



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Oct 29, 2019 – 03:06 PM EDT

PDB ID : 6J2C
EMDB ID: : EMD-9769
Title : Yeast proteasome in translocation competent state (C3-a)
Authors : Cong, Y.
Deposited on : 2019-01-01
Resolution : 7.00 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

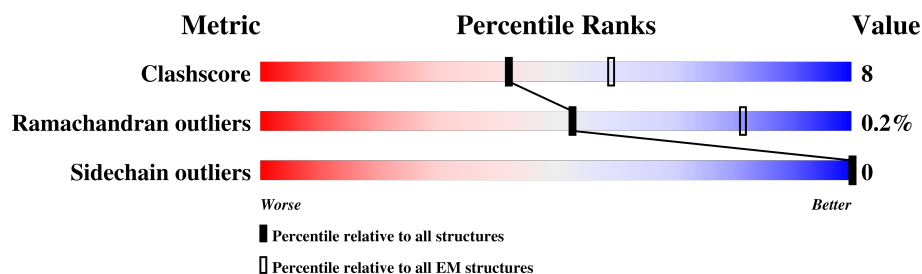
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.00 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.









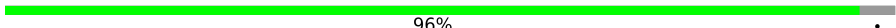

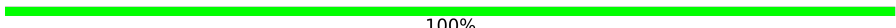

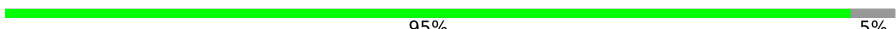

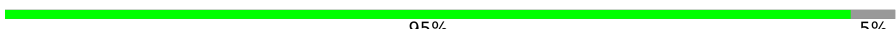



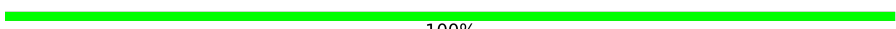








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	215	73% 18% 9%
1	b	215	91% 9%
2	2	261	69% 18% 13%
2	i	261	87% 13%
3	3	205	72% 27%
3	h	205	99%
4	4	198	78% 21% .
4	g	198	98% .
5	5	287	64% 9% 26%







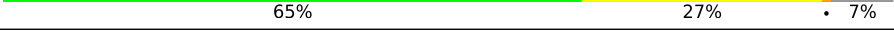
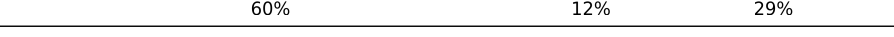
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	f	287	 74%26%
6	6	241	 74%18%8%
6	e	241	 92%8%
7	7	266	 70%16%14%
7	a	266	 87%13%
8	A	252	 79%17%.
8	c	252	 96%.
9	B	250	 72%28%
9	j	250	 100%
10	C	258	 76%19%5%
10	d	258	 95%5%
11	D	254	 78%17%6%
11	n	254	 95%5%
12	E	260	 79%14%7%
12	m	260	 93%7%
13	F	234	 81%19%
13	l	234	 100%
14	G	288	 68%16%16%
14	k	288	 85%15%
15	H	467	 55%21%23%
16	I	437	 60%23%17%
17	J	405	 72%20%8%
18	K	428	 64%24%11%
19	L	437	 63%20%17%
20	M	434	 64%20%. 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
21	N	945	 75%15%10%
22	O	393	 81%18%.
23	P	445	 81%16%.
24	Q	434	 83%17%.
25	R	429	 73%20%7%
26	S	523	 77%14%9%
27	T	274	 85%14%.
28	U	338	 56%20%25%
29	V	306	 65%27%.7%
30	W	268	 56%17%26%
31	X	156	 60%12%29%
32	Y	89	 20%9%.70%
33	Z	993	 68%14%18%

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 106149 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		
1	b	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		

- Molecule 2 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		
2	i	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		

- Molecule 3 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		
3	h	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

- Molecule 4 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		
4	g	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		

- Molecule 5 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
5	f	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		

- Molecule 6 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
6	e	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

- Molecule 7 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		
7	a	232	Total	C	N	O	S	0	0
			1815	1148	311	349	7		

- Molecule 8 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		
8	c	243	Total	C	N	O	S	0	0
			1921	1221	322	370	8		

- Molecule 9 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		
9	j	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		

- Molecule 10 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

- Molecule 11 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		
11	n	241	Total	C	N	O	S	0	0
			1890	1181	331	374	4		

- Molecule 12 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		
12	m	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		

- Molecule 13 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		
13	l	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		

- Molecule 14 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	243	Total	C	N	O	S	0	0
			1892	1203	329	356	4		
14	k	244	Total	C	N	O	S	0	0
			1896	1205	330	357	4		

- Molecule 15 is a protein called 26S protease regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	359	Total	C	N	O	S	0	0
			2792	1755	499	523	15		

- Molecule 16 is a protein called 26S protease regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	363	Total	C	N	O	S	0	0
			2831	1779	472	565	15		

- Molecule 17 is a protein called 26S protease regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	373	Total	C	N	O	S	0	0
			2928	1837	527	547	17		

- Molecule 18 is a protein called 26S protease regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	381	Total	C	N	O	S	0	0
			3019	1898	530	581	10		

- Molecule 19 is a protein called 26S protease subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	361	Total	C	N	O	S	0	0
			2853	1798	507	536	12		

- Molecule 20 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	367	Total	C	N	O	S	0	0
			2866	1799	503	553	11		

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	849	Total	C	N	O	S	0	0
			6562	4174	1099	1261	28		

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	387	Total	C	N	O	S	0	0
			3182	2047	520	606	9		

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	432	Total	C	N	O	S	0	0
			3545	2260	592	684	9		

- Molecule 24 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	431	Total	C	N	O	S	0	0
			3471	2205	574	676	16		

- Molecule 25 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	400	Total	C	N	O	S	0	0
			3218	2051	527	630	10		

- Molecule 26 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	475	Total	C	N	O	S	0	0
			3894	2488	653	738	15		

- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	272	Total	C	N	O	S	0	0
			2235	1432	355	441	7		

- Molecule 28 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	255	Total	C	N	O	S	0	0
			2061	1312	352	391	6		

- Molecule 29 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	284	Total	C	N	O	S	0	0
			2236	1405	381	436	14		

- Molecule 30 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	197	Total	C	N	O	S	0	0
			1534	962	269	300	3		

- Molecule 31 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	111	Total	C	N	O	S	0	0
			906	586	148	169	3		

- Molecule 32 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y	27	Total	C	N	O	0	0
			236	143	39	54		

- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN1.

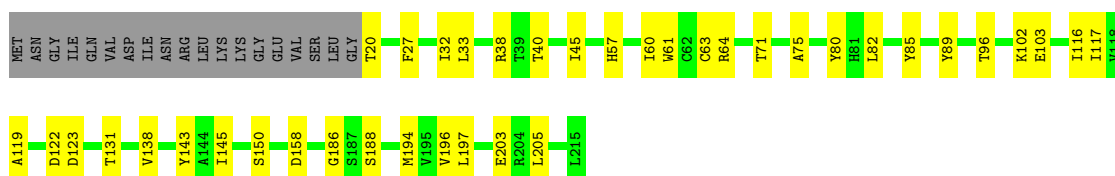
Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	813	Total	C	N	O	S	0	0
			6290	3995	1029	1237	29		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

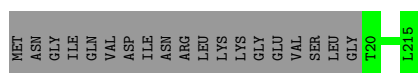
- Molecule 1: Proteasome subunit beta type-1

Chain 1: 



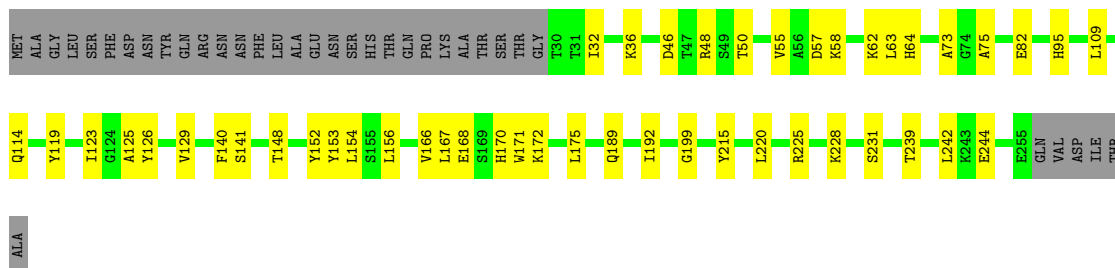
- Molecule 1: Proteasome subunit beta type-1

Chain b: 




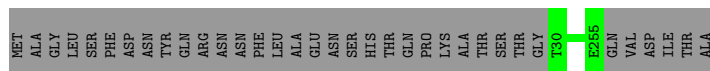
- Molecule 2: Proteasome subunit beta type-2

Chain 2: 



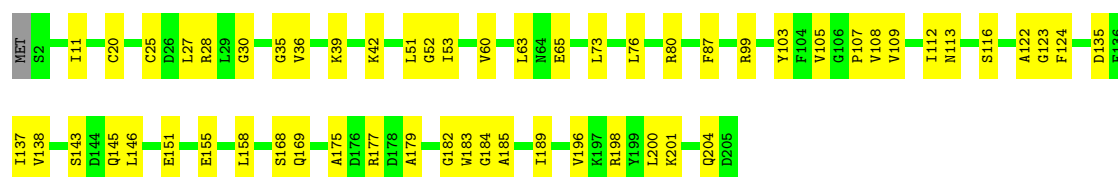
- Molecule 2: Proteasome subunit beta type-2

Chain i: 



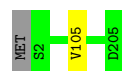
- Molecule 3: Proteasome subunit beta type-3

Chain 3: 



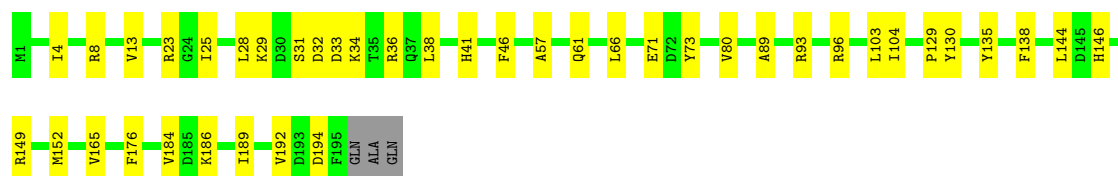
• Molecule 3: Proteasome subunit beta type-3

Chain h: 99%



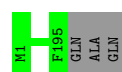
• Molecule 4: Proteasome subunit beta type-4

Chain 4: 78% 21%



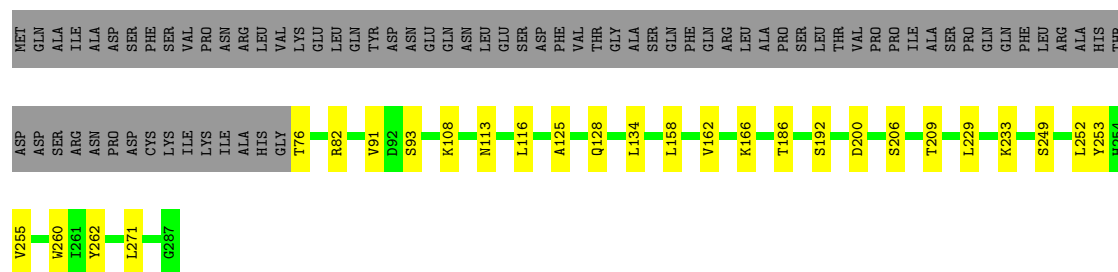
• Molecule 4: Proteasome subunit beta type-4

Chain g: 98%



• Molecule 5: Proteasome subunit beta type-5

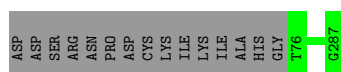
Chain 5: 64% 9% 26%



• Molecule 5: Proteasome subunit beta type-5

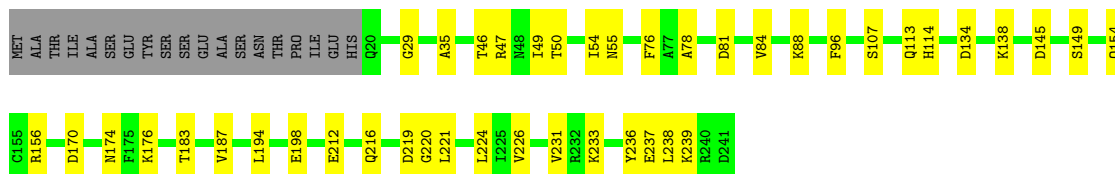
Chain f: 74% 26%





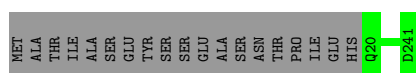
• Molecule 6: Proteasome subunit beta type-6

Chain 6: 74% 18% 8%



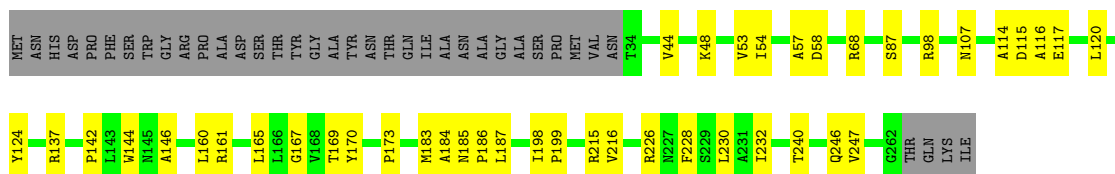
• Molecule 6: Proteasome subunit beta type-6

Chain e: 92% 8%



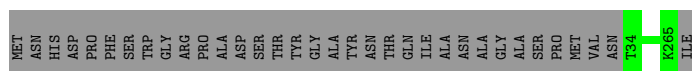
• Molecule 7: Proteasome subunit beta type-7

Chain 7: 70% 16% 14%



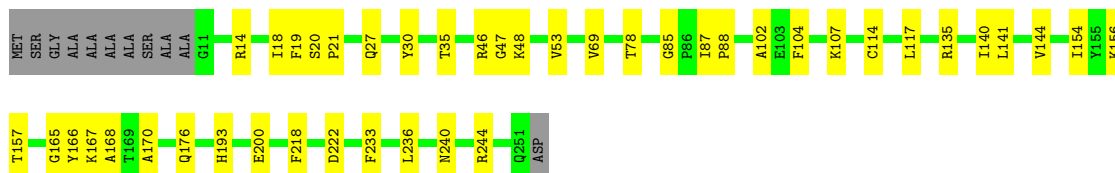
• Molecule 7: Proteasome subunit beta type-7

Chain a: 87% 13%



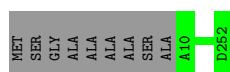
• Molecule 8: Proteasome subunit alpha type-1

Chain A: 79% 17%



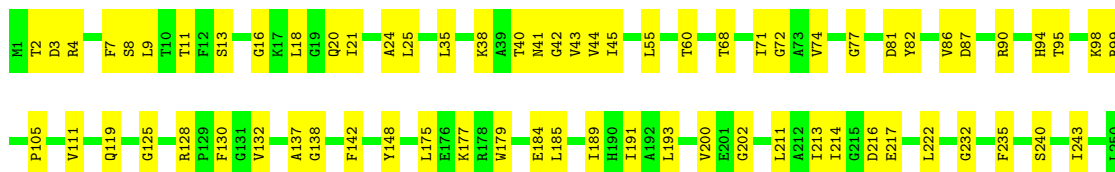
• Molecule 8: Proteasome subunit alpha type-1

Chain c: 96%



- Molecule 9: Proteasome subunit alpha type-2

Chain B: 72% 28%



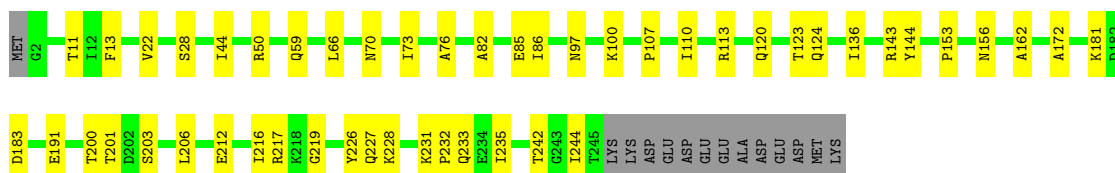
- Molecule 9: Proteasome subunit alpha type-2

Chain j: 100%

There are no outlier residues recorded for this chain.

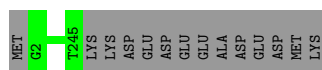
- Molecule 10: Proteasome subunit alpha type-3

Chain C: 76% 19% 5%



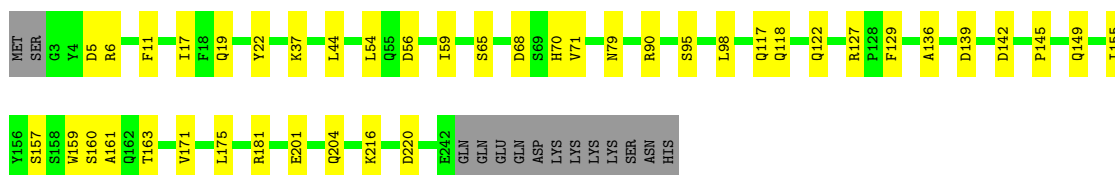
- Molecule 10: Proteasome subunit alpha type-3

Chain d: 95% 5%



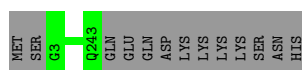
- Molecule 11: Proteasome subunit alpha type-4

Chain D: 78% 17% 6%



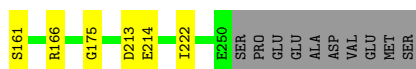
- Molecule 11: Proteasome subunit alpha type-4

Chain n: 95% 5%



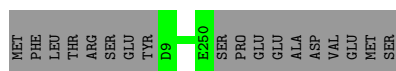
- Molecule 12: Proteasome subunit alpha type-5

Chain E: 79% 14% 7%



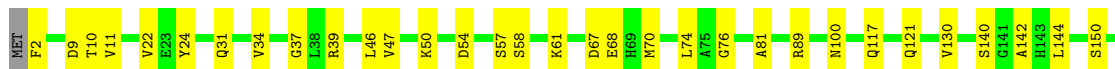
- Molecule 12: Proteasome subunit alpha type-5

Chain m: 93% 7%



- Molecule 13: Proteasome subunit alpha type-6

Chain F: 81% 19%



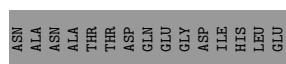
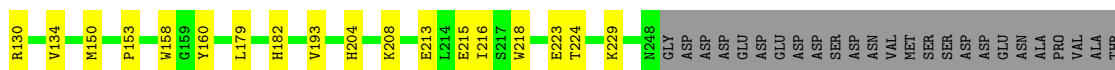
- Molecule 13: Proteasome subunit alpha type-6

