Full wwPDB EM Validation Report

Jun 3, 2025 – 04:23 PM EDT

PDB ID	:	9BV1 / pdb_00009bv1
EMDB ID	:	EMD-44927
Title	:	M2A Midnolin-Proteasome (translocating)
Authors	:	Gao, J.; Yip, M.C.J.; Shao, S.
Deposited on	:	2024-05-19
Resolution	:	3.10 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:

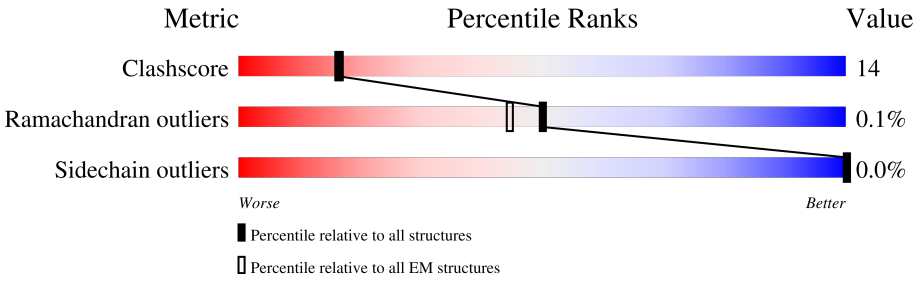
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	U	953	6% 66% 24% 10%
2	V	534	12% 49% 30% 21%
3	W	456	9% 60% 35% 5%
4	X	422	24% 77% 23%
5	Y	389	5% 72% 25%
6	Z	324	65% 24% 11%
7	a	376	18% 67% 32%
8	b	377	16% 32% 19% 49%

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Mol	Chain	Length	Quality of chain
9	c	310	6% 65% 24% 11%
10	d	350	16% 50% 24% 26%
11	e	70	33% 19% 49%
12	A	433	5% 70% 24% 6%
13	B	440	65% 23% 11%
14	C	406	73% 23%
15	D	418	64% 25% 11%
16	E	389	29% 50% 30% 20%
17	F	439	8% 61% 23% 16%
18	G	246	77% 21%
19	H	234	76% 23%
20	I	261	6% 81% 18%
21	J	248	73% 24%
22	K	241	78% 20%
23	L	263	66% 24% 10%
24	M	255	74% 22%
25	N	239	64% 19% 17%
25	n	239	13% 51% 24% 25%
26	O	277	63% 17% 20%
26	o	277	21% 49% 14% 36%
27	P	205	68% 32%
27	p	205	34% 63% 17% 20%
28	Q	201	70% 28%
28	q	201	29% 61% 25% 14%
29	R	263	57% 19% 24%

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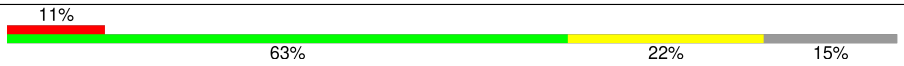
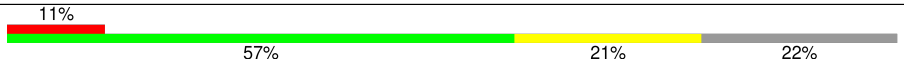
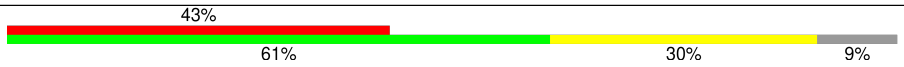
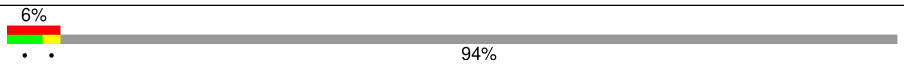
Mol	Chain	Length	Quality of chain
29	r	263	
30	S	241	
30	s	241	
31	T	264	
31	t	264	
32	f	908	
33	y	505	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 90308 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	856	Total	C	N	O	S	0	0
			6676	4237	1134	1260	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	421	Total	C	N	O	S	0	0
			3434	2192	613	617	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	434	Total	C	N	O	S	0	0
			3535	2238	606	668	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	421	Total	C	N	O	S	0	0
			3327	2111	566	638	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	379	Total	C	N	O	S	0	0
			3123	1993	534	579	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	287	Total	C	N	O	S	0	0
			2290	1462	394	429	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	375	Total	C	N	O	S	0	0
			3012	1921	513	563	15		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	b	191	Total	C	N	O	S	0	0
			1459	910	261	281	7		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	c	277	Total	C	N	O	S	0	0
			2184	1382	375	408	19		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	258	Total	C	N	O	S	0	0
			2099	1362	341	387	9		

- Molecule 11 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	e	36	Total	C	N	O	0	0
			314	193	50	71		

- Molecule 12 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	405	Total	C	N	O	S	0	0
			3183	2002	561	602	18		

- Molecule 13 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	390	Total	C	N	O	S	0	0
			3065	1931	521	598	15		

- Molecule 14 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	389	Total	C	N	O	S	0	0
			3071	1932	550	571	18		

- Molecule 15 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	D	373	Total	C	N	O	S	0	0
			2990	1894	517	567	12		

- Molecule 16 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E	311	Total	C	N	O	S	0	0
			2469	1553	439	461	16		

- Molecule 17 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F	367	Total	C	N	O	S	0	0
			2870	1812	495	546	17		

- Molecule 18 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	G	241	Total	C	N	O	S	0	0
			1885	1196	314	362	13		

- Molecule 19 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	H	233	Total	C	N	O	S	0	0
			1818	1161	308	343	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	I	258	Total	C	N	O	S	0	0
			2044	1290	350	394	10		

- Molecule 21 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	J	239	Total	C	N	O	S	0	0
			1887	1183	334	365	5		

- Molecule 22 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	K	235	Total	C	N	O	S	0	0
			1804	1132	299	362	11		

- Molecule 23 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	237	Total	C	N	O	S	0	0
			1868	1168	338	351	11		

- Molecule 24 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	245	Total	C	N	O	S	0	0
			1920	1214	326	369	11		

- Molecule 25 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	N	198	Total	C	N	O	S	0	0
			1487	931	254	290	12		
25	n	179	Total	C	N	O	S	0	0
			1336	836	230	258	12		

- Molecule 26 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	O	221	Total	C	N	O	S	0	0
			1667	1050	284	321	12		
26	o	176	Total	C	N	O	S	0	0
			1315	823	228	253	11		

- Molecule 27 is a protein called Proteasome subunit beta type-3.

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
27	p	164	Total	C	N	O	S	0	0
			1264	802	210	235	17		

- Molecule 28 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Q	197	Total	C	N	O	S	0	0
			1578	1011	268	290	9		
28	q	173	Total	C	N	O	S	0	0
			1380	890	234	248	8		

- Molecule 29 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	R	199	Total	C	N	O	S	0	0
			1549	977	272	291	9		
29	r	187	Total	C	N	O	S	0	0
			1432	904	248	271	9		

- Molecule 30 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	S	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		
30	s	206	Total	C	N	O	S	0	0
			1597	1015	269	303	10		

- Molecule 31 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	T	213	Total	C	N	O	S	0	0
			1665	1050	288	316	11		
31	t	206	Total	C	N	O	S	0	0
			1609	1016	279	302	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	828	Total	C	N	O	S	0	0
			6412	4058	1085	1225	44		

- Molecule 33 is a protein called Midnolin.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	y	31	Total	C	N	O	S	0	0
			273	164	66	42	1		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	-36	MET	-	initiating methionine	UNP Q504T8
y	-35	ASP	-	expression tag	UNP Q504T8
y	-34	TYR	-	expression tag	UNP Q504T8
y	-33	LYS	-	expression tag	UNP Q504T8
y	-32	ASP	-	expression tag	UNP Q504T8
y	-31	ASP	-	expression tag	UNP Q504T8
y	-30	ASP	-	expression tag	UNP Q504T8
y	-29	ASP	-	expression tag	UNP Q504T8
y	-28	LYS	-	expression tag	UNP Q504T8
y	-27	ASP	-	expression tag	UNP Q504T8
y	-26	TYR	-	expression tag	UNP Q504T8
y	-25	LYS	-	expression tag	UNP Q504T8
y	-24	ASP	-	expression tag	UNP Q504T8
y	-23	ASP	-	expression tag	UNP Q504T8
y	-22	ASP	-	expression tag	UNP Q504T8
y	-21	ASP	-	expression tag	UNP Q504T8
y	-20	LYS	-	expression tag	UNP Q504T8
y	-19	GLY	-	expression tag	UNP Q504T8
y	-18	GLY	-	expression tag	UNP Q504T8
y	-17	GLY	-	expression tag	UNP Q504T8
y	-16	GLY	-	expression tag	UNP Q504T8
y	-15	SER	-	expression tag	UNP Q504T8
y	-14	GLY	-	expression tag	UNP Q504T8
y	-13	GLY	-	expression tag	UNP Q504T8
y	-12	GLY	-	expression tag	UNP Q504T8
y	-11	GLY	-	expression tag	UNP Q504T8
y	-10	PHE	-	expression tag	UNP Q504T8
y	-9	GLU	-	expression tag	UNP Q504T8
y	-8	THR	-	expression tag	UNP Q504T8
y	-7	SER	-	expression tag	UNP Q504T8
y	-6	LEU	-	expression tag	UNP Q504T8
y	-5	TYR	-	expression tag	UNP Q504T8
y	-4	LYS	-	expression tag	UNP Q504T8
y	-3	LYS	-	expression tag	UNP Q504T8
y	-2	ALA	-	expression tag	UNP Q504T8
y	-1	GLY	-	expression tag	UNP Q504T8
y	0	THR	-	expression tag	UNP Q504T8

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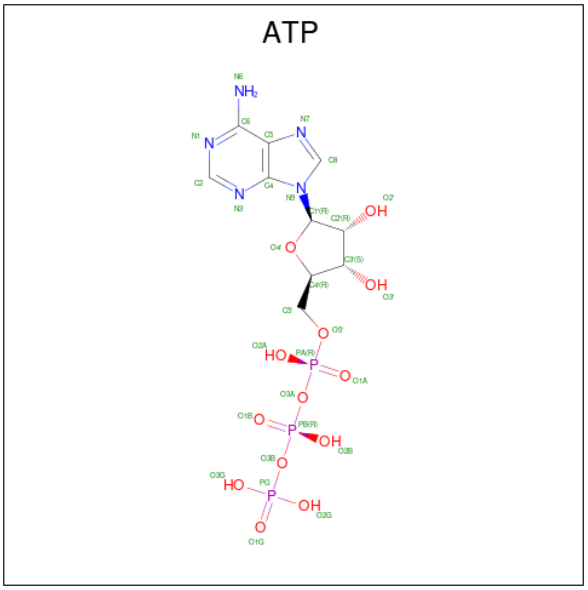
Chain	Residue	Modelled	Actual	Comment	Reference
y	457	ALA	VAL	conflict	UNP Q504T8

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

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

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
36	A	1	Total Mg 1 1	0

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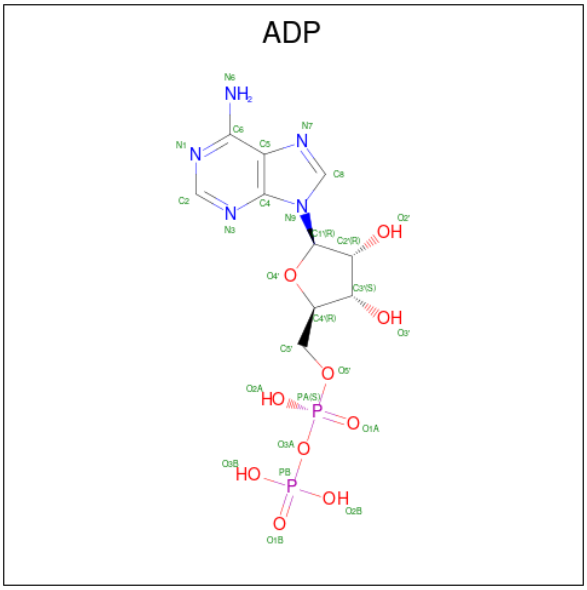
Mol	Chain	Residues	Atoms	AltConf
36	B	1	Total Mg 1 1	0
36	C	1	Total Mg 1 1	0
36	D	1	Total Mg 1 1	0

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



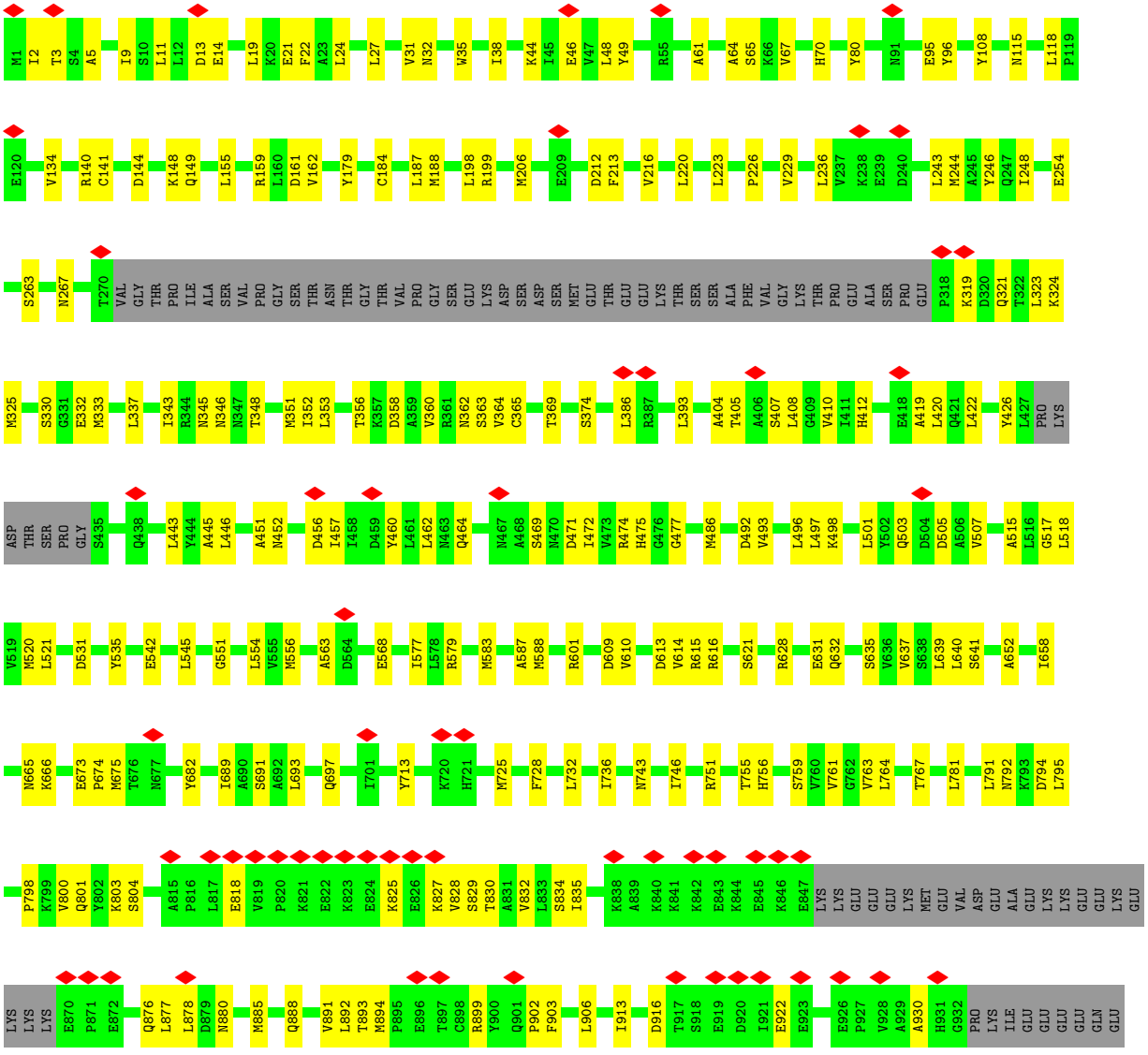
Mol	Chain	Residues	Atoms	AltConf
37	D	1	Total C N O P 27 10 5 10 2	0
37	E	1	Total C N O P 27 10 5 10 2	0

3 Residue-property plots (i)

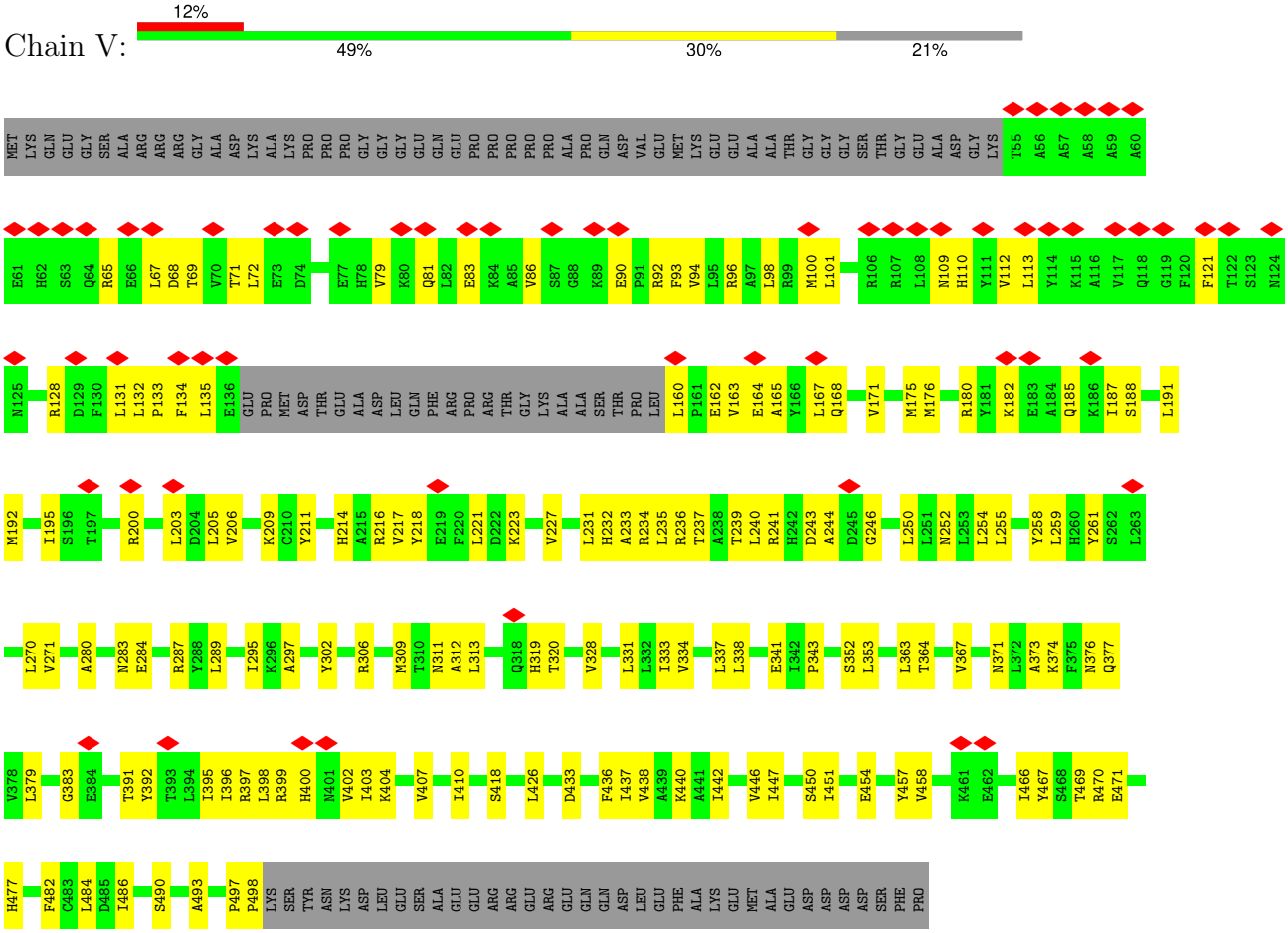
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

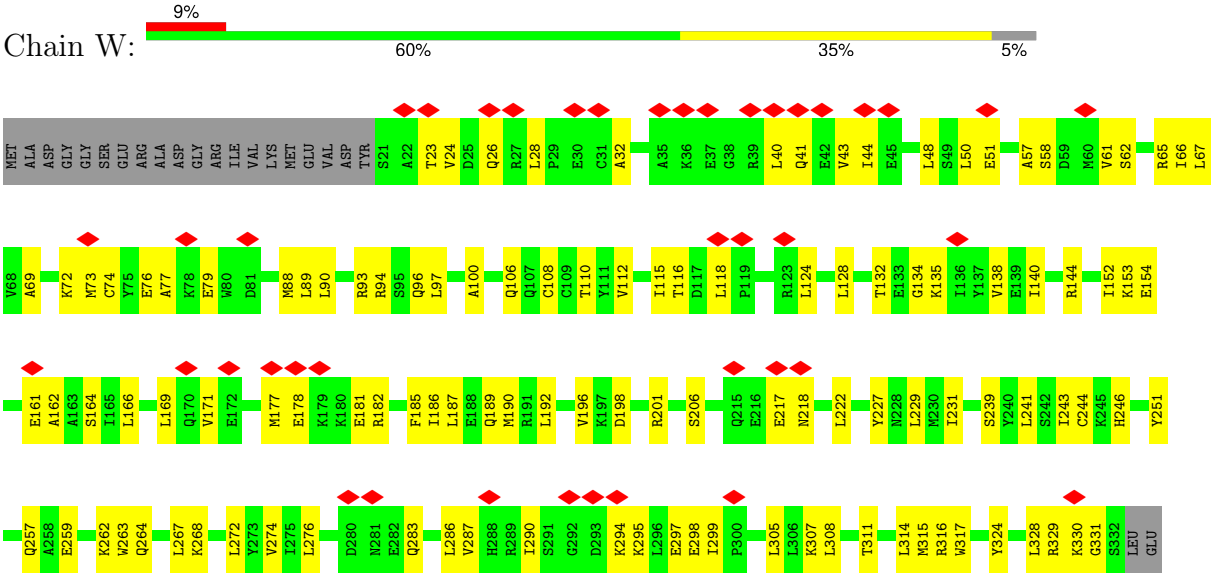
Chain U:



• Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

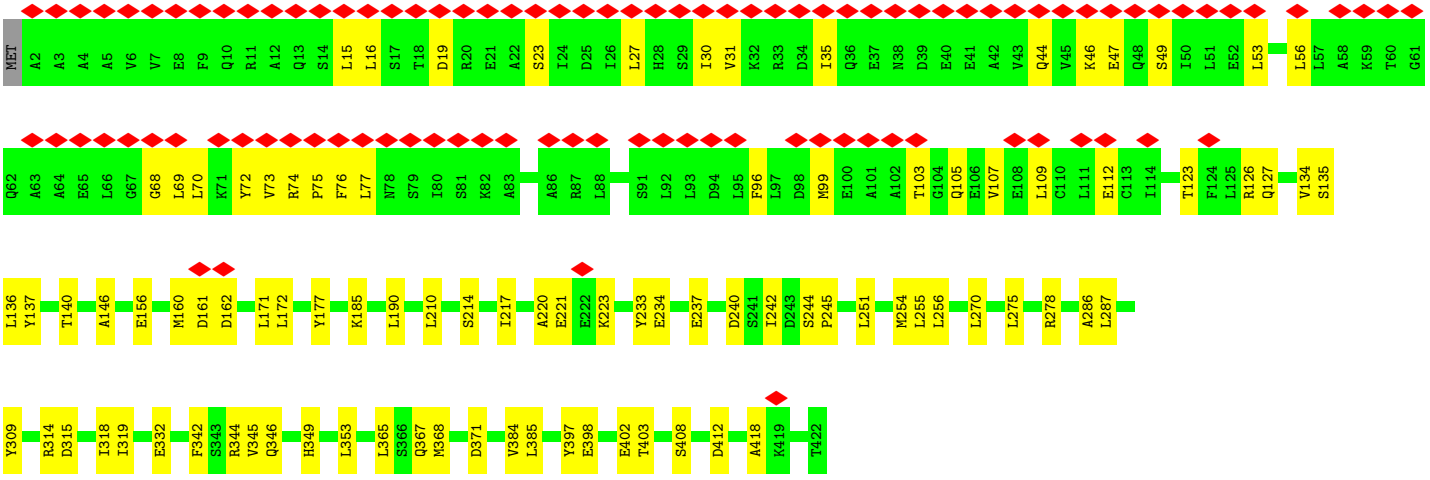


• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12



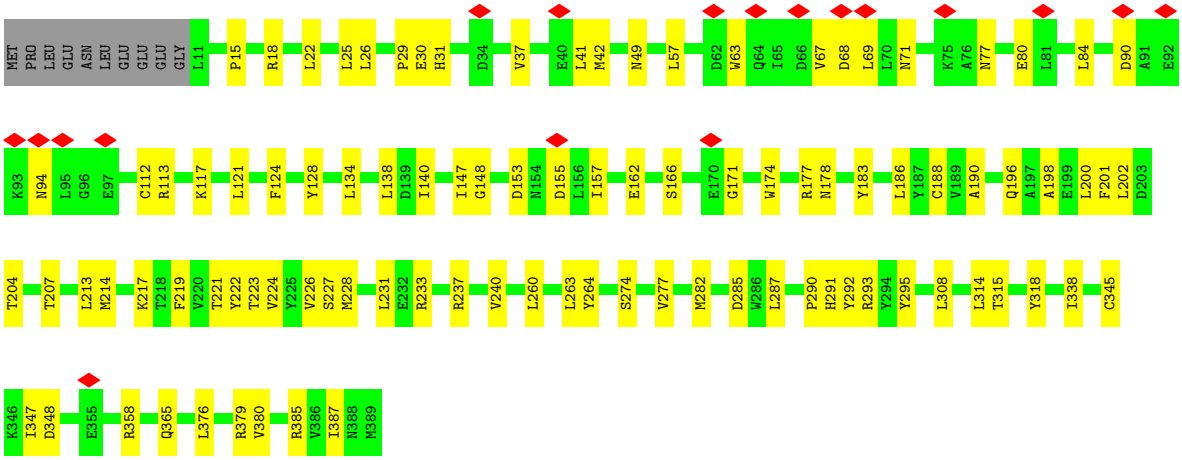
• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

Chain X:



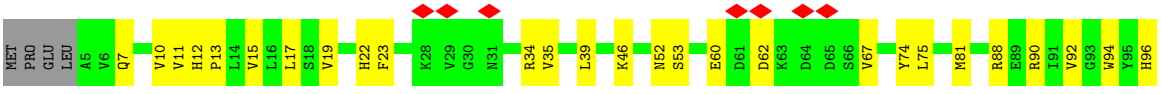
• Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

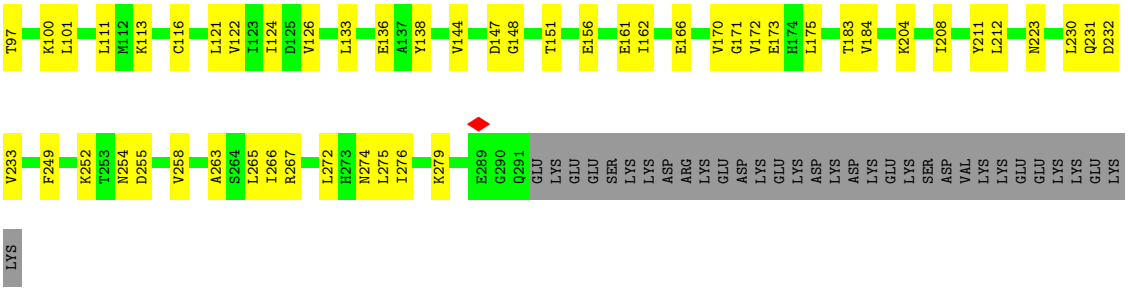
Chain Y:



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

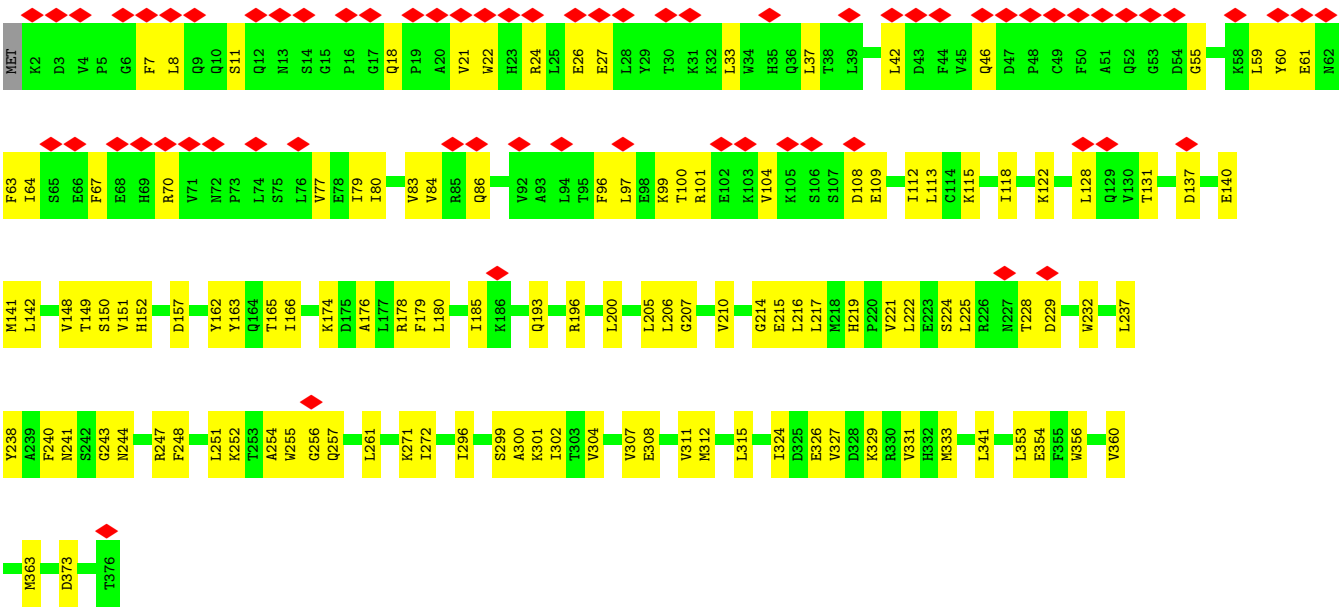
Chain Z:





