	0.40
2:B:107:ILE:HG21	2:B:112:LEU:HD12	2.02	0.40
3:C:112:LEU:C	3:C:112:LEU:HD13	2.45	0.40
4:D:243:ALA:O	4:D:244:GLU:HB2	2.22	0.40
5:E:18(D):ILE:HG23	5:E:18(E):LYS:HG3	2.04	0.40
12:L:1:GLY:HA3	12:L:33:LYS:NZ	2.36	0.40
13:M:51:ASP:O	13:M:54:HIS:HB3	2.22	0.40
13:M:186:PHE:HE1	13:M:188:LYS:HG3	1.87	0.40
1:O:134:VAL:O	1:O:153:PRO:HG3	2.21	0.40
5:S:143:LYS:HD3	13:1:71(B):GLU:O	2.21	0.40
5:S:216:GLY:O	5:S:219:THR:N	2.52	0.40
6:T:142:ASP:OD2	6:T:142:ASP:C	2.64	0.40
6:T:159:GLY:HA3	7:U:63:THR:HG21	2.03	0.40
1:A:5:THR:O	1:A:7:ARG:HG2	2.22	0.40
2:B:120:LYS:HZ1	2:B:136:PHE:HD1	1.68	0.40
3:C:89:ILE:HG22	3:C:93:ARG:HD2	2.03	0.40
6:F:109:ILE:N	6:F:110:PRO:CD	2.85	0.40
7:G:100:ARG:HG3	7:G:100:ARG:HH11	1.86	0.40
10:J:11:SER:HB3	10:J:179:ASP:HB3	2.03	0.40
13:M:164:TYR:C	13:M:165:ARG:HD2	2.46	0.40
14:N:121:LYS:O	14:N:122:LEU:HD23	2.21	0.40
14:N:161:GLN:NE2	14:N:165:TRP:HE1	2.20	0.40
2:P:5:SER:C	2:P:7:ARG:N	2.79	0.40
2:P:238:ILE:O	2:P:238:ILE:HG22	2.21	0.40
5:S:198:SER:HA	5:S:201:LEU:CD1	2.51	0.40
11:Y:124:ILE:CG2	11:Y:138:LEU:HD23	2.51	0.40
13:1:6:MET:HE3	13:1:14(A):VAL:CG2	2.51	0.40
13:1:18:ASN:HA	13:1:31:VAL:O	2.22	0.40
13:1:110:LEU:HG	13:1:125:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	228 (92%)	16 (6%)	4 (2%)	7	34
1	O	248/250 (99%)	229 (92%)	15 (6%)	4 (2%)	7	34
2	B	242/244 (99%)	218 (90%)	15 (6%)	9 (4%)	2	15
2	P	242/244 (99%)	216 (89%)	17 (7%)	9 (4%)	2	15
3	C	239/241 (99%)	219 (92%)	15 (6%)	5 (2%)	5	27
3	Q	239/241 (99%)	219 (92%)	15 (6%)	5 (2%)	5	27
4	D	240/242 (99%)	225 (94%)	10 (4%)	5 (2%)	5	27
4	R	240/242 (99%)	224 (93%)	11 (5%)	5 (2%)	5	27
5	E	231/233 (99%)	202 (87%)	20 (9%)	9 (4%)	2	14
5	S	231/233 (99%)	201 (87%)	21 (9%)	9 (4%)	2	14
6	F	242/244 (99%)	220 (91%)	18 (7%)	4 (2%)	7	32
6	T	242/244 (99%)	217 (90%)	21 (9%)	4 (2%)	7	32
7	G	241/243 (99%)	224 (93%)	15 (6%)	2 (1%)	16	50
7	U	241/243 (99%)	224 (93%)	15 (6%)	2 (1%)	16	50
8	H	220/222 (99%)	206 (94%)	12 (6%)	2 (1%)	14	48
8	V	220/222 (99%)	204 (93%)	14 (6%)	2 (1%)	14	48
9	I	202/204 (99%)	196 (97%)	5 (2%)	1 (0%)	24	60
9	W	202/204 (99%)	195 (96%)	6 (3%)	1 (0%)	24	60
10	J	196/198 (99%)	180 (92%)	12 (6%)	4 (2%)	6	28
10	X	196/198 (99%)	178 (91%)	14 (7%)	4 (2%)	6	28
11	K	210/212 (99%)	199 (95%)	11 (5%)	0	100	100
11	Y	210/212 (99%)	200 (95%)	10 (5%)	0	100	100
12	L	220/222 (99%)	206 (94%)	13 (6%)	1 (0%)	24	60
12	Z	220/222 (99%)	206 (94%)	13 (6%)	1 (0%)	24	60
13	1	231/233 (99%)	211 (91%)	20 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	231/233 (99%)	211 (91%)	20 (9%)	0	100	100
14	2	194/196 (99%)	186 (96%)	7 (4%)	1 (0%)	24	60
14	N	194/196 (99%)	186 (96%)	7 (4%)	1 (0%)	24	60
All	All	6312/6368 (99%)	5830 (92%)	388 (6%)	94 (2%)	8	35

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	LYS
2	B	20(A)	SER
3	C	58	LEU
4	D	12(G)	GLU
5	E	5	ARG
5	E	202	ARG
5	E	217	LYS
6	F	13	SER
6	F	64	ASN
7	G	239	GLN
12	L	71	ASP
1	O	167	LYS
2	P	20(A)	SER
3	Q	58	LEU
4	R	12(G)	GLU
5	S	5	ARG
5	S	202	ARG
5	S	217	LYS
6	T	13	SER
6	T	64	ASN
7	U	239	GLN
1	A	5	THR
1	A	63	THR
2	B	54	VAL
2	B	21(B)	GLY
2	B	21(C)	ASP
3	C	183	PRO
3	C	203	THR
4	D	120	ALA
4	D	18(D)	SER
5	E	64	GLN
5	E	18(A)	ASP
5	E	227	GLU