Chain l: 100%



- Molecule 14: Probable proteasome subunit alpha type-7

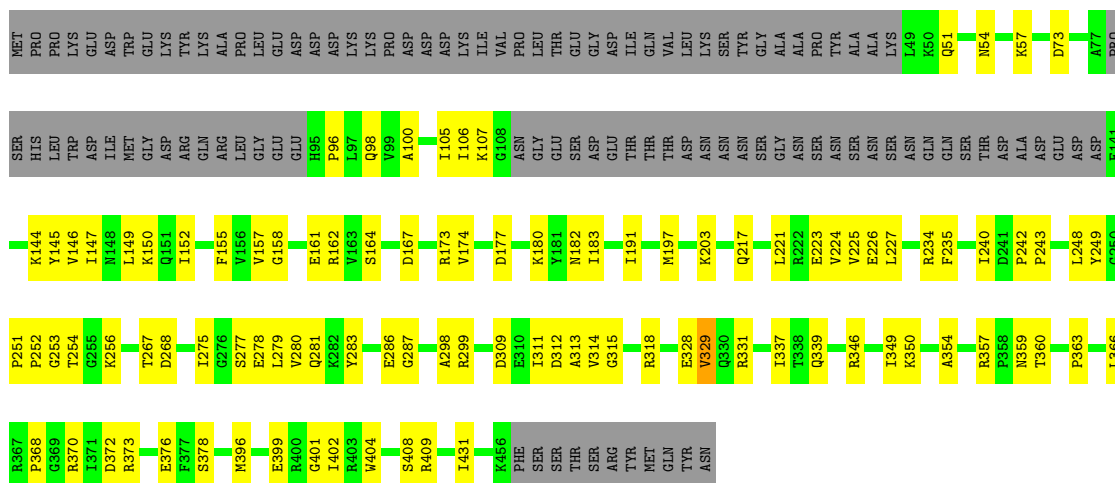
Chain G: 68% 16% 16%



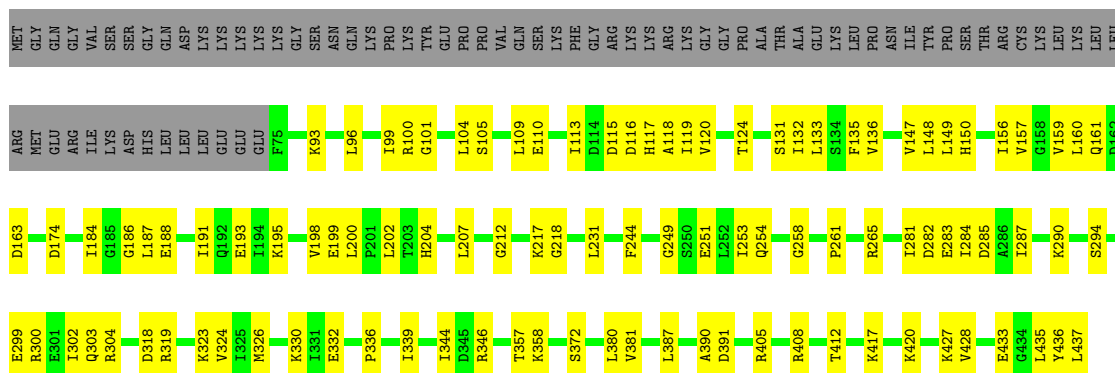
- Molecule 14: Probable proteasome subunit alpha type-7

MET	THR	SER	ILE	G5	M248	GLY	ASP	ASP	ASP	ASP	GLU	GLU	ASP	ASP	SER	ASN	VAL	MET	SER	SER	ASP	ASP	GLU	ASN	ALA	ALA	PRO	VAL	ALA	THR	ASN	ALA	ASN	ALA	THR	THR	ASP	GLN	GLU	GLY	ASP	ILE	HIS	LEU	THR
-----	-----	-----	-----	----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

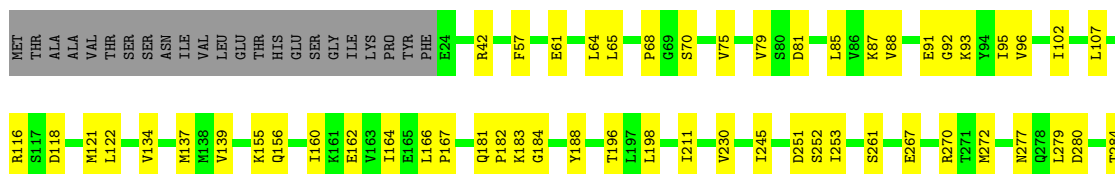
- Chain H:  55% 21% 23%



- Chain I: 60% 23% 17%



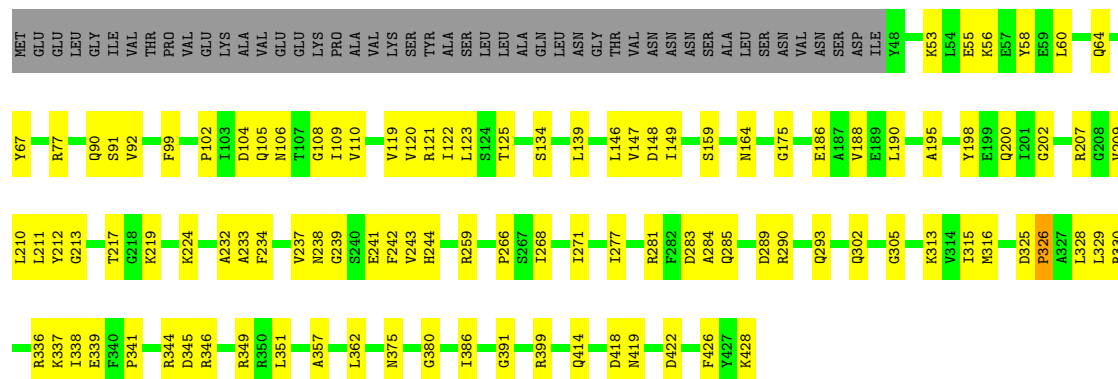
- Chain J: 72% 20% 8%





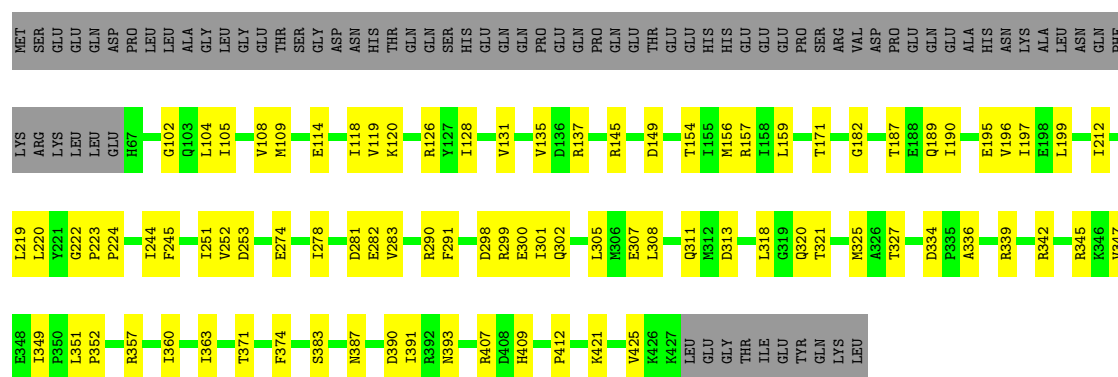
• Molecule 18: 26S protease regulatory subunit 6B homolog

Chain K: 64% 24% 11%



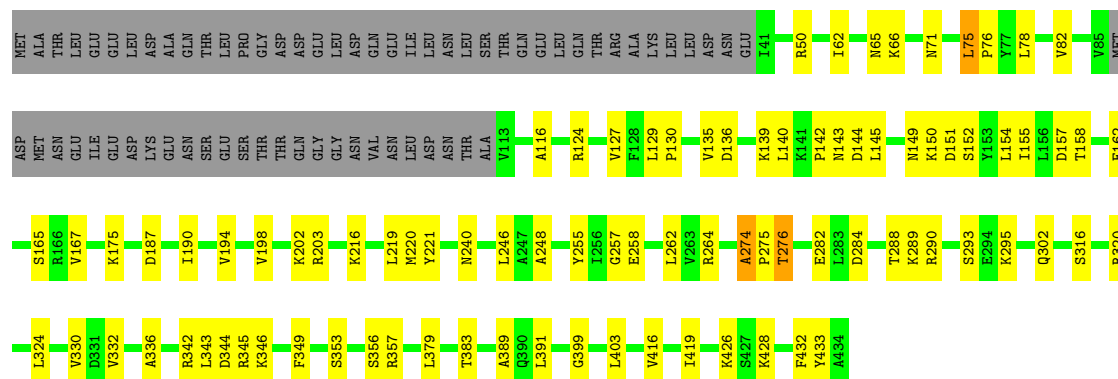
• Molecule 19: 26S protease subunit RPT4

Chain L: 63% 20% 17%

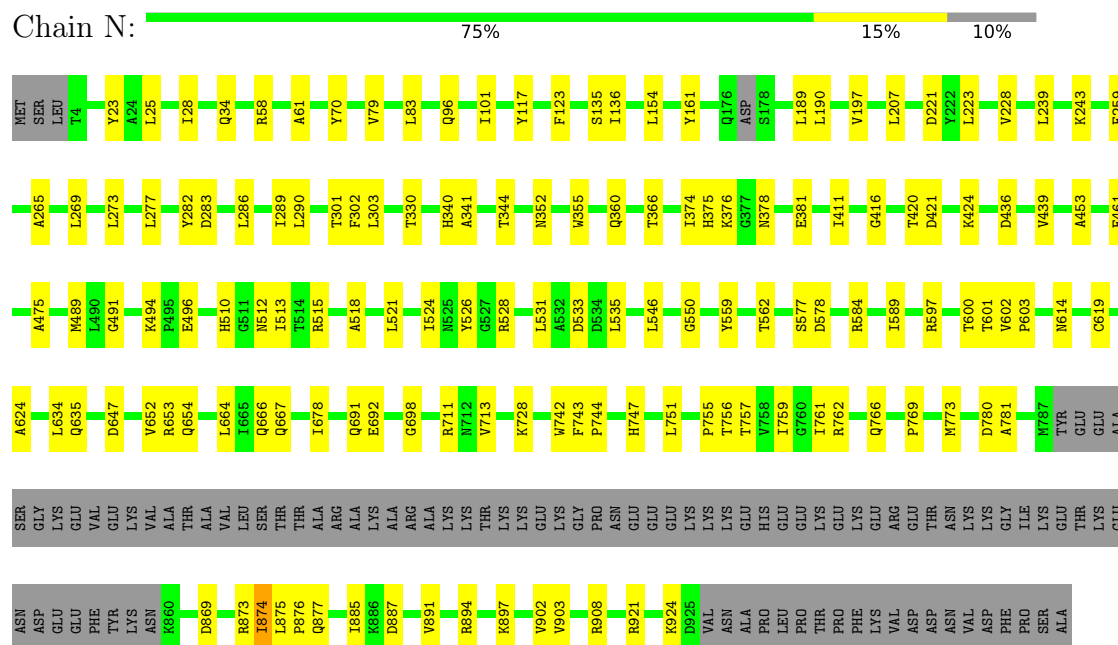


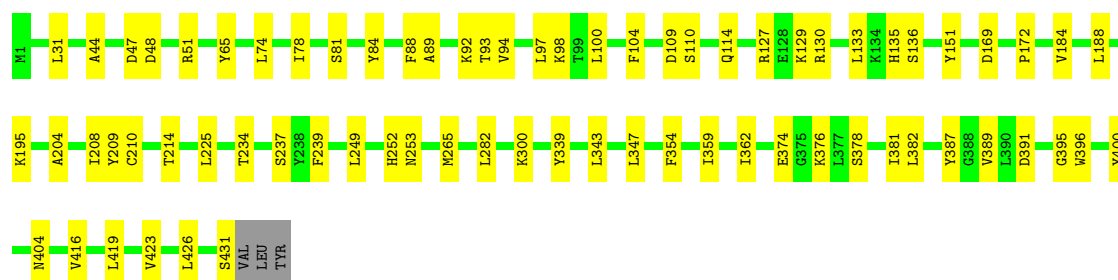
• Molecule 20: 26S protease regulatory subunit 6A

Chain M: 64% 20% 15%



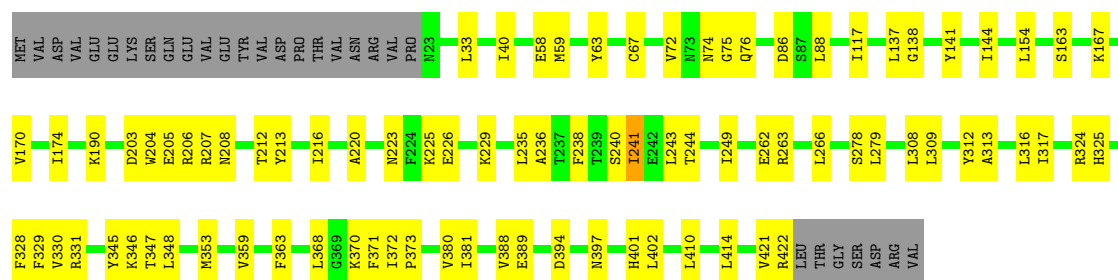
• Molecule 21: 26S proteasome regulatory subunit RPN2





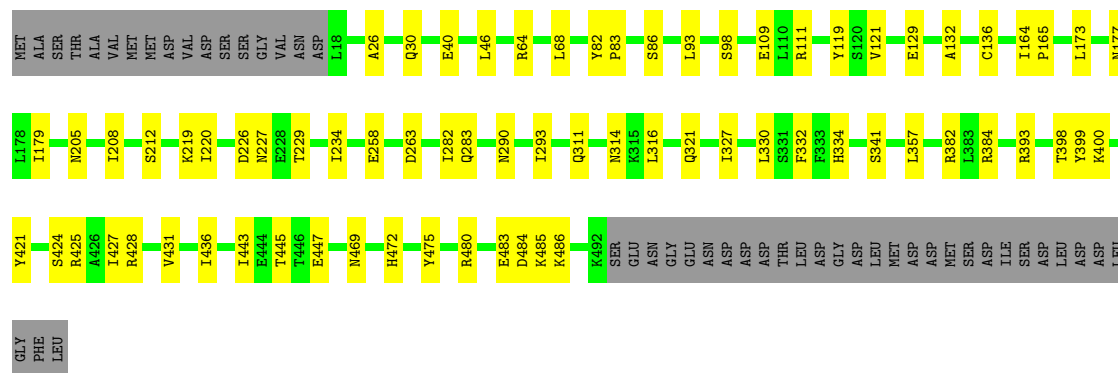
• Molecule 25: 26S proteasome regulatory subunit RPN7

Chain R: 73% 20% 7%



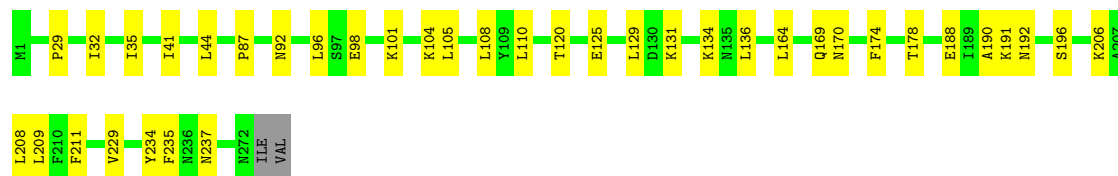
• Molecule 26: 26S proteasome regulatory subunit RPN3

Chain S: 77% 14% 9%



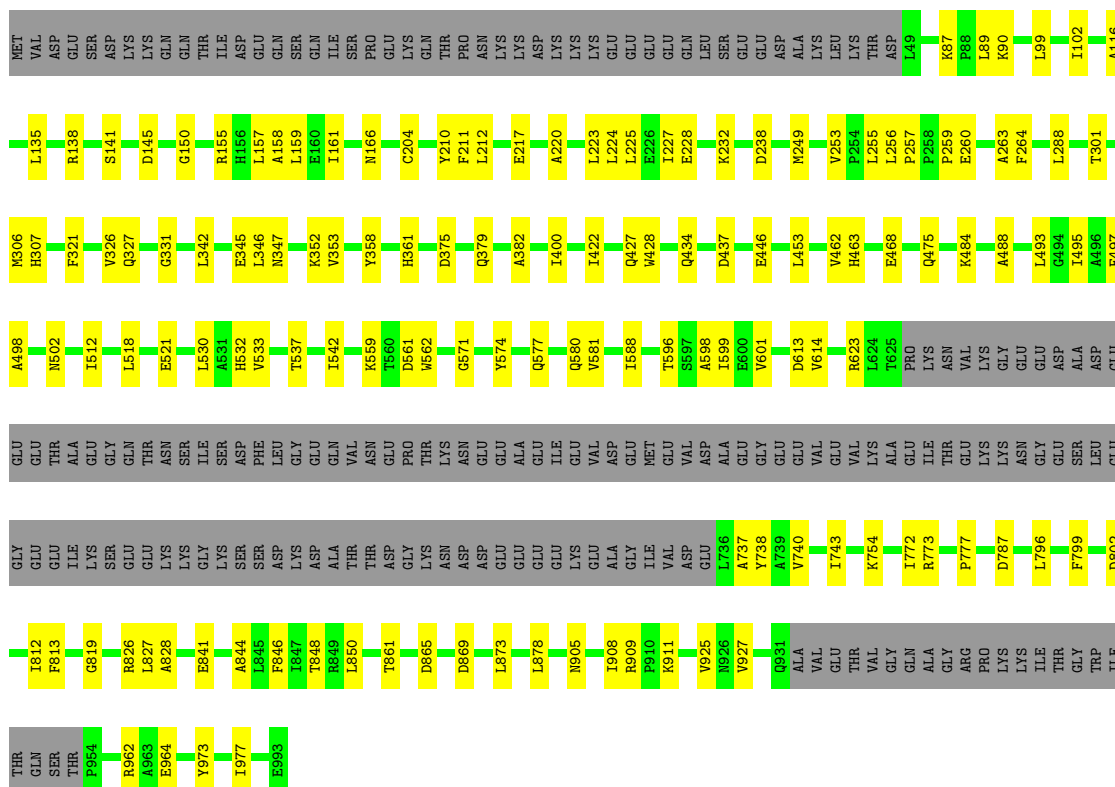
• Molecule 27: 26S proteasome regulatory subunit RPN12

Chain T: 85% 14% 1%



• Molecule 28: 26S proteasome regulatory subunit RPN8

Chain U: 56% 20% 25%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	8320	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	1	0.23	0/1541	0.41	0/2087
1	b	0.23	0/1541	0.41	0/2087
10	C	0.23	0/1934	0.40	0/2618
10	d	0.23	0/1934	0.40	0/2618
11	D	0.23	0/1910	0.39	0/2586
11	n	0.23	0/1919	0.40	0/2598
12	E	0.23	0/1886	0.40	0/2541
12	m	0.23	0/1886	0.40	0/2541
13	F	0.24	0/1823	0.41	0/2463
13	l	0.24	0/1823	0.40	0/2463
14	G	0.23	0/1932	0.38	0/2609
14	k	0.23	0/1936	0.39	0/2614
15	H	0.24	0/2831	0.41	0/3808
16	I	0.24	0/2869	0.41	0/3867
17	J	0.23	0/2964	0.40	0/3981
18	K	0.23	0/3062	0.39	0/4132
19	L	0.24	0/2896	0.39	0/3895
2	2	0.23	0/1750	0.40	0/2373
2	i	0.23	0/1750	0.42	0/2373
20	M	0.31	1/2903 (0.0%)	0.41	0/3909
21	N	0.24	0/6670	0.39	0/9023
22	O	0.23	0/3243	0.39	0/4374
23	P	0.22	0/3599	0.36	0/4854
24	Q	0.23	0/3527	0.38	0/4748
25	R	0.23	0/3272	0.39	0/4412
26	S	0.23	0/3966	0.37	0/5355
27	T	0.24	0/2279	0.40	0/3077
28	U	0.23	0/2087	0.37	0/2811
29	V	0.23	0/2271	0.44	0/3064
3	3	0.24	0/1611	0.40	0/2174
3	h	0.24	0/1611	0.41	0/2174
30	W	0.25	0/1557	0.42	0/2111
31	X	0.23	0/931	0.41	0/1262
32	Y	0.22	0/239	0.40	0/322

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
33	Z	0.26	1/6404 (0.0%)	0.40	0/8686
4	4	0.23	0/1589	0.38	0/2142
4	g	0.23	0/1589	0.39	0/2142
5	5	0.23	0/1681	0.39	0/2274
5	f	0.23	0/1681	0.40	0/2274
6	6	0.24	0/1795	0.39	0/2420
6	e	0.24	0/1795	0.39	0/2420
7	7	0.24	0/1821	0.41	0/2470
7	a	0.24	0/1846	0.42	0/2503
8	A	0.23	0/1945	0.38	0/2634
8	c	0.23	0/1959	0.39	0/2652
9	B	0.24	0/1952	0.41	0/2642
9	j	0.24	0/1952	0.40	0/2642
All	All	0.24	2/107962 (0.0%)	0.40	0/145825

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	M	75	LEU	C-N	9.87	1.53	1.34
33	Z	468	GLU	C-N	9.19	1.51	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1512	0	1478	26	0
1	b	1512	0	1478	0	0
2	2	1719	0	1716	32	0
2	i	1719	0	1716	0	0
3	3	1581	0	1571	41	0
3	h	1581	0	1571	0	0
4	4	1561	0	1569	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	g	1561	0	1569	0	0
5	5	1644	0	1592	16	0
5	f	1644	0	1592	0	0
6	6	1757	0	1708	29	0
6	e	1757	0	1708	0	0
7	7	1790	0	1790	29	0
7	a	1815	0	1818	0	0
8	A	1907	0	1901	29	0
8	c	1921	0	1910	0	0
9	B	1915	0	1929	50	0
9	j	1915	0	1929	0	0
10	C	1904	0	1901	36	0
10	d	1904	0	1901	0	0
11	D	1881	0	1892	35	0
11	n	1890	0	1900	0	0
12	E	1861	0	1836	28	0
12	m	1861	0	1836	0	0
13	F	1795	0	1797	31	0
13	l	1795	0	1797	0	0
14	G	1892	0	1883	32	0
14	k	1896	0	1886	0	0
15	H	2792	0	2879	75	0
16	I	2831	0	2881	74	0
17	J	2928	0	3057	62	0
18	K	3019	0	3084	70	0
19	L	2853	0	2926	52	0
20	M	2866	0	2938	72	0
21	N	6562	0	6625	81	0
22	O	3182	0	3207	44	0
23	P	3545	0	3629	47	0
24	Q	3471	0	3495	53	0
25	R	3218	0	3216	62	0
26	S	3894	0	3938	49	0
27	T	2235	0	2207	25	0
28	U	2061	0	2116	63	0
29	V	2236	0	2242	68	0
30	W	1534	0	1542	29	0
31	X	906	0	888	13	0
32	Y	236	0	203	13	0
33	Z	6290	0	6236	80	0
All	All	106149	0	106483	1265	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 8.