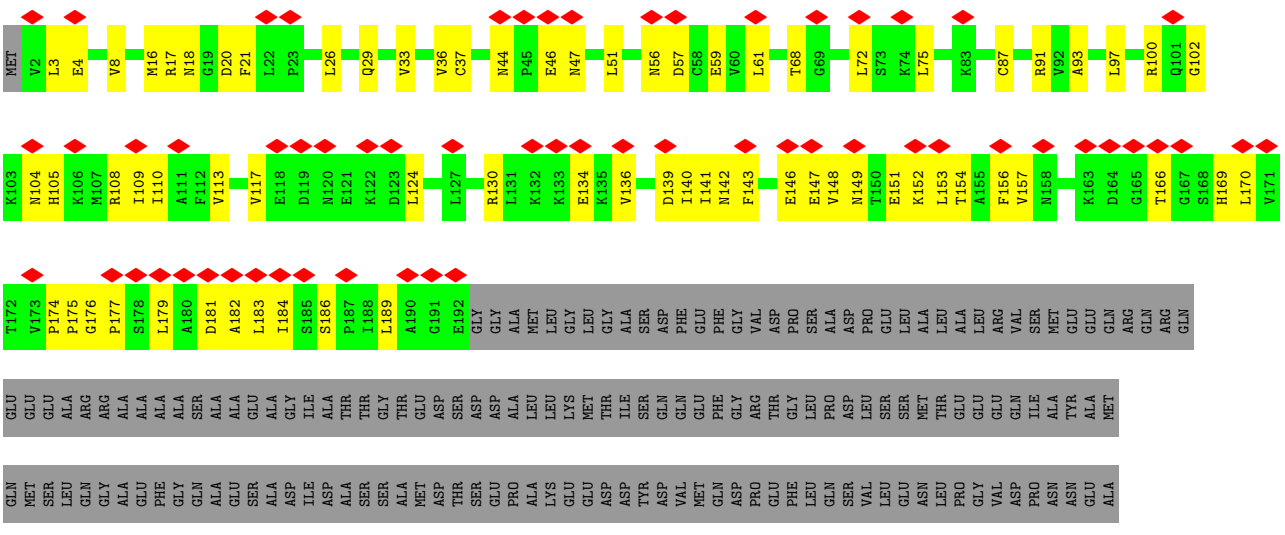
• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

Chain a:



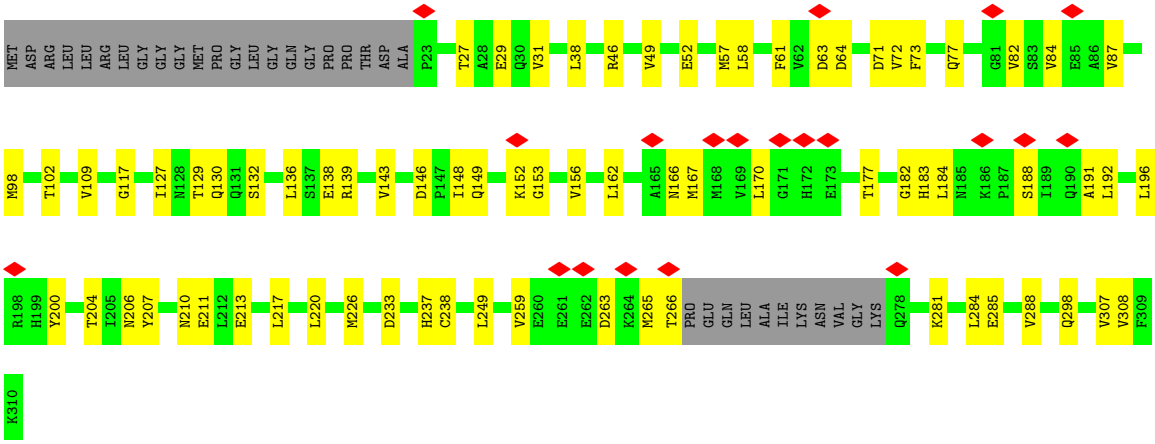
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

Chain b:



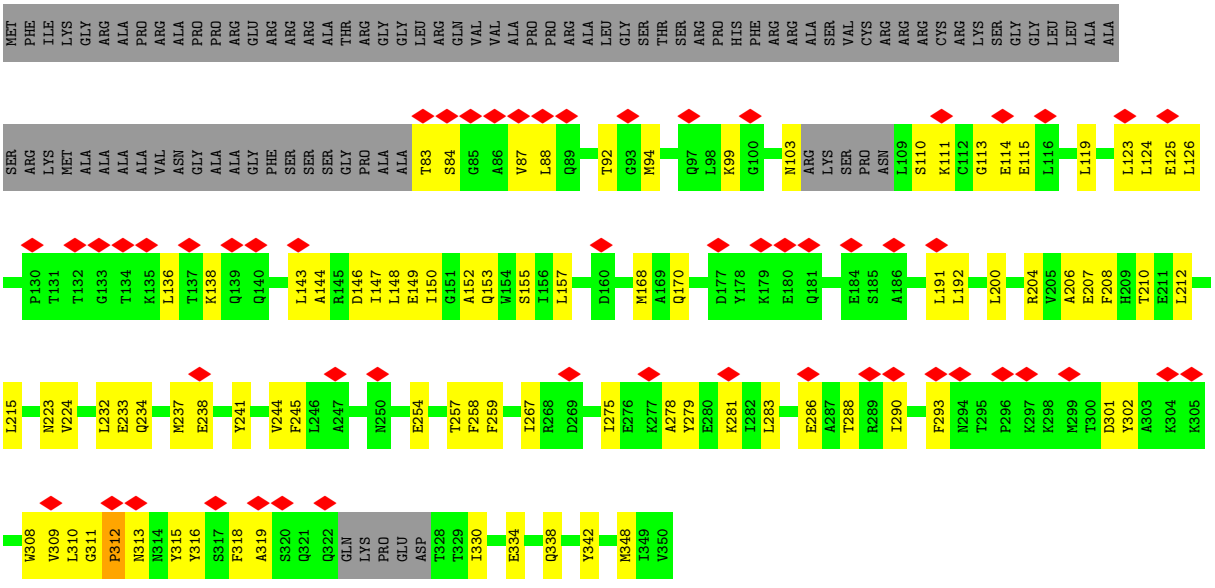
• Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

Chain c:



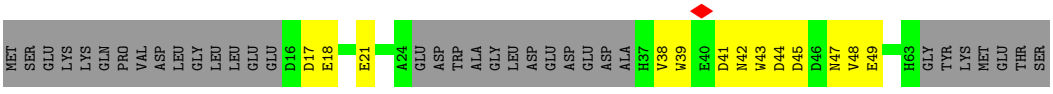
• Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

Chain d:



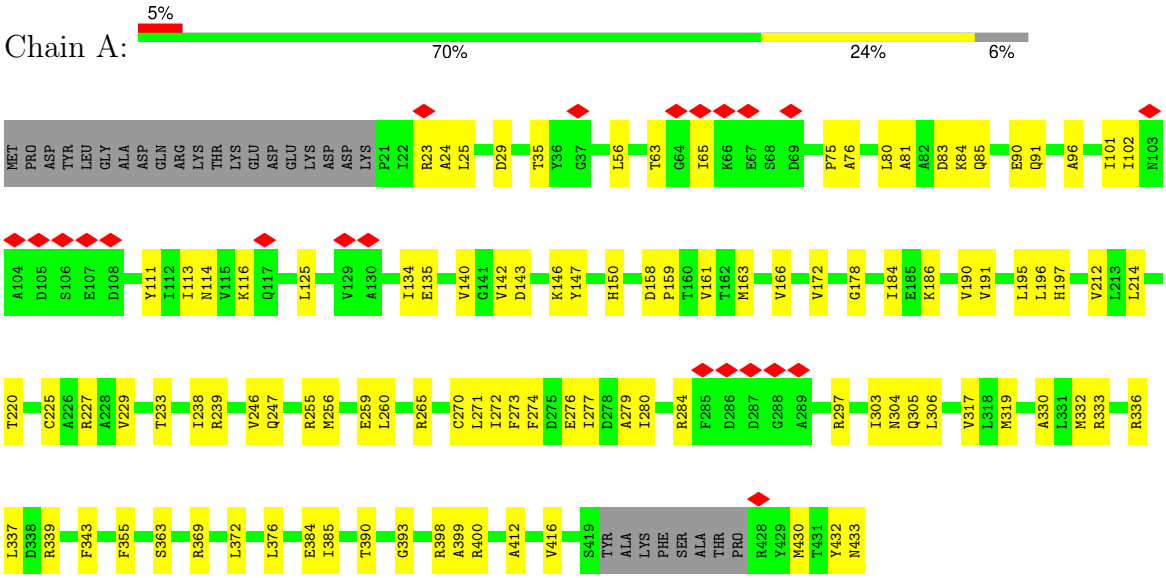
• Molecule 11: 26S proteasome complex subunit SEM1

Chain e:



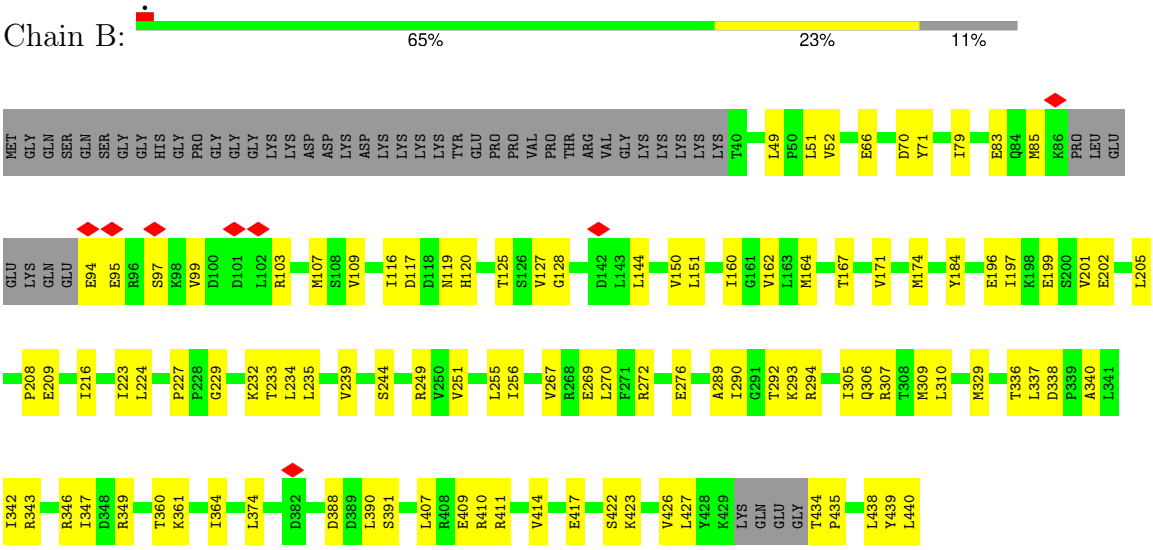
• Molecule 12: 26S proteasome regulatory subunit 7

Chain A:



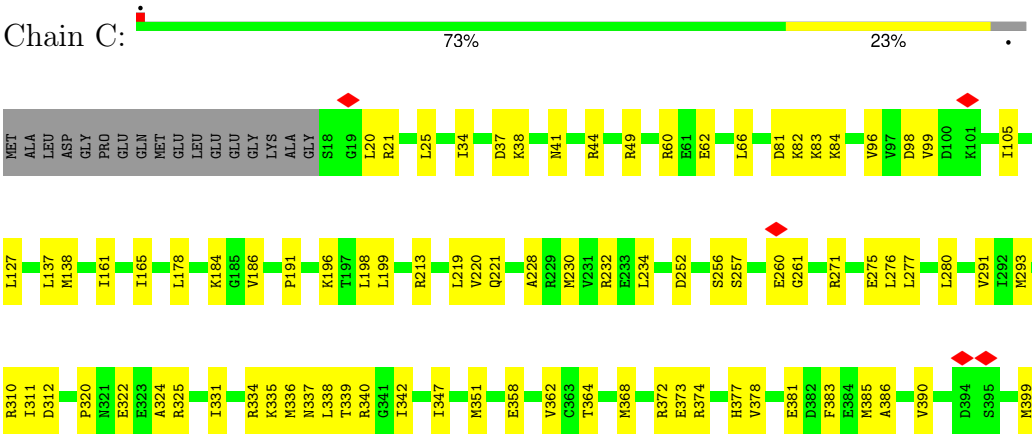
• Molecule 13: 26S proteasome regulatory subunit 4

Chain B:



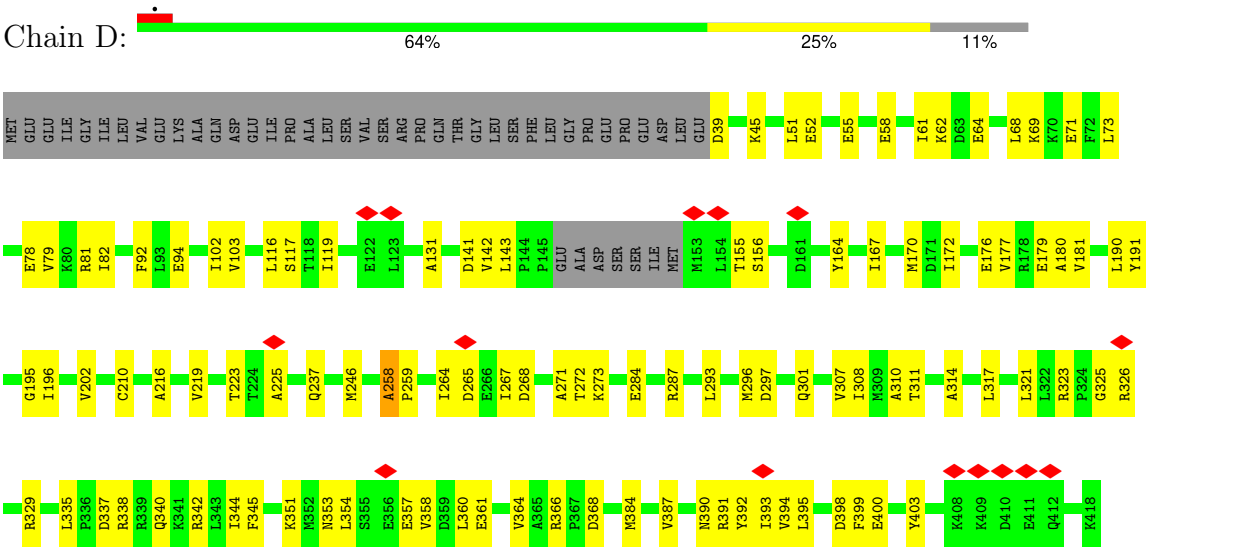
• Molecule 14: 26S protease regulatory subunit 8

Chain C:



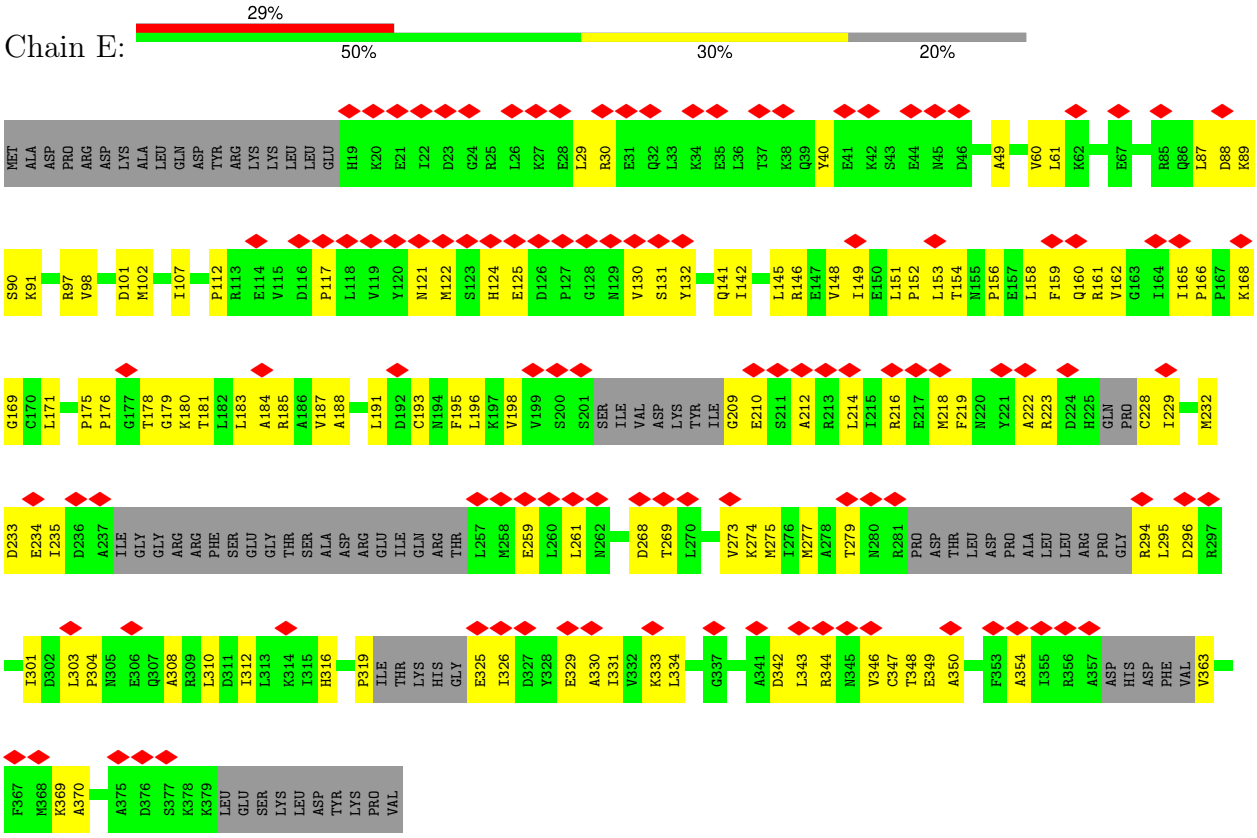
• Molecule 15: 26S proteasome regulatory subunit 6B

Chain D:



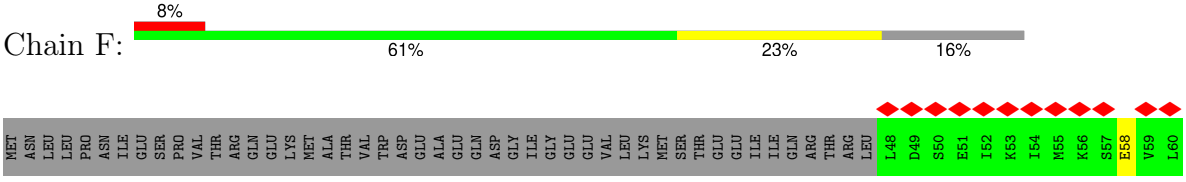
• Molecule 16: 26S protease regulatory subunit 10B

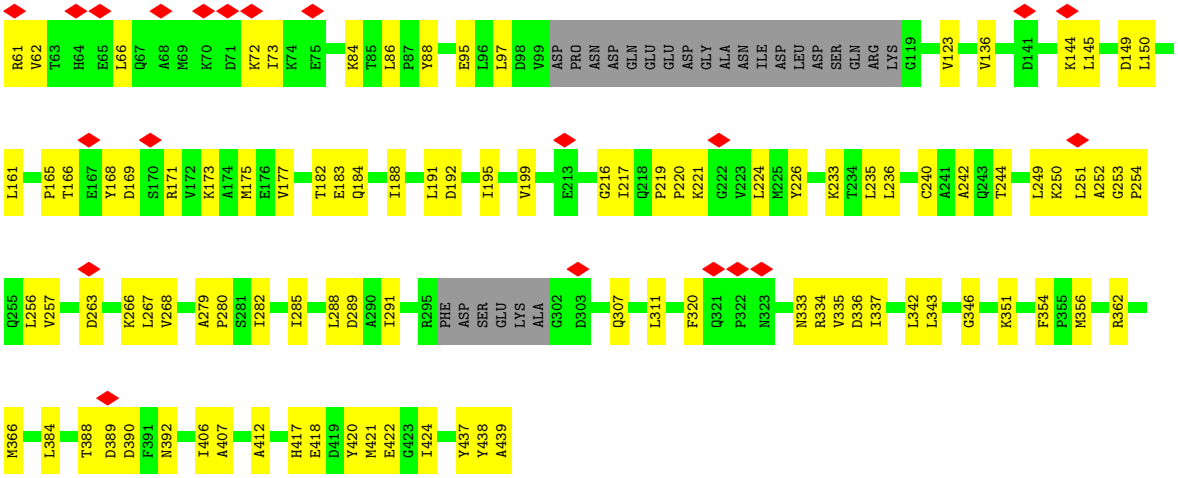
Chain E:



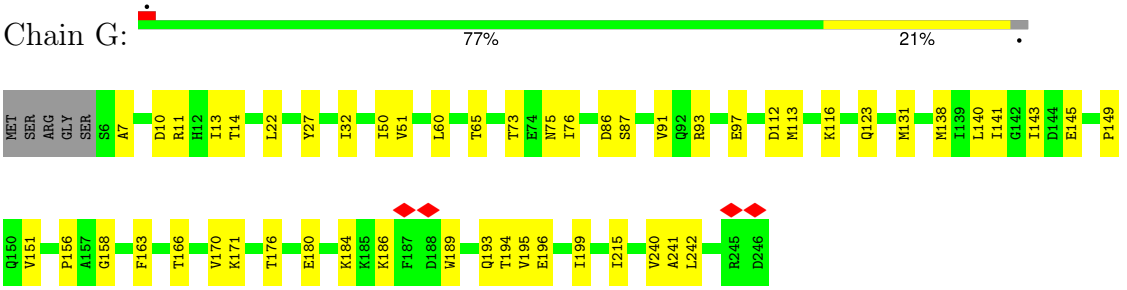
• Molecule 17: 26S proteasome regulatory subunit 6A

Chain F:

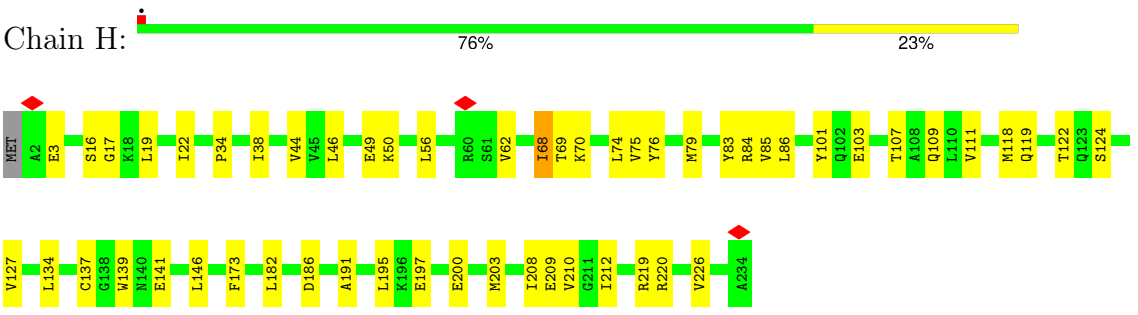




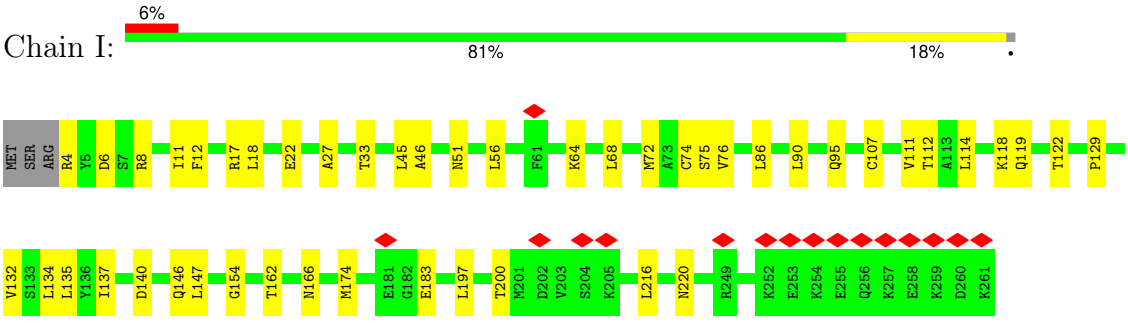
• Molecule 18: Proteasome subunit alpha type-6



• Molecule 19: Proteasome subunit alpha type-2

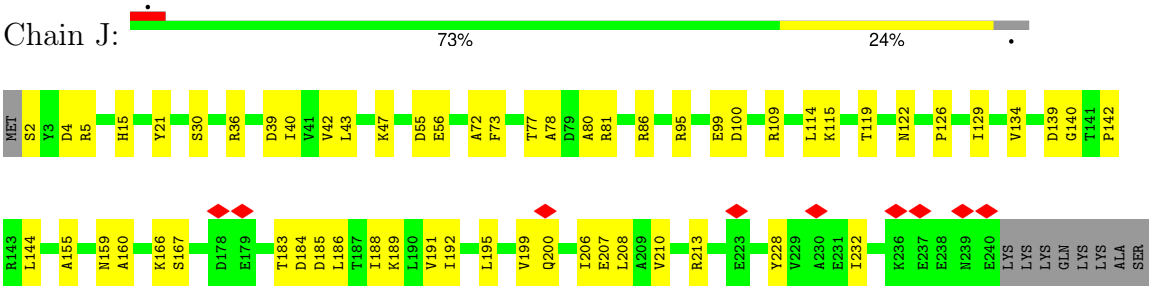


• Molecule 20: Proteasome subunit alpha type-4



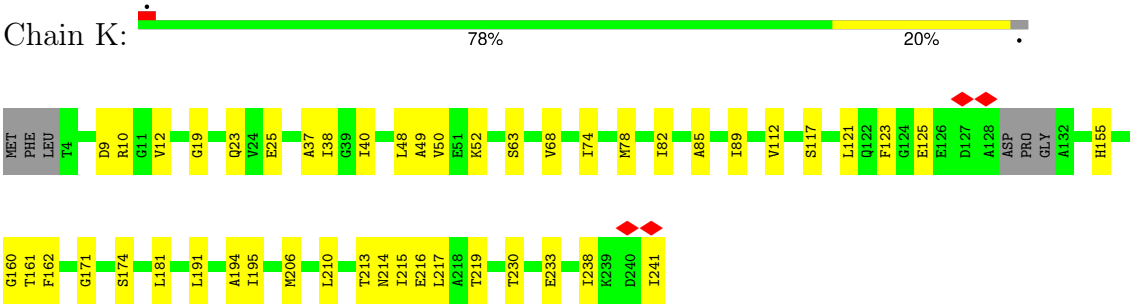
• Molecule 21: Proteasome subunit alpha type-7

Chain J:



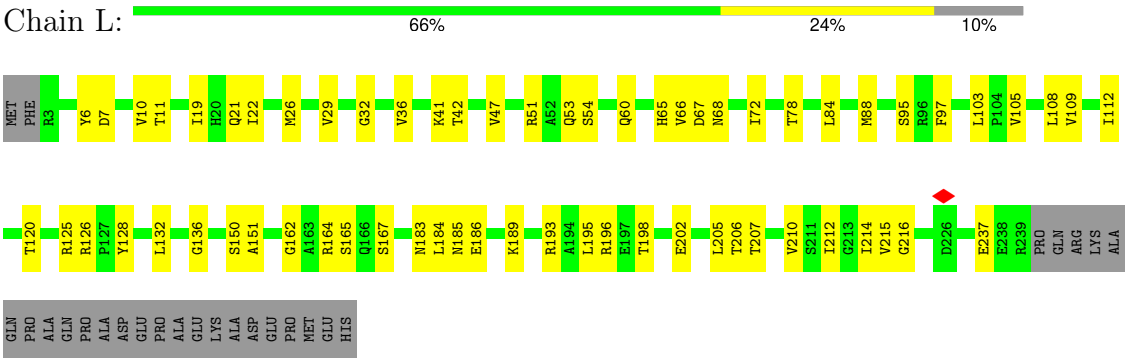
• Molecule 22: Proteasome subunit alpha type-5

Chain K:



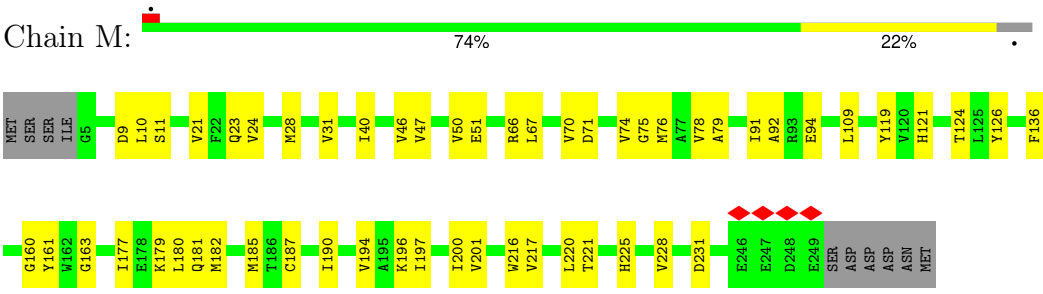
• Molecule 23: Proteasome subunit alpha type-1

Chain L:



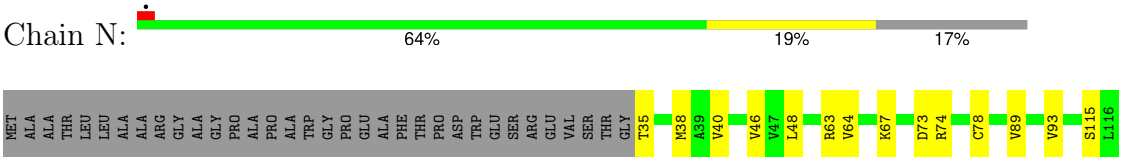
• Molecule 24: Proteasome subunit alpha type-3

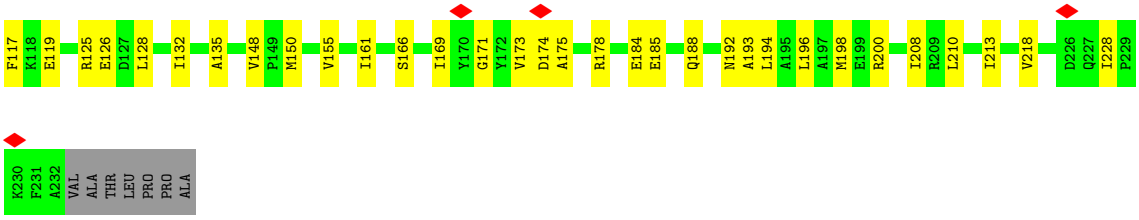
Chain M:



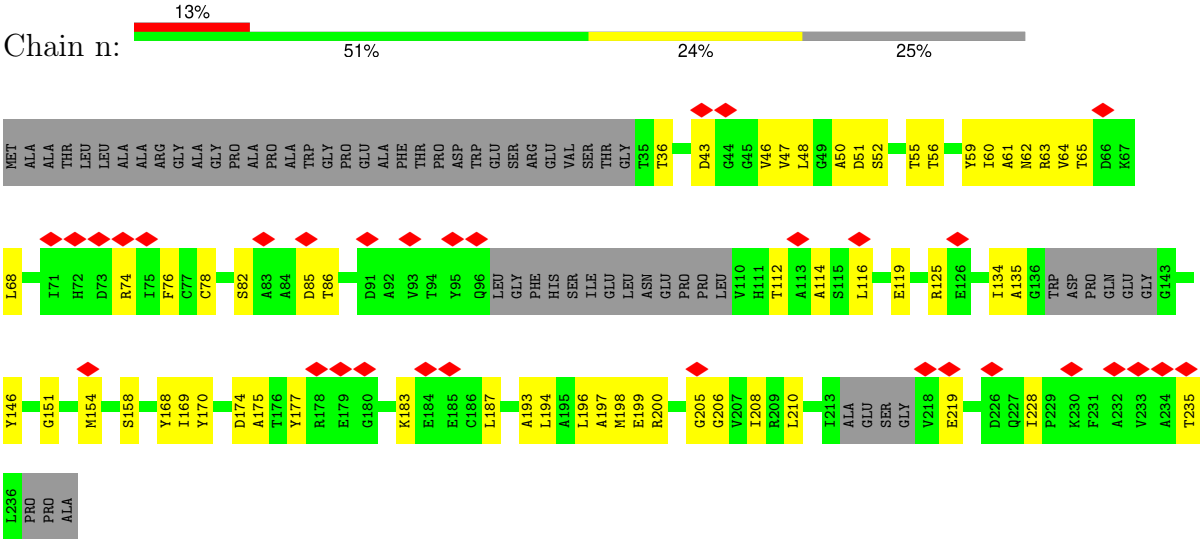
• Molecule 25: Proteasome subunit beta type-6

Chain N:

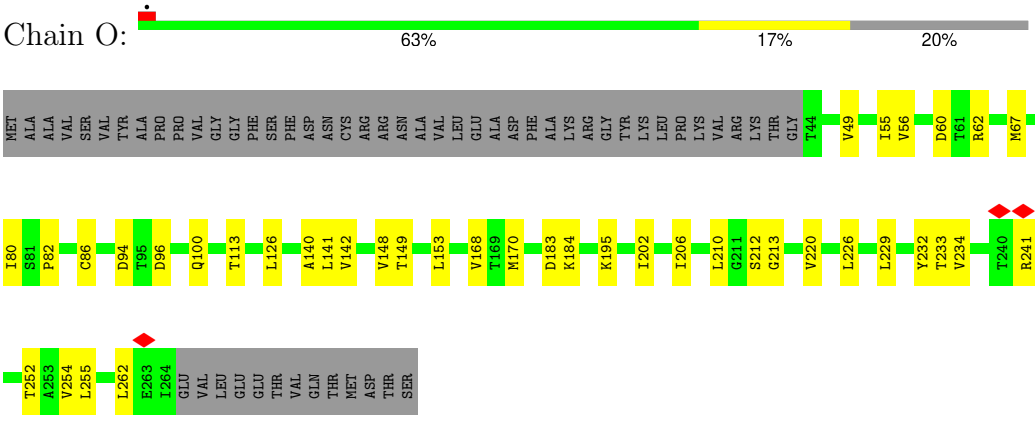




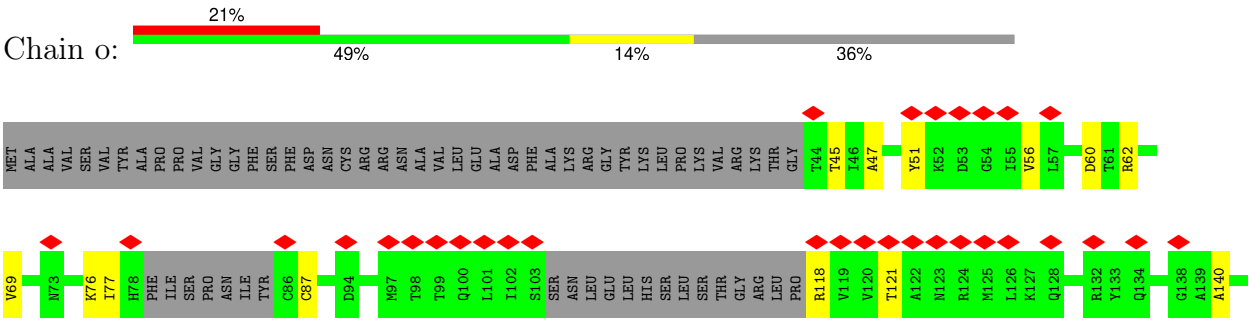
• Molecule 25: Proteasome subunit beta type-6

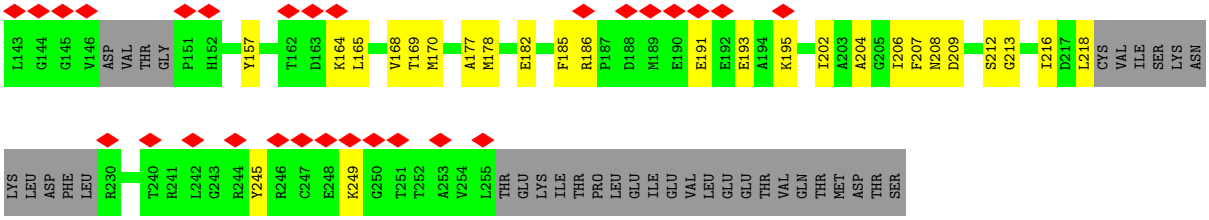


• Molecule 26: Proteasome subunit beta type-7



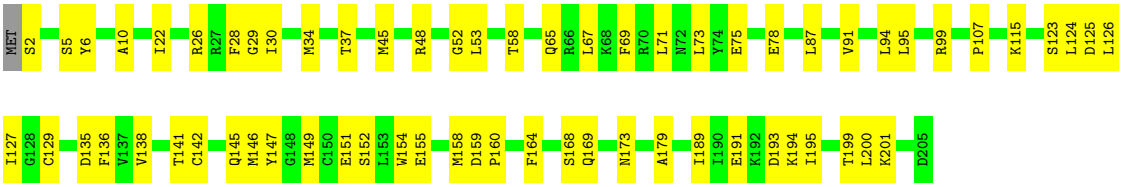
• Molecule 26: Proteasome subunit beta type-7





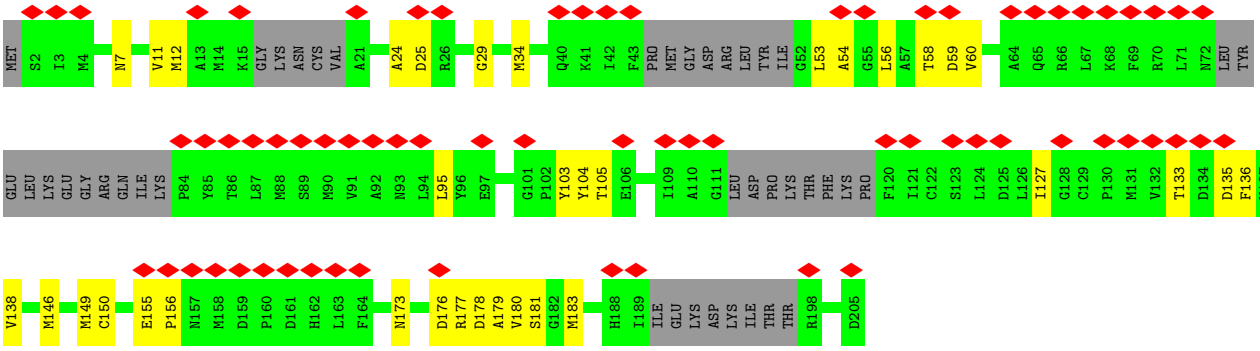
• Molecule 27: Proteasome subunit beta type-3

Chain P:



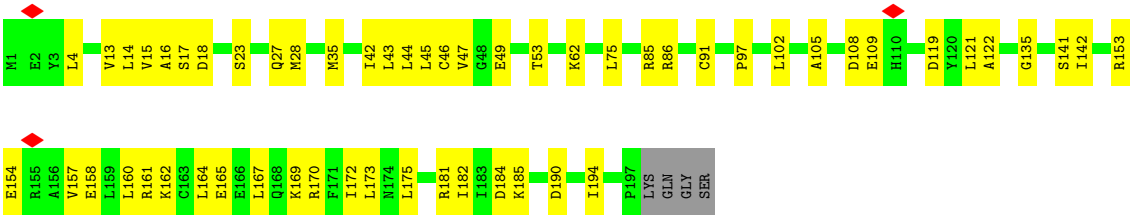
• Molecule 27: Proteasome subunit beta type-3

Chain p:



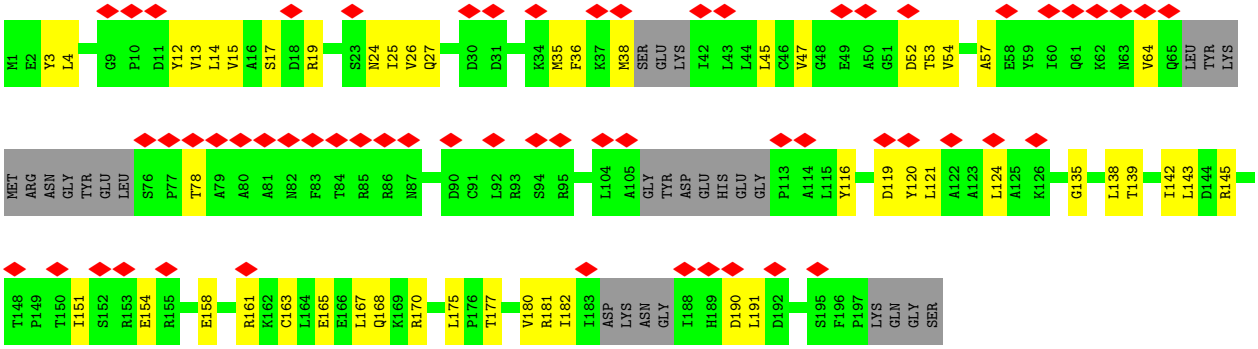
• Molecule 28: Proteasome subunit beta type-2

Chain Q:



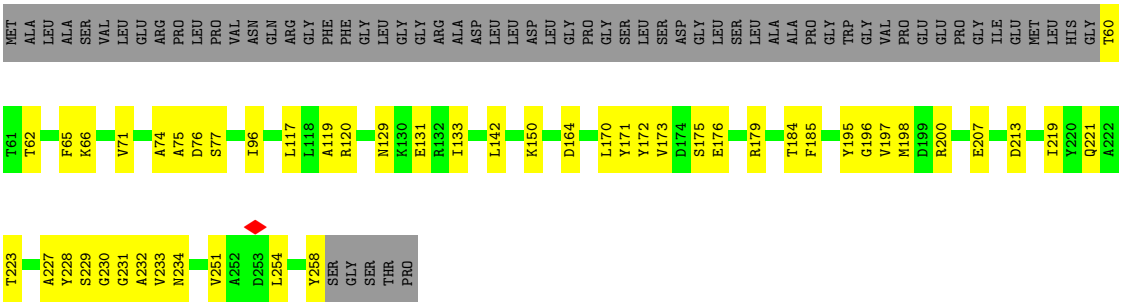
• Molecule 28: Proteasome subunit beta type-2

Chain q:



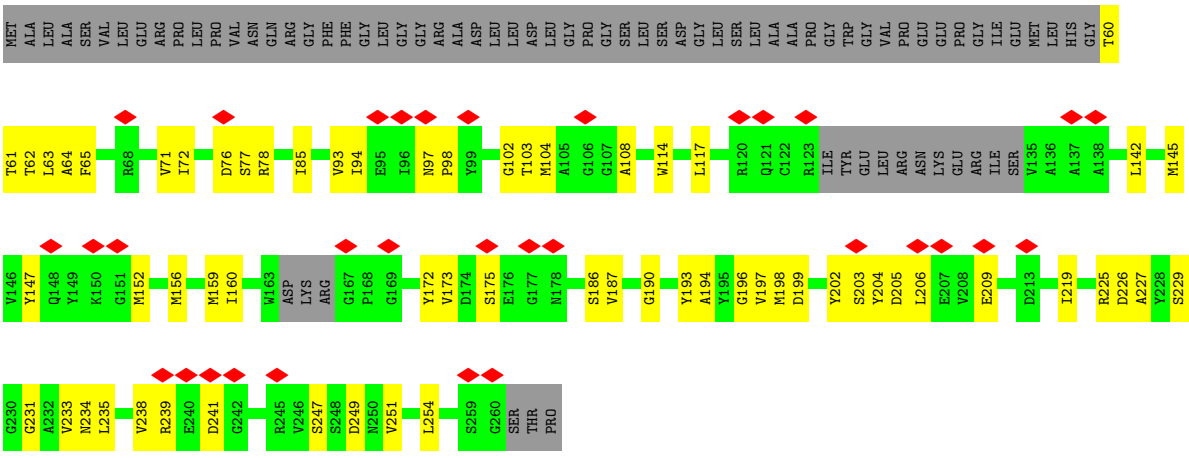
• Molecule 29: Proteasome subunit beta type-5

Chain R:



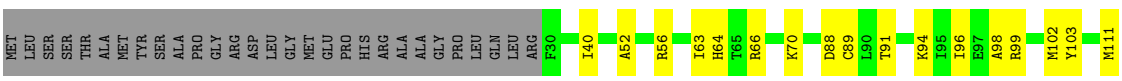
• Molecule 29: Proteasome subunit beta type-5

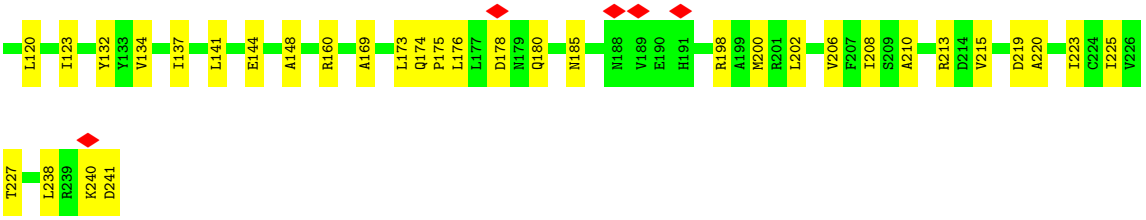
Chain r:



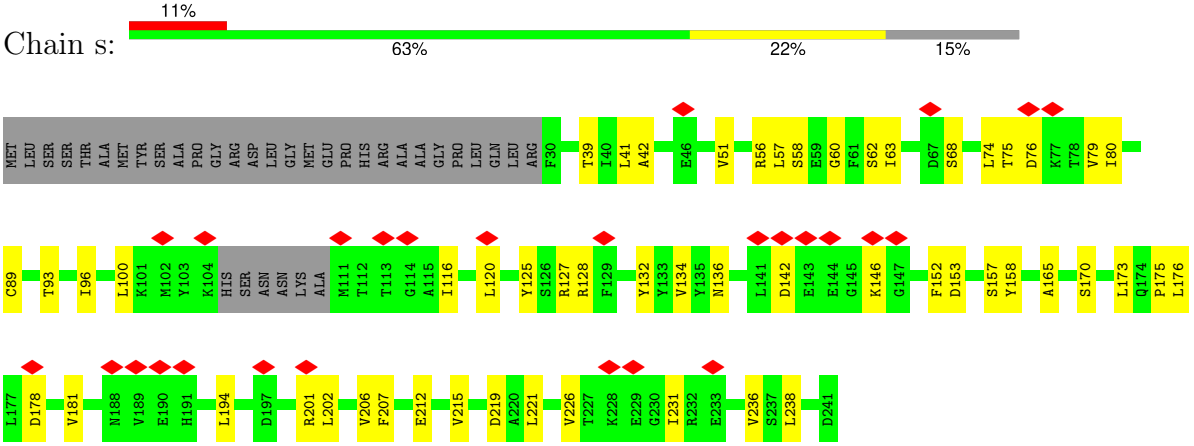
• Molecule 30: Proteasome subunit beta type-1

Chain S:

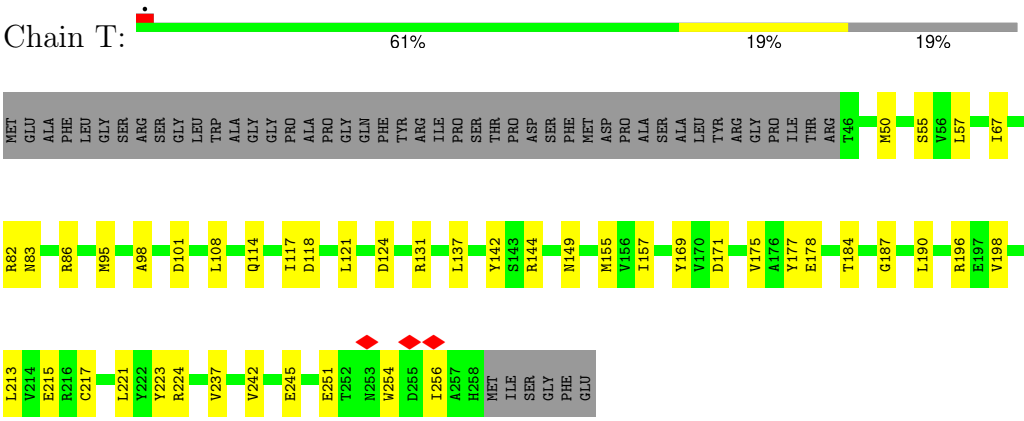




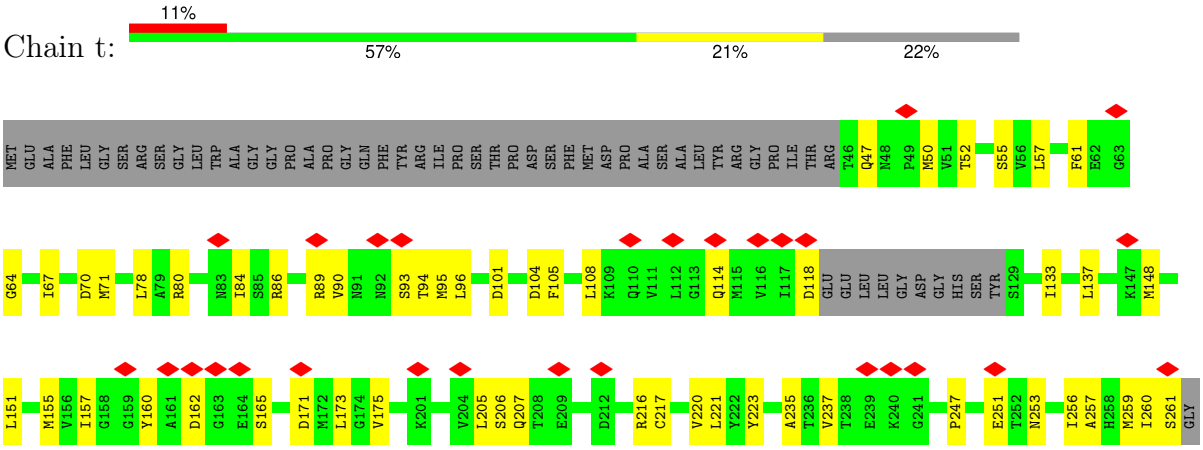
• Molecule 30: Proteasome subunit beta type-1



• Molecule 31: Proteasome subunit beta type-4



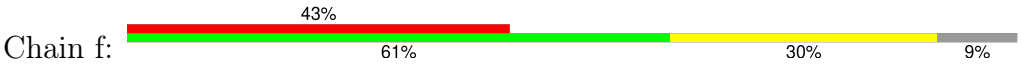
• Molecule 31: Proteasome subunit beta type-4

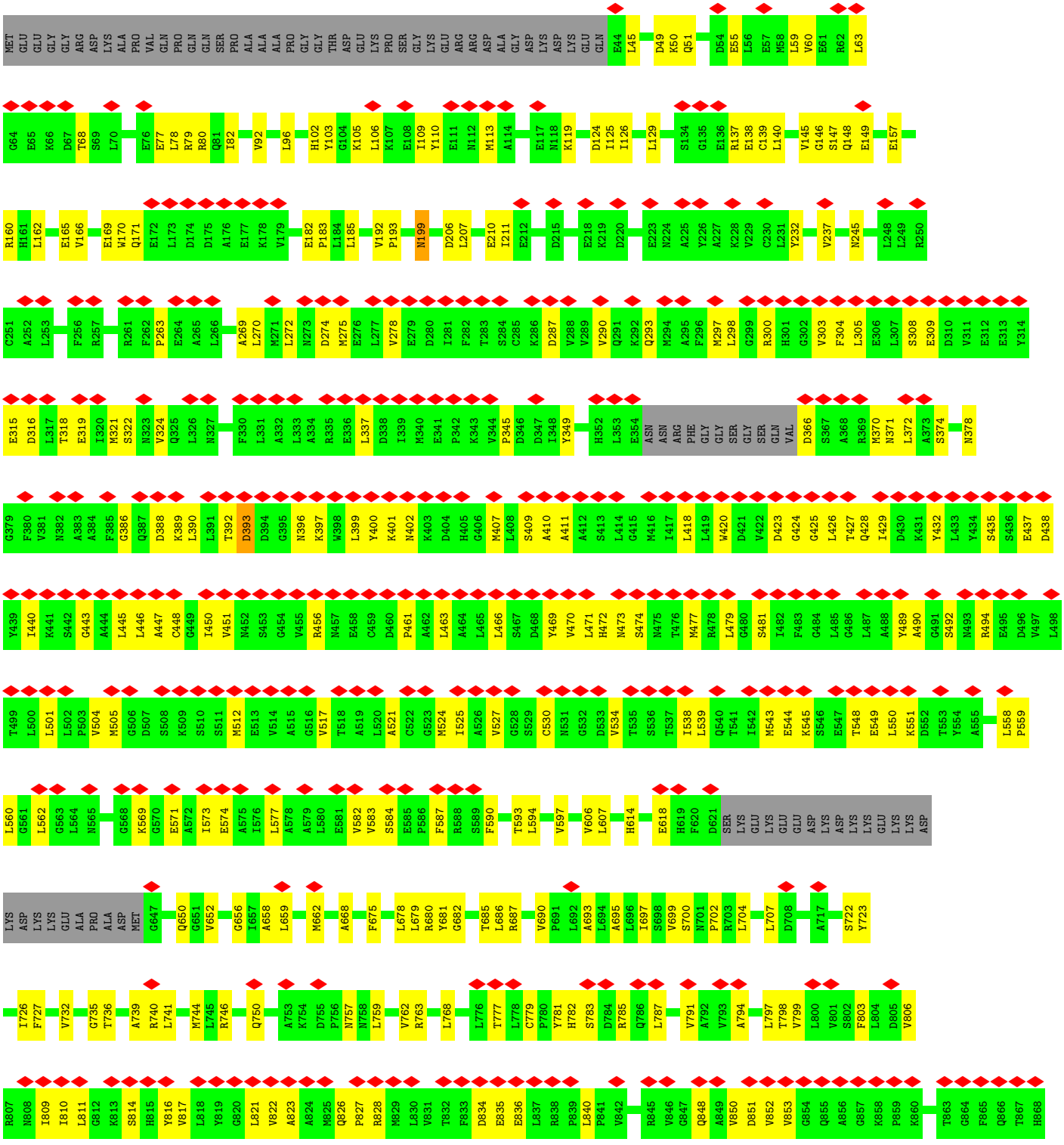


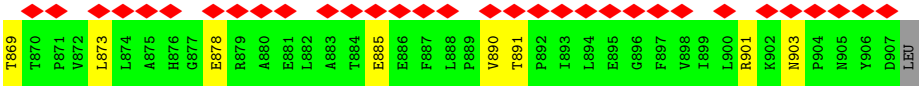
PHE
GLU

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

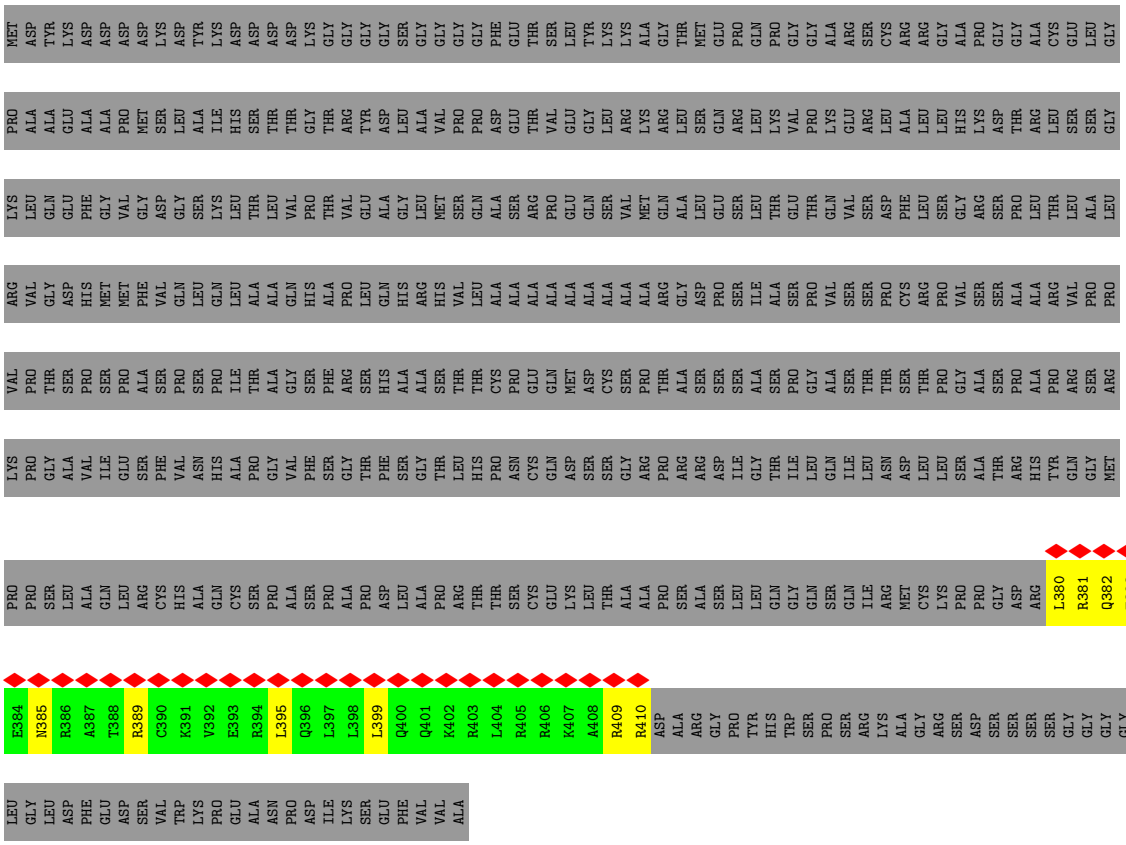
Chain f:







- Molecule 33: Midnolin



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	186489	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.445	Depositor
Minimum map value	-1.349	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	363.0, 363.0, 363.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	U	0.13	0/6791	0.29	0/9181
2	V	0.17	0/3499	0.35	0/4722
3	W	0.16	0/3581	0.35	0/4814
4	X	0.15	0/3373	0.29	0/4548
5	Y	0.17	0/3181	0.31	0/4285
6	Z	0.16	0/2333	0.30	0/3162
7	a	0.17	0/3070	0.36	0/4155
8	b	0.12	0/1479	0.31	0/2003
9	c	0.16	0/2225	0.33	0/3005
10	d	0.16	0/2141	0.36	0/2891
11	e	0.17	0/322	0.31	0/436
12	A	0.21	0/3233	0.40	0/4362
13	B	0.18	0/3109	0.33	0/4193
14	C	0.18	0/3112	0.32	0/4182
15	D	0.17	0/3039	0.35	0/4098
16	E	0.15	0/2498	0.37	0/3350
17	F	0.16	0/2907	0.36	0/3915
18	G	0.20	0/1919	0.33	0/2593
19	H	0.20	0/1857	0.35	1/2514 (0.0%)
20	I	0.19	0/2074	0.30	0/2786
21	J	0.19	0/1913	0.33	0/2581
22	K	0.19	0/1830	0.32	0/2468
23	L	0.18	0/1902	0.33	0/2569
24	M	0.18	0/1955	0.30	0/2632
25	N	0.17	0/1513	0.32	0/2047
25	n	0.14	0/1352	0.29	0/1822
26	O	0.18	0/1694	0.32	0/2293
26	o	0.13	0/1331	0.30	0/1791
27	P	0.18	0/1620	0.33	0/2184
27	p	0.13	0/1282	0.33	0/1722
28	Q	0.18	0/1611	0.35	0/2180
28	q	0.14	0/1405	0.31	0/1899