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Mol	Chain	Res	Type
7	G	55	PRO
8	H	91	GLN
1	O	5	THR
1	O	63	THR
2	P	54	VAL
2	P	21(B)	GLY
2	P	21(C)	ASP
3	Q	183	PRO
3	Q	203	THR
4	R	120	ALA
4	R	18(D)	SER
5	S	64	GLN
5	S	180	LEU
5	S	18(A)	ASP
5	S	227	GLU
7	U	55	PRO
8	V	91	GLN
12	Z	71	ASP
4	D	128	MET
5	E	180	LEU
5	E	203	ASP
10	J	8	VAL
2	P	6	ARG
4	R	128	MET
5	S	203	ASP
10	X	8	VAL
10	X	180	LYS
2	B	183	ASP
3	C	202	GLN
5	E	231	LYS
6	F	12	ASN
9	I	93	GLY
10	J	180	LYS
14	N	18(E)	ASP
2	P	183	ASP
2	P	217	ALA
3	Q	202	GLN
5	S	231	LYS
6	T	12	ASN
6	T	206	LYS
14	2	18(E)	ASP
2	B	6	ARG

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Mol	Chain	Res	Type
2	B	208	ASP
2	B	217	ALA
3	C	242	GLU
6	F	206	LYS
8	H	145	ASP
10	J	192	ALA
2	P	22	TYR
2	P	208	ASP
3	Q	242	GLU
8	V	145	ASP
9	W	93	GLY
10	X	192	ALA
1	A	204	GLY
2	B	22	TYR
10	J	49	ALA
1	O	204	GLY
10	X	49	ALA
4	R	12(F)	GLY
4	D	12(F)	GLY

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%)	197 (94%)	12 (6%)	18	52
1	O	209/209 (100%)	197 (94%)	12 (6%)	18	52
2	B	203/203 (100%)	187 (92%)	16 (8%)	11	39
2	P	203/203 (100%)	187 (92%)	16 (8%)	11	39
3	C	213/213 (100%)	199 (93%)	14 (7%)	15	46
3	Q	213/213 (100%)	198 (93%)	15 (7%)	14	44
4	D	198/198 (100%)	186 (94%)	12 (6%)	17	49
4	R	198/198 (100%)	186 (94%)	12 (6%)	17	49
5	E	192/192 (100%)	173 (90%)	19 (10%)	7	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	192/192 (100%)	173 (90%)	19 (10%)	7	30
6	F	201/201 (100%)	185 (92%)	16 (8%)	11	38
6	T	201/201 (100%)	186 (92%)	15 (8%)	12	41
7	G	207/207 (100%)	194 (94%)	13 (6%)	16	48
7	U	207/207 (100%)	194 (94%)	13 (6%)	16	48
8	H	181/181 (100%)	171 (94%)	10 (6%)	19	53
8	V	181/181 (100%)	170 (94%)	11 (6%)	17	49
9	I	172/172 (100%)	165 (96%)	7 (4%)	27	61
9	W	172/172 (100%)	165 (96%)	7 (4%)	27	61
10	J	175/175 (100%)	168 (96%)	7 (4%)	28	62
10	X	175/175 (100%)	169 (97%)	6 (3%)	32	66
11	K	169/169 (100%)	157 (93%)	12 (7%)	13	43
11	Y	169/169 (100%)	158 (94%)	11 (6%)	15	47
12	L	185/185 (100%)	160 (86%)	25 (14%)	4	18
12	Z	185/185 (100%)	160 (86%)	25 (14%)	4	18
13	1	199/199 (100%)	190 (96%)	9 (4%)	24	59
13	M	199/199 (100%)	189 (95%)	10 (5%)	22	56
14	2	162/162 (100%)	155 (96%)	7 (4%)	26	60
14	N	162/162 (100%)	155 (96%)	7 (4%)	26	60
All	All	5332/5332 (100%)	4974 (93%)	358 (7%)	15	46

All (358) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	32	LYS
1	A	33	GLN
1	A	62	GLU
1	A	69	LEU
1	A	124	THR
1	A	158	PHE
1	A	170	VAL
1	A	179	ARG
1	A	192	ILE
1	A	210	ILE

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Mol	Chain	Res	Type
1	A	214	ILE
2	B	10	SER
2	B	14	ILE
2	B	38	ILE
2	B	41	MET
2	B	58	LEU
2	B	67	LEU
2	B	107	ILE
2	B	116	LEU
2	B	135	SER
2	B	14(A)	TYR
2	B	150	THR
2	B	156	ASN
2	B	185	LYS
2	B	192	LEU
2	B	206	THR
2	B	224	PHE
3	C	10	ARG
3	C	14	ILE
3	C	33	ARG
3	C	57	LYS
3	C	66	LYS
3	C	87	ILE
3	C	135	SER
3	C	14(A)	ARG
3	C	14(B)	ASP
3	C	150	GLN
3	C	156	ILE
3	C	174	GLU
3	C	210	ILE
3	C	236	ILE
4	D	28	LEU
4	D	40	ILE
4	D	48	LEU
4	D	52	LYS
4	D	107	ILE
4	D	110	GLU
4	D	156	THR
4	D	170	GLU
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE

