



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 06:43 AM UTC

PDB ID : 5T0H / pdb_00005t0h
EMDB ID : EMD-8335
Title : Structural basis for dynamic regulation of the human 26S proteasome
Authors : Chen, S.; Wu, J.; Lu, Y.; Ma, Y.B.; Lee, B.H.; Yu, Z.; Ouyang, Q.; Finley, D.; Kirschner, M.W.; Mao, Y.
Deposited on : 2016-08-16
Resolution : 6.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

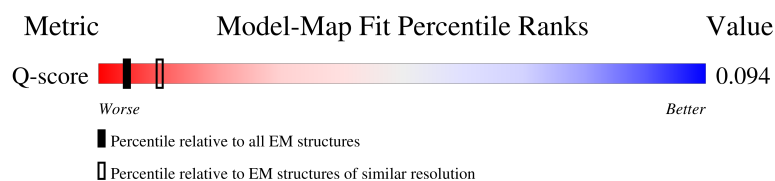
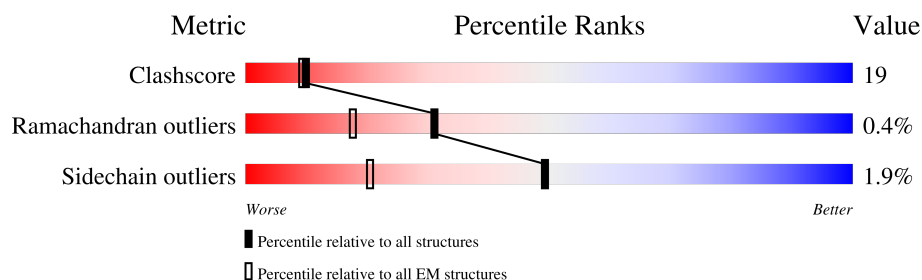
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	503 (6.30 - 7.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	440	
3	C	398	
4	D	418	

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Mol	Chain	Length	Quality of chain
5	E	403	
6	F	439	
7	G	245	
8	H	233	
9	I	260	
10	J	247	
11	K	240	
12	L	268	
13	M	254	
14	N	238	
15	O	276	
16	P	204	
17	Q	201	
18	R	262	
19	S	240	
20	T	263	
21	U	953	
22	V	533	
23	W	456	
24	X	422	
25	Y	389	
26	Z	324	
27	a	376	
28	b	377	
29	c	309	

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Mol	Chain	Length	Quality of chain
30	d	349	44%43%29%26%
31	e	70	11%14%20%66%
32	f	749	61%63%28%7%

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 73509 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 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	361	Total	C	N	O	S	0	0
			2835	1788	501	528	18		

- Molecule 2 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	341	Total	C	N	O	S	0	0
			2662	1671	453	526	12		

- Molecule 3 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	384	Total	C	N	O	S	0	0
			3015	1894	540	564	17		

- Molecule 4 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		

- Molecule 5 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	353	Total	C	N	O	S	0	0
			2790	1755	494	525	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	366	Total	C	N	O	S	0	0
			2863	1802	496	549	16		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 15 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 16 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 17 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 18 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 19 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

- Molecule 20 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	806	Total	C	N	O	S	0	0
			6287	3990	1075	1178	44		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	480	Total	C	N	O	S	0	0
			3852	2444	684	710	14		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	236	Total	C	N	O	S	0	0
			1940	1237	331	361	11		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	81	Total	C	N	O	S	0	0
			647	414	107	124	2		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 26 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

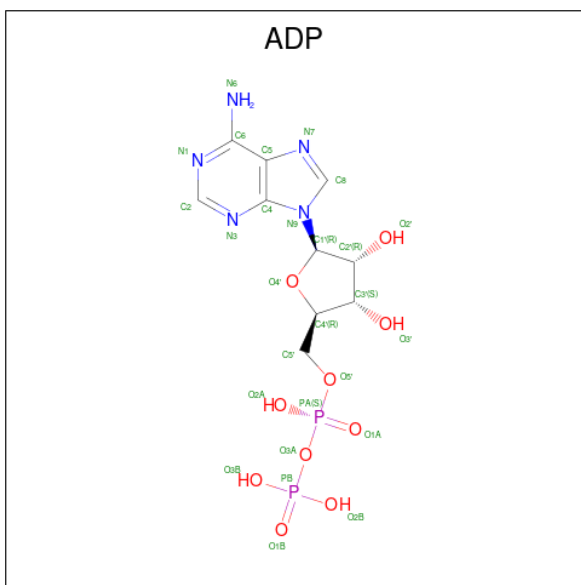
- Molecule 31 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	24	Total	C	N	O	S	0	0
			197	121	34	40	2		

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	694	Total	C	N	O	S	0	0
			5331	3364	899	1027	41		

- Molecule 33 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total 27	C 10	N 5	O 10	P 2	0
33	B	1	Total 27	C 10	N 5	O 10	P 2	0
33	C	1	Total 27	C 10	N 5	O 10	P 2	0
33	D	1	Total 27	C 10	N 5	O 10	P 2	0
33	E	1	Total 27	C 10	N 5	O 10	P 2	0
33	F	1	Total 27	C 10	N 5	O 10	P 2	0

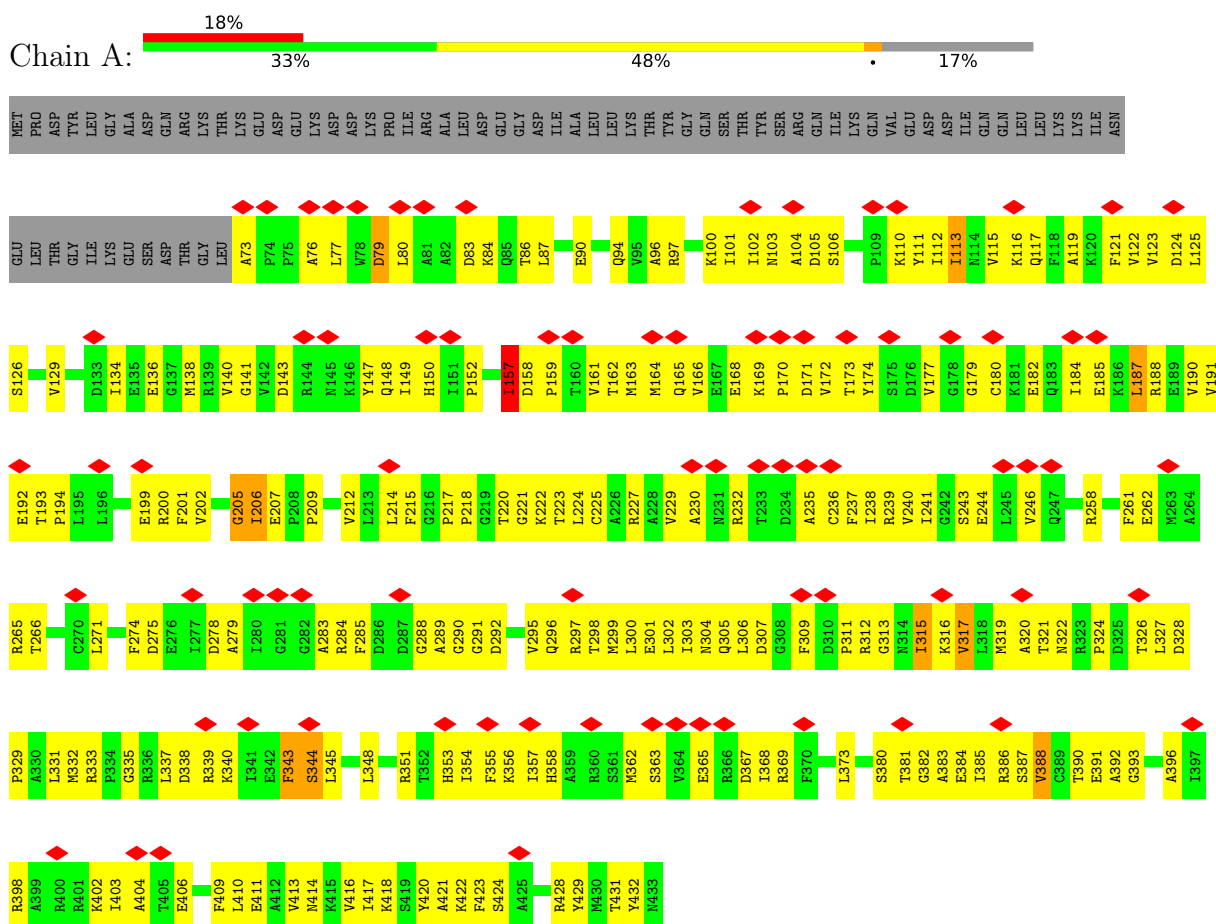
- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
34	c	1	Total Zn 1 1	0

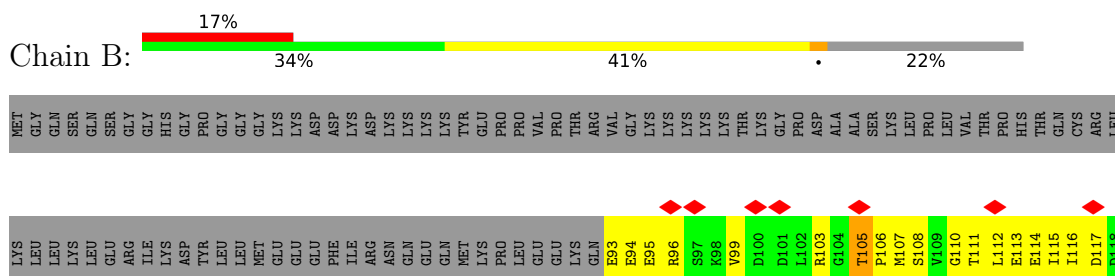
3 Residue-property plots

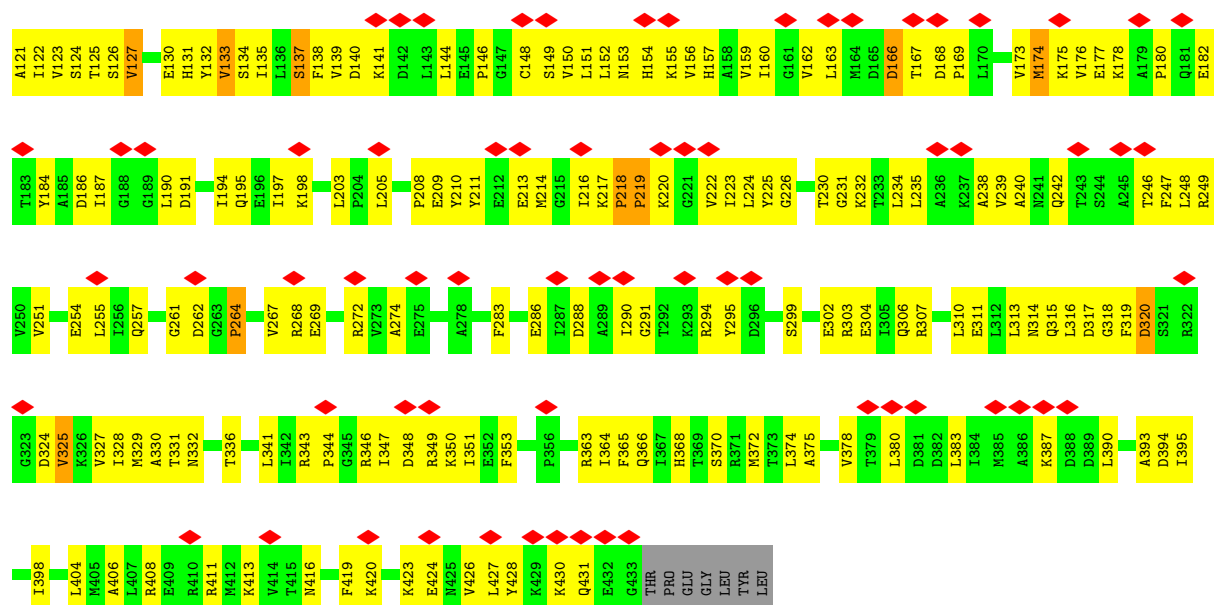
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: 26S protease regulatory subunit 7

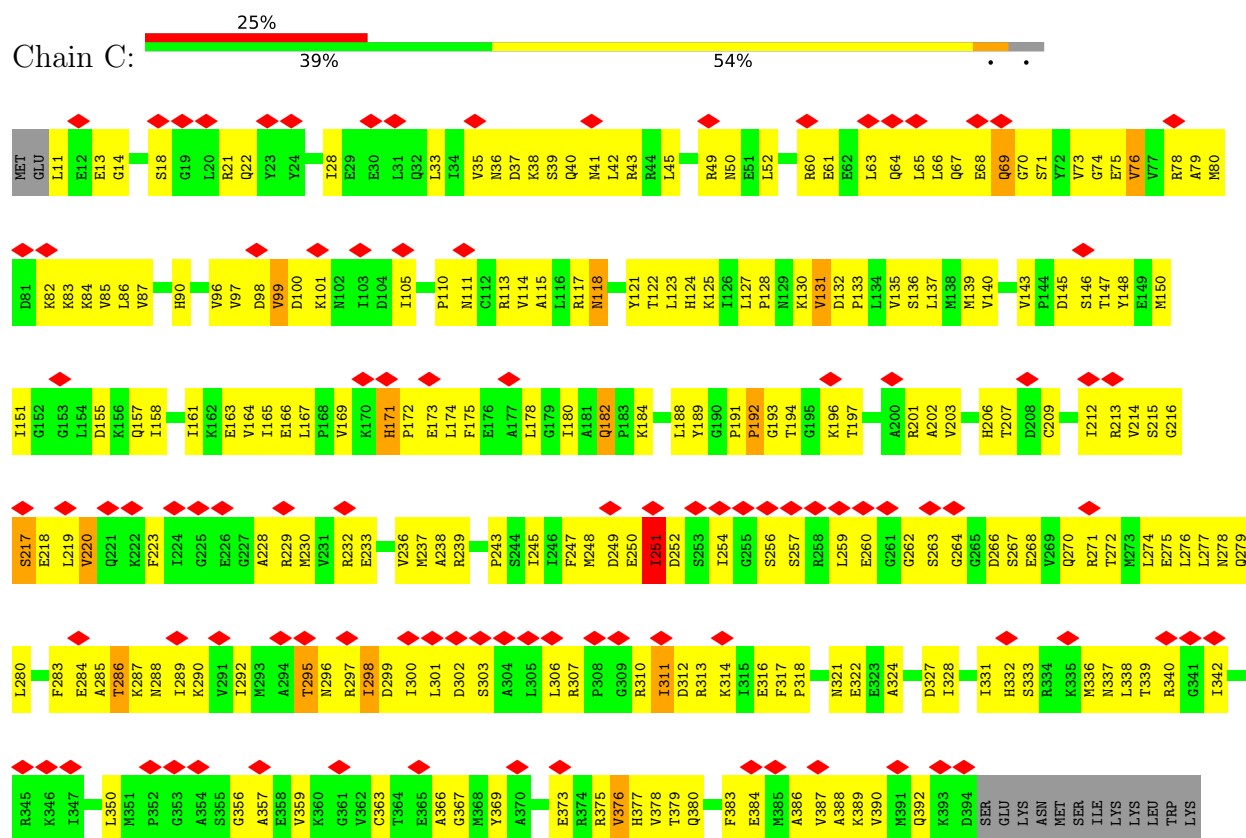


• Molecule 2: 26S protease regulatory subunit 4



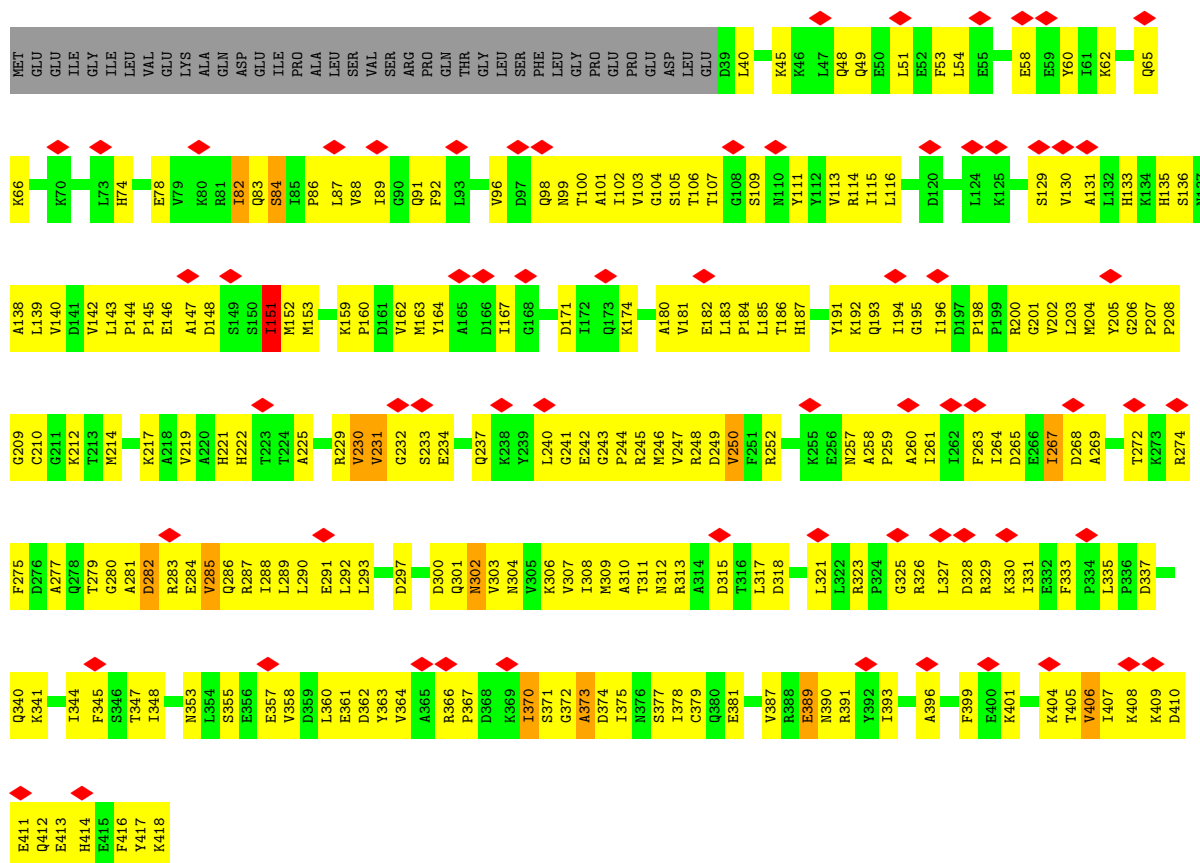


• Molecule 3: 26S protease regulatory subunit 8

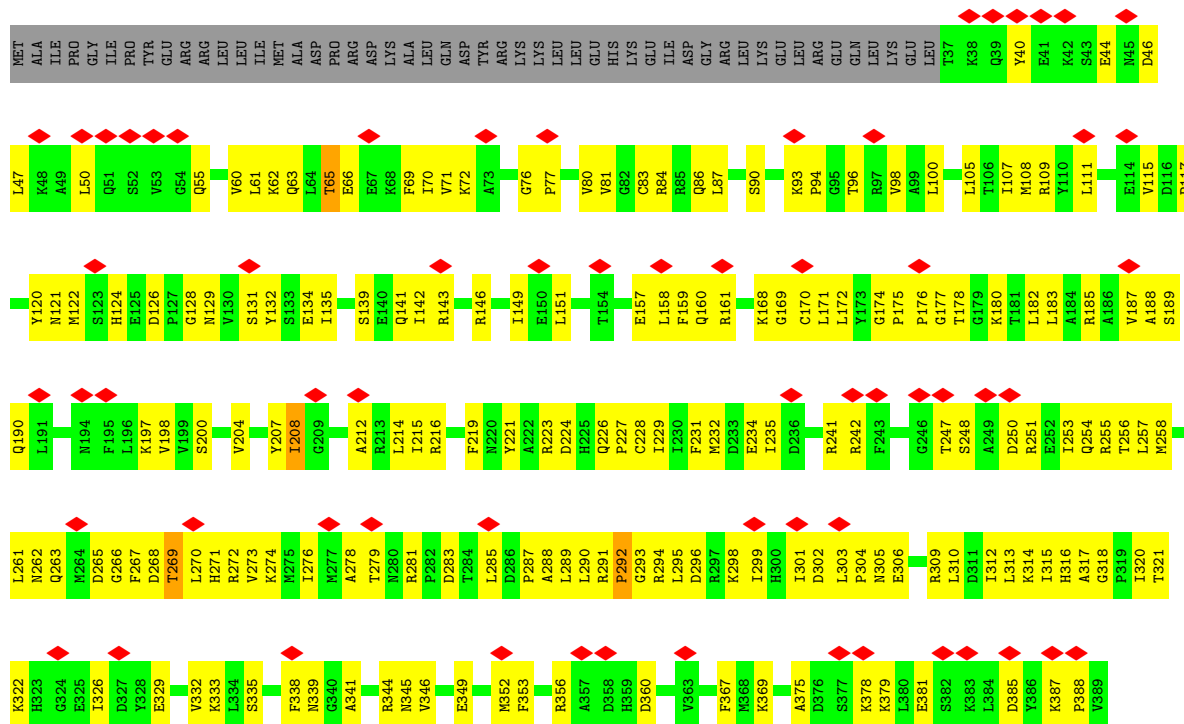
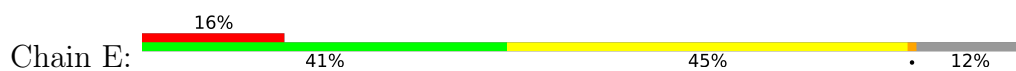


• Molecule 4: 26S protease regulatory subunit 6B

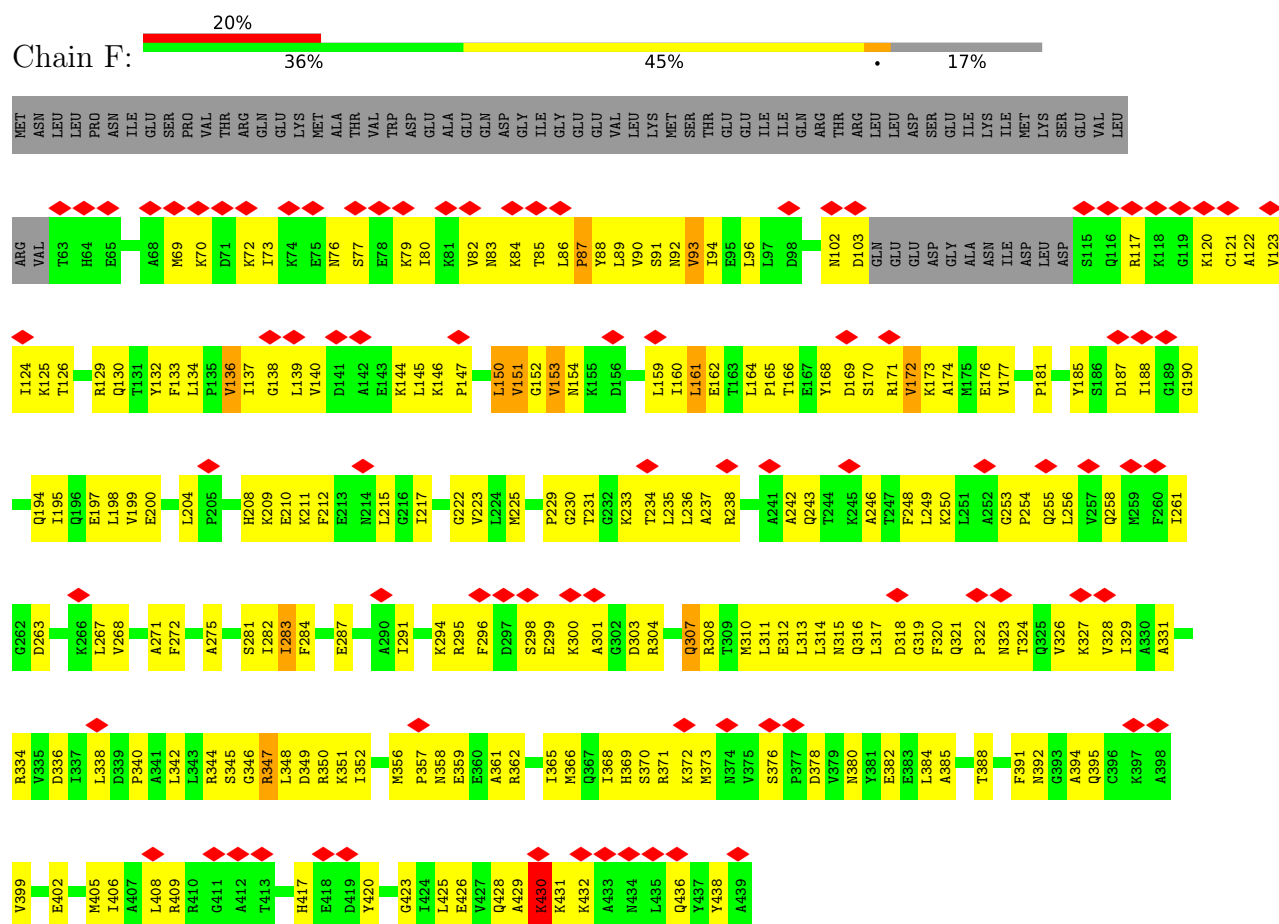




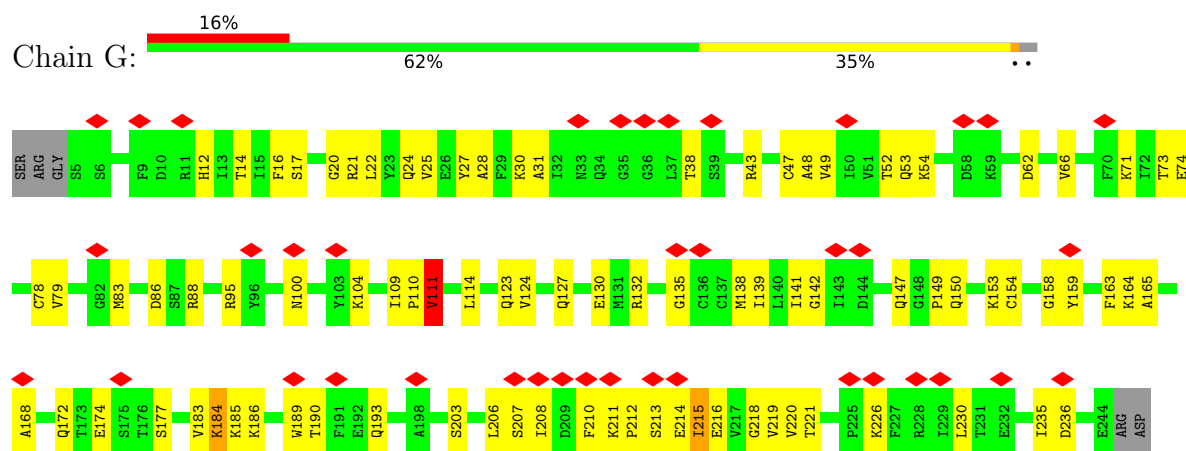
• Molecule 5: 26S protease regulatory subunit 10B



- Molecule 6: 26S protease regulatory subunit 6A

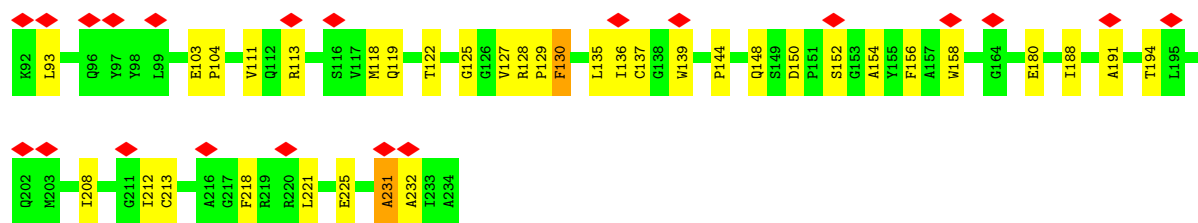


- Molecule 7: Proteasome subunit alpha type-6

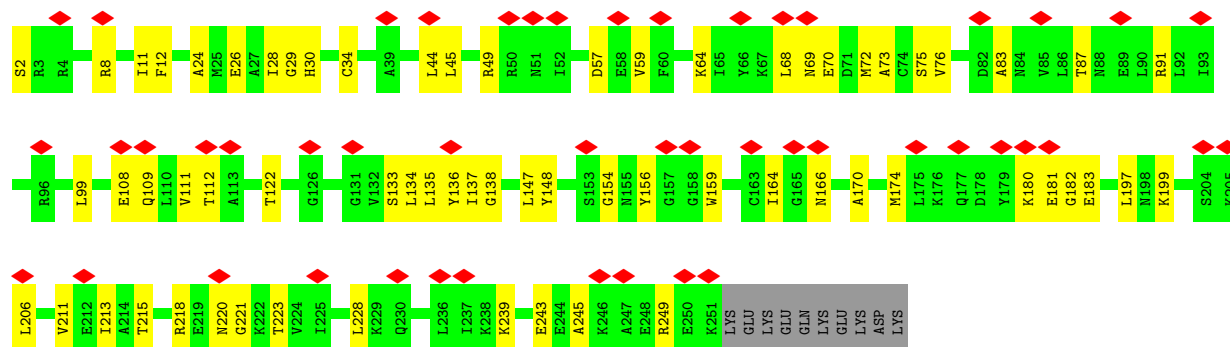


- Molecule 8: Proteasome subunit alpha type-2

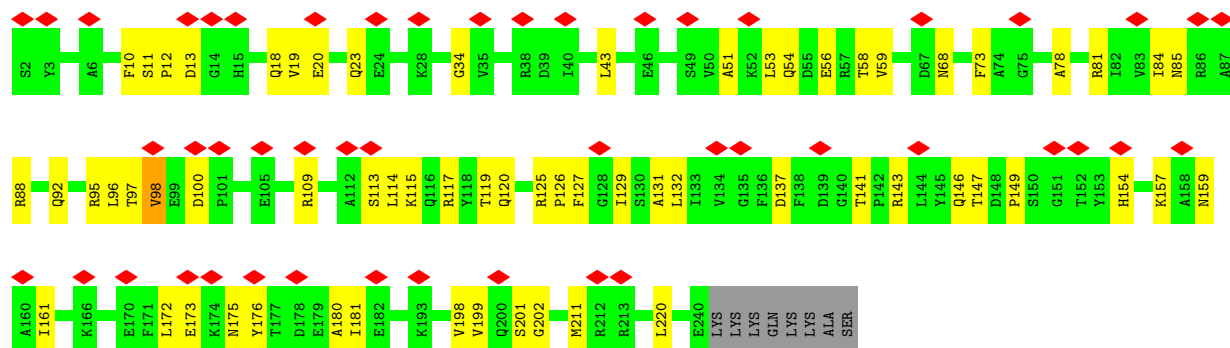




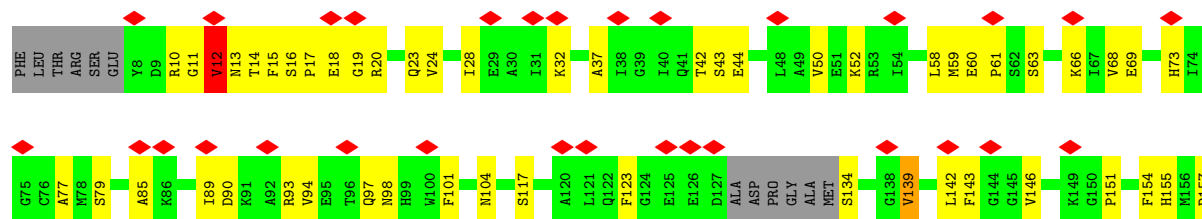
• Molecule 9: Proteasome subunit alpha type-4

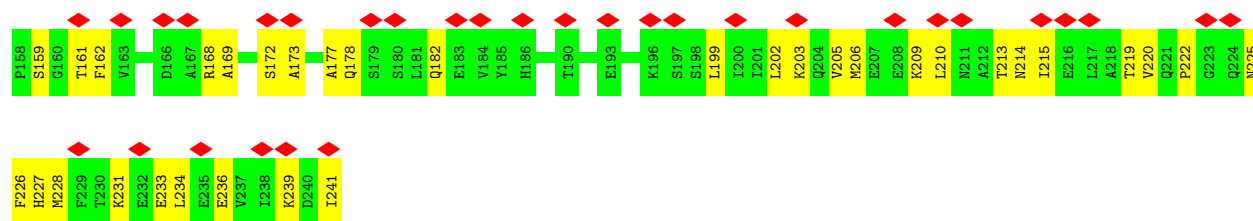


• Molecule 10: Proteasome subunit alpha type-7

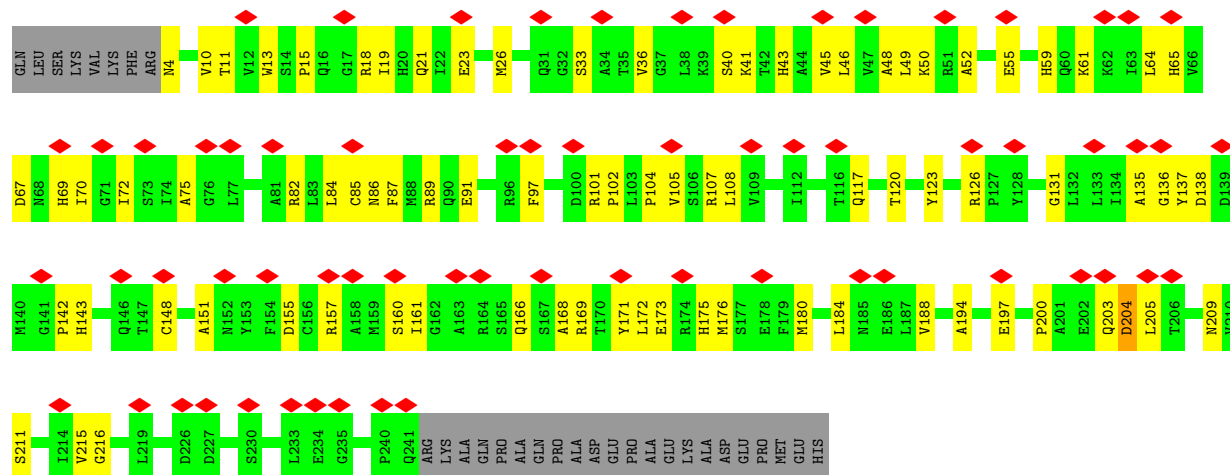


• Molecule 11: Proteasome subunit alpha type-5

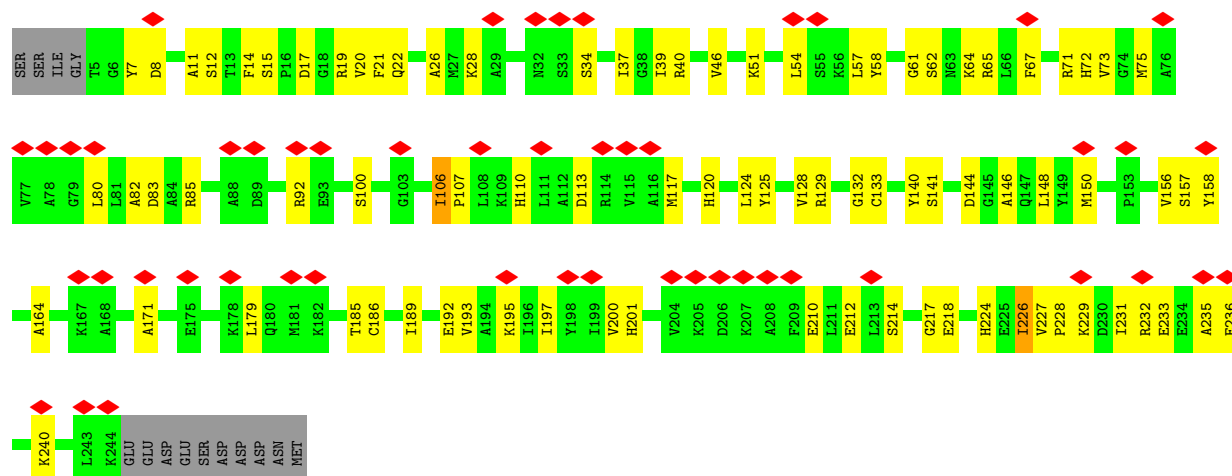




• Molecule 12: Proteasome subunit alpha type-1

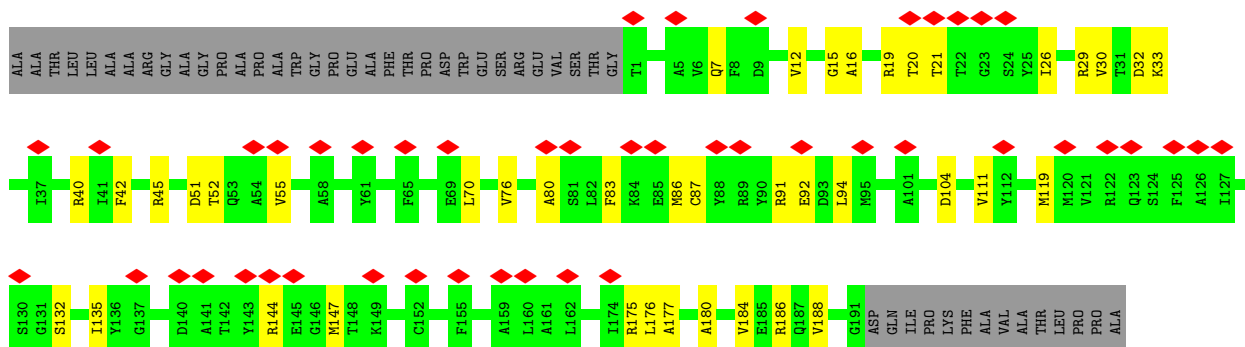


• Molecule 13: Proteasome subunit alpha type-3

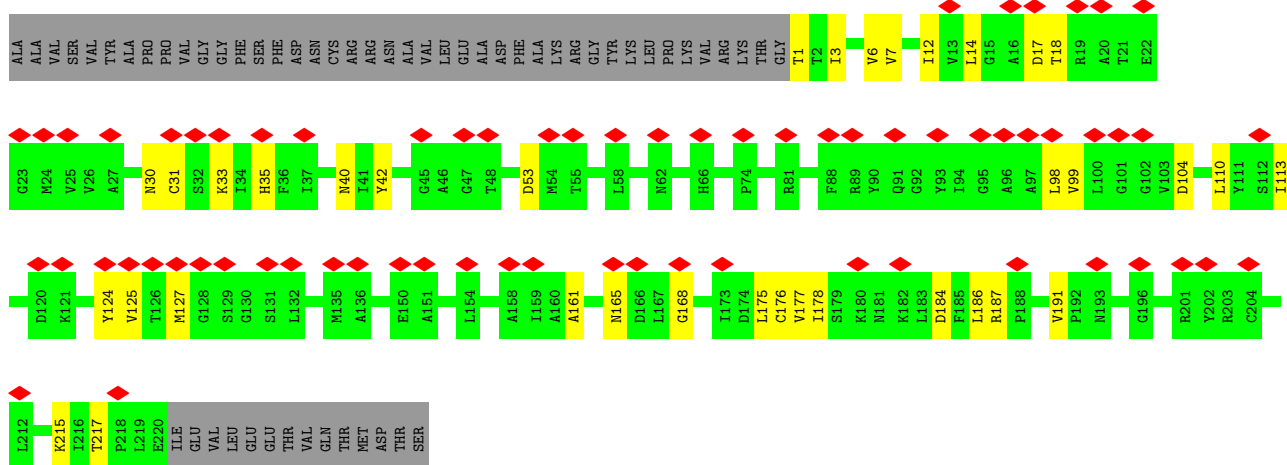


• Molecule 14: Proteasome subunit beta type-6

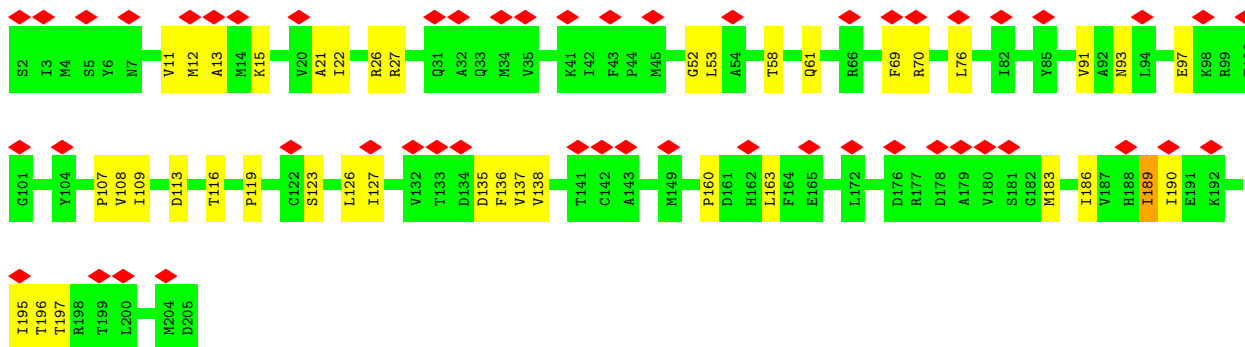
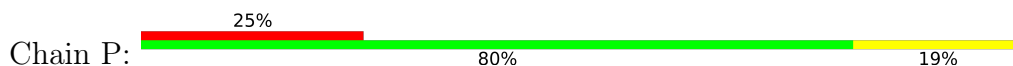




• Molecule 15: Proteasome subunit beta type-7

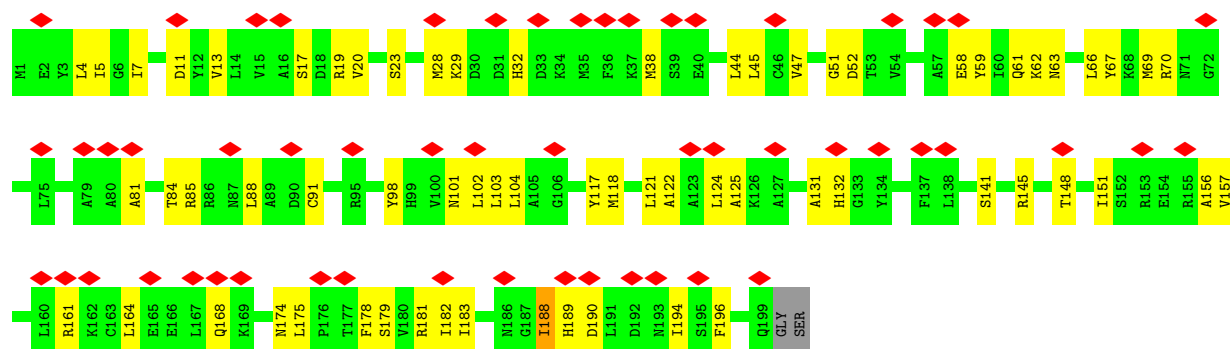


• Molecule 16: Proteasome subunit beta type-3

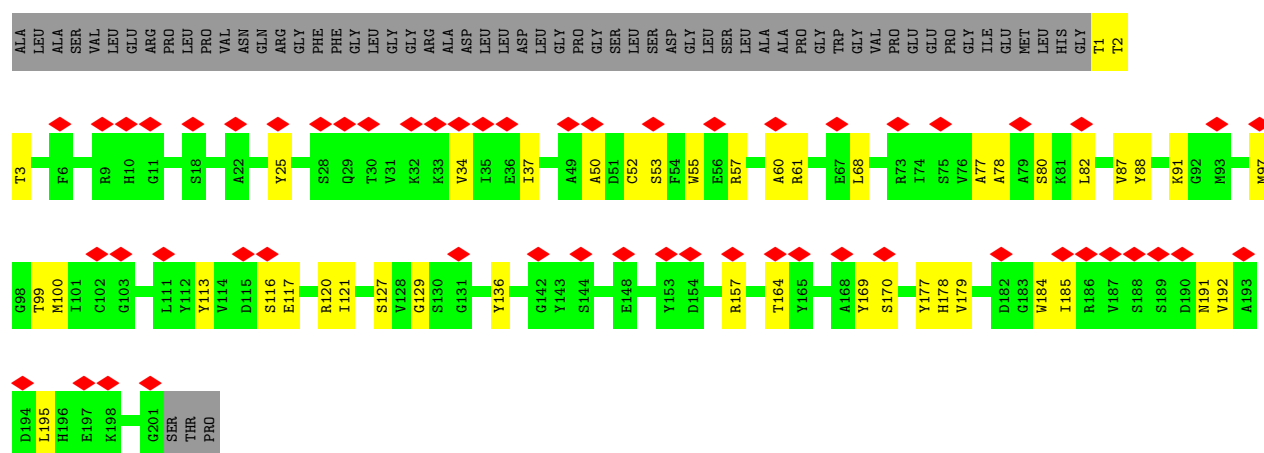


• Molecule 17: Proteasome subunit beta type-2

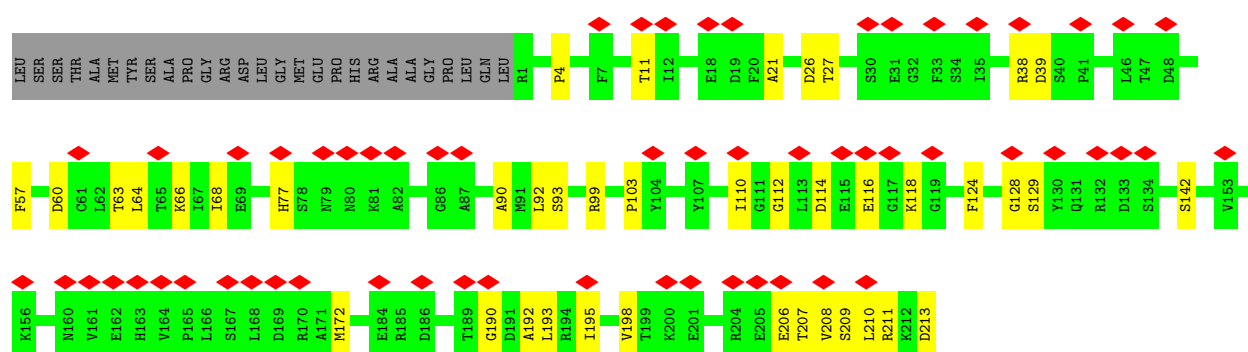




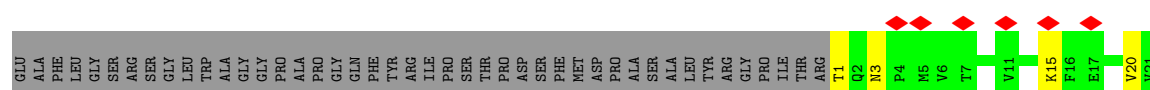
• Molecule 18: Proteasome subunit beta type-5