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
29	R	0.16	0/1580	0.30	0/2134
29	r	0.14	0/1460	0.34	0/1972
30	S	0.15	0/1673	0.32	0/2254
30	s	0.14	0/1625	0.31	0/2188
31	T	0.16	0/1698	0.31	0/2299
31	t	0.14	0/1639	0.32	0/2217
32	f	0.19	0/6521	0.41	0/8829
33	y	0.15	0/272	0.38	0/357
All	All	0.17	0/91619	0.34	1/123633 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	H	68	ILE	N-CA-C	-5.30	108.67	113.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	6676	0	6735	175	0
2	V	3434	0	3503	147	0
3	W	3535	0	3658	141	0
4	X	3327	0	3423	76	0
5	Y	3123	0	3130	77	0
6	Z	2290	0	2320	92	0
7	a	3012	0	3029	119	0
8	b	1459	0	1499	50	0
9	c	2184	0	2191	73	0
10	d	2099	0	2127	79	0
11	e	314	0	247	12	0
12	A	3183	0	3239	115	0
13	B	3065	0	3129	131	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	C	3071	0	3192	85	0
15	D	2990	0	3030	100	0
16	E	2469	0	2532	99	0
17	F	2870	0	2964	103	0
18	G	1885	0	1889	46	0
19	H	1818	0	1811	50	0
20	I	2044	0	2069	43	0
21	J	1887	0	1905	53	0
22	K	1804	0	1789	38	0
23	L	1868	0	1858	53	0
24	M	1920	0	1893	47	0
25	N	1487	0	1452	37	0
25	n	1336	0	1324	52	0
26	O	1667	0	1689	50	0
26	o	1315	0	1321	31	0
27	P	1591	0	1609	58	0
27	p	1264	0	1255	29	0
28	Q	1578	0	1580	50	0
28	q	1380	0	1399	42	0
29	R	1549	0	1512	42	0
29	r	1432	0	1384	55	0
30	S	1643	0	1640	40	0
30	s	1597	0	1597	43	0
31	T	1665	0	1638	42	0
31	t	1609	0	1597	50	0
32	f	6412	0	6433	239	0
33	y	273	0	309	11	0
34	c	1	0	0	0	0
35	A	31	0	12	3	0
35	B	31	0	12	4	0
35	C	31	0	12	4	0
35	F	31	0	12	6	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
37	D	27	0	12	1	0
37	E	27	0	12	2	0
All	All	90308	0	90973	2513	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (2513) 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)
13:B:244:SER:OG	32:f:704:LEU:HD12	1.36	1.23
12:A:25:LEU:HD23	13:B:410:ARG:CZ	1.72	1.19
1:U:179:TYR:HH	15:D:39:ASP:N	1.47	1.13
29:r:60:THR:N	29:r:229:SER:HG	1.51	1.08
12:A:23:ARG:HE	13:B:410:ARG:CG	1.72	1.02
12:A:23:ARG:HE	13:B:410:ARG:HG3	1.22	1.01
12:A:29:ASP:OD2	13:B:410:ARG:NE	1.91	1.00
23:L:164:ARG:O	23:L:198:THR:OG1	1.81	0.99
31:t:160:TYR:OH	31:t:237:VAL:O	1.83	0.96
32:f:316:ASP:OD1	33:y:409:ARG:NH1	1.99	0.95
32:f:315:GLU:OE1	33:y:409:ARG:NH1	2.01	0.94
13:B:244:SER:HG	32:f:704:LEU:HD12	1.19	0.92
12:A:23:ARG:NE	13:B:410:ARG:HG3	1.85	0.92
1:U:588:MET:HE3	1:U:764:LEU:HD22	1.50	0.90
1:U:639:LEU:HD22	15:D:61:ILE:HD11	1.54	0.90
28:q:52:ASP:OD1	29:r:147:TYR:OH	1.90	0.89
32:f:427:THR:OG1	32:f:428:GLN:OE1	1.90	0.89
23:L:97:PHE:O	30:S:94:LYS:NZ	2.06	0.89
17:F:362:ARG:NE	17:F:388:THR:OG1	2.07	0.88
12:A:25:LEU:CD2	13:B:410:ARG:CZ	2.50	0.88
3:W:51:GLU:OE1	3:W:93:ARG:NH1	2.07	0.88
21:J:2:SER:O	22:K:10:ARG:NH2	2.06	0.87
17:F:438:TYR:OH	22:K:19:GLY:O	1.93	0.87
32:f:505:MET:HE1	32:f:538:ILE:HD13	1.56	0.87
32:f:512:MET:SD	32:f:545:LYS:NZ	2.48	0.86
14:C:362:VAL:HG22	14:C:390:VAL:HG21	1.56	0.85
4:X:240:ASP:OD1	4:X:278:ARG:NH2	2.10	0.85
29:r:172:TYR:CE1	29:r:187:VAL:HG11	2.11	0.84
30:S:176:LEU:HD23	30:S:206:VAL:HG12	1.58	0.84
3:W:451:MET:HE3	6:Z:101:LEU:HD13	1.58	0.83
15:D:219:VAL:O	15:D:223:THR:OG1	1.96	0.83
8:b:100:ARG:NH1	8:b:102:GLY:O	2.11	0.83
23:L:72:ILE:HD11	23:L:132:LEU:HD22	1.58	0.83
4:X:237:GLU:OE1	15:D:338:ARG:NH1	2.10	0.83
19:H:46:LEU:HD22	19:H:75:VAL:HG12	1.59	0.83
30:S:173:LEU:HD11	30:S:210:ALA:HB2	1.60	0.83
31:t:96:LEU:HD21	31:t:155:MET:HE3	1.60	0.83
13:B:205:LEU:O	32:f:740:ARG:HD2	1.78	0.82
27:p:178:ASP:OD2	27:p:181:SER:OG	1.96	0.82
12:A:23:ARG:HH21	13:B:410:ARG:CG	1.91	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:199:ASN:O	32:f:199:ASN:ND2	2.10	0.82
15:D:284:GLU:OE1	15:D:287:ARG:NH1	2.12	0.82
25:N:174:ASP:OD2	25:n:200:ARG:NE	2.12	0.82
30:s:176:LEU:HD23	30:s:206:VAL:HG12	1.61	0.81
1:U:27:LEU:O	1:U:31:VAL:HG23	1.80	0.81
2:V:367:VAL:HG23	2:V:402:VAL:HG22	1.60	0.81
32:f:501:LEU:O	32:f:504:VAL:HG12	1.79	0.81
21:J:109:ARG:NH2	29:R:129:ASN:OD1	2.14	0.81
3:W:118:LEU:HD23	3:W:152:ILE:HG23	1.63	0.81
25:n:158:SER:HG	25:n:177:TYR:HH	0.87	0.81
26:o:140:ALA:HB1	26:o:170:MET:SD	2.21	0.81
17:F:221:LYS:NZ	17:F:346:GLY:O	2.11	0.81
1:U:321:GLN:OE1	1:U:324:LYS:NZ	2.11	0.80
15:D:391:ARG:NH1	15:D:398:ASP:OD2	2.14	0.80
28:Q:27:GLN:O	28:q:170:ARG:NH1	2.14	0.80
14:C:347:ILE:HG22	14:C:351:MET:HE2	1.64	0.80
23:L:26:MET:O	23:L:29:VAL:HG12	1.82	0.80
25:n:51:ASP:OD2	25:n:205:GLY:N	2.15	0.80
13:B:205:LEU:O	32:f:740:ARG:CD	2.30	0.80
17:F:418:GLU:OE2	23:L:167:SER:OG	2.00	0.80
29:r:60:THR:N	29:r:229:SER:OG	2.13	0.80
1:U:825:LYS:CB	13:B:85:MET:SD	2.70	0.79
4:X:233:TYR:OH	15:D:361:GLU:OE2	2.00	0.79
1:U:825:LYS:HB2	13:B:85:MET:SD	2.23	0.79
32:f:396:ASN:N	32:f:432:TYR:OH	2.14	0.79
15:D:268:ASP:OD1	15:D:311:THR:OG1	2.00	0.79
6:Z:74:TYR:HH	9:c:102:THR:HG1	1.31	0.79
10:d:223:ASN:OD1	10:d:224:VAL:N	2.16	0.79
14:C:252:ASP:OD2	14:C:297:ARG:NH1	2.16	0.79
28:Q:184:ASP:OD1	28:Q:185:LYS:N	2.14	0.79
15:D:258:ALA:HB1	15:D:259:PRO:HD2	1.62	0.78
1:U:356:THR:O	1:U:360:VAL:HG23	1.81	0.78
32:f:885:GLU:OE2	32:f:903:ASN:ND2	2.15	0.78
11:e:41:ASP:OD1	11:e:42:ASN:N	2.16	0.78
6:Z:74:TYR:OH	9:c:102:THR:OG1	2.01	0.78
30:S:56:ARG:NH2	30:S:241:ASP:O	2.17	0.77
32:f:400:TYR:O	32:f:401:LYS:HG2	1.84	0.77
8:b:36:VAL:HG23	8:b:189:LEU:HD11	1.64	0.77
17:F:420:TYR:O	17:F:424:ILE:HD12	1.84	0.77
13:B:272:ARG:NH1	13:B:276:GLU:OE2	2.16	0.77
23:L:6:TYR:OH	24:M:9:ASP:OD2	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:T:190:LEU:HD11	31:T:221:LEU:HD23	1.66	0.77
15:D:177:VAL:O	15:D:181:VAL:HG22	1.83	0.77
25:n:125:ARG:NH1	25:n:151:GLY:O	2.18	0.77
8:b:166:THR:O	8:b:169:HIS:NE2	2.18	0.77
30:S:213:ARG:O	26:o:69:VAL:HG12	1.85	0.77
15:D:167:ILE:HG21	15:D:170:MET:HE2	1.67	0.77
29:R:60:THR:N	29:R:228:TYR:O	2.18	0.77
2:V:167:LEU:O	2:V:171:VAL:HG23	1.84	0.77
28:Q:35:MET:SD	28:Q:45:LEU:HD21	2.25	0.77
32:f:319:GLU:OE1	33:y:409:ARG:NH2	2.18	0.77
26:o:45:THR:OG1	26:o:212:SER:OG	1.99	0.77
21:J:159:ASN:OD1	21:J:160:ALA:N	2.18	0.76
16:E:122:MET:HE2	16:E:214:LEU:HD12	1.66	0.76
17:F:439:ALA:OXT	23:L:60:GLN:NE2	2.18	0.76
28:Q:153:ARG:NH2	28:Q:184:ASP:OD2	2.17	0.76
1:U:49:TYR:CE1	1:U:61:ALA:HB2	2.20	0.76
7:a:240:PHE:CD1	7:a:272:ILE:HD13	2.21	0.76
31:t:95:MET:HE1	31:t:235:ALA:O	1.85	0.76
18:G:93:ARG:NH1	18:G:97:GLU:OE2	2.19	0.76
21:J:73:PHE:CZ	21:J:80:ALA:HB2	2.21	0.76
6:Z:266:ILE:CG2	9:c:284:LEU:HD21	2.16	0.76
25:n:125:ARG:NH2	31:t:101:ASP:OD2	2.19	0.76
2:V:440:LYS:NZ	10:d:237:MET:O	2.19	0.76
3:W:451:MET:HE3	6:Z:101:LEU:CD1	2.15	0.76
29:r:233:VAL:HG21	29:r:254:LEU:HD12	1.68	0.76
18:G:113:MET:HE2	18:G:113:MET:HA	1.66	0.75
27:P:58:THR:OG1	28:Q:121:LEU:O	2.02	0.75
32:f:103:TYR:OH	32:f:138:GLU:OE1	2.02	0.75
14:C:293:MET:SD	14:C:311:ILE:HD11	2.26	0.75
32:f:45:LEU:HD12	32:f:50:LYS:HD3	1.67	0.75
24:M:40:ILE:HD13	24:M:194:VAL:HG22	1.67	0.75
32:f:79:ARG:NE	32:f:124:ASP:OD2	2.18	0.75
1:U:404:ALA:O	1:U:407:SER:OG	2.04	0.75
3:W:406:VAL:HG12	3:W:413:ILE:HG12	1.69	0.75
12:A:247:GLN:NE2	12:A:256:MET:SD	2.59	0.74
7:a:232:TRP:CZ2	7:a:254:ALA:HB3	2.22	0.74
31:t:50:MET:O	31:t:52:THR:HG23	1.86	0.74
21:J:228:TYR:O	21:J:232:ILE:HD12	1.87	0.74
17:F:183:GLU:OE1	17:F:183:GLU:N	2.18	0.74
3:W:314:LEU:HD13	3:W:381:LEU:HD21	1.68	0.74
23:L:212:ILE:HG22	23:L:214:ILE:HD11	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:568:GLU:OE1	1:U:601:ARG:NH2	2.20	0.74
2:V:243:ASP:OD1	2:V:244:ALA:N	2.20	0.74
29:r:247:SER:OG	29:r:249:ASP:OD1	2.05	0.74
1:U:756:HIS:ND1	1:U:759:SER:OG	2.18	0.74
32:f:680:ARG:NH2	32:f:681:TYR:OH	2.21	0.74
1:U:798:PRO:O	1:U:880:ASN:ND2	2.20	0.74
17:F:251:LEU:HD22	17:F:285:ILE:HG23	1.68	0.74
14:C:372:ARG:NH2	15:D:179:GLU:OE1	2.21	0.74
3:W:272:LEU:HD22	3:W:341:PHE:CE2	2.22	0.73
4:X:367:GLN:NE2	4:X:371:ASP:OD2	2.21	0.73
14:C:99:VAL:HG11	14:C:105:ILE:HD11	1.70	0.73
31:T:131:ARG:NH2	31:T:178:GLU:OE2	2.20	0.73
4:X:220:ALA:O	4:X:223:LYS:NZ	2.21	0.73
32:f:659:LEU:HD12	32:f:662:MET:HE3	1.70	0.73
15:D:391:ARG:NH2	15:D:395:LEU:HD13	2.04	0.73
25:n:46:VAL:HG11	25:n:135:ALA:HB1	1.70	0.73
30:s:74:LEU:HD11	30:s:80:ILE:CD1	2.19	0.73
5:Y:219:PHE:O	5:Y:223:THR:HG23	1.89	0.73
6:Z:252:LYS:NZ	9:c:238:CYS:SG	2.57	0.72
13:B:103:ARG:NH2	13:B:107:MET:HE1	2.04	0.72
22:K:125:GLU:OE1	22:K:125:GLU:N	2.22	0.72
23:L:47:VAL:HG12	23:L:195:LEU:HD11	1.69	0.72
26:O:183:ASP:OD2	26:O:184:LYS:NZ	2.23	0.72
1:U:362:ASN:OD1	1:U:363:SER:N	2.22	0.72
7:a:77:VAL:HG12	7:a:113:LEU:HD22	1.72	0.72
29:r:226:ASP:O	29:r:229:SER:N	2.22	0.72
13:B:209:GLU:HB3	32:f:739:ALA:HB2	1.69	0.72
3:W:366:MET:CE	3:W:381:LEU:HD22	2.20	0.72
3:W:451:MET:HE1	6:Z:138:TYR:OH	1.90	0.72
2:V:334:VAL:O	2:V:338:LEU:HD23	1.88	0.72
5:Y:207:THR:HG21	14:C:377:HIS:CE1	2.25	0.72
16:E:344:ARG:NH1	17:F:216:GLY:O	2.23	0.72
16:E:117:PRO:O	16:E:121:ASN:ND2	2.22	0.72
32:f:618:GLU:O	32:f:650:GLN:NE2	2.23	0.71
32:f:809:ILE:O	32:f:814:SER:OG	2.04	0.71
10:d:275:ILE:HD13	10:d:279:TYR:CD2	2.25	0.71
12:A:25:LEU:CD2	13:B:410:ARG:NE	2.53	0.71
14:C:406:LYS:O	20:I:64:LYS:NZ	2.22	0.71
17:F:384:LEU:HD11	17:F:420:TYR:HB3	1.72	0.71
25:N:208:ILE:HD12	25:N:228:ILE:HD11	1.72	0.71
30:S:66:ARG:NH1	30:S:240:LYS:O	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:146:ASP:O	10:d:150:ILE:HD12	1.90	0.71
12:A:238:ILE:HG21	12:A:260:LEU:HD11	1.73	0.71
13:B:70:ASP:OD2	32:f:606:VAL:HG11	1.91	0.71
29:r:204:TYR:O	29:r:206:LEU:HD12	1.90	0.71
3:W:331:GLY:CA	3:W:337:ALA:HB2	2.21	0.71
10:d:136:LEU:HD12	10:d:138:LYS:HD2	1.72	0.71
30:S:64:HIS:O	31:T:196:ARG:NH2	2.24	0.71
28:q:24:ASN:OD1	28:q:25:ILE:N	2.23	0.71
17:F:384:LEU:O	17:F:388:THR:HG23	1.90	0.71
22:K:117:SER:OG	22:K:160:GLY:O	2.05	0.71
1:U:19:LEU:HD13	10:d:124:LEU:HD13	1.73	0.71
2:V:297:ALA:O	2:V:397:ARG:NH2	2.24	0.71
12:A:116:LYS:NZ	13:B:128:GLY:O	2.24	0.71
19:H:74:LEU:HD21	19:H:134:LEU:HD22	1.72	0.71
3:W:227:TYR:O	3:W:231:ILE:HD12	1.91	0.70
5:Y:174:TRP:CE2	5:Y:178:ASN:ND2	2.59	0.70
5:Y:376:LEU:O	5:Y:380:VAL:HG23	1.90	0.70
3:W:43:VAL:HG11	3:W:73:MET:HE1	1.71	0.70
4:X:418:ALA:HB2	6:Z:276:ILE:HD12	1.72	0.70
31:T:57:LEU:HD11	31:T:221:LEU:HD11	1.72	0.70
3:W:307:LYS:O	3:W:311:THR:HG23	1.91	0.70
3:W:409:LEU:HD22	4:X:384:VAL:HG21	1.73	0.70
14:C:399:MET:CE	20:I:56:LEU:HD11	2.21	0.70
4:X:398:GLU:OE2	5:Y:365:GLN:NE2	2.25	0.70
20:I:33:THR:OG1	20:I:166:ASN:O	2.08	0.70
5:Y:201:PHE:HB3	5:Y:223:THR:HG22	1.74	0.70
15:D:116:LEU:HB3	15:D:119:ILE:HD11	1.72	0.70
17:F:240:CYS:O	17:F:244:THR:OG1	2.08	0.70
23:L:162:GLY:O	23:L:165:SER:OG	2.09	0.70
5:Y:183:TYR:CE1	5:Y:213:LEU:HD11	2.26	0.70
12:A:229:VAL:O	12:A:233:THR:HG23	1.91	0.70
14:C:84:LYS:NZ	14:C:98:ASP:OD1	2.14	0.70
32:f:345:PRO:HD2	32:f:390:LEU:HD11	1.73	0.69
2:V:121:PHE:O	2:V:128:ARG:NH1	2.25	0.69
14:C:113:ARG:NH2	15:D:94:GLU:OE2	2.24	0.69
16:E:310:LEU:HD21	16:E:329:GLU:OE1	1.91	0.69
16:E:350:ALA:O	16:E:369:LYS:NZ	2.20	0.69
2:V:343:PRO:O	11:e:43:TRP:NE1	2.24	0.69
3:W:108:CYS:O	3:W:112:VAL:HG23	1.93	0.69
14:C:41:ASN:OD1	14:C:44:ARG:NH1	2.25	0.69
13:B:336:THR:OG1	14:C:260:GLU:OE1	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:119:ILE:O	15:D:119:ILE:HG22	1.93	0.69
25:N:208:ILE:HD12	25:N:228:ILE:CD1	2.22	0.69
32:f:199:ASN:HD22	32:f:199:ASN:C	2.01	0.69
17:F:356:MET:HE1	17:F:392:ASN:OD1	1.92	0.69
21:J:199:VAL:HG21	21:J:206:ILE:HD11	1.74	0.69
22:K:171:GLY:O	22:K:174:SER:OG	2.08	0.69
26:o:118:ARG:N	26:o:121:THR:HG1	1.91	0.69
32:f:435:SER:O	33:y:381:ARG:NH1	2.26	0.69
4:X:365:LEU:HD13	4:X:385:LEU:HD12	1.75	0.69
29:r:156:MET:N	29:r:175:SER:OG	2.25	0.69
32:f:722:SER:O	32:f:726:ILE:HD12	1.93	0.69
6:Z:172:VAL:HG22	9:c:217:LEU:CD1	2.23	0.69
23:L:47:VAL:HG12	23:L:195:LEU:CD1	2.22	0.69
5:Y:22:LEU:HD12	5:Y:37:VAL:HG13	1.75	0.68
7:a:324:ILE:HG13	7:a:331:VAL:HG22	1.75	0.68
2:V:67:LEU:O	2:V:71:THR:HG23	1.93	0.68
2:V:254:LEU:HD23	2:V:270:LEU:HD11	1.75	0.68
8:b:141:ILE:HG12	8:b:183:LEU:HD11	1.75	0.68
14:C:81:ASP:OD1	14:C:82:LYS:N	2.25	0.68
25:n:114:ALA:HB1	25:n:154:MET:HE1	1.75	0.68
21:J:195:LEU:O	21:J:199:VAL:HG22	1.93	0.68
25:N:125:ARG:NH2	31:T:101:ASP:OD2	2.26	0.68
1:U:365:CYS:O	1:U:369:THR:HG23	1.94	0.68
7:a:331:VAL:HG11	7:a:333:MET:HE2	1.74	0.68
12:A:85:GLN:NE2	13:B:119:ASN:OD1	2.25	0.68
28:Q:170:ARG:NE	29:r:199:ASP:OD2	2.26	0.68
26:o:169:THR:HG21	26:o:177:ALA:HB1	1.75	0.68
17:F:191:LEU:HD12	17:F:191:LEU:O	1.94	0.68
6:Z:35:VAL:HG22	6:Z:97:THR:OG1	1.92	0.68
1:U:471:ASP:OD1	1:U:472:ILE:HD12	1.94	0.68
3:W:381:LEU:HD23	3:W:381:LEU:O	1.93	0.68
8:b:182:ALA:O	8:b:186:SER:OG	2.11	0.68
13:B:197:ILE:HD12	13:B:235:LEU:CD2	2.24	0.68
13:B:197:ILE:HD12	13:B:235:LEU:HD23	1.75	0.68
32:f:407:MET:HE2	32:f:440:ILE:HD11	1.76	0.68
2:V:90:GLU:O	2:V:92:ARG:N	2.27	0.68
5:Y:387:ILE:O	6:Z:279:LYS:NZ	2.26	0.68
12:A:23:ARG:HH21	13:B:410:ARG:CB	2.07	0.68
30:s:74:LEU:HD11	30:s:80:ILE:HD12	1.76	0.68
32:f:530:CYS:SG	32:f:569:LYS:NZ	2.66	0.68
2:V:383:GLY:O	2:V:392:TYR:OH	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:158:ASP:OD2	12:A:255:ARG:NH1	2.27	0.68
28:q:12:TYR:HB2	28:q:182:ILE:HD11	1.75	0.68
12:A:23:ARG:HH21	13:B:410:ARG:HB2	1.57	0.67
12:A:25:LEU:HD23	13:B:410:ARG:NH1	2.06	0.67
16:E:124:HIS:O	16:E:124:HIS:ND1	2.27	0.67
32:f:305:LEU:O	32:f:321:MET:HE1	1.93	0.67
16:E:40:TYR:OH	17:F:73:ILE:N	2.28	0.67
32:f:92:VAL:HG23	32:f:92:VAL:O	1.93	0.67
32:f:418:LEU:O	32:f:451:VAL:HG22	1.94	0.67
1:U:360:VAL:HG21	1:U:369:THR:HG21	1.75	0.67
3:W:409:LEU:HD23	4:X:344:ARG:NH1	2.10	0.67
5:Y:90:ASP:OD1	5:Y:94:ASN:ND2	2.27	0.67
12:A:143:ASP:OD2	12:A:150:HIS:NE2	2.27	0.67
13:B:269:GLU:OE2	13:B:272:ARG:NH2	2.28	0.67
14:C:161:ILE:CD1	14:C:186:VAL:HG11	2.25	0.67
22:K:230:THR:N	22:K:233:GLU:OE1	2.27	0.67
1:U:609:ASP:O	1:U:615:ARG:NH1	2.27	0.67
12:A:101:ILE:O	12:A:102:ILE:HG22	1.95	0.67
1:U:148:LYS:O	1:U:149:GLN:HG2	1.94	0.67
3:W:366:MET:HE3	3:W:381:LEU:HD22	1.77	0.67
3:W:443:THR:HG21	6:Z:204:LYS:CD	2.23	0.67
7:a:360:VAL:HG22	9:c:308:VAL:CG2	2.25	0.67
1:U:899:ARG:NH2	1:U:916:ASP:OD2	2.27	0.67
13:B:70:ASP:OD1	13:B:71:TYR:N	2.28	0.67
17:F:285:ILE:HG21	17:F:288:LEU:HD13	1.76	0.67
4:X:371:ASP:OD1	5:Y:237:ARG:NH2	2.28	0.66
12:A:23:ARG:NH2	13:B:410:ARG:HG3	2.10	0.66
1:U:22:PHE:CD1	10:d:124:LEU:HD11	2.30	0.66
3:W:344:THR:O	3:W:346:GLU:N	2.29	0.66
4:X:255:LEU:HD23	4:X:270:LEU:HD23	1.78	0.66
12:A:390:THR:O	13:B:216:ILE:HD11	1.94	0.66
8:b:4:GLU:N	8:b:47:ASN:OD1	2.27	0.66
12:A:23:ARG:CZ	13:B:410:ARG:HG3	2.26	0.66
2:V:367:VAL:CG2	2:V:402:VAL:HG22	2.25	0.66
5:Y:217:LYS:O	5:Y:221:THR:HG23	1.96	0.66
8:b:56:ASN:OD1	8:b:57:ASP:N	2.29	0.66
21:J:42:VAL:HG13	21:J:191:VAL:HG21	1.77	0.66
24:M:76:MET:HE2	24:M:78:VAL:HG12	1.76	0.66
30:s:221:LEU:HD23	30:s:236:VAL:HB	1.77	0.66
2:V:497:PRO:HG2	2:V:498:PRO:HD3	1.76	0.66
12:A:63:THR:HG23	32:f:680:ARG:CZ	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:21:GLU:OE1	1:U:21:GLU:N	2.28	0.66
1:U:632:GLN:O	1:U:635:SER:OG	2.13	0.66
6:Z:151:THR:CG2	7:a:148:VAL:HG21	2.26	0.66
27:P:169:GLN:O	27:P:173:ASN:ND2	2.28	0.66
30:s:120:LEU:HD23	30:s:152:PHE:CE2	2.31	0.66
3:W:94:ARG:O	3:W:96:GLN:N	2.29	0.66
3:W:329:ARG:HE	3:W:341:PHE:HB3	1.61	0.66
30:s:56:ARG:NE	30:s:219:ASP:OD2	2.27	0.66
1:U:609:ASP:OD1	1:U:610:VAL:N	2.29	0.65
8:b:151:GLU:N	8:b:151:GLU:OE1	2.28	0.65
12:A:23:ARG:HH21	13:B:410:ARG:HG3	1.59	0.65
13:B:196:GLU:OE1	13:B:349:ARG:NE	2.28	0.65
13:B:388:ASP:OD2	13:B:423:LYS:NZ	2.27	0.65
27:p:178:ASP:OD1	27:p:179:ALA:N	2.29	0.65
14:C:49:ARG:NH1	15:D:64:GLU:OE2	2.29	0.65
14:C:325:ARG:NE	14:C:351:MET:O	2.29	0.65
3:W:166:LEU:HD23	3:W:192:LEU:HD12	1.78	0.65
8:b:8:VAL:HG11	8:b:33:VAL:HG23	1.79	0.65
8:b:157:VAL:HG21	8:b:170:LEU:HB2	1.76	0.65
9:c:166:ASN:OD1	9:c:167:MET:N	2.29	0.65
10:d:254:GLU:OE2	10:d:257:THR:OG1	2.13	0.65
13:B:234:LEU:HD11	35:B:501:ATP:H2'	1.77	0.65
25:n:183:LYS:NZ	25:n:219:GLU:OE2	2.29	0.65
32:f:679:LEU:O	32:f:687:ARG:NH1	2.29	0.65
2:V:192:MET:HE3	2:V:214:HIS:HB2	1.78	0.65
12:A:24:ALA:C	13:B:410:ARG:NH2	2.54	0.65
35:B:501:ATP:O3G	14:C:310:ARG:NH1	2.28	0.65
3:W:329:ARG:HH22	3:W:351:TRP:HB2	1.61	0.65
5:Y:26:LEU:HD21	5:Y:63:TRP:CZ2	2.32	0.65
9:c:117:GLY:N	9:c:146:ASP:OD1	2.29	0.65
13:B:103:ARG:NH1	13:B:160:ILE:O	2.29	0.65
23:L:186:GLU:OE1	23:L:186:GLU:N	2.28	0.65
32:f:113:MET:O	32:f:119:LYS:NZ	2.24	0.65
16:E:273:VAL:O	16:E:273:VAL:HG12	1.97	0.65
6:Z:274:ASN:OD1	9:c:281:LYS:NZ	2.28	0.65
26:O:206:ILE:HD12	26:O:213:GLY:O	1.97	0.65
12:A:384:GLU:OE2	12:A:416:VAL:HG12	1.96	0.65
14:C:358:GLU:O	14:C:362:VAL:HG23	1.96	0.65
22:K:52:LYS:NZ	22:K:216:GLU:OE2	2.28	0.65
26:O:60:ASP:HB2	26:O:206:ILE:HD11	1.78	0.65
26:O:242:LEU:O	30:s:201:ARG:NH1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:R:74:ALA:HB1	29:R:219:ILE:HD12	1.78	0.65
32:f:659:LEU:HD12	32:f:662:MET:CE	2.27	0.65
8:b:20:ASP:OD1	8:b:21:PHE:N	2.30	0.64
20:I:154:GLY:O	21:J:81:ARG:NH2	2.29	0.64
25:N:178:ARG:NH2	25:N:185:GLU:OE1	2.29	0.64
6:Z:172:VAL:HG22	9:c:217:LEU:HD12	1.77	0.64
19:H:46:LEU:HD22	19:H:75:VAL:CG1	2.28	0.64
6:Z:19:VAL:HG21	6:Z:124:ILE:HD13	1.80	0.64
23:L:183:ASN:OD1	23:L:184:LEU:N	2.30	0.64
27:p:149:MET:HE3	27:p:173:ASN:CB	2.27	0.64
7:a:180:LEU:HD12	7:a:221:VAL:HG21	1.78	0.64
7:a:360:VAL:HG22	9:c:308:VAL:HG22	1.79	0.64
13:B:440:LEU:O	21:J:77:THR:OG1	2.13	0.64
20:I:8:ARG:NH2	21:J:5:ARG:O	2.30	0.64
27:P:126:LEU:HD12	27:P:127:ILE:HG23	1.80	0.64
32:f:345:PRO:CD	32:f:390:LEU:HD11	2.27	0.64
11:e:17:ASP:OD1	11:e:18:GLU:N	2.30	0.64
12:A:29:ASP:OD2	13:B:410:ARG:CD	2.44	0.64
17:F:343:LEU:HD22	17:F:351:LYS:HD3	1.79	0.64
6:Z:175:LEU:HD11	9:c:38:LEU:HD23	1.80	0.64
32:f:79:ARG:HG3	32:f:125:ILE:HD11	1.78	0.64
32:f:124:ASP:OD1	32:f:125:ILE:N	2.31	0.64
10:d:237:MET:O	10:d:237:MET:HE3	1.97	0.64
21:J:188:ILE:O	21:J:192:ILE:HD12	1.97	0.64
27:P:37:THR:HG22	27:P:37:THR:O	1.97	0.64
29:R:233:VAL:HG21	29:R:254:LEU:HD12	1.79	0.64
9:c:191:ALA:HB1	9:c:196:LEU:HD12	1.80	0.64
10:d:92:THR:HG22	10:d:143:LEU:HD13	1.80	0.64
13:B:417:GLU:OE1	13:B:417:GLU:N	2.30	0.64
15:D:271:ALA:O	15:D:317:LEU:HD13	1.98	0.64
15:D:393:ILE:HD13	16:E:160:GLN:OE1	1.98	0.64
23:L:202:GLU:OE1	23:L:202:GLU:N	2.29	0.64
31:t:137:LEU:HD12	31:t:157:ILE:HD11	1.80	0.64
1:U:161:ASP:OD1	1:U:162:VAL:N	2.31	0.63
1:U:263:SER:O	1:U:267:ASN:ND2	2.31	0.63
14:C:161:ILE:HG21	14:C:199:LEU:HD21	1.79	0.63
31:t:70:ASP:O	31:t:86:ARG:NH1	2.30	0.63
32:f:538:ILE:HG21	32:f:562:LEU:HG	1.78	0.63
2:V:233:ALA:O	2:V:237:THR:HG23	1.98	0.63
25:N:73:ASP:OD1	25:N:74:ARG:N	2.30	0.63
28:Q:49:GLU:OE2	29:R:150:LYS:NZ	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:n:48:LEU:HD23	25:n:78:CYS:SG	2.38	0.63
32:f:371:ASN:O	32:f:374:SER:OG	2.15	0.63
1:U:212:ASP:O	1:U:216:VAL:HG23	1.98	0.63
7:a:100:THR:O	7:a:104:VAL:HG12	1.98	0.63
25:N:175:ALA:HB2	25:n:196:LEU:HD11	1.80	0.63
28:q:168:GLN:NE2	28:q:175:LEU:O	2.32	0.63
1:U:155:LEU:HD22	1:U:188:MET:HE1	1.81	0.63
12:A:195:LEU:HD11	12:A:271:LEU:HD11	1.81	0.63
7:a:70:ARG:NH1	8:b:17:ARG:O	2.32	0.63
24:M:121:HIS:HA	24:M:124:THR:HG22	1.79	0.63
2:V:176:MET:HE1	2:V:216:ARG:HB2	1.80	0.63
12:A:101:ILE:O	12:A:101:ILE:HG22	1.98	0.63
14:C:336:MET:HE2	15:D:196:ILE:HD11	1.81	0.63
15:D:394:VAL:HG23	16:E:161:ARG:HD2	1.79	0.63
21:J:191:VAL:CG1	21:J:208:LEU:HD11	2.29	0.63
7:a:331:VAL:CG1	7:a:333:MET:HE2	2.29	0.63
27:p:56:LEU:HD11	28:q:121:LEU:HD21	1.79	0.63
32:f:109:ILE:HG22	32:f:113:MET:CE	2.29	0.63
18:G:138:MET:HE3	18:G:140:LEU:HD11	1.81	0.63
32:f:479:LEU:HD11	32:f:816:TYR:OH	1.99	0.63
3:W:57:ALA:O	3:W:58:SER:OG	2.15	0.63
16:E:223:ARG:CZ	16:E:273:VAL:HG11	2.28	0.63
32:f:550:LEU:HD11	32:f:587:PHE:CE2	2.33	0.63
8:b:68:THR:HG22	8:b:72:LEU:CD1	2.28	0.62
20:I:86:LEU:HD12	20:I:132:VAL:HG11	1.81	0.62
20:I:95:GLN:HG3	27:P:73:LEU:HD22	1.81	0.62
23:L:67:ASP:OD1	23:L:68:ASN:N	2.32	0.62
31:T:117:ILE:O	31:T:121:LEU:HD13	1.98	0.62
31:T:251:GLU:OE1	31:T:251:GLU:N	2.32	0.62
30:s:153:ASP:OD2	30:s:157:SER:OG	2.17	0.62
32:f:702:PRO:HG3	32:f:736:THR:HG21	1.79	0.62