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Mol	Chain	Res	Type
4	D	233	ILE
5	E	12	THR
5	E	13	VAL
5	E	28	LEU
5	E	32	LYS
5	E	57	GLU
5	E	59	SER
5	E	76	LEU
5	E	97	ASN
5	E	139	ILE
5	E	197	ILE
5	E	199	GLN
5	E	207	LEU
5	E	2(B)	THR
5	E	2(C)	VAL
5	E	2(D)	ASP
5	E	2(E)	ASN
5	E	227	GLU
5	E	231	LYS
5	E	233	ILE
6	F	35	THR
6	F	36	THR
6	F	38	ILE
6	F	43	ASN
6	F	54	ILE
6	F	72	ARG
6	F	74	ILE
6	F	98	SER
6	F	105	THR
6	F	121	GLN
6	F	127	ASN
6	F	169	ARG
6	F	187	ARG
6	F	203	GLU
6	F	205	ASN
6	F	233	ILE
7	G	35	ILE
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	124	THR
7	G	169	GLN

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Mol	Chain	Res	Type
7	G	184	ASN
7	G	192	PHE
7	G	197	MET
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
7	G	236	ILE
8	H	34	LEU
8	H	38	SER
8	H	56	THR
8	H	121	VAL
8	H	144	GLN
8	H	159	ILE
8	H	163	ILE
8	H	197	ARG
8	H	221	ILE
8	H	223	ASP
9	I	-3	ILE
9	I	29	ASN
9	I	104	ILE
9	I	113	PHE
9	I	155	ILE
9	I	160	LEU
9	I	181	LYS
10	J	6	ILE
10	J	13	ILE
10	J	68	ILE
10	J	70	GLU
10	J	121	GLU
10	J	155	LEU
10	J	177	ILE
11	K	4	LEU
11	K	7	ARG
11	K	9	GLN
11	K	35	ILE
11	K	69	ARG
11	K	74	ILE
11	K	82	ILE
11	K	101	ILE
11	K	110	ILE
11	K	138	LEU
11	K	146	LEU

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Mol	Chain	Res	Type
11	K	185	ILE
12	L	-9	GLN
12	L	14	LEU
12	L	40	ASN
12	L	43	MET
12	L	58	ARG
12	L	98	HIS
12	L	99	THR
12	L	120	GLU
12	L	134	ILE
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	146	LEU
13	M	-4	ILE
13	M	4	ILE
13	M	29	ASN
13	M	40	ASN
13	M	55	ILE
13	M	62	LEU
13	M	65	GLU
13	M	79	ILE
13	M	91	ARG
13	M	178	ILE
14	N	41	ILE
14	N	55	ILE
14	N	70	TYR
14	N	84	LYS
14	N	89	GLU
14	N	119	VAL

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Mol	Chain	Res	Type
14	N	126	ILE
1	O	24	ILE
1	O	32	LYS
1	O	33	GLN
1	O	62	GLU
1	O	69	LEU
1	O	124	THR
1	O	158	PHE
1	O	170	VAL
1	O	179	ARG
1	O	192	ILE
1	O	210	ILE
1	O	214	ILE
2	P	10	SER
2	P	14	ILE
2	P	38	ILE
2	P	41	MET
2	P	58	LEU
2	P	67	LEU
2	P	107	ILE
2	P	116	LEU
2	P	135	SER
2	P	14(A)	TYR
2	P	150	THR
2	P	156	ASN
2	P	185	LYS
2	P	192	LEU
2	P	206	THR
2	P	224	PHE
3	Q	10	ARG
3	Q	14	ILE
3	Q	33	ARG
3	Q	57	LYS
3	Q	66	LYS
3	Q	87	ILE
3	Q	89	ILE
3	Q	135	SER
3	Q	14(A)	ARG
3	Q	14(B)	ASP
3	Q	150	GLN
3	Q	156	ILE
3	Q	174	GLU

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Mol	Chain	Res	Type
3	Q	210	ILE
3	Q	236	ILE
4	R	28	LEU
4	R	40	ILE
4	R	48	LEU
4	R	52	LYS
4	R	107	ILE
4	R	110	GLU
4	R	156	THR
4	R	170	GLU
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
4	R	233	ILE
5	S	12	THR
5	S	13	VAL
5	S	28	LEU
5	S	32	LYS
5	S	57	GLU
5	S	59	SER
5	S	76	LEU
5	S	97	ASN
5	S	123	ASN
5	S	197	ILE
5	S	199	GLN
5	S	207	LEU
5	S	2(B)	THR
5	S	2(C)	VAL
5	S	2(D)	ASP
5	S	2(E)	ASN
5	S	227	GLU
5	S	231	LYS
5	S	233	ILE
6	T	36	THR
6	T	38	ILE
6	T	43	ASN
6	T	54	ILE
6	T	72	ARG
6	T	74	ILE
6	T	98	SER
6	T	105	THR
6	T	121	GLN

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Mol	Chain	Res	Type
6	T	127	ASN
6	T	169	ARG
6	T	187	ARG
6	T	203	GLU
6	T	205	ASN
6	T	233	ILE
7	U	35	ILE
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	124	THR
7	U	169	GLN
7	U	184	ASN
7	U	192	PHE
7	U	197	MET
7	U	217	LYS
7	U	232	ARG
7	U	233	LEU
7	U	236	ILE
8	V	34	LEU
8	V	38	SER
8	V	56	THR
8	V	68	LEU
8	V	121	VAL
8	V	144	GLN
8	V	159	ILE
8	V	163	ILE
8	V	197	ARG
8	V	221	ILE
8	V	223	ASP
9	W	-3	ILE
9	W	29	ASN
9	W	104	ILE
9	W	113	PHE
9	W	155	ILE
9	W	160	LEU
9	W	181	LYS
10	X	6	ILE
10	X	13	ILE
10	X	68	ILE
10	X	121	GLU
10	X	155	LEU