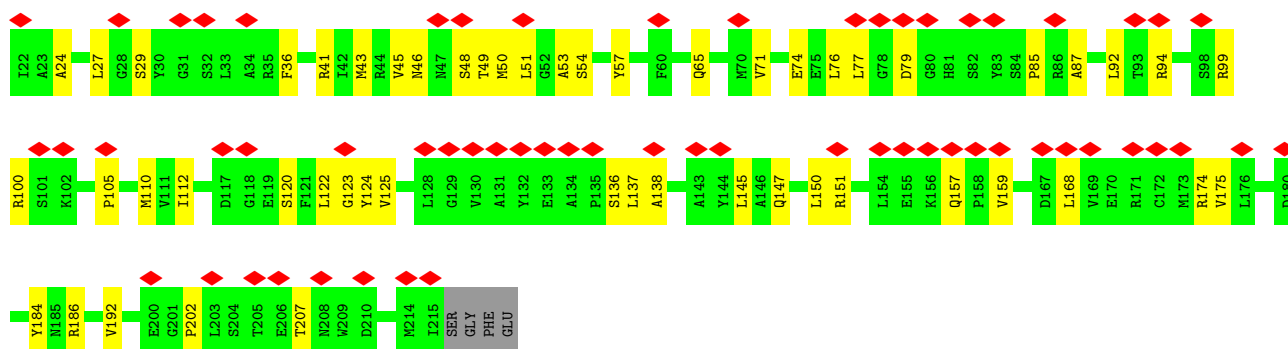


• Molecule 19: Proteasome subunit beta type-1

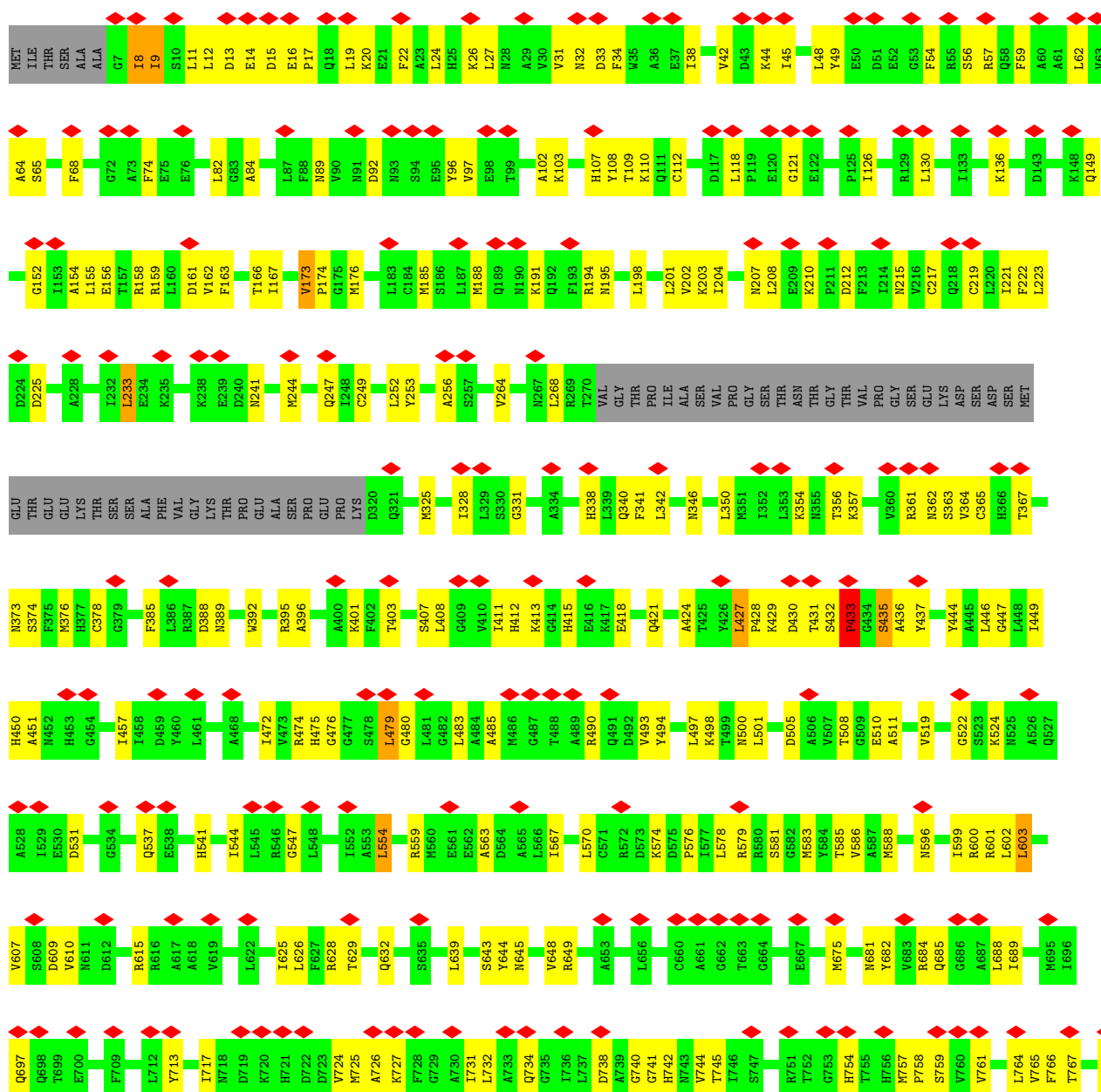


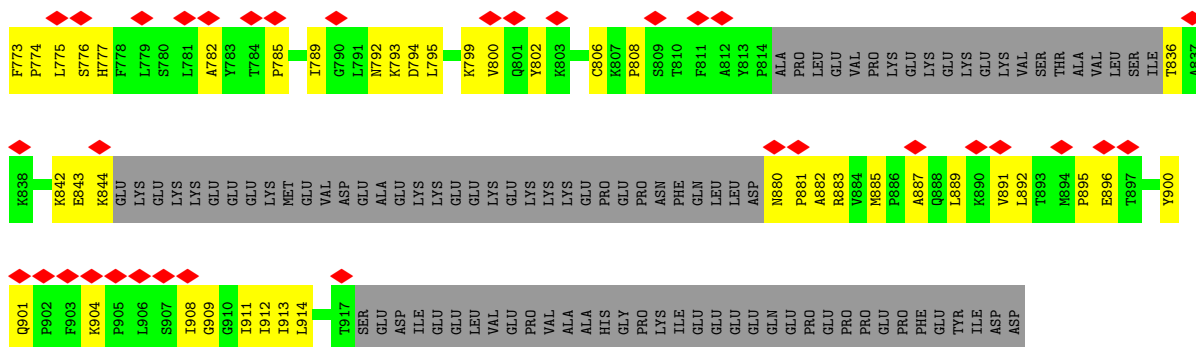
• Molecule 20: Proteasome subunit beta type-4



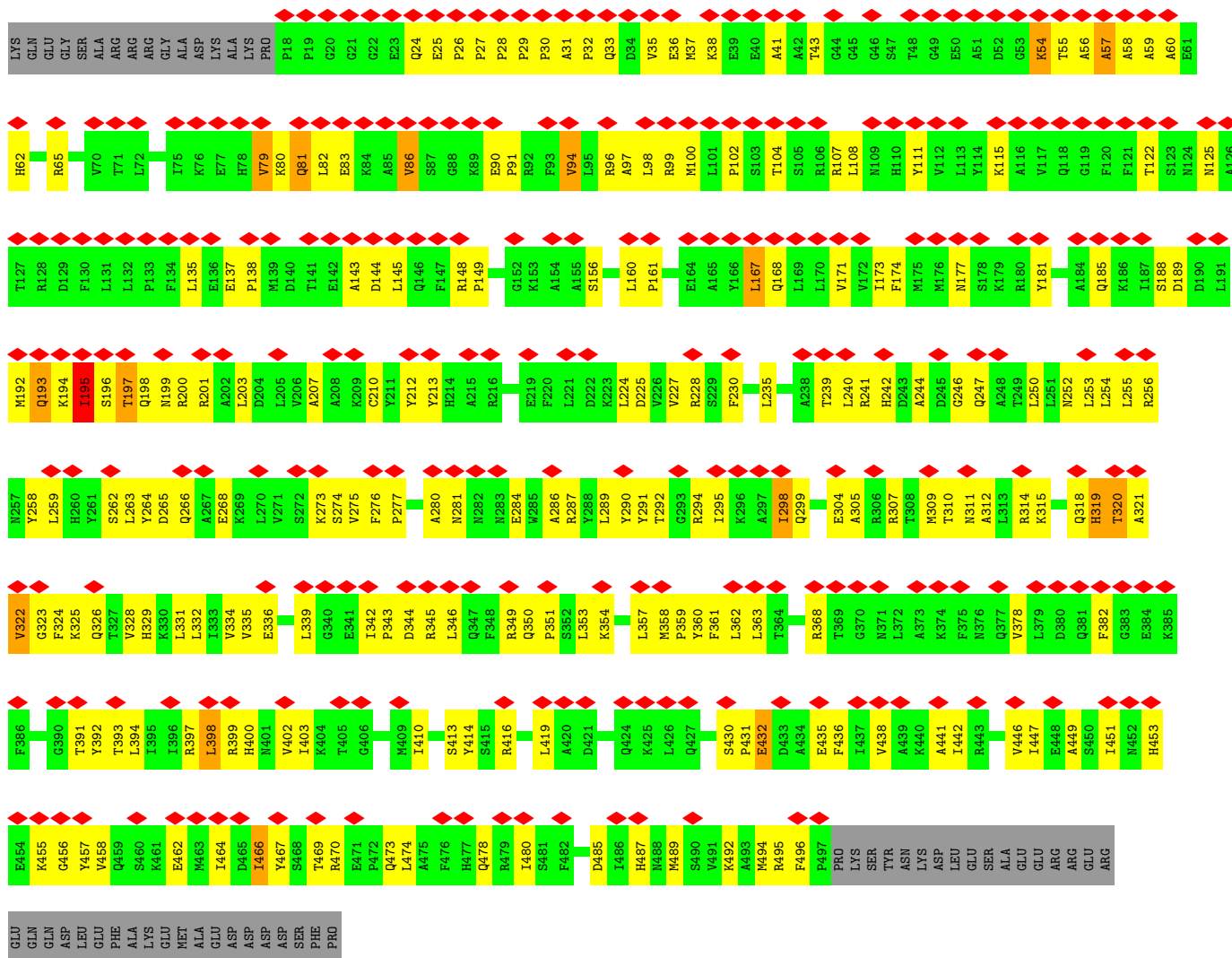


- Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

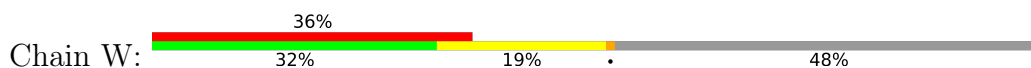


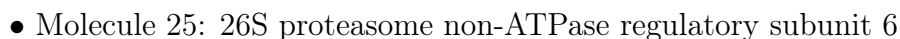
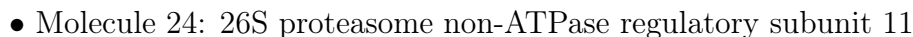


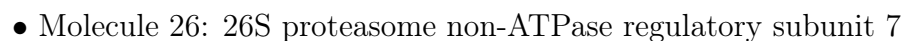
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 3



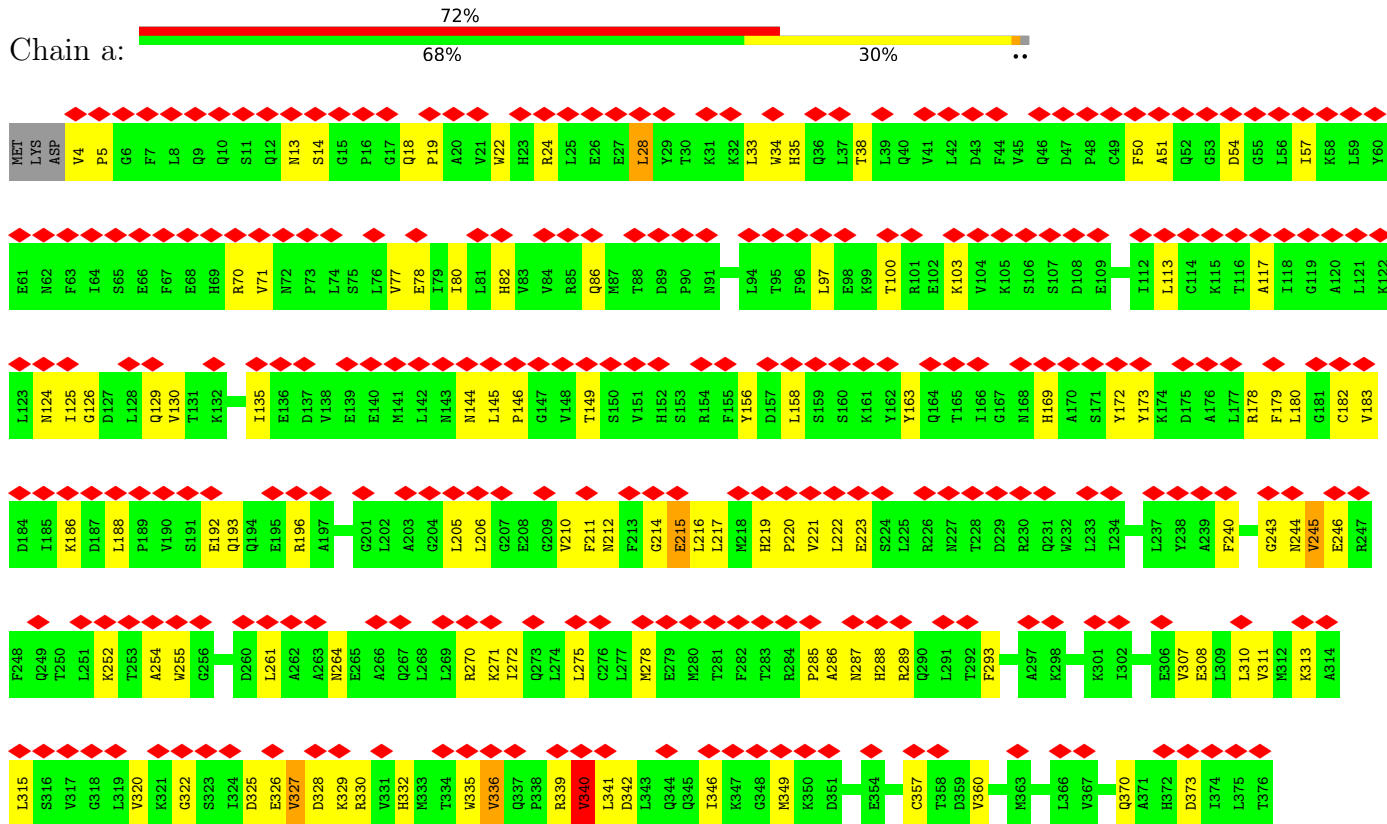
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 12



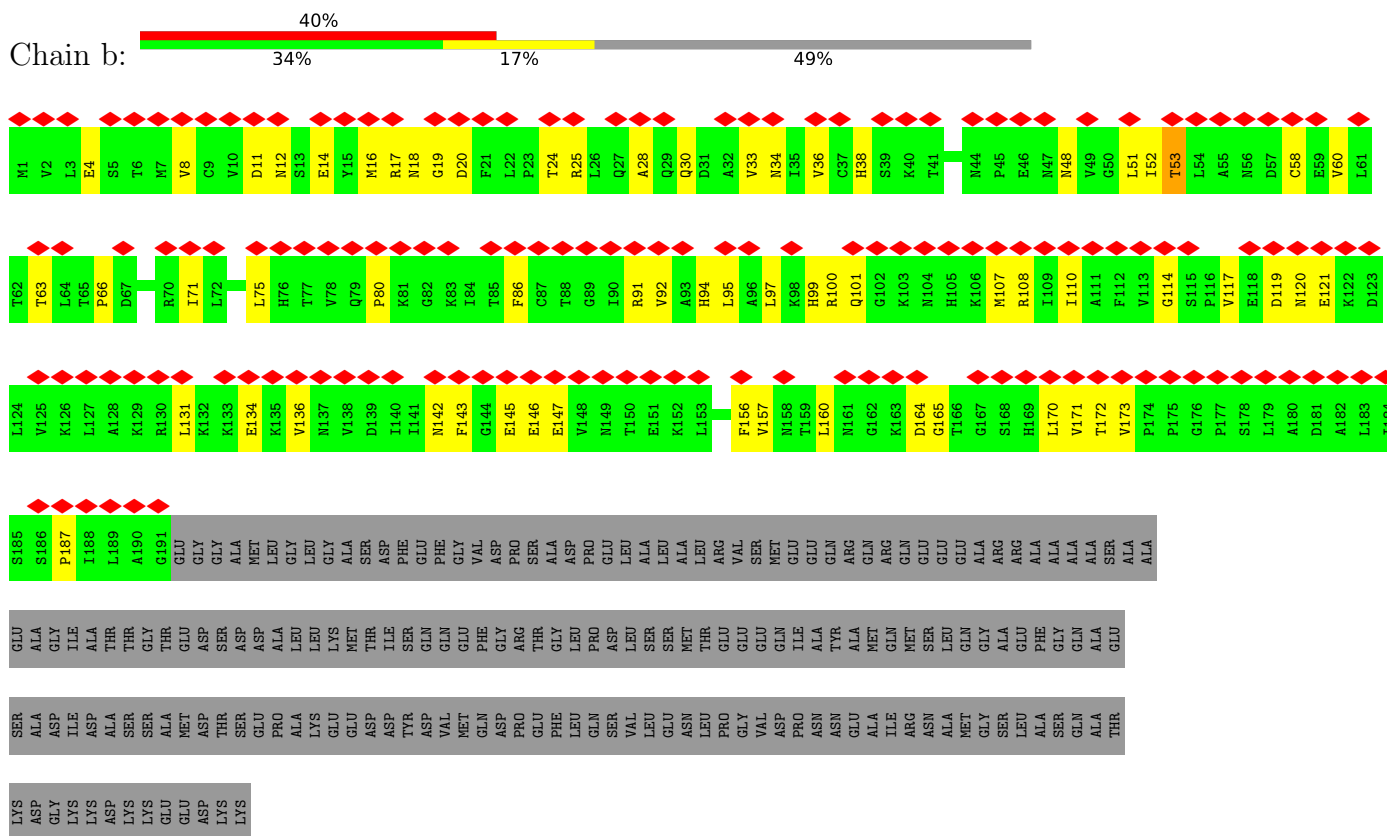


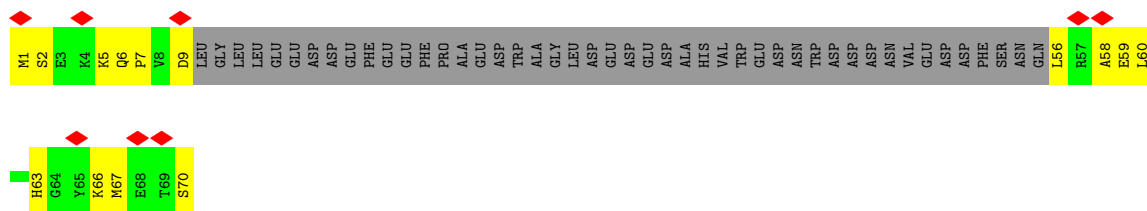


• Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

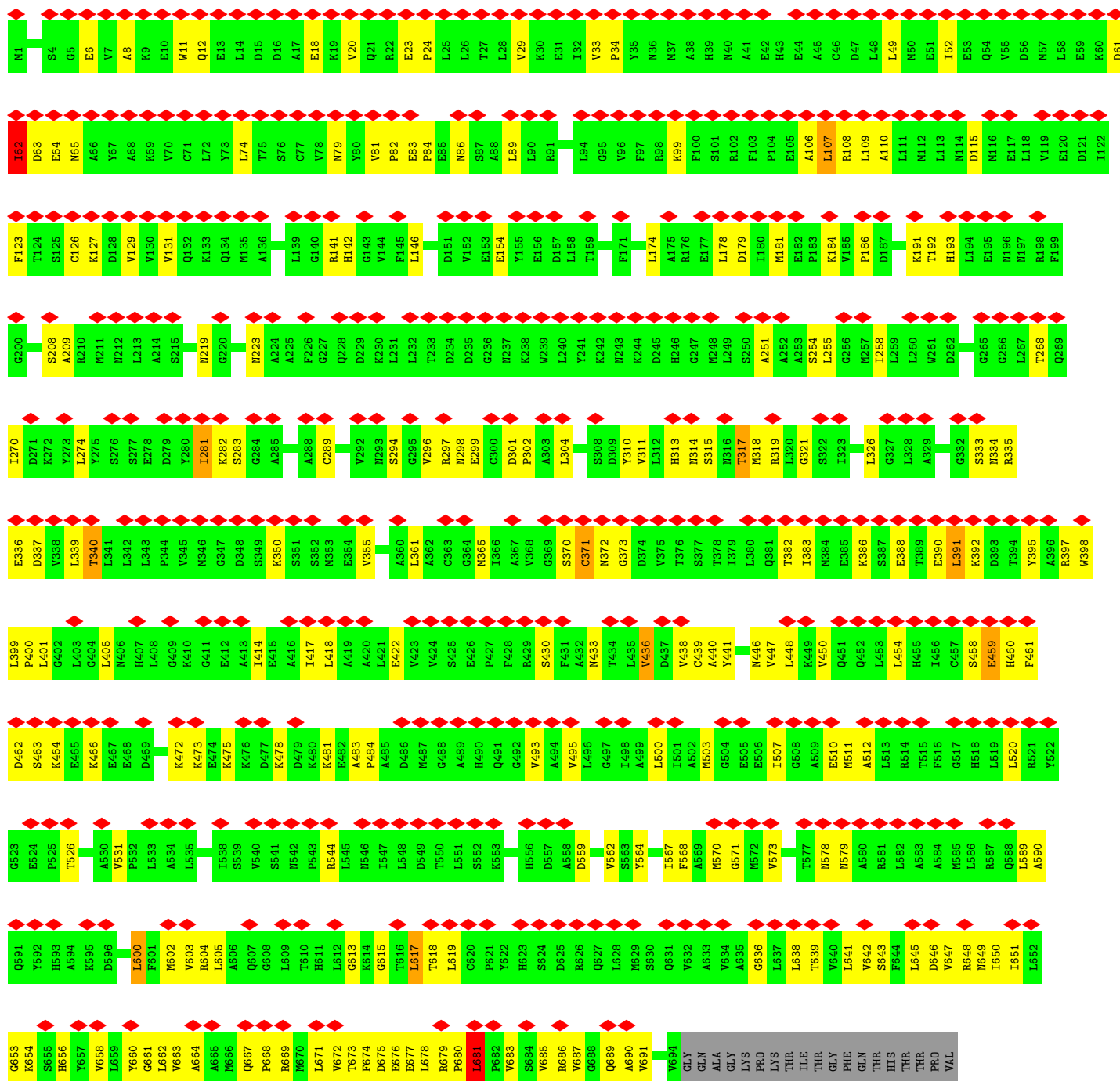


• Molecule 28: 26S proteasome non-ATPase regulatory subunit 4





• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2



LEU
LEU
ALA
HIS
GLY
GLU
ARG
ALA
GLU
LEU
ALA
THR
GLU
GLU
PHE
LEU
PRO
VAL
THR
PRO
ILE
LEU
GLY
GLY
PHE
VAL
ILE
LEU
ARG
LYS
ASN
PRO
ASN
TYR
ASP
LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18443	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.005	Depositor
Minimum map value	-0.002	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0015	Depositor
Map size (Å)	309.6, 309.6, 309.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.21	0/2886	0.58	7/3899 (0.2%)
2	B	0.21	0/2700	0.59	4/3645 (0.1%)
3	C	0.19	0/3054	0.55	2/4107 (0.0%)
4	D	0.23	0/3090	0.61	11/4168 (0.3%)
5	E	0.15	0/2835	0.48	0/3821
6	F	0.19	0/2903	0.58	1/3912 (0.0%)
7	G	0.10	0/1859	0.39	2/2523 (0.1%)
8	H	0.14	0/1743	0.43	2/2372 (0.1%)
9	I	0.10	0/1942	0.35	0/2628
10	J	0.11	0/1728	0.33	0/2358
11	K	0.12	0/1747	0.37	0/2364
12	L	0.12	0/1885	0.37	2/2552 (0.1%)
13	M	0.10	0/1891	0.31	0/2552
14	N	0.10	0/1454	0.25	0/1967
15	O	0.08	0/1670	0.26	0/2265
16	P	0.08	0/1614	0.24	0/2177
17	Q	0.09	0/1603	0.28	0/2174
18	R	0.08	0/1579	0.25	0/2134
19	S	0.08	0/1671	0.26	0/2253
20	T	0.11	0/1700	0.29	0/2305
21	U	0.12	0/6396	0.36	0/8646
22	V	0.20	0/3929	0.60	8/5309 (0.2%)
23	W	0.16	0/1975	0.48	0/2659
24	X	0.10	0/655	0.35	0/877
25	Y	0.14	0/3173	0.47	4/4273 (0.1%)
26	Z	1.01	6/2324 (0.3%)	0.54	5/3150 (0.2%)
27	a	0.91	1/3052 (0.0%)	0.48	3/4130 (0.1%)
28	b	0.14	0/1478	0.33	0/2001
29	c	0.19	0/2302	0.57	2/3110 (0.1%)
30	d	0.19	0/2162	0.53	1/2919 (0.0%)
31	e	0.21	0/198	0.62	0/258
32	f	0.20	1/5413 (0.0%)	0.57	10/7317 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.30	8/74611 (0.0%)	0.47	64/100825 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
3	C	0	1
5	E	0	1
6	F	0	2
21	U	0	3
22	V	0	2
25	Y	0	1
30	d	0	1
32	f	0	2
All	All	0	15

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	215	GLU	CG-CD	49.50	2.75	1.52
26	Z	228	TYR	CD2-CE2	23.28	2.08	1.38
26	Z	228	TYR	CD1-CE1	22.86	2.07	1.38
26	Z	228	TYR	CE1-CZ	18.93	1.83	1.38
26	Z	228	TYR	CE2-CZ	18.25	1.82	1.38
26	Z	228	TYR	CG-CD1	16.42	1.73	1.39
26	Z	228	TYR	CG-CD2	16.22	1.73	1.39
32	f	681	LEU	C-N	5.32	1.46	1.33

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	215	GLU	CB-CG-CD	10.74	130.86	112.60
32	f	636	GLY	N-CA-C	10.68	126.28	113.79
27	a	215	GLU	OE1-CD-OE2	-9.40	100.35	122.90
32	f	459	GLU	N-CA-C	9.24	127.56	113.51
29	c	243	SER	CA-C-N	8.59	137.17	121.70
29	c	243	SER	C-N-CA	8.59	137.17	121.70
3	C	217	SER	CA-C-N	8.31	136.67	121.70
3	C	217	SER	C-N-CA	8.31	136.67	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	63	TRP	CA-C-N	8.05	136.19	121.70
25	Y	63	TRP	C-N-CA	8.05	136.19	121.70
26	Z	63	LYS	N-CA-C	7.46	119.20	111.14
22	V	195	ILE	CA-C-N	7.39	135.00	121.70
22	V	195	ILE	C-N-CA	7.39	135.00	121.70
22	V	81	GLN	CA-C-N	7.04	134.37	121.70
22	V	81	GLN	C-N-CA	7.04	134.37	121.70
22	V	57	ALA	CA-C-N	6.79	133.92	121.70
22	V	57	ALA	C-N-CA	6.79	133.92	121.70
30	d	228	GLN	N-CA-C	6.75	123.98	113.72
32	f	459	GLU	CA-C-N	6.75	133.84	121.70
32	f	459	GLU	C-N-CA	6.75	133.84	121.70
26	Z	222	ILE	CA-C-N	6.61	133.60	121.70
26	Z	222	ILE	C-N-CA	6.61	133.60	121.70
4	D	373	ALA	CA-C-N	6.37	133.17	121.70
4	D	373	ALA	C-N-CA	6.37	133.17	121.70
25	Y	356	THR	CA-C-N	6.14	132.75	121.70
25	Y	356	THR	C-N-CA	6.14	132.75	121.70
32	f	459	GLU	N-CA-CB	-6.08	108.02	114.10
1	A	344	SER	CA-C-N	6.05	132.59	121.70
1	A	344	SER	C-N-CA	6.05	132.59	121.70
26	Z	63	LYS	CA-C-N	5.98	132.47	121.70
26	Z	63	LYS	C-N-CA	5.98	132.47	121.70
32	f	617	LEU	CA-C-N	5.97	132.46	121.70
32	f	617	LEU	C-N-CA	5.97	132.46	121.70
8	H	231	ALA	CA-C-N	5.97	132.44	121.70
8	H	231	ALA	C-N-CA	5.97	132.44	121.70
32	f	617	LEU	N-CA-C	5.91	117.41	110.97
4	D	389	GLU	CA-C-N	5.82	132.18	121.70
4	D	389	GLU	C-N-CA	5.82	132.18	121.70
4	D	206	GLY	CA-C-N	-5.76	114.45	120.38
4	D	206	GLY	C-N-CA	-5.76	114.45	120.38
4	D	302	ASN	CB-CA-C	-5.76	109.40	117.23
1	A	157	ILE	N-CA-C	-5.62	99.69	108.95
1	A	205	GLY	CA-C-N	5.59	131.77	121.70
1	A	205	GLY	C-N-CA	5.59	131.77	121.70
27	a	215	GLU	CG-CD-OE1	5.48	131.00	118.40
32	f	459	GLU	CB-CA-C	-5.47	104.41	109.83
6	F	430	LYS	CB-CA-C	-5.43	109.85	117.23
2	B	166	ASP	CA-C-N	5.34	131.32	121.70
2	B	166	ASP	C-N-CA	5.34	131.32	121.70
32	f	459	GLU	CA-C-O	-5.24	114.89	119.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	324	ASP	CA-C-N	5.22	131.09	121.70
2	B	324	ASP	C-N-CA	5.22	131.09	121.70
7	G	184	LYS	CA-C-N	5.17	131.00	121.70
7	G	184	LYS	C-N-CA	5.17	131.00	121.70
22	V	54	LYS	CA-C-N	5.15	130.97	121.70
22	V	54	LYS	C-N-CA	5.15	130.97	121.70
4	D	151	ILE	CA-C-N	5.13	130.93	121.70
4	D	151	ILE	C-N-CA	5.13	130.93	121.70
12	L	204	ASP	CA-C-N	5.08	130.84	121.70
12	L	204	ASP	C-N-CA	5.08	130.84	121.70
1	A	343	PHE	CA-C-N	5.01	130.72	121.70
1	A	343	PHE	C-N-CA	5.01	130.72	121.70
4	D	84	SER	CA-C-N	5.00	130.70	121.70
4	D	84	SER	C-N-CA	5.00	130.70	121.70

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	133	VAL	Peptide
2	B	264	PRO	Peptide
3	C	171	HIS	Peptide
5	E	292	PRO	Peptide
6	F	294	LYS	Peptide
6	F	87	PRO	Peptide
21	U	432	SER	Peptide
21	U	433	PRO	Peptide
21	U	435	SER	Peptide
22	V	193	GLN	Peptide
22	V	319	HIS	Peptide
25	Y	357	ASN	Peptide
30	d	3	GLU	Peptide
32	f	667	GLN	Peptide
32	f	681	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2835	0	2879	234	0
2	B	2662	0	2702	199	0
3	C	3015	0	3125	213	0
4	D	3040	0	3076	230	0
5	E	2790	0	2846	189	0
6	F	2863	0	2931	211	0
7	G	1826	0	1796	77	0
8	H	1708	0	1594	46	0
9	I	1912	0	1851	47	0
10	J	1704	0	1517	52	0
11	K	1722	0	1673	71	0
12	L	1850	0	1822	65	0
13	M	1856	0	1814	69	0
14	N	1430	0	1398	25	0
15	O	1643	0	1644	21	0
16	P	1585	0	1598	27	0
17	Q	1570	0	1547	50	0
18	R	1548	0	1499	32	0
19	S	1641	0	1618	26	0
20	T	1667	0	1628	43	0
21	U	6287	0	6338	200	0
22	V	3852	0	3893	197	0
23	W	1940	0	1978	82	0
24	X	647	0	676	22	0
25	Y	3115	0	3120	107	0
26	Z	2281	0	2312	156	0
27	a	2995	0	3011	122	0
28	b	1458	0	1505	47	0
29	c	2260	0	2276	109	0
30	d	2116	0	2146	99	0
31	e	197	0	199	14	0
32	f	5331	0	5344	165	0
33	A	27	0	12	5	0
33	B	27	0	12	8	0
33	C	27	0	12	3	0
33	D	27	0	12	5	0
33	E	27	0	12	7	0
33	F	27	0	12	4	0
34	c	1	0	0	0	0
All	All	73509	0	73428	2863	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 19.

