



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:09 AM UTC

PDB ID : 9E8L / pdb_00009e8l
EMDB ID : EMD-47724
Title : Nub1/Fat10-processing human 26S proteasome bound to Txnl1 with Rpt4 at top of spiral staircase
Authors : Arkinson, C.; Gee, C.L.; Martin, A.
Deposited on : 2024-11-05
Resolution : 3.59 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:

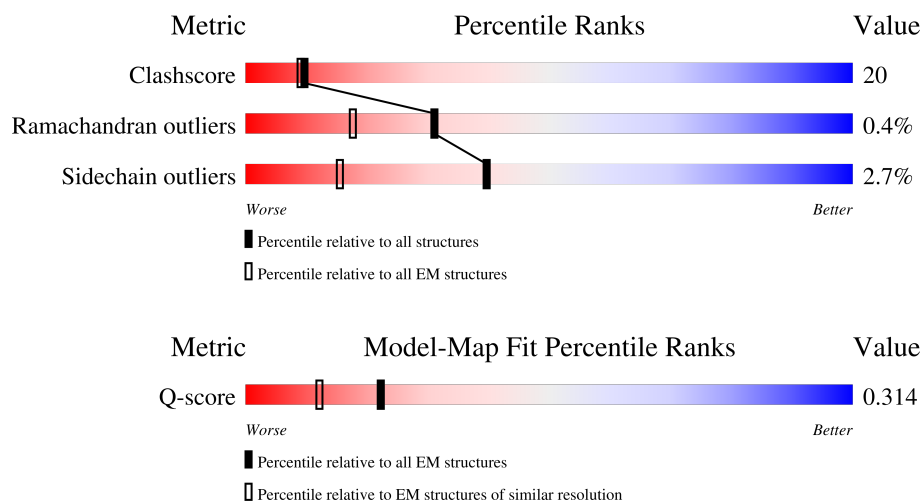
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.59 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	12565 (3.09 - 4.09)

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

Mol	Chain	Length	Quality of chain
1	A	433	23% 52% 41% 6%
2	B	440	25% 44% 37% 16%
3	C	406	33% 52% 41% 5%
4	D	418	30% 46% 39% 13%

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Mol	Chain	Length	Quality of chain
5	E	389	
6	F	439	
7	G	246	
8	H	234	
9	I	261	
10	J	248	
11	K	241	
12	L	263	
13	M	255	
14	U	953	
15	V	534	
16	W	456	
17	X	422	
18	Y	389	
19	Z	324	
20	a	376	
21	b	377	
22	c	424	
23	d	350	
24	e	70	
25	f	908	
26	g	601	
27	u	289	
28	v	14	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 70522 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 regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	407	Total	C	N	O	S	0	0
			3196	2012	561	605	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	371	Total	C	N	O	S	0	0
			2917	1840	498	565	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	386	Total	C	N	O	S	0	0
			3053	1921	547	567	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	362	Total	C	N	O	S	0	0
			2889	1828	503	547	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	368	Total	C	N	O	S	0	0
			2932	1846	522	548	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	367	Total	C	N	O	S	0	0
			2877	1818	498	544	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1820	1157	304	346	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	230	Total	C	N	O	S	0	0
			1717	1091	291	330	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	163	HIS	MET	conflict	UNP P25787

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	248	Total	C	N	O	S	0	0
			1895	1195	324	368	8		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	228	Total	C	N	O	S	0	0
			1729	1086	284	349	10		

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

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

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

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

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	839	Total	C	N	O	S	0	0
			6538	4150	1111	1233	44		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	439	Total	C	N	O	S	0	0
			3525	2239	623	650	13		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	438	Total	C	N	O	S	0	0
			3570	2261	609	677	23		

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	378	Total	C	N	O	S	0	0
			2994	1909	507	566	12		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	380	Total	C	N	O	S	0	0
			3127	1995	535	580	17		

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	272	Total	C	N	O	S	0	0
			2153	1363	370	403	17		

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	311	LEU	-	expression tag	UNP O00487
c	312	ILE	-	expression tag	UNP O00487
c	313	ASN	-	expression tag	UNP O00487
c	314	HIS	-	expression tag	UNP O00487
c	315	HIS	-	expression tag	UNP O00487
c	316	HIS	-	expression tag	UNP O00487
c	317	HIS	-	expression tag	UNP O00487
c	318	HIS	-	expression tag	UNP O00487
c	319	HIS	-	expression tag	UNP O00487
c	320	ASP	-	expression tag	UNP O00487
c	321	TYR	-	expression tag	UNP O00487
c	322	ASP	-	expression tag	UNP O00487
c	323	ILE	-	expression tag	UNP O00487
c	324	PRO	-	expression tag	UNP O00487
c	325	THR	-	expression tag	UNP O00487
c	326	THR	-	expression tag	UNP O00487
c	327	ALA	-	expression tag	UNP O00487
c	328	SER	-	expression tag	UNP O00487
c	329	GLU	-	expression tag	UNP O00487
c	330	ASN	-	expression tag	UNP O00487
c	331	LEU	-	expression tag	UNP O00487
c	332	TYR	-	expression tag	UNP O00487
c	333	PHE	-	expression tag	UNP O00487
c	334	GLN	-	expression tag	UNP O00487
c	335	GLY	-	expression tag	UNP O00487

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Chain	Residue	Modelled	Actual	Comment	Reference
c	336	GLU	-	expression tag	UNP O00487
c	337	LEU	-	expression tag	UNP O00487
c	338	GLY	-	expression tag	UNP O00487
c	339	MET	-	expression tag	UNP O00487
c	340	ARG	-	expression tag	UNP O00487
c	341	GLY	-	expression tag	UNP O00487
c	342	SER	-	expression tag	UNP O00487
c	343	ALA	-	expression tag	UNP O00487
c	344	GLY	-	expression tag	UNP O00487
c	345	LYS	-	expression tag	UNP O00487
c	346	ALA	-	expression tag	UNP O00487
c	347	GLY	-	expression tag	UNP O00487
c	348	GLU	-	expression tag	UNP O00487
c	349	GLY	-	expression tag	UNP O00487
c	350	GLU	-	expression tag	UNP O00487
c	351	ILE	-	expression tag	UNP O00487
c	352	PRO	-	expression tag	UNP O00487
c	353	ALA	-	expression tag	UNP O00487
c	354	PRO	-	expression tag	UNP O00487
c	355	LEU	-	expression tag	UNP O00487
c	356	ALA	-	expression tag	UNP O00487
c	357	GLY	-	expression tag	UNP O00487
c	358	THR	-	expression tag	UNP O00487
c	359	VAL	-	expression tag	UNP O00487
c	360	SER	-	expression tag	UNP O00487
c	361	LYS	-	expression tag	UNP O00487
c	362	ILE	-	expression tag	UNP O00487
c	363	LEU	-	expression tag	UNP O00487
c	364	VAL	-	expression tag	UNP O00487
c	365	LYS	-	expression tag	UNP O00487
c	366	GLU	-	expression tag	UNP O00487
c	367	GLY	-	expression tag	UNP O00487
c	368	ASP	-	expression tag	UNP O00487
c	369	THR	-	expression tag	UNP O00487
c	370	VAL	-	expression tag	UNP O00487
c	371	LYS	-	expression tag	UNP O00487
c	372	ALA	-	expression tag	UNP O00487
c	373	GLY	-	expression tag	UNP O00487
c	374	GLN	-	expression tag	UNP O00487
c	375	THR	-	expression tag	UNP O00487
c	376	VAL	-	expression tag	UNP O00487
c	377	LEU	-	expression tag	UNP O00487

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Chain	Residue	Modelled	Actual	Comment	Reference
c	378	VAL	-	expression tag	UNP O00487
c	379	LEU	-	expression tag	UNP O00487
c	380	GLU	-	expression tag	UNP O00487
c	381	ALA	-	expression tag	UNP O00487
c	382	MET	-	expression tag	UNP O00487
c	383	LYS	-	expression tag	UNP O00487
c	384	MET	-	expression tag	UNP O00487
c	385	GLU	-	expression tag	UNP O00487
c	386	THR	-	expression tag	UNP O00487
c	387	GLU	-	expression tag	UNP O00487
c	388	ILE	-	expression tag	UNP O00487
c	389	ASN	-	expression tag	UNP O00487
c	390	ALA	-	expression tag	UNP O00487
c	391	PRO	-	expression tag	UNP O00487
c	392	THR	-	expression tag	UNP O00487
c	393	ASP	-	expression tag	UNP O00487
c	394	GLY	-	expression tag	UNP O00487
c	395	LYS	-	expression tag	UNP O00487
c	396	VAL	-	expression tag	UNP O00487
c	397	GLU	-	expression tag	UNP O00487
c	398	LYS	-	expression tag	UNP O00487
c	399	VAL	-	expression tag	UNP O00487
c	400	LEU	-	expression tag	UNP O00487
c	401	VAL	-	expression tag	UNP O00487
c	402	LYS	-	expression tag	UNP O00487
c	403	GLU	-	expression tag	UNP O00487
c	404	ARG	-	expression tag	UNP O00487
c	405	ASP	-	expression tag	UNP O00487
c	406	ALA	-	expression tag	UNP O00487
c	407	VAL	-	expression tag	UNP O00487
c	408	GLN	-	expression tag	UNP O00487
c	409	GLY	-	expression tag	UNP O00487
c	410	GLY	-	expression tag	UNP O00487
c	411	GLN	-	expression tag	UNP O00487
c	412	GLY	-	expression tag	UNP O00487
c	413	LEU	-	expression tag	UNP O00487
c	414	ILE	-	expression tag	UNP O00487
c	415	LYS	-	expression tag	UNP O00487
c	416	ILE	-	expression tag	UNP O00487
c	417	GLY	-	expression tag	UNP O00487
c	418	VAL	-	expression tag	UNP O00487
c	419	HIS	-	expression tag	UNP O00487

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Chain	Residue	Modelled	Actual	Comment	Reference
c	420	HIS	-	expression tag	UNP O00487
c	421	HIS	-	expression tag	UNP O00487
c	422	HIS	-	expression tag	UNP O00487
c	423	HIS	-	expression tag	UNP O00487
c	424	HIS	-	expression tag	UNP O00487

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	269	Total	C	N	O	S	0	0
			2188	1414	359	406	9		

- Molecule 24 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	e	42	Total	C	N	O	0	0
			361	221	56	84		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	842	Total	C	N	O	S	0	0
			6511	4117	1105	1244	45		

- Molecule 26 is a protein called Isoform 2 of NEDD8 ultimate buster 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	95	Total	C	N	O	S	0	0
			771	487	139	144	1		

- Molecule 27 is a protein called Thioredoxin-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	u	172	Total	C	N	O	S	0	0
			1376	865	226	276	9		

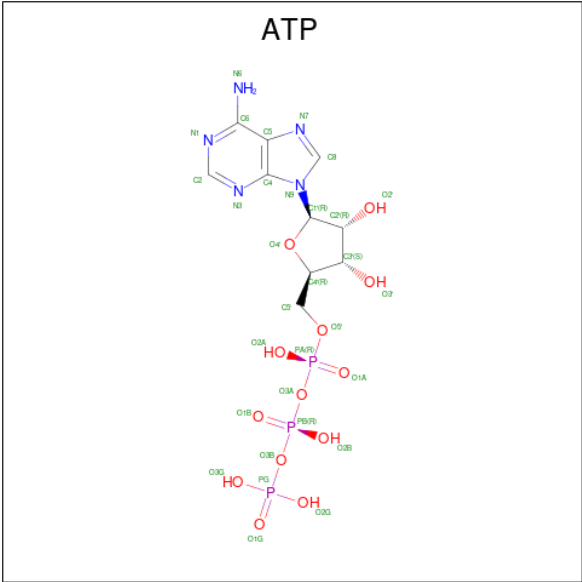
- Molecule 28 is a protein called substrate peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	v	13	Total	C	N	O	0	0
			65	39	13	13		

- # ADP

- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

- Molecule 31 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



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

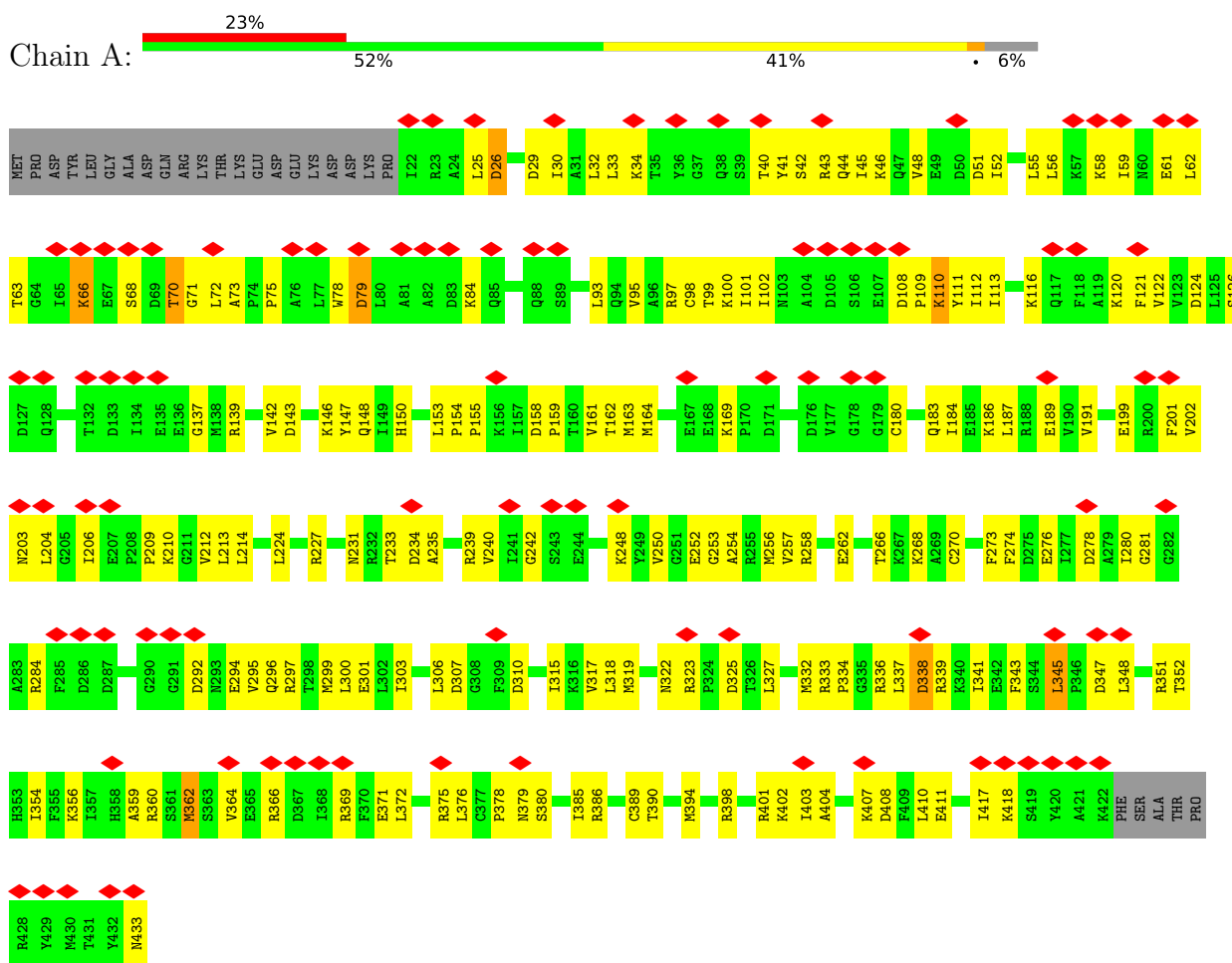
- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

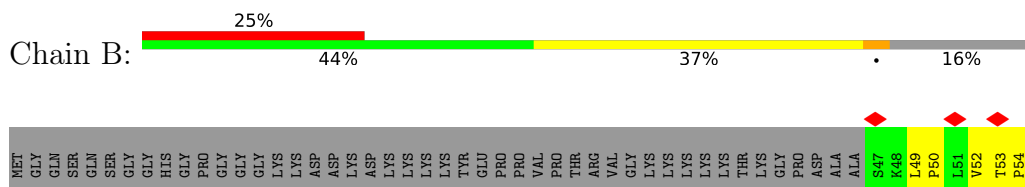
3 Residue-property plots

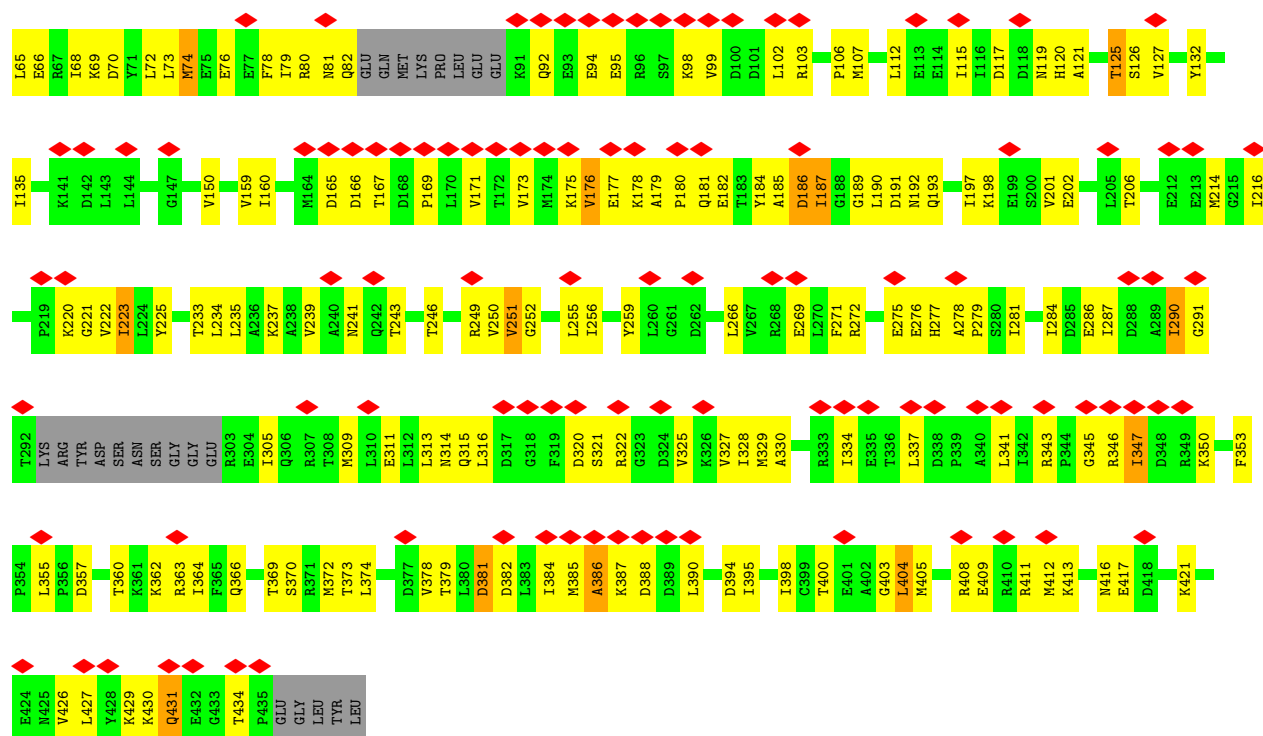
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 regulatory subunit 7

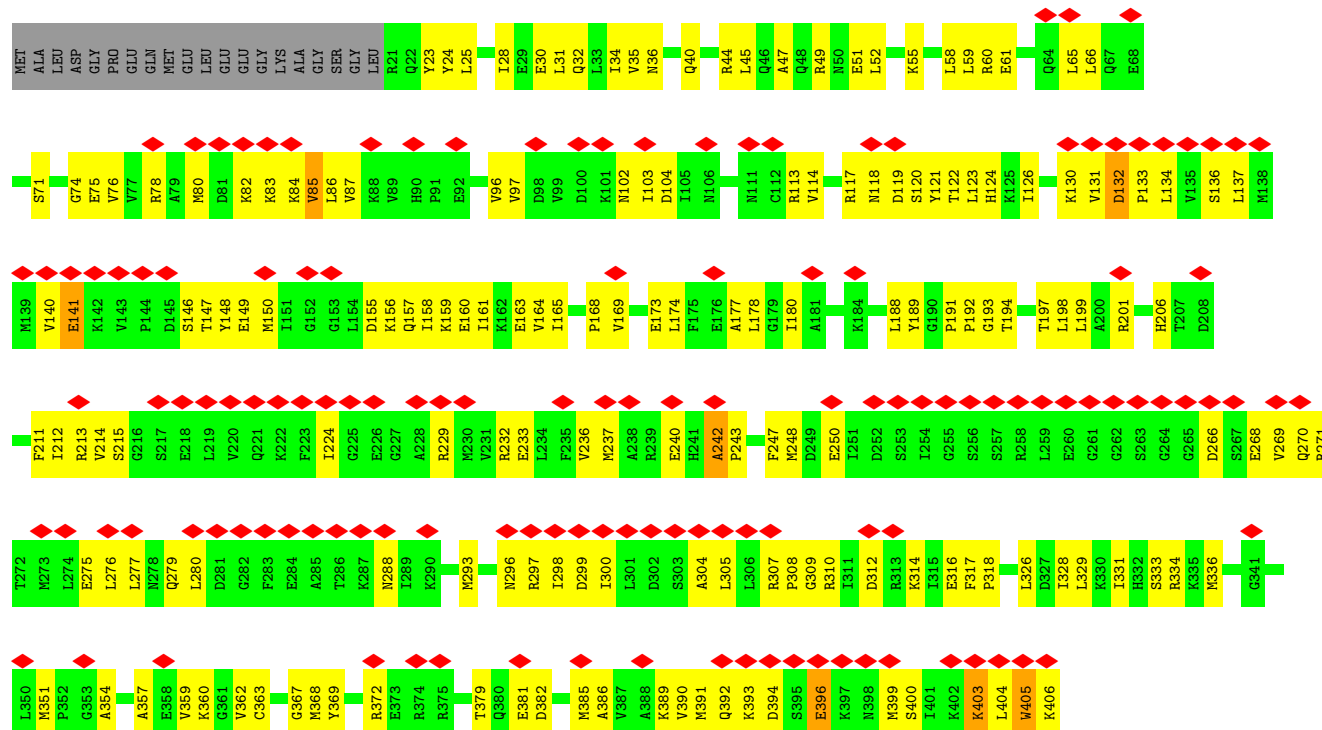


• Molecule 2: 26S proteasome regulatory subunit 4

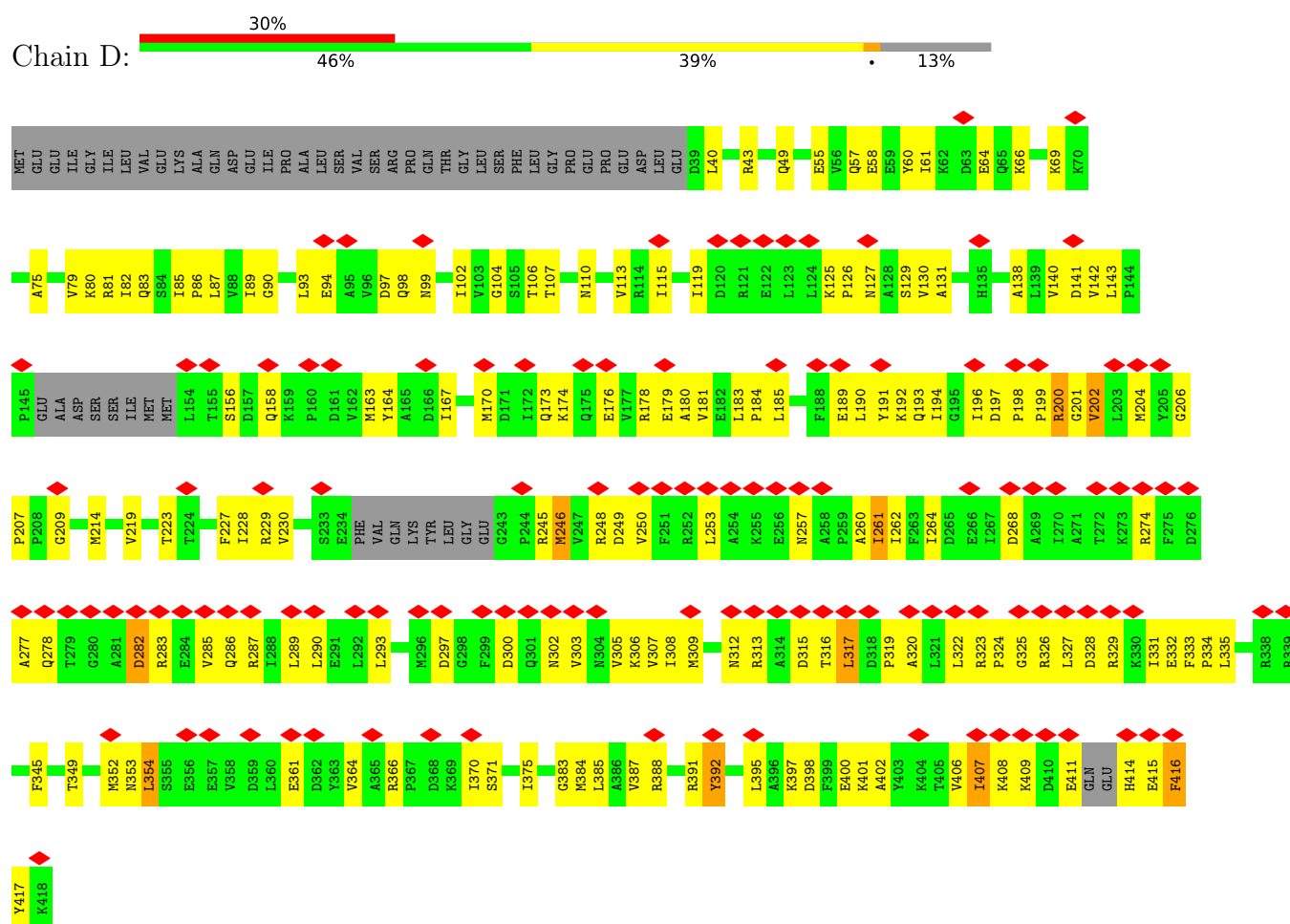




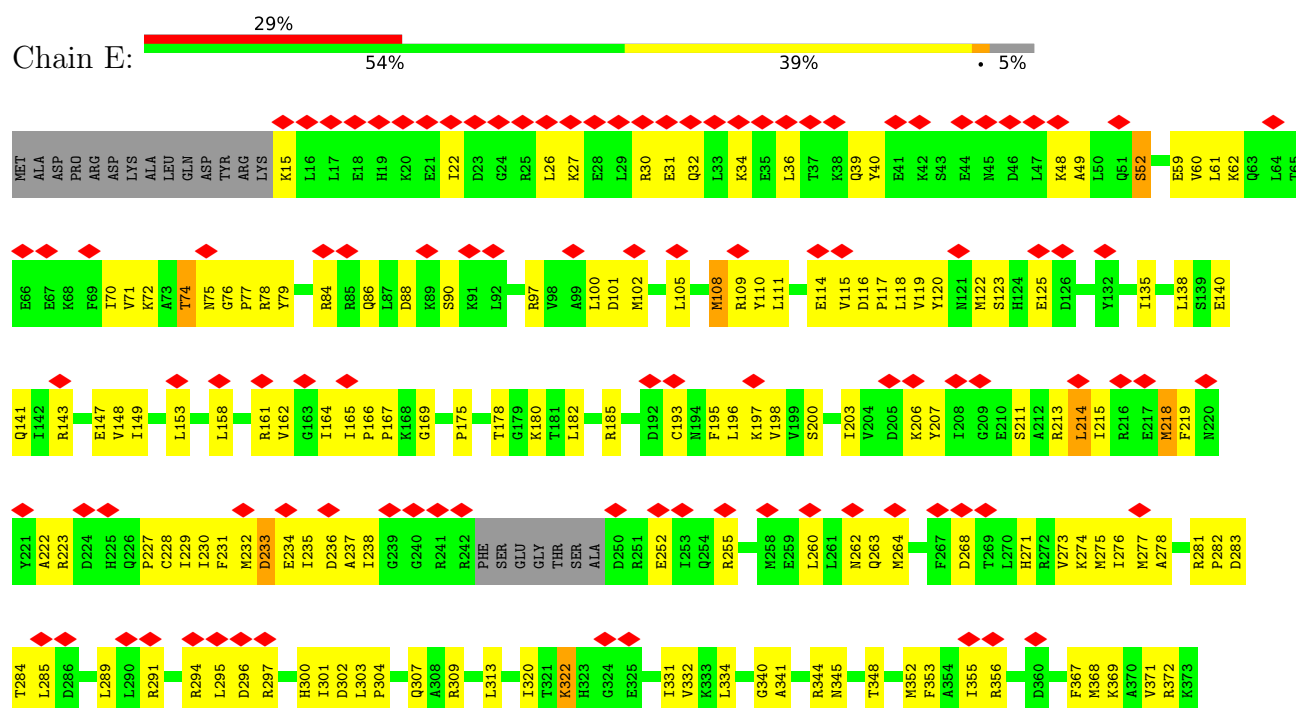
• Molecule 3: 26S protease regulatory subunit 8

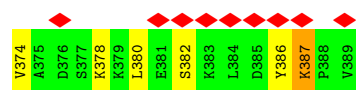


• Molecule 4: 26S proteasome regulatory subunit 6B

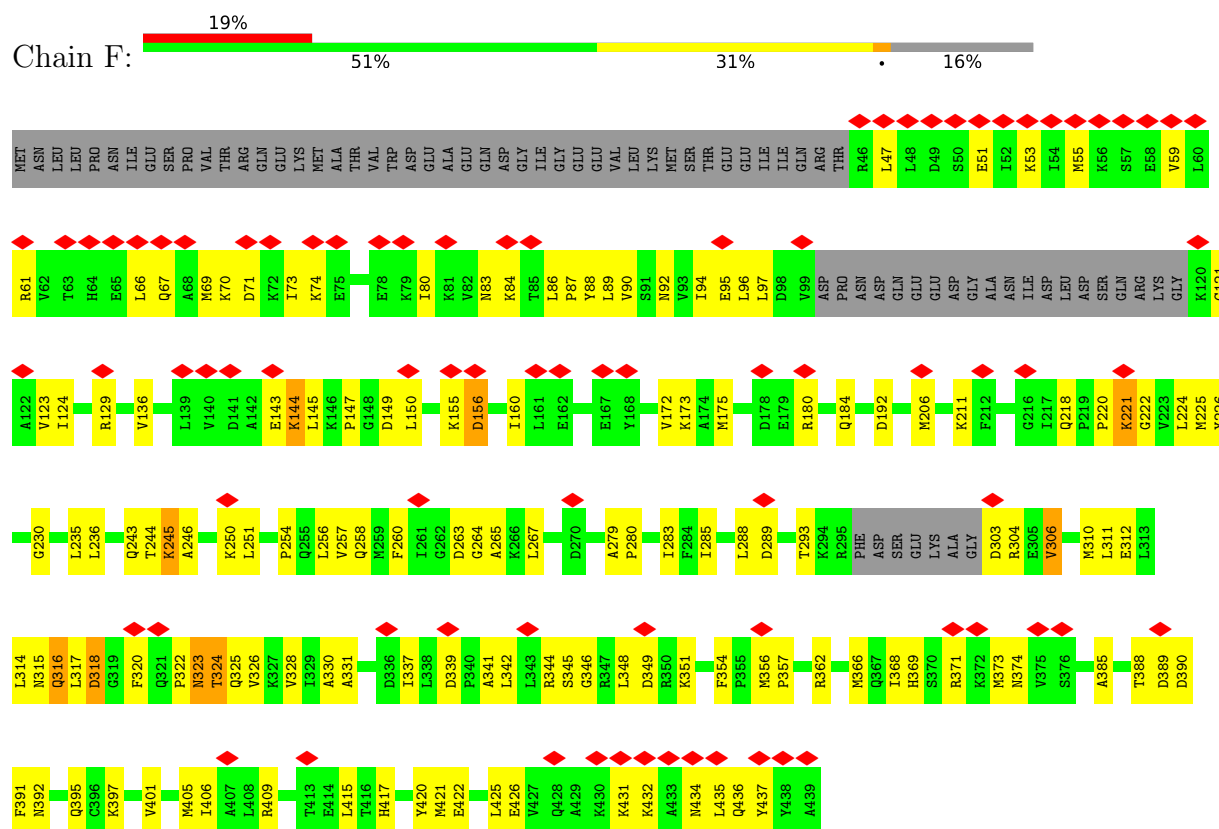


• Molecule 5: 26S protease regulatory subunit 10B

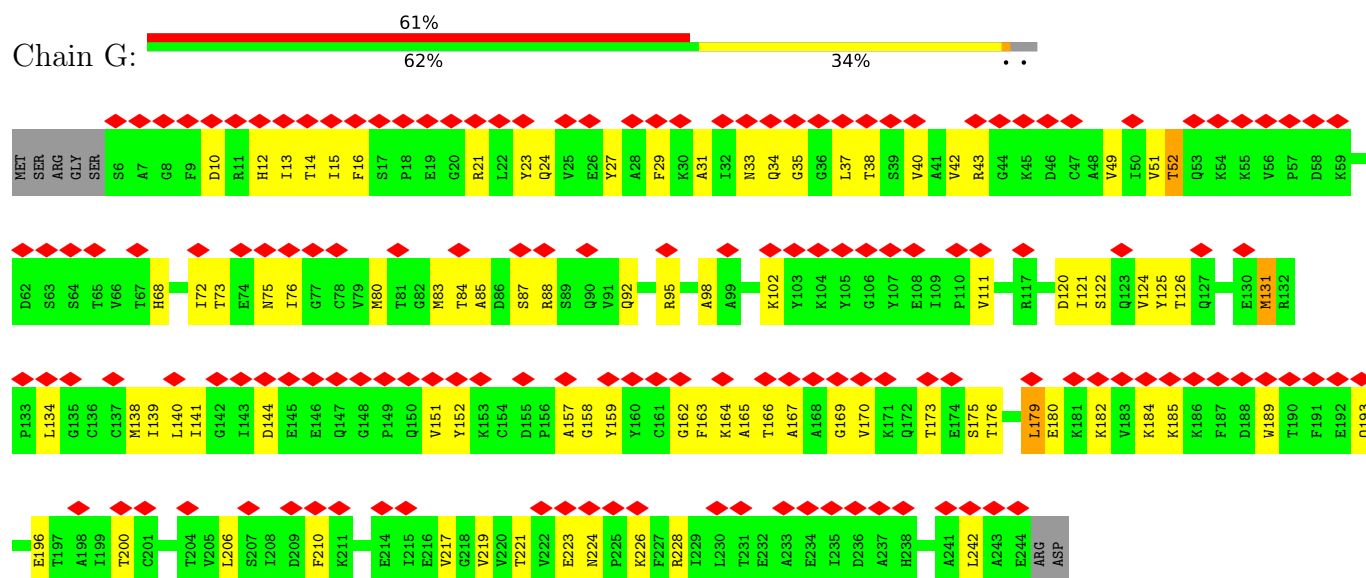




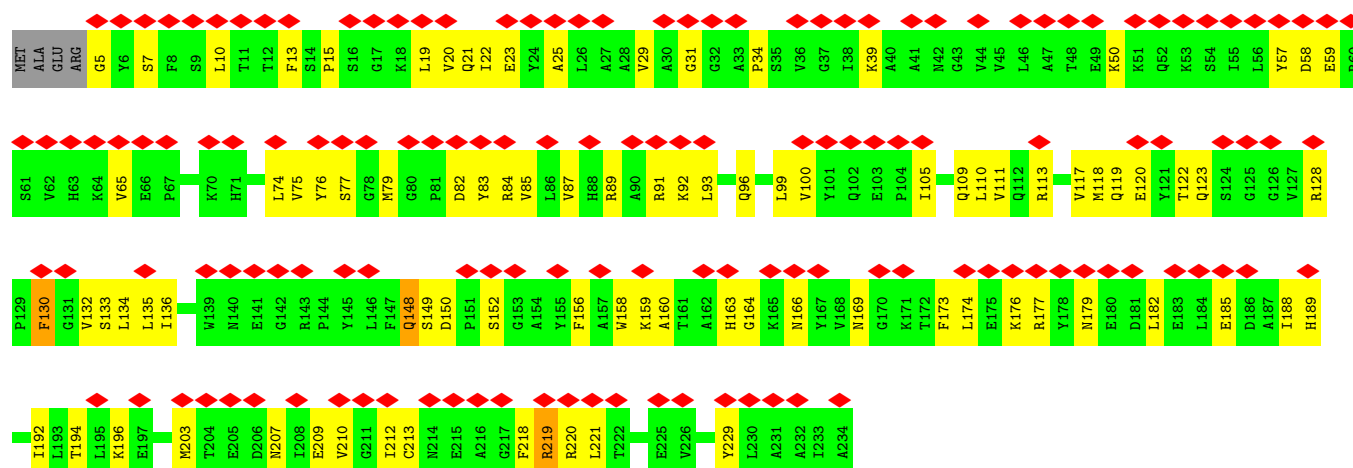
• Molecule 6: 26S proteasome regulatory subunit 6A



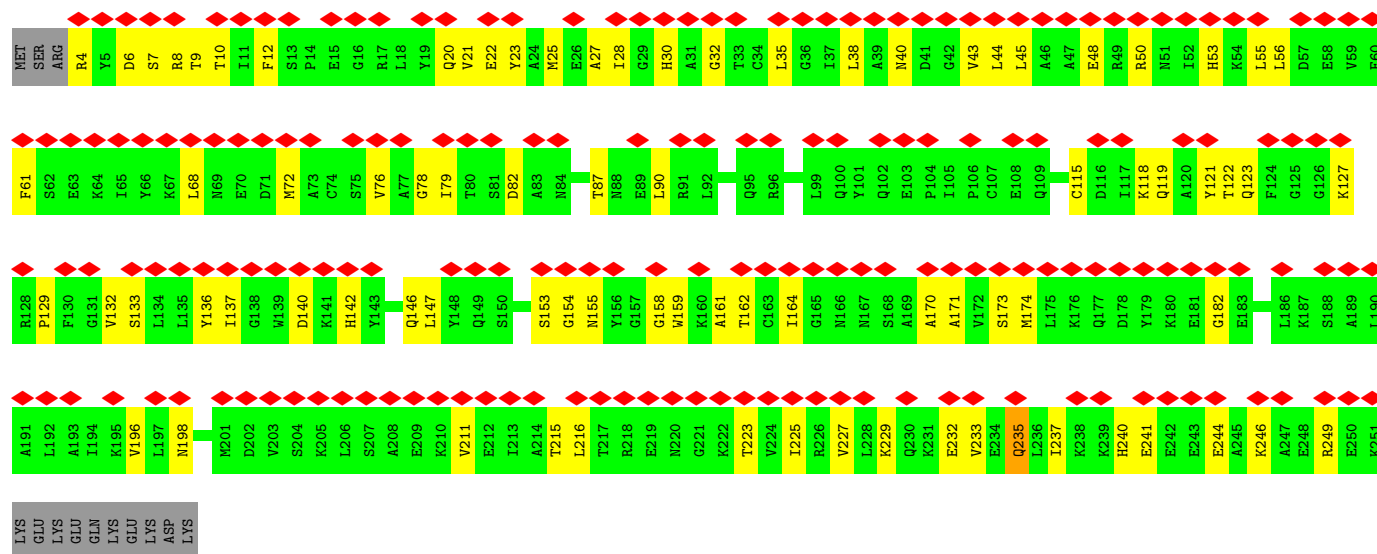
• Molecule 7: Proteasome subunit alpha type-6



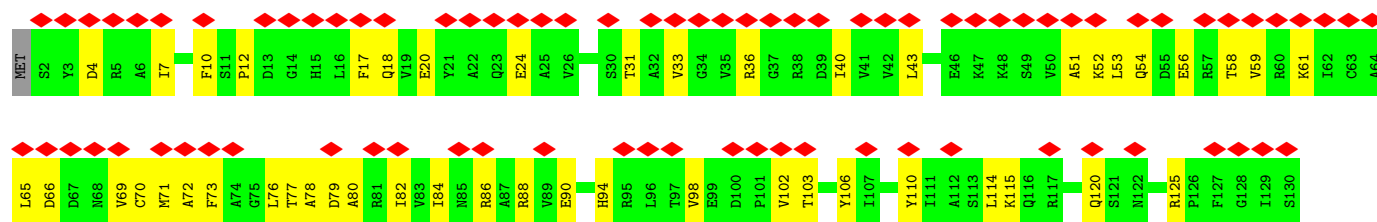
• Molecule 8: Proteasome subunit alpha type-2

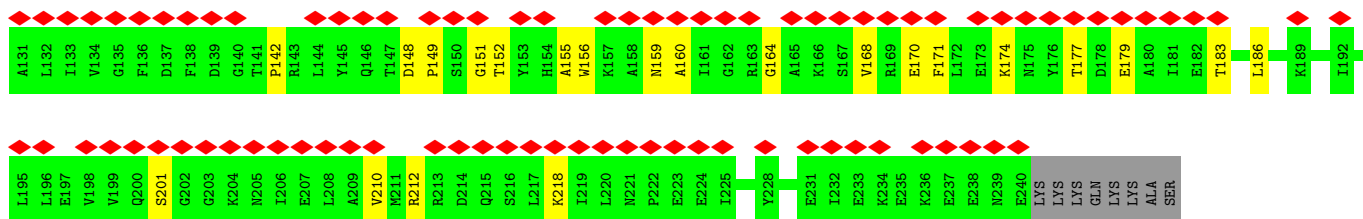


• Molecule 9: Proteasome subunit alpha type-4

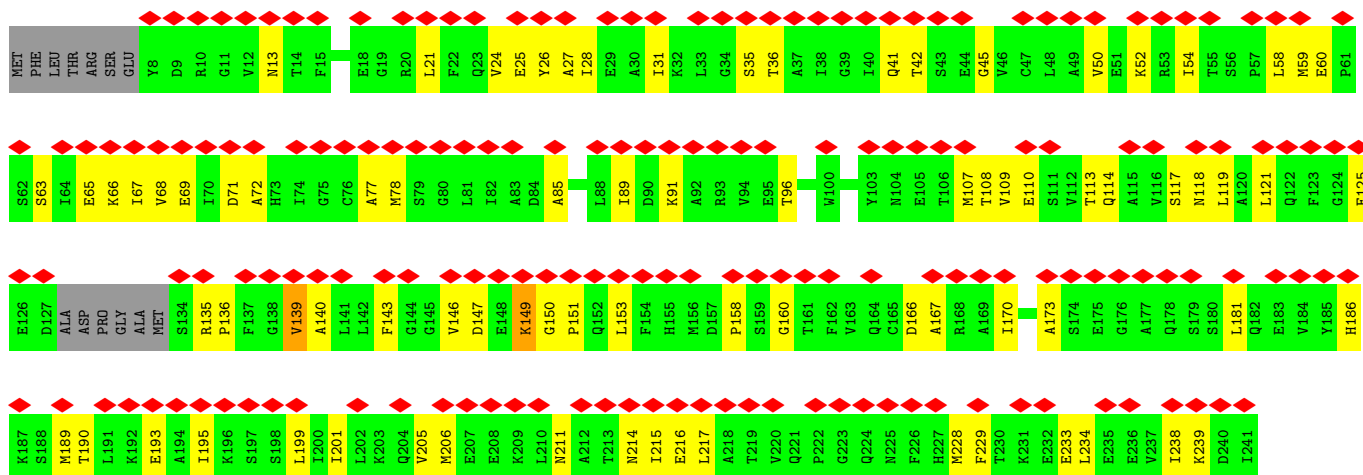
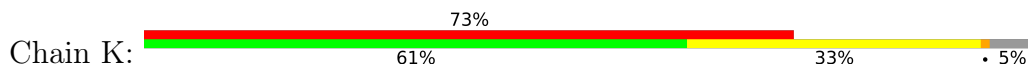


• Molecule 10: Proteasome subunit alpha type-7





• Molecule 11: Proteasome subunit alpha type-5

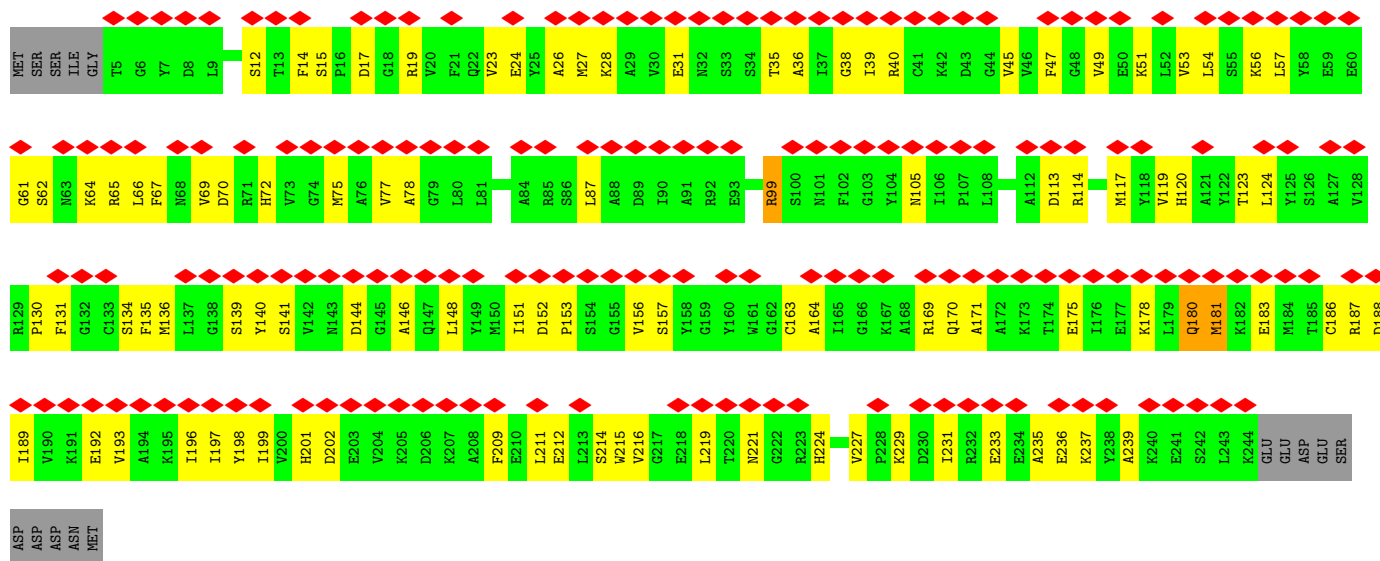


• Molecule 12: Proteasome subunit alpha type-1

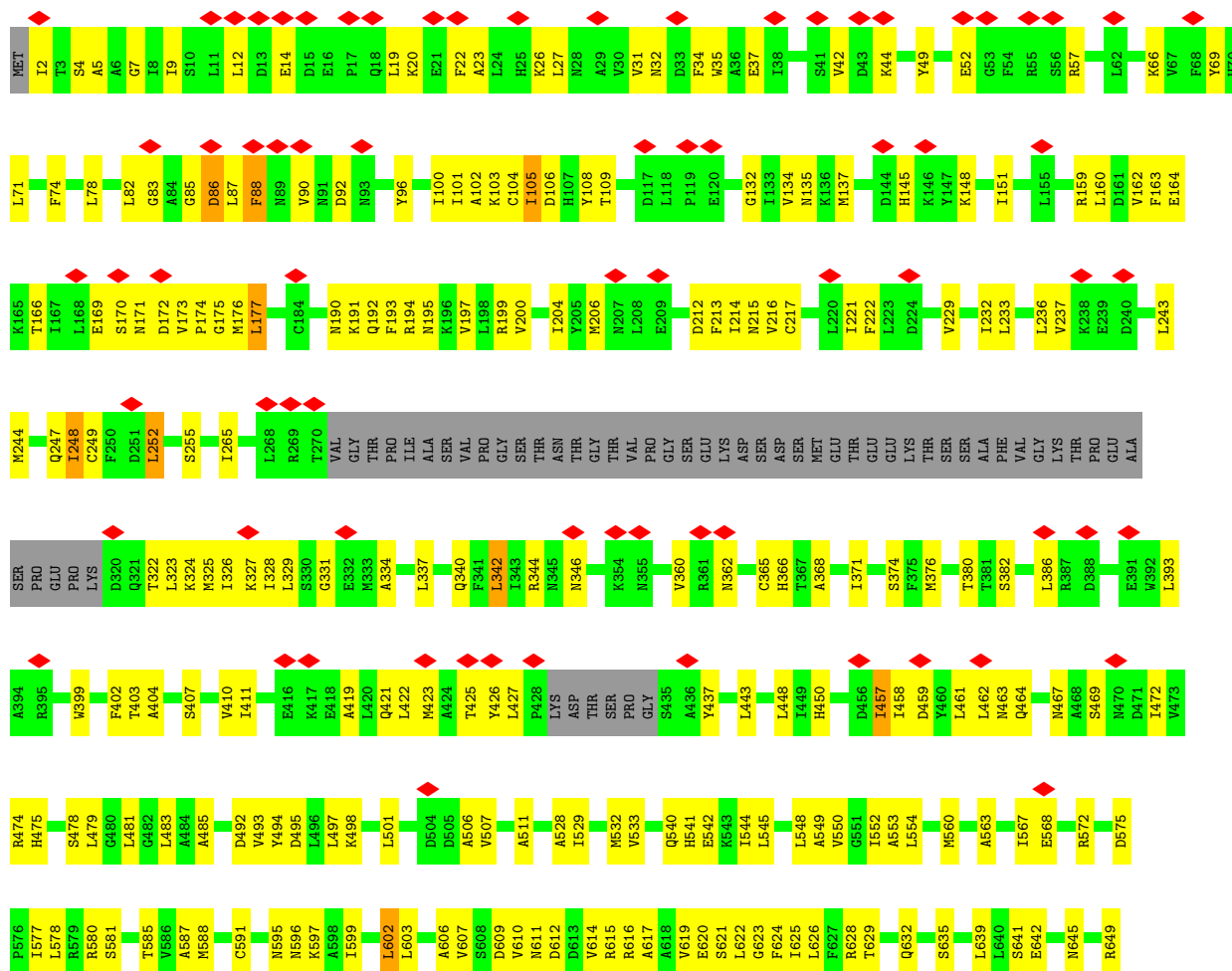


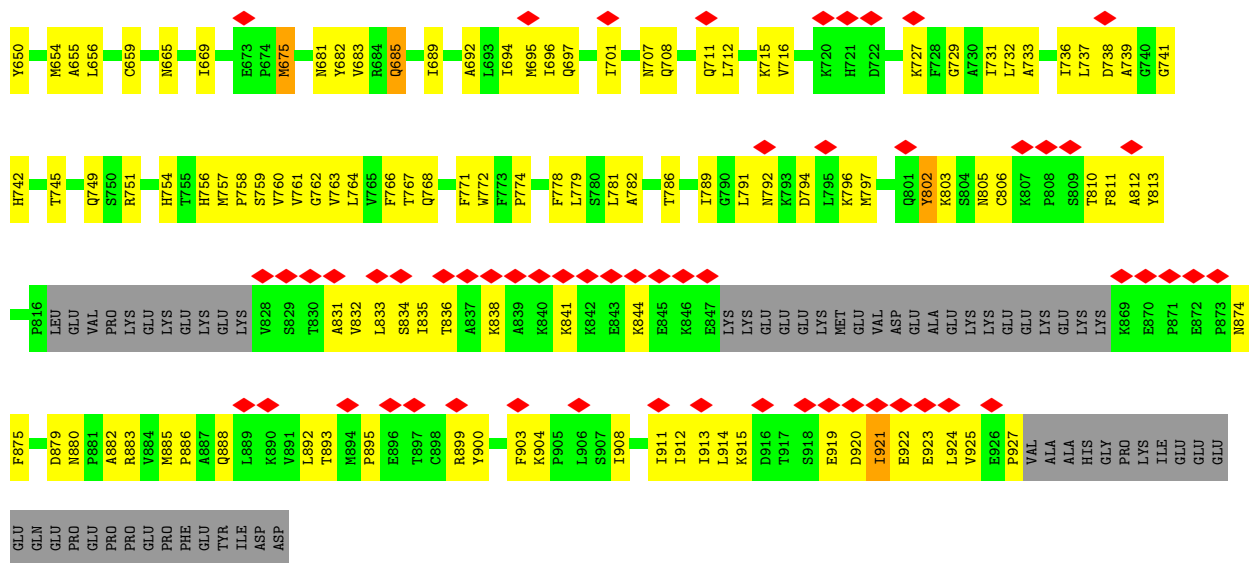
• Molecule 13: Proteasome subunit alpha type-3