10:d:94:MET:HE2	10:d:119:LEU:HD22	1.82	0.62
12:A:23:ARG:NH2	13:B:410:ARG:CG	2.62	0.62
12:A:393:GLY:HA3	13:B:216:ILE:HD12	1.79	0.62
15:D:258:ALA:HB1	15:D:259:PRO:CD	2.28	0.62
17:F:224:LEU:HD22	17:F:343:LEU:HD21	1.81	0.62
21:J:73:PHE:CE1	21:J:80:ALA:HB2	2.34	0.62
32:f:794:ALA:O	32:f:798:THR:HG23	1.99	0.62
2:V:110:HIS:NE2	2:V:135:LEU:O	2.32	0.62
6:Z:148:GLY:O	7:a:219:HIS:NE2	2.31	0.62
21:J:191:VAL:HG11	21:J:208:LEU:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:304:PHE:CD2	32:f:321:MET:HE3	2.34	0.62
1:U:443:LEU:HD21	1:U:464:GLN:NE2	2.14	0.62
8:b:140:ILE:HD13	8:b:156:PHE:HD2	1.65	0.62
12:A:333:ARG:NH1	35:F:501:ATP:O3G	2.32	0.62
17:F:58:GLU:OE1	17:F:61:ARG:NH2	2.31	0.62
1:U:95:GLU:OE1	2:V:237:THR:HG22	1.99	0.62
5:Y:183:TYR:HE1	5:Y:213:LEU:HD11	1.63	0.62
7:a:185:ILE:O	7:a:193:GLN:NE2	2.33	0.62
10:d:110:SER:O	10:d:114:GLU:OE1	2.18	0.62
12:A:246:VAL:HG21	13:B:307:ARG:HD3	1.80	0.62
14:C:37:ASP:OD1	14:C:38:LYS:N	2.32	0.62
18:G:22:LEU:CD1	19:H:79:MET:HE1	2.30	0.62
25:N:169:ILE:HG21	25:N:193:ALA:O	1.98	0.62
32:f:668:ALA:HA	32:f:697:ILE:HD11	1.82	0.62
2:V:94:VAL:HG21	2:V:205:LEU:HD13	1.82	0.62
3:W:298:GLU:OE1	3:W:298:GLU:N	2.33	0.62
5:Y:112:CYS:SG	5:Y:147:ILE:HD11	2.39	0.62
14:C:399:MET:HE3	20:I:56:LEU:HD11	1.81	0.62
26:O:60:ASP:OD1	26:O:76:LYS:NZ	2.27	0.62
32:f:781:TYR:O	32:f:785:ARG:NH2	2.32	0.62
9:c:71:ASP:OD1	9:c:72:VAL:N	2.33	0.62
12:A:63:THR:O	32:f:680:ARG:NH2	2.32	0.62
27:P:191:GLU:OE1	27:P:194:LYS:NZ	2.32	0.62
30:S:175:PRO:HB2	27:p:149:MET:HE2	1.81	0.62
5:Y:174:TRP:NE1	5:Y:178:ASN:HD21	1.96	0.62
12:A:25:LEU:CD2	13:B:410:ARG:HD3	2.29	0.62
14:C:219:LEU:HD23	14:C:230:MET:HE2	1.81	0.62
28:Q:15:VAL:HG21	28:Q:43:LEU:HD23	1.80	0.62
28:Q:181:ARG:NH1	28:Q:190:ASP:OD2	2.32	0.62
1:U:65:SER:OG	1:U:96:TYR:OH	2.16	0.61
10:d:311:GLY:O	10:d:313:ASN:N	2.31	0.61
20:I:90:LEU:HG	20:I:114:LEU:HD13	1.81	0.61
23:L:32:GLY:O	23:L:51:ARG:NH2	2.32	0.61
25:n:198:MET:HE1	25:n:206:GLY:O	2.00	0.61
26:o:186:ARG:NH2	26:o:193:GLU:OE1	2.33	0.61
7:a:216:LEU:HD22	7:a:237:LEU:CD2	2.30	0.61
17:F:86:LEU:O	17:F:88:TYR:N	2.32	0.61
17:F:171:ARG:HD2	17:F:267:LEU:HD21	1.81	0.61
21:J:36:ARG:NE	21:J:142:PRO:O	2.33	0.61
1:U:732:LEU:O	1:U:736:ILE:HD12	1.99	0.61
16:E:165:ILE:O	16:E:168:LYS:NZ	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E:223:ARG:NH2	16:E:273:VAL:HG11	2.16	0.61
18:G:7:ALA:O	18:G:11:ARG:NH1	2.33	0.61
25:N:48:LEU:HD23	25:N:78:CYS:SG	2.40	0.61
27:P:2:SER:N	27:P:5:SER:HG	1.98	0.61
29:R:62:THR:HG22	29:R:75:ALA:CB	2.30	0.61
28:q:119:ASP:OD1	28:q:120:TYR:N	2.33	0.61
1:U:2:ILE:O	1:U:3:THR:OG1	2.15	0.61
10:d:283:LEU:HB3	10:d:315:TYR:CE1	2.35	0.61
19:H:119:GLN:HA	19:H:122:THR:HG22	1.83	0.61
25:N:148:VAL:HG23	25:N:148:VAL:O	1.99	0.61
25:N:155:VAL:HG11	31:T:81:PHE:CD2	2.35	0.61
30:s:51:VAL:HG21	30:s:79:VAL:HG23	1.81	0.61
1:U:246:TYR:CD1	1:U:325:MET:HE1	2.35	0.61
2:V:168:GLN:HG3	2:V:191:LEU:HD21	1.83	0.61
2:V:466:ILE:O	2:V:466:ILE:HG23	2.01	0.61
15:D:237:GLN:HG3	15:D:246:MET:HE1	1.82	0.61
20:I:86:LEU:HD12	20:I:132:VAL:CG1	2.30	0.61
6:Z:94:TRP:CE2	6:Z:121:LEU:HD13	2.36	0.61
21:J:4:ASP:OD1	21:J:5:ARG:N	2.28	0.61
1:U:825:LYS:HB3	13:B:85:MET:SD	2.40	0.61
3:W:409:LEU:HD23	4:X:344:ARG:HH12	1.65	0.61
7:a:244:ASN:O	7:a:247:ARG:N	2.34	0.61
18:G:60:LEU:HD23	24:M:163:GLY:O	2.00	0.61
2:V:98:LEU:HD13	2:V:209:LYS:HE2	1.83	0.61
5:Y:148:GLY:O	5:Y:157:ILE:HD11	2.01	0.61
10:d:153:GLN:HE22	10:d:191:LEU:HD21	1.66	0.61
14:C:99:VAL:HG11	14:C:105:ILE:CD1	2.31	0.61
18:G:196:GLU:CG	18:G:242:LEU:HD13	2.30	0.61
24:M:9:ASP:O	24:M:23:GLN:NE2	2.31	0.61
29:r:62:THR:HG21	29:r:103:THR:HB	1.82	0.61
32:f:489:TYR:O	32:f:492:SER:OG	2.15	0.61
1:U:5:ALA:O	1:U:9:ILE:HD12	2.00	0.60
1:U:792:ASN:ND2	1:U:922:GLU:OE2	2.33	0.60
14:C:351:MET:SD	14:C:362:VAL:HG21	2.40	0.60
16:E:316:HIS:NE2	37:E:401:ADP:N3	2.49	0.60
32:f:450:ILE:HG23	32:f:822:VAL:HG21	1.81	0.60
4:X:240:ASP:OD2	4:X:275:LEU:HD22	2.01	0.60
12:A:23:ARG:NE	13:B:410:ARG:CG	2.49	0.60
17:F:390:ASP:OD1	17:F:390:ASP:O	2.20	0.60
26:O:96:ASP:OD1	26:O:100:GLN:NE2	2.34	0.60
27:p:135:ASP:OD1	27:p:136:PHE:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:467:TYR:O	6:Z:254:ASN:ND2	2.34	0.60
15:D:368:ASP:OD2	15:D:403:TYR:OH	2.11	0.60
23:L:66:VAL:HG12	23:L:67:ASP:H	1.66	0.60
27:P:135:ASP:OD1	27:P:136:PHE:N	2.33	0.60
16:E:210:GLU:O	16:E:214:LEU:HD23	2.02	0.60
30:S:66:ARG:NH2	26:o:207:PHE:O	2.35	0.60
30:S:180:GLN:O	30:S:198:ARG:NH2	2.35	0.60
2:V:482:PHE:CZ	2:V:486:ILE:HD11	2.36	0.60
15:D:78:GLU:OE1	15:D:81:ARG:NH2	2.34	0.60
15:D:167:ILE:HG21	15:D:170:MET:CE	2.30	0.60
16:E:112:PRO:HD2	17:F:97:LEU:HD21	1.83	0.60
31:T:86:ARG:NH1	31:T:98:ALA:O	2.35	0.60
1:U:665:ASN:OD1	1:U:666:LYS:N	2.35	0.60
26:O:206:ILE:HD13	26:O:212:SER:HB3	1.84	0.60
18:G:50:ILE:HG23	18:G:141:ILE:HG21	1.82	0.60
35:A:501:ATP:O1G	13:B:346:ARG:NH1	2.33	0.60
26:O:140:ALA:HB1	26:O:170:MET:CE	2.32	0.60
29:R:231:GLY:O	29:R:251:VAL:HG23	2.01	0.60
31:t:57:LEU:HD21	31:t:221:LEU:HD11	1.82	0.60
7:a:163:TYR:HA	7:a:166:ILE:HG22	1.83	0.60
26:o:62:ARG:O	26:o:76:LYS:NZ	2.29	0.60
32:f:145:VAL:HG23	32:f:145:VAL:O	2.02	0.60
2:V:309:MET:HE1	2:V:331:LEU:CG	2.32	0.59
15:D:358:VAL:O	15:D:358:VAL:HG22	2.02	0.59
19:H:75:VAL:HG22	19:H:76:TYR:H	1.67	0.59
22:K:195:ILE:HG23	22:K:217:LEU:HD21	1.83	0.59
29:R:76:ASP:OD2	29:R:229:SER:OG	2.16	0.59
29:r:239:ARG:NH2	29:r:241:ASP:OD2	2.35	0.59
30:s:226:VAL:HG22	30:s:231:ILE:CD1	2.32	0.59
31:t:223:TYR:OH	31:t:253:ASN:N	2.35	0.59
31:t:251:GLU:OE1	31:t:251:GLU:N	2.35	0.59
1:U:216:VAL:O	1:U:220:LEU:HD23	2.03	0.59
1:U:446:LEU:HD21	1:U:457:ILE:HD13	1.84	0.59
2:V:469:THR:HG22	2:V:470:ARG:H	1.67	0.59
2:V:482:PHE:CE2	2:V:486:ILE:HD11	2.37	0.59
22:K:238:ILE:HA	22:K:241:ILE:HG23	1.84	0.59
29:r:233:VAL:O	29:r:233:VAL:HG12	2.00	0.59
2:V:484:LEU:HD23	6:Z:267:ARG:HH21	1.66	0.59
20:I:45:LEU:HD12	20:I:137:ILE:HD13	1.84	0.59
2:V:171:VAL:HG12	2:V:175:MET:HE1	1.84	0.59
2:V:467:TYR:OH	4:X:397:TYR:OH	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:259:GLU:OE1	3:W:262:LYS:N	2.33	0.59
6:Z:96:HIS:HD2	6:Z:121:LEU:HD11	1.67	0.59
8:b:68:THR:HG22	8:b:72:LEU:HD13	1.83	0.59
13:B:205:LEU:O	32:f:740:ARG:HD3	2.03	0.59
1:U:446:LEU:HD21	1:U:457:ILE:CD1	2.32	0.59
5:Y:22:LEU:CD1	5:Y:37:VAL:HG13	2.33	0.59
16:E:165:ILE:HG22	16:E:168:LYS:HE3	1.85	0.59
29:R:175:SER:OG	29:R:176:GLU:OE1	2.21	0.59
7:a:232:TRP:CE2	7:a:254:ALA:HB3	2.37	0.59
8:b:37:CYS:SG	8:b:68:THR:HG23	2.43	0.59
13:B:184:TYR:OH	13:B:202:GLU:OE2	2.13	0.59
14:C:362:VAL:CG2	14:C:390:VAL:HG21	2.30	0.59
2:V:86:VAL:HG11	2:V:162:GLU:HG2	1.84	0.59
3:W:32:ALA:HA	3:W:73:MET:HE3	1.85	0.59
4:X:69:LEU:O	4:X:73:VAL:HG22	2.03	0.59
5:Y:227:SER:HB3	5:Y:231:LEU:HD12	1.84	0.59
9:c:213:GLU:O	9:c:217:LEU:HD23	2.02	0.59
29:R:170:LEU:HD22	29:R:185:PHE:HD2	1.68	0.59
2:V:280:ALA:O	5:Y:385:ARG:NH2	2.36	0.59
3:W:374:THR:N	7:a:326:GLU:OE2	2.27	0.59
19:H:195:LEU:CD1	19:H:208:ILE:HD11	2.33	0.59
32:f:146:GLY:O	32:f:148:GLN:NE2	2.34	0.59
32:f:678:LEU:HD22	32:f:686:LEU:HD13	1.85	0.59
3:W:274:VAL:CG1	3:W:287:VAL:HG22	2.33	0.59
27:p:149:MET:HE3	27:p:173:ASN:HB3	1.85	0.59
28:q:78:THR:HG22	28:q:116:TYR:OH	2.02	0.59
29:r:61:THR:N	29:r:76:ASP:OD2	2.36	0.59
2:V:259:LEU:HD21	2:V:295:ILE:HD11	1.84	0.59
9:c:84:VAL:O	9:c:87:VAL:HG12	2.02	0.59
10:d:149:GLU:O	10:d:153:GLN:NE2	2.30	0.59
16:E:88:ASP:OD2	16:E:91:LYS:NZ	2.36	0.59
13:B:125:THR:O	13:B:125:THR:HG22	2.02	0.58
23:L:72:ILE:HD12	23:L:88:MET:SD	2.43	0.58
27:P:65:GLN:OE1	28:Q:86:ARG:NH2	2.34	0.58
6:Z:13:PRO:O	6:Z:17:LEU:HD23	2.03	0.58
14:C:138:MET:CE	14:C:234:LEU:HD12	2.33	0.58
17:F:279:ALA:HB3	17:F:280:PRO:HD3	1.84	0.58
18:G:32:ILE:HD11	18:G:156:PRO:CD	2.34	0.58
23:L:88:MET:HE3	23:L:112:ILE:HD11	1.84	0.58
26:O:183:ASP:OD2	31:t:216:ARG:NH2	2.36	0.58
28:Q:108:ASP:OD1	28:Q:109:GLU:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:S:178:ASP:OD2	27:p:177:ARG:NH2	2.36	0.58
25:n:36:THR:HG21	25:n:197:ALA:HB3	1.84	0.58
26:o:245:TYR:O	26:o:249:LYS:NZ	2.33	0.58
1:U:682:TYR:CD1	9:c:184:LEU:HD22	2.38	0.58
2:V:466:ILE:HD11	2:V:471:GLU:HB2	1.85	0.58
14:C:96:VAL:HG23	14:C:96:VAL:O	2.02	0.58
16:E:154:THR:HG23	16:E:156:PRO:CD	2.33	0.58
28:Q:42:ILE:HD11	28:Q:75:LEU:O	2.03	0.58
29:R:170:LEU:HD22	29:R:185:PHE:CD2	2.38	0.58
3:W:72:LYS:NZ	3:W:76:GLU:OE2	2.29	0.58
7:a:296:ILE:HG21	7:a:307:VAL:HG13	1.85	0.58
13:B:390:LEU:HD21	13:B:427:LEU:HD11	1.85	0.58
16:E:98:VAL:HB	16:E:107:ILE:HG23	1.85	0.58
17:F:406:ILE:HD13	17:F:422:GLU:HB2	1.85	0.58
29:r:142:LEU:HD23	29:r:173:VAL:HG21	1.85	0.58
7:a:180:LEU:HD12	7:a:221:VAL:CG2	2.34	0.58
20:I:135:LEU:HD21	20:I:162:THR:HG23	1.85	0.58
23:L:72:ILE:CD1	23:L:132:LEU:HD22	2.32	0.58
17:F:182:THR:HG23	17:F:182:THR:O	2.04	0.58
29:R:65:PHE:CB	29:R:184:THR:HG22	2.34	0.58
29:r:117:LEU:O	29:r:117:LEU:HD23	2.02	0.58
31:t:108:LEU:HD21	31:t:151:LEU:HD13	1.86	0.58
32:f:848:GLN:NE2	32:f:878:GLU:OE2	2.37	0.58
9:c:166:ASN:O	9:c:170:LEU:HD13	2.04	0.58
10:d:232:LEU:HD13	10:d:244:VAL:HG23	1.85	0.58
12:A:297:ARG:CD	17:F:257:VAL:HG21	2.34	0.58
1:U:70:HIS:O	2:V:236:ARG:NH1	2.37	0.58
8:b:124:LEU:HD21	8:b:156:PHE:CE1	2.38	0.58
13:B:109:VAL:HG22	13:B:151:LEU:HD23	1.85	0.58
31:T:190:LEU:HD11	31:T:221:LEU:CD2	2.33	0.58
26:o:157:TYR:CE1	26:o:170:MET:HE2	2.38	0.58
28:q:4:LEU:HD11	28:q:47:VAL:HG13	1.85	0.58
2:V:68:ASP:O	2:V:72:LEU:HD23	2.04	0.58
7:a:176:ALA:HB3	7:a:200:LEU:HD21	1.84	0.58
8:b:46:GLU:OE1	8:b:46:GLU:N	2.36	0.58
16:E:196:LEU:HD13	16:E:222:ALA:HB1	1.86	0.58
32:f:679:LEU:HG	32:f:690:VAL:HG11	1.86	0.58
1:U:462:LEU:HG	1:U:496:LEU:HD13	1.85	0.58
2:V:400:HIS:O	2:V:403:ILE:HG22	2.03	0.58
4:X:27:LEU:HD12	4:X:56:LEU:HD12	1.86	0.58
4:X:418:ALA:CB	6:Z:276:ILE:HD12	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:e:44:ASP:OD1	11:e:47:ASN:ND2	2.37	0.58
12:A:63:THR:HG1	32:f:681:TYR:HE2	1.51	0.58
12:A:190:VAL:HG11	12:A:212:VAL:HG21	1.86	0.58
29:r:233:VAL:HG21	29:r:254:LEU:CD1	2.32	0.58
7:a:216:LEU:HD22	7:a:237:LEU:HD23	1.86	0.57
10:d:204:ARG:NE	10:d:207:GLU:OE1	2.27	0.57
18:G:51:VAL:HG21	18:G:215:ILE:HD11	1.85	0.57
2:V:396:ILE:O	2:V:400:HIS:ND1	2.36	0.57
6:Z:183:THR:O	6:Z:183:THR:HG22	2.03	0.57
18:G:141:ILE:HG22	18:G:151:VAL:HG22	1.86	0.57
21:J:43:LEU:HD11	21:J:134:VAL:HG22	1.86	0.57
32:f:479:LEU:HD11	32:f:517:VAL:HG21	1.86	0.57
32:f:682:GLY:HA3	32:f:686:LEU:HD11	1.85	0.57
1:U:159:ARG:HE	1:U:162:VAL:HG23	1.69	0.57
2:V:134:PHE:O	2:V:180:ARG:NH2	2.37	0.57
7:a:77:VAL:CG1	7:a:113:LEU:HD22	2.33	0.57
8:b:51:LEU:HD11	8:b:75:LEU:HD12	1.86	0.57
16:E:188:ALA:HB3	16:E:195:PHE:HE1	1.70	0.57
21:J:55:ASP:OD1	21:J:56:GLU:N	2.35	0.57
25:N:194:LEU:HB2	25:N:208:ILE:HD13	1.86	0.57
29:r:93:VAL:HG23	29:r:93:VAL:O	2.03	0.57
6:Z:263:ALA:HB1	9:c:288:VAL:HG23	1.86	0.57
13:B:439:TYR:O	13:B:440:LEU:HB2	2.05	0.57
23:L:105:VAL:O	23:L:109:VAL:HG23	2.05	0.57
27:P:34:MET:O	29:r:225:ARG:NH1	2.38	0.57
3:W:112:VAL:HA	3:W:115:ILE:HD12	1.86	0.57
3:W:443:THR:HG21	6:Z:204:LYS:HD3	1.86	0.57
9:c:109:VAL:HG23	9:c:109:VAL:O	2.04	0.57
13:B:409:GLU:OE1	13:B:411:ARG:NE	2.37	0.57
14:C:21:ARG:O	14:C:25:LEU:HD23	2.03	0.57
19:H:109:GLN:NE2	27:P:78:GLU:OE1	2.37	0.57
27:P:69:PHE:O	27:P:73:LEU:HD23	2.04	0.57
1:U:22:PHE:CG	10:d:124:LEU:HD11	2.40	0.57
1:U:443:LEU:HD13	1:U:477:GLY:CA	2.34	0.57
6:Z:94:TRP:CZ2	6:Z:121:LEU:HD13	2.39	0.57
7:a:104:VAL:O	7:a:104:VAL:HG13	2.05	0.57
9:c:127:ILE:HG23	9:c:162:LEU:HD21	1.86	0.57
9:c:191:ALA:CB	9:c:196:LEU:HD12	2.34	0.57
14:C:386:ALA:O	14:C:390:VAL:HG22	2.05	0.57
30:S:185:ASN:ND2	27:p:176:ASP:OD2	2.35	0.57
29:r:60:THR:O	29:r:60:THR:HG22	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:835:GLU:OE2	32:f:901:ARG:NE	2.36	0.57
5:Y:26:LEU:HD21	5:Y:63:TRP:CH2	2.39	0.57
15:D:293:LEU:HD21	15:D:321:LEU:HB2	1.86	0.57
15:D:337:ASP:OD1	15:D:338:ARG:N	2.35	0.57
28:Q:4:LEU:HD11	28:Q:47:VAL:HG13	1.86	0.57
28:q:36:PHE:HD2	28:q:57:ALA:HB1	1.69	0.57
16:E:130:VAL:HG23	16:E:131:SER:H	1.70	0.57
1:U:658:ILE:HG23	1:U:763:VAL:HG11	1.86	0.57
6:Z:23:PHE:CE2	6:Z:126:VAL:HG21	2.40	0.57
12:A:102:ILE:HD11	17:F:165:PRO:HD3	1.86	0.57
13:B:107:MET:HB2	14:C:96:VAL:HG22	1.87	0.57
17:F:175:MET:HE3	17:F:251:LEU:HA	1.86	0.57
1:U:492:ASP:OD1	1:U:493:VAL:N	2.37	0.57
7:a:214:GLY:O	7:a:215:GLU:HB3	2.04	0.57
13:B:338:ASP:OD1	13:B:340:ALA:N	2.35	0.57
15:D:264:ILE:HG21	15:D:267:ILE:HD13	1.87	0.57
15:D:391:ARG:HH22	15:D:395:LEU:HD13	1.70	0.57
19:H:50:LYS:NZ	19:H:62:VAL:O	2.28	0.57
29:r:114:TRP:NE1	30:s:125:TYR:OH	2.38	0.57
28:Q:18:ASP:OD2	28:Q:175:LEU:HD22	2.04	0.56
29:R:170:LEU:HD23	29:R:171:TYR:N	2.19	0.56
32:f:539:LEU:O	32:f:543:MET:HG2	2.05	0.56
32:f:779:CYS:SG	32:f:785:ARG:NH1	2.78	0.56
16:E:142:ILE:HD13	16:E:183:LEU:HD12	1.86	0.56
2:V:446:VAL:HG23	2:V:447:ILE:HG23	1.86	0.56
10:d:99:LYS:O	10:d:103:ASN:N	2.38	0.56
12:A:246:VAL:HG21	13:B:307:ARG:CD	2.35	0.56
16:E:122:MET:CE	16:E:214:LEU:HD12	2.34	0.56
32:f:505:MET:HE1	32:f:538:ILE:CD1	2.30	0.56
7:a:18:GLN:HG3	7:a:21:VAL:HB	1.87	0.56
18:G:196:GLU:HG2	18:G:242:LEU:HD13	1.87	0.56
28:Q:44:LEU:HD21	28:Q:102:LEU:HD23	1.87	0.56
30:S:56:ARG:NH1	30:S:215:VAL:O	2.38	0.56
3:W:244:CYS:SG	3:W:274:VAL:HG23	2.46	0.56
3:W:438:LEU:HD21	6:Z:232:ASP:HB3	1.86	0.56
7:a:214:GLY:N	7:a:241:ASN:OD1	2.38	0.56
9:c:265:MET:SD	9:c:266:THR:HG23	2.45	0.56
17:F:88:TYR:CD1	17:F:161:LEU:HD12	2.40	0.56
17:F:224:LEU:CD2	17:F:343:LEU:HD21	2.35	0.56
29:R:66:LYS:HG2	29:R:71:VAL:HG22	1.87	0.56
12:A:265:ARG:NH2	12:A:305:GLN:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:164:TYR:OH	15:D:219:VAL:HG12	2.06	0.56
24:M:109:LEU:HD12	24:M:140:SER:HB3	1.88	0.56
29:R:62:THR:HG22	29:R:75:ALA:HB1	1.87	0.56
31:T:131:ARG:NH1	31:T:178:GLU:OE1	2.37	0.56
25:n:48:LEU:HD22	25:n:76:PHE:HB3	1.87	0.56
30:s:57:LEU:HD13	30:s:68:SER:OG	2.04	0.56
2:V:454:GLU:OE1	2:V:454:GLU:N	2.39	0.56
7:a:324:ILE:HG23	7:a:324:ILE:O	2.05	0.56
10:d:309:VAL:HG22	10:d:309:VAL:O	2.06	0.56
13:B:208:PRO:HG2	32:f:740:ARG:HB3	1.87	0.56
13:B:438:LEU:HD23	13:B:438:LEU:O	2.06	0.56
14:C:138:MET:HE1	14:C:234:LEU:HD12	1.85	0.56
14:C:381:GLU:O	14:C:385:MET:HE3	2.06	0.56
18:G:112:ASP:OD1	18:G:113:MET:N	2.39	0.56
1:U:332:GLU:OE1	1:U:332:GLU:N	2.38	0.56
2:V:176:MET:HE1	2:V:216:ARG:CB	2.34	0.56
2:V:436:PHE:HE1	10:d:290:ILE:HG23	1.70	0.56
3:W:408:ARG:NH1	4:X:346:GLN:OE1	2.39	0.56
14:C:60:ARG:NH2	15:D:71:GLU:OE1	2.39	0.56
16:E:89:LYS:O	16:E:90:SER:OG	2.22	0.56
23:L:205:LEU:HD22	23:L:210:VAL:HG22	1.88	0.56
32:f:372:LEU:HD11	32:f:409:SER:OG	2.04	0.56
2:V:287:ARG:NE	11:e:21:GLU:OE2	2.38	0.56
2:V:306:ARG:NH2	2:V:341:GLU:OE2	2.39	0.56
3:W:171:VAL:O	3:W:182:ARG:NH1	2.39	0.56
3:W:190:MET:HE2	3:W:206:SER:OG	2.06	0.56
12:A:25:LEU:CD2	13:B:410:ARG:CD	2.83	0.56
14:C:184:LYS:N	14:C:312:ASP:OD2	2.37	0.56
18:G:86:ASP:OD1	24:M:121:HIS:NE2	2.39	0.56
1:U:226:PRO:HA	1:U:229:VAL:HG12	1.88	0.56
6:Z:52:ASN:OD1	6:Z:53:SER:N	2.37	0.56
22:K:213:THR:O	22:K:214:ASN:OD1	2.23	0.56
25:N:200:ARG:NE	25:n:174:ASP:OD2	2.39	0.56
32:f:293:GLN:HG2	32:f:891:THR:HG23	1.87	0.56
16:E:232:MET:SD	16:E:235:ILE:HD11	2.45	0.55
25:n:194:LEU:HD13	25:n:208:ILE:HG23	1.88	0.55
27:p:7:ASN:ND2	27:p:29:GLY:O	2.37	0.55
2:V:227:VAL:HG12	2:V:231:LEU:HD12	1.88	0.55
7:a:60:TYR:CE1	7:a:64:ILE:HG21	2.41	0.55
7:a:207:GLY:O	7:a:271:LYS:NZ	2.19	0.55
7:a:228:THR:HG22	7:a:229:ASP:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:61:PHE:CE2	9:c:109:VAL:HG12	2.41	0.55
31:t:90:VAL:HG11	31:t:133:ILE:HD13	1.88	0.55
1:U:456:ASP:OD1	1:U:457:ILE:N	2.40	0.55
5:Y:15:PRO:HD3	5:Y:147:ILE:HD13	1.88	0.55
8:b:33:VAL:HG11	8:b:75:LEU:HD13	1.87	0.55
17:F:366:MET:HE1	17:F:388:THR:CG2	2.36	0.55
28:Q:135:GLY:HA3	28:Q:167:LEU:HD11	1.87	0.55
32:f:571:GLU:O	32:f:573:ILE:N	2.39	0.55
6:Z:231:GLN:NE2	7:a:341:LEU:HD21	2.21	0.55
27:P:152:SER:CB	30:s:176:LEU:HD22	2.37	0.55
29:r:103:THR:OG1	29:r:159:MET:N	2.34	0.55
7:a:149:THR:HG22	7:a:150:SER:N	2.22	0.55
12:A:330:ALA:O	12:A:336:ARG:NH1	2.40	0.55
32:f:463:LEU:N	32:f:489:TYR:OH	2.39	0.55
32:f:746:ARG:O	32:f:750:GLN:OE1	2.24	0.55
9:c:188:SER:O	9:c:192:LEU:HD23	2.07	0.55
9:c:210:ASN:OD1	9:c:211:GLU:N	2.39	0.55
20:I:122:THR:HG22	20:I:129:PRO:HB3	1.89	0.55
27:P:149:MET:HA	27:P:149:MET:HE2	1.89	0.55
31:t:171:ASP:OD2	31:t:175:VAL:HG22	2.06	0.55
32:f:550:LEU:HD11	32:f:587:PHE:CD2	2.42	0.55
1:U:891:VAL:O	1:U:891:VAL:HG13	2.06	0.55
3:W:374:THR:OG1	7:a:327:VAL:HG22	2.06	0.55
16:E:146:ARG:O	16:E:149:ILE:HG22	2.06	0.55
17:F:233:LYS:N	35:F:501:ATP:O1B	2.39	0.55
26:O:140:ALA:HB1	26:O:170:MET:HE2	1.89	0.55
28:Q:44:LEU:HD21	28:Q:46:CYS:SG	2.47	0.55
1:U:187:LEU:HD12	15:D:45:LYS:HB3	1.87	0.55
12:A:433:ASN:H	22:K:82:ILE:HD11	1.72	0.55
14:C:161:ILE:HD12	14:C:186:VAL:HG11	1.88	0.55
14:C:234:LEU:HD23	14:C:234:LEU:C	2.31	0.55
17:F:235:LEU:HD13	35:F:501:ATP:H2'	1.89	0.55
17:F:236:LEU:HD23	17:F:354:PHE:HZ	1.71	0.55
23:L:205:LEU:HD22	23:L:210:VAL:CG2	2.37	0.55
25:n:62:ASN:OD1	26:o:165:LEU:HD21	2.06	0.55
30:s:100:LEU:HD11	30:s:116:ILE:HD11	1.87	0.55
32:f:658:ALA:HB2	32:f:693:ALA:HB1	1.89	0.55
3:W:422:ASN:OD1	6:Z:252:LYS:NZ	2.34	0.55
7:a:373:ASP:HB3	10:d:348:MET:HE1	1.89	0.55
14:C:198:LEU:HD22	35:C:501:ATP:H2'	1.88	0.55
29:R:233:VAL:O	29:R:233:VAL:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:322:SER:OG	32:f:324:VAL:HG23	2.07	0.55
26:O:252:THR:HG21	27:P:168:SER:CB	2.36	0.54
28:Q:16:ALA:HB3	28:Q:160:LEU:HD11	1.87	0.54
3:W:442:THR:HG21	6:Z:230:LEU:CD2	2.38	0.54
7:a:8:LEU:HD22	7:a:26:GLU:HB3	1.87	0.54
17:F:123:VAL:O	17:F:123:VAL:HG12	2.06	0.54
20:I:119:GLN:HG3	21:J:78:ALA:HB1	1.89	0.54
26:O:262:LEU:HD21	27:P:195:ILE:CD1	2.36	0.54
30:S:96:ILE:HD11	30:S:120:LEU:HD13	1.90	0.54
31:t:94:THR:HG21	31:t:133:ILE:HD12	1.89	0.54
31:t:260:ILE:O	31:t:261:SER:OG	2.17	0.54
32:f:505:MET:CE	32:f:538:ILE:HD13	2.33	0.54
3:W:112:VAL:HG22	3:W:124:LEU:HD21	1.87	0.54
3:W:344:THR:O	3:W:347:GLY:N	2.38	0.54
5:Y:200:LEU:O	5:Y:204:THR:HG22	2.08	0.54
5:Y:290:PRO:O	5:Y:291:HIS:ND1	2.40	0.54
7:a:137:ASP:O	7:a:141:MET:HG3	2.07	0.54
17:F:165:PRO:O	17:F:166:THR:HG23	2.06	0.54
19:H:69:THR:HG22	19:H:70:LYS:N	2.22	0.54
27:P:168:SER:CB	27:P:200:LEU:HD21	2.37	0.54
3:W:257:GLN:OE1	3:W:295:LYS:NZ	2.35	0.54
12:A:297:ARG:HD3	17:F:257:VAL:HG11	1.89	0.54
16:E:145:LEU:O	16:E:145:LEU:HD23	2.07	0.54
17:F:384:LEU:HD12	17:F:424:ILE:HD11	1.90	0.54
28:q:25:ILE:HG23	28:q:26:VAL:HG13	1.89	0.54
18:G:176:THR:HG23	19:H:56:LEU:HD12	1.89	0.54
21:J:77:THR:O	21:J:80:ALA:HB3	2.06	0.54
30:s:96:ILE:O	30:s:100:LEU:HD23	2.07	0.54
32:f:411:ALA:HB3	32:f:443:GLY:HA3	1.89	0.54
1:U:19:LEU:CD1	10:d:124:LEU:HD13	2.37	0.54
1:U:27:LEU:HD11	1:U:38:ILE:HG12	1.89	0.54
3:W:331:GLY:HA3	3:W:337:ALA:HB2	1.88	0.54
7:a:243:GLY:HA2	7:a:272:ILE:HD11	1.90	0.54
17:F:84:LYS:HG3	17:F:84:LYS:O	2.08	0.54
29:R:184:THR:HB	29:R:198:MET:HE3	1.90	0.54
31:T:67:ILE:HG23	31:T:95:MET:HE3	1.88	0.54
26:o:56:VAL:CG1	26:o:218:LEU:HD21	2.38	0.54
28:q:138:LEU:H	28:q:138:LEU:HD12	1.73	0.54
32:f:397:LYS:O	32:f:401:LYS:NZ	2.38	0.54
13:B:227:PRO:O	13:B:232:LYS:NZ	2.39	0.54
18:G:32:ILE:HD11	18:G:156:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:G:189:TRP:HB3	18:G:194:THR:HG23	1.90	0.54
23:L:41:LYS:HG3	23:L:42:THR:HG23	1.90	0.54
26:o:204:ALA:O	26:o:208:ASN:ND2	2.37	0.54
3:W:135:LYS:HB2	3:W:138:VAL:HG12	1.89	0.54
4:X:126:ARG:NH2	4:X:156:GLU:OE2	2.39	0.54
5:Y:188:CYS:SG	5:Y:196:GLN:NE2	2.79	0.54
14:C:342:ILE:HD11	14:C:383:PHE:CE2	2.43	0.54
20:I:107:CYS:O	20:I:111:VAL:HG23	2.07	0.54
20:I:135:LEU:HD21	20:I:162:THR:CG2	2.37	0.54
21:J:139:ASP:OD1	21:J:140:GLY:N	2.40	0.54
2:V:440:LYS:HZ3	10:d:238:GLU:C	2.16	0.54
3:W:283:GLN:O	3:W:287:VAL:HG23	2.08	0.54
12:A:142:VAL:HG23	12:A:147:TYR:O	2.08	0.54
12:A:172:VAL:HG21	12:A:227:ARG:HE	1.72	0.54
3:W:51:GLU:HB2	3:W:66:ILE:HG21	1.90	0.53
3:W:443:THR:HG21	6:Z:204:LYS:HD2	1.89	0.53
5:Y:25:LEU:HD21	5:Y:31:HIS:NE2	2.23	0.53