All (2863) 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)
26:Z:228:TYR:CE1	26:Z:228:TYR:CZ	1.83	1.63
26:Z:228:TYR:CZ	26:Z:228:TYR:CE2	1.82	1.60
26:Z:228:TYR:CE2	26:Z:228:TYR:CD2	2.08	1.42
26:Z:228:TYR:CE1	26:Z:228:TYR:CD1	2.07	1.40
27:a:13:ASN:OD1	27:a:19:PRO:CG	1.68	1.39
26:Z:228:TYR:CE1	27:a:215:GLU:CD	2.22	1.18
27:a:13:ASN:OD1	27:a:19:PRO:HG3	0.98	1.14
26:Z:228:TYR:CZ	27:a:215:GLU:CD	2.25	1.14
26:Z:228:TYR:CE2	27:a:215:GLU:CD	2.25	1.14
26:Z:228:TYR:CD1	27:a:215:GLU:CD	2.26	1.13
26:Z:228:TYR:CD2	27:a:215:GLU:CD	2.28	1.11
26:Z:228:TYR:CD2	27:a:215:GLU:CG	2.34	1.11
26:Z:228:TYR:CE2	27:a:215:GLU:CG	2.36	1.08
26:Z:228:TYR:CG	27:a:215:GLU:CD	2.36	1.04
26:Z:228:TYR:CD1	27:a:215:GLU:CG	2.39	1.04
26:Z:228:TYR:CG	27:a:215:GLU:CG	2.40	1.04
26:Z:228:TYR:CZ	27:a:215:GLU:CG	2.42	1.02
26:Z:228:TYR:CG	27:a:215:GLU:HG3	1.96	1.00
26:Z:228:TYR:CE1	27:a:215:GLU:CG	2.45	0.98
1:A:362:MET:HB2	2:B:216:ILE:HD11	1.47	0.97
3:C:217:SER:HB3	3:C:218:GLU:HB3	1.45	0.96
27:a:13:ASN:CG	27:a:19:PRO:HG3	1.92	0.95
26:Z:228:TYR:CE2	27:a:215:GLU:HG2	2.02	0.93
26:Z:63:LYS:HB2	26:Z:64:ASP:HB2	1.52	0.91
5:E:50:LEU:HD13	6:F:138:GLY:HA2	1.50	0.91
3:C:70:GLY:O	3:C:118:ASN:ND2	2.05	0.89
26:Z:224:HIS:HB3	26:Z:225:GLN:HA	1.56	0.88
4:D:151:ILE:HB	4:D:152:MET:HA	1.54	0.88
26:Z:228:TYR:CZ	27:a:215:GLU:OE1	2.27	0.87
1:A:205:GLY:HA2	1:A:206:ILE:HG22	1.58	0.83
26:Z:228:TYR:CD2	27:a:215:GLU:HG2	2.14	0.83
4:D:83:GLN:HE22	4:D:140:VAL:HG21	1.44	0.83
3:C:84:LYS:HA	3:C:98:ASP:HA	1.61	0.82
23:W:416:GLN:HB3	23:W:417:ARG:HA	1.60	0.82
3:C:299:ASP:HA	3:C:302:ASP:HB3	1.61	0.82
6:F:299:GLU:HG3	6:F:300:LYS:HB3	1.61	0.82
32:f:371:CYS:SG	32:f:372:ASN:N	2.52	0.82
27:a:13:ASN:OD1	27:a:19:PRO:CB	2.29	0.81
1:A:271:LEU:HA	1:A:315:ILE:HB	1.61	0.81
29:c:174:PRO:HB2	29:c:175:ARG:HD3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:286:ALA:HB1	27:a:287:ASN:HA	1.63	0.80
32:f:663:VAL:HG13	32:f:664:ALA:HB2	1.62	0.80
1:A:385:ILE:HA	1:A:388:VAL:HB	1.62	0.80
22:V:57:ALA:HB3	22:V:58:ALA:HB3	1.64	0.80
4:D:89:ILE:HA	4:D:131:ALA:HA	1.64	0.80
4:D:389:GLU:HB2	4:D:391:ARG:HB2	1.64	0.80
26:Z:228:TYR:CG	27:a:215:GLU:OE2	2.34	0.80
4:D:113:VAL:HG11	4:D:138:ALA:HA	1.64	0.79
32:f:615:GLY:HA2	32:f:619:LEU:H	1.47	0.79
32:f:617:LEU:HB3	32:f:618:THR:HB	1.62	0.79
4:D:184:PRO:HB2	4:D:306:LYS:HE2	1.63	0.79
11:K:225:ASN:HA	11:K:227:HIS:HB3	1.65	0.79
3:C:99:VAL:HA	3:C:100:ASP:HB2	1.63	0.79
6:F:316:GLN:HA	6:F:320:PHE:HB2	1.64	0.79
22:V:193:GLN:HB3	22:V:194:LYS:HA	1.64	0.79
4:D:243:GLY:HA3	4:D:288:ILE:HD13	1.65	0.79
5:E:126:ASP:HB2	5:E:185:ARG:HG2	1.62	0.79
26:Z:233:VAL:HA	26:Z:236:LEU:HD13	1.64	0.79
1:A:344:SER:N	1:A:345:LEU:HB2	1.98	0.78
5:E:250:ASP:HB2	6:F:300:LYS:HD3	1.66	0.78
26:Z:228:TYR:CD1	27:a:215:GLU:HG3	2.17	0.78
22:V:148:ARG:HG3	22:V:149:PRO:HD3	1.67	0.77
3:C:157:GLN:NE2	3:C:316:GLU:O	2.18	0.77
2:B:387:LYS:HB3	2:B:390:LEU:HD11	1.65	0.77
27:a:270:ARG:HH11	27:a:313:LYS:HB3	1.50	0.77
32:f:296:VAL:HG12	32:f:297:ARG:HG2	1.66	0.77
32:f:391:LEU:HD12	32:f:392:LYS:H	1.50	0.77
5:E:262:ASN:HA	5:E:265:ASP:HB2	1.67	0.77
6:F:120:LYS:HD2	6:F:136:VAL:HG21	1.68	0.76
2:B:232:LYS:N	33:B:501:ADP:O1A	2.19	0.76
6:F:84:LYS:N	6:F:85:THR:HA	1.98	0.76
3:C:41:ASN:HD21	22:V:492:LYS:HD3	1.48	0.76
5:E:320:ILE:HD13	6:F:217:ILE:HD11	1.67	0.76
30:d:3:GLU:HB3	30:d:4:GLN:HA	1.66	0.75
32:f:436:VAL:HA	32:f:439:CYS:HB2	1.69	0.75
26:Z:150:PRO:HD3	27:a:182:CYS:HA	1.67	0.75
4:D:279:THR:O	4:D:283:ARG:N	2.17	0.75
22:V:287:ARG:HD2	31:e:5:LYS:HB2	1.68	0.74
30:d:147:SER:OG	30:d:151:VAL:N	2.19	0.74
2:B:261:GLY:HA2	2:B:262:ASP:HB3	1.69	0.74
5:E:60:VAL:HG23	5:E:98:VAL:HG21	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:94:ILE:HB	6:F:123:VAL:HB	1.70	0.74
22:V:192:MET:HA	22:V:193:GLN:HB2	1.68	0.74
1:A:90:GLU:O	1:A:94:GLN:HB2	1.87	0.74
2:B:105:THR:HG23	2:B:106:PRO:HD3	1.68	0.73
5:E:109:ARG:HH12	6:F:121:CYS:HB2	1.53	0.73
1:A:157:ILE:HG22	1:A:158:ASP:HA	1.69	0.73
5:E:290:LEU:HA	5:E:295:LEU:HD12	1.70	0.73
2:B:131:HIS:NE2	2:B:156:VAL:O	2.22	0.73
23:W:257:GLN:HA	23:W:258:ALA:HB3	1.71	0.73
7:G:219:VAL:HG12	7:G:230:LEU:HD11	1.70	0.73
24:X:417:LYS:HD2	25:Y:383:LEU:HD23	1.70	0.73
3:C:65:LEU:O	3:C:69:GLN:NE2	2.22	0.72
3:C:118:ASN:OD1	3:C:118:ASN:N	2.21	0.72
26:Z:97:THR:HA	26:Z:124:ILE:HG13	1.70	0.72
26:Z:201:LEU:HD22	27:a:357:CYS:HA	1.70	0.72
8:H:71:HIS:HA	8:H:218:PHE:H	1.52	0.72
12:L:105:VAL:HG21	12:L:136:GLY:HA3	1.71	0.72
32:f:317:THR:HG21	32:f:689:GLN:HG3	1.70	0.72
29:c:180:ASN:HB2	29:c:204:THR:HG21	1.71	0.72
22:V:435:GLU:HG2	22:V:453:HIS:CE1	2.24	0.72
22:V:195:ILE:H	22:V:196:SER:HB3	1.53	0.72
4:D:133:HIS:HB3	4:D:138:ALA:H	1.53	0.72
6:F:233:LYS:N	33:F:501:ADP:O1A	2.23	0.72
23:W:418:PRO:HA	23:W:419:LYS:HB2	1.72	0.72
27:a:70:ARG:HE	28:b:80:PRO:HD2	1.55	0.72
3:C:263:SER:O	3:C:267:SER:N	2.20	0.71
4:D:83:GLN:HG3	4:D:133:HIS:CD2	2.25	0.71
6:F:168:TYR:HB2	6:F:169:ASP:HB2	1.72	0.71
3:C:137:LEU:HA	3:C:140:VAL:HG12	1.71	0.71
2:B:264:PRO:HG3	2:B:311:GLU:HG2	1.72	0.71
6:F:86:LEU:HD12	6:F:87:PRO:HD2	1.72	0.71
1:A:90:GLU:HG3	1:A:94:GLN:HE21	1.53	0.71
6:F:267:LEU:O	6:F:271:ALA:N	2.22	0.71
22:V:326:GLN:HB3	22:V:353:LEU:HD13	1.73	0.71
26:Z:167:ALA:HB1	29:c:42:LEU:HB2	1.73	0.71
2:B:307:ARG:HA	2:B:310:LEU:HB3	1.73	0.71
10:J:115:LYS:HE3	10:J:127:PHE:HB2	1.70	0.71
32:f:311:VAL:HB	32:f:319:ARG:HG2	1.72	0.71
4:D:185:LEU:HD11	4:D:259:PRO:HB3	1.71	0.71
21:U:799:LYS:HA	21:U:843:GLU:HG3	1.72	0.71
6:F:85:THR:H	6:F:159:LEU:HD11	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:740:GLY:HA3	21:U:744:VAL:HG22	1.74	0.70
1:A:284:ARG:O	1:A:296:GLN:NE2	2.24	0.70
5:E:266:GLY:HA2	5:E:267:PHE:HB2	1.71	0.70
25:Y:272:PHE:HB2	31:e:67:MET:HE3	1.74	0.70
24:X:407:MET:HE1	25:Y:375:LEU:HB3	1.73	0.70
9:I:29:GLY:O	9:I:166:ASN:ND2	2.25	0.70
27:a:320:VAL:HG22	27:a:322:GLY:H	1.56	0.70
26:Z:33:LYS:NZ	26:Z:34:ARG:O	2.25	0.70
4:D:167:ILE:HG21	33:D:501:ADP:HN62	1.55	0.70
4:D:285:VAL:HA	4:D:288:ILE:HB	1.74	0.70
16:P:61:GLN:HE22	17:Q:124:LEU:HB2	1.57	0.70
2:B:111:THR:OG1	2:B:124:SER:O	2.10	0.69
4:D:401:LYS:HG3	4:D:404:LYS:HE2	1.74	0.69
18:R:52:CYS:HA	18:R:97:MET:HE3	1.72	0.69
21:U:191:LYS:HG3	21:U:194:ARG:HE	1.57	0.69
7:G:16:PHE:HB2	8:H:128:ARG:HH22	1.56	0.69
21:U:842:LYS:HA	21:U:843:GLU:HB3	1.72	0.69
26:Z:150:PRO:HG2	27:a:149:THR:HG23	1.74	0.69
27:a:211:PHE:HA	27:a:271:LYS:HE3	1.73	0.69
1:A:380:SER:HB3	1:A:385:ILE:HG21	1.74	0.69
2:B:378:VAL:HG22	2:B:416:ASN:HB2	1.73	0.69
26:Z:128:PRO:HG3	29:c:216:MET:HB3	1.72	0.69
4:D:246:MET:O	4:D:250:VAL:N	2.25	0.69
17:Q:117:TYR:HB3	17:Q:125:ALA:HB3	1.75	0.69
3:C:328:ILE:HG23	3:C:359:VAL:HG11	1.75	0.69
4:D:230:VAL:HG23	4:D:264:ILE:HA	1.73	0.69
32:f:399:LEU:HD23	32:f:418:LEU:HD21	1.74	0.69
1:A:232:ARG:HH12	1:A:271:LEU:HD13	1.56	0.69
1:A:384:GLU:H	2:B:343:ARG:HH11	1.40	0.69
3:C:113:ARG:NH1	3:C:128:PRO:O	2.25	0.69
8:H:25:ALA:HB2	8:H:128:ARG:HE	1.58	0.69
12:L:75:ALA:HB3	12:L:131:GLY:HA3	1.74	0.69
21:U:112:CYS:SG	21:U:159:ARG:NH1	2.66	0.69
23:W:432:LEU:HD23	23:W:435:LEU:HD22	1.74	0.69
3:C:145:ASP:HB3	3:C:201:ARG:HG2	1.75	0.69
4:D:248:ARG:NH2	4:D:291:GLU:OE2	2.26	0.69
21:U:356:THR:HG21	21:U:731:ILE:HD13	1.72	0.69
23:W:407:ASP:H	23:W:413:ILE:HG22	1.58	0.69
1:A:240:VAL:HB	1:A:274:PHE:HA	1.74	0.68
4:D:194:ILE:HG13	4:D:196:ILE:H	1.58	0.68
5:E:207:TYR:HD1	5:E:208:ILE:HD12	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:183:VAL:HG12	7:G:184:LYS:HG2	1.72	0.68
22:V:275:VAL:HB	22:V:277:PRO:HD3	1.73	0.68
28:b:12:ASN:ND2	28:b:53:THR:OG1	2.26	0.68
1:A:409:PHE:O	1:A:413:VAL:N	2.25	0.68
12:L:157:ARG:HG3	12:L:176:MET:HE2	1.75	0.68
22:V:413:SER:OG	25:Y:335:SER:OG	2.09	0.68
32:f:361:LEU:HD13	32:f:398:TRP:HB3	1.74	0.68
1:A:112:ILE:HA	1:A:122:VAL:HA	1.75	0.68
8:H:231:ALA:HB3	8:H:232:ALA:HB3	1.74	0.68
11:K:209:LYS:O	11:K:214:ASN:ND2	2.25	0.68
25:Y:138:LEU:HD11	25:Y:180:LEU:HD11	1.75	0.68
1:A:413:VAL:HA	1:A:416:VAL:HG12	1.74	0.68
2:B:103:ARG:HG2	2:B:160:ILE:HG21	1.76	0.68
24:X:395:LYS:HD3	26:Z:258:VAL:HG13	1.75	0.68
25:Y:64:GLN:HG2	25:Y:65:ILE:HG22	1.74	0.68
11:K:16:SER:HB3	11:K:20:ARG:H	1.59	0.68
21:U:155:LEU:O	21:U:158:ARG:NH1	2.26	0.68
21:U:446:LEU:O	21:U:450:HIS:ND1	2.26	0.68
22:V:259:LEU:HD11	22:V:294:ARG:HD2	1.76	0.68
6:F:308:ARG:HA	6:F:311:LEU:HB2	1.76	0.68
26:Z:228:TYR:CE1	27:a:215:GLU:CB	2.77	0.68
1:A:410:LEU:O	1:A:414:ASN:ND2	2.27	0.68
29:c:154:LYS:HG2	29:c:156:VAL:H	1.57	0.68
32:f:372:ASN:N	32:f:373:GLY:HA2	2.09	0.68
1:A:80:LEU:HD22	2:B:99:VAL:HG11	1.75	0.68
1:A:182:GLU:HA	1:A:185:GLU:HB3	1.73	0.68
2:B:175:LYS:O	3:C:232:ARG:NH1	2.27	0.68
21:U:418:GLU:HG3	21:U:421:GLN:HE21	1.59	0.68
22:V:262:SER:HB2	22:V:263:LEU:HB2	1.74	0.68
30:d:160:ALA:HB3	30:d:161:GLU:HA	1.75	0.68
21:U:108:TYR:OH	21:U:159:ARG:NH2	2.27	0.67
23:W:441:LYS:HE3	26:Z:233:VAL:HG12	1.75	0.67
1:A:398:ARG:NH1	2:B:195:GLN:O	2.21	0.67
2:B:294:ARG:NH1	2:B:295:TYR:O	2.26	0.67
23:W:373:ILE:HG12	23:W:374:THR:H	1.59	0.67
32:f:294:SER:O	32:f:298:ASN:ND2	2.27	0.67
32:f:390:GLU:HG3	32:f:395:TYR:HB3	1.76	0.67
1:A:123:VAL:HG21	1:A:147:TYR:HB2	1.74	0.67
3:C:218:GLU:OE2	4:D:286:GLN:NE2	2.25	0.67
4:D:260:ALA:H	4:D:304:ASN:HD22	1.40	0.67
32:f:154:GLU:HB3	32:f:184:LYS:HD3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:LYS:HB3	2:B:176:VAL:HB	1.76	0.67
6:F:249:LEU:HB2	6:F:283:ILE:HG13	1.76	0.67
21:U:808:PRO:HD3	21:U:836:THR:HB	1.76	0.67
9:I:76:VAL:HG23	9:I:134:LEU:HB3	1.76	0.67
17:Q:183:ILE:HG12	17:Q:188:ILE:HG13	1.75	0.67
22:V:255:LEU:HD22	22:V:291:TYR:HB3	1.76	0.67
23:W:420:ASP:HB3	23:W:422:ASN:HB3	1.76	0.67
1:A:258:ARG:NH2	6:F:255:GLN:OE1	2.28	0.67
1:A:292:ASP:O	1:A:296:GLN:N	2.25	0.67
15:O:30:ASN:OD1	15:O:187:ARG:NH2	2.27	0.67
22:V:321:ALA:HB1	22:V:322:VAL:HB	1.75	0.67
30:d:147:SER:HG	30:d:151:VAL:H	1.42	0.67
26:Z:16:LEU:HD13	29:c:220:LEU:HD21	1.76	0.66
26:Z:208:ILE:HD11	27:a:349:MET:HG2	1.77	0.66
2:B:174:MET:HA	2:B:248:LEU:HD13	1.76	0.66
4:D:249:ASP:HA	4:D:252:ARG:HG2	1.77	0.66
4:D:345:PHE:HB3	4:D:360:LEU:HD13	1.76	0.66
9:I:12:PHE:HB2	10:J:18:GLN:HB3	1.78	0.66
16:P:58:THR:OG1	17:Q:121:LEU:O	2.12	0.66
3:C:64:GLN:O	29:c:190:GLN:NE2	2.28	0.66
7:G:43:ARG:HB3	7:G:164:LYS:HA	1.76	0.66
12:L:151:ALA:O	13:M:85:ARG:NH2	2.27	0.66
29:c:124:GLY:O	29:c:128:ASN:ND2	2.28	0.66
27:a:205:LEU:O	27:a:271:LYS:NZ	2.28	0.66
1:A:140:VAL:HA	1:A:152:PRO:HA	1.77	0.66
6:F:263:ASP:O	6:F:267:LEU:N	2.22	0.66
21:U:474:ARG:NH1	21:U:500:ASN:O	2.24	0.66
1:A:304:ASN:HD22	6:F:254:PRO:HG2	1.59	0.66
22:V:349:ARG:HH12	22:V:361:PHE:HB2	1.59	0.66
26:Z:220:LEU:HB3	26:Z:221:PRO:HA	1.78	0.66
30:d:147:SER:HA	30:d:148:TYR:HB2	1.77	0.66
1:A:410:LEU:HA	1:A:413:VAL:HB	1.77	0.66
3:C:38:LYS:HA	22:V:492:LYS:HB3	1.77	0.66
5:E:178:THR:HG23	33:E:401:ADP:C8	2.31	0.66
1:A:362:MET:HG2	1:A:363:SER:H	1.61	0.66
4:D:355:SER:HB2	4:D:393:ILE:HG21	1.78	0.65
6:F:209:LYS:NZ	6:F:217:ILE:O	2.28	0.65
26:Z:133:LEU:HB2	29:c:229:LEU:HA	1.78	0.65
15:O:42:TYR:HB2	15:O:178:ILE:HD11	1.79	0.65
3:C:182:GLN:NE2	3:C:286:THR:O	2.30	0.65
3:C:268:GLU:HA	3:C:271:ARG:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:287:ARG:O	4:D:291:GLU:N	2.27	0.65
10:J:68:ASN:HA	10:J:211:MET:HE1	1.78	0.65
2:B:191:ASP:HA	2:B:194:ILE:HG22	1.77	0.65
2:B:416:ASN:HA	2:B:419:PHE:HB3	1.77	0.65
4:D:89:ILE:O	4:D:106:THR:OG1	2.15	0.65
32:f:503:MET:SD	32:f:669:ARG:NH1	2.69	0.65
21:U:341:PHE:HB2	21:U:881:PRO:HD2	1.77	0.65
1:A:122:VAL:HG21	6:F:150:LEU:HD21	1.79	0.65
1:A:348:LEU:HD21	11:K:32:LYS:HE3	1.79	0.65
3:C:188:LEU:HB3	3:C:317:PHE:HB2	1.78	0.65
4:D:335:LEU:HD11	4:D:372:GLY:HA2	1.78	0.65
29:c:260:GLU:HA	29:c:263:ASP:HB2	1.77	0.65
4:D:373:ALA:HB1	4:D:374:ASP:HB3	1.77	0.65
5:E:47:LEU:HA	5:E:50:LEU:HD12	1.78	0.65
7:G:109:ILE:HD11	7:G:114:LEU:HB2	1.79	0.65
25:Y:79:ASP:HA	25:Y:82:LYS:HG2	1.78	0.65
3:C:169:VAL:HG21	3:C:207:THR:HG21	1.78	0.65
5:E:281:ARG:HD3	5:E:387:LYS:HE3	1.78	0.65
6:F:417:HIS:HA	6:F:420:TYR:HB2	1.78	0.65
9:I:26:GLU:O	9:I:30:HIS:ND1	2.27	0.65
22:V:298:ILE:HG13	30:d:116:HIS:HB3	1.77	0.65
29:c:191:ALA:O	29:c:195:GLY:N	2.29	0.65
1:A:303:ILE:HD12	1:A:332:MET:HG2	1.77	0.65
22:V:81:GLN:HB3	22:V:82:LEU:C	2.22	0.65
4:D:129:SER:HB2	4:D:252:ARG:HH12	1.62	0.65
2:B:291:GLY:HA2	2:B:336:THR:HG21	1.79	0.64
3:C:182:GLN:HE21	3:C:287:LYS:HG2	1.61	0.64
8:H:135:LEU:HD23	8:H:148:GLN:HB2	1.78	0.64
32:f:146:LEU:HG	32:f:178:LEU:HD13	1.79	0.64
1:A:290:GLY:O	6:F:295:ARG:NH1	2.30	0.64
4:D:406:VAL:HG23	4:D:407:ILE:HB	1.79	0.64
5:E:309:ARG:NH2	5:E:338:PHE:O	2.30	0.64
21:U:208:LEU:HD23	21:U:210:LYS:H	1.62	0.64
25:Y:63:TRP:HB3	25:Y:64:GLN:HB3	1.79	0.64
25:Y:251:HIS:HA	25:Y:257:ARG:HD3	1.79	0.64
26:Z:241:SER:HB3	26:Z:245:PHE:HB3	1.79	0.64
4:D:100:THR:HB	4:D:114:ARG:HD2	1.78	0.64
4:D:229:ARG:NH2	5:E:267:PHE:O	2.29	0.64
6:F:138:GLY:O	6:F:160:ILE:N	2.31	0.64
6:F:150:LEU:HD22	6:F:164:LEU:HB3	1.78	0.64
30:d:182:ILE:HG12	30:d:213:ARG:HH12	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:LYS:C	2:B:219:PRO:HD3	2.23	0.64
21:U:376:MET:O	21:U:741:GLY:N	2.31	0.64
22:V:362:LEU:HB3	22:V:382:PHE:HE2	1.63	0.64
23:W:432:LEU:HA	23:W:435:LEU:HB2	1.80	0.64
2:B:112:LEU:HB2	2:B:150:VAL:HG13	1.80	0.64
14:N:144:ARG:H	14:N:147:MET:HE3	1.62	0.64
20:T:51:LEU:HD11	20:T:110:MET:HB3	1.80	0.64
22:V:281:ASN:ND2	25:Y:389:MET:SD	2.71	0.64
32:f:405:LEU:HG	32:f:671:LEU:HD13	1.80	0.64
22:V:97:ALA:HB3	22:V:98:LEU:HA	1.79	0.64
22:V:344:ASP:HB2	22:V:368:ARG:HH11	1.62	0.64
3:C:14:GLY:O	3:C:18:SER:N	2.31	0.64
5:E:310:LEU:O	5:E:314:LYS:NZ	2.27	0.64
11:K:93:ARG:NH1	18:R:68:LEU:O	2.31	0.64
21:U:249:CYS:HB3	21:U:328:ILE:HD12	1.78	0.64
29:c:299:CYS:SG	29:c:300:LEU:N	2.71	0.64
32:f:62:ILE:HD12	32:f:99:LYS:HB3	1.79	0.64
20:T:99:ARG:HG3	20:T:105:PRO:HA	1.80	0.64
1:A:339:ARG:NH2	6:F:402:GLU:OE1	2.32	0.63
5:E:86:GLN:OE1	6:F:117:ARG:NH2	2.31	0.63
21:U:444:TYR:HB2	21:U:476:GLY:HA3	1.81	0.63
6:F:298:SER:HB3	6:F:299:GLU:HB2	1.80	0.63
23:W:331:GLY:HA2	23:W:332:SER:HB3	1.79	0.63
27:a:370:GLN:O	30:d:251:ARG:NH1	2.32	0.63
4:D:284:GLU:O	4:D:288:ILE:N	2.31	0.63
9:I:45:LEU:HD11	9:I:137:ILE:HG12	1.80	0.63
16:P:11:VAL:HG11	16:P:52:GLY:HA3	1.81	0.63
22:V:37:MET:HE2	22:V:115:LYS:HE3	1.81	0.63
1:A:103:ASN:HB2	1:A:112:ILE:HG23	1.78	0.63
1:A:205:GLY:HA2	1:A:206:ILE:CG2	2.29	0.63
20:T:174:ARG:HG3	20:T:207:THR:HG22	1.79	0.63
28:b:14:GLU:HB2	28:b:17:ARG:HH21	1.64	0.63
30:d:12:LYS:HG2	30:d:57:ILE:HD11	1.79	0.63
32:f:676:GLU:HB3	32:f:691:VAL:HG13	1.80	0.63
2:B:317:ASP:HB3	2:B:318:GLY:HA2	1.79	0.63
3:C:22:GLN:HB3	22:V:195:ILE:HD13	1.81	0.63
11:K:32:LYS:NZ	11:K:172:SER:O	2.30	0.63
27:a:186:LYS:HD2	27:a:193:GLN:HE22	1.64	0.63
1:A:168:GLU:HA	1:A:236:CYS:HB2	1.79	0.63
6:F:79:LYS:HA	6:F:82:VAL:HG22	1.80	0.63
7:G:211:LYS:NZ	7:G:213:SER:OG	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:VAL:HG21	2:B:159:VAL:HG12	1.81	0.63
16:P:27:ARG:HB2	16:P:183:MET:HB2	1.79	0.63
1:A:333:ARG:HB2	1:A:337:LEU:HB2	1.81	0.63
5:E:171:LEU:HD22	5:E:295:LEU:HD13	1.81	0.63
7:G:86:ASP:OD2	7:G:132:ARG:NH2	2.32	0.63
17:Q:178:PHE:HB2	17:Q:194:ILE:HB	1.80	0.63
32:f:604:ARG:HD2	32:f:649:ASN:HB3	1.81	0.63
2:B:225:TYR:CE2	2:B:350:LYS:HE3	2.34	0.62
2:B:398:ILE:HG22	2:B:426:VAL:HG11	1.80	0.62
5:E:177:GLY:H	5:E:303:LEU:HD12	1.63	0.62
5:E:288:ALA:O	5:E:294:ARG:NH1	2.32	0.62
11:K:203:LYS:HD3	11:K:241:ILE:HD11	1.81	0.62
27:a:13:ASN:CG	27:a:19:PRO:CG	2.61	0.62
27:a:129:GLN:HG3	27:a:130:VAL:H	1.64	0.62
4:D:286:GLN:HA	4:D:289:LEU:HB3	1.80	0.62
5:E:131:SER:HA	5:E:134:GLU:HB2	1.79	0.62
21:U:685:GLN:HB2	21:U:726:ALA:HA	1.80	0.62
22:V:324:PHE:HB3	31:e:6:GLN:HA	1.81	0.62
30:d:227:SER:C	30:d:229:GLN:HA	2.24	0.62
13:M:236:GLU:O	13:M:240:LYS:NZ	2.27	0.62
1:A:122:VAL:O	6:F:88:TYR:HA	1.99	0.62
1:A:353:HIS:HA	1:A:356:LYS:HB2	1.82	0.62
3:C:63:LEU:HD11	4:D:133:HIS:CD2	2.34	0.62
3:C:171:HIS:O	3:C:173:GLU:N	2.32	0.62
7:G:22:LEU:HD13	7:G:25:VAL:HB	1.81	0.62
9:I:181:GLU:C	9:I:183:GLU:HB2	2.25	0.62
3:C:313:ARG:NH1	3:C:314:LYS:O	2.32	0.62
4:D:269:ALA:HB2	5:E:258:MET:HG3	1.80	0.62
11:K:10:ARG:NH2	12:L:4:ASN:O	2.31	0.62
21:U:247:GLN:HE22	21:U:912:ILE:HG22	1.64	0.62
1:A:115:VAL:HG13	1:A:117:GLN:H	1.65	0.62
1:A:206:ILE:HG23	1:A:207:GLU:H	1.64	0.62
6:F:392:ASN:HB2	6:F:395:GLN:HG3	1.80	0.62
21:U:842:LYS:HG2	21:U:882:ALA:HB2	1.81	0.62
30:d:49:ILE:HD11	30:d:89:LEU:HD22	1.81	0.62
7:G:49:VAL:HG22	7:G:219:VAL:HG23	1.81	0.62
10:J:23:GLN:HG2	10:J:149:PRO:HG2	1.81	0.62
15:O:215:LYS:HB3	16:P:197:THR:HB	1.81	0.62
21:U:800:VAL:HG21	21:U:914:LEU:HD21	1.81	0.62
25:Y:232:GLU:HG2	25:Y:234:PRO:HD2	1.81	0.62
26:Z:33:LYS:HE2	26:Z:59:ASP:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:127:ILE:HA	29:c:130:GLN:HB2	1.81	0.62
3:C:386:ALA:HA	3:C:389:LYS:HB2	1.80	0.62
4:D:414:HIS:NE2	7:G:21:ARG:HB2	2.15	0.62
5:E:292:PRO:HA	5:E:295:LEU:O	2.00	0.62
6:F:137:ILE:HG21	6:F:160:ILE:HB	1.80	0.62
24:X:420:LYS:HD2	26:Z:283:ARG:HD2	1.81	0.62
32:f:20:VAL:HG12	32:f:24:PRO:HD3	1.80	0.62
1:A:184:ILE:HD13	1:A:224:LEU:HD22	1.82	0.62
5:E:329:GLU:HA	5:E:332:VAL:HB	1.82	0.62
6:F:121:CYS:SG	6:F:122:ALA:N	2.73	0.62
8:H:93:LEU:HD21	8:H:113:ARG:HE	1.64	0.62
21:U:374:SER:HA	21:U:411:ILE:HG12	1.81	0.62
3:C:83:LYS:HA	3:C:105:ILE:HD11	1.81	0.62
25:Y:173:ASP:HB2	25:Y:177:ARG:HG3	1.82	0.62
29:c:298:GLN:HE22	30:d:246:VAL:HB	1.64	0.62
25:Y:312:ARG:HG3	25:Y:313:SER:H	1.65	0.61
28:b:164:ASP:N	28:b:165:GLY:HA2	2.14	0.61
2:B:107:MET:HG3	3:C:96:VAL:HG13	1.82	0.61
5:E:178:THR:HG22	5:E:339:ASN:HB3	1.82	0.61
6:F:303:ASP:O	6:F:307:GLN:N	2.33	0.61
28:b:34:ASN:O	28:b:38:HIS:ND1	2.25	0.61
29:c:263:ASP:OD1	29:c:283:HIS:ND1	2.32	0.61
31:e:1:MET:H3	31:e:2:SER:HA	1.65	0.61
1:A:111:TYR:HE2	1:A:125:LEU:HD23	1.64	0.61
4:D:151:ILE:CB	4:D:152:MET:HA	2.29	0.61
10:J:88:ARG:HH22	17:Q:69:MET:HB2	1.66	0.61
17:Q:13:VAL:HB	17:Q:183:ILE:HB	1.81	0.61
17:Q:45:LEU:HB3	17:Q:102:LEU:HD13	1.83	0.61
21:U:792:ASN:HA	21:U:914:LEU:HB3	1.81	0.61
25:Y:112:CYS:SG	25:Y:120:ALA:N	2.73	0.61
6:F:229:PRO:HB3	33:F:501:ADP:H5'1	1.82	0.61
19:S:57:PHE:HD2	19:S:60:ASP:H	1.49	0.61
22:V:262:SER:HB3	30:d:121:ARG:HA	1.82	0.61
26:Z:191:ILE:HG22	29:c:226:MET:HE1	1.83	0.61
27:a:315:LEU:HD23	27:a:320:VAL:HG13	1.82	0.61
1:A:191:VAL:HG13	1:A:192:GLU:H	1.66	0.61
21:U:429:LYS:HA	21:U:430:ASP:HB3	1.82	0.61
25:Y:323:PHE:HD2	25:Y:326:GLY:HA3	1.66	0.61
26:Z:7:GLN:OE1	26:Z:46:LYS:NZ	2.32	0.61
4:D:247:VAL:HA	4:D:250:VAL:HB	1.82	0.61
8:H:75:VAL:HG23	8:H:135:LEU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:12:LEU:HD22	21:U:20:LYS:HG3	1.80	0.61
22:V:224:LEU:O	22:V:227:VAL:N	2.29	0.61
26:Z:235:ASN:HD22	27:a:341:LEU:HD11	1.64	0.61
29:c:159:ALA:HB1	29:c:203:ILE:HG22	1.80	0.61
3:C:192:PRO:HG3	3:C:296:ASN:HD21	1.64	0.61
3:C:236:VAL:HG22	3:C:239:ARG:HH12	1.64	0.61
3:C:271:ARG:HD3	3:C:274:LEU:HB2	1.81	0.61
6:F:233:LYS:O	6:F:237:ALA:N	2.29	0.61
21:U:388:ASP:OD1	21:U:389:ASN:ND2	2.34	0.61
25:Y:357:ASN:HB2	25:Y:358:ARG:HA	1.82	0.61
26:Z:124:ILE:HA	26:Z:135:THR:HA	1.83	0.61
32:f:673:THR:O	32:f:677:GLU:N	2.31	0.61
4:D:212:LYS:HE3	4:D:310:ALA:HB1	1.83	0.61
6:F:366:MET:O	6:F:370:SER:N	2.29	0.61
21:U:789:ILE:HB	21:U:911:ILE:HA	1.83	0.61
26:Z:72:HIS:ND1	28:b:63:THR:OG1	2.31	0.61
26:Z:148:GLY:HA3	27:a:178:ARG:HA	1.82	0.61
32:f:383:ILE:HG21	32:f:414:ILE:HD11	1.82	0.61
2:B:346:ARG:NH1	2:B:348:ASP:OD2	2.33	0.61
3:C:67:GLN:HB2	4:D:135:HIS:HB3	1.82	0.61
4:D:207:PRO:HB3	4:D:210:CYS:HA	1.83	0.61
5:E:178:THR:OG1	33:E:401:ADP:O5'	2.18	0.61
6:F:284:PHE:HD1	6:F:329:ILE:HB	1.64	0.61
13:M:141:SER:HB3	13:M:144:ASP:HB2	1.83	0.61
23:W:416:GLN:HB3	23:W:417:ARG:CA	2.29	0.61
29:c:242:GLU:HA	29:c:245:VAL:HB	1.83	0.61
1:A:305:GLN:O	1:A:312:ARG:NE	2.33	0.61
1:A:386:ARG:NH2	33:A:501:ADP:O2'	2.34	0.61
11:K:225:ASN:HB2	11:K:226:PHE:CG	2.36	0.61
27:a:35:HIS:CE1	28:b:17:ARG:HB2	2.36	0.61
5:E:60:VAL:HA	5:E:71:VAL:HG12	1.82	0.60
26:Z:69:PHE:HE1	28:b:60:VAL:H	1.49	0.60
1:A:313:GLY:C	1:A:315:ILE:H	2.08	0.60
4:D:87:LEU:HD11	4:D:133:HIS:HA	1.82	0.60
11:K:199:LEU:HD13	11:K:241:ILE:HD12	1.83	0.60
30:d:254:GLU:HA	30:d:257:VAL:HG23	1.83	0.60
1:A:232:ARG:HE	1:A:235:ALA:H	1.47	0.60
6:F:388:THR:HG22	6:F:391:PHE:HD2	1.65	0.60
11:K:94:VAL:O	11:K:98:ASN:ND2	2.32	0.60
21:U:252:LEU:HD21	21:U:264:VAL:HG11	1.82	0.60
27:a:19:PRO:HA	27:a:22:TRP:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:458:SER:HB2	32:f:461:PHE:HA	1.83	0.60
5:E:229:ILE:HG23	5:E:274:LYS:HB3	1.82	0.60
30:d:198:LEU:HD22	30:d:205:LYS:HE3	1.81	0.60
1:A:299:MET:HE2	1:A:300:LEU:HG	1.83	0.60
5:E:241:ARG:O	5:E:242:ARG:HG2	2.02	0.60
20:T:1:THR:HG22	20:T:3:ASN:H	1.67	0.60
21:U:757:MET:HG3	21:U:758:PRO:HD3	1.84	0.60
23:W:390:GLU:HG3	23:W:408:ARG:HH21	1.66	0.60
30:d:151:VAL:O	30:d:155:LYS:N	2.35	0.60
4:D:203:LEU:O	4:D:331:ILE:HB	2.02	0.60
12:L:160:SER:O	12:L:169:ARG:NH2	2.35	0.60
23:W:374:THR:HG23	27:a:327:VAL:HA	1.82	0.60
30:d:82:TYR:HE2	30:d:98:LEU:HD21	1.65	0.60
3:C:85:VAL:N	3:C:97:VAL:O	2.33	0.60
4:D:202:VAL:HB	4:D:308:ILE:HA	1.83	0.60
4:D:261:ILE:HG23	4:D:306:LYS:HB2	1.83	0.60
17:Q:19:ARG:HD2	17:Q:179:SER:HB3	1.83	0.60
21:U:188:MET:HG2	21:U:194:ARG:HD3	1.83	0.60
26:Z:14:LEU:HA	29:c:39:LEU:HD13	1.84	0.60
28:b:51:LEU:HD23	28:b:71:ILE:HG23	1.83	0.60
3:C:76:VAL:O	3:C:111:ASN:N	2.30	0.60
4:D:130:VAL:HA	4:D:142:VAL:HA	1.84	0.60
22:V:195:ILE:N	22:V:196:SER:HB3	2.17	0.60
2:B:173:VAL:HA	3:C:232:ARG:HG2	1.83	0.60
6:F:230:GLY:H	6:F:392:ASN:HB3	1.65	0.60
21:U:221:ILE:HB	21:U:754:HIS:HB2	1.83	0.60
21:U:233:LEU:HD22	21:U:268:LEU:HD21	1.83	0.60
22:V:143:ALA:HB3	22:V:145:LEU:HB3	1.83	0.60
22:V:252:ASN:ND2	22:V:284:GLU:OE2	2.35	0.60
4:D:91:GLN:NE2	4:D:244:PRO:HB2	2.16	0.60
4:D:348:ILE:HG21	4:D:379:CYS:HB3	1.83	0.60
5:E:172:LEU:HB2	5:E:278:ALA:HB2	1.84	0.60
9:I:239:LYS:NZ	9:I:243:GLU:OE2	2.35	0.60
25:Y:308:LEU:HB3	25:Y:356:THR:HG21	1.84	0.60
1:A:365:GLU:HB3	1:A:368:ILE:HG13	1.84	0.59
4:D:181:VAL:O	4:D:306:LYS:NZ	2.32	0.59
5:E:50:LEU:CD1	6:F:138:GLY:HA2	2.30	0.59
7:G:38:THR:HB	7:G:53:GLN:HE22	1.67	0.59
13:M:100:SER:O	20:T:65:GLN:NE2	2.35	0.59
20:T:51:LEU:HD13	20:T:112:ILE:HG12	1.84	0.59
22:V:122:THR:O	22:V:125:ASN:ND2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:279:GLU:HB3	31:e:60:LEU:HD13	1.84	0.59
27:a:215:GLU:CD	27:a:215:GLU:CG	2.75	0.59
28:b:8:VAL:HA	28:b:110:ILE:HG13	1.84	0.59
1:A:303:ILE:HA	1:A:306:LEU:HB2	1.85	0.59
3:C:171:HIS:HB3	3:C:174:LEU:HG	1.84	0.59
27:a:14:SER:HB2	27:a:18:GLN:HG2	1.85	0.59
1:A:327:LEU:O	1:A:331:LEU:N	2.32	0.59
1:A:381:THR:OG1	2:B:343:ARG:NH1	2.35	0.59
4:D:408:LYS:HB3	4:D:409:LYS:HB2	1.83	0.59
6:F:314:LEU:O	6:F:318:ASP:N	2.35	0.59
10:J:120:GLN:OE1	11:K:134:SER:N	2.34	0.59
18:R:91:LYS:NZ	18:R:117:GLU:OE1	2.35	0.59
32:f:398:TRP:HE1	32:f:690:ALA:HB1	1.67	0.59
2:B:224:LEU:HB2	2:B:330:ALA:HB2	1.85	0.59
25:Y:300:ARG:HH22	31:e:56:LEU:HD13	1.68	0.59
28:b:25:ARG:NH2	28:b:145:GLU:OE1	2.29	0.59
29:c:273:LYS:HD2	29:c:277:LYS:HG3	1.85	0.59
32:f:333:SER:O	32:f:334:ASN:ND2	2.35	0.59
11:K:16:SER:OG	11:K:18:GLU:OE1	2.19	0.59
25:Y:12:PRO:O	25:Y:146:ARG:NH1	2.35	0.59
26:Z:242:LEU:O	27:a:288:HIS:N	2.35	0.59
32:f:294:SER:OG	32:f:321:GLY:O	2.20	0.59
3:C:69:GLN:HB2	3:C:118:ASN:HB2	1.84	0.59
4:D:337:ASP:H	4:D:340:GLN:HB2	1.67	0.59
6:F:181:PRO:HG2	6:F:242:ALA:HB2	1.84	0.59
9:I:49:ARG:NH1	9:I:211:VAL:O	2.36	0.59
12:L:204:ASP:HB3	12:L:205:LEU:C	2.28	0.59
20:T:1:THR:N	20:T:105:PRO:O	2.26	0.59
22:V:263:LEU:HD13	30:d:121:ARG:HD3	1.84	0.59
22:V:394:LEU:HD23	30:d:116:HIS:HE1	1.68	0.59
23:W:237:GLU:HG2	23:W:238:GLY:H	1.67	0.59
26:Z:17:LEU:HD12	29:c:217:LEU:HD13	1.85	0.59
32:f:673:THR:O	32:f:677:GLU:HG2	2.01	0.59
3:C:307:ARG:HE	3:C:312:ASP:HB2	1.66	0.59
5:E:128:GLY:HA2	5:E:129:ASN:HB2	1.85	0.59
17:Q:88:LEU:HD23	17:Q:122:ALA:HA	1.84	0.59
25:Y:170:GLU:N	25:Y:171:GLY:HA3	2.17	0.59
1:A:159:PRO:O	1:A:162:THR:OG1	2.20	0.59
21:U:194:ARG:HH22	21:U:222:PHE:HB3	1.68	0.59
21:U:361:ARG:HG3	21:U:365:CYS:HB2	1.84	0.59
28:b:171:VAL:HG21	28:b:187:PRO:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:PRO:HD2	1:A:313:GLY:HA2	1.83	0.59
3:C:60:ARG:O	3:C:64:GLN:N	2.33	0.59
4:D:171:ASP:HA	4:D:174:LYS:HE2	1.84	0.59
4:D:318:ASP:HB2	4:D:321:LEU:HG	1.85	0.59
30:d:105:PHE:HA	30:d:170:LEU:HD12	1.85	0.59
4:D:237:GLN:HG3	4:D:242:GLU:HB3	1.85	0.58
4:D:410:ASP:HA	4:D:411:GLU:HB2	1.84	0.58
5:E:335:SER:HB3	5:E:338:PHE:CE2	2.37	0.58
6:F:406:ILE:HA	6:F:409:ARG:HG2	1.84	0.58
23:W:373:ILE:HG12	23:W:374:THR:N	2.16	0.58
24:X:379:ASP:N	24:X:384:VAL:O	2.32	0.58
27:a:182:CYS:SG	27:a:183:VAL:N	2.75	0.58
32:f:483:ALA:HB1	32:f:500:LEU:HG	1.85	0.58
3:C:165:ILE:HA	3:C:290:LYS:HE3	1.85	0.58
4:D:153:MET:SD	4:D:257:ASN:ND2	2.76	0.58
5:E:223:ARG:NE	5:E:268:ASP:OD2	2.36	0.58
22:V:275:VAL:H	22:V:276:PHE:HA	1.67	0.58
27:a:286:ALA:HA	27:a:288:HIS:HB2	1.85	0.58
12:L:120:THR:O	13:M:129:ARG:NH1	2.26	0.58
14:N:20:THR:OG1	14:N:33:LYS:NZ	2.34	0.58
29:c:282:ARG:N	29:c:283:HIS:HB2	2.18	0.58
3:C:148:TYR:H	3:C:206:HIS:HE2	1.50	0.58
4:D:89:ILE:HG21	4:D:143:LEU:HD11	1.86	0.58
16:P:123:SER:HB3	16:P:137:VAL:HB	1.86	0.58
23:W:423:ASN:HA	26:Z:251:LEU:HD21	1.85	0.58
27:a:125:ILE:N	27:a:126:GLY:HA2	2.19	0.58
32:f:615:GLY:HA2	32:f:619:LEU:N	2.18	0.58
3:C:202:ALA:O	3:C:206:HIS:N	2.30	0.58
4:D:284:GLU:HA	4:D:287:ARG:HB2	1.85	0.58
6:F:195:ILE:HG13	6:F:198:LEU:HD23	1.86	0.58
6:F:320:PHE:HB3	6:F:322:PRO:HD2	1.84	0.58
8:H:67:PRO:O	8:H:91:ARG:NH2	2.36	0.58
21:U:599:ILE:O	21:U:603:LEU:HB3	2.03	0.58
23:W:436:MET:O	23:W:440:ASN:ND2	2.26	0.58
2:B:220:LYS:HB2	2:B:346:ARG:HH21	1.69	0.58
2:B:404:LEU:O	2:B:408:ARG:N	2.32	0.58
3:C:67:GLN:HA	4:D:136:SER:HA	1.85	0.58
3:C:338:LEU:HD13	3:C:383:PHE:HE2	1.68	0.58
9:I:180:LYS:HB2	9:I:183:GLU:HG2	1.85	0.58
18:R:97:MET:H	18:R:116:SER:HB3	1.69	0.58
2:B:120:HIS:HB3	2:B:132:TYR:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:159:TRP:HB3	10:J:54:GLN:HG3	1.85	0.58
21:U:792:ASN:OD1	21:U:793:LYS:N	2.36	0.58
25:Y:108:ALA:O	25:Y:112:CYS:N	2.35	0.58
28:b:91:ARG:NH1	28:b:134:GLU:OE1	2.35	0.58
30:d:122:LEU:HD11	30:d:125:LYS:HG2	1.84	0.58
30:d:246:VAL:HA	30:d:249:TYR:HB3	1.84	0.58
5:E:200:SER:O	6:F:308:ARG:NH1	2.36	0.58
5:E:316:HIS:CE1	5:E:344:ARG:HB2	2.39	0.58
7:G:147:GLN:HB2	7:G:150:GLN:HE21	1.67	0.58
21:U:649:ARG:HB3	21:U:675:MET:HE1	1.86	0.58
24:X:420:LYS:HD3	25:Y:387:ILE:HG21	1.86	0.58
29:c:161:ARG:NH1	29:c:162:LEU:O	2.37	0.58
31:e:63:HIS:HA	31:e:66:LYS:HE2	1.84	0.58
3:C:214:VAL:HG12	3:C:249:ASP:H	1.68	0.58
3:C:270:GLN:HB3	3:C:306:LEU:HD21	1.86	0.58
5:E:197:LYS:NZ	5:E:198:VAL:O	2.37	0.58
30:d:114:GLU:HA	30:d:117:THR:HG22	1.85	0.58
1:A:102:ILE:HA	1:A:113:ILE:HA	1.86	0.57
1:A:119:ALA:HB1	1:A:121:PHE:HE2	1.70	0.57
1:A:303:ILE:O	1:A:307:ASP:N	2.34	0.57
1:A:390:THR:HA	2:B:216:ILE:HG21	1.86	0.57
4:D:183:LEU:HA	4:D:186:THR:HG22	1.85	0.57
13:M:192:GLU:HA	13:M:195:LYS:HE3	1.86	0.57
17:Q:7:ILE:HD13	17:Q:156:ALA:HB1	1.85	0.57
1:A:343:PHE:HB3	1:A:344:SER:C	2.29	0.57
2:B:349:ARG:HE	2:B:351:ILE:HG22	1.68	0.57
4:D:83:GLN:HG2	4:D:84:SER:N	2.19	0.57
7:G:14:THR:HG22	7:G:24:GLN:HB2	1.85	0.57
15:O:1:THR:N	15:O:168:GLY:O	2.36	0.57
21:U:493:VAL:O	21:U:497:LEU:HB2	2.05	0.57
22:V:174:PHE:HA	22:V:177:ASN:HD22	1.68	0.57
32:f:436:VAL:HG22	32:f:679:ARG:HH22	1.69	0.57
2:B:223:ILE:HG13	2:B:346:ARG:HB3	1.86	0.57
4:D:201:GLY:HA3	4:D:328:ASP:H	1.69	0.57
17:Q:52:ASP:OD1	18:R:88:TYR:OH	2.21	0.57
18:R:3:THR:O	18:R:127:SER:OG	2.21	0.57
21:U:576:PRO:HA	21:U:579:ARG:HE	1.68	0.57
32:f:106:ALA:HB1	32:f:107:LEU:HA	1.86	0.57
32:f:392:LYS:O	32:f:433:ASN:ND2	2.37	0.57
1:A:333:ARG:HH22	1:A:340:LYS:HD3	1.69	0.57
1:A:406:GLU:HA	1:A:409:PHE:CE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:ARG:HB3	3:C:264:GLY:H	1.70	0.57
5:E:149:ILE:HG23	5:E:274:LYS:HG2	1.87	0.57
8:H:128:ARG:HB2	8:H:129:PRO:HD2	1.85	0.57
12:L:117:GLN:NE2	13:M:83:ASP:OD1	2.37	0.57
15:O:17:ASP:O	15:O:33:LYS:NZ	2.31	0.57
22:V:480:ILE:HG23	26:Z:271:ALA:HB2	1.84	0.57
26:Z:16:LEU:HD21	29:c:216:MET:HE2	1.86	0.57
30:d:30:LEU:HA	30:d:34:ASN:HA	1.86	0.57
30:d:215:TRP:CD1	30:d:216:VAL:H	2.21	0.57
32:f:600:LEU:HD13	32:f:600:LEU:H	1.68	0.57
3:C:67:GLN:CB	4:D:135:HIS:HB3	2.35	0.57
3:C:299:ASP:O	3:C:303:SER:N	2.36	0.57
6:F:185:TYR:HE2	6:F:243:GLN:HG3	1.68	0.57
21:U:14:GLU:O	21:U:20:LYS:NZ	2.26	0.57
26:Z:101:LEU:HD23	26:Z:123:ILE:HD11	1.86	0.57
27:a:244:ASN:HB2	27:a:272:ILE:HB	1.87	0.57
1:A:206:ILE:H	6:F:373:MET:HE3	1.69	0.57
1:A:223:THR:O	1:A:227:ARG:N	2.30	0.57
4:D:115:ILE:HA	4:D:139:LEU:HB2	1.85	0.57
4:D:283:ARG:HA	4:D:286:GLN:HG2	1.87	0.57
9:I:136:TYR:HB2	9:I:148:TYR:HB2	1.87	0.57
11:K:90:ASP:HA	11:K:93:ARG:HD2	1.85	0.57
21:U:17:PRO:HA	21:U:20:LYS:HD3	1.86	0.57
27:a:327:VAL:HG13	27:a:328:ASP:H	1.69	0.57
1:A:383:ALA:HB3	2:B:343:ARG:HE	1.68	0.57
22:V:331:LEU:HD12	22:V:334:VAL:HG21	1.85	0.57
23:W:268:LYS:HE2	23:W:301:LYS:HE2	1.87	0.57
1:A:246:VAL:HG21	2:B:307:ARG:HD2	1.87	0.57
2:B:119:ASN:O	2:B:134:SER:OG	2.19	0.57
2:B:269:GLU:HA	2:B:272:ARG:HG2	1.87	0.57
5:E:345:ASN:HB3	6:F:345:SER:HB2	1.87	0.57
17:Q:29:LYS:HE2	18:R:121:ILE:HB	1.87	0.57
22:V:441:ALA:HB1	22:V:446:VAL:HB	1.85	0.57
2:B:286:GLU:HA	2:B:331:THR:HA	1.87	0.57
5:E:151:LEU:HD11	5:E:158:LEU:HD12	1.87	0.57
6:F:301:ALA:HB3	6:F:304:ARG:HB2	1.87	0.57
25:Y:78:GLU:O	25:Y:82:LYS:N	2.33	0.57
32:f:397:ARG:HG2	32:f:433:ASN:HA	1.85	0.57
1:A:358:HIS:HE1	1:A:386:ARG:HA	1.69	0.57
3:C:99:VAL:HG13	3:C:100:ASP:C	2.30	0.57
11:K:101:PHE:O	18:R:57:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:10:VAL:HG13	12:L:19:ILE:HG21	1.86	0.57
17:Q:20:VAL:HG21	17:Q:175:LEU:HA	1.87	0.57
21:U:26:LYS:HG2	30:d:36:LEU:HG	1.87	0.57
22:V:419:LEU:HD22	22:V:431:PRO:HA	1.87	0.57
29:c:168:MET:HA	29:c:172:HIS:HE1	1.70	0.57
4:D:282:ASP:HA	4:D:285:VAL:HG22	1.87	0.56
5:E:385:ASP:OD1	6:F:340:PRO:HB2	2.04	0.56
10:J:201:SER:HB3	10:J:202:GLY:CA	2.35	0.56
21:U:203:LYS:O	21:U:207:ASN:ND2	2.38	0.56
21:U:908:ILE:HG12	21:U:909:GLY:H	1.70	0.56
22:V:227:VAL:HA	22:V:230:PHE:HB3	1.87	0.56
22:V:287:ARG:HB2	31:e:5:LYS:HD3	1.87	0.56
32:f:401:LEU:HD23	32:f:672:VAL:HG12	1.86	0.56
3:C:336:MET:HA	4:D:195:GLY:HA3	1.86	0.56
4:D:146:GLU:HG2	4:D:148:ASP:H	1.70	0.56
15:O:161:ALA:O	15:O:165:ASN:ND2	2.34	0.56
21:U:185:MET:HE3	21:U:628:ARG:HH12	1.70	0.56
25:Y:182:VAL:HA	25:Y:201:PHE:HE1	1.70	0.56
32:f:283:SER:OG	32:f:643:SER:OG	2.23	0.56
2:B:139:VAL:HA	2:B:140:ASP:HB3	1.87	0.56
2:B:182:GLU:HB2	2:B:239:VAL:HG11	1.86	0.56
3:C:132:ASP:O	3:C:136:SER:N	2.29	0.56
4:D:411:GLU:HA	4:D:412:GLN:HB2	1.87	0.56
5:E:169:GLY:N	5:E:296:ASP:OD2	2.39	0.56
5:E:187:VAL:HA	5:E:190:GLN:HB3	1.88	0.56
5:E:313:LEU:O	5:E:317:ALA:N	2.31	0.56
6:F:190:GLY:HA3	6:F:361:ALA:HB2	1.86	0.56
6:F:384:LEU:O	6:F:388:THR:N	2.38	0.56
8:H:119:GLN:NE2	8:H:152:SER:O	2.37	0.56
8:H:150:ASP:OD1	8:H:154:ALA:N	2.38	0.56
15:O:6:VAL:HG23	15:O:124:TYR:HB3	1.88	0.56
20:T:112:ILE:O	20:T:123:GLY:N	2.34	0.56
21:U:198:LEU:HD21	21:U:219:CYS:HA	1.86	0.56
21:U:494:TYR:OH	21:U:531:ASP:OD2	2.24	0.56
22:V:173:ILE:O	22:V:177:ASN:ND2	2.38	0.56
26:Z:228:TYR:CD2	27:a:215:GLU:OE2	2.58	0.56
28:b:17:ARG:HG2	28:b:80:PRO:HG2	1.86	0.56
30:d:142:TYR:O	30:d:147:SER:N	2.38	0.56
32:f:6:GLU:HG2	32:f:8:ALA:H	1.70	0.56
5:E:305:ASN:O	5:E:309:ARG:N	2.33	0.56
15:O:177:VAL:HB	15:O:184:ASP:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:108:SER:HB2	30:d:170:LEU:HD11	1.87	0.56
32:f:255:LEU:HD23	32:f:258:ILE:HD11	1.86	0.56
32:f:335:ARG:N	32:f:336:GLU:OE1	2.30	0.56
3:C:340:ARG:HH11	25:Y:97:GLU:HB2	1.71	0.56
5:E:247:THR:OG1	5:E:248:SER:N	2.39	0.56
6:F:365:ILE:HG13	6:F:366:MET:H	1.70	0.56
11:K:43:SER:HA	11:K:151:PRO:HG3	1.86	0.56
11:K:199:LEU:HA	11:K:202:LEU:HB2	1.86	0.56
22:V:212:TYR:HE1	22:V:256:ARG:HE	1.52	0.56
25:Y:141:VAL:HG21	25:Y:164:ALA:HB2	1.88	0.56
1:A:170:PRO:HA	1:A:229:VAL:HG12	1.87	0.56
2:B:133:VAL:HG13	2:B:135:ILE:HG23	1.86	0.56
4:D:405:THR:O	5:E:298:LYS:NZ	2.37	0.56
6:F:249:LEU:HD12	6:F:283:ILE:HD11	1.88	0.56
7:G:78:CYS:SG	7:G:79:VAL:N	2.78	0.56
24:X:351:SER:HA	24:X:354:ILE:HG22	1.88	0.56
3:C:43:ARG:HG2	21:U:639:LEU:HD22	1.86	0.56
4:D:243:GLY:O	4:D:247:VAL:N	2.31	0.56
4:D:285:VAL:HA	4:D:288:ILE:HD12	1.86	0.56
21:U:554:LEU:HG	21:U:588:MET:HE1	1.86	0.56
23:W:237:GLU:HG2	23:W:238:GLY:N	2.20	0.56
26:Z:241:SER:HB2	26:Z:242:LEU:HA	1.88	0.56
2:B:96:ARG:HH22	3:C:82:LYS:HB2	1.70	0.56
5:E:61:LEU:HD11	5:E:72:LYS:HB2	1.88	0.56
17:Q:59:TYR:O	17:Q:63:ASN:ND2	2.29	0.56
19:S:64:LEU:HD21	19:S:92:LEU:HD11	1.88	0.56
19:S:68:ILE:HD11	19:S:92:LEU:HD13	1.87	0.56
32:f:662:LEU:H	32:f:664:ALA:HA	1.70	0.56
3:C:212:ILE:N	3:C:245:ILE:O	2.35	0.56
4:D:96:VAL:HG22	4:D:101:ALA:HA	1.87	0.56
16:P:58:THR:O	17:Q:85:ARG:NH2	2.39	0.56
26:Z:228:TYR:CZ	27:a:215:GLU:CB	2.89	0.56
27:a:188:LEU:HD11	27:a:193:GLN:HG3	1.86	0.56
29:c:232:GLN:O	29:c:236:GLU:N	2.36	0.56
3:C:266:ASP:O	3:C:270:GLN:N	2.27	0.56
7:G:71:LYS:O	7:G:95:ARG:NH2	2.39	0.56
9:I:69:ASN:OD1	9:I:70:GLU:N	2.38	0.56
9:I:91:ARG:HD3	16:P:76:LEU:HB3	1.87	0.56
20:T:45:VAL:HG11	20:T:71:VAL:HG21	1.88	0.56
30:d:225:PHE:HB3	30:d:226:ALA:HB2	1.86	0.56
31:e:1:MET:N	31:e:2:SER:HA	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:181:MET:HE1	32:f:511:MET:HE1	1.88	0.56
3:C:297:ARG:HG3	3:C:298:ILE:H	1.72	0.55
5:E:221:TYR:HA	5:E:224:ASP:HB3	1.87	0.55
21:U:583:MET:HE1	21:U:602:LEU:HA	1.87	0.55
25:Y:102:ASP:HA	25:Y:105:MET:HG2	1.88	0.55
26:Z:201:LEU:HD21	27:a:360:VAL:HB	1.88	0.55
1:A:162:THR:O	1:A:166:VAL:N	2.28	0.55
6:F:176:GLU:HB2	6:F:250:LYS:HB2	1.88	0.55
10:J:132:LEU:HG	10:J:146:GLN:HA	1.88	0.55
14:N:45:ARG:HB2	14:N:52:THR:HG21	1.88	0.55
23:W:273:TYR:HA	23:W:276:LEU:HD13	1.87	0.55
26:Z:219:LYS:HG3	26:Z:220:LEU:HD23	1.88	0.55
28:b:117:VAL:HG22	28:b:119:ASP:H	1.71	0.55
1:A:73:ALA:O	1:A:77:LEU:N	2.36	0.55
3:C:350:LEU:HD23	3:C:387:VAL:HG11	1.88	0.55
4:D:287:ARG:HA	4:D:290:LEU:HB3	1.88	0.55
13:M:12:SER:OG	13:M:124:LEU:O	2.20	0.55
27:a:212:ASN:HD21	27:a:339:ARG:HG3	1.70	0.55
3:C:135:VAL:HG22	3:C:223:PHE:HE2	1.72	0.55
6:F:283:ILE:HG22	6:F:328:VAL:HG13	1.87	0.55
6:F:430:LYS:NZ	11:K:17:PRO:HB2	2.22	0.55
8:H:128:ARG:HG3	8:H:130:PHE:H	1.71	0.55
10:J:34:GLY:HA2	10:J:43:LEU:HA	1.87	0.55
10:J:157:LYS:N	11:K:58:LEU:O	2.39	0.55
12:L:166:GLN:OE1	12:L:169:ARG:NH1	2.39	0.55
21:U:225:ASP:OD1	21:U:225:ASP:N	2.39	0.55
22:V:56:ALA:O	22:V:59:ALA:HB3	2.07	0.55
24:X:346:GLN:HE21	24:X:349:HIS:HB2	1.71	0.55
1:A:324:PRO:HD3	1:A:432:TYR:HB2	1.89	0.55
2:B:106:PRO:HG2	2:B:154:HIS:CD2	2.41	0.55
3:C:115:ALA:HB3	3:C:125:LYS:H	1.71	0.55
11:K:154:PHE:HB3	11:K:162:PHE:HE1	1.72	0.55
23:W:436:MET:HE3	29:c:239:LYS:HD3	1.87	0.55
1:A:232:ARG:NE	1:A:235:ALA:O	2.39	0.55
3:C:376:VAL:HG13	3:C:377:HIS:H	1.71	0.55
5:E:241:ARG:HD3	6:F:298:SER:HB2	1.88	0.55
6:F:91:SER:OG	6:F:125:LYS:O	2.17	0.55
6:F:208:HIS:HB3	6:F:211:LYS:HD3	1.89	0.55
6:F:376:SER:O	6:F:378:ASP:N	2.39	0.55
11:K:182:GLN:NE2	12:L:55:GLU:OE1	2.39	0.55
12:L:97:PHE:O	19:S:66:LYS:NZ	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:18:THR:HB	15:O:31:CYS:H	1.72	0.55
22:V:100:MET:HG2	22:V:102:PRO:HD2	1.88	0.55
22:V:394:LEU:HA	22:V:397:ARG:HG2	1.89	0.55
26:Z:72:HIS:HD1	28:b:63:THR:HG1	1.53	0.55
2:B:113:GLU:HB3	2:B:123:VAL:HA	1.89	0.55
2:B:133:VAL:HG21	2:B:159:VAL:H	1.71	0.55
3:C:35:VAL:HA	3:C:38:LYS:HD3	1.89	0.55
4:D:341:LYS:O	4:D:345:PHE:N	2.32	0.55
6:F:130:GLN:OE1	6:F:132:TYR:OH	2.17	0.55
22:V:54:LYS:N	22:V:55:THR:OG1	2.39	0.55
22:V:79:VAL:HG13	22:V:80:LYS:H	1.72	0.55
22:V:210:CYS:HA	22:V:213:TYR:HB2	1.87	0.55
23:W:420:ASP:CG	23:W:421:PRO:HD2	2.31	0.55
2:B:383:LEU:HB3	2:B:387:LYS:HZ1	1.72	0.55
3:C:247:PHE:HD1	3:C:292:ILE:HB	1.72	0.55
4:D:204:MET:HE3	4:D:310:ALA:HB2	1.89	0.55
9:I:28:ILE:HG21	9:I:133:SER:HB2	1.87	0.55
9:I:218:ARG:NH1	9:I:223:THR:OG1	2.39	0.55
19:S:114:ASP:OD1	19:S:118:LYS:N	2.39	0.55
1:A:239:ARG:HD3	2:B:319:PHE:HD2	1.71	0.55
1:A:373:LEU:HD22	1:A:409:PHE:HE1	1.72	0.55
4:D:133:HIS:HE1	4:D:135:HIS:HB2	1.72	0.55
7:G:47:CYS:HB3	7:G:221:THR:HG23	1.89	0.55
11:K:11:GLY:C	11:K:13:ASN:H	2.14	0.55
12:L:171:TYR:O	12:L:175:HIS:ND1	2.40	0.55
1:A:143:ASP:H	1:A:148:GLN:HG2	1.72	0.55
5:E:312:ILE:HD12	5:E:315:ILE:HD11	1.89	0.55
17:Q:29:LYS:HD3	18:R:121:ILE:HD12	1.88	0.55
21:U:161:ASP:OD1	21:U:162:VAL:N	2.35	0.55
22:V:80:LYS:HA	22:V:81:GLN:HB2	1.88	0.55
30:d:35:PHE:HD2	30:d:36:LEU:HD23	1.71	0.55
30:d:215:TRP:CG	30:d:216:VAL:H	2.25	0.55
1:A:355:PHE:HE1	1:A:385:ILE:HB	1.72	0.54
2:B:177:GLU:H	2:B:178:LYS:HA	1.72	0.54
2:B:374:LEU:HB2	2:B:378:VAL:HB	1.89	0.54
4:D:391:ARG:NE	4:D:393:ILE:O	2.35	0.54
8:H:7:SER:HA	8:H:125:GLY:HA3	1.88	0.54
12:L:50:LYS:HB3	12:L:59:HIS:HB3	1.89	0.54
22:V:320:THR:HG23	22:V:321:ALA:HB2	1.89	0.54
23:W:429:SER:O	23:W:433:ASN:HB2	2.07	0.54
29:c:98:MET:O	29:c:102:THR:OG1	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:LEU:HD22	2:B:341:LEU:HD23	1.89	0.54
7:G:141:ILE:HD13	7:G:220:VAL:HG11	1.90	0.54
13:M:8:ASP:HB2	13:M:21:PHE:HB2	1.88	0.54
17:Q:141:SER:O	17:Q:145:ARG:HB3	2.07	0.54
26:Z:229:GLN:N	27:a:215:GLU:OE2	2.38	0.54
29:c:131:GLN:HA	29:c:134:GLU:HG2	1.87	0.54
29:c:157:ILE:HG12	29:c:158:ASP:H	1.72	0.54
32:f:559:ASP:HB3	32:f:562:VAL:HG22	1.87	0.54
1:A:122:VAL:N	6:F:88:TYR:O	2.29	0.54
9:I:44:LEU:HA	9:I:215:THR:HA	1.89	0.54
11:K:215:ILE:HD12	11:K:234:LEU:HD11	1.88	0.54
27:a:28:LEU:HG	27:a:33:LEU:HD11	1.89	0.54
2:B:303:ARG:HA	2:B:306:GLN:HB3	1.90	0.54
4:D:268:ASP:OD1	4:D:268:ASP:N	2.41	0.54
5:E:90:SER:O	5:E:93:LYS:NZ	2.36	0.54
14:N:16:ALA:HB1	14:N:33:LYS:HB2	1.88	0.54
17:Q:38:MET:HE3	17:Q:61:GLN:HA	1.90	0.54
23:W:373:ILE:HG23	23:W:413:ILE:HG13	1.88	0.54
26:Z:228:TYR:CE1	27:a:215:GLU:OE1	2.57	0.54
32:f:82:PRO:O	32:f:86:ASN:ND2	2.40	0.54
2:B:251:VAL:HG11	3:C:271:ARG:HD2	1.89	0.54
2:B:268:ARG:HA	2:B:315:GLN:HE22	1.73	0.54
3:C:373:GLU:HG2	3:C:375:ARG:NH1	2.22	0.54
5:E:212:ALA:HB2	5:E:256:THR:HA	1.88	0.54
5:E:356:ARG:NH2	6:F:197:GLU:OE1	2.40	0.54
7:G:127:GLN:HE22	8:H:130:PHE:HZ	1.56	0.54
8:H:66:GLU:HG3	8:H:91:ARG:HH22	1.71	0.54
8:H:139:TRP:HA	8:H:144:PRO:HA	1.89	0.54
3:C:375:ARG:HH21	3:C:378:VAL:HG13	1.72	0.54
5:E:81:VAL:HG11	5:E:105:LEU:HB2	1.88	0.54
5:E:281:ARG:HH22	6:F:296:PHE:HD1	1.55	0.54
7:G:215:ILE:HD11	7:G:235:ILE:HG21	1.87	0.54
13:M:26:ALA:HB1	13:M:132:GLY:HA2	1.90	0.54
22:V:349:ARG:HB3	22:V:354:LYS:HB2	1.88	0.54
30:d:93:ALA:O	30:d:97:GLN:NE2	2.41	0.54
2:B:255:LEU:HD11	2:B:267:VAL:HG23	1.88	0.54
3:C:68:GLU:HG3	29:c:190:GLN:HG3	1.90	0.54
4:D:208:PRO:HD2	5:E:287:PRO:HB2	1.90	0.54
4:D:353:ASN:HB3	4:D:393:ILE:HG12	1.89	0.54
7:G:16:PHE:HB3	7:G:20:GLY:HA2	1.90	0.54
13:M:189:ILE:HA	13:M:192:GLU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:2:THR:HA	18:R:129:GLY:HA3	1.88	0.54
22:V:254:LEU:O	22:V:258:TYR:HB2	2.08	0.54
25:Y:191:ILE:HG13	25:Y:192:ARG:H	1.72	0.54
25:Y:377:LEU:HA	25:Y:380:VAL:HG22	1.90	0.54
2:B:166:ASP:N	2:B:166:ASP:OD1	2.40	0.54
2:B:249:ARG:HB3	3:C:283:PHE:HE2	1.72	0.54
2:B:313:LEU:O	2:B:317:ASP:N	2.40	0.54
3:C:267:SER:O	3:C:271:ARG:N	2.36	0.54
5:E:44:GLU:HB3	6:F:76:ASN:HD22	1.73	0.54
22:V:149:PRO:HG2	22:V:199:ASN:HB3	1.88	0.54
22:V:235:LEU:HD11	22:V:247:GLN:HG3	1.90	0.54
22:V:349:ARG:NH2	22:V:358:MET:SD	2.81	0.54
25:Y:356:THR:HA	25:Y:357:ASN:CG	2.32	0.54
26:Z:228:TYR:HB2	27:a:340:VAL:HA	1.89	0.54
29:c:27:THR:HB	29:c:65:TYR:HB3	1.90	0.54
29:c:243:SER:N	29:c:245:VAL:H	2.05	0.54
3:C:248:MET:HE1	3:C:272:THR:HB	1.89	0.54
3:C:257:SER:C	3:C:259:LEU:H	2.16	0.54
4:D:323:ARG:HE	4:D:326:ARG:NE	2.04	0.54
21:U:8:ILE:HD11	21:U:27:LEU:HG	1.90	0.54
22:V:455:LYS:N	22:V:456:GLY:HA2	2.22	0.54
26:Z:182:THR:N	26:Z:183:THR:HA	2.22	0.54
30:d:45:LYS:HG2	30:d:48:LEU:HD12	1.89	0.54
4:D:60:TYR:CG	21:U:603:LEU:HD11	2.42	0.54
4:D:92:PHE:HA	4:D:103:VAL:HG23	1.88	0.54
5:E:235:ILE:HG23	5:E:285:LEU:HD21	1.90	0.54
6:F:234:THR:HB	33:F:501:ADP:H3'	1.88	0.54
17:Q:29:LYS:HE3	17:Q:32:HIS:HB2	1.90	0.54
21:U:429:LYS:HB3	21:U:431:THR:HG23	1.89	0.54
22:V:81:GLN:HB3	22:V:83:GLU:N	2.22	0.54
22:V:399:ARG:HG2	30:d:141:GLN:HE22	1.73	0.54
23:W:412:ILE:HG22	24:X:344:ARG:HH22	1.73	0.54
25:Y:190:ALA:HA	25:Y:287:LEU:HD13	1.90	0.54
2:B:264:PRO:O	2:B:267:VAL:N	2.36	0.53
3:C:388:ALA:O	3:C:392:GLN:HG2	2.08	0.53
4:D:200:ARG:NH2	4:D:325:GLY:O	2.35	0.53
4:D:389:GLU:HB3	4:D:390:ASN:C	2.32	0.53
21:U:772:TRP:HB3	21:U:775:LEU:HG	1.88	0.53
22:V:357:LEU:O	22:V:360:TYR:N	2.41	0.53
27:a:135:ILE:HG12	27:a:158:LEU:HD13	1.90	0.53
29:c:278:GLN:N	29:c:279:ASP:HB2	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:225:ALA:HB1	4:D:260:ALA:HA	1.90	0.53
14:N:32:ASP:O	14:N:45:ARG:NH1	2.41	0.53
14:N:175:ARG:HG2	14:N:188:VAL:HG13	1.90	0.53
21:U:109:THR:OG1	21:U:156:GLU:O	2.18	0.53
22:V:195:ILE:HG13	22:V:196:SER:HB3	1.90	0.53
22:V:200:ARG:HH11	22:V:242:HIS:CE1	2.26	0.53
23:W:438:LEU:HD21	26:Z:237:LEU:HD21	1.89	0.53
1:A:420:TYR:HA	1:A:423:PHE:CE2	2.43	0.53
33:D:501:ADP:H1'	5:E:291:ARG:CZ	2.38	0.53
5:E:322:LYS:HD2	5:E:367:PHE:HE2	1.74	0.53
11:K:61:PRO:HB3	11:K:213:THR:HG22	1.90	0.53
17:Q:182:ILE:HG23	17:Q:189:HIS:HB2	1.91	0.53
21:U:403:THR:HG23	21:U:777:HIS:HE2	1.73	0.53
9:I:137:ILE:HG22	9:I:147:LEU:HD22	1.90	0.53
11:K:227:HIS:HA	11:K:228:MET:C	2.33	0.53
13:M:228:PRO:HB2	13:M:231:ILE:HB	1.90	0.53
19:S:38:ARG:HH22	20:T:151:ARG:HD3	1.74	0.53
23:W:274:VAL:O	23:W:283:GLN:NE2	2.41	0.53
25:Y:229:ILE:HG23	25:Y:298:GLU:HG2	1.90	0.53
27:a:71:VAL:HG22	28:b:17:ARG:HH12	1.74	0.53
29:c:111:TRP:NE1	29:c:130:GLN:OE1	2.29	0.53
29:c:209:LYS:HA	29:c:210:ASN:HB2	1.91	0.53
3:C:277:LEU:HD13	3:C:311:ILE:HG13	1.90	0.53
4:D:293:LEU:O	4:D:326:ARG:NH2	2.42	0.53
5:E:207:TYR:OH	6:F:129:ARG:NH1	2.41	0.53
6:F:380:ASN:C	6:F:382:GLU:H	2.16	0.53
22:V:59:ALA:N	22:V:60:ALA:HB3	2.24	0.53
22:V:419:LEU:HD21	22:V:456:GLY:H	1.73	0.53
32:f:520:LEU:HB3	32:f:531:VAL:HG11	1.91	0.53
3:C:276:LEU:O	3:C:280:LEU:N	2.42	0.53
3:C:286:THR:HG23	3:C:287:LYS:H	1.74	0.53
3:C:295:THR:HG21	3:C:299:ASP:HB2	1.90	0.53
6:F:195:ILE:HG12	6:F:199:VAL:HG23	1.90	0.53
6:F:359:GLU:HB2	6:F:385:ALA:HB1	1.91	0.53
9:I:72:MET:HG2	9:I:138:GLY:HA3	1.89	0.53
13:M:54:LEU:H	13:M:57:LEU:HD11	1.72	0.53
16:P:13:ALA:HA	16:P:22:ILE:HA	1.90	0.53
21:U:645:ASN:HD21	21:U:648:VAL:HG23	1.73	0.53
23:W:343:SER:HB2	23:W:346:GLU:HB3	1.91	0.53
24:X:404:ILE:HG12	25:Y:372:LYS:HE2	1.91	0.53
32:f:65:ASN:ND2	32:f:115:ASP:OD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:310:TYR:HE2	32:f:318:MET:HG2	1.73	0.53
32:f:564:TYR:O	32:f:568:PHE:HB2	2.08	0.53
6:F:311:LEU:O	6:F:315:ASN:N	2.32	0.53
6:F:312:GLU:O	6:F:316:GLN:N	2.38	0.53
7:G:43:ARG:HA	7:G:48:ALA:HA	1.91	0.53
21:U:896:GLU:O	21:U:901:GLN:NE2	2.42	0.53
21:U:904:LYS:H	21:U:913:ILE:HD11	1.73	0.53
23:W:449:GLU:O	23:W:453:HIS:ND1	2.39	0.53
26:Z:234:PHE:CE2	27:a:349:MET:HG3	2.44	0.53
27:a:70:ARG:HG2	28:b:17:ARG:HB3	1.90	0.53
28:b:19:GLY:HA2	28:b:24:THR:HA	1.89	0.53
28:b:131:LEU:HD22	28:b:136:VAL:HB	1.89	0.53
30:d:147:SER:HG	30:d:148:TYR:C	2.17	0.53
32:f:108:ARG:HH21	32:f:141:ARG:HA	1.74	0.53
32:f:335:ARG:HB2	32:f:336:GLU:HA	1.91	0.53
2:B:316:LEU:HD11	2:B:327:VAL:HG21	1.91	0.53
6:F:308:ARG:O	6:F:312:GLU:N	2.29	0.53
7:G:43:ARG:HD2	7:G:149:PRO:HB2	1.90	0.53
8:H:50:LYS:NZ	8:H:62:VAL:O	2.42	0.53
9:I:154:GLY:HA3	10:J:78:ALA:HB2	1.90	0.53
14:N:132:SER:HA	14:N:135:ILE:HG12	1.89	0.53
22:V:416:ARG:HG2	22:V:457:TYR:HB3	1.91	0.53
22:V:462:GLU:HB3	25:Y:346:LYS:HG3	1.90	0.53
23:W:320:LEU:HD21	23:W:354:LEU:HD21	1.90	0.53