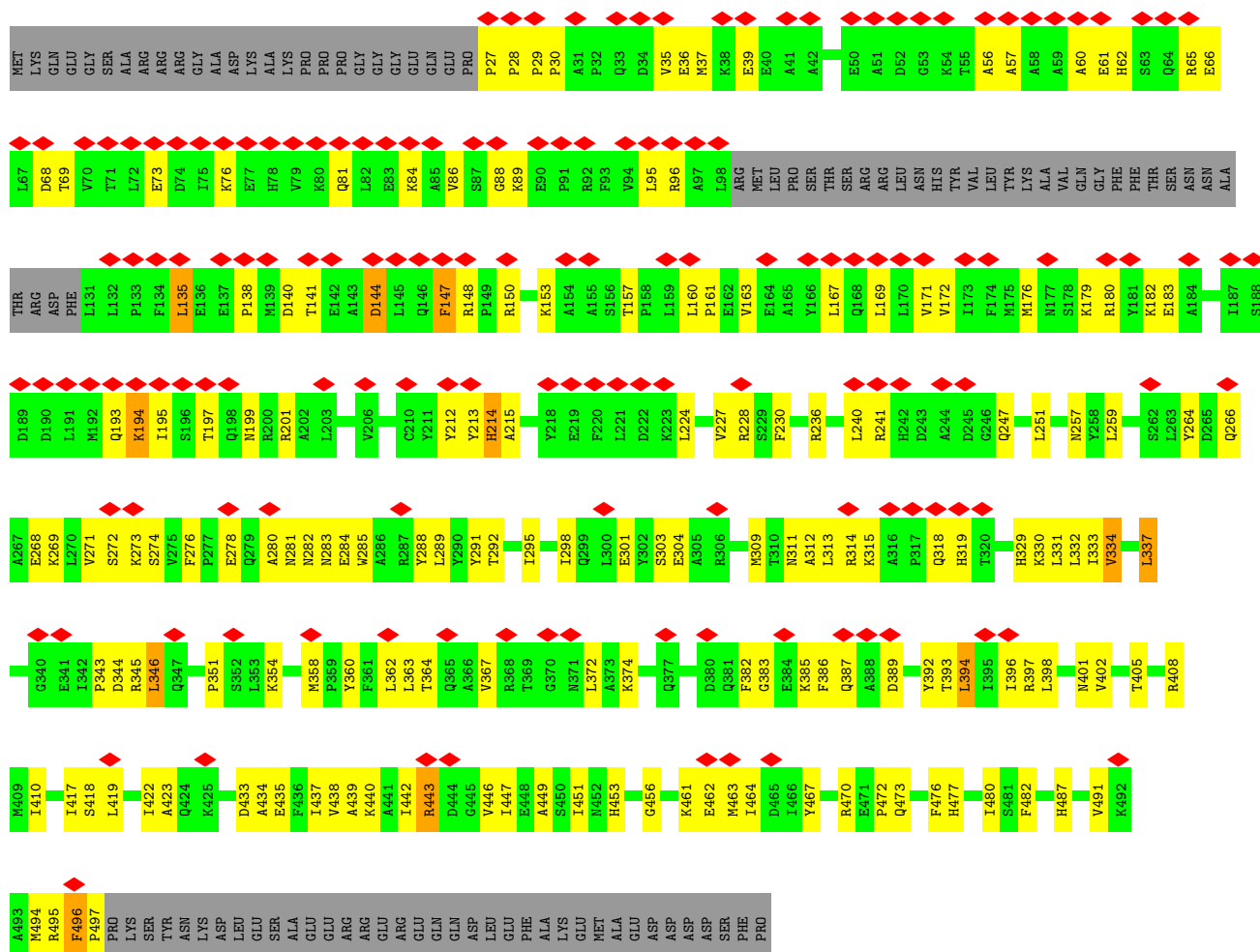


• Molecule 14: 26S proteasome non-ATPase regulatory subunit 1

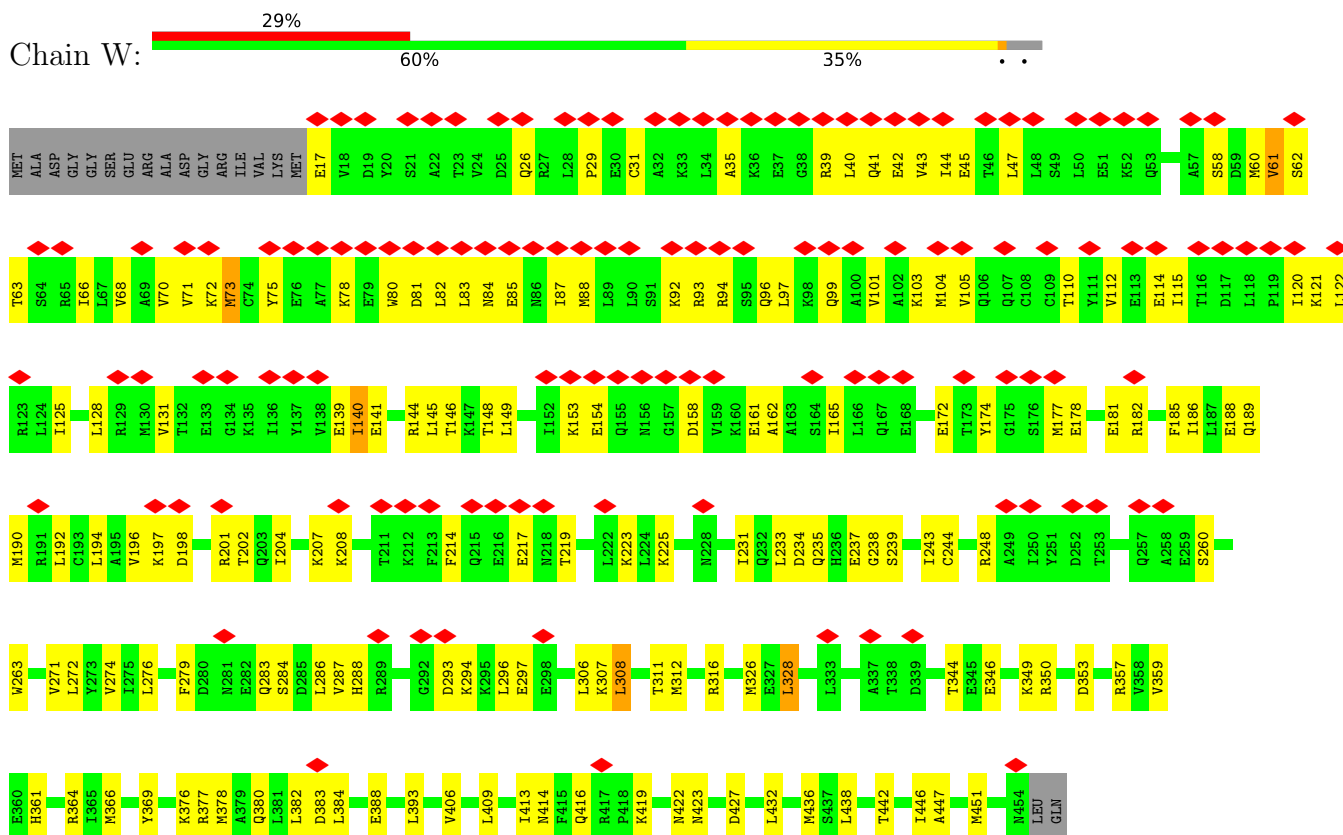




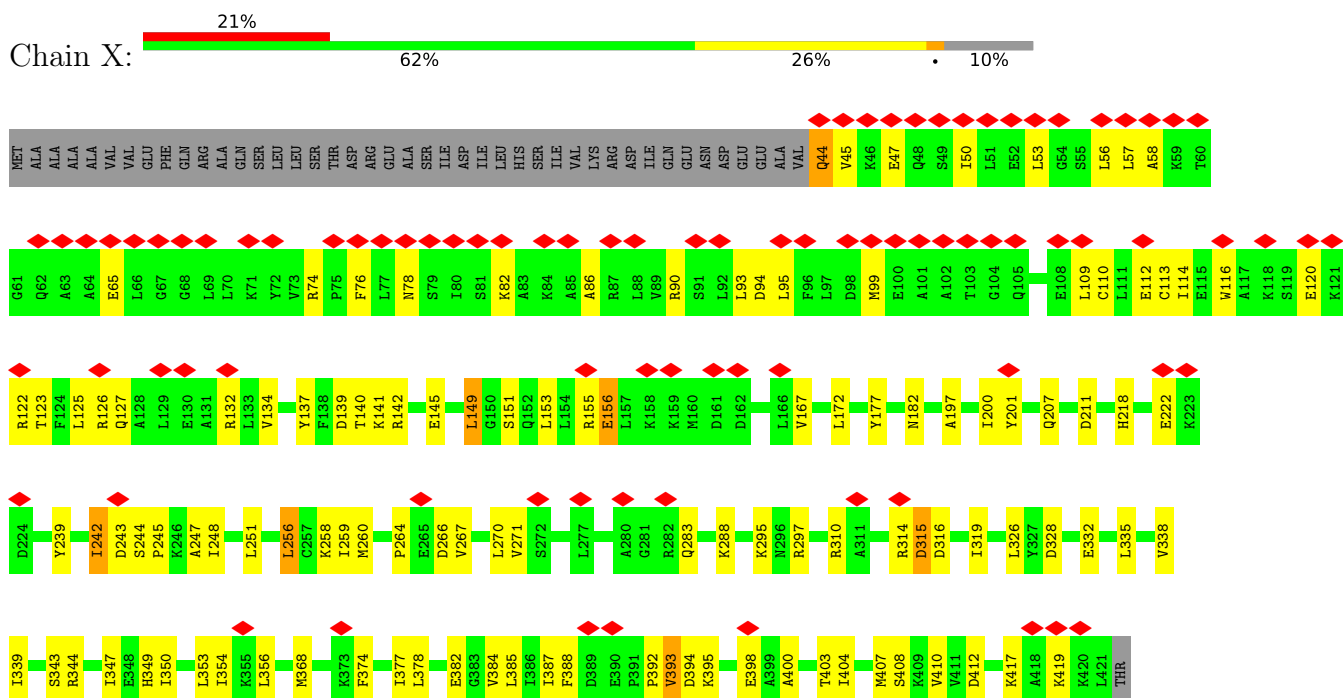
• Molecule 15: 26S proteasome non-ATPase regulatory subunit 3



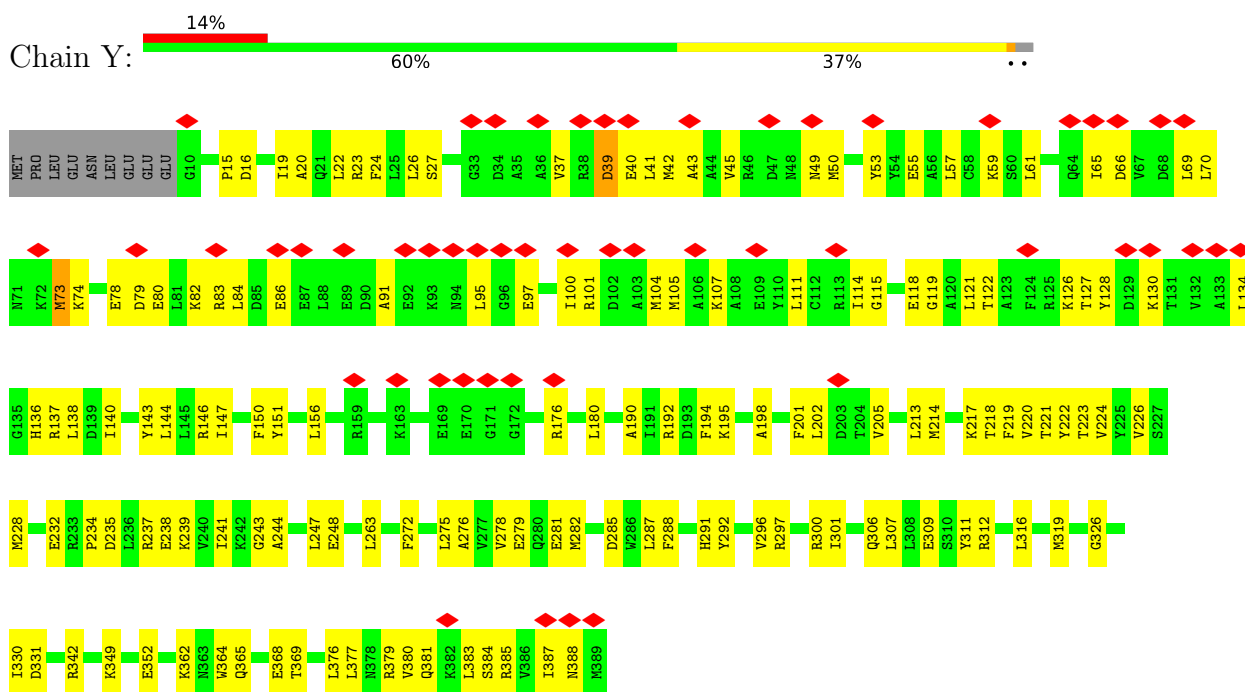
- Molecule 16: 26S proteasome non-ATPase regulatory subunit 12



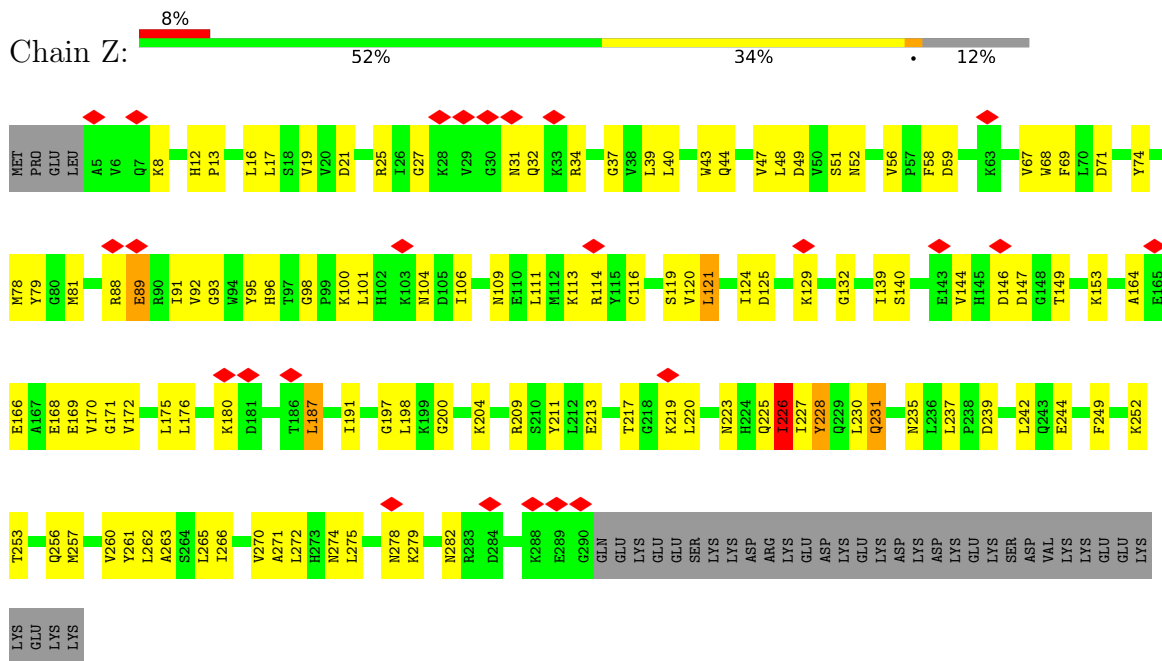
- Molecule 17: 26S proteasome non-ATPase regulatory subunit 11



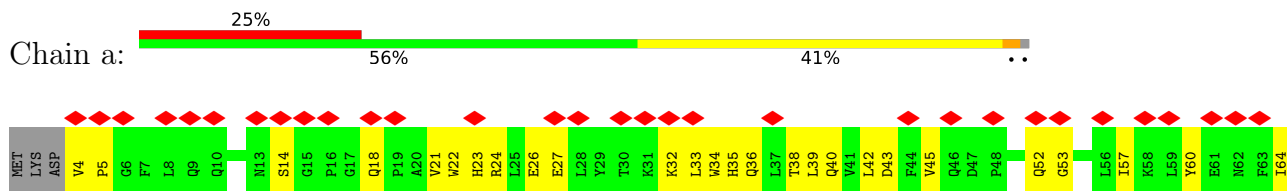
- Molecule 18: 26S proteasome non-ATPase regulatory subunit 6

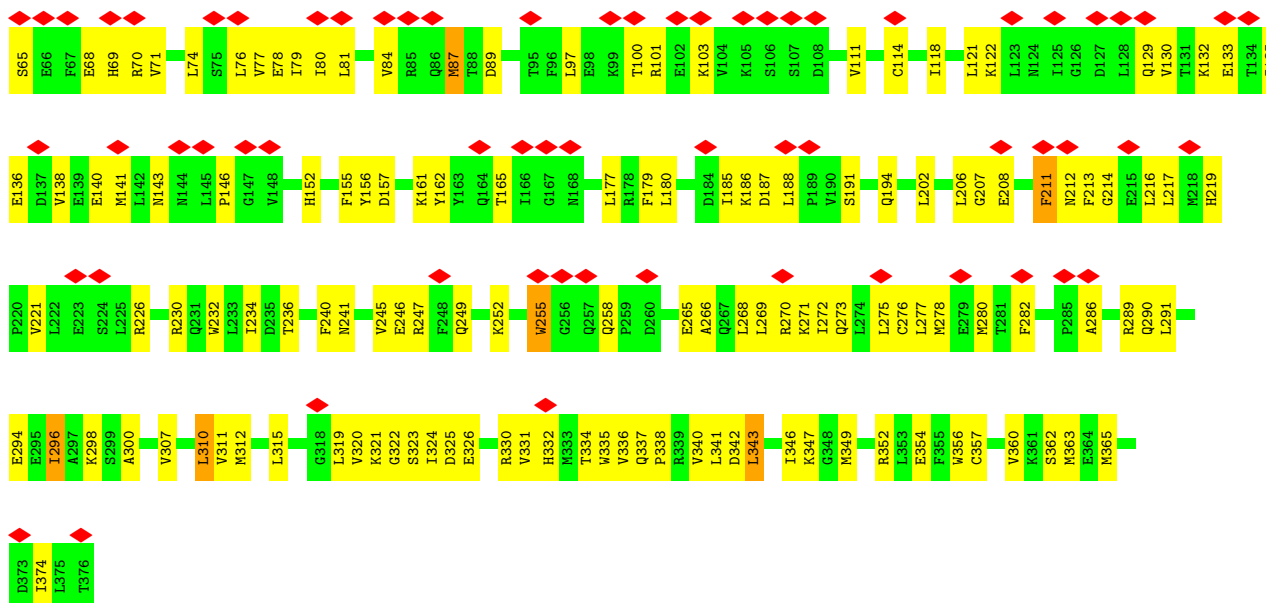


- Molecule 19: 26S proteasome non-ATPase regulatory subunit 7

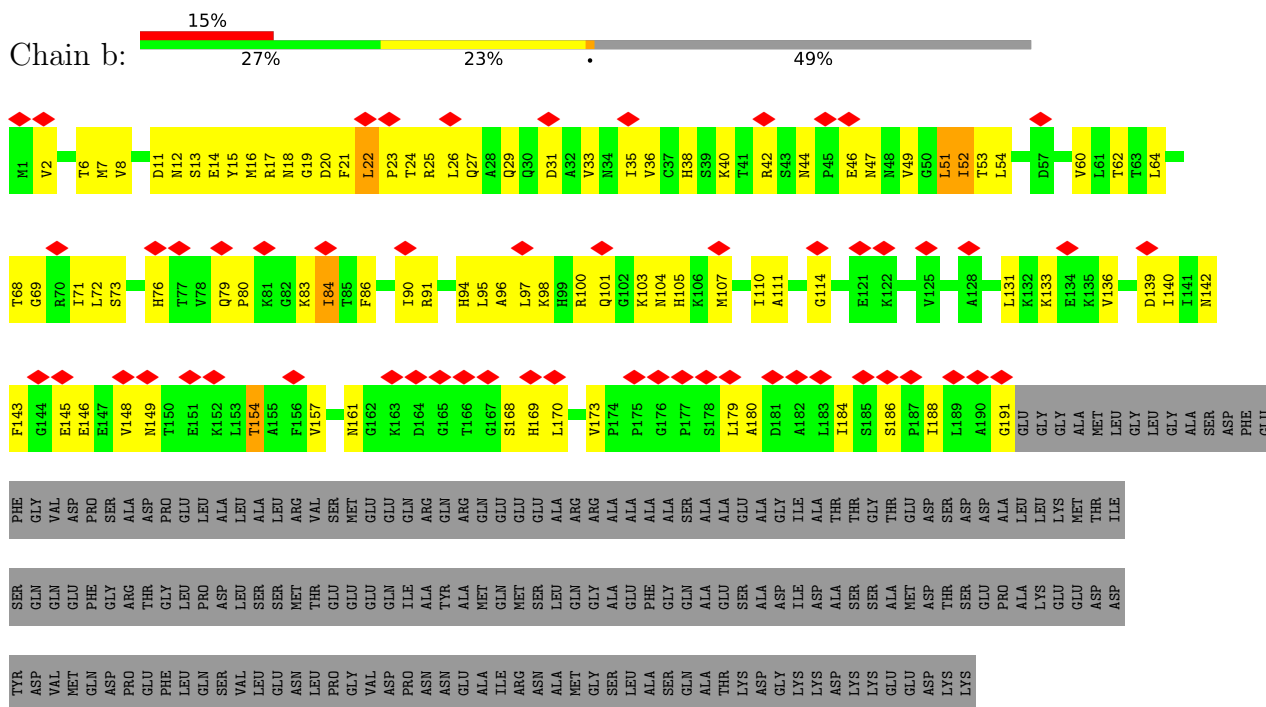


- Molecule 20: 26S proteasome non-ATPase regulatory subunit 13

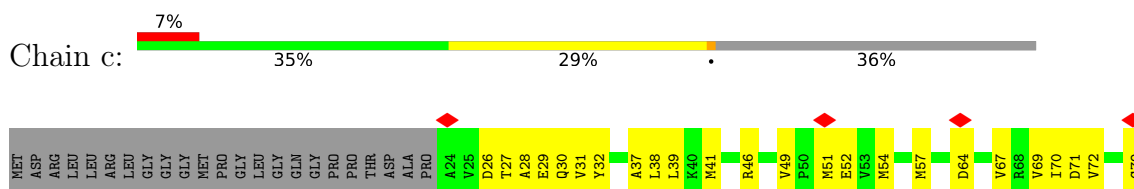




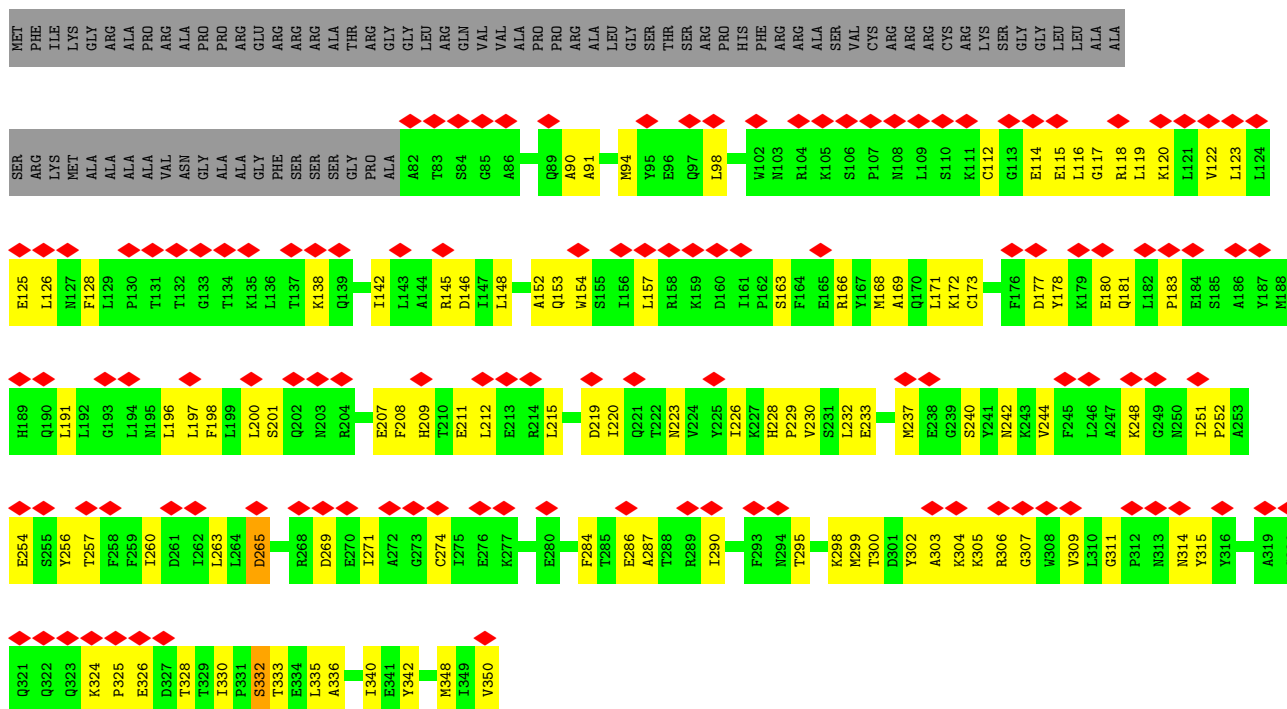
- Molecule 21: 26S proteasome non-ATPase regulatory subunit 4



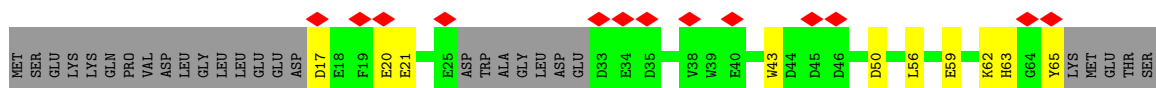
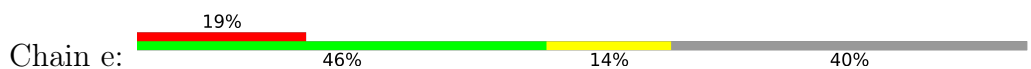
- Molecule 22: 26S proteasome non-ATPase regulatory subunit 14



- Molecule 23: 26S proteasome non-ATPase regulatory subunit 8

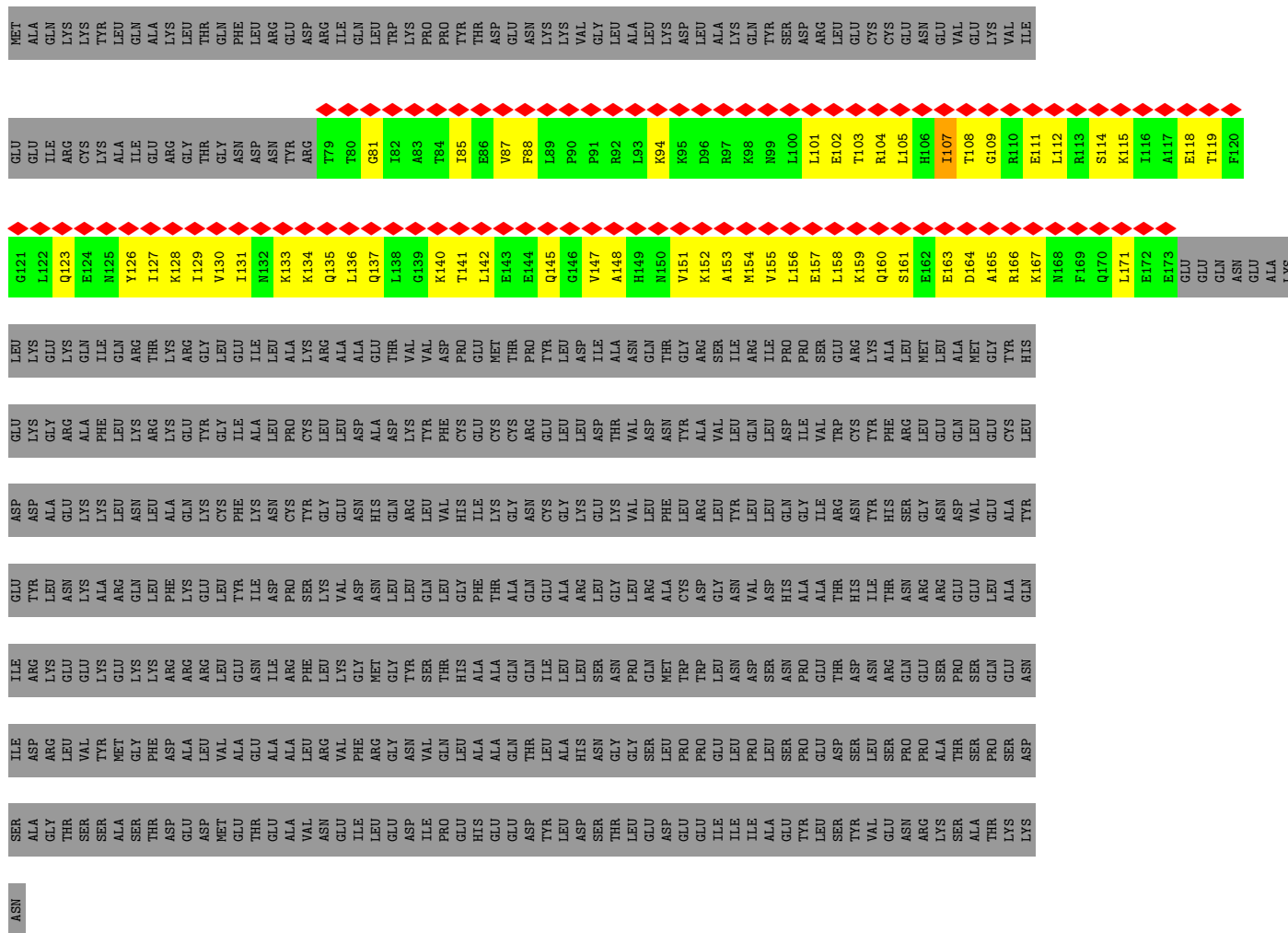


- Molecule 24: 26S proteasome complex subunit SEM1

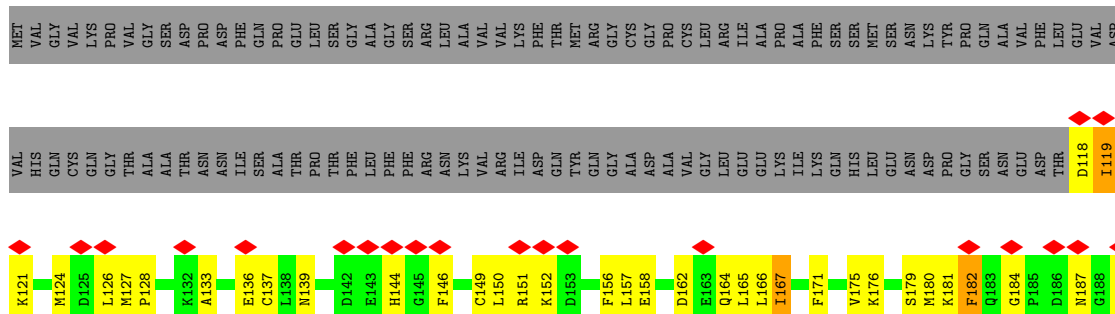
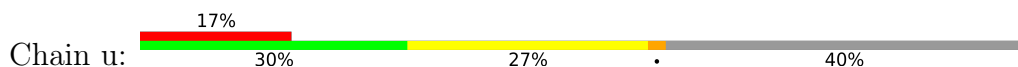


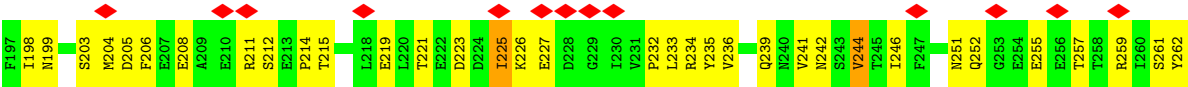
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 2



