



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 12:02 AM UTC

PDB ID : 22MM / pdb_000022mm
EMDB ID : EMD-68472
Title : Structure of human 26S proteasome complexed with midnolin(1-111+337-468)
Authors : Liang, L.; Zhu, C.; Qin, L.
Deposited on : 2026-01-16
Resolution : 3.42 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

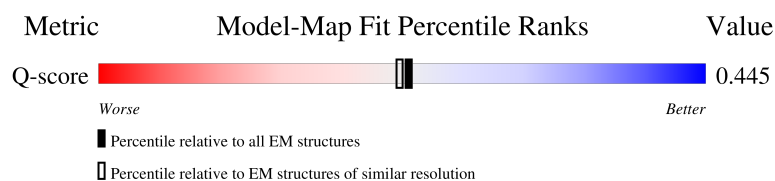
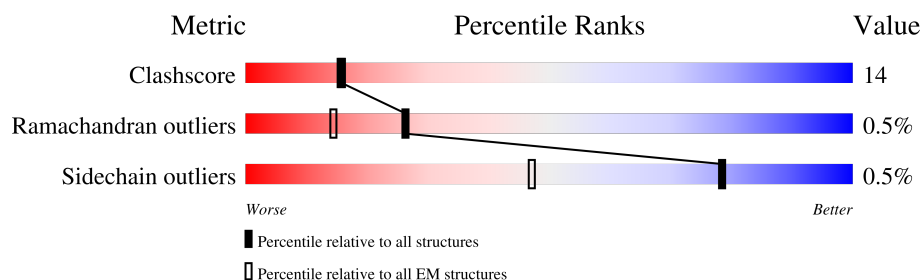
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.42 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.






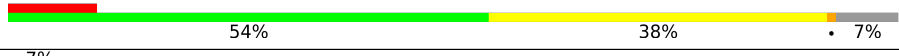
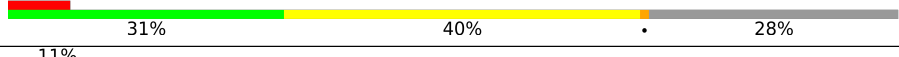
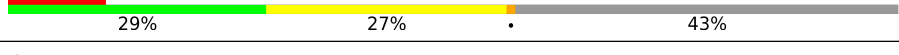


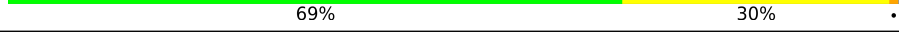
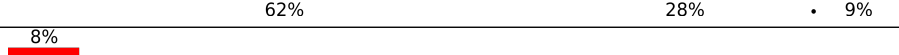

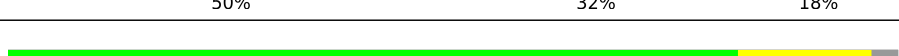

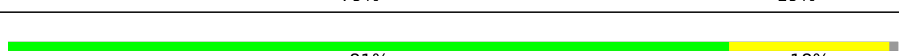
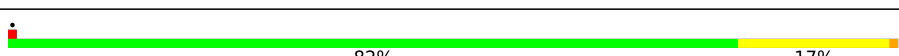
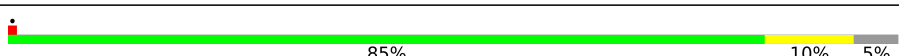





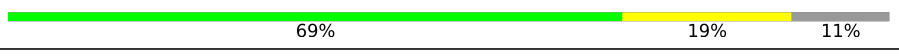

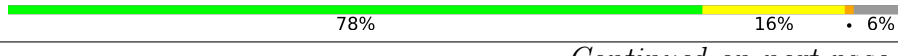

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13959 (2.92 - 3.92)

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	U	953	
2	V	533	
3	W	456	
4	X	422	


















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Mol	Chain	Length	Quality of chain
5	Y	389	
6	Z	324	
7	a	376	
8	c	309	
9	d	349	
10	e	70	
11	A	433	
12	B	440	
13	C	398	
14	D	418	
15	E	403	
16	F	439	
17	G	245	
17	g	245	
18	H	233	
18	h	233	
19	I	260	
19	i	260	
20	J	248	
21	K	241	
21	k	241	
22	L	268	
22	l	268	
23	M	254	
23	m	254	

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Mol	Chain	Length	Quality of chain
24	N	238	
24	n	238	
25	O	276	
25	o	276	
26	P	204	
26	p	204	
27	Q	201	
27	q	201	
28	R	262	
28	r	262	
29	S	240	
29	s	240	
30	T	263	
30	t	263	
31	j	247	
32	f	445	
33	u	908	

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 103249 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 proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	845	Total	C	N	O	S	0	0
			6595	4186	1120	1245	44		

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

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

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	452	Total	C	N	O	S	0	0
			3667	2314	631	697	25		

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	380	Total	C	N	O	S	0	0
			3009	1918	509	570	12		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	d	253	Total	C	N	O	S	0	0
			2078	1348	340	381	9		

- Molecule 10 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	e	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

- Molecule 11 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	413	Total	C	N	O	S	0	0
			3229	2034	566	611	18		

- Molecule 12 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	405	Total	C	N	O	S	0	0
			3162	1994	538	615	15		

- Molecule 13 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	396	Total	C	N	O	S	0	0
			3105	1954	558	576	17		

- Molecule 14 is a protein called 26S proteasome regulatory subunit 6B.

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

- Molecule 15 is a protein called Proteasome 26S subunit, ATPase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	352	Total	C	N	O	S	0	0
			2786	1750	496	524	16		

- Molecule 16 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	362	Total	C	N	O	S	0	0
			2834	1789	489	540	16		

- Molecule 17 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	237	Total	C	N	O	S	0	0
			1809	1151	302	343	13		
17	g	240	Total	C	N	O	S	0	0
			1830	1163	306	348	13		

- Molecule 18 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	H	231	Total	C	N	O	S	0	0
			1726	1097	293	331	5		
18	h	232	Total	C	N	O	S	0	0
			1727	1096	292	334	5		

- Molecule 19 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	248	Total	C	N	O	S	0	0
			1895	1195	324	368	8		
19	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 20 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	247	Total	C	N	O	S	0	0
			1844	1148	331	360	5		

- Molecule 21 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	K	230	Total	C	N	O	S	0	0
			1746	1096	286	353	11		
21	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 22 is a protein called Isoform Long of Proteasome subunit alpha type-1.

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

- Molecule 23 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		
23	m	240	Total	C	N	O	S	0	0
			1862	1181	317	353	11		

- Molecule 24 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	197	Total	C	N	O	S	0	0
			1482	928	253	289	12		
24	n	197	Total	C	N	O	S	0	0
			1482	928	253	289	12		

- Molecule 25 is a protein called Proteasome subunit beta type-7.

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

- Molecule 26 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
26	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 27 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
27	q	199	Total	C	N	O	S	0	0
			1574	1009	266	290	9		

- Molecule 28 is a protein called Proteasome subunit beta type-5.

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

- Molecule 29 is a protein called Proteasome subunit beta type-1.

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

- Molecule 30 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
30	t	215	Total	C	N	O	S	0	0
			1673	1055	288	318	12		

- Molecule 31 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 32 is a protein called Midnolin,MCHERRY,fusion tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	57	Total	C	N	O	S	0	0
			453	266	108	76	3		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	469	SER	-	linker	UNP Q504T8
f	470	ARG	-	linker	UNP Q504T8
f	471	GLU	-	linker	UNP Q504T8
f	472	ASN	-	linker	UNP Q504T8
f	473	LEU	-	linker	UNP Q504T8
f	474	TYR	-	linker	UNP Q504T8
f	475	PHE	-	linker	UNP Q504T8
f	476	GLN	-	linker	UNP Q504T8
f	477	GLY	-	linker	UNP Q504T8
f	478	ALA	-	linker	UNP Q504T8

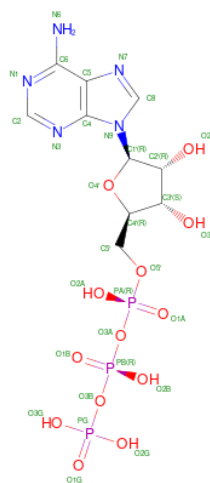
- Molecule 33 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	u	832	Total	C	N	O	S	0	0
			6439	4072	1090	1232	45		

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

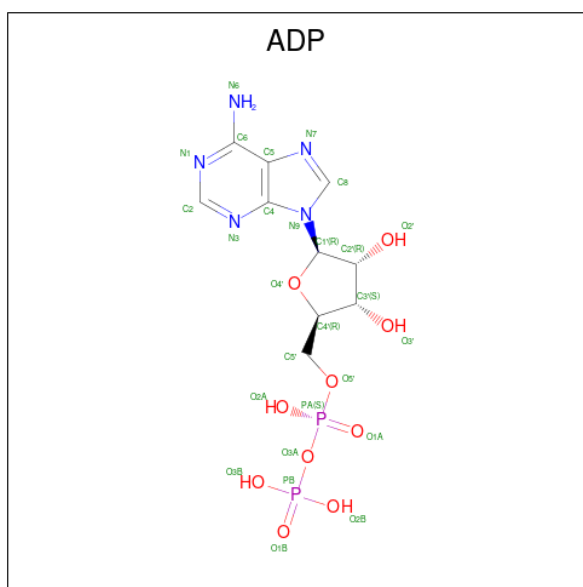


Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total 31	C 10	N 5	O 13	P 3	0
35	B	1	Total 31	C 10	N 5	O 13	P 3	0
35	C	1	Total 31	C 10	N 5	O 13	P 3	0
35	F	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
36	A	1	Total 1	Mg 1	0
36	B	1	Total 1	Mg 1	0
36	C	1	Total 1	Mg 1	0
36	D	1	Total 1	Mg 1	0
36	F	1	Total 1	Mg 1	0

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms				AltConf
38	O	1	Total 34	C 26	N 3	O 5	0
38	R	1	Total 34	C 26	N 3	O 5	0
38	n	1	Total 34	C 26	N 3	O 5	0
38	o	1	Total 34	C 26	N 3	O 5	0
38	r	1	Total 34	C 26	N 3	O 5	0

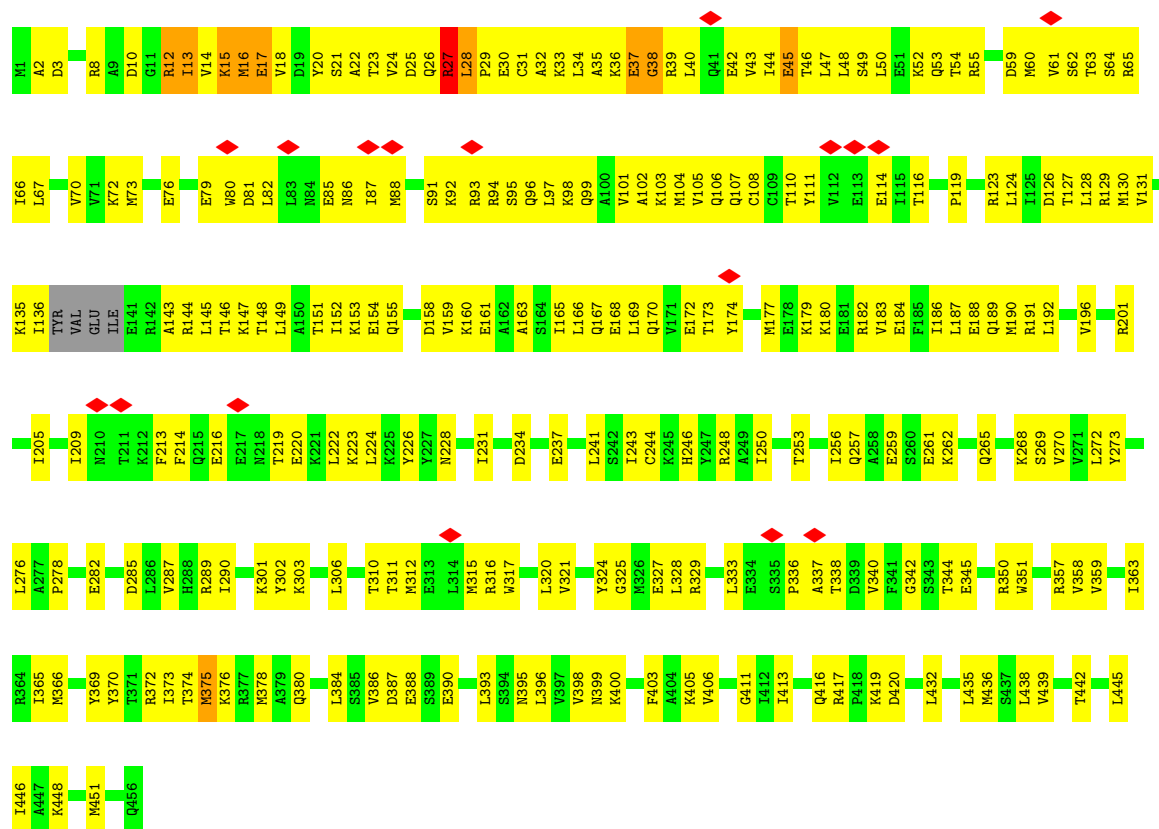
3 Residue-property plots

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 proteasome non-ATPase regulatory subunit 1

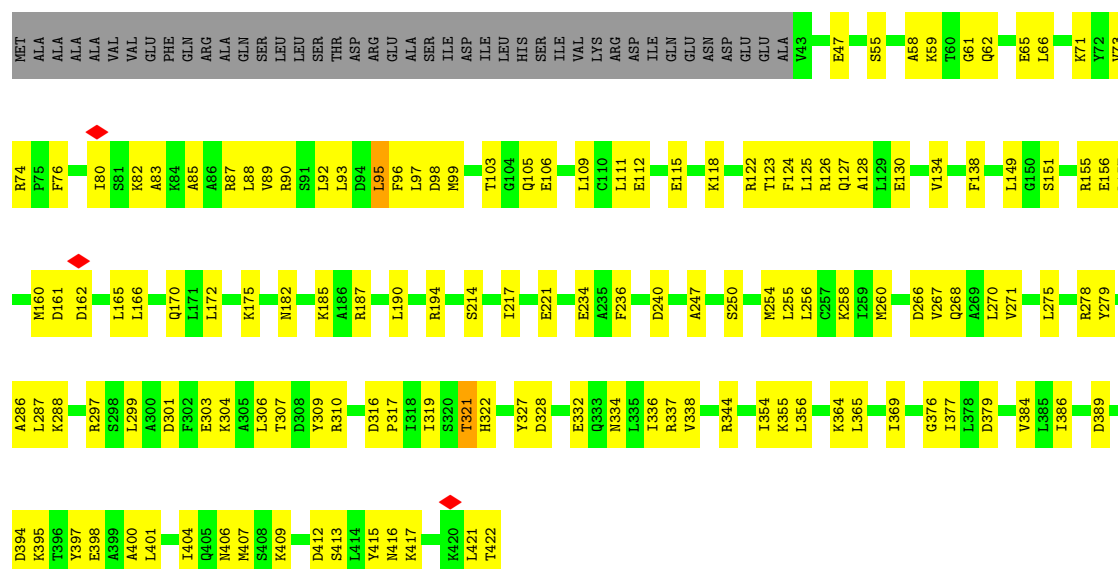






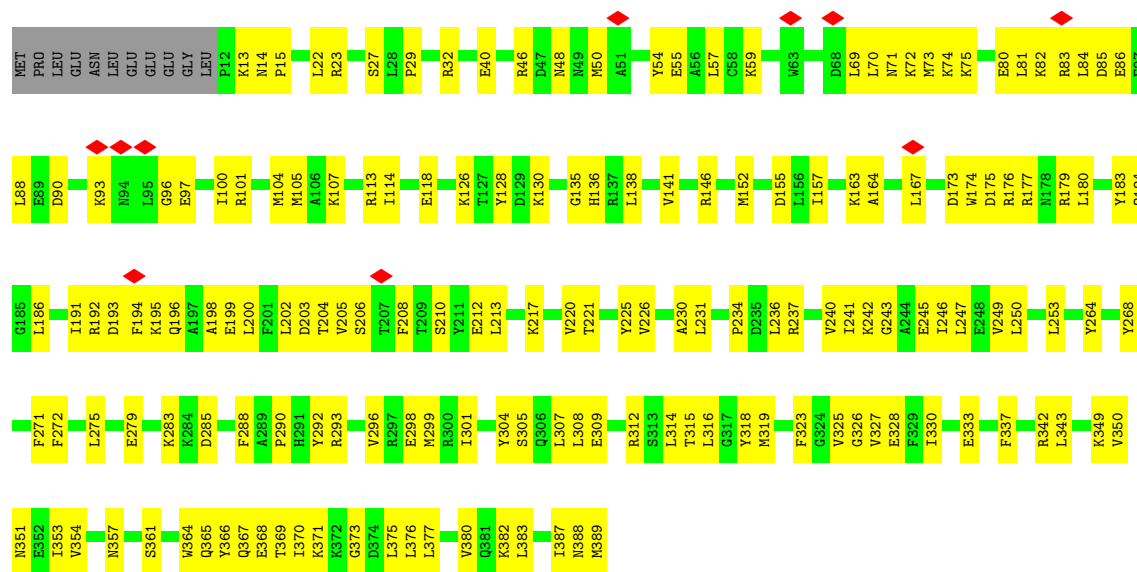
- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

Chain X: 57% 32% 10%



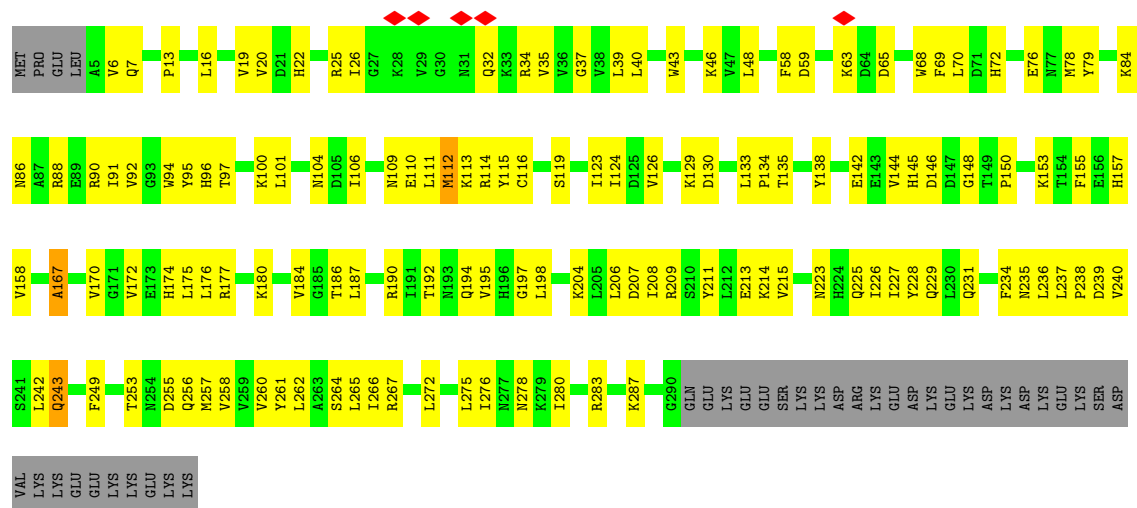
- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 54% 43% 3%



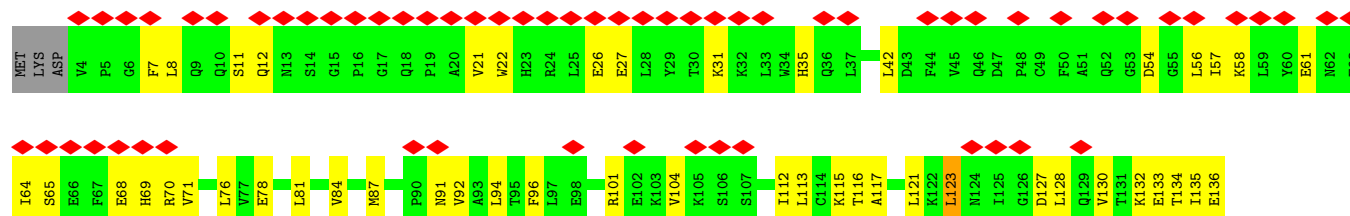
• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

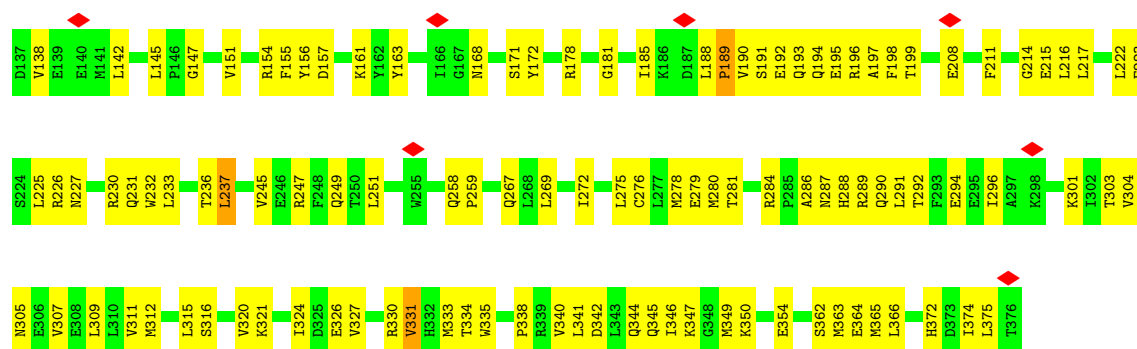
Chain Z: 47% 40% 12%



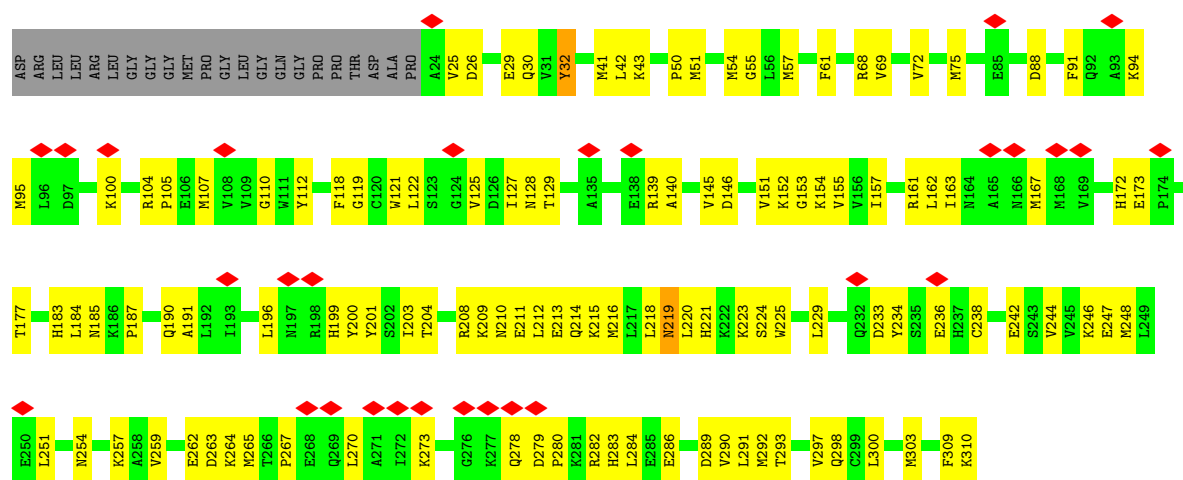
• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

Chain a: 18% 57% 41%

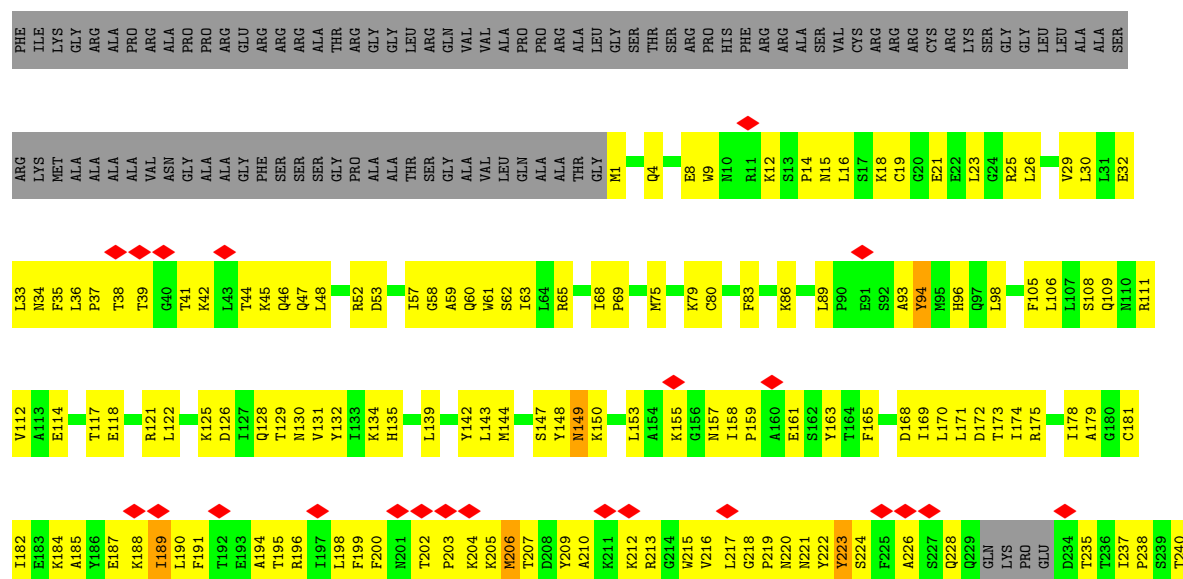




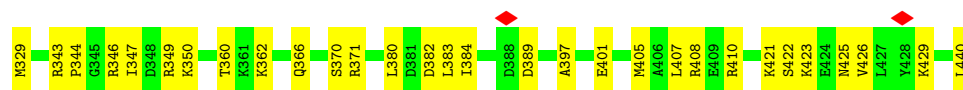
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 14



• Molecule 9: 26S proteasome non-ATPase regulatory subunit 8

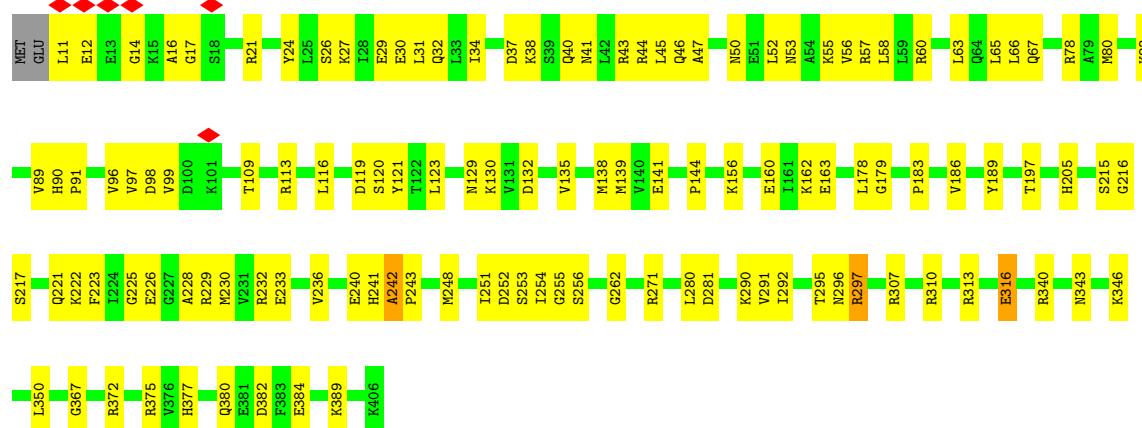






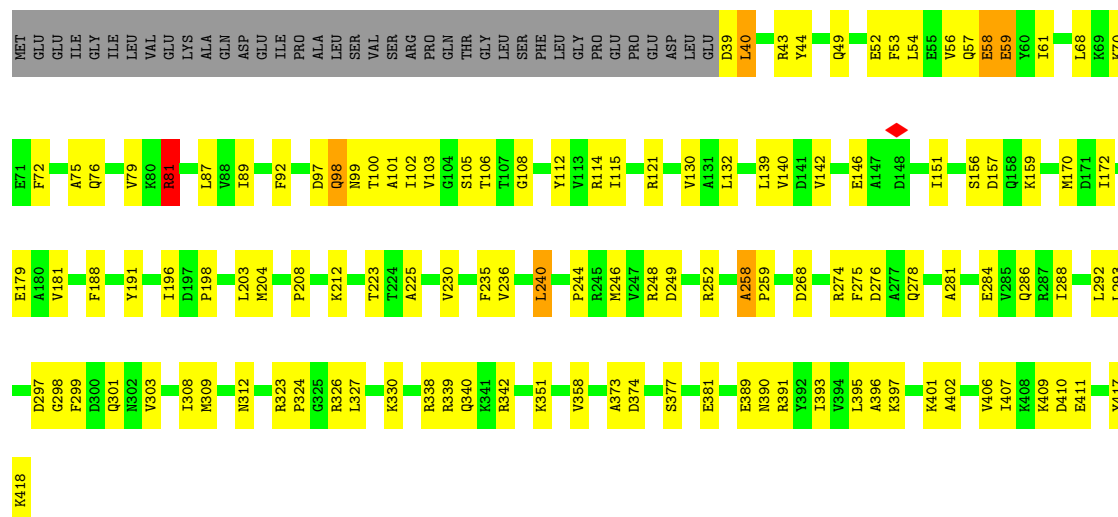
• Molecule 13: 26S proteasome regulatory subunit 8

Chain C: 69% 30%



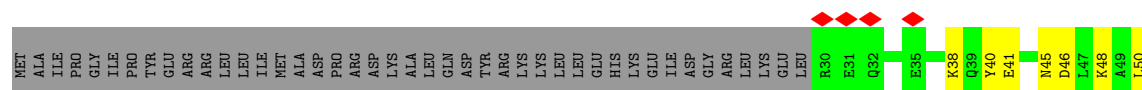
• Molecule 14: 26S proteasome regulatory subunit 6B

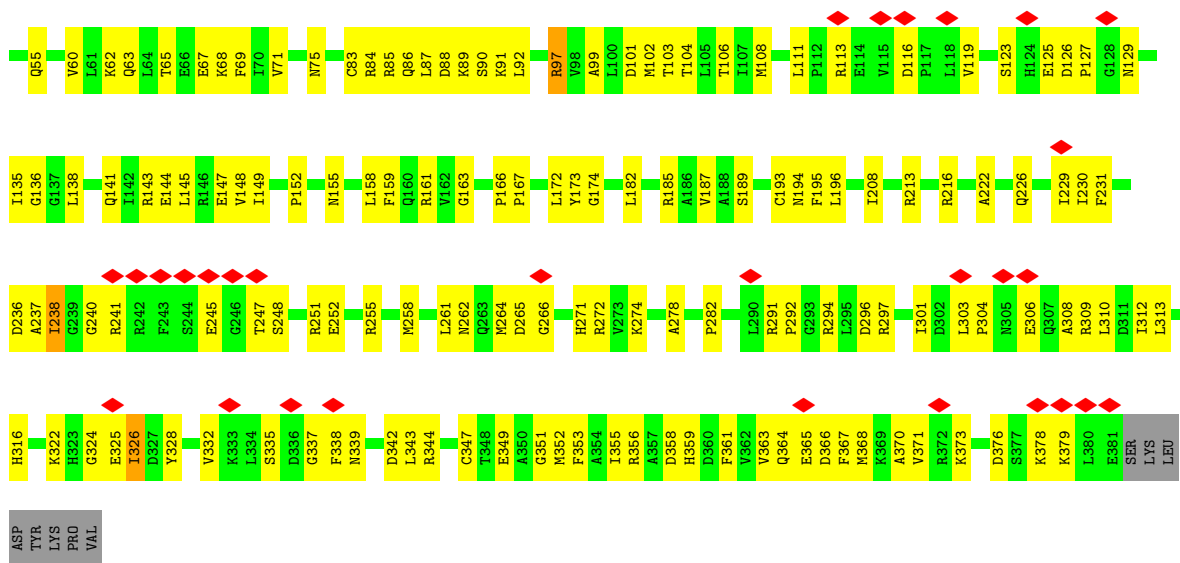
Chain D: 62% 28% 9%



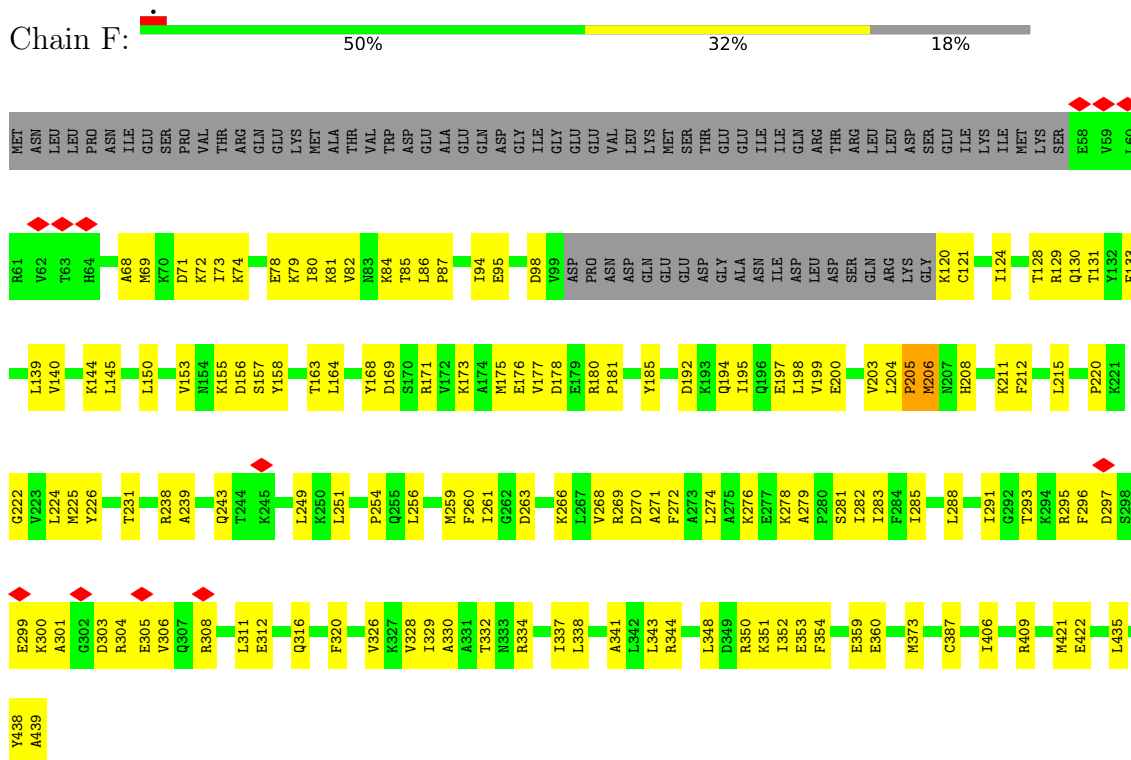
• Molecule 15: Proteasome 26S subunit, ATPase 6

Chain E: 8% 49% 37% 13%

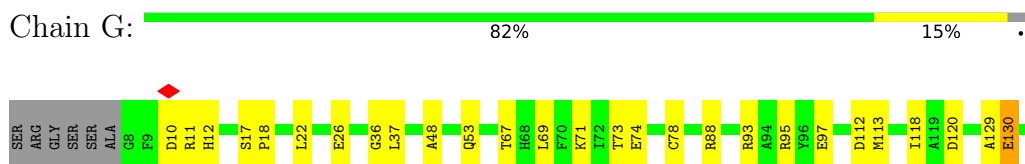




- Molecule 16: 26S proteasome regulatory subunit 6A

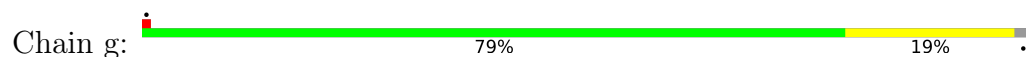


- Molecule 17: Proteasome subunit alpha type-6

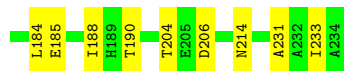
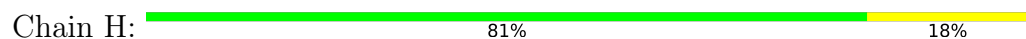




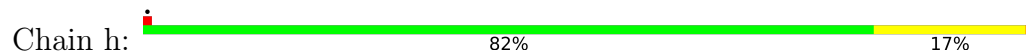
• Molecule 17: Proteasome subunit alpha type-6



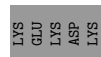
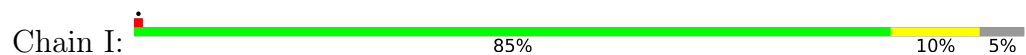
• Molecule 18: Proteasome subunit alpha type-2



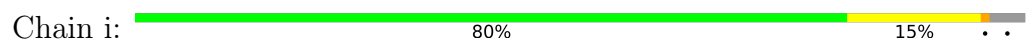
• Molecule 18: Proteasome subunit alpha type-2



• Molecule 19: Proteasome subunit alpha type-4

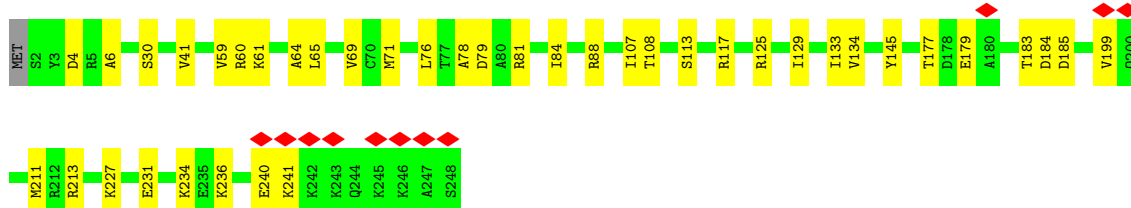
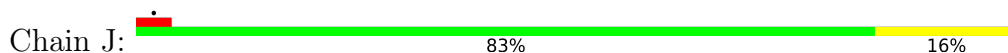


• Molecule 19: Proteasome subunit alpha type-4

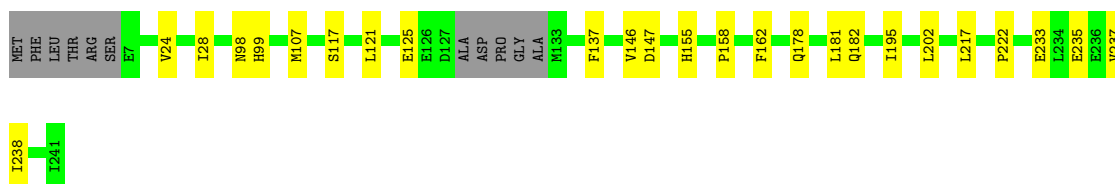
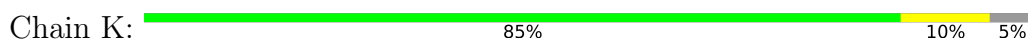




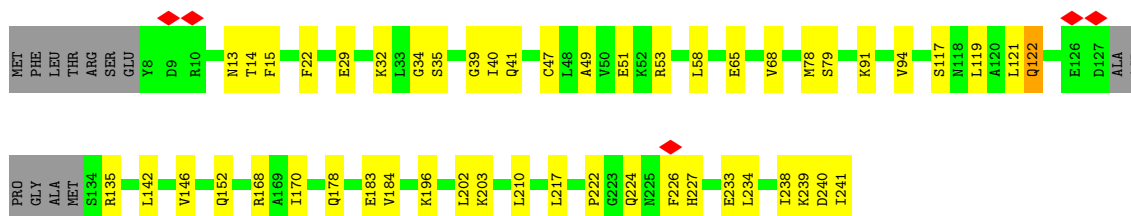
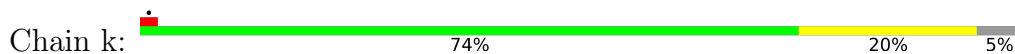
- Molecule 20: Proteasome subunit alpha type-7



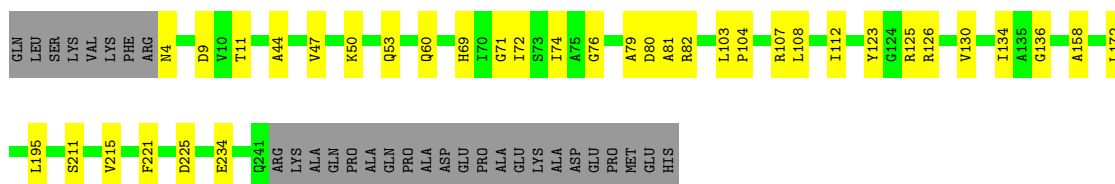
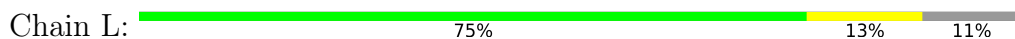
- Molecule 21: Proteasome subunit alpha type-5



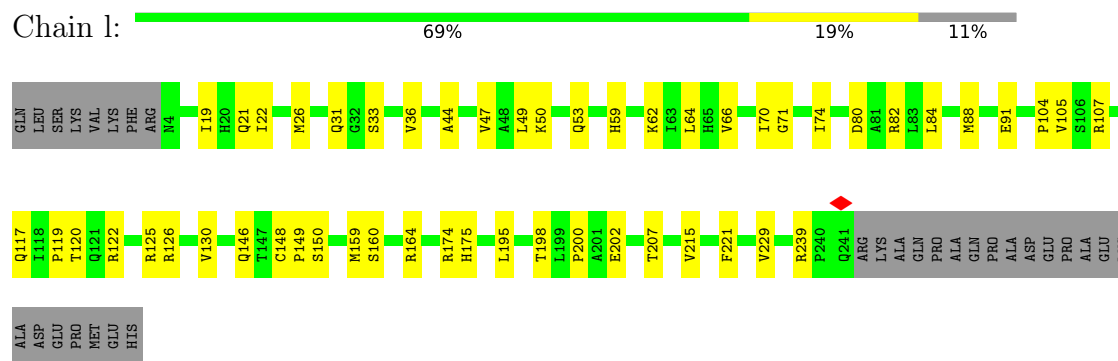
- Molecule 21: Proteasome subunit alpha type-5



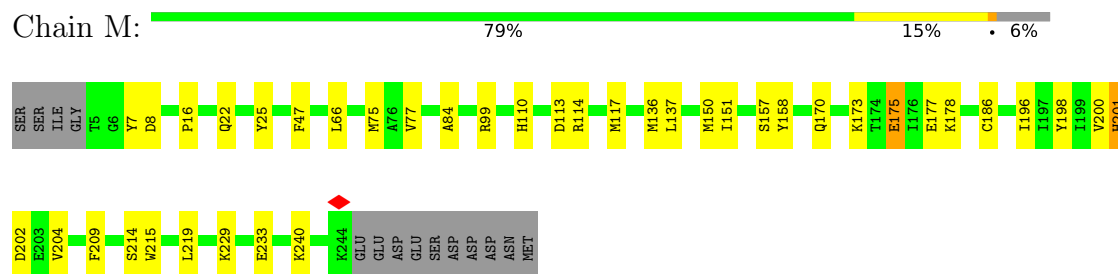
- Molecule 22: Isoform Long of Proteasome subunit alpha type-1



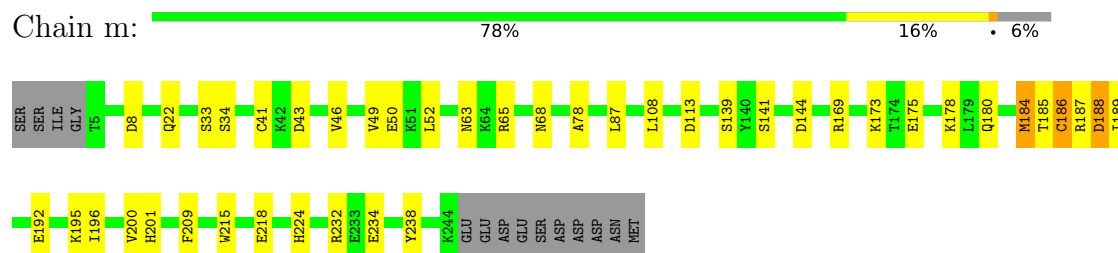
- Molecule 22: Isoform Long of Proteasome subunit alpha type-1



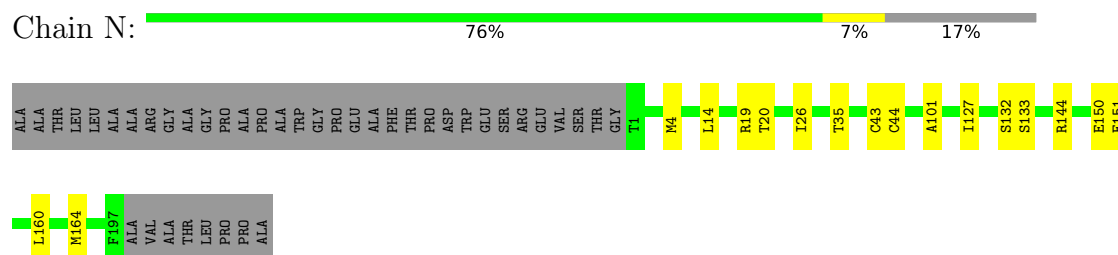
- Molecule 23: Proteasome subunit alpha type-3



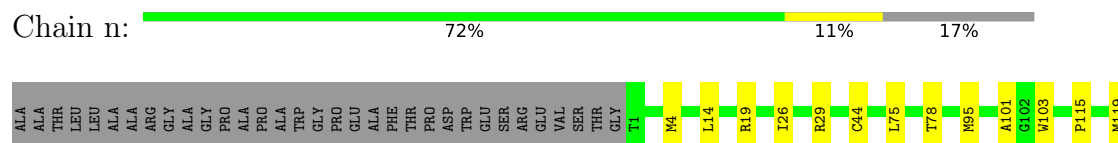
- Molecule 23: Proteasome subunit alpha type-3

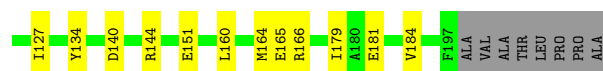


- Molecule 24: Proteasome subunit beta type-6

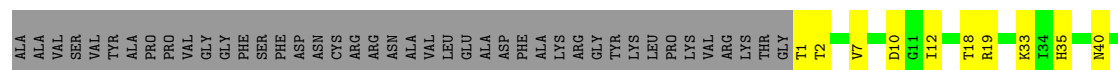


- Molecule 24: Proteasome subunit beta type-6

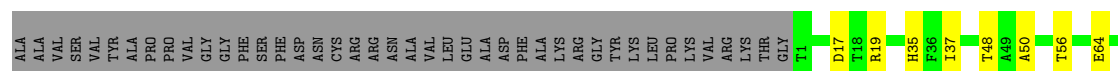




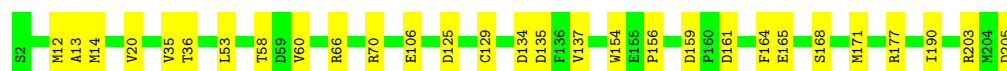
- Molecule 25: Proteasome subunit beta type-7



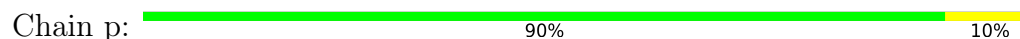
- Molecule 25: Proteasome subunit beta type-7



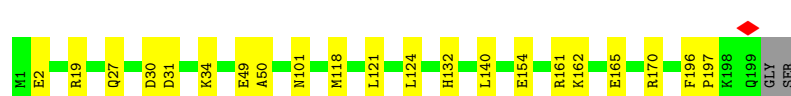
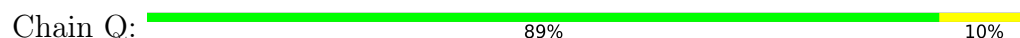
- Molecule 26: Proteasome subunit beta type-3



- Molecule 26: Proteasome subunit beta type-3



- Molecule 27: Proteasome subunit beta type-2



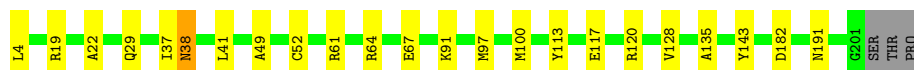
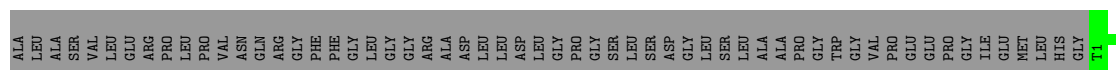
- Molecule 27: Proteasome subunit beta type-2

Chain q:  91% 8%



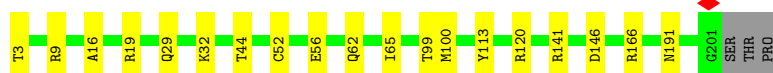
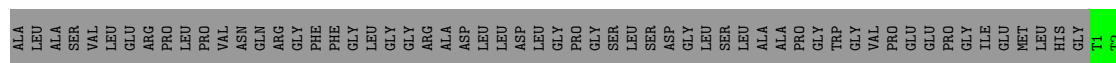
- Molecule 28: Proteasome subunit beta type-5

Chain R:  68% 8% 23%




- Molecule 28: Proteasome subunit beta type-5

Chain r:  69% 7% 23%




- Molecule 29: Proteasome subunit beta type-1

Chain S:  82% 6% 11%



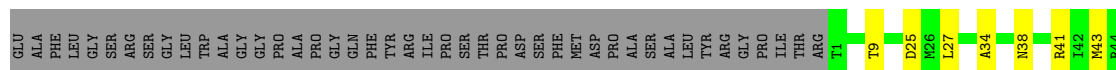
- Molecule 29: Proteasome subunit beta type-1

Chain s:  81% 8% 11%

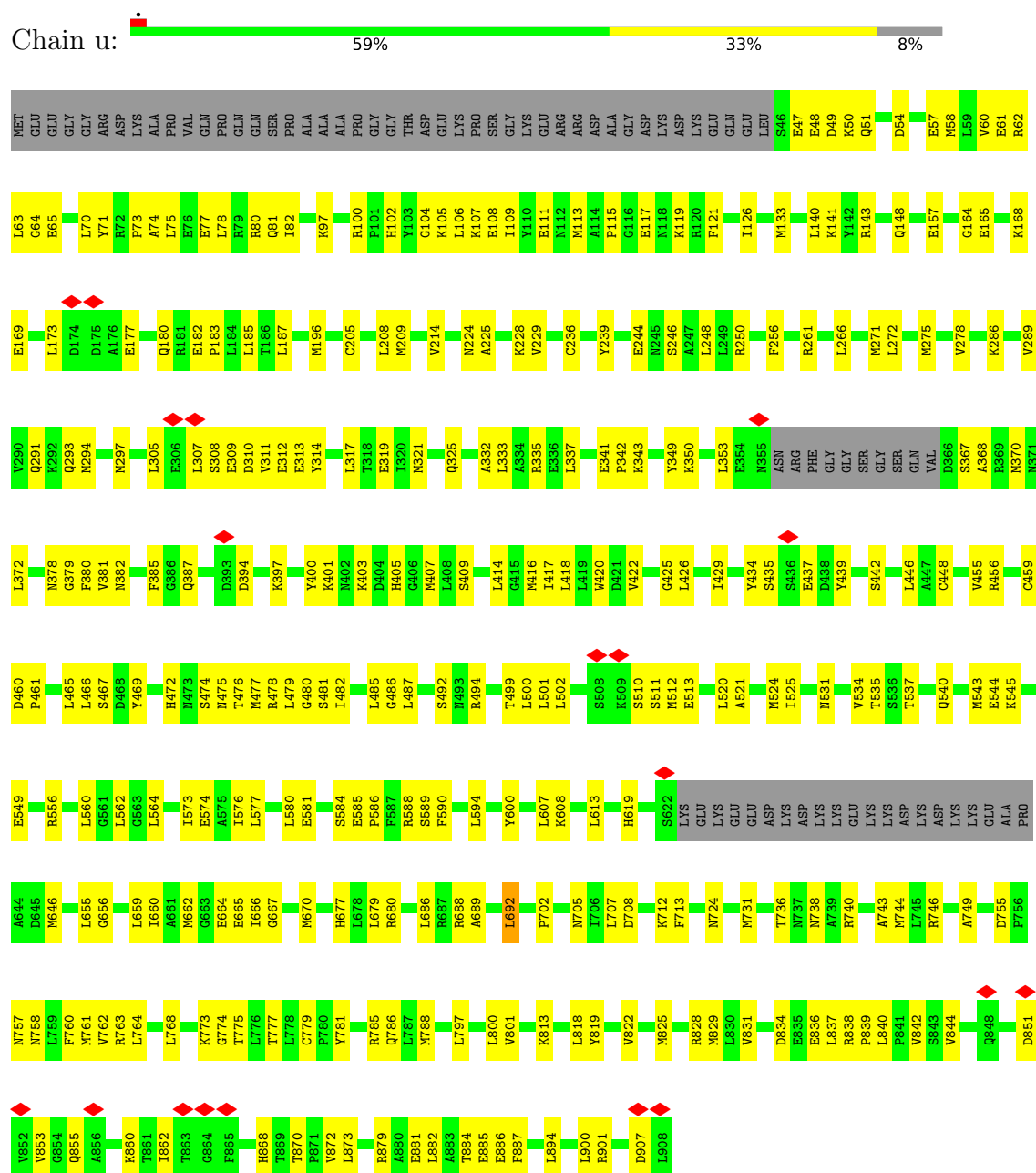


- Molecule 30: Proteasome subunit beta type-4

Chain T:  70% 12% 18%



• Molecule 33: 26S proteasome non-ATPase regulatory subunit 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17418	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	20.957	Depositor
Minimum map value	-0.182	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.550	Depositor
Recommended contour level	1.6	Depositor
Map size (Å)	510.0, 510.0, 510.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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, MG, LDZ, ADP, ATP

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	U	0.17	0/6710	0.45	0/9074
2	V	0.21	0/3929	0.55	0/5309
3	W	0.32	0/3713	0.67	0/4988
4	X	0.18	0/3053	0.47	1/4115 (0.0%)
5	Y	0.18	0/3173	0.49	0/4273
6	Z	0.22	0/2324	0.58	1/3150 (0.0%)
7	a	0.19	0/3053	0.55	2/4133 (0.0%)
8	c	0.20	0/2302	0.57	0/3110
9	d	0.21	0/2122	0.60	0/2864
10	e	0.21	0/338	0.64	0/450
11	A	0.18	0/3283	0.47	0/4433
12	B	0.19	0/3208	0.46	0/4327
13	C	0.22	0/3146	0.50	0/4226
14	D	0.25	0/3090	0.55	3/4168 (0.1%)
15	E	0.20	0/2829	0.51	0/3812
16	F	0.21	0/2873	0.54	1/3872 (0.0%)
17	G	0.16	0/1842	0.37	0/2500
17	g	0.14	0/1863	0.34	0/2527
18	H	0.18	0/1762	0.38	0/2394
18	h	0.25	0/1764	0.44	0/2399
19	I	0.16	0/1925	0.37	0/2606
19	i	0.16	0/1942	0.41	0/2628
20	J	0.16	0/1869	0.39	0/2531
21	K	0.14	0/1772	0.31	0/2397
21	k	0.18	0/1747	0.40	1/2364 (0.0%)
22	L	0.15	0/1885	0.34	0/2552
22	l	0.15	0/1885	0.36	0/2552
23	M	0.15	0/1891	0.35	0/2552
23	m	0.25	0/1897	0.42	0/2559
24	N	0.15	0/1508	0.34	0/2040
24	n	0.14	0/1508	0.33	0/2040
25	O	0.16	0/1670	0.37	0/2265

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
25	o	0.15	0/1670	0.41	0/2265
26	P	0.15	0/1620	0.33	0/2184
26	p	0.15	0/1620	0.32	0/2184
27	Q	0.14	0/1603	0.33	0/2174
27	q	0.14	0/1607	0.34	0/2178
28	R	0.14	0/1579	0.32	0/2134
28	r	0.14	0/1579	0.32	0/2134
29	S	0.16	0/1671	0.35	0/2253
29	s	0.15	0/1671	0.34	0/2253
30	T	0.15	0/1700	0.35	0/2305
30	t	0.15	0/1706	0.34	0/2312
31	j	0.15	0/1728	0.38	0/2358
32	f	0.24	0/455	0.72	0/600
33	u	0.18	0/6548	0.45	0/8864
All	All	0.19	0/104633	0.45	9/141408 (0.0%)

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
3	W	0	1
9	d	0	1
14	D	0	1
All	All	0	3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	F	205	PRO	CA-N-CD	-9.74	98.36	112.00
7	a	189	PRO	CA-N-CD	-7.01	102.19	112.00
7	a	259	PRO	CA-N-CD	-6.45	102.97	112.00
14	D	58	GLU	CA-C-N	-5.92	111.66	122.38
14	D	58	GLU	C-N-CA	-5.92	111.66	122.38
6	Z	112	MET	CA-CB-CG	5.68	125.46	114.10
21	k	122	GLN	CB-CG-CD	5.50	121.95	112.60
4	X	95	LEU	CA-CB-CG	5.41	135.24	116.30
14	D	59	GLU	CA-CB-CG	5.07	124.25	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	D	81	ARG	Sidechain
3	W	27	ARG	Sidechain
9	d	189	ILE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	6595	0	6650	305	0
2	V	3852	0	3893	205	0
3	W	3667	0	3786	271	0
4	X	3009	0	3113	124	0
5	Y	3115	0	3120	156	0
6	Z	2281	0	2312	144	0
7	a	2995	0	3012	133	0
8	c	2260	0	2276	108	0
9	d	2078	0	2107	154	0
10	e	334	0	294	19	0
11	A	3229	0	3263	116	0
12	B	3162	0	3225	110	0
13	C	3105	0	3219	126	0
14	D	3040	0	3076	115	0
15	E	2786	0	2843	147	0
16	F	2834	0	2912	127	0
17	G	1809	0	1781	23	0
17	g	1830	0	1807	30	0
18	H	1726	0	1646	31	0
18	h	1727	0	1619	28	0
19	I	1895	0	1833	19	0
19	i	1912	0	1851	36	0
20	J	1844	0	1747	29	0
21	K	1746	0	1695	18	0
21	k	1722	0	1673	37	0
22	L	1850	0	1822	28	0
22	l	1850	0	1822	36	0
23	M	1856	0	1816	25	0
23	m	1862	0	1827	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	N	1482	0	1450	12	0
24	n	1482	0	1450	15	0
25	O	1643	0	1644	28	0
25	o	1643	0	1644	20	0
26	P	1591	0	1609	20	0
26	p	1591	0	1609	12	0
27	Q	1570	0	1547	17	0
27	q	1574	0	1558	13	0
28	R	1548	0	1499	16	0
28	r	1548	0	1499	16	0
29	S	1641	0	1618	12	0
29	s	1641	0	1618	13	0
30	T	1667	0	1628	21	0
30	t	1673	0	1639	19	0
31	j	1704	0	1517	36	0
32	f	453	0	481	30	0
33	u	6439	0	6456	245	0
34	c	1	0	0	0	0
35	A	31	0	12	0	0
35	B	31	0	12	3	0
35	C	31	0	12	0	0
35	F	31	0	12	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
36	F	1	0	0	0	0
37	D	27	0	12	0	0
37	E	27	0	12	2	0
38	N	34	0	41	3	0
38	O	34	0	41	4	0
38	R	34	0	41	3	0
38	n	34	0	41	2	0
38	o	34	0	41	1	0
38	r	34	0	41	2	0
All	All	103249	0	102824	2984	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 14.