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Mol	Chain	Res	Type
10	X	177	ILE
11	Y	4	LEU
11	Y	7	ARG
11	Y	9	GLN
11	Y	35	ILE
11	Y	69	ARG
11	Y	74	ILE
11	Y	82	ILE
11	Y	110	ILE
11	Y	138	LEU
11	Y	146	LEU
11	Y	185	ILE
12	Z	-9	GLN
12	Z	14	LEU
12	Z	40	ASN
12	Z	43	MET
12	Z	58	ARG
12	Z	98	HIS
12	Z	99	THR
12	Z	120	GLU
12	Z	134	ILE
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	146	LEU
13	1	-4	ILE
13	1	4	ILE
13	1	29	ASN
13	1	40	ASN
13	1	62	LEU

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Mol	Chain	Res	Type
13	1	65	GLU
13	1	79	ILE
13	1	91	ARG
13	1	178	ILE
14	2	41	ILE
14	2	55	ILE
14	2	70	TYR
14	2	84	LYS
14	2	89	GLU
14	2	119	VAL
14	2	126	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (229) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	145	ASN
1	A	150	GLN
2	B	23	GLN
2	B	33	HIS
2	B	71	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	59	GLN
3	C	82	ASN
3	C	97	GLN
3	C	120	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
4	D	108	ASN
4	D	218	GLN

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Mol	Chain	Res	Type
4	D	226	ASN
5	E	33	GLN
5	E	64	GLN
5	E	73	HIS
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	170	GLN
5	E	185	ASN
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	144	ASN
6	F	192	GLN
6	F	205	ASN
6	F	221	HIS
7	G	32	ASN
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	85	GLN
8	H	114	HIS
8	H	141	HIS
8	H	144	GLN
8	H	165	ASN

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Mol	Chain	Res	Type
8	H	172	ASN
8	H	190	ASN
8	H	201	GLN
9	I	29	ASN
9	I	161	ASN
9	I	193	GLN
10	J	40	HIS
10	J	54	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
11	K	9	GLN
11	K	85	ASN
11	K	131	GLN
11	K	174	ASN
11	K	190	HIS
11	K	207	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	27	ASN
12	L	40	ASN
12	L	61	ASN
12	L	70(A)	ASN
12	L	82	ASN
12	L	85	HIS
12	L	123	GLN
12	L	14(C)	GLN
12	L	1(I)	ASN
12	L	166	HIS
13	M	10	ASN
13	M	29	ASN
13	M	40	ASN
13	M	54	HIS
13	M	89	GLN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
13	M	191	GLN
14	N	69	GLN

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Mol	Chain	Res	Type
14	N	141	ASN
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
1	O	97	HIS
1	O	145	ASN
1	O	150	GLN
2	P	23	GLN
2	P	71	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	59	GLN
3	Q	82	ASN
3	Q	97	GLN
3	Q	120	GLN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	209	ASN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	218	GLN
4	R	226	ASN
5	S	64	GLN
5	S	73	HIS
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	170	GLN
5	S	185	ASN
5	S	199	GLN

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Mol	Chain	Res	Type
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	144	ASN
6	T	147	HIS
6	T	192	GLN
6	T	205	ASN
6	T	221	HIS
7	U	11	HIS
7	U	32	ASN
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	114	HIS
8	V	141	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
8	V	201	GLN
9	W	29	ASN
9	W	56	ASN
9	W	64	ASN
9	W	81	GLN
9	W	161	ASN
10	X	40	HIS
10	X	54	GLN
10	X	62	ASN
10	X	77	GLN

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Mol	Chain	Res	Type
10	X	85	GLN
10	X	112	GLN
10	X	140	HIS
10	X	186	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	131	GLN
11	Y	174	ASN
11	Y	190	HIS
11	Y	207	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	27	ASN
12	Z	40	ASN
12	Z	61	ASN
12	Z	70(A)	ASN
12	Z	82	ASN
12	Z	85	HIS
12	Z	123	GLN
12	Z	14(C)	GLN
12	Z	1(I)	ASN
12	Z	166	HIS
12	Z	168	GLN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN
13	1	191	GLN
14	2	69	GLN
14	2	145	ASN
14	2	157	HIS
14	2	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	ESY	Y	2000	11	44,44,44	2.23	13 (29%)	52,56,56	2.21	10 (19%)
15	ESY	K	2000	11	44,44,44	2.29	18 (40%)	52,56,56	2.31	7 (13%)