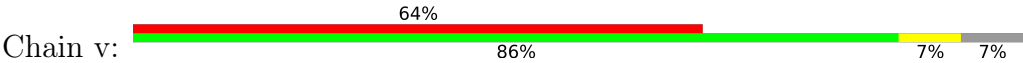


- Molecule 27: Thioredoxin-like protein 1





• Molecule 28: substrate peptide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29525	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.517	Depositor
Minimum map value	-0.222	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	356.32, 356.32, 356.32	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.19	0/3246	0.54	0/4380
2	B	0.20	0/2958	0.55	0/3991
3	C	0.20	0/3094	0.58	0/4158
4	D	0.19	0/2934	0.50	0/3955
5	E	0.17	0/2976	0.45	0/4004
6	F	0.18	0/2914	0.51	0/3925
7	G	0.17	0/1853	0.48	0/2515
8	H	0.18	0/1754	0.47	0/2384
9	I	0.18	0/1925	0.46	0/2606
10	J	0.16	0/1728	0.45	0/2358
11	K	0.16	0/1755	0.47	0/2375
12	L	0.17	0/1885	0.45	0/2552
13	M	0.19	0/1891	0.52	2/2552 (0.1%)
14	U	0.17	0/6650	0.49	1/8993 (0.0%)
15	V	0.18	0/3591	0.53	0/4849
16	W	0.15	0/3618	0.44	0/4868
17	X	0.17	0/3038	0.47	1/4095 (0.0%)
18	Y	0.18	0/3185	0.42	0/4290
19	Z	0.18	0/2324	0.50	0/3150
20	a	0.18	0/3053	0.51	0/4133
21	b	0.18	0/1478	0.53	0/2001
22	c	0.21	0/2193	0.55	0/2962
23	d	0.18	0/2234	0.48	0/3018
24	e	0.18	0/370	0.51	0/501
25	f	0.16	0/6622	0.48	1/8965 (0.0%)
26	g	0.20	0/778	0.60	0/1041
27	u	0.19	0/1403	0.50	0/1892
All	All	0.18	0/71450	0.50	5/96513 (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
2	B	0	1
10	J	0	1
15	V	0	1
21	b	0	1
22	c	0	1
All	All	0	5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	180	GLN	CA-CB-CG	7.79	129.67	114.10
14	U	812	ALA	CB-CA-C	-5.77	109.90	116.54
17	X	242	ILE	N-CA-C	-5.55	107.33	112.83
25	f	339	ILE	N-CA-C	-5.45	107.06	111.91
13	M	180	GLN	CB-CG-CD	5.13	121.32	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	53	THR	Peptide
10	J	70	CYS	Peptide
15	V	195	ILE	Peptide
21	b	22	LEU	Peptide
22	c	279	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3196	0	3250	178	0
2	B	2917	0	2987	161	0
3	C	3053	0	3173	161	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2889	0	2920	139	0
5	E	2932	0	3011	154	0
6	F	2877	0	2977	147	0
7	G	1820	0	1789	77	0
8	H	1717	0	1629	82	0
9	I	1895	0	1833	61	0
10	J	1704	0	1517	50	0
11	K	1729	0	1680	70	0
12	L	1850	0	1822	62	0
13	M	1856	0	1814	83	0
14	U	6538	0	6575	262	0
15	V	3525	0	3579	156	0
16	W	3570	0	3685	128	0
17	X	2994	0	3097	89	0
18	Y	3127	0	3133	113	0
19	Z	2281	0	2312	113	0
20	a	2995	0	3012	126	0
21	b	1458	0	1505	81	0
22	c	2153	0	2156	115	0
23	d	2188	0	2216	94	0
24	e	361	0	280	15	0
25	f	6511	0	6529	258	0
26	g	771	0	815	49	0
27	u	1376	0	1324	72	0
28	v	65	0	18	3	0
29	A	27	0	12	2	0
29	B	27	0	12	1	0
29	C	27	0	12	3	0
29	D	27	0	12	2	0
30	C	1	0	0	0	0
30	E	1	0	0	0	0
30	F	1	0	0	0	0
31	E	31	0	12	5	0
31	F	31	0	12	1	0
32	c	1	0	0	0	0
All	All	70522	0	70710	2796	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (2796) 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)
6:F:356:MET:HE3	6:F:357:PRO:HD2	1.46	0.97
20:a:57:ILE:HA	20:a:60:TYR:HB3	1.51	0.93
8:H:79:MET:HB3	8:H:132:VAL:HG22	1.52	0.92
1:A:274:PHE:HB2	1:A:319:MET:HG3	1.53	0.91
25:f:407:MET:HB3	25:f:440:ILE:HG22	1.54	0.89
20:a:335:TRP:NE1	20:a:337:GLN:O	2.05	0.88
14:U:587:ALA:HB2	14:U:621:SER:HB3	1.58	0.86
7:G:73:THR:HB	7:G:76:ILE:HB	1.56	0.85
3:C:113:ARG:HD3	3:C:130:LYS:HB2	1.58	0.85
15:V:309:MET:HE1	15:V:331:LEU:HG	1.58	0.85
9:I:53:HIS:HE1	9:I:55:LEU:HB2	1.40	0.85
15:V:334:VAL:HA	15:V:337:LEU:HD12	1.59	0.84
18:Y:232:GLU:HG2	18:Y:234:PRO:HD2	1.59	0.84
25:f:646:MET:H	25:f:646:MET:HE3	1.41	0.84
22:c:215:LYS:HA	22:c:218:LEU:HB3	1.59	0.84
6:F:251:LEU:HD11	6:F:285:ILE:HD13	1.57	0.83
14:U:148:LYS:HE2	14:U:176:MET:HG3	1.60	0.83
23:d:348:MET:HE1	23:d:350:VAL:HB	1.59	0.83
2:B:176:VAL:HG22	2:B:178:LYS:H	1.44	0.83
25:f:407:MET:HB2	25:f:439:TYR:HB3	1.60	0.83
16:W:162:ALA:HA	16:W:165:ILE:HD12	1.60	0.82
11:K:35:SER:HB2	11:K:66:LYS:HZ2	1.42	0.82
19:Z:67:VAL:HG21	21:b:91:ARG:HD2	1.61	0.82
3:C:146:SER:HB2	3:C:201:ARG:HG2	1.62	0.81
14:U:461:LEU:HB3	14:U:481:LEU:HD12	1.61	0.81
15:V:201:ARG:NH1	15:V:201:ARG:O	2.12	0.81
9:I:53:HIS:CE1	9:I:55:LEU:HB2	2.15	0.81
14:U:811:PHE:HE1	14:U:885:MET:HE1	1.45	0.81
17:X:410:VAL:HG23	22:c:259:VAL:HG11	1.61	0.81
19:Z:231:GLN:HA	20:a:349:MET:HE1	1.63	0.81
25:f:422:VAL:O	25:f:426:LEU:HB2	1.81	0.80
15:V:330:LYS:HG3	15:V:360:TYR:HE1	1.46	0.80
14:U:641:SER:HB2	14:U:675:MET:HE1	1.64	0.80
23:d:248:LYS:HZ3	23:d:260:ILE:HG21	1.47	0.80
3:C:277:LEU:HD21	3:C:305:LEU:HA	1.64	0.79
8:H:74:LEU:HD11	8:H:134:LEU:HD12	1.65	0.79
15:V:148:ARG:HH21	15:V:199:ASN:H	1.27	0.79
14:U:805:ASN:ND2	14:U:893:THR:OG1	2.15	0.79
22:c:29:GLU:HG3	22:c:30:GLN:H	1.46	0.79
9:I:27:ALA:O	9:I:30:HIS:ND1	2.16	0.79
15:V:69:THR:HA	15:V:73:GLU:HB2	1.65	0.78
17:X:398:GLU:OE1	17:X:398:GLU:N	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:a:70:ARG:HH21	21:b:17:ARG:HA	1.50	0.78
5:E:300:HIS:HE2	5:E:386:TYR:HH	1.21	0.77
13:M:51:LYS:NZ	13:M:62:SER:O	2.17	0.77
19:Z:48:LEU:HD11	19:Z:92:VAL:HG21	1.66	0.77
1:A:364:VAL:HG12	1:A:404:ALA:HB3	1.65	0.77
25:f:521:ALA:HA	25:f:524:MET:HE2	1.66	0.77
3:C:140:VAL:HG23	3:C:212:ILE:HG13	1.65	0.77
10:J:56:GLU:O	10:J:61:LYS:NZ	2.18	0.77
3:C:114:VAL:HG23	3:C:126:ILE:HA	1.67	0.76
7:G:152:TYR:HA	7:G:162:GLY:HA3	1.67	0.76
1:A:233:THR:HG22	1:A:235:ALA:H	1.48	0.76
3:C:137:LEU:HA	3:C:140:VAL:HG12	1.65	0.76
14:U:386:LEU:HD12	14:U:393:LEU:HD11	1.67	0.76
2:B:220:LYS:NZ	2:B:325:VAL:O	2.17	0.76
1:A:32:LEU:HB3	25:f:92:VAL:HG12	1.67	0.76
20:a:226:ARG:HH22	20:a:230:ARG:HE	1.30	0.76
21:b:142:ASN:ND2	21:b:149:ASN:OD1	2.19	0.76
20:a:319:LEU:HD12	20:a:320:VAL:HG23	1.68	0.75
2:B:281:ILE:HD11	2:B:328:ILE:HG12	1.67	0.75
9:I:171:ALA:HA	9:I:174:MET:HE3	1.68	0.75
23:d:168:MET:HE2	23:d:172:LYS:HZ3	1.49	0.75
20:a:286:ALA:HA	20:a:289:ARG:HB2	1.67	0.75
4:D:97:ASP:OD1	4:D:98:GLN:N	2.20	0.75
25:f:474:SER:HB3	25:f:477:MET:HG2	1.67	0.75
16:W:214:PHE:HA	16:W:219:THR:HG21	1.69	0.75
14:U:695:MET:HA	14:U:695:MET:HE3	1.67	0.75
25:f:131:MET:HE1	25:f:158:TYR:HA	1.68	0.75
19:Z:263:ALA:HB1	22:c:288:VAL:HG23	1.69	0.74
2:B:66:GLU:HA	2:B:69:LYS:HG2	1.68	0.74
7:G:38:THR:HA	7:G:169:GLY:HA3	1.68	0.74
13:M:24:GLU:HA	13:M:27:MET:HG2	1.68	0.74
15:V:289:LEU:HB3	15:V:312:ALA:HB2	1.68	0.74
21:b:64:LEU:HD21	21:b:97:LEU:HA	1.69	0.74
9:I:32:GLY:HA2	9:I:50:ARG:HH21	1.52	0.74
16:W:93:ARG:HE	16:W:94:ARG:H	1.33	0.74
1:A:146:LYS:NZ	1:A:148:GLN:NE2	2.36	0.74
18:Y:144:LEU:HA	18:Y:147:ILE:HD12	1.70	0.74
23:d:116:LEU:HA	23:d:119:LEU:HD12	1.70	0.74
5:E:345:ASN:HD21	6:F:349:ASP:HA	1.53	0.73
18:Y:282:MET:HG3	18:Y:292:TYR:HB2	1.70	0.73
1:A:52:ILE:HG12	2:B:69:LYS:HE3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:307:ARG:HH12	3:C:309:GLY:H	1.34	0.73
19:Z:252:LYS:NZ	22:c:238:CYS:SG	2.60	0.73
25:f:412:ALA:HA	25:f:447:ALA:HB2	1.70	0.73
19:Z:244:GLU:OE1	19:Z:244:GLU:N	2.22	0.73
6:F:435:LEU:HG	6:F:437:TYR:HB2	1.71	0.73
10:J:65:LEU:HD22	10:J:88:ARG:HG3	1.71	0.72
22:c:158:ASP:OD1	22:c:159:ALA:N	2.22	0.72
4:D:81:ARG:HH21	22:c:153:GLY:HA3	1.54	0.72
17:X:44:GLN:N	17:X:44:GLN:HE21	1.87	0.72
21:b:44:ASN:HD21	21:b:46:GLU:HB3	1.53	0.72
15:V:311:ASN:OD1	15:V:314:ARG:NH1	2.22	0.72
4:D:391:ARG:NH2	4:D:398:ASP:OD1	2.22	0.72
7:G:42:VAL:HA	7:G:164:LYS:HZ3	1.55	0.72
14:U:322:THR:HA	14:U:325:MET:HE3	1.72	0.72
3:C:49:ARG:HD2	14:U:639:LEU:HD23	1.72	0.71
5:E:165:ILE:HD12	5:E:166:PRO:HD2	1.70	0.71
3:C:45:LEU:HB3	4:D:61:ILE:HG21	1.71	0.71
9:I:21:VAL:HG12	9:I:25:MET:HE3	1.71	0.71
21:b:107:MET:HG3	21:b:136:VAL:HG22	1.73	0.71
22:c:151:VAL:HG13	22:c:152:LYS:HG3	1.71	0.71
2:B:103:ARG:NH2	2:B:160:ILE:O	2.23	0.71
18:Y:128:TYR:O	18:Y:137:ARG:NH1	2.24	0.71
23:d:215:LEU:HD21	23:d:219:ASP:HB2	1.73	0.71
3:C:161:ILE:HG21	3:C:199:LEU:HD21	1.72	0.70
3:C:198:LEU:HD22	29:C:501:ADP:H2'	1.72	0.70
7:G:84:THR:HB	13:M:156:VAL:HG22	1.72	0.70
24:e:62:LYS:HG2	24:e:63:HIS:HD2	1.56	0.70
9:I:119:GLN:NE2	10:J:79:ASP:OD1	2.23	0.70
19:Z:17:LEU:HD12	22:c:39:LEU:HD12	1.73	0.70
20:a:208:GLU:OE1	20:a:208:GLU:N	2.24	0.70
2:B:182:GLU:O	2:B:241:ASN:ND2	2.24	0.70
7:G:158:GLY:O	8:H:84:ARG:NH2	2.24	0.70
9:I:21:VAL:HG11	9:I:153:SER:HB3	1.72	0.70
13:M:39:ILE:HD13	13:M:193:VAL:HG22	1.73	0.70
18:Y:23:ARG:HH12	18:Y:27:SER:HB3	1.55	0.70
25:f:237:VAL:HG21	25:f:249:LEU:HG	1.73	0.70
2:B:70:ASP:O	2:B:74:MET:HG2	1.90	0.70
2:B:191:ASP:OD1	2:B:192:ASN:N	2.25	0.70
20:a:216:LEU:HA	20:a:219:HIS:HB2	1.72	0.70
2:B:405:MET:HA	2:B:408:ARG:HE	1.56	0.70
3:C:114:VAL:HG22	3:C:123:LEU:HD11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:48:GLU:HA	9:I:211:VAL:HA	1.74	0.70
11:K:13:ASN:HA	12:L:126:ARG:HB3	1.72	0.70
18:Y:307:LEU:HD23	18:Y:319:MET:HE3	1.72	0.69
21:b:26:LEU:O	21:b:29:GLN:NE2	2.24	0.69
13:M:123:THR:HG22	13:M:130:PRO:HB3	1.74	0.69
16:W:177:MET:HB3	16:W:182:ARG:HE	1.57	0.69
20:a:140:GLU:OE1	20:a:140:GLU:N	2.25	0.69
23:d:299:MET:O	23:d:303:ALA:N	2.23	0.69
25:f:552:ASP:OD2	25:f:553:THR:N	2.25	0.69
1:A:390:THR:O	1:A:394:MET:HE2	1.92	0.69
3:C:333:SER:HA	3:C:336:MET:HG2	1.72	0.69
1:A:102:ILE:HD11	1:A:112:ILE:HD11	1.73	0.69
3:C:71:SER:H	3:C:118:ASN:HB2	1.56	0.69
23:d:128:PHE:O	23:d:178:TYR:OH	2.09	0.69
1:A:213:LEU:HB2	1:A:337:LEU:HD13	1.75	0.69
9:I:38:LEU:HB2	9:I:161:ALA:HB2	1.75	0.69
14:U:751:ARG:HD3	14:U:908:ILE:HB	1.75	0.69
16:W:35:ALA:HB1	16:W:73:MET:HG2	1.74	0.69
25:f:233:LEU:HB3	25:f:248:LEU:HD21	1.74	0.69
27:u:176:LYS:HG3	27:u:270:VAL:HG12	1.74	0.69
1:A:362:MET:HE1	1:A:389:CYS:HB3	1.75	0.69
11:K:54:ILE:HD11	11:K:59:MET:HB3	1.73	0.69
14:U:151:ILE:H	14:U:151:ILE:HD12	1.58	0.69
18:Y:42:MET:HA	18:Y:45:VAL:HB	1.73	0.69
1:A:242:GLY:HA2	1:A:280:ILE:HD11	1.74	0.68
25:f:702:PRO:HD3	25:f:736:THR:HG21	1.75	0.68
5:E:234:GLU:HG2	6:F:315:ASN:HD21	1.59	0.68
5:E:331:ILE:HG23	5:E:371:VAL:HG21	1.76	0.68
14:U:371:ILE:O	14:U:374:SER:OG	2.10	0.68
26:g:81:GLY:O	26:g:104:ARG:NH1	2.27	0.68
2:B:378:VAL:HA	2:B:416:ASN:HB2	1.76	0.68
4:D:388:ARG:NH1	5:E:147:GLU:OE2	2.26	0.68
5:E:207:TYR:HE1	6:F:129:ARG:HD3	1.58	0.68
5:E:252:GLU:HA	5:E:255:ARG:HE	1.59	0.68
23:d:138:LYS:HE2	23:d:181:GLN:HB3	1.75	0.68
2:B:373:THR:OG1	2:B:412:MET:O	2.11	0.68
11:K:50:VAL:HG11	11:K:67:ILE:HB	1.74	0.68
16:W:153:LYS:HB3	16:W:158:ASP:HB2	1.75	0.68
25:f:688:ARG:O	25:f:724:ASN:ND2	2.25	0.68
5:E:352:MET:HE3	6:F:220:PRO:HD3	1.76	0.68
6:F:288:LEU:HD21	6:F:330:ALA:HB1	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:421:MET:HE2	6:F:421:MET:H	1.59	0.68
15:V:153:LYS:O	15:V:157:THR:OG1	2.12	0.68
20:a:363:MET:HE1	22:c:307:VAL:HG22	1.75	0.68
3:C:357:ALA:HB1	4:D:323:ARG:HH22	1.58	0.68
23:d:299:MET:HA	23:d:302:TYR:HB2	1.75	0.68
1:A:280:ILE:HG22	1:A:299:MET:HB3	1.74	0.68
3:C:396:GLU:HG2	3:C:399:MET:HE3	1.76	0.68
2:B:320:ASP:OD2	2:B:321:SER:N	2.26	0.67
14:U:609:ASP:O	14:U:615:ARG:NH1	2.27	0.67
17:X:394:ASP:OD2	18:Y:362:LYS:NZ	2.27	0.67
7:G:43:ARG:NH2	7:G:163:PHE:O	2.26	0.67
13:M:134:SER:HB2	13:M:153:PRO:HD3	1.75	0.67
10:J:7:ILE:HG12	10:J:18:GLN:HG2	1.74	0.67
21:b:52:ILE:HD11	21:b:60:VAL:HG22	1.76	0.67
25:f:901:ARG:HH12	25:f:904:PRO:HD3	1.57	0.67
5:E:149:ILE:HD12	5:E:274:LYS:HB3	1.75	0.67
7:G:120:ASP:OD1	8:H:84:ARG:NH1	2.28	0.67
7:G:221:THR:HG22	7:G:223:GLU:H	1.59	0.67
25:f:504:VAL:HB	25:f:518:THR:HG21	1.76	0.67
4:D:416:PHE:HZ	7:G:21:ARG:HG3	1.59	0.67
16:W:234:ASP:HB2	16:W:243:ILE:HD11	1.77	0.67
18:Y:326:GLY:N	24:e:59:GLU:OE1	2.28	0.67
21:b:104:ASN:HB3	27:u:133:ALA:HA	1.76	0.67
1:A:345:LEU:HD22	1:A:379:ASN:HB3	1.76	0.67
4:D:411:GLU:OE2	4:D:414:HIS:N	2.28	0.67
16:W:146:THR:HG23	16:W:165:ILE:HG22	1.75	0.67
14:U:213:PHE:HB2	14:U:244:MET:HE2	1.76	0.67
20:a:291:LEU:HD22	20:a:296:ILE:HG22	1.77	0.67
1:A:224:LEU:HD22	29:A:501:ADP:H2'	1.77	0.67
14:U:164:GLU:HG3	14:U:204:ILE:HD11	1.75	0.67
25:f:319:GLU:OE1	25:f:325:GLN:NE2	2.27	0.67
8:H:159:LYS:NZ	9:I:56:LEU:O	2.28	0.67
12:L:196:ARG:HG3	12:L:239:ARG:HH21	1.60	0.67
27:u:157:LEU:HD22	27:u:165:LEU:HD11	1.76	0.67
3:C:147:THR:H	3:C:150:MET:HE3	1.60	0.66
3:C:192:PRO:HB3	3:C:296:ASN:HD21	1.60	0.66
5:E:31:GLU:HA	5:E:34:LYS:HD2	1.77	0.66
27:u:189:GLN:HG2	27:u:255:GLU:HG3	1.76	0.66
8:H:92:LYS:O	8:H:96:GLN:HG3	1.96	0.66
14:U:789:ILE:HB	14:U:911:ILE:HA	1.78	0.66
22:c:52:GLU:CD	27:u:289:HIS:HE1	2.03	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:ILE:HD11	2:B:239:VAL:HG11	1.77	0.66
25:f:879:ARG:NH1	25:f:895:GLU:OE2	2.28	0.66
10:J:61:LYS:H	10:J:61:LYS:HD2	1.61	0.66
12:L:24:TYR:HA	12:L:27:GLU:HG2	1.78	0.66
25:f:446:LEU:HD13	25:f:483:PHE:HB3	1.76	0.66
6:F:94:ILE:HG22	6:F:95:GLU:H	1.60	0.66
11:K:114:GLN:O	11:K:118:ASN:ND2	2.21	0.66
15:V:179:LYS:NZ	15:V:183:GLU:OE2	2.27	0.66
17:X:392:PRO:O	17:X:394:ASP:N	2.24	0.66
2:B:214:MET:HE2	2:B:214:MET:HA	1.78	0.66
14:U:12:LEU:O	14:U:20:LYS:NZ	2.28	0.66
5:E:117:PRO:HD3	6:F:94:ILE:HG23	1.77	0.66
15:V:214:HIS:CE1	15:V:227:VAL:HG22	2.29	0.66
16:W:283:GLN:O	16:W:287:VAL:HG23	1.96	0.66
4:D:384:MET:HA	4:D:384:MET:HE3	1.78	0.66
12:L:146:GLN:HB3	12:L:159:MET:HE1	1.75	0.66
14:U:549:ALA:HA	14:U:581:SER:HB3	1.77	0.66
22:c:277:LYS:O	22:c:282:ARG:NE	2.28	0.66
27:u:227:GLU:OE2	27:u:227:GLU:N	2.29	0.66
11:K:31:ILE:HD11	11:K:158:PRO:HD2	1.78	0.66
20:a:296:ILE:HD11	20:a:307:VAL:HB	1.78	0.66
1:A:186:LYS:NZ	6:F:426:GLU:OE2	2.29	0.66
7:G:73:THR:HG22	7:G:75:ASN:H	1.61	0.66
19:Z:93:GLY:CA	19:Z:120:VAL:O	2.44	0.66
23:d:324:LYS:NZ	23:d:328:THR:OG1	2.29	0.66
25:f:666:ILE:HD12	25:f:667:GLY:N	2.11	0.66
2:B:184:TYR:HE2	2:B:198:LYS:HE2	1.61	0.65
14:U:811:PHE:CE1	14:U:885:MET:HE1	2.30	0.65
15:V:433:ASP:OD1	23:d:242:ASN:ND2	2.28	0.65
25:f:463:LEU:HD22	26:g:133:LYS:HB3	1.78	0.65
16:W:140:ILE:HG23	16:W:141:GLU:OE1	1.96	0.65
3:C:82:LYS:HE2	3:C:82:LYS:H	1.60	0.65
13:M:77:VAL:HG12	13:M:135:PHE:HB3	1.79	0.65
20:a:34:TRP:HH2	20:a:64:ILE:HG13	1.60	0.65
23:d:119:LEU:HA	23:d:122:VAL:HG12	1.78	0.65
6:F:417:HIS:CD2	6:F:421:MET:HE1	2.30	0.65
26:g:159:LYS:HA	26:g:159:LYS:HE3	1.78	0.65
12:L:109:VAL:HG22	12:L:134:ILE:HD12	1.79	0.65
13:M:215:TRP:HB2	13:M:227:VAL:HG22	1.79	0.65
3:C:131:VAL:HG12	3:C:133:PRO:HG3	1.79	0.65
4:D:141:ASP:OD1	4:D:142:VAL:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:41:GLN:HB2	11:K:153:LEU:HB3	1.77	0.65
22:c:130:GLN:HE21	22:c:142:ALA:HB2	1.60	0.65
23:d:260:ILE:HA	23:d:263:LEU:HD12	1.78	0.65
25:f:809:ILE:HD11	25:f:817:VAL:HG21	1.78	0.65
1:A:159:PRO:HA	1:A:162:THR:HG22	1.79	0.65
13:M:66:LEU:HD22	13:M:212:GLU:HB2	1.79	0.65
3:C:23:TYR:CZ	14:U:105:ILE:HG12	2.32	0.65
11:K:107:MET:N	11:K:107:MET:SD	2.70	0.65
15:V:439:ALA:O	15:V:443:ARG:HG2	1.96	0.65
20:a:34:TRP:N	21:b:18:ASN:OD1	2.30	0.65
1:A:73:ALA:O	1:A:78:TRP:NE1	2.24	0.65
1:A:398:ARG:NH1	1:A:398:ARG:O	2.30	0.65
2:B:287:ILE:HD12	2:B:290:ILE:HG23	1.79	0.65
14:U:602:LEU:HD12	14:U:621:SER:HB2	1.79	0.65
25:f:534:VAL:O	25:f:538:ILE:HG12	1.97	0.65
11:K:195:ILE:O	11:K:199:LEU:HG	1.97	0.64
12:L:214:ILE:O	12:L:221:PHE:HA	1.97	0.64
25:f:138:GLU:HG3	25:f:142:TYR:CE2	2.33	0.64
2:B:417:GLU:O	2:B:421:LYS:HG3	1.97	0.64
4:D:40:LEU:HD22	4:D:43:ARG:HH21	1.63	0.64
25:f:263:PRO:HB3	25:f:297:MET:HE1	1.77	0.64
14:U:35:TRP:HH2	15:V:274:SER:HB2	1.62	0.64
20:a:335:TRP:CD1	20:a:337:GLN:H	2.15	0.64
3:C:141:GLU:OE1	3:C:201:ARG:NH1	2.31	0.64
6:F:53:LYS:HZ3	21:b:23:PRO:HB2	1.62	0.64
20:a:100:THR:HA	20:a:103:LYS:HE2	1.78	0.64
25:f:177:GLU:OE2	25:f:180:GLN:NE2	2.31	0.64
25:f:720:GLU:OE1	25:f:807:ARG:NH1	2.30	0.64
15:V:410:ILE:HG21	15:V:422:ILE:HG22	1.79	0.64
23:d:91:ALA:HB2	23:d:122:VAL:HG21	1.80	0.64
25:f:670:MET:HE2	25:f:670:MET:HA	1.78	0.64
14:U:169:GLU:O	14:U:171:ASN:ND2	2.30	0.64
15:V:280:ALA:HB1	15:V:284:GLU:HB2	1.78	0.64
17:X:222:GLU:N	17:X:222:GLU:OE2	2.31	0.64
1:A:214:LEU:HG	1:A:343:PHE:HE1	1.63	0.64
15:V:309:MET:HE3	15:V:332:LEU:HA	1.78	0.64
21:b:161:ASN:ND2	21:b:168:SER:O	2.31	0.64
14:U:31:VAL:HG21	14:U:66:LYS:HE2	1.80	0.64
17:X:182:ASN:ND2	18:Y:248:GLU:OE1	2.27	0.64
3:C:76:VAL:HA	3:C:87:VAL:HA	1.80	0.64
5:E:109:ARG:NH2	5:E:110:TYR:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:12:SER:OG	13:M:124:LEU:O	2.13	0.64
27:u:196:ILE:O	27:u:215:THR:N	2.31	0.64
1:A:307:ASP:O	1:A:336:ARG:NH2	2.28	0.63
3:C:314:LYS:N	3:C:314:LYS:HD2	2.13	0.63
16:W:406:VAL:HG22	16:W:413:ILE:HG12	1.80	0.63
3:C:23:TYR:OH	14:U:106:ASP:N	2.30	0.63
5:E:352:MET:HA	5:E:355:ILE:HG22	1.80	0.63
15:V:318:GLN:HG2	15:V:319:HIS:H	1.63	0.63
27:u:195:LYS:HB3	27:u:214:PRO:HB3	1.80	0.63
6:F:258:GLN:HG3	6:F:267:LEU:HD11	1.78	0.63
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.80	0.63
17:X:207:GLN:NE2	17:X:211:ASP:OD1	2.32	0.63
26:g:102:GLU:OE1	26:g:102:GLU:N	2.29	0.63
2:B:291:GLY:HA2	2:B:309:MET:HE1	1.79	0.63
10:J:36:ARG:NH1	10:J:142:PRO:O	2.31	0.63
21:b:38:HIS:HB3	21:b:42:ARG:HH21	1.63	0.63
7:G:224:ASN:HD21	7:G:228:ARG:HH12	1.47	0.63
22:c:279:ASP:HB2	22:c:280:PRO:HD3	1.81	0.63
26:g:123:GLN:HB2	26:g:126:TYR:HB2	1.80	0.63
26:g:160:GLN:HB3	26:g:164:ASP:HB3	1.80	0.63
27:u:235:TYR:O	27:u:239:GLN:NE2	2.31	0.63
12:L:27:GLU:HA	12:L:30:LYS:HG2	1.81	0.63
25:f:216:MET:HB3	25:f:219:LYS:HE2	1.79	0.63
1:A:146:LYS:CE	1:A:148:GLN:HE21	2.11	0.63
2:B:313:LEU:HD11	2:B:343:ARG:HD3	1.80	0.63
6:F:224:LEU:HB2	6:F:348:LEU:HD22	1.81	0.63
13:M:36:ALA:HB1	13:M:49:VAL:HG22	1.81	0.63
22:c:27:THR:OG1	22:c:28:ALA:N	2.31	0.63
2:B:198:LYS:NZ	2:B:202:GLU:OE2	2.32	0.63
5:E:158:LEU:HD23	5:E:161:ARG:HH21	1.64	0.63
9:I:6:ASP:O	9:I:20:GLN:NE2	2.31	0.63
13:M:72:HIS:NE2	13:M:105:ASN:OD1	2.32	0.63
18:Y:201:PHE:HB3	18:Y:223:THR:HG23	1.80	0.63
19:Z:78:MET:HE2	22:c:98:MET:HE3	1.80	0.63
23:d:287:ALA:HA	23:d:290:ILE:HG12	1.79	0.63
3:C:307:ARG:HG2	3:C:308:PRO:HD2	1.81	0.63
5:E:97:ARG:HD3	5:E:111:LEU:HB2	1.81	0.62
14:U:838:LYS:HA	14:U:841:LYS:HG2	1.80	0.62
14:U:879:ASP:H	14:U:882:ALA:HB2	1.64	0.62
7:G:49:VAL:HG22	7:G:219:VAL:HG23	1.81	0.62
22:c:71:ASP:OD1	22:c:72:VAL:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:250:GLU:HG2	3:C:250:GLU:O	1.98	0.62
3:C:312:ASP:O	3:C:314:LYS:NZ	2.33	0.62
12:L:173:GLU:HB2	13:M:56:LYS:HG3	1.80	0.62
14:U:7:GLY:HA3	23:d:169:ALA:HB1	1.81	0.62
13:M:180:GLN:HE22	13:M:183:GLU:HB2	1.65	0.62
16:W:40:LEU:HD12	16:W:43:VAL:HB	1.80	0.62
25:f:693:ALA:O	25:f:697:ILE:HG13	2.00	0.62
2:B:193:GLN:O	2:B:197:ILE:HG22	1.98	0.62
13:M:119:VAL:HA	13:M:131:PHE:HE2	1.64	0.62
16:W:201:ARG:HA	16:W:204:ILE:HG22	1.81	0.62
17:X:90:ARG:HE	17:X:93:LEU:HD21	1.65	0.62
25:f:407:MET:N	25:f:407:MET:SD	2.73	0.62
5:E:355:ILE:HD11	6:F:211:LYS:HB3	1.82	0.62
14:U:553:ALA:HA	14:U:585:THR:HG22	1.80	0.62
1:A:56:LEU:HD11	2:B:49:LEU:HD21	1.80	0.62
16:W:378:MET:HE1	16:W:393:LEU:HD22	1.81	0.62
18:Y:202:LEU:HD23	18:Y:239:LYS:HD2	1.80	0.62
26:g:157:GLU:N	26:g:157:GLU:OE2	2.31	0.62
20:a:76:LEU:O	20:a:80:ILE:HG23	2.00	0.62
25:f:163:ALA:HB1	25:f:207:LEU:HD12	1.82	0.62
12:L:103:LEU:HD12	12:L:104:PRO:HD2	1.82	0.62
14:U:789:ILE:HG22	14:U:791:LEU:H	1.65	0.62
26:g:137:GLN:HB3	26:g:140:LYS:HD3	1.82	0.62
11:K:201:ILE:O	11:K:205:VAL:HG12	2.00	0.62
15:V:344:ASP:OD1	15:V:345:ARG:N	2.33	0.62
16:W:31:CYS:HB3	16:W:43:VAL:HG13	1.82	0.61
16:W:366:MET:HE1	16:W:378:MET:HG3	1.81	0.61
25:f:464:ALA:O	26:g:135:GLN:NE2	2.28	0.61
27:u:139:ASN:ND2	27:u:164:GLN:O	2.33	0.61
7:G:80:MET:HE1	7:G:138:MET:HG2	1.81	0.61
18:Y:122:THR:O	18:Y:126:LYS:HE3	1.99	0.61
2:B:106:PRO:HG3	3:C:121:TYR:CD1	2.35	0.61
14:U:255:SER:O	14:U:754:HIS:NE2	2.33	0.61
19:Z:69:PHE:CD2	21:b:96:ALA:HA	2.34	0.61
21:b:103:LYS:HB3	27:u:136:GLU:OE2	2.01	0.61
4:D:417:TYR:HA	8:H:79:MET:HE1	1.83	0.61
16:W:188:GLU:OE2	16:W:225:LYS:NZ	2.34	0.61
22:c:284:LEU:O	22:c:288:VAL:HG12	1.99	0.61
11:K:125:GLU:OE2	12:L:126:ARG:NH2	2.29	0.61
18:Y:111:LEU:HD23	18:Y:114:ILE:HD11	1.82	0.61
20:a:77:VAL:HA	20:a:80:ILE:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:g:130:VAL:HG22	26:g:154:MET:HB3	1.82	0.61
5:E:213:ARG:HH22	5:E:214:LEU:HD13	1.64	0.61
14:U:443:LEU:HD11	14:U:464:GLN:HG2	1.82	0.61
16:W:47:LEU:HD22	16:W:66:ILE:HG13	1.82	0.61
17:X:407:MET:HA	17:X:410:VAL:HG12	1.82	0.61
18:Y:301:ILE:H	18:Y:301:ILE:HD12	1.66	0.61
20:a:24:ARG:NH2	20:a:27:GLU:OE1	2.33	0.61
25:f:278:VAL:HG11	25:f:298:LEU:HD21	1.81	0.61
25:f:470:VAL:HG21	25:f:500:LEU:HD21	1.82	0.61
1:A:51:ASP:HB2	2:B:69:LYS:HZ1	1.66	0.61
12:L:26:MET:HE1	12:L:148:CYS:HB2	1.81	0.61
13:M:229:LYS:HZ1	13:M:236:GLU:H	1.49	0.61
18:Y:45:VAL:HA	18:Y:50:MET:HE1	1.83	0.61
1:A:300:LEU:O	1:A:303:ILE:HG22	2.01	0.61
11:K:228:MET:HA	11:K:228:MET:HE3	1.81	0.61
22:c:281:LYS:HB3	22:c:282:ARG:NH1	2.16	0.61
25:f:220:ASP:C	25:f:221:ILE:HD13	2.26	0.61
5:E:72:LYS:NZ	5:E:76:GLY:O	2.31	0.61
12:L:23:GLU:HA	12:L:26:MET:HG2	1.83	0.61
15:V:37:MET:HE1	15:V:89:LYS:HE3	1.83	0.61
15:V:337:LEU:HD22	15:V:367:VAL:HG11	1.82	0.61
17:X:47:GLU:CD	17:X:47:GLU:H	2.09	0.61
20:a:60:TYR:O	20:a:64:ILE:HG22	2.01	0.61
10:J:71:MET:HE3	10:J:72:ALA:C	2.25	0.61
15:V:440:LYS:HA	15:V:443:ARG:HG3	1.82	0.61
18:Y:190:ALA:HB2	18:Y:287:LEU:HD11	1.83	0.61
3:C:102:ASN:O	3:C:104:ASP:N	2.33	0.60
8:H:185:GLU:O	8:H:189:HIS:ND1	2.34	0.60
12:L:143:HIS:HB3	12:L:145:PHE:CE1	2.36	0.60
20:a:129:GLN:HG3	20:a:130:VAL:H	1.66	0.60
4:D:406:VAL:HG23	4:D:407:ILE:HG13	1.83	0.60
11:K:113:THR:HG22	11:K:143:PHE:HD2	1.66	0.60
16:W:293:ASP:HB3	16:W:296:LEU:HD13	1.83	0.60
19:Z:223:ASN:O	19:Z:225:GLN:N	2.34	0.60
25:f:794:ALA:O	25:f:798:THR:HG23	1.99	0.60
25:f:862:ILE:HG22	25:f:865:PHE:HB3	1.82	0.60
1:A:51:ASP:HB2	2:B:69:LYS:NZ	2.16	0.60
11:K:91:LYS:HE2	11:K:119:LEU:CB	2.31	0.60
26:g:129:ILE:HB	26:g:136:LEU:HD23	1.83	0.60
5:E:36:LEU:HD11	6:F:70:LYS:HD3	1.82	0.60
8:H:82:ASP:HB3	8:H:130:PHE:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:g:161:SER:O	26:g:165:ALA:N	2.34	0.60
27:u:144:HIS:HB2	27:u:158:GLU:HG2	1.82	0.60
7:G:182:LYS:HA	7:G:185:LYS:HE2	1.82	0.60
17:X:86:ALA:HB2	17:X:125:LEU:HD21	1.84	0.60
22:c:139:ARG:HA	22:c:161:ARG:HH22	1.66	0.60
23:d:295:THR:HB	23:d:298:LYS:HE2	1.83	0.60
25:f:253:LEU:HB2	25:f:268:LEU:HD22	1.84	0.60
14:U:921:ILE:HG13	14:U:923:GLU:HB2	1.84	0.60
19:Z:12:HIS:NE2	19:Z:49:ASP:OD1	2.34	0.60
19:Z:227:ILE:HG13	20:a:341:LEU:HD23	1.83	0.60
2:B:187:ILE:HD11	2:B:190:LEU:HB2	1.82	0.60
15:V:443:ARG:HH11	23:d:274:CYS:HB2	1.67	0.60
25:f:287:ASP:HB3	25:f:290:VAL:HB	1.84	0.60
8:H:65:VAL:HG22	8:H:75:VAL:HG22	1.84	0.60
8:H:212:ILE:HB	8:H:219:ARG:HH22	1.66	0.60
15:V:66:GLU:O	15:V:69:THR:OG1	2.14	0.60
18:Y:383:LEU:HD22	19:Z:272:LEU:HD13	1.83	0.60
23:d:145:ARG:NH1	23:d:183:PRO:O	2.33	0.60
5:E:15:LYS:HG2	6:F:47:LEU:HD12	1.84	0.60
7:G:80:MET:HG2	7:G:87:SER:CB	2.32	0.60
14:U:463:ASN:O	14:U:467:ASN:ND2	2.34	0.60
21:b:97:LEU:HD22	21:b:107:MET:SD	2.41	0.60
25:f:402:ASN:HB2	25:f:407:MET:HE1	1.83	0.60
25:f:505:MET:HE1	25:f:518:THR:HB	1.83	0.60
5:E:307:GLN:OE1	5:E:307:GLN:N	2.34	0.60
10:J:73:PHE:HD2	10:J:80:ALA:HA	1.67	0.60
15:V:494:MET:O	19:Z:278:ASN:ND2	2.35	0.60
18:Y:279:GLU:HG3	18:Y:296:VAL:HG21	1.83	0.60
20:a:258:GLN:OE1	20:a:258:GLN:N	2.35	0.60
6:F:373:MET:HB3	6:F:415:LEU:HD21	1.84	0.59
14:U:796:LYS:HE3	14:U:921:ILE:HD13	1.84	0.59
18:Y:326:GLY:HA3	24:e:63:HIS:CE1	2.37	0.59
23:d:215:LEU:HD22	23:d:220:ILE:HG23	1.84	0.59
27:u:126:LEU:HD12	27:u:265:PHE:HB3	1.83	0.59
2:B:250:VAL:HG13	2:B:284:ILE:HG22	1.83	0.59
2:B:311:GLU:HA	2:B:314:ASN:ND2	2.17	0.59
2:B:334:ILE:HA	2:B:337:LEU:HD23	1.83	0.59
2:B:400:THR:O	2:B:404:LEU:HD22	2.02	0.59
4:D:349:THR:HB	4:D:354:LEU:HD11	1.83	0.59
8:H:160:ALA:HB1	8:H:174:LEU:HD13	1.83	0.59
14:U:707:ASN:O	14:U:711:GLN:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:849:ALA:HB2	25:f:879:ARG:HG3	1.82	0.59
25:f:866:GLN:OE1	25:f:866:GLN:N	2.35	0.59
12:L:143:HIS:HB3	12:L:145:PHE:HE1	1.67	0.59
2:B:385:MET:HE2	2:B:386:ALA:H	1.67	0.59
14:U:588:MET:HA	14:U:591:CYS:HB2	1.85	0.59
16:W:141:GLU:OE1	16:W:141:GLU:N	2.35	0.59
17:X:260:MET:HE1	17:X:326:LEU:HB2	1.84	0.59
7:G:10:ASP:O	7:G:24:GLN:NE2	2.35	0.59
14:U:469:SER:HA	27:u:121:LYS:HE2	1.85	0.59
15:V:433:ASP:O	15:V:437:ILE:HG12	2.02	0.59
19:Z:175:LEU:HD21	22:c:38:LEU:HD23	1.83	0.59
22:c:122:LEU:HD22	22:c:126:ASP:HB3	1.82	0.59
4:D:316:THR:O	4:D:317:LEU:HB2	2.02	0.59
25:f:220:ASP:O	25:f:221:ILE:HD13	2.02	0.59
27:u:146:PHE:HA	27:u:157:LEU:HD12	1.84	0.59
1:A:30:ILE:HD12	1:A:30:ILE:H	1.68	0.59
3:C:23:TYR:CE1	14:U:102:ALA:HA	2.36	0.59
5:E:196:LEU:N	5:E:229:ILE:O	2.35	0.59
11:K:36:THR:O	11:K:66:LYS:NZ	2.36	0.59
14:U:925:VAL:HG12	14:U:927:PRO:HD3	1.84	0.59
17:X:44:GLN:N	17:X:44:GLN:NE2	2.50	0.59
20:a:232:TRP:O	20:a:236:THR:HG23	2.03	0.59
25:f:369:ARG:NH1	25:f:757:ASN:OD1	2.35	0.59
2:B:379:THR:OG1	2:B:382:ASP:OD2	2.20	0.59
5:E:234:GLU:HB3	6:F:311:LEU:HD13	1.85	0.59
12:L:157:ARG:HH12	12:L:180:MET:HB3	1.67	0.59
18:Y:80:GLU:OE2	18:Y:83:ARG:NH1	2.36	0.59
20:a:42:LEU:HD11	20:a:78:GLU:HG3	1.85	0.59
4:D:89:ILE:HD11	4:D:129:SER:HB2	1.85	0.59
4:D:192:LYS:NZ	4:D:302:ASN:HA	2.18	0.59
7:G:72:ILE:HG12	7:G:95:ARG:HA	1.84	0.59
10:J:76:LEU:HD23	10:J:76:LEU:H	1.68	0.59
18:Y:376:LEU:HD23	19:Z:265:LEU:HD11	1.85	0.59
21:b:107:MET:HB3	21:b:136:VAL:HA	1.84	0.59
25:f:340:MET:O	25:f:387:GLN:NE2	2.36	0.59
27:u:150:LEU:HD23	27:u:151:ARG:HD2	1.85	0.59
1:A:386:ARG:HH21	29:A:501:ADP:H4'	1.67	0.59
14:U:23:ALA:O	14:U:27:LEU:HD22	2.03	0.59
14:U:697:GLN:HE22	14:U:786:THR:HG21	1.68	0.59
15:V:487:HIS:O	15:V:491:VAL:HG23	2.01	0.59
23:d:284:PHE:HB3	23:d:314:ASN:HD21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:685:THR:HG23	25:f:686:LEU:HD22	1.85	0.59
2:B:360:THR:O	2:B:364:ILE:HG12	2.02	0.58
4:D:207:PRO:HG2	4:D:335:LEU:HG	1.85	0.58
7:G:51:VAL:HG23	7:G:217:VAL:HG22	1.83	0.58
18:Y:26:LEU:HB3	18:Y:61:LEU:HD13	1.85	0.58
18:Y:97:GLU:HA	18:Y:100:ILE:HG12	1.85	0.58
18:Y:140:ILE:HA	18:Y:143:TYR:HD2	1.68	0.58
1:A:268:LYS:O	1:A:268:LYS:HD3	2.03	0.58
13:M:40:ARG:HG3	13:M:45:VAL:HG22	1.84	0.58
14:U:629:THR:OG1	14:U:632:GLN:OE1	2.19	0.58
19:Z:69:PHE:HE1	19:Z:71:ASP:HA	1.68	0.58
20:a:356:TRP:O	20:a:360:VAL:HG23	2.02	0.58
7:G:159:TYR:HA	8:H:84:ARG:NH2	2.18	0.58
23:d:302:TYR:HA	23:d:305:LYS:HE3	1.84	0.58
26:g:128:LYS:HD2	26:g:129:ILE:N	2.18	0.58
1:A:398:ARG:NH2	25:f:867:THR:O	2.37	0.58
2:B:189:GLY:HA3	2:B:360:THR:HG22	1.85	0.58
3:C:75:GLU:HG3	3:C:113:ARG:HA	1.84	0.58
8:H:118:MET:HA	8:H:130:PHE:HE1	1.67	0.58
11:K:91:LYS:HE2	11:K:119:LEU:HB2	1.85	0.58
15:V:491:VAL:HA	15:V:494:MET:HE1	1.84	0.58
17:X:53:LEU:HA	17:X:56:LEU:HG	1.85	0.58
22:c:52:GLU:OE2	27:u:289:HIS:HE1	1.86	0.58
23:d:332:SER:O	23:d:335:LEU:N	2.34	0.58
2:B:276:GLU:OE1	2:B:277:HIS:ND1	2.36	0.58
3:C:224:ILE:HD12	3:C:224:ILE:H	1.68	0.58
9:I:119:GLN:NE2	9:I:123:GLN:OE1	2.37	0.58
11:K:121:LEU:HD21	11:K:160:GLY:HA3	1.83	0.58
12:L:66:VAL:HG11	12:L:89:ARG:HA	1.86	0.58
19:Z:68:TRP:HD1	19:Z:104:ASN:HD21	1.52	0.58
20:a:246:GLU:CD	20:a:249:GLN:H	2.12	0.58
25:f:852:VAL:O	25:f:855:GLN:NE2	2.37	0.58
1:A:25:LEU:HD12	1:A:30:ILE:HG13	1.85	0.58
5:E:27:LYS:NZ	5:E:31:GLU:OE2	2.34	0.58
9:I:136:TYR:O	9:I:147:LEU:HA	2.04	0.58
14:U:792:ASN:HA	14:U:913:ILE:HG22	1.86	0.58
21:b:68:THR:HA	21:b:71:ILE:HD13	1.86	0.58
27:u:137:CYS:HA	27:u:167:ILE:HA	1.84	0.58
10:J:82:ILE:O	10:J:86:ARG:HG2	2.04	0.58
14:U:14:GLU:OE2	23:d:166:ARG:NH1	2.36	0.58
23:d:180:GLU:OE2	23:d:181:GLN:NE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LYS:NZ	1:A:148:GLN:HE22	2.00	0.58
5:E:233:ASP:N	5:E:233:ASP:OD2	2.35	0.58
5:E:380:LEU:HD11	6:F:226:TYR:CZ	2.39	0.58
13:M:119:VAL:O	13:M:123:THR:HG23	2.04	0.58
16:W:271:VAL:HG23	16:W:306:LEU:HD13	1.85	0.58
1:A:248:LYS:HZ3	28:v:19:UNK:HA	1.67	0.58
1:A:401:ARG:NH2	1:A:408:ASP:OD1	2.35	0.58
3:C:233:GLU:O	3:C:237:MET:HE2	2.04	0.58
4:D:297:ASP:OD2	4:D:326:ARG:NH1	2.37	0.58
14:U:174:PRO:HA	14:U:177:LEU:HG	1.85	0.58
19:Z:164:ALA:HB2	22:c:220:LEU:HD11	1.86	0.58
1:A:62:LEU:HB3	2:B:79:ILE:HD13	1.86	0.57
12:L:158:ALA:HB1	12:L:172:LEU:HB3	1.86	0.57
19:Z:59:ASP:HB3	21:b:95:LEU:HD21	1.85	0.57
19:Z:226:ILE:O	19:Z:230:LEU:N	2.35	0.57
22:c:191:ALA:O	22:c:196:LEU:N	2.36	0.57
2:B:176:VAL:HG13	2:B:177:GLU:H	1.69	0.57
15:V:462:GLU:HG3	15:V:464:ILE:HG23	1.86	0.57
13:M:216:VAL:HG12	13:M:224:HIS:HA	1.85	0.57
14:U:323:LEU:HB3	14:U:327:LYS:HZ2	1.69	0.57
15:V:215:ALA:HB1	15:V:224:LEU:HD13	1.87	0.57
1:A:169:LYS:HZ1	1:A:234:ASP:H	1.52	0.57
2:B:119:ASN:O	2:B:135:ILE:N	2.34	0.57
8:H:196:LYS:HE2	8:H:203:MET:HE1	1.85	0.57
11:K:167:ALA:HB1	11:K:181:LEU:HG	1.86	0.57
14:U:233:LEU:HD12	14:U:325:MET:SD	2.44	0.57
15:V:236:ARG:O	15:V:240:LEU:HG	2.05	0.57
16:W:316:ARG:NH2	16:W:380:GLN:O	2.36	0.57
22:c:29:GLU:HG3	22:c:30:GLN:N	2.18	0.57
25:f:99:LEU:HD13	25:f:129:LEU:HD12	1.85	0.57
12:L:225:ASP:O	12:L:229:VAL:N	2.24	0.57
7:G:200:THR:HG23	7:G:242:LEU:HD23	1.86	0.57
14:U:764:LEU:O	14:U:767:THR:OG1	2.21	0.57
26:g:94:LYS:H	26:g:94:LYS:HD3	1.68	0.57
8:H:166:ASN:OD1	8:H:169:ASN:HB2	2.05	0.57
14:U:596:ASN:OD1	14:U:597:LYS:N	2.37	0.57
14:U:712:LEU:O	14:U:716:VAL:HG22	2.04	0.57
20:a:79:ILE:H	20:a:79:ILE:HD12	1.69	0.57
21:b:31:ASP:O	21:b:35:ILE:HG12	2.05	0.57
25:f:418:LEU:HD13	25:f:425:GLY:HA2	1.86	0.57
16:W:87:ILE:HG23	16:W:104:MET:HE2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:b:114:GLY:HA2	21:b:143:PHE:HB2	1.87	0.57
2:B:117:ASP:HB2	2:B:120:HIS:HB2	1.87	0.57
9:I:123:GLN:OE1	10:J:125:ARG:NH1	2.38	0.57
9:I:155:ASN:OD1	10:J:77:THR:OG1	2.16	0.57
11:K:239:LYS:HD3	11:K:239:LYS:N	2.20	0.57
14:U:580:ARG:HH12	14:U:768:GLN:HE22	1.52	0.57
25:f:434:TYR:HB3	26:g:166:ARG:HG3	1.85	0.57
25:f:788:MET:HE2	25:f:793:VAL:HG21	1.87	0.57
1:A:210:LYS:N	1:A:338:ASP:OD1	2.32	0.57
3:C:25:LEU:HD13	15:V:193:GLN:HB2	1.87	0.57
10:J:66:ASP:HB2	10:J:69:VAL:HG12	1.86	0.57
13:M:39:ILE:HG23	13:M:181:MET:HE3	1.86	0.57
18:Y:39:ASP:OD2	18:Y:39:ASP:N	2.36	0.57
18:Y:205:VAL:HA	18:Y:219:PHE:HE2	1.69	0.57
19:Z:93:GLY:HA2	19:Z:120:VAL:O	2.04	0.57
1:A:97:ARG:HG2	1:A:116:LYS:HE3	1.87	0.56
3:C:71:SER:HA	3:C:118:ASN:N	2.19	0.56
4:D:277:ALA:HB1	4:D:282:ASP:HB2	1.87	0.56
14:U:222:PHE:HE1	14:U:754:HIS:HB2	1.70	0.56
15:V:280:ALA:HB3	15:V:285:TRP:CD1	2.39	0.56
19:Z:266:ILE:O	19:Z:270:VAL:HG12	2.05	0.56
1:A:146:LYS:HE2	1:A:148:GLN:HE21	1.68	0.56
7:G:166:THR:HA	7:G:176:THR:HG22	1.87	0.56
1:A:121:PHE:HE1	6:F:89:LEU:HD13	1.70	0.56
2:B:287:ILE:O	2:B:291:GLY:N	2.31	0.56
3:C:114:VAL:CG2	3:C:123:LEU:HD11	2.36	0.56
3:C:359:VAL:O	3:C:362:VAL:HG12	2.06	0.56
15:V:330:LYS:HG3	15:V:360:TYR:CE1	2.35	0.56
18:Y:364:TRP:O	18:Y:368:GLU:HG2	2.05	0.56
20:a:212:ASN:ND2	20:a:241:ASN:OD1	2.38	0.56
25:f:512:MET:HE2	25:f:554:TYR:C	2.30	0.56
2:B:256:ILE:HD12	2:B:305:ILE:HG12	1.87	0.56
2:B:409:GLU:OE1	2:B:411:ARG:NH1	2.38	0.56
4:D:227:PHE:HA	4:D:261:ILE:HG23	1.88	0.56
4:D:245:ARG:HG3	4:D:248:ARG:HH22	1.70	0.56
5:E:175:PRO:HD2	5:E:178:THR:HG21	1.87	0.56
8:H:173:PHE:HA	8:H:176:LYS:HZ2	1.69	0.56
14:U:14:GLU:O	14:U:20:LYS:NZ	2.34	0.56
15:V:147:PHE:HB2	15:V:150:ARG:HB3	1.87	0.56
18:Y:326:GLY:O	18:Y:330:ILE:HG22	2.05	0.56
25:f:307:LEU:HD13	25:f:321:MET:HE1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:LEU:HD12	29:B:501:ADP:H2'	1.86	0.56
9:I:87:THR:HA	9:I:90:LEU:HG	1.87	0.56
13:M:65:ARG:HH12	13:M:78:ALA:HA	1.71	0.56
14:U:191:LYS:HA	14:U:194:ARG:HB3	1.88	0.56
14:U:642:GLU:N	14:U:642:GLU:OE2	2.39	0.56
22:c:41:MET:HE1	22:c:143:VAL:HG11	1.87	0.56
22:c:107:MET:HE3	27:u:272:ALA:HA	1.87	0.56
5:E:200:SER:O	5:E:203:ILE:HG12	2.06	0.56
7:G:10:ASP:HB2	7:G:27:TYR:HE2	1.71	0.56
11:K:69:GLU:HB2	11:K:229:PHE:HE2	1.70	0.56
14:U:78:LEU:HD21	14:U:103:LYS:HB2	1.87	0.56
5:E:118:LEU:HD22	5:E:214:LEU:HD11	1.86	0.56
9:I:158:GLY:HA3	10:J:58:THR:HG21	1.88	0.56
17:X:239:TYR:HD1	17:X:244:SER:HB3	1.71	0.56
18:Y:83:ARG:HA	18:Y:86:GLU:HG2	1.87	0.56
3:C:369:TYR:HD1	3:C:372:ARG:HE	1.52	0.56
8:H:185:GLU:HG3	8:H:189:HIS:HE1	1.71	0.56
15:V:212:TYR:CZ	24:e:21:GLU:HG2	2.41	0.56
21:b:2:VAL:O	21:b:47:ASN:ND2	2.31	0.56
26:g:85:ILE:HD11	26:g:153:ALA:HB2	1.87	0.56
5:E:61:LEU:N	5:E:70:ILE:O	2.39	0.56
7:G:14:THR:HB	8:H:128:ARG:HB3	1.87	0.56
14:U:365:CYS:O	14:U:368:ALA:HB3	2.06	0.56
15:V:167:LEU:HD21	15:V:171:VAL:HG21	1.88	0.56
18:Y:65:ILE:HG23	18:Y:70:LEU:HD13	1.87	0.56
23:d:254:GLU:HA	23:d:257:THR:HG23	1.88	0.56
25:f:694:LEU:HD12	25:f:706:ILE:HG23	1.87	0.56
14:U:501:LEU:HD21	14:U:548:LEU:HD21	1.87	0.56
16:W:384:LEU:HD13	16:W:388:GLU:HG3	1.88	0.56
23:d:232:LEU:HD11	23:d:244:VAL:HG13	1.88	0.56
25:f:478:ARG:NH1	25:f:510:SER:OG	2.38	0.56
27:u:167:ILE:HG23	27:u:246:ILE:HB	1.87	0.56
4:D:352:MET:HE2	4:D:352:MET:HA	1.87	0.55
5:E:203:ILE:HD11	5:E:238:ILE:HD13	1.87	0.55
5:E:277:MET:N	5:E:277:MET:SD	2.79	0.55
15:V:144:ASP:HB2	15:V:147:PHE:CE1	2.41	0.55
16:W:101:VAL:O	16:W:104:MET:HG2	2.06	0.55
17:X:239:TYR:HB3	17:X:247:ALA:HB2	1.88	0.55
17:X:410:VAL:HG21	22:c:255:TYR:CE2	2.41	0.55