5:Y:186:LEU:HD21	5:Y:214:MET:CE	2.38	0.53
6:Z:15:VAL:O	6:Z:19:VAL:HG23	2.08	0.53
6:Z:81:MET:HE2	9:c:98:MET:HE2	1.90	0.53
10:d:87:VAL:HG11	10:d:125:GLU:OE1	2.07	0.53
19:H:44:VAL:HG11	19:H:137:CYS:SG	2.47	0.53
26:O:252:THR:HG21	27:P:168:SER:HB2	1.91	0.53
29:R:213:ASP:OD1	29:R:258:TYR:OH	2.24	0.53
28:q:135:GLY:O	28:q:139:THR:HG23	2.08	0.53
2:V:493:ALA:HB3	6:Z:275:LEU:HD11	1.90	0.53
16:E:216:ARG:HD3	16:E:219:PHE:HE2	1.73	0.53
21:J:86:ARG:HD3	21:J:114:LEU:HD11	1.91	0.53
26:O:60:ASP:OD2	26:O:213:GLY:N	2.40	0.53
32:f:777:THR:HG23	32:f:828:ARG:HB3	1.90	0.53
32:f:791:VAL:HG12	32:f:823:ALA:HB1	1.90	0.53
3:W:276:LEU:HD11	3:W:341:PHE:CE1	2.44	0.53
3:W:377:ARG:NE	7:a:308:GLU:OE1	2.40	0.53
9:c:49:VAL:HG21	9:c:148:ILE:HD11	1.90	0.53
16:E:354:ALA:HB3	16:E:369:LYS:HZ1	1.73	0.53
28:Q:14:LEU:HD21	28:Q:160:LEU:HD13	1.90	0.53
31:T:80:ARG:O	25:n:200:ARG:NH1	2.41	0.53
31:t:64:GLY:HA2	31:t:160:TYR:OH	2.08	0.53
8:b:117:VAL:O	8:b:152:LYS:NZ	2.40	0.53
14:C:221:GLN:NE2	14:C:230:MET:SD	2.82	0.53
27:P:95:LEU:HD11	27:P:107:PRO:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:R:223:THR:HG23	29:R:230:GLY:HA2	1.91	0.53
27:p:59:ASP:OD2	27:p:104:TYR:N	2.41	0.53
32:f:59:LEU:O	32:f:63:LEU:HD23	2.07	0.53
7:a:112:ILE:HG21	7:a:142:LEU:HD13	1.91	0.53
12:A:284:ARG:NH1	17:F:289:ASP:OD2	2.42	0.53
15:D:323:ARG:O	15:D:325:GLY:N	2.39	0.53
24:M:76:MET:HE2	24:M:78:VAL:CG1	2.39	0.53
28:Q:172:ILE:HG23	28:Q:173:LEU:HD12	1.90	0.53
28:q:139:THR:HG22	28:q:167:LEU:HD11	1.89	0.53
28:q:154:GLU:O	28:q:158:GLU:OE1	2.27	0.53
2:V:258:TYR:HE2	2:V:270:LEU:HD12	1.73	0.53
6:Z:255:ASP:O	6:Z:258:VAL:HG12	2.08	0.53
9:c:61:PHE:CZ	9:c:109:VAL:HG12	2.44	0.53
12:A:214:LEU:HD22	12:A:343:PHE:HE1	1.73	0.53
15:D:225:ALA:HB1	15:D:259:PRO:O	2.09	0.53
21:J:42:VAL:CG1	21:J:191:VAL:HG21	2.38	0.53
28:Q:4:LEU:HD13	28:Q:45:LEU:HB3	1.91	0.53
29:r:203:SER:H	29:r:206:LEU:HD11	1.72	0.53
33:y:380:LEU:HD12	33:y:381:ARG:N	2.24	0.53
4:X:96:PHE:HE2	4:X:109:LEU:HD22	1.74	0.53
5:Y:134:LEU:O	5:Y:138:LEU:HD23	2.08	0.53
6:Z:172:VAL:HG11	9:c:220:LEU:HD23	1.90	0.53
10:d:245:PHE:HE1	10:d:267:ILE:HG21	1.74	0.53
12:A:191:VAL:HG13	12:A:271:LEU:HD21	1.90	0.53
16:E:165:ILE:HG22	16:E:168:LYS:CE	2.38	0.53
22:K:37:ALA:HB1	22:K:50:VAL:HG12	1.90	0.53
31:T:169:TYR:CG	31:T:169:TYR:O	2.61	0.53
25:n:48:LEU:HD21	25:n:135:ALA:HB3	1.91	0.53
32:f:399:LEU:HG	32:f:440:ILE:HD12	1.91	0.53
2:V:185:GLN:OE1	2:V:221:LEU:HD22	2.07	0.53
4:X:287:LEU:HD21	4:X:319:ILE:HD11	1.89	0.53
9:c:27:THR:HG22	9:c:177:THR:HA	1.89	0.53
18:G:22:LEU:HD12	19:H:79:MET:HE1	1.89	0.53
25:N:93:VAL:HG11	25:N:117:PHE:CE2	2.43	0.53
26:O:262:LEU:HD21	27:P:195:ILE:HD11	1.90	0.53
28:Q:18:ASP:OD2	28:Q:175:LEU:HD13	2.07	0.53
29:r:190:GLY:N	29:r:226:ASP:OD2	2.42	0.53
32:f:293:GLN:CG	32:f:891:THR:HG23	2.39	0.53
32:f:388:ASP:OD1	32:f:389:LYS:N	2.38	0.53
32:f:471:LEU:HD23	32:f:504:VAL:HG23	1.91	0.53
1:U:24:LEU:HD11	1:U:48:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:340:GLN:O	15:D:344:ILE:HG12	2.08	0.53
16:E:130:VAL:HG23	16:E:131:SER:N	2.24	0.53
17:F:251:LEU:CD2	17:F:285:ILE:HG23	2.39	0.53
24:M:179:LYS:O	24:M:180:LEU:HD12	2.09	0.53
27:P:125:ASP:OD1	27:P:129:CYS:N	2.37	0.53
29:R:65:PHE:HB2	29:R:184:THR:HG22	1.91	0.53
25:n:187:LEU:HD23	25:n:210:LEU:HD23	1.91	0.53
30:s:165:ALA:O	30:s:170:SER:OG	2.15	0.53
1:U:206:MET:HA	1:U:206:MET:HE3	1.90	0.53
3:W:329:ARG:HD2	3:W:342:GLY:O	2.08	0.53
12:A:35:THR:O	12:A:35:THR:HG22	2.09	0.53
13:B:233:THR:OG1	35:B:501:ATP:O2B	2.27	0.53
23:L:7:ASP:O	23:L:21:GLN:NE2	2.40	0.53
28:Q:154:GLU:O	28:Q:158:GLU:OE1	2.27	0.53
2:V:236:ARG:O	2:V:240:LEU:HD23	2.09	0.52
3:W:177:MET:SD	3:W:178:GLU:N	2.82	0.52
5:Y:387:ILE:HG21	6:Z:276:ILE:HD13	1.91	0.52
29:r:72:ILE:HD11	29:r:235:LEU:HD11	1.91	0.52
1:U:556:MET:HE3	1:U:556:MET:HA	1.91	0.52
10:d:88:LEU:HD23	10:d:126:LEU:HD21	1.91	0.52
16:E:325:GLU:OE1	16:E:325:GLU:N	2.42	0.52
17:F:307:GLN:O	17:F:311:LEU:HD23	2.09	0.52
22:K:191:LEU:HD21	22:K:219:THR:OG1	2.08	0.52
26:O:241:ARG:NH2	27:P:154:TRP:O	2.42	0.52
16:E:154:THR:HG23	16:E:156:PRO:HD3	1.91	0.52
31:t:64:GLY:O	31:t:165:SER:OG	2.20	0.52
32:f:479:LEU:CD1	32:f:517:VAL:HG21	2.40	0.52
2:V:164:GLU:HG2	2:V:165:ALA:N	2.25	0.52
3:W:88:MET:HA	3:W:88:MET:HE3	1.91	0.52
15:D:116:LEU:HD12	15:D:117:SER:H	1.73	0.52
23:L:72:ILE:HD11	23:L:132:LEU:CD2	2.37	0.52
28:Q:85:ARG:NH1	28:Q:122:ALA:O	2.42	0.52
29:R:200:ARG:HG3	28:q:142:ILE:HD12	1.91	0.52
31:T:114:GLN:NE2	31:T:118:ASP:OD1	2.42	0.52
31:t:160:TYR:HE1	31:t:237:VAL:HG13	1.73	0.52
1:U:337:LEU:HD21	1:U:791:LEU:HD11	1.92	0.52
10:d:206:ALA:O	10:d:210:THR:HG23	2.09	0.52
16:E:158:LEU:HG	16:E:159:PHE:H	1.74	0.52
16:E:277:MET:HE2	16:E:295:LEU:HD13	1.92	0.52
17:F:333:ASN:ND2	35:F:501:ATP:O2G	2.36	0.52
23:L:195:LEU:HA	23:L:198:THR:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:198:LEU:CB	1:U:223:LEU:HD11	2.39	0.52
1:U:583:MET:HE2	1:U:583:MET:HA	1.91	0.52
2:V:65:ARG:O	2:V:69:THR:HG23	2.09	0.52
2:V:192:MET:HA	2:V:195:ILE:HG22	1.92	0.52
2:V:484:LEU:HD23	6:Z:267:ARG:NH2	2.24	0.52
3:W:276:LEU:HD21	3:W:341:PHE:CZ	2.45	0.52
4:X:408:SER:HA	5:Y:376:LEU:HD13	1.91	0.52
7:a:326:GLU:O	7:a:329:LYS:NZ	2.29	0.52
20:I:112:THR:HG23	21:J:81:ARG:HD2	1.92	0.52
23:L:88:MET:HG2	23:L:112:ILE:HD11	1.91	0.52
26:O:60:ASP:CB	26:O:206:ILE:HD11	2.40	0.52
3:W:440:ASN:O	3:W:443:THR:HG22	2.08	0.52
4:X:15:LEU:O	4:X:19:ASP:C	2.52	0.52
4:X:99:MET:SD	4:X:103:THR:HG22	2.50	0.52
9:c:156:VAL:HG13	9:c:156:VAL:O	2.09	0.52
12:A:25:LEU:CD2	13:B:410:ARG:NH1	2.69	0.52
16:E:334:LEU:HD23	16:E:334:LEU:H	1.74	0.52
28:Q:14:LEU:HD11	28:Q:157:VAL:HG22	1.91	0.52
32:f:407:MET:CE	32:f:440:ILE:HD11	2.39	0.52
1:U:641:SER:OG	1:U:675:MET:SD	2.62	0.52
2:V:395:ILE:HG22	2:V:395:ILE:O	2.09	0.52
6:Z:208:ILE:HG22	7:a:353:LEU:HD11	1.92	0.52
9:c:38:LEU:HD22	9:c:207:TYR:CE1	2.44	0.52
14:C:34:ILE:HG21	15:D:51:LEU:HD11	1.92	0.52
15:D:296:MET:HE2	15:D:307:VAL:HG11	1.92	0.52
17:F:244:THR:O	17:F:244:THR:HG22	2.08	0.52
29:r:204:TYR:O	29:r:205:ASP:OD1	2.28	0.52
31:t:52:THR:HG22	31:t:101:ASP:HA	1.92	0.52
3:W:330:LYS:O	3:W:330:LYS:HG2	2.09	0.52
12:A:273:PHE:CG	12:A:273:PHE:O	2.63	0.52
16:E:141:GLN:OE1	16:E:141:GLN:N	2.42	0.52
21:J:119:THR:HG22	21:J:126:PRO:HB3	1.91	0.52
23:L:10:VAL:O	23:L:10:VAL:HG12	2.09	0.52
27:P:141:THR:HG22	27:P:142:CYS:N	2.25	0.52
29:r:238:VAL:HG23	29:r:238:VAL:O	2.09	0.52
1:U:588:MET:CE	1:U:764:LEU:HD22	2.32	0.52
2:V:309:MET:HE1	2:V:331:LEU:HD23	1.92	0.52
3:W:435:LEU:HD23	3:W:435:LEU:C	2.35	0.52
12:A:63:THR:CG2	32:f:680:ARG:CZ	2.88	0.52
7:a:185:ILE:HD12	7:a:221:VAL:CG2	2.40	0.51
7:a:356:TRP:O	7:a:360:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:329:MET:SD	13:B:347:ILE:HD11	2.51	0.51
32:f:407:MET:HE2	32:f:440:ILE:CD1	2.39	0.51
10:d:192:LEU:HD13	10:d:215:LEU:CD2	2.39	0.51
17:F:149:ASP:OD1	17:F:150:LEU:N	2.44	0.51
17:F:336:ASP:OD1	17:F:336:ASP:N	2.43	0.51
29:R:129:ASN:O	29:R:131:GLU:N	2.40	0.51
28:q:4:LEU:HD23	28:q:17:SER:HB2	1.93	0.51
1:U:587:ALA:HB2	1:U:621:SER:CB	2.40	0.51
5:Y:293:ARG:NH2	11:e:49:GLU:O	2.44	0.51
19:H:3:GLU:OE2	19:H:16:SER:OG	2.24	0.51
24:M:197:ILE:O	24:M:201:VAL:HG22	2.11	0.51
31:t:93:SER:O	31:t:94:THR:OG1	2.23	0.51
32:f:170:TRP:CH2	32:f:185:LEU:HD21	2.45	0.51
3:W:412:ILE:HG22	3:W:412:ILE:O	2.11	0.51
7:a:304:VAL:HG23	7:a:304:VAL:O	2.10	0.51
12:A:276:GLU:HB3	13:B:310:LEU:HD23	1.91	0.51
17:F:168:TYR:O	17:F:173:LYS:NZ	2.38	0.51
25:n:61:ALA:HB1	26:o:157:TYR:OH	2.10	0.51
32:f:558:LEU:HB2	32:f:559:PRO:HD3	1.93	0.51
33:y:382:GLN:NE2	33:y:383:THR:HG23	2.25	0.51
5:Y:376:LEU:HD23	6:Z:265:LEU:HD21	1.92	0.51
17:F:235:LEU:HD13	35:F:501:ATP:C2'	2.41	0.51
18:G:186:LYS:NZ	18:G:193:GLN:OE1	2.39	0.51
19:H:107:THR:O	19:H:111:VAL:HG23	2.10	0.51
21:J:95:ARG:HG3	28:Q:62:LYS:HE3	1.91	0.51
31:t:114:GLN:NE2	31:t:118:ASP:OD1	2.43	0.51
32:f:803:PHE:CE1	32:f:810:ILE:HD13	2.45	0.51
1:U:330:SER:OG	1:U:332:GLU:OE1	2.29	0.51
7:a:80:ILE:HD13	7:a:100:THR:HB	1.92	0.51
13:B:167:THR:HG22	13:B:171:VAL:HG13	1.92	0.51
28:Q:142:ILE:HD11	29:r:196:GLY:C	2.36	0.51
29:r:63:LEU:HD21	29:r:65:PHE:HD2	1.76	0.51
31:t:171:ASP:OD1	31:t:173:LEU:N	2.43	0.51
32:f:727:PHE:CZ	32:f:768:LEU:HD11	2.46	0.51
32:f:803:PHE:O	32:f:806:VAL:HG23	2.11	0.51
2:V:302:TYR:OH	2:V:397:ARG:NE	2.36	0.51
3:W:40:LEU:HD23	3:W:41:GLN:HG3	1.91	0.51
7:a:176:ALA:O	7:a:180:LEU:HD23	2.10	0.51
29:r:219:ILE:HB	29:r:233:VAL:HG13	1.93	0.51
32:f:423:ASP:O	32:f:427:THR:HG23	2.11	0.51
3:W:438:LEU:HD23	6:Z:233:VAL:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:144:LEU:HD21	13:B:162:VAL:HG22	1.92	0.51
17:F:334:ARG:HE	17:F:337:ILE:HD11	1.75	0.51
24:M:76:MET:HE3	24:M:136:PHE:CD2	2.46	0.51
27:p:133:THR:HG21	27:p:136:PHE:O	2.11	0.51
2:V:289:LEU:HB3	2:V:312:ALA:HB2	1.92	0.51
5:Y:222:TYR:OH	5:Y:285:ASP:OD2	2.15	0.51
6:Z:23:PHE:CD2	6:Z:126:VAL:HG21	2.46	0.51
15:D:342:ARG:HA	15:D:364:VAL:HG11	1.92	0.51
17:F:251:LEU:HD11	17:F:256:LEU:HD21	1.91	0.51
18:G:186:LYS:O	18:G:186:LYS:HD2	2.10	0.51
19:H:75:VAL:HG22	19:H:76:TYR:N	2.26	0.51
22:K:9:ASP:O	22:K:23:GLN:NE2	2.39	0.51
28:q:3:TYR:OH	28:q:139:THR:HG21	2.11	0.51
30:s:219:ASP:O	30:s:238:LEU:N	2.44	0.51
1:U:486:MET:HE1	1:U:781:LEU:CD2	2.41	0.51
28:Q:13:VAL:HG11	28:Q:105:ALA:HB1	1.92	0.51
25:n:170:TYR:OH	31:t:80:ARG:NE	2.44	0.51
32:f:445:LEU:HB3	32:f:466:LEU:HD23	1.93	0.51
1:U:827:LYS:HE2	32:f:614:HIS:HB3	1.93	0.50
3:W:257:GLN:HG3	3:W:257:GLN:O	2.10	0.50
4:X:256:LEU:HD22	4:X:319:ILE:HG13	1.93	0.50
5:Y:186:LEU:HD21	5:Y:214:MET:HE1	1.91	0.50
7:a:83:VAL:O	7:a:86:GLN:NE2	2.43	0.50
10:d:316:TYR:O	10:d:318:PHE:N	2.45	0.50
12:A:161:VAL:HG11	12:A:259:GLU:OE1	2.11	0.50
13:B:234:LEU:HD11	35:B:501:ATP:C4	2.46	0.50
23:L:47:VAL:HG22	23:L:212:ILE:HG23	1.93	0.50
28:q:12:TYR:OH	28:q:151:ILE:HG23	2.10	0.50
2:V:79:VAL:HG13	2:V:163:VAL:HG22	1.93	0.50
2:V:458:VAL:HG23	2:V:458:VAL:O	2.11	0.50
5:Y:285:ASP:OD1	5:Y:287:LEU:N	2.44	0.50
19:H:46:LEU:HD21	19:H:137:CYS:SG	2.51	0.50
19:H:212:ILE:HD11	19:H:219:ARG:HH21	1.76	0.50
22:K:161:THR:OG1	23:L:78:THR:HG21	2.11	0.50
26:O:126:LEU:HD22	26:O:141:LEU:CD1	2.41	0.50
29:R:221:GLN:OE1	28:q:145:ARG:HA	2.11	0.50
32:f:171:GLN:HE22	32:f:210:GLU:HG2	1.76	0.50
2:V:81:GLN:OE1	2:V:96:ARG:NH1	2.44	0.50
4:X:107:VAL:HG13	4:X:137:TYR:HE1	1.77	0.50
4:X:171:LEU:HD13	4:X:210:LEU:HD23	1.93	0.50
13:B:289:ALA:HB1	14:C:271:ARG:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:360:THR:O	13:B:364:ILE:HG12	2.11	0.50
17:F:406:ILE:HD13	17:F:422:GLU:CB	2.41	0.50
21:J:73:PHE:CE1	21:J:129:ILE:HB	2.47	0.50
28:Q:17:SER:OG	28:Q:45:LEU:HD22	2.11	0.50
2:V:68:ASP:HB3	2:V:112:VAL:HG22	1.94	0.50
2:V:379:LEU:HD13	2:V:395:ILE:HG21	1.93	0.50
7:a:55:GLY:O	7:a:59:LEU:HD13	2.12	0.50
7:a:301:LYS:O	7:a:302:ILE:HG23	2.11	0.50
9:c:129:THR:O	9:c:132:SER:OG	2.26	0.50
13:B:197:ILE:O	13:B:201:VAL:HG22	2.12	0.50
23:L:95:SER:HB2	23:L:103:LEU:HD13	1.94	0.50
25:n:56:THR:N	25:n:59:TYR:O	2.42	0.50
32:f:424:GLY:O	32:f:428:GLN:OE1	2.29	0.50
1:U:475:HIS:ND1	1:U:507:VAL:O	2.34	0.50
5:Y:177:ARG:NH1	14:C:337:ASN:OD1	2.43	0.50
6:Z:133:LEU:HD22	6:Z:162:ILE:HG12	1.93	0.50
13:B:305:ILE:HD13	14:C:271:ARG:CZ	2.41	0.50
19:H:195:LEU:HD13	19:H:208:ILE:HD11	1.92	0.50
26:O:255:LEU:HD11	27:P:201:LYS:CG	2.42	0.50
3:W:449:GLU:OE1	6:Z:223:ASN:ND2	2.44	0.50
6:Z:147:ASP:HA	7:a:215:GLU:OE2	2.11	0.50
7:a:60:TYR:O	7:a:61:GLU:C	2.53	0.50
12:A:430:MET:HA	12:A:430:MET:HE2	1.92	0.50
13:B:79:ILE:O	13:B:83:GLU:OE1	2.29	0.50
13:B:337:LEU:CD1	13:B:342:ILE:HD11	2.42	0.50
16:E:303:LEU:HB3	16:E:304:PRO:HD3	1.94	0.50
22:K:37:ALA:CB	22:K:50:VAL:HG12	2.41	0.50
30:s:74:LEU:HD11	30:s:80:ILE:HD11	1.93	0.50
32:f:799:VAL:HG21	32:f:821:LEU:HG	1.94	0.50
3:W:28:LEU:HD11	3:W:69:ALA:CB	2.42	0.50
3:W:393:LEU:O	3:W:397:VAL:HG23	2.12	0.50
13:B:116:ILE:HG22	13:B:117:ASP:N	2.26	0.50
18:G:145:GLU:OE1	18:G:145:GLU:HA	2.12	0.50
32:f:582:VAL:HG22	32:f:582:VAL:O	2.09	0.50
1:U:554:LEU:HD21	1:U:764:LEU:HD23	1.93	0.50
5:Y:42:MET:HE1	5:Y:63:TRP:HZ3	1.76	0.50
7:a:363:MET:SD	9:c:307:VAL:HG11	2.51	0.50
8:b:151:GLU:O	8:b:154:THR:OG1	2.25	0.50
12:A:111:TYR:CE1	12:A:134:ILE:HG21	2.47	0.50
13:B:109:VAL:HG22	13:B:151:LEU:CD2	2.41	0.50
18:G:113:MET:HE1	18:G:116:LYS:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:216:TRP:CE3	24:M:228:VAL:HG22	2.47	0.50
30:S:98:ALA:O	30:S:102:MET:HG3	2.12	0.50
31:T:137:LEU:HD22	31:T:157:ILE:HD11	1.93	0.50
32:f:109:ILE:HG22	32:f:113:MET:HE2	1.94	0.50
32:f:298:LEU:HD22	32:f:303:VAL:HG11	1.93	0.50
6:Z:34:ARG:NH2	6:Z:60:GLU:OE2	2.41	0.50
7:a:299:SER:O	7:a:300:ALA:C	2.55	0.50
17:F:285:ILE:HG21	17:F:288:LEU:CD1	2.42	0.50
18:G:196:GLU:HG3	18:G:242:LEU:HD13	1.94	0.50
30:s:142:ASP:OD1	30:s:146:LYS:N	2.36	0.50
32:f:659:LEU:HD13	32:f:797:LEU:HD21	1.94	0.50
7:a:108:ASP:O	7:a:112:ILE:HG12	2.12	0.49
16:E:87:LEU:HD23	16:E:88:ASP:O	2.12	0.49
21:J:47:LYS:NZ	21:J:207:GLU:OE2	2.35	0.49
26:O:67:MET:HE3	30:s:215:VAL:HG21	1.93	0.49
27:P:149:MET:HE1	30:s:176:LEU:HA	1.93	0.49
25:n:36:THR:HG21	25:n:197:ALA:CB	2.42	0.49
27:p:149:MET:HE3	27:p:173:ASN:HB2	1.93	0.49
28:q:3:TYR:CZ	28:q:139:THR:HG21	2.47	0.49
32:f:583:VAL:HG12	32:f:584:SER:N	2.26	0.49
2:V:436:PHE:CE1	10:d:290:ILE:HG23	2.47	0.49
6:Z:39:LEU:HD11	6:Z:122:VAL:HB	1.94	0.49
8:b:130:ARG:O	8:b:134:GLU:OE1	2.30	0.49
12:A:25:LEU:HD22	13:B:410:ARG:NE	2.26	0.49
12:A:279:ALA:O	13:B:307:ARG:NH1	2.44	0.49
19:H:141:GLU:CD	27:P:115:LYS:HZ3	2.20	0.49
29:R:233:VAL:HG21	29:R:254:LEU:CD1	2.42	0.49
28:q:116:TYR:HD2	28:q:124:LEU:HD11	1.76	0.49
3:W:315:MET:HE3	3:W:358:VAL:HG22	1.93	0.49
6:Z:172:VAL:HG13	9:c:217:LEU:HD12	1.94	0.49
13:B:255:LEU:HD13	13:B:267:VAL:HG22	1.94	0.49
25:N:63:ARG:CZ	31:t:256:ILE:HD11	2.42	0.49
26:O:148:VAL:HG23	26:O:149:THR:HG23	1.94	0.49
32:f:162:LEU:O	32:f:166:VAL:HG23	2.13	0.49
32:f:727:PHE:CE2	32:f:803:PHE:HE2	2.29	0.49
1:U:689:ILE:O	1:U:693:LEU:HD23	2.11	0.49
3:W:362:ASN:O	3:W:366:MET:HG3	2.13	0.49
7:a:157:ASP:OD1	7:a:196:ARG:NH2	2.41	0.49
12:A:25:LEU:HD21	13:B:410:ARG:HD3	1.94	0.49
13:B:440:LEU:HD11	21:J:30:SER:H	1.76	0.49
17:F:88:TYR:CE1	17:F:161:LEU:HD12	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:G:196:GLU:OE2	18:G:242:LEU:HD22	2.11	0.49
23:L:196:ARG:HG3	23:L:205:LEU:HD12	1.94	0.49
24:M:190:ILE:O	24:M:194:VAL:HG23	2.12	0.49
25:N:169:ILE:O	25:N:173:VAL:HG13	2.12	0.49
28:Q:28:MET:HE1	29:R:172:TYR:CE2	2.47	0.49
26:o:186:ARG:NE	26:o:193:GLU:OE2	2.46	0.49
31:t:47:GLN:NE2	31:t:148:MET:O	2.46	0.49
3:W:115:ILE:HG22	3:W:116:THR:N	2.27	0.49
3:W:426:ASN:ND2	9:c:233:ASP:OD1	2.45	0.49
6:Z:212:LEU:HD12	7:a:353:LEU:HD12	1.94	0.49
12:A:279:ALA:HB2	13:B:310:LEU:HD22	1.95	0.49
12:A:306:LEU:CD2	12:A:317:VAL:HG21	2.42	0.49
20:I:197:LEU:HA	20:I:200:THR:HG22	1.94	0.49
2:V:309:MET:HE1	2:V:331:LEU:HB3	1.94	0.49
4:X:137:TYR:HB3	4:X:146:ALA:HB2	1.93	0.49
5:Y:162:GLU:OE2	5:Y:166:SER:OG	2.30	0.49
7:a:33:LEU:O	8:b:18:ASN:HA	2.12	0.49
18:G:87:SER:O	18:G:91:VAL:HG23	2.12	0.49
19:H:38:ILE:HD12	19:H:191:ALA:HB2	1.94	0.49
19:H:209:GLU:OE2	19:H:220:ARG:HD3	2.13	0.49
29:r:104:MET:HE2	29:r:108:ALA:HA	1.94	0.49
1:U:803:LYS:N	1:U:893:THR:O	2.41	0.49
3:W:61:VAL:O	3:W:65:ARG:HD3	2.12	0.49
3:W:144:ARG:NH2	3:W:181:GLU:OE2	2.44	0.49
3:W:294:LYS:O	3:W:294:LYS:NZ	2.28	0.49
10:d:281:LYS:HG3	10:d:315:TYR:CE2	2.48	0.49
12:A:178:GLY:O	35:A:501:ATP:N6	2.44	0.49
22:K:230:THR:OG1	22:K:233:GLU:OE1	2.25	0.49
24:M:179:LYS:C	24:M:180:LEU:HD12	2.38	0.49
2:V:337:LEU:HD22	2:V:367:VAL:HG11	1.95	0.49
5:Y:282:MET:HE1	5:Y:295:TYR:CG	2.48	0.49
20:I:46:ALA:HB1	20:I:197:LEU:HD11	1.95	0.49
22:K:40:ILE:HG21	22:K:194:ALA:HB1	1.94	0.49
25:N:196:LEU:HD21	25:n:175:ALA:HB2	1.95	0.49
26:O:62:ARG:CB	26:O:213:GLY:HA2	2.42	0.49
1:U:764:LEU:O	1:U:767:THR:OG1	2.25	0.49
2:V:469:THR:HG22	2:V:470:ARG:N	2.27	0.49
3:W:97:LEU:N	3:W:97:LEU:HD12	2.28	0.49
4:X:135:SER:HB2	4:X:172:LEU:HD11	1.94	0.49
5:Y:240:VAL:HG12	5:Y:260:LEU:HD21	1.95	0.49
6:Z:7:GLN:HG2	6:Z:46:LYS:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E:121:ASN:ND2	17:F:311:LEU:HD12	2.27	0.49
26:o:209:ASP:OD2	26:o:212:SER:N	2.41	0.49
32:f:139:CYS:HB3	32:f:165:GLU:OE1	2.13	0.49
32:f:263:PRO:CB	32:f:891:THR:HG22	2.43	0.49
32:f:399:LEU:HD23	32:f:432:TYR:CD1	2.48	0.49
32:f:420:TRP:CH2	32:f:827:PRO:HD3	2.48	0.49
2:V:352:SER:C	2:V:353:LEU:HD12	2.38	0.49
2:V:490:SER:O	6:Z:275:LEU:HD12	2.12	0.49
3:W:438:LEU:HD23	6:Z:233:VAL:CG2	2.42	0.49
10:d:313:ASN:O	10:d:315:TYR:N	2.44	0.49
12:A:25:LEU:HD22	13:B:410:ARG:CD	2.42	0.49
12:A:272:ILE:HG21	12:A:274:PHE:CE2	2.48	0.49
14:C:115:ALA:C	14:C:116:LEU:HD12	2.38	0.49
17:F:188:ILE:O	17:F:188:ILE:HG23	2.12	0.49
27:p:34:MET:HE2	27:p:183:MET:HE2	1.95	0.49
32:f:571:GLU:O	32:f:574:GLU:OE1	2.30	0.49
3:W:62:SER:O	3:W:66:ILE:HD12	2.13	0.48
10:d:123:LEU:O	10:d:126:LEU:C	2.55	0.48
12:A:143:ASP:HB2	12:A:146:LYS:O	2.13	0.48
13:B:292:THR:HG21	14:C:261:GLY:HA3	1.94	0.48
15:D:258:ALA:O	15:D:259:PRO:C	2.55	0.48
16:E:145:LEU:O	16:E:148:VAL:HG22	2.13	0.48
17:F:279:ALA:HB3	17:F:280:PRO:CD	2.42	0.48
18:G:10:ASP:OD2	18:G:27:TYR:OH	2.29	0.48
20:I:76:VAL:HG12	20:I:134:LEU:CD2	2.43	0.48
25:N:64:VAL:HG11	31:t:256:ILE:HG13	1.95	0.48
32:f:521:ALA:O	32:f:525:ILE:HG12	2.13	0.48
1:U:631:GLU:OE1	1:U:631:GLU:N	2.41	0.48
1:U:835:ILE:HG13	32:f:607:LEU:HD21	1.95	0.48
6:Z:113:LYS:HA	6:Z:116:CYS:O	2.13	0.48
12:A:29:ASP:OD2	13:B:410:ARG:HD2	2.11	0.48
12:A:303:ILE:HG23	12:A:336:ARG:CZ	2.43	0.48
15:D:155:THR:HG22	15:D:156:SER:N	2.28	0.48
19:H:86:LEU:CD1	19:H:118:MET:HE2	2.43	0.48
26:O:202:ILE:O	26:O:206:ILE:HG12	2.13	0.48
30:S:208:ILE:HD13	30:S:238:LEU:CD2	2.43	0.48
32:f:269:ALA:O	32:f:272:LEU:O	2.30	0.48
32:f:806:VAL:HG12	32:f:811:LEU:CD1	2.43	0.48
32:f:853:VAL:O	32:f:853:VAL:HG13	2.13	0.48
1:U:804:SER:OG	1:U:876:GLN:HB2	2.14	0.48
4:X:134:VAL:HG12	4:X:172:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:190:LEU:HD21	4:X:214:SER:HA	1.94	0.48
6:Z:170:VAL:HG23	9:c:152:LYS:HA	1.95	0.48
13:B:94:GLU:O	13:B:97:SER:OG	2.27	0.48
14:C:331:ILE:O	14:C:334:ARG:NH1	2.41	0.48
14:C:364:THR:HA	15:D:196:ILE:HD12	1.95	0.48
15:D:64:GLU:O	15:D:68:LEU:HD23	2.13	0.48
17:F:144:LYS:O	17:F:145:LEU:C	2.55	0.48
17:F:177:VAL:O	17:F:177:VAL:HG23	2.13	0.48
18:G:73:THR:HG22	18:G:76:ILE:HB	1.95	0.48
24:M:187:CYS:HA	24:M:190:ILE:HG22	1.95	0.48
26:O:255:LEU:HD11	27:P:201:LYS:HG3	1.95	0.48
32:f:810:ILE:HD11	32:f:817:VAL:CG1	2.43	0.48
2:V:185:GLN:HB2	2:V:218:TYR:HE1	1.77	0.48
2:V:477:HIS:ND1	10:d:342:TYR:OH	2.29	0.48
3:W:344:THR:O	3:W:345:GLU:C	2.56	0.48
12:A:63:THR:OG1	32:f:681:TYR:HE2	1.96	0.48
16:E:344:ARG:O	16:E:348:THR:HG22	2.12	0.48
17:F:288:LEU:HD21	17:F:342:LEU:HD21	1.95	0.48
25:n:208:ILE:HD12	25:n:228:ILE:HG23	1.96	0.48
26:o:47:ALA:CB	26:o:202:ILE:HD11	2.44	0.48
32:f:77:GLU:OE2	32:f:80:ARG:NH2	2.46	0.48
2:V:450:SER:OG	2:V:451:ILE:N	2.45	0.48
4:X:23:SER:OG	4:X:56:LEU:HD11	2.13	0.48
9:c:132:SER:O	9:c:136:LEU:HD23	2.13	0.48
13:B:52:VAL:O	13:B:52:VAL:HG23	2.13	0.48
13:B:309:MET:HE1	13:B:338:ASP:CB	2.43	0.48
13:B:337:LEU:HD13	13:B:342:ILE:HD11	1.94	0.48
15:D:297:ASP:OD1	15:D:301:GLN:NE2	2.46	0.48
21:J:115:LYS:O	21:J:119:THR:HG23	2.13	0.48
29:R:223:THR:HG21	29:R:251:VAL:HG21	1.95	0.48
29:r:190:GLY:CA	29:r:226:ASP:OD2	2.62	0.48
31:t:67:ILE:HD13	31:t:95:MET:HE3	1.96	0.48
32:f:51:GLN:NE2	32:f:55:GLU:OE2	2.39	0.48
32:f:727:PHE:CD2	32:f:803:PHE:CE2	3.02	0.48
32:f:826:GLN:OE1	32:f:827:PRO:HD2	2.14	0.48
1:U:728:PHE:O	1:U:732:LEU:HD23	2.14	0.48
2:V:168:GLN:HG3	2:V:191:LEU:HD11	1.96	0.48
2:V:255:LEU:HD21	2:V:271:VAL:HG23	1.95	0.48
3:W:154:GLU:OE1	3:W:192:LEU:HD21	2.14	0.48
13:B:244:SER:OG	32:f:704:LEU:CD1	2.31	0.48
13:B:422:SER:O	13:B:426:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:277:LEU:CD2	14:C:305:LEU:HD23	2.44	0.48
16:E:295:LEU:HD23	16:E:295:LEU:O	2.14	0.48
26:O:94:ASP:OD1	27:P:99:ARG:NE	2.47	0.48