25:Y:323:PHE:CD2	25:Y:326:GLY:HA3	2.44	0.53
2:B:111:THR:HA	2:B:149:SER:HA	1.90	0.53
3:C:285:ALA:HB1	3:C:286:THR:HB	1.91	0.53
4:D:133:HIS:CB	4:D:138:ALA:H	2.22	0.53
12:L:45:VAL:HG11	12:L:188:VAL:HA	1.90	0.53
29:c:242:GLU:OE2	29:c:297:VAL:HA	2.08	0.53
2:B:424:GLU:O	2:B:428:TYR:N	2.29	0.53
4:D:217:LYS:NZ	5:E:266:GLY:O	2.42	0.53
8:H:50:LYS:HD2	8:H:64:LYS:HG2	1.91	0.53
13:M:15:SER:OG	13:M:19:ARG:O	2.27	0.53
20:T:138:ALA:HB3	20:T:147:GLN:HB2	1.91	0.53
21:U:485:ALA:HB3	21:U:519:VAL:HG12	1.91	0.53
22:V:273:LYS:HA	22:V:274:SER:HB2	1.91	0.53
22:V:319:HIS:HB2	22:V:320:THR:HA	1.90	0.53
23:W:393:LEU:HD23	23:W:406:VAL:HG11	1.91	0.53
23:W:412:ILE:O	24:X:344:ARG:NH2	2.42	0.53
27:a:34:TRP:O	27:a:38:THR:OG1	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:106:LEU:HD11	30:d:114:GLU:HB3	1.91	0.53
15:O:3:ILE:HG13	15:O:127:MET:HB2	1.90	0.52
21:U:31:VAL:HA	21:U:34:PHE:HB2	1.91	0.52
22:V:495:ARG:NH1	26:Z:282:ASN:OD1	2.41	0.52
1:A:284:ARG:HG3	1:A:285:PHE:HD2	1.73	0.52
3:C:283:PHE:CD1	3:C:284:GLU:HG2	2.44	0.52
5:E:253:ILE:O	5:E:256:THR:OG1	2.26	0.52
5:E:360:ASP:OD1	5:E:360:ASP:N	2.34	0.52
7:G:71:LYS:HE3	7:G:74:GLU:HA	1.91	0.52
23:W:259:GLU:HG2	23:W:262:LYS:HB3	1.89	0.52
26:Z:91:ILE:HD11	26:Z:115:TYR:HB3	1.90	0.52
27:a:13:ASN:OD1	27:a:19:PRO:HB3	2.07	0.52
29:c:241:ASN:HD21	29:c:300:LEU:HB3	1.73	0.52
32:f:301:ASP:OD1	32:f:302:PRO:HD3	2.08	0.52
3:C:74:GLY:N	3:C:114:VAL:O	2.39	0.52
22:V:33:GLN:HG2	22:V:86:VAL:HG21	1.90	0.52
26:Z:186:THR:HG23	26:Z:187:LEU:H	1.74	0.52
1:A:76:ALA:HA	1:A:79:ASP:HB2	1.92	0.52
1:A:100:LYS:HG2	1:A:113:ILE:HG22	1.92	0.52
3:C:71:SER:HA	3:C:118:ASN:HB3	1.91	0.52
3:C:143:VAL:HG11	3:C:197:THR:HG22	1.91	0.52
11:K:13:ASN:HD21	12:L:126:ARG:HH11	1.57	0.52
12:L:18:ARG:NH1	12:L:23:GLU:OE2	2.42	0.52
18:R:77:ALA:HA	18:R:120:ARG:HH22	1.74	0.52
22:V:349:ARG:HE	22:V:354:LYS:HG3	1.74	0.52
25:Y:304:TYR:OH	25:Y:333:GLU:OE2	2.28	0.52
25:Y:349:LYS:O	25:Y:350:VAL:HG22	2.09	0.52
26:Z:214:LYS:HB3	26:Z:222:ILE:HD13	1.90	0.52
26:Z:254:ASN:HA	26:Z:257:MET:HG3	1.91	0.52
29:c:145:VAL:HA	29:c:157:ILE:HA	1.90	0.52
29:c:191:ALA:HA	29:c:194:HIS:ND1	2.24	0.52
32:f:392:LYS:HG2	32:f:422:GLU:HA	1.92	0.52
2:B:230:THR:HG21	2:B:353:PHE:CE2	2.45	0.52
4:D:366:ARG:HB3	4:D:367:PRO:HD3	1.92	0.52
4:D:387:VAL:HG21	5:E:159:PHE:HE1	1.74	0.52
6:F:126:THR:OG1	6:F:130:GLN:N	2.42	0.52
6:F:253:GLY:H	6:F:287:GLU:HB2	1.74	0.52
21:U:325:MET:HA	21:U:328:ILE:HG12	1.91	0.52
21:U:765:VAL:HG12	21:U:775:LEU:HD22	1.91	0.52
22:V:193:GLN:HB3	22:V:194:LYS:CA	2.38	0.52
23:W:236:HIS:HB3	23:W:237:GLU:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:424:LEU:O	23:W:428:TRP:HB2	2.10	0.52
27:a:163:TYR:HH	27:a:169:HIS:HD1	1.58	0.52
29:c:267:PRO:HA	29:c:270:LEU:HD12	1.91	0.52
30:d:228:GLN:N	30:d:229:GLN:HA	2.24	0.52
2:B:372:MET:HE3	3:C:178:LEU:HD11	1.92	0.52
2:B:383:LEU:HD21	2:B:420:LYS:HG2	1.91	0.52
3:C:13:GLU:N	3:C:14:GLY:HA3	2.25	0.52
5:E:65:THR:HG22	5:E:66:GLU:H	1.75	0.52
6:F:310:MET:HA	6:F:313:LEU:HB3	1.90	0.52
13:M:231:ILE:HG22	13:M:232:ARG:HG3	1.92	0.52
14:N:40:ARG:NH1	14:N:180:ALA:O	2.42	0.52
18:R:25:TYR:OH	19:S:142:SER:O	2.27	0.52
22:V:318:GLN:O	22:V:319:HIS:ND1	2.42	0.52
27:a:214:GLY:HA2	27:a:217:LEU:HD22	1.91	0.52
29:c:121:TRP:HB3	29:c:193:ILE:HD13	1.90	0.52
32:f:314:ASN:HD21	32:f:355:VAL:HG13	1.74	0.52
1:A:274:PHE:HB2	1:A:319:MET:SD	2.50	0.52
1:A:297:ARG:O	1:A:301:GLU:N	2.31	0.52
3:C:166:GLU:OE2	3:C:207:THR:OG1	2.22	0.52
5:E:180:LYS:NZ	5:E:279:THR:O	2.43	0.52
5:E:242:ARG:HB3	5:E:254:GLN:HG3	1.91	0.52
5:E:306:GLU:HA	5:E:309:ARG:HB3	1.91	0.52
6:F:195:ILE:HD12	6:F:236:LEU:HD21	1.92	0.52
7:G:210:PHE:CE1	7:G:215:ILE:HG23	2.45	0.52
10:J:95:ARG:HG3	17:Q:62:LYS:HE3	1.91	0.52
11:K:37:ALA:HB2	11:K:50:VAL:HG23	1.92	0.52
11:K:42:THR:HG22	11:K:44:GLU:H	1.73	0.52
12:L:155:ASP:HB3	13:M:62:SER:HB2	1.91	0.52
22:V:342:ILE:HD12	22:V:343:PRO:HD2	1.91	0.52
25:Y:367:GLN:HG3	25:Y:371:LYS:HG2	1.92	0.52
29:c:168:MET:HA	29:c:172:HIS:CE1	2.45	0.52
31:e:58:ALA:HB3	31:e:59:GLU:HA	1.91	0.52
32:f:365:MET:HE3	32:f:672:VAL:HG11	1.91	0.52
1:A:106:SER:HB3	1:A:110:LYS:HD2	1.92	0.52
5:E:135:ILE:HD11	5:E:142:ILE:HG12	1.92	0.52
5:E:335:SER:HB3	5:E:338:PHE:HE2	1.74	0.52
9:I:73:ALA:HB3	9:I:137:ILE:HD11	1.91	0.52
10:J:115:LYS:NZ	10:J:129:ILE:O	2.42	0.52
21:U:522:GLY:O	21:U:559:ARG:NH2	2.43	0.52
21:U:774:PRO:HA	21:U:777:HIS:HD2	1.75	0.52
22:V:324:PHE:HD1	31:e:9:ASP:HB2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:393:THR:HB	30:d:115:PHE:HE2	1.74	0.52
23:W:373:ILE:HD13	23:W:378:MET:HE3	1.92	0.52
27:a:205:LEU:HD11	27:a:240:PHE:CG	2.45	0.52
28:b:25:ARG:HA	28:b:28:ALA:HB3	1.91	0.52
28:b:30:GLN:HG3	28:b:75:LEU:HD13	1.90	0.52
30:d:145:GLU:N	30:d:146:GLY:HA2	2.22	0.52
32:f:18:GLU:OE1	32:f:79:ASN:ND2	2.43	0.52
32:f:430:SER:HA	32:f:433:ASN:HB3	1.91	0.52
2:B:194:ILE:O	2:B:198:LYS:N	2.43	0.52
11:K:16:SER:O	11:K:19:GLY:HA3	2.09	0.52
18:R:100:MET:HG2	18:R:113:TYR:HD1	1.75	0.52
19:S:116:GLU:OE1	19:S:118:LYS:NZ	2.38	0.52
26:Z:69:PHE:HB2	28:b:99:HIS:CE1	2.44	0.52
29:c:227:GLU:HB3	29:c:233:ASP:HB2	1.91	0.52
32:f:108:ARG:HG2	32:f:141:ARG:HH21	1.74	0.52
1:A:297:ARG:NH1	6:F:303:ASP:OD1	2.41	0.52
1:A:388:VAL:HG13	1:A:413:VAL:HG22	1.92	0.52
3:C:39:SER:O	3:C:43:ARG:HG3	2.10	0.52
4:D:242:GLU:HG3	4:D:246:MET:HE2	1.91	0.52
5:E:329:GLU:O	5:E:333:LYS:N	2.37	0.52
6:F:430:LYS:HZ2	11:K:17:PRO:HB2	1.75	0.52
10:J:19:VAL:HG22	10:J:126:PRO:HG2	1.92	0.52
11:K:157:ASP:OD2	11:K:159:SER:OG	2.27	0.52
20:T:24:ALA:HB1	20:T:41:ARG:HH12	1.75	0.52
21:U:212:ASP:O	21:U:215:ASN:ND2	2.43	0.52
21:U:625:ILE:HG13	21:U:626:LEU:HG	1.91	0.52
22:V:451:ILE:HG12	22:V:458:VAL:HG22	1.91	0.52
29:c:229:LEU:O	29:c:230:THR:OG1	2.24	0.52
4:D:277:ALA:C	4:D:280:GLY:H	2.18	0.51
4:D:281:ALA:O	4:D:285:VAL:HG13	2.09	0.51
12:L:15:PRO:O	13:M:28:LYS:NZ	2.32	0.51
14:N:7:GLN:HB3	14:N:111:VAL:HG23	1.92	0.51
25:Y:224:VAL:HG13	25:Y:256:VAL:HG11	1.92	0.51
25:Y:233:ARG:NH1	25:Y:306:GLN:OE1	2.43	0.51
25:Y:386:VAL:HG12	25:Y:387:ILE:HG23	1.92	0.51
29:c:63:ASP:OD1	29:c:66:THR:OG1	2.21	0.51
32:f:11:TRP:HB3	32:f:12:GLN:HB3	1.90	0.51
1:A:316:LYS:O	1:A:317:VAL:HG13	2.11	0.51
3:C:189:TYR:O	3:C:317:PHE:N	2.31	0.51
3:C:298:ILE:O	3:C:301:LEU:N	2.42	0.51
5:E:176:PRO:HB2	5:E:302:ASP:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:18:GLU:HB2	11:K:19:GLY:HA2	1.92	0.51
29:c:250:GLU:HA	29:c:253:LYS:HG2	1.90	0.51
30:d:159:PRO:N	30:d:160:ALA:HA	2.25	0.51
1:A:80:LEU:HD22	2:B:99:VAL:HG21	1.92	0.51
4:D:289:LEU:O	4:D:293:LEU:HB2	2.09	0.51
4:D:337:ASP:O	4:D:341:LYS:N	2.28	0.51
4:D:377:SER:O	4:D:381:GLU:N	2.42	0.51
5:E:115:VAL:HG22	5:E:117:PRO:HD2	1.92	0.51
10:J:137:ASP:N	10:J:141:THR:O	2.43	0.51
22:V:244:ALA:C	22:V:246:GLY:H	2.18	0.51
29:c:275:VAL:HG13	29:c:276:GLY:H	1.75	0.51
30:d:214:GLY:N	30:d:215:TRP:HB3	2.26	0.51
32:f:675:ASP:OD1	32:f:679:ARG:NH1	2.44	0.51
32:f:680:PRO:CG	32:f:691:VAL:HG21	2.41	0.51
32:f:685:VAL:HG23	32:f:686:ARG:H	1.75	0.51
1:A:80:LEU:HG	2:B:137:SER:OG	2.10	0.51
2:B:224:LEU:HA	2:B:351:ILE:HG13	1.91	0.51
4:D:98:GLN:HG3	4:D:99:ASN:HD22	1.76	0.51
5:E:111:LEU:HD22	6:F:96:LEU:HD23	1.92	0.51
7:G:28:ALA:HB1	7:G:135:GLY:HA3	1.92	0.51
8:H:119:GLN:O	8:H:122:THR:OG1	2.28	0.51
11:K:79:SER:H	11:K:139:VAL:HG23	1.75	0.51
22:V:266:GLN:HG3	22:V:295:ILE:HG23	1.92	0.51
23:W:452:ILE:HG21	26:Z:226:ILE:H	1.75	0.51
25:Y:301:ILE:HG13	25:Y:343:LEU:HB2	1.92	0.51
26:Z:48:LEU:HD11	26:Z:92:VAL:HG21	1.93	0.51
26:Z:136:GLU:OE2	26:Z:157:HIS:ND1	2.40	0.51
27:a:206:LEU:HD22	27:a:264:ASN:HB2	1.92	0.51
1:A:126:SER:OG	1:A:149:ILE:O	2.23	0.51
3:C:254:ILE:HG23	3:C:296:ASN:HD22	1.76	0.51
3:C:307:ARG:HE	3:C:312:ASP:CB	2.23	0.51
3:C:337:ASN:ND2	4:D:193:GLN:O	2.43	0.51
7:G:138:MET:HB3	7:G:154:CYS:HB3	1.93	0.51
11:K:202:LEU:HA	11:K:205:VAL:HG22	1.92	0.51
16:P:52:GLY:N	16:P:108:VAL:O	2.39	0.51
21:U:45:ILE:HG21	21:U:64:ALA:HB2	1.93	0.51
22:V:26:PRO:O	22:V:29:PRO:HD2	2.10	0.51
27:a:54:ASP:HA	27:a:57:ILE:HG22	1.92	0.51
30:d:94:TYR:HD1	30:d:97:GLN:HE21	1.58	0.51
32:f:83:GLU:HB3	32:f:84:PRO:HD3	1.93	0.51
32:f:339:LEU:HD12	32:f:340:THR:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:PHE:O	1:A:265:ARG:N	2.38	0.51
5:E:126:ASP:OD1	5:E:185:ARG:NE	2.36	0.51
6:F:92:ASN:HB3	6:F:125:LYS:HB2	1.92	0.51
6:F:174:ALA:HB1	6:F:177:VAL:HG23	1.92	0.51
6:F:229:PRO:O	6:F:392:ASN:ND2	2.44	0.51
7:G:31:ALA:HB1	7:G:83:MET:HE3	1.92	0.51
10:J:132:LEU:HD13	10:J:161:ILE:HG12	1.93	0.51
12:L:137:TYR:CZ	12:L:142:PRO:HB3	2.46	0.51
21:U:154:ALA:HB2	21:U:166:THR:HG21	1.93	0.51
22:V:200:ARG:HA	22:V:203:LEU:HB2	1.93	0.51
25:Y:358:ARG:HH21	25:Y:359:PRO:HD2	1.76	0.51
32:f:371:CYS:C	32:f:373:GLY:HA2	2.35	0.51
1:A:279:ALA:O	2:B:307:ARG:NH1	2.43	0.51
2:B:366:GLN:O	2:B:370:SER:OG	2.23	0.51
3:C:131:VAL:HG13	3:C:132:ASP:H	1.76	0.51
4:D:311:THR:HG21	4:D:317:LEU:HD11	1.93	0.51
6:F:204:LEU:O	6:F:209:LYS:N	2.44	0.51
7:G:172:GLN:OE1	7:G:172:GLN:N	2.44	0.51
8:H:39:LYS:HE3	8:H:144:PRO:HG2	1.93	0.51
21:U:490:ARG:HH11	21:U:493:VAL:HB	1.75	0.51
23:W:414:ASN:N	23:W:414:ASN:OD1	2.43	0.51
29:c:219:ASN:HA	29:c:222:LYS:HB2	1.92	0.51
32:f:438:VAL:HG13	32:f:472:LYS:HD3	1.93	0.51
32:f:674:PHE:O	32:f:678:LEU:HG	2.11	0.51
2:B:235:LEU:HA	2:B:238:ALA:HB3	1.93	0.51
5:E:281:ARG:NE	5:E:283:ASP:OD2	2.35	0.51
8:H:44:VAL:O	8:H:213:CYS:N	2.39	0.51
11:K:146:VAL:HG11	11:K:222:PRO:HG3	1.93	0.51
22:V:79:VAL:HG22	22:V:80:LYS:HG2	1.93	0.51
22:V:478:GLN:HE22	30:d:245:GLN:HE22	1.59	0.51
25:Y:77:ASN:HD21	25:Y:114:ILE:HG13	1.74	0.51
26:Z:228:TYR:CD1	27:a:215:GLU:OE2	2.60	0.51
32:f:647:VAL:O	32:f:650:ILE:HG13	2.11	0.51
1:A:362:MET:HE3	1:A:404:ALA:H	1.76	0.51
2:B:180:PRO:HD2	2:B:242:GLN:NE2	2.26	0.51
3:C:117:ARG:N	3:C:122:THR:O	2.30	0.51
33:E:401:ADP:O1B	6:F:347:ARG:NH2	2.44	0.51
6:F:84:LYS:H	6:F:85:THR:HA	1.76	0.51
12:L:41:LYS:HG3	12:L:180:MET:HB3	1.91	0.51
13:M:15:SER:OG	13:M:17:ASP:OD1	2.19	0.51
13:M:39:ILE:HG21	13:M:193:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:168:GLN:NE2	17:Q:174:ASN:O	2.44	0.51
22:V:148:ARG:NH2	22:V:192:MET:O	2.44	0.51
23:W:232:GLN:O	23:W:236:HIS:HB2	2.11	0.51
25:Y:42:MET:HE3	25:Y:46:ARG:HH12	1.76	0.51
28:b:97:LEU:O	28:b:100:ARG:NE	2.43	0.51
32:f:304:LEU:HD11	32:f:326:LEU:HD12	1.93	0.51
3:C:49:ARG:HA	3:C:52:LEU:HB2	1.93	0.51
3:C:165:ILE:HG13	3:C:203:VAL:HG11	1.92	0.51
6:F:246:ALA:HB3	6:F:282:ILE:HG12	1.92	0.51
7:G:206:LEU:HB3	7:G:208:ILE:HG12	1.92	0.51
7:G:210:PHE:HE1	7:G:215:ILE:HG23	1.74	0.51
10:J:98:VAL:HG12	10:J:100:ASP:OD1	2.11	0.51
13:M:37:ILE:HG22	13:M:164:ALA:HA	1.92	0.51
17:Q:148:THR:HB	17:Q:151:ILE:HB	1.93	0.51
18:R:164:THR:HG22	18:R:170:SER:HB3	1.93	0.51
26:Z:32:GLN:HG3	26:Z:33:LYS:H	1.75	0.51
26:Z:228:TYR:CZ	27:a:215:GLU:HB3	2.45	0.51
27:a:156:TYR:CG	27:a:179:PHE:HB2	2.46	0.51
30:d:49:ILE:HG13	30:d:90:PRO:HD2	1.92	0.51
1:A:100:LYS:HG3	1:A:115:VAL:HB	1.92	0.50
2:B:139:VAL:HB	2:B:141:LYS:N	2.26	0.50
2:B:364:ILE:HG12	33:B:501:ADP:N6	2.27	0.50
3:C:238:ALA:HB1	3:C:289:ILE:HD12	1.92	0.50
5:E:128:GLY:O	5:E:189:SER:OG	2.16	0.50
6:F:204:LEU:HD13	6:F:212:PHE:CE2	2.46	0.50
8:H:231:ALA:HB3	8:H:232:ALA:CB	2.39	0.50
9:I:75:SER:HB2	9:I:135:LEU:HB2	1.92	0.50
22:V:319:HIS:HB3	22:V:325:LYS:HD3	1.93	0.50
26:Z:164:ALA:HB1	26:Z:168:GLU:HG3	1.93	0.50
2:B:151:LEU:O	2:B:159:VAL:HA	2.10	0.50
2:B:151:LEU:HD11	2:B:163:LEU:HD13	1.93	0.50
5:E:157:GLU:HA	5:E:160:GLN:HG2	1.92	0.50
5:E:174:GLY:HA2	5:E:176:PRO:HD2	1.93	0.50
5:E:369:LYS:HZ1	13:M:171:ALA:HA	1.75	0.50
22:V:310:THR:HA	22:V:332:LEU:HD11	1.91	0.50
27:a:270:ARG:NH1	27:a:310:LEU:O	2.44	0.50
3:C:268:GLU:O	3:C:272:THR:OG1	2.22	0.50
4:D:407:ILE:HG13	4:D:408:LYS:H	1.76	0.50
5:E:281:ARG:HD2	5:E:388:PRO:HD2	1.93	0.50
6:F:80:ILE:HA	6:F:83:ASN:O	2.11	0.50
6:F:342:LEU:HA	6:F:347:ARG:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:15:PHE:HE1	12:L:126:ARG:HD2	1.75	0.50
12:L:157:ARG:HD2	12:L:176:MET:HG3	1.94	0.50
19:S:99:ARG:HB3	19:S:103:PRO:HA	1.91	0.50
20:T:46:ASN:OD1	20:T:48:SER:N	2.41	0.50
22:V:311:ASN:HA	22:V:314:ARG:HG2	1.94	0.50
25:Y:232:GLU:O	25:Y:236:LEU:N	2.41	0.50
32:f:463:SER:HA	32:f:466:LYS:HE3	1.92	0.50
1:A:102:ILE:HG22	1:A:113:ILE:HG23	1.94	0.50
1:A:163:MET:SD	2:B:146:PRO:HG2	2.52	0.50
1:A:302:LEU:O	1:A:306:LEU:N	2.40	0.50
5:E:313:LEU:HD12	5:E:316:HIS:HB2	1.94	0.50
6:F:336:ASP:OD1	6:F:336:ASP:N	2.43	0.50
10:J:98:VAL:HG22	18:R:78:ALA:HB1	1.94	0.50
21:U:126:ILE:HG23	21:U:130:LEU:HD11	1.93	0.50
22:V:314:ARG:HD2	25:Y:378:ASN:OD1	2.11	0.50
23:W:312:MET:SD	23:W:361:HIS:ND1	2.85	0.50
27:a:373:ASP:HB2	30:d:251:ARG:HH12	1.75	0.50
32:f:436:VAL:HG21	32:f:675:ASP:CG	2.36	0.50
1:A:206:ILE:N	6:F:373:MET:HE3	2.27	0.50
2:B:144:LEU:HD22	2:B:162:VAL:HG21	1.93	0.50
3:C:41:ASN:ND2	22:V:492:LYS:HD3	2.22	0.50
4:D:53:PHE:HB2	21:U:632:GLN:HE22	1.76	0.50
4:D:62:LYS:HA	4:D:65:GLN:HE21	1.77	0.50
6:F:225:MET:O	6:F:331:ALA:HA	2.11	0.50
13:M:67:PHE:HB2	13:M:75:MET:HB2	1.92	0.50
16:P:70:ARG:NH2	16:P:97:GLU:OE2	2.45	0.50
17:Q:23:SER:H	17:Q:28:MET:HE2	1.77	0.50
21:U:62:LEU:HD12	21:U:84:ALA:HB1	1.94	0.50
21:U:436:ALA:HB1	21:U:472:ILE:HD13	1.93	0.50
22:V:38:LYS:HA	22:V:41:ALA:HB3	1.93	0.50
24:X:416:ASN:HB3	26:Z:283:ARG:HH21	1.76	0.50
25:Y:179:ARG:NH2	25:Y:212:GLU:OE2	2.38	0.50
1:A:328:ASP:HA	1:A:331:LEU:HG	1.93	0.50
3:C:130:LYS:HG3	3:C:133:PRO:HG2	1.92	0.50
4:D:207:PRO:HD2	4:D:312:ASN:HA	1.93	0.50
5:E:47:LEU:HD13	6:F:80:ILE:HG12	1.93	0.50
5:E:305:ASN:OD1	5:E:306:GLU:N	2.45	0.50
6:F:139:LEU:N	6:F:160:ILE:O	2.45	0.50
6:F:223:VAL:HG23	6:F:350:ARG:HB2	1.94	0.50
11:K:97:GLN:HG2	18:R:61:ARG:HG3	1.94	0.50
15:O:14:LEU:HB2	15:O:176:CYS:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:103:LEU:HB3	17:Q:118:MET:H	1.76	0.50
20:T:43:MET:HE2	20:T:51:LEU:HB3	1.94	0.50
21:U:154:ALA:HB1	21:U:163:PHE:HD1	1.77	0.50
21:U:474:ARG:NH1	21:U:500:ASN:OD1	2.45	0.50
22:V:167:LEU:HD11	22:V:171:VAL:HB	1.92	0.50
29:c:64:ASP:HA	29:c:139:ARG:HH21	1.76	0.50
32:f:370:SER:HA	32:f:371:CYS:SG	2.52	0.50
1:A:402:LYS:HD2	1:A:402:LYS:N	2.27	0.50
3:C:43:ARG:HB3	21:U:639:LEU:HD13	1.94	0.50
5:E:216:ARG:HG3	5:E:263:GLN:HE21	1.77	0.50
13:M:57:LEU:HB2	13:M:58:TYR:CD1	2.47	0.50
16:P:91:VAL:HG21	16:P:109:ILE:HD11	1.93	0.50
17:Q:4:LEU:HD22	17:Q:17:SER:HA	1.92	0.50
21:U:82:LEU:HD21	21:U:130:LEU:HB3	1.94	0.50
21:U:427:LEU:HG	21:U:428:PRO:HD2	1.93	0.50
30:d:182:ILE:HG23	30:d:183:GLU:H	1.77	0.50
32:f:475:LYS:HG3	32:f:503:MET:HG2	1.94	0.50
1:A:329:PRO:HA	1:A:332:MET:HB3	1.94	0.50
1:A:384:GLU:HA	2:B:347:ILE:HG12	1.94	0.50
3:C:295:THR:HB	3:C:300:ILE:HG12	1.94	0.50
4:D:83:GLN:HG2	4:D:84:SER:H	1.77	0.50
12:L:36:VAL:HG22	12:L:160:SER:HB2	1.94	0.50
3:C:217:SER:HB3	3:C:218:GLU:CB	2.31	0.50
6:F:181:PRO:HG3	6:F:238:ARG:O	2.12	0.50
7:G:123:GLN:O	7:G:127:GLN:HG2	2.12	0.50
12:L:48:ALA:HB3	12:L:211:SER:HB2	1.94	0.50
14:N:15:GLY:HA2	14:N:176:LEU:HD22	1.94	0.50
15:O:40:ASN:ND2	15:O:104:ASP:OD1	2.37	0.50
16:P:160:PRO:HA	16:P:163:LEU:HB3	1.94	0.50
17:Q:164:LEU:HB3	17:Q:196:PHE:HE2	1.76	0.50
20:T:49:THR:HB	20:T:85:PRO:HG3	1.92	0.50
21:U:54:PHE:CZ	21:U:56:SER:HB2	2.46	0.50
2:B:406:ALA:O	2:B:411:ARG:N	2.44	0.49
5:E:63:GLN:HA	5:E:69:PHE:HA	1.93	0.49
9:I:245:ALA:O	9:I:249:ARG:NH2	2.44	0.49
11:K:157:ASP:OD1	11:K:161:THR:N	2.45	0.49
12:L:200:PRO:HD2	12:L:203:GLN:HE22	1.76	0.49
20:T:50:MET:HE2	20:T:192:VAL:HG13	1.94	0.49
23:W:334:GLU:OE1	23:W:338:THR:OG1	2.29	0.49
25:Y:357:ASN:HB2	25:Y:359:PRO:HD3	1.92	0.49
29:c:96:LEU:HD23	29:c:99:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:192:THR:HA	32:f:193:HIS:HB2	1.93	0.49
4:D:49:GLN:OE1	4:D:49:GLN:N	2.45	0.49
5:E:121:ASN:HB3	5:E:197:LYS:O	2.13	0.49
6:F:194:GLN:HB2	6:F:352:ILE:HG21	1.94	0.49
21:U:19:LEU:HD13	30:d:27:LYS:HZ3	1.77	0.49
21:U:367:THR:HG21	21:U:773:PHE:HB3	1.94	0.49
22:V:436:PHE:HB2	30:d:146:GLY:H	1.78	0.49
23:W:285:ASP:OD1	23:W:285:ASP:N	2.46	0.49
28:b:120:ASN:OD1	28:b:121:GLU:N	2.45	0.49
32:f:660:TYR:HB2	32:f:663:VAL:HG23	1.94	0.49
12:L:138:ASP:OD1	12:L:143:HIS:NE2	2.43	0.49
22:V:304:GLU:HA	22:V:307:ARG:HG2	1.93	0.49
23:W:447:ALA:O	23:W:451:MET:HG2	2.12	0.49
1:A:111:TYR:CE2	1:A:125:LEU:HD23	2.46	0.49
4:D:106:THR:HB	5:E:77:PRO:HA	1.95	0.49
4:D:230:VAL:O	4:D:265:ASP:N	2.46	0.49
4:D:373:ALA:HB3	4:D:375:ILE:HG12	1.95	0.49
5:E:349:GLU:HA	5:E:352:MET:HE3	1.95	0.49
6:F:169:ASP:N	6:F:173:LYS:HB2	2.26	0.49
12:L:50:LYS:N	12:L:209:ASN:O	2.41	0.49
13:M:106:ILE:HD12	13:M:107:PRO:HD2	1.93	0.49
20:T:41:ARG:NH2	20:T:53:ALA:O	2.46	0.49
20:T:124:TYR:HB2	20:T:137:LEU:HD13	1.95	0.49
26:Z:185:GLY:O	29:c:292:MET:HB3	2.12	0.49
29:c:234:TYR:HA	29:c:237:HIS:HB2	1.94	0.49
1:A:190:VAL:HG23	1:A:209:PRO:HG2	1.93	0.49
1:A:328:ASP:HB3	1:A:329:PRO:HD3	1.94	0.49
2:B:224:LEU:N	2:B:329:MET:O	2.45	0.49
2:B:290:ILE:HG23	2:B:336:THR:HB	1.93	0.49
3:C:363:CYS:HA	3:C:366:ALA:HB3	1.95	0.49
4:D:344:ILE:HA	4:D:347:THR:HG22	1.94	0.49
7:G:183:VAL:HG13	7:G:189:TRP:HZ2	1.77	0.49
13:M:229:LYS:HE2	13:M:235:ALA:HB3	1.94	0.49
23:W:420:ASP:OD2	23:W:425:LEU:HB3	2.12	0.49
32:f:680:PRO:O	32:f:683:VAL:N	2.46	0.49
1:A:115:VAL:HG12	1:A:119:ALA:O	2.12	0.49
5:E:108:MET:HG2	5:E:109:ARG:HG3	1.95	0.49
6:F:84:LYS:HZ3	6:F:139:LEU:HD23	1.77	0.49
6:F:342:LEU:HB3	6:F:348:LEU:HG	1.93	0.49
7:G:218:GLY:HA2	7:G:230:LEU:HD13	1.93	0.49
8:H:69:THR:HG22	8:H:70:LYS:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:7:VAL:HG13	15:O:12:ILE:HG12	1.94	0.49
18:R:97:MET:HE2	18:R:99:THR:HG21	1.93	0.49
26:Z:9:VAL:HG12	26:Z:48:LEU:HB3	1.94	0.49
27:a:78:GLU:O	27:a:82:HIS:ND1	2.38	0.49
29:c:32:TYR:HB3	29:c:208:ARG:HD3	1.94	0.49
30:d:147:SER:OG	30:d:150:LYS:N	2.46	0.49
1:A:271:LEU:HG	1:A:315:ILE:O	2.13	0.49
1:A:292:ASP:O	1:A:296:GLN:HG2	2.13	0.49
2:B:286:GLU:OE1	2:B:332:ASN:N	2.45	0.49
6:F:394:ALA:HB2	33:F:501:ADP:H1'	1.95	0.49
16:P:126:LEU:HD12	16:P:127:ILE:HG23	1.94	0.49
21:U:599:ILE:HD12	21:U:602:LEU:HD22	1.95	0.49
23:W:452:ILE:HD13	26:Z:226:ILE:HG22	1.94	0.49
25:Y:312:ARG:HG3	25:Y:313:SER:N	2.28	0.49
25:Y:355:GLU:HG3	25:Y:357:ASN:ND2	2.27	0.49
1:A:79:ASP:HB3	2:B:137:SER:HA	1.95	0.49
1:A:115:VAL:HG13	1:A:117:GLN:N	2.28	0.49
1:A:355:PHE:CE1	1:A:385:ILE:HB	2.48	0.49
2:B:307:ARG:O	2:B:311:GLU:N	2.33	0.49
5:E:170:CYS:SG	5:E:171:LEU:N	2.85	0.49
5:E:227:PRO:HD3	5:E:272:ARG:HH11	1.78	0.49
16:P:113:ASP:OD2	16:P:116:THR:OG1	2.29	0.49
21:U:27:LEU:O	21:U:31:VAL:HB	2.13	0.49
22:V:160:LEU:HB2	22:V:161:PRO:HD3	1.95	0.49
22:V:349:ARG:HH21	22:V:354:LYS:HG3	1.77	0.49
22:V:485:ASP:O	22:V:489:MET:HG2	2.13	0.49
26:Z:263:ALA:O	26:Z:267:ARG:HG2	2.13	0.49
30:d:54:ILE:HA	30:d:57:ILE:HG22	1.95	0.49
1:A:218:PRO:O	1:A:221:GLY:N	2.45	0.49
1:A:295:VAL:HG21	2:B:303:ARG:HH12	1.78	0.49
2:B:394:ASP:O	2:B:398:ILE:N	2.45	0.49
3:C:87:VAL:HG21	3:C:123:LEU:HD11	1.95	0.49
3:C:157:GLN:HE22	3:C:318:PRO:HD3	1.77	0.49
3:C:194:THR:HG21	3:C:357:ALA:N	2.28	0.49
4:D:62:LYS:HD2	4:D:65:GLN:HE21	1.78	0.49
4:D:204:MET:SD	4:D:212:LYS:HA	2.53	0.49
4:D:374:ASP:HA	5:E:291:ARG:CZ	2.42	0.49
5:E:228:CYS:O	5:E:273:VAL:HA	2.13	0.49
5:E:269:THR:OG1	5:E:271:HIS:ND1	2.41	0.49
8:H:19:LEU:HD12	8:H:22:ILE:HD12	1.95	0.49
12:L:82:ARG:O	12:L:86:ASN:ND2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:179:VAL:HA	18:R:184:TRP:HA	1.94	0.49
21:U:14:GLU:OE1	21:U:16:GLU:HG2	2.13	0.49
22:V:91:PRO:HA	22:V:94:VAL:HG12	1.94	0.49
22:V:97:ALA:N	22:V:98:LEU:HB2	2.27	0.49
25:Y:190:ALA:O	25:Y:291:HIS:NE2	2.36	0.49
29:c:217:LEU:HA	29:c:220:LEU:HB2	1.95	0.49
32:f:33:VAL:HG23	32:f:34:PRO:HD3	1.93	0.49
1:A:96:ALA:HB3	2:B:132:TYR:CE2	2.47	0.49
2:B:394:ASP:O	2:B:398:ILE:HG23	2.13	0.49
5:E:182:LEU:H	33:E:401:ADP:H3'	1.78	0.49
5:E:304:PRO:HD2	5:E:309:ARG:HH22	1.77	0.49
7:G:124:VAL:HA	7:G:127:GLN:HG3	1.94	0.49
10:J:201:SER:HB3	10:J:202:GLY:HA3	1.94	0.49
12:L:50:LYS:HE2	12:L:61:LYS:HA	1.95	0.49
12:L:69:HIS:HE2	12:L:102:PRO:HB2	1.78	0.49
21:U:396:ALA:O	21:U:401:LYS:NZ	2.45	0.49
22:V:413:SER:HB2	25:Y:339:ALA:HB2	1.95	0.49
23:W:372:ARG:HG2	23:W:414:ASN:HB3	1.94	0.49
26:Z:238:PRO:HB2	26:Z:239:ASP:HA	1.95	0.49
32:f:49:LEU:HD23	32:f:74:LEU:HD22	1.94	0.49
1:A:190:VAL:HG22	1:A:316:LYS:HD2	1.94	0.48
1:A:220:THR:HB	33:A:501:ADP:C4	2.47	0.48
1:A:316:LYS:HG2	1:A:317:VAL:H	1.78	0.48
1:A:421:ALA:HA	1:A:424:SER:O	2.13	0.48
4:D:82:ILE:HG23	4:D:83:GLN:HB3	1.95	0.48
4:D:375:ILE:HD13	4:D:378:ILE:HD12	1.93	0.48
7:G:208:ILE:HB	7:G:210:PHE:HD2	1.77	0.48
11:K:50:VAL:HG11	11:K:66:LYS:HB2	1.95	0.48
16:P:15:LYS:HE2	16:P:119:PRO:HB2	1.95	0.48
22:V:290:TYR:OH	22:V:294:ARG:NH2	2.46	0.48
24:X:414:LEU:HD23	25:Y:383:LEU:HD11	1.95	0.48
25:Y:51:ALA:HA	25:Y:54:TYR:HD2	1.78	0.48
32:f:223:ASN:HA	32:f:254:SER:HB3	1.94	0.48
1:A:333:ARG:O	1:A:337:LEU:N	2.46	0.48
1:A:392:ALA:HB2	1:A:409:PHE:HB3	1.95	0.48
3:C:117:ARG:O	3:C:121:TYR:HA	2.13	0.48
5:E:349:GLU:O	5:E:353:PHE:N	2.35	0.48
7:G:73:THR:HG22	7:G:74:GLU:H	1.77	0.48
12:L:204:ASP:HA	12:L:205:LEU:HB3	1.95	0.48
21:U:724:VAL:HA	21:U:727:LYS:HG2	1.95	0.48
22:V:197:THR:HG21	22:V:200:ARG:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:410:ILE:HG23	22:V:414:TYR:CD2	2.47	0.48
23:W:425:LEU:O	23:W:429:SER:OG	2.19	0.48
26:Z:271:ALA:O	26:Z:275:LEU:HB2	2.13	0.48
1:A:105:ASP:OD1	1:A:105:ASP:N	2.46	0.48
1:A:184:ILE:HD12	1:A:187:LEU:HD21	1.94	0.48
6:F:69:MET:HA	6:F:72:LYS:HG2	1.95	0.48
6:F:272:PHE:HA	6:F:275:ALA:HB3	1.95	0.48
21:U:435:SER:O	21:U:437:TYR:N	2.45	0.48
22:V:263:LEU:HG	22:V:264:TYR:H	1.78	0.48
26:Z:181:ASP:OD1	26:Z:181:ASP:N	2.46	0.48
32:f:89:LEU:HD21	32:f:126:CYS:SG	2.54	0.48
1:A:429:TYR:CZ	10:J:12:PRO:HD2	2.48	0.48
2:B:224:LEU:HD22	2:B:351:ILE:HG12	1.95	0.48
2:B:235:LEU:O	2:B:239:VAL:N	2.31	0.48
2:B:364:ILE:HG22	2:B:368:HIS:HE1	1.78	0.48
3:C:86:LEU:HD23	3:C:96:VAL:HB	1.94	0.48
6:F:164:LEU:HD12	6:F:165:PRO:HD2	1.96	0.48
7:G:54:LYS:HD3	7:G:66:VAL:HG13	1.96	0.48
12:L:172:LEU:O	12:L:176:MET:N	2.30	0.48
18:R:1:THR:N	18:R:169:TYR:O	2.45	0.48
25:Y:292:TYR:HA	25:Y:295:TYR:HB3	1.95	0.48
29:c:100:LYS:HA	29:c:105:PRO:HB3	1.95	0.48
1:A:157:ILE:CG2	1:A:158:ASP:HA	2.42	0.48
1:A:177:VAL:HG22	1:A:179:GLY:H	1.77	0.48
1:A:184:ILE:O	1:A:188:ARG:N	2.47	0.48
1:A:417:ILE:HG13	1:A:418:LYS:N	2.28	0.48
3:C:65:LEU:HA	29:c:190:GLN:HE22	1.78	0.48
3:C:295:THR:HG22	3:C:296:ASN:H	1.78	0.48
4:D:288:ILE:O	4:D:292:LEU:N	2.30	0.48
6:F:315:ASN:O	6:F:320:PHE:N	2.47	0.48
7:G:24:GLN:OE1	13:M:14:PHE:N	2.41	0.48
7:G:43:ARG:HH21	7:G:164:LYS:HG3	1.79	0.48
21:U:340:GLN:HG3	21:U:880:ASN:HB3	1.96	0.48
22:V:194:LYS:HB3	22:V:195:ILE:HG23	1.96	0.48
22:V:322:VAL:HG13	22:V:323:GLY:H	1.78	0.48
22:V:480:ILE:HG13	26:Z:267:ARG:HB3	1.95	0.48
23:W:435:LEU:HG	23:W:438:LEU:HD12	1.96	0.48
27:a:33:LEU:HA	28:b:18:ASN:HD22	1.77	0.48
30:d:182:ILE:HG13	30:d:183:GLU:HG3	1.96	0.48
32:f:219:ASN:O	32:f:223:ASN:ND2	2.46	0.48
1:A:180:CYS:SG	1:A:344:SER:HB2	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:PHE:HA	2:B:328:ILE:O	2.13	0.48
3:C:250:GLU:O	3:C:251:ILE:HG22	2.14	0.48
4:D:113:VAL:HB	4:D:139:LEU:HG	1.95	0.48
6:F:152:GLY:O	6:F:160:ILE:HA	2.14	0.48
6:F:223:VAL:HG13	6:F:329:ILE:HG23	1.96	0.48
7:G:79:VAL:HG13	7:G:139:ILE:HB	1.94	0.48
10:J:180:ALA:HA	10:J:181:ILE:HA	1.47	0.48
21:U:413:LYS:HA	21:U:449:ILE:HG12	1.94	0.48
22:V:27:PRO:O	22:V:30:PRO:HD2	2.14	0.48
22:V:416:ARG:CZ	22:V:457:TYR:HB2	2.44	0.48
1:A:384:GLU:O	1:A:388:VAL:N	2.45	0.48
2:B:318:GLY:O	2:B:320:ASP:HA	2.13	0.48
6:F:388:THR:HG22	6:F:391:PHE:CD2	2.47	0.48
9:I:34:CYS:HB2	9:I:164:ILE:HB	1.95	0.48
13:M:185:THR:O	13:M:189:ILE:HG12	2.13	0.48
14:N:119:MET:HB2	20:T:57:TYR:HD2	1.79	0.48
19:S:192:ALA:HA	19:S:209:SER:HA	1.95	0.48
21:U:74:PHE:HD1	21:U:103:LYS:HD2	1.78	0.48
21:U:253:TYR:CZ	21:U:331:GLY:HA3	2.49	0.48
21:U:388:ASP:OD1	21:U:389:ASN:N	2.47	0.48
21:U:403:THR:HG23	21:U:777:HIS:NE2	2.29	0.48
28:b:114:GLY:HA2	28:b:143:PHE:O	2.13	0.48
2:B:431:GLN:NE2	9:I:170:ALA:HA	2.28	0.48
3:C:167:LEU:HG	3:C:171:HIS:HB2	1.95	0.48
3:C:271:ARG:HA	3:C:274:LEU:HB2	1.94	0.48
5:E:204:VAL:HG13	6:F:308:ARG:HH22	1.79	0.48
8:H:111:VAL:HG22	8:H:136:ILE:HD12	1.95	0.48
12:L:104:PRO:HD2	12:L:107:ARG:HH12	1.77	0.48
16:P:189:ILE:HG23	16:P:196:THR:HB	1.94	0.48
22:V:210:CYS:HA	22:V:213:TYR:HD2	1.78	0.48
22:V:289:LEU:HA	22:V:292:THR:HG22	1.96	0.48
23:W:262:LYS:HA	23:W:265:GLN:HG2	1.95	0.48
27:a:50:PHE:O	27:a:86:GLN:NE2	2.46	0.48
29:c:174:PRO:HB2	29:c:175:ARG:HH11	1.78	0.48
1:A:215:PHE:HB3	1:A:321:THR:HG23	1.95	0.48
3:C:191:PRO:O	3:C:193:GLY:HA3	2.13	0.48
4:D:104:GLY:HA2	4:D:109:SER:O	2.14	0.48
4:D:214:MET:HE1	33:D:501:ADP:C4	2.48	0.48
4:D:303:VAL:CG2	4:D:304:ASN:HB2	2.44	0.48
4:D:315:ASP:OD1	4:D:315:ASP:N	2.45	0.48
5:E:84:ARG:HD2	5:E:108:MET:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:139:SER:O	5:E:143:ARG:N	2.32	0.48
5:E:157:GLU:O	5:E:161:ARG:N	2.45	0.48
5:E:204:VAL:HB	6:F:261:ILE:HD12	1.95	0.48
6:F:230:GLY:HA2	6:F:231:THR:HB	1.96	0.48
8:H:45:VAL:HG22	8:H:212:ILE:HG22	1.96	0.48
10:J:120:GLN:O	11:K:134:SER:OG	2.25	0.48
12:L:69:HIS:HB2	12:L:137:TYR:HB2	1.96	0.48
32:f:191:LYS:HD2	32:f:478:LYS:HE2	1.96	0.48
2:B:151:LEU:HD13	3:C:96:VAL:HG11	1.96	0.48
4:D:162:VAL:O	4:D:221:HIS:NE2	2.44	0.48
4:D:244:PRO:HA	4:D:248:ARG:H	1.78	0.48
10:J:96:LEU:HA	17:Q:62:LYS:HE2	1.95	0.48
21:U:689:ILE:HG12	21:U:732:LEU:HD22	1.95	0.48
21:U:759:SER:HA	21:U:782:ALA:HA	1.95	0.48
23:W:435:LEU:HA	23:W:438:LEU:HB2	1.96	0.48
26:Z:239:ASP:O	29:c:308:VAL:HG13	2.13	0.48
29:c:290:VAL:O	29:c:293:THR:OG1	2.23	0.48
1:A:194:PRO:HB3	1:A:201:PHE:HE2	1.78	0.47
3:C:213:ARG:HH21	3:C:249:ASP:CG	2.22	0.47
3:C:256:SER:O	3:C:262:GLY:HA3	2.14	0.47
5:E:134:GLU:O	5:E:315:ILE:HD12	2.14	0.47
6:F:88:TYR:HB2	6:F:154:ASN:OD1	2.14	0.47
6:F:195:ILE:HA	6:F:198:LEU:HB3	1.94	0.47
18:R:50:ALA:HB2	19:S:129:SER:HB2	1.96	0.47
25:Y:178:ASN:HB3	25:Y:207:THR:HG22	1.96	0.47
32:f:617:LEU:HB3	32:f:618:THR:CB	2.36	0.47
3:C:233:GLU:O	3:C:237:MET:HG2	2.13	0.47
4:D:231:VAL:HA	4:D:265:ASP:O	2.14	0.47
4:D:244:PRO:O	4:D:248:ARG:HB3	2.14	0.47
6:F:170:SER:OG	6:F:171:ARG:N	2.47	0.47
7:G:54:LYS:HG2	7:G:214:GLU:O	2.15	0.47
9:I:76:VAL:HG21	9:I:83:ALA:HB1	1.96	0.47
12:L:11:THR:HG23	13:M:129:ARG:HB3	1.95	0.47
14:N:76:VAL:HG23	14:N:104:ASP:HB2	1.96	0.47
21:U:586:VAL:HG11	21:U:601:ARG:HH12	1.78	0.47
26:Z:83:LYS:NZ	26:Z:87:ALA:O	2.40	0.47
28:b:94:HIS:HD2	28:b:136:VAL:HG21	1.78	0.47
28:b:157:VAL:HG21	28:b:170:LEU:HB2	1.97	0.47
1:A:193:THR:O	1:A:200:ARG:NH1	2.47	0.47
2:B:155:LYS:HA	2:B:156:VAL:HA	1.55	0.47
4:D:147:ALA:O	5:E:62:LYS:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:346:VAL:HA	5:E:349:GLU:HB3	1.96	0.47
6:F:428:GLN:HG2	6:F:429:ALA:HB2	1.96	0.47
7:G:185:LYS:HB3	7:G:186:LYS:H	1.44	0.47
9:I:122:THR:O	10:J:125:ARG:NH1	2.47	0.47
21:U:541:HIS:HB2	21:U:544:ILE:HG22	1.96	0.47
22:V:96:ARG:HB2	22:V:107:ARG:HD2	1.96	0.47
25:Y:89:GLU:HA	25:Y:92:GLU:HG2	1.96	0.47
26:Z:63:LYS:CB	26:Z:64:ASP:HB2	2.33	0.47
28:b:97:LEU:HD23	28:b:107:MET:HB3	1.95	0.47
29:c:243:SER:HB2	29:c:244:VAL:HB	1.97	0.47
30:d:97:GLN:HB2	30:d:101:LEU:HG	1.96	0.47
30:d:164:THR:O	30:d:167:ILE:HG12	2.14	0.47
32:f:106:ALA:HB1	32:f:107:LEU:CA	2.44	0.47
32:f:371:CYS:O	32:f:372:ASN:HB2	2.13	0.47
2:B:167:THR:OG1	2:B:168:ASP:N	2.46	0.47
2:B:169:PRO:HB3	3:C:228:ALA:HB2	1.96	0.47
4:D:83:GLN:NE2	4:D:140:VAL:HG21	2.23	0.47
5:E:44:GLU:HB3	6:F:76:ASN:ND2	2.29	0.47
6:F:368:ILE:O	6:F:371:ARG:HG2	2.14	0.47
11:K:117:SER:HB3	12:L:82:ARG:HH22	1.79	0.47
13:M:40:ARG:HH11	13:M:148:LEU:HB3	1.78	0.47
13:M:80:LEU:HD23	13:M:82:ALA:H	1.80	0.47
21:U:241:ASN:HD21	21:U:244:MET:HG3	1.80	0.47
23:W:403:PHE:CD2	23:W:419:LYS:HE3	2.49	0.47
26:Z:96:HIS:HE1	26:Z:121:LEU:HD13	1.79	0.47
29:c:293:THR:O	29:c:297:VAL:HG23	2.14	0.47
1:A:97:ARG:HD3	2:B:130:GLU:O	2.15	0.47
1:A:111:TYR:O	1:A:123:VAL:N	2.47	0.47
1:A:187:LEU:O	1:A:191:VAL:HG12	2.14	0.47
2:B:375:ALA:HA	2:B:413:LYS:HD2	1.96	0.47
3:C:172:PRO:O	3:C:175:PHE:HB2	2.14	0.47
5:E:268:ASP:OD1	5:E:269:THR:N	2.47	0.47
14:N:7:GLN:HA	14:N:12:VAL:HG12	1.97	0.47
21:U:610:VAL:O	26:Z:177:ARG:NH2	2.47	0.47
26:Z:239:ASP:OD1	26:Z:239:ASP:N	2.47	0.47
26:Z:262:LEU:O	26:Z:266:ILE:HD12	2.13	0.47
30:d:167:ILE:HA	30:d:170:LEU:HB3	1.96	0.47
32:f:313:HIS:ND1	32:f:315:SER:HB2	2.29	0.47
32:f:568:PHE:HE2	32:f:677:GLU:HB3	1.80	0.47
2:B:178:LYS:HE2	3:C:285:ALA:HB2	1.97	0.47
2:B:274:ALA:HB1	2:B:325:VAL:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:68:GLU:HG3	29:c:190:GLN:HE21	1.80	0.47
3:C:194:THR:HB	33:C:501:ADP:C8	2.49	0.47
3:C:229:ARG:NH1	3:C:279:GLN:HE22	2.13	0.47
4:D:417:TYR:OH	7:G:22:LEU:HG	2.14	0.47
8:H:9:SER:O	8:H:11:THR:N	2.47	0.47
8:H:221:LEU:HD13	8:H:225:GLU:HB2	1.96	0.47
21:U:89:ASN:HB3	21:U:136:LYS:NZ	2.29	0.47
22:V:224:LEU:HD13	22:V:227:VAL:HB	1.96	0.47
26:Z:102:HIS:CD2	26:Z:104:ASN:HB3	2.49	0.47
26:Z:178:ASP:HB2	29:c:218:LEU:HD11	1.95	0.47
26:Z:228:TYR:CE2	27:a:215:GLU:OE1	2.66	0.47
27:a:335:TRP:CG	27:a:336:VAL:H	2.33	0.47
32:f:436:VAL:HG22	32:f:679:ARG:NH2	2.30	0.47
1:A:237:PHE:HB2	1:A:271:LEU:O	2.14	0.47
3:C:117:ARG:HD3	3:C:122:THR:OG1	2.15	0.47
3:C:194:THR:OG1	3:C:356:GLY:HA3	2.15	0.47
3:C:214:VAL:HG22	3:C:215:SER:H	1.80	0.47
4:D:86:PRO:HB3	5:E:81:VAL:HG12	1.96	0.47
4:D:282:ASP:OD1	5:E:251:ARG:NH2	2.47	0.47
5:E:44:GLU:OE2	6:F:77:SER:OG	2.33	0.47
5:E:55:GLN:N	6:F:133:PHE:O	2.48	0.47
5:E:62:LYS:O	5:E:70:ILE:N	2.47	0.47
5:E:215:ILE:HB	5:E:263:GLN:HE22	1.79	0.47
6:F:428:GLN:HA	6:F:429:ALA:HA	1.69	0.47
7:G:132:ARG:HB2	13:M:124:LEU:HA	1.96	0.47
11:K:52:LYS:HB3	11:K:59:MET:HE1	1.97	0.47
11:K:68:VAL:HG21	11:K:89:ILE:HG13	1.97	0.47
12:L:101:ARG:HH12	20:T:87:ALA:HB2	1.80	0.47
15:O:217:THR:HB	16:P:195:ILE:HB	1.97	0.47
17:Q:117:TYR:N	17:Q:125:ALA:O	2.47	0.47
18:R:127:SER:N	18:R:136:TYR:OH	2.43	0.47
19:S:11:THR:N	19:S:26:ASP:OD1	2.48	0.47
19:S:110:ILE:HG13	19:S:124:PHE:HE2	1.79	0.47
21:U:22:PHE:HE2	30:d:31:LEU:HD12	1.79	0.47
21:U:738:ASP:OD1	21:U:742:HIS:NE2	2.47	0.47
22:V:336:GLU:HA	22:V:339:LEU:HD12	1.96	0.47
27:a:97:LEU:HD11	27:a:117:ALA:HB1	1.97	0.47
29:c:255:TYR:HB2	29:c:287:HIS:HE1	1.80	0.47
29:c:261:GLU:HA	29:c:264:LYS:HE3	1.96	0.47
30:d:125:LYS:HD2	30:d:128:GLN:HE22	1.80	0.47
32:f:400:PRO:HB2	32:f:440:ALA:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:414:ILE:HG12	32:f:418:LEU:HD13	1.96	0.47
1:A:243:SER:HB3	2:B:264:PRO:HD3	1.96	0.47
2:B:314:ASN:HA	2:B:317:ASP:HB2	1.96	0.47
2:B:363:ARG:NH1	2:B:363:ARG:O	2.48	0.47
4:D:300:ASP:HA	4:D:301:GLN:HA	1.51	0.47
5:E:289:LEU:HD23	5:E:294:ARG:HD3	1.96	0.47
7:G:110:PRO:O	7:G:111:VAL:HG12	2.14	0.47
10:J:73:PHE:HA	10:J:131:ALA:HA	1.96	0.47
11:K:231:LYS:C	11:K:233:GLU:H	2.23	0.47
21:U:92:ASP:OD1	21:U:92:ASP:N	2.48	0.47
22:V:344:ASP:HB2	22:V:368:ARG:NH1	2.29	0.47
26:Z:195:VAL:HG11	29:c:230:THR:HB	1.97	0.47
29:c:243:SER:CB	29:c:244:VAL:HB	2.44	0.47
30:d:155:LYS:O	30:d:158:ILE:HD11	2.15	0.47
1:A:288:GLY:HA2	1:A:289:ALA:HA	1.65	0.47
1:A:384:GLU:H	2:B:343:ARG:NH1	2.09	0.47
3:C:184:LYS:HG3	3:C:311:ILE:HD12	1.96	0.47
4:D:133:HIS:CE1	4:D:135:HIS:HB2	2.49	0.47
5:E:47:LEU:HA	5:E:50:LEU:CD1	2.45	0.47
6:F:93:VAL:HG22	6:F:151:VAL:HG21	1.97	0.47
14:N:80:ALA:HA	14:N:83:PHE:HD2	1.80	0.47
17:Q:5:ILE:HG13	17:Q:7:ILE:HG13	1.96	0.47
21:U:118:LEU:HD23	21:U:121:GLY:O	2.15	0.47
21:U:167:ILE:HD12	21:U:204:ILE:HG21	1.97	0.47
21:U:581:SER:O	21:U:585:THR:OG1	2.27	0.47
22:V:432:GLU:HB3	30:d:196:ARG:HB3	1.96	0.47
25:Y:204:THR:HB	25:Y:246:ILE:HD13	1.96	0.47
25:Y:221:THR:HA	25:Y:224:VAL:HG12	1.97	0.47
27:a:145:LEU:HD12	27:a:146:PRO:HD2	1.97	0.47
1:A:83:ASP:HA	1:A:86:THR:HB	1.97	0.47
1:A:104:ALA:H	1:A:112:ILE:HG23	1.80	0.47
6:F:222:GLY:O	6:F:349:ASP:HB3	2.15	0.47
6:F:299:GLU:CG	6:F:300:LYS:HB3	2.40	0.47
6:F:344:ARG:HB3	6:F:347:ARG:HG3	1.97	0.47
7:G:17:SER:OG	7:G:21:ARG:HG2	2.15	0.47
10:J:84:ILE:O	10:J:88:ARG:HG3	2.14	0.47
13:M:34:SER:OG	13:M:65:ARG:NH2	2.36	0.47
19:S:211:ARG:NH2	19:S:213:ASP:OD2	2.46	0.47
22:V:280:ALA:HB1	22:V:281:ASN:ND2	2.30	0.47
25:Y:240:VAL:HG23	25:Y:241:ILE:HG13	1.97	0.47
26:Z:133:LEU:HB3	29:c:229:LEU:HG	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:ILE:O	2:B:350:LYS:HA	2.15	0.46
2:B:365:PHE:HD2	2:B:380:LEU:HD12	1.79	0.46
4:D:202:VAL:HG11	4:D:308:ILE:HG22	1.96	0.46
4:D:205:TYR:HA	4:D:311:THR:O	2.15	0.46
4:D:401:LYS:HA	4:D:404:LYS:HG2	1.96	0.46
5:E:381:GLU:HG2	6:F:351:LYS:HZ2	1.80	0.46
7:G:190:THR:H	7:G:193:GLN:HB3	1.80	0.46
10:J:85:ASN:OD1	17:Q:70:ARG:NH1	2.48	0.46
10:J:154:HIS:CE1	11:K:59:MET:HG3	2.50	0.46
11:K:11:GLY:O	11:K:12:VAL:HG22	2.14	0.46
11:K:203:LYS:HA	11:K:206:MET:HG2	1.96	0.46
13:M:20:VAL:HG12	13:M:22:GLN:H	1.80	0.46
21:U:32:ASN:OD1	21:U:33:ASP:N	2.44	0.46
25:Y:101:ARG:HA	25:Y:104:MET:HG2	1.96	0.46
25:Y:311:TYR:HD2	25:Y:314:LEU:HG	1.80	0.46
32:f:298:ASN:HA	32:f:299:GLU:HA	1.79	0.46
1:A:380:SER:HB3	1:A:385:ILE:CG2	2.45	0.46
2:B:187:ILE:HB	2:B:190:LEU:HD21	1.98	0.46
3:C:78:ARG:HB3	3:C:86:LEU:HD12	1.97	0.46
3:C:219:LEU:HD21	4:D:287:ARG:HG2	1.97	0.46
4:D:192:LYS:NZ	4:D:302:ASN:OD1	2.40	0.46
4:D:280:GLY:HA2	4:D:283:ARG:HD3	1.97	0.46
5:E:83:CYS:HA	5:E:107:ILE:HB	1.97	0.46
6:F:93:VAL:HA	6:F:124:ILE:HD12	1.97	0.46
10:J:10:PHE:HD2	11:K:23:GLN:HE21	1.62	0.46
13:M:197:ILE:HA	13:M:200:VAL:HG12	1.97	0.46
20:T:186:ARG:HE	20:T:202:PRO:HB2	1.81	0.46
22:V:58:ALA:HB2	22:V:201:ARG:HD2	1.97	0.46
23:W:299:ILE:HG22	23:W:301:LYS:H	1.79	0.46
27:a:325:ASP:O	27:a:330:ARG:N	2.49	0.46
28:b:156:PHE:O	28:b:160:LEU:HB2	2.16	0.46
29:c:226:MET:O	29:c:227:GLU:HG2	2.16	0.46
29:c:269:GLN:O	29:c:273:LYS:HG2	2.16	0.46
32:f:314:ASN:HA	32:f:319:ARG:HD2	1.95	0.46
32:f:600:LEU:HD11	32:f:641:LEU:HD13	1.96	0.46
1:A:125:LEU:HB3	1:A:149:ILE:HD12	1.98	0.46
1:A:388:VAL:HG13	1:A:413:VAL:CG2	2.45	0.46
2:B:111:THR:H	2:B:125:THR:HB	1.79	0.46
3:C:271:ARG:O	3:C:275:GLU:HG2	2.15	0.46
4:D:208:PRO:HA	4:D:209:GLY:C	2.39	0.46
5:E:356:ARG:NE	6:F:200:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:26:ARG:HD3	16:P:186:ILE:HB	1.98	0.46
19:S:93:SER:OG	19:S:128:GLY:O	2.28	0.46
22:V:250:LEU:HA	22:V:253:LEU:HD12	1.95	0.46
22:V:474:LEU:HD13	30:d:245:GLN:HG3	1.98	0.46
23:W:444:HIS:O	23:W:448:LYS:NZ	2.46	0.46
25:Y:357:ASN:OD1	25:Y:358:ARG:N	2.48	0.46
30:d:101:LEU:HD11	30:d:161:GLU:CD	2.41	0.46
32:f:390:GLU:HB3	32:f:391:LEU:HA	1.97	0.46
32:f:493:VAL:HG12	32:f:495:VAL:HG23	1.97	0.46
2:B:249:ARG:HG3	2:B:283:PHE:HD2	1.80	0.46
3:C:37:ASP:OD2	22:V:496:PHE:N	2.49	0.46
4:D:82:ILE:HA	4:D:83:GLN:HA	1.47	0.46
5:E:146:ARG:HH22	5:E:190:GLN:HG2	1.80	0.46
6:F:392:ASN:H	6:F:395:GLN:CD	2.23	0.46
11:K:69:GLU:HB2	11:K:228:MET:HE1	1.96	0.46
11:K:77:ALA:HB3	11:K:142:LEU:HB2	1.97	0.46
12:L:10:VAL:HG22	12:L:21:GLN:HG3	1.97	0.46
12:L:89:ARG:HE	19:S:77:HIS:CD2	2.33	0.46
21:U:49:TYR:O	21:U:57:ARG:NH2	2.48	0.46
22:V:241:ARG:HG3	22:V:242:HIS:H	1.81	0.46
23:W:431:LYS:O	23:W:434:SER:OG	2.21	0.46
25:Y:78:GLU:HA	25:Y:81:LEU:HB3	1.96	0.46
1:A:141:GLY:C	1:A:150:HIS:HB3	2.41	0.46
1:A:221:GLY:C	1:A:223:THR:H	2.23	0.46
1:A:382:GLY:HA3	33:A:501:ADP:C8	2.51	0.46
2:B:126:SER:HA	2:B:127:VAL:HA	1.42	0.46
6:F:92:ASN:OD1	6:F:93:VAL:N	2.43	0.46
6:F:334:ARG:HD3	6:F:336:ASP:HB3	1.97	0.46
8:H:93:LEU:HD11	8:H:113:ARG:HB3	1.97	0.46
13:M:57:LEU:HB2	13:M:58:TYR:HD1	1.81	0.46
16:P:135:ASP:OD1	16:P:136:PHE:N	2.44	0.46
17:Q:11:ASP:OD1	17:Q:11:ASP:N	2.47	0.46
17:Q:47:VAL:HB	17:Q:102:LEU:HG	1.97	0.46
22:V:100:MET:O	22:V:104:THR:HG23	2.15	0.46
25:Y:324:GLY:N	25:Y:325:VAL:HA	2.30	0.46
26:Z:193:ASN:HA	26:Z:196:HIS:CE1	2.49	0.46
26:Z:197:GLY:O	26:Z:201:LEU:HG	2.15	0.46
32:f:109:LEU:HA	32:f:110:ALA:HB3	1.96	0.46
32:f:446:ASN:C	32:f:448:LEU:H	2.23	0.46
32:f:645:LEU:HA	32:f:648:ARG:HB3	1.97	0.46
1:A:343:PHE:HA	1:A:344:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:TYR:CE1	10:J:12:PRO:HD2	2.50	0.46
2:B:220:LYS:HB2	2:B:346:ARG:NH2	2.30	0.46
4:D:269:ALA:HB1	5:E:255:ARG:HG2	1.97	0.46
6:F:102:ASN:HA	6:F:103:ASP:HA	1.69	0.46
10:J:88:ARG:NH2	17:Q:66:LEU:O	2.49	0.46
10:J:131:ALA:H	10:J:147:THR:HG1	1.60	0.46
19:S:27:THR:HB	19:S:39:ASP:HA	1.96	0.46
22:V:55:THR:HB	22:V:198:GLN:CD	2.41	0.46
22:V:363:LEU:HA	22:V:378:VAL:HG11	1.97	0.46
24:X:365:LEU:O	24:X:369:ILE:HD12	2.16	0.46
24:X:378:LEU:HA	24:X:385:LEU:HA	1.97	0.46
2:B:117:ASP:OD1	2:B:117:ASP:N	2.49	0.46
4:D:408:LYS:HB3	4:D:409:LYS:CB	2.45	0.46
4:D:413:GLU:HA	4:D:416:PHE:CG	2.50	0.46
6:F:358:ASN:HA	6:F:362:ARG:NH1	2.30	0.46
10:J:198:VAL:HA	10:J:199:VAL:HA	1.62	0.46
22:V:286:ALA:HB2	22:V:315:LYS:HB3	1.98	0.46
22:V:394:LEU:HD23	30:d:116:HIS:CE1	2.50	0.46
22:V:469:THR:HG21	26:Z:257:MET:SD	2.56	0.46
25:Y:108:ALA:HA	25:Y:111:LEU:HB2	1.97	0.46
25:Y:329:PHE:HZ	31:e:70:SER:HB2	1.80	0.46
26:Z:138:TYR:HB3	26:Z:155:PHE:HB3	1.98	0.46
29:c:49:VAL:HG22	29:c:116:PRO:HB3	1.97	0.46
29:c:54:MET:HE2	29:c:82:VAL:HG13	1.97	0.46
2:B:166:ASP:HB2	2:B:167:THR:O	2.16	0.46
3:C:97:VAL:HG11	3:C:122:THR:HA	1.97	0.46
4:D:244:PRO:HD3	4:D:288:ILE:CD1	2.45	0.46
4:D:258:ALA:HA	4:D:259:PRO:C	2.41	0.46
5:E:55:GLN:NE2	5:E:108:MET:SD	2.89	0.46
5:E:128:GLY:HA3	5:E:131:SER:H	1.81	0.46
5:E:375:ALA:O	5:E:379:LYS:N	2.46	0.46
6:F:138:GLY:O	6:F:159:LEU:HB2	2.16	0.46
11:K:123:PHE:HB2	11:K:134:SER:C	2.41	0.46
12:L:52:ALA:HB2	12:L:59:HIS:HA	1.98	0.46
21:U:363:SER:C	21:U:365:CYS:H	2.24	0.46
21:U:524:LYS:HB3	21:U:559:ARG:HE	1.81	0.46
23:W:420:ASP:HB3	23:W:422:ASN:CB	2.44	0.46
25:Y:50:MET:HE2	25:Y:74:LYS:HD2	1.98	0.46
32:f:281:ILE:HG23	32:f:282:LYS:H	1.81	0.46
1:A:100:LYS:HE2	1:A:115:VAL:HB	1.97	0.46
1:A:129:VAL:HG21	1:A:149:ILE:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:146:SER:HB2	3:C:150:MET:HB2	1.97	0.46
3:C:151:ILE:HD11	33:C:501:ADP:N7	2.31	0.46
4:D:60:TYR:HB2	21:U:603:LEU:HD21	1.98	0.46
4:D:91:GLN:N	4:D:104:GLY:O	2.49	0.46
4:D:105:SER:HB3	4:D:111:TYR:HE2	1.80	0.46
4:D:231:VAL:HG12	4:D:232:GLY:H	1.81	0.46
4:D:263:PHE:HB2	4:D:308:ILE:HD11	1.97	0.46
7:G:109:ILE:HG12	7:G:111:VAL:H	1.80	0.46
9:I:108:GLU:OE2	9:I:148:TYR:OH	2.33	0.46
12:L:33:SER:HB2	12:L:49:LEU:HD23	1.97	0.46
12:L:107:ARG:HE	20:T:77:LEU:HD13	1.79	0.46
13:M:83:ASP:HB2	13:M:133:CYS:SG	2.56	0.46
18:R:37:ILE:HG23	18:R:60:ALA:HB2	1.98	0.46
21:U:885:MET:HG2	21:U:887:ALA:H	1.81	0.46
22:V:258:TYR:HB3	22:V:265:ASP:OD2	2.15	0.46
25:Y:77:ASN:O	25:Y:81:LEU:N	2.49	0.46
32:f:301:ASP:OD1	32:f:301:ASP:N	2.44	0.46
32:f:662:LEU:H	32:f:664:ALA:CA	2.28	0.46
32:f:664:ALA:HB3	32:f:668:PRO:HD2	1.96	0.46
3:C:338:LEU:HD21	3:C:342:ILE:HG21	1.98	0.46
4:D:414:HIS:CE1	7:G:21:ARG:HB2	2.50	0.46
6:F:314:LEU:HG	6:F:347:ARG:HE	1.80	0.46
32:f:297:ARG:HA	32:f:298:ASN:C	2.41	0.46
32:f:350:LYS:HD2	32:f:390:GLU:HA	1.98	0.46
2:B:110:GLY:N	2:B:150:VAL:O	2.47	0.45
6:F:122:ALA:N	6:F:134:LEU:O	2.43	0.45
6:F:436:GLN:C	6:F:438:TYR:H	2.23	0.45
10:J:119:THR:HG22	10:J:126:PRO:HG3	1.99	0.45
12:L:137:TYR:CZ	12:L:216:GLY:HA2	2.51	0.45
13:M:58:TYR:CE2	13:M:62:SER:HB3	2.51	0.45
14:N:19:ARG:HH21	14:N:26:ILE:HG12	1.82	0.45
26:Z:45:LYS:HG3	26:Z:46:LYS:H	1.80	0.45
26:Z:67:VAL:HG13	28:b:92:VAL:HG23	1.98	0.45
27:a:245:VAL:HA	27:a:246:GLU:C	2.41	0.45
30:d:6:LYS:HD3	30:d:50:LEU:HG	1.97	0.45
32:f:653:GLY:O	32:f:656:HIS:NE2	2.49	0.45
1:A:338:ASP:OD1	1:A:339:ARG:N	2.45	0.45
1:A:411:GLU:HA	1:A:414:ASN:HD21	1.82	0.45
4:D:45:LYS:O	4:D:48:GLN:NE2	2.49	0.45
6:F:231:THR:HG22	6:F:233:LYS:HG3	1.99	0.45
6:F:310:MET:O	6:F:314:LEU:N	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:139:ILE:HG13	7:G:153:LYS:HG3	1.98	0.45
14:N:92:GLU:OE1	20:T:3:ASN:ND2	2.49	0.45
17:Q:47:VAL:O	17:Q:101:ASN:N	2.48	0.45
17:Q:91:CYS:SG	17:Q:98:TYR:HB2	2.56	0.45
20:T:27:LEU:HD13	20:T:184:TYR:HB3	1.98	0.45
21:U:20:LYS:HG2	21:U:48:LEU:HD21	1.97	0.45
22:V:156:SER:HB2	22:V:160:LEU:HG	1.98	0.45
25:Y:387:ILE:HA	25:Y:388:ASN:HA	1.70	0.45
26:Z:67:VAL:HG12	28:b:95:LEU:HD23	1.97	0.45
28:b:146:GLU:HG2	28:b:147:GLU:H	1.81	0.45
30:d:187:GLU:CD	30:d:188:LYS:H	2.23	0.45
30:d:201:ASN:OD1	30:d:201:ASN:N	2.49	0.45
32:f:400:PRO:HG3	32:f:441:TYR:CE1	2.51	0.45
32:f:568:PHE:CE2	32:f:677:GLU:HB3	2.51	0.45
2:B:115:ILE:HA	2:B:121:ALA:HA	1.98	0.45
2:B:140:ASP:O	2:B:144:LEU:HG	2.17	0.45
3:C:182:GLN:H	3:C:182:GLN:CD	2.24	0.45
3:C:378:VAL:HG12	3:C:379:THR:H	1.81	0.45
4:D:180:ALA:C	4:D:184:PRO:HG2	2.41	0.45
4:D:272:THR:HB	5:E:251:ARG:HE	1.81	0.45
5:E:174:GLY:C	5:E:176:PRO:HD2	2.42	0.45
6:F:225:MET:HE2	6:F:233:LYS:HG2	1.97	0.45
7:G:174:GLU:O	7:G:177:SER:OG	2.32	0.45
10:J:11:SER:OG	10:J:13:ASP:OD1	2.27	0.45
11:K:206:MET:HE1	11:K:210:LEU:HD13	1.97	0.45
13:M:72:HIS:CD2	13:M:73:VAL:HG23	2.52	0.45
21:U:900:TYR:HB3	21:U:914:LEU:HG	1.97	0.45
22:V:62:HIS:HA	22:V:65:ARG:HB3	1.98	0.45
26:Z:68:TRP:CE3	26:Z:108:ILE:HG13	2.51	0.45
26:Z:245:PHE:CE2	29:c:308:VAL:HG11	2.51	0.45
2:B:112:LEU:N	2:B:148:CYS:O	2.49	0.45
2:B:222:VAL:HA	2:B:346:ARG:HG2	1.98	0.45
3:C:114:VAL:HG21	3:C:123:LEU:HD13	1.97	0.45
6:F:70:LYS:HD2	6:F:73:ILE:HD11	1.98	0.45
6:F:312:GLU:HA	6:F:315:ASN:HB3	1.98	0.45
10:J:132:LEU:HD22	10:J:159:ASN:OD1	2.17	0.45
10:J:172:LEU:HD22	10:J:175:ASN:HD22	1.81	0.45
11:K:85:ALA:HB2	11:K:139:VAL:HG21	1.99	0.45
21:U:65:SER:HB3	21:U:96:TYR:OH	2.16	0.45
21:U:447:GLY:HA3	21:U:480:GLY:HA2	1.97	0.45
21:U:697:GLN:HG3	21:U:745:THR:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:794:ASP:OD1	21:U:795:LEU:N	2.49	0.45
22:V:31:ALA:HB3	22:V:32:PRO:HD3	1.97	0.45
22:V:305:ALA:HB1	22:V:335:VAL:HG11	1.99	0.45
26:Z:34:ARG:HB2	26:Z:97:THR:HG22	1.97	0.45
27:a:178:ARG:O	27:a:182:CYS:HB3	2.16	0.45
29:c:227:GLU:CD	29:c:234:TYR:HB2	2.40	0.45
30:d:122:LEU:HD12	30:d:125:LYS:H	1.82	0.45
1:A:261:PHE:HD2	1:A:305:GLN:HE21	1.64	0.45
1:A:299:MET:O	1:A:303:ILE:HG12	2.16	0.45
2:B:166:ASP:HA	2:B:167:THR:OG1	2.17	0.45
2:B:349:ARG:NE	2:B:351:ILE:HG22	2.32	0.45
2:B:365:PHE:HD1	2:B:395:ILE:HG12	1.82	0.45
3:C:209:CYS:HB3	3:C:243:PRO:HG2	1.99	0.45
5:E:62:LYS:HA	5:E:94:PRO:HB3	1.98	0.45
5:E:168:LYS:NZ	5:E:293:GLY:HA2	2.31	0.45
6:F:425:LEU:HA	6:F:428:GLN:O	2.17	0.45
7:G:12:HIS:HD2	13:M:7:TYR:HA	1.81	0.45
11:K:225:ASN:HB2	11:K:226:PHE:CD1	2.51	0.45
11:K:236:GLU:HG3	11:K:239:LYS:HE3	1.99	0.45
13:M:186:CYS:HA	13:M:189:ILE:HB	1.98	0.45
17:Q:81:ALA:HA	17:Q:104:LEU:HD12	1.98	0.45
18:R:80:SER:OG	18:R:120:ARG:NH2	2.36	0.45
21:U:342:LEU:O	21:U:346:ASN:HB2	2.16	0.45
21:U:415:HIS:NE2	21:U:418:GLU:HB3	2.32	0.45
21:U:563:ALA:O	21:U:567:ILE:HG12	2.17	0.45
22:V:192:MET:O	22:V:200:ARG:NH2	2.49	0.45
23:W:247:TYR:HB3	23:W:270:VAL:HG23	1.97	0.45
27:a:272:ILE:HA	27:a:275:LEU:HB3	1.98	0.45
1:A:168:GLU:HG2	1:A:169:LYS:HG2	1.97	0.45
3:C:82:LYS:HG3	3:C:84:LYS:HG3	1.98	0.45
4:D:87:LEU:HD12	4:D:87:LEU:HA	1.81	0.45
4:D:275:PHE:O	4:D:283:ARG:HD2	2.17	0.45
4:D:280:GLY:HA2	4:D:283:ARG:HB2	1.99	0.45
5:E:40:TYR:O	5:E:44:GLU:HG2	2.17	0.45
6:F:233:LYS:HA	6:F:236:LEU:HB3	1.97	0.45
9:I:182:GLY:N	9:I:183:GLU:HB2	2.31	0.45
13:M:150:MET:N	13:M:158:TYR:O	2.34	0.45
13:M:214:SER:HA	13:M:226:ILE:HA	1.98	0.45
21:U:152:GLY:O	21:U:156:GLU:HG2	2.16	0.45
22:V:309:MET:HB3	22:V:332:LEU:HG	1.99	0.45
22:V:416:ARG:CB	25:Y:349:LYS:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:349:LYS:C	25:Y:351:ASN:H	2.23	0.45
25:Y:357:ASN:CB	25:Y:358:ARG:HA	2.46	0.45
26:Z:181:ASP:HA	26:Z:182:THR:HA	1.72	0.45
27:a:243:GLY:HA3	27:a:244:ASN:HA	1.67	0.45
29:c:149:GLN:HB2	29:c:156:VAL:HG13	1.99	0.45
29:c:176:GLN:O	29:c:177:THR:OG1	2.30	0.45
1:A:187:LEU:O	1:A:190:VAL:HG12	2.16	0.45
1:A:298:THR:HA	1:A:301:GLU:HB3	1.98	0.45