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	ESY	Y	2000	11	-	9/50/50/50	0/2/2/2
15	ESY	K	2000	11	-	11/50/50/50	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	K	2000	ESY	C10-N11	6.89	1.48	1.34
15	Y	2000	ESY	C10-N11	6.51	1.48	1.34
15	Y	2000	ESY	C20-C19	5.28	1.59	1.54
15	K	2000	ESY	C12-N11	4.82	1.55	1.45
15	Y	2000	ESY	C12-N11	4.60	1.55	1.45
15	K	2000	ESY	C20-C19	4.13	1.58	1.54
15	K	2000	ESY	C2-C3	3.57	1.45	1.38
15	Y	2000	ESY	O6-C5	3.55	1.53	1.45
15	K	2000	ESY	C43-C1	3.40	1.45	1.38
15	Y	2000	ESY	C40-C9	3.34	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	2000	ESY	C43-C42	3.22	1.44	1.38
15	K	2000	ESY	C20-C21	3.03	1.55	1.50
15	K	2000	ESY	O6-C5	2.94	1.51	1.45
15	Y	2000	ESY	C43-C1	2.87	1.44	1.38
15	K	2000	ESY	C43-C42	2.81	1.43	1.38
15	Y	2000	ESY	C20-C21	2.66	1.54	1.50
15	Y	2000	ESY	C2-C3	2.40	1.43	1.38
15	K	2000	ESY	C40-C9	2.40	1.58	1.52
15	K	2000	ESY	C13-C12	2.36	1.59	1.53
15	Y	2000	ESY	C2-C1	2.33	1.43	1.38
15	K	2000	ESY	C3-C4	2.33	1.43	1.38
15	K	2000	ESY	C34-C33	2.32	1.42	1.38
15	K	2000	ESY	C33-C32	2.25	1.43	1.38
15	K	2000	ESY	C7-N8	2.23	1.40	1.34
15	K	2000	ESY	C42-C4	2.22	1.43	1.38
15	Y	2000	ESY	C18-N17	2.12	1.38	1.33
15	Y	2000	ESY	C13-C12	2.10	1.58	1.53
15	Y	2000	ESY	C3-C4	2.10	1.43	1.38
15	K	2000	ESY	C18-N17	2.06	1.38	1.33
15	K	2000	ESY	C37-C32	2.05	1.43	1.38
15	K	2000	ESY	C36-C35	2.03	1.42	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K	2000	ESY	C9-N8-C7	10.22	139.92	120.59
15	Y	2000	ESY	C9-N8-C7	9.43	138.43	120.59
15	K	2000	ESY	C10-C9-N8	-8.84	89.70	111.59
15	Y	2000	ESY	C10-C9-N8	-8.07	91.59	111.59
15	K	2000	ESY	C5-O6-C7	-4.67	105.41	115.93
15	Y	2000	ESY	C5-O6-C7	-4.35	106.14	115.93
15	Y	2000	ESY	O30-C31-C32	-3.43	101.09	109.40
15	K	2000	ESY	O30-C31-C32	-2.95	102.24	109.40
15	Y	2000	ESY	C40-C9-N8	2.89	115.68	110.38
15	K	2000	ESY	C31-O30-C29	2.87	121.65	116.28
15	K	2000	ESY	O6-C7-N8	2.54	115.88	110.45
15	Y	2000	ESY	O6-C7-N8	2.49	115.78	110.45
15	Y	2000	ESY	O6-C7-O41	-2.47	119.52	124.26
15	Y	2000	ESY	C31-O30-C29	2.27	120.54	116.28
15	Y	2000	ESY	C1-C2-C3	-2.24	117.47	120.24
15	Y	2000	ESY	O6-C5-C4	2.16	114.64	109.40
15	K	2000	ESY	C5-C4-C3	-2.00	116.03	120.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

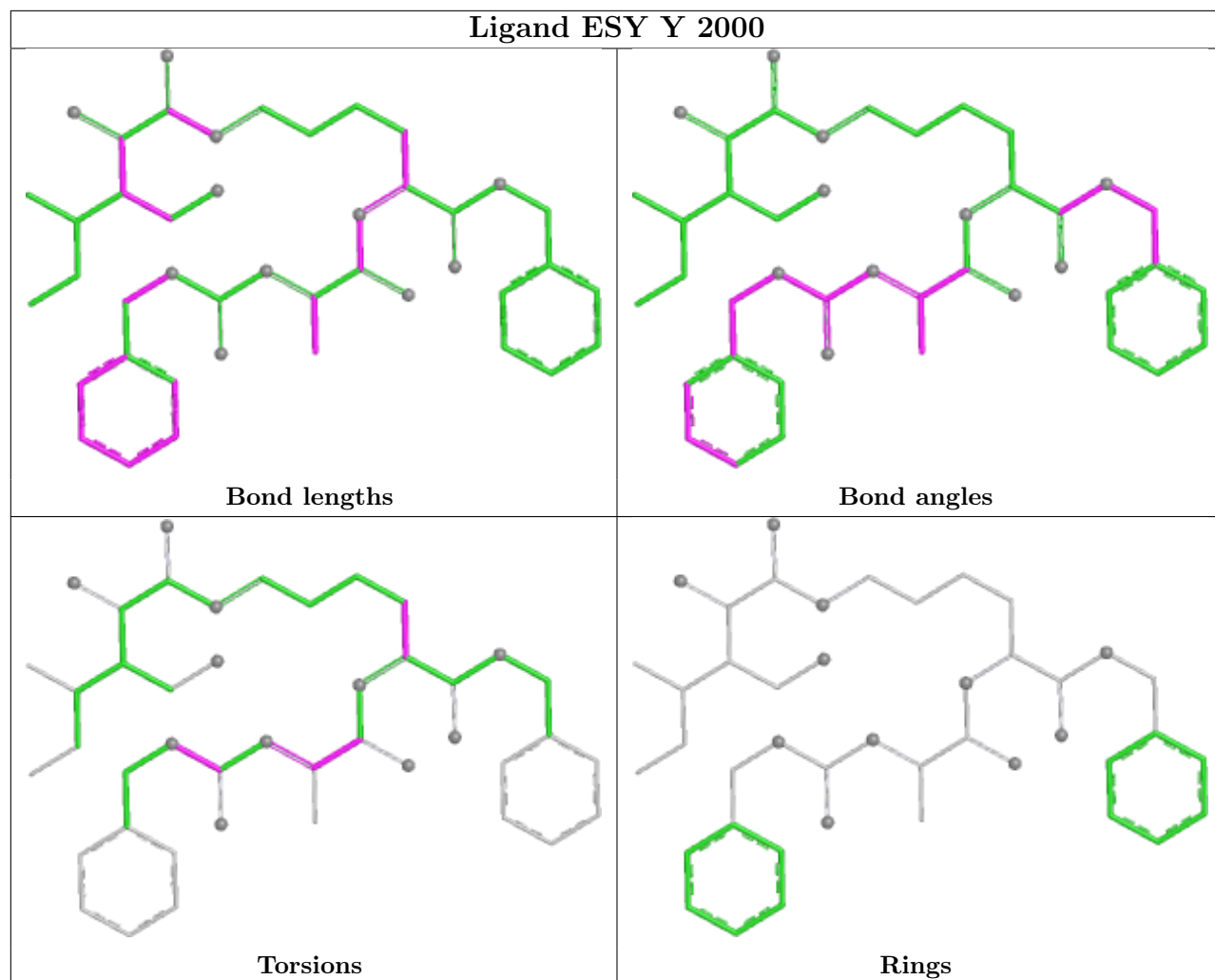
Mol	Chain	Res	Type	Atoms
15	K	2000	ESY	C40-C9-N8-C7
15	K	2000	ESY	N11-C12-C13-C14
15	Y	2000	ESY	C40-C9-N8-C7
15	Y	2000	ESY	N11-C12-C13-C14
15	K	2000	ESY	O41-C7-O6-C5
15	Y	2000	ESY	O41-C7-O6-C5
15	K	2000	ESY	N8-C7-O6-C5
15	Y	2000	ESY	N8-C7-O6-C5
15	Y	2000	ESY	N11-C10-C9-N8
15	K	2000	ESY	N11-C10-C9-N8
15	K	2000	ESY	C29-C12-C13-C14
15	Y	2000	ESY	C29-C12-C13-C14
15	Y	2000	ESY	O39-C10-C9-N8
15	K	2000	ESY	O39-C10-C9-N8
15	K	2000	ESY	N17-C18-C19-O27
15	K	2000	ESY	O39-C10-C9-C40
15	Y	2000	ESY	O39-C10-C9-C40
15	Y	2000	ESY	N11-C10-C9-C40
15	K	2000	ESY	N11-C10-C9-C40
15	K	2000	ESY	O28-C18-C19-O27