All (1265) 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)
20:M:275:PRO:HG3	20:M:320:ARG:HG2	1.19	1.14
20:M:275:PRO:HB3	20:M:320:ARG:HA	1.32	1.08
25:R:348:LEU:HB2	25:R:388:VAL:HB	1.50	0.94
28:U:210:TYR:HH	28:U:223:HIS:N	1.74	0.85
20:M:274:ALA:HB1	20:M:275:PRO:CD	2.07	0.85
1:1:20:THR:N	1:1:188:SER:HG	1.74	0.84
30:W:162:ASN:HA	30:W:168:THR:HG21	1.60	0.82
20:M:274:ALA:HB1	20:M:275:PRO:HD3	1.64	0.80
29:V:62:THR:O	29:V:63:VAL:HG23	1.81	0.80
16:I:186:GLY:H	16:I:357:THR:HG23	1.48	0.78
21:N:221:ASP:HA	21:N:894:ARG:HH22	1.48	0.77
29:V:23:THR:HG21	29:V:171:ARG:HE	1.49	0.77
15:H:313:ALA:HA	16:I:304:ARG:HE	1.50	0.76
20:M:275:PRO:CG	20:M:320:ARG:HG2	2.09	0.75
22:O:15:ARG:HD2	30:W:18:ASN:HD21	1.51	0.75
29:V:50:MET:HG3	29:V:71:MET:HB2	1.70	0.73
15:H:180:LYS:HE3	15:H:331:ARG:HH11	1.54	0.73
21:N:875:LEU:HD12	21:N:876:PRO:HD2	1.70	0.72
19:L:171:THR:HB	19:L:245:PHE:HB3	1.70	0.71
21:N:781:ALA:O	21:N:873:ARG:NH2	2.23	0.71
7:7:215:ARG:HG2	7:7:247:VAL:HG13	1.71	0.71
16:I:148:LEU:HG	16:I:157:VAL:HG23	1.71	0.71
30:W:98:LEU:HD13	30:W:108:GLN:HB3	1.71	0.71
18:K:188:VAL:HG22	18:K:313:LYS:HE2	1.72	0.70
8:A:135:ARG:HB2	14:G:13:SER:HB3	1.71	0.70
15:H:224:VAL:HG11	15:H:373:ARG:HG3	1.73	0.70
21:N:773:MET:HB2	21:N:869:ASP:HB2	1.72	0.70
1:1:131:THR:HG21	7:7:68:ARG:HH21	1.56	0.70
17:J:252:SER:HB2	17:J:295:ASN:H	1.56	0.70
17:J:85:LEU:HD11	17:J:93:LYS:HB3	1.75	0.69
29:V:61:TYR:CD1	29:V:172:GLN:NE2	2.60	0.69
12:E:18:GLU:HG2	20:M:426:LYS:HD3	1.75	0.69
3:3:27:LEU:HB3	3:3:39:LYS:HA	1.73	0.69
19:L:149:ASP:HB3	19:L:154:THR:H	1.56	0.69
9:B:40:THR:HG22	9:B:45:ILE:HG12	16.71	0.68
28:U:195:LYS:HB3	29:V:226:LYS:HB3	1.75	0.68
16:I:285:ASP:HB2	17:J:270:ARG:HE	1.58	0.68
20:M:275:PRO:HA	20:M:320:ARG:HB3	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:V:61:TYR:HD1	29:V:172:GLN:HE21	1.41	0.68
7:7:98:ARG:HD2	14:G:101:LYS:HA	1.74	0.68
15:H:242:PRO:HD2	15:H:346:ARG:HE	1.58	0.68
16:I:290:LYS:HD2	16:I:303:GLN:HG2	1.75	0.68
21:N:528:ARG:HB3	21:N:531:LEU:HB2	1.76	0.68
29:V:62:THR:O	29:V:63:VAL:CG2	2.42	0.68
31:X:38:ASN:HD22	31:X:42:GLU:H	1.42	0.68
33:Z:453:LEU:HB2	33:Z:488:ALA:HB1	1.74	0.68
4:4:184:VAL:HG22	4:4:189:ILE:HG12	1.76	0.68
1:1:80:TYR:HB2	8:A:102:ALA:HB1	1.76	0.68
16:I:204:HIS:HB3	16:I:207:LEU:HD13	1.76	0.68
17:J:338:THR:HA	25:R:203:ASP:HB3	1.76	0.68
25:R:359:VAL:HA	32:Y:81:LEU:HD22	1.76	0.67
29:V:188:LEU:HB3	29:V:192:LEU:HA	1.75	0.67
22:O:353:VAL:HG23	22:O:354:GLN:H	1.59	0.67
33:Z:530:LEU:HB3	33:Z:542:ILE:HD11	1.75	0.67
8:A:176:GLN:NE2	18:K:422:ASP:OD2	2.28	0.67
11:D:37:LYS:HE2	11:D:160:SER:HA	1.77	0.67
11:D:6:ARG:NH2	12:E:9:ASP:O	2.28	0.67
20:M:289:LYS:HB3	20:M:295:LYS:HE3	1.77	0.67
29:V:232:GLU:HA	29:V:236:SER:HB2	1.77	0.67
1:1:57:HIS:HB3	1:1:60:ILE:HB	1.75	0.66
15:H:98:GLN:HB2	16:I:119:ILE:HG21	1.75	0.66
18:K:90:GLN:HG2	18:K:147:VAL:HG13	1.77	0.66
27:T:92:ASN:HD21	27:T:96:LEU:HD13	1.59	0.66
1:1:40:THR:HG22	1:1:45:ILE:HG12	1.78	0.66
5:5:82:ARG:HH11	5:5:186:THR:HA	1.60	0.66
28:U:210:TYR:OH	28:U:223:HIS:N	2.29	0.66
10:C:124:GLN:NE2	11:D:127:ARG:O	2.28	0.66
20:M:275:PRO:CB	20:M:320:ARG:HA	2.20	0.66
2:2:141:SER:HB3	2:2:154:LEU:HD13	1.78	0.66
18:K:289:ASP:OD1	19:L:299:ARG:NH2	2.29	0.65
23:P:432:LEU:HD13	28:U:225:ILE:HG13	1.78	0.65
9:B:42:GLY:HA3	9:B:185:LEU:HD22	1.76	0.65
16:I:132:ILE:HG12	16:I:156:ILE:HD12	1.77	0.65
19:L:393:ASN:ND2	20:M:344:ASP:OD2	2.30	0.65
21:N:421:ASP:HA	21:N:424:LYS:HE2	1.79	0.65
15:H:275:ILE:HA	15:H:309:ASP:HB3	1.79	0.65
11:D:216:LYS:HB2	11:D:220:ASP:HB3	1.79	0.64
29:V:259:LYS:HB2	29:V:279:HIS:HD2	1.63	0.64
33:Z:257:PRO:HB2	33:Z:259:PRO:HD2	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:306:MET:HG2	33:Z:973:TYR:HB3	1.79	0.64
17:J:339:ARG:NH2	25:R:205:GLU:OE1	2.30	0.64
23:P:28:ALA:H	23:P:30:ASN:HD22	1.45	0.64
22:O:2:PHE:HB3	22:O:5:HIS:HB3	1.79	0.64
25:R:348:LEU:N	25:R:388:VAL:O	2.31	0.64
26:S:173:LEU:O	26:S:177:ASN:ND2	2.30	0.64
22:O:70:TYR:O	22:O:120:LYS:NZ	2.30	0.64
1:1:194:MET:HB2	1:1:205:LEU:HB2	1.80	0.64
29:V:67:ASP:OD2	29:V:100:ARG:NH1	2.31	0.64
8:A:46:ARG:HH21	8:A:167:LYS:HA	1.63	0.64
25:R:223:ASN:HB3	25:R:226:GLU:HB2	1.79	0.64
33:Z:204:CYS:HA	33:Z:232:LYS:HE2	1.79	0.64
3:3:109:VAL:HB	3:3:122:ALA:HB3	1.80	0.63
21:N:584:ARG:NH1	21:N:614:ASN:OD1	2.31	0.63
25:R:380:VAL:HB	25:R:389:GLU:HB3	1.80	0.63
21:N:635:GLN:NE2	21:N:667:GLN:OE1	2.31	0.63
1:1:38:ARG:HD2	1:1:45:ILE:HD13	1.80	0.63
2:2:228:LYS:HE2	2:2:231:SER:HA	1.79	0.63
29:V:60:ASP:O	29:V:61:TYR:HB3	1.98	0.63
18:K:134:SER:O	18:K:259:ARG:NH2	2.31	0.63
10:C:216:ILE:HG12	10:C:227:GLN:HG2	1.79	0.63
17:J:336:ASN:OD1	25:R:207:ARG:NH2	2.31	0.63
23:P:248:ASP:HA	23:P:252:SER:HB3	1.81	0.63
33:Z:773:ARG:NH1	33:Z:802:ASP:OD2	2.31	0.63
8:A:14:ARG:NH2	8:A:30:TYR:OH	2.29	0.62
21:N:780:ASP:HB2	21:N:874:ILE:HA	1.81	0.62
22:O:98:TYR:HB2	22:O:102:LEU:HD13	1.80	0.62
26:S:421:TYR:HE1	27:T:208:LEU:HG	1.64	0.62
2:2:225:ARG:NH2	3:3:151:GLU:O	2.33	0.62
14:G:68:GLN:OE1	14:G:93:ARG:NH2	2.33	0.62
17:J:336:ASN:ND2	18:K:200:GLN:O	2.32	0.62
25:R:348:LEU:CB	25:R:388:VAL:HB	2.28	0.62
6:6:174:ASN:HB3	6:6:176:LYS:HE2	1.82	0.62
17:J:160:ILE:HG23	17:J:164:ILE:HD12	1.82	0.62
20:M:151:ASP:HB3	29:V:46:PRO:HB2	1.82	0.62
15:H:203:LYS:HE2	15:H:268:ASP:HB3	1.82	0.61
24:Q:426:LEU:HD21	28:U:292:ILE:HG23	1.82	0.61
31:X:91:PHE:H	31:X:96:ARG:HD3	1.63	0.61
22:O:350:ILE:O	28:U:234:ASN:ND2	2.33	0.61
30:W:132:LEU:HB3	30:W:137:VAL:HB	1.82	0.61
9:B:119:GLN:HE22	10:C:85:GLU:HB2	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:W:2:VAL:HG22	30:W:196:SER:HB2	1.82	0.61
30:W:38:GLN:HG3	30:W:42:ASN:HD22	1.65	0.61
17:J:139:VAL:HG22	17:J:211:ILE:HG12	1.82	0.61
26:S:314:ASN:HB3	26:S:332:PHE:HZ	1.66	0.61
29:V:104:VAL:O	29:V:133:ASN:ND2	2.34	0.61
29:V:53:MET:HA	29:V:68:VAL:HG12	1.83	0.61
24:Q:31:LEU:HB3	24:Q:44:ALA:HB1	1.81	0.61
3:3:185:ALA:HB3	3:3:200:LEU:HB2	1.82	0.61
21:N:494:LYS:HE2	21:N:496:GLU:HB3	1.81	0.61
33:Z:135:LEU:HB3	33:Z:161:ILE:HD13	1.82	0.61
9:B:94:HIS:HA	9:B:98:LYS:HB2	1.83	0.61
19:L:283:VAL:HG21	19:L:325:MET:HB3	1.83	0.61
23:P:286:ASN:HA	23:P:293:LEU:HD11	1.82	0.61
8:A:47:GLY:O	8:A:193:HIS:ND1	2.33	0.60
26:S:227:ASN:HD22	26:S:263:ASP:HB2	1.66	0.60
32:Y:69:VAL:HG12	32:Y:70:ASP:H	1.66	0.60
26:S:283:GLN:HE22	27:T:120:THR:HG23	1.66	0.60
30:W:21:PHE:HB2	30:W:22:PRO:HD3	1.82	0.60
5:5:128:GLN:HB2	6:6:113:GLN:HE22	1.65	0.60
21:N:273:LEU:HB3	21:N:290:LEU:HD13	1.84	0.60
21:N:34:GLN:NE2	26:S:212:SER:OG	2.35	0.60
2:2:153:TYR:HB2	2:2:167:LEU:HD13	1.83	0.60
6:6:212:GLU:OE2	6:6:239:LYS:NZ	2.35	0.60
28:U:171:VAL:HB	29:V:217:HIS:HD2	1.66	0.60
7:7:114:ALA:HB1	7:7:117:GLU:HB2	1.84	0.60
10:C:66:LEU:HD23	10:C:76:ALA:HB2	1.84	0.60
16:I:100:ARG:HH11	16:I:133:LEU:HD23	1.67	0.60
29:V:228:TYR:HA	29:V:231:GLU:HB3	1.84	0.60
1:1:64:ARG:HD2	1:1:71:THR:HB	1.83	0.60
17:J:75:VAL:HG11	17:J:107:LEU:HB3	1.84	0.60
16:I:294:SER:HB3	16:I:300:ARG:HG3	1.83	0.60
17:J:267:GLU:OE1	18:K:290:ARG:NH2	2.27	0.60
3:3:28:ARG:NH1	3:3:179:ALA:O	2.35	0.59
11:D:201:GLU:O	11:D:204:GLN:NE2	2.33	0.59
16:I:100:ARG:HB3	16:I:157:VAL:HG12	1.84	0.59
17:J:181:GLN:HE22	17:J:287:ASN:H	1.49	0.59
33:Z:754:LYS:NZ	33:Z:787:ASP:OD2	2.32	0.59
10:C:162:ALA:HB3	11:D:54:LEU:HD13	1.84	0.59
20:M:71:ASN:HB3	29:V:74:SER:HA	1.84	0.59
21:N:653:ARG:NH1	21:N:691:GLN:OE1	2.35	0.59
4:4:146:HIS:O	4:4:149:ARG:NH1	2.30	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:574:TYR:HB2	33:Z:581:VAL:HG12	1.83	0.59
33:Z:813:PHE:HB2	33:Z:850:LEU:HD13	1.83	0.59
22:O:4:ASN:ND2	22:O:39:PHE:O	2.36	0.59
22:O:39:PHE:HB2	22:O:52:ALA:HB2	1.83	0.59
25:R:313:ALA:HA	25:R:317:ILE:HD12	1.84	0.59
25:R:33:LEU:HB3	25:R:74:ASN:HD22	1.66	0.59
2:2:239:THR:OG1	3:3:169:GLN:NE2	2.35	0.59
26:S:327:ILE:HG21	32:Y:64:TRP:HE1	1.68	0.59
28:U:125:LYS:HB3	28:U:127:GLN:HE21	1.66	0.59
33:Z:327:GLN:HE22	33:Z:463:HIS:HB2	1.66	0.59
33:Z:87:LYS:HE2	33:Z:89:LEU:HB2	1.84	0.59
16:I:147:VAL:HG12	16:I:159:VAL:HG23	1.83	0.59
18:K:207:ARG:NH2	18:K:302:GLN:O	2.36	0.59
21:N:341:ALA:HA	21:N:374:ILE:HA	1.83	0.59
22:O:30:GLU:OE2	22:O:58:ARG:NH1	2.35	0.59
24:Q:416:VAL:HG23	25:R:410:LEU:HD21	1.85	0.59
11:D:118:GLN:NE2	12:E:83:ALA:O	2.36	0.59
16:I:147:VAL:HA	16:I:160:LEU:H	1.66	0.59
23:P:48:GLN:O	23:P:88:GLN:NE2	2.31	0.59
17:J:164:ILE:HG12	17:J:289:LYS:HE2	1.84	0.59
21:N:875:LEU:HG	21:N:877:GLN:H	1.68	0.59
22:O:74:ASN:OD1	22:O:75:GLN:N	2.36	0.59
9:B:177:LYS:HG3	24:Q:209:TYR:CZ	2.38	0.59
1:1:117:ILE:HG12	1:1:131:THR:HG23	1.85	0.58
11:D:155:ILE:HG22	12:E:82:THR:HB	1.85	0.58
4:4:149:ARG:HB2	4:4:152:MET:HG3	1.85	0.58
10:C:120:GLN:NE2	10:C:123:THR:OG1	2.35	0.58
10:C:201:THR:HG22	10:C:203:SER:H	1.69	0.58
16:I:358:LYS:NZ	16:I:380:LEU:O	2.34	0.58
25:R:154:LEU:HD13	25:R:170:VAL:HA	1.85	0.58
7:7:87:SER:HB3	7:7:146:ALA:HB3	1.83	0.58
9:B:71:ILE:HG12	9:B:138:GLY:HA3	1.85	0.58
21:N:666:GLN:NE2	21:N:711:ARG:O	2.37	0.58
23:P:392:LYS:HB2	23:P:401:ASN:HB2	1.85	0.58
33:Z:358:TYR:HE1	33:Z:962:ARG:HB2	1.67	0.58
3:3:175:ALA:HB1	3:3:182:GLY:HA2	1.83	0.58
16:I:319:ARG:HH21	33:Z:828:ALA:HB2	1.68	0.58
15:H:223:GLU:HG2	20:M:403:LEU:HD23	1.85	0.58
22:O:343:GLN:HB3	23:P:360:ILE:HA	1.85	0.58
17:J:335:MET:HA	18:K:202:GLY:HA3	1.85	0.58
16:I:195:LYS:HG3	16:I:199:GLU:HB3	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:218:SER:HA	22:O:251:LEU:HD21	1.86	0.58
7:7:144:TRP:HA	7:7:165:LEU:HD23	1.86	0.58
23:P:52:LEU:HD23	23:P:55:SER:HB3	1.85	0.58
25:R:308:LEU:HD13	25:R:330:VAL:HG13	1.84	0.58
33:Z:116:ALA:HB3	33:Z:141:SER:HB2	1.86	0.58
23:P:23:LYS:HA	23:P:27:LEU:HD11	1.86	0.58
4:4:96:ARG:HH22	5:5:166:LYS:HB3	1.69	0.58
15:H:145:TYR:CZ	15:H:174:VAL:HA	2.38	0.58
22:O:143:LEU:HD13	22:O:178:TYR:HA	1.86	0.58
10:C:156:ASN:HB2	16:I:437:LEU:HD22	1.86	0.57
13:F:47:VAL:HG22	13:F:213:ILE:HG12	1.84	0.57
29:V:194:ARG:HG2	29:V:195:HIS:CD2	2.39	0.57
11:D:122:GLN:HA	12:E:136:ARG:HE	1.68	0.57
17:J:183:LYS:NZ	17:J:280:ASP:OD1	2.36	0.57
21:N:330:THR:HG21	21:N:744:PRO:HG2	1.85	0.57
24:Q:51:ARG:HD2	24:Q:88:PHE:HA	1.85	0.57
26:S:136:CYS:HB3	26:S:179:ILE:HG21	1.86	0.57
7:7:226:ARG:HE	7:7:246:GLN:HB3	1.68	0.57
21:N:489:MET:HB3	21:N:524:ILE:HG13	1.86	0.57
16:I:218:GLY:HA3	16:I:344:ILE:HG12	1.86	0.57
23:P:269:VAL:HG13	23:P:303:PHE:HZ	1.69	0.57
15:H:144:LYS:HE3	20:M:75:LEU:HG	1.87	0.57
18:K:210:LEU:HD12	18:K:337:LYS:HG2	1.86	0.57
19:L:253:ASP:HB3	20:M:293:SER:HB2	1.86	0.57
21:N:223:LEU:HD11	21:N:897:LYS:HE3	1.86	0.57
33:Z:737:ALA:HA	33:Z:772:ILE:HD13	1.87	0.57
2:2:242:LEU:HB2	3:3:201:LYS:HB2	1.85	0.57
3:3:145:GLN:HE22	3:3:177:ARG:HB2	1.69	0.57
33:Z:588:ILE:HG12	33:Z:596:THR:HB	1.85	0.57
15:H:337:ILE:HG23	15:H:370:ARG:HH21	1.69	0.57
23:P:392:LYS:HG3	23:P:403:GLU:HB2	1.86	0.57
26:S:485:LYS:HB2	28:U:305:ARG:HH21	1.69	0.57
27:T:104:LYS:NZ	27:T:169:GLN:OE1	2.38	0.57
28:U:279:SER:HB3	29:V:287:THR:HG23	1.87	0.57
14:G:9:ASP:O	14:G:23:GLN:NE2	2.37	0.57
20:M:175:LYS:HE2	20:M:240:ASN:HB3	1.86	0.57
33:Z:321:PHE:HB3	33:Z:326:VAL:HG21	1.86	0.57
15:H:243:PRO:HB3	15:H:372:ASP:HB2	1.87	0.56
21:N:562:THR:HA	21:N:597:ARG:HE	1.70	0.56
23:P:377:GLU:OE1	23:P:395:ARG:NH2	2.38	0.56
27:T:170:ASN:HA	27:T:174:PHE:HB2	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:U:49:ASN:OD1	28:U:50:SER:N	2.38	0.56
30:W:130:LYS:HA	30:W:133:LYS:HE2	1.87	0.56
3:3:63:LEU:HD22	3:3:105:VAL:HG11	1.85	0.56
9:B:41:ASN:ND2	9:B:184:GLU:OE1	2.37	0.56
21:N:762:ARG:NH2	21:N:766:GLN:O	2.38	0.56
24:Q:426:LEU:HD13	28:U:295:LYS:HD2	1.87	0.56
8:A:19:PHE:HB2	9:B:20:GLN:HE21	1.69	0.56
21:N:619:CYS:HB2	21:N:652:VAL:HG22	1.86	0.56
31:X:91:PHE:HB3	31:X:94:ASN:HD22	1.69	0.56
16:I:249:GLY:HA3	16:I:284:ILE:HG12	1.88	0.56
25:R:372:ILE:HB	26:S:398:THR:HG22	1.87	0.56
9:B:2:THR:HG22	9:B:3:ASP:H	1.71	0.56
13:F:67:ASP:HB3	13:F:70:MET:HB2	1.87	0.56
15:H:225:VAL:HA	15:H:350:LYS:HE2	1.88	0.56
16:I:118:ALA:HB2	16:I:132:ILE:HD11	1.86	0.56
18:K:195:ALA:HA	18:K:198:TYR:HD2	1.70	0.56
27:T:98:GLU:HB2	27:T:101:LYS:HG2	1.87	0.56
8:A:144:VAL:HG12	8:A:154:ILE:HG12	1.87	0.56
26:S:400:LYS:HG3	26:S:445:THR:HB	1.85	0.56
28:U:31:ARG:NH1	28:U:97:LYS:O	2.38	0.56
17:J:277:ASN:HB2	17:J:309:ARG:HE	1.71	0.56
18:K:224:LYS:NZ	19:L:313:ASP:O	2.38	0.56
22:O:120:LYS:HG2	30:W:81:ILE:HB	1.88	0.56
22:O:283:HIS:HA	22:O:286:PHE:HD2	1.70	0.56
23:P:392:LYS:HE3	23:P:403:GLU:HA	1.87	0.56
29:V:147:VAL:HG12	29:V:149:GLY:H	1.71	0.56
20:M:143:ASN:HD21	20:M:257:GLY:HA2	1.70	0.56
21:N:330:THR:HG23	21:N:366:THR:HG21	1.88	0.56
19:L:118:ILE:HG12	19:L:128:ILE:HG12	1.88	0.56
29:V:52:LEU:HD11	29:V:104:VAL:HG13	1.88	0.56
2:2:75:ALA:HB3	2:2:126:TYR:HB2	1.88	0.56
19:L:195:GLU:HA	19:L:199:LEU:HD13	1.88	0.56
22:O:377:VAL:HG22	28:U:197:LEU:HD22	1.87	0.56
29:V:221:TRP:NE1	29:V:223:SER:OG	2.39	0.56
16:I:330:LYS:HG2	16:I:332:GLU:H	1.71	0.56
19:L:407:ARG:HG2	19:L:409:HIS:H	1.70	0.56
21:N:366:THR:HG22	21:N:747:HIS:HE1	1.70	0.56
29:V:163:ALA:H	29:V:166:ASN:HD21	1.54	0.56
23:P:424:GLU:HB2	28:U:232:VAL:HG11	1.88	0.55
23:P:409:SER:HB3	23:P:412:LEU:HD12	1.88	0.55
24:Q:65:TYR:HD2	24:Q:74:LEU:HD13	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:29:LYS:HE3	4:4:31:SER:HB2	1.88	0.55
16:I:174:ASP:HB3	16:I:244:PHE:HB3	1.88	0.55
25:R:373:PRO:HB2	32:Y:64:TRP:HZ3	1.71	0.55
3:3:20:CYS:HA	3:3:112:ILE:HD11	1.88	0.55
8:A:156:LYS:NZ	8:A:170:ALA:O	2.39	0.55
11:D:68:ASP:HB3	11:D:71:VAL:HB	1.88	0.55
13:F:34:VAL:HA	13:F:162:GLY:HA3	1.88	0.55
19:L:305:LEU:HD13	19:L:334:ASP:HB2	1.89	0.55
20:M:129:LEU:HD11	20:M:155:ILE:HD12	1.87	0.55
22:O:75:GLN:OE1	22:O:114:GLN:NE2	2.39	0.55
24:Q:104:PHE:HB3	24:Q:114:GLN:HE21	1.71	0.55
29:V:124:ASN:OD1	29:V:194:ARG:NH1	2.36	0.55
33:Z:812:ILE:HD13	33:Z:848:THR:HA	1.88	0.55
9:B:111:VAL:HG21	9:B:148:TYR:HD2	1.72	0.55
19:L:357:ARG:NH2	19:L:383:SER:O	2.39	0.55
33:Z:861:THR:OG1	33:Z:962:ARG:NH1	2.39	0.55
1:1:33:LEU:HD21	1:1:119:ALA:HB3	1.88	0.55
3:3:11:ILE:HD12	3:3:146:LEU:HD11	1.88	0.55
25:R:174:ILE:HG21	25:R:190:LYS:HB2	1.88	0.55
3:3:73:LEU:HD23	3:3:76:LEU:HD12	1.89	0.55
10:C:217:ARG:HG2	10:C:219:GLY:H	1.71	0.55
20:M:219:LEU:HD23	20:M:346:LYS:HG2	1.89	0.55
30:W:11:ASP:HA	30:W:55:ALA:HB3	1.89	0.55
33:Z:150:GLY:H	33:Z:210:TYR:HE1	1.53	0.55
33:Z:347:ASN:HB3	33:Z:353:VAL:HG23	1.89	0.55
7:7:48:LYS:HD2	7:7:173:PRO:HA	1.88	0.55
17:J:357:ASP:OD2	18:K:330:ARG:NH1	2.40	0.55
21:N:70:TYR:HE2	26:S:219:LYS:HD2	1.72	0.55
24:Q:127:ARG:HA	24:Q:130:ARG:HB2	1.89	0.55
12:E:71:ASP:HB3	12:E:74:ILE:HB	1.89	0.55
15:H:147:ILE:HD11	15:H:157:VAL:HG23	1.89	0.55