All (2984) 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)
15:E:303:LEU:HD12	15:E:304:PRO:HD2	1.41	1.03
3:W:320:LEU:O	3:W:324:TYR:HB3	1.61	1.01
3:W:35:ALA:HB1	3:W:48:LEU:HD22	1.43	1.00
8:c:55:GLY:HA2	8:c:75:MET:HG2	1.49	0.95
2:V:148:ARG:HD2	2:V:149:PRO:HD3	1.47	0.94
3:W:375:MET:HE1	3:W:413:ILE:HG23	1.47	0.93
9:d:68:ILE:HG13	9:d:69:PRO:HD3	1.50	0.93
3:W:36:LYS:HE2	3:W:85:GLU:HG2	1.50	0.92
32:f:385:ASN:HB3	32:f:386:ARG:HH21	1.34	0.92
2:V:409:MET:HE3	2:V:412:LEU:HD21	1.51	0.91
2:V:91:PRO:HA	2:V:94:VAL:HG12	1.51	0.90
3:W:95:SER:HA	3:W:98:LYS:HB3	1.52	0.90
1:U:503:GLN:HE22	1:U:505:ASP:HB2	1.37	0.89
3:W:366:MET:O	3:W:370:TYR:HB2	1.72	0.89
14:D:92:PHE:HE1	14:D:101:ALA:HB1	1.38	0.89
1:U:7:GLY:N	9:d:80:CYS:HG	1.69	0.89
25:O:2:THR:HG21	25:O:162:GLY:HA3	1.54	0.89
3:W:152:ILE:HG13	3:W:161:GLU:HB3	1.53	0.88
1:U:325:MET:HA	1:U:328:ILE:HG22	1.56	0.87
3:W:20:TYR:HD1	3:W:22:ALA:H	1.19	0.86
7:a:222:LEU:HB2	7:a:226:ARG:HH12	1.41	0.85
16:F:439:ALA:CB	22:L:60:GLN:HE22	1.91	0.84
2:V:309:MET:HE2	2:V:332:LEU:HB2	1.58	0.83
9:d:12:LYS:HG2	9:d:14:PRO:HD3	1.60	0.83
8:c:233:ASP:OD1	8:c:234:TYR:N	2.10	0.83
15:E:158:LEU:HD23	15:E:161:ARG:HH22	1.42	0.83
33:u:664:GLU:HG2	33:u:667:GLY:H	1.44	0.83
15:E:148:VAL:HG21	15:E:297:ARG:HG3	1.61	0.83
13:C:17:GLY:HA2	13:C:21:ARG:HB2	1.60	0.82
33:u:104:GLY:HA2	33:u:107:LYS:HE2	1.60	0.82
3:W:154:GLU:HG2	3:W:155:GLN:H	1.40	0.82
15:E:102:MET:HG3	15:E:103:THR:HG23	1.60	0.82
6:Z:214:LYS:HA	6:Z:214:LYS:HE3	1.61	0.82
8:c:68:ARG:HG3	8:c:208:ARG:HH12	1.45	0.81
13:C:367:GLY:HA3	14:D:196:ILE:HG21	1.62	0.81
15:E:355:ILE:HG12	16:F:215:LEU:HD21	1.60	0.81
11:A:425:ALA:HB1	11:A:428:ARG:HB2	1.62	0.81
23:m:41:CYS:HB3	23:m:189:ILE:HD12	1.63	0.81
9:d:106:LEU:HA	9:d:111:ARG:HH21	1.45	0.80
15:E:127:PRO:HG2	15:E:185:ARG:HE	1.46	0.80
13:C:55:LYS:HD2	13:C:56:VAL:N	1.97	0.80
23:m:41:CYS:HB3	23:m:189:ILE:CD1	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:294:GLU:H	32:f:12:ARG:HH22	1.29	0.79
1:U:328:ILE:HA	1:U:333:MET:HE1	1.62	0.79
13:C:63:LEU:HD21	14:D:79:VAL:HG22	1.63	0.78
1:U:82:LEU:HB3	1:U:129:ARG:HH21	1.48	0.78
3:W:30:GLU:O	3:W:33:LYS:HG3	1.83	0.78
7:a:275:LEU:HA	7:a:278:MET:HG2	1.65	0.78
14:D:223:THR:HG22	14:D:225:ALA:H	1.47	0.77
15:E:182:LEU:HD22	37:E:401:ADP:H2'	1.66	0.77
30:T:45:VAL:HB	30:T:49:THR:HG23	1.66	0.77
9:d:14:PRO:HA	9:d:65:ARG:HH12	1.49	0.77
16:F:439:ALA:HB1	22:L:60:GLN:HE22	1.50	0.77
33:u:75:LEU:HD12	33:u:121:PHE:HB3	1.67	0.77
1:U:146:LYS:HD2	13:C:21:ARG:HH22	1.50	0.76
2:V:496:PHE:HA	13:C:43:ARG:HH12	1.49	0.76
3:W:154:GLU:CG	3:W:155:GLN:H	1.99	0.76
15:E:50:LEU:HD21	16:F:80:ILE:HD11	1.67	0.76
1:U:715:LYS:HA	1:U:718:ASN:HD21	1.50	0.76
3:W:21:SER:HA	3:W:24:VAL:HB	1.67	0.76
24:n:75:LEU:HB2	24:n:78:THR:HG23	1.68	0.76
1:U:557:TYR:HD1	1:U:588:MET:HG3	1.50	0.76
2:V:359:PRO:HB3	2:V:382:PHE:HD2	1.50	0.76
1:U:462:LEU:HD21	1:U:490:ARG:HH22	1.51	0.76
8:c:280:PRO:HG2	8:c:282:ARG:HH21	1.49	0.76
19:i:8:ARG:HG2	19:i:9:THR:H	1.50	0.76
25:o:163:ILE:HG12	25:o:169:SER:HB3	1.66	0.76
24:n:160:LEU:O	24:n:164:MET:HG3	1.86	0.75
33:u:333:LEU:HD22	33:u:829:MET:HG3	1.67	0.75
9:d:172:ASP:HA	9:d:175:ARG:HD2	1.69	0.75
2:V:346:LEU:HA	2:V:357:LEU:HD22	1.69	0.75
11:A:166:VAL:HG12	11:A:168:GLU:H	1.52	0.75
20:J:236:LYS:NZ	20:J:240:GLU:HB2	2.01	0.75
11:A:116:LYS:NZ	12:B:128:GLY:O	2.20	0.75
32:f:406:ARG:HH22	33:u:325:GLN:HB3	1.52	0.74
33:u:585:GLU:HA	33:u:588:ARG:HG2	1.67	0.74
4:X:354:ILE:HG23	4:X:356:LEU:HG	1.68	0.74
16:F:251:LEU:HD11	16:F:256:LEU:HG	1.69	0.74
1:U:162:VAL:HA	1:U:165:LYS:HG2	1.68	0.74
6:Z:242:LEU:HD13	9:d:235:THR:HG21	1.70	0.74
12:B:287:ILE:HG12	12:B:329:MET:HE3	1.69	0.74
19:I:174:MET:HE1	19:I:199:LYS:HG2	1.69	0.74
1:U:102:ALA:HA	1:U:105:ILE:HD12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:188:MET:SD	1:U:190:ASN:N	2.60	0.74
11:A:87:LEU:HB2	11:A:91:GLN:HE22	1.53	0.74
16:F:197:GLU:HG2	16:F:352:ILE:HD11	1.70	0.73
30:t:45:VAL:HB	30:t:49:THR:HG23	1.70	0.73
1:U:903:PHE:HB2	1:U:915:LYS:HB2	1.70	0.73
31:j:7:ILE:HD11	31:j:126:PRO:HD3	1.71	0.73
6:Z:68:TRP:HZ3	6:Z:70:LEU:HG	1.53	0.73
1:U:105:ILE:HG12	1:U:134:VAL:HG22	1.69	0.73
4:X:334:ASN:HB3	4:X:354:ILE:HD11	1.69	0.73
11:A:84:LYS:O	11:A:88:GLN:NE2	2.20	0.73
14:D:236:VAL:HG11	15:E:255:ARG:HH22	1.52	0.73
3:W:395:ASN:O	3:W:399:ASN:ND2	2.22	0.73
16:F:332:THR:HG21	16:F:338:LEU:HD11	1.69	0.73
21:k:203:LYS:HB2	21:k:210:LEU:HD22	1.69	0.73
1:U:633:CYS:HG	1:U:659:CYS:HG	1.31	0.73
2:V:43:THR:HG22	2:V:65:ARG:HH11	1.54	0.73
30:T:50:MET:HE2	30:T:192:VAL:HG23	1.69	0.73
7:a:247:ARG:HD2	7:a:247:ARG:H	1.54	0.72
16:F:341:ALA:HA	16:F:344:ARG:HH21	1.53	0.72
28:R:19:ARG:HH21	28:R:29:GLN:HE22	1.37	0.72
1:U:7:GLY:N	9:d:80:CYS:SG	2.62	0.72
5:Y:174:TRP:HD1	13:C:340:ARG:NH1	1.85	0.72
7:a:315:LEU:HD13	7:a:321:LYS:HA	1.71	0.72
18:h:12:THR:OG1	19:i:20:GLN:NE2	2.23	0.72
1:U:639:LEU:HD23	13:C:46:GLN:HE21	1.53	0.72
9:d:142:TYR:HB3	9:d:147:SER:HB2	1.71	0.72
20:J:236:LYS:HZ1	20:J:240:GLU:HB2	1.53	0.72
5:Y:293:ARG:HH12	10:e:57:ARG:HB3	1.55	0.72
8:c:292:MET:HE3	9:d:253:LEU:HD11	1.72	0.72
14:D:130:VAL:HG21	14:D:139:LEU:HD12	1.72	0.72
4:X:62:GLN:O	4:X:66:LEU:HB2	1.90	0.72
33:u:47:GLU:OE1	33:u:47:GLU:N	2.21	0.72
3:W:35:ALA:HB1	3:W:48:LEU:CD2	2.18	0.72
6:Z:111:LEU:O	6:Z:114:ARG:NH1	2.23	0.72
15:E:135:ILE:HG23	15:E:182:LEU:HD23	1.72	0.72
16:F:259:MET:HE3	16:F:260:PHE:HB2	1.72	0.71
3:W:436:MET:HE2	3:W:436:MET:HA	1.73	0.71
12:B:371:ARG:NH2	13:C:178:LEU:O	2.22	0.71
5:Y:175:ASP:HA	13:C:340:ARG:HH22	1.56	0.71
15:E:222:ALA:HA	15:E:230:ILE:HG13	1.72	0.71
16:F:121:CYS:HB3	16:F:133:PHE:HE1	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:600:ARG:CZ	14:D:56:VAL:HA	2.21	0.71
3:W:12:ARG:HA	3:W:15:LYS:HG2	1.71	0.71
6:Z:209:ARG:NH2	7:a:350:LYS:O	2.24	0.71
23:m:187:ARG:HG3	23:m:232:ARG:HH12	1.55	0.71
1:U:619:VAL:HG21	1:U:648:VAL:HG13	1.72	0.71
3:W:154:GLU:HG2	3:W:155:GLN:N	2.06	0.71
16:F:200:GLU:HA	16:F:204:LEU:HD13	1.73	0.71
18:H:119:GLN:HG3	19:I:81:SER:HB2	1.72	0.71
3:W:268:LYS:HD2	3:W:301:LYS:HD2	1.72	0.71
1:U:173:VAL:HG22	1:U:175:GLY:H	1.56	0.70
4:X:157:LEU:HD21	4:X:165:LEU:HB3	1.73	0.70
6:Z:184:VAL:HG12	6:Z:186:THR:H	1.54	0.70
14:D:389:GLU:OE2	14:D:391:ARG:HG3	1.90	0.70
16:F:263:ASP:OD1	16:F:266:LYS:NZ	2.24	0.70
8:c:100:LYS:HD2	8:c:105:PRO:HG3	1.71	0.70
24:n:19:ARG:HD3	24:n:26:ILE:HG12	1.74	0.70
33:u:531:ASN:HB3	33:u:534:VAL:HG22	1.72	0.70
2:V:176:MET:HE1	2:V:180:ARG:HH21	1.57	0.70
3:W:49:SER:HA	3:W:52:LYS:HD2	1.73	0.70
14:D:278:GLN:OE1	14:D:278:GLN:N	2.24	0.70
1:U:902:PRO:HB3	1:U:914:LEU:HD23	1.71	0.70
15:E:60:VAL:HG22	15:E:71:VAL:HG22	1.73	0.70
32:f:409:ARG:NH2	33:u:319:GLU:OE1	2.25	0.70
1:U:596:ASN:HD21	14:D:52:GLU:HB2	1.57	0.70
6:Z:223:ASN:OD1	6:Z:225:GLN:NE2	2.25	0.70
1:U:841:LYS:HA	1:U:841:LYS:HE3	1.74	0.70
7:a:81:LEU:HD21	7:a:154:ARG:HH22	1.57	0.70
11:A:238:ILE:HG21	11:A:260:LEU:HD11	1.74	0.70
14:D:410:ASP:OD1	14:D:411:GLU:N	2.25	0.70
18:H:185:GLU:N	18:H:185:GLU:OE2	2.24	0.70
2:V:443:ARG:NH1	9:d:181:CYS:SG	2.64	0.70
8:c:184:LEU:HD22	8:c:185:ASN:H	1.57	0.70
9:d:32:GLU:OE1	9:d:47:GLN:NE2	2.24	0.70
7:a:133:GLU:HA	7:a:136:GLU:HG3	1.74	0.69
22:l:200:PRO:O	22:l:239:ARG:NH2	2.25	0.69
7:a:290:GLN:O	7:a:330:ARG:NH2	2.25	0.69
33:u:486:GLY:HA2	33:u:525:ILE:HD11	1.73	0.69
21:k:227:HIS:NE2	21:k:233:GLU:OE1	2.23	0.69
27:Q:118:MET:HE2	27:Q:124:LEU:HD13	1.74	0.69
1:U:120:GLU:O	1:U:123:LYS:HE3	1.93	0.69
3:W:173:THR:HG23	3:W:182:ARG:HH21	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:287:ASN:OD1	7:a:288:HIS:ND1	2.25	0.69
16:F:300:LYS:O	16:F:304:ARG:NH1	2.26	0.69
26:P:66:ARG:HH12	26:P:70:ARG:HH21	1.38	0.69
23:m:187:ARG:HD3	23:m:232:ARG:HH22	1.58	0.69
33:u:446:LEU:HD21	33:u:480:GLY:HA2	1.75	0.69
3:W:315:MET:HE1	3:W:320:LEU:HD22	1.74	0.69
5:Y:325:VAL:HG22	5:Y:326:GLY:H	1.57	0.69
9:d:147:SER:HB3	9:d:150:LYS:HB3	1.75	0.69
12:B:429:LYS:H	12:B:429:LYS:HD3	1.58	0.69
24:N:127:ILE:HD12	24:N:132:SER:HB2	1.73	0.69
6:Z:197:GLY:HA2	8:c:225:TRP:CD1	2.28	0.69
7:a:216:LEU:HB2	7:a:222:LEU:HD21	1.75	0.69
8:c:187:PRO:HB3	8:c:196:LEU:HD23	1.74	0.69
23:M:175:GLU:HA	23:M:178:LYS:HG3	1.75	0.69
30:T:38:ASN:OD1	30:T:186:ARG:NH2	2.26	0.69
30:t:126:ASP:OD1	30:t:127:MET:N	2.26	0.69
4:X:256:LEU:HD13	4:X:319:ILE:HG23	1.75	0.69
5:Y:301:ILE:HG12	5:Y:342:ARG:HH21	1.58	0.69
10:e:40:GLU:OE1	10:e:40:GLU:N	2.26	0.69
11:A:119:ALA:HB2	16:F:128:THR:HG23	1.75	0.69
15:E:352:MET:HA	15:E:355:ILE:HD12	1.74	0.68
12:B:113:GLU:HB2	12:B:122:ILE:HG23	1.74	0.68
33:u:165:GLU:O	33:u:169:GLU:HG2	1.93	0.68
12:B:401:GLU:HB3	12:B:422:SER:HB2	1.76	0.68
1:U:471:ASP:OD1	1:U:472:ILE:N	2.26	0.68
2:V:464:ILE:HG13	2:V:465:ASP:N	2.08	0.68
14:D:98:GLN:CB	14:D:121:ARG:HH22	2.07	0.68
33:u:286:LYS:HE2	33:u:286:LYS:HA	1.75	0.68
8:c:91:PHE:O	8:c:95:MET:HG2	1.94	0.68
13:C:197:THR:HG21	14:D:298:GLY:HA2	1.75	0.68
21:k:234:LEU:O	21:k:238:ILE:HG13	1.93	0.68
7:a:112:ILE:HD11	7:a:138:VAL:HA	1.75	0.68
12:B:322:ARG:NH1	12:B:325:VAL:O	2.27	0.68
1:U:715:LYS:HA	1:U:718:ASN:ND2	2.08	0.68
2:V:30:PRO:HA	2:V:33:GLN:HB2	1.75	0.68
2:V:91:PRO:HA	2:V:94:VAL:CG1	2.24	0.68
3:W:12:ARG:HD2	3:W:24:VAL:HG13	1.74	0.68
33:u:401:LYS:O	33:u:403:LYS:NZ	2.25	0.68
4:X:255:LEU:HD22	4:X:267:VAL:HG13	1.75	0.68
31:j:56:GLU:N	31:j:56:GLU:OE1	2.23	0.68
1:U:259:GLN:HA	1:U:262:SER:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:27:GLU:OE1	11:A:27:GLU:N	2.23	0.68
12:B:120:HIS:HB3	12:B:132:TYR:HE2	1.59	0.68
3:W:93:ARG:H	3:W:96:GLN:HE21	1.41	0.67
8:c:209:LYS:HG2	8:c:214:GLN:HE21	1.59	0.67
19:I:209:GLU:N	19:I:209:GLU:OE2	2.26	0.67
21:k:146:VAL:HG21	21:k:222:PRO:HA	1.75	0.67
1:U:813:TYR:HB3	1:U:883:ARG:HH22	1.58	0.67
4:X:301:ASP:HA	4:X:304:LYS:HG2	1.75	0.67
11:A:213:LEU:HB2	11:A:337:LEU:HD22	1.76	0.67
16:F:85:THR:HG22	16:F:87:PRO:HD2	1.75	0.67
3:W:60:MET:SD	3:W:107:GLN:NE2	2.68	0.67
9:d:75:MET:O	9:d:79:LYS:HG2	1.95	0.67
33:u:853:VAL:HG12	33:u:855:GLN:HG2	1.75	0.67
7:a:278:MET:HE1	7:a:320:VAL:HG13	1.77	0.67
9:d:143:LEU:HD23	9:d:148:TYR:HE1	1.59	0.67
3:W:111:TYR:HA	3:W:114:GLU:HG3	1.76	0.67
12:B:165:ASP:OD1	12:B:166:ASP:N	2.24	0.67
2:V:33:GLN:NE2	2:V:83:GLU:O	2.28	0.67
2:V:111:TYR:OH	2:V:150:ARG:NH2	2.28	0.67
3:W:107:GLN:N	3:W:107:GLN:OE1	2.27	0.67
5:Y:175:ASP:OD1	13:C:340:ARG:NH2	2.28	0.67
19:i:246:LYS:HA	19:i:246:LYS:HE3	1.76	0.67
3:W:33:LYS:HA	3:W:36:LYS:HG3	1.75	0.67
3:W:163:ALA:HA	3:W:166:LEU:HD12	1.76	0.67
3:W:311:THR:HG23	7:a:316:SER:HB2	1.77	0.67
8:c:254:ASN:HA	8:c:257:LYS:HZ3	1.60	0.67
11:A:59:ILE:HD11	12:B:79:ILE:HD12	1.77	0.67
3:W:170:GLN:OE1	3:W:170:GLN:N	2.21	0.66
15:E:238:ILE:H	15:E:241:ARG:HG2	1.59	0.66
2:V:29:PRO:HA	2:V:32:PRO:HG2	1.77	0.66
7:a:349:MET:O	7:a:349:MET:HE3	1.95	0.66
12:B:258:LYS:HE3	13:C:223:PHE:HD1	1.60	0.66
13:C:45:LEU:HB3	14:D:61:ILE:HG21	1.78	0.66
1:U:28:ASN:HD22	1:U:63:VAL:HG12	1.61	0.66
3:W:237:GLU:OE1	3:W:237:GLU:N	2.27	0.66
7:a:138:VAL:O	7:a:142:LEU:HB2	1.95	0.66
14:D:373:ALA:O	15:E:291:ARG:NH2	2.28	0.66
33:u:460:ASP:OD2	33:u:494:ARG:NH1	2.29	0.66
5:Y:316:LEU:HB2	5:Y:330:ILE:HD11	1.77	0.66
15:E:229:ILE:HG13	15:E:272:ARG:HB3	1.78	0.66
23:M:170:GLN:OE1	23:M:170:GLN:N	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:52:LYS:HA	3:W:55:ARG:HD3	1.77	0.66
3:W:220:GLU:OE2	3:W:257:GLN:NE2	2.29	0.66
12:B:41:LYS:HE2	12:B:41:LYS:HA	1.77	0.66
13:C:57:ARG:HD3	13:C:60:ARG:HH12	1.61	0.66
15:E:303:LEU:HD11	15:E:338:PHE:O	1.94	0.66
30:T:9:THR:O	30:T:41:ARG:NH2	2.28	0.66
1:U:162:VAL:HG12	1:U:165:LYS:HE2	1.76	0.66
1:U:639:LEU:HD11	13:C:50:ASN:ND2	2.10	0.66
3:W:188:GLU:HA	3:W:191:ARG:HH21	1.59	0.66
2:V:182:LYS:O	2:V:182:LYS:NZ	2.29	0.66
3:W:374:THR:O	3:W:376:LYS:N	2.29	0.66
17:G:158:GLY:O	18:H:84:ARG:NH2	2.28	0.66
33:u:466:LEU:HD23	33:u:481:SER:HA	1.77	0.66
4:X:47:GLU:HA	4:X:76:PHE:HZ	1.60	0.66
5:Y:113:ARG:HG3	5:Y:114:ILE:HG12	1.77	0.66
11:A:251:GLY:N	11:A:294:GLU:OE2	2.27	0.66
22:l:146:GLN:HE22	22:l:159:MET:HE2	1.60	0.66
2:V:81:GLN:HB2	2:V:85:ALA:HB3	1.78	0.66
2:V:313:LEU:HD11	2:V:329:HIS:CD2	2.31	0.66
3:W:93:ARG:H	3:W:96:GLN:NE2	1.94	0.66
2:V:495:ARG:HG2	2:V:497:PRO:HD3	1.77	0.65
10:e:45:ASP:O	10:e:47:ASN:N	2.28	0.65
13:C:186:VAL:HG12	13:C:313:ARG:HB2	1.79	0.65
12:B:177:GLU:N	12:B:177:GLU:OE2	2.29	0.65
16:F:249:LEU:HD22	16:F:274:LEU:HD11	1.78	0.65
29:s:184:GLU:OE2	29:s:211:ARG:NH1	2.28	0.65
2:V:391:THR:OG1	2:V:397:ARG:NH2	2.29	0.65
5:Y:97:GLU:HA	5:Y:101:ARG:HG2	1.76	0.65
7:a:303:THR:OG1	7:a:305:ASN:ND2	2.29	0.65
31:j:66:ASP:HA	27:q:69:MET:HE3	1.77	0.65
33:u:115:PRO:HA	33:u:119:LYS:HD2	1.78	0.65
1:U:416:GLU:HB2	1:U:417:LYS:HD2	1.79	0.65
15:E:41:GLU:O	15:E:45:ASN:ND2	2.30	0.65
8:c:254:ASN:HA	8:c:257:LYS:NZ	2.12	0.65
9:d:242:LEU:O	9:d:246:VAL:HG23	1.97	0.65
17:G:118:ILE:HG13	17:G:138:MET:HE1	1.78	0.65
25:O:121:LYS:HD3	30:t:215:ILE:HG21	1.79	0.65
33:u:117:GLU:OE1	33:u:117:GLU:N	2.23	0.65
5:Y:174:TRP:CH2	13:C:377:HIS:HD2	2.15	0.65
14:D:240:LEU:HD23	14:D:240:LEU:H	1.60	0.65
16:F:296:PHE:HE1	16:F:311:LEU:HD21	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:359:PRO:HG3	2:V:385:LYS:HE3	1.77	0.65
11:A:64:GLY:O	33:u:680:ARG:NH2	2.28	0.65
1:U:323:LEU:O	1:U:327:LYS:HG2	1.96	0.65
2:V:495:ARG:O	13:C:43:ARG:NH2	2.30	0.65
5:Y:101:ARG:HD2	5:Y:105:MET:HG2	1.79	0.65
8:c:216:MET:HG3	8:c:220:LEU:HD12	1.78	0.65
18:h:119:GLN:HG3	19:i:81:SER:HB2	1.78	0.65
9:d:135:HIS:HD2	9:d:139:LEU:HD11	1.62	0.65
15:E:252:GLU:OE1	15:E:255:ARG:NH2	2.29	0.65
22:L:80:ASP:OD1	22:L:125:ARG:NH2	2.26	0.65
33:u:885:GLU:OE1	33:u:885:GLU:N	2.26	0.65
15:E:291:ARG:HD2	15:E:292:PRO:HD2	1.79	0.65
23:m:196:ILE:O	23:m:200:VAL:HG23	1.97	0.65
2:V:300:LEU:CD1	9:d:112:VAL:HG12	2.28	0.64
2:V:480:ILE:HD11	6:Z:260:VAL:HG22	1.79	0.64
3:W:177:MET:O	3:W:179:LYS:NZ	2.30	0.64
25:o:17:ASP:HB2	25:o:169:SER:HB2	1.78	0.64
9:d:125:LYS:O	9:d:130:ASN:ND2	2.26	0.64
13:C:233:GLU:HA	13:C:236:VAL:HG12	1.77	0.64
29:S:162:GLU:OE1	29:S:162:GLU:N	2.27	0.64
33:u:183:PRO:O	33:u:187:LEU:HG	1.97	0.64
8:c:32:TYR:HE2	8:c:208:ARG:HB3	1.62	0.64
12:B:49:LEU:HD11	33:u:670:MET:SD	2.38	0.64
15:E:271:HIS:HB3	15:E:272:ARG:HH11	1.62	0.64
1:U:475:HIS:HD2	1:U:511:ALA:HB2	1.61	0.64
4:X:255:LEU:HB2	4:X:287:LEU:HD13	1.80	0.64
6:Z:39:LEU:HD21	6:Z:95:TYR:HB3	1.78	0.64
16:F:194:GLN:HE22	16:F:354:PHE:HA	1.62	0.64
21:k:117:SER:OG	22:l:82:ARG:NH2	2.30	0.64
33:u:760:PHE:O	33:u:764:LEU:HD12	1.97	0.64
4:X:151:SER:O	4:X:155:ARG:HG2	1.97	0.64
10:e:49:GLU:OE1	10:e:49:GLU:N	2.29	0.64
13:C:242:ALA:HB1	13:C:243:PRO:HD2	1.79	0.64
25:O:162:GLY:O	25:O:165:ASN:ND2	2.31	0.64
3:W:189:GLN:HE22	3:W:205:ILE:HD12	1.62	0.64
12:B:223:ILE:HB	12:B:347:ILE:HD13	1.80	0.64
12:B:371:ARG:CZ	13:C:179:GLY:HA3	2.28	0.64
15:E:328:TYR:O	15:E:332:VAL:HG23	1.98	0.64
28:R:49:ALA:HA	38:R:301:LDZ:H22	1.80	0.64
2:V:285:TRP:HB2	2:V:315:LYS:HZ1	1.63	0.64
14:D:417:TYR:HB3	18:H:79:MET:HG2	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:E:38:LYS:HE2	15:E:38:LYS:HA	1.80	0.64
15:E:358:ASP:OD2	16:F:211:LYS:NZ	2.31	0.64
32:f:1:MET:O	32:f:1:MET:HE3	1.98	0.64
1:U:92:ASP:OD1	1:U:140:ARG:NH2	2.31	0.64
1:U:675:MET:HE1	1:U:687:ALA:HB2	1.80	0.64
2:V:247:GLN:OE1	2:V:247:GLN:N	2.29	0.64
5:Y:315:THR:H	5:Y:318:TYR:HE2	1.46	0.64
7:a:333:MET:SD	7:a:334:THR:N	2.71	0.64
17:g:141:ILE:HG22	17:g:151:VAL:HG22	1.80	0.64
3:W:262:LYS:HA	3:W:265:GLN:HG2	1.80	0.64
4:X:379:ASP:OD1	5:Y:312:ARG:HG2	1.98	0.64
15:E:45:ASN:OD1	15:E:48:LYS:NZ	2.28	0.64
19:i:196:VAL:O	19:i:200:THR:HG22	1.98	0.64
31:j:215:GLN:HG2	31:j:216:SER:N	2.13	0.64
21:k:91:LYS:HG3	21:k:119:LEU:HD22	1.80	0.64
32:f:401:GLN:OE1	32:f:405:ARG:NH1	2.30	0.64
33:u:49:ASP:OD1	33:u:50:LYS:N	2.32	0.64
33:u:378:ASN:OD1	33:u:382:ASN:ND2	2.31	0.64
1:U:545:LEU:HB3	1:U:577:ILE:HG21	1.80	0.63
1:U:798:PRO:O	1:U:880:ASN:ND2	2.29	0.63
2:V:139:MET:HA	2:V:143:ALA:H	1.63	0.63
2:V:409:MET:CE	2:V:412:LEU:HD21	2.27	0.63
4:X:415:TYR:OH	5:Y:382:LYS:HG3	1.98	0.63
8:c:162:LEU:HD13	8:c:200:TYR:HB3	1.80	0.63
12:B:85:MET:HE1	33:u:619:HIS:HB2	1.79	0.63
1:U:45:ILE:HG21	1:U:64:ALA:HB2	1.81	0.63
1:U:609:ASP:O	1:U:615:ARG:NH1	2.31	0.63
3:W:82:LEU:HD11	3:W:96:GLN:OE1	1.97	0.63
5:Y:118:GLU:OE1	5:Y:118:GLU:N	2.26	0.63
11:A:119:ALA:HB3	11:A:121:PHE:HE1	1.63	0.63
13:C:52:LEU:HB3	14:D:68:LEU:HD21	1.80	0.63
5:Y:104:MET:HE3	5:Y:126:LYS:HZ1	1.63	0.63
9:d:213:ARG:HB2	9:d:215:TRP:NE1	2.13	0.63
31:j:38:ARG:HH21	31:j:180:ALA:HA	1.62	0.63
22:l:202:GLU:N	22:l:202:GLU:OE1	2.32	0.63
33:u:590:PHE:CE1	33:u:594:LEU:HD21	2.33	0.63
7:a:280:MET:HE1	7:a:291:LEU:HG	1.80	0.63
15:E:310:LEU:HD13	15:E:332:VAL:HG21	1.81	0.63
17:g:67:THR:HG22	17:g:69:LEU:H	1.64	0.63
2:V:99:ARG:HB2	2:V:142:GLU:OE2	1.99	0.63
6:Z:236:LEU:HD21	7:a:335:TRP:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:197:ALA:HB3	7:a:226:ARG:HH22	1.63	0.63
8:c:32:TYR:CE2	8:c:208:ARG:HB3	2.33	0.63
15:E:196:LEU:HD21	15:E:230:ILE:HG23	1.81	0.63
29:s:116:GLU:OE1	29:s:116:GLU:N	2.32	0.63
1:U:236:LEU:HG	1:U:244:MET:HE1	1.80	0.63
1:U:506:ALA:HA	1:U:544:ILE:HD11	1.81	0.63
3:W:386:VAL:O	3:W:390:GLU:HG2	1.99	0.63
13:C:144:PRO:O	13:C:205:HIS:ND1	2.31	0.63
25:o:143:ARG:NH2	25:o:150:GLU:OE1	2.30	0.63
9:d:237:ILE:H	9:d:237:ILE:HD12	1.62	0.63
13:C:66:LEU:HA	14:D:114:ARG:NH2	2.14	0.63
2:V:486:ILE:HA	2:V:489:MET:SD	2.39	0.62
3:W:219:THR:HG21	3:W:222:LEU:HB3	1.81	0.62
5:Y:206:SER:HB3	5:Y:213:LEU:HD13	1.81	0.62
11:A:66:LYS:HE2	11:A:68:SER:H	1.64	0.62
1:U:226:PRO:HB2	1:U:267:ASN:HD21	1.63	0.62
2:V:494:MET:SD	13:C:44:ARG:HG2	2.38	0.62
5:Y:96:GLY:O	5:Y:130:LYS:NZ	2.32	0.62
9:d:9:TRP:CH2	9:d:60:GLN:HB2	2.33	0.62
1:U:405:THR:HG23	1:U:441:GLY:HA3	1.80	0.62
3:W:166:LEU:HA	3:W:169:LEU:HD23	1.81	0.62
6:Z:172:VAL:O	6:Z:176:LEU:HG	1.99	0.62
7:a:278:MET:N	7:a:278:MET:SD	2.72	0.62
9:d:9:TRP:CZ2	9:d:60:GLN:HB2	2.34	0.62
1:U:40:GLU:O	1:U:41:SER:OG	2.15	0.62
1:U:490:ARG:NE	1:U:492:ASP:OD1	2.33	0.62
1:U:568:GLU:O	1:U:572:ARG:HG2	1.98	0.62
15:E:65:THR:HG23	15:E:67:GLU:H	1.64	0.62
16:F:261:ILE:HD13	16:F:305:GLU:HA	1.80	0.62
7:a:190:VAL:HG13	7:a:225:LEU:HB3	1.81	0.62
33:u:475:ASN:ND2	33:u:511:SER:OG	2.32	0.62
4:X:398:GLU:HA	4:X:401:LEU:HD12	1.79	0.62
7:a:84:VAL:HA	7:a:87:MET:HG3	1.81	0.62
18:H:19:LEU:H	18:H:19:LEU:HD12	1.62	0.62
33:u:545:LYS:HB3	33:u:549:GLU:OE1	1.97	0.62
2:V:79:VAL:HA	2:V:161:PRO:HB3	1.81	0.62
7:a:258:GLN:OE1	7:a:258:GLN:N	2.22	0.62
8:c:75:MET:HA	8:c:75:MET:HE3	1.81	0.62
9:d:135:HIS:CD2	9:d:139:LEU:HD11	2.35	0.62
15:E:261:LEU:HG	15:E:294:ARG:HH21	1.64	0.62
19:i:8:ARG:HH21	19:i:19:TYR:HD2	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:148:THR:O	3:W:152:ILE:HD13	1.98	0.62
4:X:268:GLN:OE1	4:X:288:LYS:NZ	2.32	0.62
9:d:200:PHE:HB3	9:d:205:LYS:HB2	1.81	0.62
19:i:245:ALA:O	19:i:249:ARG:NH1	2.32	0.62
23:m:185:THR:HG22	23:m:186:CYS:H	1.63	0.62
33:u:224:ASN:O	33:u:228:LYS:NZ	2.33	0.62
2:V:92:ARG:HD3	2:V:115:LYS:HG3	1.81	0.62
3:W:26:GLN:C	3:W:29:PRO:HD2	2.25	0.62
12:B:41:LYS:NZ	12:B:244:SER:O	2.32	0.62
27:Q:154:GLU:OE1	27:Q:154:GLU:N	2.26	0.62
33:u:48:GLU:HA	33:u:51:GLN:HE21	1.63	0.62
2:V:194:LYS:HD2	2:V:198:GLN:HA	1.82	0.62
2:V:495:ARG:HB2	6:Z:278:ASN:HD21	1.65	0.62
3:W:92:LYS:HB3	3:W:94:ARG:HG2	1.81	0.62
5:Y:220:VAL:HG21	5:Y:249:VAL:HG21	1.82	0.62
11:A:31:ALA:O	11:A:35:THR:HG22	2.00	0.62
33:u:289:VAL:HB	33:u:901:ARG:HH21	1.64	0.62
3:W:12:ARG:O	3:W:13:ILE:C	2.42	0.61
16:F:439:ALA:HB1	22:L:60:GLN:NE2	2.15	0.61
19:I:44:LEU:HD22	19:I:190:LEU:HD22	1.82	0.61
23:M:229:LYS:O	23:M:233:GLU:HG2	1.99	0.61
28:R:100:MET:HE2	28:R:128:VAL:HG23	1.82	0.61
19:i:32:GLY:N	19:i:50:ARG:HH21	1.97	0.61
29:s:169:ASP:O	29:s:173:ARG:HG3	1.99	0.61
32:f:410:ARG:HH22	33:u:838:ARG:HH21	1.47	0.61
1:U:8:ILE:HG21	1:U:26:LYS:HD3	1.82	0.61
1:U:555:VAL:HG13	1:U:556:MET:HE2	1.82	0.61
15:E:264:MET:HG2	15:E:294:ARG:HD2	1.82	0.61
30:T:108:ASN:HB3	30:T:110:MET:HE2	1.81	0.61
22:l:84:LEU:O	22:l:88:MET:HG3	2.01	0.61
33:u:469:TYR:HB2	33:u:481:SER:OG	2.00	0.61
3:W:144:ARG:HH12	3:W:172:GLU:HG3	1.65	0.61
16:F:212:PHE:HA	16:F:215:LEU:HB2	1.82	0.61
33:u:577:LEU:HA	33:u:580:LEU:HG	1.82	0.61
1:U:423:MET:HG2	1:U:446:LEU:HD21	1.82	0.61
1:U:807:LYS:HB2	1:U:808:PRO:HD3	1.83	0.61
2:V:452:ASN:HB3	2:V:457:TYR:HB2	1.82	0.61
7:a:145:LEU:HD12	7:a:147:GLY:H	1.64	0.61
15:E:84:ARG:HG2	15:E:85:ARG:N	2.15	0.61
33:u:205:CYS:O	33:u:209:MET:HG3	2.01	0.61
33:u:228:LYS:HD3	33:u:228:LYS:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:50:PRO:HD3	15:E:102:MET:HE1	1.82	0.61
1:U:678:ASP:O	1:U:684:ARG:NH1	2.29	0.61
5:Y:387:ILE:HG13	6:Z:276:ILE:HD11	1.82	0.61
8:c:68:ARG:CZ	8:c:208:ARG:HH22	2.14	0.61
27:Q:2:GLU:HG2	27:Q:34:LYS:HE2	1.82	0.61
23:m:43:ASP:OD1	23:m:218:GLU:HB3	2.00	0.61
33:u:540:GLN:O	33:u:544:GLU:HG3	2.00	0.61
3:W:130:MET:SD	3:W:130:MET:N	2.67	0.61
4:X:82:LYS:HG2	4:X:122:ARG:HH11	1.66	0.61
9:d:188:LYS:H	9:d:220:ASN:HB2	1.65	0.61
19:I:163:CYS:SG	19:I:164:ILE:N	2.72	0.61
1:U:885:MET:HE2	1:U:885:MET:N	2.16	0.61
5:Y:85:ASP:OD1	5:Y:86:GLU:N	2.34	0.61
6:Z:231:GLN:HA	6:Z:234:PHE:HD1	1.65	0.61
23:M:202:ASP:OD1	23:M:202:ASP:N	2.34	0.61
33:u:437:GLU:OE1	33:u:439:TYR:N	2.33	0.61
4:X:138:PHE:HE2	4:X:175:LYS:HE3	1.66	0.61
6:Z:110:GLU:HA	6:Z:113:LYS:HD3	1.83	0.61
11:A:294:GLU:OE1	11:A:297:ARG:NH1	2.34	0.61
20:J:177:THR:HG22	20:J:179:GLU:H	1.66	0.61
33:u:731:MET:HE2	33:u:731:MET:HA	1.83	0.61
33:u:764:LEU:O	33:u:768:LEU:HG	2.00	0.61
2:V:265:ASP:O	2:V:269:LYS:HG3	2.01	0.60
3:W:28:LEU:HG	3:W:29:PRO:HD3	1.81	0.60
7:a:151:VAL:HA	7:a:154:ARG:HG2	1.84	0.60
2:V:345:ARG:HD2	2:V:364:THR:HG21	1.81	0.60
4:X:96:PHE:HE1	4:X:105:GLN:HE22	1.48	0.60
9:d:196:ARG:O	9:d:196:ARG:NE	2.34	0.60
13:C:253:SER:O	13:C:255:GLY:N	2.29	0.60
1:U:96:TYR:CD2	1:U:97:VAL:HG23	2.36	0.60
1:U:587:ALA:HB2	1:U:621:SER:HB3	1.83	0.60
3:W:172:GLU:OE1	3:W:172:GLU:N	2.28	0.60
6:Z:116:CYS:O	6:Z:119:SER:OG	2.20	0.60
7:a:189:PRO:HD2	7:a:192:GLU:HB3	1.83	0.60
21:K:233:GLU:O	21:K:237:VAL:HG23	2.00	0.60
1:U:708:GLN:O	1:U:712:LEU:HG	2.02	0.60
12:B:222:VAL:HG22	12:B:349:ARG:HB2	1.84	0.60
24:N:35:THR:HG1	24:N:43:CYS:HG	1.47	0.60
19:i:70:GLU:OE1	19:i:70:GLU:N	2.35	0.60
21:k:41:GLN:HE21	21:k:152:GLN:HA	1.66	0.60
33:u:182:GLU:OE1	33:u:182:GLU:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:108:ASP:HB3	11:A:110:LYS:HD2	1.83	0.60
12:B:78:PHE:O	12:B:82:GLN:HG2	2.01	0.60
16:F:171:ARG:O	16:F:175:MET:HB2	2.02	0.60
1:U:490:ARG:CZ	1:U:493:VAL:HG23	2.31	0.60
1:U:744:VAL:HA	1:U:785:PRO:HA	1.83	0.60
11:A:156:LYS:HE2	11:A:156:LYS:HA	1.84	0.60
15:E:69:PHE:HE2	15:E:83:CYS:HB2	1.66	0.60
23:m:8:ASP:O	23:m:22:GLN:NE2	2.34	0.60
3:W:39:ARG:HD2	3:W:42:GLU:HB2	1.83	0.60
4:X:157:LEU:HD11	4:X:162:ASP:HB3	1.83	0.60
5:Y:212:GLU:HG3	5:Y:213:LEU:HG	1.83	0.60
5:Y:292:TYR:CZ	5:Y:293:ARG:HD3	2.36	0.60
9:d:16:LEU:HD23	9:d:16:LEU:H	1.67	0.60
1:U:503:GLN:NE2	1:U:505:ASP:HB2	2.14	0.60
2:V:81:GLN:H	2:V:86:VAL:HB	1.67	0.60
26:P:12:MET:HE3	26:P:171:MET:HG2	1.84	0.60
5:Y:192:ARG:NH1	5:Y:192:ARG:HA	2.16	0.60
7:a:81:LEU:HD21	7:a:154:ARG:NH2	2.17	0.60
11:A:309:PHE:HD2	11:A:315:ILE:HG23	1.65	0.60
12:B:118:ASP:O	12:B:120:HIS:ND1	2.33	0.60
13:C:375:ARG:NH2	13:C:382:ASP:OD2	2.35	0.60
15:E:69:PHE:CE2	15:E:83:CYS:HB2	2.37	0.60
15:E:119:VAL:HA	15:E:123:SER:HB3	1.84	0.60
15:E:152:PRO:HG3	15:E:159:PHE:HE2	1.65	0.60
16:F:69:MET:HA	16:F:72:LYS:HE2	1.83	0.60
20:J:64:ALA:O	20:J:88:ARG:NH1	2.34	0.60
23:m:187:ARG:CD	23:m:232:ARG:HH22	2.14	0.60
23:m:234:GLU:N	23:m:234:GLU:OE2	2.35	0.60
33:u:246:SER:O	33:u:250:ARG:HG2	2.00	0.60
33:u:743:ALA:HA	33:u:746:ARG:HD2	1.83	0.60
1:U:97:VAL:HA	1:U:100:ILE:HG22	1.84	0.60
1:U:144:ASP:HA	13:C:12:GLU:HG2	1.82	0.60
3:W:47:LEU:HD12	3:W:50:LEU:HD23	1.82	0.60
6:Z:58:PHE:HB2	6:Z:70:LEU:HD23	1.84	0.60
8:c:41:MET:HE1	8:c:112:TYR:CG	2.37	0.60
11:A:292:ASP:OD1	12:B:307:ARG:NH2	2.27	0.60
14:D:115:ILE:HD11	14:D:121:ARG:HE	1.65	0.60
22:l:119:PRO:HB3	22:l:125:ARG:HG3	1.82	0.60
33:u:372:LEU:HD11	33:u:409:SER:HB2	1.84	0.60
1:U:151:ILE:HD11	1:U:163:PHE:HD1	1.66	0.59
2:V:200:ARG:HB3	2:V:201:ARG:HH21	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:400:LYS:HA	3:W:400:LYS:HE3	1.82	0.59
9:d:36:LEU:HB3	9:d:37:PRO:HD3	1.84	0.59
33:u:512:MET:SD	33:u:512:MET:N	2.72	0.59
1:U:263:SER:O	1:U:267:ASN:ND2	2.36	0.59
3:W:395:ASN:OD1	3:W:396:LEU:N	2.34	0.59
5:Y:204:THR:OG1	5:Y:245:GLU:OE2	2.20	0.59
7:a:91:ASN:OD1	7:a:92:VAL:N	2.35	0.59
17:g:71:LYS:O	17:g:95:ARG:NH1	2.34	0.59
1:U:108:TYR:HD2	1:U:126:ILE:HG21	1.67	0.59
1:U:554:LEU:HD22	1:U:588:MET:HE1	1.85	0.59
3:W:273:TYR:HB2	3:W:276:LEU:HB2	1.83	0.59
7:a:127:ASP:OD1	7:a:127:ASP:N	2.33	0.59
15:E:91:LYS:HE2	15:E:91:LYS:HA	1.84	0.59
16:F:295:ARG:HH12	16:F:304:ARG:HH22	1.49	0.59
33:u:851:ASP:HB2	33:u:860:LYS:HG2	1.85	0.59
2:V:163:VAL:HA	2:V:216:ARG:HH12	1.65	0.59
12:B:70:ASP:O	12:B:74:MET:HG2	2.03	0.59
14:D:53:PHE:O	14:D:56:VAL:HG12	2.01	0.59
16:F:337:ILE:HD12	16:F:337:ILE:H	1.67	0.59
17:g:158:GLY:O	18:h:84:ARG:NH2	2.35	0.59
24:n:140:ASP:OD1	24:n:140:ASP:N	2.35	0.59
6:Z:19:VAL:HG11	6:Z:124:ILE:HG21	1.84	0.59
11:A:24:ALA:H	11:A:25:LEU:HD22	1.66	0.59
15:E:60:VAL:HG21	15:E:92:LEU:HD21	1.85	0.59
12:B:401:GLU:OE2	12:B:425:ASN:ND2	2.35	0.59
16:F:84:LYS:HE3	16:F:139:LEU:HD12	1.85	0.59
4:X:404:ILE:HD12	6:Z:265:LEU:HD12	1.85	0.59
11:A:398:ARG:HD2	12:B:195:GLN:HE21	1.67	0.59
15:E:127:PRO:HB2	15:E:185:ARG:HH21	1.68	0.59
17:G:138:MET:HE3	17:G:140:LEU:HD11	1.83	0.59
19:i:53:HIS:HB3	19:i:56:LEU:HD23	1.83	0.59
25:o:97:ALA:HB1	25:o:127:MET:SD	2.43	0.59
9:d:171:LEU:HB3	9:d:175:ARG:NH1	2.17	0.59
13:C:229:ARG:O	13:C:233:GLU:HG2	2.02	0.59
14:D:281:ALA:HB1	15:E:208:ILE:HD12	1.85	0.59
33:u:60:VAL:HG11	33:u:102:HIS:CD2	2.38	0.59
6:Z:16:LEU:O	6:Z:19:VAL:HG12	2.03	0.59
7:a:112:ILE:HA	7:a:115:LYS:HE2	1.85	0.59
17:G:93:ARG:NH1	17:G:97:GLU:OE2	2.35	0.59
31:j:8:THR:HG23	21:k:135:ARG:HB3	1.84	0.59
1:U:69:TYR:CE1	1:U:96:TYR:HB2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:602:LEU:HD11	1:U:621:SER:HB2	1.83	0.59
2:V:300:LEU:HD11	9:d:112:VAL:HG12	1.84	0.59
5:Y:71:ASN:O	5:Y:75:LYS:HG2	2.03	0.59
6:Z:72:HIS:O	6:Z:76:GLU:HG2	2.03	0.59
33:u:305:LEU:H	33:u:321:MET:HE2	1.67	0.59
5:Y:82:LYS:O	5:Y:86:GLU:HG3	2.03	0.58
9:d:79:LYS:HB3	9:d:83:PHE:CE1	2.38	0.58
23:m:195:LYS:HD2	23:m:238:TYR:HE1	1.67	0.58
33:u:143:ARG:HH21	33:u:148:GLN:HA	1.68	0.58
33:u:350:LYS:HB3	33:u:353:LEU:HD13	1.84	0.58
3:W:92:LYS:NZ	3:W:96:GLN:OE1	2.35	0.58
3:W:223:LYS:HG3	3:W:224:LEU:HD22	1.84	0.58
7:a:168:ASN:ND2	7:a:171:SER:OG	2.35	0.58
8:c:122:LEU:HD23	8:c:127:ILE:HG13	1.84	0.58
15:E:84:ARG:HH22	15:E:108:MET:HE2	1.68	0.58
15:E:99:ALA:HB3	15:E:108:MET:HB3	1.84	0.58
31:j:104:VAL:HG11	31:j:143:ARG:HB2	1.85	0.58
3:W:28:LEU:HG	3:W:29:PRO:CD	2.33	0.58
14:D:92:PHE:CE1	14:D:101:ALA:HB1	2.29	0.58
14:D:358:VAL:HB	14:D:396:ALA:HB2	1.84	0.58
15:E:308:ALA:O	15:E:309:ARG:HB3	2.02	0.58
17:G:88:ARG:NH2	23:M:113:ASP:OD2	2.36	0.58
29:s:148:LEU:HD23	29:s:178:VAL:HG12	1.84	0.58
2:V:278:GLU:O	2:V:285:TRP:NE1	2.35	0.58
14:D:292:LEU:HD21	14:D:309:MET:HE1	1.85	0.58
15:E:136:GLY:HA2	15:E:312:ILE:HG12	1.84	0.58
2:V:254:LEU:HD23	2:V:255:LEU:HD12	1.85	0.58
2:V:493:ALA:O	6:Z:275:LEU:HD13	2.04	0.58
5:Y:184:GLN:HG2	5:Y:200:LEU:HB2	1.85	0.58
5:Y:285:ASP:HB3	5:Y:288:PHE:HB3	1.86	0.58
28:R:37:ILE:O	28:R:41:LEU:HB2	2.02	0.58
18:h:111:VAL:HG22	18:h:136:ILE:HD13	1.85	0.58
26:p:22:ILE:HG22	26:p:188:HIS:HB2	1.85	0.58
33:u:708:ASP:O	33:u:712:LYS:HG2	2.04	0.58
5:Y:141:VAL:HG11	5:Y:164:ALA:HB2	1.85	0.58
6:Z:79:TYR:CZ	6:Z:91:ILE:HG13	2.39	0.58
9:d:143:LEU:HD23	9:d:148:TYR:CE1	2.37	0.58
12:B:67:ARG:HH22	33:u:239:TYR:HA	1.69	0.58
13:C:83:LYS:HA	13:C:83:LYS:HE3	1.85	0.58
27:Q:19:ARG:NH2	27:Q:31:ASP:OD1	2.37	0.58
1:U:836:THR:HG22	33:u:607:LEU:HD21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:334:ASN:O	4:X:338:VAL:HG22	2.04	0.58
6:Z:255:ASP:OD2	8:c:298:GLN:NE2	2.37	0.58
15:E:316:HIS:ND1	15:E:347:CYS:SG	2.76	0.58
16:F:304:ARG:O	16:F:308:ARG:HG2	2.03	0.58
27:q:45:LEU:HD22	27:q:103:LEU:HD11	1.85	0.58
2:V:29:PRO:HB3	2:V:85:ALA:HB2	1.84	0.58
2:V:440:LYS:HE2	9:d:148:TYR:CZ	2.39	0.58
4:X:328:ASP:O	4:X:332:GLU:HG2	2.04	0.58
5:Y:90:ASP:O	5:Y:93:LYS:NZ	2.35	0.58
11:A:139:ARG:NH1	11:A:156:LYS:HB2	2.19	0.58
13:C:236:VAL:O	13:C:240:GLU:HG3	2.03	0.58
14:D:418:LYS:NZ	18:H:78:GLY:H	2.02	0.58
17:g:221:THR:HG23	17:g:224:ASN:H	1.67	0.58
2:V:289:LEU:HA	2:V:292:THR:HG22	1.84	0.58
3:W:406:VAL:HA	3:W:413:ILE:HG22	1.85	0.58
14:D:281:ALA:HA	14:D:284:GLU:HB3	1.84	0.58
17:G:141:ILE:HG22	17:G:151:VAL:HG22	1.86	0.58
21:K:146:VAL:HG11	21:K:222:PRO:HA	1.86	0.58
8:c:57:MET:HE3	8:c:112:TYR:HB3	1.85	0.57
8:c:88:ASP:OD2	8:c:91:PHE:HB2	2.03	0.57
8:c:118:PHE:HB3	8:c:121:TRP:CZ2	2.39	0.57
9:d:219:PRO:HD2	9:d:223:TYR:HB2	1.84	0.57
3:W:31:CYS:O	3:W:34:LEU:HG	2.04	0.57
3:W:152:ILE:HG21	3:W:165:ILE:HD11	1.86	0.57
9:d:15:ASN:HB3	9:d:18:LYS:NZ	2.19	0.57
9:d:114:GLU:O	9:d:118:GLU:HG2	2.04	0.57
32:f:388:THR:HA	32:f:391:LYS:HG2	1.85	0.57
3:W:387:ASP:N	3:W:387:ASP:OD1	2.34	0.57
5:Y:184:GLN:NE2	5:Y:200:LEU:HD13	2.18	0.57
9:d:33:LEU:HD23	9:d:48:LEU:HG	1.86	0.57
16:F:194:GLN:NE2	16:F:354:PHE:HA	2.19	0.57
33:u:182:GLU:HA	33:u:185:LEU:HD12	1.85	0.57
4:X:62:GLN:HB3	4:X:65:GLU:HB2	1.85	0.57
4:X:126:ARG:O	4:X:130:GLU:HG2	2.04	0.57
7:a:135:ILE:HG13	7:a:155:PHE:HE1	1.69	0.57
12:B:103:ARG:NH2	12:B:160:ILE:O	2.37	0.57
1:U:108:TYR:CD2	1:U:126:ILE:HG21	2.39	0.57
5:Y:179:ARG:HB3	5:Y:183:TYR:CZ	2.39	0.57
8:c:30:GLN:HA	8:c:204:THR:HG23	1.86	0.57
9:d:215:TRP:HB3	9:d:222:TYR:CE1	2.38	0.57
11:A:42:SER:O	11:A:46:LYS:NZ	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:398:ARG:HD2	12:B:195:GLN:NE2	2.19	0.57
32:f:379:ARG:O	32:f:383:THR:HG23	2.05	0.57
32:f:385:ASN:HB3	32:f:386:ARG:NH2	2.12	0.57
1:U:142:LEU:HG	1:U:165:LYS:HE3	1.86	0.57
1:U:541:HIS:HB2	1:U:544:ILE:HG12	1.86	0.57
2:V:34:ASP:O	2:V:38:LYS:HG3	2.04	0.57
2:V:353:LEU:O	2:V:357:LEU:HG	2.05	0.57
5:Y:105:MET:HE2	5:Y:105:MET:N	2.19	0.57
7:a:211:PHE:CZ	7:a:278:MET:HG3	2.39	0.57
12:B:205:LEU:HA	33:u:740:ARG:HH22	1.67	0.57
14:D:418:LYS:HZ1	18:H:78:GLY:H	1.53	0.57
15:E:83:CYS:SG	15:E:84:ARG:N	2.78	0.57
23:M:186:CYS:HB3	23:M:215:TRP:HE1	1.70	0.57
27:Q:30:ASP:OD1	27:Q:30:ASP:N	2.36	0.57
33:u:414:LEU:HA	33:u:417:ILE:HD12	1.87	0.57
2:V:203:LEU:HA	2:V:206:VAL:HG22	1.86	0.57
3:W:44:ILE:O	3:W:46:THR:N	2.37	0.57
4:X:187:ARG:HH21	4:X:221:GLU:HG3	1.70	0.57
4:X:415:TYR:CZ	5:Y:383:LEU:HD23	2.40	0.57
5:Y:192:ARG:HA	5:Y:192:ARG:HH11	1.69	0.57
6:Z:25:ARG:HG3	8:c:104:ARG:HH21	1.69	0.57
13:C:139:MET:HE1	13:C:241:HIS:CD2	2.40	0.57
15:E:353:PHE:HA	15:E:356:ARG:HG2	1.87	0.57
16:F:225:MET:HG2	16:F:352:ILE:HB	1.86	0.57
2:V:51:ALA:HB1	2:V:146:GLN:HE22	1.70	0.57
13:C:296:ASN:O	13:C:297:ARG:HB3	2.05	0.57
24:N:20:THR:HG23	38:N:301:LDZ:H13	1.86	0.57
26:P:58:THR:OG1	27:Q:121:LEU:O	2.23	0.57
26:P:134:ASP:OD1	26:P:134:ASP:N	2.37	0.57
1:U:899:ARG:NH2	1:U:923:GLU:OE2	2.34	0.57
2:V:175:MET:HE1	2:V:217:VAL:HG21	1.86	0.57
3:W:16:MET:HB2	3:W:24:VAL:HG11	1.86	0.57
4:X:240:ASP:OD2	4:X:275:LEU:HD11	2.05	0.57
11:A:189:GLU:OE1	16:F:409:ARG:NH2	2.38	0.57
13:C:55:LYS:HD2	13:C:55:LYS:C	2.29	0.57
13:C:253:SER:C	13:C:255:GLY:H	2.12	0.57
15:E:309:ARG:HH12	15:E:335:SER:HB2	1.70	0.57
18:h:145:TYR:HB3	18:h:147:PHE:HE1	1.70	0.57
33:u:77:GLU:HA	33:u:80:ARG:HG2	1.85	0.57
3:W:95:SER:O	3:W:99:GLN:HG3	2.05	0.57
3:W:174:TYR:HE1	15:E:143:ARG:HG2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:65:GLU:H	4:X:65:GLU:CD	2.13	0.57
7:a:112:ILE:O	7:a:116:THR:HG23	2.05	0.57
11:A:324:PRO:HA	11:A:327:LEU:HD23	1.86	0.57
31:j:67:ASP:OD2	31:j:68:ASN:ND2	2.37	0.57
33:u:749:ALA:HB2	33:u:762:VAL:HG11	1.86	0.57
1:U:266:GLN:HA	1:U:269:ARG:HG2	1.85	0.56
1:U:374:SER:OG	1:U:407:SER:HB2	2.05	0.56
1:U:468:ALA:HB1	1:U:473:VAL:HG11	1.87	0.56
5:Y:198:ALA:HB2	5:Y:226:VAL:HG12	1.86	0.56
6:Z:142:GLU:OE1	6:Z:153:LYS:HD2	2.05	0.56
7:a:54:ASP:HA	7:a:57:ILE:HG22	1.87	0.56
7:a:68:GLU:HG3	7:a:71:VAL:HB	1.86	0.56
8:c:128:ASN:OD1	8:c:129:THR:N	2.38	0.56
9:d:34:ASN:OD1	9:d:35:PHE:N	2.36	0.56
23:m:49:VAL:HG13	23:m:65:ARG:HH11	1.69	0.56
1:U:78:LEU:HD22	1:U:101:ILE:HD13	1.87	0.56
3:W:66:ILE:H	3:W:66:ILE:HD12	1.70	0.56
3:W:448:LYS:HZ3	6:Z:155:PHE:C	2.13	0.56
9:d:109:GLN:HE22	9:d:169:ILE:HD11	1.71	0.56
9:d:135:HIS:O	9:d:139:LEU:HD12	2.05	0.56
13:C:375:ARG:HG2	13:C:377:HIS:H	1.69	0.56
15:E:75:ASN:ND2	16:F:129:ARG:O	2.33	0.56
18:H:184:LEU:O	18:H:188:ILE:HG13	2.05	0.56
26:P:203:ARG:HH12	28:r:191:ASN:HD21	1.53	0.56
27:q:49:GLU:HG3	27:q:50:ALA:H	1.70	0.56
27:q:182:ILE:HG22	27:q:189:HIS:HB2	1.86	0.56
1:U:69:TYR:CZ	1:U:96:TYR:HB2	2.40	0.56
1:U:95:GLU:HG2	1:U:96:TYR:HD1	1.71	0.56
1:U:397:THR:OG1	1:U:401:LYS:NZ	2.38	0.56
2:V:99:ARG:HB2	2:V:142:GLU:CD	2.30	0.56
2:V:100:MET:H	2:V:103:SER:HB3	1.70	0.56
3:W:36:LYS:C	3:W:38:GLY:N	2.64	0.56
9:d:15:ASN:HB3	9:d:18:LYS:HZ2	1.71	0.56
17:G:71:LYS:O	17:G:95:ARG:NH1	2.38	0.56
38:O:301:LDZ:H15	38:O:301:LDZ:H11	1.87	0.56
22:l:26:MET:HE2	22:l:150:SER:HB3	1.87	0.56
24:n:4:MET:HG3	24:n:127:ILE:HG22	1.87	0.56
1:U:131:GLU:HG3	1:U:135:ASN:HD21	1.69	0.56
2:V:473:GLN:HE21	6:Z:253:THR:HG22	1.70	0.56
7:a:68:GLU:O	7:a:69:HIS:ND1	2.39	0.56
8:c:110:GLY:HA2	8:c:140:ALA:HB1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:125:LEU:HD12	11:A:129:VAL:HG23	1.87	0.56
15:E:364:GLN:HA	15:E:367:PHE:CD2	2.40	0.56
16:F:439:ALA:HB3	22:L:60:GLN:HE22	1.66	0.56
17:g:11:ARG:O	17:g:24:GLN:NE2	2.38	0.56
33:u:308:SER:OG	33:u:310:ASP:OD1	2.24	0.56
2:V:91:PRO:CA	2:V:94:VAL:HG12	2.30	0.56
3:W:124:LEU:HD12	3:W:147:LYS:HB3	1.88	0.56
3:W:442:THR:HG21	6:Z:234:PHE:HE1	1.69	0.56
5:Y:22:LEU:HD23	5:Y:40:GLU:HB2	1.86	0.56
5:Y:337:PHE:HB3	5:Y:343:LEU:HD13	1.87	0.56
7:a:208:GLU:OE2	7:a:267:GLN:NE2	2.32	0.56
11:A:30:ILE:HG22	11:A:34:LYS:HZ2	1.70	0.56
15:E:364:GLN:HA	15:E:367:PHE:HD2	1.71	0.56
30:T:43:MET:HE2	30:T:45:VAL:HG22	1.85	0.56
18:h:39:LYS:NZ	19:i:57:ASP:OD2	2.38	0.56
1:U:262:SER:O	1:U:266:GLN:HG3	2.05	0.56
2:V:68:ASP:O	2:V:73:GLU:N	2.38	0.56
4:X:334:ASN:HA	4:X:337:ARG:HD3	1.87	0.56
4:X:344:ARG:HG3	4:X:386:ILE:HG12	1.88	0.56
7:a:27:GLU:HG3	7:a:31:LYS:HD2	1.88	0.56
8:c:41:MET:HE1	8:c:112:TYR:CD2	2.40	0.56
11:A:99:THR:O	11:A:139:ARG:HA	2.06	0.56
13:C:215:SER:OG	13:C:216:GLY:N	2.36	0.56
15:E:145:LEU:HD21	15:E:187:VAL:HG21	1.86	0.56
15:E:309:ARG:NH1	15:E:335:SER:HB2	2.20	0.56
15:E:367:PHE:O	15:E:371:VAL:HG23	2.05	0.56
1:U:580:ARG:HH11	1:U:584:TYR:HE2	1.53	0.56
2:V:39:GLU:O	2:V:43:THR:HG23	2.05	0.56
5:Y:389:MET:N	5:Y:389:MET:HE2	2.20	0.56
8:c:236:GLU:OE1	8:c:236:GLU:N	2.37	0.56
23:m:52:LEU:HD23	23:m:52:LEU:H	1.71	0.56
4:X:394:ASP:OD1	4:X:394:ASP:N	2.35	0.56
11:A:65:ILE:HD12	11:A:65:ILE:H	1.71	0.56
24:N:14:LEU:HD21	24:N:101:ALA:HB3	1.87	0.56
38:n:301:LDZ:H26	38:n:301:LDZ:H8	1.71	0.56
33:u:309:GLU:HA	33:u:314:TYR:CD2	2.41	0.56
33:u:884:THR:HG23	33:u:886:GLU:OE1	2.05	0.56
1:U:475:HIS:CD2	1:U:511:ALA:HB2	2.41	0.56
1:U:708:GLN:NE2	1:U:712:LEU:HD21	2.21	0.56
4:X:73:VAL:HB	4:X:76:PHE:HD2	1.69	0.56
4:X:271:VAL:HG21	4:X:288:LYS:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:344:ARG:HG2	4:X:384:VAL:HG21	1.87	0.56
9:d:109:GLN:HB2	9:d:111:ARG:NE	2.21	0.56
9:d:200:PHE:CD2	9:d:205:LYS:HD3	2.41	0.56
12:B:205:LEU:HA	33:u:740:ARG:NH2	2.21	0.56
13:C:99:VAL:HG12	13:C:123:LEU:HB2	1.88	0.56
15:E:85:ARG:HA	15:E:89:LYS:HE3	1.87	0.56
30:t:184:TYR:CE2	30:t:186:ARG:HD3	2.41	0.56
1:U:883:ARG:NE	1:U:885:MET:HE1	2.21	0.56
11:A:187:LEU:O	11:A:191:VAL:HG22	2.06	0.56
14:D:99:ASN:HA	14:D:115:ILE:HG12	1.87	0.56
19:I:108:GLU:OE2	20:J:60:ARG:NH2	2.39	0.56
33:u:482:ILE:HD12	33:u:501:LEU:HD23	1.87	0.56
3:W:36:LYS:HG2	3:W:85:GLU:HA	1.88	0.55
4:X:299:LEU:HD13	4:X:356:LEU:HD21	1.88	0.55
5:Y:195:LYS:NZ	5:Y:230:ALA:HA	2.21	0.55
5:Y:237:ARG:HD3	5:Y:264:TYR:OH	2.07	0.55
12:B:301:GLY:O	12:B:305:ILE:HG12	2.06	0.55
13:C:119:ASP:OD1	13:C:120:SER:N	2.39	0.55
20:J:113:SER:O	20:J:117:ARG:HG3	2.06	0.55
7:a:280:MET:HE3	7:a:296:ILE:HD11	1.87	0.55
9:d:212:LYS:HG3	9:d:213:ARG:HG2	1.87	0.55
9:d:219:PRO:O	9:d:222:TYR:N	2.32	0.55
14:D:249:ASP:HA	14:D:252:ARG:HG2	1.88	0.55
15:E:251:ARG:HD3	15:E:251:ARG:H	1.72	0.55
1:U:600:ARG:NH1	14:D:56:VAL:HA	2.21	0.55
2:V:106:ARG:O	2:V:110:HIS:ND1	2.39	0.55
2:V:224:LEU:HD23	2:V:257:ASN:HB3	1.88	0.55
2:V:495:ARG:C	13:C:43:ARG:HH22	2.15	0.55
3:W:25:ASP:O	3:W:29:PRO:HG2	2.06	0.55
6:Z:283:ARG:O	6:Z:287:LYS:HG2	2.06	0.55
7:a:290:GLN:HB3	7:a:330:ARG:HH21	1.71	0.55
11:A:220:THR:HG21	11:A:343:PHE:HB3	1.88	0.55
18:h:69:THR:HG22	18:h:70:LYS:H	1.70	0.55
31:j:4:ASP:O	31:j:123:GLY:N	2.38	0.55
3:W:231:ILE:HA	3:W:243:ILE:HG22	1.89	0.55
4:X:260:MET:HE2	4:X:322:HIS:HB3	1.88	0.55
19:I:119:GLN:HG3	20:J:78:ALA:HB1	1.88	0.55
2:V:235:LEU:HB2	2:V:250:LEU:HD13	1.89	0.55
2:V:290:TYR:HE1	2:V:331:LEU:HD21	1.72	0.55
2:V:350:GLN:H	2:V:353:LEU:HB3	1.70	0.55
9:d:18:LYS:HB3	9:d:61:TRP:CZ3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:d:108:SER:HA	9:d:170:LEU:HD13	1.89	0.55
30:T:27:LEU:HD11	30:T:34:ALA:HB1	1.88	0.55
2:V:28:PRO:O	2:V:32:PRO:HD2	2.07	0.55
2:V:397:ARG:HA	2:V:400:HIS:HE2	1.72	0.55
5:Y:377:LEU:HA	5:Y:380:VAL:HG12	1.89	0.55
7:a:341:LEU:HD13	7:a:345:GLN:HB2	1.88	0.55
11:A:252:GLU:O	11:A:256:MET:HG3	2.05	0.55
16:F:199:VAL:HA	16:F:203:VAL:HG23	1.88	0.55
33:u:313:GLU:O	33:u:317:LEU:HG	2.06	0.55
1:U:31:VAL:HG22	1:U:35:TRP:CD1	2.41	0.55
4:X:413:SER:HA	4:X:416:ASN:ND2	2.22	0.55
13:C:252:ASP:O	13:C:256:SER:HB2	2.07	0.55
14:D:268:ASP:N	14:D:268:ASP:OD1	2.40	0.55
20:J:65:LEU:HB2	20:J:69:VAL:HG23	1.87	0.55
31:j:228:TYR:HA	31:j:231:GLU:OE1	2.06	0.55
1:U:167:ILE:HD11	1:U:204:ILE:HD13	1.89	0.55
1:U:401:LYS:O	1:U:405:THR:HG22	2.07	0.55
2:V:228:ARG:HG3	2:V:257:ASN:HD21	1.72	0.55
3:W:136:ILE:HG22	3:W:143:ALA:HB3	1.89	0.55
24:N:160:LEU:O	24:N:164:MET:HG3	2.07	0.55
19:i:8:ARG:HG2	19:i:9:THR:N	2.20	0.55
3:W:91:SER:HB2	3:W:96:GLN:HE22	1.71	0.55
3:W:446:ILE:HD13	6:Z:227:ILE:HD12	1.89	0.55
4:X:96:PHE:CE2	4:X:109:LEU:HD22	2.42	0.55
12:B:48:LYS:C	12:B:49:LEU:HD12	2.32	0.55
13:C:47:ALA:HA	13:C:50:ASN:OD1	2.06	0.55
15:E:351:GLY:O	15:E:355:ILE:HG13	2.07	0.55
1:U:8:ILE:HD12	1:U:27:LEU:HG	1.88	0.55
2:V:400:HIS:NE2	9:d:144:MET:HE1	2.22	0.55
5:Y:196:GLN:O	5:Y:200:LEU:HD12	2.07	0.55
5:Y:237:ARG:HA	5:Y:241:ILE:HB	1.89	0.55
7:a:222:LEU:HD12	7:a:223:GLU:HG3	1.88	0.55
9:d:15:ASN:H	9:d:65:ARG:HH22	1.54	0.55
9:d:18:LYS:HB3	9:d:61:TRP:HZ3	1.72	0.55
18:h:9:SER:HA	18:h:125:GLY:HA2	1.88	0.55
33:u:535:THR:HG23	33:u:562:LEU:HD11	1.88	0.55
33:u:757:ASN:O	33:u:761:MET:HG2	2.07	0.55
1:U:115:ASN:O	1:U:123:LYS:NZ	2.35	0.54
2:V:144:ASP:HB3	2:V:147:PHE:HB2	1.89	0.54
4:X:417:LYS:HZ1	6:Z:280:ILE:HG13	1.72	0.54
5:Y:174:TRP:CH2	13:C:377:HIS:CD2	2.94	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:d:46:GLN:OE1	9:d:46:GLN:N	2.28	0.54
13:C:156:LYS:O	13:C:160:GLU:HG3	2.07	0.54
14:D:236:VAL:HG11	15:E:255:ARG:NH2	2.20	0.54
21:K:125:GLU:OE2	22:L:126:ARG:NH1	2.40	0.54
26:p:142:CYS:O	26:p:146:MET:HG3	2.07	0.54
33:u:312:GLU:OE2	33:u:313:GLU:HG2	2.07	0.54
2:V:483:CYS:HA	2:V:486:ILE:HG22	1.87	0.54
5:Y:304:TYR:OH	5:Y:333:GLU:OE1	2.25	0.54
6:Z:253:THR:O	6:Z:257:MET:HE3	2.07	0.54
9:d:200:PHE:O	9:d:202:THR:N	2.36	0.54
9:d:204:LYS:HG3	9:d:207:THR:OG1	2.07	0.54
13:C:30:GLU:O	13:C:34:ILE:HG12	2.07	0.54
15:E:296:ASP:HB2	15:E:297:ARG:HG2	1.90	0.54
20:J:236:LYS:NZ	20:J:236:LYS:O	2.40	0.54
19:i:244:GLU:O	19:i:248:GLU:HG2	2.08	0.54
9:d:29:VAL:HA	9:d:32:GLU:HG3	1.88	0.54
13:C:38:LYS:HZ1	14:D:54:LEU:C	2.16	0.54
1:U:111:GLN:O	1:U:114:GLU:HG2	2.08	0.54
2:V:95:LEU:HD13	2:V:107:ARG:NH2	2.22	0.54
3:W:269:SER:HA	3:W:272:LEU:HD12	1.90	0.54
5:Y:342:ARG:HB2	5:Y:343:LEU:HD12	1.89	0.54
6:Z:112:MET:O	6:Z:112:MET:HE3	2.07	0.54
12:B:288:ASP:OD1	12:B:288:ASP:N	2.39	0.54
16:F:140:VAL:CG1	16:F:145:LEU:HD21	2.37	0.54
21:k:35:SER:HB3	21:k:51:GLU:HG2	1.88	0.54
28:r:3:THR:HG23	28:r:16:ALA:HB2	1.89	0.54
33:u:228:LYS:HD3	33:u:228:LYS:H	1.73	0.54
2:V:246:GLY:O	2:V:250:LEU:HG	2.08	0.54
3:W:12:ARG:O	3:W:15:LYS:N	2.40	0.54
3:W:108:CYS:HA	3:W:123:ARG:NH2	2.22	0.54
5:Y:388:ASN:ND2	5:Y:388:ASN:O	2.40	0.54
9:d:61:TRP:O	9:d:65:ARG:HG2	2.07	0.54
16:F:435:LEU:HD12	16:F:438:TYR:HE2	1.73	0.54
24:N:144:ARG:NH2	24:N:151:GLU:OE2	2.41	0.54
25:O:10:ASP:OD1	25:O:10:ASP:N	2.40	0.54
1:U:878:LEU:HD13	1:U:882:ALA:HB1	1.87	0.54
2:V:211:TYR:OH	2:V:234:ARG:NH1	2.40	0.54
3:W:201:ARG:O	3:W:205:ILE:HG12	2.07	0.54
3:W:373:ILE:HD13	3:W:378:MET:HB3	1.90	0.54
6:Z:211:TYR:O	6:Z:215:VAL:HG12	2.07	0.54
8:c:219:ASN:HB2	8:c:223:LYS:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:e:56:LEU:O	10:e:56:LEU:HD23	2.07	0.54
11:A:258:ARG:O	11:A:262:GLU:HG2	2.08	0.54
11:A:294:GLU:H	32:f:12:ARG:NH2	2.02	0.54
25:O:35:HIS:HB2	25:O:56:THR:HG21	1.90	0.54
33:u:822:VAL:HA	33:u:825:MET:SD	2.47	0.54
1:U:838:LYS:HD2	1:U:838:LYS:C	2.33	0.54
4:X:377:ILE:HG22	5:Y:312:ARG:HH11	1.73	0.54
5:Y:315:THR:HA	5:Y:353:ILE:HA	1.88	0.54
7:a:133:GLU:OE1	7:a:133:GLU:N	2.29	0.54
9:d:19:CYS:O	9:d:23:LEU:HG	2.06	0.54
9:d:121:ARG:HE	9:d:122:LEU:HG	1.72	0.54
12:B:165:ASP:OD2	13:C:78:ARG:NH2	2.41	0.54
13:C:89:VAL:HG12	13:C:91:PRO:HD2	1.90	0.54
15:E:376:ASP:HA	15:E:379:LYS:HG2	1.90	0.54
26:P:203:ARG:NH2	26:P:205:ASP:OD2	2.40	0.54
21:k:15:PHE:H	22:l:21:GLN:NE2	2.04	0.54
22:l:70:ILE:HD11	22:l:105:VAL:HG22	1.90	0.54
33:u:487:LEU:HD21	33:u:822:VAL:HG11	1.90	0.54
6:Z:228:TYR:OH	7:a:340:VAL:HA	2.07	0.54
27:Q:101:ASN:HB3	27:Q:132:HIS:CE1	2.42	0.54
21:k:196:LYS:HZ3	21:k:241:ILE:HD13	1.72	0.54
3:W:146:THR:HG23	3:W:147:LYS:HD2	1.90	0.54
3:W:448:LYS:HD3	6:Z:157:HIS:HB2	1.90	0.54
4:X:61:GLY:HA2	4:X:99:MET:HE2	1.90	0.54
8:c:57:MET:HA	8:c:72:VAL:HG12	1.90	0.54
11:A:24:ALA:HA	12:B:410:ARG:NH2	2.23	0.54
22:L:9:ASP:OD2	22:L:11:THR:OG1	2.21	0.54
23:m:175:GLU:O	23:m:178:LYS:NZ	2.41	0.54
1:U:748:LEU:HD23	1:U:760:VAL:HG22	1.90	0.54
3:W:2:ALA:HA	3:W:47:LEU:HD13	1.90	0.54
3:W:36:LYS:O	3:W:38:GLY:N	2.41	0.54
4:X:395:LYS:HE3	8:c:242:GLU:HG3	1.89	0.54
8:c:57:MET:HB3	8:c:69:VAL:HG21	1.90	0.54
12:B:204:PRO:O	33:u:740:ARG:NH2	2.38	0.54
12:B:380:LEU:O	12:B:384:ILE:HD12	2.08	0.54
27:Q:49:GLU:HG3	27:Q:50:ALA:H	1.72	0.54
19:i:16:GLY:HA3	31:j:24:GLU:OE1	2.07	0.54
26:p:65:GLN:OE1	27:q:86:ARG:NH2	2.40	0.54
1:U:139:GLN:OE1	1:U:165:LYS:NZ	2.41	0.53
2:V:496:PHE:CE1	13:C:40:GLN:HB2	2.43	0.53
4:X:55:SER:HA	4:X:95:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:d:182:ILE:HD13	9:d:198:LEU:HD11	1.90	0.53
9:d:218:GLY:HA3	9:d:222:TYR:CD1	2.43	0.53
14:D:188:PHE:HD1	14:D:188:PHE:O	1.91	0.53
1:U:460:TYR:HA	1:U:463:ASN:ND2	2.22	0.53
2:V:94:VAL:HG23	2:V:137:GLU:OE1	2.08	0.53
2:V:257:ASN:HA	2:V:260:HIS:HB3	1.88	0.53
2:V:393:THR:O	2:V:396:ILE:HG13	2.07	0.53
3:W:187:LEU:HD13	3:W:226:TYR:CG	2.43	0.53
6:Z:238:PRO:HB2	8:c:310:LYS:HD3	1.90	0.53
6:Z:264:SER:HA	6:Z:267:ARG:CZ	2.38	0.53
7:a:344:GLN:HA	7:a:347:LYS:HD3	1.90	0.53
2:V:78:HIS:HB3	2:V:164:GLU:OE1	2.08	0.53
2:V:89:LYS:HB3	2:V:93:PHE:CD2	2.43	0.53
3:W:445:LEU:HD13	6:Z:226:ILE:HD11	1.91	0.53
12:B:343:ARG:NH1	12:B:344:PRO:O	2.41	0.53
14:D:230:VAL:HG11	14:D:235:PHE:CZ	2.43	0.53
33:u:379:GLY:O	33:u:416:MET:HE1	2.09	0.53
33:u:520:LEU:O	33:u:524:MET:HG2	2.07	0.53
1:U:654:MET:N	1:U:654:MET:SD	2.82	0.53
3:W:107:GLN:HG3	3:W:111:TYR:CE1	2.43	0.53
4:X:89:VAL:HG11	4:X:125:LEU:HD21	1.89	0.53
4:X:365:LEU:O	4:X:369:ILE:HG12	2.07	0.53
6:Z:34:ARG:HA	6:Z:97:THR:O	2.07	0.53
6:Z:101:LEU:HD13	6:Z:123:ILE:HD11	1.89	0.53
7:a:276:CYS:O	7:a:279:GLU:HG3	2.08	0.53
7:a:309:LEU:O	7:a:312:MET:HE3	2.08	0.53
19:i:232:GLU:OE1	19:i:232:GLU:N	2.33	0.53
32:f:406:ARG:NH1	33:u:325:GLN:OE1	2.36	0.53
2:V:65:ARG:O	2:V:69:THR:HG23	2.08	0.53
3:W:36:LYS:O	3:W:37:GLU:C	2.51	0.53
3:W:438:LEU:HD13	6:Z:234:PHE:CE2	2.44	0.53
12:B:317:ASP:OD2	12:B:343:ARG:NH2	2.42	0.53
32:f:405:ARG:HG3	32:f:406:ARG:N	2.23	0.53
2:V:290:TYR:CE1	2:V:331:LEU:HD21	2.44	0.53
4:X:397:TYR:HD2	5:Y:365:GLN:HG2	1.73	0.53
7:a:286:ALA:HB1	7:a:289:ARG:CZ	2.39	0.53
9:d:4:GLN:HE21	9:d:21:GLU:HG2	1.74	0.53
9:d:126:ASP:O	9:d:134:LYS:NZ	2.42	0.53
11:A:26:ASP:HB2	11:A:29:ASP:HB2	1.89	0.53
14:D:98:GLN:CG	14:D:121:ARG:HH22	2.22	0.53
18:H:91:ARG:HD3	25:O:68:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:M:8:ASP:O	23:M:22:GLN:NE2	2.40	0.53
23:M:99:ARG:HD2	30:T:69:GLN:HE22	1.73	0.53
23:M:136:MET:HG2	23:M:150:MET:HG3	1.90	0.53
19:i:119:GLN:HG3	31:j:78:ALA:HB1	1.91	0.53
1:U:505:ASP:HB3	1:U:508:THR:HG22	1.91	0.53
1:U:695:MET:HE2	1:U:695:MET:HA	1.90	0.53
2:V:417:ILE:HD11	2:V:421:ASP:HB2	1.90	0.53
3:W:384:LEU:HD12	3:W:388:GLU:HB2	1.91	0.53
4:X:328:ASP:OD2	4:X:364:LYS:NZ	2.41	0.53
6:Z:190:ARG:O	6:Z:194:GLN:HG3	2.08	0.53
7:a:227:ASN:O	7:a:231:GLN:NE2	2.41	0.53
9:d:149:ASN:HA	9:d:199:PHE:HE2	1.74	0.53
25:O:78:THR:O	25:O:82:MET:HG3	2.09	0.53
32:f:385:ASN:HD22	32:f:386:ARG:NH2	2.07	0.53
1:U:633:CYS:HG	1:U:659:CYS:CB	2.22	0.53
2:V:410:ILE:HD12	2:V:425:LYS:HD3	1.90	0.53
16:F:69:MET:O	16:F:73:ILE:HG13	2.09	0.53
19:i:106:PRO:O	19:i:107:CYS:HB2	2.08	0.53
33:u:788:MET:SD	33:u:788:MET:N	2.78	0.53
1:U:409:GLY:HA3	1:U:445:ALA:HB1	1.91	0.53
1:U:903:PHE:HB2	1:U:915:LYS:HE3	1.91	0.53
2:V:337:LEU:O	2:V:401:ASN:ND2	2.41	0.53
2:V:409:MET:O	2:V:412:LEU:HG	2.09	0.53
3:W:12:ARG:HH21	3:W:27:ARG:CB	2.22	0.53
5:Y:174:TRP:HD1	13:C:340:ARG:HH11	1.56	0.53
5:Y:316:LEU:HD13	5:Y:327:VAL:HG13	1.91	0.53