18:Y:198:ALA:HB2	18:Y:226:VAL:HG22	1.87	0.55
14:U:560:MET:HA	14:U:560:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:270:VAL:O	19:Z:274:ASN:ND2	2.40	0.55
25:f:267:ARG:NH1	25:f:783:SER:OG	2.31	0.55
25:f:389:LYS:HG3	25:f:390:LEU:HD22	1.87	0.55
13:M:24:GLU:OE1	13:M:24:GLU:N	2.26	0.55
14:U:85:GLY:O	14:U:87:LEU:N	2.39	0.55
14:U:206:MET:HA	14:U:206:MET:HE3	1.88	0.55
2:B:357:ASP:N	2:B:360:THR:OG1	2.40	0.55
15:V:344:ASP:OD1	15:V:346:LEU:N	2.32	0.55
21:b:71:ILE:H	21:b:71:ILE:HD12	1.71	0.55
1:A:40:THR:C	1:A:41:TYR:HD1	2.15	0.55
1:A:281:GLY:HA3	1:A:327:LEU:HD12	1.88	0.55
8:H:7:SER:OG	8:H:21:GLN:NE2	2.40	0.55
12:L:80:ASP:HB3	12:L:128:TYR:HB3	1.88	0.55
13:M:31:GLU:OE1	13:M:169:ARG:NH1	2.40	0.55
14:U:540:GLN:OE1	22:c:208:ARG:NH2	2.38	0.55
15:V:462:GLU:OE2	15:V:463:MET:N	2.39	0.55
18:Y:84:LEU:HB3	18:Y:107:LYS:HG2	1.88	0.55
18:Y:326:GLY:HA3	24:e:63:HIS:HE1	1.70	0.55
20:a:135:ILE:HG23	20:a:155:PHE:HE2	1.72	0.55
25:f:164:GLY:O	25:f:168:LYS:HG3	2.06	0.55
1:A:42:SER:HA	1:A:46:LYS:NZ	2.22	0.55
5:E:237:ALA:HB2	6:F:311:LEU:HD12	1.88	0.55
5:E:282:PRO:HA	5:E:285:LEU:HD23	1.87	0.55
19:Z:19:VAL:HG11	19:Z:124:ILE:HD12	1.88	0.55
20:a:23:HIS:HA	20:a:26:GLU:HB3	1.88	0.55
27:u:193:TYR:HD1	27:u:219:GLU:HG2	1.72	0.55
3:C:61:GLU:O	3:C:65:LEU:HD22	2.07	0.55
4:D:130:VAL:HG12	4:D:142:VAL:HG22	1.88	0.55
5:E:169:GLY:HA3	5:E:275:MET:HB2	1.89	0.55
6:F:325:GLN:NE2	6:F:325:GLN:O	2.35	0.55
9:I:4:ARG:HG3	9:I:7:SER:HB3	1.89	0.55
11:K:109:VAL:O	11:K:113:THR:HG23	2.06	0.55
13:M:120:HIS:CE1	13:M:124:LEU:HD11	2.41	0.55
14:U:337:LEU:HD12	14:U:789:ILE:HG13	1.88	0.55
16:W:161:GLU:H	16:W:161:GLU:CD	2.15	0.55
23:d:123:LEU:HD23	23:d:126:LEU:HD12	1.88	0.55
1:A:334:PRO:HG2	6:F:395:GLN:HG2	1.89	0.55
3:C:97:VAL:HG22	3:C:123:LEU:H	1.72	0.55
11:K:146:VAL:HG12	11:K:151:PRO:HB3	1.89	0.55
19:Z:52:ASN:HD22	19:Z:89:GLU:CD	2.14	0.55
19:Z:69:PHE:CE2	21:b:96:ALA:HA	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:d:197:LEU:HA	23:d:200:LEU:HG	1.89	0.55
25:f:266:LEU:HD13	25:f:294:MET:HB2	1.88	0.55
27:u:274:ASN:HB3	27:u:277:ASP:HB2	1.89	0.55
2:B:225:TYR:CE2	2:B:350:LYS:HB2	2.42	0.55
8:H:10:LEU:HD12	8:H:19:LEU:HD21	1.89	0.55
20:a:362:SER:HA	20:a:365:MET:HE2	1.88	0.55
25:f:461:PRO:O	25:f:465:LEU:HG	2.07	0.55
6:F:180:ARG:NH2	6:F:246:ALA:O	2.34	0.55
15:V:351:PRO:O	15:V:354:LYS:HG3	2.07	0.55
16:W:93:ARG:O	16:W:96:GLN:HG3	2.07	0.55
21:b:157:VAL:HG21	21:b:170:LEU:HD13	1.88	0.55
22:c:265:MET:HE2	22:c:265:MET:N	2.22	0.55
25:f:670:MET:O	25:f:674:THR:HG23	2.07	0.55
4:D:202:VAL:HG22	4:D:308:ILE:HG22	1.89	0.54
5:E:48:LYS:NZ	19:Z:88:ARG:HH11	2.04	0.54
5:E:236:ASP:OD2	5:E:236:ASP:N	2.38	0.54
6:F:74:LYS:HE2	6:F:74:LYS:HA	1.89	0.54
7:G:72:ILE:HB	7:G:95:ARG:HG2	1.89	0.54
17:X:109:LEU:HA	17:X:112:GLU:OE2	2.08	0.54
23:d:260:ILE:HG23	23:d:263:LEU:HD12	1.89	0.54
25:f:755:ASP:OD2	25:f:758:ASN:ND2	2.39	0.54
25:f:818:LEU:O	25:f:821:LEU:HG	2.07	0.54
9:I:68:LEU:HB2	9:I:72:MET:HB3	1.90	0.54
14:U:802:TYR:HB3	14:U:895:PRO:HD3	1.89	0.54
16:W:244:CYS:SG	16:W:274:VAL:HB	2.47	0.54
20:a:286:ALA:HA	20:a:289:ARG:HD3	1.89	0.54
25:f:538:ILE:HD12	25:f:562:LEU:HA	1.88	0.54
25:f:655:LEU:H	25:f:655:LEU:HD12	1.71	0.54
27:u:208:GLU:HA	27:u:211:ARG:HG2	1.90	0.54
1:A:254:ALA:O	1:A:258:ARG:HG3	2.08	0.54
2:B:382:ASP:HA	2:B:385:MET:HG3	1.88	0.54
4:D:383:GLY:HA3	5:E:164:ILE:HD11	1.90	0.54
6:F:283:ILE:HG22	6:F:328:VAL:HG23	1.88	0.54
7:G:163:PHE:HD1	7:G:164:LYS:H	1.55	0.54
7:G:163:PHE:HB2	8:H:58:ASP:H	1.73	0.54
8:H:7:SER:HB2	8:H:20:VAL:HG12	1.90	0.54
10:J:177:THR:HB	10:J:179:GLU:HG3	1.89	0.54
13:M:56:LYS:HG2	13:M:57:LEU:HD13	1.89	0.54
14:U:82:LEU:HA	14:U:88:PHE:CE2	2.42	0.54
15:V:153:LYS:HZ2	15:V:157:THR:HA	1.73	0.54
1:A:359:ALA:HA	1:A:362:MET:HE3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:LYS:HA	2:B:202:GLU:HB3	1.90	0.54
3:C:242:ALA:HB3	3:C:243:PRO:HD3	1.88	0.54
4:D:353:ASN:HB2	5:E:162:VAL:HA	1.89	0.54
4:D:385:LEU:HG	4:D:388:ARG:HH21	1.72	0.54
5:E:40:TYR:HD1	6:F:73:ILE:HG13	1.73	0.54
13:M:87:LEU:HD23	13:M:135:PHE:CE2	2.42	0.54
25:f:426:LEU:HD11	25:f:465:LEU:HD11	1.88	0.54
25:f:512:MET:HG3	25:f:554:TYR:HB2	1.88	0.54
12:L:158:ALA:HB2	12:L:179:PHE:HE2	1.71	0.54
20:a:40:GLN:NE2	20:a:43:ASP:OD2	2.41	0.54
2:B:95:GLU:O	2:B:99:VAL:HG22	2.06	0.54
5:E:117:PRO:HG3	6:F:94:ILE:HA	1.89	0.54
14:U:481:LEU:HD21	14:U:493:VAL:HG23	1.89	0.54
16:W:260:SER:HA	16:W:263:TRP:NE1	2.23	0.54
19:Z:176:LEU:HD11	22:c:218:LEU:HB2	1.90	0.54
20:a:21:VAL:HG23	20:a:22:TRP:CD1	2.43	0.54
20:a:315:LEU:HD11	20:a:324:ILE:HD11	1.90	0.54
2:B:78:PHE:HE2	25:f:678:LEU:HB2	1.70	0.54
3:C:149:GLU:N	3:C:149:GLU:OE2	2.41	0.54
5:E:71:VAL:HG21	5:E:100:LEU:HD11	1.89	0.54
11:K:85:ALA:HB2	11:K:139:VAL:HG21	1.87	0.54
16:W:101:VAL:O	16:W:105:VAL:HG22	2.07	0.54
21:b:149:ASN:HB3	21:b:154:THR:HG23	1.88	0.54
23:d:196:LEU:HB3	23:d:208:PHE:HE1	1.73	0.54
26:g:109:GLY:HA2	26:g:112:LEU:HG	1.90	0.54
1:A:33:LEU:HG	2:B:412:MET:HE2	1.90	0.54
2:B:271:PHE:CE2	2:B:315:GLN:HB3	2.43	0.54
4:D:131:ALA:HB3	4:D:141:ASP:HB3	1.88	0.54
13:M:135:PHE:CE1	13:M:151:ILE:HB	2.42	0.54
15:V:313:LEU:HD11	15:V:329:HIS:CE1	2.42	0.54
2:B:322:ARG:HA	2:B:322:ARG:CZ	2.38	0.54
3:C:82:LYS:H	3:C:82:LYS:CE	2.21	0.54
4:D:192:LYS:HZ3	4:D:302:ASN:HA	1.73	0.54
12:L:175:HIS:ND1	12:L:178:GLU:OE2	2.28	0.54
18:Y:365:GLN:O	18:Y:369:THR:OG1	2.20	0.54
22:c:148:ILE:HD12	22:c:149:GLN:N	2.23	0.54
22:c:191:ALA:HB3	22:c:196:LEU:HD12	1.89	0.54
1:A:199:GLU:HA	1:A:202:VAL:HG12	1.89	0.54
2:B:169:PRO:O	2:B:173:VAL:HG23	2.08	0.54
3:C:49:ARG:HE	4:D:64:GLU:CD	2.15	0.54
6:F:415:LEU:HD23	6:F:415:LEU:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:344:ARG:NH2	17:X:382:GLU:OE1	2.41	0.54
19:Z:13:PRO:HG3	22:c:220:LEU:HD12	1.89	0.54
19:Z:252:LYS:O	19:Z:256:GLN:HG2	2.08	0.54
3:C:242:ALA:CB	3:C:243:PRO:HD3	2.39	0.53
4:D:219:VAL:O	4:D:223:THR:OG1	2.22	0.53
6:F:431:LYS:NZ	6:F:434:ASN:OD1	2.41	0.53
7:G:111:VAL:HG23	7:G:140:LEU:HD12	1.89	0.53
13:M:47:PHE:HB2	13:M:214:SER:HB3	1.89	0.53
13:M:119:VAL:HA	13:M:131:PHE:CE2	2.44	0.53
25:f:196:MET:HE1	25:f:201:GLU:HA	1.90	0.53
25:f:378:ASN:OD1	25:f:382:ASN:ND2	2.37	0.53
27:u:127:MET:HE1	27:u:150:LEU:O	2.08	0.53
1:A:169:LYS:NZ	1:A:234:ASP:H	2.06	0.53
1:A:262:GLU:O	1:A:266:THR:HG23	2.08	0.53
5:E:232:MET:HB2	5:E:277:MET:HA	1.89	0.53
6:F:310:MET:SD	6:F:311:LEU:HD23	2.48	0.53
7:G:163:PHE:CB	8:H:58:ASP:H	2.20	0.53
15:V:439:ALA:HB1	15:V:443:ARG:HH21	1.71	0.53
16:W:178:GLU:OE2	16:W:178:GLU:N	2.38	0.53
16:W:451:MET:SD	19:Z:100:LYS:HA	2.48	0.53
19:Z:52:ASN:ND2	19:Z:89:GLU:OE2	2.40	0.53
19:Z:79:TYR:CD2	19:Z:91:ILE:HD11	2.44	0.53
22:c:189:ILE:HA	22:c:192:LEU:HB2	1.91	0.53
1:A:26:ASP:O	1:A:29:ASP:N	2.41	0.53
1:A:372:LEU:O	1:A:376:LEU:HG	2.08	0.53
2:B:175:LYS:O	2:B:177:GLU:N	2.41	0.53
3:C:229:ARG:HD2	3:C:233:GLU:HG3	1.91	0.53
3:C:403:LYS:HB3	8:H:156:PHE:HE2	1.74	0.53
6:F:362:ARG:HB3	6:F:366:MET:HE3	1.90	0.53
7:G:16:PHE:CD2	8:H:25:ALA:HA	2.44	0.53
14:U:609:ASP:OD1	14:U:610:VAL:N	2.41	0.53
15:V:367:VAL:HG23	15:V:402:VAL:HG23	1.90	0.53
16:W:85:GLU:HA	16:W:88:MET:SD	2.48	0.53
17:X:295:LYS:O	17:X:297:ARG:NH1	2.41	0.53
17:X:407:MET:HA	17:X:407:MET:HE2	1.90	0.53
18:Y:331:ASP:OD2	18:Y:349:LYS:NZ	2.41	0.53
19:Z:109:ASN:ND2	19:Z:140:SER:HB2	2.23	0.53
19:Z:217:THR:HB	19:Z:219:LYS:HE2	1.90	0.53
23:d:94:MET:HE3	23:d:115:GLU:HG3	1.89	0.53
25:f:108:GLU:OE1	25:f:112:ASN:ND2	2.40	0.53
25:f:450:ILE:HG13	25:f:487:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:361:GLU:HA	4:D:364:VAL:HG12	1.90	0.53
7:G:80:MET:HG2	7:G:87:SER:HB2	1.89	0.53
14:U:532:MET:HG2	14:U:548:LEU:HD22	1.91	0.53
25:f:802:SER:O	25:f:809:ILE:HG21	2.07	0.53
27:u:282:VAL:HG22	27:u:283:GLY:H	1.73	0.53
3:C:277:LEU:HD23	3:C:280:LEU:HD11	1.90	0.53
4:D:415:GLU:HG3	7:G:159:TYR:HB3	1.90	0.53
5:E:122:MET:HB3	5:E:197:LYS:O	2.09	0.53
8:H:109:GLN:O	8:H:113:ARG:HD3	2.09	0.53
11:K:91:LYS:HD3	11:K:119:LEU:HD22	1.91	0.53
13:M:201:HIS:O	13:M:201:HIS:ND1	2.42	0.53
14:U:707:ASN:OD1	14:U:708:GLN:N	2.42	0.53
16:W:436:MET:HE3	22:c:226:MET:HB3	1.89	0.53
17:X:167:VAL:HG21	17:X:197:ALA:HB2	1.90	0.53
20:a:156:TYR:HB3	20:a:179:PHE:HB2	1.91	0.53
21:b:69:GLY:O	21:b:72:LEU:HD12	2.08	0.53
25:f:115:PRO:HA	25:f:119:LYS:HD2	1.89	0.53
25:f:348:ILE:HD13	25:f:381:VAL:HG21	1.89	0.53
4:D:191:TYR:HA	4:D:194:ILE:HD12	1.91	0.53
12:L:84:LEU:O	12:L:88:MET:HG3	2.09	0.53
12:L:148:CYS:SG	12:L:150:SER:OG	2.63	0.53
14:U:101:ILE:HA	14:U:104:CYS:SG	2.48	0.53
14:U:265:ILE:HG23	14:U:326:ILE:HD12	1.91	0.53
14:U:685:GLN:O	14:U:689:ILE:HG12	2.09	0.53
15:V:496:PHE:H	15:V:497:PRO:CD	2.22	0.53
16:W:172:GLU:H	16:W:208:LYS:HZ3	1.56	0.53
19:Z:93:GLY:HA3	19:Z:120:VAL:O	2.09	0.53
25:f:151:LEU:HB3	25:f:159:VAL:HG22	1.90	0.53
25:f:466:LEU:O	25:f:470:VAL:HG13	2.09	0.53
1:A:34:LYS:NZ	3:C:173:GLU:OE2	2.38	0.53
3:C:367:GLY:HA3	4:D:196:ILE:HG21	1.91	0.53
13:M:186:CYS:HA	13:M:189:ILE:HB	1.91	0.53
16:W:172:GLU:HA	16:W:182:ARG:HD3	1.90	0.53
16:W:234:ASP:O	16:W:238:GLY:N	2.42	0.53
17:X:354:ILE:HG22	17:X:356:LEU:HD23	1.90	0.53
17:X:403:THR:OG1	19:Z:262:LEU:HD21	2.09	0.53
18:Y:235:ASP:OD1	18:Y:239:LYS:NZ	2.34	0.53
21:b:12:ASN:OD1	21:b:53:THR:OG1	2.26	0.53
22:c:52:GLU:OE2	27:u:289:HIS:CE1	2.62	0.53
22:c:57:MET:HB3	22:c:72:VAL:HG22	1.89	0.53
23:d:265:ASP:OD1	23:d:265:ASP:N	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:233:LEU:HD12	25:f:248:LEU:HD11	1.91	0.53
27:u:221:THR:HG23	27:u:223:ASP:H	1.72	0.53
1:A:78:TRP:HE3	1:A:79:ASP:HB2	1.72	0.53
7:G:88:ARG:NH1	13:M:157:SER:OG	2.41	0.53
8:H:74:LEU:HD13	8:H:136:ILE:HG13	1.88	0.53
15:V:282:ASN:H	15:V:285:TRP:HD1	1.57	0.53
16:W:198:ASP:OD2	16:W:201:ARG:NH1	2.32	0.53
20:a:268:LEU:O	20:a:272:ILE:HG13	2.09	0.53
25:f:803:PHE:CE1	25:f:810:ILE:HG13	2.44	0.53
3:C:386:ALA:O	3:C:390:VAL:HG22	2.09	0.53
4:D:190:LEU:O	4:D:193:GLN:HG3	2.08	0.53
14:U:9:ILE:HG13	14:U:44:LYS:HE2	1.90	0.53
14:U:578:LEU:O	14:U:581:SER:OG	2.23	0.53
15:V:387:GLN:HA	15:V:392:TYR:CD1	2.44	0.53
17:X:316:ASP:HB3	17:X:319:ILE:HB	1.90	0.53
19:Z:225:GLN:O	19:Z:227:ILE:N	2.38	0.53
19:Z:237:LEU:HD23	22:c:309:PHE:O	2.09	0.53
25:f:56:LEU:HD11	25:f:95:PRO:HB3	1.91	0.53
25:f:263:PRO:HG3	25:f:290:VAL:HG13	1.91	0.53
1:A:296:GLN:HA	1:A:299:MET:HG3	1.91	0.53
1:A:327:LEU:HB2	1:A:332:MET:SD	2.49	0.53
1:A:378:PRO:O	1:A:380:SER:N	2.42	0.53
5:E:353:PHE:HD1	5:E:356:ARG:HH12	1.57	0.53
7:G:159:TYR:HA	8:H:84:ARG:HH21	1.73	0.53
11:K:41:GLN:NE2	11:K:166:ASP:OD1	2.41	0.53
14:U:324:LYS:O	14:U:328:ILE:HG12	2.09	0.53
17:X:94:ASP:OD1	17:X:132:ARG:NH1	2.42	0.53
20:a:186:LYS:O	20:a:188:LEU:HD23	2.08	0.53
25:f:117:GLU:OE2	25:f:120:ARG:NH1	2.42	0.53
25:f:666:ILE:HD12	25:f:667:GLY:H	1.73	0.53
1:A:164:MET:HG2	1:A:239:ARG:O	2.10	0.52
1:A:184:ILE:HA	1:A:187:LEU:HG	1.91	0.52
4:D:89:ILE:HG22	5:E:78:ARG:O	2.08	0.52
5:E:86:GLN:OE1	5:E:86:GLN:N	2.42	0.52
5:E:196:LEU:O	5:E:231:PHE:N	2.38	0.52
6:F:184:GLN:OE1	6:F:243:GLN:NE2	2.41	0.52
8:H:76:TYR:HB3	8:H:83:TYR:CD1	2.44	0.52
8:H:77:SER:HB3	8:H:133:SER:HB3	1.89	0.52
9:I:61:PHE:HE2	9:I:227:VAL:HG13	1.74	0.52
14:U:599:ILE:HA	14:U:602:LEU:HD22	1.91	0.52
16:W:231:ILE:O	16:W:235:GLN:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:b:169:HIS:HE1	21:b:191:GLY:HA3	1.73	0.52
25:f:885:GLU:OE1	25:f:885:GLU:N	2.35	0.52
1:A:292:ASP:O	1:A:294:GLU:N	2.40	0.52
3:C:390:VAL:HA	4:D:324:PRO:HG2	1.90	0.52
6:F:318:ASP:OD2	6:F:344:ARG:NH1	2.42	0.52
9:I:25:MET:HA	9:I:28:ILE:HD12	1.91	0.52
9:I:232:GLU:HA	9:I:235:GLN:OE1	2.09	0.52
12:L:36:VAL:HG13	12:L:172:LEU:HD11	1.92	0.52
14:U:606:ALA:HB1	14:U:619:VAL:HG23	1.91	0.52
15:V:360:TYR:HA	15:V:363:LEU:HB3	1.91	0.52
17:X:57:LEU:HD11	17:X:65:GLU:HB2	1.91	0.52
19:Z:21:ASP:OD2	22:c:104:ARG:NH1	2.42	0.52
25:f:63:LEU:HA	25:f:70:LEU:HD13	1.91	0.52
25:f:542:ILE:HG22	25:f:558:LEU:HB3	1.91	0.52
2:B:125:THR:HG23	2:B:127:VAL:HG12	1.91	0.52
2:B:311:GLU:HA	2:B:314:ASN:HD21	1.75	0.52
6:F:83:ASN:OD1	22:c:79:GLY:N	2.42	0.52
8:H:105:ILE:HG12	8:H:110:LEU:HB2	1.91	0.52
14:U:544:ILE:HD12	14:U:544:ILE:H	1.74	0.52
20:a:70:ARG:NH2	21:b:17:ARG:HA	2.22	0.52
24:e:20:GLU:CD	24:e:20:GLU:H	2.18	0.52
3:C:403:LYS:C	3:C:404:LEU:HD23	2.33	0.52
14:U:545:LEU:HB3	14:U:577:ILE:HG21	1.91	0.52
14:U:792:ASN:HB3	14:U:914:LEU:H	1.73	0.52
16:W:39:ARG:HG3	16:W:40:LEU:H	1.75	0.52
20:a:214:GLY:HA3	20:a:340:VAL:HG11	1.90	0.52
22:c:94:LYS:O	22:c:98:MET:HG3	2.09	0.52
1:A:352:THR:O	1:A:356:LYS:HG2	2.10	0.52
3:C:307:ARG:NH1	3:C:309:GLY:H	2.07	0.52
11:K:96:THR:HA	11:K:107:MET:HG2	1.91	0.52
13:M:69:VAL:HG23	13:M:75:MET:HG2	1.92	0.52
13:M:197:ILE:HG21	13:M:211:LEU:HD13	1.92	0.52
15:V:396:ILE:HD11	23:d:230:VAL:HG11	1.92	0.52
16:W:419:LYS:HZ2	16:W:423:ASN:HB3	1.74	0.52
16:W:447:ALA:O	16:W:451:MET:HB2	2.10	0.52
18:Y:104:MET:SD	18:Y:130:LYS:NZ	2.83	0.52
25:f:728:ALA:O	25:f:732:VAL:HG12	2.08	0.52
3:C:237:MET:HA	3:C:240:GLU:CD	2.35	0.52
5:E:367:PHE:O	5:E:371:VAL:HG23	2.10	0.52
15:V:247:GLN:O	15:V:251:LEU:HG	2.09	0.52
19:Z:279:LYS:HA	19:Z:282:ASN:ND2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:c:219:ASN:HA	22:c:222:LYS:HB2	1.92	0.52
25:f:425:GLY:O	25:f:429:ILE:HG12	2.09	0.52
25:f:785:ARG:NH2	25:f:895:GLU:OE1	2.39	0.52
3:C:394:ASP:N	3:C:394:ASP:OD1	2.42	0.52
8:H:213:CYS:SG	8:H:218:PHE:HB2	2.50	0.52
13:M:136:MET:HE3	13:M:148:LEU:HD21	1.92	0.52
15:V:148:ARG:NE	15:V:197:THR:HB	2.24	0.52
22:c:206:ASN:OD1	22:c:207:TYR:N	2.43	0.52
25:f:470:VAL:HG23	25:f:471:LEU:HD22	1.90	0.52
3:C:52:LEU:HA	3:C:55:LYS:NZ	2.25	0.52
6:F:317:LEU:HD11	6:F:328:VAL:HG11	1.92	0.52
11:K:50:VAL:HG13	11:K:216:GLU:HB2	1.90	0.52
17:X:310:ARG:HD2	17:X:314:ARG:HG3	1.91	0.52
18:Y:40:GLU:O	18:Y:43:ALA:HB3	2.10	0.52
18:Y:41:LEU:HB3	18:Y:42:MET:HE2	1.92	0.52
18:Y:228:MET:HE3	18:Y:263:LEU:HD22	1.90	0.52
23:d:142:ILE:O	23:d:145:ARG:HB3	2.10	0.52
5:E:40:TYR:CD1	6:F:73:ILE:HG13	2.44	0.52
17:X:338:VAL:HG23	17:X:339:ILE:HD13	1.92	0.52
18:Y:49:ASN:HA	18:Y:73:MET:SD	2.50	0.52
4:D:93:LEU:HD12	4:D:102:ILE:HG22	1.91	0.52
5:E:206:LYS:HB2	6:F:260:PHE:HB3	1.91	0.52
6:F:225:MET:O	6:F:331:ALA:HA	2.09	0.52
8:H:120:GLU:O	8:H:123:GLN:NE2	2.23	0.52
11:K:41:GLN:HB3	11:K:166:ASP:HA	1.92	0.52
12:L:155:ASP:HB3	13:M:62:SER:HB2	1.92	0.52
13:M:233:GLU:O	13:M:237:LYS:HG2	2.10	0.52
14:U:265:ILE:HD11	14:U:329:LEU:HB3	1.92	0.52
14:U:766:PHE:CG	14:U:779:LEU:HD12	2.45	0.52
16:W:207:LYS:O	16:W:207:LYS:NZ	2.36	0.52
17:X:153:LEU:HA	17:X:156:GLU:OE2	2.10	0.52
22:c:282:ARG:O	22:c:286:GLU:HG2	2.09	0.52
23:d:228:HIS:CE1	23:d:251:ILE:HG22	2.45	0.52
4:D:409:LYS:HB3	7:G:173:THR:HG21	1.93	0.51
5:E:22:ILE:HD11	6:F:59:VAL:HG21	1.92	0.51
5:E:158:LEU:HD23	5:E:161:ARG:NH2	2.25	0.51
6:F:289:ASP:OD1	6:F:289:ASP:N	2.42	0.51
6:F:344:ARG:HG2	6:F:346:GLY:H	1.75	0.51
8:H:65:VAL:N	8:H:209:GLU:OE2	2.25	0.51
11:K:113:THR:HG22	11:K:143:PHE:CD2	2.45	0.51
13:M:27:MET:SD	13:M:27:MET:N	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:217:CYS:O	14:U:221:ILE:HG23	2.10	0.51
15:V:65:ARG:O	15:V:68:ASP:HB3	2.10	0.51
19:Z:68:TRP:HD1	19:Z:104:ASN:ND2	2.08	0.51
19:Z:129:LYS:HD2	22:c:215:LYS:HE2	1.92	0.51
20:a:226:ARG:HB2	20:a:234:ILE:HD12	1.90	0.51
21:b:98:LYS:HD2	27:u:203:SER:HB2	1.92	0.51
23:d:125:GLU:N	23:d:125:GLU:OE2	2.41	0.51
1:A:407:LYS:HA	1:A:410:LEU:HG	1.91	0.51
4:D:183:LEU:HB3	4:D:191:TYR:OH	2.10	0.51
6:F:263:ASP:O	6:F:267:LEU:HD12	2.10	0.51
14:U:148:LYS:HE3	14:U:151:ILE:HD11	1.91	0.51
18:Y:15:PRO:HD2	18:Y:146:ARG:HB3	1.93	0.51
25:f:71:TYR:OH	25:f:109:ILE:HG12	2.10	0.51
3:C:316:GLU:HG3	3:C:318:PRO:HD3	1.92	0.51
8:H:148:GLN:NE2	8:H:150:ASP:OD2	2.43	0.51
10:J:33:VAL:HG21	10:J:168:VAL:HG11	1.91	0.51
12:L:26:MET:HE1	12:L:149:PRO:HD2	1.92	0.51
14:U:603:LEU:HD13	14:U:622:LEU:HD21	1.90	0.51
14:U:665:ASN:H	14:U:694:ILE:HD11	1.76	0.51
15:V:61:GLU:HG2	15:V:65:ARG:HB2	1.93	0.51
25:f:380:PHE:HE1	25:f:821:LEU:HD11	1.74	0.51
1:A:97:ARG:NH1	1:A:139:ARG:HB2	2.26	0.51
10:J:51:ALA:O	10:J:53:LEU:N	2.44	0.51
13:M:171:ALA:O	13:M:175:GLU:HG2	2.10	0.51
14:U:399:TRP:CH2	14:U:472:ILE:HG23	2.45	0.51
16:W:409:LEU:HD22	17:X:384:VAL:HG21	1.91	0.51
17:X:200:ILE:HG22	17:X:201:TYR:H	1.75	0.51
17:X:256:LEU:HA	17:X:259:ILE:HD12	1.92	0.51
19:Z:209:ARG:O	19:Z:213:GLU:HG2	2.10	0.51
1:A:48:VAL:HG13	2:B:69:LYS:HZ3	1.75	0.51
1:A:111:TYR:C	1:A:112:ILE:HD13	2.36	0.51
1:A:386:ARG:HH22	2:B:345:GLY:HA3	1.74	0.51
2:B:68:ILE:O	2:B:72:LEU:HG	2.11	0.51
3:C:360:LYS:HA	3:C:363:CYS:SG	2.51	0.51
5:E:275:MET:HA	5:E:275:MET:HE3	1.91	0.51
5:E:380:LEU:HD11	6:F:226:TYR:CE1	2.46	0.51
7:G:92:GLN:HB3	13:M:117:MET:HE1	1.93	0.51
8:H:79:MET:HE2	8:H:79:MET:HA	1.92	0.51
19:Z:37:GLY:HA2	19:Z:56:VAL:HG22	1.92	0.51
20:a:42:LEU:HD13	20:a:79:ILE:HG13	1.92	0.51
20:a:335:TRP:CD1	20:a:337:GLN:N	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:u:184:GLY:HA2	27:u:261:SER:H	1.74	0.51
1:A:371:GLU:OE1	1:A:375:ARG:NH1	2.43	0.51
3:C:155:ASP:HA	3:C:158:ILE:HG22	1.92	0.51
4:D:125:LYS:HD2	4:D:127:ASN:H	1.75	0.51
5:E:52:SER:HA	19:Z:88:ARG:HH22	1.75	0.51
5:E:122:MET:SD	5:E:122:MET:N	2.84	0.51
6:F:236:LEU:HD23	6:F:354:PHE:CZ	2.46	0.51
18:Y:213:LEU:HB3	18:Y:214:MET:HG3	1.93	0.51
18:Y:380:VAL:O	18:Y:384:SER:N	2.40	0.51
19:Z:16:LEU:HA	19:Z:19:VAL:HG12	1.93	0.51
20:a:252:LYS:HA	20:a:255:TRP:CE3	2.44	0.51
20:a:320:VAL:HG12	20:a:322:GLY:H	1.75	0.51
23:d:207:GLU:H	23:d:207:GLU:CD	2.17	0.51
25:f:646:MET:H	25:f:646:MET:CE	2.18	0.51
26:g:131:ILE:O	26:g:134:LYS:N	2.42	0.51
2:B:94:GLU:O	2:B:98:LYS:HG2	2.10	0.51
3:C:55:LYS:HA	3:C:58:LEU:HG	1.92	0.51
3:C:351:MET:HG3	3:C:354:ALA:HB2	1.92	0.51
6:F:155:LYS:HG3	6:F:156:ASP:OD1	2.10	0.51
14:U:575:ASP:HB3	14:U:578:LEU:HD23	1.91	0.51
16:W:154:GLU:OE2	16:W:192:LEU:HD21	2.11	0.51
19:Z:68:TRP:CD1	19:Z:104:ASN:HD21	2.29	0.51
26:g:107:ILE:HG13	26:g:142:LEU:HD13	1.92	0.51
1:A:417:ILE:HG22	1:A:418:LYS:HD2	1.92	0.51
3:C:174:LEU:O	3:C:178:LEU:N	2.30	0.51
9:I:121:TYR:CE1	9:I:127:LYS:HB3	2.45	0.51
10:J:71:MET:HE3	10:J:72:ALA:O	2.10	0.51
13:M:113:ASP:OD2	13:M:114:ARG:N	2.43	0.51
13:M:120:HIS:O	13:M:123:THR:OG1	2.26	0.51
15:V:477:HIS:ND1	23:d:342:TYR:OH	2.31	0.51
19:Z:242:LEU:HG	19:Z:244:GLU:OE1	2.11	0.51
20:a:33:LEU:H	20:a:33:LEU:HD23	1.74	0.51
22:c:139:ARG:C	22:c:161:ARG:HH12	2.19	0.51
25:f:735:GLY:HA3	25:f:776:LEU:O	2.11	0.51
1:A:146:LYS:HZ3	1:A:148:GLN:HE22	1.59	0.51
1:A:307:ASP:HB3	1:A:336:ARG:HG2	1.92	0.51
3:C:30:GLU:O	3:C:34:ILE:HG12	2.11	0.51
3:C:224:ILE:HG23	3:C:268:GLU:OE1	2.11	0.51
13:M:229:LYS:HE3	13:M:235:ALA:H	1.76	0.51
14:U:212:ASP:OD2	14:U:215:ASN:ND2	2.32	0.51
14:U:541:HIS:HB2	14:U:544:ILE:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:222:TYR:OH	18:Y:285:ASP:OD2	2.17	0.51
18:Y:306:GLN:O	18:Y:309:GLU:HB2	2.09	0.51
19:Z:172:VAL:HG23	22:c:217:LEU:HB3	1.93	0.51
20:a:354:GLU:HA	20:a:357:CYS:SG	2.51	0.51
22:c:191:ALA:O	22:c:195:GLY:N	2.43	0.51
1:A:364:VAL:O	1:A:366:ARG:NH2	2.44	0.51
3:C:80:MET:HB2	3:C:84:LYS:HB2	1.93	0.51
15:V:224:LEU:HD23	15:V:224:LEU:H	1.76	0.51
17:X:151:SER:O	17:X:155:ARG:HG2	2.11	0.51
18:Y:55:GLU:O	18:Y:59:LYS:HG2	2.11	0.51
26:g:85:ILE:HG23	26:g:101:LEU:HB3	1.93	0.51
27:u:118:ASP:O	27:u:119:ILE:HG12	2.11	0.51
1:A:227:ARG:NH1	2:B:320:ASP:O	2.43	0.50
2:B:201:VAL:HG11	2:B:328:ILE:HD11	1.93	0.50
6:F:224:LEU:HA	6:F:330:ALA:HB3	1.93	0.50
8:H:19:LEU:O	8:H:22:ILE:HG22	2.11	0.50
8:H:192:ILE:HD13	8:H:229:TYR:HB3	1.92	0.50
11:K:189:MET:HE2	11:K:193:GLU:HG3	1.92	0.50
12:L:156:CYS:HB2	12:L:159:MET:HE3	1.93	0.50
14:U:160:LEU:HD22	14:U:200:VAL:HG21	1.92	0.50
14:U:919:GLU:HG3	14:U:920:ASP:H	1.76	0.50
15:V:374:LYS:O	15:V:374:LYS:NZ	2.41	0.50
18:Y:23:ARG:NH1	18:Y:27:SER:HB3	2.24	0.50
18:Y:220:VAL:O	18:Y:224:VAL:HG12	2.11	0.50
18:Y:297:ARG:O	18:Y:301:ILE:HD12	2.11	0.50
21:b:107:MET:CB	21:b:136:VAL:HA	2.41	0.50
21:b:179:LEU:HG	21:b:180:ALA:H	1.76	0.50
1:A:348:LEU:HD13	1:A:351:ARG:HH21	1.77	0.50
4:D:201:GLY:HA2	4:D:307:VAL:O	2.12	0.50
5:E:232:MET:HE2	5:E:232:MET:HA	1.93	0.50
5:E:352:MET:O	5:E:355:ILE:HG22	2.12	0.50
9:I:43:VAL:HG12	9:I:216:LEU:HB3	1.93	0.50
20:a:53:GLY:O	20:a:57:ILE:HG12	2.11	0.50
20:a:114:CYS:O	20:a:118:ILE:HG22	2.11	0.50
22:c:303:MET:O	22:c:307:VAL:HG12	2.10	0.50
25:f:346:ASP:OD2	25:f:351:THR:OG1	2.27	0.50
25:f:460:ASP:OD2	25:f:494:ARG:NH1	2.41	0.50
5:E:158:LEU:HA	5:E:161:ARG:HH21	1.76	0.50
8:H:220:ARG:NH1	8:H:221:LEU:O	2.44	0.50
12:L:116:THR:HG22	12:L:128:TYR:HD1	1.76	0.50
14:U:108:TYR:CG	14:U:134:VAL:HG21	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:a:294:GLU:O	20:a:298:LYS:HG2	2.11	0.50
25:f:77:GLU:O	25:f:81:GLN:HG2	2.12	0.50
25:f:657:ILE:H	25:f:657:ILE:HD12	1.76	0.50
1:A:180:CYS:HB3	1:A:183:GLN:HB2	1.93	0.50
3:C:232:ARG:NH1	3:C:279:GLN:OE1	2.42	0.50
4:D:99:ASN:OD1	4:D:99:ASN:N	2.44	0.50
5:E:116:ASP:O	5:E:119:VAL:N	2.42	0.50
6:F:51:GLU:HG2	6:F:55:MET:HG2	1.92	0.50
14:U:458:ILE:HD12	14:U:485:ALA:HB2	1.93	0.50
16:W:122:LEU:O	16:W:125:ILE:HG13	2.12	0.50
16:W:214:PHE:CZ	16:W:223:LYS:HA	2.47	0.50
20:a:35:HIS:NE2	21:b:14:GLU:HG3	2.27	0.50
20:a:335:TRP:HD1	20:a:337:GLN:H	1.58	0.50
23:d:251:ILE:HD11	23:d:257:THR:HG22	1.93	0.50
25:f:802:SER:HB2	25:f:809:ILE:HG12	1.93	0.50
25:f:828:ARG:HD2	25:f:874:LEU:O	2.11	0.50
1:A:201:PHE:HE1	6:F:405:MET:HE1	1.75	0.50
3:C:403:LYS:HB3	8:H:156:PHE:CE2	2.46	0.50
4:D:164:TYR:HA	4:D:167:ILE:HG12	1.93	0.50
4:D:300:ASP:OD1	4:D:300:ASP:N	2.39	0.50
7:G:180:GLU:O	7:G:184:LYS:N	2.42	0.50
13:M:236:GLU:HG3	13:M:237:LYS:HE2	1.94	0.50
14:U:757:MET:HE3	14:U:758:PRO:HD3	1.93	0.50
14:U:792:ASN:HB3	14:U:914:LEU:N	2.26	0.50
17:X:50:ILE:HA	17:X:53:LEU:HB2	1.93	0.50
21:b:8:VAL:HA	21:b:110:ILE:HG23	1.94	0.50
23:d:112:CYS:HB2	23:d:154:TRP:HE1	1.76	0.50
3:C:44:ARG:HH22	23:d:350:VAL:HG13	1.76	0.50
3:C:47:ALA:O	3:C:51:GLU:HG2	2.11	0.50
3:C:393:LYS:HA	3:C:396:GLU:HB2	1.93	0.50
4:D:214:MET:SD	29:D:501:ADP:H2'	2.51	0.50
5:E:232:MET:N	5:E:276:ILE:O	2.28	0.50
7:G:37:LEU:HD22	7:G:52:THR:OG1	2.11	0.50
10:J:4:ASP:HB3	10:J:17:PHE:HB2	1.93	0.50
14:U:581:SER:O	14:U:585:THR:HG23	2.11	0.50
15:V:95:LEU:HD12	15:V:141:THR:HB	1.93	0.50
15:V:467:TYR:HA	15:V:472:PRO:HG2	1.94	0.50
17:X:368:MET:HG2	17:X:374:PHE:HB3	1.93	0.50
21:b:13:SER:HB2	21:b:83:LYS:HA	1.93	0.50
21:b:139:ASP:OD1	21:b:169:HIS:N	2.44	0.50
25:f:213:GLN:HB3	25:f:216:MET:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:410:ALA:O	25:f:413:SER:HB3	2.12	0.50
1:A:146:LYS:CE	1:A:148:GLN:NE2	2.75	0.50
2:B:390:LEU:HD12	2:B:394:ASP:HB2	1.93	0.50
4:D:125:LYS:HG2	4:D:126:PRO:HD2	1.93	0.50
6:F:421:MET:O	6:F:425:LEU:HG	2.12	0.50
7:G:10:ASP:HB3	7:G:23:TYR:CD2	2.46	0.50
13:M:170:GLN:OE1	13:M:170:GLN:N	2.45	0.50
14:U:757:MET:O	14:U:761:VAL:HG12	2.12	0.50
17:X:56:LEU:HD12	17:X:57:LEU:N	2.27	0.50
19:Z:270:VAL:HG23	22:c:281:LYS:NZ	2.27	0.50
23:d:90:ALA:O	23:d:94:MET:HG2	2.12	0.50
1:A:206:ILE:HB	6:F:373:MET:HE1	1.94	0.50
3:C:80:MET:H	3:C:85:VAL:HA	1.77	0.50
3:C:161:ILE:HG21	3:C:199:LEU:CD2	2.41	0.50
4:D:113:VAL:HG13	4:D:138:ALA:HA	1.94	0.50
5:E:52:SER:HA	19:Z:88:ARG:NH2	2.26	0.50
6:F:406:ILE:HA	6:F:409:ARG:HE	1.76	0.50
8:H:185:GLU:HG3	8:H:189:HIS:CE1	2.47	0.50
9:I:32:GLY:HA2	9:I:50:ARG:NH2	2.25	0.50
14:U:148:LYS:HB3	14:U:176:MET:HE3	1.92	0.50
14:U:681:ASN:OD1	14:U:682:TYR:N	2.45	0.50
20:a:65:SER:HA	20:a:68:GLU:HB3	1.94	0.50
24:e:63:HIS:HB2	24:e:65:TYR:CE1	2.47	0.50
27:u:285:LYS:N	27:u:285:LYS:HD2	2.27	0.50
1:A:433:ASN:HD21	11:K:78:MET:HG2	1.77	0.50
3:C:193:GLY:N	29:C:501:ADP:O3B	2.42	0.50
3:C:336:MET:HE1	4:D:196:ILE:HA	1.93	0.50
5:E:309:ARG:NH1	5:E:332:VAL:O	2.34	0.50
11:K:28:ILE:HA	11:K:31:ILE:HD12	1.94	0.50
14:U:232:ILE:O	14:U:236:LEU:HG	2.12	0.50
14:U:757:MET:HA	14:U:760:VAL:HG12	1.93	0.50
15:V:283:ASN:ND2	24:e:17:ASP:OD2	2.45	0.50
25:f:672:LEU:HD11	25:f:703:ARG:HH21	1.76	0.50
25:f:859:PRO:HD2	25:f:860:LYS:HZ3	1.77	0.50
1:A:59:ILE:O	1:A:63:THR:HG22	2.12	0.49
1:A:108:ASP:O	1:A:110:LYS:NZ	2.45	0.49
15:V:314:ARG:NH1	18:Y:381:GLN:OE1	2.45	0.49
25:f:776:LEU:HB3	25:f:825:MET:CE	2.42	0.49
1:A:394:MET:HE1	2:B:216:ILE:HG21	1.94	0.49
2:B:121:ALA:HB2	2:B:135:ILE:HD11	1.93	0.49
3:C:275:GLU:O	3:C:279:GLN:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:368:ILE:HG12	6:F:371:ARG:HH21	1.77	0.49
15:V:405:THR:O	15:V:408:ARG:HB2	2.12	0.49
15:V:443:ARG:HD3	23:d:274:CYS:HB2	1.94	0.49
25:f:165:GLU:O	25:f:169:GLU:HG2	2.12	0.49
25:f:774:GLY:O	25:f:828:ARG:NH2	2.45	0.49
7:G:83:MET:HE1	7:G:85:ALA:HB3	1.94	0.49
14:U:27:LEU:O	14:U:31:VAL:HG13	2.13	0.49
15:V:315:LYS:HD2	18:Y:385:ARG:NH1	2.27	0.49
19:Z:219:LYS:N	19:Z:219:LYS:HD3	2.28	0.49
21:b:54:LEU:HB2	21:b:84:ILE:HD12	1.95	0.49
27:u:151:ARG:NH1	27:u:151:ARG:HA	2.28	0.49
1:A:100:LYS:HD3	6:F:173:LYS:NZ	2.27	0.49
1:A:158:ASP:HB3	1:A:161:VAL:HG23	1.93	0.49
2:B:76:GLU:O	2:B:80:ARG:HG3	2.12	0.49
2:B:322:ARG:HA	2:B:322:ARG:NE	2.27	0.49
4:D:156:SER:N	4:D:158:GLN:OE1	2.44	0.49
4:D:262:ILE:HD13	4:D:307:VAL:HG22	1.94	0.49
4:D:320:ALA:O	4:D:326:ARG:NH2	2.43	0.49
8:H:173:PHE:CD1	8:H:194:THR:HB	2.48	0.49
15:V:37:MET:HE2	15:V:37:MET:HA	1.94	0.49
15:V:292:THR:HA	15:V:295:ILE:HG12	1.94	0.49
19:Z:101:LEU:HD21	19:Z:121:LEU:HD21	1.94	0.49
20:a:74:LEU:HA	20:a:77:VAL:HG12	1.94	0.49
22:c:214:GLN:O	22:c:215:LYS:HG2	2.12	0.49
25:f:196:MET:N	25:f:196:MET:HE2	2.27	0.49
25:f:675:PHE:HD1	25:f:678:LEU:HD23	1.76	0.49
26:g:148:ALA:H	26:g:151:VAL:HG21	1.77	0.49
1:A:75:PRO:HA	1:A:78:TRP:CE2	2.47	0.49
3:C:133:PRO:C	3:C:137:LEU:HG	2.38	0.49
14:U:628:ARG:CZ	14:U:749:GLN:HE22	2.26	0.49
23:d:209:HIS:HA	23:d:212:LEU:HG	1.94	0.49
25:f:63:LEU:HD23	25:f:70:LEU:HB3	1.94	0.49
2:B:316:LEU:HB3	2:B:346:ARG:HG2	1.95	0.49
3:C:119:ASP:OD2	3:C:120:SER:N	2.46	0.49
4:D:79:VAL:O	4:D:82:ILE:HG22	2.12	0.49
4:D:199:PRO:HB2	4:D:306:LYS:HZ1	1.78	0.49
9:I:119:GLN:OE1	10:J:82:ILE:HG13	2.12	0.49
11:K:52:LYS:HB2	11:K:214:ASN:HA	1.94	0.49
14:U:195:ASN:O	14:U:199:ARG:HG2	2.13	0.49
20:a:97:LEU:HB2	20:a:114:CYS:SG	2.52	0.49
1:A:78:TRP:CE3	1:A:79:ASP:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LYS:HD3	6:F:173:LYS:HZ2	1.76	0.49
3:C:148:TYR:CG	3:C:158:ILE:HD11	2.48	0.49
6:F:96:LEU:HD21	6:F:145:LEU:HD11	1.95	0.49
7:G:152:TYR:HA	7:G:162:GLY:CA	2.40	0.49
11:K:24:VAL:O	11:K:28:ILE:HD12	2.13	0.49
16:W:192:LEU:HA	16:W:192:LEU:HD23	1.61	0.49
20:a:157:ASP:O	20:a:161:LYS:HG2	2.12	0.49
23:d:196:LEU:HB3	23:d:208:PHE:CE1	2.47	0.49
25:f:479:LEU:HD21	25:f:514:VAL:HA	1.95	0.49
25:f:655:LEU:HD11	25:f:804:LEU:HD21	1.94	0.49
26:g:108:THR:HA	26:g:141:THR:HA	1.95	0.49
1:A:270:CYS:HB3	1:A:315:ILE:HD12	1.95	0.49
1:A:352:THR:HG22	1:A:371:GLU:HA	1.94	0.49
4:D:179:GLU:HA	4:D:183:LEU:HD23	1.95	0.49
4:D:257:ASN:HB3	4:D:260:ALA:HB2	1.94	0.49
4:D:414:HIS:O	4:D:414:HIS:ND1	2.44	0.49
5:E:348:THR:O	5:E:352:MET:HG2	2.13	0.49
6:F:61:ARG:HH12	21:b:76:HIS:N	2.10	0.49
7:G:120:ASP:O	7:G:124:VAL:HG13	2.12	0.49
9:I:40:ASN:ND2	9:I:182:GLY:O	2.46	0.49
13:M:51:LYS:HZ3	13:M:64:LYS:HA	1.77	0.49
14:U:101:ILE:O	14:U:105:ILE:HG23	2.13	0.49
16:W:344:THR:OG1	16:W:346:GLU:OE2	2.29	0.49
17:X:410:VAL:HG21	22:c:255:TYR:HE2	1.78	0.49
20:a:324:ILE:HG23	20:a:331:VAL:HG12	1.95	0.49
22:c:195:GLY:HA2	22:c:198:ARG:HB2	1.94	0.49
25:f:109:ILE:O	25:f:113:MET:HB3	2.13	0.49
27:u:198:ILE:HD12	27:u:199:ASN:HB2	1.94	0.49
1:A:70:THR:HB	1:A:72:LEU:HD23	1.95	0.49
1:A:276:GLU:OE2	1:A:322:ASN:ND2	2.46	0.49
3:C:132:ASP:OD1	3:C:132:ASP:N	2.46	0.49
4:D:268:ASP:OD2	4:D:313:ARG:NH1	2.44	0.49
5:E:178:THR:N	31:E:402:ATP:O1B	2.46	0.49
7:G:21:ARG:HG2	7:G:21:ARG:HH11	1.78	0.49
7:G:122:SER:HB2	7:G:158:GLY:HA2	1.95	0.49
9:I:45:LEU:HD22	9:I:137:ILE:HG12	1.94	0.49
17:X:110:CYS:O	17:X:114:ILE:HG12	2.12	0.49
17:X:283:GLN:OE1	17:X:283:GLN:N	2.44	0.49
20:a:335:TRP:HD1	20:a:337:GLN:N	2.11	0.49
20:a:337:GLN:NE2	20:a:338:PRO:O	2.45	0.49
25:f:815:HIS:O	25:f:818:LEU:HG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ASP:O	1:A:30:ILE:HD12	2.12	0.49
7:G:40:VAL:HA	7:G:167:ALA:HB2	1.95	0.49
7:G:80:MET:CE	7:G:138:MET:HG2	2.43	0.49
11:K:42:THR:OG1	11:K:45:GLY:O	2.22	0.49
15:V:393:THR:HG23	15:V:397:ARG:HE	1.78	0.49
22:c:303:MET:HE1	23:d:332:SER:C	2.38	0.49
26:g:112:LEU:HD23	26:g:142:LEU:HD11	1.94	0.49
26:g:137:GLN:HB2	26:g:145:GLN:HE21	1.78	0.49
2:B:235:LEU:HD23	2:B:353:PHE:HZ	1.78	0.48
4:D:164:TYR:HB3	4:D:174:LYS:HE2	1.95	0.48
6:F:67:GLN:NE2	6:F:71:ASP:OD2	2.46	0.48
6:F:374:ASN:O	6:F:374:ASN:ND2	2.44	0.48
7:G:138:MET:SD	7:G:140:LEU:HD23	2.53	0.48
9:I:8:ARG:HG3	9:I:10:THR:H	1.78	0.48
9:I:119:GLN:HG3	10:J:78:ALA:HB1	1.95	0.48
10:J:59:VAL:HB	10:J:61:LYS:HE3	1.95	0.48
14:U:450:HIS:CE1	14:U:457:ILE:HG12	2.48	0.48
14:U:617:ALA:O	14:U:621:SER:OG	2.31	0.48
15:V:423:ALA:HB2	15:V:434:ALA:HB2	1.94	0.48
16:W:217:GLU:N	16:W:217:GLU:OE1	2.46	0.48
17:X:86:ALA:HA	17:X:125:LEU:HD11	1.94	0.48
18:Y:234:PRO:O	18:Y:238:GLU:HG2	2.13	0.48
25:f:846:VAL:O	25:f:865:PHE:HA	2.13	0.48
2:B:176:VAL:HG11	2:B:249:ARG:HG2	1.95	0.48
4:D:395:LEU:HD12	4:D:397:LYS:HE2	1.95	0.48
5:E:260:LEU:HD21	5:E:289:LEU:HD21	1.95	0.48
15:V:301:GLU:OE2	15:V:304:GLU:HB3	2.14	0.48
15:V:473:GLN:HG2	19:Z:257:MET:HG3	1.95	0.48
18:Y:111:LEU:HD13	18:Y:119:GLY:C	2.38	0.48
20:a:101:ARG:HG3	20:a:111:VAL:HG23	1.94	0.48
25:f:350:LYS:HD2	25:f:353:LEU:HD23	1.95	0.48
25:f:650:GLN:O	25:f:653:ALA:HB3	2.13	0.48
4:D:246:MET:O	4:D:250:VAL:HG12	2.12	0.48
4:D:387:VAL:HG22	5:E:158:LEU:HB3	1.95	0.48
5:E:283:ASP:HB3	5:E:387:LYS:HD3	1.94	0.48
6:F:221:LYS:N	6:F:349:ASP:OD2	2.42	0.48
6:F:264:GLY:HA2	6:F:267:LEU:HD13	1.95	0.48
9:I:53:HIS:HB3	9:I:56:LEU:HG	1.94	0.48
12:L:8:ASN:N	12:L:8:ASN:OD1	2.45	0.48
14:U:170:SER:C	14:U:172:ASP:H	2.21	0.48
15:V:443:ARG:HD3	23:d:274:CYS:CB	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:37:GLY:HA3	19:Z:95:TYR:CZ	2.48	0.48
25:f:557:TRP:N	25:f:557:TRP:CD1	2.81	0.48
1:A:45:ILE:HG13	2:B:65:LEU:HD22	1.95	0.48
2:B:125:THR:OG1	2:B:126:SER:N	2.46	0.48
5:E:88:ASP:OD1	5:E:90:SER:N	2.45	0.48
6:F:222:GLY:HA3	6:F:348:LEU:HA	1.96	0.48
9:I:140:ASP:OD2	9:I:146:GLN:OE1	2.30	0.48
17:X:271:VAL:HG11	17:X:288:LYS:HD2	1.95	0.48
27:u:189:GLN:HE22	27:u:257:THR:HG23	1.79	0.48
2:B:233:THR:O	2:B:237:LYS:HG3	2.13	0.48
5:E:334:LEU:HD12	5:E:368:MET:HE1	1.95	0.48
7:G:10:ASP:OD1	7:G:10:ASP:N	2.45	0.48
13:M:140:TYR:HD1	13:M:146:ALA:HB2	1.77	0.48
14:U:69:TYR:HE2	15:V:240:LEU:HD11	1.78	0.48
14:U:922:GLU:O	14:U:924:LEU:N	2.47	0.48
15:V:160:LEU:HB2	15:V:161:PRO:HD3	1.94	0.48
15:V:176:MET:SD	15:V:179:LYS:HE3	2.53	0.48
16:W:60:MET:SD	16:W:61:VAL:N	2.86	0.48
16:W:307:LYS:O	16:W:311:THR:HG23	2.14	0.48
22:c:305:ASP:O	22:c:309:PHE:HB2	2.14	0.48
23:d:348:MET:HE2	23:d:348:MET:HB2	1.67	0.48
25:f:315:GLU:N	25:f:315:GLU:OE2	2.45	0.48
6:F:61:ARG:HD2	21:b:73:SER:HA	1.94	0.48
6:F:369:HIS:CE1	6:F:397:LYS:HB2	2.48	0.48
9:I:12:PHE:HE1	10:J:125:ARG:HD3	1.78	0.48
12:L:132:LEU:O	12:L:146:GLN:HA	2.13	0.48
13:M:70:ASP:OD2	13:M:99:ARG:NH2	2.45	0.48
13:M:141:SER:OG	13:M:144:ASP:OD1	2.21	0.48
14:U:52:GLU:HA	14:U:57:ARG:HD2	1.94	0.48
14:U:595:ASN:O	14:U:599:ILE:HD12	2.13	0.48
15:V:278:GLU:HA	15:V:285:TRP:HZ2	1.78	0.48
16:W:185:PHE:O	16:W:189:GLN:HG3	2.13	0.48
17:X:134:VAL:HG12	17:X:172:LEU:HD13	1.94	0.48
19:Z:44:GLN:O	19:Z:47:VAL:HG12	2.13	0.48
23:d:248:LYS:NZ	23:d:260:ILE:HG21	2.22	0.48
27:u:180:MET:HE1	27:u:182:PHE:CG	2.48	0.48
1:A:213:LEU:HD12	1:A:214:LEU:N	2.29	0.48
5:E:185:ARG:HH11	6:F:320:PHE:HA	1.79	0.48
6:F:323:ASN:O	6:F:326:VAL:HG12	2.14	0.48
7:G:13:ILE:HG23	7:G:14:THR:HG23	1.95	0.48
8:H:74:LEU:HD12	8:H:75:VAL:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:176:LYS:HD2	8:H:177:ARG:N	2.29	0.48
11:K:24:VAL:HG12	11:K:136:PRO:HG2	1.96	0.48
11:K:65:GLU:OE1	11:K:65:GLU:N	2.36	0.48
12:L:157:ARG:HB3	12:L:176:MET:HE3	1.94	0.48
14:U:86:ASP:O	14:U:90:VAL:HG22	2.13	0.48
14:U:669:ILE:HG12	14:U:695:MET:SD	2.54	0.48
15:V:271:VAL:HG22	15:V:272:SER:H	1.79	0.48
25:f:437:GLU:HB2	25:f:440:ILE:HG12	1.96	0.48
25:f:731:MET:HE2	25:f:731:MET:HA	1.95	0.48
25:f:790:GLN:CD	25:f:790:GLN:H	2.22	0.48
1:A:284:ARG:NH2	6:F:289:ASP:OD2	2.26	0.48
4:D:209:GLY:O	4:D:371:SER:HB2	2.14	0.48
4:D:283:ARG:HB2	4:D:287:ARG:HH22	1.77	0.48
5:E:125:GLU:OE2	5:E:197:LYS:NZ	2.46	0.48
5:E:228:CYS:O	5:E:273:VAL:HA	2.14	0.48
7:G:121:ILE:O	7:G:125:TYR:HD2	1.97	0.48
13:M:175:GLU:HA	13:M:178:LYS:NZ	2.29	0.48
16:W:41:GLN:O	16:W:45:GLU:HG2	2.14	0.48
17:X:86:ALA:CB	17:X:125:LEU:HD21	2.43	0.48
18:Y:101:ARG:NH2	18:Y:130:LYS:O	2.47	0.48
18:Y:316:LEU:HG	18:Y:352:GLU:HB3	1.96	0.48
19:Z:197:GLY:HA2	22:c:225:TRP:HB2	1.95	0.48
22:c:37:ALA:O	22:c:41:MET:HG3	2.13	0.48
25:f:304:PHE:CE2	25:f:321:MET:HE3	2.49	0.48
25:f:656:GLY:O	25:f:660:ILE:HG12	2.14	0.48