20:M:202:LYS:HG2	20:M:203:ARG:HG2	1.87	0.55
21:N:713:VAL:HA	21:N:755:PRO:HA	1.88	0.55
22:O:43:GLU:HA	22:O:82:LEU:HD21	1.89	0.55
26:S:109:GLU:OE2	26:S:111:ARG:NE	2.38	0.55
28:U:283:ARG:HB2	29:V:287:THR:HG21	1.89	0.55
24:Q:188:LEU:HD11	25:R:278:SER:HA	1.87	0.55
27:T:206:LYS:HG3	27:T:211:PHE:HB2	1.89	0.55
10:C:181:LYS:HE2	10:C:183:ASP:HB2	1.89	0.54
13:F:117:GLN:HE21	13:F:121:GLN:HG3	1.72	0.54
33:Z:869:ASP:HB2	33:Z:977:ILE:HG13	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:32:ILE:HD13	2:2:73:ALA:HB1	1.90	0.54
8:A:18:ILE:HG22	9:B:128:ARG:HB3	1.88	0.54
15:H:275:ILE:HG22	15:H:277:SER:H	1.72	0.54
20:M:295:LYS:HB3	20:M:302:GLN:HB2	1.89	0.54
28:U:273:LEU:HD23	28:U:276:ILE:HD12	1.89	0.54
28:U:66:PHE:HB2	30:W:96:LEU:HD13	1.89	0.54
15:H:96:PRO:HA	15:H:191:ILE:HG13	1.89	0.54
1:1:196:VAL:HB	1:1:203:GLU:HB3	1.90	0.54
13:F:22:VAL:HG11	13:F:150:SER:HB3	1.88	0.54
21:N:83:LEU:HD11	21:N:136:ILE:HG13	1.89	0.54
21:N:154:LEU:HD22	21:N:189:LEU:HD21	1.88	0.54
28:U:47:VAL:HG22	28:U:89:ILE:HD11	1.90	0.54
28:U:81:LYS:HB3	29:V:72:PRO:HB3	1.90	0.54
26:S:330:LEU:HD12	32:Y:65:ASP:H	1.72	0.54
16:I:161:GLN:NE2	16:I:163:ASP:OD2	2.41	0.54
29:V:61:TYR:CD2	29:V:62:THR:N	2.76	0.54
8:A:141:LEU:HB2	8:A:157:THR:HB	1.90	0.54
9:B:81:ASP:HB3	9:B:130:PHE:HB3	1.89	0.54
11:D:44:LEU:HD11	11:D:136:ALA:HB3	1.89	0.54
16:I:281:ILE:HB	16:I:326:MET:HG2	1.90	0.54
2:2:109:LEU:HD21	2:2:148:THR:HB	1.89	0.54
3:3:103:TYR:OH	4:4:93:ARG:NH1	2.33	0.54
16:I:417:LYS:HA	16:I:420:LYS:HE2	1.90	0.54
21:N:265:ALA:HB1	21:N:269:LEU:HB2	1.89	0.54
21:N:378:ASN:HD21	21:N:381:GLU:HB2	1.73	0.54
23:P:425:HIS:HE2	28:U:233:PHE:HE1	1.56	0.54
20:M:136:ASP:OD2	20:M:139:LYS:NZ	2.36	0.54
33:Z:99:LEU:HD23	33:Z:102:ILE:HD12	1.90	0.54
2:2:114:GLN:HE22	8:A:107:LYS:HA	1.70	0.54
28:U:189:ARG:HG3	29:V:296:LEU:HD11	1.90	0.54
3:3:138:VAL:HG11	3:3:146:LEU:HB2	1.89	0.53
9:B:20:GLN:O	9:B:24:ALA:N	2.35	0.53
11:D:37:LYS:HD2	11:D:145:PRO:HB2	1.90	0.53
13:F:31:GLN:NE2	20:M:428:LYS:O	2.40	0.53
15:H:283:TYR:HD2	15:H:286:GLU:HB2	1.73	0.53
16:I:372:SER:HB3	16:I:412:THR:HA	1.91	0.53
17:J:301:ASP:HB3	17:J:304:LEU:HG	1.90	0.53
24:Q:382:LEU:O	25:R:263:ARG:NH1	2.40	0.53
24:Q:404:ASN:O	25:R:397:ASN:ND2	2.41	0.53
14:G:73:HIS:ND1	14:G:74:ILE:HG13	2.23	0.53
19:L:351:LEU:HD12	19:L:352:PRO:HD2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:251:ASP:OD1	17:J:253:ILE:HG12	2.07	0.53
19:L:131:VAL:HB	19:L:135:VAL:HG21	1.89	0.53
17:J:155:LYS:HD3	17:J:317:PRO:HG3	1.90	0.53
20:M:290:ARG:H	20:M:332:VAL:HG21	1.73	0.53
18:K:77:ARG:HH22	21:N:577:SER:HA	1.74	0.53
25:R:312:TYR:HA	25:R:316:LEU:HD12	1.89	0.53
28:U:265:LEU:HB3	28:U:268:LYS:HE2	1.90	0.53
13:F:2:PHE:N	13:F:24:TYR:HH	2.07	0.53
15:H:399:GLU:HB3	15:H:402:ILE:HG23	1.89	0.53
28:U:276:ILE:O	28:U:280:ASN:ND2	2.42	0.53
4:4:4:ILE:HG12	4:4:103:LEU:HD12	1.90	0.53
20:M:219:LEU:HD21	20:M:330:VAL:HG21	1.90	0.53
21:N:510:HIS:HB3	21:N:513:ILE:HB	1.90	0.53
24:Q:431:SER:HA	25:R:422:ARG:HG3	1.91	0.53
29:V:97:GLN:HG3	29:V:98:THR:HG23	1.90	0.53
1:1:89:TYR:HD1	14:G:111:ALA:HB1	1.74	0.53
7:7:161:ARG:HE	7:7:169:THR:HB	1.74	0.53
20:M:357:ARG:NH2	20:M:383:THR:O	2.42	0.53
33:Z:596:THR:HA	33:Z:599:ILE:HD12	1.91	0.53
8:A:48:LYS:HG2	8:A:53:VAL:HG12	18.07	0.53
16:I:93:LYS:H	16:I:96:LEU:HD13	1.73	0.53
18:K:281:ARG:NH2	18:K:285:GLN:H	2.07	0.53
20:M:357:ARG:HD2	20:M:391:LEU:HD21	1.90	0.53
9:B:13:SER:HB2	9:B:18:LEU:HD23	1.91	0.52
27:T:129:LEU:HD12	27:T:136:LEU:HD12	1.91	0.52
33:Z:512:ILE:HG23	33:Z:521:GLU:HB3	1.91	0.52
8:A:114:CYS:HA	8:A:117:LEU:HB3	1.90	0.52
12:E:146:GLY:HA2	12:E:222:ILE:HG21	1.90	0.52
15:H:299:ARG:NH2	15:H:339:GLN:OE1	2.42	0.52
18:K:99:PHE:HA	18:K:110:VAL:HG12	1.92	0.52
13:F:76:GLY:HA3	13:F:130:VAL:HA	1.90	0.52
13:F:153:VAL:HB	14:G:86:ARG:HH12	1.74	0.52
15:H:279:LEU:HD22	15:H:287:GLY:HA2	1.90	0.52
21:N:259:PHE:HB2	21:N:902:VAL:HG13	1.90	0.52
3:3:28:ARG:HB2	3:3:183:TRP:HB2	1.92	0.52
10:C:97:ASN:HA	10:C:100:LYS:HD3	1.90	0.52
12:E:166:ARG:HB3	13:F:58:SER:HB2	1.91	0.52
25:R:363:PHE:HD2	32:Y:81:LEU:HD21	1.73	0.52
29:V:29:ILE:HG23	29:V:33:ALA:HB3	1.92	0.52
8:A:156:LYS:HB3	8:A:166:TYR:HE2	1.75	0.52
9:B:44:VAL:HG21	9:B:189:ILE:HG12	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:8:SER:HA	9:B:11:THR:O	2.10	0.52
15:H:100:ALA:HB1	15:H:173:ARG:O	2.10	0.52
26:S:311:GLN:NE2	26:S:341:SER:OG	2.42	0.52
29:V:62:THR:C	29:V:63:VAL:HG23	2.30	0.52
1:1:27:PHE:HE2	1:1:32:ILE:HG13	1.73	0.52
4:4:8:ARG:HG3	4:4:13:VAL:HG22	1.91	0.52
6:6:145:ASP:OD1	6:6:156:ARG:NH2	2.43	0.52
15:H:157:VAL:O	15:H:182:ASN:ND2	2.42	0.52
15:H:314:VAL:O	15:H:318:ARG:NH1	2.42	0.52
20:M:221:TYR:HE1	20:M:346:LYS:HB3	1.74	0.52
28:U:46:ARG:NH2	28:U:164:GLU:OE2	2.37	0.52
6:6:107:SER:HB3	12:E:103:TYR:HD1	1.75	0.52
28:U:19:ASP:OD2	28:U:23:ARG:NE	2.42	0.52
9:B:7:PHE:HB2	9:B:9:LEU:HG	1.91	0.52
12:E:99:HIS:ND1	12:E:105:GLU:O	2.38	0.52
20:M:246:LEU:HD22	20:M:262:LEU:HD13	1.92	0.52
21:N:589:ILE:HA	21:N:624:ALA:HB2	1.92	0.52
23:P:55:SER:HA	23:P:59:LEU:HB3	1.90	0.52
7:7:137:ARG:HA	7:7:142:PRO:HG3	1.90	0.52
15:H:251:PRO:HG2	15:H:254:THR:HB	1.91	0.52
16:I:101:GLY:HA3	16:I:150:HIS:CD2	2.45	0.52
21:N:647:ASP:O	21:N:653:ARG:NE	2.43	0.52
33:Z:446:GLU:HG2	33:Z:484:LYS:HG3	1.91	0.52
16:I:202:LEU:O	33:Z:826:ARG:NH2	2.43	0.52
26:S:393:ARG:NH1	26:S:431:VAL:O	2.43	0.52
26:S:475:TYR:OH	28:U:295:LYS:HG3	2.10	0.52
3:3:123:GLY:HA3	3:3:137:ILE:HG21	1.93	0.51
17:J:160:ILE:HD11	17:J:198:LEU:HD21	1.91	0.51
22:O:292:CYS:O	22:O:295:THR:OG1	2.26	0.51
22:O:72:LYS:HG2	22:O:73:ILE:HG12	1.92	0.51
25:R:240:SER:HB2	25:R:244:THR:HG22	1.91	0.51
31:X:48:PHE:HB2	31:X:66:LEU:HB3	1.92	0.51
2:2:123:ILE:HG22	2:2:125:ALA:H	1.76	0.51
8:A:14:ARG:O	8:A:27:GLN:NE2	2.43	0.51
13:F:74:LEU:HD13	13:F:81:ALA:HB1	1.92	0.51
19:L:283:VAL:HB	19:L:327:THR:HB	1.91	0.51
21:N:424:LYS:NZ	21:N:461:GLU:OE1	2.42	0.51
24:Q:249:LEU:HB2	24:Q:253:ASN:HB2	1.92	0.51
25:R:347:THR:O	25:R:348:LEU:HD23	2.10	0.51
26:S:425:ARG:NH1	27:T:188:GLU:OE2	2.42	0.51
27:T:190:ALA:HB2	27:T:209:LEU:HD21	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:366:MET:HE3	28:U:233:PHE:HE2	1.75	0.51
3:3:30:GLY:HA2	3:3:36:VAL:HG23	1.92	0.51
9:B:21:ILE:O	9:B:25:LEU:N	2.33	0.51
16:I:198:VAL:HG13	16:I:323:LYS:HG3	1.92	0.51
3:3:51:LEU:HD22	3:3:87:PHE:HZ	1.76	0.51
4:4:80:VAL:HG12	4:4:104:ILE:HD13	1.92	0.51
10:C:206:LEU:HD23	10:C:244:ILE:HG21	1.91	0.51
18:K:109:ILE:HG12	18:K:119:VAL:HG22	1.92	0.51
18:K:341:PRO:O	18:K:344:ARG:NH1	2.34	0.51
20:M:275:PRO:HB3	20:M:320:ARG:CA	2.22	0.51
27:T:131:LYS:HB3	27:T:134:LYS:HB2	1.92	0.51
28:U:64:VAL:HG22	30:W:92:GLN:HG2	1.92	0.51
28:U:56:GLU:HB2	28:U:66:PHE:HB3	1.92	0.51
29:V:225:LEU:O	29:V:228:TYR:N	2.44	0.51
33:Z:873:LEU:HD13	33:Z:878:LEU:HD21	1.91	0.51
2:2:57:ASP:OD1	2:2:58:LYS:N	2.44	0.51
9:B:87:ASP:OD1	9:B:90:ARG:NH2	2.44	0.51
12:E:142:LEU:HB2	12:E:158:ALA:HB3	1.92	0.51
23:P:304:THR:HA	23:P:352:VAL:HG21	1.92	0.51
26:S:82:TYR:CD2	26:S:86:SER:HB3	2.46	0.51
15:H:155:PHE:HZ	20:M:150:LYS:HD2	1.75	0.51
15:H:158:GLY:HA2	20:M:162:GLU:HG3	1.92	0.51
21:N:742:TRP:CE3	21:N:743:PHE:HB3	2.46	0.51
33:Z:352:LYS:HG2	33:Z:462:VAL:HG23	1.91	0.51
14:G:150:MET:HB3	14:G:160:TYR:CE2	2.46	0.51
16:I:148:LEU:HB2	16:I:160:LEU:HG	1.93	0.51
25:R:325:HIS:HB3	25:R:328:PHE:HB2	1.93	0.51
33:Z:217:GLU:HA	33:Z:220:ALA:HB3	1.93	0.51
6:6:221:LEU:N	6:6:236:TYR:O	2.41	0.51
6:6:49:ILE:HG22	6:6:54:ILE:HA	1.93	0.51
14:G:54:ILE:HD11	14:G:213:GLU:HG3	1.92	0.51
20:M:116:ALA:HA	20:M:130:PRO:HA	1.93	0.51
28:U:37:LEU:HB2	28:U:49:ASN:HB3	1.92	0.51
33:Z:327:GLN:HG3	33:Z:346:LEU:HD11	1.93	0.51
10:C:172:ALA:HB2	10:C:200:THR:HG21	1.93	0.51
9:B:16:GLY:O	10:C:28:SER:OG	2.26	0.51
12:E:213:ASP:OD1	12:E:214:GLU:N	2.44	0.51
20:M:274:ALA:CB	20:M:275:PRO:CD	2.86	0.51
24:Q:426:LEU:HD11	28:U:292:ILE:HG12	1.92	0.51
29:V:28:TYR:CE1	29:V:202:ASP:OD2	2.63	0.51
30:W:109:ARG:HH22	30:W:195:GLY:HA3	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:27:LEU:HD12	3:3:184:GLY:HA3	1.92	0.51
4:4:73:TYR:HB2	10:C:143:ARG:HH21	1.75	0.51
7:7:58:ASP:HA	7:7:228:PHE:HA	1.93	0.51
18:K:120:VAL:HG11	18:K:139:LEU:HD22	1.93	0.51
15:H:227:LEU:HD22	20:M:403:LEU:HD22	1.92	0.51
20:M:62:ILE:HG13	20:M:66:LYS:HG3	1.92	0.51
24:Q:195:LYS:HG2	24:Q:225:LEU:HD13	1.93	0.51
7:7:54:ILE:HD11	7:7:230:LEU:HD21	1.93	0.50
14:G:150:MET:HB3	14:G:160:TYR:HE2	1.75	0.50
14:G:224:THR:HG22	14:G:229:LYS:HD2	1.93	0.50
16:I:390:ALA:HB1	17:J:307:PRO:HD2	1.93	0.50
17:J:42:ARG:NE	26:S:484:ASP:OD2	2.44	0.50
25:R:58:GLU:HB3	25:R:144:ILE:HA	1.92	0.50
26:S:129:GLU:OE2	26:S:132:ALA:N	2.44	0.50
7:7:107:ASN:HD22	7:7:120:LEU:HG	1.76	0.50
16:I:336:PRO:HA	16:I:339:ILE:HD12	1.92	0.50
19:L:196:VAL:HG23	19:L:197:ILE:HG12	1.92	0.50
19:L:189:GLN:OE1	19:L:345:ARG:NH2	2.43	0.50
24:Q:172:PRO:HA	24:Q:208:ILE:HD13	1.92	0.50
24:Q:419:LEU:HD22	25:R:414:LEU:HD13	1.93	0.50
1:1:102:LYS:HD2	1:1:138:VAL:HG23	1.93	0.50
6:6:47:ARG:HB2	6:6:219:ASP:HB2	1.93	0.50
6:6:78:ALA:HB2	7:7:167:GLY:HA3	1.93	0.50
10:C:44:ILE:HB	10:C:216:ILE:HD12	1.94	0.50
16:I:124:THR:HG22	17:J:91:GLU:HB3	1.94	0.50
17:J:304:LEU:HD23	17:J:309:ARG:HD3	1.91	0.50
29:V:61:TYR:CG	29:V:62:THR:N	2.77	0.50
33:Z:537:THR:O	33:Z:577:GLN:NE2	2.44	0.50
33:Z:559:LYS:HG3	33:Z:561:ASP:H	1.76	0.50
33:Z:601:VAL:HG21	33:Z:623:ARG:HD3	1.92	0.50
18:K:123:LEU:HG	18:K:125:THR:H	1.76	0.50
18:K:345:ASP:OD1	18:K:346:ARG:N	2.44	0.50
23:P:283:LYS:HD2	23:P:286:ASN:HD21	1.77	0.50
26:S:436:ILE:HG12	26:S:443:ILE:HG12	1.93	0.50
17:J:336:ASN:HB3	17:J:376:HIS:ND1	2.27	0.50
21:N:533:ASP:OD1	21:N:559:TYR:OH	2.29	0.50
21:N:436:ASP:HB2	21:N:439:VAL:HG23	1.93	0.50
2:2:63:LEU:HD12	2:2:215:TYR:HE1	1.76	0.50
9:B:200:VAL:HG22	9:B:202:GLY:H	1.76	0.50
11:D:79:ASN:HB2	16:I:437:LEU:HD23	1.93	0.50
15:H:73:ASP:OD1	15:H:173:ARG:NH2	2.39	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:183:LYS:N	17:J:311:ASP:OD2	2.40	0.50
22:O:290:LYS:NZ	22:O:354:GLN:HE21	2.10	0.50
33:Z:138:ARG:HH21	33:Z:157:LEU:HB2	1.76	0.50
5:5:253:TYR:HE1	5:5:262:TYR:HD1	1.58	0.50
13:F:67:ASP:OD1	13:F:68:GLU:N	2.44	0.50
17:J:88:VAL:HB	17:J:92:GLY:H	1.76	0.50
19:L:298:ASP:HB3	19:L:302:GLN:HG2	1.94	0.50
24:Q:391:ASP:HB3	24:Q:396:TRP:H	1.76	0.50
15:H:399:GLU:HG2	15:H:401:GLY:H	1.77	0.50
21:N:891:VAL:HB	21:N:908:ARG:HD3	1.94	0.50
25:R:347:THR:HA	25:R:389:GLU:HA	1.94	0.50
19:L:425:VAL:HG21	20:M:345:ARG:HA	1.94	0.49
29:V:250:GLN:HE22	29:V:253:LYS:HD3	1.77	0.49
29:V:25:GLU:HB3	29:V:63:VAL:HG21	1.94	0.49
30:W:114:VAL:HG21	30:W:141:ILE:HG23	1.94	0.49
2:2:192:ILE:HG23	2:2:199:GLY:HA2	1.94	0.49
7:7:48:LYS:HG2	7:7:53:VAL:HG12	1.93	0.49
11:D:181:ARG:NH1	12:E:59:LEU:O	2.45	0.49
12:E:71:ASP:OD1	12:E:72:ARG:N	2.44	0.49
13:F:226:ASP:OD1	13:F:227:GLY:N	2.45	0.49
18:K:241:GLU:O	18:K:243:VAL:HG23	2.12	0.49
19:L:219:LEU:HD11	19:L:327:THR:HG22	1.95	0.49
25:R:236:ALA:HB1	25:R:279:LEU:HD21	1.94	0.49
29:V:259:LYS:HB2	29:V:279:HIS:CD2	2.45	0.49
29:V:95:LEU:HG	29:V:100:ARG:NE	2.27	0.49
31:X:85:ARG:HD2	31:X:101:LEU:HD12	1.94	0.49
15:H:431:ILE:HG21	16:I:200:LEU:HD21	1.95	0.49
15:H:96:PRO:HB3	15:H:191:ILE:HG21	1.94	0.49
24:Q:339:TYR:HE2	24:Q:376:LYS:HE2	1.77	0.49
26:S:330:LEU:N	32:Y:62:GLU:O	2.44	0.49
30:W:36:ILE:HG12	30:W:191:ILE:HD11	1.94	0.49
7:7:185:ASN:HB3	7:7:186:PRO:HD3	1.93	0.49
8:A:168:ALA:HB3	9:B:55:LEU:HD13	1.94	0.49
11:D:117:GLN:HE22	11:D:129:PHE:HB2	1.78	0.49
12:E:130:GLU:HB3	12:E:132:ARG:HH12	1.77	0.49
13:F:39:ARG:NH2	13:F:155:GLU:OE2	2.46	0.49
6:6:84:VAL:HG12	6:6:88:LYS:HE3	1.94	0.49
9:B:222:LEU:HD13	9:B:232:GLY:HA2	1.94	0.49
16:I:251:GLU:O	16:I:254:GLN:NE2	2.43	0.49
18:K:238:ASN:HB2	18:K:241:GLU:HG3	1.94	0.49
18:K:386:ILE:HG12	18:K:414:GLN:HG3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:318:LEU:HB3	19:L:321:THR:HB	1.94	0.49
25:R:40:ILE:HG12	25:R:88:LEU:HD13	1.95	0.49
26:S:30:GLN:OE1	26:S:64:ARG:NH2	2.46	0.49
27:T:29:PRO:HA	27:T:32:ILE:HD12	1.94	0.49
7:7:232:ILE:HB	7:7:240:THR:HB	1.94	0.49
9:B:119:GLN:HB3	10:C:86:ILE:HD11	1.95	0.49
15:H:177:ASP:OD1	15:H:283:TYR:OH	2.22	0.49
17:J:79:VAL:HG12	17:J:81:ASP:H	1.78	0.49
18:K:148:ASP:OD1	18:K:149:ILE:N	2.45	0.49
18:K:213:GLY:O	18:K:219:LYS:NZ	2.42	0.49
24:Q:81:SER:HA	24:Q:84:TYR:HD2	1.76	0.49
33:Z:518:LEU:HB2	33:Z:562:TRP:HH2	1.77	0.49
5:5:93:SER:OG	5:5:249:SER:N	2.31	0.49
18:K:283:ASP:OD1	18:K:284:ALA:N	2.44	0.49
19:L:105:ILE:HD11	19:L:145:ARG:HD2	1.94	0.49
21:N:654:GLN:HG3	21:N:698:GLY:HA3	1.95	0.49
27:T:41:ILE:HG23	27:T:87:PRO:HG3	1.95	0.49
14:G:204:HIS:CE1	14:G:208:LYS:HA	2.47	0.49
16:I:101:GLY:HA3	16:I:150:HIS:HD2	1.78	0.49
18:K:426:PHE:HB3	18:K:428:LYS:NZ	2.28	0.49
21:N:190:LEU:HD13	21:N:207:LEU:HD21	1.93	0.49
24:Q:387:TYR:HB3	24:Q:400:TYR:HD2	1.78	0.49
33:Z:400:ILE:HD13	33:Z:422:ILE:HG23	1.93	0.49
24:Q:92:LYS:HA	24:Q:129:LYS:HE2	1.95	0.49
26:S:293:ILE:HD13	26:S:316:LEU:HD23	1.95	0.49
26:S:424:SER:HB3	27:T:192:ASN:HB3	1.95	0.49
29:V:55:GLY:HA2	29:V:66:VAL:HG23	1.95	0.49
31:X:66:LEU:HD11	31:X:91:PHE:HE2	1.78	0.49
33:Z:382:ALA:HA	33:Z:846:PHE:HD1	1.76	0.49
16:I:294:SER:HA	16:I:299:GLU:HA	1.93	0.49
15:H:57:LYS:HZ1	16:I:99:ILE:HB	1.78	0.49
19:L:244:ILE:HB	19:L:278:ILE:HA	1.95	0.49
23:P:177:ILE:HG23	23:P:203:ILE:HD12	1.94	0.49
28:U:226:LEU:HD23	28:U:229:LEU:HD12	1.94	0.49
11:D:17:ILE:HG22	11:D:19:GLN:H	1.77	0.48
15:H:363:PRO:HA	15:H:366:LEU:HB3	1.95	0.48
16:I:408:ARG:NH1	16:I:412:THR:OG1	2.46	0.48
18:K:217:THR:OG1	18:K:380:GLY:N	2.46	0.48
18:K:244:HIS:O	19:L:299:ARG:NH1	2.44	0.48
19:L:108:VAL:HG22	19:L:119:VAL:HG12	1.94	0.48
21:N:521:LEU:HB3	21:N:535:LEU:HD21	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:664:LEU:HD13	21:N:678:ILE:HG21	1.95	0.48
29:V:228:TYR:HB3	29:V:232:GLU:HB2	1.95	0.48
6:6:76:PHE:CE2	6:6:78:ALA:HB3	2.48	0.48
18:K:271:ILE:N	18:K:315:ILE:O	2.41	0.48
18:K:91:SER:OG	18:K:92:VAL:N	2.45	0.48
20:M:135:VAL:HG12	20:M:158:THR:HG23	1.94	0.48
20:M:220:MET:HB3	20:M:349:PHE:HE2	1.77	0.48
15:H:368:PRO:HD2	20:M:389:ALA:HB1	1.95	0.48
21:N:239:LEU:HG	21:N:243:LYS:HE3	1.95	0.48
23:P:361:THR:HG22	23:P:363:LEU:H	1.78	0.48
24:Q:97:LEU:HB3	24:Q:130:ARG:HH21	1.78	0.48
26:S:486:LYS:HE2	28:U:301:ILE:HG22	1.95	0.48
23:P:411:LEU:HD13	29:V:297:THR:HG21	1.95	0.48
5:5:162:VAL:HG11	5:5:192:SER:HA	1.95	0.48
18:K:271:ILE:HB	18:K:316:MET:HA	1.95	0.48
18:K:418:ASP:OD1	18:K:419:ASN:N	2.45	0.48
19:L:104:LEU:HD23	20:M:127:VAL:HG12	1.95	0.48
21:N:756:THR:HG21	21:N:876:PRO:HD3	1.95	0.48
21:N:96:GLN:HG3	26:S:220:ILE:HG12	1.94	0.48