9:d:1:MET:SD	9:d:1:MET:N	2.82	0.53
12:B:371:ARG:NH1	13:C:179:GLY:HA3	2.24	0.53
13:C:37:ASP:OD1	13:C:38:LYS:N	2.42	0.53
26:P:14:MET:HE3	26:P:154:TRP:HD1	1.74	0.53
33:u:165:GLU:O	33:u:168:LYS:HG2	2.09	0.53
2:V:256:ARG:NH2	10:e:4:LYS:O	2.41	0.53
3:W:12:ARG:HH21	3:W:27:ARG:HB2	1.73	0.53
5:Y:333:GLU:HG2	5:Y:337:PHE:HE2	1.73	0.53
9:d:161:GLU:HG3	9:d:163:TYR:CE1	2.44	0.53
14:D:401:LYS:HE2	14:D:401:LYS:HA	1.91	0.53
15:E:143:ARG:O	15:E:147:GLU:HG3	2.09	0.53
16:F:197:GLU:HG2	16:F:352:ILE:CD1	2.38	0.53
18:H:86:LEU:HD13	18:H:134:LEU:HD11	1.91	0.53
18:h:75:VAL:HG12	18:h:135:LEU:HB2	1.90	0.53
23:m:187:ARG:CG	23:m:232:ARG:HH12	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:t:27:LEU:HD11	30:t:34:ALA:HB1	1.91	0.53
1:U:188:MET:HE2	1:U:194:ARG:HB2	1.90	0.52
2:V:373:ALA:O	2:V:377:GLN:HG2	2.09	0.52
3:W:376:LYS:NZ	3:W:380:GLN:HB3	2.24	0.52
4:X:88:LEU:O	4:X:92:LEU:HG	2.08	0.52
8:c:145:VAL:HG22	8:c:157:ILE:HG12	1.91	0.52
9:d:108:SER:OG	9:d:109:GLN:NE2	2.42	0.52
9:d:175:ARG:HG2	9:d:200:PHE:HE1	1.73	0.52
11:A:166:VAL:HG12	11:A:168:GLU:N	2.24	0.52
11:A:420:TYR:CZ	12:B:350:LYS:HE3	2.44	0.52
13:C:389:LYS:HB2	13:C:389:LYS:NZ	2.24	0.52
16:F:251:LEU:HD23	16:F:285:ILE:HG12	1.91	0.52
25:O:163:ILE:HG23	25:O:169:SER:HB2	1.91	0.52
33:u:836:GLU:OE1	33:u:836:GLU:N	2.29	0.52
3:W:213:PHE:CD1	3:W:214:PHE:N	2.76	0.52
8:c:251:LEU:HD21	8:c:284:LEU:N	2.25	0.52
26:P:164:PHE:O	26:P:168:SER:OG	2.22	0.52
27:q:154:GLU:OE1	27:q:154:GLU:N	2.41	0.52
33:u:57:GLU:HA	33:u:60:VAL:HG12	1.90	0.52
33:u:486:GLY:HA3	33:u:521:ALA:HB1	1.90	0.52
1:U:611:ASN:HB3	1:U:614:VAL:HG12	1.90	0.52
2:V:238:ALA:C	2:V:240:LEU:H	2.17	0.52
4:X:394:ASP:HB2	5:Y:365:GLN:HE22	1.74	0.52
5:Y:268:TYR:HA	5:Y:271:PHE:HB3	1.91	0.52
6:Z:260:VAL:O	6:Z:264:SER:OG	2.25	0.52
7:a:245:VAL:HG11	7:a:301:LYS:HE3	1.89	0.52
8:c:121:TRP:CZ3	8:c:190:GLN:HG3	2.44	0.52
8:c:125:VAL:O	8:c:129:THR:HG22	2.09	0.52
15:E:309:ARG:CZ	15:E:337:GLY:H	2.22	0.52
16:F:181:PRO:HB3	16:F:238:ARG:HD2	1.90	0.52
20:J:41:VAL:CG2	20:J:211:MET:HB3	2.40	0.52
1:U:529:ILE:HD13	1:U:556:MET:HE1	1.91	0.52
3:W:327:GLU:N	3:W:327:GLU:OE1	2.42	0.52
3:W:375:MET:H	3:W:375:MET:HE2	1.75	0.52
6:Z:26:ILE:HD13	6:Z:35:VAL:HG22	1.91	0.52
7:a:8:LEU:HD23	7:a:8:LEU:H	1.73	0.52
14:D:146:GLU:OE1	14:D:146:GLU:N	2.43	0.52
19:I:68:LEU:HD11	19:I:74:CYS:HB3	1.92	0.52
33:u:862:ILE:HD11	33:u:879:ARG:HB3	1.91	0.52
1:U:642:GLU:O	13:C:53:ASN:ND2	2.42	0.52
2:V:176:MET:HE3	2:V:214:HIS:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:287:VAL:HA	3:W:290:ILE:HG22	1.90	0.52
4:X:190:LEU:HD22	4:X:217:ILE:HD12	1.91	0.52
6:Z:198:LEU:HD23	7:a:363:MET:HE1	1.90	0.52
7:a:123:LEU:HD22	7:a:127:ASP:OD2	2.10	0.52
12:B:258:LYS:HE3	13:C:223:PHE:CD1	2.43	0.52
3:W:79:GLU:HG3	3:W:97:LEU:HD11	1.91	0.52
5:Y:283:LYS:HD3	5:Y:288:PHE:CE2	2.44	0.52
6:Z:134:PRO:HB3	8:c:220:LEU:HD13	1.90	0.52
16:F:266:LYS:HA	16:F:269:ARG:HE	1.75	0.52
16:F:285:ILE:O	16:F:330:ALA:HA	2.10	0.52
2:V:470:ARG:HA	2:V:473:GLN:HE22	1.75	0.52
3:W:170:GLN:H	3:W:170:GLN:CD	2.14	0.52
6:Z:13:PRO:HA	6:Z:16:LEU:HG	1.92	0.52
6:Z:192:THR:HA	6:Z:195:VAL:HG12	1.91	0.52
8:c:152:LYS:HG3	8:c:153:GLY:H	1.74	0.52
8:c:210:ASN:O	8:c:213:GLU:HG2	2.10	0.52
11:A:87:LEU:HD23	11:A:87:LEU:H	1.75	0.52
13:C:226:GLU:O	13:C:230:MET:HG3	2.09	0.52
16:F:150:LEU:O	16:F:164:LEU:HD13	2.10	0.52
22:L:72:ILE:HG22	22:L:134:ILE:HG12	1.91	0.52
25:o:48:THR:O	25:o:50:ALA:N	2.42	0.52
33:u:478:ARG:O	33:u:482:ILE:HG22	2.09	0.52
33:u:655:LEU:HD21	33:u:800:LEU:HD12	1.90	0.52
1:U:99:THR:O	1:U:103:LYS:HG2	2.10	0.52
1:U:636:VAL:HA	14:D:57:GLN:HE22	1.75	0.52
16:F:205:PRO:HD2	16:F:206:MET:N	2.23	0.52
20:J:41:VAL:HB	20:J:134:VAL:HG13	1.91	0.52
23:M:7:TYR:CE1	23:M:16:PRO:HD3	2.45	0.52
23:M:117:MET:HA	23:M:117:MET:HE3	1.92	0.52
30:T:99:ARG:HD2	30:T:104:ASN:O	2.10	0.52
33:u:448:CYS:SG	33:u:465:LEU:HD12	2.50	0.52
1:U:35:TRP:HB3	1:U:70:HIS:CE1	2.44	0.52
1:U:542:GLU:N	1:U:542:GLU:OE1	2.43	0.52
3:W:317:TRP:CD1	3:W:358:VAL:HG21	2.44	0.52
5:Y:50:MET:HE1	5:Y:70:LEU:HD23	1.91	0.52
5:Y:383:LEU:HD12	6:Z:272:LEU:HD11	1.92	0.52
13:C:248:MET:HE3	13:C:251:ILE:HD13	1.92	0.52
15:E:84:ARG:HD2	15:E:86:GLN:HB2	1.92	0.52
16:F:185:TYR:CE2	16:F:243:GLN:HG3	2.45	0.52
16:F:387:CYS:SG	16:F:421:MET:HE1	2.50	0.52
25:O:159:ILE:O	25:O:163:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:359:PRO:HB3	2:V:382:PHE:CD2	2.39	0.52
3:W:67:LEU:HD12	3:W:67:LEU:O	2.10	0.52
5:Y:293:ARG:HH22	10:e:57:ARG:HD2	1.73	0.52
6:Z:13:PRO:HG3	8:c:221:HIS:CE1	2.45	0.52
6:Z:264:SER:HA	6:Z:267:ARG:NE	2.25	0.52
9:d:26:LEU:HA	9:d:29:VAL:HG12	1.92	0.52
9:d:111:ARG:HB3	9:d:114:GLU:OE1	2.10	0.52
14:D:130:VAL:HG23	14:D:142:VAL:HG12	1.92	0.52
17:g:206:LEU:HB3	17:g:208:ILE:HG12	1.92	0.52
31:j:121:SER:OG	31:j:122:ASN:N	2.43	0.52
27:q:49:GLU:HG3	27:q:50:ALA:N	2.24	0.52
3:W:64:SER:HB2	3:W:65:ARG:HH22	1.75	0.51
3:W:324:TYR:O	3:W:324:TYR:CG	2.64	0.51
6:Z:229:GLN:NE2	7:a:338:PRO:HB2	2.25	0.51
6:Z:276:ILE:O	6:Z:280:ILE:HG12	2.10	0.51
12:B:389:ASP:OD1	12:B:389:ASP:N	2.36	0.51
14:D:49:GLN:O	14:D:52:GLU:HG3	2.10	0.51
16:F:295:ARG:HH12	16:F:303:ASP:HB2	1.75	0.51
19:i:3:ARG:HD2	31:j:5:ARG:HH22	1.75	0.51
33:u:590:PHE:O	33:u:594:LEU:HD22	2.10	0.51
1:U:841:LYS:O	1:U:845:GLU:HG2	2.10	0.51
3:W:33:LYS:HD2	3:W:33:LYS:C	2.35	0.51
5:Y:333:GLU:HG2	5:Y:337:PHE:CE2	2.45	0.51
7:a:135:ILE:HG13	7:a:155:PHE:CE1	2.46	0.51
12:B:316:LEU:HD21	12:B:327:VAL:HG21	1.93	0.51
14:D:417:TYR:HA	18:H:79:MET:HA	1.92	0.51
15:E:292:PRO:HA	15:E:296:ASP:OD1	2.09	0.51
27:Q:161:ARG:O	27:Q:165:GLU:HG3	2.10	0.51
1:U:233:LEU:HD21	1:U:325:MET:HE1	1.93	0.51
1:U:567:ILE:HG12	1:U:586:VAL:HG23	1.92	0.51
2:V:130:PHE:O	2:V:133:PRO:HD2	2.10	0.51
4:X:266:ASP:O	4:X:270:LEU:HG	2.10	0.51
5:Y:157:ILE:HG21	5:Y:186:LEU:HG	1.92	0.51
6:Z:134:PRO:HG3	8:c:220:LEU:HD22	1.92	0.51
9:d:21:GLU:O	9:d:25:ARG:HG3	2.10	0.51
9:d:37:PRO:HB2	9:d:39:THR:HG23	1.93	0.51
15:E:226:GLN:NE2	15:E:272:ARG:HD3	2.24	0.51
33:u:62:ARG:HH12	33:u:71:TYR:HD1	1.58	0.51
33:u:662:MET:HG3	33:u:781:TYR:CE1	2.45	0.51
1:U:605:VAL:O	1:U:609:ASP:HB2	2.10	0.51
3:W:16:MET:HA	3:W:24:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:33:LYS:HD2	3:W:34:LEU:N	2.25	0.51
9:d:15:ASN:H	9:d:65:ARG:NH2	2.08	0.51
11:A:101:ILE:HG22	11:A:138:MET:O	2.10	0.51
23:M:196:ILE:O	23:M:200:VAL:HG23	2.10	0.51
18:h:95:GLN:NE2	25:o:64:GLU:OE1	2.44	0.51
33:u:540:GLN:HA	33:u:543:MET:HG3	1.92	0.51
1:U:162:VAL:O	1:U:166:THR:HG23	2.11	0.51
9:d:93:ALA:O	9:d:94:TYR:HB2	2.11	0.51
9:d:155:LYS:HE2	9:d:171:LEU:HD11	1.92	0.51
15:E:237:ALA:O	15:E:238:ILE:HB	2.09	0.51
21:K:117:SER:OG	22:L:82:ARG:NH2	2.28	0.51
28:r:52:CYS:O	28:r:56:GLU:HG3	2.11	0.51
33:u:688:ARG:O	33:u:724:ASN:ND2	2.44	0.51
2:V:200:ARG:HA	2:V:203:LEU:HB3	1.91	0.51
2:V:213:TYR:O	2:V:217:VAL:HG23	2.11	0.51
2:V:480:ILE:O	2:V:484:LEU:HG	2.10	0.51
2:V:496:PHE:HA	13:C:43:ARG:NH1	2.23	0.51
3:W:52:LYS:HA	3:W:55:ARG:CD	2.39	0.51
3:W:186:ILE:O	3:W:189:GLN:NE2	2.29	0.51
15:E:108:MET:HE2	15:E:108:MET:HA	1.93	0.51
1:U:95:GLU:O	1:U:97:VAL:N	2.43	0.51
1:U:96:TYR:CE2	1:U:97:VAL:HG23	2.46	0.51
1:U:492:ASP:OD1	1:U:492:ASP:N	2.39	0.51
3:W:93:ARG:HG2	3:W:135:LYS:HG3	1.93	0.51
6:Z:177:ARG:NH1	6:Z:177:ARG:HA	2.26	0.51
7:a:195:GLU:O	7:a:199:THR:HG23	2.10	0.51
9:d:217:LEU:O	9:d:219:PRO:HD3	2.10	0.51
9:d:219:PRO:HD2	9:d:223:TYR:H	1.76	0.51
11:A:43:ARG:HH21	11:A:46:LYS:HE2	1.76	0.51
11:A:84:LYS:C	11:A:88:GLN:HE21	2.16	0.51
11:A:113:ILE:HD12	11:A:113:ILE:O	2.10	0.51
14:D:244:PRO:HD3	14:D:288:ILE:HG12	1.92	0.51
25:O:1:THR:HG23	38:O:301:LDZ:C22	2.40	0.51
33:u:58:MET:HA	33:u:58:MET:HE3	1.93	0.51
33:u:70:LEU:HD12	33:u:73:PRO:HG2	1.93	0.51
1:U:462:LEU:O	1:U:466:LYS:HG2	2.11	0.51
2:V:96:ARG:HB2	2:V:150:ARG:HH12	1.76	0.51
5:Y:376:LEU:HD23	6:Z:265:LEU:HD13	1.93	0.51
9:d:8:GLU:CD	9:d:18:LYS:HE2	2.36	0.51
18:H:179:ASN:OD1	18:H:180:GLU:N	2.41	0.51
24:N:133:SER:O	24:n:134:TYR:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:P:159:ASP:OD1	26:P:159:ASP:N	2.41	0.51
18:h:184:LEU:O	18:h:188:ILE:HG13	2.10	0.51
22:l:33:SER:HB2	22:l:62:LYS:HE2	1.93	0.51
30:t:51:LEU:HD21	30:t:110:MET:HE2	1.92	0.51
33:u:108:GLU:O	33:u:111:GLU:HG2	2.11	0.51
2:V:183:GLU:O	2:V:186:LYS:HG3	2.11	0.51
3:W:17:GLU:OE1	3:W:18:VAL:N	2.44	0.51
3:W:23:THR:O	3:W:26:GLN:HB2	2.11	0.51
4:X:317:PRO:O	4:X:321:THR:OG1	2.26	0.51
6:Z:13:PRO:HG3	8:c:221:HIS:HE1	1.76	0.51
14:D:87:LEU:HG	14:D:140:VAL:HG21	1.91	0.51
15:E:167:PRO:O	15:E:274:LYS:NZ	2.42	0.51
21:k:40:ILE:HB	21:k:47:CYS:SG	2.51	0.51
23:m:68:ASN:OD1	23:m:224:HIS:ND1	2.43	0.51
23:m:192:GLU:O	23:m:196:ILE:HG13	2.11	0.51
25:o:19:ARG:HB2	25:o:170:GLY:H	1.75	0.51
33:u:61:GLU:HA	33:u:105:LYS:NZ	2.26	0.51
3:W:158:ASP:OD2	3:W:160:LYS:NZ	2.43	0.51
4:X:109:LEU:O	4:X:112:GLU:HG2	2.11	0.51
4:X:122:ARG:HG3	4:X:125:LEU:CB	2.40	0.51
5:Y:46:ARG:NH1	5:Y:46:ARG:HA	2.26	0.51
9:d:222:TYR:O	9:d:224:SER:N	2.44	0.51
12:B:366:GLN:O	12:B:370:SER:HB3	2.10	0.51
14:D:99:ASN:O	14:D:114:ARG:HG3	2.11	0.51
14:D:156:SER:HA	14:D:159:LYS:HZ2	1.76	0.51
14:D:275:PHE:N	14:D:286:GLN:OE1	2.41	0.51
16:F:71:ASP:O	16:F:74:LYS:HG2	2.11	0.51
27:Q:27:GLN:O	27:q:170:ARG:NH1	2.44	0.51
19:i:172:VAL:O	19:i:176:LYS:HG3	2.11	0.51
26:p:135:ASP:OD1	26:p:135:ASP:N	2.43	0.51
33:u:492:SER:HB2	33:u:494:ARG:HG3	1.92	0.51
1:U:115:ASN:HB3	1:U:123:LYS:HD3	1.93	0.50
3:W:375:MET:HE3	3:W:411:GLY:C	2.36	0.50
5:Y:101:ARG:HH21	5:Y:136:HIS:HD2	1.59	0.50
6:Z:112:MET:CE	6:Z:116:CYS:HB3	2.41	0.50
8:c:163:ILE:N	8:c:199:HIS:O	2.44	0.50
11:A:268:LYS:HD3	11:A:269:ALA:N	2.26	0.50
12:B:40:THR:HB	33:u:712:LYS:HE3	1.92	0.50
15:E:322:LYS:NZ	15:E:328:TYR:OH	2.41	0.50
33:u:48:GLU:H	33:u:48:GLU:CD	2.19	0.50
1:U:469:SER:HB3	1:U:473:VAL:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:48:LEU:HD13	3:W:86:ASN:HD21	1.75	0.50
5:Y:70:LEU:O	5:Y:73:MET:HG3	2.10	0.50
6:Z:68:TRP:CG	6:Z:104:ASN:HD21	2.29	0.50
11:A:300:LEU:O	11:A:303:ILE:HG22	2.11	0.50
15:E:99:ALA:O	15:E:108:MET:N	2.35	0.50
5:Y:174:TRP:C	13:C:340:ARG:HH12	2.20	0.50
9:d:204:LYS:HG3	9:d:207:THR:HG1	1.75	0.50
11:A:139:ARG:HH12	11:A:156:LYS:HB2	1.74	0.50
12:B:234:LEU:HD22	35:B:501:ATP:H2'	1.92	0.50
15:E:125:GLU:HB2	15:E:195:PHE:HB3	1.92	0.50
19:i:50:ARG:NH1	19:i:50:ARG:HG2	2.27	0.50
31:j:80:ALA:HA	31:j:129:ILE:HD13	1.93	0.50
33:u:405:HIS:CD2	33:u:813:LYS:HB3	2.46	0.50
1:U:71:LEU:HD23	1:U:73:ALA:H	1.75	0.50
1:U:636:VAL:HA	14:D:57:GLN:NE2	2.26	0.50
3:W:53:GLN:HE22	3:W:103:LYS:HG2	1.76	0.50
7:a:188:LEU:HD11	7:a:193:GLN:HG3	1.94	0.50
7:a:214:GLY:O	7:a:216:LEU:N	2.45	0.50
16:F:185:TYR:CE1	16:F:195:ILE:HG12	2.46	0.50
22:L:103:LEU:HD12	22:L:104:PRO:HD2	1.93	0.50
19:i:249:ARG:HA	19:i:249:ARG:NE	2.26	0.50
1:U:510:GLU:HA	1:U:547:GLY:HA3	1.92	0.50
1:U:568:GLU:HA	1:U:601:ARG:NH2	2.27	0.50
2:V:289:LEU:HD23	2:V:312:ALA:HB2	1.93	0.50
2:V:342:ILE:HD12	2:V:343:PRO:HD2	1.94	0.50
2:V:381:GLN:C	2:V:382:PHE:HD1	2.19	0.50
4:X:278:ARG:HD2	4:X:279:TYR:CZ	2.46	0.50
7:a:116:THR:HG1	7:a:154:ARG:HH11	1.60	0.50
7:a:116:THR:OG1	7:a:154:ARG:HD3	2.11	0.50
7:a:156:TYR:OH	7:a:178:ARG:NH1	2.44	0.50
9:d:68:ILE:HG13	9:d:69:PRO:CD	2.33	0.50
11:A:206:ILE:HG12	16:F:373:MET:HE2	1.92	0.50
12:B:49:LEU:HD13	12:B:68:ILE:CD1	2.42	0.50
15:E:193:CYS:SG	15:E:229:ILE:HG22	2.52	0.50
17:g:97:GLU:HG2	17:g:117:ARG:HG2	1.92	0.50
21:k:79:SER:HB2	21:k:170:ILE:HD12	1.94	0.50
33:u:838:ARG:HD3	33:u:839:PRO:HD2	1.92	0.50
1:U:230:SER:O	1:U:234:GLU:HG2	2.12	0.50
1:U:348:THR:HG21	1:U:377:HIS:CD2	2.47	0.50
1:U:427:LEU:HB2	1:U:430:ASP:HB2	1.93	0.50
2:V:351:PRO:O	2:V:355:ARG:NE	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:26:GLN:O	3:W:30:GLU:HG3	2.11	0.50
5:Y:246:ILE:HG12	5:Y:250:LEU:HD23	1.94	0.50
5:Y:325:VAL:HG22	5:Y:326:GLY:N	2.26	0.50
6:Z:231:GLN:HA	6:Z:234:PHE:CD1	2.46	0.50
12:B:46:ALA:HB2	12:B:178:LYS:HA	1.93	0.50
12:B:125:THR:O	12:B:128:GLY:N	2.42	0.50
15:E:97:ARG:HD2	15:E:113:ARG:HB3	1.94	0.50
33:u:689:ALA:HA	33:u:692:LEU:HD23	1.94	0.50
1:U:801:GLN:HB3	1:U:877:LEU:HD11	1.93	0.50
2:V:88:GLY:HA2	2:V:118:GLN:OE1	2.12	0.50
2:V:324:PHE:HZ	10:e:3:GLU:H	1.59	0.50
3:W:80:TRP:NE1	17:G:244:GLU:OE1	2.44	0.50
5:Y:365:GLN:HA	5:Y:368:GLU:CD	2.36	0.50
9:d:210:ALA:HB1	9:d:216:VAL:HG22	1.94	0.50
13:C:132:ASP:HB3	13:C:135:VAL:HG22	1.94	0.50
15:E:373:LYS:O	15:E:373:LYS:HD3	2.12	0.50
16:F:224:LEU:HB2	16:F:348:LEU:HD12	1.93	0.50
26:P:135:ASP:OD1	26:P:135:ASP:N	2.43	0.50
17:g:88:ARG:NH2	23:m:113:ASP:OD2	2.45	0.50
22:l:148:CYS:SG	22:l:150:SER:OG	2.60	0.50
26:p:12:MET:HG3	26:p:138:VAL:HG12	1.94	0.50
33:u:705:ASN:N	33:u:705:ASN:OD1	2.43	0.50
1:U:521:LEU:HD21	1:U:757:MET:HG3	1.93	0.50
1:U:797:MET:N	1:U:797:MET:HE3	2.27	0.50
3:W:145:LEU:HD22	3:W:172:GLU:HG2	1.94	0.50
4:X:166:LEU:O	4:X:170:GLN:HG3	2.12	0.50
8:c:270:LEU:HA	8:c:273:LYS:HG2	1.94	0.50
11:A:66:LYS:HE2	11:A:68:SER:HB3	1.93	0.50
13:C:346:LYS:O	13:C:350:LEU:HG	2.12	0.50
16:F:78:GLU:O	16:F:82:VAL:HG12	2.12	0.50
27:Q:170:ARG:NH1	27:q:27:GLN:O	2.44	0.50
28:R:64:ARG:NH1	28:R:67:GLU:OE1	2.45	0.50
28:r:113:TYR:O	28:r:120:ARG:HA	2.11	0.50
1:U:421:GLN:O	1:U:425:THR:HG23	2.11	0.50
1:U:796:LYS:HE2	1:U:798:PRO:HG3	1.94	0.50
1:U:827:LYS:HZ1	1:U:830:THR:HG23	1.76	0.50
3:W:12:ARG:HG3	3:W:27:ARG:HH21	1.76	0.50
3:W:359:VAL:O	3:W:363:ILE:HG13	2.11	0.50
4:X:250:SER:O	4:X:254:MET:HG3	2.12	0.50
6:Z:186:THR:OG1	6:Z:187:LEU:N	2.45	0.50
13:C:135:VAL:HG11	13:C:233:GLU:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:E:55:GLN:HG2	15:E:108:MET:HG2	1.94	0.50
15:E:149:ILE:HG21	15:E:231:PHE:CZ	2.46	0.50
22:L:76:GLY:HA3	22:L:130:VAL:HA	1.94	0.50
26:P:177:ARG:NH2	29:s:150:ASP:OD2	2.30	0.50
33:u:307:LEU:HB2	33:u:314:TYR:CE1	2.47	0.50
1:U:774:PRO:HD3	8:c:177:THR:HB	1.94	0.49
2:V:137:GLU:HA	2:V:140:ASP:OD2	2.12	0.49
2:V:245:ASP:H	2:V:247:GLN:HE22	1.58	0.49
3:W:76:GLU:OE1	3:W:129:ARG:NH1	2.45	0.49
4:X:286:ALA:HB2	4:X:309:TYR:CD2	2.47	0.49
5:Y:104:MET:HE3	5:Y:126:LYS:NZ	2.26	0.49
9:d:42:LYS:HA	9:d:45:LYS:HG3	1.93	0.49
16:F:87:PRO:HB2	16:F:155:LYS:HD3	1.94	0.49
17:G:37:LEU:HD22	17:G:53:GLN:HG3	1.93	0.49
25:O:155:VAL:O	25:O:159:ILE:HG12	2.12	0.49
22:l:36:VAL:HG22	22:l:160:SER:HB2	1.94	0.49
22:l:53:GLN:CD	22:l:53:GLN:H	2.20	0.49
22:l:174:ARG:HE	22:l:175:HIS:CE1	2.29	0.49
1:U:225:ASP:O	1:U:229:VAL:HG23	2.12	0.49
2:V:332:LEU:HG	2:V:336:GLU:OE2	2.12	0.49
3:W:104:MET:HE1	3:W:127:THR:HB	1.94	0.49
4:X:87:ARG:HH12	4:X:90:ARG:HD3	1.76	0.49
4:X:394:ASP:CB	5:Y:365:GLN:HE22	2.24	0.49
5:Y:29:PRO:HB2	5:Y:32:ARG:HB2	1.94	0.49
7:a:269:LEU:O	7:a:272:ILE:HG13	2.13	0.49
11:A:325:ASP:OD1	11:A:325:ASP:N	2.43	0.49
15:E:309:ARG:H	15:E:312:ILE:HG13	1.77	0.49
17:G:22:LEU:O	17:G:26:GLU:HG3	2.11	0.49
33:u:140:LEU:HB3	33:u:141:LYS:HZ2	1.75	0.49
1:U:149:GLN:OE1	13:C:21:ARG:NH1	2.46	0.49
1:U:883:ARG:CZ	1:U:885:MET:HE1	2.42	0.49
2:V:176:MET:HE1	2:V:180:ARG:NH2	2.25	0.49
4:X:123:THR:HA	4:X:126:ARG:HG2	1.95	0.49
7:a:198:PHE:CD1	7:a:233:LEU:HD22	2.47	0.49
9:d:60:GLN:HE22	9:d:98:LEU:HD11	1.77	0.49
11:A:165:GLN:HE22	11:A:267:LYS:HE3	1.77	0.49
12:B:196:GLU:OE1	12:B:349:ARG:NH1	2.45	0.49
12:B:271:PHE:O	12:B:275:GLU:HG3	2.12	0.49
15:E:264:MET:HG3	15:E:265:ASP:OD1	2.12	0.49
31:j:99:GLU:OE2	28:r:120:ARG:NH2	2.43	0.49
21:k:13:ASN:HB3	22:l:126:ARG:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:s:19:ASP:N	29:s:19:ASP:OD1	2.45	0.49
33:u:414:LEU:O	33:u:418:LEU:HD12	2.12	0.49
1:U:813:TYR:CG	1:U:813:TYR:O	2.65	0.49
2:V:476:PHE:HE1	5:Y:370:ILE:HD12	1.75	0.49
4:X:122:ARG:HG3	4:X:125:LEU:HB3	1.93	0.49
4:X:194:ARG:NH1	4:X:214:SER:OG	2.45	0.49
5:Y:389:MET:HE2	5:Y:389:MET:H	1.78	0.49
6:Z:225:GLN:H	6:Z:225:GLN:CD	2.21	0.49
13:C:97:VAL:HB	13:C:121:TYR:O	2.12	0.49
14:D:203:LEU:HB2	14:D:327:LEU:HD13	1.94	0.49
25:O:18:THR:OG1	25:O:171:SER:O	2.30	0.49
25:O:163:ILE:HG23	25:O:169:SER:CB	2.43	0.49
33:u:600:TYR:CE2	33:u:608:LYS:HE3	2.47	0.49
1:U:213:PHE:HB2	1:U:248:ILE:HG22	1.94	0.49
2:V:132:LEU:HB3	2:V:133:PRO:HD3	1.95	0.49
4:X:297:ARG:HH21	4:X:337:ARG:NH1	2.11	0.49
4:X:316:ASP:OD2	4:X:319:ILE:HG13	2.12	0.49
11:A:156:LYS:HD3	11:A:157:ILE:H	1.77	0.49
11:A:317:VAL:HG11	11:A:319:MET:HE2	1.94	0.49
11:A:351:ARG:NH1	11:A:378:PRO:O	2.46	0.49
15:E:144:GLU:HB3	15:E:297:ARG:NH2	2.26	0.49
15:E:309:ARG:NE	15:E:343:LEU:HD11	2.28	0.49
21:K:121:LEU:HD22	22:L:79:ALA:HB2	1.95	0.49
24:N:26:ILE:O	30:t:179:ARG:NH1	2.43	0.49
23:m:200:VAL:O	23:m:201:HIS:HB3	2.12	0.49
25:o:35:HIS:HB2	25:o:56:THR:HG21	1.94	0.49
32:f:391:LYS:NZ	33:u:465:LEU:HA	2.27	0.49
3:W:82:LEU:HD22	3:W:97:LEU:CD2	2.43	0.49
3:W:395:ASN:HA	3:W:398:VAL:HG22	1.95	0.49
6:Z:237:LEU:HD12	6:Z:237:LEU:O	2.13	0.49
7:a:286:ALA:O	7:a:289:ARG:NH1	2.45	0.49
9:d:185:ALA:HB2	9:d:226:ALA:HA	1.93	0.49
10:e:56:LEU:HD11	10:e:62:LYS:HB3	1.95	0.49
11:A:66:LYS:HD3	11:A:66:LYS:C	2.37	0.49
13:C:343:ASN:HB3	13:C:346:LYS:HE2	1.94	0.49
17:g:48:ALA:HB3	17:g:220:VAL:HG12	1.95	0.49
19:i:15:GLU:OE2	19:i:17:ARG:NE	2.32	0.49
22:l:71:GLY:HA3	22:l:221:PHE:CZ	2.48	0.49
3:W:183:VAL:O	3:W:187:LEU:HG	2.12	0.49
4:X:134:VAL:HG13	4:X:172:LEU:HD13	1.93	0.49
4:X:236:PHE:CE1	4:X:247:ALA:HB1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:415:TYR:CE1	5:Y:383:LEU:HD23	2.47	0.49
7:a:281:THR:O	7:a:284:ARG:HG3	2.12	0.49
7:a:304:VAL:O	7:a:307:VAL:HG22	2.12	0.49
7:a:324:ILE:HG22	7:a:331:VAL:HB	1.95	0.49
9:d:188:LYS:N	9:d:220:ASN:H	2.11	0.49
9:d:198:LEU:HD13	9:d:205:LYS:HZ1	1.78	0.49
14:D:323:ARG:NH1	14:D:324:PRO:O	2.45	0.49
15:E:40:TYR:CE1	16:F:72:LYS:HG3	2.46	0.49
16:F:130:GLN:OE1	16:F:131:THR:N	2.45	0.49
16:F:222:GLY:HA3	16:F:328:VAL:HG23	1.94	0.49
17:G:67:THR:HG22	17:G:69:LEU:H	1.77	0.49
17:g:80:MET:SD	17:g:138:MET:HE3	2.52	0.49
21:k:122:GLN:OE1	21:k:122:GLN:O	2.30	0.49
26:p:107:PRO:HG2	26:p:124:LEU:HB2	1.95	0.49
5:Y:231:LEU:HB2	5:Y:234:PRO:HG2	1.95	0.49
5:Y:314:LEU:O	5:Y:354:VAL:N	2.25	0.49
6:Z:111:LEU:O	6:Z:114:ARG:HG2	2.13	0.49
6:Z:145:HIS:ND1	6:Z:150:PRO:O	2.38	0.49
11:A:289:ALA:HA	16:F:301:ALA:HB2	1.93	0.49
12:B:36:LYS:C	12:B:38:LYS:HZ2	2.21	0.49
12:B:107:MET:HB2	12:B:160:ILE:HD11	1.94	0.49
13:C:186:VAL:HG23	13:C:292:ILE:HG23	1.95	0.49
16:F:343:LEU:O	16:F:343:LEU:HG	2.13	0.49
18:H:204:THR:HG22	18:H:206:ASP:H	1.77	0.49
2:V:384:GLU:OE1	2:V:384:GLU:N	2.44	0.49
3:W:32:ALA:O	3:W:35:ALA:HB3	2.12	0.49
3:W:60:MET:HA	3:W:64:SER:OG	2.13	0.49
4:X:122:ARG:HH21	4:X:124:PHE:HB2	1.78	0.49
4:X:412:ASP:HA	4:X:415:TYR:HB2	1.94	0.49
11:A:158:ASP:OD2	11:A:255:ARG:NH2	2.42	0.49
15:E:129:ASN:HA	15:E:189:SER:OG	2.12	0.49
15:E:173:TYR:HB2	15:E:282:PRO:HG3	1.95	0.49
15:E:363:VAL:HG13	15:E:365:GLU:H	1.78	0.49
17:G:112:ASP:OD1	17:G:113:MET:N	2.46	0.49
20:J:30:SER:HB2	20:J:61:LYS:HZ3	1.78	0.49
28:R:37:ILE:O	28:R:41:LEU:CB	2.61	0.49
24:n:14:LEU:HD21	24:n:101:ALA:HB3	1.94	0.49
33:u:305:LEU:H	33:u:321:MET:CE	2.25	0.49
3:W:102:ALA:HA	3:W:105:VAL:HG22	1.94	0.49
3:W:243:ILE:HG13	3:W:273:TYR:HE2	1.77	0.49
6:Z:20:VAL:HG22	6:Z:126:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:113:LEU:HB2	7:a:154:ARG:CZ	2.43	0.49
8:c:251:LEU:CD2	8:c:283:HIS:HB2	2.43	0.49
11:A:74:PRO:HD2	11:A:77:LEU:HD13	1.94	0.49
15:E:309:ARG:HE	15:E:343:LEU:HD11	1.78	0.49
18:H:179:ASN:O	18:H:180:GLU:HB2	2.13	0.49
24:n:144:ARG:NH2	24:n:151:GLU:OE1	2.45	0.49
33:u:349:TYR:HE1	33:u:763:ARG:HD2	1.78	0.49
33:u:581:GLU:OE1	33:u:581:GLU:N	2.46	0.49
33:u:662:MET:HG3	33:u:781:TYR:HE1	1.78	0.49
33:u:777:THR:HB	33:u:828:ARG:HD3	1.95	0.49
1:U:18:GLN:OE1	9:d:30:LEU:HD13	2.13	0.48
1:U:247:GLN:NE2	1:U:904:LYS:HB2	2.28	0.48
1:U:495:ASP:O	1:U:499:THR:HG23	2.13	0.48
5:Y:101:ARG:HH21	5:Y:136:HIS:CD2	2.30	0.48
6:Z:148:GLY:HA2	7:a:181:GLY:HA3	1.94	0.48
6:Z:204:LYS:O	6:Z:208:ILE:HG23	2.13	0.48
6:Z:256:GLN:O	6:Z:260:VAL:HG23	2.12	0.48
8:c:139:ARG:HG2	8:c:139:ARG:O	2.13	0.48
9:d:129:THR:OG1	9:d:130:ASN:N	2.42	0.48
12:B:405:MET:HE3	12:B:421:LYS:HE2	1.95	0.48
15:E:313:LEU:HD12	15:E:332:VAL:HG22	1.95	0.48
18:H:148:GLN:OE1	18:H:158:TRP:NE1	2.44	0.48
23:M:173:LYS:O	23:M:177:GLU:HG3	2.12	0.48
25:O:173:ILE:HB	25:O:190:THR:HG22	1.95	0.48
29:S:190:GLY:O	29:S:191:ASP:HB2	2.13	0.48
22:l:122:ARG:HG3	22:l:122:ARG:HH11	1.78	0.48
23:m:50:GLU:HG2	23:m:209:PHE:CD2	2.48	0.48
1:U:86:ASP:O	1:U:90:VAL:HG12	2.13	0.48
1:U:643:SER:OG	1:U:648:VAL:HB	2.13	0.48
1:U:894:MET:HE1	1:U:906:LEU:HD23	1.95	0.48
3:W:37:GLU:CD	3:W:38:GLY:N	2.71	0.48
5:Y:243:GLY:O	5:Y:247:LEU:HB2	2.12	0.48
5:Y:271:PHE:HZ	5:Y:299:MET:HG3	1.77	0.48
5:Y:366:TYR:HA	5:Y:369:THR:HG22	1.94	0.48
6:Z:133:LEU:HD12	6:Z:134:PRO:HD2	1.95	0.48
7:a:362:SER:HA	7:a:365:MET:SD	2.53	0.48
18:h:51:LYS:HD2	18:h:199:PHE:CZ	2.47	0.48
22:l:26:MET:HG2	22:l:149:PRO:HG2	1.95	0.48
23:m:187:ARG:HG3	23:m:232:ARG:NH1	2.23	0.48
33:u:266:LEU:HD23	33:u:294:MET:HB2	1.94	0.48
33:u:537:THR:O	33:u:540:GLN:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:111:GLN:HG3	1:U:126:ILE:HD11	1.94	0.48
2:V:336:GLU:HG3	2:V:342:ILE:HD13	1.95	0.48
2:V:378:VAL:HA	2:V:381:GLN:NE2	2.28	0.48
3:W:269:SER:HA	3:W:272:LEU:CD1	2.44	0.48
30:T:92:LEU:O	30:T:96:MET:HG2	2.13	0.48
17:g:13:ILE:HD11	19:i:5:TYR:CE1	2.48	0.48
21:k:68:VAL:HG22	21:k:78:MET:HE1	1.96	0.48
23:m:50:GLU:HG2	23:m:209:PHE:HD2	1.78	0.48
23:m:188:ASP:OD1	23:m:188:ASP:N	2.32	0.48
24:n:103:TRP:CH2	24:n:181:GLU:HG3	2.48	0.48
25:o:110:LEU:HD21	25:o:125:VAL:HG22	1.96	0.48
25:o:194:LYS:HB2	25:o:194:LYS:NZ	2.28	0.48
32:f:394:ARG:O	32:f:397:LEU:HD12	2.13	0.48
33:u:844:VAL:HG12	33:u:882:LEU:HA	1.95	0.48
1:U:565:ALA:O	1:U:568:GLU:HG2	2.13	0.48
2:V:358:MET:O	2:V:362:LEU:HG	2.12	0.48
2:V:487:HIS:ND1	6:Z:267:ARG:HG3	2.28	0.48
6:Z:109:ASN:HD22	6:Z:155:PHE:HE1	1.61	0.48
15:E:161:ARG:HB2	15:E:161:ARG:HH11	1.78	0.48
20:J:30:SER:HB2	20:J:61:LYS:NZ	2.29	0.48
1:U:21:GLU:HA	1:U:24:LEU:CD2	2.43	0.48
6:Z:167:ALA:HB1	8:c:42:LEU:HD21	1.95	0.48
16:F:266:LYS:O	16:F:269:ARG:HG2	2.13	0.48
20:J:4:ASP:OD1	20:J:4:ASP:N	2.38	0.48
38:n:301:LDZ:H26	38:n:301:LDZ:N10	2.28	0.48
33:u:54:ASP:O	33:u:57:GLU:HG2	2.13	0.48
33:u:588:ARG:HG3	33:u:589:SER:N	2.28	0.48
1:U:707:ASN:O	1:U:711:GLN:HG2	2.14	0.48
3:W:28:LEU:HD13	3:W:55:ARG:HB3	1.95	0.48
3:W:124:LEU:HA	3:W:127:THR:HG22	1.95	0.48
3:W:303:LYS:O	3:W:306:LEU:HD12	2.13	0.48
3:W:416:GLN:NE2	3:W:416:GLN:O	2.46	0.48
7:a:101:ARG:HA	7:a:104:VAL:HG12	1.96	0.48
8:c:265:MET:HB2	8:c:270:LEU:HD13	1.95	0.48
9:d:57:ILE:O	9:d:61:TRP:CD1	2.67	0.48
16:F:140:VAL:HG12	16:F:145:LEU:HD21	1.95	0.48
26:P:203:ARG:HH12	28:r:191:ASN:ND2	2.12	0.48
31:j:196:LEU:O	31:j:201:SER:OG	2.30	0.48
33:u:332:ALA:HA	33:u:335:ARG:HE	1.78	0.48
33:u:332:ALA:HA	33:u:335:ARG:NE	2.28	0.48
33:u:584:SER:OG	33:u:586:PRO:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:700:GLU:H	1:U:700:GLU:CD	2.22	0.48
3:W:87:ILE:HG13	3:W:88:MET:O	2.13	0.48
5:Y:128:TYR:OH	5:Y:163:LYS:HD2	2.13	0.48
6:Z:239:ASP:OD1	6:Z:239:ASP:N	2.45	0.48
11:A:401:ARG:HG3	11:A:401:ARG:HH11	1.78	0.48
14:D:98:GLN:HB2	14:D:121:ARG:HH22	1.79	0.48
15:E:145:LEU:HD12	15:E:172:LEU:HD21	1.95	0.48
15:E:322:LYS:HD2	15:E:326:ILE:HG13	1.96	0.48
15:E:367:PHE:HA	15:E:370:ALA:HB3	1.95	0.48
17:G:73:THR:HG22	17:G:74:GLU:H	1.78	0.48
33:u:646:MET:HA	33:u:646:MET:HE3	1.96	0.48
1:U:160:LEU:HD22	1:U:163:PHE:CD2	2.48	0.48
1:U:715:LYS:NZ	1:U:719:ASP:OD2	2.36	0.48
2:V:69:THR:HA	2:V:73:GLU:HB2	1.95	0.48
3:W:101:VAL:O	3:W:105:VAL:HG13	2.14	0.48
3:W:148:THR:HA	3:W:151:THR:HG22	1.95	0.48
5:Y:82:LYS:HE2	5:Y:107:LYS:HZ2	1.78	0.48
5:Y:174:TRP:HH2	13:C:377:HIS:CD2	2.31	0.48
7:a:342:ASP:O	7:a:346:ILE:HG12	2.13	0.48
8:c:286:GLU:O	8:c:290:VAL:HG12	2.13	0.48
9:d:41:THR:HB	9:d:44:THR:HG23	1.95	0.48
9:d:238:PRO:HB2	9:d:242:LEU:HG	1.96	0.48
15:E:255:ARG:O	15:E:258:MET:HG3	2.14	0.48
16:F:238:ARG:HG2	16:F:238:ARG:HH11	1.79	0.48
22:l:207:THR:HG22	22:l:229:VAL:HG23	1.96	0.48
33:u:208:LEU:HB3	33:u:214:VAL:HA	1.96	0.48
33:u:556:ARG:HD2	33:u:590:PHE:CZ	2.48	0.48
1:U:460:TYR:HA	1:U:463:ASN:HD21	1.79	0.48
4:X:96:PHE:HE2	4:X:109:LEU:HD22	1.78	0.48
9:d:114:GLU:HA	9:d:117:THR:HG22	1.96	0.48
9:d:170:LEU:O	9:d:174:ILE:HG13	2.13	0.48
15:E:262:ASN:OD1	15:E:266:GLY:HA3	2.14	0.48
19:I:40:ASN:ND2	19:I:182:GLY:O	2.47	0.48
23:M:201:HIS:NE2	23:M:204:VAL:HB	2.29	0.48
32:f:385:ASN:HD22	32:f:386:ARG:HH21	1.62	0.48
33:u:797:LEU:O	33:u:801:VAL:HG22	2.14	0.48
1:U:439:GLU:CD	1:U:473:VAL:HG13	2.39	0.48
1:U:633:CYS:HB2	1:U:659:CYS:SG	2.54	0.48
2:V:77:GLU:HB2	2:V:86:VAL:HG21	1.95	0.48
2:V:194:LYS:O	2:V:198:GLN:NE2	2.47	0.48
2:V:419:LEU:H	2:V:419:LEU:HD12	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:376:LYS:HZ1	3:W:380:GLN:HB3	1.77	0.48
3:W:451:MET:SD	6:Z:101:LEU:HB2	2.53	0.48
5:Y:74:LYS:NZ	5:Y:114:ILE:HG13	2.29	0.48
8:c:289:ASP:O	8:c:293:THR:HG23	2.14	0.48
16:F:185:TYR:HE1	16:F:195:ILE:HG12	1.78	0.48
33:u:271:MET:HE2	33:u:786:GLN:HB3	1.96	0.48
33:u:385:PHE:CE1	33:u:773:LYS:HD3	2.49	0.48
1:U:588:MET:HA	1:U:591:CYS:SG	2.54	0.47
1:U:646:PRO:HA	1:U:649:ARG:HE	1.79	0.47
4:X:421:LEU:CD2	6:Z:280:ILE:HD12	2.43	0.47
5:Y:118:GLU:H	5:Y:118:GLU:CD	2.16	0.47
6:Z:22:HIS:O	6:Z:26:ILE:HG22	2.13	0.47
6:Z:249:PHE:HE2	8:c:303:MET:HE1	1.79	0.47
8:c:51:MET:SD	8:c:51:MET:N	2.87	0.47
9:d:220:ASN:O	9:d:221:ASN:ND2	2.45	0.47
16:F:208:HIS:HB3	16:F:211:LYS:HB3	1.96	0.47
19:I:19:TYR:HA	19:I:22:GLU:HG3	1.95	0.47
19:i:198:ASN:HD22	19:i:240:HIS:HE1	1.62	0.47
2:V:132:LEU:O	2:V:136:GLU:HG2	2.14	0.47
2:V:406:GLY:O	2:V:410:ILE:HG22	2.13	0.47
3:W:3:ASP:OD1	3:W:3:ASP:N	2.44	0.47
3:W:16:MET:HB2	3:W:24:VAL:CG1	2.44	0.47
4:X:90:ARG:CZ	4:X:128:ALA:HB1	2.44	0.47
12:B:114:GLU:O	12:B:122:ILE:HG22	2.14	0.47
13:C:99:VAL:HG12	13:C:123:LEU:CB	2.45	0.47
16:F:175:MET:HE3	16:F:251:LEU:HA	1.95	0.47
33:u:62:ARG:HH22	33:u:63:LEU:HD12	1.78	0.47
33:u:573:ILE:HD12	33:u:576:ILE:HD13	1.96	0.47
1:U:138:PHE:O	1:U:142:LEU:HD23	2.14	0.47
1:U:728:PHE:O	1:U:732:LEU:HD23	2.14	0.47
2:V:193:GLN:HB3	2:V:241:ARG:NH2	2.29	0.47
2:V:426:LEU:O	2:V:427:GLN:HG2	2.14	0.47
3:W:136:ILE:HG21	3:W:144:ARG:HD2	1.96	0.47
3:W:321:VAL:HA	3:W:324:TYR:HD2	1.79	0.47
5:Y:152:MET:N	5:Y:152:MET:SD	2.87	0.47
5:Y:173:ASP:OD1	5:Y:174:TRP:N	2.47	0.47
6:Z:240:VAL:HG13	8:c:310:LYS:HE2	1.96	0.47
7:a:127:ASP:O	7:a:128:LEU:HD23	2.13	0.47
7:a:130:VAL:O	7:a:134:THR:HG23	2.14	0.47
7:a:163:TYR:HD2	7:a:172:TYR:HA	1.80	0.47
7:a:258:GLN:H	7:a:258:GLN:CD	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:d:174:ILE:O	9:d:178:ILE:HG23	2.15	0.47
12:B:41:LYS:HB3	12:B:41:LYS:HZ3	1.79	0.47
12:B:107:MET:HG2	13:C:96:VAL:HB	1.94	0.47
13:C:280:LEU:HD23	13:C:310:ARG:HG3	1.96	0.47
15:E:359:HIS:ND1	15:E:361:PHE:O	2.47	0.47
15:E:365:GLU:HA	15:E:368:MET:HG2	1.95	0.47
17:G:48:ALA:HB3	17:G:220:VAL:HG12	1.96	0.47
18:H:107:THR:HG21	18:H:138:GLY:HA3	1.95	0.47
17:g:73:THR:HG22	17:g:74:GLU:H	1.79	0.47
21:k:196:LYS:NZ	21:k:241:ILE:HD13	2.29	0.47
1:U:469:SER:HB3	1:U:473:VAL:CG2	2.45	0.47
2:V:172:VAL:O	2:V:175:MET:HE2	2.14	0.47
2:V:383:GLY:HA2	2:V:386:PHE:CD2	2.50	0.47
3:W:312:MET:HB2	3:W:365:ILE:HG13	1.95	0.47
9:d:190:LEU:HA	9:d:219:PRO:HA	1.97	0.47
10:e:52:PHE:CE1	10:e:55:GLN:HB2	2.49	0.47
13:C:11:LEU:HD22	13:C:14:GLY:HA3	1.96	0.47
16:F:205:PRO:HB3	16:F:212:PHE:HE2	1.79	0.47
30:T:96:MET:HE3	30:T:127:MET:HA	1.97	0.47
19:i:50:ARG:HG2	19:i:50:ARG:HH11	1.79	0.47
1:U:31:VAL:HG23	1:U:38:ILE:HD11	1.96	0.47
1:U:548:LEU:O	1:U:552:ILE:HG23	2.15	0.47
3:W:248:ARG:HD2	3:W:270:VAL:HG21	1.97	0.47
4:X:92:LEU:HA	4:X:95:LEU:HD23	1.97	0.47
4:X:303:GLU:HA	4:X:306:LEU:HG	1.96	0.47
6:Z:72:HIS:CE1	6:Z:111:LEU:HD11	2.49	0.47
6:Z:249:PHE:CE2	8:c:303:MET:HE1	2.50	0.47
7:a:363:MET:O	7:a:366:LEU:HD12	2.14	0.47
12:B:382:ASP:N	12:B:382:ASP:OD1	2.46	0.47
13:C:217:SER:O	14:D:248:ARG:NH2	2.48	0.47
17:G:129:ALA:O	17:G:130:GLU:HG3	2.14	0.47
22:L:158:ALA:HB1	22:L:172:LEU:HD13	1.96	0.47
31:j:21:TYR:O	31:j:24:GLU:HG3	2.15	0.47
26:p:15:LYS:HG3	26:p:119:PRO:HB2	1.95	0.47
28:r:32:LYS:HE2	28:r:32:LYS:HB3	1.66	0.47
1:U:74:PHE:HB3	1:U:100:ILE:HG12	1.96	0.47
1:U:148:LYS:O	1:U:151:ILE:HG22	2.15	0.47
1:U:766:PHE:HE1	1:U:778:PHE:H	1.61	0.47
14:D:39:ASP:O	14:D:43:ARG:HG3	2.14	0.47
14:D:105:SER:OG	14:D:108:GLY:O	2.32	0.47
15:E:213:ARG:HA	15:E:216:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:E:324:GLY:O	15:E:325:GLU:HG2	2.14	0.47
18:H:118:MET:HE2	18:H:151:PRO:HA	1.96	0.47
1:U:462:LEU:HD11	1:U:490:ARG:HH22	1.80	0.47
1:U:465:LEU:HD11	1:U:477:GLY:HA3	1.95	0.47
1:U:697:GLN:NE2	1:U:744:VAL:O	2.47	0.47
1:U:766:PHE:CE2	1:U:779:LEU:HB2	2.49	0.47
2:V:358:MET:HE2	2:V:358:MET:HA	1.97	0.47
3:W:12:ARG:CZ	3:W:24:VAL:HA	2.44	0.47
3:W:28:LEU:HG	3:W:29:PRO:N	2.29	0.47
4:X:355:LYS:O	4:X:356:LEU:HD23	2.15	0.47
5:Y:54:TYR:O	5:Y:57:LEU:HG	2.15	0.47
5:Y:69:LEU:O	5:Y:72:LYS:HG2	2.14	0.47
6:Z:106:ILE:O	6:Z:110:GLU:HG2	2.15	0.47
11:A:116:LYS:HE2	11:A:116:LYS:HB3	1.73	0.47
11:A:240:VAL:HG12	11:A:274:PHE:HA	1.97	0.47
15:E:46:ASP:OD1	16:F:80:ILE:HD13	2.14	0.47
16:F:205:PRO:HB3	16:F:212:PHE:CE2	2.49	0.47
17:G:165:ALA:HB1	17:G:179:LEU:HD13	1.97	0.47
19:I:18:LEU:O	19:I:22:GLU:HG2	2.14	0.47
21:K:178:GLN:O	21:K:182:GLN:HG3	2.15	0.47
25:O:135:MET:HE3	30:t:179:ARG:NH2	2.29	0.47
29:S:184:GLU:OE2	25:o:195:LYS:HB2	2.15	0.47
31:j:26:VAL:HG21	31:j:130:SER:HB2	1.96	0.47
21:k:49:ALA:HB2	21:k:217:LEU:HD12	1.97	0.47
22:l:47:VAL:HG12	22:l:195:LEU:HD22	1.96	0.47
30:t:151:ARG:O	30:t:155:GLU:HG3	2.14	0.47
33:u:342:PRO:HB3	33:u:387:GLN:HG3	1.96	0.47
33:u:524:MET:HB3	33:u:564:LEU:HD21	1.96	0.47
1:U:357:LYS:HE3	1:U:392:TRP:CD1	2.50	0.47
1:U:542:GLU:O	1:U:546:ARG:HG2	2.14	0.47
3:W:327:GLU:O	3:W:337:ALA:HB1	2.15	0.47
4:X:138:PHE:C	4:X:138:PHE:CD1	2.93	0.47
4:X:160:MET:HE2	4:X:160:MET:HA	1.97	0.47
4:X:260:MET:CE	4:X:322:HIS:HB3	2.45	0.47
5:Y:275:LEU:HD21	5:Y:296:VAL:HG13	1.96	0.47
6:Z:111:LEU:HG	6:Z:114:ARG:NH1	2.30	0.47
6:Z:236:LEU:HD11	7:a:335:TRP:HB3	1.97	0.47
7:a:190:VAL:HG22	7:a:225:LEU:HD12	1.96	0.47
7:a:374:ILE:HG23	7:a:375:LEU:HD23	1.97	0.47
8:c:26:ASP:H	8:c:172:HIS:CE1	2.33	0.47
8:c:29:GLU:HB2	8:c:203:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:K:155:HIS:O	21:K:162:PHE:HA	2.15	0.47
21:K:235:GLU:HA	21:K:238:ILE:HG22	1.97	0.47
24:N:35:THR:OG1	24:N:43:CYS:SG	2.67	0.47
17:g:19:GLU:HG3	17:g:21:ARG:HG3	1.96	0.47
31:j:132:LEU:HD21	31:j:159:ASN:HB3	1.97	0.47
22:l:66:VAL:HB	22:l:70:ILE:HG22	1.96	0.47
27:q:31:ASP:N	27:q:31:ASP:OD1	2.48	0.47
29:s:169:ASP:OD1	29:s:169:ASP:N	2.47	0.47
33:u:309:GLU:HA	33:u:314:TYR:HD2	1.79	0.47
1:U:196:LYS:O	1:U:199:ARG:HG2	2.14	0.47
1:U:462:LEU:HD21	1:U:490:ARG:NH2	2.23	0.47
1:U:636:VAL:HG13	1:U:637:VAL:HG23	1.97	0.47
2:V:228:ARG:HB2	2:V:257:ASN:HD21	1.79	0.47
2:V:241:ARG:HH12	13:C:26:SER:HB3	1.78	0.47
3:W:23:THR:HA	3:W:26:GLN:HB2	1.97	0.47
3:W:158:ASP:OD2	3:W:160:LYS:HG2	2.14	0.47
5:Y:193:ASP:OD1	5:Y:226:VAL:HG22	2.15	0.47
7:a:211:PHE:HZ	7:a:278:MET:HG3	1.77	0.47
9:d:157:ASN:O	9:d:158:ILE:HD13	2.14	0.47
9:d:189:ILE:HG12	9:d:220:ASN:OD1	2.14	0.47
9:d:191:PHE:HA	9:d:194:ALA:HB3	1.96	0.47
15:E:141:GLN:H	15:E:141:GLN:CD	2.20	0.47
20:J:234:LYS:HB2	20:J:234:LYS:NZ	2.29	0.47
18:h:118:MET:O	18:h:122:THR:HG23	2.15	0.47
18:h:179:ASN:HB3	18:h:182:LEU:HD13	1.97	0.47
18:h:231:ALA:O	18:h:233:ILE:N	2.47	0.47
31:j:16:LEU:O	31:j:20:GLU:HG2	2.14	0.47
31:j:184:ASP:O	31:j:188:ILE:HG22	2.14	0.47
33:u:106:LEU:HG	33:u:126:ILE:HG12	1.97	0.47
33:u:381:VAL:O	33:u:773:LYS:HD2	2.14	0.47
1:U:516:LEU:CD1	1:U:520:MET:HE1	2.45	0.47
2:V:348:PHE:HB2	2:V:353:LEU:HD23	1.97	0.47
2:V:397:ARG:HA	2:V:400:HIS:NE2	2.30	0.47
5:Y:191:ILE:HB	10:e:43:TRP:CH2	2.50	0.47
8:c:41:MET:HE3	8:c:57:MET:HE2	1.97	0.47
16:F:312:GLU:O	16:F:316:GLN:HG2	2.15	0.47
19:I:151:ASP:OD1	19:I:153:SER:OG	2.28	0.47
22:l:107:ARG:NH2	30:t:79:ASP:OD2	2.30	0.47
25:o:167:LEU:O	25:o:167:LEU:HD13	2.14	0.47
33:u:256:PHE:HD1	33:u:261:ARG:HB2	1.80	0.47
33:u:477:MET:HE3	33:u:477:MET:HB2	1.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:u:573:ILE:HA	33:u:576:ILE:HD13	1.97	0.47
1:U:58:GLN:HG3	1:U:84:ALA:C	2.40	0.46
1:U:410:VAL:HG23	1:U:448:LEU:HD13	1.96	0.46
2:V:289:LEU:HG	2:V:308:THR:HG23	1.97	0.46
3:W:64:SER:HB2	3:W:65:ARG:NH2	2.30	0.46
5:Y:177:ARG:NH2	5:Y:205:VAL:O	2.48	0.46
6:Z:78:MET:HE2	6:Z:78:MET:HA	1.96	0.46
12:B:67:ARG:NH2	33:u:239:TYR:HA	2.30	0.46
14:D:391:ARG:NH1	14:D:393:ILE:O	2.49	0.46
23:M:110:HIS:O	23:M:114:ARG:HG3	2.15	0.46
28:R:182:ASP:OD1	28:R:182:ASP:N	2.45	0.46
31:j:5:ARG:HD3	31:j:8:THR:HB	1.97	0.46
25:o:190:THR:HG22	25:o:192:PRO:HD3	1.96	0.46
33:u:472:HIS:CD2	33:u:474:SER:HB3	2.50	0.46
33:u:544:GLU:OE2	33:u:545:LYS:HE2	2.15	0.46
1:U:616:ARG:HD2	1:U:650:TYR:CD1	2.50	0.46
2:V:349:ARG:NH2	10:e:40:GLU:OE1	2.48	0.46
2:V:418:SER:O	2:V:422:ILE:HG13	2.15	0.46
3:W:12:ARG:HA	3:W:12:ARG:HD3	1.81	0.46
3:W:25:ASP:HA	3:W:28:LEU:HD23	1.97	0.46
3:W:344:THR:HG23	3:W:345:GLU:H	1.80	0.46
5:Y:104:MET:C	5:Y:105:MET:HE2	2.39	0.46
6:Z:228:TYR:HE2	7:a:341:LEU:HG	1.79	0.46
12:B:408:ARG:HH21	13:C:163:GLU:CD	2.23	0.46
16:F:144:LYS:O	16:F:144:LYS:HD3	2.15	0.46
16:F:239:ALA:O	16:F:243:GLN:HG2	2.15	0.46
21:K:98:ASN:OD1	28:R:61:ARG:NH1	2.48	0.46
28:R:191:ASN:HD21	26:p:203:ARG:NH1	2.13	0.46
21:k:34:GLY:O	21:k:53:ARG:NH2	2.48	0.46
33:u:485:LEU:HD23	33:u:501:LEU:HD11	1.97	0.46
1:U:336:GLU:O	1:U:339:LEU:HG	2.15	0.46
1:U:554:LEU:HA	1:U:588:MET:SD	2.55	0.46
3:W:173:THR:HG22	3:W:177:MET:SD	2.56	0.46
4:X:217:ILE:O	4:X:221:GLU:HG2	2.15	0.46
4:X:389:ASP:OD1	4:X:389:ASP:N	2.47	0.46
5:Y:83:ARG:HA	5:Y:86:GLU:OE2	2.15	0.46
5:Y:174:TRP:CD1	13:C:340:ARG:NH1	2.76	0.46
5:Y:272:PHE:HE2	5:Y:323:PHE:HE1	1.63	0.46
9:d:206:MET:H	9:d:206:MET:HE2	1.80	0.46
10:e:41:ASP:OD1	10:e:43:TRP:N	2.48	0.46
13:C:31:LEU:HD22	14:D:44:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:F:226:TYR:HA	16:F:332:THR:O	2.16	0.46
22:L:53:GLN:H	22:L:53:GLN:CD	2.21	0.46
26:P:125:ASP:OD1	26:P:129:CYS:HB3	2.16	0.46
27:q:13:VAL:HG11	27:q:105:ALA:HB1	1.97	0.46
2:V:157:THR:OG1	2:V:158:PRO:HD3	2.15	0.46
2:V:440:LYS:HE2	9:d:148:TYR:CE2	2.50	0.46
3:W:37:GLU:C	3:W:39:ARG:H	2.23	0.46
3:W:241:LEU:HD21	3:W:282:GLU:HG3	1.97	0.46
4:X:406:ASN:O	4:X:409:LYS:HG3	2.16	0.46
7:a:347:LYS:HA	7:a:350:LYS:HE3	1.97	0.46
9:d:63:ILE:HB	9:d:165:PHE:CE2	2.50	0.46
9:d:187:GLU:C	9:d:219:PRO:HB2	2.41	0.46
11:A:164:MET:HE2	11:A:241:ILE:H	1.80	0.46
12:B:46:ALA:HB3	12:B:179:ALA:H	1.81	0.46
12:B:256:ILE:HD12	13:C:271:ARG:HD3	1.97	0.46
15:E:261:LEU:CD1	15:E:294:ARG:HE	2.27	0.46
15:E:363:VAL:N	15:E:366:ASP:OD2	2.48	0.46
20:J:227:LYS:HD2	20:J:227:LYS:O	2.16	0.46
18:h:179:ASN:OD1	18:h:180:GLU:N	2.49	0.46
19:i:249:ARG:HG2	19:i:249:ARG:HH11	1.80	0.46
23:m:63:ASN:N	23:m:63:ASN:OD1	2.48	0.46
1:U:202:VAL:HG13	1:U:206:MET:HE3	1.97	0.46
1:U:722:ASP:OD1	1:U:722:ASP:N	2.48	0.46
2:V:68:ASP:O	2:V:72:LEU:N	2.49	0.46
2:V:256:ARG:HH12	10:e:5:LYS:HB2	1.81	0.46
3:W:320:LEU:HD12	3:W:320:LEU:HA	1.75	0.46
5:Y:82:LYS:HE2	5:Y:107:LYS:NZ	2.30	0.46
6:Z:242:LEU:HB2	6:Z:243:GLN:NE2	2.31	0.46
12:B:60:LEU:HD13	33:u:236:CYS:HB3	1.96	0.46
14:D:103:VAL:HG21	14:D:132:LEU:HD21	1.98	0.46
16:F:169:ASP:O	16:F:173:LYS:HG2	2.15	0.46
16:F:256:LEU:HD12	16:F:291:ILE:HG12	1.98	0.46
20:J:76:LEU:H	20:J:129:ILE:HG22	1.81	0.46
25:O:201:ARG:HG3	25:O:201:ARG:HH11	1.81	0.46
30:T:211:ILE:HG12	24:n:29:ARG:HH21	1.80	0.46
31:j:136:PHE:HA	31:j:142:PRO:HA	1.96	0.46
33:u:140:LEU:CD2	33:u:169:GLU:HG3	2.46	0.46
33:u:291:GLN:HA	33:u:294:MET:HE2	1.97	0.46
2:V:227:VAL:O	2:V:231:LEU:HG	2.15	0.46
3:W:180:LYS:O	3:W:184:GLU:HG3	2.15	0.46
3:W:259:GLU:OE1	3:W:262:LYS:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:290:PRO:HB3	10:e:43:TRP:CE2	2.51	0.46
5:Y:373:GLY:O	5:Y:377:LEU:HG	2.15	0.46
6:Z:86:ASN:OD1	6:Z:88:ARG:NH1	2.49	0.46
7:a:12:GLN:HG3	7:a:22:TRP:CD1	2.51	0.46
9:d:179:ALA:O	9:d:182:ILE:HG22	2.16	0.46
13:C:65:LEU:O	14:D:114:ARG:NH1	2.48	0.46
18:H:29:VAL:HG11	18:H:133:SER:HB2	1.98	0.46
24:N:4:MET:HG3	24:N:127:ILE:HG22	1.98	0.46
31:j:41:VAL:HG23	31:j:211:MET:HB2	1.98	0.46
23:m:141:SER:HB3	23:m:144:ASP:HB2	1.98	0.46
33:u:278:VAL:HG12	33:u:305:LEU:HD11	1.96	0.46
1:U:144:ASP:OD2	13:C:16:ALA:HB2	2.16	0.46
3:W:73:MET:O	3:W:76:GLU:HB2	2.15	0.46
3:W:92:LYS:HB2	3:W:96:GLN:CD	2.41	0.46
3:W:188:GLU:HA	3:W:191:ARG:NH2	2.29	0.46
5:Y:179:ARG:HB3	5:Y:183:TYR:CE1	2.50	0.46
12:B:198:LYS:NZ	12:B:202:GLU:OE1	2.37	0.46
12:B:317:ASP:O	12:B:346:ARG:NH1	2.45	0.46
15:E:226:GLN:HE21	15:E:272:ARG:HD3	1.79	0.46
15:E:356:ARG:HA	15:E:356:ARG:CZ	2.46	0.46
20:J:108:THR:HG22	20:J:133:ILE:HD13	1.98	0.46
25:O:7:VAL:HG22	25:O:12:ILE:HD13	1.96	0.46
19:i:21:VAL:HG12	19:i:25:MET:HE3	1.98	0.46
31:j:158:ALA:O	21:k:58:LEU:HD13	2.16	0.46
21:k:168:ARG:HD2	21:k:178:GLN:HE21	1.80	0.46
22:l:19:ILE:HB	22:l:22:ILE:HD12	1.97	0.46
33:u:62:ARG:NH2	33:u:63:LEU:HD12	2.30	0.46
1:U:15:ASP:HA	1:U:20:LYS:HE3	1.97	0.46
2:V:315:LYS:HD3	2:V:316:ALA:N	2.31	0.46
3:W:165:ILE:HD12	3:W:192:LEU:HD12	1.98	0.46
3:W:338:THR:HA	3:W:342:GLY:HA3	1.98	0.46
6:Z:35:VAL:O	6:Z:96:HIS:HA	2.16	0.46
6:Z:209:ARG:HD2	6:Z:213:GLU:HG2	1.97	0.46
7:a:133:GLU:HA	7:a:136:GLU:CG	2.45	0.46
8:c:278:GLN:HG2	8:c:279:ASP:OD1	2.16	0.46
15:E:97:ARG:HB2	15:E:111:LEU:HB2	1.98	0.46
25:O:19:ARG:HB2	25:O:170:GLY:N	2.30	0.46
26:P:20:VAL:HG12	26:P:190:ILE:HB	1.97	0.46
21:k:58:LEU:HD23	21:k:58:LEU:HA	1.78	0.46
28:r:19:ARG:HH21	28:r:29:GLN:NE2	2.13	0.46
32:f:401:GLN:CD	32:f:405:ARG:HH12	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:106:ASP:O	1:U:109:THR:HB	2.16	0.46
2:V:32:PRO:HA	2:V:36:GLU:HG2	1.98	0.46
2:V:37:MET:C	2:V:37:MET:HE2	2.41	0.46
4:X:122:ARG:HE	4:X:125:LEU:H	1.64	0.46
5:Y:177:ARG:HA	5:Y:180:LEU:HB2	1.97	0.46
7:a:307:VAL:O	7:a:311:VAL:HG23	2.15	0.46
11:A:106:SER:C	11:A:108:ASP:H	2.24	0.46
12:B:52:VAL:O	12:B:52:VAL:HG23	2.16	0.46
12:B:68:ILE:HD13	33:u:670:MET:HE2	1.96	0.46
13:C:113:ARG:NE	13:C:130:LYS:HB2	2.31	0.46
14:D:395:LEU:HD12	14:D:397:LYS:HZ2	1.81	0.46
16:F:220:PRO:HG3	16:F:350:ARG:NH2	2.31	0.46
18:H:38:ILE:HD13	18:H:190:THR:HG23	1.98	0.46
28:R:4:LEU:HD21	28:R:135:ALA:HB1	1.98	0.46
29:S:24:ALA:HB1	29:S:193:LEU:HD11	1.96	0.46
22:l:91:GLU:HA	22:l:91:GLU:OE2	2.16	0.46
22:l:164:ARG:O	22:l:198:THR:HG23	2.16	0.46
32:f:388:THR:HA	32:f:391:LYS:CE	2.46	0.46
33:u:425:GLY:O	33:u:429:ILE:HG13	2.16	0.46
1:U:101:ILE:HD12	1:U:104:CYS:HB2	1.97	0.46
1:U:497:LEU:HB2	1:U:516:LEU:HD13	1.98	0.46
1:U:571:CYS:HB3	1:U:601:ARG:HH22	1.80	0.46
1:U:791:LEU:O	1:U:913:ILE:HD13	2.16	0.46
1:U:792:ASN:C	1:U:793:LYS:HD3	2.40	0.46
5:Y:80:GLU:O	5:Y:83:ARG:HG2	2.16	0.46
5:Y:180:LEU:HD12	5:Y:180:LEU:HA	1.79	0.46
6:Z:174:HIS:O	6:Z:177:ARG:HG2	2.15	0.46
9:d:219:PRO:HG2	9:d:223:TYR:HD2	1.81	0.46
11:A:174:TYR:HD2	11:A:232:ARG:HH21	1.64	0.46
11:A:218:PRO:HB2	12:B:343:ARG:HD3	1.98	0.46
12:B:105:THR:HG23	13:C:98:ASP:OD1	2.16	0.46
14:D:181:VAL:HG11	14:D:308:ILE:HD11	1.98	0.46
14:D:225:ALA:HB1	14:D:259:PRO:O	2.16	0.46
18:H:10:LEU:HD13	18:H:21:GLN:HB2	1.97	0.46
20:J:241:LYS:HD2	20:J:241:LYS:HA	1.77	0.46
1:U:583:MET:HA	1:U:583:MET:HE3	1.98	0.45
2:V:73:GLU:O	2:V:77:GLU:HG3	2.16	0.45
2:V:461:LYS:HA	2:V:461:LYS:HE2	1.98	0.45
3:W:82:LEU:O	3:W:85:GLU:N	2.49	0.45
3:W:272:LEU:HD11	3:W:336:PRO:HB2	1.98	0.45
4:X:344:ARG:CG	4:X:386:ILE:HG12	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:d:96:HIS:HB3	9:d:132:TYR:HD2	1.80	0.45
14:D:191:TYR:CD2	14:D:198:PRO:HB3	2.50	0.45
14:D:244:PRO:O	14:D:248:ARG:HG3	2.16	0.45
15:E:104:THR:HG22	15:E:106:THR:HG23	1.99	0.45
16:F:155:LYS:HB2	16:F:155:LYS:HE3	1.73	0.45
16:F:192:ASP:HA	16:F:195:ILE:HD12	1.98	0.45
20:J:79:ASP:OD2	20:J:125:ARG:NH2	2.49	0.45
26:P:35:VAL:HG12	26:P:36:THR:HG23	1.98	0.45
32:f:381:ARG:O	32:f:385:ASN:HB2	2.16	0.45
33:u:333:LEU:HD12	33:u:337:LEU:HD23	1.98	0.45
2:V:188:SER:O	2:V:192:MET:HG3	2.17	0.45
2:V:400:HIS:CD2	9:d:144:MET:HE1	2.51	0.45
4:X:111:LEU:O	4:X:115:GLU:HG2	2.16	0.45
6:Z:19:VAL:HG23	6:Z:95:TYR:CE1	2.51	0.45
9:d:128:GLN:HB2	9:d:130:ASN:ND2	2.30	0.45
17:G:78:CYS:HA	17:G:139:ILE:O	2.17	0.45
20:J:236:LYS:HZ2	20:J:240:GLU:HB2	1.81	0.45
22:l:117:GLN:O	22:l:120:THR:OG1	2.30	0.45
25:o:179:SER:OG	25:o:180:LYS:N	2.50	0.45
1:U:221:ILE:HG22	1:U:260:PHE:HE2	1.82	0.45
1:U:418:GLU:HG2	1:U:418:GLU:O	2.16	0.45
1:U:670:ASN:HA	1:U:673:GLU:OE1	2.16	0.45
2:V:34:ASP:HA	2:V:37:MET:SD	2.55	0.45
2:V:105:SER:O	2:V:108:LEU:HG	2.16	0.45
2:V:139:MET:SD	2:V:139:MET:N	2.85	0.45
2:V:263:LEU:HD12	2:V:264:TYR:H	1.80	0.45
2:V:332:LEU:O	2:V:336:GLU:HG2	2.16	0.45
2:V:416:ARG:NH1	5:Y:351:ASN:OD1	2.49	0.45
4:X:334:ASN:O	4:X:337:ARG:HG2	2.15	0.45
5:Y:81:LEU:HA	5:Y:84:LEU:HG	1.99	0.45
8:c:244:VAL:O	8:c:247:GLU:HG2	2.17	0.45
9:d:4:GLN:O	9:d:25:ARG:NH1	2.49	0.45
9:d:128:GLN:O	9:d:134:LYS:NZ	2.47	0.45
9:d:218:GLY:CA	9:d:222:TYR:HA	2.46	0.45
9:d:237:ILE:N	9:d:238:PRO:HD3	2.31	0.45
11:A:70:THR:HG21	12:B:164:MET:SD	2.56	0.45
12:B:316:LEU:HD23	12:B:316:LEU:HA	1.80	0.45
12:B:362:LYS:HG2	12:B:384:ILE:HD13	1.98	0.45
15:E:88:ASP:OD1	15:E:90:SER:OG	2.34	0.45
19:I:116:ASP:OD1	20:J:81:ARG:NH1	2.48	0.45
24:N:150:GLU:H	24:N:150:GLU:CD	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Q:165:GLU:HG2	27:Q:196:PHE:CE1	2.51	0.45
29:S:16:ALA:HB2	29:S:121:VAL:HG23	1.98	0.45
23:m:180:GLN:O	23:m:184:MET:HG2	2.16	0.45
33:u:380:PHE:CZ	33:u:818:LEU:HD21	2.50	0.45
1:U:334:ALA:O	1:U:337:LEU:HG	2.15	0.45
1:U:633:CYS:HG	1:U:659:CYS:HB2	1.82	0.45
3:W:144:ARG:HH22	3:W:172:GLU:HG3	1.82	0.45
3:W:224:LEU:HD12	3:W:250:ILE:HG22	1.98	0.45
3:W:340:VAL:HA	3:W:350:ARG:CZ	2.45	0.45
3:W:372:ARG:HH12	7:a:327:VAL:HG11	1.82	0.45
7:a:69:HIS:ND1	7:a:70:ARG:HG2	2.32	0.45
7:a:344:GLN:OE1	7:a:347:LYS:NZ	2.30	0.45
8:c:55:GLY:HA3	8:c:112:TYR:CE2	2.51	0.45
12:B:231:GLY:N	35:B:501:ATP:O2A	2.49	0.45
13:C:24:TYR:HA	13:C:27:LYS:HE3	1.99	0.45
13:C:225:GLY:O	13:C:229:ARG:HG2	2.16	0.45
15:E:101:ASP:OD1	15:E:102:MET:N	2.48	0.45
15:E:363:VAL:HG13	15:E:365:GLU:N	2.31	0.45
16:F:79:LYS:HZ2	16:F:80:ILE:HD12	1.81	0.45
16:F:281:SER:O	16:F:326:VAL:HA	2.17	0.45
21:K:195:ILE:HG23	21:K:217:LEU:HD11	1.99	0.45
21:k:224:GLN:NE2	21:k:226:PHE:HB3	2.31	0.45
1:U:417:LYS:HD2	1:U:417:LYS:N	2.32	0.45
1:U:669:ILE:HG21	1:U:705:LYS:HG2	1.98	0.45
2:V:188:SER:HA	2:V:191:LEU:HB2	1.98	0.45
2:V:334:VAL:HG23	2:V:360:TYR:CE2	2.52	0.45
2:V:397:ARG:HG3	2:V:398:LEU:HD22	1.97	0.45
3:W:31:CYS:HA	3:W:34:LEU:CD2	2.46	0.45
3:W:167:GLN:OE1	3:W:168:GLU:N	2.49	0.45
4:X:83:ALA:HA	4:X:122:ARG:HH12	1.81	0.45
6:Z:114:ARG:HG2	6:Z:114:ARG:HH11	1.82	0.45
7:a:8:LEU:HD11	7:a:26:GLU:HB2	1.98	0.45
9:d:209:TYR:HD1	9:d:215:TRP:HD1	1.63	0.45
9:d:218:GLY:HA3	9:d:222:TYR:HA	1.98	0.45
16:F:156:ASP:OD1	16:F:157:SER:N	2.48	0.45
22:L:104:PRO:HB2	22:L:107:ARG:HG3	1.97	0.45
29:S:173:ARG:HG2	25:o:199:LEU:HB3	1.98	0.45
17:g:213:SER:O	17:g:213:SER:OG	2.34	0.45
21:k:14:THR:HB	21:k:22:PHE:HE1	1.81	0.45
1:U:244:MET:HA	1:U:247:GLN:OE1	2.16	0.45
1:U:439:GLU:OE1	1:U:473:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:703:CYS:SG	1:U:706:VAL:HG23	2.57	0.45
1:U:772:TRP:HB3	1:U:775:LEU:HG	1.99	0.45
4:X:417:LYS:NZ	6:Z:280:ILE:HG13	2.31	0.45
6:Z:6:VAL:HG23	6:Z:158:VAL:HG11	1.98	0.45
6:Z:96:HIS:NE2	6:Z:123:ILE:HG12	2.32	0.45
8:c:26:ASP:H	8:c:172:HIS:HE1	1.65	0.45
8:c:263:ASP:HB2	8:c:265:MET:HE1	1.97	0.45
8:c:282:ARG:O	8:c:286:GLU:HG2	2.17	0.45
12:B:115:ILE:HG21	12:B:144:LEU:HD21	1.99	0.45
12:B:193:GLN:OE1	12:B:193:GLN:N	2.48	0.45
13:C:65:LEU:HG	14:D:114:ARG:HH12	1.81	0.45
15:E:84:ARG:HH22	15:E:108:MET:CE	2.29	0.45
16:F:249:LEU:HD21	16:F:271:ALA:HB1	1.99	0.45
28:r:9:ARG:NH2	28:r:146:ASP:OD1	2.45	0.45
3:W:87:ILE:HD13	3:W:94:ARG:NH2	2.32	0.45
3:W:302:TYR:O	3:W:306:LEU:HG	2.17	0.45
4:X:95:LEU:HA	4:X:98:ASP:OD1	2.17	0.45
4:X:306:LEU:HD12	4:X:307:THR:N	2.31	0.45
7:a:292:THR:HG22	7:a:294:GLU:OE1	2.16	0.45
11:A:66:LYS:HE3	13:C:78:ARG:NH1	2.32	0.45
13:C:297:ARG:HH21	14:D:274:ARG:HH11	1.65	0.45
13:C:372:ARG:NH2	14:D:179:GLU:OE1	2.49	0.45
14:D:299:PHE:O	14:D:301:GLN:HG3	2.17	0.45
16:F:353:GLU:OE1	16:F:353:GLU:N	2.36	0.45
22:L:108:LEU:O	22:L:112:ILE:HG13	2.17	0.45
25:O:167:LEU:HG	25:O:167:LEU:O	2.17	0.45
28:R:37:ILE:O	28:R:38:ASN:HB2	2.17	0.45
29:S:28:ARG:NE	29:S:191:ASP:OD2	2.33	0.45
17:g:161:CYS:SG	17:g:162:GLY:N	2.89	0.45
30:t:25:ASP:HA	30:t:187:PHE:HA	1.97	0.45
32:f:395:LEU:HD23	32:f:398:LEU:HD21	1.98	0.45
33:u:140:LEU:HB3	33:u:141:LYS:NZ	2.30	0.45
1:U:28:ASN:ND2	1:U:63:VAL:HG12	2.28	0.45
1:U:639:LEU:CD2	13:C:46:GLN:HE21	2.27	0.45
2:V:169:LEU:C	2:V:171:VAL:H	2.25	0.45
2:V:170:LEU:O	2:V:173:ILE:HG22	2.17	0.45
2:V:236:ARG:NE	2:V:236:ARG:O	2.50	0.45
2:V:409:MET:HE3	2:V:409:MET:HA	1.98	0.45
3:W:20:TYR:HD1	3:W:22:ALA:N	2.00	0.45
3:W:182:ARG:O	3:W:186:ILE:HG23	2.17	0.45
4:X:122:ARG:NH2	4:X:124:PHE:HB2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:409:LYS:HA	4:X:412:ASP:OD2	2.17	0.45
7:a:191:SER:O	7:a:195:GLU:HG2	2.17	0.45
8:c:242:GLU:O	8:c:246:LYS:HG2	2.17	0.45
11:A:199:GLU:HA	11:A:202:VAL:HG12	1.99	0.45
12:B:294:ARG:NH1	12:B:309:MET:HE2	2.32	0.45
13:C:27:LYS:HE3	13:C:27:LYS:HB3	1.79	0.45
13:C:60:ARG:HH11	13:C:60:ARG:HB2	1.81	0.45
15:E:245:GLU:HB3	17:G:18:PRO:HG2	1.99	0.45
15:E:353:PHE:N	15:E:353:PHE:CD1	2.84	0.45
23:M:151:ILE:HG13	23:M:157:SER:HB2	1.99	0.45
23:M:229:LYS:NZ	23:M:233:GLU:OE2	2.43	0.45
28:R:191:ASN:HD21	26:p:203:ARG:HH12	1.65	0.45
21:k:14:THR:HB	21:k:22:PHE:CE1	2.51	0.45
30:t:99:ARG:HD2	30:t:104:ASN:O	2.16	0.45
1:U:118:LEU:HB2	1:U:123:LYS:NZ	2.31	0.45