1:A:428:ARG:HD3	1:A:431:THR:OG1	2.17	0.45
2:B:283:PHE:HB2	2:B:328:ILE:HB	1.99	0.45
2:B:294:ARG:HD2	2:B:295:TYR:H	1.82	0.45
6:F:84:LYS:NZ	6:F:139:LEU:HD23	2.31	0.45
7:G:62:ASP:CG	13:M:40:ARG:HH22	2.25	0.45
7:G:138:MET:O	7:G:154:CYS:N	2.49	0.45
9:I:197:LEU:HB3	9:I:206:LEU:HD11	1.99	0.45
23:W:428:TRP:HE1	26:Z:252:LYS:HD3	1.81	0.45
26:Z:165:GLU:H	26:Z:168:GLU:HG3	1.81	0.45
27:a:77:VAL:HA	27:a:80:ILE:HG22	1.99	0.45
30:d:191:PHE:HB2	30:d:220:ASN:HA	1.99	0.45
32:f:680:PRO:HB3	32:f:683:VAL:HB	1.99	0.45
1:A:174:TYR:OH	1:A:192:GLU:OE1	2.28	0.45
1:A:222:LYS:HZ3	2:B:319:PHE:HB2	1.82	0.45
5:E:188:ALA:HB2	5:E:231:PHE:CE2	2.52	0.45
10:J:115:LYS:O	10:J:119:THR:HG23	2.17	0.45
12:L:107:ARG:NH2	20:T:79:ASP:OD2	2.50	0.45
19:S:172:MET:HE1	19:S:195:ILE:HG21	1.99	0.45
20:T:136:SER:HB2	20:T:150:LEU:HD13	1.99	0.45
22:V:416:ARG:HA	22:V:458:VAL:O	2.17	0.45
23:W:268:LYS:HA	23:W:271:VAL:HG12	1.98	0.45
27:a:50:PHE:N	27:a:51:ALA:HA	2.32	0.45
28:b:11:ASP:OD2	28:b:114:GLY:N	2.39	0.45
28:b:86:PHE:HB2	28:b:117:VAL:HG21	1.98	0.45
29:c:170:LEU:HG	29:c:171:GLY:H	1.82	0.45
29:c:258:ALA:O	29:c:261:GLU:HG2	2.17	0.45
29:c:268:GLU:O	29:c:272:ILE:HD12	2.16	0.45
30:d:118:GLU:HA	30:d:121:ARG:HH12	1.81	0.45
31:e:56:LEU:O	31:e:59:GLU:HB2	2.16	0.45
32:f:268:THR:OG1	32:f:654:LYS:O	2.33	0.45
2:B:95:GLU:O	2:B:99:VAL:HG22	2.16	0.45
2:B:131:HIS:CD2	2:B:157:HIS:HB2	2.52	0.45
3:C:76:VAL:HG22	3:C:110:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:229:ARG:HH11	3:C:279:GLN:HE22	1.63	0.45
4:D:375:ILE:O	4:D:379:CYS:N	2.36	0.45
5:E:84:ARG:HH22	6:F:117:ARG:HH12	1.65	0.45
6:F:161:LEU:HG	6:F:162:GLU:N	2.32	0.45
7:G:88:ARG:NH1	13:M:156:VAL:HA	2.32	0.45
13:M:71:ARG:O	13:M:224:HIS:N	2.47	0.45
13:M:140:TYR:HE2	13:M:218:GLU:HB2	1.82	0.45
14:N:26:ILE:HG21	14:N:29:ARG:HE	1.82	0.45
18:R:34:VAL:HG11	18:R:177:TYR:HD2	1.82	0.45
22:V:94:VAL:HG22	22:V:138:PRO:HD3	1.99	0.45
25:Y:131:THR:O	25:Y:137:ARG:NH1	2.50	0.45
27:a:100:THR:HA	27:a:103:LYS:HE2	1.99	0.45
27:a:144:ASN:HA	27:a:145:LEU:HA	1.58	0.45
30:d:36:LEU:HB2	30:d:37:PRO:HA	1.99	0.45
32:f:481:LYS:O	32:f:484:PRO:HD2	2.17	0.45
32:f:571:GLY:HA2	32:f:605:LEU:HD21	1.99	0.45
1:A:96:ALA:HB3	2:B:132:TYR:HE2	1.79	0.45
1:A:112:ILE:HB	1:A:122:VAL:HG13	1.98	0.45
1:A:164:MET:O	1:A:239:ARG:NH2	2.50	0.45
3:C:11:LEU:HD23	3:C:14:GLY:HA2	1.99	0.45
4:D:240:LEU:HB2	4:D:284:GLU:OE1	2.16	0.45
6:F:365:ILE:HG13	6:F:366:MET:N	2.31	0.45
15:O:98:LEU:HB2	15:O:113:ILE:HD12	1.98	0.45
21:U:505:ASP:HB3	21:U:508:THR:HG22	1.99	0.45
21:U:607:VAL:O	21:U:615:ARG:NH1	2.49	0.45
21:U:742:HIS:HB2	21:U:883:ARG:HH12	1.82	0.45
22:V:225:ASP:HA	22:V:228:ARG:HG3	1.98	0.45
22:V:451:ILE:HB	22:V:453:HIS:CE1	2.52	0.45
25:Y:101:ARG:HD3	25:Y:130:LYS:HD3	1.99	0.45
25:Y:286:TRP:O	25:Y:287:LEU:HG	2.17	0.45
26:Z:185:GLY:O	26:Z:189:GLN:NE2	2.50	0.45
26:Z:196:HIS:HA	29:c:231:LEU:HG	1.99	0.45
26:Z:253:THR:O	26:Z:257:MET:HG2	2.17	0.45
27:a:254:ALA:HA	27:a:261:LEU:HD23	1.99	0.45
32:f:589:LEU:HD13	32:f:602:MET:HE3	1.99	0.45
3:C:274:LEU:HD21	3:C:306:LEU:HD23	1.99	0.44
4:D:362:ASP:OD1	4:D:363:TYR:N	2.50	0.44
4:D:418:LYS:HE2	8:H:33:ALA:N	2.32	0.44
6:F:327:LYS:N	6:F:327:LYS:HD2	2.32	0.44
6:F:423:GLY:HA2	6:F:426:GLU:HB3	1.98	0.44
7:G:212:PRO:HG3	7:G:236:ASP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:169:ALA:HB3	11:K:178:GLN:HG2	1.99	0.44
13:M:110:HIS:NE2	14:N:70:LEU:HA	2.32	0.44
14:N:177:ALA:HA	14:N:186:ARG:HA	1.98	0.44
16:P:93:ASN:O	16:P:97:GLU:HG3	2.17	0.44
21:U:501:LEU:HD11	21:U:544:ILE:HD11	1.98	0.44
22:V:98:LEU:HA	22:V:99:ARG:HA	1.69	0.44
23:W:432:LEU:HD13	29:c:241:ASN:HB3	1.98	0.44
26:Z:68:TRP:HD1	26:Z:104:ASN:HD21	1.64	0.44
26:Z:258:VAL:O	26:Z:262:LEU:HG	2.17	0.44
29:c:213:GLU:HA	29:c:216:MET:HG2	1.99	0.44
32:f:570:MET:O	32:f:573:VAL:HG12	2.17	0.44
1:A:166:VAL:HG22	1:A:238:ILE:HG12	2.00	0.44
3:C:161:ILE:HD12	3:C:164:VAL:HB	1.99	0.44
4:D:289:LEU:HA	4:D:292:LEU:HG	1.99	0.44
6:F:300:LYS:HD2	6:F:304:ARG:HH21	1.82	0.44
9:I:220:ASN:HA	9:I:221:GLY:HA2	1.55	0.44
14:N:21:THR:HG22	14:N:26:ILE:HG13	1.98	0.44
18:R:55:TRP:CD2	18:R:87:VAL:HG22	2.53	0.44
18:R:157:ARG:HD3	18:R:195:LEU:HD22	1.99	0.44
20:T:122:LEU:HG	20:T:137:LEU:HD12	1.98	0.44
20:T:145:LEU:HD13	20:T:175:VAL:HG12	2.00	0.44
21:U:9:ILE:HG12	21:U:38:ILE:HG23	1.99	0.44
22:V:25:GLU:O	22:V:28:PRO:HD2	2.17	0.44
22:V:266:GLN:HB3	22:V:299:GLN:HE22	1.83	0.44
25:Y:318:TYR:HA	25:Y:321:GLU:HG3	1.99	0.44
29:c:295:ASN:HA	29:c:298:GLN:HG2	1.98	0.44
32:f:662:LEU:N	32:f:663:VAL:HA	2.32	0.44
2:B:153:ASN:O	2:B:157:HIS:HA	2.17	0.44
2:B:249:ARG:NH1	3:C:278:ASN:O	2.50	0.44
3:C:268:GLU:O	3:C:272:THR:N	2.47	0.44
4:D:105:SER:OG	4:D:107:THR:OG1	2.25	0.44
6:F:255:GLN:O	6:F:258:GLN:NE2	2.50	0.44
7:G:168:ALA:O	7:G:172:GLN:NE2	2.50	0.44
9:I:68:LEU:HD12	9:I:69:ASN:HB2	1.99	0.44
11:K:117:SER:HB2	12:L:82:ARG:HH12	1.82	0.44
21:U:424:ALA:HA	21:U:427:LEU:HD13	2.00	0.44
21:U:889:LEU:HD23	21:U:892:LEU:HD21	1.98	0.44
22:V:188:SER:O	22:V:200:ARG:NH2	2.40	0.44
22:V:194:LYS:HA	22:V:195:ILE:HA	1.54	0.44
23:W:367:ALA:HB1	23:W:416:GLN:OE1	2.18	0.44
28:b:164:ASP:H	28:b:165:GLY:HA2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:238:CYS:HA	29:c:241:ASN:ND2	2.32	0.44
1:A:301:GLU:HG3	6:F:254:PRO:HG3	1.98	0.44
2:B:184:TYR:HD2	2:B:240:ALA:HB1	1.82	0.44
3:C:28:ILE:HG22	4:D:51:LEU:HD11	1.99	0.44
3:C:73:VAL:HA	3:C:115:ALA:HA	1.99	0.44
3:C:216:GLY:O	3:C:220:VAL:HG22	2.16	0.44
3:C:363:CYS:O	3:C:367:GLY:N	2.43	0.44
4:D:201:GLY:O	4:D:329:ARG:HB2	2.17	0.44
4:D:274:ARG:HD2	4:D:274:ARG:HA	1.76	0.44
5:E:117:PRO:HG2	5:E:214:LEU:HD11	1.98	0.44
7:G:52:THR:O	7:G:216:GLU:N	2.37	0.44
7:G:62:ASP:O	7:G:66:VAL:HG23	2.17	0.44
9:I:156:TYR:HE2	10:J:58:THR:HB	1.82	0.44
21:U:407:SER:O	21:U:411:ILE:HG13	2.17	0.44
25:Y:80:GLU:HA	25:Y:83:ARG:HG2	2.00	0.44
25:Y:268:TYR:CZ	25:Y:307:LEU:HD12	2.52	0.44
25:Y:363:ASN:O	25:Y:367:GLN:HB2	2.17	0.44
26:Z:96:HIS:CE1	26:Z:123:ILE:HG12	2.53	0.44
26:Z:242:LEU:HB2	27:a:288:HIS:NE2	2.32	0.44
28:b:20:ASP:OD1	28:b:25:ARG:NE	2.49	0.44
30:d:3:GLU:HB3	30:d:4:GLN:CA	2.42	0.44
30:d:123:PRO:O	30:d:127:ILE:HG12	2.18	0.44
1:A:170:PRO:HB2	1:A:230:ALA:HA	2.00	0.44
1:A:206:ILE:HG23	1:A:207:GLU:N	2.29	0.44
2:B:313:LEU:HD22	2:B:341:LEU:HA	1.98	0.44
3:C:380:GLN:O	3:C:384:GLU:N	2.40	0.44
4:D:186:THR:HG23	4:D:187:HIS:CD2	2.53	0.44
4:D:263:PHE:CD1	4:D:308:ILE:HG13	2.52	0.44
4:D:371:SER:HA	4:D:372:GLY:HA3	1.72	0.44
6:F:338:LEU:HD13	6:F:342:LEU:HD12	2.00	0.44
8:H:87:VAL:O	8:H:91:ARG:HG2	2.17	0.44
10:J:173:GLU:HA	10:J:176:TYR:HD2	1.82	0.44
13:M:92:ARG:CZ	20:T:76:LEU:HD12	2.48	0.44
16:P:53:LEU:HD23	16:P:107:PRO:HA	2.00	0.44
16:P:190:ILE:HG22	16:P:195:ILE:HG23	2.00	0.44
24:X:411:VAL:HA	24:X:414:LEU:HD12	1.97	0.44
25:Y:283:LYS:HE2	25:Y:292:TYR:CZ	2.53	0.44
27:a:219:HIS:ND1	27:a:221:VAL:HG22	2.33	0.44
32:f:283:SER:HG	32:f:643:SER:HG	1.60	0.44
32:f:458:SER:O	32:f:459:GLU:HB2	2.17	0.44
32:f:567:ILE:HG21	32:f:602:MET:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:638:LEU:HA	32:f:639:THR:C	2.42	0.44
1:A:143:ASP:O	1:A:147:TYR:N	2.46	0.44
1:A:244:GLU:HG2	2:B:268:ARG:NH2	2.32	0.44
2:B:203:LEU:HD21	2:B:211:TYR:HB2	2.00	0.44
2:B:230:THR:HA	33:B:501:ADP:O2A	2.17	0.44
2:B:343:ARG:HA	2:B:347:ILE:HD13	2.00	0.44
3:C:115:ALA:O	3:C:124:HIS:N	2.33	0.44
3:C:203:VAL:HA	3:C:206:HIS:HB2	2.00	0.44
3:C:228:ALA:O	3:C:230:MET:HG2	2.18	0.44
3:C:260:GLU:O	3:C:263:SER:OG	2.32	0.44
3:C:300:ILE:HD13	3:C:300:ILE:HA	1.84	0.44
5:E:270:LEU:O	5:E:273:VAL:HG12	2.16	0.44
5:E:349:GLU:OE2	6:F:350:ARG:NH1	2.50	0.44
6:F:76:ASN:O	6:F:80:ILE:HG13	2.18	0.44
7:G:16:PHE:CZ	8:H:130:PHE:HB3	2.53	0.44
7:G:86:ASP:OD1	13:M:120:HIS:NE2	2.50	0.44
11:K:219:THR:O	11:K:228:MET:N	2.50	0.44
12:L:168:ALA:HB1	12:L:194:ALA:HB1	2.00	0.44
14:N:55:VAL:HA	14:N:86:MET:HE1	1.99	0.44
15:O:110:LEU:HD21	15:O:125:VAL:HG22	1.98	0.44
20:T:45:VAL:HG12	20:T:46:ASN:ND2	2.33	0.44
21:U:107:HIS:HA	21:U:110:LYS:HE3	1.99	0.44
21:U:431:THR:C	21:U:433:PRO:HD3	2.43	0.44
25:Y:34:ASP:OD1	25:Y:34:ASP:N	2.47	0.44
25:Y:238:GLU:O	25:Y:242:LYS:HB2	2.18	0.44
26:Z:176:LEU:HD12	26:Z:177:ARG:N	2.33	0.44
30:d:103:LEU:HD12	30:d:106:LEU:HD22	1.98	0.44
32:f:268:THR:HB	32:f:656:HIS:HD2	1.82	0.44
32:f:391:LEU:CD1	32:f:392:LYS:H	2.24	0.44
1:A:306:LEU:HA	1:A:312:ARG:NE	2.33	0.44
2:B:178:LYS:HB3	2:B:180:PRO:HD3	1.99	0.44
3:C:113:ARG:HG2	3:C:127:LEU:HB2	2.00	0.44
3:C:151:ILE:HD12	3:C:151:ILE:HA	1.88	0.44
3:C:243:PRO:HA	3:C:288:ASN:HB3	1.99	0.44
4:D:145:PRO:HB2	4:D:146:GLU:HB2	1.99	0.44
4:D:232:GLY:HA3	4:D:269:ALA:HB3	1.99	0.44
4:D:337:ASP:C	4:D:341:LYS:HG2	2.43	0.44
5:E:289:LEU:HA	5:E:294:ARG:HD2	1.99	0.44
6:F:145:LEU:HG	6:F:146:LYS:HG2	2.00	0.44
7:G:165:ALA:HB3	8:H:56:LEU:HD22	2.00	0.44
11:K:146:VAL:HG22	11:K:151:PRO:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:154:PHE:HB3	11:K:162:PHE:CE1	2.50	0.44
17:Q:85:ARG:HD2	17:Q:124:LEU:HD11	1.99	0.44
22:V:239:THR:HA	22:V:240:LEU:HA	1.65	0.44
22:V:328:VAL:O	22:V:332:LEU:HB2	2.18	0.44
23:W:306:LEU:O	23:W:310:THR:HG22	2.17	0.44
27:a:219:HIS:HB3	27:a:222:LEU:HG	2.00	0.44
32:f:251:ALA:HA	32:f:254:SER:HB2	1.98	0.44
4:D:229:ARG:CZ	5:E:267:PHE:HB3	2.47	0.44
4:D:263:PHE:HD1	4:D:308:ILE:HG13	1.83	0.44
4:D:348:ILE:HG12	4:D:379:CYS:HB3	1.99	0.44
5:E:232:MET:N	5:E:276:ILE:O	2.47	0.44
5:E:257:LEU:O	5:E:261:LEU:HG	2.18	0.44
6:F:93:VAL:HB	6:F:147:PRO:HB3	1.99	0.44
7:G:183:VAL:HG13	7:G:189:TRP:CZ2	2.52	0.44
8:H:191:ALA:HA	8:H:194:THR:HG22	1.99	0.44
12:L:197:GLU:OE1	12:L:197:GLU:N	2.51	0.44
19:S:206:GLU:HG2	19:S:207:THR:H	1.83	0.44
21:U:74:PHE:CD1	21:U:103:LYS:HD2	2.53	0.44
21:U:554:LEU:HD11	21:U:761:VAL:HG13	1.99	0.44
22:V:470:ARG:HD2	30:d:242:LEU:HD21	1.99	0.44
23:W:407:ASP:HB2	24:X:344:ARG:HG2	1.99	0.44
25:Y:46:ARG:C	25:Y:48:ASN:H	2.26	0.44
29:c:242:GLU:CA	29:c:245:VAL:HB	2.48	0.44
32:f:483:ALA:HB3	32:f:484:PRO:HD3	1.99	0.44
1:A:262:GLU:O	1:A:266:THR:N	2.50	0.44
2:B:211:TYR:CD1	2:B:218:PRO:HD2	2.52	0.44
2:B:427:LEU:HD12	2:B:430:LYS:HD2	1.99	0.44
4:D:355:SER:HB3	4:D:358:VAL:HG23	2.00	0.44
5:E:124:HIS:CE1	6:F:320:PHE:HA	2.53	0.44
5:E:378:LYS:HZ2	6:F:351:LYS:HE2	1.82	0.44
7:G:27:TYR:HD1	7:G:30:LYS:HE2	1.83	0.44
10:J:92:GLN:HG3	17:Q:62:LYS:HB3	1.99	0.44
12:L:91:GLU:HB3	12:L:108:LEU:HD11	2.00	0.44
13:M:140:TYR:HB3	13:M:217:GLY:HA2	2.00	0.44
22:V:416:ARG:HB3	25:Y:349:LYS:HB3	1.99	0.44
28:b:101:GLN:HB3	29:c:101:GLN:HB3	1.98	0.44
32:f:672:VAL:HG23	32:f:673:THR:H	1.83	0.44
1:A:214:LEU:HB2	1:A:320:ALA:HA	2.00	0.43
1:A:311:PRO:N	1:A:312:ARG:HA	2.33	0.43
2:B:194:ILE:HA	2:B:197:ILE:HG22	2.00	0.43
2:B:295:TYR:CG	2:B:299:SER:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:GLU:O	3:C:65:LEU:N	2.44	0.43
3:C:229:ARG:NH1	3:C:232:ARG:HB2	2.33	0.43
4:D:89:ILE:HG12	4:D:143:LEU:HD21	1.99	0.43
4:D:164:TYR:HE2	4:D:222:HIS:HE1	1.65	0.43
4:D:260:ALA:H	4:D:304:ASN:ND2	2.12	0.43
5:E:178:THR:HG23	33:E:401:ADP:H8	1.82	0.43
9:I:24:ALA:O	9:I:28:ILE:HD12	2.18	0.43
22:V:137:GLU:N	22:V:138:PRO:HD2	2.33	0.43
22:V:167:LEU:HD12	22:V:168:GLN:N	2.33	0.43
22:V:265:ASP:HA	22:V:268:GLU:HB3	2.00	0.43
22:V:451:ILE:HG23	22:V:458:VAL:HA	1.99	0.43
22:V:455:LYS:HD2	22:V:457:TYR:HE2	1.83	0.43
22:V:495:ARG:HH12	26:Z:282:ASN:HA	1.82	0.43
27:a:18:GLN:HG3	27:a:22:TRP:CD1	2.53	0.43
30:d:191:PHE:O	30:d:194:ALA:N	2.51	0.43
32:f:52:ILE:HG13	32:f:64:GLU:HG2	2.00	0.43
1:A:217:PRO:HA	1:A:428:ARG:NE	2.33	0.43
1:A:384:GLU:HB2	2:B:347:ILE:HD11	2.00	0.43
2:B:116:ILE:O	2:B:119:ASN:N	2.47	0.43
3:C:369:TYR:O	3:C:373:GLU:N	2.49	0.43
6:F:366:MET:HA	6:F:369:HIS:HB2	2.00	0.43
9:I:99:LEU:HD13	16:P:69:PHE:HB2	1.99	0.43
13:M:11:ALA:HA	13:M:20:VAL:HG11	2.00	0.43
21:U:570:LEU:HD22	21:U:578:LEU:HD11	2.00	0.43
26:Z:30:GLY:HA3	26:Z:31:ASN:OD1	2.18	0.43
27:a:100:THR:HA	27:a:103:LYS:HG2	2.01	0.43
27:a:192:GLU:OE2	27:a:196:ARG:NH2	2.49	0.43
27:a:346:ILE:HA	27:a:349:MET:HE2	2.00	0.43
30:d:233:GLU:HB3	30:d:235:THR:HG23	1.99	0.43
2:B:249:ARG:HG3	2:B:283:PHE:CD2	2.53	0.43
3:C:41:ASN:ND2	22:V:492:LYS:HA	2.34	0.43
4:D:274:ARG:HE	5:E:248:SER:HB3	1.82	0.43
7:G:130:GLU:HG3	8:H:4:ARG:HD3	2.01	0.43
13:M:51:LYS:HB3	13:M:210:GLU:HB3	2.00	0.43
19:S:112:GLY:HA2	19:S:198:VAL:HG11	1.99	0.43
20:T:20:VAL:HG23	20:T:120:SER:HB3	2.00	0.43
21:U:681:ASN:OD1	21:U:681:ASN:N	2.51	0.43
23:W:423:ASN:HB2	26:Z:255:ASP:OD1	2.18	0.43
25:Y:295:TYR:O	25:Y:299:MET:HG2	2.18	0.43
26:Z:105:ASP:HA	26:Z:108:ILE:HD13	1.99	0.43
27:a:278:MET:HE1	27:a:339:ARG:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:33:ILE:HD11	29:c:207:TYR:CD1	2.54	0.43
2:B:302:GLU:O	2:B:306:GLN:N	2.44	0.43
3:C:43:ARG:HD3	21:U:639:LEU:HB2	1.99	0.43
3:C:196:LYS:HE3	3:C:252:ASP:OD2	2.18	0.43
4:D:143:LEU:HB3	4:D:144:PRO:HD2	2.00	0.43
6:F:222:GLY:HA3	6:F:347:ARG:O	2.18	0.43
6:F:300:LYS:HD2	6:F:304:ARG:NH2	2.33	0.43
10:J:96:LEU:HG	17:Q:58:GLU:HB3	2.00	0.43
21:U:764:LEU:HA	21:U:767:THR:HG23	2.00	0.43
23:W:312:MET:HG3	23:W:365:ILE:HD13	2.00	0.43
24:X:406:ASN:HA	24:X:409:LYS:HB2	1.99	0.43
32:f:462:ASP:C	32:f:464:LYS:H	2.25	0.43
32:f:680:PRO:O	32:f:681:LEU:C	2.62	0.43
1:A:173:THR:OG1	1:A:174:TYR:N	2.50	0.43
1:A:417:ILE:O	1:A:421:ALA:N	2.51	0.43
2:B:288:ASP:OD2	3:C:271:ARG:NH2	2.52	0.43
4:D:341:LYS:HA	4:D:344:ILE:HG22	2.00	0.43
5:E:135:ILE:HD12	5:E:183:LEU:HD12	1.99	0.43
7:G:12:HIS:CD2	13:M:7:TYR:HA	2.54	0.43
9:I:57:ASP:HB3	9:I:59:VAL:HG13	2.00	0.43
19:S:193:LEU:N	19:S:208:VAL:O	2.41	0.43
21:U:742:HIS:O	21:U:883:ARG:NH2	2.52	0.43
21:U:842:LYS:HE3	21:U:843:GLU:O	2.18	0.43
22:V:32:PRO:O	22:V:36:GLU:HB3	2.19	0.43
22:V:487:HIS:ND1	26:Z:279:LYS:HD2	2.33	0.43
23:W:276:LEU:HD21	23:W:350:ARG:NH1	2.34	0.43
23:W:373:ILE:HG13	27:a:326:GLU:HB2	2.00	0.43
25:Y:63:TRP:HB3	25:Y:64:GLN:CB	2.47	0.43
29:c:55:GLY:HA3	29:c:112:TYR:CZ	2.53	0.43
30:d:188:LYS:HG3	30:d:221:ASN:HD21	1.82	0.43
32:f:336:GLU:HG3	32:f:337:ASP:H	1.83	0.43
1:A:102:ILE:HD11	1:A:136:GLU:HA	2.00	0.43
1:A:134:ILE:HD12	1:A:152:PRO:HG3	1.99	0.43
1:A:171:ASP:C	1:A:230:ALA:HB2	2.43	0.43
1:A:299:MET:HG3	1:A:300:LEU:H	1.83	0.43
1:A:322:ASN:OD1	1:A:428:ARG:NH2	2.52	0.43
1:A:335:GLY:HA2	6:F:394:ALA:HB3	1.99	0.43
3:C:42:LEU:HD12	3:C:45:LEU:HB2	2.00	0.43
4:D:293:LEU:HG	4:D:326:ARG:CZ	2.49	0.43
4:D:303:VAL:HG23	4:D:304:ASN:HB2	2.01	0.43
6:F:188:ILE:HD11	6:F:236:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:229:PRO:HA	6:F:230:GLY:HA2	1.77	0.43
7:G:88:ARG:CZ	13:M:157:SER:H	2.31	0.43
14:N:19:ARG:HE	14:N:26:ILE:HG12	1.84	0.43
22:V:31:ALA:O	22:V:35:VAL:HG22	2.18	0.43
22:V:90:GLU:OE1	22:V:90:GLU:N	2.50	0.43
22:V:329:HIS:HD2	22:V:353:LEU:HD21	1.84	0.43
24:X:405:GLN:O	24:X:409:LYS:HD3	2.19	0.43
27:a:124:ASN:C	27:a:126:GLY:HA2	2.43	0.43
27:a:220:PRO:O	27:a:223:GLU:HG2	2.17	0.43
29:c:247:GLU:OE1	29:c:247:GLU:N	2.51	0.43
29:c:263:ASP:O	29:c:266:THR:OG1	2.36	0.43
32:f:662:LEU:N	32:f:664:ALA:HA	2.33	0.43
2:B:93:GLU:HG3	2:B:94:GLU:H	1.82	0.43
2:B:114:GLU:HG3	2:B:122:ILE:HB	2.00	0.43
2:B:304:GLU:HA	2:B:307:ARG:HG2	2.00	0.43
4:D:99:ASN:O	4:D:115:ILE:N	2.36	0.43
5:E:60:VAL:N	5:E:96:THR:O	2.49	0.43
5:E:309:ARG:O	5:E:312:ILE:HG22	2.19	0.43
7:G:142:GLY:N	7:G:150:GLN:O	2.52	0.43
18:R:53:SER:O	18:R:57:ARG:HG2	2.18	0.43
20:T:15:LYS:HE2	20:T:122:LEU:H	1.83	0.43
21:U:163:PHE:CE2	21:U:201:LEU:HD21	2.54	0.43
21:U:338:HIS:CE1	21:U:785:PRO:HB3	2.54	0.43
21:U:356:THR:HG22	21:U:717:ILE:HD13	2.00	0.43
22:V:25:GLU:HB2	22:V:26:PRO:HD3	2.00	0.43
22:V:275:VAL:N	22:V:276:PHE:HA	2.32	0.43
23:W:244:CYS:HA	23:W:273:TYR:CE1	2.54	0.43
23:W:436:MET:HG2	29:c:239:LYS:HG2	2.01	0.43
25:Y:145:LEU:HD13	25:Y:183:TYR:CD1	2.54	0.43
28:b:4:GLU:HG3	28:b:108:ARG:HE	1.84	0.43
30:d:148:TYR:CE2	30:d:178:ILE:HD13	2.54	0.43
32:f:510:GLU:C	32:f:512:ALA:H	2.27	0.43
1:A:283:ALA:HA	1:A:284:ARG:HA	1.69	0.43
3:C:215:SER:HA	3:C:216:GLY:HA3	1.51	0.43
12:L:84:LEU:HA	12:L:87:PHE:HB3	2.01	0.43
19:S:21:ALA:HB3	19:S:198:VAL:HB	2.00	0.43
22:V:290:TYR:HB2	22:V:312:ALA:HB1	2.01	0.43
22:V:359:PRO:HB3	22:V:382:PHE:CG	2.53	0.43
22:V:435:GLU:HG2	22:V:453:HIS:NE2	2.32	0.43
23:W:340:VAL:HG22	23:W:350:ARG:HH11	1.82	0.43
28:b:33:VAL:HA	28:b:36:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:36:LEU:HD11	29:c:71:ASP:HA	2.01	0.43
32:f:663:VAL:HA	32:f:664:ALA:HA	1.56	0.43
32:f:673:THR:C	32:f:677:GLU:HG2	2.43	0.43
1:A:222:LYS:HD2	2:B:319:PHE:HB2	2.00	0.43
4:D:396:ALA:HA	4:D:399:PHE:CD2	2.54	0.43
5:E:379:LYS:HA	5:E:379:LYS:HD2	1.83	0.43
6:F:187:ASP:HB3	6:F:368:ILE:HG21	2.00	0.43
6:F:356:MET:HE2	6:F:362:ARG:HH11	1.83	0.43
7:G:74:GLU:HB3	7:G:226:LYS:HD2	2.00	0.43
8:H:156:PHE:HB2	8:H:158:TRP:CZ3	2.53	0.43
9:I:45:LEU:HD21	9:I:137:ILE:HG21	2.01	0.43
11:K:60:GLU:OE1	11:K:63:SER:N	2.52	0.43
13:M:179:LEU:HD13	13:M:189:ILE:HG23	2.00	0.43
15:O:35:HIS:NE2	15:O:53:ASP:OD1	2.52	0.43
17:Q:131:ALA:O	17:Q:132:HIS:ND1	2.52	0.43
19:S:190:GLY:HA2	19:S:210:LEU:HD12	2.00	0.43
21:U:429:LYS:HA	21:U:430:ASP:CB	2.46	0.43
22:V:438:VAL:O	22:V:442:ILE:HG13	2.19	0.43
25:Y:97:GLU:C	25:Y:99:GLU:H	2.26	0.43
25:Y:210:SER:HB3	25:Y:213:LEU:HG	2.01	0.43
26:Z:254:ASN:HA	26:Z:257:MET:CG	2.49	0.43
29:c:243:SER:OG	29:c:244:VAL:HB	2.18	0.43
29:c:282:ARG:NH1	29:c:284:LEU:O	2.52	0.43
32:f:123:PHE:CE2	32:f:127:LYS:HD3	2.53	0.43
1:A:309:PHE:HZ	6:F:235:LEU:HA	1.84	0.43
2:B:108:SER:N	2:B:152:LEU:O	2.37	0.43
2:B:209:GLU:HG2	2:B:210:TYR:N	2.34	0.43
6:F:395:GLN:O	6:F:399:VAL:HG23	2.19	0.43
9:I:213:ILE:HG22	9:I:228:LEU:HD21	2.01	0.43
16:P:21:ALA:HB2	16:P:189:ILE:HD13	2.01	0.43
21:U:173:VAL:N	21:U:174:PRO:HD3	2.34	0.43
21:U:385:PHE:CE2	21:U:411:ILE:HD13	2.54	0.43
21:U:451:ALA:HB2	21:U:483:LEU:HG	2.01	0.43
22:V:80:LYS:HB3	22:V:81:GLN:O	2.19	0.43
26:Z:14:LEU:HD23	29:c:43:LYS:HD3	2.01	0.43
26:Z:40:LEU:HD22	26:Z:89:GLU:HG3	2.00	0.43
26:Z:96:HIS:NE2	26:Z:123:ILE:HG12	2.34	0.43
32:f:672:VAL:HG23	32:f:673:THR:N	2.34	0.43
1:A:241:ILE:HD12	2:B:268:ARG:CZ	2.49	0.42
1:A:312:ARG:HA	1:A:313:GLY:HA2	1.64	0.42
2:B:387:LYS:HE3	2:B:423:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:ASN:HD21	21:U:644:TYR:N	2.17	0.42
3:C:115:ALA:HB3	3:C:124:HIS:HB3	2.00	0.42
4:D:74:HIS:O	4:D:78:GLU:HG2	2.19	0.42
6:F:89:LEU:HG	6:F:153:VAL:O	2.19	0.42
11:K:143:PHE:HB2	11:K:154:PHE:HB2	2.00	0.42
21:U:362:ASN:HA	21:U:395:ARG:NH1	2.34	0.42
23:W:310:THR:C	23:W:312:MET:H	2.27	0.42
23:W:428:TRP:CH2	26:Z:255:ASP:HB3	2.54	0.42
26:Z:54:PHE:HB3	26:Z:82:PHE:HE2	1.84	0.42
26:Z:109:ASN:O	26:Z:113:LYS:HG3	2.19	0.42
26:Z:241:SER:HB2	26:Z:246:VAL:HG23	2.01	0.42
27:a:270:ARG:NH2	27:a:270:ARG:O	2.52	0.42
28:b:142:ASN:HD22	28:b:172:THR:HG22	1.83	0.42
30:d:101:LEU:HD13	30:d:161:GLU:H	1.85	0.42
1:A:174:TYR:HE1	1:A:227:ARG:HH21	1.68	0.42
1:A:409:PHE:O	1:A:413:VAL:HG23	2.19	0.42
3:C:75:GLU:HG2	3:C:90:HIS:NE2	2.34	0.42
3:C:80:MET:HE3	3:C:86:LEU:HG	2.01	0.42
3:C:147:THR:OG1	3:C:206:HIS:NE2	2.42	0.42
3:C:155:ASP:HA	3:C:158:ILE:HG12	2.02	0.42
3:C:324:ALA:O	3:C:328:ILE:HG22	2.19	0.42
4:D:163:MET:HA	4:D:221:HIS:NE2	2.34	0.42
4:D:309:MET:HE3	4:D:309:MET:HB2	1.98	0.42
5:E:83:CYS:SG	5:E:107:ILE:HD13	2.60	0.42
6:F:283:ILE:O	6:F:328:VAL:HA	2.19	0.42
8:H:46:LEU:HD11	8:H:137:CYS:SG	2.59	0.42
12:L:135:ALA:HA	12:L:143:HIS:O	2.19	0.42
16:P:12:MET:HA	16:P:138:VAL:HG12	2.00	0.42
20:T:136:SER:HB2	20:T:150:LEU:HB3	2.01	0.42
21:U:600:ARG:HD3	21:U:600:ARG:HA	1.75	0.42
22:V:398:LEU:O	22:V:402:VAL:HG23	2.19	0.42
23:W:337:ALA:O	23:W:342:GLY:N	2.51	0.42
27:a:173:TYR:CZ	27:a:216:LEU:HD13	2.54	0.42
29:c:145:VAL:HB	29:c:157:ILE:HG13	2.00	0.42
30:d:184:LYS:HB2	30:d:185:ALA:HB2	2.00	0.42
32:f:642:VAL:HA	32:f:645:LEU:HG	2.01	0.42
1:A:392:ALA:HB2	1:A:409:PHE:CD2	2.54	0.42
2:B:254:GLU:HA	2:B:257:GLN:HG2	2.01	0.42
3:C:219:LEU:HD11	4:D:287:ARG:HG3	2.01	0.42
4:D:297:ASP:OD2	4:D:326:ARG:NH2	2.52	0.42
4:D:375:ILE:HA	4:D:378:ILE:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:444:TYR:CE1	21:U:479:LEU:HD23	2.54	0.42
21:U:596:ASN:O	21:U:600:ARG:HG2	2.19	0.42
22:V:30:PRO:HA	22:V:33:GLN:HB2	2.01	0.42
22:V:345:ARG:HH12	22:V:357:LEU:HD22	1.85	0.42
23:W:433:ASN:HA	23:W:436:MET:HG3	2.00	0.42
26:Z:126:VAL:HG23	26:Z:127:LYS:HG3	2.02	0.42
26:Z:247:LYS:HA	26:Z:250:TYR:CE2	2.54	0.42
29:c:236:GLU:HG2	29:c:239:LYS:HD2	2.00	0.42
30:d:226:ALA:HA	30:d:227:SER:HA	1.66	0.42
1:A:84:LYS:O	1:A:87:LEU:HG	2.19	0.42
1:A:123:VAL:HG23	6:F:88:TYR:CE1	2.54	0.42
1:A:243:SER:CB	2:B:264:PRO:HD3	2.49	0.42
1:A:261:PHE:HE2	1:A:305:GLN:HB3	1.84	0.42
1:A:313:GLY:C	1:A:315:ILE:N	2.76	0.42
2:B:187:ILE:HA	33:B:501:ADP:N6	2.34	0.42
2:B:316:LEU:HD11	2:B:327:VAL:HG11	2.01	0.42
4:D:233:SER:HB2	5:E:255:ARG:HB3	2.00	0.42
4:D:313:ARG:NH2	5:E:242:ARG:O	2.52	0.42
4:D:340:GLN:H	4:D:340:GLN:CD	2.25	0.42
5:E:69:PHE:O	5:E:80:VAL:HA	2.20	0.42
5:E:115:VAL:HG22	5:E:117:PRO:CD	2.50	0.42
5:E:132:TYR:O	5:E:135:ILE:HG12	2.19	0.42
5:E:320:ILE:HD12	6:F:215:LEU:HB3	2.01	0.42
11:K:85:ALA:O	11:K:89:ILE:HG12	2.19	0.42
14:N:87:CYS:O	14:N:91:ARG:N	2.52	0.42
21:U:789:ILE:HG23	21:U:844:LYS:HG2	2.01	0.42
23:W:370:TYR:HA	23:W:371:THR:HB	2.02	0.42
26:Z:15:VAL:O	26:Z:19:VAL:HG23	2.19	0.42
27:a:163:TYR:CE1	27:a:172:TYR:HB2	2.55	0.42
29:c:289:ASP:HA	29:c:292:MET:HG2	2.01	0.42
32:f:414:ILE:HG13	32:f:417:ILE:HD11	2.02	0.42
1:A:122:VAL:HG23	6:F:90:VAL:HG22	2.01	0.42
2:B:138:PHE:HE2	2:B:162:VAL:H	1.67	0.42
3:C:157:GLN:NE2	3:C:318:PRO:HD3	2.34	0.42
3:C:249:ASP:HA	3:C:250:GLU:HA	1.56	0.42
5:E:111:LEU:HD23	6:F:133:PHE:HE1	1.84	0.42
5:E:120:TYR:OH	6:F:147:PRO:HD2	2.20	0.42
5:E:124:HIS:NE2	6:F:319:GLY:O	2.52	0.42
5:E:149:ILE:HG12	5:E:274:LYS:HE2	2.01	0.42
5:E:314:LYS:O	5:E:318:GLY:N	2.53	0.42
6:F:93:VAL:C	6:F:147:PRO:HB3	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:137:ASP:HA	10:J:143:ARG:HH21	1.84	0.42
12:L:137:TYR:HE1	12:L:215:VAL:HG13	1.85	0.42
13:M:125:TYR:HB2	13:M:128:VAL:HG22	2.01	0.42
17:Q:38:MET:SD	17:Q:44:LEU:HB2	2.59	0.42
19:S:4:PRO:O	20:T:100:ARG:NH2	2.51	0.42
22:V:144:ASP:N	22:V:145:LEU:HA	2.34	0.42
23:W:227:TYR:O	23:W:231:ILE:HG23	2.20	0.42
23:W:440:ASN:O	23:W:444:HIS:ND1	2.53	0.42
25:Y:237:ARG:HB2	25:Y:241:ILE:HD12	2.00	0.42
29:c:288:VAL:O	29:c:292:MET:HG2	2.19	0.42
30:d:47:GLN:HA	30:d:50:LEU:HB2	2.02	0.42
30:d:182:ILE:HG23	30:d:183:GLU:N	2.35	0.42
1:A:170:PRO:CB	1:A:230:ALA:HA	2.50	0.42
1:A:414:ASN:HA	1:A:417:ILE:HG12	2.00	0.42
2:B:393:ALA:HB2	33:B:501:ADP:H4'	2.02	0.42
4:D:201:GLY:HA2	4:D:327:LEU:HA	2.01	0.42
4:D:203:LEU:HB3	4:D:330:LYS:HA	2.02	0.42
4:D:207:PRO:HG2	4:D:312:ASN:HB3	2.01	0.42
5:E:226:GLN:CD	5:E:272:ARG:HD3	2.44	0.42
5:E:242:ARG:HB3	5:E:254:GLN:CD	2.44	0.42
5:E:261:LEU:O	5:E:265:ASP:N	2.52	0.42
6:F:204:LEU:HA	6:F:208:HIS:HB2	2.02	0.42
6:F:246:ALA:HB1	6:F:281:SER:HA	2.01	0.42
7:G:100:ASN:O	7:G:104:LYS:HG2	2.19	0.42
8:H:74:LEU:HD12	8:H:136:ILE:HG12	2.01	0.42
12:L:26:MET:HE1	12:L:148:CYS:HB2	2.01	0.42
17:Q:157:VAL:O	17:Q:161:ARG:HG2	2.20	0.42
21:U:24:LEU:HA	21:U:27:LEU:HB2	2.01	0.42
21:U:603:LEU:O	21:U:607:VAL:HG23	2.20	0.42
22:V:346:LEU:HB3	22:V:361:PHE:CE1	2.54	0.42
23:W:377:ARG:NH2	27:a:308:GLU:OE2	2.37	0.42
25:Y:52:PRO:HD3	25:Y:115:GLY:HA2	2.02	0.42
25:Y:356:THR:HA	25:Y:357:ASN:OD1	2.18	0.42
28:b:18:ASN:HD21	28:b:25:ARG:NH2	2.17	0.42
30:d:106:LEU:O	30:d:109:GLN:HG2	2.20	0.42
32:f:23:GLU:HB3	32:f:24:PRO:HD3	2.02	0.42
32:f:270:ILE:HD12	32:f:274:LEU:HD12	2.02	0.42
1:A:101:ILE:HA	1:A:138:MET:O	2.20	0.42
1:A:220:THR:HB	33:A:501:ADP:C5	2.55	0.42
1:A:354:ILE:O	1:A:357:ILE:HG22	2.19	0.42
2:B:249:ARG:HB3	3:C:283:PHE:CE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:317:LEU:HD13	6:F:346:GLY:O	2.20	0.42
7:G:163:PHE:CD2	8:H:57:TYR:HA	2.54	0.42
11:K:225:ASN:HA	11:K:226:PHE:HA	1.82	0.42
12:L:67:ASP:HB3	12:L:70:ILE:HB	2.00	0.42
13:M:120:HIS:O	13:M:124:LEU:HG	2.20	0.42
17:Q:7:ILE:HG21	17:Q:156:ALA:HB1	2.01	0.42
20:T:92:LEU:HG	20:T:125:VAL:HG11	2.01	0.42
22:V:378:VAL:HG13	22:V:382:PHE:CD2	2.55	0.42
22:V:494:MET:SD	26:Z:282:ASN:ND2	2.92	0.42
23:W:449:GLU:HG3	26:Z:211:TYR:HE1	1.85	0.42
29:c:245:VAL:O	29:c:249:LEU:HG	2.20	0.42
30:d:193:GLU:HG3	30:d:196:ARG:HD2	2.01	0.42
32:f:283:SER:HB3	32:f:289:CYS:SG	2.60	0.42
32:f:673:THR:O	32:f:674:PHE:C	2.63	0.42
1:A:351:ARG:O	1:A:355:PHE:N	2.50	0.42
1:A:393:GLY:HA2	1:A:396:ALA:HB3	2.01	0.42
2:B:294:ARG:C	3:C:264:GLY:HA3	2.44	0.42
3:C:180:ILE:HD12	3:C:180:ILE:HA	1.95	0.42
3:C:327:ASP:O	3:C:331:ILE:N	2.49	0.42
4:D:103:VAL:HG11	4:D:139:LEU:HD21	2.01	0.42
4:D:130:VAL:HB	4:D:142:VAL:HG12	2.02	0.42
4:D:231:VAL:H	4:D:234:GLU:CD	2.27	0.42
4:D:267:ILE:HG12	4:D:309:MET:HG3	2.01	0.42
4:D:357:GLU:OE2	4:D:396:ALA:N	2.52	0.42
5:E:76:GLY:N	5:E:77:PRO:HD2	2.35	0.42
5:E:83:CYS:HB3	5:E:87:LEU:HD21	2.01	0.42
5:E:170:CYS:HB3	5:E:276:ILE:CD1	2.50	0.42
6:F:256:LEU:HD13	6:F:291:ILE:HD13	2.01	0.42
18:R:191:ASN:OD1	18:R:192:VAL:N	2.53	0.42
20:T:41:ARG:HH21	20:T:54:SER:HA	1.84	0.42
21:U:494:TYR:O	21:U:498:LYS:HG3	2.20	0.42
21:U:510:GLU:HA	21:U:547:GLY:HA3	2.01	0.42
21:U:579:ARG:O	21:U:583:MET:HG2	2.19	0.42
22:V:24:GLN:C	22:V:27:PRO:HD2	2.44	0.42
23:W:285:ASP:O	23:W:289:ARG:HG3	2.20	0.42
26:Z:33:LYS:HE3	26:Z:33:LYS:HB3	1.81	0.42
30:d:244:LYS:HA	30:d:247:ILE:HD12	2.01	0.42
32:f:142:HIS:HB2	32:f:174:LEU:HD22	2.01	0.42
1:A:289:ALA:HB1	6:F:295:ARG:HD3	2.01	0.42
2:B:197:ILE:HG13	2:B:222:VAL:HG11	2.01	0.42
2:B:231:GLY:HA2	2:B:234:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:ARG:HB2	2:B:344:PRO:HD3	2.02	0.42
4:D:205:TYR:O	4:D:333:PHE:HB2	2.20	0.42
5:E:83:CYS:SG	5:E:87:LEU:HD11	2.60	0.42
6:F:248:PHE:CE1	6:F:284:PHE:HB3	2.55	0.42
9:I:49:ARG:H	9:I:211:VAL:HA	1.85	0.42
9:I:83:ALA:O	9:I:87:THR:HG23	2.19	0.42
9:I:111:VAL:HG22	9:I:136:TYR:CE1	2.54	0.42
12:L:50:LYS:HB2	12:L:209:ASN:HA	2.01	0.42
13:M:40:ARG:HD2	13:M:146:ALA:HB1	2.01	0.42
13:M:64:LYS:HD2	13:M:212:GLU:HG2	2.02	0.42
15:O:7:VAL:HG22	15:O:12:ILE:HG23	2.02	0.42
19:S:63:THR:OG1	20:T:94:ARG:NH1	2.45	0.42
21:U:15:ASP:O	21:U:20:LYS:NZ	2.53	0.42
21:U:42:VAL:HG11	21:U:68:PHE:CZ	2.55	0.42
21:U:252:LEU:O	21:U:256:ALA:HB3	2.19	0.42
21:U:474:ARG:HG2	21:U:500:ASN:HD21	1.85	0.42
21:U:713:TYR:HB2	21:U:734:GLN:HE21	1.84	0.42
27:a:307:VAL:O	27:a:311:VAL:HG22	2.20	0.42
27:a:342:ASP:O	27:a:346:ILE:HD12	2.20	0.42
29:c:157:ILE:HG23	29:c:158:ASP:N	2.35	0.42
30:d:184:LYS:HA	30:d:185:ALA:HA	1.76	0.42
2:B:152:LEU:HD23	2:B:157:HIS:HB3	2.02	0.42
2:B:180:PRO:HD2	2:B:242:GLN:HE22	1.83	0.42
2:B:211:TYR:CZ	2:B:217:LYS:HA	2.55	0.42
3:C:243:PRO:HB3	3:C:288:ASN:HB3	2.02	0.42
3:C:388:ALA:O	3:C:392:GLN:N	2.52	0.42
4:D:267:ILE:HG12	4:D:309:MET:CG	2.50	0.42
5:E:250:ASP:O	5:E:254:GLN:HG2	2.20	0.42
9:I:8:ARG:HB3	9:I:11:ILE:HB	2.02	0.42
9:I:112:THR:HB	10:J:81:ARG:HD3	2.01	0.42
12:L:101:ARG:NH1	20:T:87:ALA:HB2	2.35	0.42
20:T:74:GLU:HA	20:T:77:LEU:HD12	2.01	0.42
21:U:338:HIS:NE2	21:U:342:LEU:HD11	2.34	0.42
22:V:350:GLN:HB3	22:V:351:PRO:HD2	2.02	0.42
22:V:466:ILE:HG23	22:V:467:TYR:HB2	2.01	0.42
25:Y:14:ASN:HA	25:Y:17:LEU:HB3	2.02	0.42
27:a:180:LEU:HD11	27:a:222:LEU:HB3	2.02	0.42
27:a:287:ASN:HA	27:a:288:HIS:C	2.44	0.42
29:c:256:ASN:O	29:c:260:GLU:HB2	2.20	0.42
30:d:148:TYR:HB3	30:d:199:PHE:CE2	2.55	0.42
1:A:165:GLN:HE21	1:A:240:VAL:HG13	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LYS:HG2	2:B:319:PHE:CD1	2.55	0.41
1:A:418:LYS:O	1:A:422:LYS:N	2.52	0.41
2:B:214:MET:HB3	2:B:216:ILE:HG12	2.01	0.41
3:C:214:VAL:HG23	3:C:272:THR:HG21	2.02	0.41
4:D:159:LYS:HB3	4:D:160:PRO:HA	2.02	0.41
4:D:361:GLU:O	4:D:364:VAL:HG12	2.19	0.41
5:E:234:GLU:OE1	6:F:308:ARG:HD3	2.20	0.41
9:I:11:ILE:H	9:I:11:ILE:HD12	1.85	0.41
13:M:61:GLY:O	13:M:64:LYS:NZ	2.52	0.41
21:U:11:LEU:HB3	21:U:19:LEU:HG	2.02	0.41
21:U:195:ASN:HB2	21:U:223:LEU:HD13	2.01	0.41
21:U:408:LEU:O	21:U:412:HIS:ND1	2.53	0.41
21:U:457:ILE:HD12	21:U:457:ILE:H	1.86	0.41
21:U:684:ARG:O	21:U:688:LEU:HG	2.20	0.41
24:X:378:LEU:O	25:Y:312:ARG:HG2	2.19	0.41
25:Y:203:ASP:HB2	25:Y:206:SER:OG	2.20	0.41
27:a:293:PHE:HB3	27:a:329:LYS:O	2.20	0.41
31:e:6:GLN:N	31:e:7:PRO:HD2	2.34	0.41
32:f:370:SER:HB3	32:f:372:ASN:HD22	1.85	0.41
1:A:212:VAL:HG12	1:A:339:ARG:HB3	2.02	0.41
2:B:226:GLY:HA3	2:B:353:PHE:HB3	2.01	0.41
4:D:191:TYR:HB3	4:D:198:PRO:HD3	2.01	0.41
5:E:122:MET:HE3	5:E:122:MET:HB3	1.87	0.41
5:E:124:HIS:NE2	5:E:185:ARG:HD2	2.35	0.41
5:E:341:ALA:HB2	33:E:401:ADP:N3	2.35	0.41
13:M:189:ILE:HG22	13:M:193:VAL:HG23	2.02	0.41
17:Q:181:ARG:NH1	17:Q:190:ASP:OD1	2.52	0.41
22:V:96:ARG:HA	22:V:98:LEU:HB2	2.02	0.41
23:W:264:GLN:NE2	23:W:299:ILE:HD11	2.35	0.41
32:f:590:ALA:HB2	32:f:603:VAL:HG11	2.02	0.41
32:f:613:GLY:HA2	32:f:656:HIS:HA	2.03	0.41
1:A:115:VAL:HG22	1:A:116:LYS:H	1.85	0.41
1:A:275:ASP:CG	2:B:314:ASN:HD21	2.28	0.41
2:B:123:VAL:O	2:B:130:GLU:HA	2.20	0.41
2:B:175:LYS:NZ	2:B:247:PHE:O	2.52	0.41
3:C:80:MET:HB3	3:C:82:LYS:HG2	2.02	0.41
3:C:97:VAL:HG22	3:C:98:ASP:H	1.85	0.41
3:C:306:LEU:O	3:C:307:ARG:NH2	2.49	0.41
4:D:54:LEU:O	4:D:58:GLU:HG2	2.20	0.41
4:D:200:ARG:O	4:D:307:VAL:HB	2.19	0.41
4:D:203:LEU:HB3	4:D:331:ILE:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:370:ILE:HG23	4:D:371:SER:H	1.84	0.41
5:E:84:ARG:HG2	5:E:87:LEU:HD23	2.02	0.41
5:E:141:GLN:HE22	5:E:301:ILE:HA	1.85	0.41
5:E:378:LYS:NZ	6:F:349:ASP:O	2.31	0.41
8:H:50:LYS:HD3	8:H:59:GLU:OE1	2.20	0.41
9:I:64:LYS:O	9:I:76:VAL:HG12	2.19	0.41
10:J:114:LEU:HA	10:J:117:ARG:HG2	2.02	0.41
20:T:92:LEU:HD21	20:T:110:MET:SD	2.60	0.41
21:U:574:LYS:H	21:U:574:LYS:HG2	1.70	0.41
21:U:806:CYS:SG	21:U:891:VAL:HG21	2.60	0.41
22:V:487:HIS:CG	26:Z:275:LEU:HG	2.55	0.41
29:c:53:VAL:HG22	29:c:114:SER:HB2	2.02	0.41
30:d:43:LEU:HA	30:d:46:GLN:HG2	2.01	0.41
32:f:281:ILE:HG13	32:f:282:LYS:H	1.86	0.41
32:f:460:HIS:HB3	32:f:461:PHE:H	1.50	0.41
32:f:647:VAL:O	32:f:651:ILE:HG12	2.20	0.41
1:A:304:ASN:HD22	6:F:254:PRO:CG	2.31	0.41
1:A:367:ASP:O	1:A:369:ARG:NH1	2.53	0.41
3:C:161:ILE:O	3:C:165:ILE:HG12	2.21	0.41
4:D:40:LEU:HB2	21:U:149:GLN:OE1	2.20	0.41
4:D:297:ASP:OD1	4:D:326:ARG:NH1	2.54	0.41
9:I:174:MET:HE3	9:I:199:LYS:HD2	2.01	0.41
10:J:137:ASP:OD1	10:J:143:ARG:NE	2.54	0.41
18:R:127:SER:HB3	18:R:136:TYR:CE2	2.56	0.41
20:T:157:GLN:HG2	20:T:159:VAL:O	2.21	0.41
22:V:207:ALA:HA	22:V:210:CYS:SG	2.60	0.41
22:V:353:LEU:HG	22:V:357:LEU:HD23	2.00	0.41
23:W:340:VAL:HG13	23:W:350:ARG:HD2	2.02	0.41
25:Y:367:GLN:HG3	25:Y:371:LYS:CG	2.51	0.41
28:b:52:ILE:HD11	28:b:58:CYS:HB3	2.01	0.41
29:c:37:ALA:O	29:c:41:MET:HG2	2.20	0.41
32:f:281:ILE:HG23	32:f:282:LYS:N	2.35	0.41
1:A:225:CYS:O	1:A:229:VAL:HG23	2.20	0.41
3:C:310:ARG:HA	3:C:311:ILE:HA	1.77	0.41
3:C:333:SER:HA	3:C:336:MET:HE3	2.02	0.41
4:D:159:LYS:HD3	4:D:159:LYS:HA	1.89	0.41
7:G:203:SER:O	7:G:207:SER:HB3	2.21	0.41
11:K:24:VAL:O	11:K:28:ILE:HG12	2.20	0.41
14:N:42:PHE:CE2	14:N:184:VAL:HG11	2.55	0.41
15:O:215:LYS:N	16:P:197:THR:O	2.41	0.41
20:T:20:VAL:HG11	20:T:122:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:59:PHE:HA	21:U:62:LEU:HD13	2.02	0.41
21:U:342:LEU:HD13	21:U:378:CYS:O	2.19	0.41
21:U:766:PHE:CD1	21:U:776:SER:HA	2.56	0.41
21:U:842:LYS:HA	21:U:843:GLU:CB	2.46	0.41
22:V:43:THR:HG23	22:V:62:HIS:HB3	2.01	0.41
22:V:195:ILE:H	22:V:195:ILE:HG13	1.73	0.41
25:Y:101:ARG:HH21	25:Y:126:LYS:HG3	1.86	0.41
27:a:24:ARG:O	27:a:28:LEU:HD13	2.20	0.41
27:a:156:TYR:HE2	27:a:196:ARG:HH11	1.68	0.41
30:d:40:GLY:HA3	30:d:41:THR:C	2.45	0.41
30:d:142:TYR:HB3	30:d:147:SER:HB3	2.03	0.41
32:f:382:THR:HG22	32:f:386:LYS:NZ	2.35	0.41
32:f:544:ARG:NH2	32:f:578:ASN:O	2.53	0.41
1:A:94:GLN:OE1	2:B:131:HIS:NE2	2.53	0.41
1:A:123:VAL:HG22	1:A:124:ASP:H	1.86	0.41
1:A:278:ASP:HB3	1:A:321:THR:OG1	2.21	0.41
3:C:158:ILE:HA	3:C:161:ILE:HG22	2.02	0.41
3:C:163:GLU:OE1	3:C:163:GLU:N	2.49	0.41
4:D:116:LEU:HB2	4:D:140:VAL:HA	2.02	0.41
4:D:182:GLU:HG3	4:D:183:LEU:H	1.85	0.41
5:E:170:CYS:SG	5:E:299:ILE:HD13	2.60	0.41
5:E:216:ARG:HA	5:E:219:PHE:HB2	2.02	0.41
5:E:321:THR:HG23	6:F:215:LEU:HD22	2.03	0.41
6:F:402:GLU:HA	6:F:405:MET:HB2	2.01	0.41
6:F:405:MET:O	6:F:408:LEU:HB3	2.20	0.41
6:F:431:LYS:HB2	6:F:432:LYS:HA	2.02	0.41
10:J:20:GLU:OE1	10:J:20:GLU:N	2.52	0.41
10:J:97:THR:HG22	18:R:82:LEU:HD21	2.03	0.41
10:J:109:ARG:O	10:J:113:SER:OG	2.32	0.41
11:K:225:ASN:HB2	11:K:226:PHE:CD2	2.55	0.41
12:L:82:ARG:HA	12:L:85:CYS:HB3	2.03	0.41
12:L:173:GLU:HA	12:L:176:MET:SD	2.61	0.41
17:Q:5:ILE:HD12	17:Q:5:ILE:HA	1.97	0.41
17:Q:84:THR:HG21	17:Q:104:LEU:HD11	2.02	0.41
18:R:178:HIS:O	18:R:185:ILE:N	2.52	0.41
21:U:682:TYR:HB3	21:U:725:MET:SD	2.61	0.41
25:Y:236:LEU:O	25:Y:240:VAL:HG22	2.20	0.41
26:Z:221:PRO:CB	26:Z:222:ILE:HA	2.50	0.41
27:a:252:LYS:HA	27:a:255:TRP:HD1	1.85	0.41
27:a:287:ASN:HB3	27:a:289:ARG:HB3	2.02	0.41
29:c:235:SER:O	29:c:239:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:660:TYR:HA	32:f:661:GLY:HA3	1.62	0.41
1:A:262:GLU:HA	1:A:265:ARG:HB2	2.02	0.41
1:A:387:SER:O	1:A:391:GLU:HG2	2.20	0.41
2:B:208:PRO:O	2:B:211:TYR:HB3	2.21	0.41
3:C:33:LEU:HG	22:V:496:PHE:CZ	2.56	0.41
3:C:99:VAL:HG13	3:C:101:LYS:HA	2.02	0.41
4:D:102:ILE:HA	4:D:111:TYR:O	2.21	0.41
4:D:146:GLU:CG	4:D:148:ASP:H	2.33	0.41
4:D:241:GLY:O	4:D:244:PRO:HD2	2.20	0.41
5:E:46:ASP:O	5:E:50:LEU:HG	2.20	0.41
5:E:215:ILE:O	5:E:219:PHE:N	2.42	0.41
6:F:140:VAL:HG13	6:F:161:LEU:O	2.21	0.41
6:F:144:LYS:HA	6:F:145:LEU:HA	1.70	0.41
6:F:357:PRO:O	6:F:362:ARG:NH1	2.53	0.41
7:G:28:ALA:HB2	13:M:14:PHE:HE2	1.85	0.41
9:I:109:GLN:HE22	17:Q:67:TYR:HE2	1.69	0.41
10:J:56:GLU:O	10:J:59:VAL:HG12	2.20	0.41
11:K:10:ARG:O	11:K:14:THR:OG1	2.27	0.41
22:V:273:LYS:HB3	22:V:274:SER:O	2.21	0.41
26:Z:195:VAL:O	26:Z:199:LYS:HB2	2.20	0.41
26:Z:229:GLN:O	26:Z:233:VAL:HG23	2.20	0.41
27:a:289:ARG:HG3	27:a:332:HIS:CE1	2.55	0.41
29:c:113:HIS:O	29:c:144:VAL:HG13	2.21	0.41
30:d:133:ILE:O	30:d:137:VAL:HG22	2.21	0.41
32:f:61:ASP:C	32:f:63:ASP:H	2.28	0.41
2:B:186:ASP:O	33:B:501:ADP:N6	2.53	0.41
2:B:209:GLU:HB3	32:f:579:ASN:OD1	2.20	0.41
3:C:21:ARG:NH2	21:U:102:ALA:HA	2.36	0.41
6:F:317:LEU:HG	6:F:323:ASN:ND2	2.36	0.41
7:G:215:ILE:H	7:G:215:ILE:HG13	1.63	0.41
12:L:64:LEU:HG	12:L:72:ILE:HD11	2.03	0.41
15:O:175:LEU:HB2	15:O:186:LEU:HB2	2.03	0.41
21:U:173:VAL:HG13	21:U:176:MET:HB2	2.03	0.41
32:f:661:GLY:N	32:f:662:LEU:HA	2.36	0.41
1:A:119:ALA:HB1	1:A:121:PHE:CE2	2.52	0.41
1:A:191:VAL:HG13	1:A:192:GLU:N	2.33	0.41
1:A:292:ASP:HB3	1:A:296:GLN:HE21	1.86	0.41
1:A:403:ILE:HA	2:B:214:MET:HE1	2.02	0.41
2:B:303:ARG:HH21	2:B:307:ARG:NH1	2.19	0.41
2:B:346:ARG:CZ	2:B:348:ASP:HB3	2.51	0.41
2:B:346:ARG:HG3	2:B:349:ARG:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:ASP:OD1	3:C:122:THR:HB	2.21	0.41
3:C:196:LYS:NZ	33:C:501:ADP:O3B	2.48	0.41
3:C:328:ILE:O	3:C:332:HIS:ND1	2.31	0.41
5:E:285:LEU:HB3	5:E:289:LEU:HD12	2.01	0.41
6:F:321:GLN:O	6:F:324:THR:HG23	2.21	0.41
7:G:158:GLY:O	8:H:84:ARG:NH2	2.54	0.41
8:H:45:VAL:HG11	8:H:188:ILE:HG12	2.03	0.41
12:L:65:HIS:O	12:L:89:ARG:NH2	2.54	0.41
13:M:113:ASP:O	13:M:117:MET:HG2	2.21	0.41
20:T:29:SER:HA	20:T:36:PHE:H	1.85	0.41
21:U:22:PHE:HB3	30:d:34:ASN:ND2	2.36	0.41
21:U:357:LYS:HE2	21:U:389:ASN:HA	2.03	0.41
21:U:373:ASN:HB2	21:U:385:PHE:CE1	2.56	0.41
21:U:537:GLN:N	21:U:537:GLN:OE1	2.54	0.41
21:U:643:SER:O	21:U:649:ARG:NH1	2.42	0.41
21:U:774:PRO:HA	21:U:777:HIS:CD2	2.54	0.41
22:V:436:PHE:CB	30:d:146:GLY:H	2.34	0.41
22:V:447:ILE:HG13	22:V:449:ALA:H	1.86	0.41
25:Y:141:VAL:HG22	25:Y:160:ASN:HB2	2.02	0.41
25:Y:323:PHE:HD1	25:Y:323:PHE:HA	1.73	0.41
26:Z:23:PHE:HA	26:Z:35:VAL:HG21	2.02	0.41
26:Z:58:PHE:CZ	26:Z:60:GLU:HB2	2.56	0.41
26:Z:238:PRO:HG2	27:a:285:PRO:O	2.21	0.41
27:a:4:VAL:HB	27:a:5:PRO:HD3	2.02	0.41
28:b:16:MET:SD	28:b:114:GLY:HA3	2.61	0.41
30:d:82:TYR:CZ	30:d:95:MET:HG3	2.55	0.41
30:d:215:TRP:CG	30:d:216:VAL:N	2.89	0.41
32:f:282:LYS:NZ	32:f:283:SER:O	2.54	0.41
32:f:388:GLU:O	32:f:391:LEU:HB3	2.21	0.41
32:f:450:VAL:HG21	32:f:473:LYS:HD3	2.03	0.41
32:f:458:SER:CB	32:f:461:PHE:HA	2.51	0.41
32:f:656:HIS:C	32:f:658:VAL:H	2.29	0.41
1:A:138:MET:O	1:A:140:VAL:HG13	2.21	0.41
1:A:283:ALA:HB3	1:A:326:THR:HB	2.03	0.41
1:A:413:VAL:O	1:A:417:ILE:HG12	2.19	0.41
2:B:224:LEU:HB2	2:B:330:ALA:CB	2.51	0.41
4:D:409:LYS:O	4:D:411:GLU:HB2	2.21	0.41
5:E:55:GLN:HB3	5:E:100:LEU:O	2.21	0.41
5:E:141:GLN:NE2	5:E:301:ILE:HA	2.36	0.41
6:F:230:GLY:HA2	6:F:231:THR:CB	2.51	0.41
6:F:231:THR:HG21	6:F:233:LYS:NZ	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:356:MET:HE2	6:F:362:ARG:NH1	2.36	0.41
6:F:372:LYS:HG2	6:F:373:MET:HE2	2.03	0.41
9:I:2:SER:HB3	12:L:123:TYR:CZ	2.56	0.41
11:K:104:ASN:HD21	19:S:90:ALA:HB2	1.86	0.41
12:L:40:SER:OG	12:L:43:HIS:O	2.37	0.41
21:U:392:TRP:NE1	21:U:395:ARG:HH21	2.19	0.41
22:V:185:GLN:O	22:V:189:ASP:HB2	2.21	0.41
22:V:253:LEU:HD23	22:V:256:ARG:HH21	1.86	0.41
22:V:400:HIS:O	22:V:403:ILE:HG22	2.20	0.41
22:V:430:SER:HB2	22:V:431:PRO:HD2	2.02	0.41
26:Z:72:HIS:NE2	26:Z:111:LEU:HD21	2.36	0.41
26:Z:166:GLU:O	26:Z:170:VAL:HG23	2.20	0.41
28:b:48:ASN:HA	28:b:66:PRO:HA	2.02	0.41
30:d:82:TYR:CE2	30:d:98:LEU:HD21	2.52	0.41
1:A:123:VAL:HG11	1:A:147:TYR:HB3	2.02	0.40
2:B:175:LYS:NZ	2:B:246:THR:HG22	2.36	0.40
3:C:147:THR:HG22	3:C:150:MET:HG2	2.02	0.40
4:D:167:ILE:HD13	33:D:501:ADP:HN62	1.85	0.40
5:E:182:LEU:HD12	33:E:401:ADP:H2'	2.02	0.40
6:F:344:ARG:O	6:F:349:ASP:HB2	2.21	0.40
7:G:16:PHE:HE2	8:H:79:MET:HE1	1.86	0.40
10:J:51:ALA:C	10:J:53:LEU:H	2.29	0.40
13:M:200:VAL:HG22	13:M:201:HIS:H	1.85	0.40
21:U:188:MET:HE3	21:U:194:ARG:HG3	2.03	0.40
22:V:108:LEU:HD23	22:V:111:TYR:HE2	1.85	0.40
22:V:310:THR:HG22	22:V:314:ARG:HD3	2.03	0.40
23:W:407:ASP:N	23:W:413:ILE:HG22	2.32	0.40
26:Z:78:MET:HE3	29:c:98:MET:SD	2.61	0.40
30:d:197:ILE:HG22	30:d:198:LEU:HG	2.03	0.40
32:f:179:ASP:HB2	32:f:186:PRO:HD3	2.03	0.40
32:f:646:ASP:OD1	32:f:647:VAL:N	2.54	0.40
1:A:386:ARG:NH1	33:A:501:ADP:O3'	2.49	0.40
3:C:42:LEU:HD12	3:C:42:LEU:HA	1.84	0.40
3:C:135:VAL:O	3:C:139:MET:HG2	2.21	0.40
4:D:163:MET:HA	4:D:221:HIS:HE2	1.86	0.40
4:D:341:LYS:NZ	4:D:375:ILE:HG13	2.36	0.40
4:D:412:GLN:HB3	4:D:414:HIS:HB3	2.02	0.40
5:E:266:GLY:CA	5:E:267:PHE:HB2	2.46	0.40
6:F:356:MET:HE2	6:F:362:ARG:HD3	2.02	0.40
11:K:73:HIS:HA	11:K:226:PHE:CE1	2.56	0.40
12:L:13:TRP:NE1	13:M:129:ARG:HD2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:184:LEU:O	12:L:188:VAL:HG23	2.21	0.40
13:M:51:LYS:HE2	13:M:212:GLU:OE2	2.22	0.40
15:O:3:ILE:HD12	15:O:99:VAL:HG23	2.02	0.40
21:U:14:GLU:HB3	21:U:19:LEU:HD23	2.03	0.40
21:U:479:LEU:HD13	21:U:511:ALA:HA	2.02	0.40
22:V:469:THR:O	22:V:473:GLN:HG2	2.21	0.40
24:X:394:ASP:OD1	24:X:394:ASP:N	2.54	0.40
25:Y:71:ASN:HA	25:Y:74:LYS:HG2	2.04	0.40
25:Y:122:THR:O	25:Y:126:LYS:HB2	2.21	0.40
25:Y:186:LEU:HA	25:Y:189:VAL:HG12	2.04	0.40
32:f:208:SER:HA	32:f:209:ALA:HA	1.76	0.40
32:f:454:LEU:O	32:f:458:SER:OG	2.32	0.40
1:A:290:GLY:HA2	1:A:291:GLY:HA3	1.82	0.40
2:B:211:TYR:OH	2:B:217:LYS:HG3	2.21	0.40
2:B:239:VAL:HA	2:B:242:GLN:CD	2.47	0.40
3:C:36:ASN:O	3:C:40:GLN:HG2	2.21	0.40
3:C:321:ASN:OD1	3:C:322:GLU:N	2.50	0.40
4:D:207:PRO:HG3	4:D:212:LYS:NZ	2.37	0.40
6:F:405:MET:HB3	6:F:409:ARG:HH22	1.85	0.40
7:G:159:TYR:HB3	8:H:81:PRO:HG3	2.03	0.40
8:H:118:MET:HG3	8:H:129:PRO:HB3	2.03	0.40
13:M:39:ILE:HG23	13:M:46:VAL:HB	2.02	0.40
13:M:231:ILE:C	13:M:233:GLU:H	2.29	0.40
21:U:13:ASP:OD1	21:U:44:LYS:NZ	2.38	0.40
21:U:362:ASN:HA	21:U:395:ARG:HH11	1.85	0.40
21:U:802:TYR:HB3	21:U:895:PRO:HD3	2.02	0.40
24:X:344:ARG:HA	24:X:385:LEU:O	2.21	0.40
26:Z:69:PHE:CE1	28:b:60:VAL:HB	2.56	0.40
26:Z:221:PRO:HB2	26:Z:224:HIS:O	2.22	0.40
27:a:100:THR:HG22	27:a:103:LYS:HE2	2.03	0.40
29:c:270:LEU:HB3	29:c:275:VAL:HG23	2.02	0.40
32:f:678:LEU:O	32:f:681:LEU:HG	2.21	0.40
1:A:199:GLU:HA	1:A:202:VAL:HG23	2.04	0.40
1:A:232:ARG:NH1	1:A:271:LEU:HD13	2.30	0.40
1:A:327:LEU:HD12	1:A:328:ASP:N	2.36	0.40
2:B:210:TYR:HA	2:B:213:GLU:HB2	2.03	0.40
2:B:232:LYS:HB2	33:B:501:ADP:O1B	2.21	0.40
2:B:349:ARG:HD2	2:B:349:ARG:HA	1.84	0.40
3:C:386:ALA:O	3:C:390:VAL:HG22	2.21	0.40
4:D:313:ARG:NH1	5:E:241:ARG:O	2.55	0.40
5:E:62:LYS:H	5:E:70:ILE:HB	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:144:LYS:HB2	6:F:145:LEU:HB2	2.04	0.40
6:F:172:VAL:HG13	6:F:267:LEU:HG	2.02	0.40
8:H:103:GLU:HG2	8:H:104:PRO:HD2	2.04	0.40
11:K:155:HIS:CG	11:K:168:ARG:HG2	2.56	0.40
14:N:51:ASP:HB3	14:N:94:LEU:HD13	2.04	0.40
21:U:202:VAL:HG11	21:U:219:CYS:SG	2.61	0.40
21:U:472:ILE:HA	21:U:475:HIS:CE1	2.56	0.40
22:V:470:ARG:HD3	22:V:470:ARG:HA	1.96	0.40
26:Z:39:LEU:HB2	26:Z:95:TYR:HD2	1.87	0.40
30:d:45:LYS:O	30:d:49:ILE:HG12	2.21	0.40
1:A:140:VAL:HG12	1:A:152:PRO:HB3	2.03	0.40
1:A:381:THR:HG1	2:B:343:ARG:NH1	2.19	0.40
2:B:232:LYS:HD2	33:B:501:ADP:O3'	2.21	0.40
3:C:79:ALA:C	3:C:80:MET:HE2	2.46	0.40
3:C:264:GLY:HA2	3:C:267:SER:HB3	2.04	0.40
3:C:338:LEU:HG	3:C:339:THR:O	2.21	0.40
4:D:66:LYS:NZ	30:d:254:GLU:O	2.53	0.40
4:D:241:GLY:O	4:D:245:ARG:HG3	2.21	0.40
33:D:501:ADP:O3B	5:E:294:ARG:NH2	2.48	0.40
5:E:174:GLY:HA3	5:E:175:PRO:HA	1.86	0.40
6:F:77:SER:HA	6:F:80:ILE:HB	2.03	0.40
6:F:299:GLU:HA	6:F:300:LYS:HA	1.92	0.40
11:K:173:ALA:O	11:K:177:ALA:N	2.36	0.40
13:M:192:GLU:O	13:M:195:LYS:HG2	2.21	0.40
17:Q:51:GLY:HA3	18:R:88:TYR:CE1	2.57	0.40
21:U:350:LEU:O	21:U:354:LYS:HG2	2.22	0.40
21:U:609:ASP:O	21:U:615:ARG:HD2	2.21	0.40
21:U:688:LEU:HD22	21:U:713:TYR:HE1	1.86	0.40
22:V:135:LEU:HB3	22:V:181:TYR:HE2	1.85	0.40
25:Y:347:ILE:HG13	25:Y:354:VAL:HG22	2.02	0.40
26:Z:176:LEU:HD12	26:Z:177:ARG:H	1.87	0.40
27:a:125:ILE:HG22	27:a:126:GLY:C	2.47	0.40
30:d:109:GLN:HB2	30:d:173:THR:HG21	2.03	0.40
32:f:438:VAL:HA	32:f:441:TYR:CD2	2.56	0.40
32:f:648:ARG:HA	32:f:651:ILE:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A	359/433 (83%)	304 (85%)	53 (15%)	2 (1%)	21	59
2	B	339/440 (77%)	298 (88%)	38 (11%)	3 (1%)	14	51
3	C	382/398 (96%)	317 (83%)	62 (16%)	3 (1%)	16	54
4	D	378/418 (90%)	328 (87%)	49 (13%)	1 (0%)	36	72
5	E	351/403 (87%)	299 (85%)	51 (14%)	1 (0%)	36	72
6	F	362/439 (82%)	316 (87%)	45 (12%)	1 (0%)	36	72
7	G	238/245 (97%)	221 (93%)	16 (7%)	1 (0%)	30	67
8	H	230/233 (99%)	210 (91%)	19 (8%)	1 (0%)	30	67
9	I	248/260 (95%)	230 (93%)	18 (7%)	0	100	100
10	J	237/247 (96%)	221 (93%)	15 (6%)	1 (0%)	30	67
11	K	224/240 (93%)	203 (91%)	20 (9%)	1 (0%)	30	67
12	L	236/268 (88%)	222 (94%)	14 (6%)	0	100	100
13	M	238/254 (94%)	218 (92%)	20 (8%)	0	100	100
14	N	189/238 (79%)	175 (93%)	14 (7%)	0	100	100
15	O	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
16	P	202/204 (99%)	188 (93%)	14 (7%)	0	100	100
17	Q	197/201 (98%)	183 (93%)	14 (7%)	0	100	100
18	R	199/262 (76%)	190 (96%)	9 (4%)	0	100	100
19	S	211/240 (88%)	199 (94%)	12 (6%)	0	100	100
20	T	213/263 (81%)	204 (96%)	9 (4%)	0	100	100
21	U	798/953 (84%)	729 (91%)	67 (8%)	2 (0%)	36	72
22	V	478/533 (90%)	416 (87%)	60 (13%)	2 (0%)	30	67
23	W	234/456 (51%)	213 (91%)	21 (9%)	0	100	100
24	X	79/422 (19%)	75 (95%)	4 (5%)	0	100	100
25	Y	376/389 (97%)	336 (89%)	38 (10%)	2 (0%)	24	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	284/324 (88%)	251 (88%)	32 (11%)	1 (0%)	30	67
27	a	369/376 (98%)	340 (92%)	27 (7%)	2 (0%)	24	63
28	b	189/377 (50%)	178 (94%)	11 (6%)	0	100	100
29	c	285/309 (92%)	242 (85%)	39 (14%)	4 (1%)	9	40
30	d	255/349 (73%)	219 (86%)	34 (13%)	2 (1%)	16	54
31	e	20/70 (29%)	16 (80%)	4 (20%)	0	100	100
32	f	686/749 (92%)	574 (84%)	108 (16%)	4 (1%)	21	59
All	All	9304/11269 (83%)	8324 (90%)	946 (10%)	34 (0%)	31	67