24:Q:129:LYS:HG3	24:Q:133:LEU:HD12	1.95	0.48
11:D:161:ALA:HB1	11:D:175:LEU:HD22	1.95	0.48
13:F:9:ASP:OD1	13:F:10:THR:N	2.47	0.48
16:I:184:ILE:HB	16:I:187:LEU:HD12	1.94	0.48
17:J:134:VAL:HG22	17:J:137:MET:HE2	1.96	0.48
17:J:162:GLU:HA	17:J:166:LEU:HD13	1.95	0.48
18:K:102:PRO:HA	18:K:108:GLY:HA2	1.94	0.48
23:P:89:LEU:HG	23:P:91:LEU:H	1.78	0.48
29:V:225:LEU:O	29:V:229:ASP:N	2.47	0.48
9:B:35:LEU:HD22	9:B:175:LEU:HD21	1.95	0.48
14:G:80:GLY:HA3	14:G:134:VAL:HG12	1.94	0.48
13:F:176:LEU:HD13	14:G:58:LEU:HD23	1.95	0.48
15:H:217:GLN:NE2	15:H:378:SER:H	2.11	0.48
16:I:282:ASP:OD1	16:I:283:GLU:N	2.46	0.48
17:J:61:GLU:OE2	18:K:121:ARG:NH2	2.45	0.48
20:M:324:LEU:HA	20:M:343:LEU:HD21	1.94	0.48
18:K:60:LEU:HD21	21:N:601:THR:HB	1.95	0.48
18:K:399:ARG:HD3	23:P:198:VAL:HG11	1.95	0.48
23:P:94:GLN:HA	23:P:97:ILE:HD12	1.96	0.48
33:Z:475:GLN:HE22	33:Z:502:ASN:HD22	1.61	0.48
4:4:33:ASP:OD1	4:4:34:LYS:N	2.46	0.48
6:6:50:THR:OG1	6:6:55:ASN:ND2	2.36	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:81:ALA:HB2	13:F:130:VAL:HG21	1.96	0.48
15:H:240:ILE:HD13	20:M:399:GLY:HA3	1.95	0.48
29:V:38:LEU:O	29:V:42:ARG:HG3	2.13	0.48
3:3:113:ASN:ND2	3:3:116:SER:OG	2.47	0.48
14:G:68:GLN:O	14:G:76:CYS:N	2.46	0.48
15:H:357:ARG:HH21	15:H:359:ASN:HD22	1.62	0.48
21:N:25:LEU:HD23	21:N:28:ILE:HD12	1.96	0.48
21:N:301:THR:HG21	21:N:921:ARG:HB3	1.96	0.48
21:N:303:LEU:HD21	21:N:755:PRO:HB3	1.96	0.48
29:V:51:GLY:HA3	29:V:108:TYR:CZ	2.48	0.48
33:Z:598:ALA:HB3	33:Z:738:TYR:HB3	1.96	0.48
5:5:91:VAL:HG21	5:5:108:LYS:HB2	1.94	0.48
10:C:144:TYR:HB3	11:D:59:ILE:HG22	1.94	0.48
17:J:156:GLN:HE21	17:J:198:LEU:HD22	1.78	0.48
31:X:17:TYR:HH	31:X:97:TYR:HH	1.60	0.48
21:N:728:LYS:HB3	21:N:751:LEU:HB3	1.95	0.48
25:R:240:SER:HB3	25:R:243:LEU:HB2	1.96	0.48
29:V:59:ASP:O	29:V:60:ASP:CB	2.62	0.48
4:4:29:LYS:HE3	4:4:32:ASP:H	1.78	0.47
4:4:36:ARG:HG2	4:4:46:PHE:HE1	1.79	0.47
8:A:200:GLU:HB3	8:A:244:ARG:HH12	1.79	0.47
13:F:121:GLN:NE2	14:G:84:ASP:OD1	2.46	0.47
15:H:107:LYS:HB2	15:H:144:LYS:HG3	1.95	0.47
16:I:105:SER:O	16:I:149:LEU:HB2	2.14	0.47
20:M:165:SER:HB3	20:M:258:GLU:HG2	1.96	0.47
21:N:416:GLY:HA3	21:N:453:ALA:HB1	1.96	0.47
21:N:600:THR:HA	21:N:634:LEU:HD22	1.96	0.47
9:B:44:VAL:HG23	9:B:213:ILE:HG22	1.95	0.47
17:J:64:LEU:HB3	18:K:121:ARG:HD2	1.95	0.47
20:M:78:LEU:HD22	20:M:150:LYS:HA	1.96	0.47
18:K:212:TYR:HB2	18:K:339:GLU:HA	1.96	0.47
26:S:119:TYR:CE2	26:S:121:VAL:HB	2.50	0.47
29:V:197:TYR:CE2	29:V:199:LEU:HB2	2.49	0.47
12:E:161:SER:HB2	20:M:433:TYR:HD2	1.79	0.47
26:S:428:ARG:NH1	27:T:191:LYS:O	2.48	0.47
30:W:186:ALA:HA	30:W:191:ILE:HD12	1.97	0.47
25:R:331:ARG:NH2	32:Y:72:ASP:O	2.47	0.47
33:Z:342:LEU:HB2	33:Z:345:GLU:HG2	1.96	0.47
10:C:44:ILE:H	10:C:216:ILE:HB	1.78	0.47
10:C:50:ARG:NH1	10:C:59:GLN:O	2.29	0.47
18:K:325:ASP:OD2	18:K:329:LEU:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S:26:ALA:HB2	26:S:68:LEU:HD12	1.96	0.47
28:U:175:LEU:HD23	29:V:205:LYS:HE3	1.97	0.47
5:5:113:ASN:OD1	5:5:116:LEU:N	2.47	0.47
9:B:94:HIS:O	9:B:99:ARG:N	2.43	0.47
11:D:139:ASP:HB2	11:D:142:ASP:HB3	1.96	0.47
18:K:268:ILE:HG12	18:K:313:LYS:HB3	1.97	0.47
24:Q:419:LEU:HD12	25:R:410:LEU:HD13	1.97	0.47
26:S:480:ARG:HD2	26:S:483:GLU:HB2	1.95	0.47
33:Z:358:TYR:HA	33:Z:361:HIS:HD2	1.80	0.47
8:A:78:THR:H	8:A:233:PHE:HB2	1.79	0.47
13:F:39:ARG:NH1	13:F:142:ALA:O	2.48	0.47
18:K:281:ARG:HH22	18:K:285:GLN:H	1.62	0.47
20:M:187:ASP:HA	20:M:190:ILE:HB	1.96	0.47
21:N:360:GLN:HG3	29:V:168:LEU:HD12	1.97	0.47
4:4:36:ARG:HG3	4:4:57:ALA:HB1	1.97	0.47
16:I:100:ARG:HD3	16:I:133:LEU:HD23	1.97	0.47
15:H:98:GLN:HG3	16:I:110:GLU:HB3	1.96	0.47
16:I:135:PHE:CD2	16:I:136:VAL:HG13	2.50	0.47
20:M:144:ASP:OD1	20:M:145:LEU:N	2.47	0.47
20:M:149:ASN:OD1	20:M:150:LYS:N	2.47	0.47
23:P:119:ILE:HG23	23:P:125:VAL:HG11	1.96	0.47
3:3:80:ARG:HE	9:B:142:PHE:HB3	1.79	0.47
18:K:123:LEU:H	18:K:146:LEU:HD23	1.79	0.47
18:K:357:ALA:HB1	18:K:362:LEU:HD11	1.97	0.47
19:L:371:THR:HG22	19:L:407:ARG:HH21	1.80	0.47
21:N:286:LEU:HD23	21:N:289:ILE:HD12	1.97	0.47
22:O:76:LEU:HA	22:O:79:VAL:HG12	1.97	0.47
25:R:213:TYR:HD1	25:R:216:ILE:HD12	1.80	0.47
28:U:262:GLN:HG2	28:U:265:LEU:HD12	1.95	0.47
29:V:159:ILE:HB	29:V:195:HIS:HB3	1.97	0.47
33:Z:331:GLY:HA3	33:Z:346:LEU:HD22	1.96	0.47
6:6:81:ASP:OD2	7:7:169:THR:OG1	2.33	0.47
10:C:156:ASN:ND2	16:I:436:TYR:O	2.48	0.47
33:Z:249:MET:HG3	33:Z:253:VAL:HG21	1.96	0.47
33:Z:577:GLN:HB3	33:Z:580:GLN:HB2	1.96	0.47
3:3:107:PRO:HG2	3:3:124:PHE:HB2	1.97	0.47
24:Q:47:ASP:OD1	24:Q:48:ASP:N	2.47	0.47
2:2:189:GLN:HB2	2:2:220:LEU:HD21	1.97	0.46
29:V:59:ASP:O	29:V:60:ASP:HB3	2.16	0.46
6:6:29:GLY:H	6:6:216:GLN:HG3	1.79	0.46
14:G:218:TRP:HH2	14:G:223:GLU:HB2	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:217:LYS:NZ	16:I:318:ASP:OD1	2.40	0.46
16:I:358:LYS:HD3	16:I:381:VAL:HA	1.98	0.46
18:K:326:PRO:HD2	18:K:328:LEU:HG	1.98	0.46
23:P:123:ARG:HA	23:P:126:THR:HB	1.97	0.46
24:Q:426:LEU:HD22	28:U:295:LYS:HB2	1.96	0.46
25:R:381:ILE:HB	26:S:399:TYR:HD1	1.80	0.46
28:U:82:ILE:HG23	29:V:70:ALA:HB3	1.95	0.46
30:W:163:ASN:HB3	30:W:164:PRO:HD3	1.96	0.46
33:Z:613:ASP:OD1	33:Z:614:VAL:N	2.48	0.46
4:4:165:VAL:HG13	4:4:176:PHE:HZ	1.80	0.46
4:4:89:ALA:O	4:4:93:ARG:NE	2.48	0.46
9:B:38:LYS:HA	9:B:43:VAL:HG22	1.98	0.46
3:3:65:GLU:HG2	10:C:100:LYS:HA	1.97	0.46
10:C:50:ARG:HH21	10:C:212:GLU:HG2	1.80	0.46
22:O:114:GLN:HG2	22:O:118:GLY:HA3	1.95	0.46
23:P:393:VAL:H	24:Q:354:PHE:HB3	1.80	0.46
23:P:47:ARG:HG2	23:P:52:LEU:HG	1.97	0.46
24:Q:135:HIS:ND1	24:Q:169:ASP:OD2	2.49	0.46
28:U:15:LEU:HD22	29:V:213:LEU:HD21	1.96	0.46
33:Z:87:LYS:HD3	33:Z:90:LYS:HG3	1.98	0.46
9:B:77:GLY:HA3	9:B:132:VAL:HG12	1.98	0.46
11:D:149:GLN:NE2	11:D:157:SER:OG	2.48	0.46
15:H:106:ILE:HG12	20:M:76:PRO:HD3	1.97	0.46
15:H:226:GLU:HA	15:H:267:THR:HG22	1.97	0.46
24:Q:374:GLU:O	25:R:345:TYR:OH	2.33	0.46
25:R:117:ILE:HD12	25:R:137:LEU:HD22	1.98	0.46
22:O:306:ARG:NH2	28:U:234:ASN:OD1	2.49	0.46
3:3:53:ILE:HG22	3:3:60:VAL:HG22	1.97	0.46
10:C:226:TYR:CE2	10:C:228:LYS:HB2	2.51	0.46
13:F:54:ASP:H	13:F:57:SER:HB3	1.81	0.46
1:1:103:GLU:HG3	14:G:102:LEU:HA	1.97	0.46
15:H:248:LEU:HB2	15:H:354:ALA:HA	1.97	0.46
15:H:396:MET:HA	16:I:212:GLY:HA3	1.98	0.46
22:O:341:ILE:HG22	22:O:348:VAL:HG13	1.98	0.46
23:P:388:ILE:HG22	23:P:389:ILE:HG23	1.97	0.46
29:V:67:ASP:OD1	29:V:68:VAL:N	2.48	0.46
2:2:126:TYR:HB3	2:2:156:LEU:HD21	1.97	0.46
6:6:220:GLY:H	6:6:238:LEU:HB2	1.80	0.46
19:L:182:GLY:HA2	19:L:363:ILE:HD13	1.97	0.46
21:N:602:VAL:HB	21:N:603:PRO:HD3	1.98	0.46
24:Q:109:ASP:OD1	24:Q:110:SER:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:911:LYS:HE3	33:Z:964:GLU:HB3	1.97	0.46
2:2:36:LYS:HD2	2:2:152:TYR:HD1	1.81	0.46
15:H:311:ILE:HD12	15:H:314:VAL:HB	1.97	0.46
19:L:298:ASP:O	19:L:301:ILE:N	2.48	0.46
23:P:144:VAL:HG12	23:P:148:LYS:HE3	1.98	0.46
24:Q:249:LEU:HB3	24:Q:252:HIS:HB2	1.96	0.46
24:Q:98:LYS:HD2	24:Q:136:SER:HB3	1.98	0.46
26:S:357:LEU:HB3	26:S:384:ARG:HH22	1.80	0.46
28:U:273:LEU:HA	28:U:276:ILE:HD12	1.98	0.46
33:Z:256:LEU:HB3	33:Z:257:PRO:HD3	1.97	0.46
33:Z:841:GLU:H	33:Z:844:ALA:HB3	1.81	0.46
22:O:2:PHE:HE1	22:O:35:GLU:HA	1.81	0.46
9:B:68:THR:HG21	9:B:105:PRO:HD2	1.98	0.46
9:B:90:ARG:O	9:B:94:HIS:ND1	2.29	0.46
15:H:105:ILE:HB	15:H:146:VAL:HG22	1.97	0.46
18:K:211:LEU:HD23	18:K:338:ILE:HB	1.97	0.46
19:L:374:PHE:HA	19:L:412:PRO:HG3	1.98	0.46
3:3:138:VAL:HG12	3:3:143:SER:HB2	1.98	0.46
10:C:70:ASN:OD1	10:C:73:ILE:N	2.49	0.46
23:P:59:LEU:HD21	23:P:82:LEU:HD13	1.97	0.46
30:W:143:ASN:ND2	30:W:149:GLN:O	2.49	0.46
1:1:143:TYR:OH	1:1:158:ASP:OD1	2.33	0.45
11:D:79:ASN:HD22	16:I:437:LEU:HG	1.81	0.45
12:E:19:GLY:HA2	13:F:24:TYR:HB3	1.98	0.45
14:G:68:GLN:HB2	14:G:76:CYS:HB3	1.98	0.45
26:S:445:THR:HG22	26:S:447:GLU:H	1.81	0.45
28:U:289:ASP:O	28:U:293:GLU:N	2.45	0.45
25:R:331:ARG:HH12	32:Y:69:VAL:HG12	1.80	0.45
33:Z:301:THR:O	33:Z:307:HIS:NE2	2.48	0.45
1:1:122:ASP:OD1	1:1:123:ASP:N	2.49	0.45
9:B:35:LEU:HB2	9:B:175:LEU:HD11	1.97	0.45
9:B:45:ILE:HD12	9:B:74:VAL:HB	1.98	0.45
18:K:212:TYR:N	18:K:338:ILE:O	2.49	0.45
19:L:145:ARG:HH21	19:L:159:LEU:HB3	1.81	0.45
23:P:164:GLN:HG3	23:P:168:TYR:HE2	1.82	0.45
24:Q:423:VAL:HA	24:Q:426:LEU:HD12	1.99	0.45
1:1:64:ARG:HG2	1:1:116:ILE:HG12	1.98	0.45
5:5:134:LEU:HD22	5:5:158:LEU:HB2	1.97	0.45
9:B:214:ILE:HG13	9:B:235:PHE:HD1	1.81	0.45
12:E:41:ALA:HA	12:E:46:VAL:HG22	1.98	0.45
13:F:39:ARG:HD3	13:F:144:LEU:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:653:ARG:NH1	21:N:692:GLU:OE1	2.50	0.45
21:N:885:ILE:HG12	21:N:887:ASP:H	1.81	0.45
22:O:270:ILE:HD12	22:O:274:ILE:HG13	1.98	0.45
24:Q:93:THR:O	24:Q:130:ARG:NH2	2.50	0.45
26:S:164:ILE:HB	26:S:165:PRO:HD3	1.98	0.45
1:1:145:ILE:HD12	1:1:150:SER:HB2	1.97	0.45
11:D:56:ASP:HB3	11:D:59:ILE:HG12	1.98	0.45
17:J:188:TYR:HB2	17:J:315:GLU:HA	1.98	0.45
17:J:335:MET:SD	17:J:362:CYS:HB3	2.56	0.45
18:K:175:GLY:HA3	18:K:351:LEU:HB3	1.98	0.45
21:N:376:LYS:HA	21:N:411:ILE:HG12	1.97	0.45
23:P:90:LYS:HG3	23:P:129:LYS:HB3	1.98	0.45
25:R:220:ALA:HA	25:R:324:ARG:HE	1.82	0.45
30:W:30:ILE:HG23	30:W:73:LEU:HD22	1.98	0.45
12:E:175:GLY:O	15:H:409:ARG:NH2	2.50	0.45
16:I:261:PRO:HB2	16:I:265:ARG:HH12	1.82	0.45
19:L:222:GLY:HA3	19:L:349:ILE:HB	1.97	0.45
19:L:360:ILE:HG22	19:L:391:ILE:HD13	1.98	0.45
21:N:277:LEU:HG	21:N:282:TYR:HB3	1.99	0.45
25:R:348:LEU:HD13	25:R:353:MET:SD	2.57	0.45
3:3:25:CYS:HB2	3:3:42:LYS:NZ	2.32	0.45
7:7:187:LEU:HD11	7:7:216:VAL:HG11	1.98	0.45
19:L:156:MET:HG2	19:L:157:ARG:HG2	1.99	0.45
20:M:124:ARG:HH22	20:M:255:TYR:HE1	1.64	0.45
22:O:137:TYR:HB2	22:O:146:ALA:HB2	1.97	0.45
24:Q:97:LEU:HB3	24:Q:130:ARG:NH2	2.32	0.45
28:U:93:HIS:HE1	28:U:121:ILE:HG12	1.81	0.45
33:Z:865:ASP:HB3	33:Z:909:ARG:HD3	1.98	0.45
4:4:135:TYR:HA	4:4:138:PHE:HE2	1.81	0.45
8:A:35:THR:HG21	8:A:140:ILE:HG13	1.99	0.45
10:C:76:ALA:HB3	10:C:136:ILE:HD12	1.98	0.45
21:N:161:TYR:HE1	21:N:197:VAL:HG22	1.82	0.45
25:R:370:LYS:NZ	32:Y:70:ASP:OD1	2.36	0.45
7:7:44:VAL:HG13	7:7:57:ALA:HB2	1.97	0.45
17:J:167:PRO:HG3	17:J:182:PRO:HG2	1.99	0.45
25:R:394:ASP:O	25:R:397:ASN:ND2	2.49	0.45
28:U:293:GLU:HA	28:U:296:ILE:HD12	1.99	0.45
1:1:63:CYS:HB2	1:1:117:ILE:HB	1.99	0.45
2:2:129:VAL:HB	2:2:140:PHE:HB2	1.98	0.45
2:2:153:TYR:OH	2:2:168:GLU:OE1	2.29	0.45
16:I:287:ILE:HG13	16:I:302:ILE:HG23	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:427:LYS:HG3	16:I:428:VAL:H	1.82	0.45
17:J:87:LYS:HA	17:J:93:LYS:HA	1.98	0.45
18:K:237:VAL:O	18:K:271:ILE:HA	2.17	0.45
21:N:578:ASP:O	21:N:584:ARG:NE	2.42	0.45
27:T:164:LEU:HB3	27:T:178:THR:HG23	1.98	0.45
27:T:235:PHE:CZ	27:T:237:ASN:HB2	2.51	0.45
28:U:140:GLU:OE2	28:U:152:LYS:NZ	2.39	0.45
3:3:189:ILE:HB	3:3:196:VAL:HB	1.99	0.45
9:B:8:SER:OG	9:B:18:LEU:HD21	2.17	0.45
21:N:491:GLY:H	21:N:526:TYR:HB3	1.81	0.45
25:R:204:TRP:CG	25:R:235:LEU:HD12	2.52	0.45
27:T:110:LEU:HD21	27:T:125:GLU:HB2	1.99	0.45
33:Z:571:GLY:HA2	33:Z:574:TYR:HE2	1.82	0.45
4:4:192:VAL:HG12	4:4:194:ASP:H	1.82	0.44
5:5:82:ARG:HH21	5:5:200:ASP:HA	1.80	0.44
9:B:193:LEU:HD21	9:B:211:LEU:HD22	1.99	0.44
13:F:11:VAL:HA	14:G:130:ARG:HD3	1.99	0.44
16:I:116:ASP:HA	16:I:132:ILE:HB	2.00	0.44
16:I:387:LEU:HD22	16:I:391:ASP:HB2	1.99	0.44
18:K:106:ASN:HA	18:K:122:ILE:HB	1.98	0.44
19:L:187:THR:HA	19:L:190:ILE:HB	1.99	0.44
20:M:82:VAL:HG21	20:M:140:LEU:HB3	1.99	0.44
22:O:376:GLN:O	22:O:381:GLY:N	2.43	0.44
32:Y:69:VAL:HG12	32:Y:70:ASP:N	2.30	0.44
33:Z:347:ASN:HA	33:Z:352:LYS:HD2	1.99	0.44
3:3:108:VAL:HA	3:3:123:GLY:HA2	1.98	0.44
6:6:134:ASP:OD1	6:6:138:LYS:N	2.50	0.44
15:H:149:LEU:HD23	15:H:177:ASP:HB2	1.99	0.44
18:K:210:LEU:HD23	18:K:316:MET:HB2	1.99	0.44
21:N:207:LEU:HB3	21:N:228:VAL:HG13	1.98	0.44
21:N:302:PHE:HB3	21:N:757:THR:HG21	2.00	0.44
28:U:93:HIS:CE1	28:U:121:ILE:HG12	2.52	0.44
30:W:30:ILE:HG12	30:W:76:LEU:HD13	2.00	0.44
9:B:9:LEU:HB3	9:B:125:GLY:HA2	1.98	0.44
11:D:163:THR:HG21	11:D:171:VAL:HB	1.99	0.44
17:J:252:SER:H	17:J:294:THR:HA	1.82	0.44
17:J:61:GLU:O	17:J:65:LEU:HG	2.17	0.44
18:K:349:ARG:NH2	18:K:375:ASN:O	2.50	0.44
20:M:248:ALA:HB2	20:M:282:GLU:HB2	2.00	0.44
20:M:62:ILE:HD12	20:M:65:ASN:HB2	1.98	0.44
23:P:438:ILE:HD11	28:U:98:LEU:HD12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:224:LEU:HD21	33:Z:232:LYS:HB2	1.98	0.44
10:C:22:VAL:HG13	10:C:153:PRO:HG2	1.97	0.44
17:J:68:PRO:HB2	17:J:118:ASP:HB2	2.00	0.44
17:J:297:LEU:HD21	17:J:302:PRO:HA	2.00	0.44
18:K:164:ASN:HB3	18:K:234:PHE:HD2	1.82	0.44
19:L:281:ASP:OD1	19:L:282:GLU:N	2.50	0.44
21:N:416:GLY:O	21:N:420:THR:N	2.51	0.44
33:Z:819:GLY:HA2	33:Z:827:LEU:HD13	2.00	0.44
1:1:85:TYR:CZ	1:1:96:THR:HG21	2.53	0.44
5:5:76:THR:N	5:5:206:SER:HG	2.15	0.44
10:C:107:PRO:HD2	10:C:110:ILE:HD12	2.00	0.44
17:J:184:GLY:HA3	17:J:309:ARG:O	2.17	0.44
19:L:220:LEU:HD23	19:L:347:VAL:HB	1.99	0.44
23:P:364:ARG:NH1	23:P:367:GLU:OE1	2.50	0.44
26:S:93:LEU:O	26:S:98:SER:OG	2.27	0.44
30:W:166:GLU:HB3	30:W:195:GLY:HA2	1.99	0.44
31:X:37:PRO:HB3	31:X:46:TRP:HD1	1.82	0.44
31:X:48:PHE:HD2	31:X:66:LEU:HD23	1.82	0.44
33:Z:159:LEU:HD21	33:Z:223:LEU:HD22	1.99	0.44
6:6:170:ASP:O	6:6:176:LYS:N	2.36	0.44
15:H:311:ILE:O	15:H:315:GLY:N	2.51	0.44
15:H:57:LYS:NZ	16:I:99:ILE:HB	2.33	0.44
17:J:329:ARG:HG2	17:J:343:LEU:HD13	1.99	0.44
22:O:222:LEU:HB3	22:O:280:LEU:HD13	1.99	0.44
30:W:9:VAL:HB	30:W:112:ALA:HA	2.00	0.44
33:Z:740:VAL:HA	33:Z:743:ILE:HD12	1.99	0.44
3:3:109:VAL:N	3:3:122:ALA:O	2.41	0.44
3:3:28:ARG:HG3	3:3:183:TRP:CE3	2.51	0.44
8:A:20:SER:HB2	8:A:21:PRO:HD2	1.99	0.44
8:A:165:GLY:H	9:B:60:THR:HG21	1.83	0.44
11:D:5:ASP:HB3	11:D:22:TYR:HE2	1.82	0.44
17:J:267:GLU:HG3	17:J:270:ARG:HH12	1.83	0.44
18:K:232:ALA:HA	18:K:266:PRO:HB2	1.99	0.44
19:L:252:VAL:HG13	19:L:300:GLU:HB2	2.00	0.44
30:W:110:ILE:HD12	30:W:139:VAL:HG22	1.98	0.44
30:W:52:ILE:HG22	30:W:61:VAL:HG13	2.00	0.44
16:I:184:ILE:HG22	16:I:231:LEU:HB3	1.99	0.44
16:I:104:LEU:HD23	17:J:95:ILE:HG21	1.98	0.44
15:H:146:VAL:HG11	20:M:76:PRO:HB3	1.98	0.44
24:Q:426:LEU:HB3	28:U:295:LYS:HD3	1.99	0.44
25:R:138:GLY:HA2	25:R:141:TYR:HD2	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:228:GLU:HA	33:Z:264:PHE:HZ	1.82	0.44
33:Z:400:ILE:HG12	33:Z:422:ILE:HG12	1.99	0.44
9:B:2:THR:HG22	9:B:3:ASP:N	2.33	0.44
12:E:120:ALA:HB1	12:E:160:PRO:HA	1.99	0.44
13:F:187:ASP:OD1	13:F:233:TYR:OH	2.32	0.44
19:L:387:ASN:OD1	19:L:390:ASP:N	2.46	0.44
21:N:117:TYR:HD1	21:N:123:PHE:HE2	1.66	0.44
21:N:475:ALA:O	21:N:512:ASN:ND2	2.46	0.44