25:f:782:HIS:HA	25:f:785:ARG:HH21	1.79	0.48
25:f:805:ASP:O	25:f:809:ILE:HG22	2.14	0.48
2:B:70:ASP:OD1	14:U:834:SER:OG	2.29	0.48
5:E:300:HIS:NE2	5:E:386:TYR:OH	2.22	0.48
10:J:12:PRO:HA	11:K:26:TYR:CD1	2.48	0.48
13:M:72:HIS:CE1	13:M:105:ASN:HD21	2.32	0.48
16:W:63:THR:HA	16:W:66:ILE:HG22	1.96	0.48
18:Y:42:MET:SD	18:Y:42:MET:N	2.86	0.48
25:f:76:GLU:HG3	25:f:121:PHE:HE2	1.77	0.48
2:B:179:ALA:O	2:B:181:GLN:N	2.45	0.48
2:B:184:TYR:CE2	2:B:198:LYS:HE2	2.45	0.48
5:E:48:LYS:HZ3	19:Z:88:ARG:HH11	1.62	0.48
5:E:84:ARG:HD3	5:E:108:MET:HG2	1.96	0.48
6:F:265:ALA:HB1	6:F:312:GLU:OE1	2.13	0.48
11:K:71:ASP:OD2	11:K:72:ALA:N	2.47	0.48
14:U:620:GLU:HG2	14:U:654:MET:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:79:ASP:O	18:Y:83:ARG:HG2	2.14	0.48
18:Y:281:GLU:OE1	18:Y:281:GLU:N	2.44	0.48
19:Z:249:PHE:HD1	23:d:330:ILE:HD13	1.77	0.48
20:a:211:PHE:HD1	20:a:212:ASN:H	1.61	0.48
21:b:15:TYR:HB3	21:b:145:GLU:OE1	2.14	0.48
21:b:133:LYS:NZ	27:u:162:ASP:OD1	2.46	0.48
25:f:208:LEU:HD22	25:f:213:GLN:O	2.14	0.48
1:A:146:LYS:HZ3	1:A:148:GLN:NE2	2.12	0.47
2:B:99:VAL:O	2:B:103:ARG:HG2	2.13	0.47
2:B:252:GLY:O	2:B:255:LEU:HG	2.13	0.47
2:B:374:LEU:HD12	2:B:378:VAL:HG11	1.96	0.47
2:B:405:MET:HG2	2:B:408:ARG:HH21	1.79	0.47
3:C:134:LEU:HD22	3:C:137:LEU:HD12	1.96	0.47
6:F:316:GLN:N	6:F:316:GLN:OE1	2.47	0.47
14:U:620:GLU:HA	14:U:655:ALA:HB2	1.96	0.47
14:U:763:VAL:O	14:U:767:THR:HG23	2.14	0.47
16:W:121:LYS:O	16:W:125:ILE:HG12	2.14	0.47
16:W:294:LYS:O	16:W:297:GLU:HG2	2.13	0.47
17:X:349:HIS:O	17:X:353:LEU:HG	2.14	0.47
20:a:140:GLU:O	20:a:143:ASN:ND2	2.47	0.47
25:f:76:GLU:HB3	25:f:80:ARG:HH21	1.78	0.47
25:f:577:LEU:HA	25:f:580:LEU:HG	1.96	0.47
25:f:694:LEU:HA	25:f:697:ILE:HD12	1.96	0.47
25:f:700:SER:HB2	25:f:779:CYS:SG	2.54	0.47
27:u:282:VAL:HG22	27:u:283:GLY:N	2.28	0.47
15:V:36:GLU:HA	15:V:39:GLU:HG3	1.94	0.47
17:X:408:SER:HA	18:Y:376:LEU:HD13	1.97	0.47
23:d:219:ASP:O	23:d:223:ASN:ND2	2.47	0.47
25:f:440:ILE:HG13	25:f:441:LYS:N	2.29	0.47
27:u:184:GLY:N	27:u:225:ILE:HG22	2.29	0.47
13:M:56:LYS:HE2	13:M:57:LEU:HD22	1.95	0.47
14:U:78:LEU:HD11	14:U:103:LYS:HB3	1.96	0.47
14:U:879:ASP:OD1	14:U:880:ASN:N	2.42	0.47
17:X:182:ASN:HA	18:Y:244:ALA:HB1	1.96	0.47
18:Y:275:LEU:HA	18:Y:278:VAL:HG12	1.96	0.47
2:B:150:VAL:HG11	2:B:159:VAL:HG22	1.95	0.47
5:E:138:LEU:HB3	5:E:141:GLN:HB2	1.97	0.47
5:E:193:CYS:SG	5:E:229:ILE:HD13	2.54	0.47
5:E:268:ASP:HB3	5:E:271:HIS:HD1	1.79	0.47
6:F:143:GLU:OE2	6:F:144:LYS:HD2	2.13	0.47
6:F:226:TYR:O	6:F:354:PHE:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:389:ASP:OD2	6:F:389:ASP:N	2.46	0.47
10:J:156:TRP:CG	10:J:159:ASN:HB2	2.49	0.47
14:U:331:GLY:HA2	14:U:334:ALA:HB3	1.96	0.47
16:W:346:GLU:HA	16:W:349:LYS:HE3	1.97	0.47
18:Y:387:ILE:HA	19:Z:279:LYS:NZ	2.29	0.47
19:Z:43:TRP:CZ3	19:Z:48:LEU:HB2	2.48	0.47
20:a:343:LEU:HD12	20:a:347:LYS:HE2	1.96	0.47
25:f:850:VAL:HG12	25:f:852:VAL:H	1.78	0.47
1:A:78:TRP:HZ3	2:B:98:LYS:HE2	1.80	0.47
1:A:300:LEU:HA	1:A:303:ILE:HG22	1.96	0.47
1:A:362:MET:HB2	1:A:364:VAL:HG13	1.95	0.47
2:B:223:ILE:HG23	2:B:329:MET:HE3	1.96	0.47
2:B:409:GLU:OE2	2:B:411:ARG:HG3	2.14	0.47
2:B:429:LYS:HD2	3:C:308:PRO:HA	1.96	0.47
3:C:49:ARG:NH2	14:U:639:LEU:O	2.48	0.47
5:E:74:THR:OG1	5:E:75:ASN:N	2.44	0.47
5:E:148:VAL:HG13	5:E:167:PRO:HG2	1.95	0.47
6:F:80:ILE:HG22	6:F:84:LYS:HE3	1.97	0.47
11:K:69:GLU:HB2	11:K:229:PHE:CE2	2.49	0.47
14:U:323:LEU:O	14:U:327:LYS:HG3	2.14	0.47
14:U:602:LEU:HD23	14:U:603:LEU:N	2.28	0.47
18:Y:79:ASP:OD1	18:Y:80:GLU:N	2.47	0.47
19:Z:231:GLN:CA	20:a:349:MET:HE1	2.39	0.47
20:a:14:SER:OG	20:a:52:GLN:OE1	2.29	0.47
21:b:7:MET:HG2	21:b:64:LEU:HD11	1.97	0.47
23:d:112:CYS:O	23:d:116:LEU:HG	2.14	0.47
2:B:50:PRO:HD3	25:f:670:MET:HE3	1.96	0.47
2:B:206:THR:HA	25:f:740:ARG:HH21	1.78	0.47
5:E:119:VAL:HG22	5:E:218:MET:HG3	1.95	0.47
7:G:196:GLU:HA	7:G:242:LEU:HD21	1.95	0.47
8:H:34:PRO:HA	8:H:164:GLY:HA3	1.97	0.47
10:J:31:THR:HG22	10:J:164:GLY:H	1.80	0.47
15:V:148:ARG:HE	15:V:199:ASN:HB2	1.79	0.47
16:W:361:HIS:HA	16:W:364:ARG:HE	1.79	0.47
1:A:146:LYS:HZ1	1:A:148:GLN:NE2	2.09	0.47
1:A:189:GLU:OE1	1:A:339:ARG:NH1	2.34	0.47
2:B:59:ARG:HE	25:f:206:ASP:HB3	1.79	0.47
3:C:191:PRO:O	3:C:194:THR:OG1	2.26	0.47
5:E:135:ILE:HD11	5:E:138:LEU:HD23	1.96	0.47
5:E:219:PHE:HE1	5:E:264:MET:HB3	1.79	0.47
6:F:264:GLY:HA2	6:F:267:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:324:THR:OG1	6:F:325:GLN:N	2.47	0.47
7:G:35:GLY:HA2	7:G:170:VAL:HG21	1.96	0.47
8:H:79:MET:HG3	8:H:82:ASP:HB2	1.96	0.47
8:H:179:ASN:OD1	8:H:182:LEU:HG	2.15	0.47
12:L:61:LYS:NZ	12:L:211:SER:OG	2.46	0.47
12:L:180:MET:SD	12:L:181:GLU:HG2	2.55	0.47
14:U:2:ILE:N	23:d:177:ASP:OD1	2.47	0.47
14:U:340:GLN:HE21	14:U:927:PRO:HG2	1.79	0.47
14:U:376:MET:HA	14:U:739:ALA:HA	1.96	0.47
14:U:467:ASN:O	27:u:121:LYS:NZ	2.47	0.47
14:U:803:LYS:HD3	14:U:875:PHE:HB3	1.96	0.47
15:V:76:LYS:O	15:V:81:GLN:NE2	2.31	0.47
16:W:88:MET:C	16:W:88:MET:HE2	2.39	0.47
17:X:343:SER:HA	17:X:387:ILE:HB	1.95	0.47
18:Y:105:MET:SD	18:Y:127:THR:HG21	2.55	0.47
22:c:105:PRO:HB2	27:u:242:ASN:ND2	2.30	0.47
22:c:286:GLU:O	22:c:290:VAL:HG12	2.15	0.47
25:f:478:ARG:O	25:f:482:ILE:HG22	2.14	0.47
26:g:167:LYS:O	26:g:171:LEU:HG	2.13	0.47
27:u:208:GLU:O	27:u:212:SER:N	2.37	0.47
2:B:186:ASP:OD1	2:B:186:ASP:N	2.48	0.47
2:B:225:TYR:CD1	2:B:334:ILE:HG21	2.50	0.47
4:D:119:ILE:HD11	4:D:140:VAL:C	2.40	0.47
4:D:371:SER:O	4:D:375:ILE:HG12	2.15	0.47
5:E:101:ASP:O	5:E:105:LEU:HD22	2.15	0.47
5:E:178:THR:HB	5:E:301:ILE:HG22	1.96	0.47
8:H:132:VAL:HG12	8:H:134:LEU:HD22	1.96	0.47
8:H:135:LEU:HG	8:H:163:HIS:CE1	2.49	0.47
12:L:158:ALA:HB2	12:L:179:PHE:CE2	2.49	0.47
14:U:12:LEU:HA	14:U:20:LYS:HG2	1.97	0.47
14:U:419:ALA:HA	14:U:422:LEU:HB3	1.96	0.47
15:V:259:LEU:HD11	15:V:295:ILE:HD11	1.95	0.47
15:V:392:TYR:H	15:V:392:TYR:HD1	1.63	0.47
16:W:369:TYR:CD2	20:a:312:MET:HG2	2.50	0.47
19:Z:132:GLY:HA2	22:c:222:LYS:HE2	1.96	0.47
20:a:68:GLU:HB2	20:a:71:VAL:HG23	1.97	0.47
20:a:84:VAL:HA	20:a:87:MET:HE3	1.97	0.47
25:f:47:GLU:O	25:f:51:GLN:HG2	2.15	0.47
25:f:398:TRP:O	25:f:401:LYS:HG2	2.14	0.47
25:f:486:GLY:C	25:f:524:MET:HE3	2.40	0.47
1:A:325:ASP:OD2	1:A:325:ASP:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:LEU:O	2:B:69:LYS:HG2	2.13	0.47
5:E:115:VAL:CG1	6:F:95:GLU:HB3	2.44	0.47
5:E:222:ALA:HB2	5:E:230:ILE:HD11	1.96	0.47
7:G:31:ALA:HA	13:M:19:ARG:HH21	1.79	0.47
14:U:483:LEU:HD12	14:U:778:PHE:CZ	2.49	0.47
15:V:29:PRO:HB2	15:V:30:PRO:HD3	1.97	0.47
15:V:496:PHE:H	15:V:497:PRO:HD2	1.79	0.47
16:W:326:MET:HA	16:W:326:MET:HE3	1.96	0.47
19:Z:198:LEU:HD22	22:c:229:LEU:HD21	1.97	0.47
21:b:44:ASN:ND2	21:b:46:GLU:HB3	2.26	0.47
21:b:111:ALA:HB3	21:b:140:ILE:HD12	1.96	0.47
25:f:55:GLU:HA	25:f:58:MET:SD	2.55	0.47
26:g:104:ARG:NH1	26:g:105:LEU:H	2.13	0.47
6:F:144:LYS:HE3	6:F:144:LYS:HB3	1.76	0.47
8:H:118:MET:O	8:H:122:THR:HG23	2.15	0.47
9:I:159:TRP:CD1	9:I:162:THR:HB	2.50	0.47
13:M:72:HIS:HD1	13:M:139:SER:HG	1.58	0.47
15:V:385:LYS:HE3	15:V:385:LYS:HB2	1.72	0.47
16:W:110:THR:O	16:W:114:GLU:HG3	2.14	0.47
18:Y:118:GLU:OE1	18:Y:118:GLU:N	2.44	0.47
21:b:6:THR:HB	21:b:49:VAL:HG22	1.97	0.47
22:c:303:MET:HE2	23:d:336:ALA:N	2.30	0.47
23:d:117:GLY:O	23:d:120:LYS:HB2	2.14	0.47
25:f:309:GLU:N	25:f:309:GLU:OE2	2.48	0.47
25:f:396:ASN:HB3	25:f:400:TYR:CZ	2.50	0.47
8:H:87:VAL:O	8:H:91:ARG:HG3	2.13	0.46
15:V:318:GLN:HG2	15:V:319:HIS:N	2.28	0.46
16:W:80:TRP:NE1	16:W:120:ILE:HD12	2.30	0.46
16:W:248:ARG:HD2	16:W:286:LEU:HD11	1.96	0.46
20:a:252:LYS:HA	20:a:255:TRP:CZ3	2.50	0.46
25:f:293:GLN:O	25:f:297:MET:HG3	2.15	0.46
25:f:684:PRO:HA	25:f:687:ARG:HB2	1.97	0.46
25:f:702:PRO:HA	25:f:732:VAL:HG22	1.97	0.46
26:g:152:LYS:HD3	26:g:152:LYS:N	2.30	0.46
1:A:169:LYS:HD3	1:A:231:ASN:HA	1.96	0.46
3:C:133:PRO:O	3:C:137:LEU:HG	2.15	0.46
5:E:114:GLU:OE1	5:E:114:GLU:N	2.35	0.46
5:E:340:GLY:HA3	31:E:402:ATP:C8	2.50	0.46
6:F:86:LEU:HD23	6:F:88:TYR:CE2	2.50	0.46
11:K:36:THR:HA	11:K:170:ILE:O	2.15	0.46
11:K:147:ASP:OD1	11:K:150:GLY:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:53:VAL:H	13:M:209:PHE:HA	1.80	0.46
14:U:741:GLY:O	14:U:813:TYR:OH	2.29	0.46
18:Y:218:THR:O	18:Y:221:THR:OG1	2.29	0.46
23:d:237:MET:N	23:d:237:MET:SD	2.88	0.46
25:f:85:SER:O	25:f:88:SER:OG	2.32	0.46
26:g:107:ILE:H	26:g:107:ILE:HG12	1.50	0.46
1:A:252:GLU:O	1:A:256:MET:HG3	2.16	0.46
1:A:319:MET:HE2	1:A:337:LEU:HD11	1.98	0.46
3:C:163:GLU:HG2	3:C:164:VAL:N	2.29	0.46
3:C:390:VAL:O	3:C:392:GLN:HG2	2.14	0.46
5:E:32:GLN:HG2	6:F:66:LEU:HD11	1.98	0.46
5:E:36:LEU:HA	5:E:39:GLN:OE1	2.15	0.46
7:G:42:VAL:HA	7:G:164:LYS:NZ	2.27	0.46
11:K:91:LYS:HE3	11:K:91:LYS:HB3	1.61	0.46
12:L:155:ASP:H	13:M:62:SER:HG	1.64	0.46
12:L:207:THR:HB	12:L:226:ASP:HA	1.97	0.46
18:Y:19:ILE:HG23	18:Y:41:LEU:HD11	1.97	0.46
18:Y:138:LEU:HB3	18:Y:176:ARG:HG2	1.96	0.46
20:a:33:LEU:HD12	20:a:36:GLN:HG3	1.98	0.46
20:a:87:MET:SD	20:a:89:ASP:N	2.81	0.46
20:a:273:GLN:HB3	20:a:310:LEU:HD11	1.97	0.46
22:c:292:MET:HE3	22:c:292:MET:HB2	1.87	0.46
7:G:131:MET:HE2	7:G:131:MET:HB3	1.75	0.46
9:I:118:LYS:O	9:I:122:THR:HG23	2.15	0.46
13:M:198:TYR:CG	13:M:239:ALA:HB1	2.51	0.46
14:U:217:CYS:SG	14:U:248:ILE:HG13	2.56	0.46
14:U:766:PHE:CD2	14:U:779:LEU:HD12	2.50	0.46
17:X:393:VAL:HG22	17:X:398:GLU:OE2	2.15	0.46
18:Y:41:LEU:HD23	18:Y:42:MET:HE1	1.97	0.46
19:Z:12:HIS:CG	19:Z:51:SER:HB3	2.51	0.46
21:b:16:MET:HB3	21:b:80:PRO:HB3	1.98	0.46
25:f:143:ARG:HH12	25:f:154:TRP:HE1	1.63	0.46
25:f:346:ASP:OD1	25:f:352:HIS:NE2	2.48	0.46
25:f:654:VAL:HG11	25:f:690:VAL:HA	1.98	0.46
25:f:753:ALA:HB3	25:f:754:LYS:NZ	2.30	0.46
27:u:234:ARG:HH21	27:u:236:VAL:HG11	1.79	0.46
1:A:356:LYS:O	1:A:360:ARG:HG3	2.15	0.46
2:B:55:HIS:ND1	25:f:855:GLN:HG3	2.31	0.46
5:E:196:LEU:HD12	5:E:218:MET:HE2	1.98	0.46
6:F:303:ASP:CG	6:F:304:ARG:H	2.23	0.46
12:L:20:HIS:HA	12:L:23:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:157:ARG:HD2	12:L:179:PHE:HB2	1.98	0.46
14:U:625:ILE:HD12	14:U:626:LEU:HG	1.98	0.46
15:V:84:LYS:HA	15:V:88:GLY:HA3	1.98	0.46
15:V:289:LEU:HA	15:V:292:THR:HG22	1.98	0.46
17:X:82:LYS:HB2	17:X:82:LYS:HE3	1.66	0.46
21:b:157:VAL:HG11	21:b:170:LEU:HB2	1.97	0.46
24:e:62:LYS:HG2	24:e:63:HIS:CD2	2.43	0.46
1:A:354:ILE:HG23	1:A:385:ILE:HG21	1.97	0.46
2:B:107:MET:HG2	3:C:96:VAL:HB	1.97	0.46
2:B:225:TYR:HE2	2:B:350:LYS:HB2	1.81	0.46
3:C:123:LEU:HD12	3:C:124:HIS:N	2.31	0.46
4:D:197:ASP:O	4:D:200:ARG:NH1	2.48	0.46
5:E:283:ASP:N	5:E:283:ASP:OD1	2.47	0.46
6:F:437:TYR:CZ	11:K:25:GLU:HG3	2.51	0.46
10:J:71:MET:SD	10:J:72:ALA:N	2.89	0.46
11:K:173:ALA:HB3	11:K:206:MET:HE1	1.98	0.46
14:U:374:SER:HB2	14:U:410:VAL:CG1	2.45	0.46
16:W:68:VAL:HA	16:W:71:VAL:HG22	1.98	0.46
17:X:86:ALA:O	17:X:90:ARG:HG2	2.15	0.46
18:Y:297:ARG:O	18:Y:300:ARG:HB2	2.16	0.46
19:Z:144:VAL:HG23	19:Z:146:ASP:H	1.81	0.46
22:c:113:HIS:CE1	22:c:144:VAL:HG22	2.50	0.46
22:c:146:ASP:O	22:c:150:SER:OG	2.23	0.46
25:f:398:TRP:CD1	25:f:401:LYS:HE3	2.50	0.46
27:u:152:LYS:HG2	27:u:262:TYR:CE1	2.50	0.46
27:u:187:ASN:HD21	27:u:259:ARG:HD2	1.81	0.46
2:B:363:ARG:NH1	2:B:363:ARG:HA	2.31	0.46
3:C:102:ASN:C	3:C:104:ASP:H	2.23	0.46
3:C:307:ARG:HG2	3:C:307:ARG:HH11	1.80	0.46
5:E:300:HIS:CE1	5:E:302:ASP:HB2	2.50	0.46
10:J:115:LYS:HD3	10:J:149:PRO:HA	1.96	0.46
12:L:66:VAL:O	12:L:67:ASP:HB2	2.16	0.46
13:M:39:ILE:HG21	13:M:189:ILE:HD12	1.96	0.46
14:U:229:VAL:HG21	14:U:252:LEU:HD11	1.98	0.46
18:Y:237:ARG:HA	18:Y:241:ILE:HB	1.98	0.46
21:b:27:GLN:OE1	21:b:27:GLN:HA	2.14	0.46
21:b:97:LEU:HD23	21:b:97:LEU:O	2.16	0.46
25:f:388:ASP:O	25:f:392:THR:OG1	2.18	0.46
25:f:391:LEU:HD12	25:f:395:GLY:HA2	1.97	0.46
25:f:491:GLY:N	25:f:524:MET:O	2.42	0.46
27:u:182:PHE:HD1	27:u:182:PHE:HA	1.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:u:205:ASP:OD1	27:u:206:PHE:N	2.49	0.46
1:A:253:GLY:O	1:A:257:VAL:HG23	2.16	0.46
2:B:165:ASP:OD1	2:B:167:THR:HG22	2.15	0.46
2:B:395:ILE:HA	2:B:398:ILE:HD12	1.97	0.46
4:D:85:ILE:HG22	4:D:86:PRO:HA	1.97	0.46
4:D:397:LYS:HG3	4:D:401:LYS:HE2	1.97	0.46
5:E:77:PRO:HG2	5:E:79:TYR:CE2	2.50	0.46
6:F:236:LEU:HD23	6:F:354:PHE:HZ	1.80	0.46
7:G:84:THR:O	7:G:87:SER:OG	2.25	0.46
12:L:36:VAL:HG22	12:L:160:SER:HB2	1.97	0.46
12:L:50:LYS:N	12:L:209:ASN:O	2.44	0.46
14:U:340:GLN:NE2	14:U:927:PRO:O	2.46	0.46
14:U:899:ARG:HD3	14:U:900:TYR:CZ	2.50	0.46
15:V:453:HIS:CD2	23:d:286:GLU:HG2	2.50	0.46
16:W:99:GLN:O	16:W:103:LYS:HG2	2.16	0.46
17:X:82:LYS:HE2	17:X:122:ARG:HG2	1.97	0.46
17:X:123:THR:O	17:X:127:GLN:HG2	2.16	0.46
18:Y:57:LEU:HD12	18:Y:61:LEU:HD12	1.98	0.46
20:a:42:LEU:O	20:a:45:VAL:HG12	2.15	0.46
20:a:138:VAL:HA	20:a:141:MET:HG3	1.98	0.46
22:c:162:LEU:HD23	22:c:200:TYR:HB3	1.96	0.46
22:c:279:ASP:HB2	22:c:280:PRO:CD	2.44	0.46
23:d:197:LEU:HB2	23:d:229:PRO:HB3	1.97	0.46
23:d:226:ILE:O	23:d:230:VAL:HG23	2.15	0.46
25:f:388:ASP:OD1	25:f:389:LYS:N	2.49	0.46
1:A:66:LYS:NZ	1:A:68:SER:HA	2.30	0.46
1:A:126:SER:HB3	1:A:150:HIS:HB3	1.97	0.46
3:C:331:ILE:O	3:C:334:ARG:NH1	2.49	0.46
3:C:404:LEU:HB3	8:H:152:SER:HB2	1.97	0.46
4:D:66:LYS:HA	4:D:69:LYS:HZ3	1.81	0.46
13:M:152:ASP:OD1	13:M:156:VAL:N	2.40	0.46
14:U:37:GLU:OE2	15:V:266:GLN:HB3	2.16	0.46
16:W:316:ARG:NH2	16:W:383:ASP:OD1	2.47	0.46
20:a:132:LYS:HD2	20:a:162:TYR:OH	2.15	0.46
22:c:263:ASP:CG	22:c:265:MET:HE3	2.41	0.46
26:g:158:LEU:HD23	26:g:165:ALA:HB2	1.98	0.46
3:C:165:ILE:O	3:C:168:PRO:HD2	2.15	0.46
5:E:344:ARG:HH21	6:F:218:GLN:HB3	1.81	0.46
7:G:226:LYS:C	7:G:226:LYS:HD3	2.41	0.46
8:H:210:VAL:HB	8:H:221:LEU:HD12	1.97	0.46
11:K:147:ASP:OD1	11:K:149:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:203:GLN:O	12:L:239:ARG:NH1	2.49	0.46
14:U:371:ILE:HD11	14:U:403:THR:HG21	1.98	0.46
14:U:450:HIS:NE2	14:U:457:ILE:HG12	2.31	0.46
14:U:733:ALA:HA	14:U:736:ILE:HD12	1.98	0.46
15:V:251:LEU:HD12	15:V:276:PHE:CD2	2.51	0.46
25:f:512:MET:HE1	25:f:558:LEU:CD1	2.45	0.46
25:f:707:LEU:HD21	25:f:741:LEU:HD12	1.98	0.46
26:g:109:GLY:O	26:g:112:LEU:HD12	2.16	0.46
27:u:176:LYS:HG2	27:u:239:GLN:HA	1.97	0.46
2:B:165:ASP:OD1	2:B:166:ASP:N	2.48	0.45
2:B:180:PRO:HA	2:B:241:ASN:HD21	1.81	0.45
2:B:309:MET:HE2	2:B:341:LEU:HD22	1.98	0.45
2:B:355:LEU:HD12	2:B:355:LEU:HA	1.83	0.45
2:B:386:ALA:C	2:B:387:LYS:HD2	2.40	0.45
3:C:328:ILE:HG12	29:C:501:ADP:C6	2.51	0.45
3:C:400:SER:OG	3:C:403:LYS:HD2	2.16	0.45
4:D:248:ARG:NH2	4:D:249:ASP:OD1	2.49	0.45
4:D:345:PHE:CE2	4:D:375:ILE:HD12	2.52	0.45
4:D:409:LYS:HA	4:D:409:LYS:HD2	1.75	0.45
5:E:49:ALA:HB1	6:F:136:VAL:HG21	1.98	0.45
6:F:61:ARG:HH12	21:b:76:HIS:H	1.64	0.45
6:F:390:ASP:OD1	6:F:390:ASP:O	2.35	0.45
8:H:111:VAL:HG22	8:H:136:ILE:HD13	1.99	0.45
12:L:71:GLY:HA3	12:L:221:PHE:CZ	2.51	0.45
12:L:112:ILE:HG22	12:L:147:THR:HG21	1.98	0.45
14:U:340:GLN:NE2	14:U:927:PRO:HG2	2.31	0.45
14:U:599:ILE:HA	14:U:602:LEU:CD2	2.46	0.45
15:V:288:TYR:CD1	15:V:289:LEU:HD12	2.51	0.45
15:V:393:THR:HG23	15:V:397:ARG:HH21	1.81	0.45
17:X:412:ASP:OD1	18:Y:379:ARG:NH1	2.42	0.45
21:b:100:ARG:HD2	21:b:105:HIS:HB2	1.99	0.45
22:c:232:GLN:HG2	22:c:233:ASP:H	1.81	0.45
23:d:119:LEU:HA	23:d:122:VAL:CG1	2.46	0.45
26:g:130:VAL:O	26:g:153:ALA:HA	2.16	0.45
27:u:149:CYS:SG	27:u:157:LEU:HB2	2.56	0.45
5:E:223:ARG:NH2	5:E:263:GLN:OE1	2.48	0.45
16:W:128:LEU:HA	16:W:131:VAL:HG22	1.99	0.45
19:Z:13:PRO:HG3	22:c:220:LEU:CD1	2.46	0.45
19:Z:147:ASP:OD1	19:Z:149:THR:OG1	2.25	0.45
23:d:325:PRO:HB2	23:d:326:GLU:CD	2.41	0.45
3:C:213:ARG:HH21	3:C:215:SER:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:310:MET:HE2	6:F:310:MET:HB2	1.88	0.45
6:F:392:ASN:OD1	6:F:395:GLN:N	2.41	0.45
10:J:65:LEU:HD11	10:J:84:ILE:HG12	1.98	0.45
14:U:206:MET:SD	14:U:216:VAL:HG21	2.56	0.45
14:U:421:GLN:O	14:U:425:THR:HG23	2.16	0.45
16:W:231:ILE:HA	16:W:243:ILE:HD12	1.99	0.45
16:W:279:PHE:CD2	16:W:364:ARG:HD3	2.50	0.45
18:Y:222:TYR:O	18:Y:226:VAL:HG12	2.17	0.45
23:d:168:MET:O	23:d:168:MET:HE3	2.16	0.45
25:f:468:ASP:HB3	26:g:134:LYS:HZ3	1.80	0.45
25:f:571:GLU:O	25:f:574:GLU:HB2	2.16	0.45
1:A:143:ASP:OD1	1:A:147:TYR:N	2.45	0.45
2:B:246:THR:HG21	2:B:277:HIS:HD2	1.81	0.45
3:C:141:GLU:HB2	3:C:211:PHE:HB3	1.99	0.45
3:C:197:THR:HA	3:C:247:PHE:HE2	1.82	0.45
3:C:391:MET:O	3:C:393:LYS:HD2	2.17	0.45
11:K:78:MET:N	11:K:78:MET:HE3	2.32	0.45
14:U:495:ASP:HA	14:U:498:LYS:HB2	1.99	0.45
16:W:414:ASN:OD1	16:W:416:GLN:HG2	2.15	0.45
19:Z:187:LEU:HD12	19:Z:187:LEU:HA	1.78	0.45
19:Z:271:ALA:HA	19:Z:274:ASN:HD22	1.81	0.45
25:f:173:LEU:HD11	25:f:177:GLU:OE2	2.15	0.45
25:f:445:LEU:HD23	25:f:445:LEU:HA	1.84	0.45
26:g:88:PHE:O	26:g:155:VAL:HG12	2.16	0.45
3:C:351:MET:HE2	3:C:351:MET:HA	1.98	0.45
5:E:116:ASP:O	5:E:118:LEU:N	2.49	0.45
5:E:117:PRO:O	5:E:120:TYR:HB3	2.16	0.45
5:E:120:TYR:CD1	6:F:147:PRO:HG2	2.52	0.45
11:K:68:VAL:HG11	11:K:89:ILE:HD13	1.96	0.45
16:W:312:MET:HE2	16:W:312:MET:HA	1.98	0.45
18:Y:66:ASP:HB2	18:Y:69:LEU:HB2	1.98	0.45
18:Y:272:PHE:HB3	24:e:56:LEU:HD21	1.99	0.45
19:Z:257:MET:HA	19:Z:260:VAL:HG12	1.99	0.45
20:a:240:PHE:CE1	20:a:272:ILE:HG12	2.51	0.45
22:c:139:ARG:HG3	22:c:161:ARG:CZ	2.47	0.45
23:d:248:LYS:NZ	23:d:260:ILE:HD13	2.32	0.45
25:f:250:ARG:NH2	25:f:272:LEU:HD21	2.32	0.45
25:f:514:VAL:O	25:f:518:THR:OG1	2.27	0.45
26:g:114:SER:O	26:g:118:GLU:HG3	2.17	0.45
2:B:107:MET:HE2	2:B:107:MET:HB3	1.85	0.45
3:C:277:LEU:HD23	3:C:277:LEU:HA	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:40:LEU:HD13	4:D:43:ARG:HE	1.81	0.45
5:E:182:LEU:HD22	31:E:402:ATP:H2'	1.98	0.45
6:F:94:ILE:HB	6:F:123:VAL:HB	1.98	0.45
11:K:190:THR:HG23	11:K:193:GLU:H	1.82	0.45
14:U:247:GLN:HE21	14:U:904:LYS:HD3	1.81	0.45
14:U:833:LEU:HA	14:U:836:THR:HG22	1.98	0.45
15:V:169:LEU:C	15:V:171:VAL:H	2.23	0.45
16:W:62:SER:O	16:W:66:ILE:HG22	2.16	0.45
16:W:181:GLU:HG2	16:W:185:PHE:CE2	2.52	0.45
21:b:101:GLN:OE1	21:b:101:GLN:N	2.43	0.45
22:c:123:SER:O	22:c:127:ILE:HG12	2.17	0.45
25:f:155:GLY:O	25:f:159:VAL:HG23	2.15	0.45
25:f:433:LEU:HD21	25:f:448:CYS:SG	2.56	0.45
27:u:184:GLY:HA2	27:u:261:SER:HB2	1.99	0.45
1:A:30:ILE:HG23	3:C:174:LEU:HD11	1.98	0.45
1:A:113:ILE:HG12	1:A:121:PHE:HB2	1.99	0.45
1:A:203:ASN:OD1	1:A:204:LEU:N	2.50	0.45
1:A:254:ALA:HB1	1:A:301:GLU:HG3	1.98	0.45
7:G:88:ARG:HH11	13:M:157:SER:HG	1.63	0.45
9:I:78:GLY:HA3	9:I:132:VAL:HA	1.99	0.45
14:U:5:ALA:HB3	23:d:173:CYS:SG	2.56	0.45
14:U:35:TRP:CD1	14:U:35:TRP:H	2.34	0.45
14:U:692:ALA:HB1	14:U:736:ILE:HB	1.99	0.45
15:V:419:LEU:HD23	15:V:435:GLU:HB2	1.99	0.45
16:W:186:ILE:O	16:W:190:MET:HE2	2.17	0.45
16:W:194:LEU:O	16:W:197:LYS:HD2	2.17	0.45
16:W:272:LEU:HD21	16:W:328:LEU:HD11	1.99	0.45
17:X:116:TRP:NE1	17:X:120:GLU:OE2	2.49	0.45
18:Y:214:MET:HE1	18:Y:219:PHE:CA	2.47	0.45
19:Z:139:ILE:HD12	19:Z:139:ILE:HA	1.84	0.45
1:A:137:GLY:O	1:A:139:ARG:N	2.49	0.45
2:B:266:LEU:O	2:B:269:GLU:HG2	2.17	0.45
2:B:355:LEU:HD23	2:B:388:ASP:O	2.16	0.45
3:C:188:LEU:HB3	3:C:317:PHE:CE1	2.52	0.45
3:C:214:VAL:O	3:C:248:MET:HA	2.16	0.45
4:D:313:ARG:HB2	4:D:315:ASP:OD1	2.17	0.45
4:D:327:LEU:HD23	4:D:327:LEU:HA	1.79	0.45
13:M:38:GLY:HA3	13:M:136:MET:HE1	1.97	0.45
14:U:915:LYS:HA	14:U:915:LYS:HE2	1.98	0.45
15:V:364:THR:O	15:V:367:VAL:HG12	2.17	0.45
15:V:470:ARG:NE	15:V:473:GLN:OE1	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:301:ILE:HG21	18:Y:342:ARG:HB3	1.99	0.45
20:a:18:GLN:H	20:a:18:GLN:HG2	1.60	0.45
21:b:146:GLU:OE1	21:b:149:ASN:N	2.49	0.45
21:b:169:HIS:CE1	21:b:191:GLY:HA3	2.51	0.45
22:c:216:MET:HA	22:c:216:MET:HE2	1.98	0.45
25:f:59:LEU:HD12	25:f:78:LEU:HG	1.98	0.45
25:f:830:LEU:HD12	25:f:830:LEU:HA	1.75	0.45
1:A:240:VAL:N	1:A:273:PHE:O	2.50	0.45
2:B:81:ASN:O	2:B:82:GLN:NE2	2.49	0.45
2:B:277:HIS:O	2:B:279:PRO:HD2	2.16	0.45
2:B:405:MET:HA	2:B:408:ARG:NE	2.27	0.45
6:F:314:LEU:HD11	6:F:342:LEU:HG	1.99	0.45
9:I:44:LEU:HA	9:I:215:THR:HA	1.99	0.45
9:I:237:ILE:O	9:I:241:GLU:HG3	2.17	0.45
14:U:49:TYR:OH	14:U:83:GLY:HA3	2.16	0.45
18:Y:23:ARG:HG2	18:Y:53:TYR:OH	2.17	0.45
18:Y:276:ALA:HB2	24:e:56:LEU:HD23	1.99	0.45
22:c:46:ARG:NH2	22:c:147:PRO:O	2.49	0.45
23:d:287:ALA:C	23:d:299:MET:HE1	2.42	0.45
25:f:477:MET:HA	25:f:477:MET:HE3	1.98	0.45
1:A:45:ILE:HD13	2:B:57:GLN:HE22	1.81	0.45
1:A:139:ARG:O	1:A:153:LEU:HB2	2.17	0.45
4:D:55:GLU:HA	4:D:58:GLU:OE1	2.17	0.45
5:E:40:TYR:CD2	6:F:69:MET:HE1	2.52	0.45
5:E:369:LYS:HA	5:E:372:ARG:NH1	2.32	0.45
14:U:563:ALA:O	14:U:567:ILE:HG12	2.17	0.45
14:U:838:LYS:HA	14:U:841:LYS:HE2	1.99	0.45
15:V:194:LYS:HD2	15:V:241:ARG:HH22	1.81	0.45
16:W:234:ASP:HB3	16:W:239:SER:HB3	1.99	0.45
17:X:145:GLU:O	17:X:149:LEU:HD22	2.17	0.45
18:Y:237:ARG:NH1	18:Y:238:GLU:OE1	2.46	0.45
18:Y:285:ASP:OD1	18:Y:288:PHE:N	2.47	0.45
20:a:266:ALA:O	20:a:270:ARG:HG2	2.17	0.45
25:f:268:LEU:O	25:f:271:MET:HB2	2.17	0.45
25:f:482:ILE:HD11	25:f:518:THR:HG23	1.98	0.45
27:u:198:ILE:HB	27:u:241:VAL:HG22	1.97	0.45
1:A:143:ASP:OD2	1:A:148:GLN:N	2.38	0.44
2:B:363:ARG:HA	2:B:363:ARG:HH11	1.81	0.44
3:C:389:LYS:HB2	3:C:389:LYS:HE3	1.70	0.44
4:D:366:ARG:HH22	4:D:400:GLU:CD	2.25	0.44
7:G:16:PHE:HD2	8:H:25:ALA:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:84:ARG:O	8:H:87:VAL:HG12	2.17	0.44
10:J:149:PRO:C	10:J:151:GLY:H	2.25	0.44
11:K:234:LEU:O	11:K:238:ILE:HG13	2.17	0.44
12:L:146:GLN:CB	12:L:159:MET:HE1	2.46	0.44
14:U:888:GLN:OE1	14:U:888:GLN:N	2.50	0.44
15:V:60:ALA:HB3	15:V:62:HIS:CE1	2.52	0.44
20:a:202:LEU:O	20:a:206:LEU:HB2	2.17	0.44
20:a:246:GLU:OE1	20:a:249:GLN:N	2.49	0.44
23:d:207:GLU:O	23:d:211:GLU:HG2	2.18	0.44
25:f:182:GLU:O	25:f:186:THR:HG23	2.17	0.44
26:g:163:GLU:O	26:g:167:LYS:HG2	2.17	0.44
1:A:348:LEU:HD12	1:A:348:LEU:HA	1.81	0.44
3:C:132:ASP:O	3:C:134:LEU:N	2.46	0.44
3:C:160:GLU:O	3:C:164:VAL:HG23	2.16	0.44
3:C:173:GLU:O	3:C:177:ALA:N	2.39	0.44
3:C:403:LYS:HE2	8:H:156:PHE:CE2	2.53	0.44
5:E:97:ARG:NH1	6:F:95:GLU:OE2	2.38	0.44
5:E:97:ARG:NH2	6:F:123:VAL:HG11	2.32	0.44
5:E:161:ARG:CZ	5:E:161:ARG:HB2	2.47	0.44
5:E:294:ARG:O	5:E:295:LEU:HD23	2.17	0.44
7:G:138:MET:C	7:G:138:MET:HE3	2.43	0.44
8:H:109:GLN:HB3	8:H:113:ARG:NH1	2.32	0.44
14:U:611:ASN:HB3	14:U:614:VAL:HG22	2.00	0.44
14:U:695:MET:HB2	14:U:737:LEU:HD21	1.99	0.44
14:U:791:LEU:HD13	14:U:797:MET:SD	2.57	0.44
16:W:432:LEU:HD21	22:c:305:ASP:HB3	1.99	0.44
17:X:47:GLU:HG3	17:X:76:PHE:CZ	2.53	0.44
17:X:47:GLU:HG3	17:X:76:PHE:HZ	1.83	0.44
18:Y:136:HIS:O	18:Y:140:ILE:HG12	2.17	0.44
18:Y:192:ARG:HB2	18:Y:291:HIS:CE1	2.53	0.44
19:Z:27:GLY:HA2	19:Z:31:ASN:HA	1.98	0.44
21:b:6:THR:O	21:b:49:VAL:HA	2.17	0.44
21:b:8:VAL:HG23	21:b:110:ILE:HG23	1.99	0.44
26:g:94:LYS:H	26:g:94:LYS:CD	2.30	0.44
1:A:58:LYS:HA	1:A:61:GLU:HG2	1.99	0.44
1:A:369:ARG:HE	1:A:372:LEU:HD11	1.82	0.44
1:A:372:LEU:O	1:A:375:ARG:HG2	2.17	0.44
2:B:271:PHE:CD2	2:B:315:GLN:HB3	2.52	0.44
4:D:392:TYR:HE1	16:W:207:LYS:HZ1	1.65	0.44
5:E:153:LEU:HD21	5:E:227:PRO:HB2	2.00	0.44
5:E:232:MET:HG3	5:E:235:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:E:402:ATP:PG	6:F:344:ARG:HH22	2.39	0.44
9:I:22:GLU:HA	9:I:25:MET:SD	2.57	0.44
14:U:78:LEU:HD13	14:U:104:CYS:HA	1.99	0.44
14:U:772:TRP:CD1	14:U:774:PRO:HD2	2.52	0.44
15:V:259:LEU:HD11	15:V:295:ILE:CD1	2.48	0.44
15:V:447:ILE:HG22	15:V:449:ALA:H	1.83	0.44
16:W:141:GLU:O	16:W:145:LEU:N	2.41	0.44
19:Z:263:ALA:HB2	22:c:291:LEU:HD22	1.98	0.44
25:f:901:ARG:HH11	25:f:901:ARG:HG3	1.82	0.44
27:u:196:ILE:CD1	27:u:246:ILE:HG13	2.48	0.44
1:A:248:LYS:NZ	28:v:19:UNK:HA	2.31	0.44
3:C:58:LEU:HD12	3:C:59:LEU:N	2.32	0.44
3:C:120:SER:O	3:C:122:THR:N	2.51	0.44
3:C:406:LYS:HZ2	9:I:76:VAL:HG12	1.83	0.44
4:D:89:ILE:HG23	4:D:106:THR:HG21	1.98	0.44
5:E:232:MET:O	5:E:278:ALA:N	2.50	0.44
6:F:156:ASP:HB2	22:c:51:MET:HG3	1.99	0.44
12:L:50:LYS:HD3	12:L:211:SER:HB2	2.00	0.44
14:U:74:PHE:CG	14:U:103:LYS:HE2	2.52	0.44
14:U:106:ASP:O	14:U:109:THR:HG22	2.17	0.44
14:U:214:ILE:HG13	14:U:244:MET:HE1	1.99	0.44
15:V:269:LYS:NZ	15:V:274:SER:HB3	2.32	0.44
16:W:186:ILE:HG22	16:W:190:MET:HE2	1.99	0.44
21:b:51:LEU:N	21:b:62:THR:OG1	2.51	0.44
23:d:300:THR:HG22	23:d:304:LYS:HE2	2.00	0.44
23:d:336:ALA:O	23:d:340:ILE:HG12	2.17	0.44
25:f:502:LEU:O	25:f:505:MET:HG2	2.17	0.44
1:A:348:LEU:O	1:A:352:THR:HG23	2.18	0.44
2:B:381:ASP:HA	2:B:384:ILE:HD12	1.99	0.44
3:C:36:ASN:O	3:C:40:GLN:HG2	2.18	0.44
4:D:85:ILE:CG2	4:D:86:PRO:HA	2.47	0.44
4:D:230:VAL:O	4:D:264:ILE:HA	2.17	0.44
5:E:289:LEU:O	5:E:295:LEU:HB2	2.18	0.44
5:E:331:ILE:HG23	5:E:371:VAL:CG2	2.46	0.44
6:F:251:LEU:HD13	6:F:256:LEU:HD21	1.99	0.44
7:G:126:THR:HG22	8:H:128:ARG:HH12	1.81	0.44
14:U:32:ASN:OD1	14:U:32:ASN:N	2.47	0.44
14:U:612:ASP:OD1	14:U:645:ASN:ND2	2.34	0.44
14:U:623:GLY:HA2	14:U:659:CYS:HB2	1.99	0.44
14:U:669:ILE:HD12	14:U:669:ILE:H	1.83	0.44
14:U:712:LEU:HA	14:U:715:LYS:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:291:TYR:O	15:V:295:ILE:HG12	2.18	0.44
16:W:198:ASP:O	16:W:202:THR:OG1	2.29	0.44
19:Z:74:TYR:CE2	22:c:98:MET:HB3	2.52	0.44
19:Z:211:TYR:CE1	19:Z:220:LEU:HD23	2.52	0.44
20:a:216:LEU:HD23	20:a:217:LEU:HD12	1.99	0.44
21:b:84:ILE:HD13	21:b:84:ILE:HA	1.79	0.44
23:d:98:LEU:HD21	23:d:115:GLU:HB3	1.99	0.44
25:f:404:ASP:CG	25:f:405:HIS:H	2.25	0.44
1:A:209:PRO:HB3	1:A:338:ASP:HB2	1.98	0.44
1:A:214:LEU:HA	1:A:341:ILE:HG22	1.99	0.44
1:A:248:LYS:HE3	2:B:259:TYR:CD1	2.53	0.44
4:D:191:TYR:CD1	4:D:191:TYR:N	2.86	0.44
5:E:297:ARG:NH1	5:E:297:ARG:HA	2.32	0.44
6:F:192:ASP:OD2	6:F:192:ASP:N	2.47	0.44
6:F:405:MET:HE3	6:F:405:MET:HA	1.99	0.44
8:H:50:LYS:O	8:H:207:ASN:HA	2.18	0.44
13:M:120:HIS:O	13:M:124:LEU:HG	2.17	0.44
14:U:762:GLY:HA3	14:U:781:LEU:HB2	1.98	0.44
14:U:792:ASN:ND2	14:U:914:LEU:O	2.50	0.44
15:V:27:PRO:C	15:V:30:PRO:HD2	2.42	0.44
16:W:353:ASP:O	16:W:357:ARG:NH1	2.51	0.44
16:W:442:THR:O	16:W:446:ILE:HG12	2.18	0.44
18:Y:243:GLY:O	18:Y:247:LEU:HD12	2.17	0.44
22:c:26:ASP:OD1	22:c:201:TYR:OH	2.23	0.44
22:c:220:LEU:HD23	22:c:221:HIS:ND1	2.32	0.44
23:d:284:PHE:HB3	23:d:314:ASN:ND2	2.33	0.44
24:e:50:ASP:N	24:e:50:ASP:OD1	2.50	0.44
1:A:75:PRO:HA	1:A:78:TRP:CZ2	2.53	0.44
1:A:163:MET:HE2	1:A:163:MET:C	2.42	0.44
3:C:32:GLN:HA	3:C:35:VAL:HG12	1.99	0.44
3:C:277:LEU:HD22	3:C:310:ARG:HD3	2.00	0.44
3:C:297:ARG:O	3:C:300:ILE:HG12	2.18	0.44
3:C:406:LYS:HE2	3:C:406:LYS:HB2	1.84	0.44
4:D:64:GLU:HA	14:U:607:VAL:HG21	2.00	0.44
4:D:303:VAL:HG12	4:D:305:VAL:HG13	1.99	0.44
4:D:387:VAL:HG13	5:E:158:LEU:HD13	2.00	0.44
5:E:60:VAL:HA	5:E:71:VAL:HA	2.00	0.44
6:F:92:ASN:HA	6:F:149:ASP:O	2.18	0.44
13:M:15:SER:OG	13:M:19:ARG:O	2.36	0.44
14:U:159:ARG:HB3	14:U:162:VAL:HG12	1.99	0.44
14:U:654:MET:HE1	14:U:689:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:482:PHE:CD2	18:Y:377:LEU:HD12	2.53	0.44
16:W:97:LEU:HD23	16:W:97:LEU:HA	1.89	0.44
16:W:284:SER:OG	16:W:288:HIS:NE2	2.50	0.44
17:X:245:PRO:O	17:X:248:ILE:HG22	2.18	0.44
17:X:335:LEU:O	17:X:339:ILE:HG12	2.18	0.44
21:b:18:ASN:HB3	21:b:25:ARG:HD3	2.00	0.44
21:b:64:LEU:H	21:b:64:LEU:HD22	1.82	0.44
22:c:179:SER:OG	22:c:180:ASN:N	2.50	0.44
22:c:193:ILE:HG13	22:c:194:HIS:CD2	2.52	0.44
1:A:250:VAL:HG13	28:v:19:UNK:CB	2.48	0.44
3:C:25:LEU:HD22	15:V:193:GLN:HB3	1.99	0.44
4:D:173:GLN:HE21	4:D:333:PHE:HA	1.83	0.44
4:D:183:LEU:HB3	4:D:191:TYR:HH	1.82	0.44
4:D:307:VAL:HG12	4:D:309:MET:SD	2.58	0.44
4:D:402:ALA:O	4:D:406:VAL:HG22	2.17	0.44
6:F:87:PRO:HD2	6:F:155:LYS:HD2	1.99	0.44
6:F:417:HIS:O	6:F:420:TYR:N	2.50	0.44
9:I:28:ILE:HD13	9:I:133:SER:HB3	2.00	0.44
10:J:20:GLU:O	10:J:24:GLU:HG2	2.18	0.44
14:U:137:MET:HE2	14:U:137:MET:HA	1.99	0.44
15:V:28:PRO:HB2	15:V:29:PRO:HD3	1.99	0.44
15:V:140:ASP:O	15:V:141:THR:OG1	2.31	0.44
15:V:194:LYS:H	15:V:194:LYS:HE2	1.81	0.44
16:W:432:LEU:CD2	22:c:305:ASP:HB3	2.47	0.44
19:Z:32:GLN:HG3	19:Z:34:ARG:H	1.83	0.44
20:a:191:SER:O	20:a:194:GLN:HG3	2.17	0.44
21:b:157:VAL:HG21	21:b:170:LEU:HB2	2.00	0.44
22:c:304:LEU:O	22:c:308:VAL:HG12	2.17	0.44
23:d:207:GLU:OE2	23:d:207:GLU:N	2.30	0.44
23:d:254:GLU:OE1	23:d:254:GLU:N	2.49	0.44
26:g:103:THR:OG1	26:g:115:LYS:NZ	2.34	0.44
1:A:301:GLU:C	1:A:301:GLU:OE1	2.60	0.44
2:B:343:ARG:O	2:B:347:ILE:N	2.47	0.44
3:C:74:GLY:O	3:C:114:VAL:N	2.51	0.44
4:D:170:MET:SD	29:D:501:ADP:N6	2.91	0.44
6:F:225:MET:O	6:F:225:MET:HG3	2.18	0.44
6:F:251:LEU:HD11	6:F:285:ILE:CD1	2.40	0.44
6:F:388:THR:O	6:F:391:PHE:HB2	2.18	0.44
7:G:12:HIS:HB2	7:G:15:ILE:HD12	2.00	0.44
8:H:148:GLN:HB3	8:H:158:TRP:CD1	2.53	0.44
12:L:196:ARG:NH1	12:L:239:ARG:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:23:VAL:O	13:M:26:ALA:N	2.51	0.44
13:M:38:GLY:C	13:M:39:ILE:HD12	2.43	0.44
14:U:192:GLN:OE1	14:U:192:GLN:N	2.49	0.44
14:U:362:ASN:O	14:U:362:ASN:ND2	2.51	0.44
16:W:66:ILE:O	16:W:70:VAL:HG12	2.17	0.44
20:a:207:GLY:O	20:a:271:LYS:NZ	2.36	0.44
20:a:321:LYS:O	20:a:334:THR:OG1	2.30	0.44
22:c:264:LYS:HE2	22:c:267:PRO:HG3	2.00	0.44
25:f:247:ALA:O	25:f:250:ARG:HG2	2.17	0.44
25:f:776:LEU:HB3	25:f:825:MET:HE2	2.00	0.44
1:A:95:VAL:O	1:A:116:LYS:NZ	2.50	0.43
1:A:402:LYS:O	2:B:214:MET:HE1	2.18	0.43
2:B:246:THR:HG21	2:B:277:HIS:CD2	2.52	0.43
4:D:206:GLY:O	4:D:312:ASN:HA	2.18	0.43
4:D:283:ARG:CB	4:D:287:ARG:HH12	2.31	0.43
5:E:101:ASP:HB2	5:E:108:MET:HE1	2.00	0.43
5:E:268:ASP:HB3	5:E:271:HIS:ND1	2.33	0.43
6:F:421:MET:HE2	6:F:421:MET:N	2.30	0.43
11:K:186:HIS:NE2	11:K:189:MET:HG2	2.33	0.43
14:U:190:ASN:HD22	14:U:192:GLN:HE22	1.66	0.43
14:U:411:ILE:HD13	14:U:411:ILE:HA	1.88	0.43
14:U:548:LEU:O	14:U:552:ILE:HG12	2.18	0.43
14:U:789:ILE:O	14:U:912:ILE:N	2.36	0.43
15:V:383:GLY:O	15:V:387:GLN:HG3	2.17	0.43
17:X:377:ILE:HD11	18:Y:311:TYR:C	2.43	0.43
18:Y:79:ASP:HA	18:Y:82:LYS:HE3	1.99	0.43
20:a:35:HIS:H	21:b:18:ASN:HA	1.82	0.43
20:a:280:MET:HE3	20:a:280:MET:HB2	1.93	0.43
22:c:54:MET:HG2	22:c:82:VAL:HG13	2.00	0.43
27:u:182:PHE:HD1	27:u:263:PHE:HB2	1.83	0.43
27:u:252:GLN:CD	27:u:252:GLN:H	2.25	0.43
1:A:201:PHE:CE1	6:F:405:MET:HE1	2.52	0.43
2:B:363:ARG:HH12	2:B:366:GLN:HB2	1.83	0.43
7:G:175:SER:O	7:G:179:LEU:HD22	2.17	0.43
10:J:170:GLU:O	10:J:174:LYS:N	2.50	0.43
12:L:9:ASP:C	12:L:9:ASP:OD2	2.61	0.43
13:M:87:LEU:HD23	13:M:135:PHE:HE2	1.83	0.43
14:U:173:VAL:HG13	14:U:175:GLY:N	2.33	0.43
14:U:340:GLN:HE22	14:U:344:ARG:HE	1.66	0.43
14:U:399:TRP:HB2	22:c:176:GLN:OE1	2.17	0.43
15:V:57:ALA:O	15:V:62:HIS:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:a:247:ARG:HH22	20:a:265:GLU:CD	2.26	0.43
21:b:22:LEU:O	21:b:24:THR:N	2.51	0.43
26:g:142:LEU:O	26:g:145:GLN:HG2	2.18	0.43
1:A:109:PRO:HG2	1:A:111:TYR:CE2	2.53	0.43
1:A:137:GLY:C	1:A:139:ARG:H	2.26	0.43
1:A:212:VAL:HB	1:A:318:LEU:HD23	2.00	0.43
2:B:385:MET:HE2	2:B:386:ALA:N	2.32	0.43
4:D:228:ILE:HD13	4:D:253:LEU:HD22	2.00	0.43
8:H:196:LYS:HA	8:H:203:MET:HE1	1.99	0.43
9:I:45:LEU:HD12	9:I:45:LEU:HA	1.83	0.43
12:L:137:TYR:CE2	12:L:142:PRO:HG3	2.54	0.43
14:U:738:ASP:OD2	14:U:742:HIS:NE2	2.49	0.43
14:U:771:PHE:HD1	22:c:181:LEU:HD11	1.83	0.43
15:V:182:LYS:O	15:V:182:LYS:HD3	2.18	0.43
15:V:278:GLU:HA	15:V:285:TRP:CZ2	2.53	0.43
15:V:333:ILE:HD11	15:V:360:TYR:HD1	1.82	0.43
16:W:78:LYS:HA	16:W:80:TRP:CH2	2.53	0.43
16:W:359:VAL:HB	16:W:382:LEU:HD13	2.00	0.43
18:Y:115:GLY:O	18:Y:151:TYR:OH	2.37	0.43
20:a:4:VAL:HB	20:a:5:PRO:HD3	2.00	0.43
20:a:69:HIS:O	20:a:70:ARG:HD2	2.17	0.43
20:a:146:PRO:HA	20:a:152:HIS:CE1	2.53	0.43
22:c:70:ILE:HG13	22:c:104:ARG:NH2	2.33	0.43
25:f:103:TYR:OH	25:f:142:TYR:OH	2.18	0.43
25:f:447:ALA:HA	25:f:450:ILE:HG22	1.99	0.43
25:f:479:LEU:HD23	25:f:479:LEU:HA	1.79	0.43
25:f:505:MET:SD	25:f:505:MET:N	2.92	0.43
1:A:306:LEU:HD21	1:A:317:VAL:HG21	2.01	0.43
4:D:98:GLN:N	4:D:98:GLN:OE1	2.36	0.43
8:H:188:ILE:O	8:H:192:ILE:HG12	2.19	0.43
9:I:35:LEU:HD13	9:I:196:VAL:HG11	1.99	0.43
9:I:170:ALA:O	9:I:173:SER:OG	2.25	0.43
14:U:233:LEU:O	14:U:237:VAL:HG12	2.18	0.43
15:V:419:LEU:HD13	15:V:456:GLY:HA2	1.99	0.43
16:W:47:LEU:O	16:W:66:ILE:HD11	2.18	0.43
21:b:44:ASN:ND2	21:b:47:ASN:OD1	2.42	0.43
23:d:223:ASN:HD21	23:d:226:ILE:HB	1.83	0.43
25:f:304:PHE:HB3	25:f:456:ARG:CZ	2.47	0.43
25:f:470:VAL:HG23	25:f:471:LEU:CD2	2.49	0.43
25:f:611:GLN:O	25:f:615:ILE:HG12	2.18	0.43
25:f:654:VAL:HG23	25:f:686:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:825:MET:HE3	25:f:826:GLN:N	2.33	0.43
26:g:127:ILE:HA	26:g:156:LEU:O	2.19	0.43
26:g:131:ILE:HD12	26:g:131:ILE:HA	1.84	0.43
27:u:233:LEU:HD23	27:u:233:LEU:HA	1.87	0.43
1:A:122:VAL:O	6:F:87:PRO:HA	2.19	0.43
2:B:185:ALA:CB	25:f:850:VAL:HG11	2.49	0.43
2:B:251:VAL:HG23	2:B:286:GLU:OE2	2.18	0.43
3:C:52:LEU:HA	3:C:55:LYS:HZ3	1.82	0.43
3:C:78:ARG:O	3:C:86:LEU:HB3	2.18	0.43
3:C:368:MET:HE3	4:D:328:ASP:OD2	2.19	0.43
4:D:286:GLN:O	4:D:290:LEU:HG	2.19	0.43
6:F:391:PHE:HA	6:F:395:GLN:OE1	2.18	0.43