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	111	VAL
11	K	12	VAL
21	U	364	VAL
25	Y	350	VAL
29	c	244	VAL
32	f	62	ILE
32	f	447	VAL
1	A	206	ILE
32	f	131	VAL
3	C	298	ILE
29	c	157	ILE
4	D	151	ILE
8	H	10	LEU
25	Y	67	VAL
26	Z	144	VAL
27	a	336	VAL
27	a	340	VAL
29	c	156	VAL
32	f	281	ILE
30	d	121	ARG
22	V	466	ILE
30	d	213	ARG
21	U	433	PRO
2	B	218	PRO
2	B	219	PRO
2	B	325	VAL
5	E	208	ILE
22	V	86	VAL

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Mol	Chain	Res	Type
3	C	192	PRO
3	C	251	ILE
10	J	98	VAL
29	c	189	ILE
1	A	172	VAL
6	F	326	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	308/372 (83%)	300 (97%)	8 (3%)	40	62
2	B	298/385 (77%)	292 (98%)	6 (2%)	48	67
3	C	332/346 (96%)	319 (96%)	13 (4%)	28	49
4	D	333/366 (91%)	322 (97%)	11 (3%)	33	55
5	E	308/353 (87%)	305 (99%)	3 (1%)	68	78
6	F	312/379 (82%)	298 (96%)	14 (4%)	24	46
7	G	193/209 (92%)	191 (99%)	2 (1%)	68	78
8	H	164/190 (86%)	160 (98%)	4 (2%)	43	64
9	I	193/220 (88%)	193 (100%)	0	100	100
10	J	152/210 (72%)	151 (99%)	1 (1%)	76	81
11	K	186/202 (92%)	183 (98%)	3 (2%)	55	70
12	L	198/229 (86%)	196 (99%)	2 (1%)	68	78
13	M	192/211 (91%)	189 (98%)	3 (2%)	55	70
14	N	148/180 (82%)	147 (99%)	1 (1%)	76	81
15	O	177/227 (78%)	176 (99%)	1 (1%)	78	83
16	P	172/173 (99%)	171 (99%)	1 (1%)	78	83
17	Q	164/171 (96%)	163 (99%)	1 (1%)	78	83
18	R	153/201 (76%)	153 (100%)	0	100	100
19	S	174/198 (88%)	174 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	T	175/214 (82%)	174 (99%)	1 (1%)	78	83
21	U	685/816 (84%)	674 (98%)	11 (2%)	55	70
22	V	414/459 (90%)	401 (97%)	13 (3%)	35	56
23	W	218/416 (52%)	210 (96%)	8 (4%)	30	51
24	X	74/362 (20%)	71 (96%)	3 (4%)	27	49
25	Y	334/344 (97%)	330 (99%)	4 (1%)	63	75
26	Z	257/295 (87%)	251 (98%)	6 (2%)	44	64
27	a	333/336 (99%)	327 (98%)	6 (2%)	51	68
28	b	167/312 (54%)	165 (99%)	2 (1%)	63	75
29	c	252/267 (94%)	244 (97%)	8 (3%)	34	56
30	d	231/293 (79%)	229 (99%)	2 (1%)	70	79
31	e	22/63 (35%)	22 (100%)	0	100	100
32	f	582/628 (93%)	568 (98%)	14 (2%)	43	64
All	All	7901/9627 (82%)	7749 (98%)	152 (2%)	49	67