22:O:189:TYR:HB2	22:O:220:SER:HB2	2.00	0.44
24:Q:389:VAL:CG2	25:R:346:LYS:HB2	2.47	0.44
24:Q:51:ARG:NH1	24:Q:89:ALA:H	2.16	0.44
26:S:226:ASP:OD2	26:S:229:THR:OG1	2.31	0.44
28:U:166:ALA:HB3	29:V:42:ARG:HE	1.81	0.44
33:Z:375:ASP:H	33:Z:379:GLN:HE21	1.64	0.44
33:Z:427:GLN:HG2	33:Z:428:TRP:CD1	2.53	0.44
1:1:64:ARG:HD3	1:1:75:ALA:HB2	1.99	0.43
2:2:244:GLU:HG3	3:3:198:ARG:HG2	1.99	0.43
7:7:198:ILE:HB	7:7:199:PRO:HD3	1.99	0.43
9:B:217:GLU:OE1	9:B:232:GLY:N	2.36	0.43
18:K:53:LYS:HA	18:K:56:LYS:HD3	1.99	0.43
20:M:149:ASN:ND2	20:M:152:SER:OG	2.51	0.43
20:M:216:LYS:NZ	20:M:316:SER:O	2.47	0.43
23:P:94:GLN:HB3	23:P:135:GLU:HG2	1.99	0.43
25:R:347:THR:O	25:R:348:LEU:HG	2.18	0.43
26:S:475:TYR:OH	28:U:294:ASN:HB2	2.18	0.43
28:U:280:ASN:HA	28:U:283:ARG:HB3	2.00	0.43
2:2:58:LYS:NZ	3:3:135:ASP:OD2	2.37	0.43
9:B:82:TYR:CZ	9:B:86:VAL:HG21	2.53	0.43
21:N:352:ASN:HB3	21:N:355:TRP:CE3	2.53	0.43
23:P:392:LYS:HD2	23:P:401:ASN:HB2	1.99	0.43
11:D:95:SER:HA	11:D:98:LEU:HB3	2.00	0.43
15:H:221:LEU:O	15:H:225:VAL:HB	2.19	0.43
18:K:391:GLY:HA3	19:L:212:ILE:HG21	1.99	0.43
33:Z:905:ASN:HA	33:Z:908:ILE:HD12	2.00	0.43
1:1:61:TRP:HD1	1:1:197:LEU:HD11	1.83	0.43
15:H:105:ILE:HG22	15:H:107:LYS:HG2	2.00	0.43
16:I:188:GLU:HA	16:I:191:ILE:HB	2.01	0.43
22:O:127:LEU:HD22	22:O:167:ILE:HG12	2.00	0.43
22:O:40:GLN:O	22:O:58:ARG:NH2	2.38	0.43
25:R:225:LYS:O	25:R:229:LYS:HG3	2.18	0.43
9:B:179:TRP:HB2	9:B:191:ILE:HG21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:102:GLY:H	20:M:154:LEU:HD21	1.84	0.43
23:P:125:VAL:O	23:P:136:ARG:NE	2.51	0.43
23:P:350:LEU:HD11	23:P:369:LEU:HD21	2.01	0.43
33:Z:796:LEU:HA	33:Z:799:PHE:HB3	1.99	0.43
33:Z:911:LYS:HG3	33:Z:964:GLU:HB2	2.00	0.43
15:H:57:LYS:HE3	16:I:96:LEU:HA	2.00	0.43
17:J:116:ARG:HG2	17:J:118:ASP:H	1.84	0.43
28:U:52:ALA:O	29:V:97:GLN:NE2	2.52	0.43
10:C:11:THR:HG22	11:D:127:ARG:HB2	2.00	0.43
14:G:65:VAL:HG12	14:G:67:ILE:H	1.82	0.43
16:I:433:GLU:CG	16:I:435:LEU:HD13	2.48	0.43
21:N:344:THR:HG22	21:N:375:HIS:HA	2.01	0.43
21:N:340:HIS:HB2	21:N:374:ILE:HG12	1.99	0.43
23:P:19:GLU:HB3	23:P:58:VAL:HG11	2.01	0.43
24:Q:359:ILE:HA	24:Q:362:ILE:HD12	2.00	0.43
26:S:427:ILE:HD12	27:T:196:SER:HB3	2.01	0.43
28:U:126:GLN:HE22	29:V:212:MET:HA	1.83	0.43
33:Z:255:LEU:HD13	33:Z:260:GLU:HB2	2.00	0.43
2:2:46:ASP:OD1	2:2:62:LYS:NZ	2.45	0.43
4:4:34:LYS:HB3	4:4:46:PHE:CE2	2.54	0.43
5:5:229:LEU:HD22	5:5:252:LEU:HD13	2.00	0.43
15:H:162:ARG:HB2	15:H:183:ILE:HD12	2.01	0.43
15:H:328:GLU:CD	15:H:329:VAL:HG23	2.39	0.43
17:J:181:GLN:HE21	17:J:183:LYS:HE2	1.82	0.43
17:J:96:VAL:HB	17:J:121:MET:HA	2.00	0.43
18:K:233:ALA:O	18:K:268:ILE:N	2.39	0.43
25:R:208:ASN:O	25:R:212:THR:N	2.50	0.43
28:U:168:GLU:O	29:V:217:HIS:NE2	2.51	0.43
28:U:34:GLY:HA3	28:U:92:TYR:CZ	2.54	0.43
3:3:52:GLY:O	3:3:107:PRO:HA	2.18	0.43
8:A:236:LEU:HD22	8:A:240:ASN:HB3	2.01	0.43
15:H:298:ALA:HB1	15:H:349:ILE:HG12	2.01	0.43
19:L:109:MET:N	19:L:118:ILE:O	2.51	0.43
19:L:308:LEU:HB3	19:L:342:ARG:HH21	1.83	0.43
20:M:142:PRO:HG2	20:M:264:ARG:HH22	1.83	0.43
25:R:59:MET:O	25:R:63:TYR:N	2.39	0.43
26:S:428:ARG:HD3	27:T:192:ASN:HA	2.01	0.43
22:O:357:ILE:HB	28:U:223:HIS:HB2	1.99	0.43
3:3:35:GLY:HA3	3:3:183:TRP:HH2	1.83	0.42
4:4:23:ARG:HG3	4:4:28:LEU:HD12	2.00	0.42
11:D:122:GLN:HA	12:E:136:ARG:NE	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:150:LYS:HG2	15:H:152:ILE:H	1.84	0.42
20:M:379:LEU:HD21	20:M:416:VAL:HG22	2.00	0.42
25:R:238:PHE:HD2	25:R:249:ILE:HG13	1.84	0.42
25:R:316:LEU:HD13	25:R:329:PHE:CD2	2.54	0.42
28:U:163:ALA:HB3	28:U:168:GLU:HG3	2.00	0.42
29:V:42:ARG:CZ	29:V:145:GLN:HE21	2.32	0.42
31:X:91:PHE:HB3	31:X:94:ASN:ND2	2.34	0.42
33:Z:263:ALA:HA	33:Z:288:LEU:HD11	2.01	0.42
2:2:166:VAL:O	2:2:170:HIS:ND1	2.45	0.42
4:4:38:LEU:HD23	4:4:61:GLN:HG3	2.00	0.42
12:E:99:HIS:HE1	12:E:105:GLU:HB3	1.83	0.42
14:G:91:ARG:HG2	14:G:119:TYR:CE1	2.54	0.42
15:H:197:MET:SD	15:H:278:GLU:HB2	2.59	0.42
18:K:64:GLN:HA	18:K:67:TYR:HB3	2.01	0.42
21:N:283:ASP:HB3	21:N:286:LEU:HB2	2.00	0.42
23:P:126:THR:O	23:P:136:ARG:NH2	2.52	0.42
23:P:319:GLU:OE1	23:P:323:ASN:HB3	2.19	0.42
26:S:234:ILE:HD11	26:S:258:GLU:HG2	2.01	0.42
33:Z:498:ALA:HA	33:Z:533:VAL:HA	2.00	0.42
5:5:233:LYS:HD2	5:5:271:LEU:HD11	2.01	0.42
8:A:69:VAL:HG22	14:G:158:TRP:CD1	2.53	0.42
15:H:164:SER:OG	15:H:167:ASP:O	2.35	0.42
21:N:518:ALA:HB1	21:N:550:GLY:HA3	2.00	0.42
28:U:36:ILE:HG23	28:U:92:TYR:HD2	1.84	0.42
30:W:143:ASN:HD21	30:W:149:GLN:H	1.65	0.42
30:W:115:CYS:HA	30:W:144:PHE:HB2	2.01	0.42
33:Z:225:LEU:HD21	33:Z:253:VAL:HA	2.02	0.42
2:2:239:THR:HG21	3:3:168:SER:HB3	2.01	0.42
3:3:105:VAL:HG23	3:3:107:PRO:HD3	2.01	0.42
7:7:48:LYS:HE3	7:7:160:LEU:HB3	2.00	0.42
10:C:232:PRO:HA	10:C:235:ILE:HD12	2.01	0.42
13:F:168:ALA:N	13:F:200:SER:OG	2.53	0.42
15:H:253:GLY:HA2	15:H:256:LYS:HE2	2.01	0.42
24:Q:94:VAL:HB	24:Q:133:LEU:HD13	2.01	0.42
25:R:241:ILE:N	25:R:244:THR:O	2.53	0.42
15:H:106:ILE:HD12	29:V:76:THR:HG22	2.01	0.42
4:4:135:TYR:HA	4:4:138:PHE:CE2	2.54	0.42
4:4:71:GLU:OE2	10:C:113:ARG:NH2	2.41	0.42
6:6:221:LEU:HB2	6:6:238:LEU:HD11	2.01	0.42
8:A:35:THR:HA	8:A:85:GLY:HA2	2.00	0.42
14:G:179:LEU:HA	14:G:182:HIS:HD2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:312:ASP:OD1	15:H:360:THR:OG1	2.34	0.42
17:J:230:VAL:HG11	17:J:272:MET:HA	2.01	0.42
17:J:267:GLU:O	17:J:270:ARG:HG2	2.19	0.42
18:K:209:VAL:HG23	18:K:336:ARG:HB2	2.00	0.42
19:L:290:ARG:HG2	19:L:291:PHE:H	1.84	0.42
22:O:130:ASP:HA	22:O:133:ILE:HD12	2.00	0.42
24:Q:239:PHE:HB3	24:Q:265:MET:HG2	2.00	0.42
24:Q:343:LEU:O	24:Q:347:LEU:N	2.48	0.42
28:U:36:ILE:HD11	28:U:118:LEU:HB3	2.01	0.42
29:V:173:THR:HG22	29:V:174:THR:HG23	2.00	0.42
31:X:85:ARG:HH22	31:X:104:LYS:HG3	1.85	0.42
4:4:41:HIS:NE2	4:4:186:LYS:O	2.52	0.42
10:C:13:PHE:CD2	11:D:19:GLN:HB3	2.54	0.42
11:D:70:HIS:ND1	11:D:71:VAL:HG23	2.35	0.42
19:L:421:LYS:HB3	20:M:345:ARG:HH22	1.84	0.42
29:V:126:GLN:NE2	29:V:130:GLU:OE2	2.53	0.42
9:B:4:ARG:HH21	9:B:11:THR:HG21	1.84	0.42
16:I:104:LEU:HD13	16:I:148:LEU:HD12	2.02	0.42
24:Q:210:CYS:HB3	24:Q:214:THR:HB	2.00	0.42
18:K:351:LEU:HD22	24:Q:234:THR:HA	2.01	0.42
33:Z:211:PHE:CG	33:Z:220:ALA:HB2	2.54	0.42
4:4:8:ARG:N	4:4:129:PRO:O	2.44	0.42
6:6:35:ALA:HB3	6:6:154:GLN:HA	2.02	0.42
7:7:107:ASN:ND2	7:7:120:LEU:HG	2.35	0.42
9:B:119:GLN:HE21	10:C:82:ALA:HA	1.85	0.42
15:H:51:GLN:HA	15:H:54:ASN:HD22	1.85	0.42
16:I:253:ILE:HG13	16:I:302:ILE:HG12	2.01	0.42
17:J:102:ILE:HG21	17:J:122:LEU:HD21	2.02	0.42
16:I:405:ARG:NH2	17:J:162:GLU:OE2	2.50	0.42
17:J:70:SER:O	18:K:119:VAL:HG23	2.20	0.42
18:K:239:GLY:HA2	18:K:277:ILE:HG13	2.02	0.42
19:L:114:GLU:OE1	19:L:137:ARG:NH1	2.53	0.42
23:P:54:SER:HA	23:P:58:VAL:HB	2.00	0.42
25:R:401:HIS:CD2	25:R:402:LEU:HG	2.55	0.42
29:V:114:PHE:H	29:V:118:LEU:HG	1.85	0.42
1:1:38:ARG:NH2	1:1:186:GLY:O	2.53	0.42
4:4:25:ILE:HD11	5:5:209:THR:HG21	2.02	0.42
12:E:125:GLU:OE2	12:E:135:SER:OG	2.33	0.42
12:E:123:PHE:CD1	12:E:137:PRO:HA	2.54	0.42
18:K:55:GLU:HA	18:K:58:TYR:HD2	1.85	0.42
20:M:432:PHE:CG	20:M:433:TYR:N	2.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:83:LEU:HD13	21:N:135:SER:HB3	2.02	0.42
22:O:22:LEU:HD22	22:O:26:PHE:CG	2.55	0.42
24:Q:78:ILE:HG12	24:Q:100:LEU:HD13	2.02	0.42
25:R:262:GLU:O	25:R:266:LEU:HG	2.20	0.42
33:Z:925:VAL:HG12	33:Z:927:VAL:HG13	2.00	0.42
2:2:171:TRP:HA	2:2:175:LEU:HD11	2.02	0.42
7:7:184:ALA:HA	7:7:187:LEU:HD12	2.01	0.42
7:7:183:MET:O	7:7:186:PRO:HD2	2.20	0.42
14:G:68:GLN:HG3	14:G:89:VAL:HG21	2.01	0.42
17:J:279:LEU:O	17:J:284:THR:N	2.53	0.42
18:K:159:SER:HA	18:K:242:PHE:HA	2.01	0.42
19:L:307:GLU:OE2	19:L:311:GLN:NE2	2.52	0.42
22:O:51:ASP:OD1	22:O:52:ALA:N	2.53	0.42
2:2:95:HIS:HE1	8:A:104:PHE:CZ	2.38	0.41
8:A:87:ILE:N	8:A:88:PRO:HD2	2.35	0.41
9:B:18:LEU:HB2	9:B:21:ILE:HD12	2.02	0.41
11:D:159:TRP:CZ3	12:E:56:SER:HB3	2.55	0.41
13:F:50:LYS:HG2	13:F:61:LYS:HA	2.02	0.41
19:L:274:GLU:HB3	19:L:320:GLN:HG3	2.00	0.41
8:A:218:PHE:HB3	8:A:222:ASP:HB2	2.02	0.41
12:E:21:LEU:HD12	20:M:433:TYR:CE1	2.56	0.41
14:G:16:SER:OG	14:G:20:ARG:O	2.29	0.41
17:J:196:THR:HG21	18:K:305:GLY:HA2	2.02	0.41
20:M:284:ASP:O	20:M:288:THR:OG1	2.29	0.41
21:N:759:ILE:HD11	21:N:769:PRO:HD2	2.00	0.41
22:O:308:LEU:HD23	22:O:348:VAL:HB	2.02	0.41
24:Q:151:TYR:HB2	24:Q:184:VAL:HG13	2.02	0.41
29:V:57:PHE:O	29:V:135:ARG:NH1	2.53	0.41
6:6:183:THR:HG21	6:6:187:VAL:HB	2.02	0.41
6:6:194:LEU:HB3	6:6:198:GLU:HB2	2.01	0.41
15:H:157:VAL:HB	15:H:182:ASN:HD22	1.85	0.41
15:H:161:GLU:HG3	15:H:183:ILE:HG22	2.02	0.41
16:I:117:HIS:HA	16:I:131:SER:HA	2.01	0.41
17:J:261:SER:HA	18:K:293:GLN:HG3	2.02	0.41
20:M:157:ASP:OD1	20:M:158:THR:N	2.53	0.41
28:U:296:ILE:HG12	29:V:266:LEU:HD22	2.02	0.41
31:X:7:VAL:HG12	31:X:8:ILE:HG13	2.02	0.41
2:2:64:HIS:CE1	2:2:82:GLU:HG2	2.55	0.41
3:3:51:LEU:HD22	3:3:87:PHE:CZ	2.56	0.41
5:5:255:VAL:HA	5:5:260:TRP:HA	2.03	0.41
8:A:14:ARG:HH21	8:A:30:TYR:HH	1.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:216:ASP:OD1	9:B:217:GLU:N	2.53	0.41
15:H:249:TYR:HD2	15:H:376:GLU:HG2	1.84	0.41
17:J:339:ARG:HD3	25:R:206:ARG:HE	1.85	0.41
25:R:76:GLN:HB2	25:R:86:ASP:HB3	2.02	0.41
26:S:205:ASN:HA	26:S:208:ILE:HD12	2.01	0.41
26:S:40:GLU:HA	26:S:46:LEU:HD12	2.02	0.41
29:V:235:GLU:HG2	29:V:297:THR:HA	2.02	0.41
4:4:130:TYR:HB2	4:4:144:LEU:HD13	2.02	0.41
14:G:119:TYR:CZ	14:G:123:HIS:HE1	2.38	0.41
15:H:147:ILE:HA	15:H:155:PHE:HB2	2.02	0.41
15:H:251:PRO:HA	15:H:252:PRO:HD3	1.97	0.41
21:N:58:ARG:HA	21:N:61:ALA:HB3	2.03	0.41
22:O:44:SER:O	22:O:47:LYS:N	2.54	0.41
23:P:265:VAL:HG21	23:P:296:GLN:HB3	2.02	0.41
25:R:316:LEU:HD13	25:R:329:PHE:HD2	1.85	0.41
25:R:368:LEU:HD23	25:R:371:PHE:HD2	1.86	0.41
2:2:109:LEU:HD22	2:2:140:PHE:HB3	2.02	0.41
2:2:48:ARG:HE	2:2:199:GLY:HA3	1.85	0.41
3:3:184:GLY:N	3:3:204:GLN:HE21	2.18	0.41
9:B:72:GLY:N	9:B:137:ALA:O	2.47	0.41
15:H:227:LEU:HD11	15:H:234:ARG:HD2	2.01	0.41
15:H:235:PHE:CZ	15:H:242:PRO:HG3	2.55	0.41
16:I:218:GLY:HA2	16:I:324:VAL:O	2.21	0.41
20:M:336:ALA:O	20:M:342:ARG:NH1	2.48	0.41
30:W:9:VAL:HG22	30:W:52:ILE:HD11	2.01	0.41
33:Z:495:ILE:HA	33:Z:532:HIS:CE1	2.56	0.41
5:5:125:ALA:HB2	6:6:149:SER:N	2.35	0.41
13:F:37:GLY:HA3	13:F:46:LEU:HD23	2.02	0.41
17:J:57:PHE:O	17:J:61:GLU:HG2	2.21	0.41
21:N:23:TYR:HB3	27:T:35:ILE:HG21	2.01	0.41
21:N:79:VAL:HG22	21:N:101:ILE:HG23	2.01	0.41
23:P:122:ILE:HG22	23:P:124:VAL:H	1.86	0.41
24:Q:282:LEU:HD23	24:Q:300:LYS:HD2	2.01	0.41
24:Q:359:ILE:HD12	24:Q:395:GLY:HA2	2.02	0.41
26:S:469:ASN:HA	26:S:472:HIS:ND1	2.36	0.41
33:Z:777:PRO:HB3	33:Z:796:LEU:HD21	2.02	0.41
6:6:114:HIS:CD2	12:E:102:TYR:HA	2.55	0.41
6:6:226:VAL:HG22	6:6:231:VAL:HG22	2.01	0.41
11:D:79:ASN:N	16:I:437:LEU:O	2.40	0.41
17:J:211:ILE:HB	17:J:245:ILE:HA	2.02	0.41
19:L:336:ALA:HA	19:L:339:ARG:NH1	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:166:ASN:HB2	33:Z:227:ILE:HG22	2.03	0.41
2:2:172:LYS:H	2:2:175:LEU:HD11	1.85	0.41
2:2:119:TYR:OH	3:3:99:ARG:NH1	2.53	0.41
6:6:55:ASN:HB3	7:7:170:TYR:CZ	2.55	0.41
14:G:28:VAL:HG22	14:G:153:PRO:HG2	2.03	0.41
16:I:113:ILE:HD12	16:I:115:ASP:HB2	2.02	0.41
18:K:104:ASP:OD1	18:K:105:GLN:N	2.46	0.41
20:M:353:SER:N	20:M:356:SER:OG	2.54	0.41
21:N:378:ASN:HA	21:N:924:LYS:HG3	2.02	0.41
22:O:294:MET:SD	22:O:356:ARG:NE	2.94	0.41
25:R:163:SER:O	25:R:167:LYS:HG2	2.20	0.41
28:U:35:VAL:HA	28:U:91:TRP:HA	2.03	0.41
29:V:37:MET:HG3	29:V:68:VAL:HG21	2.03	0.41
32:Y:67:VAL:O	32:Y:69:VAL:HG23	2.21	0.41
33:Z:493:LEU:HB3	33:Z:497:PHE:CE2	2.55	0.41
4:4:66:LEU:HD11	11:D:90:ARG:HB3	2.03	0.41
7:7:115:ASP:OD1	7:7:116:ALA:N	2.54	0.41
10:C:191:GLU:HG2	10:C:242:THR:HG22	2.03	0.41
10:C:231:LYS:HE3	10:C:233:GLN:HB2	2.03	0.41
7:7:124:TYR:HD1	13:F:100:ASN:HB3	1.86	0.41
6:6:96:PHE:HB3	13:F:89:ARG:NH1	2.36	0.41
15:H:280:VAL:HG22	15:H:313:ALA:HB1	2.03	0.41
17:J:388:LYS:O	17:J:392:LYS:N	2.49	0.41
18:K:351:LEU:HD21	24:Q:237:SER:HB3	2.03	0.41
24:Q:204:ALA:O	24:Q:208:ILE:HG13	2.21	0.41
25:R:67:CYS:HA	25:R:75:GLY:HA2	2.03	0.41
26:S:208:ILE:HD13	27:T:44:LEU:HB3	2.03	0.41
31:X:73:THR:HG23	31:X:90:VAL:H	1.85	0.41
33:Z:434:GLN:HA	33:Z:437:ASP:OD2	2.21	0.41
6:6:46:THR:OG1	6:6:219:ASP:O	2.38	0.41
11:D:11:PHE:HZ	12:E:138:PHE:HA	1.85	0.41
7:7:117:GLU:HG2	13:F:140:SER:HA	2.03	0.41
13:F:157:TYR:CZ	14:G:60:VAL:HG22	2.56	0.41
26:S:330:LEU:HB3	26:S:334:HIS:CE1	2.56	0.41
27:T:92:ASN:ND2	27:T:96:LEU:HD13	2.32	0.41
20:M:50:ARG:HH21	30:W:30:ILE:HD13	1.85	0.41
33:Z:212:LEU:HD11	33:Z:238:ASP:HB3	2.03	0.41
1:1:61:TRP:CD1	1:1:197:LEU:HD21	2.55	0.40
1:1:82:LEU:HA	1:1:85:TYR:HB3	2.02	0.40
3:3:155:GLU:O	3:3:158:LEU:HG	2.21	0.40
6:6:220:GLY:HA2	6:6:237:GLU:HA	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:11:THR:HA	11:D:127:ARG:HB2	2.02	0.40
16:I:109:LEU:HD23	16:I:120:VAL:HG12	2.03	0.40
16:I:427:LYS:HG3	16:I:428:VAL:N	2.36	0.40
18:K:186:GLU:HA	18:K:190:LEU:HD13	2.03	0.40
19:L:120:LYS:HA	19:L:126:ARG:HA	2.02	0.40
21:N:515:ARG:HB2	21:N:546:LEU:HD22	2.03	0.40
23:P:254:GLU:HA	23:P:257:TRP:HB3	2.02	0.40
14:G:193:VAL:HG13	14:G:216:ILE:HG21	2.04	0.40
15:H:404:TRP:O	15:H:408:SER:OG	2.30	0.40
17:J:327:ILE:HG22	17:J:358:VAL:HG11	2.03	0.40
20:M:194:VAL:HA	20:M:198:VAL:HB	2.03	0.40
20:M:275:PRO:O	20:M:276:THR:HB	2.21	0.40
26:S:290:ASN:OD1	26:S:321:GLN:NE2	2.54	0.40
33:Z:145:ASP:HB3	33:Z:210:TYR:HD1	1.86	0.40
2:2:50:THR:HG22	2:2:55:VAL:HG13	2.03	0.40
6:6:224:LEU:HG	6:6:233:LYS:HG2	2.04	0.40
9:B:95:THR:HA	9:B:99:ARG:HD2	2.03	0.40
11:D:65:SER:HB3	11:D:90:ARG:HH21	1.86	0.40
15:H:145:TYR:CD1	15:H:174:VAL:HG13	2.56	0.40
19:L:223:PRO:HA	19:L:224:PRO:HD3	2.00	0.40
28:U:121:ILE:HD12	28:U:136:TYR:HE2	1.84	0.40
25:R:309:LEU:HD21	32:Y:78:LYS:HD3	2.03	0.40
14:G:41:LYS:HA	14:G:46:VAL:HG12	2.04	0.40
14:G:65:VAL:HG22	14:G:215:GLU:OE2	2.21	0.40
20:M:379:LEU:HD13	20:M:419:ILE:HD12	2.04	0.40
22:O:74:ASN:ND2	30:W:82:GLU:OE1	2.55	0.40
24:Q:378:SER:HA	24:Q:381:ILE:HD12	2.03	0.40
26:S:282:ILE:HA	26:S:382:ARG:HH12	1.85	0.40
9:B:240:SER:HA	9:B:243:ILE:HD12	2.03	0.40
15:H:281:GLN:HE22	16:I:258:GLY:HA3	1.87	0.40
16:I:193:GLU:HB3	16:I:346:ARG:HD2	2.04	0.40
19:L:251:ILE:N	20:M:293:SER:OG	2.54	0.40
22:O:157:LEU:HD12	22:O:171:PHE:HD2	1.87	0.40
22:O:20:PRO:HD2	22:O:22:LEU:HG	2.03	0.40
27:T:105:LEU:HD12	27:T:108:LEU:HD12	2.03	0.40
27:T:229:VAL:HG21	27:T:234:TYR:CE2	2.56	0.40
28:U:12:LEU:HD13	29:V:35:LEU:HB2	2.02	0.40
33:Z:155:ARG:HA	33:Z:158:ALA:HB3	2.04	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 PDB entries followed by that with respect to all EM entries.