1:U:612:ASP:HB3	1:U:647:HIS:CG	2.52	0.45
1:U:766:PHE:CZ	1:U:779:LEU:HB2	2.52	0.45
1:U:815:ALA:N	1:U:816:PRO:HD3	2.32	0.45
8:c:61:PHE:HB2	8:c:107:MET:SD	2.56	0.45
9:d:188:LYS:H	9:d:220:ASN:H	1.65	0.45
11:A:87:LEU:HG	11:A:88:GLN:HE22	1.81	0.45
11:A:91:GLN:HB2	11:A:92:PRO:HD3	1.98	0.45
11:A:220:THR:CG2	11:A:343:PHE:HB3	2.47	0.45
13:C:65:LEU:HG	14:D:114:ARG:NH1	2.32	0.45
15:E:353:PHE:CE2	15:E:373:LYS:HB2	2.52	0.45
19:I:41:ASP:OD1	19:I:41:ASP:N	2.50	0.45
22:L:50:LYS:HE2	22:L:211:SER:HB2	1.99	0.45
28:R:113:TYR:O	28:R:120:ARG:HA	2.17	0.45
31:j:38:ARG:NH2	31:j:181:ILE:H	2.15	0.45
29:s:176:LYS:HE2	29:s:208:VAL:HG21	1.99	0.45
32:f:400:GLN:O	32:f:404:LEU:HD22	2.17	0.45
33:u:164:GLY:O	33:u:168:LYS:HE3	2.16	0.45
33:u:439:TYR:CD1	33:u:476:THR:HG21	2.52	0.45
33:u:520:LEU:HD21	33:u:560:LEU:HD21	1.99	0.45
33:u:656:GLY:O	33:u:660:ILE:HG13	2.16	0.45
33:u:881:GLU:OE1	33:u:881:GLU:HA	2.17	0.45
1:U:219:CYS:O	1:U:223:LEU:HG	2.16	0.45
1:U:894:MET:HE1	1:U:906:LEU:HB3	1.98	0.45
2:V:248:ALA:HB1	2:V:284:GLU:HG3	1.99	0.45
2:V:341:GLU:HA	2:V:368:ARG:HH12	1.80	0.45
3:W:70:VAL:HA	3:W:73:MET:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:165:LEU:HD12	4:X:165:LEU:HA	1.79	0.45
9:d:58:GLY:O	9:d:62:SER:OG	2.25	0.45
12:B:126:SER:C	12:B:128:GLY:H	2.25	0.45
12:B:275:GLU:HG2	12:B:325:VAL:HG21	1.99	0.45
22:l:80:ASP:HB2	22:l:130:VAL:HG13	1.98	0.45
22:l:122:ARG:HG3	22:l:122:ARG:NH1	2.32	0.45
1:U:803:LYS:HB3	1:U:875:PHE:CD1	2.52	0.44
3:W:12:ARG:O	3:W:14:VAL:N	2.50	0.44
3:W:20:TYR:C	3:W:22:ALA:N	2.73	0.44
5:Y:298:GLU:HA	5:Y:301:ILE:HD12	1.98	0.44
5:Y:371:LYS:O	5:Y:375:LEU:HD22	2.16	0.44
9:d:9:TRP:HH2	9:d:60:GLN:HB2	1.82	0.44
9:d:114:GLU:H	9:d:114:GLU:CD	2.18	0.44
11:A:41:TYR:O	11:A:44:GLN:HG2	2.17	0.44
11:A:57:LYS:C	11:A:57:LYS:HD3	2.42	0.44
12:B:49:LEU:HD13	12:B:68:ILE:HD11	1.99	0.44
14:D:395:LEU:HD12	14:D:397:LYS:NZ	2.32	0.44
18:H:93:LEU:HD13	18:H:113:ARG:HB3	1.99	0.44
25:O:136:ALA:HB1	30:t:149:LEU:HD11	1.98	0.44
33:u:774:GLY:O	33:u:828:ARG:NH2	2.49	0.44
1:U:52:GLU:HA	1:U:57:ARG:HD2	1.99	0.44
1:U:164:GLU:O	1:U:167:ILE:HG12	2.17	0.44
2:V:212:TYR:O	2:V:216:ARG:HG3	2.16	0.44
2:V:419:LEU:HD22	2:V:435:GLU:HG2	1.98	0.44
3:W:21:SER:HA	3:W:24:VAL:CB	2.44	0.44
4:X:55:SER:O	4:X:59:LYS:HG2	2.17	0.44
4:X:58:ALA:HB3	4:X:95:LEU:HD12	1.99	0.44
5:Y:307:LEU:HD12	5:Y:319:MET:HE3	1.99	0.44
7:a:363:MET:HE2	7:a:363:MET:C	2.42	0.44
9:d:9:TRP:CZ3	9:d:57:ILE:HA	2.52	0.44
11:A:347:ASP:OD1	11:A:347:ASP:N	2.34	0.44
12:B:68:ILE:HD13	12:B:68:ILE:HA	1.82	0.44
12:B:170:LEU:O	12:B:173:VAL:HG12	2.17	0.44
35:B:501:ATP:O2G	13:C:310:ARG:NH2	2.50	0.44
13:C:135:VAL:HA	13:C:138:MET:SD	2.57	0.44
16:F:334:ARG:NH1	16:F:337:ILE:HD11	2.33	0.44
17:G:10:ASP:OD1	17:G:17:SER:HB2	2.16	0.44
21:K:117:SER:O	21:K:121:LEU:HG	2.18	0.44
21:K:202:LEU:HD23	21:K:202:LEU:HA	1.87	0.44
23:M:77:VAL:HG11	23:M:84:ALA:HB1	2.00	0.44
38:N:301:LDZ:H13	38:N:301:LDZ:H19	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:u:48:GLU:CA	33:u:51:GLN:HE21	2.30	0.44
33:u:456:ARG:NH2	33:u:492:SER:HB3	2.31	0.44
33:u:482:ILE:CD1	33:u:501:LEU:HD23	2.47	0.44
1:U:246:TYR:OH	1:U:794:ASP:HB3	2.18	0.44
1:U:490:ARG:NE	1:U:493:VAL:HG23	2.32	0.44
1:U:524:LYS:NZ	1:U:562:GLU:O	2.48	0.44
1:U:546:ARG:HD2	1:U:580:ARG:NH2	2.32	0.44
1:U:902:PRO:HA	1:U:915:LYS:H	1.81	0.44
2:V:126:ALA:HB2	2:V:130:PHE:HD2	1.82	0.44
2:V:169:LEU:HD12	2:V:169:LEU:HA	1.81	0.44
3:W:16:MET:O	3:W:17:GLU:C	2.59	0.44
3:W:60:MET:HE3	3:W:103:LYS:HG3	1.99	0.44
3:W:104:MET:O	3:W:107:GLN:HB2	2.17	0.44
4:X:407:MET:HA	4:X:407:MET:HE3	1.98	0.44
5:Y:195:LYS:HZ1	5:Y:230:ALA:HA	1.80	0.44
5:Y:237:ARG:C	5:Y:242:LYS:HG2	2.43	0.44
5:Y:293:ARG:HD2	5:Y:293:ARG:HA	1.55	0.44
8:c:218:LEU:CG	8:c:219:ASN:H	2.29	0.44
8:c:251:LEU:HD22	8:c:283:HIS:HB2	1.99	0.44
8:c:282:ARG:HB2	8:c:282:ARG:NH1	2.33	0.44
9:d:168:ASP:HA	9:d:171:LEU:HD12	1.98	0.44
11:A:248:LYS:HE2	11:A:248:LYS:HB3	1.72	0.44
12:B:99:VAL:O	12:B:103:ARG:HG2	2.16	0.44
14:D:102:ILE:HD13	14:D:112:TYR:HA	2.00	0.44
15:E:378:LYS:HD3	15:E:378:LYS:HA	1.71	0.44
16:F:406:ILE:HD13	16:F:422:GLU:HG2	1.98	0.44
25:O:193:ASN:OD1	29:s:213:ASP:HB3	2.17	0.44
33:u:478:ARG:NH1	33:u:510:SER:OG	2.50	0.44
2:V:318:GLN:O	2:V:319:HIS:ND1	2.50	0.44
3:W:268:LYS:HB2	3:W:336:PRO:HG2	2.00	0.44
5:Y:237:ARG:O	5:Y:242:LYS:HG2	2.18	0.44
7:a:191:SER:O	7:a:194:GLN:HG2	2.17	0.44
8:c:212:LEU:HA	8:c:215:LYS:HG3	1.99	0.44
8:c:219:ASN:HB2	8:c:223:LYS:HD3	2.00	0.44
28:R:22:ALA:HB2	38:R:301:LDZ:H39	1.98	0.44
18:h:74:LEU:HD23	18:h:87:VAL:HG22	2.00	0.44
31:j:5:ARG:HG3	31:j:6:ALA:H	1.83	0.44
33:u:80:ARG:HG3	33:u:81:GLN:N	2.31	0.44
33:u:225:ALA:HA	33:u:228:LYS:NZ	2.32	0.44
33:u:666:ILE:O	33:u:670:MET:HG2	2.17	0.44
3:W:37:GLU:O	3:W:39:ARG:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:244:CYS:O	3:W:248:ARG:HG2	2.17	0.44
3:W:435:LEU:HD23	3:W:436:MET:HE3	1.99	0.44
3:W:436:MET:HG3	8:c:229:LEU:HD11	2.00	0.44
4:X:103:THR:HA	4:X:106:GLU:HB2	1.99	0.44
4:X:400:ALA:O	4:X:404:ILE:HG12	2.17	0.44
6:Z:258:VAL:CG1	8:c:291:LEU:HD21	2.48	0.44
8:c:172:HIS:CG	8:c:173:GLU:H	2.35	0.44
8:c:196:LEU:HD12	8:c:196:LEU:HA	1.87	0.44
11:A:262:GLU:O	11:A:266:THR:HG22	2.17	0.44
12:B:124:SER:HA	12:B:130:GLU:HA	1.98	0.44
12:B:371:ARG:HE	12:B:371:ARG:HB3	1.70	0.44
13:C:60:ARG:HB2	13:C:60:ARG:NH1	2.33	0.44
14:D:156:SER:O	14:D:157:ASP:HB3	2.18	0.44
14:D:390:ASN:O	14:D:390:ASN:OD1	2.35	0.44
18:h:6:TYR:HB2	18:h:8:PHE:CE2	2.52	0.44
33:u:50:LYS:HD2	33:u:50:LYS:HA	1.76	0.44
2:V:32:PRO:HB2	2:V:85:ALA:HB1	2.00	0.44
2:V:292:THR:O	2:V:295:ILE:HG13	2.18	0.44
2:V:326:GLN:OE1	2:V:326:GLN:N	2.50	0.44
3:W:106:GLN:O	3:W:110:THR:HG22	2.17	0.44
3:W:325:GLY:HA2	3:W:329:ARG:NH1	2.32	0.44
5:Y:208:PHE:CD2	5:Y:210:SER:HB2	2.52	0.44
6:Z:48:LEU:HD21	6:Z:92:VAL:HB	2.00	0.44
6:Z:223:ASN:HB3	6:Z:227:ILE:HG13	1.99	0.44
6:Z:228:TYR:O	6:Z:231:GLN:HG3	2.17	0.44
11:A:84:LYS:HA	11:A:87:LEU:HD21	1.99	0.44
14:D:236:VAL:HG21	15:E:255:ARG:CZ	2.48	0.44
15:E:144:GLU:O	15:E:148:VAL:HG23	2.17	0.44
17:G:120:ASP:OD1	18:H:84:ARG:NH1	2.51	0.44
20:J:236:LYS:HA	20:J:236:LYS:HD2	1.90	0.44
22:L:4:ASN:OD1	22:L:4:ASN:N	2.50	0.44
25:O:110:LEU:HD21	25:O:125:VAL:HG22	1.99	0.44
1:U:790:GLY:HA3	1:U:880:ASN:HD22	1.83	0.44
2:V:306:ARG:HH22	2:V:307:ARG:HB2	1.82	0.44
3:W:10:ASP:OD1	3:W:10:ASP:N	2.48	0.44
6:Z:43:TRP:CH2	6:Z:48:LEU:HD22	2.51	0.44
18:H:75:VAL:HG13	18:H:135:LEU:HB2	1.99	0.44
20:J:107:ILE:HD12	20:J:107:ILE:HA	1.86	0.44
20:J:183:THR:O	20:J:185:ASP:N	2.51	0.44
18:h:4:ARG:O	31:j:3:TYR:OH	2.29	0.44
23:m:41:CYS:HB3	23:m:189:ILE:HD11	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:u:47:GLU:O	33:u:51:GLN:HG3	2.18	0.44
33:u:196:MET:HE2	33:u:196:MET:HA	1.99	0.44
1:U:258:GLN:C	1:U:260:PHE:H	2.26	0.44
1:U:333:MET:SD	1:U:333:MET:N	2.87	0.44
1:U:550:VAL:HG22	1:U:768:GLN:HE21	1.83	0.44
1:U:570:LEU:HD12	1:U:578:LEU:O	2.17	0.44
3:W:272:LEU:HD21	3:W:337:ALA:HA	1.99	0.44
4:X:115:GLU:O	4:X:118:LYS:HG2	2.18	0.44
7:a:113:LEU:O	7:a:154:ARG:NH1	2.51	0.44
9:d:109:GLN:HB2	9:d:111:ARG:CZ	2.48	0.44
18:H:111:VAL:HG22	18:H:136:ILE:HD12	1.99	0.44
22:L:47:VAL:HG12	22:L:195:LEU:HD22	2.00	0.44
21:k:224:GLN:HE22	21:k:226:PHE:HB3	1.82	0.44
22:l:104:PRO:HB2	22:l:107:ARG:HG2	1.98	0.44
24:n:115:PRO:HD2	24:n:119:MET:O	2.18	0.44
28:r:62:GLN:O	28:r:65:ILE:HG22	2.18	0.44
32:f:382:GLN:O	32:f:386:ARG:HG2	2.18	0.44
33:u:54:ASP:O	33:u:58:MET:HG2	2.18	0.44
1:U:104:CYS:HA	1:U:107:HIS:HB3	2.00	0.44
1:U:483:LEU:HD11	1:U:781:LEU:HD11	2.00	0.44
3:W:46:THR:OG1	3:W:47:LEU:N	2.50	0.44
5:Y:135:GLY:O	5:Y:138:LEU:HG	2.17	0.44
5:Y:279:GLU:HG3	5:Y:296:VAL:HG21	2.00	0.44
7:a:157:ASP:O	7:a:161:LYS:HG2	2.18	0.44
7:a:303:THR:O	7:a:307:VAL:HG13	2.18	0.44
11:A:71:GLY:HA2	12:B:162:VAL:H	1.83	0.44
11:A:120:LYS:C	11:A:121:PHE:HD1	2.25	0.44
12:B:36:LYS:HE2	12:B:36:LYS:HB3	1.85	0.44
16:F:155:LYS:O	16:F:158:TYR:HE1	2.01	0.44
17:g:126:THR:HG22	18:h:128:ARG:HH21	1.82	0.44
17:g:200:THR:O	17:g:204:THR:HG23	2.17	0.44
33:u:886:GLU:OE1	33:u:886:GLU:N	2.50	0.44
1:U:107:HIS:O	1:U:111:GLN:HG2	2.18	0.43
1:U:360:VAL:C	1:U:361:ARG:HD2	2.42	0.43
1:U:794:ASP:OD1	1:U:794:ASP:N	2.51	0.43
2:V:238:ALA:HB1	2:V:243:ASP:HB3	2.00	0.43
3:W:312:MET:SD	3:W:315:MET:N	2.86	0.43
4:X:161:ASP:C	4:X:161:ASP:OD1	2.60	0.43
5:Y:221:THR:HG22	5:Y:225:TYR:CE2	2.53	0.43
6:Z:235:ASN:ND2	7:a:349:MET:SD	2.90	0.43
14:D:72:PHE:CE1	14:D:76:GLN:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:D:75:ALA:O	14:D:79:VAL:HG23	2.18	0.43
14:D:258:ALA:CB	14:D:259:PRO:HD3	2.48	0.43
15:E:238:ILE:HA	15:E:241:ARG:NE	2.33	0.43
15:E:344:ARG:HH12	37:E:401:ADP:C4'	2.31	0.43
16:F:297:ASP:C	16:F:299:GLU:H	2.26	0.43
17:G:73:THR:HG22	17:G:74:GLU:N	2.33	0.43
19:I:238:LYS:NZ	19:I:238:LYS:HB3	2.32	0.43
17:g:211:LYS:HB2	17:g:211:LYS:NZ	2.32	0.43
22:l:44:ALA:HB3	22:l:215:VAL:HG13	2.00	0.43
22:l:50:LYS:HB3	22:l:59:HIS:HB3	2.00	0.43
33:u:78:LEU:O	33:u:82:ILE:HG12	2.18	0.43
33:u:665:GLU:OE1	33:u:665:GLU:N	2.40	0.43
2:V:33:GLN:HG3	2:V:85:ALA:HA	2.01	0.43
2:V:89:LYS:HA	2:V:92:ARG:HB2	2.00	0.43
2:V:322:VAL:HG13	2:V:325:LYS:H	1.83	0.43
2:V:489:MET:C	2:V:489:MET:HE2	2.43	0.43
3:W:169:LEU:O	3:W:182:ARG:NH2	2.51	0.43
4:X:422:THR:HB	6:Z:283:ARG:HH12	1.83	0.43
8:c:264:LYS:NZ	8:c:267:PRO:HG3	2.33	0.43
9:d:9:TRP:CE3	9:d:57:ILE:HG13	2.53	0.43
10:e:6:GLN:O	10:e:8:VAL:N	2.51	0.43
11:A:66:LYS:NZ	13:C:80:MET:HA	2.33	0.43
11:A:157:ILE:HD12	11:A:157:ILE:HA	1.86	0.43
14:D:276:ASP:O	14:D:276:ASP:OD1	2.35	0.43
14:D:418:LYS:HD3	18:H:76:TYR:OH	2.18	0.43
16:F:129:ARG:HH12	16:F:261:ILE:HG23	1.83	0.43
16:F:180:ARG:HD3	16:F:180:ARG:HA	1.83	0.43
20:J:108:THR:HG21	20:J:145:TYR:HB2	1.99	0.43
17:g:174:GLU:H	17:g:174:GLU:HG3	1.59	0.43
29:s:145:LEU:HD21	29:s:182:ALA:HB2	1.98	0.43
33:u:840:LEU:HD21	33:u:887:PHE:CE2	2.53	0.43
3:W:131:VAL:HG13	3:W:144:ARG:HB3	2.00	0.43
6:Z:231:GLN:O	6:Z:234:PHE:HB2	2.19	0.43
6:Z:260:VAL:HG12	6:Z:261:TYR:CD1	2.53	0.43
7:a:8:LEU:HA	7:a:11:SER:OG	2.19	0.43
7:a:217:LEU:HD21	7:a:237:LEU:HD22	2.00	0.43
8:c:43:LYS:HD2	8:c:43:LYS:HA	1.80	0.43
8:c:191:ALA:HB1	8:c:196:LEU:HD22	1.98	0.43
11:A:32:LEU:HD12	33:u:97:LYS:HB2	2.00	0.43
11:A:115:VAL:O	11:A:118:PHE:N	2.47	0.43
11:A:127:ASP:C	11:A:127:ASP:OD1	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:256:ILE:HD13	12:B:305:ILE:HD12	2.00	0.43
18:H:59:GLU:OE1	18:H:59:GLU:N	2.49	0.43
25:O:1:THR:N	38:O:301:LDZ:O33	2.51	0.43
27:Q:162:LYS:CG	28:r:141:ARG:HD2	2.48	0.43
19:i:28:ILE:HD13	19:i:28:ILE:HA	1.86	0.43
23:m:46:VAL:HG22	23:m:215:TRP:CD1	2.53	0.43
33:u:62:ARG:HH21	33:u:74:ALA:HB3	1.84	0.43
33:u:244:GLU:O	33:u:248:LEU:HD23	2.18	0.43
33:u:294:MET:HA	33:u:297:MET:SD	2.59	0.43
1:U:78:LEU:HA	1:U:78:LEU:HD23	1.69	0.43
4:X:90:ARG:NE	4:X:128:ALA:HB1	2.34	0.43
5:Y:328:GLU:OE1	5:Y:328:GLU:N	2.43	0.43
6:Z:129:LYS:HD3	6:Z:129:LYS:HA	1.72	0.43
7:a:7:PHE:CE1	7:a:56:LEU:HD13	2.53	0.43
7:a:65:SER:HB3	7:a:76:LEU:HD11	2.00	0.43
12:B:48:LYS:HD2	12:B:48:LYS:HA	1.71	0.43
15:E:40:TYR:HE1	16:F:72:LYS:CG	2.31	0.43
15:E:84:ARG:HG2	15:E:86:GLN:H	1.83	0.43
22:L:225:ASP:OD1	22:L:225:ASP:N	2.50	0.43
27:Q:197:PRO:HA	27:q:199:GLN:H	1.83	0.43
31:j:51:ALA:O	31:j:52:LYS:HB2	2.19	0.43
21:k:121:LEU:HD23	21:k:121:LEU:HA	1.78	0.43
33:u:62:ARG:HH22	33:u:71:TYR:HA	1.83	0.43
1:U:183:LEU:HD12	1:U:187:LEU:HB2	2.01	0.43
1:U:516:LEU:HD12	1:U:520:MET:HE1	1.99	0.43
1:U:546:ARG:HD2	1:U:580:ARG:HH22	1.83	0.43
2:V:313:LEU:O	2:V:317:PRO:HG3	2.19	0.43
3:W:24:VAL:C	3:W:26:GLN:H	2.26	0.43
3:W:39:ARG:HB3	3:W:40:LEU:H	1.59	0.43
3:W:107:GLN:HB3	3:W:123:ARG:HH12	1.82	0.43
3:W:192:LEU:O	3:W:196:VAL:HG13	2.17	0.43
3:W:369:TYR:OH	7:a:312:MET:HB2	2.18	0.43
3:W:369:TYR:CE1	7:a:315:LEU:HD23	2.52	0.43
3:W:403:PHE:HE2	3:W:417:ARG:HA	1.83	0.43
5:Y:13:LYS:HD2	5:Y:146:ARG:HD2	2.00	0.43
5:Y:194:PHE:CE2	5:Y:195:LYS:HE2	2.54	0.43
6:Z:190:ARG:HH11	8:c:297:VAL:HG11	1.84	0.43
9:d:209:TYR:CD1	9:d:215:TRP:CD1	3.07	0.43
9:d:209:TYR:CD1	9:d:215:TRP:HD1	2.36	0.43
9:d:219:PRO:HG2	9:d:223:TYR:CD2	2.53	0.43
11:A:188:ARG:HD2	11:A:192:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:163:LEU:HD11	12:B:165:ASP:OD1	2.17	0.43
13:C:29:GLU:O	13:C:32:GLN:HG2	2.19	0.43
15:E:65:THR:HG22	15:E:68:LYS:HB2	2.01	0.43
19:I:239:LYS:HE3	19:I:239:LYS:HB3	1.69	0.43
24:N:14:LEU:HD23	24:N:44:CYS:SG	2.58	0.43
26:P:161:ASP:O	26:P:165:GLU:HG2	2.18	0.43
17:g:117:ARG:HA	17:g:117:ARG:HD2	1.83	0.43
31:j:202:GLY:HA3	31:j:205:ASN:ND2	2.34	0.43
23:m:65:ARG:NH2	23:m:78:ALA:HA	2.33	0.43
33:u:777:THR:O	33:u:825:MET:HA	2.17	0.43
33:u:840:LEU:HD23	33:u:900:LEU:HD12	2.00	0.43
1:U:392:TRP:HE3	1:U:393:LEU:HD22	1.84	0.43
3:W:37:GLU:OE2	3:W:43:VAL:HG11	2.19	0.43
3:W:105:VAL:HA	3:W:108:CYS:SG	2.58	0.43
3:W:159:VAL:HG13	3:W:160:LYS:HD3	2.00	0.43
3:W:190:MET:HE3	3:W:190:MET:HB3	1.85	0.43
4:X:71:LYS:HA	4:X:74:ARG:HG3	2.01	0.43
5:Y:220:VAL:HG13	5:Y:246:ILE:HG13	2.00	0.43
8:c:121:TRP:HZ3	8:c:190:GLN:HG3	1.82	0.43
12:B:112:LEU:HD12	12:B:145:GLU:O	2.19	0.43
12:B:289:ALA:HB1	13:C:271:ARG:HG3	2.00	0.43
16:F:153:VAL:HG12	16:F:158:TYR:HA	1.99	0.43
21:K:137:PHE:O	21:K:158:PRO:HB3	2.18	0.43
17:g:70:PHE:HB2	17:g:78:CYS:SG	2.58	0.43
23:m:34:SER:OG	23:m:50:GLU:OE1	2.35	0.43
32:f:415:PRO:O	33:u:838:ARG:NH2	2.51	0.43
33:u:293:GLN:O	33:u:297:MET:HG3	2.18	0.43
1:U:58:GLN:HB3	1:U:87:LEU:HD11	2.01	0.43
2:V:354:LYS:HA	2:V:357:LEU:HG	2.01	0.43
3:W:278:PRO:HG3	3:W:357:ARG:HH21	1.83	0.43
4:X:93:LEU:O	4:X:97:LEU:HG	2.18	0.43
5:Y:231:LEU:HB2	5:Y:234:PRO:CG	2.49	0.43
5:Y:308:LEU:HD13	5:Y:314:LEU:HD21	2.00	0.43
8:c:183:HIS:O	8:c:184:LEU:HB3	2.18	0.43
11:A:417:ILE:HD13	11:A:417:ILE:HA	1.87	0.43
12:B:295:TYR:OH	13:C:262:GLY:O	2.26	0.43
15:E:116:ASP:N	15:E:116:ASP:OD1	2.51	0.43
16:F:293:THR:HA	16:F:337:ILE:HG22	2.00	0.43
21:k:39:GLY:C	21:k:40:ILE:HD13	2.44	0.43
22:l:125:ARG:HD2	22:l:126:ARG:N	2.34	0.43
30:t:122:LEU:HG	30:t:137:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:u:100:ARG:HH11	33:u:133:MET:HE1	1.83	0.43
33:u:686:LEU:HD23	33:u:686:LEU:HA	1.86	0.43
33:u:775:THR:HG22	33:u:873:LEU:HD21	2.01	0.43
1:U:18:GLN:NE2	9:d:30:LEU:HD22	2.33	0.43
1:U:92:ASP:CG	1:U:140:ARG:HH21	2.27	0.43
1:U:184:CYS:SG	1:U:197:VAL:HG11	2.59	0.43
1:U:557:TYR:CD1	1:U:588:MET:HG3	2.41	0.43
2:V:463:MET:SD	2:V:464:ILE:N	2.92	0.43
3:W:81:ASP:O	3:W:85:GLU:HG3	2.18	0.43
3:W:265:GLN:OE1	3:W:333:LEU:HD12	2.18	0.43
5:Y:14:ASN:HB2	5:Y:15:PRO:HD3	2.01	0.43
5:Y:174:TRP:HA	5:Y:176:ARG:HD2	2.01	0.43
6:Z:180:LYS:HE2	14:D:70:LYS:HG2	2.00	0.43
8:c:54:MET:N	8:c:54:MET:SD	2.92	0.43
11:A:36:TYR:CE2	33:u:157:GLU:HG3	2.54	0.43
11:A:400:ARG:NE	11:A:400:ARG:HA	2.34	0.43
31:j:158:ALA:HB1	31:j:172:LEU:HD23	1.99	0.43
21:k:39:GLY:O	21:k:40:ILE:HD13	2.18	0.43
25:o:37:ILE:HD11	25:o:56:THR:HG23	2.00	0.43
29:s:81:LYS:HB3	29:s:81:LYS:HE3	1.80	0.43
33:u:738:ASN:C	33:u:738:ASN:OD1	2.61	0.43
1:U:80:TYR:N	1:U:80:TYR:CD1	2.86	0.43
2:V:353:LEU:HG	2:V:357:LEU:HD23	2.01	0.43
3:W:12:ARG:O	3:W:16:MET:N	2.34	0.43
3:W:12:ARG:HD3	3:W:15:LYS:HD2	2.01	0.43
3:W:62:SER:O	3:W:65:ARG:HG2	2.19	0.43
4:X:299:LEU:HD21	4:X:327:TYR:OH	2.18	0.43
5:Y:202:LEU:HD12	5:Y:203:ASP:N	2.34	0.43
5:Y:272:PHE:CE2	5:Y:323:PHE:CE1	3.07	0.43
7:a:117:ALA:O	7:a:121:LEU:HG	2.19	0.43
9:d:59:ALA:HB3	9:d:60:GLN:NE2	2.34	0.43
9:d:150:LYS:O	9:d:153:LEU:HD12	2.19	0.43
12:B:135:ILE:HG22	12:B:159:VAL:HB	1.99	0.43
14:D:89:ILE:O	14:D:106:THR:OG1	2.25	0.43
14:D:338:ARG:HH21	14:D:342:ARG:HH12	1.66	0.43
15:E:159:PHE:HD2	15:E:166:PRO:HB3	1.83	0.43
16:F:163:THR:C	16:F:164:LEU:HD12	2.43	0.43
16:F:272:PHE:O	16:F:276:LYS:HG2	2.19	0.43
19:I:174:MET:HE2	19:I:174:MET:HB2	1.82	0.43
19:I:181:GLU:OE1	19:I:182:GLY:N	2.52	0.43
23:M:215:TRP:CZ2	23:M:219:LEU:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:O:40:ASN:N	25:O:40:ASN:OD1	2.52	0.43
28:R:91:LYS:NZ	28:R:117:GLU:O	2.51	0.43
30:T:154:LEU:HD23	30:T:154:LEU:HA	1.89	0.43
21:k:29:GLU:HA	21:k:32:LYS:NZ	2.34	0.43
33:u:140:LEU:HD23	33:u:169:GLU:HG3	2.00	0.43
33:u:400:TYR:HD1	33:u:407:MET:HE1	1.83	0.43
1:U:110:LYS:HA	1:U:113:VAL:HG12	2.00	0.43
1:U:202:VAL:O	1:U:206:MET:HG2	2.19	0.43
2:V:470:ARG:O	2:V:470:ARG:HG3	2.19	0.43
3:W:107:GLN:HA	3:W:111:TYR:CD1	2.54	0.43
4:X:92:LEU:HA	4:X:95:LEU:CD2	2.49	0.43
5:Y:357:ASN:N	5:Y:357:ASN:OD1	2.51	0.43
6:Z:59:ASP:HB3	6:Z:69:PHE:CZ	2.54	0.43
8:c:238:CYS:O	8:c:242:GLU:HG2	2.19	0.43
9:d:108:SER:O	9:d:173:THR:HG21	2.18	0.43
11:A:417:ILE:O	11:A:421:ALA:HB3	2.18	0.43
12:B:72:LEU:HD23	12:B:72:LEU:HA	1.83	0.43
12:B:78:PHE:CD2	33:u:613:LEU:HG	2.54	0.43
15:E:83:CYS:SG	15:E:87:LEU:HD12	2.59	0.43
21:K:99:HIS:CG	21:K:107:MET:HG3	2.54	0.43
38:R:301:LDZ:H16	38:R:301:LDZ:H23	1.70	0.43
29:S:176:LYS:O	29:S:180:ILE:HG12	2.19	0.43
30:T:136:SER:OG	30:T:147:GLN:NE2	2.51	0.43
17:g:171:LYS:HE3	17:g:171:LYS:HB3	1.81	0.43
18:h:231:ALA:O	18:h:232:ALA:C	2.62	0.43
23:m:108:LEU:HD22	23:m:139:SER:HB3	2.00	0.43
24:n:14:LEU:HD23	24:n:44:CYS:SG	2.59	0.43
30:t:180:ASP:HB3	30:t:183:SER:HB2	2.01	0.43
32:f:385:ASN:HD21	33:u:434:TYR:HB3	1.84	0.43
33:u:65:GLU:OE2	33:u:65:GLU:HA	2.19	0.43
33:u:73:PRO:O	33:u:77:GLU:HG3	2.19	0.43
33:u:104:GLY:O	33:u:108:GLU:HG2	2.18	0.43
33:u:394:ASP:HB3	33:u:397:LYS:HG2	1.99	0.43
3:W:15:LYS:NZ	3:W:15:LYS:HB3	2.34	0.42
3:W:228:ASN:HA	3:W:246:HIS:HE1	1.83	0.42
3:W:265:GLN:OE1	3:W:336:PRO:HD3	2.19	0.42
7:a:21:VAL:HG23	7:a:22:TRP:CD1	2.54	0.42
7:a:196:ARG:HH22	7:a:197:ALA:HB2	1.84	0.42
8:c:244:VAL:O	8:c:248:MET:HG3	2.19	0.42
9:d:38:THR:HB	9:d:86:LYS:HD3	2.01	0.42
9:d:53:ASP:O	9:d:57:ILE:HD13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:d:209:TYR:HA	9:d:212:LYS:HB3	2.01	0.42
12:B:79:ILE:HD11	33:u:677:HIS:CD2	2.54	0.42
13:C:380:GLN:O	13:C:384:GLU:HG2	2.18	0.42
15:E:325:GLU:CG	15:E:326:ILE:H	2.32	0.42
22:L:44:ALA:HB3	22:L:215:VAL:HG12	2.01	0.42
27:Q:162:LYS:HG3	28:r:141:ARG:HD2	2.01	0.42
29:S:211:ARG:HD3	29:S:213:ASP:OD1	2.18	0.42
17:g:191:PHE:CE1	17:g:219:VAL:HG21	2.54	0.42
18:h:29:VAL:HG11	18:h:133:SER:HB3	2.00	0.42
33:u:479:LEU:HD11	33:u:513:GLU:HG2	2.01	0.42
33:u:825:MET:SD	33:u:825:MET:N	2.91	0.42
1:U:644:TYR:O	13:C:57:ARG:NH1	2.52	0.42
3:W:12:ARG:NH1	3:W:15:LYS:HD2	2.34	0.42
3:W:31:CYS:HA	3:W:34:LEU:HD21	2.01	0.42
4:X:134:VAL:HB	4:X:149:LEU:CD2	2.49	0.42
5:Y:364:TRP:O	5:Y:368:GLU:HG3	2.19	0.42
6:Z:63:LYS:HA	6:Z:63:LYS:HD3	1.75	0.42
6:Z:79:TYR:CE1	6:Z:91:ILE:HG13	2.53	0.42
7:a:163:TYR:N	7:a:163:TYR:CD1	2.85	0.42
7:a:217:LEU:HD23	7:a:217:LEU:HA	1.87	0.42
8:c:154:LYS:HE3	13:C:67:GLN:HE21	1.85	0.42
9:d:213:ARG:HB2	9:d:215:TRP:CD1	2.54	0.42
12:B:383:LEU:HD23	12:B:383:LEU:HA	1.77	0.42
14:D:381:GLU:OE1	14:D:402:ALA:HA	2.20	0.42
27:Q:162:LYS:HB2	27:Q:162:LYS:HE3	1.62	0.42
29:S:184:GLU:HG3	25:o:195:LYS:HD2	2.02	0.42
18:h:70:LYS:NZ	18:h:70:LYS:HB2	2.34	0.42
30:t:2:GLN:C	30:t:3:ASN:HD22	2.27	0.42
30:t:71:VAL:O	30:t:75:GLU:HG3	2.19	0.42
1:U:152:GLY:O	1:U:156:GLU:HG3	2.19	0.42
1:U:247:GLN:HE21	1:U:904:LYS:HB2	1.83	0.42
1:U:569:SER:HA	1:U:572:ARG:CZ	2.48	0.42
1:U:600:ARG:CZ	14:D:59:GLU:OE2	2.68	0.42
2:V:25:GLU:HB2	2:V:26:PRO:HD3	2.01	0.42
2:V:95:LEU:HA	2:V:95:LEU:HD23	1.81	0.42
2:V:209:LYS:HA	2:V:212:TYR:CD2	2.55	0.42
3:W:13:ILE:HD11	3:W:61:VAL:HG11	2.00	0.42
5:Y:247:LEU:HA	5:Y:250:LEU:HG	2.01	0.42
6:Z:100:LYS:HA	6:Z:100:LYS:HE3	2.01	0.42
7:a:168:ASN:OD1	7:a:168:ASN:N	2.52	0.42
7:a:247:ARG:O	7:a:251:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:d:106:LEU:HA	9:d:111:ARG:NH2	2.24	0.42
9:d:114:GLU:OE1	9:d:114:GLU:N	2.33	0.42
11:A:87:LEU:HB2	11:A:91:GLN:NE2	2.26	0.42
11:A:138:MET:C	11:A:138:MET:HE2	2.44	0.42
11:A:156:LYS:HD3	11:A:157:ILE:N	2.34	0.42
14:D:351:LYS:NZ	15:E:163:GLY:O	2.52	0.42
16:F:320:PHE:C	16:F:320:PHE:CD1	2.97	0.42
30:T:84:SER:O	30:T:88:ILE:HG12	2.19	0.42
33:u:368:ALA:HB2	33:u:403:LYS:HG2	2.01	0.42
33:u:456:ARG:HA	33:u:456:ARG:HD3	1.67	0.42
33:u:467:SER:HB2	33:u:500:LEU:HD11	2.02	0.42
1:U:158:ARG:O	1:U:160:LEU:N	2.52	0.42
3:W:8:ARG:HB3	3:W:27:ARG:HD2	2.01	0.42
3:W:59:ASP:O	3:W:63:THR:OG1	2.29	0.42
4:X:122:ARG:HE	4:X:124:PHE:HB2	1.83	0.42
4:X:138:PHE:CE2	4:X:175:LYS:HE3	2.52	0.42
5:Y:192:ARG:HH22	5:Y:195:LYS:HB2	1.85	0.42
6:Z:40:LEU:HD13	6:Z:90:ARG:C	2.45	0.42
7:a:365:MET:C	7:a:365:MET:HE2	2.45	0.42
11:A:22:ILE:HD12	11:A:22:ILE:O	2.19	0.42
12:B:397:ALA:HB1	12:B:426:VAL:HG21	2.02	0.42
15:E:40:TYR:HE1	16:F:72:LYS:HG3	1.84	0.42
15:E:230:ILE:HD13	15:E:230:ILE:HA	1.82	0.42
22:L:234:GLU:OE2	22:L:234:GLU:HA	2.19	0.42
23:M:240:LYS:HE2	23:M:240:LYS:HB2	1.86	0.42
24:n:179:ILE:HG12	24:n:184:VAL:HG22	2.00	0.42
1:U:54:PHE:CE2	1:U:56:SER:HB2	2.55	0.42
3:W:228:ASN:HA	3:W:246:HIS:CE1	2.55	0.42
4:X:82:LYS:HD3	4:X:122:ARG:HD3	2.02	0.42
5:Y:100:ILE:O	5:Y:104:MET:SD	2.78	0.42
6:Z:84:LYS:HD3	6:Z:85:VAL:HG23	2.02	0.42
8:c:259:VAL:HA	8:c:262:GLU:OE2	2.20	0.42
11:A:323:ARG:NH1	12:B:294:ARG:O	2.46	0.42
13:C:297:ARG:NH2	14:D:274:ARG:HD2	2.34	0.42
16:F:168:TYR:CZ	16:F:270:ASP:HB2	2.54	0.42
23:M:47:PHE:HB2	23:M:214:SER:HB2	2.02	0.42
23:M:75:MET:HB2	23:M:137:LEU:HD23	2.02	0.42
26:P:154:TRP:CH2	26:P:156:PRO:HA	2.54	0.42
33:u:382:ASN:HA	33:u:773:LYS:NZ	2.34	0.42
33:u:499:THR:HA	33:u:502:LEU:HD12	2.02	0.42
1:U:147:TYR:CE2	1:U:169:GLU:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:798:PRO:O	1:U:800:VAL:N	2.52	0.42
2:V:264:TYR:HE1	9:d:118:GLU:HA	1.84	0.42
3:W:45:GLU:OE1	3:W:94:ARG:HD2	2.19	0.42
3:W:366:MET:HG3	3:W:370:TYR:CD2	2.55	0.42
4:X:96:PHE:HZ	4:X:106:GLU:HA	1.84	0.42
5:Y:217:LYS:HG3	5:Y:253:LEU:HD11	2.01	0.42
8:c:219:ASN:HB2	8:c:223:LYS:CB	2.49	0.42
9:d:199:PHE:HB3	9:d:200:PHE:H	1.56	0.42
11:A:234:ASP:C	11:A:234:ASP:OD1	2.63	0.42
12:B:383:LEU:HD21	12:B:423:LYS:HD2	2.01	0.42
12:B:429:LYS:HD3	12:B:429:LYS:N	2.30	0.42
13:C:189:TYR:HA	13:C:295:THR:O	2.19	0.42
17:g:22:LEU:O	17:g:26:GLU:HG3	2.20	0.42
21:k:239:LYS:NZ	21:k:240:ASP:OD1	2.47	0.42
24:n:165:GLU:OE2	24:n:165:GLU:HA	2.20	0.42
38:o:301:LDZ:H10	38:o:301:LDZ:H34	1.52	0.42
28:r:44:THR:HG21	28:r:100:MET:HE3	2.00	0.42
33:u:659:LEU:O	33:u:662:MET:HE3	2.18	0.42
3:W:316:ARG:NH1	3:W:380:GLN:O	2.53	0.42
6:Z:194:GLN:HE22	8:c:300:LEU:HG	1.84	0.42
8:c:167:MET:HE3	8:c:172:HIS:HB2	2.02	0.42
14:D:170:MET:O	14:D:172:ILE:N	2.52	0.42
15:E:155:ASN:OD1	15:E:158:LEU:HD12	2.19	0.42
16:F:283:ILE:HG23	16:F:328:VAL:HG12	2.01	0.42
22:L:53:GLN:CD	22:L:53:GLN:N	2.77	0.42
22:L:71:GLY:HA3	22:L:221:PHE:CZ	2.55	0.42
23:M:66:LEU:HD13	23:M:214:SER:OG	2.20	0.42
30:T:25:ASP:HA	30:T:187:PHE:HA	2.00	0.42
22:l:49:LEU:HB2	22:l:195:LEU:HD21	2.01	0.42
23:m:33:SER:OG	23:m:34:SER:N	2.53	0.42
33:u:113:MET:SD	33:u:119:LYS:HE2	2.60	0.42
33:u:117:GLU:H	33:u:117:GLU:CD	2.20	0.42
33:u:367:SER:N	33:u:370:MET:SD	2.74	0.42
1:U:108:TYR:HA	1:U:111:GLN:HG2	2.01	0.42
1:U:216:VAL:O	1:U:220:LEU:HB2	2.20	0.42
1:U:236:LEU:HD13	1:U:236:LEU:HA	1.91	0.42
2:V:36:GLU:CD	2:V:76:LYS:HG2	2.45	0.42
4:X:82:LYS:HG2	4:X:122:ARG:NH1	2.33	0.42
4:X:182:ASN:ND2	4:X:185:LYS:HG3	2.35	0.42
4:X:369:ILE:HD12	4:X:376:GLY:O	2.19	0.42
6:Z:170:VAL:HG11	8:c:151:VAL:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:175:LEU:HD23	6:Z:175:LEU:HA	1.84	0.42
7:a:326:GLU:N	7:a:326:GLU:OE1	2.53	0.42
8:c:50:PRO:HB2	8:c:51:MET:SD	2.60	0.42
9:d:196:ARG:C	9:d:196:ARG:HE	2.27	0.42
11:A:115:VAL:O	11:A:115:VAL:HG12	2.19	0.42
11:A:304:ASN:HD22	16:F:254:PRO:HG2	1.85	0.42
12:B:107:MET:SD	12:B:151:LEU:HD13	2.60	0.42
14:D:204:MET:HE3	14:D:212:LYS:HB3	2.01	0.42
14:D:338:ARG:C	14:D:340:GLN:H	2.28	0.42
18:H:39:LYS:HE2	18:H:39:LYS:HB3	1.88	0.42
23:M:8:ASP:HB2	23:M:25:TYR:HE2	1.84	0.42
17:g:79:VAL:HG12	17:g:139:ILE:HB	2.01	0.42
21:k:142:LEU:HD23	21:k:142:LEU:HA	1.85	0.42
27:q:41:LYS:O	27:q:106:GLY:HA2	2.20	0.42
1:U:462:LEU:HD11	1:U:490:ARG:NH2	2.35	0.42
1:U:925:VAL:HG22	1:U:927:PRO:HD3	2.00	0.42
2:V:410:ILE:HD11	2:V:417:ILE:HG12	2.00	0.42
3:W:152:ILE:CG1	3:W:161:GLU:HB3	2.37	0.42
6:Z:177:ARG:HA	6:Z:177:ARG:CZ	2.50	0.42
6:Z:262:LEU:O	6:Z:266:ILE:HD13	2.20	0.42
7:a:230:ARG:HA	7:a:232:TRP:CD1	2.55	0.42
9:d:105:PHE:O	9:d:109:GLN:HG2	2.20	0.42
9:d:188:LYS:HB3	9:d:220:ASN:CG	2.44	0.42
9:d:205:LYS:HB3	9:d:206:MET:HE2	2.02	0.42
13:C:280:LEU:HD11	13:C:291:VAL:HG21	2.00	0.42
14:D:151:ILE:HD12	14:D:151:ILE:H	1.84	0.42
15:E:69:PHE:CE2	15:E:92:LEU:HD13	2.55	0.42
22:L:123:TYR:CD1	22:L:123:TYR:C	2.98	0.42
27:Q:140:LEU:HD13	28:r:166:ARG:NH2	2.35	0.42
21:k:65:GLU:OE1	21:k:65:GLU:HA	2.20	0.42
30:t:187:PHE:HE1	30:t:205:THR:HG23	1.85	0.42
33:u:60:VAL:O	33:u:105:LYS:NZ	2.52	0.42
33:u:585:GLU:N	33:u:586:PRO:HD2	2.35	0.42
1:U:145:HIS:O	1:U:145:HIS:CG	2.71	0.42
1:U:188:MET:CE	1:U:190:ASN:H	2.32	0.42
1:U:497:LEU:CB	1:U:516:LEU:HD13	2.50	0.42
1:U:559:ARG:HB3	1:U:562:GLU:HG3	2.01	0.42
2:V:136:GLU:HA	2:V:139:MET:HE1	2.02	0.42
2:V:266:GLN:CD	2:V:298:ILE:HG21	2.45	0.42
2:V:291:TYR:O	2:V:295:ILE:HG23	2.20	0.42
2:V:497:PRO:HD2	13:C:43:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:144:ARG:HA	3:W:147:LYS:HG2	2.01	0.42
3:W:439:VAL:HA	6:Z:234:PHE:HZ	1.83	0.42
4:X:127:GLN:HE21	4:X:156:GLU:CD	2.26	0.42
5:Y:293:ARG:NH1	10:e:57:ARG:HB3	2.29	0.42
6:Z:110:GLU:CD	6:Z:153:LYS:HE3	2.45	0.42
6:Z:114:ARG:HG3	6:Z:115:TYR:HD1	1.85	0.42
6:Z:206:LEU:HD12	6:Z:207:ASP:N	2.35	0.42
8:c:119:GLY:O	8:c:146:ASP:HB2	2.20	0.42
9:d:188:LYS:H	9:d:220:ASN:CB	2.32	0.42
11:A:80:LEU:O	11:A:85:GLN:NE2	2.53	0.42
12:B:440:LEU:HD11	20:J:59:VAL:HG13	2.02	0.42
13:C:233:GLU:HG2	13:C:233:GLU:H	1.73	0.42
13:C:296:ASN:HD21	14:D:274:ARG:HH22	1.68	0.42
14:D:98:GLN:CA	14:D:121:ARG:NH2	2.83	0.42
14:D:246:MET:HE2	14:D:246:MET:HB2	1.96	0.42
14:D:297:ASP:HB3	14:D:326:ARG:HH21	1.85	0.42
15:E:312:ILE:HB	15:E:343:LEU:HD22	2.01	0.42
16:F:86:LEU:N	16:F:87:PRO:HD2	2.34	0.42
29:S:213:ASP:HB3	25:o:193:ASN:OD1	2.20	0.42
17:g:224:ASN:HD21	17:g:226:LYS:HB2	1.85	0.42
23:m:49:VAL:HG11	23:m:65:ARG:HB2	2.01	0.42
33:u:250:ARG:HD2	33:u:272:LEU:HD11	2.02	0.42
33:u:829:MET:SD	33:u:831:VAL:HG23	2.60	0.42
1:U:341:PHE:CD1	1:U:881:PRO:HB2	2.55	0.41
1:U:550:VAL:O	1:U:554:LEU:HG	2.20	0.41
1:U:761:VAL:O	1:U:765:VAL:HG23	2.20	0.41
3:W:268:LYS:HE2	3:W:268:LYS:HB3	1.94	0.41
6:Z:7:GLN:HB3	6:Z:46:LYS:HG3	2.02	0.41
7:a:294:GLU:H	7:a:294:GLU:CD	2.23	0.41
7:a:363:MET:SD	7:a:364:GLU:N	2.93	0.41
11:A:50:ASP:OD1	11:A:50:ASP:C	2.62	0.41
11:A:142:VAL:HG12	11:A:149:ILE:HG12	2.02	0.41
12:B:81:ASN:OD1	12:B:81:ASN:C	2.62	0.41
14:D:98:GLN:HA	14:D:121:ARG:NH2	2.35	0.41
15:E:125:GLU:OE1	15:E:125:GLU:N	2.52	0.41
16:F:98:ASP:HA	16:F:120:LYS:N	2.35	0.41
16:F:178:ASP:OD1	16:F:178:ASP:N	2.33	0.41
17:G:36:GLY:O	17:G:37:LEU:HD23	2.20	0.41
25:O:198:ARG:HG3	29:s:177:ASP:OD1	2.20	0.41
19:i:14:PRO:HA	31:j:21:TYR:CE2	2.55	0.41
19:i:186:LEU:HD12	19:i:186:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:k:29:GLU:HA	21:k:32:LYS:CE	2.50	0.41
33:u:341:GLU:CD	33:u:343:LYS:HZ1	2.27	0.41
33:u:342:PRO:HD3	33:u:387:GLN:CD	2.44	0.41
1:U:810:THR:HG22	1:U:811:PHE:H	1.84	0.41
1:U:834:SER:OG	12:B:70:ASP:OD1	2.27	0.41
1:U:877:LEU:HD12	1:U:877:LEU:HA	1.78	0.41
2:V:374:LYS:HA	2:V:377:GLN:HG2	2.02	0.41
3:W:26:GLN:O	3:W:29:PRO:HD2	2.19	0.41
3:W:182:ARG:HA	3:W:182:ARG:HD2	1.71	0.41
3:W:250:ILE:O	3:W:253:THR:OG1	2.33	0.41
4:X:234:GLU:OE1	14:D:339:ARG:HB3	2.20	0.41
5:Y:55:GLU:O	5:Y:59:LYS:HG2	2.20	0.41
5:Y:236:LEU:O	5:Y:240:VAL:HG12	2.20	0.41
6:Z:130:ASP:C	6:Z:130:ASP:OD1	2.63	0.41
6:Z:144:VAL:HG23	6:Z:146:ASP:O	2.21	0.41
7:a:42:LEU:HD11	7:a:78:GLU:HG3	2.02	0.41
7:a:189:PRO:HD2	7:a:189:PRO:O	2.20	0.41
11:A:44:GLN:O	11:A:48:VAL:HG23	2.20	0.41
11:A:240:VAL:HG11	11:A:274:PHE:CD2	2.56	0.41
14:D:208:PRO:HD3	14:D:312:ASN:HD21	1.85	0.41
14:D:293:LEU:HD22	14:D:326:ARG:HD3	2.01	0.41
16:F:291:ILE:HG22	16:F:306:VAL:HG13	2.02	0.41
30:T:50:MET:CE	30:T:192:VAL:HG23	2.44	0.41
18:h:181:ASP:OD1	18:h:181:ASP:N	2.48	0.41
31:j:105:GLU:OE2	31:j:109:ARG:NH1	2.53	0.41
1:U:28:ASN:OD1	1:U:66:LYS:NZ	2.37	0.41
1:U:439:GLU:OE2	1:U:473:VAL:HG13	2.20	0.41
1:U:792:ASN:O	1:U:793:LYS:HD3	2.21	0.41
1:U:917:THR:HB	1:U:918:SER:H	1.75	0.41
2:V:431:PRO:O	2:V:435:GLU:HG3	2.20	0.41
3:W:144:ARG:O	3:W:148:THR:HG23	2.20	0.41
3:W:405:LYS:HD2	3:W:405:LYS:HA	1.75	0.41
5:Y:23:ARG:NH2	5:Y:27:SER:HB3	2.35	0.41
5:Y:220:VAL:HG11	5:Y:249:VAL:HG23	2.01	0.41
6:Z:94:TRP:CZ3	6:Z:96:HIS:HB3	2.55	0.41
7:a:154:ARG:HG3	7:a:155:PHE:N	2.35	0.41
7:a:372:HIS:ND1	7:a:372:HIS:C	2.79	0.41
8:c:94:LYS:HG3	8:c:95:MET:SD	2.60	0.41
9:d:61:TRP:CD1	9:d:61:TRP:N	2.88	0.41
13:C:141:GLU:OE1	13:C:141:GLU:N	2.48	0.41
16:F:212:PHE:CD1	16:F:215:LEU:HD22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:F:231:THR:HG21	16:F:354:PHE:HB3	2.01	0.41
28:R:52:CYS:SG	28:R:97:MET:HG3	2.59	0.41
17:g:185:LYS:HB3	17:g:185:LYS:HE3	1.85	0.41
19:i:229:LYS:O	19:i:233:VAL:HG23	2.20	0.41
25:o:19:ARG:HB3	25:o:169:SER:HA	2.01	0.41
25:o:113:ILE:HG23	25:o:119:THR:HG22	2.03	0.41
29:s:190:GLY:O	29:s:191:ASP:HB2	2.20	0.41
33:u:409:SER:O	33:u:819:TYR:OH	2.35	0.41
33:u:755:ASP:HB3	33:u:758:ASN:HB2	2.02	0.41
1:U:510:GLU:HG2	1:U:511:ALA:N	2.36	0.41
1:U:645:ASN:OD1	1:U:645:ASN:C	2.63	0.41
2:V:158:PRO:O	2:V:161:PRO:HG2	2.20	0.41
2:V:495:ARG:HB2	6:Z:278:ASN:ND2	2.32	0.41
3:W:12:ARG:NH1	3:W:24:VAL:HA	2.35	0.41
3:W:128:LEU:HD23	3:W:128:LEU:HA	1.79	0.41
4:X:336:ILE:HD13	4:X:336:ILE:HA	1.97	0.41
5:Y:199:GLU:O	5:Y:202:LEU:HG	2.19	0.41
7:a:8:LEU:HD11	7:a:26:GLU:CB	2.50	0.41
15:E:102:MET:HG3	15:E:103:THR:N	2.34	0.41
15:E:236:ASP:HB3	15:E:278:ALA:O	2.20	0.41
16:F:94:ILE:HG22	16:F:95:GLU:OE1	2.21	0.41
16:F:282:ILE:HD11	16:F:329:ILE:HD12	2.02	0.41
16:F:300:LYS:HD2	16:F:300:LYS:HA	1.79	0.41
26:P:13:ALA:HB3	26:P:137:VAL:HG23	2.02	0.41
22:l:64:LEU:HD11	22:l:74:ILE:HD13	2.02	0.41
33:u:472:HIS:CD2	33:u:474:SER:H	2.38	0.41
33:u:472:HIS:HD2	33:u:474:SER:HB3	1.85	0.41
1:U:22:PHE:CB	9:d:30:LEU:HD11	2.51	0.41
1:U:59:PHE:O	1:U:63:VAL:HG13	2.20	0.41
1:U:122:GLU:HG3	1:U:123:LYS:H	1.86	0.41
1:U:201:LEU:HD23	1:U:204:ILE:HD12	2.02	0.41
1:U:349:ASP:H	1:U:376:MET:HE2	1.85	0.41
1:U:691:SER:HA	1:U:694:ILE:HG22	2.03	0.41
3:W:17:GLU:HG2	3:W:18:VAL:HG23	2.03	0.41
5:Y:85:ASP:HA	5:Y:88:LEU:HG	2.03	0.41
5:Y:367:GLN:O	5:Y:370:ILE:HG22	2.20	0.41
6:Z:96:HIS:HE2	6:Z:123:ILE:HG12	1.85	0.41
6:Z:209:ARG:NH2	7:a:354:GLU:HG2	2.34	0.41
9:d:131:VAL:HG22	9:d:159:PRO:HB3	2.01	0.41
11:A:122:VAL:O	16:F:87:PRO:HA	2.20	0.41
13:C:38:LYS:NZ	14:D:58:GLU:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:D:327:LEU:HD23	14:D:327:LEU:HA	1.87	0.41
15:E:339:ASN:HB2	15:E:342:ASP:OD2	2.20	0.41
16:F:288:LEU:HA	16:F:288:LEU:HD23	1.81	0.41
16:F:293:THR:HG21	16:F:295:ARG:HE	1.86	0.41
16:F:351:LYS:O	16:F:352:ILE:HD13	2.19	0.41
19:I:232:GLU:H	19:I:232:GLU:HG3	1.66	0.41
19:i:31:ALA:C	19:i:50:ARG:HH21	2.27	0.41
33:u:173:LEU:HD23	33:u:173:LEU:HA	1.83	0.41
33:u:225:ALA:O	33:u:229:VAL:HG22	2.21	0.41
33:u:456:ARG:HH22	33:u:492:SER:HB3	1.86	0.41
1:U:22:PHE:HB2	9:d:30:LEU:HD11	2.02	0.41
1:U:247:GLN:HG2	1:U:913:ILE:HB	2.02	0.41
1:U:737:LEU:HD12	1:U:737:LEU:HA	1.79	0.41
3:W:165:ILE:HG21	3:W:189:GLN:HB3	2.03	0.41
3:W:285:ASP:O	3:W:289:ARG:HG2	2.21	0.41
4:X:255:LEU:HD23	4:X:270:LEU:HD12	2.01	0.41
5:Y:305:SER:O	5:Y:309:GLU:HG2	2.20	0.41
5:Y:342:ARG:HB2	5:Y:342:ARG:CZ	2.50	0.41
6:Z:37:GLY:HA3	6:Z:95:TYR:CE2	2.56	0.41
6:Z:63:LYS:C	6:Z:65:ASP:H	2.29	0.41
6:Z:106:ILE:CG1	6:Z:153:LYS:HG2	2.50	0.41
8:c:51:MET:HG3	16:F:156:ASP:OD2	2.21	0.41
8:c:223:LYS:HG2	8:c:224:SER:H	1.86	0.41
11:A:261:PHE:O	11:A:265:ARG:HG3	2.21	0.41
12:B:78:PHE:HB2	33:u:613:LEU:HD23	2.03	0.41
14:D:203:LEU:HD23	14:D:330:LYS:HG3	2.02	0.41
14:D:258:ALA:HB1	14:D:259:PRO:HD3	2.01	0.41
15:E:247:THR:HG23	15:E:251:ARG:HD2	2.02	0.41
15:E:353:PHE:N	15:E:353:PHE:HD1	2.17	0.41
18:H:174:LEU:HD23	18:H:174:LEU:HA	1.92	0.41
19:i:209:GLU:O	19:i:209:GLU:HG2	2.20	0.41
23:m:169:ARG:O	23:m:173:LYS:HG2	2.21	0.41
28:r:44:THR:O	28:r:99:THR:OG1	2.36	0.41
32:f:410:ARG:NH1	32:f:415:PRO:HG2	2.35	0.41
33:u:422:VAL:O	33:u:426:LEU:HD12	2.21	0.41
1:U:135:ASN:O	1:U:139:GLN:HG2	2.21	0.41
1:U:766:PHE:HE1	1:U:778:PHE:N	2.19	0.41
1:U:797:MET:HA	1:U:798:PRO:HD3	1.89	0.41
2:V:163:VAL:HG13	2:V:216:ARG:NH1	2.35	0.41
3:W:315:MET:HE1	3:W:320:LEU:CD2	2.48	0.41
3:W:435:LEU:O	3:W:438:LEU:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:87:ARG:HH22	4:X:90:ARG:HH11	1.67	0.41
4:X:115:GLU:HB3	4:X:118:LYS:NZ	2.35	0.41
4:X:258:LYS:HG3	4:X:270:LEU:HD11	2.03	0.41
4:X:268:GLN:HA	4:X:271:VAL:HG22	2.03	0.41
5:Y:46:ARG:C	5:Y:48:ASN:H	2.29	0.41
5:Y:155:ASP:OD1	5:Y:155:ASP:N	2.52	0.41
10:e:41:ASP:OD1	10:e:42:ASN:N	2.54	0.41
11:A:422:LYS:O	11:A:423:PHE:HB2	2.20	0.41
14:D:98:GLN:O	14:D:99:ASN:CB	2.69	0.41
14:D:191:TYR:CE2	14:D:198:PRO:HB3	2.56	0.41
14:D:407:ILE:HD13	14:D:407:ILE:HA	1.85	0.41
15:E:363:VAL:HG12	15:E:366:ASP:OD2	2.20	0.41
16:F:68:ALA:O	16:F:72:LYS:HD3	2.21	0.41
16:F:124:ILE:HD12	16:F:124:ILE:O	2.20	0.41
16:F:140:VAL:HG11	16:F:145:LEU:HD21	2.01	0.41
16:F:212:PHE:O	16:F:215:LEU:C	2.63	0.41
38:N:301:LDZ:H32	38:N:301:LDZ:H11	1.87	0.41
18:h:145:TYR:HB3	18:h:147:PHE:CE1	2.53	0.41
21:k:183:GLU:OE1	21:k:184:VAL:HG13	2.21	0.41
21:k:202:LEU:HD23	21:k:202:LEU:HA	1.81	0.41
23:m:87:LEU:HD23	23:m:87:LEU:HA	1.91	0.41
38:r:301:LDZ:H33	38:r:301:LDZ:H11	1.85	0.41
33:u:225:ALA:HA	33:u:228:LYS:HZ2	1.86	0.41
1:U:772:TRP:CD1	1:U:774:PRO:HD2	2.56	0.41
2:V:399:ARG:HE	2:V:399:ARG:HB3	1.66	0.41
3:W:28:LEU:HD22	3:W:55:ARG:HB2	2.02	0.41
5:Y:70:LEU:O	5:Y:74:LYS:HG2	2.20	0.41
5:Y:163:LYS:HD3	5:Y:167:LEU:HD12	2.02	0.41
6:Z:209:ARG:HA	6:Z:209:ARG:HD3	1.81	0.41
7:a:134:THR:O	7:a:138:VAL:HG23	2.20	0.41
9:d:9:TRP:CZ3	9:d:57:ILE:HG13	2.56	0.41
9:d:195:THR:HG22	9:d:205:LYS:HE3	2.03	0.41
12:B:189:GLY:HA3	12:B:360:THR:HG23	2.03	0.41
13:C:41:ASN:O	13:C:44:ARG:HB2	2.20	0.41
13:C:45:LEU:HB3	14:D:61:ILE:CG2	2.50	0.41
13:C:52:LEU:O	13:C:56:VAL:HG12	2.20	0.41
13:C:56:VAL:HG22	13:C:60:ARG:NH2	2.35	0.41
13:C:183:PRO:O	13:C:290:LYS:NZ	2.53	0.41
13:C:226:GLU:OE2	13:C:229:ARG:HD3	2.21	0.41
15:E:135:ILE:HG22	15:E:138:LEU:HD12	2.03	0.41
15:E:291:ARG:NH1	15:E:292:PRO:HB2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:E:349:GLU:HB3	15:E:373:LYS:HE3	2.02	0.41
16:F:274:LEU:O	16:F:278:LYS:HG2	2.20	0.41
21:K:147:ASP:OD1	21:K:147:ASP:N	2.54	0.41
22:L:69:HIS:O	22:L:136:GLY:HA2	2.20	0.41
26:P:106:GLU:HG2	26:P:125:ASP:HA	2.03	0.41
22:l:174:ARG:HH21	22:l:175:HIS:CE1	2.38	0.41
33:u:62:ARG:NH2	33:u:71:TYR:HA	2.35	0.41
33:u:405:HIS:HD2	33:u:813:LYS:HB3	1.83	0.41
33:u:459:CYS:SG	33:u:461:PRO:HD3	2.61	0.41
1:U:639:LEU:HD11	13:C:50:ASN:HD21	1.85	0.41
1:U:645:ASN:OD1	1:U:648:VAL:HG23	2.20	0.41
2:V:200:ARG:HB3	2:V:201:ARG:NH2	2.35	0.41
2:V:298:ILE:HD12	2:V:298:ILE:HA	1.86	0.41
2:V:357:LEU:HD12	2:V:358:MET:N	2.36	0.41
3:W:72:LYS:HD2	3:W:126:ASP:OD2	2.21	0.41
3:W:149:LEU:O	3:W:153:LYS:HG2	2.21	0.41
3:W:186:ILE:HD11	3:W:209:ILE:HG13	2.03	0.41
3:W:234:ASP:OD2	3:W:243:ILE:HG23	2.21	0.41
3:W:261:GLU:O	3:W:265:GLN:HG2	2.20	0.41
3:W:439:VAL:HA	6:Z:234:PHE:CZ	2.56	0.41
5:Y:81:LEU:CD2	5:Y:107:LYS:HD3	2.51	0.41
5:Y:314:LEU:C	5:Y:353:ILE:HG13	2.45	0.41
5:Y:326:GLY:O	5:Y:330:ILE:HG23	2.21	0.41
6:Z:96:HIS:CD2	6:Z:123:ILE:HG12	2.56	0.41
7:a:7:PHE:HZ	7:a:56:LEU:HB3	1.85	0.41
7:a:230:ARG:HA	7:a:232:TRP:NE1	2.36	0.41
7:a:280:MET:HE3	7:a:296:ILE:CD1	2.49	0.41
8:c:95:MET:SD	8:c:95:MET:N	2.94	0.41
8:c:218:LEU:HG	8:c:219:ASN:H	1.85	0.41
9:d:60:GLN:HE22	9:d:98:LEU:CD1	2.34	0.41
9:d:60:GLN:HG3	9:d:94:TYR:OH	2.21	0.41
11:A:95:VAL:HG11	12:B:156:VAL:O	2.20	0.41
11:A:345:LEU:H	11:A:345:LEU:HD22	1.86	0.41
11:A:425:ALA:O	11:A:429:TYR:HD1	2.04	0.41
13:C:113:ARG:NH2	13:C:129:ASN:O	2.37	0.41
13:C:116:LEU:HD23	13:C:123:LEU:HD22	2.03	0.41
14:D:81:ARG:HB3	14:D:81:ARG:HH21	1.85	0.41
16:F:78:GLU:HA	16:F:81:LYS:HG2	2.02	0.41
16:F:256:LEU:HD23	16:F:256:LEU:HA	1.77	0.41
16:F:271:ALA:O	16:F:274:LEU:HD12	2.21	0.41
18:H:214:ASN:HD22	18:H:214:ASN:HA	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:H:231:ALA:C	18:H:233:ILE:H	2.29	0.41
21:K:181:LEU:HD23	21:K:181:LEU:HA	1.94	0.41
22:L:74:ILE:HG21	22:L:81:ALA:HB1	2.02	0.41
22:L:107:ARG:HH22	30:T:74:GLU:CD	2.27	0.41
26:P:53:LEU:HB3	26:P:60:VAL:HG22	2.02	0.41
18:h:6:TYR:CG	18:h:7:SER:N	2.88	0.41
31:j:36:ARG:HA	31:j:41:VAL:HG12	2.02	0.41
31:j:177:THR:OG1	31:j:179:GLU:OE1	2.28	0.41
22:l:31:GLN:O	22:l:31:GLN:HG2	2.21	0.41
23:m:187:ARG:NE	23:m:232:ARG:HH22	2.19	0.41
38:r:301:LDZ:H21	38:r:301:LDZ:H13	1.86	0.41
33:u:177:GLU:OE2	33:u:180:GLN:N	2.41	0.41
33:u:679:LEU:HD13	33:u:713:PHE:CE2	2.55	0.41
33:u:779:CYS:SG	33:u:785:ARG:NH1	2.93	0.41
33:u:881:GLU:HA	33:u:894:LEU:HD22	2.03	0.41
1:U:233:LEU:O	1:U:237:VAL:HG12	2.21	0.41
1:U:661:ALA:HB1	1:U:746:ILE:HD12	2.03	0.41
3:W:37:GLU:C	3:W:39:ARG:N	2.79	0.41
3:W:42:GLU:OE1	3:W:42:GLU:N	2.52	0.41
3:W:216:GLU:HB3	3:W:223:LYS:HG2	2.03	0.41
3:W:256:ILE:H	3:W:256:ILE:HG13	1.71	0.41
3:W:436:MET:HE3	8:c:309:PHE:CZ	2.56	0.41
4:X:109:LEU:C	4:X:109:LEU:HD23	2.46	0.41
6:Z:124:ILE:HG12	6:Z:135:THR:OG1	2.20	0.41
9:d:240:THR:O	9:d:244:LYS:HG3	2.21	0.41
11:A:267:LYS:HE2	11:A:267:LYS:HB2	1.81	0.41
12:B:407:LEU:HD12	12:B:407:LEU:HA	1.91	0.41
13:C:372:ARG:HH12	14:D:179:GLU:CD	2.29	0.41
15:E:126:ASP:N	15:E:127:PRO:HD3	2.36	0.41
15:E:166:PRO:HA	15:E:167:PRO:HD3	1.95	0.41
16:F:359:GLU:OE1	16:F:360:GLU:N	2.54	0.41
21:K:24:VAL:O	21:K:28:ILE:HG12	2.21	0.41
29:S:47:THR:HG22	29:S:48:ASP:N	2.36	0.41
19:i:32:GLY:O	19:i:165:GLY:HA3	2.21	0.41
32:f:398:LEU:HA	32:f:401:GLN:HG3	2.03	0.41
32:f:410:ARG:HE	33:u:837:LEU:HD11	1.86	0.41
33:u:63:LEU:HD23	33:u:109:ILE:CD1	2.51	0.41
33:u:819:TYR:O	33:u:822:VAL:HG12	2.21	0.41
33:u:834:ASP:N	33:u:838:ARG:O	2.35	0.41
33:u:868:HIS:CE1	33:u:872:VAL:HG21	2.56	0.41
1:U:341:PHE:HD1	1:U:881:PRO:HB2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:450:HIS:CG	1:U:457:ILE:HD13	2.56	0.40
1:U:799:LYS:O	1:U:801:GLN:NE2	2.54	0.40
2:V:302:TYR:CD1	2:V:302:TYR:N	2.89	0.40
2:V:334:VAL:HG23	2:V:360:TYR:HE2	1.85	0.40
3:W:50:LEU:O	3:W:54:THR:HG23	2.21	0.40
3:W:393:LEU:HD23	3:W:393:LEU:HA	1.96	0.40
4:X:421:LEU:HD22	6:Z:280:ILE:HD12	2.03	0.40
6:Z:48:LEU:HD11	6:Z:92:VAL:HG21	2.02	0.40
6:Z:145:HIS:CD2	6:Z:145:HIS:O	2.73	0.40
7:a:35:HIS:H	7:a:35:HIS:CD2	2.38	0.40
7:a:61:GLU:O	7:a:64:ILE:HG22	2.21	0.40
8:c:155:VAL:HG12	8:c:157:ILE:HG13	2.03	0.40
9:d:52:ARG:HH22	9:d:89:LEU:HD13	1.86	0.40
9:d:184:LYS:HE3	9:d:228:GLN:HE22	1.85	0.40
10:e:59:GLU:O	10:e:60:LEU:HG	2.21	0.40
11:A:85:GLN:H	11:A:85:GLN:CD	2.28	0.40
11:A:158:ASP:HB3	11:A:161:VAL:HB	2.02	0.40
11:A:361:SER:O	11:A:361:SER:OG	2.39	0.40
14:D:374:ASP:O	14:D:377:SER:OG	2.29	0.40
16:F:205:PRO:HD2	16:F:206:MET:H	1.87	0.40
21:k:94:VAL:HG22	28:r:65:ILE:HD11	2.02	0.40
30:t:72:ILE:O	30:t:76:LEU:HG	2.21	0.40
32:f:381:ARG:NH2	33:u:435:SER:O	2.55	0.40
33:u:382:ASN:HA	33:u:773:LYS:HZ2	1.85	0.40
33:u:702:PRO:HD3	33:u:736:THR:HG21	2.02	0.40
33:u:707:LEU:HD23	33:u:707:LEU:HA	1.90	0.40
1:U:26:LYS:HE3	1:U:26:LYS:HB2	1.90	0.40
1:U:243:LEU:HG	1:U:913:ILE:HG21	2.04	0.40
2:V:244:ALA:C	2:V:246:GLY:H	2.28	0.40
2:V:333:ILE:O	2:V:337:LEU:HG	2.22	0.40
3:W:328:LEU:HD21	3:W:351:TRP:HE1	1.86	0.40
3:W:432:LEU:HD22	8:c:309:PHE:HD2	1.86	0.40
7:a:236:THR:OG1	7:a:249:GLN:NE2	2.46	0.40
8:c:211:GLU:OE2	8:c:215:LYS:HG2	2.21	0.40
13:C:11:LEU:HD23	13:C:11:LEU:HA	1.84	0.40
13:C:189:TYR:CZ	13:C:316:GLU:HB3	2.56	0.40
13:C:281:ASP:OD2	13:C:307:ARG:NH2	2.55	0.40
15:E:62:LYS:HE2	15:E:63:GLN:O	2.21	0.40
16:F:129:ARG:NH1	16:F:261:ILE:HG23	2.35	0.40
16:F:238:ARG:HG2	16:F:238:ARG:NH1	2.36	0.40
17:G:11:ARG:HH21	17:G:12:HIS:CD2	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:J:71:MET:HE2	20:J:84:ILE:HG12	2.02	0.40
25:O:43:CYS:SG	25:O:98:LEU:HB3	2.61	0.40
25:O:73:LEU:HD23	25:O:73:LEU:HA	1.91	0.40
30:T:34:ALA:O	24:n:166:ARG:NH1	2.54	0.40
30:T:176:LEU:HD23	30:T:176:LEU:HA	1.97	0.40
17:g:80:MET:HE3	17:g:80:MET:HB3	1.97	0.40
19:i:4:ARG:H	19:i:4:ARG:HG2	1.72	0.40
26:p:59:ASP:OD2	26:p:104:TYR:N	2.35	0.40
33:u:275:MET:C	33:u:275:MET:HE2	2.47	0.40
33:u:842:VAL:O	33:u:870:THR:HG23	2.21	0.40
33:u:907:ASP:OD1	33:u:907:ASP:N	2.53	0.40
1:U:76:GLU:H	1:U:76:GLU:CD	2.29	0.40
1:U:137:MET:N	1:U:137:MET:SD	2.94	0.40
1:U:146:LYS:HB2	1:U:146:LYS:HE2	1.87	0.40
1:U:196:LYS:HA	1:U:196:LYS:HD3	1.90	0.40
1:U:509:GLY:HA3	1:U:544:ILE:HD12	2.03	0.40
1:U:680:VAL:HB	1:U:683:VAL:HG12	2.03	0.40
3:W:116:THR:HG23	3:W:119:PRO:HD3	2.04	0.40
3:W:170:GLN:O	3:W:173:THR:OG1	2.35	0.40
3:W:186:ILE:O	3:W:190:MET:HG2	2.21	0.40
3:W:419:LYS:HG2	3:W:420:ASP:N	2.35	0.40
3:W:432:LEU:HD22	8:c:309:PHE:CD2	2.56	0.40
5:Y:194:PHE:O	5:Y:195:LYS:NZ	2.52	0.40
11:A:55:LEU:O	11:A:59:ILE:HG22	2.21	0.40
11:A:119:ALA:HB3	11:A:121:PHE:CE1	2.48	0.40
13:C:221:GLN:O	14:D:240:LEU:HG	2.21	0.40
14:D:406:VAL:O	14:D:409:LYS:HD3	2.21	0.40
16:F:268:VAL:HG12	16:F:316:GLN:HG3	2.02	0.40
18:H:106:PRO:HG2	18:H:109:GLN:HG3	2.02	0.40
20:J:227:LYS:NZ	20:J:231:GLU:OE1	2.42	0.40
23:M:198:TYR:CZ	23:M:209:PHE:HZ	2.38	0.40
30:T:215:ILE:HD13	30:T:215:ILE:HA	1.93	0.40
17:g:191:PHE:HE1	17:g:219:VAL:HG21	1.86	0.40
26:p:34:MET:HE3	26:p:34:MET:HB3	1.82	0.40
33:u:420:TRP:HD1	33:u:455:VAL:HG13	1.86	0.40
33:u:461:PRO:O	33:u:465:LEU:HG	2.22	0.40
1:U:188:MET:HE3	1:U:188:MET:O	2.21	0.40
1:U:427:LEU:HD13	1:U:430:ASP:HB2	2.02	0.40
1:U:516:LEU:HD12	1:U:516:LEU:HA	1.96	0.40
2:V:111:TYR:HH	2:V:150:ARG:HH21	1.64	0.40
3:W:310:THR:C	3:W:312:MET:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:80:ILE:HG23	4:X:85:ALA:HB2	2.04	0.40
5:Y:75:LYS:HA	5:Y:75:LYS:HD3	1.99	0.40
5:Y:349:LYS:O	5:Y:351:ASN:N	2.55	0.40
14:D:40:LEU:H	14:D:40:LEU:HD23	1.86	0.40
15:E:67:GLU:OE1	15:E:67:GLU:HA	2.21	0.40
15:E:174:GLY:HA3	15:E:301:ILE:HG22	2.04	0.40
16:F:198:LEU:HD23	16:F:198:LEU:C	2.46	0.40
18:h:34:PRO:HG2	18:h:49:GLU:HB3	2.03	0.40
32:f:388:THR:HA	32:f:391:LYS:HE2	2.02	0.40
33:u:64:GLY:HA3	33:u:105:LYS:NZ	2.37	0.40
33:u:308:SER:O	33:u:311:VAL:HG22	2.21	0.40
33:u:574:GLU:N	33:u:574:GLU:OE1	2.54	0.40
1:U:525:ASN:O	1:U:529:ILE:HG22	2.21	0.40
3:W:187:LEU:HA	3:W:190:MET:HG3	2.04	0.40
3:W:435:LEU:HA	3:W:438:LEU:HD11	2.04	0.40
6:Z:68:TRP:CB	6:Z:104:ASN:HD21	2.34	0.40
7:a:58:LYS:HE3	7:a:96:PHE:HZ	1.87	0.40
7:a:132:LYS:HB2	7:a:132:LYS:HE2	1.93	0.40
8:c:161:ARG:HB3	8:c:201:TYR:CE2	2.57	0.40
13:C:222:LYS:HA	14:D:240:LEU:HD21	2.03	0.40
13:C:228:ALA:O	13:C:232:ARG:HG3	2.21	0.40
14:D:377:SER:HB3	15:E:291:ARG:CZ	2.52	0.40
14:D:409:LYS:O	14:D:411:GLU:HG2	2.20	0.40
15:E:194:ASN:HB2	15:E:230:ILE:HD13	2.04	0.40
16:F:98:ASP:OD1	16:F:120:LYS:HG3	2.21	0.40
16:F:176:GLU:HG2	16:F:177:VAL:N	2.36	0.40
21:K:125:GLU:N	21:K:125:GLU:CD	2.80	0.40
25:O:33:LYS:HE2	38:O:301:LDZ:H22	2.03	0.40
18:h:171:LYS:HZ3	19:i:53:HIS:CE1	2.40	0.40
26:p:48:ARG:HA	26:p:190:ILE:HG21	2.02	0.40
33:u:442:SER:O	33:u:446:LEU:HG	2.21	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	U	839/953 (88%)	761 (91%)	75 (9%)	3 (0%)	30	59
2	V	478/533 (90%)	427 (89%)	49 (10%)	2 (0%)	30	59
3	W	448/456 (98%)	400 (89%)	42 (9%)	6 (1%)	9	33
4	X	378/422 (90%)	365 (97%)	12 (3%)	1 (0%)	36	65
5	Y	376/389 (97%)	336 (89%)	38 (10%)	2 (0%)	24	54
6	Z	284/324 (88%)	250 (88%)	32 (11%)	2 (1%)	18	47
7	a	371/376 (99%)	329 (89%)	40 (11%)	2 (0%)	24	54
8	c	285/309 (92%)	247 (87%)	36 (13%)	2 (1%)	18	47
9	d	249/349 (71%)	200 (80%)	46 (18%)	3 (1%)	10	35
10	e	36/70 (51%)	26 (72%)	8 (22%)	2 (6%)	1	10
11	A	411/433 (95%)	371 (90%)	37 (9%)	3 (1%)	18	47
12	B	403/440 (92%)	365 (91%)	36 (9%)	2 (0%)	24	54
13	C	394/398 (99%)	361 (92%)	29 (7%)	4 (1%)	12	39
14	D	378/418 (90%)	339 (90%)	36 (10%)	3 (1%)	16	44
15	E	350/403 (87%)	309 (88%)	36 (10%)	5 (1%)	9	31
16	F	358/439 (82%)	321 (90%)	36 (10%)	1 (0%)	36	65
17	G	235/245 (96%)	225 (96%)	9 (4%)	1 (0%)	30	59
17	g	238/245 (97%)	231 (97%)	7 (3%)	0	100	100
18	H	229/233 (98%)	214 (93%)	14 (6%)	1 (0%)	30	59
18	h	230/233 (99%)	222 (96%)	7 (3%)	1 (0%)	30	59
19	I	246/260 (95%)	228 (93%)	17 (7%)	1 (0%)	30	59
19	i	248/260 (95%)	235 (95%)	12 (5%)	1 (0%)	30	59
20	J	245/248 (99%)	231 (94%)	10 (4%)	4 (2%)	7	29
21	K	226/241 (94%)	220 (97%)	6 (3%)	0	100	100
21	k	224/241 (93%)	214 (96%)	10 (4%)	0	100	100
22	L	236/268 (88%)	230 (98%)	6 (2%)	0	100	100
22	l	236/268 (88%)	227 (96%)	9 (4%)	0	100	100
23	M	238/254 (94%)	233 (98%)	4 (2%)	1 (0%)	30	59
23	m	238/254 (94%)	227 (95%)	11 (5%)	0	100	100
24	N	195/238 (82%)	188 (96%)	6 (3%)	1 (0%)	24	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	n	195/238 (82%)	189 (97%)	6 (3%)	0	100	100
25	O	218/276 (79%)	209 (96%)	8 (4%)	1 (0%)	24	54
25	o	218/276 (79%)	203 (93%)	15 (7%)	0	100	100
26	P	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
26	p	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
27	Q	197/201 (98%)	186 (94%)	11 (6%)	0	100	100
27	q	197/201 (98%)	187 (95%)	10 (5%)	0	100	100
28	R	199/262 (76%)	195 (98%)	2 (1%)	2 (1%)	12	39
28	r	199/262 (76%)	193 (97%)	6 (3%)	0	100	100
29	S	211/240 (88%)	206 (98%)	4 (2%)	1 (0%)	24	54
29	s	211/240 (88%)	208 (99%)	3 (1%)	0	100	100
30	T	213/263 (81%)	207 (97%)	5 (2%)	1 (0%)	24	54
30	t	213/263 (81%)	203 (95%)	10 (5%)	0	100	100
31	j	237/247 (96%)	219 (92%)	17 (7%)	1 (0%)	30	59
32	f	53/445 (12%)	48 (91%)	4 (8%)	1 (2%)	6	26
33	u	826/908 (91%)	797 (96%)	29 (4%)	0	100	100
All	All	13093/14930 (88%)	12167 (93%)	865 (7%)	61 (0%)	26	54