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ASP
1	A	113	ILE
1	A	157	ILE
1	A	161	VAL
1	A	187	LEU
1	A	315	ILE
1	A	317	VAL
1	A	388	VAL
2	B	105	THR
2	B	127	VAL
2	B	137	SER
2	B	174	MET
2	B	205	LEU
2	B	320	ASP
3	C	66	LEU
3	C	69	GLN
3	C	76	VAL
3	C	99	VAL
3	C	118	ASN

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Mol	Chain	Res	Type
3	C	131	VAL
3	C	182	GLN
3	C	220	VAL
3	C	251	ILE
3	C	286	THR
3	C	295	THR
3	C	311	ILE
3	C	376	VAL
4	D	82	ILE
4	D	88	VAL
4	D	219	VAL
4	D	230	VAL
4	D	231	VAL
4	D	250	VAL
4	D	267	ILE
4	D	282	ASP
4	D	285	VAL
4	D	370	ILE
4	D	406	VAL
5	E	65	THR
5	E	269	THR
5	E	326	ILE
6	F	93	VAL
6	F	136	VAL
6	F	150	LEU
6	F	151	VAL
6	F	153	VAL
6	F	161	LEU
6	F	166	THR
6	F	172	VAL
6	F	210	GLU
6	F	268	VAL
6	F	283	ILE
6	F	307	GLN
6	F	347	ARG
6	F	430	LYS
7	G	111	VAL
7	G	215	ILE
8	H	127	VAL
8	H	130	PHE
8	H	180	GLU
8	H	208	ILE

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Mol	Chain	Res	Type
10	J	220	LEU
11	K	12	VAL
11	K	139	VAL
11	K	220	VAL
12	L	46	LEU
12	L	161	ILE
13	M	106	ILE
13	M	226	ILE
13	M	227	VAL
14	N	30	VAL
15	O	191	VAL
16	P	189	ILE
17	Q	188	ILE
20	T	168	LEU
21	U	8	ILE
21	U	9	ILE
21	U	97	VAL
21	U	173	VAL
21	U	217	CYS
21	U	233	LEU
21	U	427	LEU
21	U	479	LEU
21	U	554	LEU
21	U	603	LEU
21	U	629	THR
22	V	79	VAL
22	V	94	VAL
22	V	167	LEU
22	V	195	ILE
22	V	197	THR
22	V	298	ILE
22	V	320	THR
22	V	322	VAL
22	V	391	THR
22	V	392	TYR
22	V	398	LEU
22	V	432	GLU
22	V	464	ILE
23	W	333	LEU
23	W	371	THR
23	W	373	ILE
23	W	374	THR

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Mol	Chain	Res	Type
23	W	384	LEU
23	W	402	ILE
23	W	414	ASN
23	W	424	LEU
24	X	369	ILE
24	X	393	VAL
24	X	410	VAL
25	Y	315	THR
25	Y	347	ILE
25	Y	350	VAL
25	Y	356	THR
26	Z	106	ILE
26	Z	133	LEU
26	Z	186	THR
26	Z	191	ILE
26	Z	236	LEU
26	Z	266	ILE
27	a	28	LEU
27	a	113	LEU
27	a	210	VAL
27	a	245	VAL
27	a	327	VAL
27	a	340	VAL
28	b	53	THR
28	b	173	VAL
29	c	33	ILE
29	c	69	VAL
29	c	194	HIS
29	c	227	GLU
29	c	229	LEU
29	c	272	ILE
29	c	275	VAL
29	c	308	VAL
30	d	107	LEU
30	d	131	VAL
32	f	29	VAL
32	f	62	ILE
32	f	81	VAL
32	f	107	LEU
32	f	129	VAL
32	f	317	THR
32	f	340	THR

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Mol	Chain	Res	Type
32	f	371	CYS
32	f	391	LEU
32	f	436	VAL
32	f	507	ILE
32	f	526	THR
32	f	600	LEU
32	f	687	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	165	GLN
1	A	293	ASN
1	A	304	ASN
1	A	305	GLN
1	A	358	HIS
1	A	414	ASN
2	B	120	HIS
2	B	154	HIS
2	B	193	GLN
2	B	314	ASN
2	B	431	GLN
3	C	32	GLN
3	C	48	GLN
3	C	157	GLN
3	C	182	GLN
3	C	279	GLN
3	C	296	ASN
4	D	65	GLN
4	D	91	GLN
4	D	99	ASN
4	D	187	HIS
4	D	193	GLN
4	D	222	HIS
4	D	304	ASN
4	D	376	ASN
5	E	55	GLN
5	E	63	GLN
5	E	141	GLN
5	E	323	HIS
6	F	76	ASN

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Mol	Chain	Res	Type
6	F	83	ASN
6	F	194	GLN
6	F	208	HIS
6	F	218	GLN
6	F	258	GLN
6	F	392	ASN
7	G	123	GLN
7	G	127	GLN
7	G	150	GLN
7	G	193	GLN
8	H	189	HIS
9	I	40	ASN
10	J	146	GLN
11	K	23	GLN
11	K	99	HIS
11	K	178	GLN
12	L	53	GLN
13	M	32	ASN
14	N	7	GLN
14	N	66	HIS
14	N	77	HIS
14	N	154	GLN
15	O	193	ASN
16	P	93	ASN
16	P	169	GLN
17	Q	87	ASN
17	Q	193	ASN
18	R	10	HIS
18	R	62	GLN
19	S	108	ASN
20	T	108	ASN
21	U	115	ASN
21	U	267	ASN
21	U	355	ASN
21	U	421	GLN
21	U	491	GLN
21	U	632	GLN
21	U	685	GLN
21	U	698	GLN
21	U	734	GLN
21	U	754	HIS
22	V	177	ASN

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Mol	Chain	Res	Type
22	V	242	HIS
22	V	279	GLN
22	V	281	ASN
22	V	318	GLN
22	V	329	HIS
22	V	365	GLN
22	V	400	HIS
23	W	264	GLN
23	W	444	HIS
24	X	406	ASN
25	Y	77	ASN
26	Z	77	ASN
26	Z	235	ASN
26	Z	243	GLN
27	a	86	GLN
27	a	193	GLN
27	a	287	ASN
27	a	370	GLN
28	b	76	HIS
28	b	142	ASN
28	b	149	ASN
29	c	92	GLN
29	c	101	GLN
29	c	172	HIS
29	c	190	GLN
29	c	210	ASN
29	c	241	ASN
29	c	287	HIS
29	c	298	GLN
30	d	60	GLN
30	d	97	GLN
30	d	102	ASN
30	d	128	GLN
30	d	130	ASN
30	d	228	GLN
30	d	245	GLN
32	f	65	ASN
32	f	86	ASN
32	f	166	GLN
32	f	246	HIS
32	f	269	GLN
32	f	372	ASN

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Mol	Chain	Res	Type
32	f	433	ASN
32	f	611	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
33	ADP	C	501	-	28,29,29	1.44	4 (14%)	43,45,45	1.85	8 (18%)
33	ADP	F	501	-	28,29,29	1.46	5 (17%)	43,45,45	1.91	8 (18%)
33	ADP	B	501	-	28,29,29	1.44	5 (17%)	43,45,45	1.85	10 (23%)
33	ADP	D	501	-	28,29,29	1.41	5 (17%)	43,45,45	1.83	8 (18%)
33	ADP	A	501	-	28,29,29	1.43	4 (14%)	43,45,45	1.86	8 (18%)
33	ADP	E	401	-	28,29,29	1.42	4 (14%)	43,45,45	1.93	11 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	ADP	C	501	-	-	4/16/32/32	0/3/3/3
33	ADP	F	501	-	-	7/16/32/32	0/3/3/3
33	ADP	B	501	-	-	5/16/32/32	0/3/3/3
33	ADP	D	501	-	-	5/16/32/32	0/3/3/3
33	ADP	A	501	-	-	5/16/32/32	0/3/3/3
33	ADP	E	401	-	-	6/16/32/32	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	501	ADP	C5-C4	4.94	1.47	1.39
33	C	501	ADP	C5-C4	4.83	1.47	1.39
33	F	501	ADP	C5-C4	4.82	1.47	1.39
33	E	401	ADP	C5-C4	4.72	1.47	1.39
33	B	501	ADP	C5-C4	4.66	1.47	1.39
33	D	501	ADP	C5-C4	4.64	1.47	1.39
33	B	501	ADP	C5-C6	2.79	1.48	1.41
33	C	501	ADP	C5-C6	2.77	1.48	1.41
33	F	501	ADP	C5-C6	2.76	1.48	1.41
33	E	401	ADP	C5-C6	2.75	1.48	1.41
33	D	501	ADP	C5-C6	2.65	1.48	1.41
33	A	501	ADP	C5-C6	2.63	1.48	1.41
33	A	501	ADP	C5-N7	-2.45	1.34	1.39
33	B	501	ADP	PA-O3A	2.41	1.62	1.59
33	B	501	ADP	C8-N7	2.37	1.36	1.31
33	F	501	ADP	C5-N7	-2.36	1.34	1.39
33	E	401	ADP	C8-N7	2.36	1.36	1.31
33	F	501	ADP	C8-N7	2.34	1.36	1.31
33	C	501	ADP	C5-N7	-2.32	1.34	1.39
33	C	501	ADP	C8-N7	2.30	1.36	1.31
33	D	501	ADP	C8-N7	2.28	1.36	1.31
33	E	401	ADP	C5-N7	-2.27	1.34	1.39
33	F	501	ADP	PA-O3A	2.24	1.61	1.59
33	D	501	ADP	C5-N7	-2.20	1.35	1.39
33	A	501	ADP	C8-N7	2.13	1.35	1.31
33	B	501	ADP	C5-N7	-2.12	1.35	1.39
33	D	501	ADP	PA-O3A	2.04	1.61	1.59

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	A	501	ADP	C5-C4-N3	-6.48	117.79	126.72
33	F	501	ADP	C5-C4-N3	-6.36	117.95	126.72
33	C	501	ADP	C5-C4-N3	-6.08	118.34	126.72
33	D	501	ADP	C5-C4-N3	-5.87	118.63	126.72
33	E	401	ADP	C5-C4-N3	-5.83	118.69	126.72
33	B	501	ADP	C5-C4-N3	-5.73	118.83	126.72
33	A	501	ADP	N3-C4-N9	5.29	136.17	127.17
33	F	501	ADP	N3-C4-N9	5.07	135.79	127.17
33	C	501	ADP	N3-C4-N9	4.78	135.30	127.17
33	D	501	ADP	N3-C4-N9	4.73	135.21	127.17
33	B	501	ADP	N3-C4-N9	4.45	134.74	127.17
33	E	401	ADP	N3-C4-N9	4.36	134.59	127.17
33	F	501	ADP	C2-N3-C4	3.92	121.40	111.83
33	A	501	ADP	C2-N3-C4	3.85	121.24	111.83
33	E	401	ADP	O4'-C1'-N9	3.82	115.42	108.09
33	E	401	ADP	C2-N3-C4	3.75	120.98	111.83
33	C	501	ADP	C2-N3-C4	3.72	120.92	111.83
33	B	501	ADP	C2-N3-C4	3.71	120.89	111.83
33	D	501	ADP	C2-N3-C4	3.69	120.84	111.83
33	B	501	ADP	C4-C5-N7	-3.67	106.39	110.58
33	E	401	ADP	C4-C5-N7	-3.60	106.46	110.58
33	C	501	ADP	C4-C5-N7	-3.54	106.54	110.58
33	F	501	ADP	C4-C5-N7	-3.46	106.62	110.58
33	D	501	ADP	C4-C5-N7	-3.38	106.72	110.58
33	E	401	ADP	N3-C2-N1	-3.30	123.59	128.58
33	B	501	ADP	N3-C2-N1	-3.28	123.61	128.58
33	D	501	ADP	N3-C2-N1	-3.22	123.71	128.58
33	F	501	ADP	N3-C2-N1	-3.21	123.72	128.58
33	A	501	ADP	C4-C5-N7	-3.12	107.02	110.58
33	A	501	ADP	N3-C2-N1	-3.08	123.92	128.58
33	C	501	ADP	N3-C2-N1	-3.05	123.96	128.58
33	B	501	ADP	C4-N9-C8	2.77	108.65	105.74
33	D	501	ADP	C4-N9-C8	2.74	108.62	105.74
33	B	501	ADP	C5-N7-C8	2.67	107.65	103.45
33	F	501	ADP	C5-N7-C8	2.62	107.57	103.45
33	E	401	ADP	C2'-C1'-N9	-2.54	106.98	113.30
33	C	501	ADP	C5-N7-C8	2.53	107.43	103.45
33	D	501	ADP	C5-N7-C8	2.52	107.40	103.45
33	E	401	ADP	C5-N7-C8	2.41	107.24	103.45
33	C	501	ADP	C4-N9-C8	2.35	108.21	105.74
33	C	501	ADP	C3'-C2'-C1'	2.35	105.91	101.46
33	F	501	ADP	C4-N9-C8	2.34	108.20	105.74
33	B	501	ADP	C6-C5-N7	2.31	136.54	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	A	501	ADP	C3'-C2'-C1'	2.28	105.77	101.46
33	A	501	ADP	C5-N7-C8	2.25	106.99	103.45
33	D	501	ADP	C3'-C2'-C1'	2.25	105.72	101.46
33	F	501	ADP	O4'-C1'-N9	2.23	112.36	108.09
33	E	401	ADP	C6-C5-N7	2.23	136.38	132.09
33	B	501	ADP	O4'-C1'-N9	2.18	112.28	108.09
33	E	401	ADP	C3'-C2'-C1'	2.18	105.58	101.46
33	B	501	ADP	N9-C8-N7	-2.15	110.88	113.94
33	E	401	ADP	C4-N9-C8	2.12	107.96	105.74
33	A	501	ADP	C4-N9-C8	2.04	107.88	105.74