8:H:119:GLN:O	8:H:122:THR:OG1	2.35	0.43
11:K:78:MET:HB2	11:K:140:ALA:O	2.18	0.43
11:K:186:HIS:CD2	11:K:189:MET:HG2	2.53	0.43
14:U:742:HIS:O	14:U:883:ARG:NE	2.47	0.43
16:W:26:GLN:C	16:W:29:PRO:HD2	2.44	0.43
16:W:44:ILE:HD13	16:W:82:LEU:HD21	2.01	0.43
16:W:80:TRP:CD1	16:W:120:ILE:HD12	2.53	0.43
17:X:417:LYS:C	17:X:419:LYS:H	2.26	0.43
21:b:36:VAL:O	21:b:40:LYS:HG2	2.18	0.43
22:c:196:LEU:O	22:c:201:TYR:HA	2.18	0.43
23:d:208:PHE:CE2	23:d:233:GLU:HG3	2.53	0.43
23:d:269:ASP:OD2	23:d:306:ARG:NH1	2.50	0.43
25:f:332:ALA:O	25:f:335:ARG:HG2	2.18	0.43
25:f:838:ARG:HE	25:f:839:PRO:HD2	1.83	0.43
26:g:105:LEU:HD12	26:g:147:VAL:HG13	2.00	0.43
1:A:101:ILE:HG12	1:A:111:TYR:CD1	2.53	0.43
1:A:214:LEU:N	1:A:319:MET:O	2.45	0.43
1:A:407:LYS:O	1:A:411:GLU:HG3	2.18	0.43
3:C:113:ARG:HH12	4:D:102:ILE:HD13	1.84	0.43
3:C:147:THR:HG23	3:C:206:HIS:NE2	2.34	0.43
3:C:232:ARG:O	3:C:236:VAL:HG23	2.18	0.43
4:D:204:MET:HE2	4:D:204:MET:HA	1.99	0.43
6:F:285:ILE:HG21	6:F:288:LEU:HD13	2.01	0.43
12:L:91:GLU:HA	12:L:94:ASP:OD2	2.18	0.43
14:U:806:CYS:O	14:U:874:ASN:HB2	2.19	0.43
15:V:364:THR:HA	15:V:367:VAL:HG12	2.01	0.43
16:W:40:LEU:HD22	16:W:73:MET:HG3	2.00	0.43
16:W:60:MET:SD	16:W:61:VAL:HG13	2.58	0.43
16:W:92:LYS:HE3	16:W:92:LYS:HB3	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:214:PHE:CD1	16:W:223:LYS:HG3	2.54	0.43
16:W:376:LYS:HG3	16:W:377:ARG:N	2.33	0.43
16:W:422:ASN:OD1	19:Z:252:LYS:NZ	2.29	0.43
16:W:446:ILE:HD12	19:Z:211:TYR:CG	2.54	0.43
17:X:264:PRO:O	17:X:267:VAL:HB	2.17	0.43
18:Y:219:PHE:O	18:Y:223:THR:OG1	2.27	0.43
19:Z:8:LYS:CB	19:Z:47:VAL:HG23	2.49	0.43
19:Z:106:ILE:HG12	19:Z:153:LYS:HG3	2.01	0.43
23:d:251:ILE:HA	23:d:252:PRO:HD3	1.91	0.43
24:e:62:LYS:HE3	24:e:63:HIS:NE2	2.34	0.43
25:f:55:GLU:O	25:f:59:LEU:HD23	2.19	0.43
25:f:482:ILE:HD11	25:f:518:THR:HA	2.01	0.43
26:g:163:GLU:HG2	26:g:164:ASP:N	2.34	0.43
1:A:98:CYS:HB3	1:A:137:GLY:O	2.18	0.43
3:C:276:LEU:O	3:C:280:LEU:HG	2.19	0.43
4:D:138:ALA:O	4:D:140:VAL:HG13	2.19	0.43
5:E:123:SER:HA	5:E:195:PHE:O	2.18	0.43
6:F:97:LEU:HB2	6:F:121:CYS:SG	2.59	0.43
6:F:322:PRO:O	6:F:323:ASN:HB3	2.18	0.43
8:H:113:ARG:O	8:H:117:VAL:HG23	2.18	0.43
12:L:87:PHE:O	12:L:91:GLU:HG2	2.17	0.43
13:M:23:VAL:HG12	13:M:130:PRO:HG3	2.00	0.43
15:V:278:GLU:OE1	15:V:278:GLU:N	2.52	0.43
16:W:308:LEU:O	16:W:311:THR:OG1	2.34	0.43
18:Y:319:MET:HB2	18:Y:330:ILE:CD1	2.48	0.43
20:a:68:GLU:HG3	20:a:69:HIS:H	1.84	0.43
20:a:335:TRP:HD1	20:a:336:VAL:N	2.16	0.43
23:d:148:LEU:HB2	23:d:171:LEU:HD13	2.01	0.43
25:f:404:ASP:O	25:f:407:MET:HG2	2.19	0.43
1:A:48:VAL:HG13	2:B:69:LYS:NZ	2.34	0.43
1:A:52:ILE:HG12	2:B:69:LYS:CE	2.46	0.43
3:C:147:THR:HG22	3:C:149:GLU:OE2	2.18	0.43
3:C:156:LYS:O	3:C:159:LYS:HG2	2.19	0.43
4:D:181:VAL:C	4:D:184:PRO:HD2	2.43	0.43
5:E:61:LEU:HB3	5:E:70:ILE:HB	1.99	0.43
8:H:93:LEU:HD11	8:H:117:VAL:HG21	2.01	0.43
8:H:99:LEU:HD12	8:H:100:VAL:HG23	2.00	0.43
14:U:74:PHE:O	14:U:78:LEU:HG	2.19	0.43
14:U:407:SER:O	14:U:410:VAL:HG12	2.19	0.43
14:U:459:ASP:HA	14:U:462:LEU:HB2	2.01	0.43
14:U:474:ARG:O	14:U:478:SER:OG	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:494:TYR:OH	14:U:528:ALA:HA	2.18	0.43
14:U:689:ILE:HD11	14:U:729:GLY:HA2	2.00	0.43
15:V:392:TYR:C	15:V:394:LEU:N	2.76	0.43
20:a:323:SER:O	20:a:332:HIS:N	2.49	0.43
23:d:116:LEU:HD23	23:d:119:LEU:HD12	2.01	0.43
3:C:268:GLU:OE1	3:C:271:ARG:NH1	2.39	0.43
4:D:83:GLN:O	4:D:87:LEU:HD11	2.18	0.43
5:E:26:LEU:O	5:E:30:ARG:HG3	2.19	0.43
5:E:320:ILE:HG23	5:E:322:LYS:HG3	2.01	0.43
11:K:199:LEU:HD21	11:K:217:LEU:HD11	2.00	0.43
14:U:222:PHE:CE1	14:U:754:HIS:HB2	2.52	0.43
14:U:247:GLN:OE1	14:U:913:ILE:HG23	2.18	0.43
14:U:324:LYS:HA	14:U:327:LYS:HG3	2.00	0.43
14:U:475:HIS:HB2	14:U:507:VAL:HG12	2.00	0.43
16:W:287:VAL:HG13	16:W:306:LEU:HD11	1.99	0.43
17:X:95:LEU:O	17:X:99:MET:HE2	2.18	0.43
19:Z:171:GLY:O	19:Z:175:LEU:HG	2.19	0.43
19:Z:235:ASN:C	19:Z:235:ASN:OD1	2.62	0.43
20:a:35:HIS:O	20:a:39:LEU:HG	2.19	0.43
20:a:278:MET:O	20:a:282:PHE:HB2	2.19	0.43
22:c:303:MET:SD	23:d:332:SER:HA	2.59	0.43
25:f:675:PHE:CE2	25:f:697:ILE:HD11	2.54	0.43
25:f:695:ALA:HB1	25:f:731:MET:CG	2.49	0.43
1:A:306:LEU:HD23	1:A:306:LEU:HA	1.87	0.43
1:A:386:ARG:NH1	2:B:345:GLY:O	2.46	0.43
6:F:53:LYS:HE3	21:b:27:GLN:HG3	2.00	0.43
7:G:24:GLN:HA	7:G:27:TYR:HD2	1.84	0.43
8:H:50:LYS:HE3	8:H:59:GLU:HB3	2.00	0.43
9:I:140:ASP:OD1	9:I:142:HIS:N	2.51	0.43
9:I:198:ASN:OD1	9:I:240:HIS:ND1	2.52	0.43
14:U:86:ASP:C	14:U:88:PHE:N	2.77	0.43
14:U:243:LEU:HD21	14:U:913:ILE:HD12	2.01	0.43
14:U:475:HIS:ND1	14:U:511:ALA:HB2	2.33	0.43
14:U:506:ALA:HA	14:U:544:ILE:HD11	2.01	0.43
15:V:398:LEU:HA	15:V:401:ASN:HD21	1.84	0.43
16:W:279:PHE:HE1	16:W:284:SER:HB2	1.82	0.43
19:Z:200:GLY:O	19:Z:204:LYS:HG2	2.19	0.43
20:a:32:LYS:HG3	21:b:19:GLY:O	2.18	0.43
20:a:311:VAL:O	20:a:315:LEU:HG	2.19	0.43
22:c:214:GLN:C	22:c:216:MET:H	2.25	0.43
25:f:292:LYS:HD3	25:f:837:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:LEU:HD23	14:U:832:VAL:HG22	2.01	0.42
4:D:189:GLU:OE2	4:D:189:GLU:N	2.44	0.42
6:F:206:MET:HE1	6:F:280:PRO:HB2	2.00	0.42
7:G:139:ILE:HA	7:G:152:TYR:O	2.18	0.42
11:K:186:HIS:CE1	11:K:189:MET:HG2	2.53	0.42
13:M:135:PHE:HE1	13:M:151:ILE:HB	1.84	0.42
14:U:475:HIS:CG	14:U:511:ALA:HB2	2.54	0.42
14:U:624:PHE:HD1	14:U:760:VAL:HG23	1.84	0.42
14:U:701:ILE:HD13	14:U:811:PHE:CD2	2.54	0.42
14:U:759:SER:HA	14:U:782:ALA:HA	2.00	0.42
15:V:147:PHE:HD1	15:V:150:ARG:HE	1.66	0.42
17:X:315:ASP:OD2	17:X:315:ASP:N	2.32	0.42
17:X:400:ALA:O	17:X:404:ILE:HG22	2.18	0.42
19:Z:89:GLU:H	19:Z:89:GLU:HG3	1.69	0.42
21:b:12:ASN:O	21:b:80:PRO:HA	2.19	0.42
21:b:21:PHE:CZ	21:b:173:VAL:HG11	2.54	0.42
22:c:70:ILE:HG13	22:c:104:ARG:HH21	1.83	0.42
22:c:110:GLY:HA2	22:c:141:VAL:O	2.18	0.42
22:c:256:ASN:O	22:c:259:VAL:HG12	2.19	0.42
25:f:54:ASP:O	25:f:58:MET:HG3	2.19	0.42
27:u:189:GLN:NE2	27:u:257:THR:O	2.38	0.42
1:A:29:ASP:O	1:A:33:LEU:HB2	2.19	0.42
2:B:411:ARG:HD2	2:B:413:LYS:O	2.20	0.42
4:D:283:ARG:HB3	4:D:287:ARG:HH12	1.84	0.42
6:F:437:TYR:OH	11:K:21:LEU:O	2.31	0.42
10:J:33:VAL:HG13	10:J:160:ALA:HB2	2.01	0.42
13:M:215:TRP:CZ2	13:M:219:LEU:HD11	2.53	0.42
14:U:404:ALA:O	14:U:407:SER:HB3	2.19	0.42
14:U:831:ALA:O	14:U:836:THR:HG21	2.19	0.42
15:V:309:MET:HE3	15:V:332:LEU:CA	2.46	0.42
18:Y:91:ALA:HA	18:Y:95:LEU:HD23	2.01	0.42
20:a:363:MET:HE2	20:a:363:MET:HB2	1.67	0.42
21:b:86:PHE:O	21:b:90:ILE:HG22	2.20	0.42
25:f:789:SER:O	25:f:793:VAL:HG23	2.18	0.42
26:g:94:LYS:HD3	26:g:94:LYS:N	2.32	0.42
27:u:157:LEU:HD23	27:u:158:GLU:N	2.34	0.42
1:A:159:PRO:O	1:A:163:MET:HG3	2.19	0.42
2:B:98:LYS:HG2	2:B:98:LYS:H	1.70	0.42
2:B:427:LEU:HA	2:B:430:LYS:HB2	2.00	0.42
4:D:163:MET:SD	4:D:163:MET:N	2.93	0.42
4:D:319:PRO:HA	4:D:322:LEU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:101:ASP:O	5:E:105:LEU:HA	2.19	0.42
6:F:235:LEU:HD22	31:F:501:ATP:H2'	2.01	0.42
8:H:23:GLU:CD	8:H:23:GLU:H	2.27	0.42
8:H:185:GLU:HA	8:H:188:ILE:HD12	2.00	0.42
11:K:77:ALA:C	11:K:78:MET:HE3	2.44	0.42
13:M:202:ASP:OD1	13:M:202:ASP:N	2.51	0.42
14:U:529:ILE:O	14:U:533:VAL:HG22	2.20	0.42
15:V:153:LYS:HD2	15:V:153:LYS:HA	1.82	0.42
19:Z:275:LEU:O	19:Z:279:LYS:HG3	2.19	0.42
21:b:139:ASP:O	21:b:140:ILE:HD13	2.19	0.42
23:d:332:SER:OG	23:d:333:THR:N	2.52	0.42
26:g:142:LEU:O	26:g:147:VAL:HG12	2.19	0.42
2:B:52:VAL:CG1	2:B:54:PRO:HD2	2.49	0.42
3:C:157:GLN:OE1	3:C:157:GLN:N	2.49	0.42
4:D:82:ILE:HD12	4:D:82:ILE:HA	1.89	0.42
4:D:180:ALA:HB1	4:D:202:VAL:HG11	2.02	0.42
5:E:72:LYS:HE2	5:E:78:ARG:HG2	2.00	0.42
6:F:86:LEU:HD23	6:F:88:TYR:CD2	2.55	0.42
6:F:172:VAL:HA	6:F:175:MET:HG3	2.01	0.42
9:I:115:CYS:HB3	9:I:154:GLY:O	2.20	0.42
9:I:159:TRP:CZ2	10:J:54:GLN:HB2	2.54	0.42
12:L:134:ILE:O	12:L:144:ILE:HA	2.19	0.42
13:M:188:ASP:O	13:M:192:GLU:HG2	2.19	0.42
14:U:4:SER:HA	14:U:34:PHE:CE2	2.55	0.42
14:U:163:PHE:O	14:U:166:THR:OG1	2.38	0.42
14:U:481:LEU:HD22	14:U:497:LEU:HD21	2.02	0.42
14:U:597:LYS:HE2	14:U:597:LYS:HB2	1.92	0.42
14:U:696:ILE:HD12	14:U:745:THR:HA	2.00	0.42
16:W:196:VAL:HG23	16:W:198:ASP:HB2	2.01	0.42
16:W:276:LEU:HD11	16:W:350:ARG:O	2.20	0.42
17:X:74:ARG:HD3	17:X:116:TRP:CD1	2.53	0.42
17:X:200:ILE:HG22	17:X:201:TYR:N	2.34	0.42
17:X:256:LEU:HD12	17:X:319:ILE:HD13	2.02	0.42
17:X:328:ASP:O	17:X:332:GLU:HG3	2.20	0.42
19:Z:25:ARG:NE	22:c:104:ARG:HH11	2.18	0.42
19:Z:225:GLN:HA	19:Z:228:TYR:CE1	2.55	0.42
25:f:128:VAL:HA	25:f:158:TYR:HE1	1.84	0.42
25:f:208:LEU:HD21	25:f:216:MET:HE3	2.00	0.42
25:f:450:ILE:HD11	25:f:822:VAL:HG21	2.00	0.42
25:f:462:ALA:O	25:f:466:LEU:HG	2.19	0.42
27:u:171:PHE:HE2	27:u:244:VAL:HG23	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:ASN:OD1	2:B:315:GLN:N	2.52	0.42
3:C:113:ARG:NH1	4:D:102:ILE:HD13	2.34	0.42
3:C:130:LYS:HD3	3:C:132:ASP:OD1	2.19	0.42
7:G:144:ASP:OD1	7:G:144:ASP:N	2.51	0.42
12:L:38:LEU:HA	12:L:157:ARG:O	2.19	0.42
12:L:159:MET:HB2	12:L:159:MET:HE2	1.82	0.42
15:V:495:ARG:HD3	15:V:497:PRO:HD2	2.00	0.42
20:a:245:VAL:HG21	20:a:300:ALA:HA	2.00	0.42
20:a:311:VAL:HG11	20:a:324:ILE:HG12	2.02	0.42
23:d:197:LEU:HD13	23:d:256:TYR:HD2	1.84	0.42
25:f:293:GLN:OE1	25:f:899:ILE:N	2.49	0.42
27:u:144:HIS:HB3	27:u:156:PHE:O	2.20	0.42
1:A:333:ARG:HD2	6:F:230:GLY:HA2	2.02	0.42
2:B:266:LEU:HA	2:B:269:GLU:OE2	2.19	0.42
2:B:311:GLU:C	2:B:311:GLU:OE1	2.62	0.42
4:D:229:ARG:HH12	5:E:291:ARG:NH1	2.17	0.42
6:F:124:ILE:HD11	6:F:160:ILE:HD11	2.00	0.42
6:F:235:LEU:HD12	6:F:235:LEU:O	2.20	0.42
6:F:236:LEU:HD12	6:F:236:LEU:O	2.19	0.42
8:H:74:LEU:HD12	8:H:75:VAL:N	2.34	0.42
14:U:96:TYR:CZ	14:U:100:ILE:HD13	2.55	0.42
14:U:554:LEU:HD23	14:U:588:MET:HE1	2.02	0.42
14:U:727:LYS:O	14:U:731:ILE:HG22	2.19	0.42
15:V:81:GLN:N	15:V:86:VAL:HB	2.35	0.42
15:V:176:MET:O	15:V:180:ARG:NE	2.53	0.42
15:V:298:ILE:O	23:d:209:HIS:ND1	2.53	0.42
17:X:140:THR:O	17:X:140:THR:HG22	2.19	0.42
19:Z:40:LEU:HD12	19:Z:52:ASN:HB3	2.01	0.42
19:Z:169:GLU:OE1	19:Z:170:VAL:N	2.53	0.42
20:a:323:SER:N	20:a:332:HIS:O	2.33	0.42
22:c:281:LYS:HB3	22:c:282:ARG:CZ	2.48	0.42
23:d:94:MET:HE3	23:d:94:MET:HB2	1.88	0.42
25:f:398:TRP:O	25:f:398:TRP:HD1	2.02	0.42
25:f:654:VAL:HG22	25:f:678:LEU:HD21	2.01	0.42
26:g:145:GLN:HE21	26:g:145:GLN:HB3	1.61	0.42
27:u:126:LEU:HD22	27:u:175:VAL:HG21	2.01	0.42
1:A:79:ASP:CG	2:B:98:LYS:HE3	2.44	0.42
3:C:158:ILE:HA	3:C:161:ILE:HG22	2.01	0.42
3:C:381:GLU:HG3	3:C:385:MET:CE	2.50	0.42
3:C:403:LYS:C	3:C:405:TRP:H	2.26	0.42
4:D:198:PRO:O	4:D:200:ARG:NH1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:110:TYR:HD1	5:E:110:TYR:H	1.68	0.42
5:E:374:VAL:O	5:E:378:LYS:HG2	2.19	0.42
6:F:401:VAL:O	6:F:405:MET:HG2	2.20	0.42
9:I:216:LEU:HD12	9:I:225:ILE:HD11	2.02	0.42
11:K:31:ILE:HD11	11:K:158:PRO:CD	2.49	0.42
11:K:211:ASN:H	11:K:215:ILE:HD12	1.85	0.42
14:U:19:LEU:HD12	14:U:22:PHE:HD1	1.84	0.42
14:U:479:LEU:HD23	14:U:479:LEU:HA	1.90	0.42
15:V:303:SER:OG	15:V:304:GLU:N	2.52	0.42
16:W:115:ILE:HD13	16:W:115:ILE:HA	1.93	0.42
17:X:251:LEU:HD12	17:X:251:LEU:O	2.20	0.42
18:Y:16:ASP:HB3	18:Y:19:ILE:HG12	2.01	0.42
18:Y:24:PHE:O	18:Y:27:SER:OG	2.32	0.42
18:Y:217:LYS:O	18:Y:220:VAL:HG12	2.20	0.42
18:Y:282:MET:SD	18:Y:288:PHE:HB3	2.59	0.42
20:a:34:TRP:O	20:a:38:THR:HG23	2.18	0.42
20:a:290:GLN:HE21	20:a:330:ARG:CZ	2.32	0.42
22:c:122:LEU:HB3	22:c:127:ILE:HD13	2.02	0.42
23:d:153:GLN:O	23:d:157:LEU:HG	2.19	0.42
24:e:63:HIS:CD2	24:e:63:HIS:N	2.84	0.42
25:f:48:GLU:O	25:f:52:LEU:HD23	2.20	0.42
25:f:329:ASN:O	25:f:332:ALA:HB3	2.19	0.42
25:f:695:ALA:HB1	25:f:731:MET:HG3	2.01	0.42
1:A:84:LYS:HB3	2:B:102:LEU:HD21	2.01	0.42
2:B:405:MET:HG2	2:B:408:ARG:HE	1.84	0.42
3:C:379:THR:N	3:C:382:ASP:OD2	2.48	0.42
8:H:39:LYS:N	8:H:159:LYS:O	2.49	0.42
9:I:79:ILE:HB	9:I:82:ASP:HB2	2.02	0.42
10:J:148:ASP:HB3	10:J:152:THR:OG1	2.20	0.42
13:M:47:PHE:HE1	13:M:136:MET:HE2	1.85	0.42
14:U:457:ILE:HG23	14:U:461:LEU:HD23	2.01	0.42
14:U:550:VAL:HG21	14:U:768:GLN:HG3	2.01	0.42
14:U:810:THR:HG22	14:U:874:ASN:HA	2.00	0.42
15:V:65:ARG:NH1	15:V:73:GLU:OE2	2.51	0.42
17:X:50:ILE:HD12	17:X:76:PHE:HE2	1.84	0.42
17:X:58:ALA:HB3	17:X:95:LEU:HD12	2.02	0.42
19:Z:253:THR:O	19:Z:257:MET:HG2	2.20	0.42
22:c:241:ASN:ND2	22:c:295:ASN:OD1	2.51	0.42
23:d:163:SER:HA	23:d:166:ARG:HG2	2.00	0.42
23:d:303:ALA:O	23:d:307:GLY:N	2.53	0.42
23:d:311:GLY:N	23:d:315:TYR:O	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:602:GLY:N	25:f:659:LEU:O	2.40	0.42
1:A:124:ASP:HB3	6:F:86:LEU:CD1	2.50	0.42
1:A:403:ILE:HD13	1:A:403:ILE:HA	1.93	0.42
2:B:272:ARG:O	2:B:275:GLU:HG3	2.18	0.42
2:B:334:ILE:O	2:B:337:LEU:HB2	2.20	0.42
3:C:66:LEU:HD12	3:C:66:LEU:HA	1.84	0.42
3:C:372:ARG:HH12	4:D:329:ARG:HE	1.68	0.42
4:D:176:GLU:HB3	4:D:331:ILE:HG12	2.01	0.42
4:D:274:ARG:HD2	4:D:286:GLN:HG3	2.02	0.42
4:D:282:ASP:O	4:D:285:VAL:HG12	2.19	0.42
6:F:61:ARG:NH1	21:b:72:LEU:O	2.52	0.42
7:G:189:TRP:HA	7:G:193:GLN:OE1	2.20	0.42
8:H:29:VAL:C	8:H:31:GLY:H	2.28	0.42
10:J:156:TRP:CE2	11:K:59:MET:SD	3.13	0.42
14:U:342:LEU:HD12	14:U:380:THR:HG22	2.02	0.42
15:V:419:LEU:HD21	15:V:451:ILE:HD11	2.02	0.42
18:Y:74:LYS:O	18:Y:78:GLU:HG2	2.20	0.42
25:f:110:TYR:HA	25:f:113:MET:HE2	2.01	0.42
25:f:208:LEU:HD23	25:f:208:LEU:HA	1.75	0.42
25:f:339:ILE:H	25:f:339:ILE:HD12	1.84	0.42
25:f:711:SER:HA	25:f:729:MET:HE1	2.00	0.42
25:f:797:LEU:O	25:f:801:VAL:HG12	2.19	0.42
27:u:119:ILE:HG13	27:u:120:PRO:O	2.20	0.42
27:u:127:MET:HB3	27:u:128:PRO:HD3	2.01	0.42
27:u:181:LYS:HD3	27:u:262:TYR:HE2	1.85	0.42
2:B:193:GLN:H	2:B:193:GLN:CD	2.28	0.42
3:C:329:LEU:HD12	3:C:329:LEU:HA	1.94	0.42
5:E:116:ASP:OD2	5:E:213:ARG:NH1	2.48	0.42
10:J:155:ALA:N	11:K:63:SER:OG	2.52	0.42
10:J:156:TRP:CZ3	11:K:58:LEU:HB2	2.55	0.42
12:L:71:GLY:HA3	12:L:221:PHE:CE2	2.55	0.42
14:U:244:MET:SD	14:U:903:PHE:HE1	2.43	0.42
14:U:588:MET:SD	14:U:764:LEU:HD23	2.60	0.42
14:U:892:LEU:HD12	14:U:893:THR:N	2.35	0.42
15:V:476:PHE:O	15:V:480:ILE:HG12	2.19	0.42
17:X:114:ILE:HD12	17:X:126:ARG:HG2	2.01	0.42
25:f:267:ARG:HD2	25:f:783:SER:OG	2.20	0.42
25:f:327:ASN:ND2	25:f:421:ASP:HB3	2.35	0.42
25:f:398:TRP:CD1	25:f:402:ASN:HD21	2.38	0.42
25:f:722:SER:O	25:f:726:ILE:HG12	2.20	0.42
26:g:115:LYS:O	26:g:119:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HD12	1:A:33:LEU:HA	1.92	0.41
1:A:70:THR:HG22	1:A:71:GLY:H	1.85	0.41
3:C:293:MET:HE2	3:C:293:MET:HB3	1.86	0.41
4:D:66:LYS:HA	4:D:69:LYS:NZ	2.35	0.41
4:D:349:THR:HA	4:D:352:MET:HB2	2.00	0.41
6:F:172:VAL:HA	6:F:175:MET:SD	2.60	0.41
10:J:103:THR:HG23	10:J:106:TYR:H	1.85	0.41
11:K:117:SER:HB3	11:K:160:GLY:O	2.20	0.41
12:L:66:VAL:HG21	12:L:89:ARG:HG3	2.01	0.41
12:L:159:MET:H	12:L:172:LEU:HD13	1.84	0.41
14:U:461:LEU:HD12	14:U:481:LEU:HB2	2.01	0.41
15:V:266:GLN:HA	15:V:268:GLU:OE2	2.19	0.41
16:W:233:LEU:O	16:W:237:GLU:HG2	2.20	0.41
16:W:446:ILE:HG12	19:Z:226:ILE:HD11	2.01	0.41
17:X:347:ILE:O	17:X:350:ILE:HG12	2.20	0.41
18:Y:202:LEU:O	18:Y:205:VAL:HG12	2.20	0.41
19:Z:39:LEU:HB2	19:Z:92:VAL:O	2.20	0.41
20:a:133:GLU:N	20:a:133:GLU:OE2	2.51	0.41
20:a:180:LEU:HD21	20:a:221:VAL:HG21	2.02	0.41
21:b:14:GLU:OE1	21:b:17:ARG:NH2	2.53	0.41
22:c:133:PHE:O	22:c:136:LEU:HB3	2.20	0.41
22:c:232:GLN:CG	22:c:233:ASP:H	2.33	0.41
23:d:152:ALA:HB1	23:d:191:LEU:HD13	2.02	0.41
1:A:55:LEU:O	1:A:59:ILE:HG12	2.20	0.41
1:A:112:ILE:HG22	1:A:120:LYS:HE3	2.02	0.41
2:B:366:GLN:O	2:B:370:SER:HB3	2.20	0.41
2:B:426:VAL:O	2:B:430:LYS:N	2.48	0.41
4:D:107:THR:HG22	5:E:77:PRO:HG3	2.02	0.41
4:D:200:ARG:NH2	4:D:328:ASP:OD2	2.54	0.41
6:F:254:PRO:HA	6:F:257:VAL:HG23	2.02	0.41
10:J:10:PHE:CE1	11:K:135:ARG:HD2	2.55	0.41
10:J:168:VAL:HA	10:J:171:PHE:HB3	2.01	0.41
14:U:399:TRP:O	14:U:402:PHE:HB3	2.21	0.41
14:U:656:LEU:HD12	14:U:656:LEU:HA	1.89	0.41
14:U:791:LEU:HA	14:U:796:LYS:O	2.20	0.41
15:V:438:VAL:O	15:V:442:ILE:HG13	2.20	0.41
16:W:144:ARG:O	16:W:148:THR:HG23	2.20	0.41
19:Z:187:LEU:O	19:Z:191:ILE:HG12	2.20	0.41
21:b:184:ILE:HA	21:b:188:ILE:HG22	2.00	0.41
25:f:557:TRP:HZ2	25:f:809:ILE:HD13	1.86	0.41
1:A:93:LEU:O	2:B:132:TYR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASP:HB3	1:A:336:ARG:CG	2.51	0.41
2:B:178:LYS:O	2:B:181:GLN:NE2	2.39	0.41
4:D:268:ASP:OD1	4:D:268:ASP:N	2.53	0.41
5:E:97:ARG:HH12	6:F:95:GLU:CD	2.26	0.41
5:E:122:MET:HE2	5:E:198:VAL:HG23	2.01	0.41
5:E:291:ARG:HG2	5:E:294:ARG:HD2	2.02	0.41
6:F:389:ASP:O	6:F:390:ASP:HB3	2.20	0.41
7:G:27:TYR:HB3	13:M:14:PHE:HB3	2.01	0.41
7:G:125:TYR:HE1	7:G:131:MET:SD	2.44	0.41
7:G:180:GLU:O	7:G:184:LYS:HB2	2.20	0.41
9:I:9:THR:HG21	9:I:129:PRO:HD3	2.02	0.41
12:L:105:VAL:HG11	12:L:143:HIS:HB2	2.01	0.41
13:M:196:ILE:O	13:M:199:ILE:HG22	2.20	0.41
14:U:249:CYS:SG	14:U:328:ILE:HG13	2.61	0.41
15:V:271:VAL:HG22	15:V:272:SER:N	2.35	0.41
15:V:354:LYS:HG3	15:V:354:LYS:HZ3	1.66	0.41
16:W:17:GLU:HG2	16:W:58:SER:HB2	2.02	0.41
18:Y:84:LEU:HB3	18:Y:107:LYS:CG	2.49	0.41
19:Z:17:LEU:HD23	19:Z:17:LEU:HA	1.80	0.41
19:Z:58:PHE:HA	19:Z:69:PHE:O	2.19	0.41
19:Z:96:HIS:HD2	19:Z:98:GLY:H	1.68	0.41
19:Z:153:LYS:HA	19:Z:153:LYS:HD3	1.91	0.41
21:b:20:ASP:OD1	21:b:25:ARG:HD2	2.21	0.41
21:b:21:PHE:N	21:b:21:PHE:CD1	2.88	0.41
25:f:727:PHE:CD1	25:f:727:PHE:C	2.97	0.41
2:B:102:LEU:HD23	2:B:102:LEU:HA	1.81	0.41
3:C:297:ARG:NH1	3:C:299:ASP:OD2	2.46	0.41
5:E:219:PHE:CD2	5:E:219:PHE:N	2.88	0.41
5:E:223:ARG:HG2	5:E:271:HIS:CD2	2.55	0.41
10:J:40:ILE:HA	10:J:212:ARG:HA	2.03	0.41
10:J:183:THR:O	10:J:186:LEU:N	2.32	0.41
13:M:24:GLU:O	13:M:28:LYS:HG2	2.20	0.41
16:W:149:LEU:HD23	16:W:165:ILE:HG21	2.03	0.41
16:W:432:LEU:O	16:W:436:MET:HG3	2.19	0.41
20:a:307:VAL:O	20:a:311:VAL:HG12	2.21	0.41
20:a:325:ASP:HB3	20:a:330:ARG:O	2.20	0.41
20:a:325:ASP:OD1	20:a:326:GLU:N	2.53	0.41
20:a:349:MET:HA	20:a:352:ARG:HG2	2.01	0.41
21:b:131:LEU:HD12	21:b:136:VAL:HG21	2.03	0.41
23:d:114:GLU:HB3	23:d:118:ARG:NH2	2.35	0.41
25:f:367:SER:HB3	25:f:370:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:376:PHE:CE1	25:f:818:LEU:HD12	2.55	0.41
1:A:116:LYS:N	1:A:116:LYS:HD3	2.36	0.41
2:B:52:VAL:HG12	2:B:54:PRO:HD2	2.03	0.41
3:C:362:VAL:HG23	3:C:390:VAL:HG21	2.02	0.41
4:D:60:TYR:HB2	14:U:603:LEU:HD23	2.02	0.41
4:D:80:LYS:O	4:D:83:GLN:NE2	2.54	0.41
4:D:190:LEU:O	4:D:194:ILE:HG13	2.21	0.41
5:E:140:GLU:HA	5:E:143:ARG:NH1	2.35	0.41
5:E:140:GLU:OE1	5:E:143:ARG:NH2	2.42	0.41
9:I:61:PHE:CE1	9:I:229:LYS:HA	2.55	0.41
13:M:61:GLY:HA2	13:M:64:LYS:HD3	2.01	0.41
13:M:187:ARG:NE	13:M:187:ARG:O	2.54	0.41
14:U:346:ASN:HD21	14:U:382:SER:HB3	1.86	0.41
14:U:756:HIS:ND1	14:U:758:PRO:HD2	2.35	0.41
15:V:281:ASN:C	15:V:283:ASN:H	2.27	0.41
16:W:82:LEU:HD23	16:W:82:LEU:HA	1.88	0.41
16:W:419:LYS:HE3	16:W:419:LYS:HB3	1.94	0.41
17:X:378:LEU:O	18:Y:312:ARG:N	2.31	0.41
21:b:33:VAL:HA	21:b:36:VAL:HG22	2.03	0.41
22:c:57:MET:CB	22:c:72:VAL:HG22	2.51	0.41
22:c:277:LYS:HB2	22:c:282:ARG:CD	2.50	0.41
25:f:70:LEU:O	25:f:74:ALA:HB3	2.21	0.41
25:f:256:PHE:CE2	25:f:264:GLU:HB3	2.55	0.41
25:f:342:PRO:HG2	25:f:389:LYS:HG2	2.02	0.41
25:f:834:ASP:OD1	25:f:836:GLU:HB3	2.20	0.41
27:u:181:LYS:O	27:u:263:PHE:HA	2.20	0.41
2:B:78:PHE:O	2:B:82:GLN:NE2	2.48	0.41
2:B:222:VAL:HB	2:B:328:ILE:HD12	2.03	0.41
3:C:148:TYR:CD1	3:C:158:ILE:HD11	2.56	0.41
4:D:207:PRO:HD2	4:D:333:PHE:O	2.20	0.41
5:E:180:LYS:N	31:E:402:ATP:O2B	2.53	0.41
5:E:268:ASP:HB3	5:E:271:HIS:CE1	2.55	0.41
6:F:221:LYS:O	6:F:328:VAL:HG12	2.20	0.41
9:I:233:VAL:O	9:I:237:ILE:HG12	2.21	0.41
13:M:67:PHE:HB2	13:M:75:MET:SD	2.60	0.41
13:M:163:CYS:SG	13:M:164:ALA:N	2.94	0.41
14:U:132:GLY:HA2	14:U:135:ASN:HD21	1.85	0.41
14:U:649:ARG:HB3	14:U:683:VAL:HG21	2.03	0.41
14:U:732:LEU:HD13	14:U:732:LEU:HA	1.89	0.41
15:V:417:ILE:HG13	15:V:418:SER:N	2.34	0.41
16:W:75:TYR:OH	16:W:115:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:346:GLU:OE1	16:W:346:GLU:N	2.42	0.41
17:X:335:LEU:HD23	17:X:335:LEU:HA	1.83	0.41
18:Y:121:LEU:HD21	18:Y:156:LEU:HD21	2.01	0.41
19:Z:261:TYR:CD1	19:Z:261:TYR:C	2.98	0.41
19:Z:261:TYR:HD1	19:Z:261:TYR:O	2.03	0.41
25:f:380:PHE:CE1	25:f:821:LEU:HD11	2.54	0.41
26:g:107:ILE:HD12	26:g:111:GLU:OE1	2.20	0.41
1:A:248:LYS:HG2	2:B:259:TYR:CD2	2.56	0.41
1:A:278:ASP:OD2	1:A:323:ARG:NH1	2.54	0.41
3:C:113:ARG:NH2	4:D:94:GLU:OE2	2.48	0.41
3:C:117:ARG:HE	3:C:124:HIS:CE1	2.39	0.41
3:C:243:PRO:HA	3:C:288:ASN:O	2.21	0.41
4:D:57:GLN:NE2	14:U:635:SER:O	2.54	0.41
6:F:406:ILE:HD13	6:F:422:GLU:HB3	2.03	0.41
9:I:35:LEU:HB2	9:I:162:THR:O	2.21	0.41
9:I:53:HIS:CE1	9:I:55:LEU:H	2.38	0.41
11:K:108:THR:HG22	11:K:110:GLU:H	1.86	0.41
13:M:144:ASP:OD1	13:M:144:ASP:N	2.52	0.41
15:V:60:ALA:HB3	15:V:62:HIS:NE2	2.35	0.41
15:V:372:LEU:HB3	15:V:402:VAL:HG11	2.03	0.41
17:X:78:ASN:HD21	17:X:120:GLU:CD	2.27	0.41
19:Z:74:TYR:OH	22:c:102:THR:HB	2.21	0.41
20:a:342:ASP:OD1	20:a:343:LEU:N	2.54	0.41
22:c:303:MET:HE3	22:c:303:MET:HB3	1.59	0.41
1:A:187:LEU:O	1:A:191:VAL:HG22	2.21	0.41
3:C:403:LYS:H	3:C:403:LYS:HG2	1.52	0.41
4:D:278:GLN:NE2	8:H:5:GLY:O	2.53	0.41
4:D:322:LEU:HA	4:D:327:LEU:HD12	2.02	0.41
4:D:332:GLU:HG2	4:D:334:PRO:HD3	2.03	0.41
5:E:22:ILE:HG12	6:F:55:MET:HB3	2.02	0.41
5:E:313:LEU:HD21	5:E:331:ILE:HG21	2.01	0.41
14:U:193:PHE:O	14:U:197:VAL:HG23	2.20	0.41
15:V:69:THR:O	15:V:73:GLU:N	2.53	0.41
15:V:461:LYS:HG3	15:V:462:GLU:H	1.86	0.41
16:W:72:LYS:O	16:W:75:TYR:HB3	2.20	0.41
20:a:240:PHE:CZ	20:a:272:ILE:HG12	2.56	0.41
22:c:32:TYR:HD1	22:c:206:ASN:HB3	1.86	0.41
25:f:103:TYR:O	25:f:106:LEU:N	2.38	0.41
27:u:124:MET:N	27:u:124:MET:SD	2.94	0.41
27:u:225:ILE:H	27:u:225:ILE:HG13	1.52	0.41
1:A:43:ARG:HG2	1:A:44:GLN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:THR:O	25:f:680:ARG:NH2	2.46	0.41
1:A:98:CYS:SG	1:A:99:THR:N	2.94	0.41
1:A:297:ARG:NH2	6:F:306:VAL:HG11	2.36	0.41
1:A:347:ASP:OD1	1:A:347:ASP:N	2.54	0.41
2:B:287:ILE:HG22	2:B:330:ALA:O	2.20	0.41
2:B:346:ARG:HD2	2:B:346:ARG:HA	1.84	0.41
2:B:385:MET:HE1	10:J:201:SER:OG	2.21	0.41
3:C:24:TYR:O	3:C:28:ILE:HG23	2.21	0.41
3:C:36:ASN:HD21	15:V:56:ALA:HB2	1.86	0.41
4:D:49:GLN:HE22	14:U:632:GLN:HE21	1.69	0.41
5:E:219:PHE:N	5:E:219:PHE:HD2	2.19	0.41
5:E:345:ASN:ND2	6:F:345:SER:HB3	2.35	0.41
6:F:70:LYS:HE2	6:F:70:LYS:HB2	1.88	0.41
6:F:314:LEU:HD21	6:F:341:ALA:HB1	2.03	0.41
7:G:98:ALA:C	7:G:102:LYS:HZ2	2.29	0.41
7:G:134:LEU:HD23	7:G:134:LEU:HA	1.88	0.41
8:H:85:VAL:O	8:H:89:ARG:HG2	2.21	0.41
9:I:246:LYS:HA	9:I:249:ARG:HD2	2.03	0.41
10:J:120:GLN:HE22	11:K:135:ARG:HG3	1.86	0.41
12:L:90:GLN:O	12:L:94:ASP:OD2	2.39	0.41
12:L:228:ASP:O	12:L:231:PRO:HD2	2.21	0.41
14:U:86:ASP:C	14:U:88:PHE:H	2.29	0.41
14:U:568:GLU:O	14:U:572:ARG:HG2	2.21	0.41
14:U:616:ARG:HD2	14:U:650:TYR:CD1	2.56	0.41
15:V:96:ARG:HD3	15:V:96:ARG:HA	1.83	0.41
15:V:163:VAL:HG21	15:V:213:TYR:HB3	2.03	0.41
15:V:269:LYS:NZ	15:V:269:LYS:O	2.52	0.41
15:V:343:PRO:O	24:e:43:TRP:HZ2	2.04	0.41
15:V:393:THR:O	15:V:396:ILE:HG22	2.20	0.41
17:X:407:MET:SD	19:Z:266:ILE:HG12	2.60	0.41
18:Y:190:ALA:C	18:Y:291:HIS:HE2	2.29	0.41
18:Y:297:ARG:HG2	18:Y:301:ILE:HD11	2.03	0.41
19:Z:81:MET:CE	22:c:95:MET:HE2	2.50	0.41
19:Z:96:HIS:HD2	19:Z:98:GLY:N	2.18	0.41
19:Z:113:LYS:HA	19:Z:116:CYS:O	2.21	0.41
19:Z:176:LEU:O	19:Z:180:LYS:N	2.54	0.41
20:a:162:TYR:CE2	20:a:165:THR:HG21	2.56	0.41
20:a:185:ILE:HG23	20:a:187:ASP:OD1	2.20	0.41
20:a:276:CYS:SG	20:a:277:LEU:N	2.93	0.41
21:b:11:ASP:OD1	21:b:13:SER:N	2.44	0.41
25:f:245:ASN:OD1	25:f:245:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:351:THR:HA	25:f:354:GLU:HG2	2.03	0.41
25:f:384:ALA:HB1	25:f:420:TRP:CZ3	2.56	0.41
25:f:809:ILE:HD12	25:f:814:SER:HB2	2.02	0.41
25:f:842:VAL:H	25:f:870:THR:HG1	1.62	0.41
26:g:161:SER:HB3	26:g:164:ASP:HB2	2.03	0.41
27:u:126:LEU:HD21	27:u:267:GLY:C	2.45	0.41
27:u:151:ARG:HA	27:u:151:ARG:CZ	2.51	0.41
27:u:166:LEU:HD11	27:u:204:MET:HG3	2.02	0.41
27:u:179:SER:OG	27:u:232:PRO:HA	2.20	0.41
27:u:189:GLN:NE2	27:u:257:THR:HG23	2.35	0.41
27:u:251:ASN:OD1	27:u:251:ASN:N	2.52	0.41
2:B:171:VAL:HG21	2:B:269:GLU:HG3	2.02	0.41
2:B:430:LYS:O	2:B:431:GLN:HG2	2.20	0.41
3:C:197:THR:HA	3:C:247:PHE:CE2	2.56	0.41
4:D:289:LEU:O	4:D:293:LEU:HG	2.21	0.41
4:D:323:ARG:HG2	4:D:325:GLY:H	1.85	0.41
6:F:150:LEU:HD23	6:F:150:LEU:HA	1.87	0.41
6:F:225:MET:HB2	6:F:354:PHE:CE1	2.56	0.41
10:J:90:GLU:HG2	10:J:110:TYR:CG	2.56	0.41
11:K:54:ILE:HD11	11:K:59:MET:CB	2.47	0.41
12:L:45:VAL:HG22	12:L:214:ILE:HG12	2.02	0.41
13:M:64:LYS:HE3	13:M:212:GLU:HB3	2.03	0.41
14:U:22:PHE:HE2	14:U:26:LYS:HZ1	1.66	0.41
14:U:603:LEU:HA	14:U:603:LEU:HD12	1.90	0.41
14:U:885:MET:HA	14:U:886:PRO:HD3	1.90	0.41
15:V:382:PHE:HB2	15:V:386:PHE:CZ	2.56	0.41
17:X:137:TYR:CD2	17:X:142:ARG:HD3	2.56	0.41
18:Y:194:PHE:HB3	18:Y:226:VAL:HG23	2.03	0.41
20:a:70:ARG:HB3	21:b:17:ARG:O	2.21	0.41
20:a:97:LEU:HD22	20:a:118:ILE:HB	2.03	0.41
22:c:277:LYS:HB2	22:c:282:ARG:HD3	2.03	0.41
23:d:201:SER:HA	23:d:263:LEU:HD23	2.03	0.41
25:f:57:GLU:O	25:f:61:GLU:HG2	2.20	0.41
25:f:535:THR:OG1	25:f:565:ASN:OD1	2.39	0.41
25:f:740:ARG:C	25:f:744:MET:HE3	2.46	0.41
1:A:41:TYR:OH	2:B:59:ARG:NH2	2.54	0.40
1:A:142:VAL:HG22	1:A:147:TYR:HA	2.03	0.40
1:A:407:LYS:HG3	1:A:411:GLU:OE1	2.21	0.40
3:C:189:TYR:CB	3:C:298:ILE:HB	2.51	0.40
4:D:174:LYS:O	4:D:178:ARG:HB2	2.21	0.40
5:E:59:GLU:O	5:E:72:LYS:N	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:61:LEU:HG	5:E:62:LYS:H	1.86	0.40
5:E:260:LEU:O	5:E:264:MET:HG3	2.21	0.40
6:F:406:ILE:HD13	6:F:422:GLU:CB	2.51	0.40
7:G:33:ASN:OD1	7:G:34:GLN:N	2.43	0.40
8:H:15:PRO:HA	9:I:23:TYR:CD1	2.56	0.40
9:I:240:HIS:O	9:I:244:GLU:HG3	2.21	0.40
10:J:94:HIS:ND1	10:J:102:VAL:HG22	2.36	0.40
14:U:492:ASP:HA	14:U:495:ASP:OD1	2.21	0.40
15:V:271:VAL:O	15:V:273:LYS:N	2.54	0.40
15:V:358:MET:O	15:V:362:LEU:HG	2.21	0.40
16:W:81:ASP:OD1	16:W:81:ASP:N	2.53	0.40
16:W:128:LEU:HD12	16:W:145:LEU:HD11	2.03	0.40
17:X:137:TYR:HE2	17:X:142:ARG:HH11	1.68	0.40
17:X:395:LYS:H	17:X:395:LYS:HG2	1.67	0.40
18:Y:126:LYS:O	18:Y:130:LYS:HG3	2.21	0.40
18:Y:195:LYS:HA	18:Y:195:LYS:HD3	1.82	0.40
20:a:78:GLU:OE2	20:a:81:LEU:HD21	2.21	0.40
22:c:121:TRP:CD1	22:c:190:GLN:HG3	2.56	0.40
22:c:163:ILE:HG12	22:c:199:HIS:O	2.21	0.40
22:c:256:ASN:O	22:c:260:GLU:HG2	2.22	0.40
23:d:94:MET:HE1	23:d:118:ARG:HB2	2.03	0.40
25:f:196:MET:HE3	25:f:204:ALA:HB3	2.03	0.40
25:f:344:VAL:HB	25:f:347:ASP:HB3	2.03	0.40
25:f:658:ALA:HB2	25:f:693:ALA:HB1	2.03	0.40
1:A:394:MET:HE1	2:B:216:ILE:CG2	2.52	0.40
2:B:78:PHE:HB2	25:f:613:LEU:HD11	2.03	0.40
2:B:112:LEU:HD21	2:B:115:ILE:HD11	2.03	0.40
2:B:369:THR:HA	2:B:372:MET:SD	2.61	0.40
3:C:78:ARG:HG2	3:C:80:MET:SD	2.60	0.40
5:E:303:LEU:HD22	5:E:304:PRO:HD2	2.03	0.40
6:F:244:THR:O	6:F:245:LYS:HG2	2.20	0.40
8:H:50:LYS:N	8:H:207:ASN:O	2.35	0.40
12:L:116:THR:O	12:L:119:PRO:HD2	2.21	0.40
14:U:422:LEU:O	14:U:426:TYR:HD2	2.05	0.40
16:W:84:ASN:O	16:W:88:MET:HG3	2.21	0.40
16:W:112:VAL:HG21	16:W:145:LEU:HD11	2.03	0.40
19:Z:172:VAL:CG2	22:c:217:LEU:HB3	2.51	0.40
20:a:130:VAL:HG22	20:a:133:GLU:HB2	2.03	0.40
20:a:177:LEU:HA	20:a:177:LEU:HD23	1.83	0.40
20:a:343:LEU:HA	20:a:346:ILE:HG12	2.04	0.40
22:c:31:VAL:HG23	22:c:67:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:73:PRO:O	25:f:77:GLU:HG3	2.21	0.40
25:f:281:ILE:HD12	25:f:281:ILE:HA	1.95	0.40
25:f:576:ILE:HG22	25:f:580:LEU:HD21	2.03	0.40
25:f:708:ASP:OD2	25:f:709:THR:N	2.54	0.40
1:A:40:THR:O	1:A:43:ARG:NH1	2.52	0.40
2:B:403:GLY:HA3	3:C:180:ILE:HD13	2.03	0.40
3:C:117:ARG:N	3:C:121:TYR:O	2.40	0.40
3:C:165:ILE:O	3:C:169:VAL:HG12	2.22	0.40
3:C:270:GLN:H	3:C:270:GLN:HG3	1.70	0.40
3:C:304:ALA:O	3:C:310:ARG:NH1	2.55	0.40
5:E:153:LEU:HD22	5:E:229:ILE:HD11	2.03	0.40
5:E:281:ARG:HB3	5:E:284:THR:HG23	2.04	0.40
6:F:293:THR:HA	6:F:337:ILE:HG22	2.03	0.40
8:H:84:ARG:HA	8:H:87:VAL:HG12	2.02	0.40
8:H:134:LEU:HB2	8:H:149:SER:OG	2.21	0.40
9:I:21:VAL:O	9:I:25:MET:HG3	2.20	0.40
9:I:241:GLU:HA	9:I:244:GLU:OE2	2.22	0.40
10:J:210:VAL:O	10:J:218:LYS:CB	2.69	0.40
11:K:27:ALA:O	11:K:31:ILE:HG13	2.22	0.40
14:U:96:TYR:O	14:U:100:ILE:HG12	2.21	0.40
15:V:135:LEU:O	15:V:138:PRO:HD2	2.21	0.40
15:V:228:ARG:NE	15:V:257:ASN:OD1	2.43	0.40
15:V:434:ALA:O	15:V:438:VAL:HG12	2.22	0.40
15:V:446:VAL:HG23	15:V:447:ILE:HG13	2.02	0.40
16:W:39:ARG:HE	16:W:42:GLU:CD	2.30	0.40
16:W:139:GLU:HB2	16:W:174:TYR:CD2	2.57	0.40
17:X:110:CYS:HA	17:X:113:CYS:SG	2.61	0.40
17:X:242:ILE:HG13	17:X:242:ILE:O	2.21	0.40
17:X:270:LEU:HD13	17:X:270:LEU:HA	1.87	0.40
18:Y:20:ALA:HB2	18:Y:150:PHE:CD2	2.56	0.40
18:Y:22:LEU:HD22	18:Y:37:VAL:HG13	2.03	0.40
19:Z:125:ASP:OD1	19:Z:125:ASP:N	2.55	0.40
20:a:69:HIS:CE1	20:a:70:ARG:HG2	2.57	0.40
23:d:226:ILE:O	23:d:229:PRO:HD2	2.22	0.40
25:f:227:ALA:HA	25:f:230:CYS:SG	2.61	0.40
26:g:107:ILE:O	26:g:142:LEU:N	2.41	0.40
1:A:154:PRO:HA	1:A:155:PRO:HD3	1.99	0.40
3:C:60:ARG:HH21	4:D:75:ALA:HB2	1.87	0.40
3:C:266:ASP:C	3:C:268:GLU:H	2.30	0.40
4:D:90:GLY:HA2	4:D:106:THR:HG23	2.04	0.40
5:E:115:VAL:O	5:E:119:VAL:HB	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:366:MET:HE1	6:F:385:ALA:HA	2.04	0.40
7:G:163:PHE:CB	8:H:57:TYR:HA	2.52	0.40
10:J:94:HIS:CD2	10:J:98:VAL:HG21	2.55	0.40
10:J:156:TRP:HZ3	11:K:58:LEU:HB2	1.86	0.40
13:M:24:GLU:H	13:M:24:GLU:CD	2.23	0.40
14:U:437:TYR:CE1	14:U:472:ILE:HD13	2.56	0.40
15:V:179:LYS:HG3	15:V:180:ARG:N	2.36	0.40
15:V:330:LYS:HD3	15:V:389:ASP:HB3	2.04	0.40
15:V:443:ARG:NH1	23:d:271:ILE:O	2.52	0.40
16:W:80:TRP:HA	16:W:80:TRP:CE3	2.57	0.40
17:X:258:LYS:HE3	17:X:266:ASP:OD2	2.21	0.40
18:Y:134:LEU:HA	18:Y:137:ARG:HG3	2.02	0.40
19:Z:13:PRO:HD2	19:Z:168:GLU:OE2	2.22	0.40
20:a:122:LYS:NZ	20:a:130:VAL:HG13	2.37	0.40
20:a:180:LEU:HD11	20:a:221:VAL:HG21	2.03	0.40
25:f:76:GLU:O	25:f:80:ARG:NE	2.54	0.40
25:f:89:MET:H	25:f:89:MET:HE3	1.86	0.40
25:f:249:LEU:HD22	25:f:268:LEU:HG	2.03	0.40
25:f:271:MET:HE1	25:f:786:GLN:HB2	2.04	0.40
1:A:41:TYR:CD1	1:A:41:TYR:N	2.89	0.40
1:A:301:GLU:HB2	6:F:254:PRO:CB	2.51	0.40
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.66	0.40
2:B:221:GLY:HA2	2:B:327:VAL:CG2	2.51	0.40
2:B:362:LYS:HG2	2:B:366:GLN:OE1	2.21	0.40
4:D:104:GLY:HA2	4:D:110:ASN:HA	2.02	0.40
4:D:200:ARG:HD2	4:D:326:ARG:HA	2.02	0.40
5:E:211:SER:O	5:E:215:ILE:HG22	2.21	0.40
5:E:341:ALA:HB1	6:F:346:GLY:N	2.37	0.40
7:G:29:PHE:CZ	7:G:157:ALA:HB2	2.57	0.40
7:G:206:LEU:HD12	7:G:210:PHE:HZ	1.85	0.40
8:H:189:HIS:HA	8:H:192:ILE:HD11	2.03	0.40
11:K:190:THR:HG22	11:K:193:GLU:OE1	2.21	0.40
13:M:175:GLU:HA	13:M:178:LYS:HZ3	1.87	0.40
14:U:12:LEU:HD11	14:U:27:LEU:HD21	2.02	0.40
14:U:374:SER:HB3	14:U:407:SER:OG	2.22	0.40
14:U:423:MET:HE1	14:U:427:LEU:HD23	2.03	0.40
14:U:841:LYS:HA	14:U:844:LYS:HG2	2.03	0.40
15:V:315:LYS:HD2	18:Y:385:ARG:HH12	1.86	0.40
16:W:83:LEU:HA	16:W:83:LEU:HD23	1.84	0.40
17:X:139:ASP:O	17:X:141:LYS:NZ	2.44	0.40
18:Y:241:ILE:O	18:Y:247:LEU:HD11	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:111:LEU:HG	19:Z:114:ARG:NH1	2.37	0.40
20:a:68:GLU:HG3	20:a:69:HIS:N	2.37	0.40
25:f:367:SER:HB3	25:f:370:MET:HE1	2.04	0.40
25:f:479:LEU:HG	25:f:514:VAL:HG22	2.02	0.40
25:f:573:ILE:O	25:f:577:LEU:N	2.47	0.40
25:f:725:SER:O	25:f:729:MET:HG2	2.22	0.40
27:u:223:ASP:O	27:u:226:LYS:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/433 (93%)	367 (91%)	33 (8%)	3 (1%)	18	51
2	B	365/440 (83%)	343 (94%)	18 (5%)	4 (1%)	11	43
3	C	384/406 (95%)	332 (86%)	48 (12%)	4 (1%)	12	45
4	D	354/418 (85%)	330 (93%)	21 (6%)	3 (1%)	16	49
5	E	364/389 (94%)	342 (94%)	21 (6%)	1 (0%)	36	65
6	F	361/439 (82%)	326 (90%)	31 (9%)	4 (1%)	11	43
7	G	237/246 (96%)	220 (93%)	16 (7%)	1 (0%)	30	61
8	H	228/234 (97%)	220 (96%)	8 (4%)	0	100	100
9	I	246/261 (94%)	241 (98%)	5 (2%)	0	100	100
10	J	237/248 (96%)	214 (90%)	22 (9%)	1 (0%)	30	61
11	K	224/241 (93%)	215 (96%)	9 (4%)	0	100	100
12	L	236/263 (90%)	228 (97%)	8 (3%)	0	100	100
13	M	238/255 (93%)	226 (95%)	11 (5%)	1 (0%)	30	61
14	U	829/953 (87%)	764 (92%)	61 (7%)	4 (0%)	24	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	V	435/534 (82%)	391 (90%)	42 (10%)	2 (0%)	24	57
16	W	436/456 (96%)	423 (97%)	13 (3%)	0	100	100
17	X	376/422 (89%)	359 (96%)	15 (4%)	2 (0%)	24	57
18	Y	378/389 (97%)	370 (98%)	8 (2%)	0	100	100
19	Z	284/324 (88%)	261 (92%)	22 (8%)	1 (0%)	30	61
20	a	371/376 (99%)	341 (92%)	29 (8%)	1 (0%)	36	65
21	b	189/377 (50%)	170 (90%)	17 (9%)	2 (1%)	11	43
22	c	266/424 (63%)	243 (91%)	21 (8%)	2 (1%)	16	49
23	d	267/350 (76%)	251 (94%)	15 (6%)	1 (0%)	30	61
24	e	38/70 (54%)	35 (92%)	3 (8%)	0	100	100
25	f	838/908 (92%)	790 (94%)	47 (6%)	1 (0%)	48	79
26	g	93/601 (16%)	89 (96%)	4 (4%)	0	100	100
27	u	170/289 (59%)	158 (93%)	12 (7%)	0	100	100
All	All	8847/10746 (82%)	8249 (93%)	560 (6%)	38 (0%)	31	61