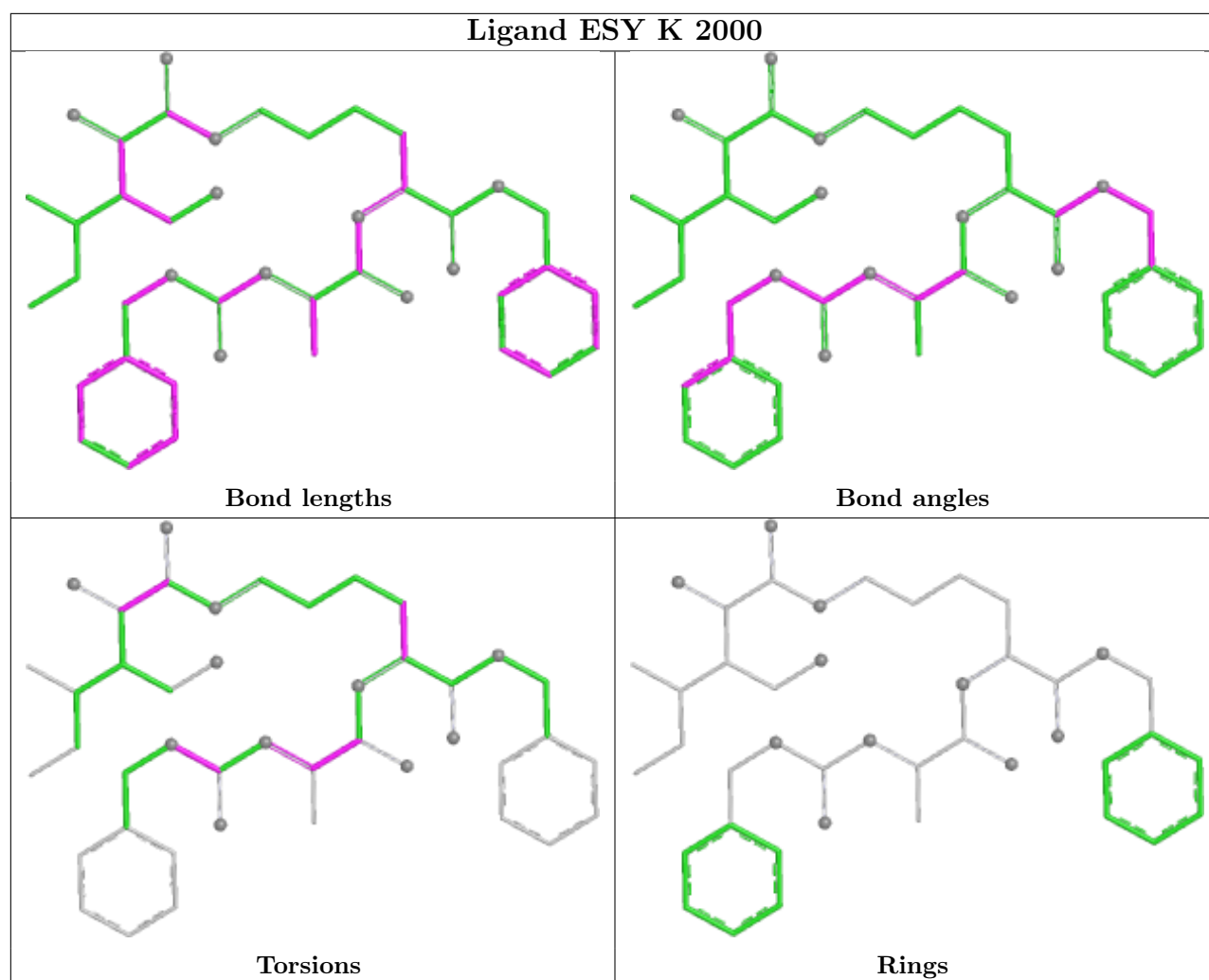
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Y	2000	ESY	5	0
15	K	2000	ESY	5	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.43	0 100 100	23, 42, 71, 96	0
1	O	250/250 (100%)	-0.31	1 (0%) 88 76	29, 49, 76, 97	0
2	B	244/244 (100%)	-0.21	5 (2%) 65 41	29, 48, 84, 112	0
2	P	244/244 (100%)	-0.12	4 (1%) 70 47	28, 50, 85, 115	0
3	C	241/241 (100%)	-0.14	4 (1%) 69 45	31, 51, 104, 118	0
3	Q	241/241 (100%)	0.04	7 (2%) 53 31	37, 56, 105, 118	0
4	D	242/242 (100%)	-0.12	8 (3%) 49 28	29, 54, 86, 116	0
4	R	242/242 (100%)	-0.10	6 (2%) 58 35	34, 54, 88, 118	0
5	E	233/233 (100%)	-0.14	2 (0%) 81 61	37, 56, 82, 105	0
5	S	233/233 (100%)	0.12	9 (3%) 43 24	37, 58, 85, 103	0
6	F	244/244 (100%)	-0.28	1 (0%) 88 76	30, 49, 84, 101	0
6	T	244/244 (100%)	-0.11	2 (0%) 82 64	26, 50, 85, 102	0
7	G	243/243 (100%)	-0.43	1 (0%) 88 76	26, 43, 68, 103	0
7	U	243/243 (100%)	-0.32	2 (0%) 82 64	30, 44, 69, 103	0
8	H	222/222 (100%)	-0.54	1 (0%) 87 72	27, 40, 62, 89	0
8	V	222/222 (100%)	-0.49	1 (0%) 87 72	29, 42, 61, 89	0
9	I	204/204 (100%)	-0.66	0 100 100	26, 40, 57, 73	0
9	W	204/204 (100%)	-0.58	0 100 100	27, 40, 59, 74	0
10	J	198/198 (100%)	-0.47	2 (1%) 79 59	25, 41, 60, 114	0
10	X	198/198 (100%)	-0.45	4 (2%) 65 41	27, 43, 62, 116	0
11	K	212/212 (100%)	-0.49	0 100 100	23, 41, 55, 69	0
11	Y	212/212 (100%)	-0.53	1 (0%) 87 72	27, 43, 58, 68	0
12	L	222/222 (100%)	-0.48	0 100 100	21, 42, 64, 79	0
12	Z	222/222 (100%)	-0.49	1 (0%) 87 72	28, 42, 65, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	233/233 (100%)	-0.53	1 (0%) 88 76	22, 41, 58, 66	0
13	M	233/233 (100%)	-0.48	0 100 100	26, 43, 59, 65	0
14	2	196/196 (100%)	-0.51	0 100 100	23, 39, 61, 74	0
14	N	196/196 (100%)	-0.57	0 100 100	26, 38, 59, 72	0
All	All	6368/6368 (100%)	-0.34	63 (0%) 79 59	21, 45, 79, 118	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	56	LEU	6.2
4	R	12(D)	ALA	6.1
7	U	240	ASP	5.6
4	D	12(D)	ALA	5.5
4	D	12(C)	GLY	5.3
10	X	193	GLN	5.0
4	R	12(E)	SER	5.0
3	Q	58	LEU	4.2
8	V	223	ASP	4.2
2	B	239	THR	4.2
4	R	127	LEU	4.1
2	B	217	ALA	3.9
3	C	56	LEU	3.7
10	J	193	GLN	3.7
10	X	192	ALA	3.7
3	C	59	GLN	3.6
7	U	6	ALA	3.5
5	S	60	SER	3.4
5	S	59	SER	3.3
4	D	126	ARG	3.3
7	G	6	ALA	3.2
2	P	217	ALA	3.1
2	P	21(B)	GLY	3.1
2	P	239	THR	3.0
4	R	12(F)	GLY	3.0
1	O	5	THR	3.0
3	C	55	THR	3.0
13	1	-8	THR	2.9
4	D	12(E)	SER	2.9
5	S	2(E)	ASN	2.8
5	E	4	PHE	2.8
3	Q	208	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	21(B)	GLY	2.7
5	S	54	ASN	2.6
3	C	54	SER	2.6
2	B	218	ASN	2.6
3	Q	63	THR	2.6
10	J	192	ALA	2.6
4	D	127	LEU	2.5
3	Q	55	THR	2.4
4	D	12(F)	GLY	2.4
4	D	242	ALA	2.4
4	R	126	ARG	2.4
4	R	12(C)	GLY	2.4
6	T	205	ASN	2.4
3	Q	54	SER	2.4
10	X	10	ASP	2.3
11	Y	145	ASP	2.3
5	E	203	ASP	2.3
5	S	58	LEU	2.3
3	Q	57	LYS	2.3
2	P	218	ASN	2.2
4	D	120	ALA	2.2
5	S	56	ASP	2.2
5	S	55	ALA	2.2
6	F	204	ASP	2.2
12	Z	145	TYR	2.1
8	H	223	ASP	2.1
5	S	63	TYR	2.1
2	B	54	VAL	2.1
5	S	32	LYS	2.1
10	X	-1	MET	2.0
6	T	241	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