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	1	194/215 (90%)	189 (97%)	5 (3%)	0	100	100
1	b	194/215 (90%)	189 (97%)	5 (3%)	0	100	100
2	2	224/261 (86%)	218 (97%)	6 (3%)	0	100	100
2	i	224/261 (86%)	220 (98%)	4 (2%)	0	100	100
3	3	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
3	h	202/205 (98%)	189 (94%)	12 (6%)	1 (0%)	31	74
4	4	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
4	g	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
5	5	210/287 (73%)	208 (99%)	2 (1%)	0	100	100
5	f	210/287 (73%)	203 (97%)	7 (3%)	0	100	100
6	6	220/241 (91%)	215 (98%)	5 (2%)	0	100	100
6	e	220/241 (91%)	213 (97%)	7 (3%)	0	100	100
7	7	227/266 (85%)	218 (96%)	9 (4%)	0	100	100
7	a	230/266 (86%)	223 (97%)	7 (3%)	0	100	100
8	A	239/252 (95%)	231 (97%)	8 (3%)	0	100	100
8	c	241/252 (96%)	234 (97%)	7 (3%)	0	100	100
9	B	248/250 (99%)	240 (97%)	8 (3%)	0	100	100
9	j	248/250 (99%)	238 (96%)	10 (4%)	0	100	100
10	C	242/258 (94%)	237 (98%)	5 (2%)	0	100	100
10	d	242/258 (94%)	233 (96%)	9 (4%)	0	100	100
11	D	238/254 (94%)	228 (96%)	10 (4%)	0	100	100
11	n	239/254 (94%)	231 (97%)	8 (3%)	0	100	100
12	E	240/260 (92%)	229 (95%)	11 (5%)	0	100	100
12	m	240/260 (92%)	233 (97%)	7 (3%)	0	100	100
13	F	231/234 (99%)	220 (95%)	11 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	I	231/234 (99%)	222 (96%)	9 (4%)	0	100	100
14	G	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
14	k	242/288 (84%)	237 (98%)	5 (2%)	0	100	100
15	H	353/467 (76%)	311 (88%)	41 (12%)	1 (0%)	43	81
16	I	361/437 (83%)	334 (92%)	27 (8%)	0	100	100
17	J	371/405 (92%)	350 (94%)	21 (6%)	0	100	100
18	K	379/428 (89%)	343 (90%)	35 (9%)	1 (0%)	43	81
19	L	359/437 (82%)	335 (93%)	24 (7%)	0	100	100
20	M	363/434 (84%)	336 (93%)	24 (7%)	3 (1%)	21	65
21	N	843/945 (89%)	793 (94%)	47 (6%)	3 (0%)	36	77
22	O	385/393 (98%)	348 (90%)	36 (9%)	1 (0%)	43	81
23	P	430/445 (97%)	390 (91%)	40 (9%)	0	100	100
24	Q	429/434 (99%)	398 (93%)	31 (7%)	0	100	100
25	R	398/429 (93%)	357 (90%)	38 (10%)	3 (1%)	21	65
26	S	473/523 (90%)	451 (95%)	21 (4%)	1 (0%)	49	85
27	T	270/274 (98%)	239 (88%)	31 (12%)	0	100	100
28	U	245/338 (72%)	240 (98%)	4 (2%)	1 (0%)	36	77
29	V	282/306 (92%)	243 (86%)	33 (12%)	6 (2%)	8	43
30	W	195/268 (73%)	174 (89%)	18 (9%)	3 (2%)	11	51
31	X	109/156 (70%)	96 (88%)	13 (12%)	0	100	100
32	Y	25/89 (28%)	18 (72%)	6 (24%)	1 (4%)	3	29
33	Z	807/993 (81%)	743 (92%)	64 (8%)	0	100	100
All	All	13382/15139 (88%)	12602 (94%)	755 (6%)	25 (0%)	53	85