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	41	SER
3	W	45	GLU
3	W	375	MET
4	X	310	ARG
5	Y	361	SER
6	Z	167	ALA
7	a	215	GLU
9	d	94	TYR
9	d	223	TYR
10	e	46	ASP
11	A	423	PHE
13	C	90	HIS
13	C	254	ILE
14	D	258	ALA
16	F	279	ALA

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Mol	Chain	Res	Type
17	G	130	GLU
18	H	180	GLU
19	I	107	CYS
20	J	199	VAL
29	S	191	ASP
19	i	107	CYS
31	j	52	LYS
1	U	96	TYR
2	V	465	ASP
3	W	12	ARG
3	W	37	GLU
3	W	38	GLY
5	Y	350	VAL
10	e	60	LEU
13	C	242	ALA
14	D	97	ASP
15	E	238	ILE
15	E	248	SER
23	M	201	HIS
30	T	46	ASN
6	Z	243	GLN
11	A	116	LYS
13	C	297	ARG
15	E	306	GLU
15	E	326	ILE
20	J	213	ARG
18	h	232	ALA
8	c	219	ASN
9	d	203	PRO
12	B	165	ASP
14	D	303	VAL
24	N	19	ARG
25	O	172	ASN
28	R	143	TYR
2	V	300	LEU
8	c	25	VAL
12	B	320	ASP
20	J	6	ALA
20	J	184	ASP
32	f	15	ALA
1	U	159	ARG
11	A	66	LYS