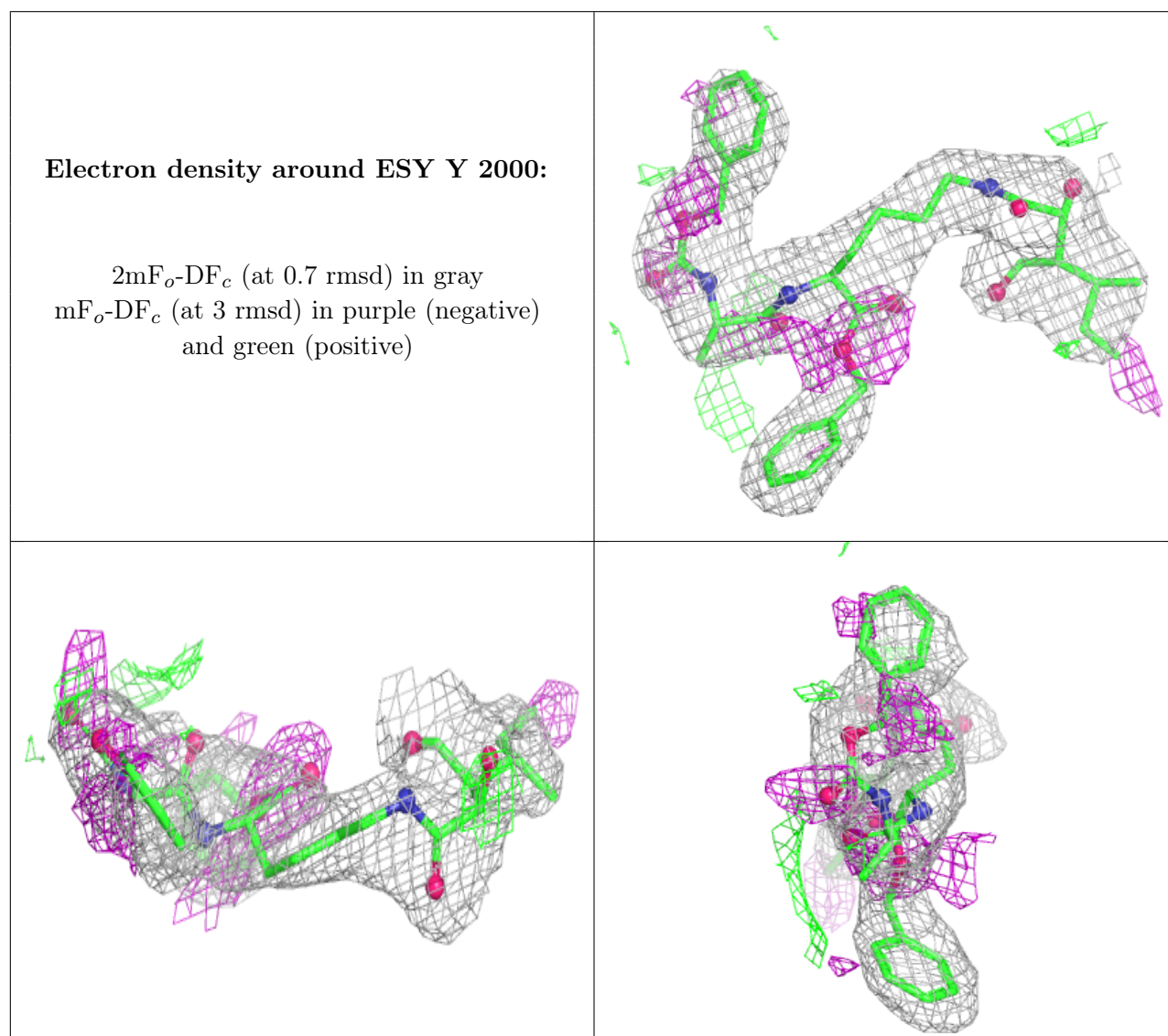
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