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	176	VAL
2	B	278	ALA
3	C	103	ILE
3	C	242	ALA
6	F	279	ALA
6	F	339	ASP
15	V	496	PHE
17	X	393	VAL
21	b	186	SER
22	c	138	GLU
22	c	279	ASP
2	B	431	GLN
3	C	85	VAL
5	E	74	THR
6	F	323	ASN
7	G	165	ALA
14	U	42	VAL
14	U	86	ASP
14	U	88	PHE

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Mol	Chain	Res	Type
20	a	213	PHE
25	f	852	VAL
1	A	110	LYS
4	D	354	LEU
6	F	324	THR
3	C	83	LYS
10	J	52	LYS
13	M	17	ASP
14	U	794	ASP
17	X	45	VAL
1	A	79	ASP
1	A	310	ASP
2	B	386	ALA
4	D	317	LEU
4	D	407	ILE
15	V	264	TYR
23	d	332	SER
19	Z	226	ILE
21	b	148	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	348/372 (94%)	341 (98%)	7 (2%)	48	66
2	B	328/385 (85%)	315 (96%)	13 (4%)	28	54
3	C	338/352 (96%)	329 (97%)	9 (3%)	39	61
4	D	314/366 (86%)	302 (96%)	12 (4%)	29	55
5	E	324/341 (95%)	313 (97%)	11 (3%)	32	57
6	F	315/379 (83%)	303 (96%)	12 (4%)	29	55
7	G	192/210 (91%)	188 (98%)	4 (2%)	47	65
8	H	168/191 (88%)	164 (98%)	4 (2%)	43	63
9	I	191/221 (86%)	188 (98%)	3 (2%)	55	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	152/211 (72%)	150 (99%)	2 (1%)	61	72
11	K	187/203 (92%)	183 (98%)	4 (2%)	47	65
12	L	198/224 (88%)	197 (100%)	1 (0%)	81	80
13	M	192/212 (91%)	186 (97%)	6 (3%)	35	59
14	U	713/816 (87%)	694 (97%)	19 (3%)	39	61
15	V	379/460 (82%)	366 (97%)	13 (3%)	32	57
16	W	403/416 (97%)	396 (98%)	7 (2%)	53	69
17	X	325/362 (90%)	315 (97%)	10 (3%)	35	59
18	Y	335/344 (97%)	331 (99%)	4 (1%)	63	73
19	Z	257/295 (87%)	248 (96%)	9 (4%)	32	57
20	a	333/336 (99%)	322 (97%)	11 (3%)	33	58
21	b	167/312 (54%)	161 (96%)	6 (4%)	31	56
22	c	241/359 (67%)	232 (96%)	9 (4%)	30	56
23	d	237/294 (81%)	232 (98%)	5 (2%)	47	65
24	e	38/63 (60%)	38 (100%)	0	100	100
25	f	709/763 (93%)	695 (98%)	14 (2%)	48	66
26	g	85/527 (16%)	83 (98%)	2 (2%)	43	63
27	u	156/253 (62%)	149 (96%)	7 (4%)	24	51
All	All	7625/9267 (82%)	7421 (97%)	204 (3%)	40	61

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASP
1	A	66	LYS
1	A	70	THR
1	A	295	VAL
1	A	338	ASP
1	A	345	LEU
1	A	362	MET
2	B	74	MET
2	B	92	GLN
2	B	125	THR
2	B	186	ASP
2	B	187	ILE
2	B	223	ILE

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Mol	Chain	Res	Type
2	B	243	THR
2	B	251	VAL
2	B	290	ILE
2	B	347	ILE
2	B	381	ASP
2	B	404	LEU
2	B	434	THR
3	C	31	LEU
3	C	132	ASP
3	C	136	SER
3	C	141	GLU
3	C	269	VAL
3	C	326	LEU
3	C	396	GLU
3	C	403	LYS
3	C	405	TRP
4	D	115	ILE
4	D	143	LEU
4	D	185	LEU
4	D	200	ARG
4	D	202	VAL
4	D	246	MET
4	D	261	ILE
4	D	282	ASP
4	D	370	ILE
4	D	392	TYR
4	D	408	LYS
4	D	416	PHE
5	E	52	SER
5	E	102	MET
5	E	108	MET
5	E	214	LEU
5	E	218	MET
5	E	233	ASP
5	E	262	ASN
5	E	296	ASP
5	E	322	LYS
5	E	382	SER
5	E	387	LYS
6	F	90	VAL
6	F	144	LYS
6	F	156	ASP

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Mol	Chain	Res	Type
6	F	221	LYS
6	F	245	LYS
6	F	250	LYS
6	F	306	VAL
6	F	316	GLN
6	F	318	ASP
6	F	351	LYS
6	F	432	LYS
6	F	436	GLN
7	G	52	THR
7	G	68	HIS
7	G	131	MET
7	G	179	LEU
8	H	13	PHE
8	H	130	PHE
8	H	148	GLN
8	H	219	ARG
9	I	164	ILE
9	I	223	THR
9	I	235	GLN
10	J	43	LEU
10	J	114	LEU
11	K	60	GLU
11	K	139	VAL
11	K	149	LYS
11	K	233	GLU
12	L	97	PHE
13	M	35	THR
13	M	54	LEU
13	M	99	ARG
13	M	181	MET
13	M	221	ASN
13	M	231	ILE
14	U	71	LEU
14	U	92	ASP
14	U	105	ILE
14	U	145	HIS
14	U	177	LEU
14	U	248	ILE
14	U	252	LEU
14	U	342	LEU
14	U	360	VAL

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Mol	Chain	Res	Type
14	U	366	HIS
14	U	448	LEU
14	U	457	ILE
14	U	542	GLU
14	U	602	LEU
14	U	675	MET
14	U	685	GLN
14	U	802	TYR
14	U	835	ILE
14	U	921	ILE
15	V	35	VAL
15	V	135	LEU
15	V	144	ASP
15	V	147	PHE
15	V	172	VAL
15	V	194	LYS
15	V	214	HIS
15	V	230	PHE
15	V	334	VAL
15	V	337	LEU
15	V	346	LEU
15	V	394	LEU
15	V	443	ARG
16	W	61	VAL
16	W	73	MET
16	W	140	ILE
16	W	308	LEU
16	W	328	LEU
16	W	427	ASP
16	W	438	LEU
17	X	44	GLN
17	X	149	LEU
17	X	156	GLU
17	X	177	TYR
17	X	218	HIS
17	X	243	ASP
17	X	256	LEU
17	X	315	ASP
17	X	385	LEU
17	X	388	PHE
18	Y	39	ASP
18	Y	73	MET

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Mol	Chain	Res	Type
18	Y	180	LEU
18	Y	388	ASN
19	Z	89	GLU
19	Z	119	SER
19	Z	121	LEU
19	Z	166	GLU
19	Z	187	LEU
19	Z	226	ILE
19	Z	228	TYR
19	Z	231	GLN
19	Z	239	ASP
20	a	87	MET
20	a	121	LEU
20	a	136	GLU
20	a	211	PHE
20	a	255	TRP
20	a	269	LEU
20	a	275	LEU
20	a	296	ILE
20	a	310	LEU
20	a	343	LEU
20	a	374	ILE
21	b	51	LEU
21	b	52	ILE
21	b	79	GLN
21	b	84	ILE
21	b	94	HIS
21	b	154	THR
22	c	49	VAL
22	c	64	ASP
22	c	69	VAL
22	c	145	VAL
22	c	179	SER
22	c	192	LEU
22	c	203	ILE
22	c	218	LEU
22	c	231	LEU
23	d	146	ASP
23	d	198	PHE
23	d	240	SER
23	d	265	ASP
23	d	309	VAL

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Mol	Chain	Res	Type
25	f	44	GLU
25	f	131	MET
25	f	149	GLU
25	f	177	GLU
25	f	256	PHE
25	f	347	ASP
25	f	397	LYS
25	f	440	ILE
25	f	446	LEU
25	f	560	LEU
25	f	808	ASN
25	f	852	VAL
25	f	898	VAL
25	f	905	ASN
26	g	87	VAL
26	g	107	ILE
27	u	119	ILE
27	u	167	ILE
27	u	182	PHE
27	u	225	ILE
27	u	244	VAL
27	u	275	MET
27	u	289	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	247	GLN
1	A	322	ASN
2	B	157	HIS
3	C	36	ASN
3	C	40	GLN
3	C	182	GLN
3	C	296	ASN
4	D	49	GLN
4	D	83	GLN
4	D	221	HIS
4	D	222	HIS
4	D	376	ASN
5	E	194	ASN
5	E	262	ASN

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Mol	Chain	Res	Type
5	E	271	HIS
5	E	345	ASN
6	F	315	ASN
6	F	417	HIS
6	F	428	GLN
9	I	53	HIS
9	I	84	ASN
9	I	109	GLN
10	J	116	GLN
10	J	146	GLN
11	K	23	GLN
12	L	31	GLN
12	L	65	HIS
12	L	69	HIS
13	M	105	ASN
14	U	70	HIS
14	U	190	ASN
14	U	218	GLN
14	U	340	GLN
14	U	373	ASN
14	U	697	GLN
14	U	749	GLN
14	U	805	ASN
15	V	214	HIS
15	V	260	HIS
15	V	347	GLN
15	V	400	HIS
15	V	427	GLN
16	W	84	ASN
16	W	86	ASN
16	W	189	GLN
16	W	416	GLN
17	X	405	GLN
18	Y	160	ASN
18	Y	258	GLN
19	Z	22	HIS
19	Z	96	HIS
19	Z	202	ASN
19	Z	224	HIS
19	Z	274	ASN
19	Z	277	ASN
20	a	36	GLN

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Mol	Chain	Res	Type
20	a	164	GLN
20	a	264	ASN
21	b	34	ASN
21	b	169	HIS
22	c	130	GLN
22	c	131	GLN
22	c	185	ASN
22	c	221	HIS
24	e	63	HIS
25	f	161	HIS
25	f	327	ASN
25	f	356	ASN
25	f	473	ASN
25	f	701	ASN
25	f	905	ASN
26	g	106	HIS
26	g	145	GLN
27	u	183	GLN
27	u	289	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
29	ADP	C	501	30	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)
29	ADP	A	501	-	28,29,29	1.42	4 (14%)	43,45,45	1.83	8 (18%)
29	ADP	B	501	-	28,29,29	1.41	4 (14%)	43,45,45	1.88	8 (18%)
29	ADP	D	501	-	28,29,29	1.42	4 (14%)	43,45,45	1.86	9 (20%)
31	ATP	F	501	30	32,33,33	0.31	0	48,52,52	0.40	0
31	ATP	E	402	30	32,33,33	0.28	0	48,52,52	0.34	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
29	ADP	C	501	30	-	1/16/32/32	0/3/3/3
29	ADP	A	501	-	-	2/16/32/32	0/3/3/3
29	ADP	B	501	-	-	3/16/32/32	0/3/3/3
29	ADP	D	501	-	-	4/16/32/32	0/3/3/3
31	ATP	F	501	30	-	2/22/38/38	0/3/3/3
31	ATP	E	402	30	-	5/22/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	501	ADP	C5-C4	4.78	1.47	1.39
29	D	501	ADP	C5-C4	4.77	1.47	1.39
29	B	501	ADP	C5-C4	4.76	1.47	1.39
29	C	501	ADP	C5-C4	4.70	1.47	1.39
29	D	501	ADP	C5-C6	2.76	1.48	1.41
29	C	501	ADP	C5-C6	2.70	1.48	1.41
29	A	501	ADP	C5-C6	2.70	1.48	1.41
29	B	501	ADP	C5-C6	2.67	1.48	1.41
29	B	501	ADP	C5-N7	-2.42	1.34	1.39
29	A	501	ADP	C5-N7	-2.36	1.34	1.39
29	D	501	ADP	C5-N7	-2.33	1.34	1.39
29	D	501	ADP	C8-N7	2.32	1.36	1.31
29	C	501	ADP	C8-N7	2.31	1.36	1.31
29	C	501	ADP	C5-N7	-2.31	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	501	ADP	C8-N7	2.24	1.36	1.31
29	B	501	ADP	C8-N7	2.17	1.35	1.31

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	501	ADP	C5-C4-N3	-6.13	118.27	126.72
29	D	501	ADP	C5-C4-N3	-6.08	118.34	126.72
29	A	501	ADP	C5-C4-N3	-5.89	118.61	126.72
29	C	501	ADP	C5-C4-N3	-5.76	118.78	126.72
29	B	501	ADP	N3-C4-N9	5.02	135.71	127.17
29	D	501	ADP	N3-C4-N9	4.74	135.23	127.17
29	A	501	ADP	N3-C4-N9	4.66	135.09	127.17
29	C	501	ADP	N3-C4-N9	4.55	134.90	127.17
29	B	501	ADP	C2-N3-C4	3.82	121.16	111.83
29	D	501	ADP	C2-N3-C4	3.72	120.91	111.83
29	A	501	ADP	C2-N3-C4	3.64	120.72	111.83
29	D	501	ADP	C4-C5-N7	-3.59	106.47	110.58
29	C	501	ADP	C2-N3-C4	3.59	120.61	111.83
29	C	501	ADP	C4-C5-N7	-3.41	106.68	110.58
29	A	501	ADP	C4-C5-N7	-3.36	106.74	110.58
29	B	501	ADP	N3-C2-N1	-3.26	123.65	128.58
29	B	501	ADP	C4-C5-N7	-3.20	106.92	110.58
29	D	501	ADP	N3-C2-N1	-3.12	123.86	128.58
29	A	501	ADP	N3-C2-N1	-3.04	123.98	128.58
29	C	501	ADP	N3-C2-N1	-2.99	124.05	128.58
29	D	501	ADP	C3'-C2'-C1'	2.73	106.63	101.46
29	B	501	ADP	C3'-C2'-C1'	2.73	106.62	101.46
29	C	501	ADP	C3'-C2'-C1'	2.71	106.58	101.46
29	A	501	ADP	C3'-C2'-C1'	2.65	106.48	101.46
29	D	501	ADP	C5-N7-C8	2.63	107.58	103.45
29	C	501	ADP	C4-N9-C8	2.56	108.43	105.74
29	B	501	ADP	C4-N9-C8	2.44	108.30	105.74
29	C	501	ADP	C5-N7-C8	2.42	107.25	103.45
29	A	501	ADP	C4-N9-C8	2.39	108.25	105.74
29	D	501	ADP	C4-N9-C8	2.38	108.24	105.74
29	B	501	ADP	C5-N7-C8	2.38	107.19	103.45
29	A	501	ADP	C5-N7-C8	2.36	107.17	103.45
29	C	501	ADP	C6-C5-N7	2.01	135.97	132.09
29	D	501	ADP	C6-C5-N7	2.01	135.97	132.09

There are no chirality outliers.

All (17) torsion outliers are listed below:

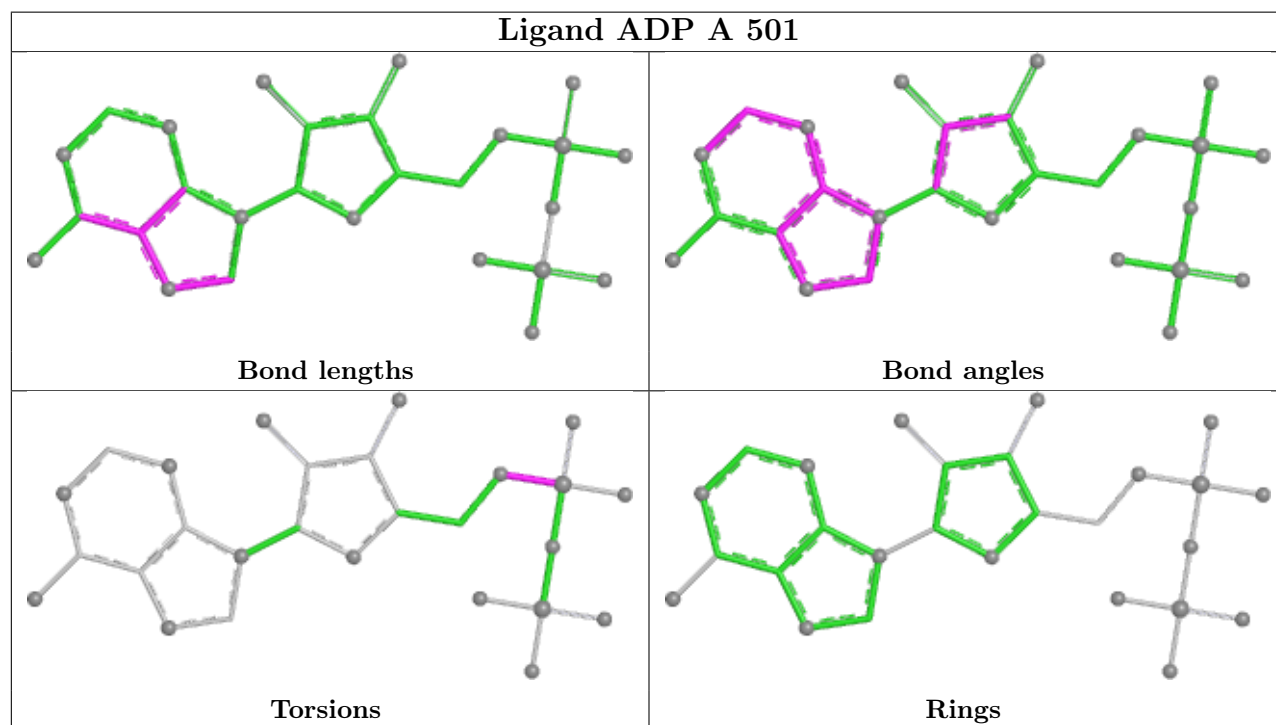
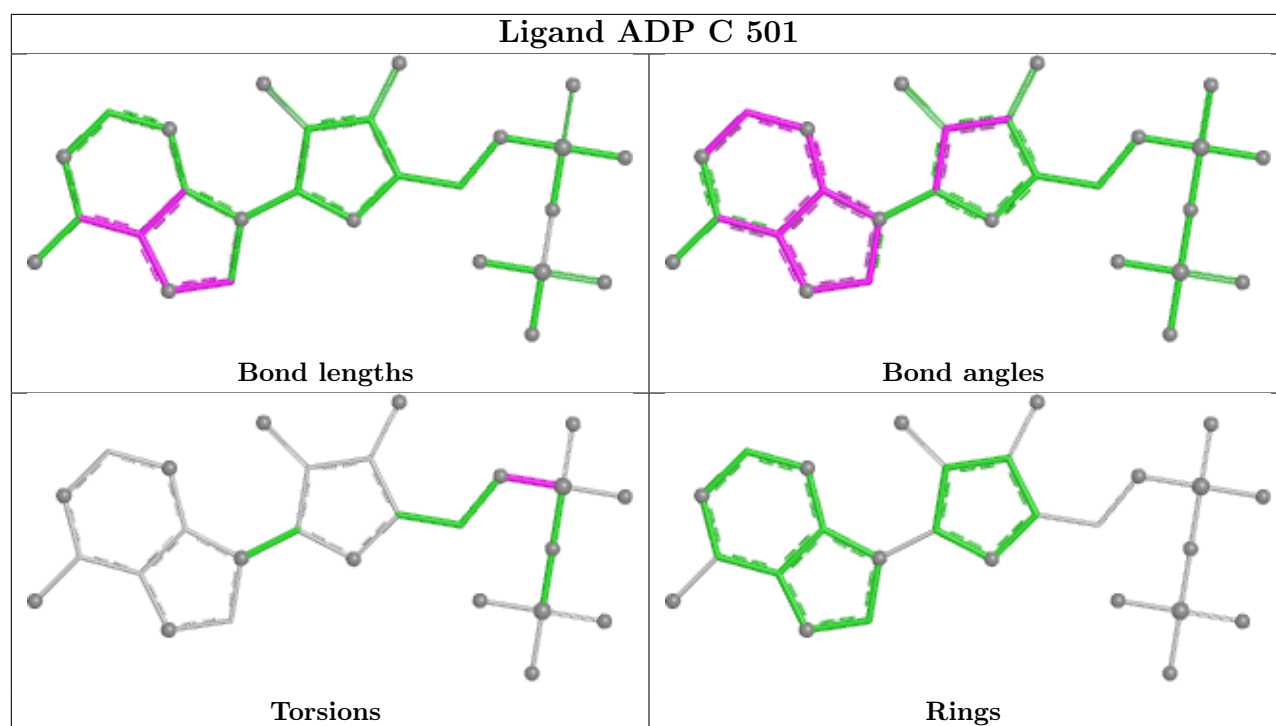
Mol	Chain	Res	Type	Atoms
29	A	501	ADP	C5'-O5'-PA-O2A
29	A	501	ADP	C5'-O5'-PA-O3A
29	B	501	ADP	C5'-O5'-PA-O1A
29	B	501	ADP	C5'-O5'-PA-O2A
29	B	501	ADP	C5'-O5'-PA-O3A
29	D	501	ADP	C5'-O5'-PA-O3A
31	E	402	ATP	C5'-O5'-PA-O2A
31	E	402	ATP	O4'-C4'-C5'-O5'
29	D	501	ADP	O4'-C4'-C5'-O5'
31	F	501	ATP	PA-O3A-PB-O2B
29	C	501	ADP	C5'-O5'-PA-O1A
29	D	501	ADP	C5'-O5'-PA-O1A
31	E	402	ATP	C5'-O5'-PA-O1A
31	E	402	ATP	C5'-O5'-PA-O3A
31	E	402	ATP	PG-O3B-PB-O2B
29	D	501	ADP	C3'-C4'-C5'-O5'
31	F	501	ATP	PA-O3A-PB-O1B

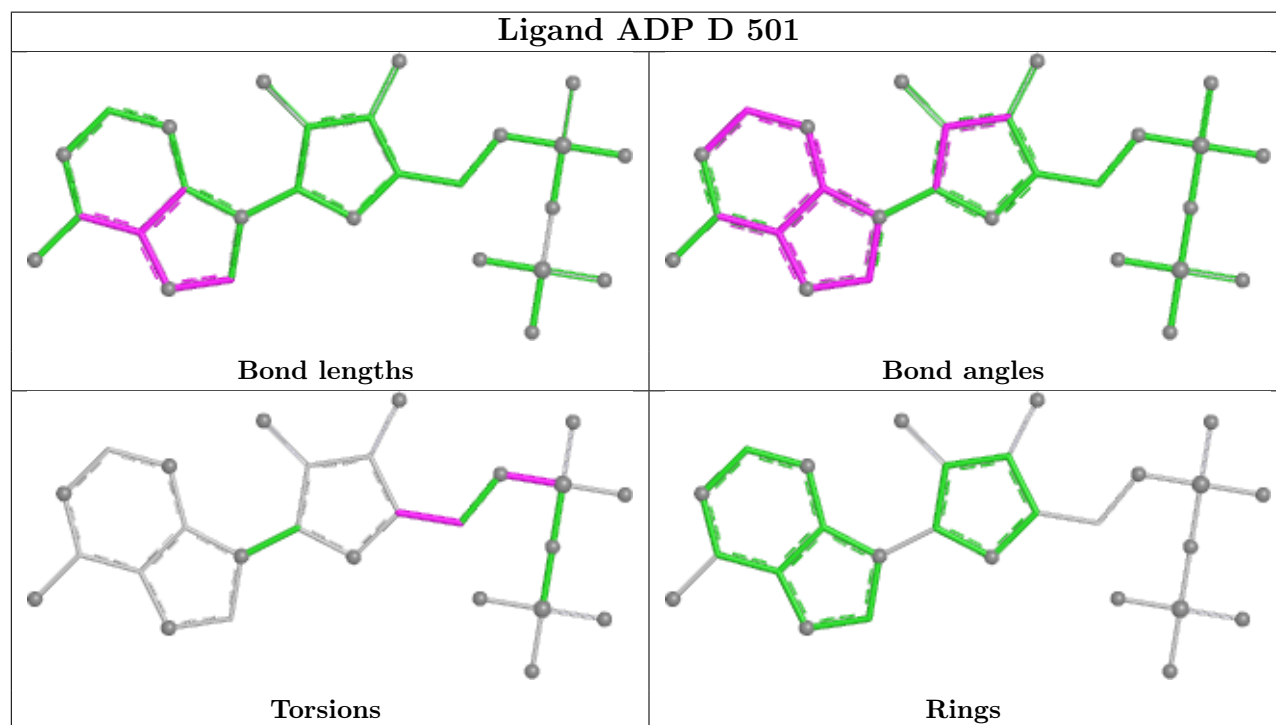
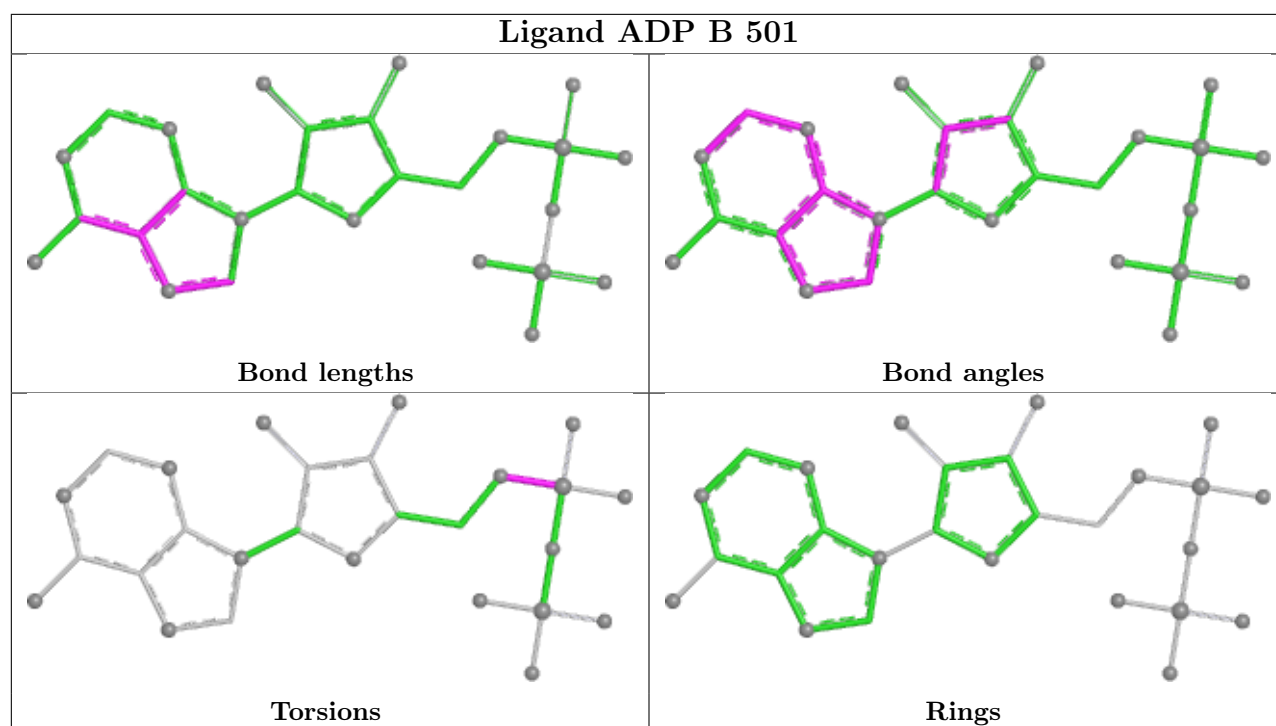
There are no ring outliers.