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Mol	Chain	Res	Type
15	E	240	GLY
3	W	13	ILE
7	a	185	ILE
28	R	38	ASN

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	U	722/816 (88%)	717 (99%)	5 (1%)	76	78
2	V	414/459 (90%)	412 (100%)	2 (0%)	81	80
3	W	412/416 (99%)	407 (99%)	5 (1%)	63	72
4	X	327/362 (90%)	326 (100%)	1 (0%)	86	84
5	Y	334/344 (97%)	334 (100%)	0	100	100
6	Z	257/295 (87%)	255 (99%)	2 (1%)	73	76
7	a	333/336 (99%)	329 (99%)	4 (1%)	63	72
8	c	252/267 (94%)	251 (100%)	1 (0%)	84	82
9	d	226/293 (77%)	224 (99%)	2 (1%)	70	75
10	e	38/63 (60%)	38 (100%)	0	100	100
11	A	348/372 (94%)	347 (100%)	1 (0%)	86	84
12	B	352/385 (91%)	352 (100%)	0	100	100
13	C	340/346 (98%)	336 (99%)	4 (1%)	63	72
14	D	333/366 (91%)	328 (98%)	5 (2%)	57	69
15	E	307/353 (87%)	306 (100%)	1 (0%)	86	84
16	F	309/379 (82%)	308 (100%)	1 (0%)	86	84
17	G	191/209 (91%)	191 (100%)	0	100	100
17	g	194/209 (93%)	192 (99%)	2 (1%)	68	74
18	H	169/190 (89%)	169 (100%)	0	100	100
18	h	167/190 (88%)	164 (98%)	3 (2%)	51	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	I	191/220 (87%)	191 (100%)	0	100	100
19	i	193/220 (88%)	192 (100%)	1 (0%)	81	80
20	J	179/211 (85%)	179 (100%)	0	100	100
21	K	189/203 (93%)	189 (100%)	0	100	100
21	k	186/203 (92%)	186 (100%)	0	100	100
22	L	198/229 (86%)	198 (100%)	0	100	100
22	l	198/229 (86%)	198 (100%)	0	100	100
23	M	192/211 (91%)	190 (99%)	2 (1%)	68	74
23	m	193/211 (92%)	190 (98%)	3 (2%)	55	68
24	N	154/180 (86%)	154 (100%)	0	100	100
24	n	154/180 (86%)	153 (99%)	1 (1%)	78	80
25	O	177/227 (78%)	177 (100%)	0	100	100
25	o	177/227 (78%)	176 (99%)	1 (1%)	78	80
26	P	173/173 (100%)	173 (100%)	0	100	100
26	p	173/173 (100%)	170 (98%)	3 (2%)	53	67
27	Q	164/171 (96%)	164 (100%)	0	100	100
27	q	165/171 (96%)	165 (100%)	0	100	100
28	R	153/201 (76%)	153 (100%)	0	100	100
28	r	153/201 (76%)	153 (100%)	0	100	100
29	S	174/198 (88%)	174 (100%)	0	100	100
29	s	174/198 (88%)	174 (100%)	0	100	100
30	T	175/214 (82%)	174 (99%)	1 (1%)	78	80
30	t	176/214 (82%)	175 (99%)	1 (1%)	78	80
31	j	152/210 (72%)	152 (100%)	0	100	100
32	f	45/364 (12%)	44 (98%)	1 (2%)	45	63
33	u	702/763 (92%)	700 (100%)	2 (0%)	86	84
All	All	10985/12652 (87%)	10930 (100%)	55 (0%)	78	80