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	H	329	VAL
29	V	61	TYR
3	h	105	VAL
20	M	274	ALA
29	V	62	THR
21	N	874	ILE
21	N	903	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	U	129	VAL
29	V	60	ASP
32	Y	69	VAL
20	M	276	THR
21	N	761	ILE
25	R	241	ILE
25	R	421	VAL
29	V	189	ILE
29	V	305	ILE
30	W	147	ILE
30	W	22	PRO
18	K	326	PRO
25	R	72	VAL
20	M	167	VAL
26	S	83	PRO
29	V	271	VAL
22	O	227	ILE
30	W	118	ILE

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 PDB entries followed by that with respect to all EM entries.

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	1	162/178 (91%)	162 (100%)	0	100	100
1	b	162/178 (91%)	162 (100%)	0	100	100
2	2	185/214 (86%)	185 (100%)	0	100	100
2	i	185/214 (86%)	185 (100%)	0	100	100
3	3	172/173 (99%)	172 (100%)	0	100	100
3	h	172/173 (99%)	172 (100%)	0	100	100
4	4	173/175 (99%)	173 (100%)	0	100	100
4	g	173/175 (99%)	173 (100%)	0	100	100
5	5	169/235 (72%)	169 (100%)	0	100	100
5	f	169/235 (72%)	169 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	6	185/201 (92%)	185 (100%)	0	100	100
6	e	185/201 (92%)	185 (100%)	0	100	100
7	7	195/224 (87%)	195 (100%)	0	100	100
7	a	198/224 (88%)	198 (100%)	0	100	100
8	A	206/210 (98%)	206 (100%)	0	100	100
8	c	207/210 (99%)	207 (100%)	0	100	100
9	B	209/209 (100%)	209 (100%)	0	100	100
9	j	209/209 (100%)	209 (100%)	0	100	100
10	C	203/216 (94%)	203 (100%)	0	100	100
10	d	203/216 (94%)	203 (100%)	0	100	100
11	D	212/226 (94%)	212 (100%)	0	100	100
11	n	213/226 (94%)	213 (100%)	0	100	100
12	E	198/215 (92%)	198 (100%)	0	100	100
12	m	198/215 (92%)	198 (100%)	0	100	100
13	F	192/193 (100%)	192 (100%)	0	100	100
13	l	192/193 (100%)	192 (100%)	0	100	100
14	G	201/239 (84%)	201 (100%)	0	100	100
14	k	201/239 (84%)	201 (100%)	0	100	100
15	H	303/399 (76%)	303 (100%)	0	100	100
16	I	320/385 (83%)	320 (100%)	0	100	100
17	J	325/352 (92%)	325 (100%)	0	100	100
18	K	334/374 (89%)	334 (100%)	0	100	100
19	L	308/377 (82%)	308 (100%)	0	100	100
20	M	315/375 (84%)	315 (100%)	0	100	100
21	N	713/797 (90%)	713 (100%)	0	100	100
22	O	363/368 (99%)	363 (100%)	0	100	100
23	P	405/415 (98%)	405 (100%)	0	100	100
24	Q	388/391 (99%)	388 (100%)	0	100	100
25	R	351/379 (93%)	351 (100%)	0	100	100
26	S	447/489 (91%)	447 (100%)	0	100	100
27	T	254/256 (99%)	254 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	U	234/308 (76%)	234 (100%)	0	100	100
29	V	249/268 (93%)	249 (100%)	0	100	100
30	W	171/230 (74%)	171 (100%)	0	100	100
31	X	101/144 (70%)	101 (100%)	0	100	100
32	Y	26/81 (32%)	26 (100%)	0	100	100
33	Z	692/850 (81%)	692 (100%)	0	100	100
All	All	11628/13054 (89%)	11628 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	214	GLN
2	2	64	HIS
2	2	95	HIS
2	2	114	GLN
3	3	89	GLN
3	3	145	GLN
3	3	169	GLN
3	3	204	GLN
5	5	104	GLN
5	5	128	GLN
5	5	254	HIS
5	5	283	ASN
6	6	55	ASN
6	6	113	GLN
7	7	107	ASN
1	b	81	HIS
2	i	51	GLN
4	g	65	GLN
4	g	86	GLN
4	g	147	HIS
4	g	191	GLN
5	f	104	GLN
5	f	208	GLN
6	e	89	ASN
6	e	113	GLN
6	e	171	ASN
7	a	95	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	a	145	ASN
9	B	20	GLN
9	B	30	GLN
9	B	119	GLN
10	C	120	GLN
10	C	227	GLN
11	D	79	ASN
11	D	122	GLN
11	D	149	GLN
11	D	178	ASN
13	F	4	ASN
13	F	43	HIS
13	F	117	GLN
13	F	143	HIS
14	G	182	HIS
8	c	92	ASN
8	c	126	GLN
10	d	94	HIS
10	d	120	GLN
11	n	19	GLN
11	n	118	GLN
11	n	162	GLN
12	m	147	HIS
13	l	93	ASN
13	l	117	GLN
14	k	12	ASN
14	k	121	GLN
14	k	127	ASN
14	k	183	HIS
15	H	54	ASN
15	H	182	ASN
15	H	281	GLN
15	H	359	ASN
15	H	413	ASN
17	J	66	GLN
17	J	181	GLN
17	J	240	HIS
18	K	72	GLN
21	N	34	GLN
21	N	375	HIS
21	N	747	HIS
22	O	4	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	O	235	HIS
22	O	354	GLN
23	P	30	ASN
23	P	263	HIS
23	P	286	ASN
23	P	418	ASN
24	Q	19	GLN
24	Q	114	GLN
24	Q	226	HIS
25	R	399	GLN
26	S	227	ASN
26	S	283	GLN
26	S	311	GLN
26	S	321	GLN
26	S	334	HIS
27	T	92	ASN
28	U	127	GLN
28	U	280	ASN
29	V	111	HIS
29	V	145	GLN
29	V	195	HIS
29	V	204	HIS
29	V	250	GLN
29	V	279	HIS
30	W	18	ASN
30	W	42	ASN
30	W	92	GLN
31	X	38	ASN
31	X	94	ASN
33	Z	327	GLN
33	Z	361	HIS
33	Z	379	GLN
33	Z	475	GLN
33	Z	801	HIS
33	Z	829	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.