6 monomers are involved in 14 short contacts:

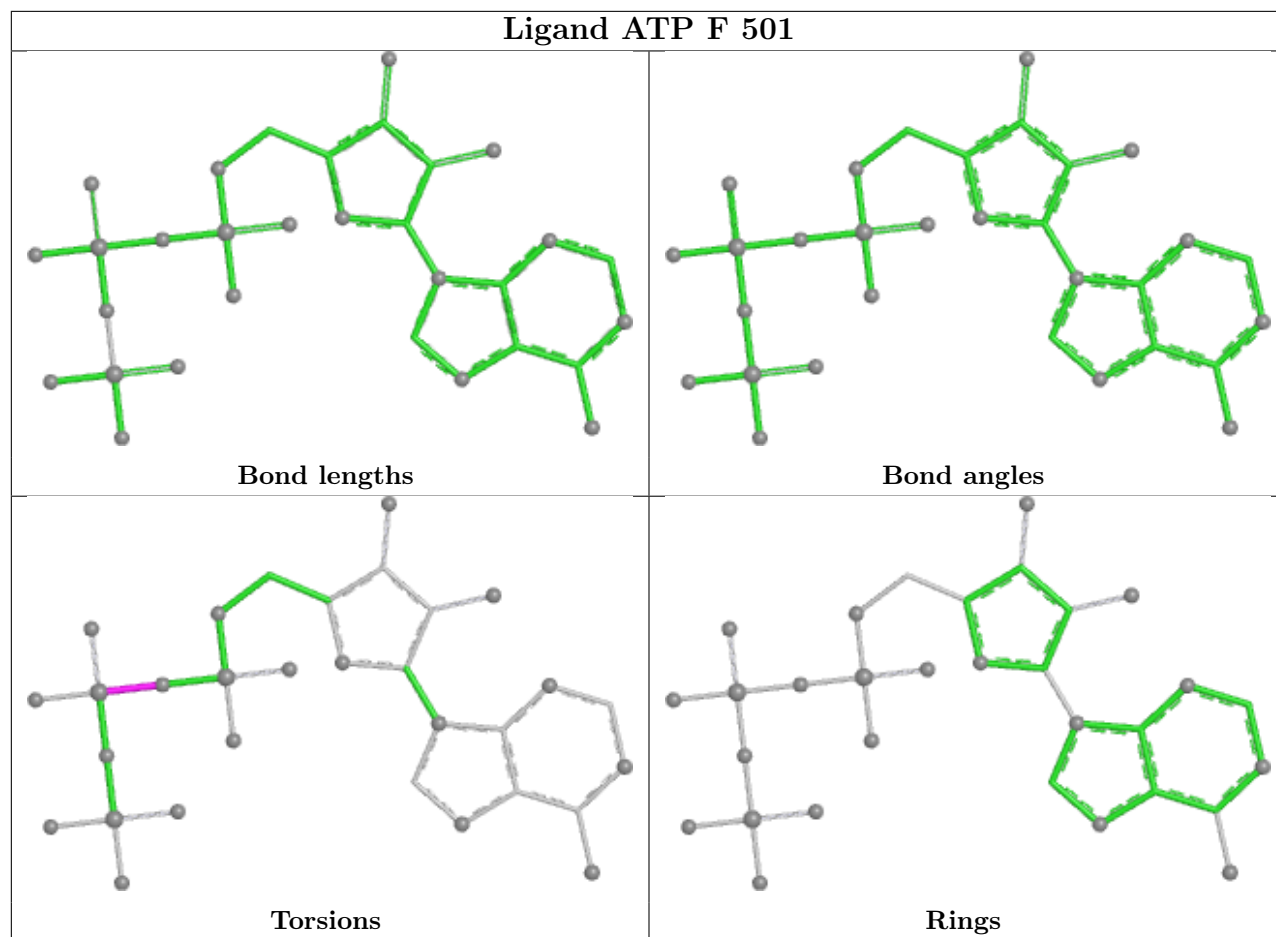
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	C	501	ADP	3	0
29	A	501	ADP	2	0
29	B	501	ADP	1	0
29	D	501	ADP	2	0
31	F	501	ATP	1	0
31	E	402	ATP	5	0

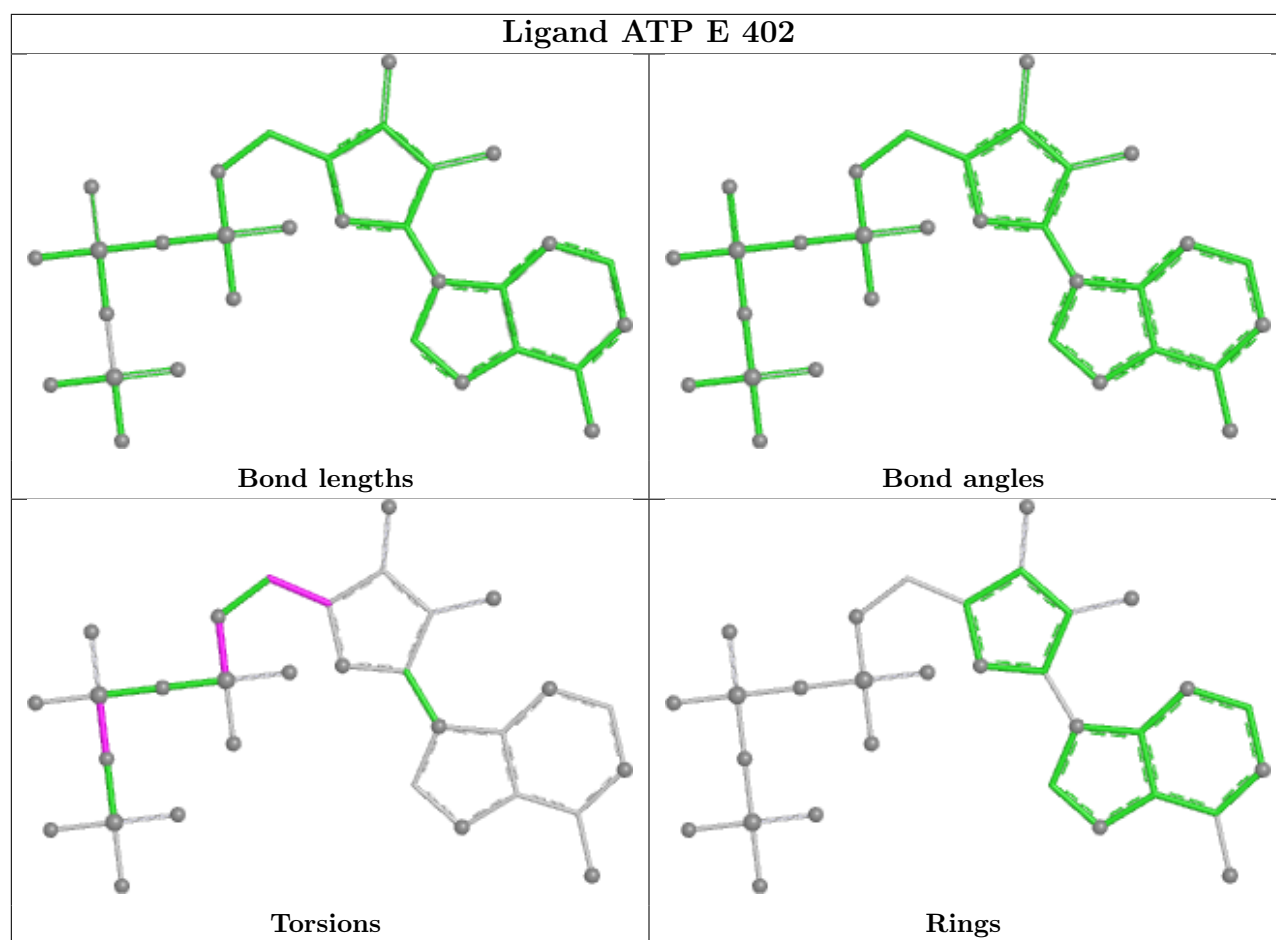
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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





Ligand ATP F 501





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.

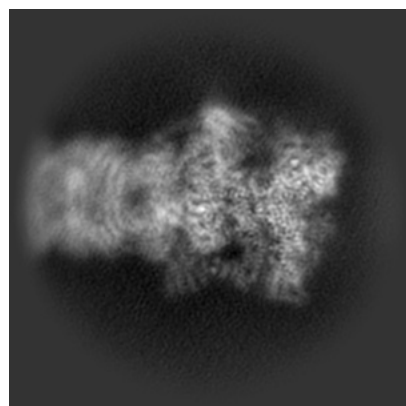
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47724. These allow visual inspection of the internal detail of the map and identification of artifacts.

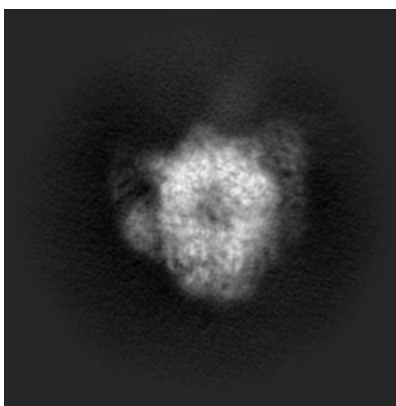
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

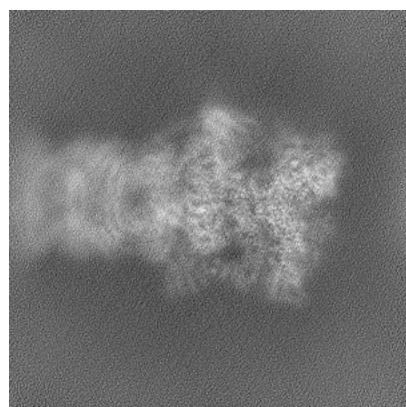


Y

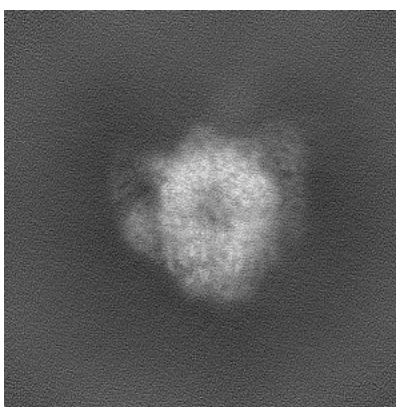


Z

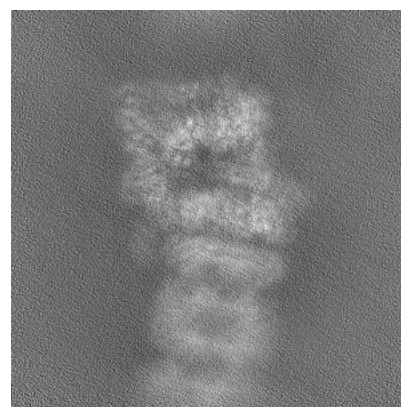
6.1.2 Raw map



X



Y

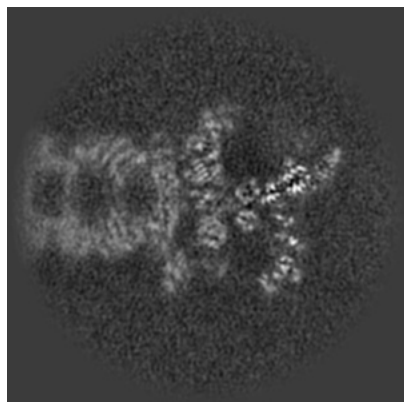


Z

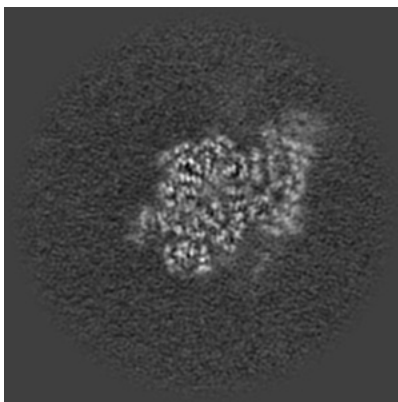
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

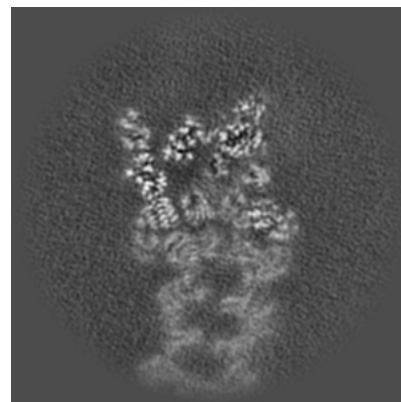
6.2.1 Primary map



X Index: 170

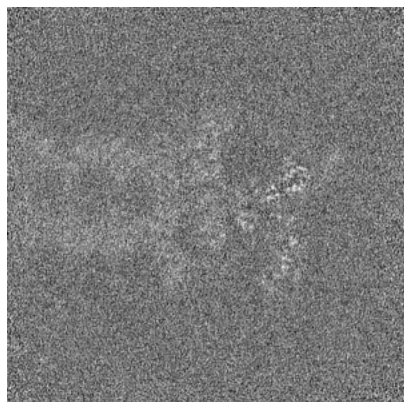


Y Index: 170

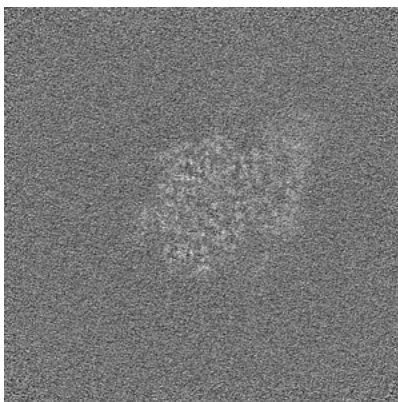


Z Index: 170

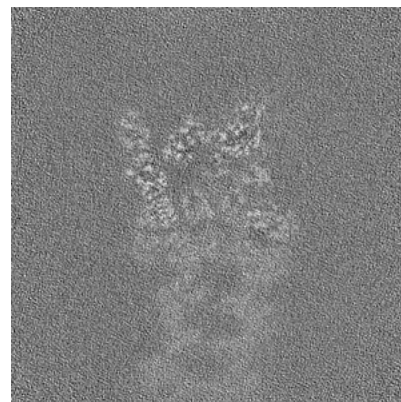
6.2.2 Raw map



X Index: 170



Y Index: 170

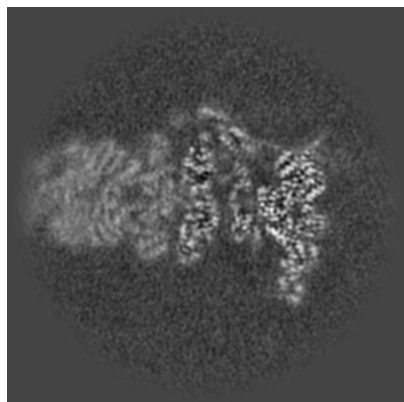


Z Index: 170

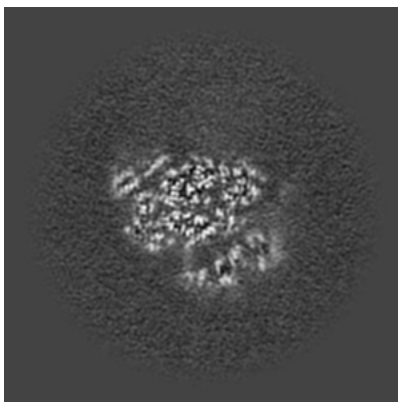
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

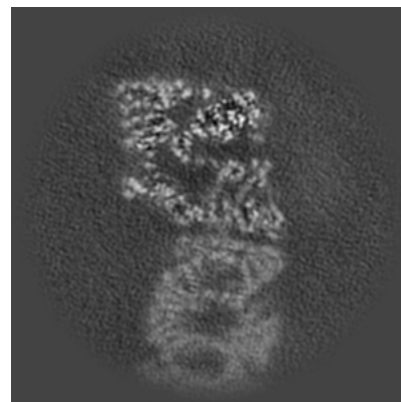
6.3.1 Primary map



X Index: 198

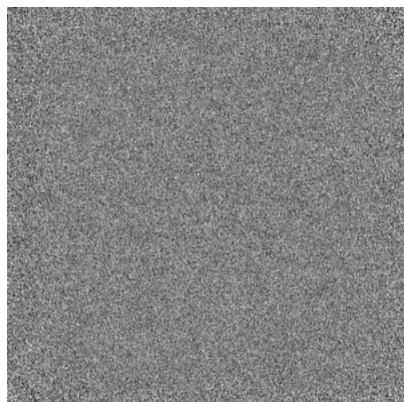


Y Index: 234

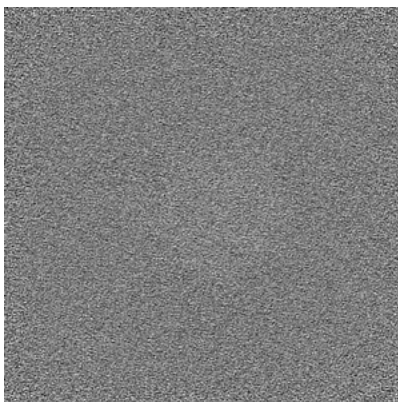


Z Index: 193

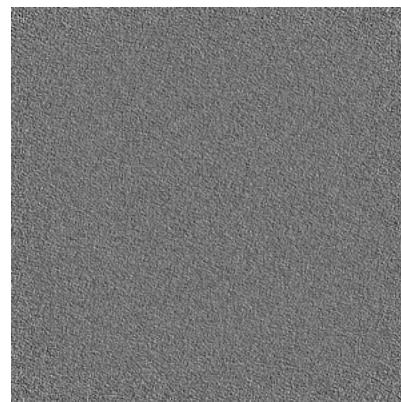
6.3.2 Raw map



X Index: 0



Y Index: 0

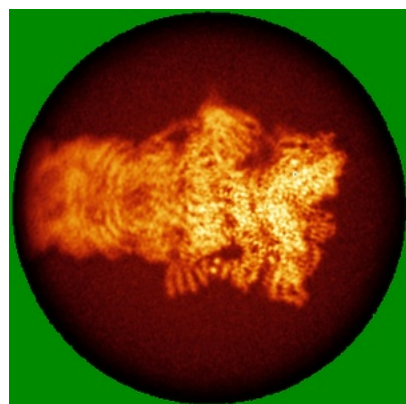


Z Index: 0

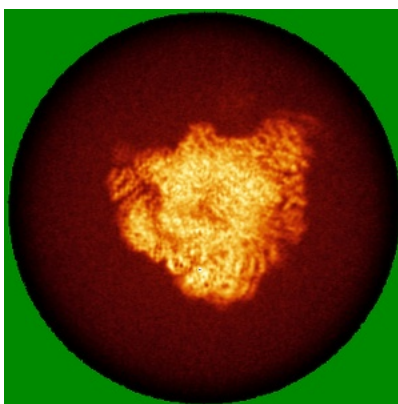
The images above show the largest variance slices of the map in three orthogonal directions.

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

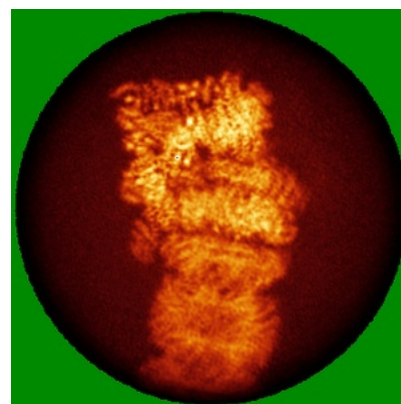
6.4.1 Primary map



X

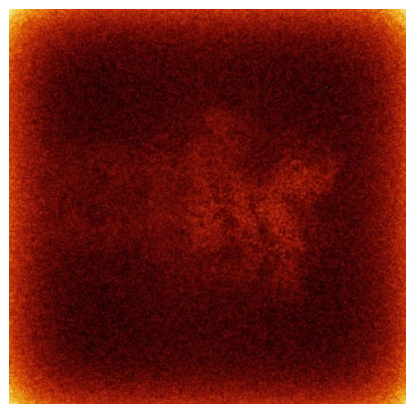


Y

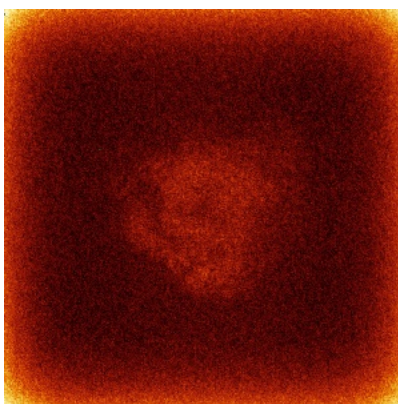


Z

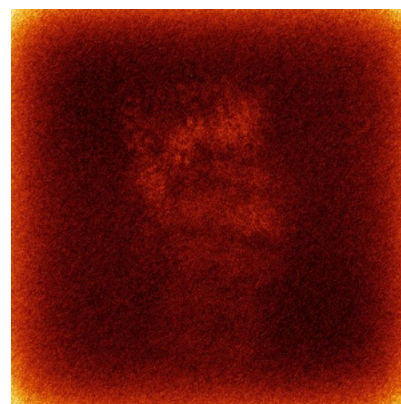
6.4.2 Raw map



X



Y

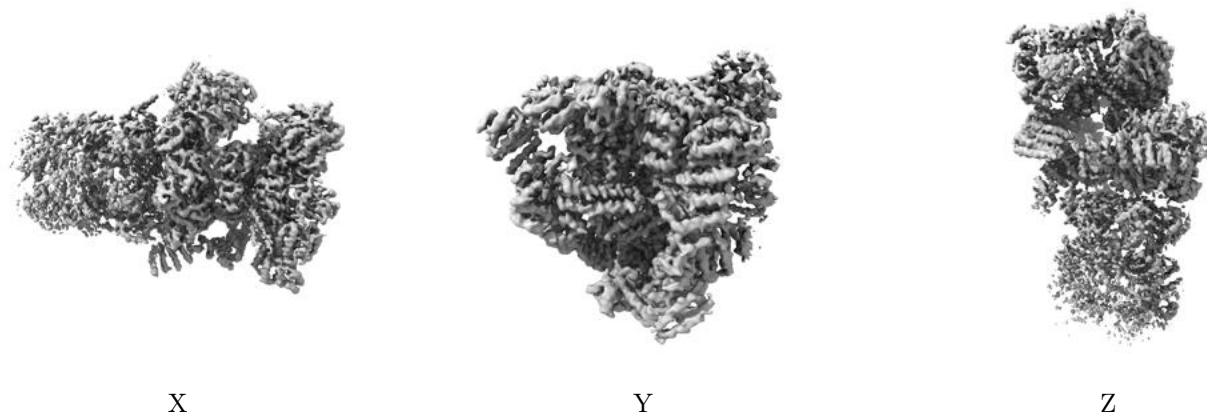


Z

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.

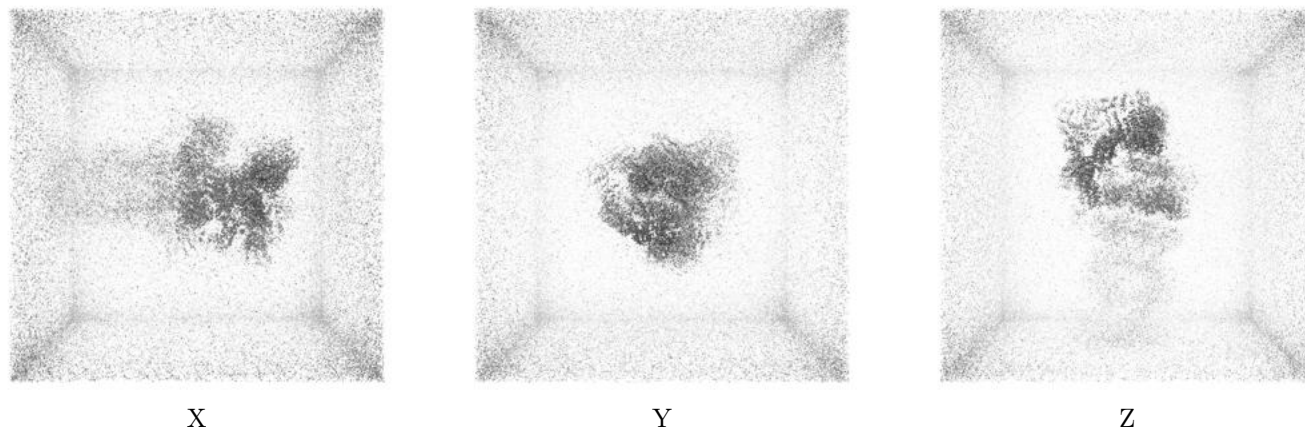
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

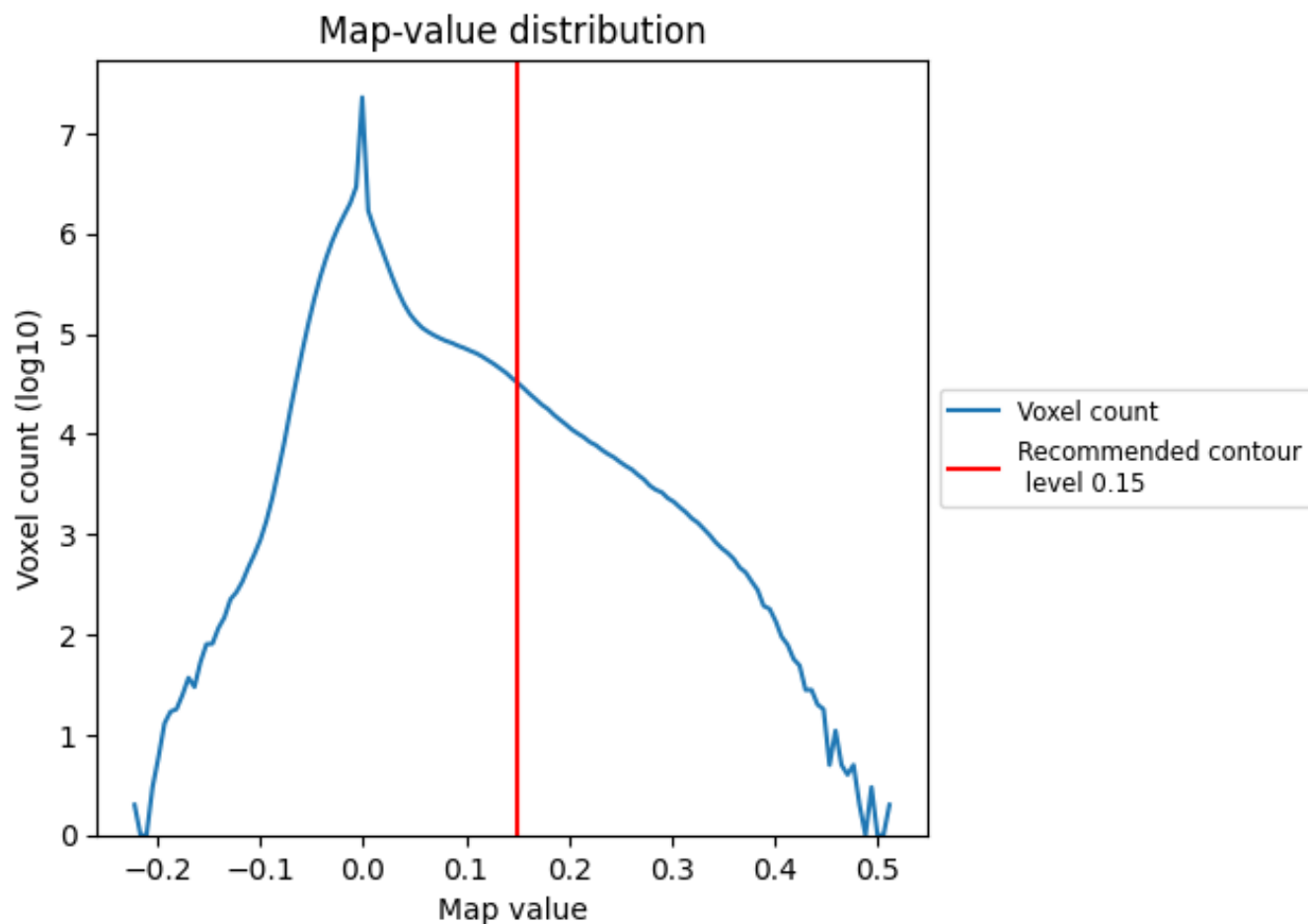
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

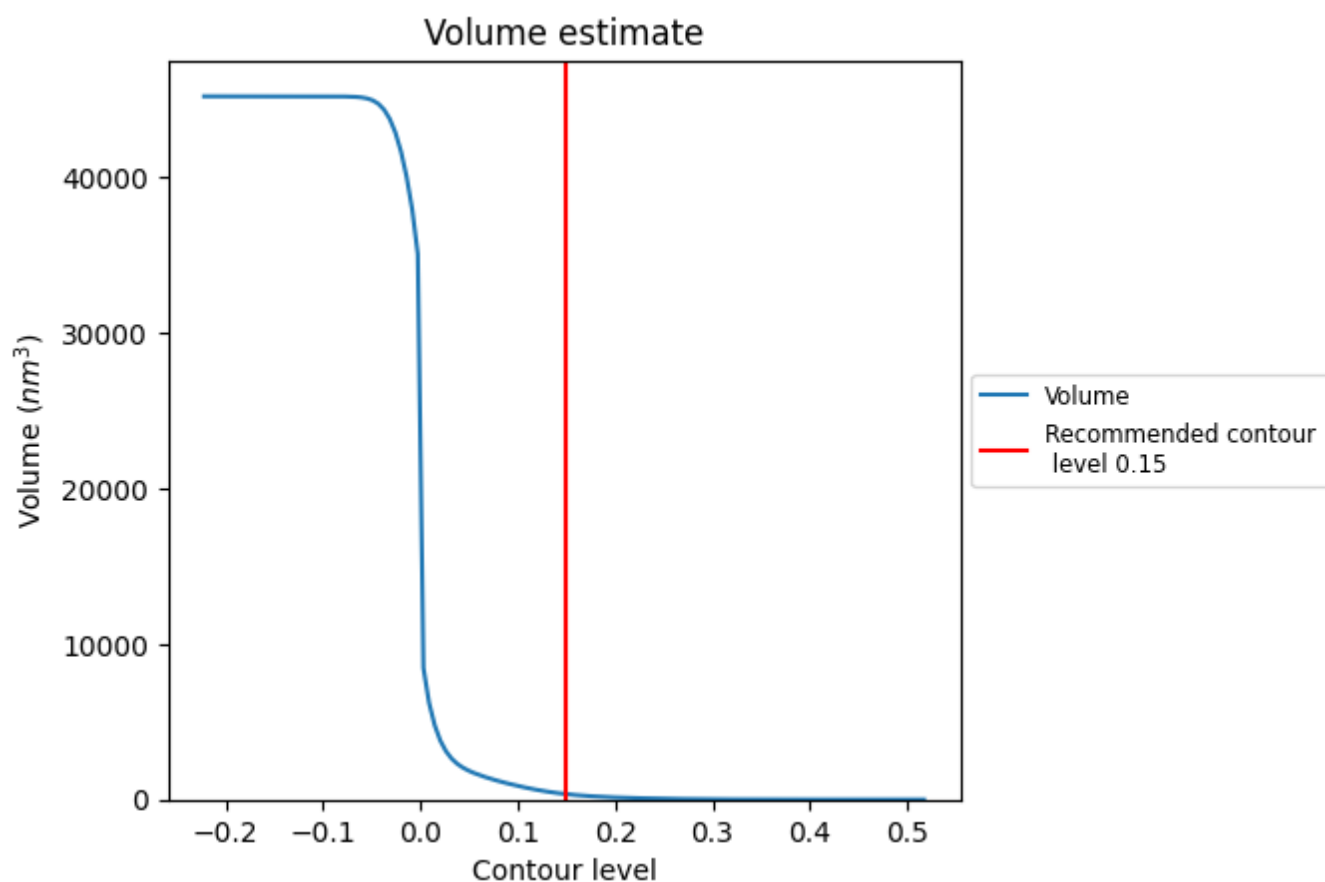
This section contains the results of statistical analysis of the map.

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.

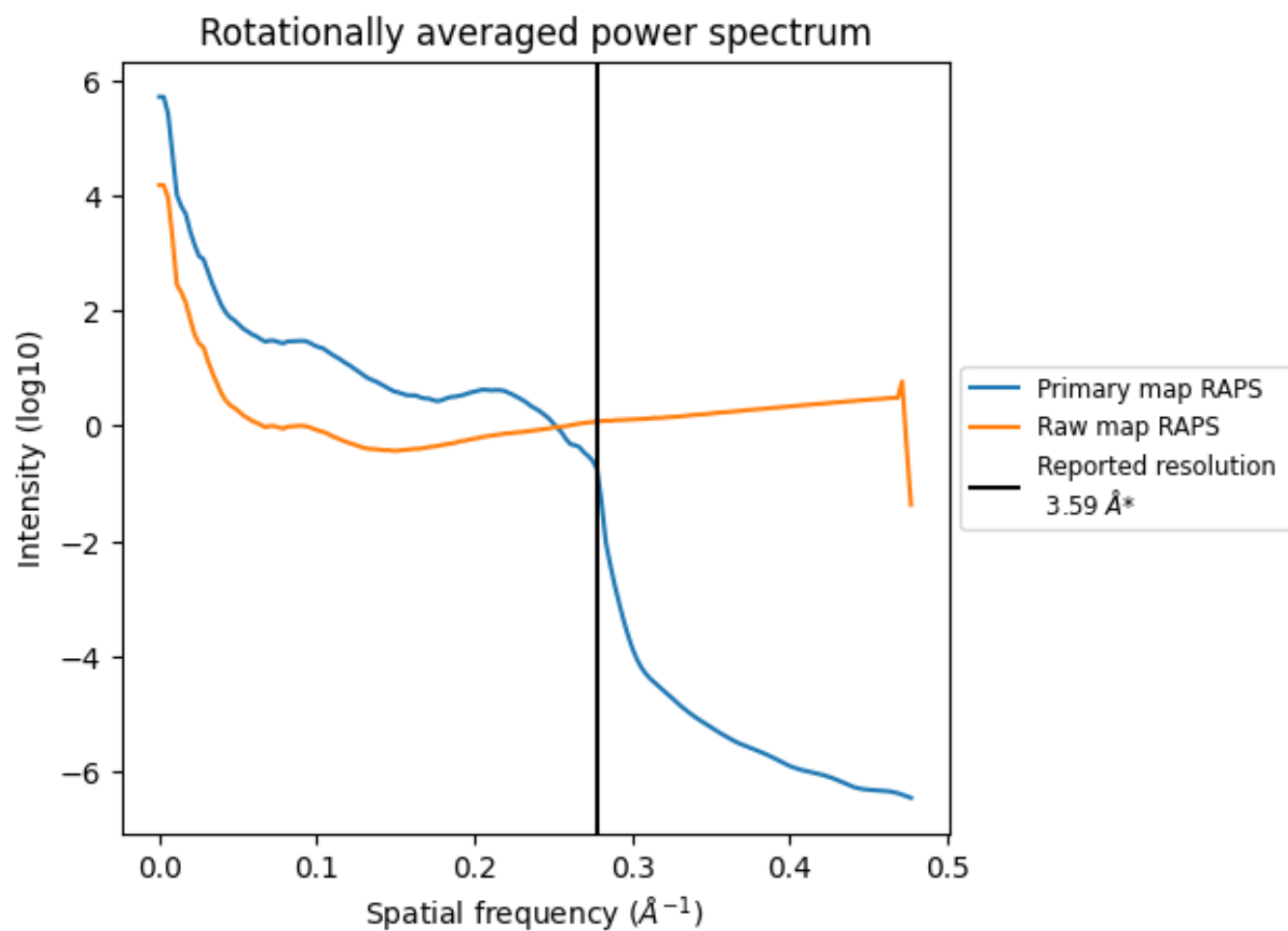
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 349 nm³; this corresponds to an approximate mass of 316 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 ⓘ

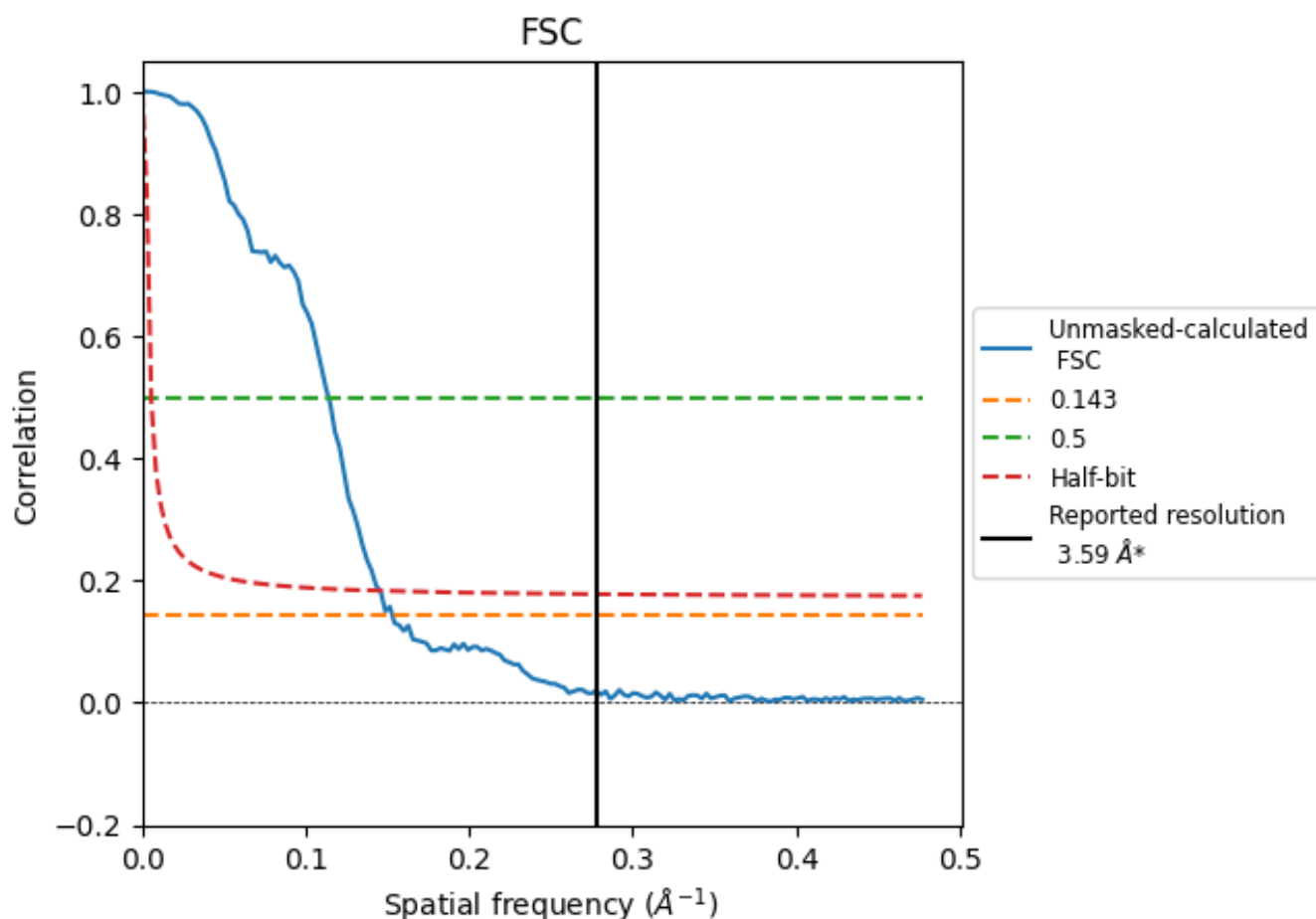


*Reported resolution corresponds to spatial frequency of 0.279 Å⁻¹

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 0.279 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

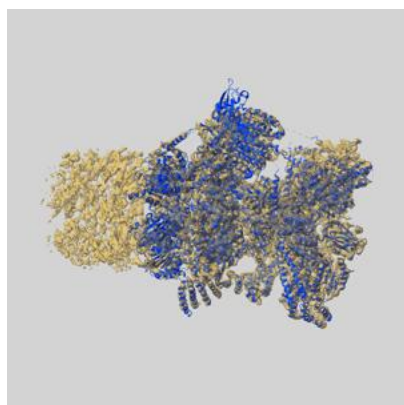
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.59	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.54	8.78	6.87

*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 6.54 differs from the reported value 3.59 by more than 10 %

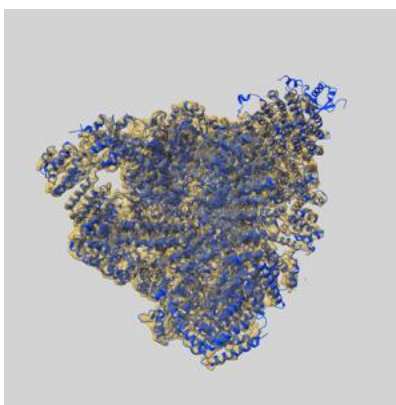
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47724 and PDB model 9E8L. Per-residue inclusion information can be found in section [3](#) on page [13](#).

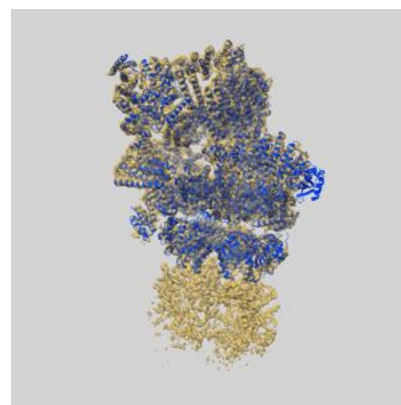
9.1 Map-model overlay [i](#)



X



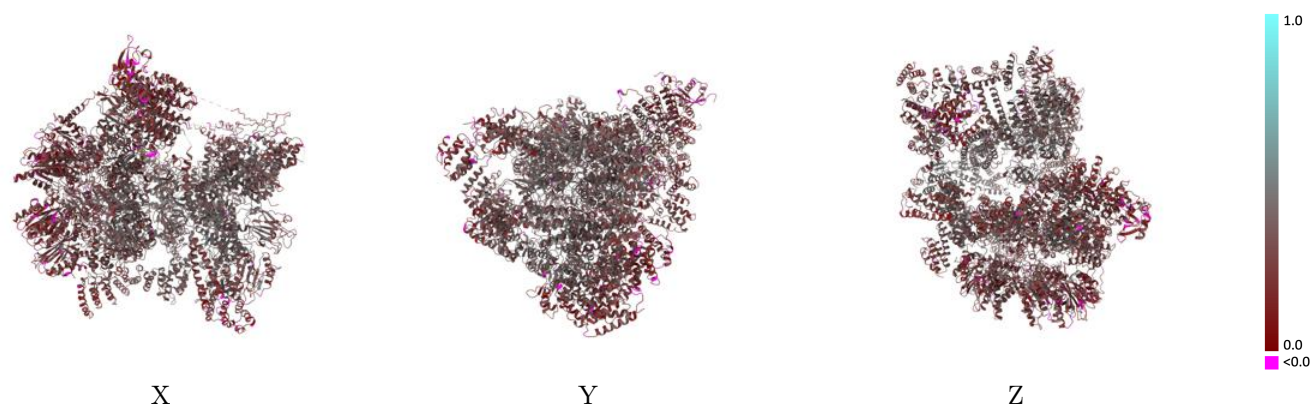
Y



Z

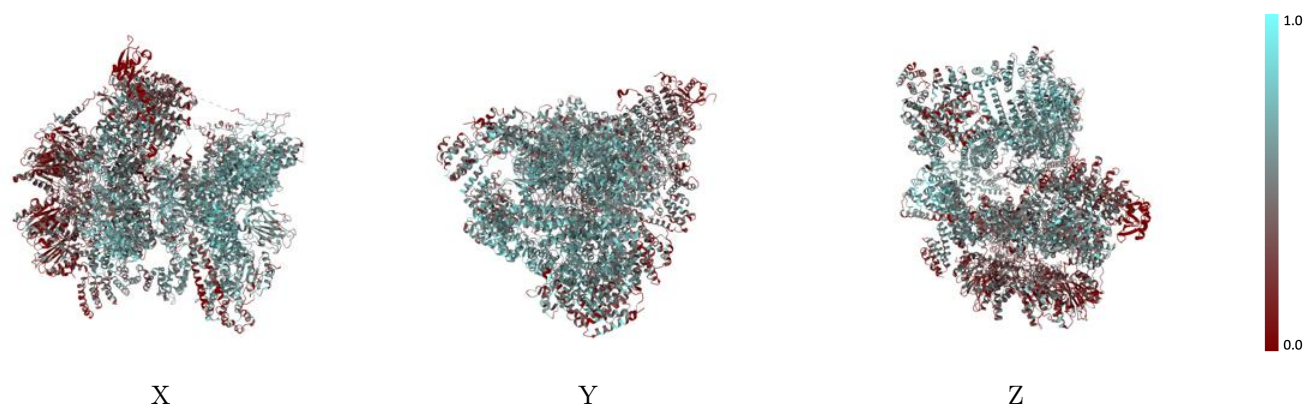
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



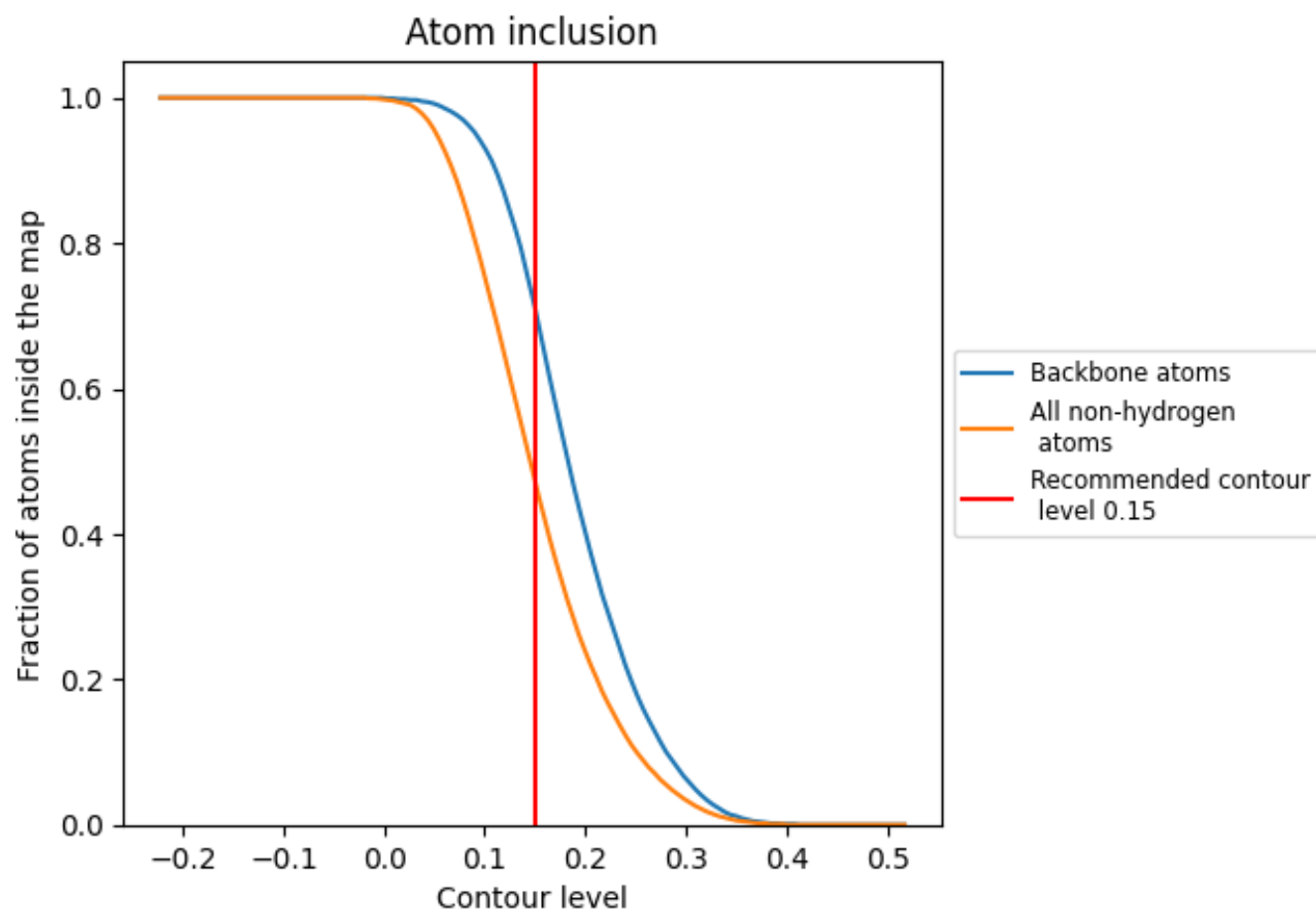
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 47% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4730	 0.3140
A	 0.5380	 0.3490
B	 0.5050	 0.3450
C	 0.4680	 0.3300
D	 0.4750	 0.3590
E	 0.5000	 0.3330
F	 0.5440	 0.3500
G	 0.3050	 0.2760
H	 0.3320	 0.2740
I	 0.2650	 0.2550
J	 0.3010	 0.2520
K	 0.2210	 0.2240
L	 0.2210	 0.2380
M	 0.2690	 0.2610
U	 0.6010	 0.3490
V	 0.4820	 0.2740
W	 0.5000	 0.3110
X	 0.5600	 0.3510
Y	 0.6530	 0.3530
Z	 0.6680	 0.4080
a	 0.5450	 0.2990
b	 0.5160	 0.3240
c	 0.6390	 0.4020
d	 0.4260	 0.2700
e	 0.5280	 0.3170
f	 0.3910	 0.2700
g	 0.0000	 0.1430
u	 0.4920	 0.3610
v	 0.3390	 0.3500