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	202	VAL
1	U	206	MET

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Mol	Chain	Res	Type
1	U	364	VAL
1	U	641	SER
1	U	766	PHE
2	V	471	GLU
2	V	473	GLN
3	W	15	LYS
3	W	16	MET
3	W	17	GLU
3	W	27	ARG
3	W	28	LEU
4	X	321	THR
6	Z	32	GLN
6	Z	138	TYR
7	a	94	LEU
7	a	123	LEU
7	a	237	LEU
7	a	331	VAL
8	c	32	TYR
9	d	149	ASN
9	d	206	MET
11	A	347	ASP
13	C	58	LEU
13	C	109	THR
13	C	162	LYS
13	C	316	GLU
14	D	40	LEU
14	D	81	ARG
14	D	98	GLN
14	D	100	THR
14	D	240	LEU
15	E	97	ARG
16	F	206	MET
23	M	158	TYR
23	M	175	GLU
30	T	150	LEU
17	g	58	ASP
17	g	192	GLU
18	h	75	VAL
18	h	203	MET
18	h	228	ASP
19	i	50	ARG
23	m	184	MET

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Mol	Chain	Res	Type
23	m	186	CYS
23	m	188	ASP
24	n	95	MET
25	o	91	GLN
26	p	85	TYR
26	p	115	LYS
26	p	191	GLU
30	t	46	ASN
32	f	405	ARG
33	u	692	LEU
33	u	744	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (179) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	89	ASN
1	U	107	HIS
1	U	115	ASN
1	U	189	GLN
1	U	195	ASN
1	U	207	ASN
1	U	467	ASN
1	U	475	HIS
1	U	491	GLN
1	U	500	ASN
1	U	503	GLN
1	U	525	ASN
1	U	596	ASN
1	U	711	GLN
1	U	743	ASN
1	U	756	HIS
1	U	768	GLN
2	V	33	GLN
2	V	146	GLN
2	V	257	ASN
2	V	311	ASN
2	V	377	GLN
3	W	53	GLN
3	W	235	GLN
3	W	236	HIS
3	W	288	HIS
3	W	416	GLN

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Mol	Chain	Res	Type
4	X	105	GLN
4	X	178	HIS
4	X	207	GLN
4	X	406	ASN
5	Y	77	ASN
5	Y	178	ASN
5	Y	280	GLN
5	Y	365	GLN
5	Y	388	ASN
6	Z	24	ASN
6	Z	104	ASN
6	Z	109	ASN
6	Z	196	HIS
6	Z	235	ASN
6	Z	256	GLN
6	Z	277	ASN
6	Z	282	ASN
7	a	35	HIS
7	a	86	GLN
7	a	257	GLN
7	a	305	ASN
8	c	210	ASN
8	c	214	GLN
8	c	240	HIS
8	c	269	GLN
8	c	295	ASN
9	d	60	GLN
9	d	96	HIS
9	d	102	ASN
9	d	109	GLN
9	d	128	GLN
9	d	135	HIS
9	d	221	ASN
11	A	88	GLN
11	A	91	GLN
11	A	165	GLN
12	B	57	GLN
12	B	153	ASN
12	B	154	HIS
12	B	207	HIS
12	B	306	GLN
13	C	46	GLN

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Mol	Chain	Res	Type
13	C	67	GLN
13	C	90	HIS
13	C	124	HIS
13	C	241	HIS
13	C	296	ASN
13	C	337	ASN
14	D	67	ASN
14	D	91	GLN
14	D	110	ASN
14	D	304	ASN
14	D	312	ASN
14	D	390	ASN
15	E	39	GLN
15	E	121	ASN
15	E	263	GLN
15	E	300	HIS
16	F	194	GLN
16	F	208	HIS
16	F	258	GLN
16	F	367	GLN
16	F	428	GLN
16	F	434	ASN
17	G	53	GLN
17	G	193	GLN
18	H	109	GLN
18	H	214	ASN
19	I	84	ASN
19	I	149	GLN
19	I	220	ASN
20	J	15	HIS
20	J	120	GLN
20	J	122	ASN
20	J	154	HIS
21	K	99	HIS
21	K	214	ASN
22	L	4	ASN
22	L	59	HIS
22	L	60	GLN
22	L	203	GLN
23	M	32	ASN
23	M	97	ASN
25	O	35	HIS

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Mol	Chain	Res	Type
26	P	7	ASN
26	P	157	ASN
26	P	169	GLN
27	Q	71	ASN
28	R	29	GLN
28	R	151	GLN
28	R	162	GLN
28	R	191	ASN
29	S	108	ASN
30	T	69	GLN
30	T	147	GLN
17	g	53	GLN
18	h	21	GLN
18	h	63	HIS
18	h	95	GLN
18	h	96	GLN
18	h	109	GLN
19	i	20	GLN
19	i	95	GLN
19	i	109	GLN
19	i	198	ASN
31	j	205	ASN
21	k	41	GLN
21	k	97	GLN
21	k	122	GLN
21	k	178	GLN
21	k	221	GLN
22	l	21	GLN
22	l	53	GLN
22	l	143	HIS
22	l	146	GLN
22	l	175	HIS
23	m	97	ASN
24	n	53	GLN
24	n	158	ASN
25	o	62	ASN
25	o	80	ASN
26	p	18	ASN
26	p	61	GLN
26	p	93	ASN
26	p	157	ASN
27	q	27	GLN

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Mol	Chain	Res	Type
27	q	71	ASN
27	q	101	ASN
27	q	168	GLN
27	q	174	ASN
28	r	29	GLN
28	r	119	ASN
28	r	162	GLN
28	r	191	ASN
29	s	8	ASN
29	s	79	ASN
30	t	3	ASN
30	t	47	ASN
30	t	147	GLN
32	f	385	ASN
33	u	51	GLN
33	u	102	HIS
33	u	161	HIS
33	u	382	ASN
33	u	387	GLN
33	u	405	HIS
33	u	472	HIS
33	u	475	ASN
33	u	565	ASN
33	u	766	GLN
33	u	808	ASN
33	u	868	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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
35	ATP	C	501	36	32,33,33	0.30	0	48,52,52	0.30	0
37	ADP	E	401	-	28,29,29	1.41	4 (14%)	43,45,45	1.85	8 (18%)
38	LDZ	n	301	-	33,34,34	0.50	0	42,44,44	1.40	3 (7%)
35	ATP	B	501	36	32,33,33	0.35	0	48,52,52	0.33	0
38	LDZ	o	301	-	33,34,34	0.49	0	42,44,44	0.70	0
37	ADP	D	501	36	28,29,29	1.41	4 (14%)	43,45,45	1.86	8 (18%)
38	LDZ	N	301	-	33,34,34	0.41	0	42,44,44	0.70	0
38	LDZ	O	301	-	33,34,34	0.39	0	42,44,44	1.53	3 (7%)
35	ATP	F	501	36	32,33,33	0.31	0	48,52,52	0.32	0
38	LDZ	r	301	-	33,34,34	0.44	0	42,44,44	0.80	2 (4%)
35	ATP	A	501	36	32,33,33	0.28	0	48,52,52	0.28	0
38	LDZ	R	301	-	33,34,34	0.47	0	42,44,44	0.58	0

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
35	ATP	C	501	36	-	4/22/38/38	0/3/3/3
37	ADP	E	401	-	-	5/16/32/32	0/3/3/3
38	LDZ	n	301	-	-	22/38/39/39	0/1/1/1
35	ATP	B	501	36	-	6/22/38/38	0/3/3/3
38	LDZ	o	301	-	-	14/38/39/39	0/1/1/1
37	ADP	D	501	36	-	0/16/32/32	0/3/3/3
38	LDZ	N	301	-	-	8/38/39/39	0/1/1/1
38	LDZ	O	301	-	-	15/38/39/39	0/1/1/1
35	ATP	F	501	36	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LDZ	r	301	-	-	13/38/39/39	0/1/1/1
35	ATP	A	501	36	-	5/22/38/38	0/3/3/3
38	LDZ	R	301	-	-	14/38/39/39	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	E	401	ADP	C5-C4	4.76	1.47	1.39
37	D	501	ADP	C5-C4	4.70	1.47	1.39
37	E	401	ADP	C5-C6	2.69	1.48	1.41
37	D	501	ADP	C5-C6	2.63	1.48	1.41
37	D	501	ADP	C5-N7	-2.37	1.34	1.39
37	E	401	ADP	C8-N7	2.37	1.36	1.31
37	E	401	ADP	C5-N7	-2.27	1.34	1.39
37	D	501	ADP	C8-N7	2.22	1.35	1.31

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	O	301	LDZ	C18-C17-N16	7.84	122.52	110.69
38	n	301	LDZ	C14-N13-C12	7.07	136.85	121.65
37	E	401	ADP	C5-C4-N3	-5.93	118.56	126.72
37	D	501	ADP	C5-C4-N3	-5.91	118.58	126.72
37	D	501	ADP	N3-C4-N9	4.76	135.26	127.17
37	E	401	ADP	N3-C4-N9	4.72	135.19	127.17
37	D	501	ADP	C2-N3-C4	3.72	120.92	111.83
37	E	401	ADP	C2-N3-C4	3.71	120.90	111.83
37	E	401	ADP	C4-C5-N7	-3.36	106.73	110.58
37	D	501	ADP	C4-C5-N7	-3.31	106.80	110.58
37	D	501	ADP	N3-C2-N1	-3.23	123.70	128.58
37	E	401	ADP	N3-C2-N1	-3.18	123.77	128.58
38	n	301	LDZ	C24-C14-N13	3.12	117.62	110.58
38	O	301	LDZ	C14-C15-N16	2.93	122.87	116.63
37	E	401	ADP	C3'-C2'-C1'	2.90	106.95	101.46
38	r	301	LDZ	C14-N13-C12	2.90	127.87	121.65
37	D	501	ADP	C3'-C2'-C1'	2.81	106.78	101.46
37	D	501	ADP	C4-N9-C8	2.59	108.46	105.74
37	E	401	ADP	C5-N7-C8	2.51	107.39	103.45
37	E	401	ADP	C4-N9-C8	2.49	108.36	105.74
37	D	501	ADP	C5-N7-C8	2.42	107.25	103.45
38	r	301	LDZ	C22-C17-N16	2.32	113.97	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	O	301	LDZ	C18-C17-C22	-2.22	107.58	110.99
38	n	301	LDZ	C11-C12-N13	2.19	121.29	116.63

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	501	ATP	PB-O3B-PG-O3G
35	A	501	ATP	C5'-O5'-PA-O1A
35	A	501	ATP	C5'-O5'-PA-O3A
35	B	501	ATP	C5'-O5'-PA-O1A
35	B	501	ATP	C5'-O5'-PA-O2A
35	B	501	ATP	C5'-O5'-PA-O3A
35	C	501	ATP	C5'-O5'-PA-O2A
35	C	501	ATP	C5'-O5'-PA-O3A
35	F	501	ATP	C5'-O5'-PA-O1A
35	F	501	ATP	C5'-O5'-PA-O3A
37	E	401	ADP	C5'-O5'-PA-O2A
37	E	401	ADP	C5'-O5'-PA-O3A
37	E	401	ADP	O4'-C4'-C5'-O5'
38	O	301	LDZ	O31-C9-O8-C7
38	O	301	LDZ	N10-C9-O8-C7
38	O	301	LDZ	C18-C17-N16-C15
38	O	301	LDZ	C22-C17-C18-C19
38	R	301	LDZ	O31-C9-O8-C7
38	R	301	LDZ	N10-C9-O8-C7
38	R	301	LDZ	C18-C17-C22-O33
38	R	301	LDZ	C22-C17-C18-C19
38	n	301	LDZ	O8-C9-N10-C11
38	n	301	LDZ	C30-C11-N10-C9
38	n	301	LDZ	C22-C17-C18-C19
38	n	301	LDZ	O31-C9-N10-C11
38	R	301	LDZ	N16-C17-C18-C19
38	o	301	LDZ	C30-C11-C12-N13
38	r	301	LDZ	C15-C14-C24-C25
38	R	301	LDZ	N13-C14-C24-C25
38	n	301	LDZ	N13-C14-C24-C25
38	r	301	LDZ	N13-C14-C24-C25
38	o	301	LDZ	C15-C14-C24-C25
38	o	301	LDZ	C30-C11-C12-O32
38	O	301	LDZ	N16-C17-C18-C19
38	R	301	LDZ	N10-C11-C30-C31

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Mol	Chain	Res	Type	Atoms
38	R	301	LDZ	C12-C11-C30-C31
38	R	301	LDZ	C15-C14-C24-C25
38	n	301	LDZ	C15-C14-C24-C25
38	n	301	LDZ	C17-C18-C19-C21
38	o	301	LDZ	C17-C18-C19-C21
38	n	301	LDZ	C11-C30-C31-C32
38	n	301	LDZ	C11-C30-C31-C33
38	n	301	LDZ	C17-C18-C19-C20
38	o	301	LDZ	C17-C18-C19-C20
38	O	301	LDZ	C14-C15-N16-C17
38	O	301	LDZ	C14-C24-C25-C27
38	O	301	LDZ	C17-C18-C19-C21
38	O	301	LDZ	O34-C15-N16-C17
38	n	301	LDZ	O32-C12-N13-C14
38	o	301	LDZ	N13-C14-C24-C25
38	O	301	LDZ	C14-C24-C25-C26
38	O	301	LDZ	C17-C18-C19-C20
38	n	301	LDZ	C11-C12-N13-C14
38	n	301	LDZ	C24-C14-N13-C12
38	n	301	LDZ	N16-C17-C18-C19
37	E	401	ADP	C3'-C4'-C5'-O5'
38	N	301	LDZ	N16-C17-C18-C19
38	N	301	LDZ	N10-C11-C30-C31
38	R	301	LDZ	C14-C24-C25-C27
38	N	301	LDZ	C14-C24-C25-C27
38	n	301	LDZ	N13-C14-C15-O34
38	n	301	LDZ	N10-C11-C12-N13
38	n	301	LDZ	N13-C14-C15-N16
38	n	301	LDZ	N10-C11-C12-O32
38	R	301	LDZ	C17-C18-C19-C21
38	r	301	LDZ	C22-C17-N16-C15
38	o	301	LDZ	N13-C14-C15-O34
38	o	301	LDZ	N13-C14-C15-N16
38	R	301	LDZ	C17-C18-C19-C20
38	r	301	LDZ	C22-C17-C18-C19
38	o	301	LDZ	C14-C24-C25-C26
38	N	301	LDZ	C18-C17-N16-C15
38	o	301	LDZ	C18-C17-N16-C15
35	C	501	ATP	PG-O3B-PB-O2B
38	r	301	LDZ	C14-C24-C25-C27
38	R	301	LDZ	C14-C24-C25-C26
38	O	301	LDZ	N13-C14-C24-C25

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Mol	Chain	Res	Type	Atoms
38	o	301	LDZ	C14-C24-C25-C27
38	o	301	LDZ	C15-C14-N13-C12
38	O	301	LDZ	C12-C11-N10-C9
35	A	501	ATP	C5'-O5'-PA-O2A
35	F	501	ATP	C5'-O5'-PA-O2A
37	E	401	ADP	C5'-O5'-PA-O1A
38	N	301	LDZ	C14-C24-C25-C26
38	o	301	LDZ	C3-C7-O8-C9
38	r	301	LDZ	N16-C17-C18-C19
38	n	301	LDZ	C3-C7-O8-C9
38	N	301	LDZ	C22-C17-N16-C15
38	o	301	LDZ	C22-C17-N16-C15
38	O	301	LDZ	C11-C30-C31-C32
38	r	301	LDZ	C15-C14-N13-C12
35	F	501	ATP	PG-O3B-PB-O1B
38	N	301	LDZ	C15-C14-C24-C25
38	r	301	LDZ	N13-C14-C15-O34
38	r	301	LDZ	N10-C11-C30-C31
38	r	301	LDZ	N13-C14-C15-N16
35	B	501	ATP	PB-O3B-PG-O1G
35	B	501	ATP	PB-O3B-PG-O2G
35	B	501	ATP	PB-O3B-PG-O3G
38	N	301	LDZ	N13-C14-C24-C25
38	n	301	LDZ	C18-C17-N16-C15
38	r	301	LDZ	C18-C17-N16-C15
38	O	301	LDZ	C11-C30-C31-C33
35	C	501	ATP	PG-O3B-PB-O1B
38	r	301	LDZ	C12-C11-C30-C31
38	n	301	LDZ	C30-C11-C12-O32
38	r	301	LDZ	C14-C24-C25-C26
38	R	301	LDZ	C3-C7-O8-C9
38	n	301	LDZ	C30-C11-C12-N13
35	A	501	ATP	PA-O3A-PB-O2B
35	F	501	ATP	PG-O3B-PB-O2B
35	F	501	ATP	PB-O3A-PA-O2A

There are no ring outliers.

8 monomers are involved in 20 short contacts:

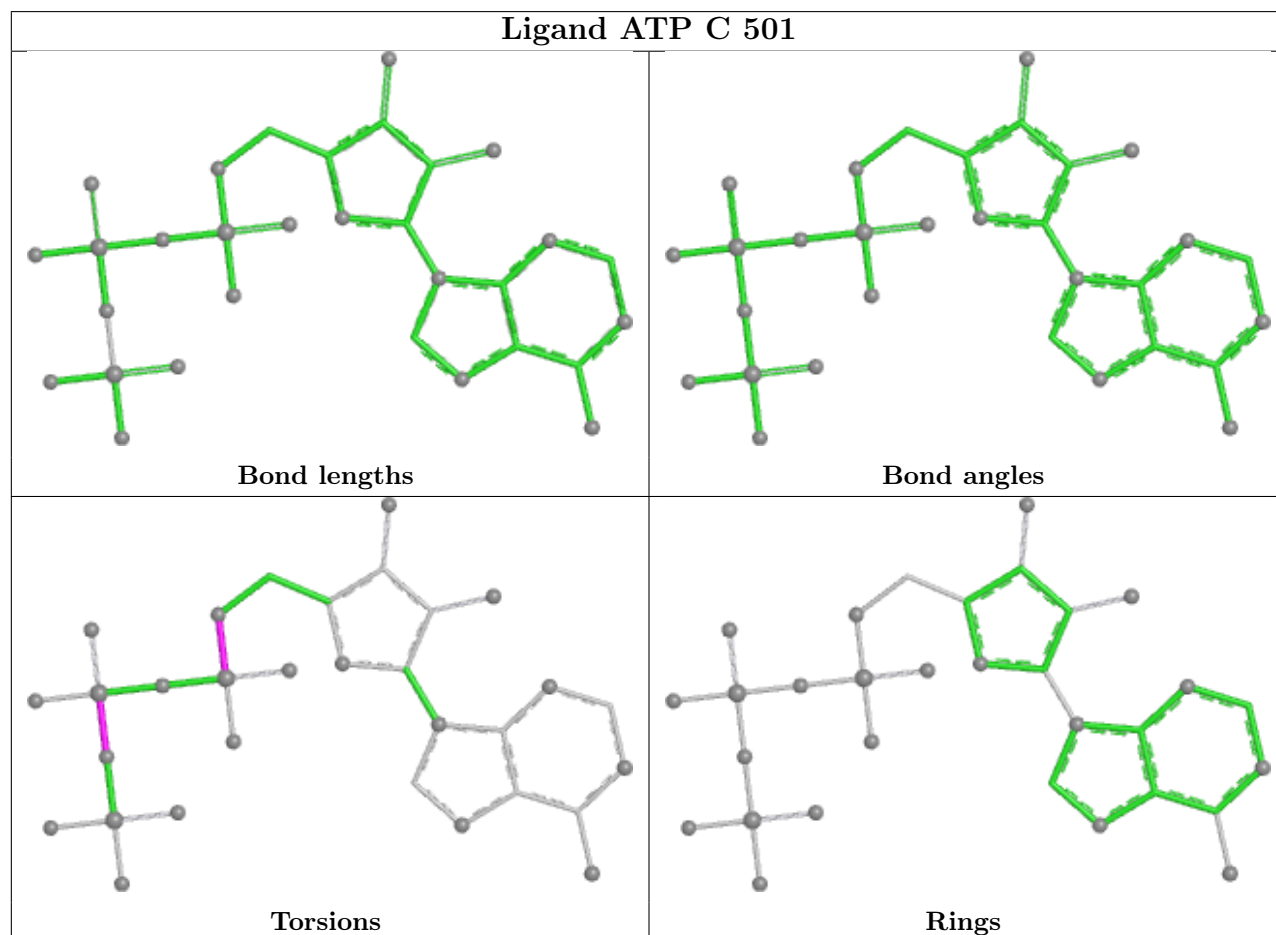
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	E	401	ADP	2	0
38	n	301	LDZ	2	0

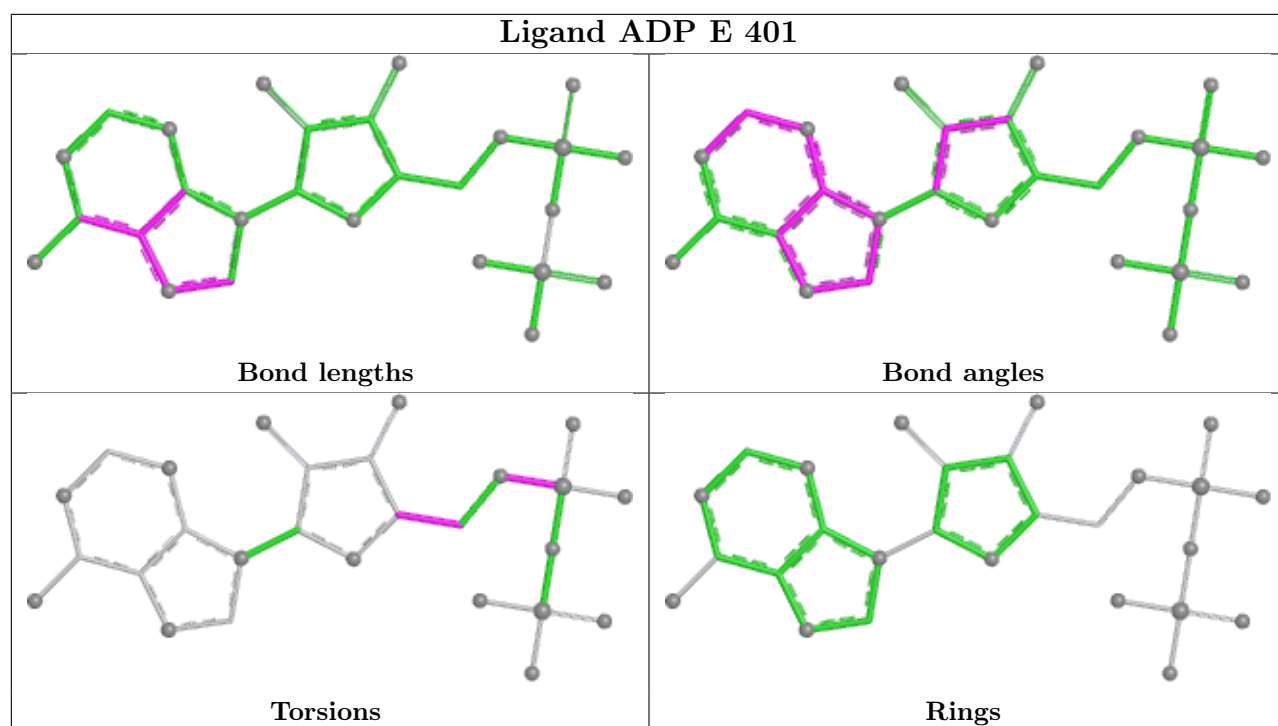
Continued on next page...

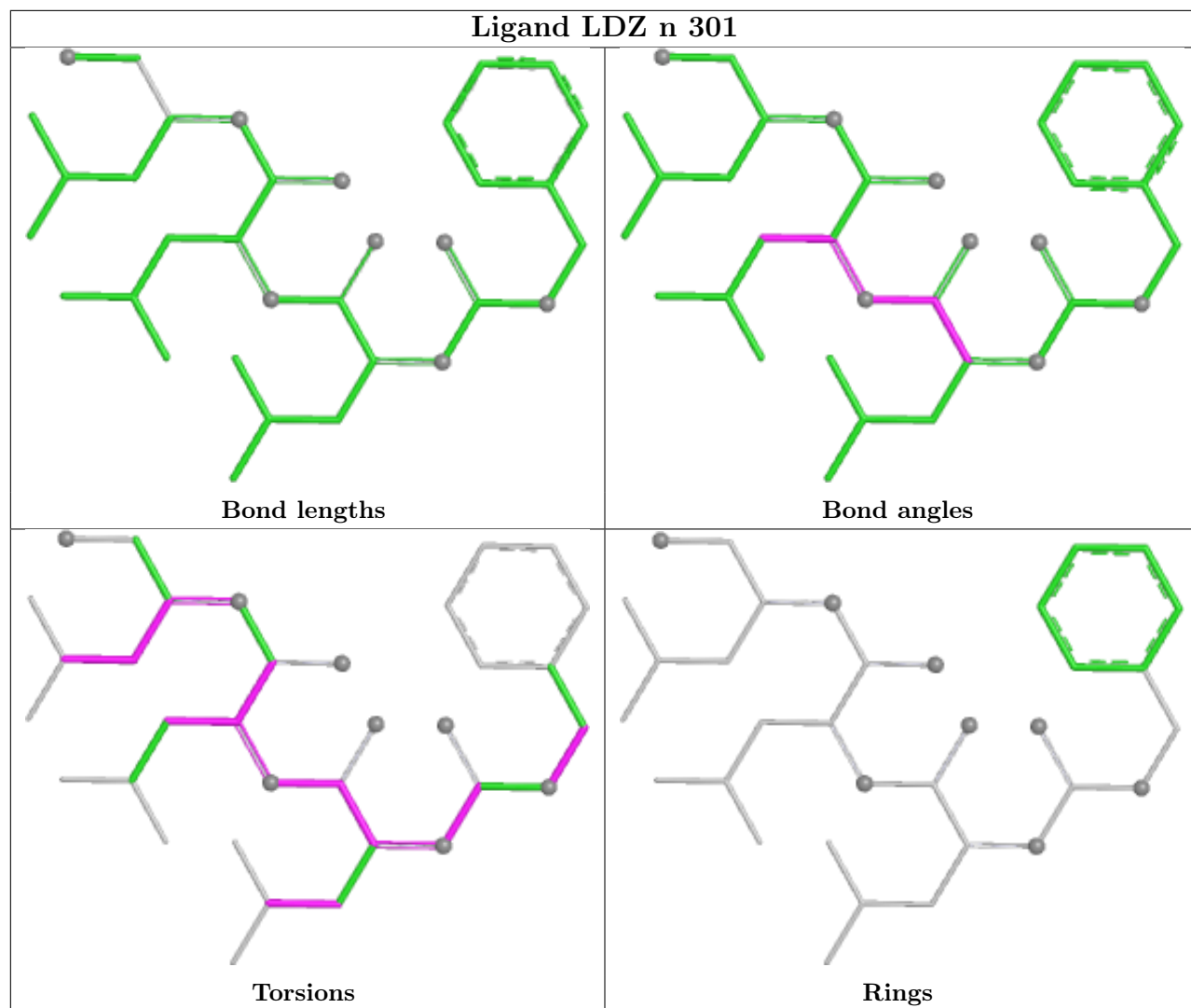
Continued from previous page...

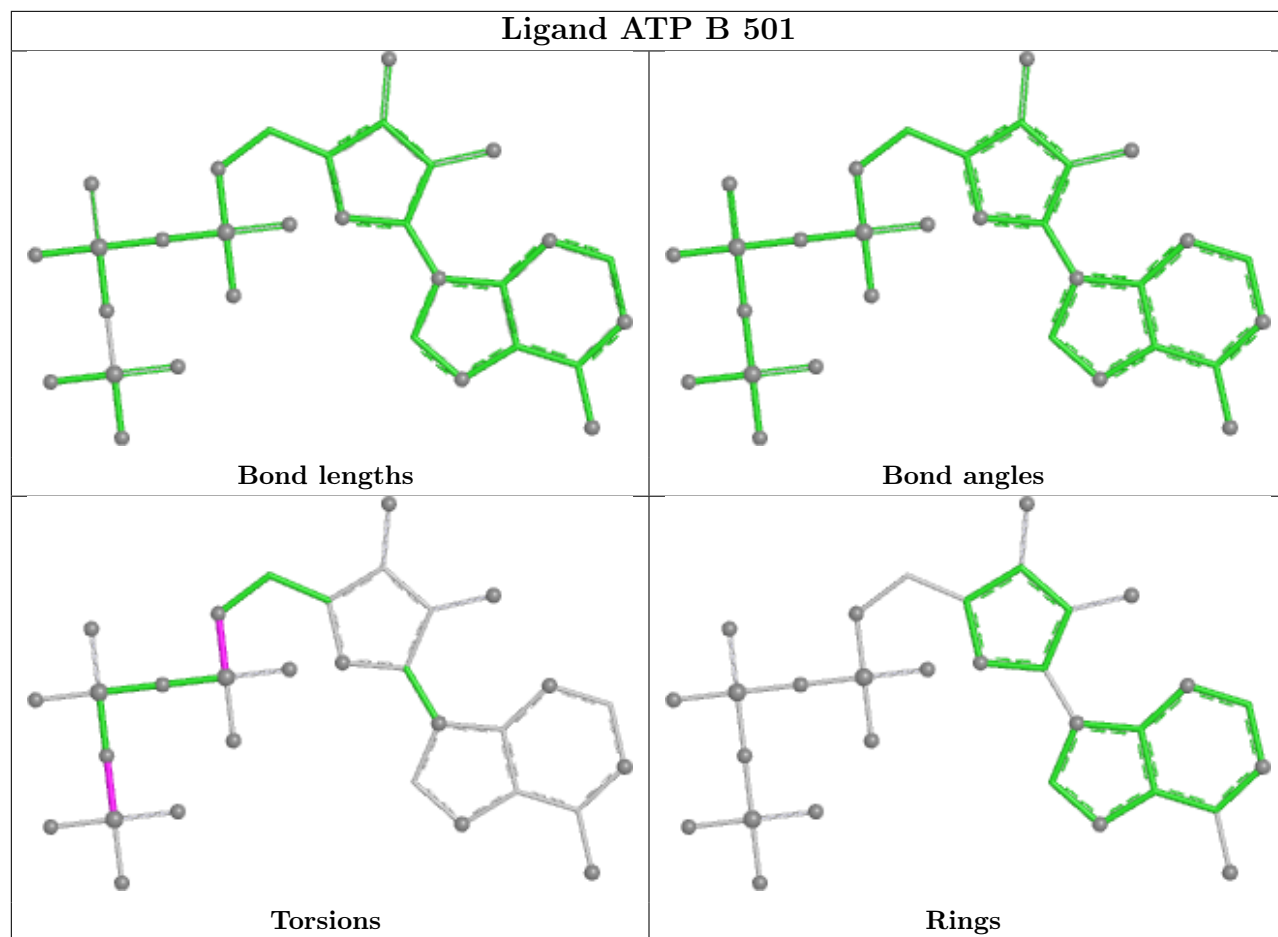
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	B	501	ATP	3	0
38	o	301	LDZ	1	0
38	N	301	LDZ	3	0
38	O	301	LDZ	4	0
38	r	301	LDZ	2	0
38	R	301	LDZ	3	0

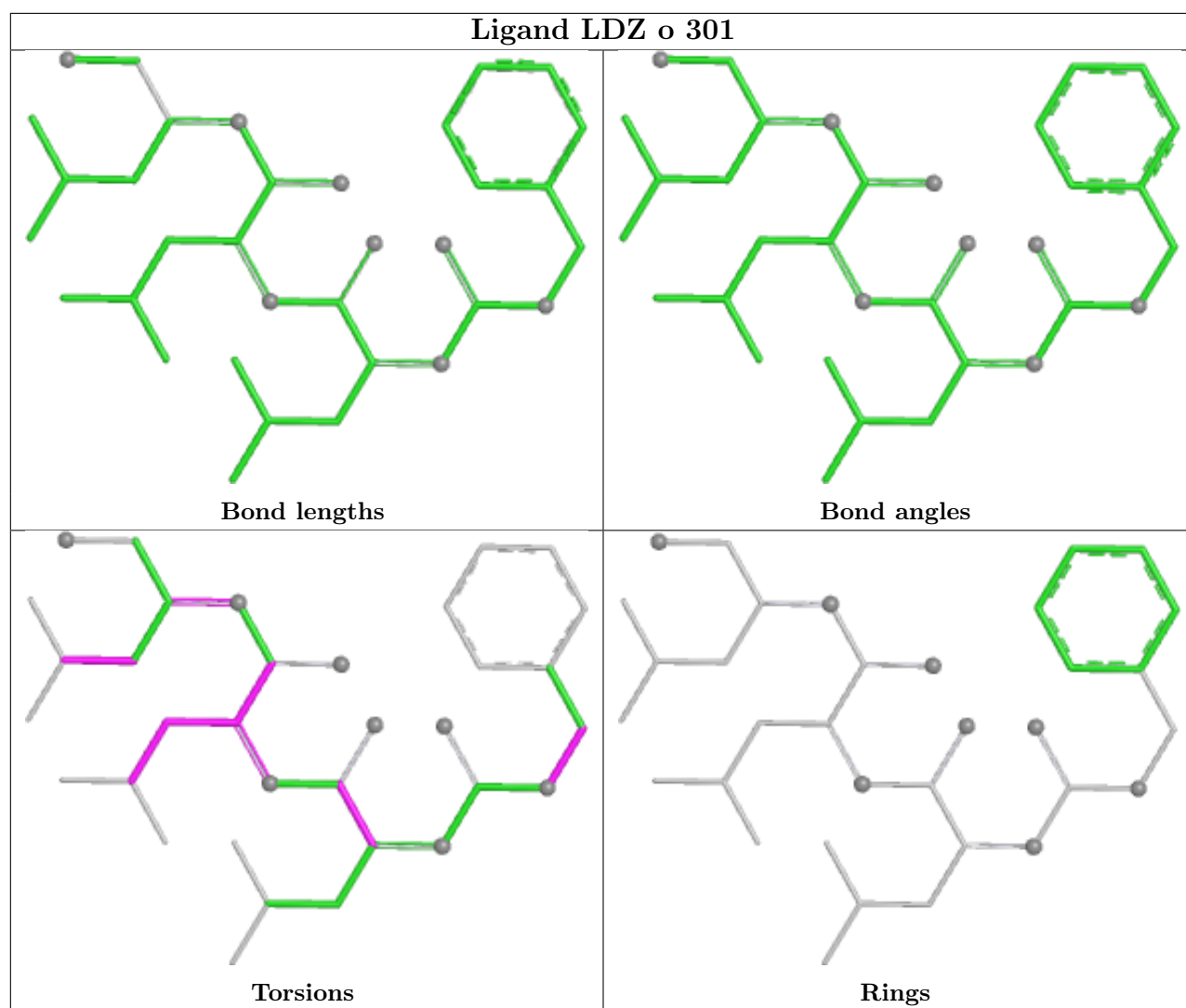
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