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	B	501	ADP	PA-O3A-PB-O3B
33	B	501	ADP	C5'-O5'-PA-O3A
33	C	501	ADP	C5'-O5'-PA-O1A
33	E	401	ADP	C5'-O5'-PA-O1A
33	E	401	ADP	C5'-O5'-PA-O3A
33	F	501	ADP	C5'-O5'-PA-O1A
33	F	501	ADP	C5'-O5'-PA-O2A
33	F	501	ADP	O4'-C4'-C5'-O5'
33	F	501	ADP	C3'-C4'-C5'-O5'
33	A	501	ADP	O4'-C4'-C5'-O5'
33	A	501	ADP	C3'-C4'-C5'-O5'
33	D	501	ADP	C2'-C1'-N9-C8
33	F	501	ADP	PA-O3A-PB-O2B
33	F	501	ADP	PA-O3A-PB-O3B
33	B	501	ADP	O4'-C4'-C5'-O5'
33	A	501	ADP	C5'-O5'-PA-O1A
33	B	501	ADP	C5'-O5'-PA-O1A
33	C	501	ADP	C5'-O5'-PA-O2A
33	C	501	ADP	C5'-O5'-PA-O3A
33	E	401	ADP	C5'-O5'-PA-O2A
33	F	501	ADP	C5'-O5'-PA-O3A
33	A	501	ADP	C2'-C1'-N9-C4
33	D	501	ADP	C2'-C1'-N9-C4
33	A	501	ADP	C2'-C1'-N9-C8
33	E	401	ADP	C4'-C5'-O5'-PA
33	D	501	ADP	C3'-C4'-C5'-O5'
33	D	501	ADP	O4'-C4'-C5'-O5'

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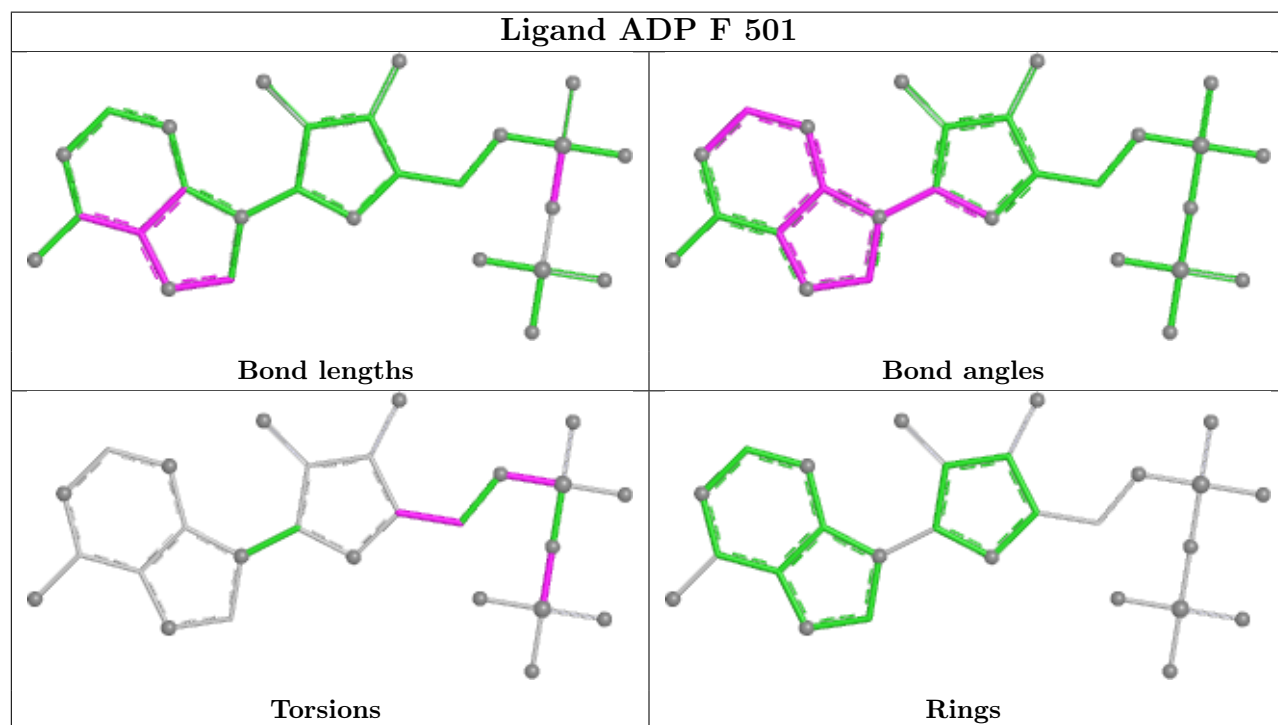
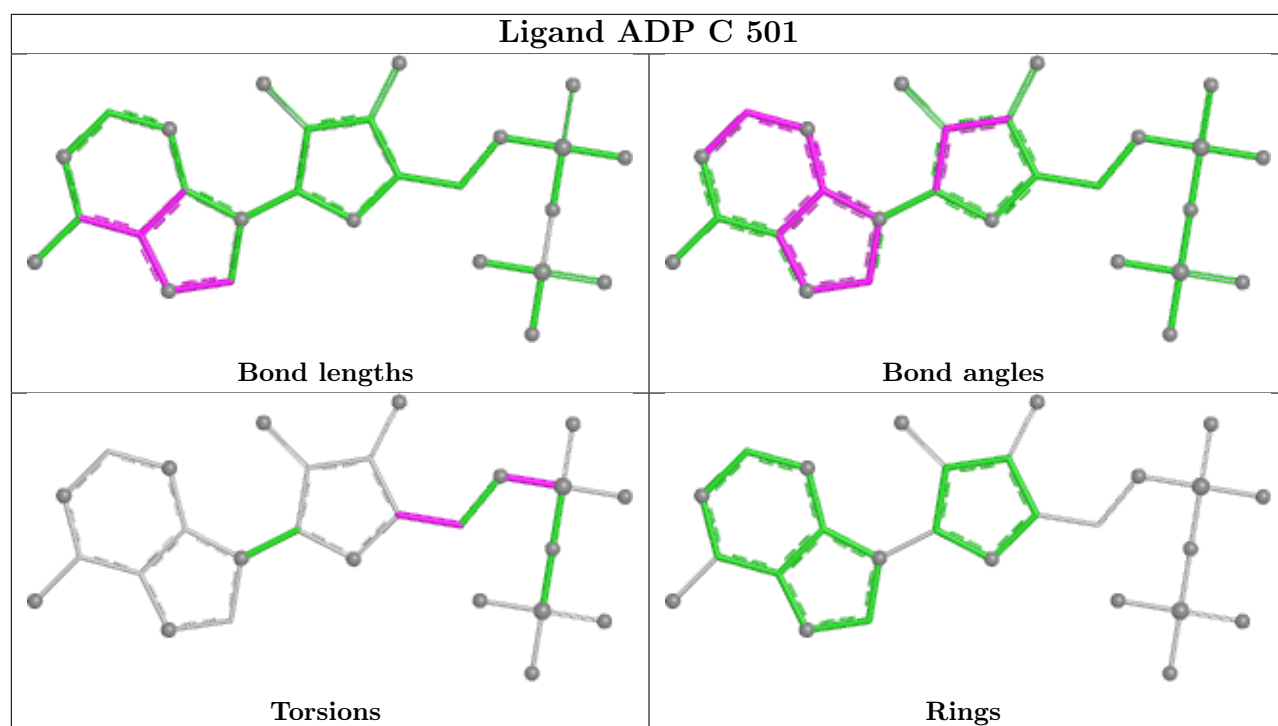
Mol	Chain	Res	Type	Atoms
33	C	501	ADP	O4'-C4'-C5'-O5'
33	B	501	ADP	PA-O3A-PB-O1B
33	D	501	ADP	O4'-C1'-N9-C8
33	E	401	ADP	PB-O3A-PA-O1A
33	E	401	ADP	PB-O3A-PA-O2A

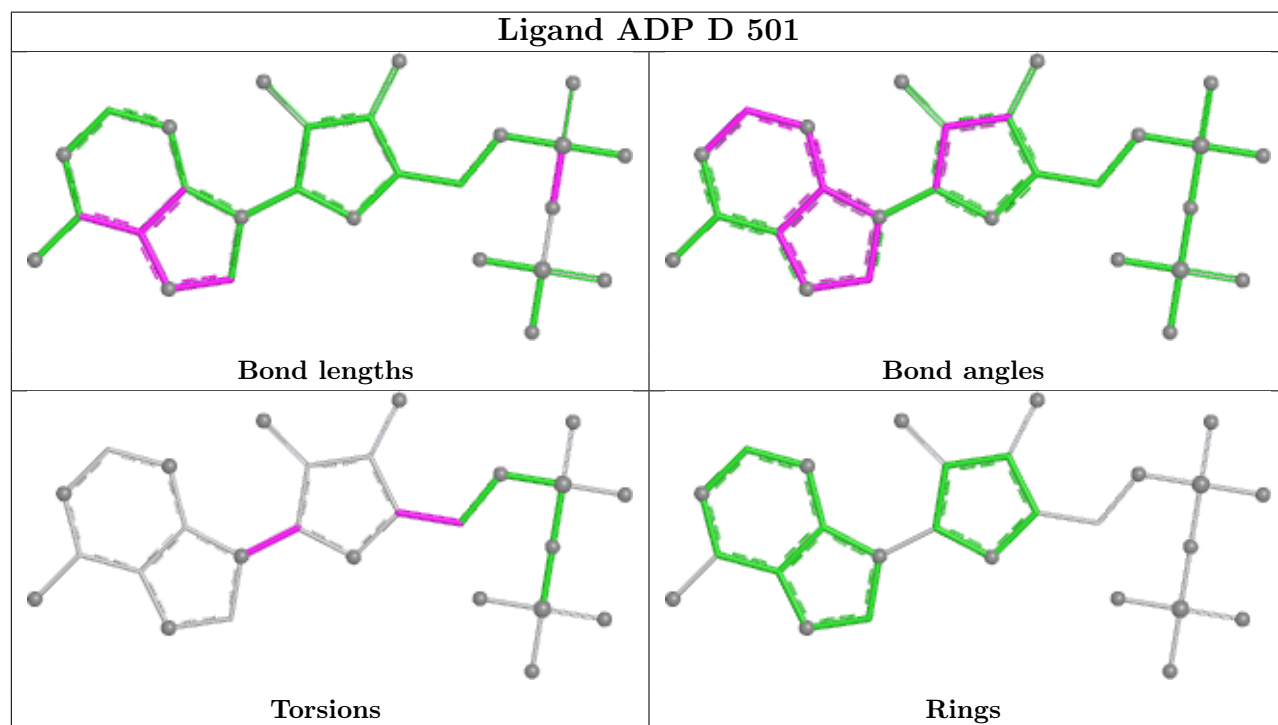
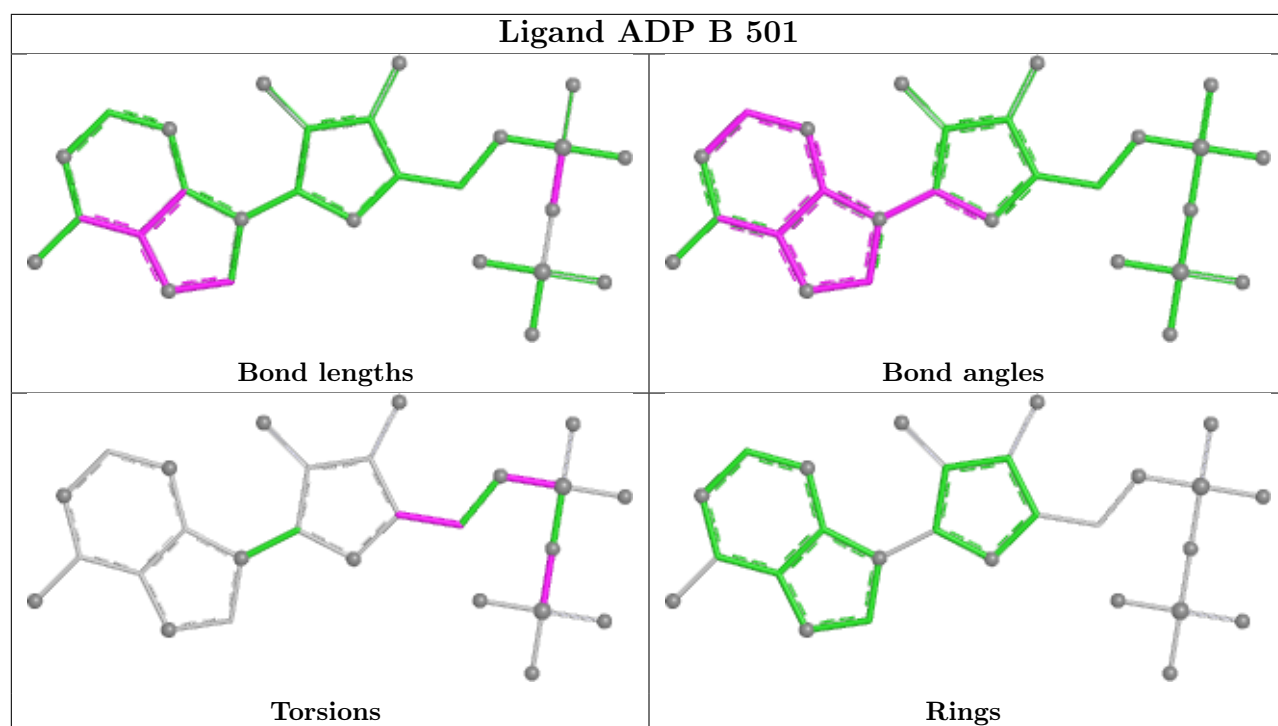
There are no ring outliers.

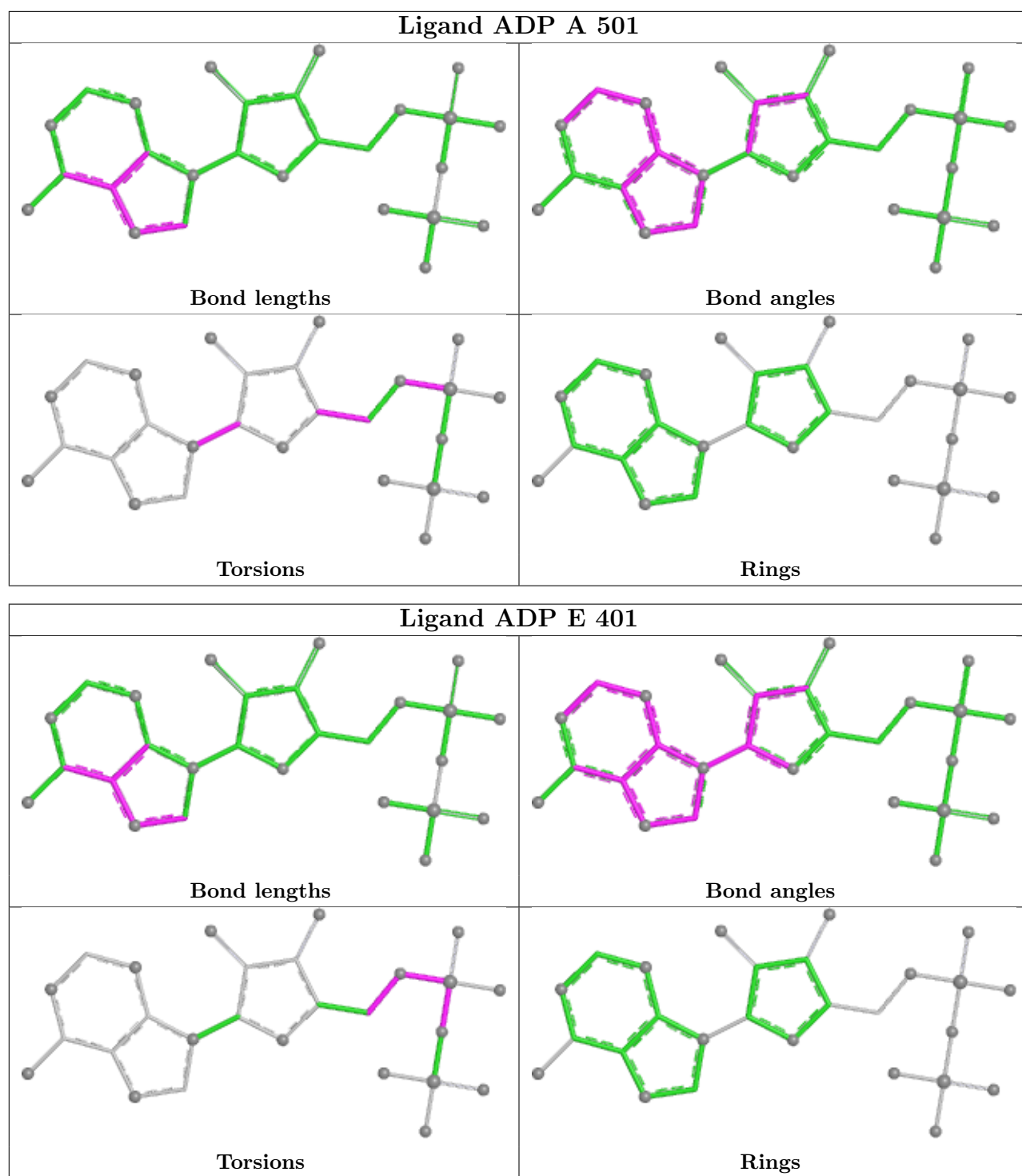
6 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	C	501	ADP	3	0
33	F	501	ADP	4	0
33	B	501	ADP	8	0
33	D	501	ADP	5	0
33	A	501	ADP	5	0
33	E	401	ADP	7	0

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







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	f	3
27	a	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	f	110:ALA	C	111:LEU	N	8.67
1	f	79:ASN	C	80:TYR	N	7.26
1	f	348:ASP	C	349:SER	N	6.44
1	a	341:LEU	C	342:ASP	N	5.77

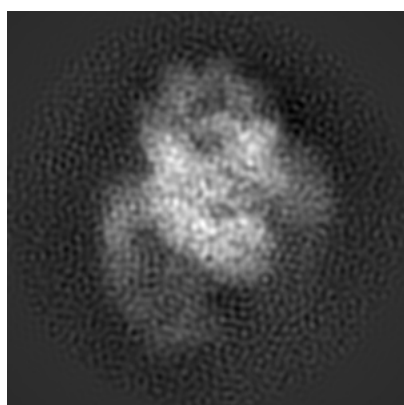
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8335. These allow visual inspection of the internal detail of the map and identification of artifacts.

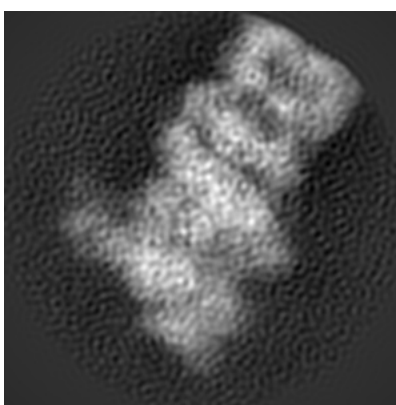
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

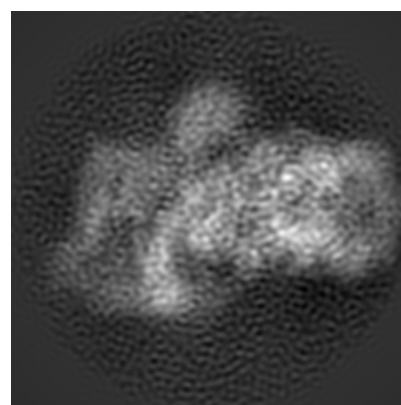
6.1.1 Primary map



X



Y

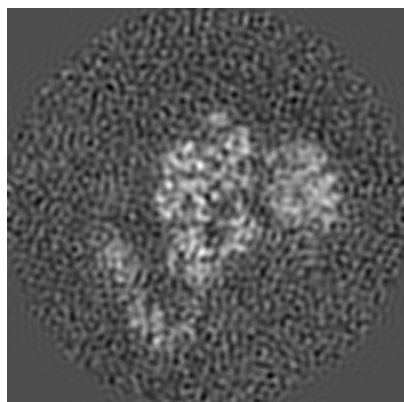


Z

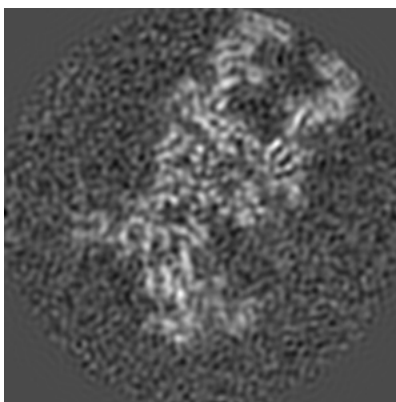
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

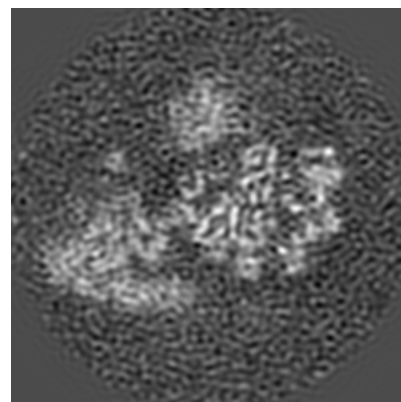
6.2.1 Primary map



X Index: 180



Y Index: 180

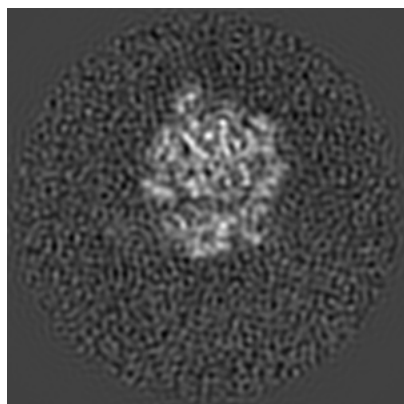


Z Index: 180

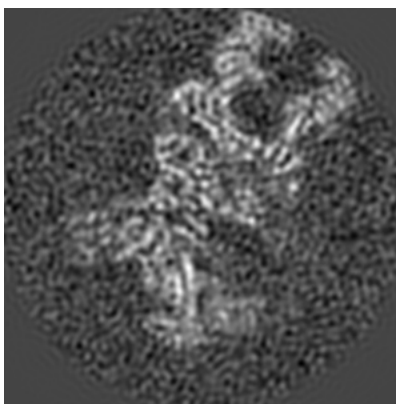
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

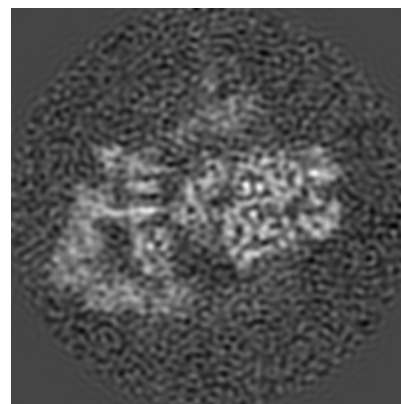
6.3.1 Primary map



X Index: 237



Y Index: 177

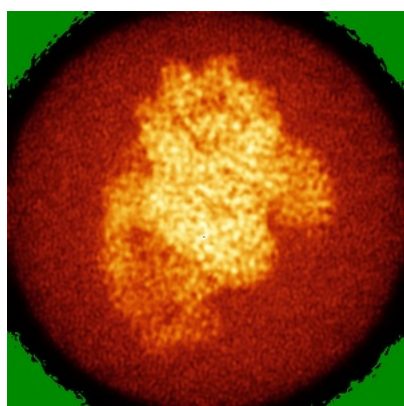


Z Index: 167

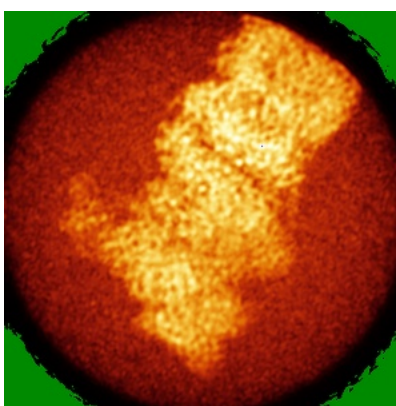
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

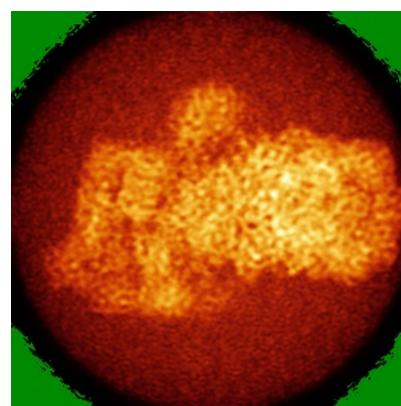
6.4.1 Primary map



X



Y

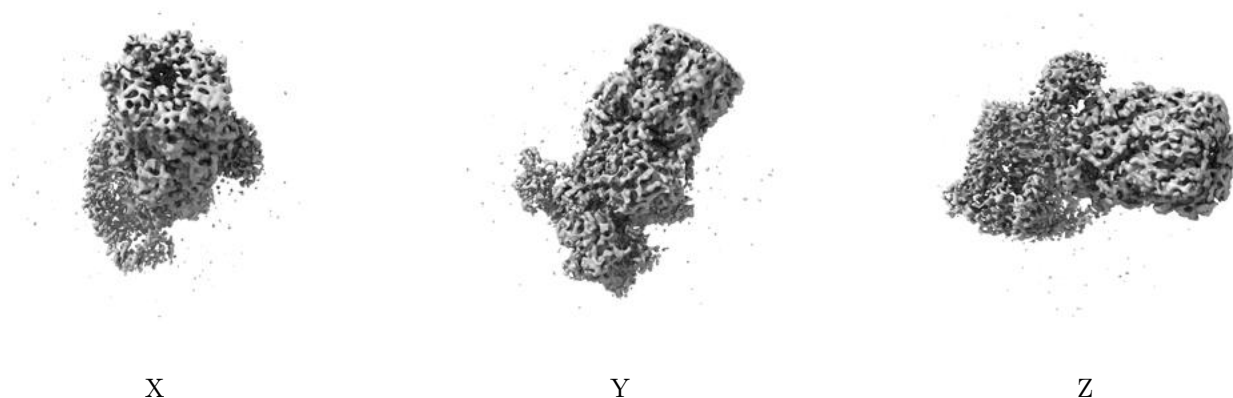


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

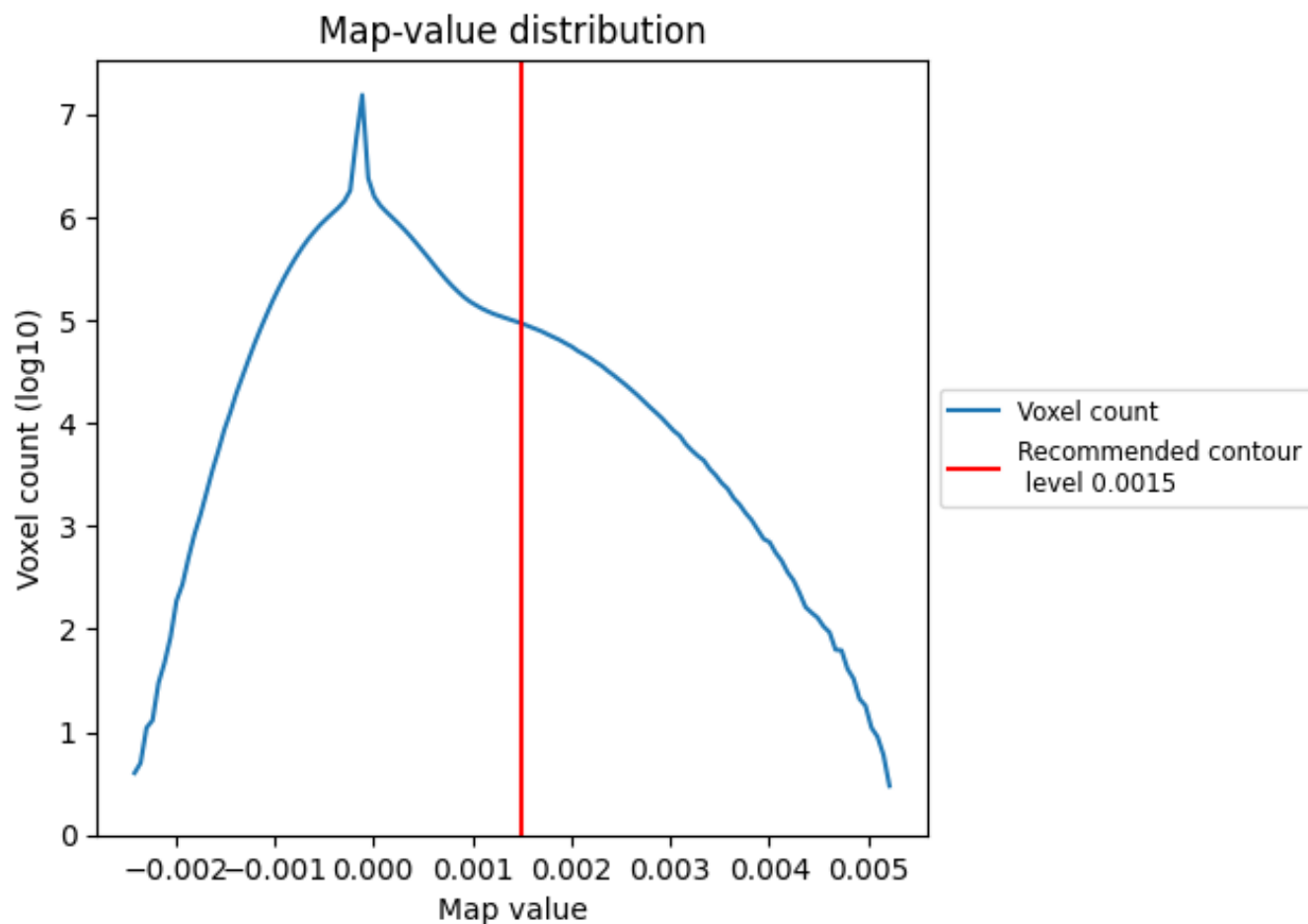
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

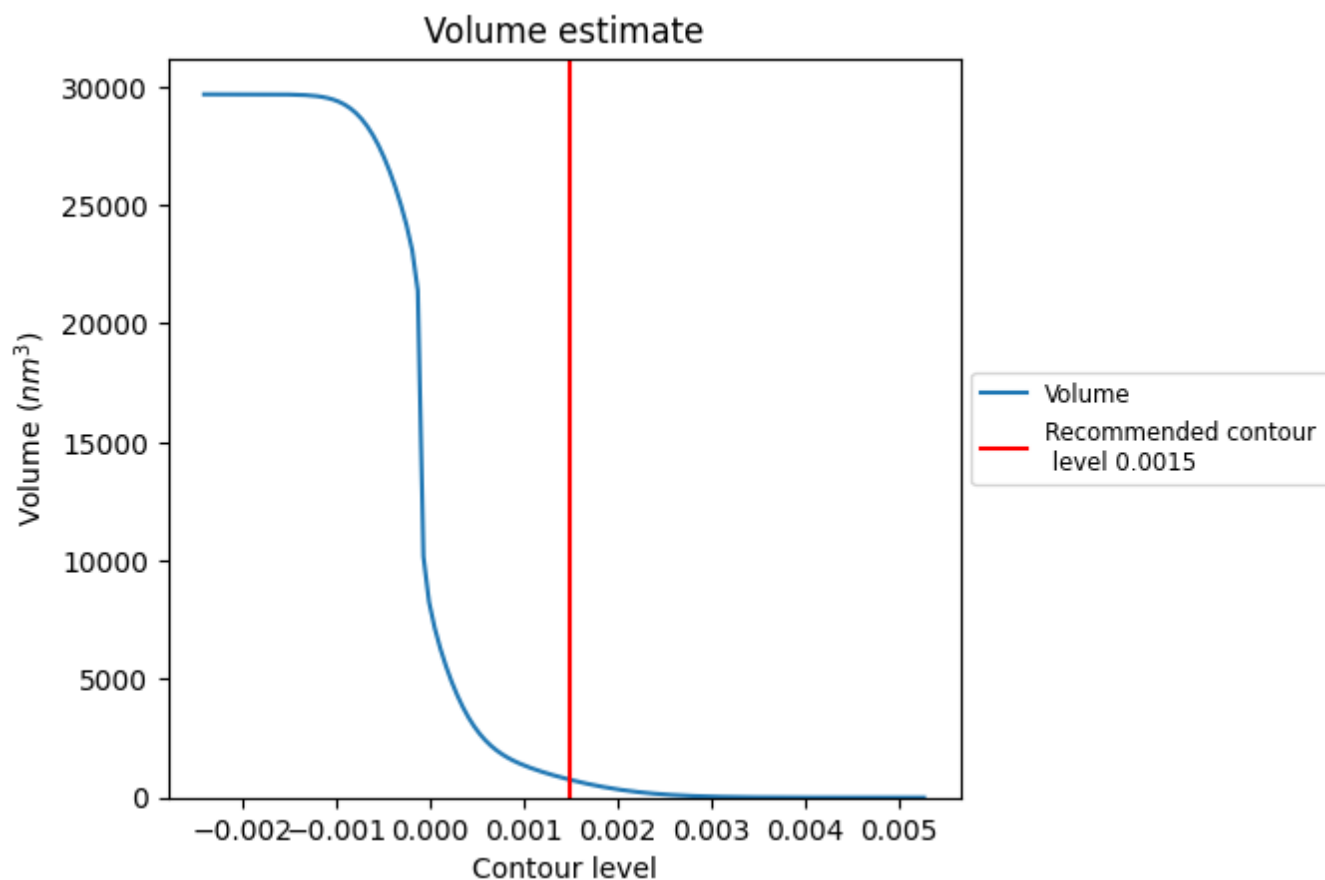
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

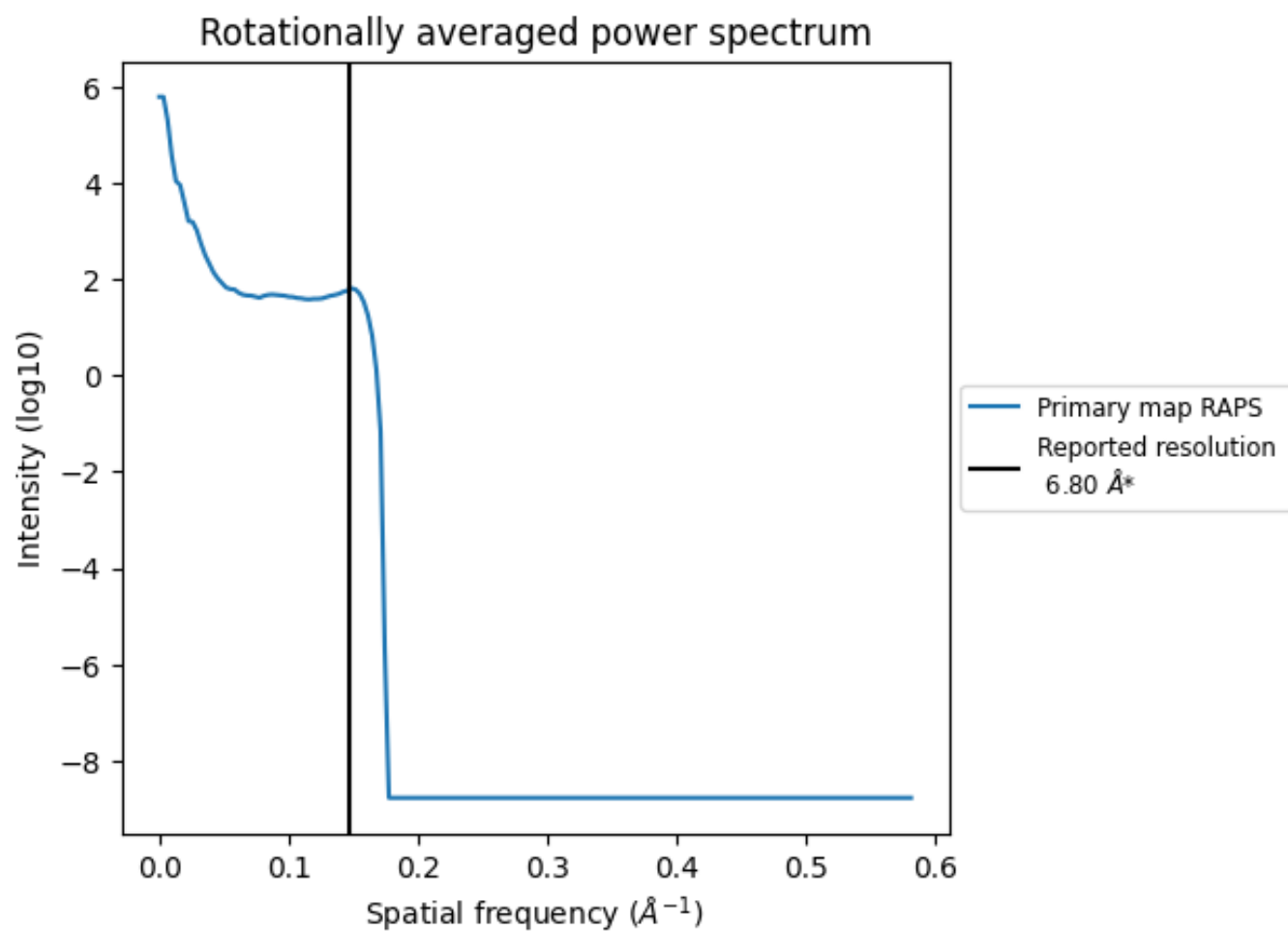
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 749 nm³; this corresponds to an approximate mass of 677 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.147 Å⁻¹

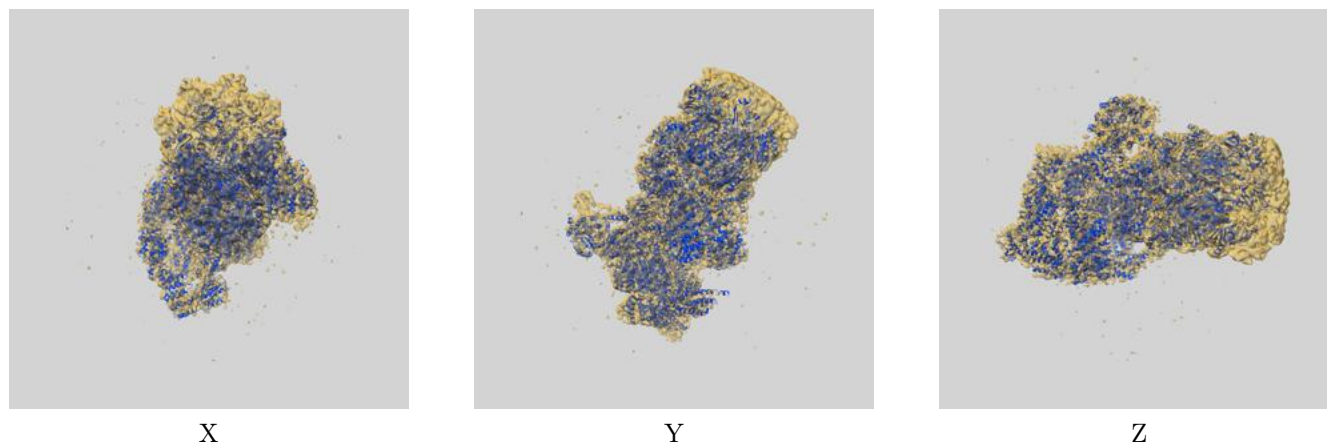
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

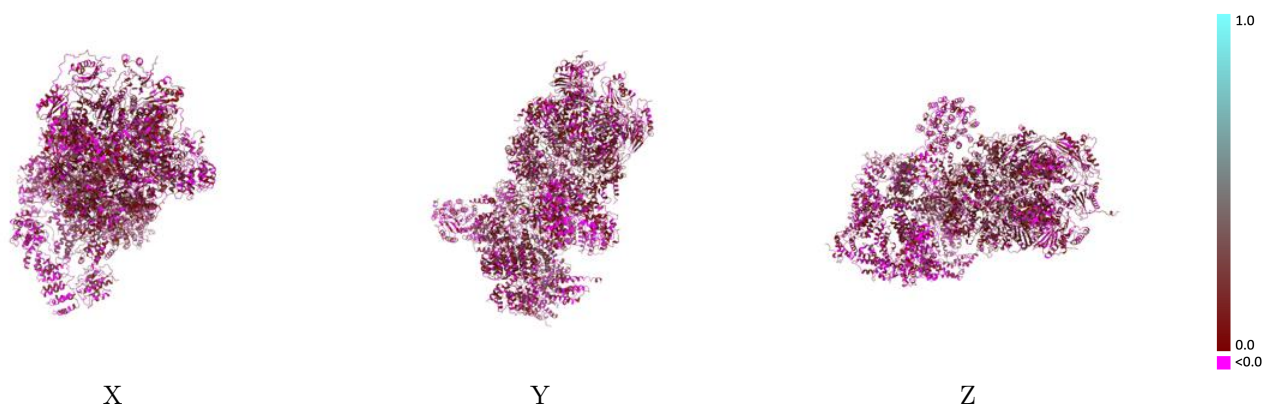
This section contains information regarding the fit between EMDB map EMD-8335 and PDB model 5T0H. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



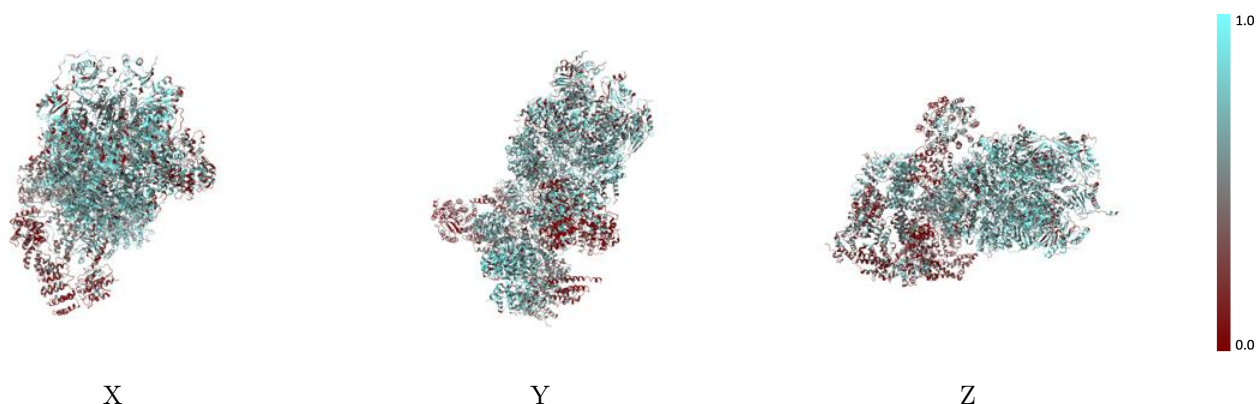
The images above show the 3D surface view of the map at the recommended contour level 0.0015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



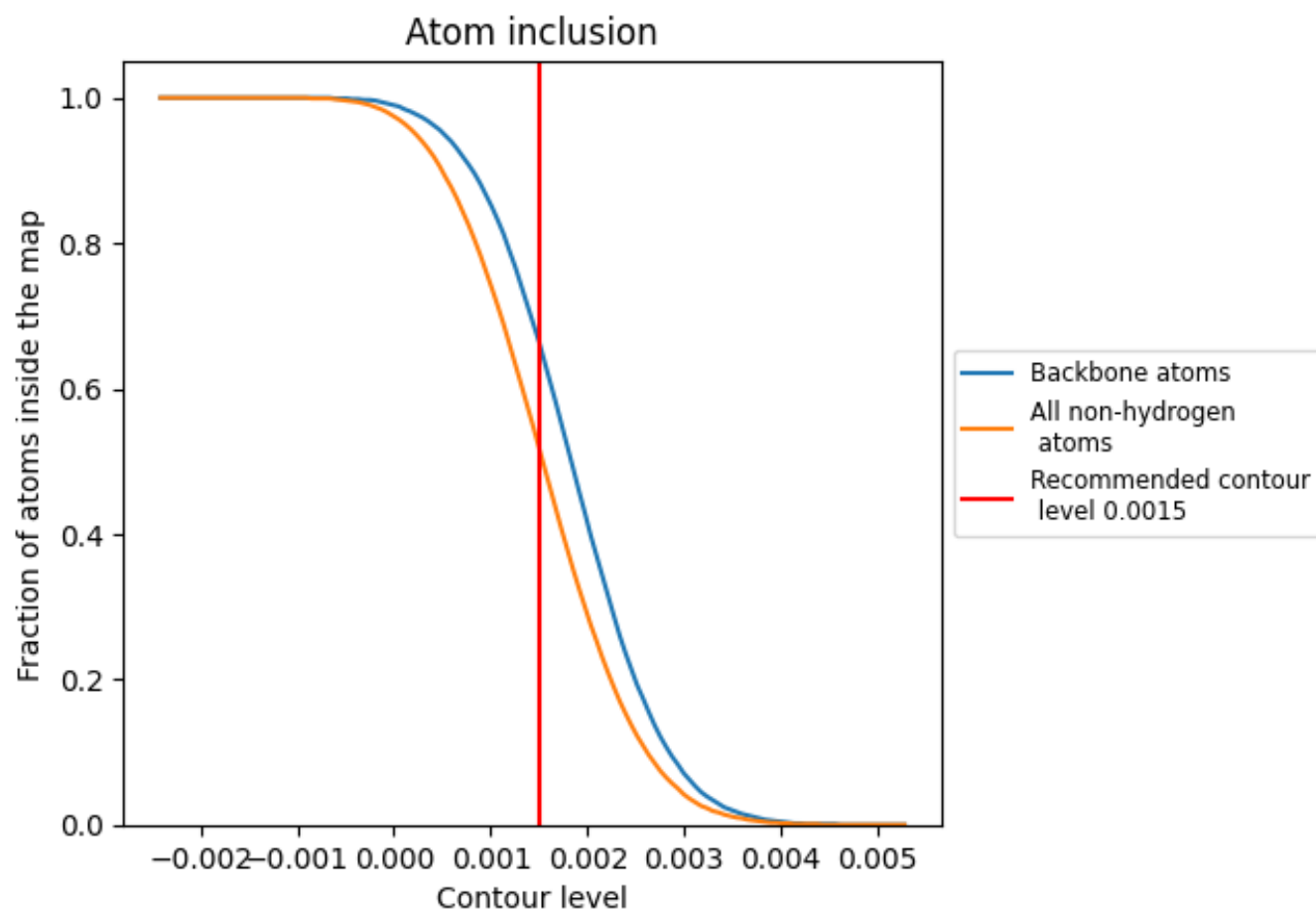
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5180	0.0940
A	0.6000	0.1350
B	0.5950	0.1460
C	0.5700	0.1290
D	0.6380	0.1430
E	0.6230	0.1420
F	0.5990	0.1360
G	0.6700	0.1350
H	0.6730	0.1420
I	0.6320	0.1350
J	0.6450	0.1320
K	0.5930	0.1010
L	0.6170	0.0950
M	0.6510	0.1320
N	0.6170	0.0820
O	0.5860	0.0800
P	0.6040	0.0920
Q	0.6100	0.1010
R	0.6060	0.1100
S	0.5770	0.1030
T	0.5710	0.0900
U	0.6110	0.1040
V	0.3610	0.0500
W	0.2710	0.0440
X	0.3850	0.0340
Y	0.3140	0.0350
Z	0.5040	0.0940
a	0.2540	0.0280
b	0.1900	0.0580
c	0.5310	0.0940
d	0.3390	0.0440
e	0.5310	0.0880
f	0.3230	0.0270