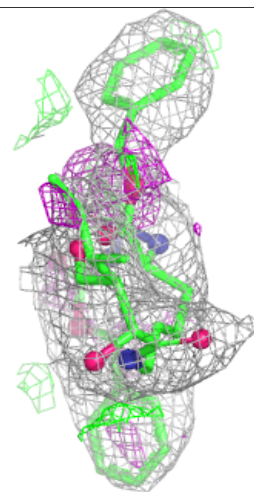
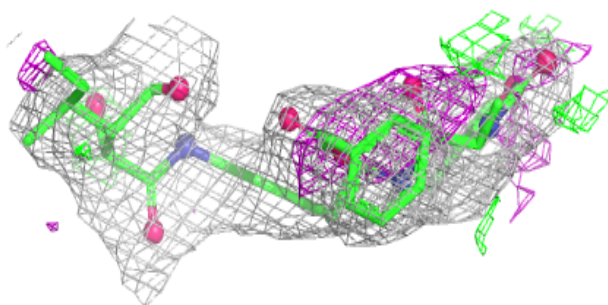
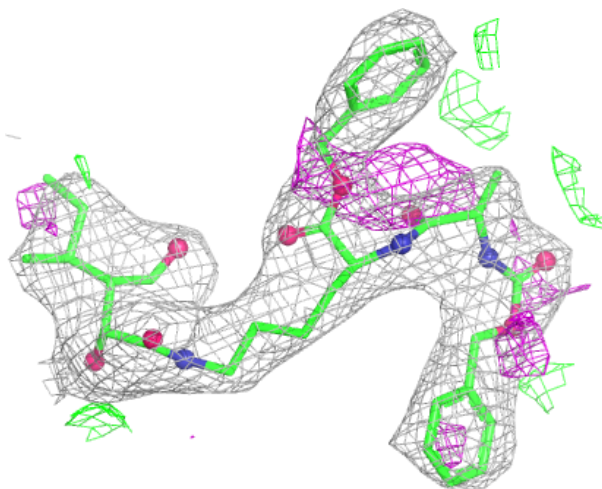
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	ESY	Y	2000	43/43	0.86	0.12	20,36,45,46	0
15	ESY	K	2000	43/43	0.88	0.10	20,36,45,46	0

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 ESY K 2000:

$2mF_o-DF_c$ (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.