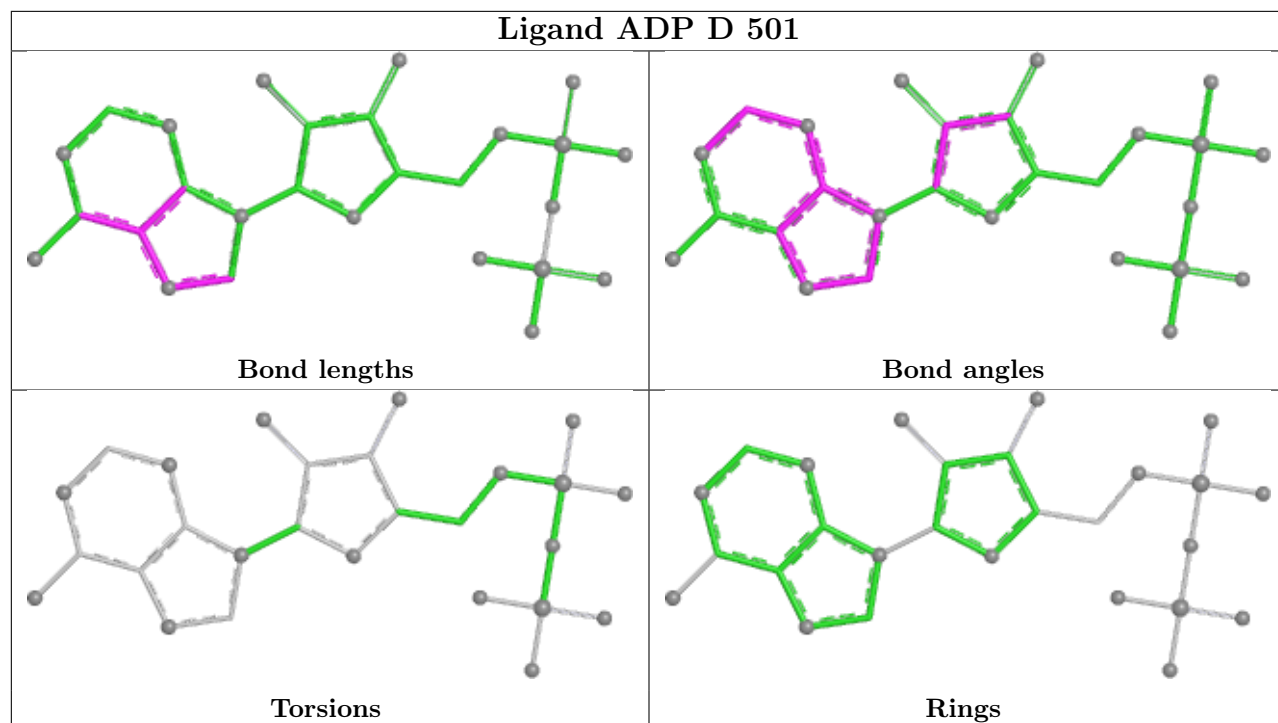


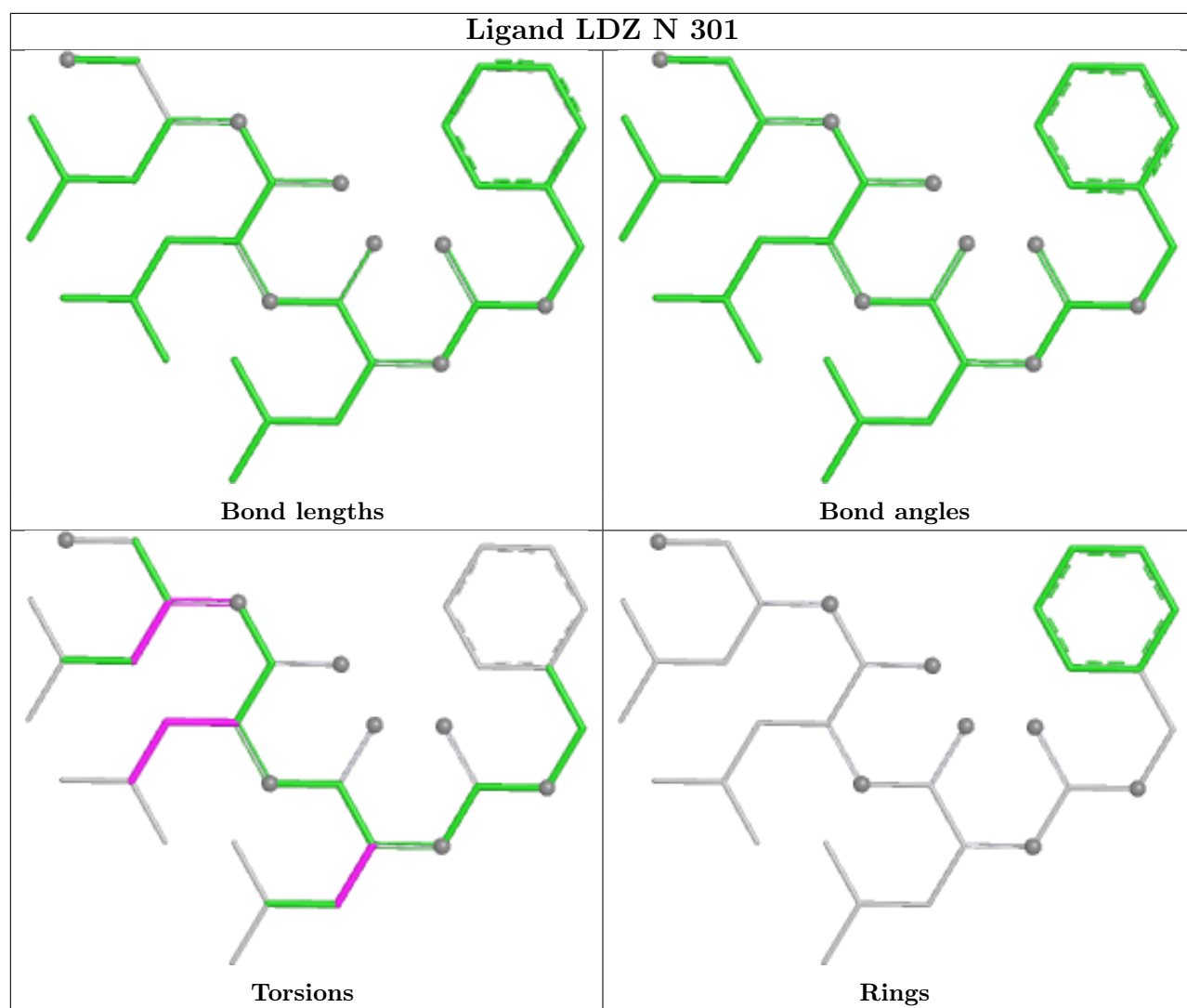


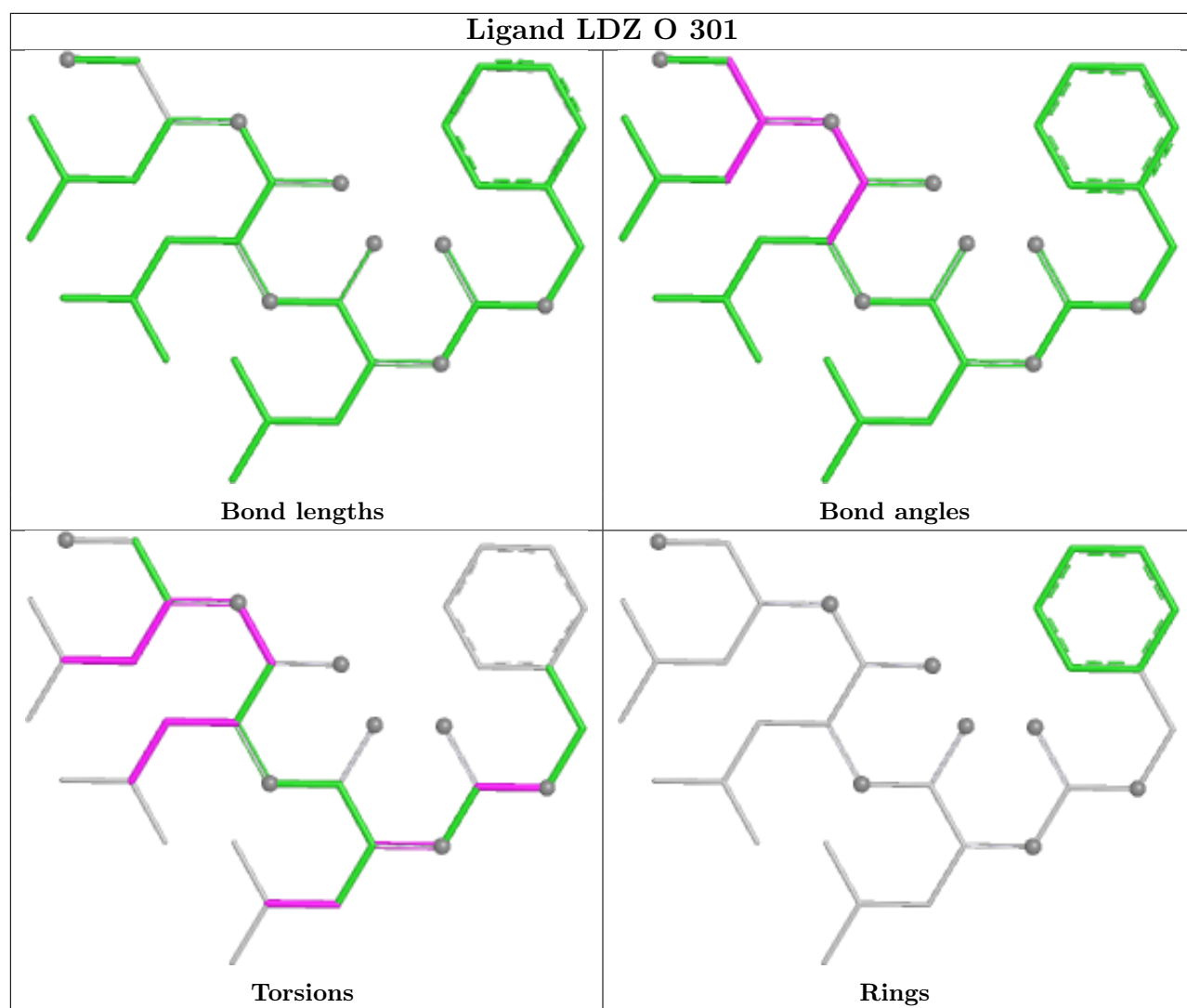


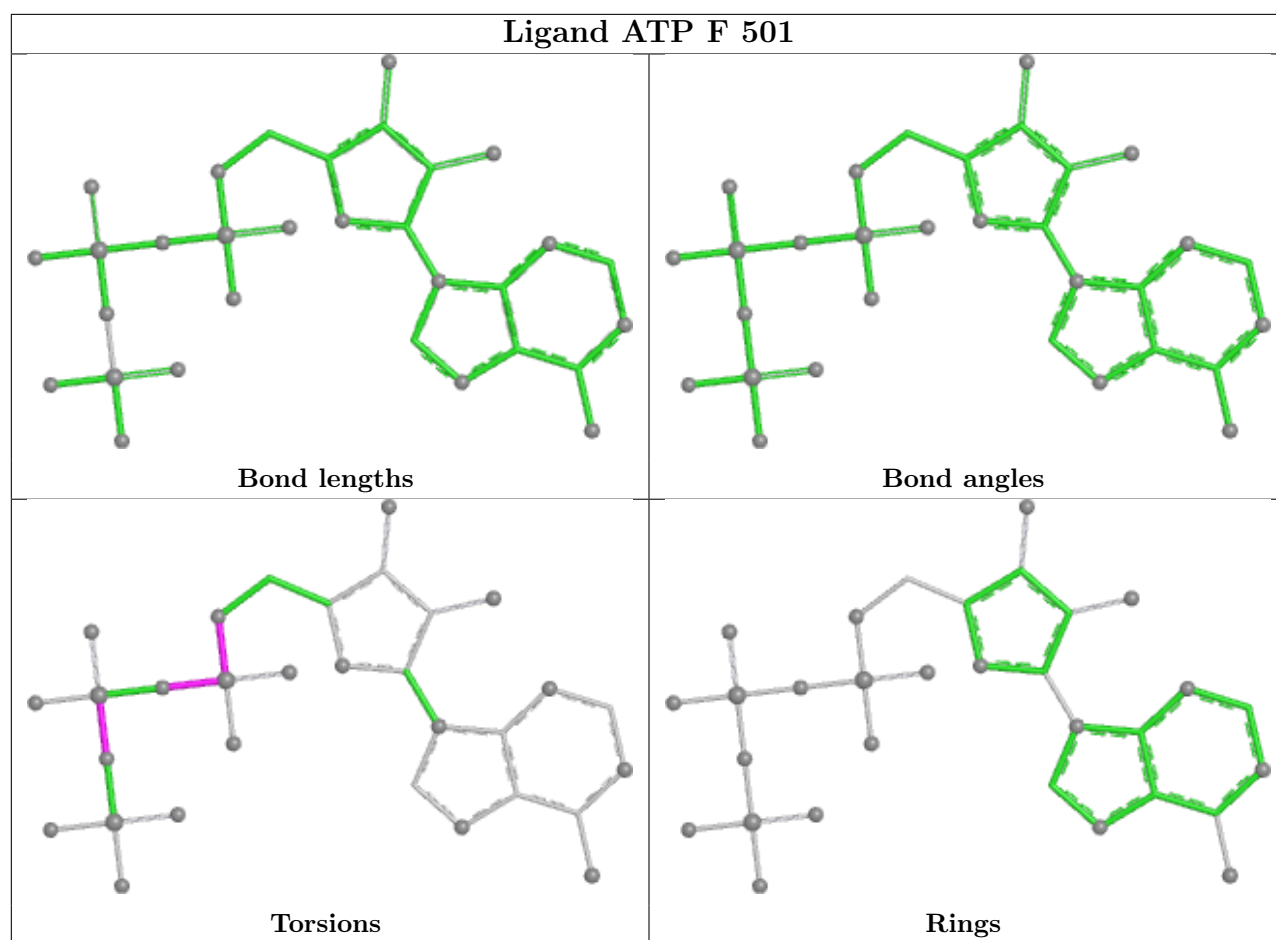


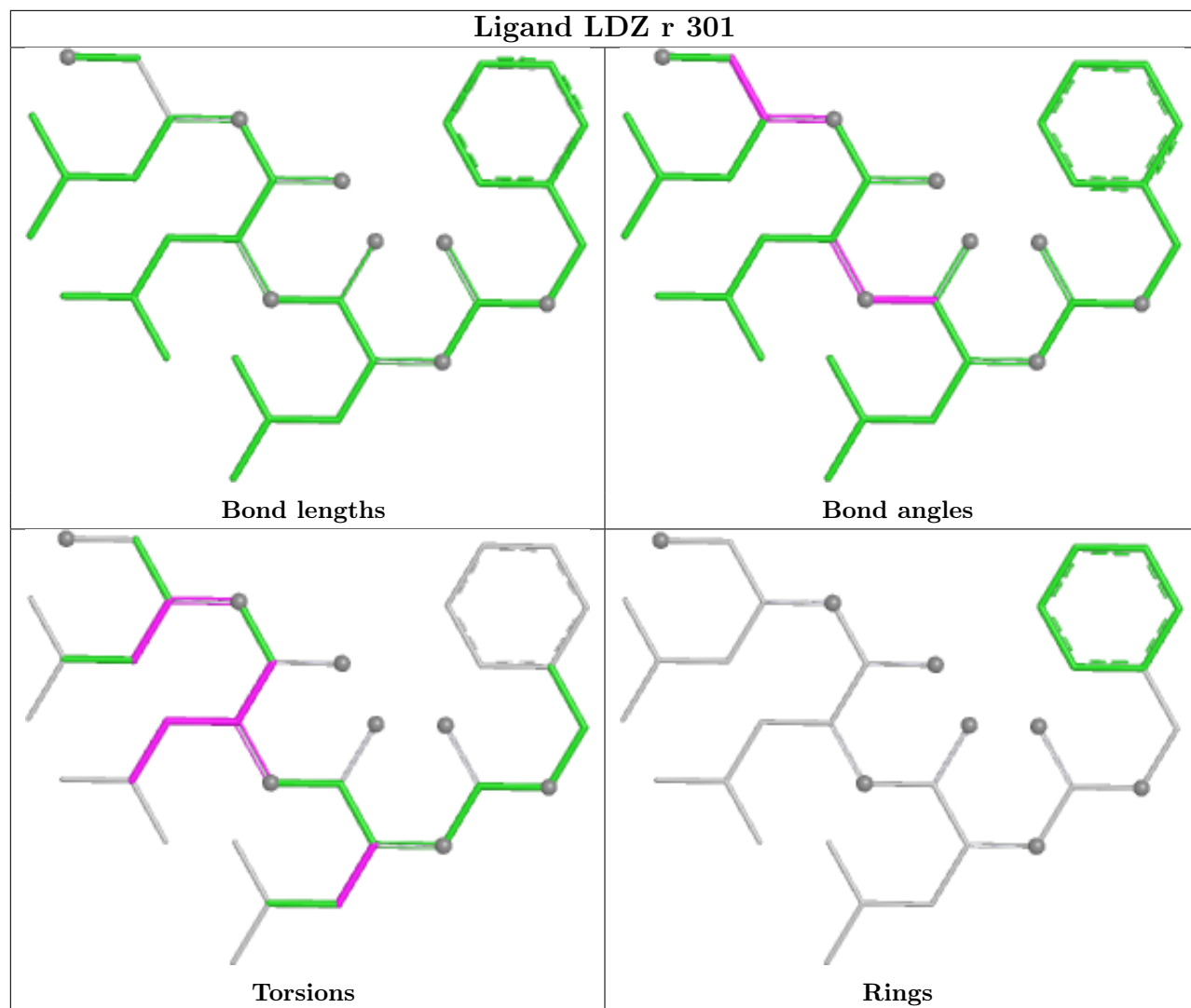


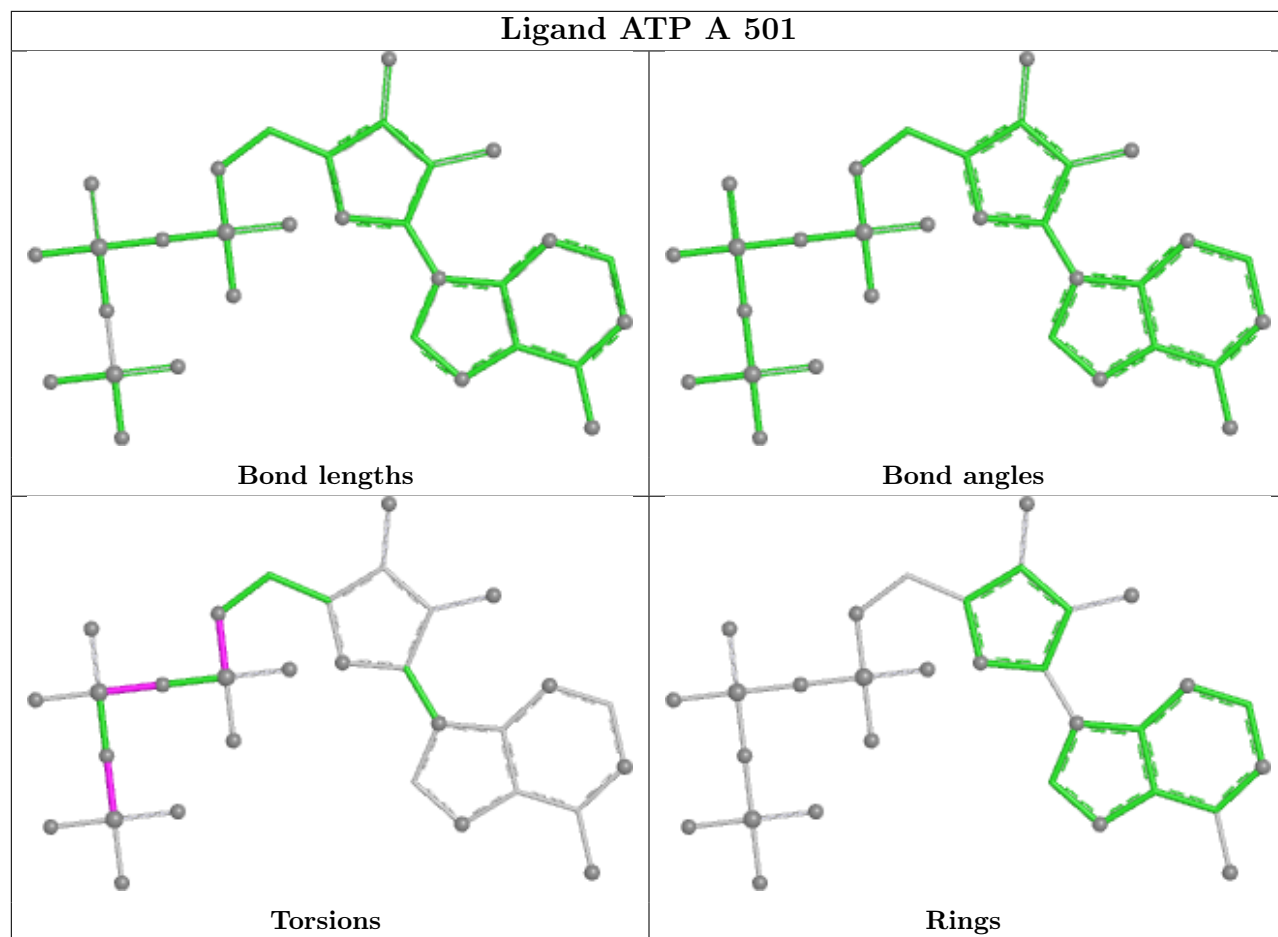


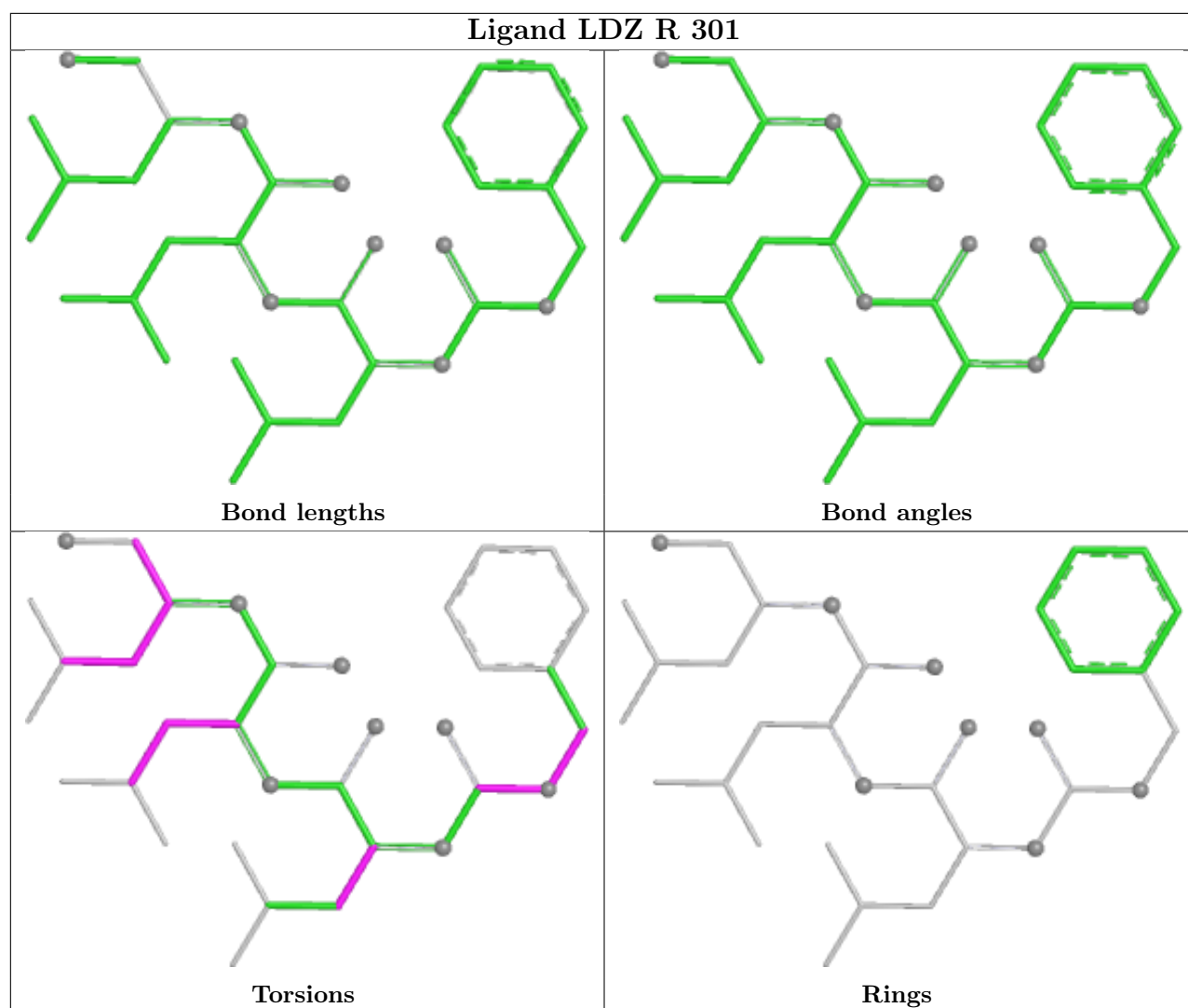












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

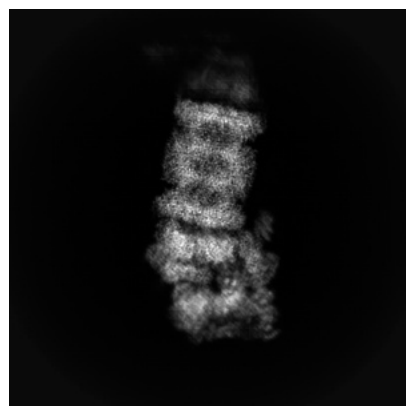
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-68472. These allow visual inspection of the internal detail of the map and identification of artifacts.

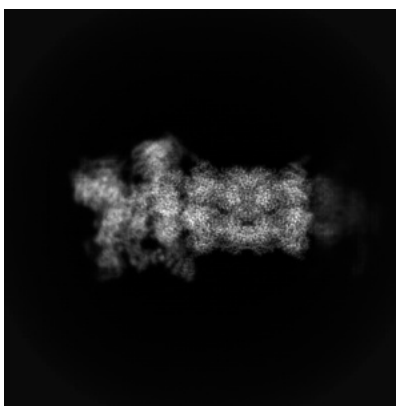
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

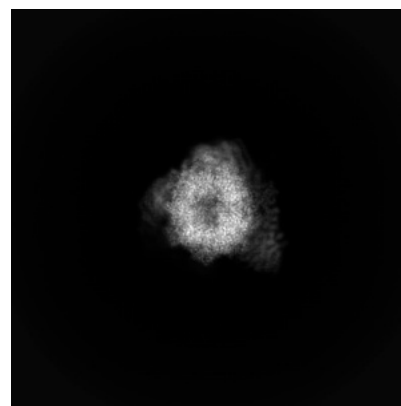
6.1.1 Primary map



X

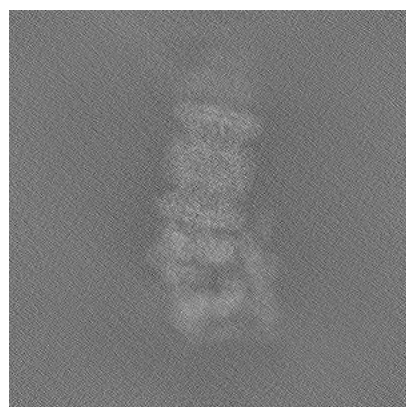


Y

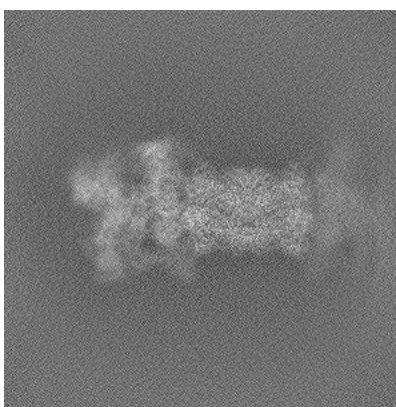


Z

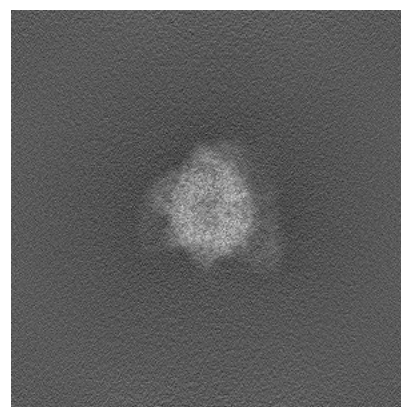
6.1.2 Raw map



X



Y

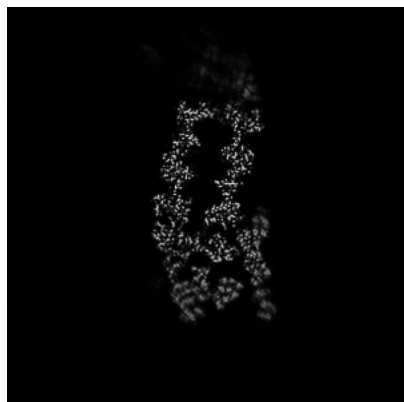


Z

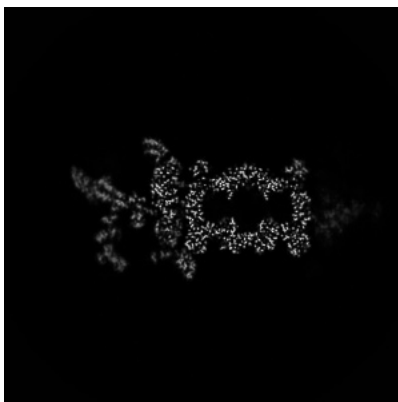
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

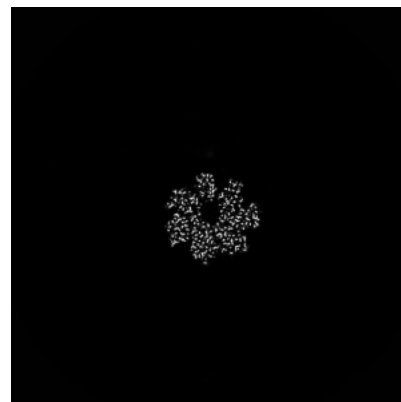
6.2.1 Primary map



X Index: 300

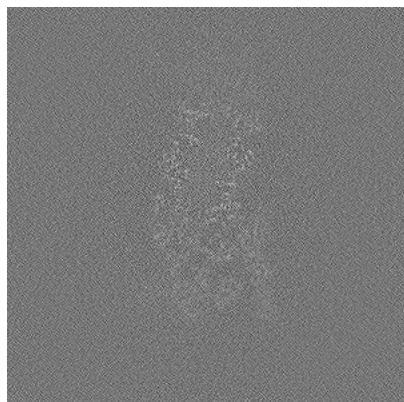


Y Index: 300

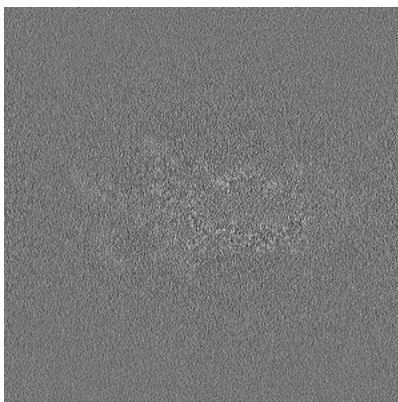


Z Index: 300

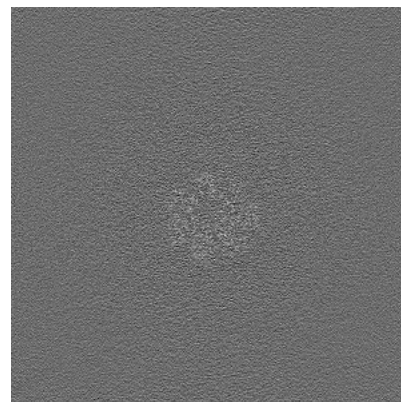
6.2.2 Raw map



X Index: 300



Y Index: 300

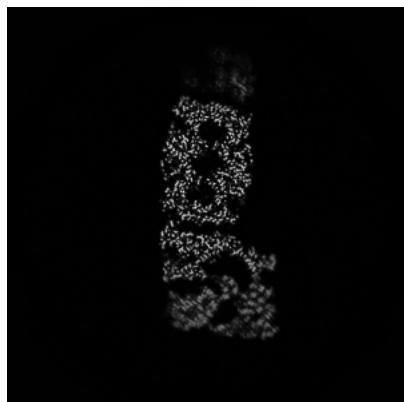


Z Index: 300

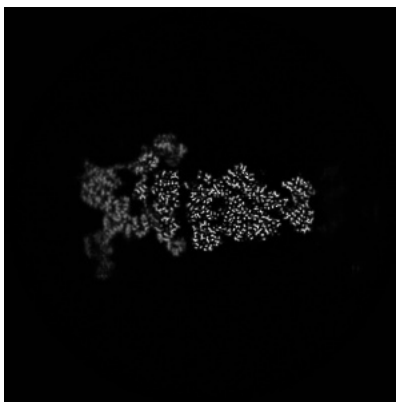
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

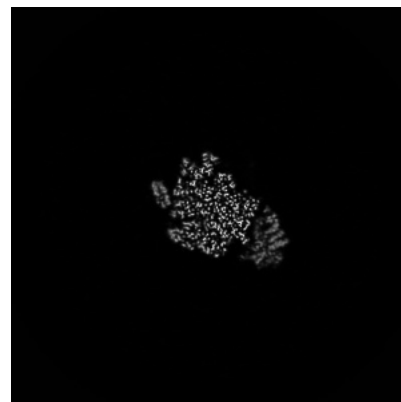
6.3.1 Primary map



X Index: 320

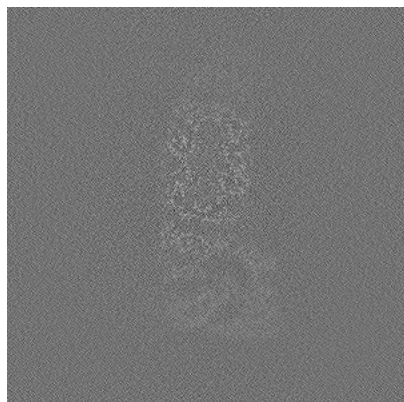


Y Index: 264

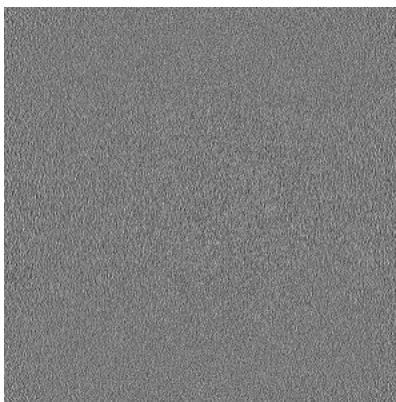


Z Index: 246

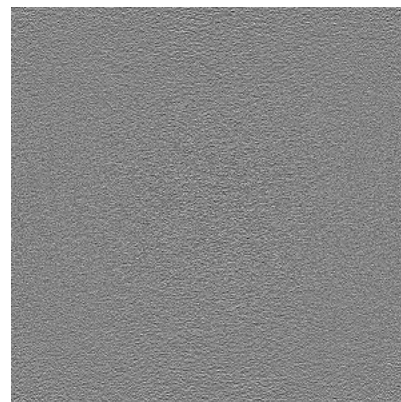
6.3.2 Raw map



X Index: 320



Y Index: 0

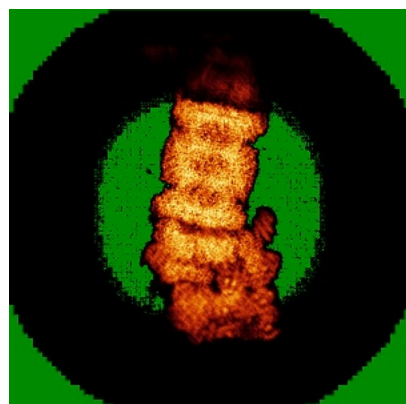


Z Index: 0

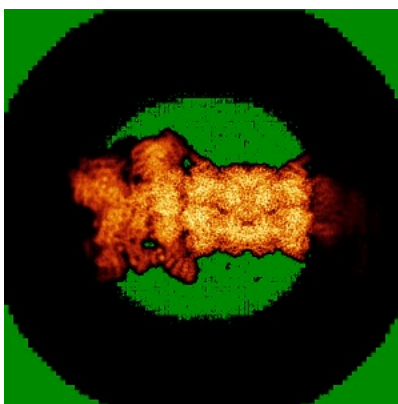
The images above show the largest variance slices of the map in three orthogonal directions.

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

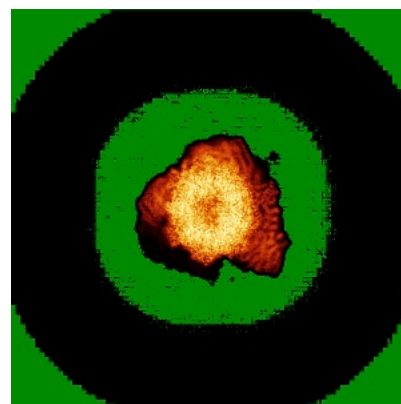
6.4.1 Primary map



X

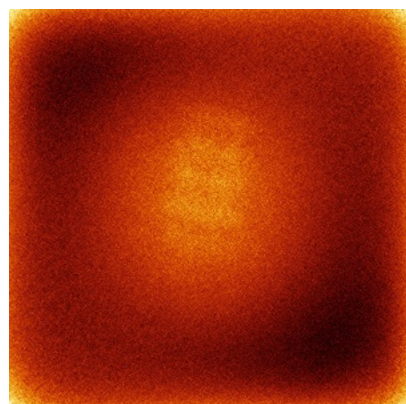


Y

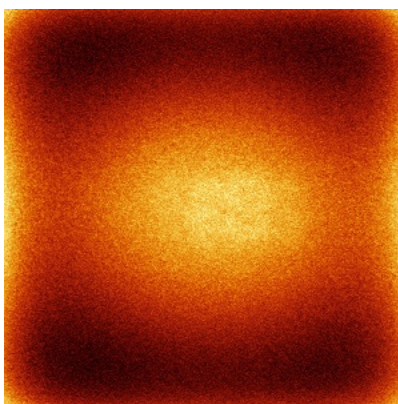


Z

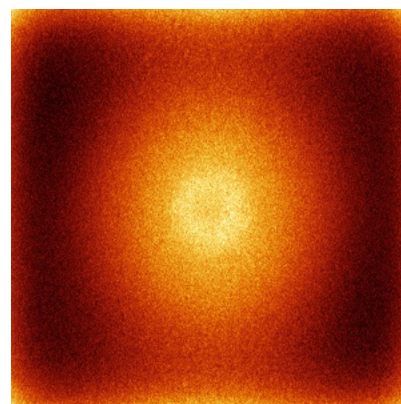
6.4.2 Raw map



X



Y

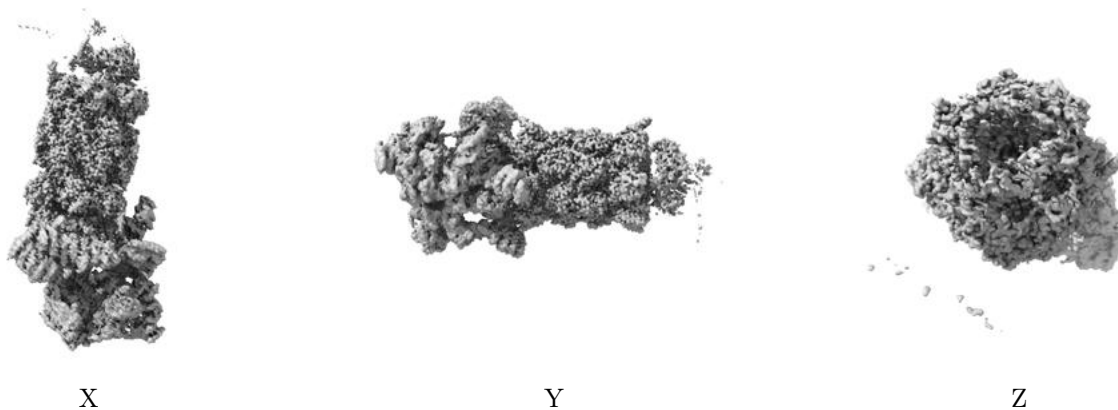


Z

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.

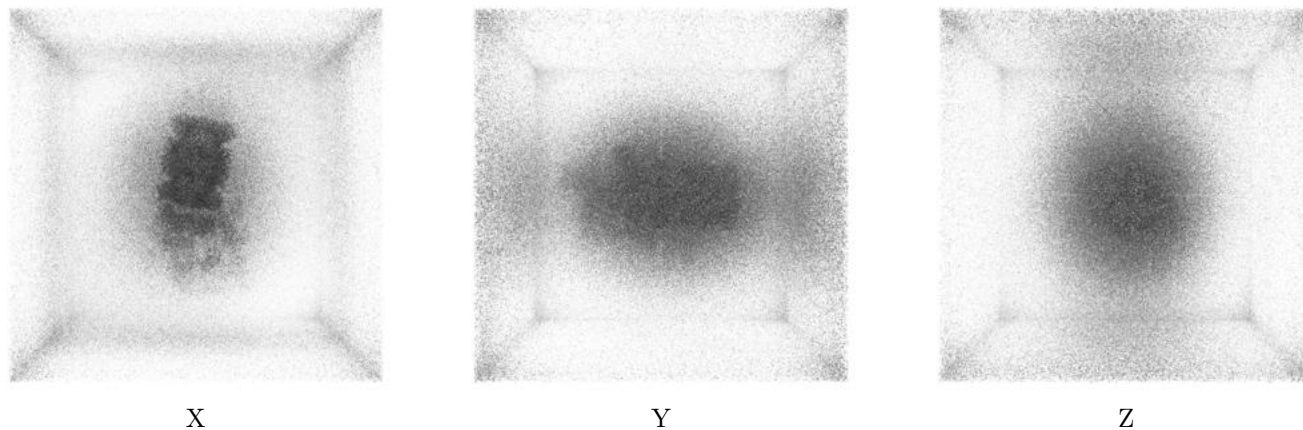
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

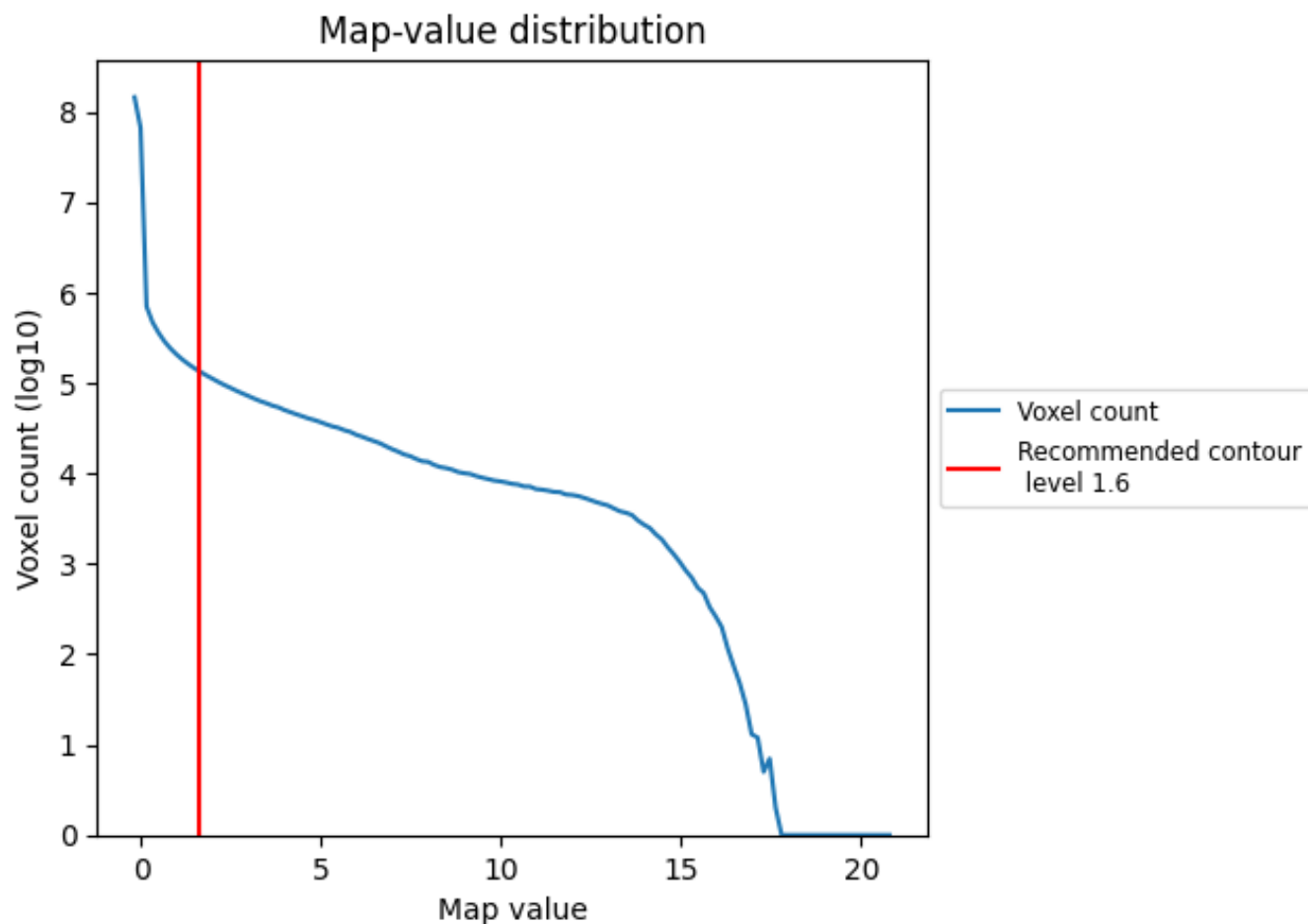
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

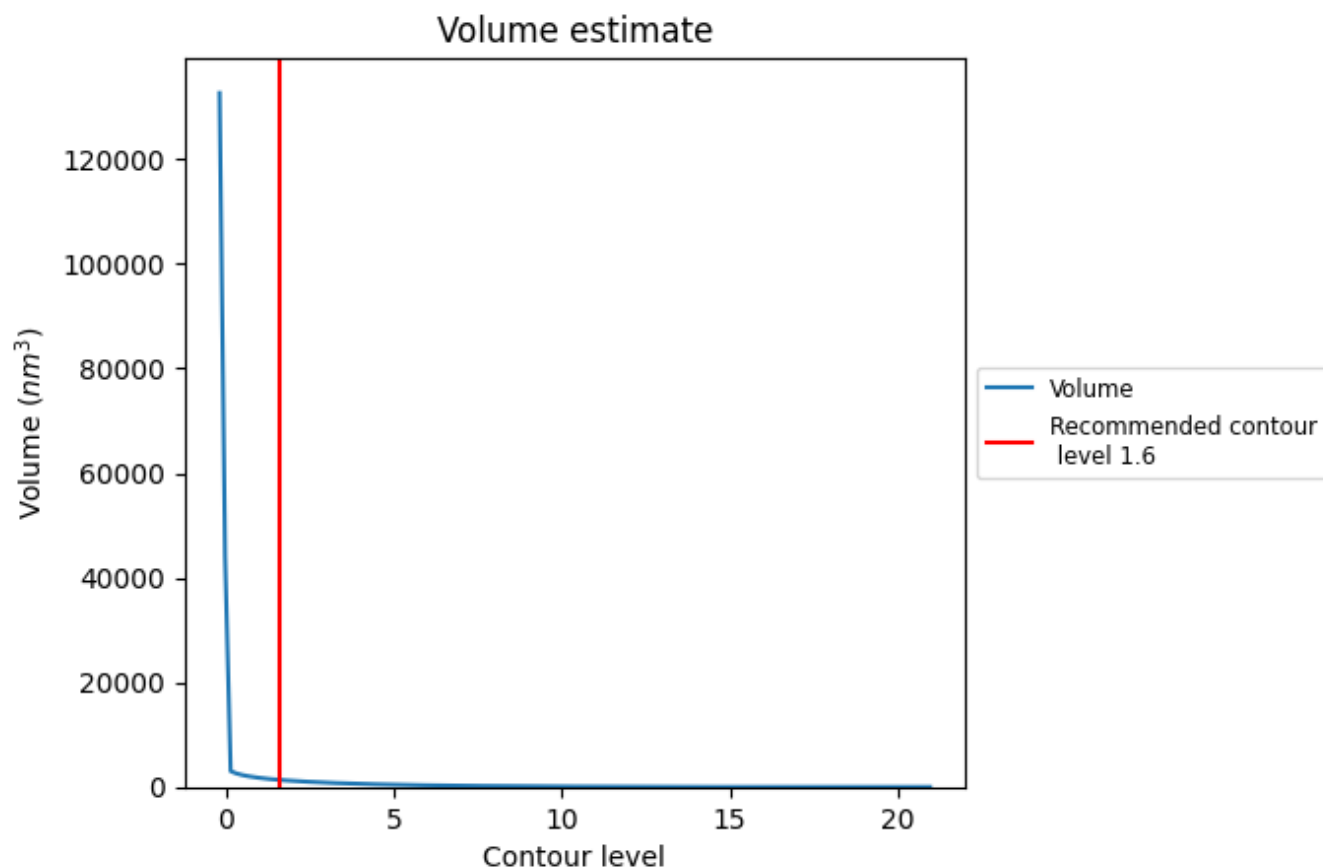
This section contains the results of statistical analysis of the map.

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.

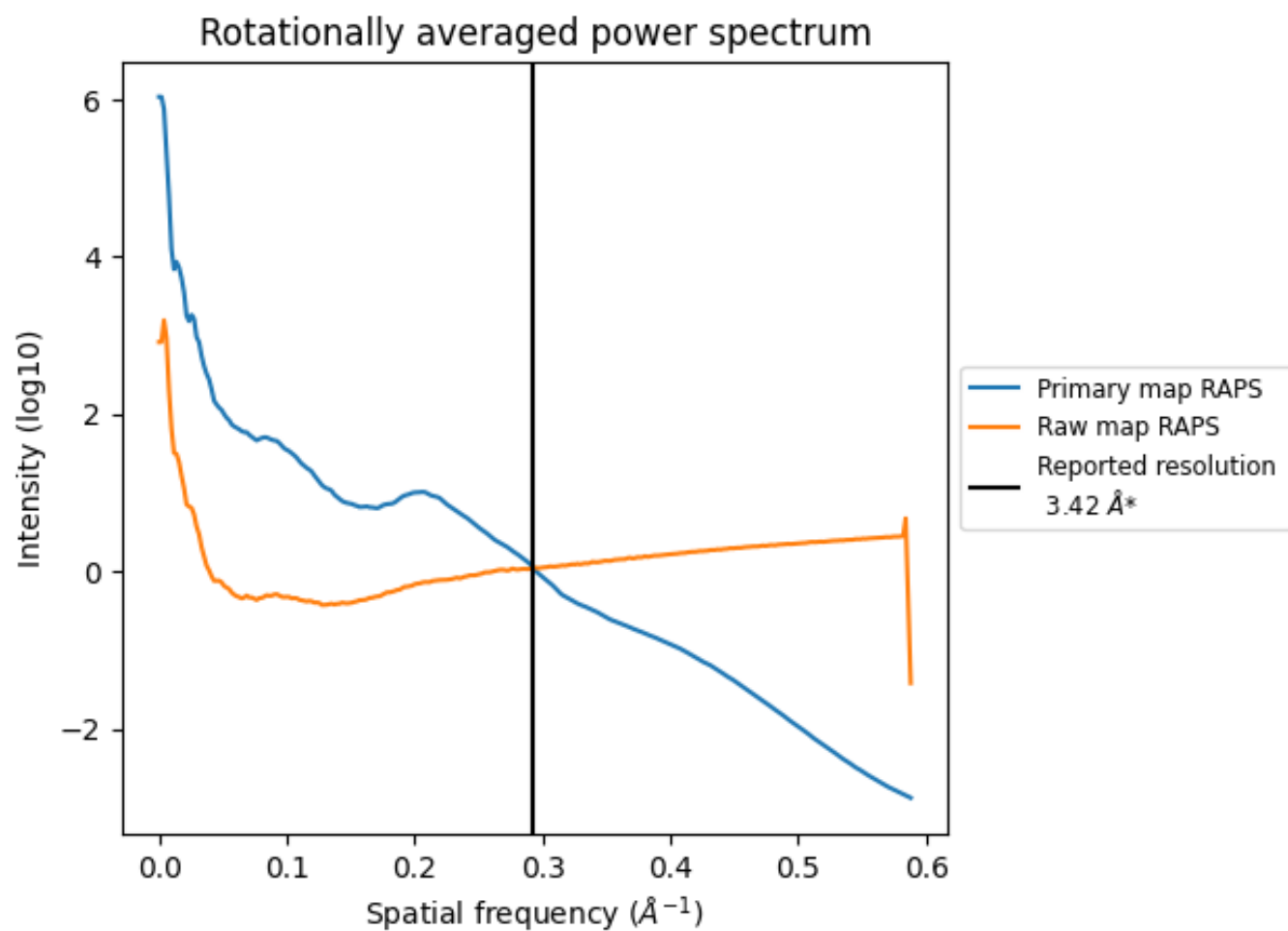
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1351 nm^3 ; this corresponds to an approximate mass of 1221 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 ⓘ

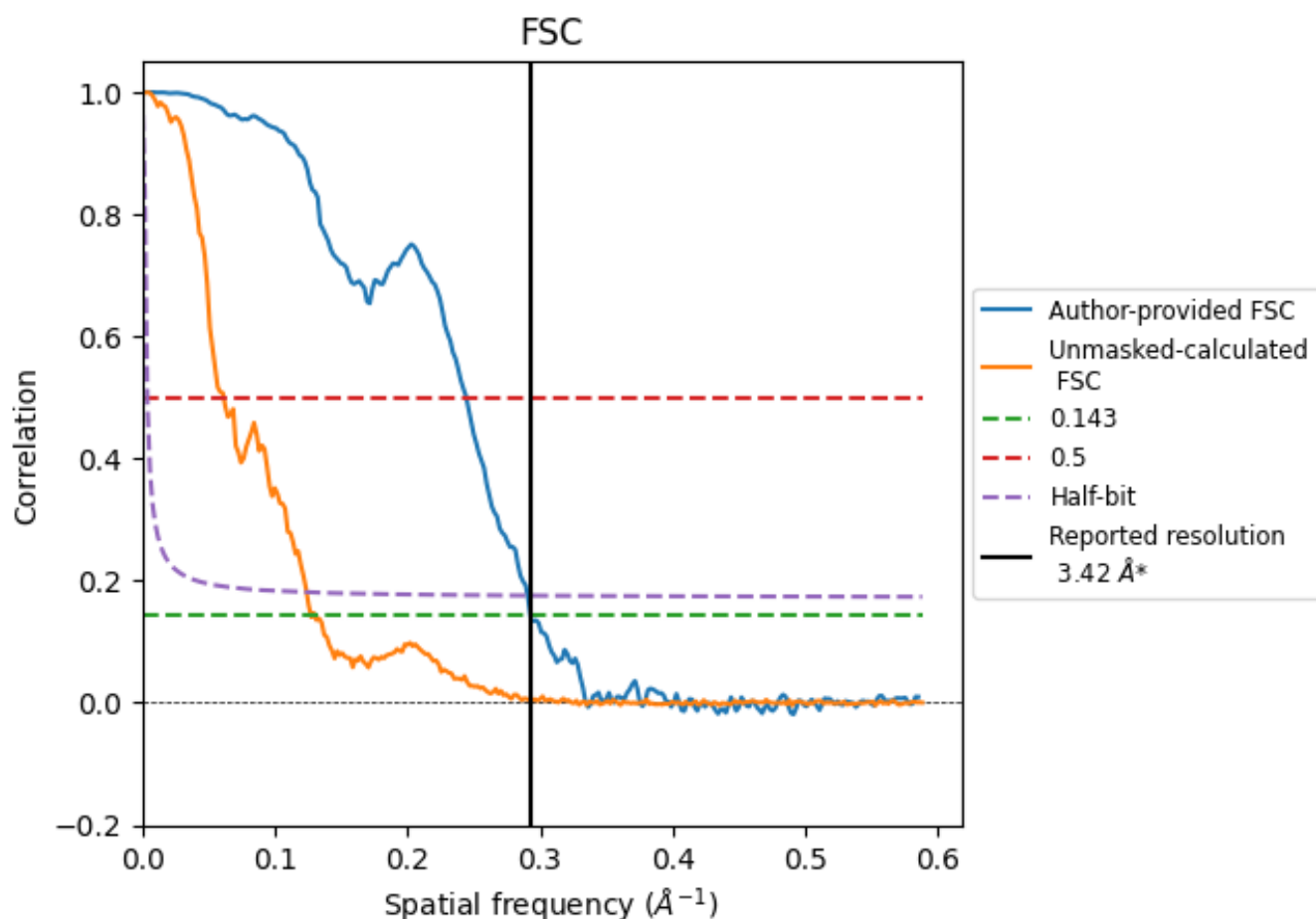


*Reported resolution corresponds to spatial frequency of 0.292 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.292 \AA^{-1}

8.2 Resolution estimates [i](#)

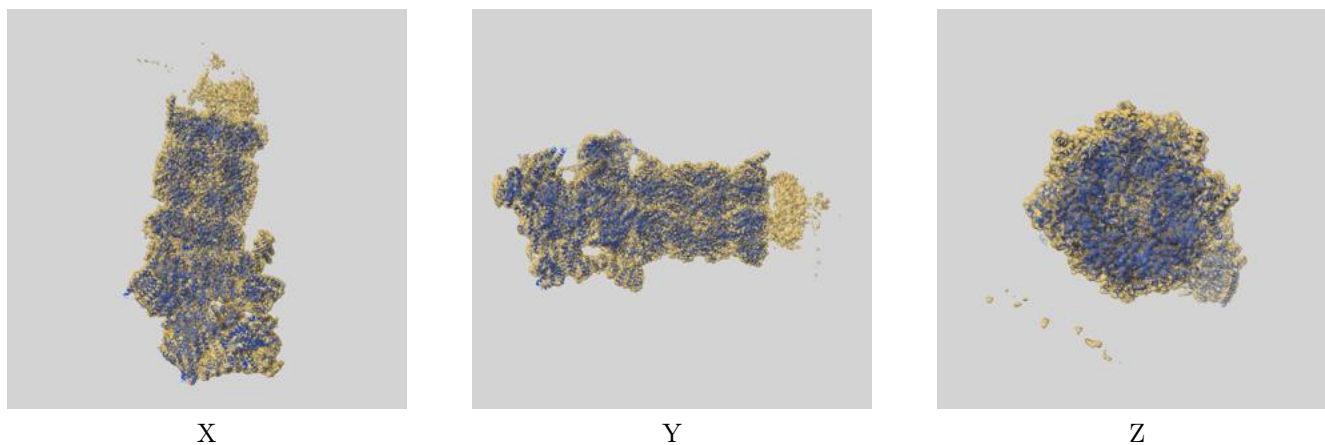
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.42	4.09	3.44
Unmasked-calculated*	7.86	16.29	8.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.86 differs from the reported value 3.42 by more than 10 %

9 Map-model fit [i](#)

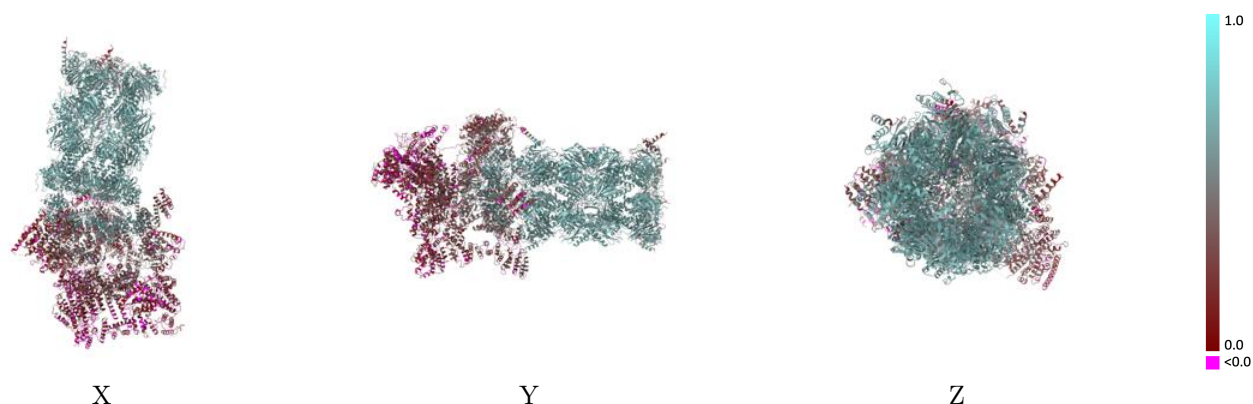
This section contains information regarding the fit between EMDB map EMD-68472 and PDB model 22MM. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



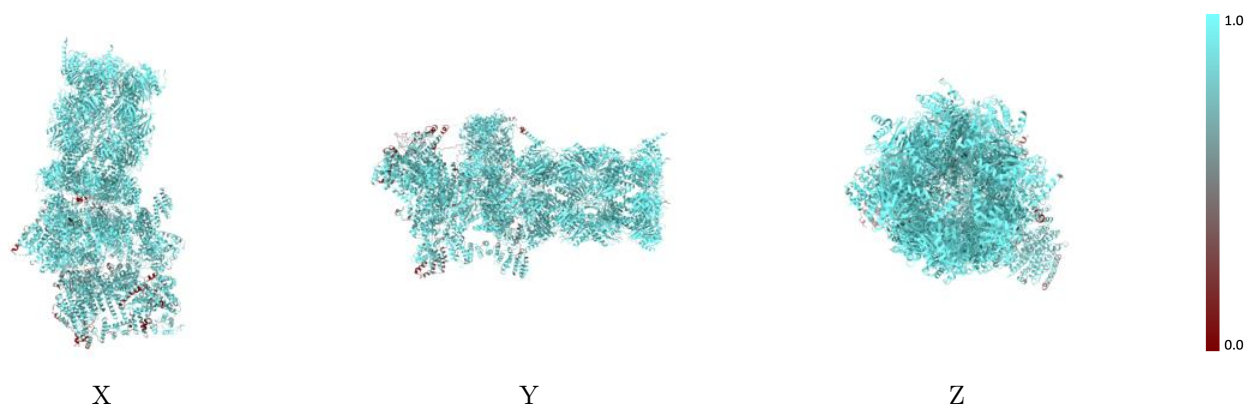
The images above show the 3D surface view of the map at the recommended contour level 1.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



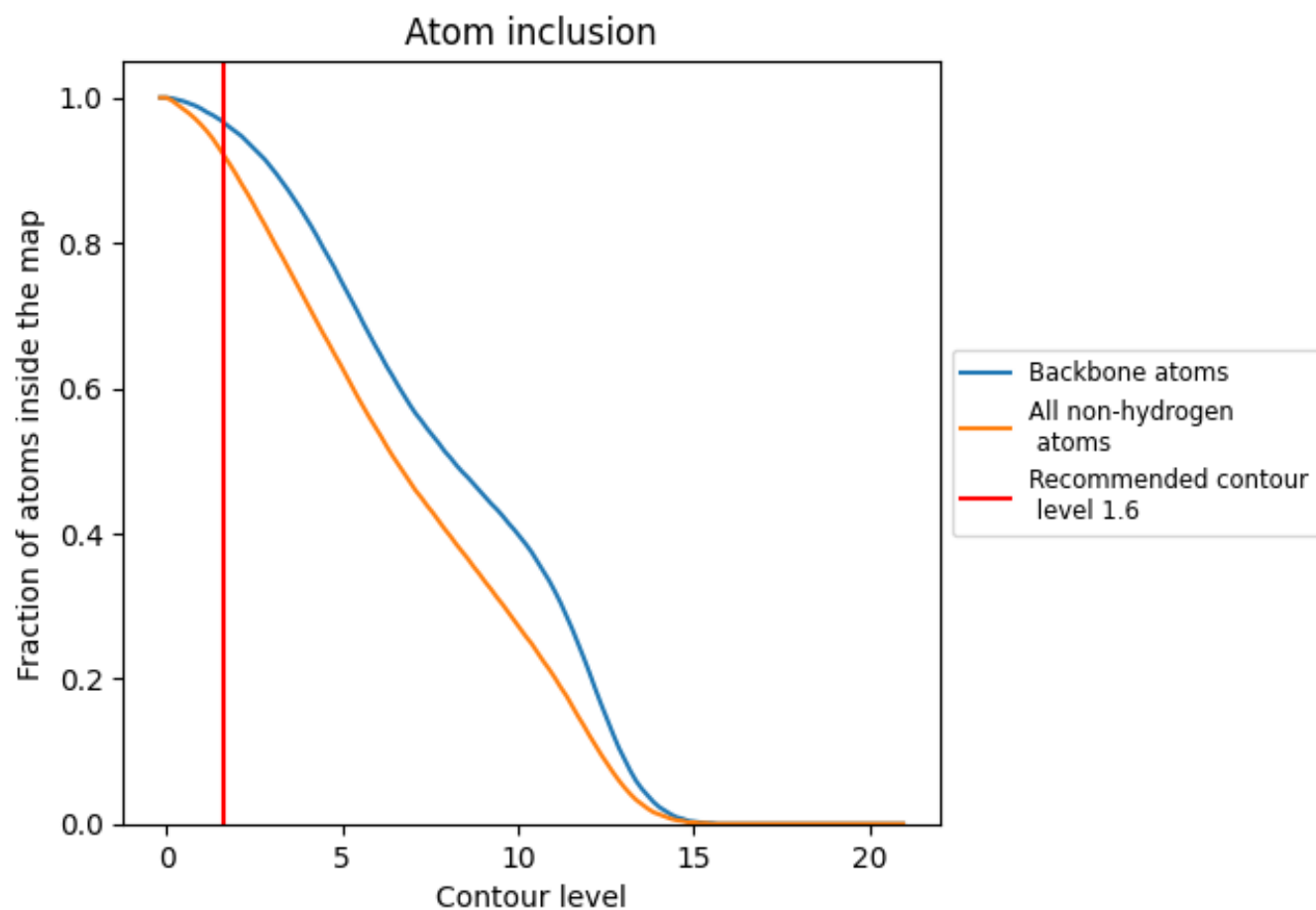
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.6).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (1.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9230	 0.4450
A	 0.9360	 0.4690
B	 0.9490	 0.5070
C	 0.9520	 0.5030
D	 0.9450	 0.4750
E	 0.8290	 0.2950
F	 0.9030	 0.3670
G	 0.9900	 0.6350
H	 0.9910	 0.6450
I	 0.9750	 0.6210
J	 0.9420	 0.5940
K	 0.9890	 0.6470
L	 0.9910	 0.6510
M	 0.9840	 0.6350
N	 0.9890	 0.6630
O	 0.9860	 0.6470
P	 0.9970	 0.6600
Q	 0.9950	 0.6610
R	 0.9890	 0.6630
S	 0.9950	 0.6680
T	 0.9970	 0.6630
U	 0.8000	 0.1400
V	 0.8090	 0.1520
W	 0.8750	 0.2220
X	 0.9300	 0.3610
Y	 0.9020	 0.2930
Z	 0.9230	 0.2240
a	 0.7090	 0.1280
c	 0.8230	 0.1570
d	 0.8210	 0.1530
e	 0.7510	 0.1290
f	 0.6350	 0.2000
g	 0.9820	 0.6120
h	 0.9730	 0.6000
i	 0.9670	 0.5660



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Chain	Atom inclusion	Q-score
j	 0.9610	 0.5210
k	 0.9530	 0.5720
l	 0.9830	 0.6150
m	 0.9810	 0.6000
n	 0.9860	 0.6600
o	 0.9890	 0.6370
p	 0.9940	 0.6560
q	 0.9950	 0.6590
r	 0.9880	 0.6560
s	 0.9940	 0.6620
t	 0.9960	 0.6650
u	 0.9050	 0.2610