2:V:93:PHE:CD1	2:V:96:ARG:HD2	2.49	0.48
2:V:309:MET:HE1	2:V:331:LEU:HG	1.95	0.48
4:X:109:LEU:O	4:X:112:GLU:HG3	2.14	0.48
4:X:403:THR:HG21	6:Z:266:ILE:HD11	1.96	0.48
18:G:22:LEU:HD11	19:H:79:MET:HE1	1.95	0.48
32:f:474:SER:HB3	32:f:477:MET:HE2	1.95	0.48
32:f:850:VAL:HG12	32:f:851:ASP:N	2.29	0.48
1:U:246:TYR:CD2	1:U:795:LEU:HD21	2.48	0.48
4:X:251:LEU:HD12	4:X:254:MET:HE3	1.95	0.48
4:X:402:GLU:HB2	9:c:249:LEU:HD11	1.94	0.48
7:a:205:LEU:HD12	7:a:240:PHE:CE2	2.47	0.48
10:d:152:ALA:O	10:d:155:SER:OG	2.26	0.48
17:F:240:CYS:O	17:F:244:THR:CB	2.61	0.48
20:I:45:LEU:HD11	20:I:137:ILE:HG12	1.96	0.48
21:J:200:GLN:OE1	21:J:200:GLN:HA	2.14	0.48
30:S:200:MET:SD	30:S:225:ILE:HD11	2.54	0.48
32:f:297:MET:SD	32:f:891:THR:HG21	2.54	0.48
32:f:446:LEU:O	32:f:450:ILE:HG13	2.14	0.48
1:U:236:LEU:HD21	1:U:244:MET:HB3	1.96	0.48
1:U:486:MET:HE2	1:U:518:LEU:HD22	1.94	0.48
15:D:258:ALA:CB	15:D:259:PRO:HD2	2.39	0.48
22:K:210:LEU:HD23	22:K:241:ILE:HD13	1.96	0.48
1:U:184:CYS:HA	1:U:188:MET:HE3	1.96	0.48
7:a:176:ALA:CB	7:a:200:LEU:HD21	2.44	0.48
12:A:63:THR:HG23	32:f:681:TYR:CE2	2.48	0.48
12:A:134:ILE:HD11	12:A:140:VAL:HG11	1.95	0.48
12:A:190:VAL:HG13	12:A:191:VAL:HG23	1.95	0.48
13:B:434:THR:N	13:B:435:PRO:HD2	2.28	0.48
22:K:74:ILE:HD13	22:K:112:VAL:HG11	1.96	0.48
32:f:504:VAL:HG22	32:f:504:VAL:O	2.14	0.48
5:Y:314:LEU:HD11	5:Y:318:TYR:CD1	2.48	0.47
6:Z:136:GLU:OE1	6:Z:138:TYR:OH	2.31	0.47
10:d:245:PHE:CE1	10:d:267:ILE:HG21	2.48	0.47
12:A:166:VAL:HG23	12:A:239:ARG:HG2	1.95	0.47
13:B:342:ILE:O	13:B:342:ILE:HG22	2.14	0.47
13:B:407:LEU:HD12	14:C:178:LEU:HD11	1.96	0.47
14:C:277:LEU:HD23	14:C:305:LEU:HD23	1.95	0.47
17:F:183:GLU:O	17:F:184:GLN:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:I:68:LEU:HD21	20:I:74:CYS:SG	2.54	0.47
31:t:96:LEU:CD2	31:t:155:MET:HE3	2.39	0.47
9:c:177:THR:HG23	9:c:177:THR:O	2.14	0.47
12:A:63:THR:HG22	32:f:680:ARG:NH1	2.29	0.47
12:A:332:MET:HA	12:A:337:LEU:HD12	1.97	0.47
13:B:294:ARG:NH1	13:B:338:ASP:OD2	2.48	0.47
15:D:314:ALA:HA	15:D:317:LEU:HD23	1.97	0.47
16:E:350:ALA:HA	16:E:369:LYS:HE2	1.95	0.47
27:P:199:THR:O	27:P:199:THR:HG22	2.13	0.47
28:q:4:LEU:HD13	28:q:45:LEU:HB3	1.96	0.47
30:s:202:LEU:O	30:s:206:VAL:HG13	2.13	0.47
31:t:70:ASP:OD1	31:t:86:ARG:NH1	2.42	0.47
32:f:392:THR:O	32:f:393:ASP:HB2	2.14	0.47
32:f:489:TYR:HB2	32:f:525:ILE:HD12	1.96	0.47
3:W:251:TYR:CZ	3:W:267:LEU:HD13	2.49	0.47
11:e:45:ASP:OD1	11:e:45:ASP:O	2.32	0.47
12:A:372:LEU:O	12:A:376:LEU:HD23	2.14	0.47
14:C:338:LEU:HD23	14:C:378:VAL:HG21	1.95	0.47
16:E:347:CYS:SG	17:F:217:ILE:HD11	2.54	0.47
27:P:145:GLN:OE1	27:P:145:GLN:N	2.44	0.47
31:t:61:PHE:HB2	31:t:205:LEU:O	2.15	0.47
32:f:207:LEU:O	32:f:211:ILE:HG12	2.15	0.47
32:f:490:ALA:O	32:f:524:MET:O	2.32	0.47
32:f:707:LEU:HD13	32:f:741:LEU:HD13	1.96	0.47
2:V:83:GLU:HA	2:V:86:VAL:HG22	1.96	0.47
10:d:115:GLU:O	10:d:119:LEU:HD23	2.15	0.47
12:A:279:ALA:HB1	13:B:307:ARG:HG3	1.96	0.47
14:C:280:LEU:HD21	14:C:291:VAL:HG21	1.96	0.47
17:F:417:HIS:NE2	17:F:421:MET:HE2	2.30	0.47
23:L:10:VAL:HG22	23:L:21:GLN:HB2	1.96	0.47
24:M:10:LEU:O	24:M:11:SER:OG	2.20	0.47
31:T:83:ASN:ND2	25:n:235:THR:O	2.45	0.47
31:T:224:ARG:HA	25:n:60:ILE:HD11	1.96	0.47
25:n:51:ASP:OD1	25:n:198:MET:HE3	2.15	0.47
32:f:445:LEU:O	32:f:466:LEU:HD21	2.14	0.47
2:V:400:HIS:H	2:V:400:HIS:HD1	1.62	0.47
3:W:217:GLU:OE1	3:W:217:GLU:N	2.39	0.47
3:W:412:ILE:O	3:W:413:ILE:C	2.57	0.47
5:Y:18:ARG:O	5:Y:22:LEU:HD23	2.15	0.47
8:b:113:VAL:O	8:b:113:VAL:HG22	2.14	0.47
12:A:220:THR:O	12:A:220:THR:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:501:ATP:O1G	13:B:346:ARG:NH2	2.47	0.47
15:D:141:ASP:OD1	15:D:142:VAL:N	2.48	0.47
17:F:58:GLU:OE1	17:F:61:ARG:NH1	2.46	0.47
20:I:147:LEU:HD21	20:I:162:THR:HG22	1.96	0.47
28:Q:16:ALA:CB	28:Q:160:LEU:HD11	2.43	0.47
30:s:41:LEU:HD12	30:s:42:ALA:H	1.78	0.47
30:s:134:VAL:O	30:s:134:VAL:HG13	2.15	0.47
1:U:319:LYS:O	1:U:323:LEU:HD13	2.15	0.47
1:U:333:MET:O	1:U:337:LEU:HD13	2.14	0.47
3:W:74:CYS:O	3:W:79:GLU:HB3	2.14	0.47
5:Y:134:LEU:HD21	5:Y:171:GLY:O	2.14	0.47
7:a:96:PHE:O	7:a:100:THR:HG23	2.15	0.47
7:a:228:THR:HG22	7:a:229:ASP:OD1	2.15	0.47
11:e:38:VAL:O	11:e:38:VAL:HG12	2.14	0.47
16:E:175:PRO:O	16:E:176:PRO:C	2.57	0.47
17:F:254:PRO:O	17:F:257:VAL:HG22	2.14	0.47
24:M:24:VAL:HG22	24:M:124:THR:OG1	2.15	0.47
31:T:169:TYR:CD1	31:T:184:THR:HG22	2.49	0.47
31:T:254:TRP:CE3	25:n:63:ARG:NH2	2.83	0.47
31:T:254:TRP:CH2	25:n:206:GLY:HA2	2.48	0.47
27:p:105:THR:HG23	27:p:105:THR:O	2.15	0.47
30:s:152:PHE:CE1	30:s:158:TYR:HB3	2.49	0.47
31:t:105:PHE:CD1	31:t:155:MET:HE1	2.49	0.47
1:U:579:ARG:NH1	1:U:609:ASP:OD1	2.48	0.47
2:V:211:TYR:OH	2:V:234:ARG:NE	2.48	0.47
2:V:333:ILE:HG23	2:V:343:PRO:HG2	1.96	0.47
2:V:363:LEU:HD21	2:V:398:LEU:CD2	2.45	0.47
2:V:466:ILE:HD11	2:V:471:GLU:OE1	2.14	0.47
3:W:414:ASN:OD1	3:W:416:GLN:N	2.47	0.47
4:X:315:ASP:C	4:X:315:ASP:OD1	2.57	0.47
8:b:181:ASP:HA	8:b:184:ILE:HG22	1.95	0.47
9:c:146:ASP:OD2	9:c:149:GLN:NE2	2.35	0.47
13:B:235:LEU:O	13:B:239:VAL:HG23	2.14	0.47
15:D:52:GLU:O	15:D:55:GLU:HG3	2.15	0.47
16:E:196:LEU:HD23	16:E:198:VAL:HG23	1.96	0.47
16:E:269:THR:HG22	16:E:269:THR:O	2.15	0.47
24:M:70:VAL:O	24:M:74:VAL:HB	2.14	0.47
24:M:149:LEU:HD23	24:M:161:TYR:HB2	1.96	0.47
29:R:196:GLY:C	28:q:142:ILE:HD11	2.40	0.47
28:q:143:LEU:HD12	28:q:163:CYS:SG	2.54	0.47
31:t:67:ILE:CD1	31:t:95:MET:HE3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:392:THR:O	32:f:393:ASP:CB	2.62	0.47
32:f:548:THR:O	32:f:549:GLU:HB3	2.14	0.47
3:W:196:VAL:O	3:W:196:VAL:HG22	2.15	0.47
19:H:34:PRO:HD2	19:H:49:GLU:OE2	2.15	0.47
20:I:119:GLN:CG	21:J:78:ALA:HB1	2.44	0.47
27:P:155:GLU:H	27:P:158:MET:HE3	1.79	0.47
28:Q:14:LEU:HD12	28:Q:182:ILE:HD11	1.97	0.47
25:n:114:ALA:CB	25:n:146:TYR:HD2	2.28	0.47
26:o:51:TYR:CE1	26:o:56:VAL:HG23	2.50	0.47
27:p:103:TYR:O	27:p:105:THR:N	2.47	0.47
1:U:637:VAL:CG1	1:U:652:ALA:HB1	2.45	0.47
2:V:223:LYS:O	2:V:261:TYR:OH	2.32	0.47
4:X:242:ILE:O	4:X:242:ILE:HG22	2.14	0.47
5:Y:207:THR:HG21	14:C:377:HIS:NE2	2.30	0.47
6:Z:17:LEU:HD21	9:c:217:LEU:HD22	1.97	0.47
7:a:118:ILE:HB	7:a:122:LYS:HZ3	1.79	0.47
7:a:216:LEU:HD23	7:a:222:LEU:HD22	1.96	0.47
10:d:168:MET:HA	10:d:168:MET:HE3	1.96	0.47
19:H:195:LEU:HD12	19:H:208:ILE:HD11	1.95	0.47
23:L:212:ILE:HG22	23:L:214:ILE:CD1	2.43	0.47
32:f:272:LEU:O	32:f:274:ASP:N	2.48	0.47
32:f:425:GLY:O	32:f:426:LEU:C	2.58	0.47
32:f:702:PRO:HA	32:f:732:VAL:HG12	1.95	0.47
2:V:162:GLU:OE2	2:V:200:ARG:HD2	2.15	0.47
3:W:190:MET:CE	3:W:206:SER:HA	2.45	0.47
3:W:317:TRP:CE3	3:W:358:VAL:HG21	2.50	0.47
5:Y:183:TYR:CD1	5:Y:213:LEU:HD11	2.49	0.47
6:Z:111:LEU:HD23	6:Z:111:LEU:C	2.40	0.47
12:A:101:ILE:HG23	12:A:111:TYR:CE1	2.49	0.47
13:B:290:ILE:O	13:B:290:ILE:HG13	2.14	0.47
15:D:155:THR:HG22	15:D:156:SER:H	1.80	0.47
29:R:197:VAL:HG21	29:R:221:GLN:NE2	2.29	0.47
31:T:223:TYR:CE1	25:n:63:ARG:NH2	2.83	0.47
26:o:165:LEU:HD12	26:o:168:VAL:HG12	1.96	0.47
1:U:95:GLU:CD	2:V:237:THR:HG22	2.40	0.46
1:U:198:LEU:HB2	1:U:223:LEU:HD11	1.96	0.46
2:V:113:LEU:HD21	2:V:171:VAL:HA	1.96	0.46
5:Y:29:PRO:O	5:Y:30:GLU:HG3	2.15	0.46
7:a:162:TYR:O	7:a:165:THR:HG22	2.15	0.46
7:a:360:VAL:HG22	9:c:308:VAL:HG23	1.97	0.46
14:C:196:LYS:NZ	35:C:501:ATP:O1B	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:391:ARG:O	15:D:393:ILE:N	2.41	0.46
16:E:319:PRO:HB2	16:E:363:VAL:HG13	1.97	0.46
17:F:256:LEU:HD23	17:F:268:VAL:CG2	2.45	0.46
25:N:89:VAL:HG21	25:N:128:LEU:HD13	1.97	0.46
26:O:140:ALA:HB1	26:O:170:MET:HE1	1.97	0.46
25:n:194:LEU:CD1	25:n:208:ILE:HG23	2.45	0.46
30:s:89:CYS:O	30:s:93:THR:HG23	2.14	0.46
32:f:806:VAL:HG12	32:f:811:LEU:HD12	1.97	0.46
2:V:100:MET:N	2:V:100:MET:SD	2.87	0.46
3:W:239:SER:O	3:W:243:ILE:HD12	2.15	0.46
8:b:124:LEU:HD23	8:b:124:LEU:C	2.40	0.46
9:c:130:GLN:CG	9:c:162:LEU:HD13	2.45	0.46
15:D:345:PHE:HD2	15:D:364:VAL:HG12	1.80	0.46
16:E:171:LEU:HD11	16:E:279:THR:HG22	1.96	0.46
19:H:69:THR:HG22	19:H:70:LYS:H	1.79	0.46
19:H:122:THR:HG23	19:H:122:THR:O	2.14	0.46
22:K:210:LEU:CD1	22:K:215:ILE:HG21	2.45	0.46
23:L:150:SER:O	23:L:151:ALA:HB3	2.16	0.46
33:y:395:LEU:O	33:y:399:LEU:HD13	2.15	0.46
1:U:697:GLN:O	1:U:885:MET:HE2	2.15	0.46
3:W:77:ALA:O	3:W:79:GLU:OE1	2.33	0.46
3:W:132:THR:HG22	3:W:138:VAL:HG11	1.96	0.46
3:W:442:THR:HG21	6:Z:230:LEU:HD21	1.98	0.46
10:d:83:THR:OG1	10:d:84:SER:N	2.48	0.46
12:A:297:ARG:HD2	17:F:257:VAL:HG21	1.96	0.46
35:C:501:ATP:O2'	15:D:326:ARG:NH2	2.42	0.46
16:E:223:ARG:NH2	16:E:268:ASP:OD1	2.49	0.46
19:H:50:LYS:HD2	19:H:209:GLU:OE1	2.16	0.46
19:H:68:ILE:HD11	19:H:74:LEU:HD13	1.97	0.46
22:K:12:VAL:O	22:K:12:VAL:HG22	2.13	0.46
25:n:208:ILE:HG22	25:n:210:LEU:CD1	2.45	0.46
31:t:104:ASP:O	31:t:108:LEU:HD23	2.15	0.46
32:f:60:VAL:HG12	32:f:105:LYS:NZ	2.31	0.46
32:f:96:LEU:HD13	32:f:129:LEU:HD23	1.95	0.46
32:f:378:ASN:ND2	32:f:390:LEU:HD12	2.29	0.46
32:f:727:PHE:CE2	32:f:803:PHE:CE2	3.03	0.46
1:U:497:LEU:HD21	1:U:515:ALA:HB1	1.97	0.46
1:U:556:MET:HE2	1:U:563:ALA:HB2	1.97	0.46
4:X:136:LEU:O	4:X:140:THR:HG22	2.15	0.46
5:Y:49:ASN:O	5:Y:77:ASN:ND2	2.46	0.46
5:Y:57:LEU:HD23	5:Y:57:LEU:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:272:LEU:O	6:Z:276:ILE:HG12	2.16	0.46
7:a:63:PHE:O	7:a:67:PHE:CB	2.64	0.46
14:C:374:ARG:HH12	15:D:190:LEU:HD11	1.80	0.46
15:D:181:VAL:HG11	15:D:308:ILE:HD11	1.98	0.46
23:L:105:VAL:HG21	23:L:136:GLY:HA3	1.98	0.46
24:M:70:VAL:O	24:M:71:ASP:CB	2.63	0.46
26:O:62:ARG:HB3	26:O:213:GLY:HA2	1.97	0.46
25:n:198:MET:HE1	25:n:206:GLY:N	2.30	0.46
27:p:56:LEU:O	27:p:60:VAL:HG23	2.16	0.46
31:t:71:MET:HE1	31:t:247:PRO:HB3	1.97	0.46
32:f:400:TYR:CE1	32:f:437:GLU:OE2	2.67	0.46
32:f:400:TYR:HD1	32:f:407:MET:HE3	1.80	0.46
1:U:446:LEU:HD23	1:U:446:LEU:C	2.40	0.46
1:U:542:GLU:OE1	1:U:542:GLU:N	2.40	0.46
1:U:583:MET:HE2	1:U:583:MET:CA	2.46	0.46
3:W:317:TRP:HE3	3:W:358:VAL:HG21	1.80	0.46
5:Y:148:GLY:HA2	5:Y:153:ASP:OD1	2.16	0.46
10:d:309:VAL:O	10:d:319:ALA:HB2	2.16	0.46
15:D:119:ILE:O	15:D:119:ILE:CG2	2.63	0.46
16:E:331:ILE:HD11	16:E:370:ALA:HB3	1.97	0.46
29:R:195:TYR:HE2	28:q:170:ARG:HE	1.63	0.46
26:o:169:THR:OG1	26:o:178:MET:HE3	2.16	0.46
32:f:287:ASP:C	32:f:287:ASP:OD1	2.58	0.46
32:f:573:ILE:O	32:f:574:GLU:C	2.58	0.46
33:y:385:ASN:O	33:y:389:ARG:HG2	2.16	0.46
1:U:419:ALA:O	1:U:420:LEU:HB2	2.15	0.46
2:V:379:LEU:CD1	2:V:395:ILE:HG21	2.45	0.46
3:W:112:VAL:HG22	3:W:124:LEU:CD2	2.46	0.46
3:W:190:MET:HB3	3:W:229:LEU:HD13	1.97	0.46
4:X:190:LEU:HD22	4:X:217:ILE:HD12	1.96	0.46
6:Z:144:VAL:O	6:Z:144:VAL:HG13	2.15	0.46
14:C:322:GLU:HA	14:C:325:ARG:HB2	1.98	0.46
15:D:390:ASN:O	15:D:391:ARG:C	2.59	0.46
24:M:76:MET:HE3	24:M:136:PHE:CG	2.50	0.46
27:P:67:LEU:HD22	27:P:91:VAL:HG22	1.96	0.46
32:f:675:PHE:HB3	32:f:690:VAL:HG13	1.97	0.46
2:V:182:LYS:O	2:V:185:GLN:HG2	2.16	0.46
2:V:289:LEU:HD23	2:V:311:ASN:HB3	1.97	0.46
2:V:371:ASN:OD1	2:V:373:ALA:N	2.49	0.46
3:W:185:PHE:O	3:W:189:GLN:HG3	2.16	0.46
4:X:342:PHE:CD1	4:X:345:VAL:HG22	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:274:SER:O	5:Y:277:VAL:HG22	2.16	0.46
7:a:112:ILE:CD1	7:a:141:MET:SD	3.03	0.46
9:c:58:LEU:HD23	9:c:73:PHE:HB2	1.98	0.46
13:B:343:ARG:HE	13:B:346:ARG:NH1	2.14	0.46
17:F:366:MET:HE1	17:F:388:THR:HG21	1.97	0.46
31:T:171:ASP:OD1	31:T:175:VAL:N	2.48	0.46
27:p:12:MET:HE1	27:p:150:CYS:HB2	1.98	0.46
29:r:226:ASP:O	29:r:227:ALA:C	2.59	0.46
1:U:161:ASP:OD1	1:U:162:VAL:HG23	2.16	0.46
3:W:90:LEU:O	3:W:96:GLN:NE2	2.47	0.46
3:W:378:MET:SD	3:W:413:ILE:HD12	2.56	0.46
9:c:27:THR:HG23	9:c:27:THR:O	2.15	0.46
10:d:288:THR:HA	10:d:293:PHE:HD2	1.80	0.46
12:A:317:VAL:HG11	12:A:319:MET:HE3	1.98	0.46
14:C:191:PRO:O	14:C:196:LYS:NZ	2.48	0.46
14:C:228:ALA:O	14:C:232:ARG:HG3	2.15	0.46
16:E:348:THR:HG23	16:E:349:GLU:N	2.31	0.46
27:P:151:GLU:OE1	30:s:212:GLU:OE1	2.34	0.46
32:f:492:SER:HB2	32:f:494:ARG:HG3	1.97	0.46
32:f:534:VAL:O	32:f:538:ILE:HG12	2.16	0.46
1:U:469:SER:O	1:U:474:ARG:NH1	2.49	0.46
7:a:37:LEU:HD11	7:a:67:PHE:CZ	2.51	0.46
10:d:192:LEU:HD13	10:d:215:LEU:HD21	1.98	0.46
13:B:95:GLU:O	13:B:99:VAL:HG23	2.16	0.46
16:E:181:THR:O	16:E:185:ARG:HG2	2.16	0.46
16:E:316:HIS:O	16:E:343:LEU:HD22	2.15	0.46
16:E:326:ILE:H	16:E:326:ILE:HD12	1.81	0.46
21:J:99:GLU:OE1	29:R:179:ARG:NH2	2.48	0.46
22:K:38:ILE:HG23	22:K:181:LEU:HD11	1.98	0.46
24:M:231:ASP:OD1	24:M:231:ASP:N	2.47	0.46
26:O:82:PRO:O	26:O:226:LEU:HD22	2.15	0.46
26:O:210:LEU:HD12	30:s:60:GLY:O	2.16	0.46
27:P:28:PHE:O	27:P:28:PHE:CG	2.67	0.46
26:o:77:ILE:HG22	26:o:87:CYS:SG	2.56	0.46
29:r:63:LEU:HD23	29:r:64:ALA:N	2.30	0.46
2:V:252:ASN:ND2	2:V:284:GLU:OE1	2.44	0.46
4:X:332:GLU:HG3	4:X:368:MET:HE3	1.98	0.46
4:X:365:LEU:HD13	4:X:385:LEU:CD1	2.44	0.46
5:Y:228:MET:HE3	5:Y:263:LEU:HD23	1.98	0.46
8:b:174:PRO:N	8:b:175:PRO:HD2	2.31	0.46
10:d:241:TYR:HA	10:d:244:VAL:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:237:GLN:HG3	15:D:246:MET:CE	2.45	0.46
16:E:29:LEU:O	16:E:30:ARG:C	2.58	0.46
16:E:218:MET:O	16:E:218:MET:HE3	2.16	0.46
23:L:19:ILE:HG21	23:L:22:ILE:HD12	1.97	0.46
26:O:262:LEU:HD11	27:P:195:ILE:HD11	1.97	0.46
30:S:88:ASP:HA	30:S:91:THR:HG22	1.98	0.46
1:U:358:ASP:C	1:U:358:ASP:OD1	2.59	0.45
1:U:587:ALA:HB2	1:U:621:SER:HB3	1.98	0.45
3:W:341:PHE:CE2	3:W:354:LEU:HD22	2.51	0.45
4:X:103:THR:HG23	4:X:105:GLN:H	1.81	0.45
6:Z:173:GLU:OE1	9:c:153:GLY:HA2	2.16	0.45
10:d:200:LEU:HD11	10:d:233:GLU:CG	2.46	0.45
12:A:238:ILE:HD12	12:A:270:CYS:SG	2.56	0.45
12:A:277:ILE:HD13	12:A:319:MET:SD	2.56	0.45
18:G:195:VAL:HG12	18:G:199:ILE:HD12	1.97	0.45
18:G:240:VAL:HG23	18:G:241:ALA:N	2.30	0.45
20:I:12:PHE:CE1	20:I:18:LEU:HD11	2.51	0.45
21:J:134:VAL:HG12	21:J:144:LEU:HD12	1.98	0.45
24:M:24:VAL:O	24:M:28:MET:HG3	2.16	0.45
26:O:262:LEU:N	27:P:193:ASP:O	2.49	0.45
25:n:112:THR:O	25:n:116:LEU:HG	2.16	0.45
26:o:169:THR:HG23	26:o:178:MET:CE	2.45	0.45
28:q:53:THR:HG23	28:q:54:VAL:N	2.31	0.45
32:f:78:LEU:O	32:f:82:ILE:HG13	2.16	0.45
32:f:171:GLN:NE2	32:f:210:GLU:HG2	2.31	0.45
2:V:94:VAL:CG2	2:V:205:LEU:HD13	2.45	0.45
3:W:140:ILE:O	3:W:144:ARG:HG3	2.17	0.45
3:W:329:ARG:CD	3:W:342:GLY:O	2.63	0.45
4:X:286:ALA:HB2	4:X:309:TYR:CD2	2.51	0.45
5:Y:117:LYS:O	5:Y:121:LEU:HD13	2.16	0.45
5:Y:198:ALA:HB2	5:Y:226:VAL:HG12	1.98	0.45
9:c:138:GLU:OE1	9:c:138:GLU:O	2.34	0.45
12:A:246:VAL:HG23	12:A:280:ILE:HD11	1.98	0.45
12:A:398:ARG:NH1	13:B:199:GLU:OE2	2.50	0.45
14:C:368:MET:HE1	15:D:191:TYR:OH	2.17	0.45
16:E:97:ARG:NH1	16:E:112:PRO:O	2.50	0.45
24:M:140:SER:HA	24:M:217:VAL:HG11	1.98	0.45
30:S:144:GLU:HA	30:S:144:GLU:OE1	2.17	0.45
30:s:181:VAL:O	30:s:181:VAL:HG13	2.16	0.45
31:t:61:PHE:CE2	31:t:64:GLY:HA3	2.50	0.45
2:V:98:LEU:HD11	2:V:206:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:69:LEU:O	4:X:73:VAL:HG13	2.16	0.45
4:X:96:PHE:CE2	4:X:109:LEU:HD22	2.51	0.45
15:D:92:PHE:HA	15:D:103:VAL:HG12	1.98	0.45
17:F:226:TYR:HB2	17:F:335:VAL:CG1	2.46	0.45
23:L:53:GLN:O	23:L:54:SER:OG	2.29	0.45
25:N:126:GLU:OE1	25:N:126:GLU:HA	2.16	0.45
26:O:229:LEU:HD22	26:O:232:TYR:CD1	2.51	0.45
28:Q:49:GLU:O	28:Q:53:THR:HG23	2.17	0.45
30:S:40:ILE:CD1	30:S:137:ILE:HD12	2.46	0.45
27:p:95:LEU:HB2	27:p:127:ILE:O	2.17	0.45
3:W:407:ASP:OD2	4:X:344:ARG:NH2	2.49	0.45
5:Y:112:CYS:SG	5:Y:124:PHE:HE2	2.40	0.45
7:a:149:THR:HB	7:a:151:VAL:HG12	1.97	0.45
7:a:308:GLU:O	7:a:312:MET:HG2	2.16	0.45
15:D:79:VAL:O	15:D:82:ILE:HG22	2.17	0.45
23:L:215:VAL:HG22	23:L:216:GLY:N	2.31	0.45
26:O:254:VAL:C	26:O:255:LEU:HD12	2.42	0.45
25:n:50:ALA:HB3	25:n:68:LEU:CD1	2.47	0.45
32:f:735:GLY:O	32:f:828:ARG:NH1	2.49	0.45
1:U:637:VAL:O	1:U:637:VAL:HG12	2.16	0.45
2:V:400:HIS:NE2	10:d:234:GLN:HA	2.31	0.45
3:W:440:ASN:ND2	9:c:226:MET:HE1	2.32	0.45
5:Y:387:ILE:HG13	6:Z:276:ILE:HD11	1.98	0.45
12:A:23:ARG:HE	13:B:410:ARG:HG2	1.71	0.45
15:D:216:ALA:O	15:D:219:VAL:HG22	2.16	0.45
16:E:184:ALA:HB1	16:E:195:PHE:HZ	1.82	0.45
16:E:212:ALA:O	16:E:216:ARG:HG2	2.16	0.45
22:K:213:THR:O	22:K:214:ASN:CG	2.60	0.45
27:P:67:LEU:CD2	27:P:91:VAL:HG22	2.46	0.45
29:R:65:PHE:HB3	29:R:184:THR:HG22	1.97	0.45
31:T:237:VAL:HG23	31:T:242:VAL:HG22	1.99	0.45
26:o:169:THR:N	26:o:178:MET:HE3	2.31	0.45
3:W:329:ARG:NH2	3:W:351:TRP:CE3	2.84	0.45
7:a:24:ARG:O	7:a:27:GLU:HG3	2.17	0.45
12:A:83:ASP:OD1	12:A:84:LYS:N	2.50	0.45
15:D:366:ARG:NH1	15:D:400:GLU:OE2	2.44	0.45
27:p:11:VAL:HG12	27:p:24:ALA:CB	2.46	0.45
32:f:571:GLU:C	32:f:573:ILE:H	2.25	0.45
3:W:24:VAL:HG13	3:W:50:LEU:HD21	1.97	0.45
4:X:74:ARG:N	4:X:75:PRO:CD	2.80	0.45
6:Z:75:LEU:HD23	6:Z:75:LEU:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:112:ILE:HD13	7:a:141:MET:SD	2.56	0.45
7:a:232:TRP:HH2	7:a:255:TRP:HB3	1.82	0.45
8:b:16:MET:N	8:b:16:MET:HE2	2.31	0.45
14:C:161:ILE:HG13	14:C:165:ILE:HD13	1.98	0.45
16:E:151:LEU:HB3	16:E:152:PRO:HD3	1.99	0.45
16:E:312:ILE:HD12	37:E:401:ADP:C6	2.52	0.45
16:E:342:ASP:O	16:E:346:VAL:HG23	2.17	0.45
27:P:26:ARG:HH12	27:P:199:THR:HG23	1.81	0.45
29:R:77:SER:OG	29:R:232:ALA:N	2.48	0.45
31:T:198:VAL:HG11	31:T:213:LEU:HD22	1.98	0.45
31:t:160:TYR:HH	31:t:237:VAL:C	2.19	0.45
32:f:560:LEU:HD21	32:f:798:THR:HA	1.98	0.45
1:U:639:LEU:HD12	1:U:640:LEU:N	2.32	0.45
3:W:187:LEU:HD12	3:W:222:LEU:HD13	1.99	0.45
6:Z:10:VAL:HG13	6:Z:10:VAL:O	2.17	0.45
7:a:42:LEU:HD13	7:a:46:GLN:HE22	1.82	0.45
7:a:148:VAL:O	7:a:149:THR:OG1	2.33	0.45
8:b:93:ALA:O	8:b:97:LEU:HD23	2.17	0.45
16:E:187:VAL:O	16:E:191:LEU:HD13	2.16	0.45
17:F:251:LEU:HD23	17:F:253:GLY:H	1.82	0.45
18:G:131:MET:HE2	24:M:126:TYR:OH	2.16	0.45
23:L:11:THR:O	23:L:11:THR:HG22	2.16	0.45
28:q:36:PHE:CD2	28:q:57:ALA:HB1	2.51	0.45
30:s:39:THR:CG2	30:s:173:LEU:HD11	2.47	0.45
31:t:206:SER:OG	31:t:207:GLN:N	2.50	0.45
32:f:68:THR:O	32:f:68:THR:HG22	2.17	0.45
1:U:35:TRP:HE1	2:V:232:HIS:CE1	2.35	0.45
1:U:451:ALA:O	1:U:452:ASN:C	2.60	0.45
1:U:725:MET:HE2	9:c:183:HIS:ND1	2.32	0.45
2:V:109:ASN:OD1	2:V:110:HIS:N	2.48	0.45
2:V:188:SER:O	2:V:192:MET:HG2	2.16	0.45
2:V:241:ARG:O	2:V:243:ASP:N	2.49	0.45
2:V:309:MET:CE	2:V:331:LEU:HD23	2.46	0.45
3:W:406:VAL:HG23	3:W:406:VAL:O	2.16	0.45
4:X:70:LEU:HA	4:X:73:VAL:HG22	1.99	0.45
5:Y:41:LEU:HD21	5:Y:57:LEU:CD1	2.47	0.45
8:b:26:LEU:O	8:b:29:GLN:HG2	2.17	0.45
8:b:36:VAL:HG21	8:b:110:ILE:HD12	1.99	0.45
13:B:107:MET:HE2	13:B:151:LEU:HB3	1.99	0.45
18:G:158:GLY:O	19:H:84:ARG:NH2	2.43	0.45
23:L:10:VAL:HG11	23:L:120:THR:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:s:173:LEU:HD13	30:s:207:PHE:HE1	1.81	0.45
32:f:659:LEU:HA	32:f:662:MET:HE3	1.99	0.45
32:f:675:PHE:CZ	32:f:693:ALA:HB1	2.52	0.45
32:f:757:ASN:OD1	32:f:811:LEU:HD22	2.17	0.45
1:U:46:GLU:OE2	1:U:80:TYR:OH	2.33	0.45
1:U:503:GLN:O	1:U:535:TYR:OH	2.35	0.45
1:U:800:VAL:HG12	1:U:801:GLN:N	2.32	0.45
2:V:168:GLN:CG	2:V:191:LEU:HD11	2.46	0.45
3:W:231:ILE:HD11	3:W:246:HIS:HB3	1.99	0.45
5:Y:190:ALA:HB2	5:Y:287:LEU:HD11	1.99	0.45
6:Z:266:ILE:HG23	9:c:284:LEU:HD21	1.98	0.45
6:Z:275:LEU:C	6:Z:275:LEU:HD23	2.42	0.45
9:c:63:ASP:OD1	9:c:64:ASP:N	2.46	0.45
12:A:159:PRO:O	12:A:163:MET:HE2	2.16	0.45
14:C:339:THR:HG22	14:C:340:ARG:N	2.32	0.45
15:D:357:GLU:OE1	15:D:357:GLU:N	2.49	0.45
16:E:101:ASP:OD1	16:E:102:MET:N	2.49	0.45
17:F:175:MET:O	17:F:249:LEU:HD13	2.17	0.45
27:p:25:ASP:HB2	27:p:181:SER:O	2.16	0.45
1:U:374:SER:OG	1:U:410:VAL:HB	2.16	0.44
1:U:412:HIS:CE1	1:U:422:LEU:HD11	2.52	0.44
3:W:217:GLU:HG2	3:W:218:ASN:N	2.32	0.44
12:A:75:PRO:O	12:A:76:ALA:HB3	2.17	0.44
12:A:102:ILE:HD11	17:F:165:PRO:CD	2.48	0.44
16:E:29:LEU:HD13	17:F:62:VAL:HG11	1.99	0.44
18:G:113:MET:SD	26:O:113:THR:HG22	2.57	0.44
19:H:86:LEU:HD13	19:H:118:MET:HE2	1.99	0.44
20:I:183:GLU:O	20:I:183:GLU:HG2	2.17	0.44
29:r:63:LEU:HD21	29:r:65:PHE:CD2	2.52	0.44
32:f:396:ASN:OD1	32:f:400:TYR:CD2	2.69	0.44
1:U:386:LEU:HD22	1:U:393:LEU:HD12	1.99	0.44
2:V:227:VAL:CG1	2:V:231:LEU:HD12	2.48	0.44
4:X:35:ILE:HD11	4:X:46:LYS:HB2	1.98	0.44
6:Z:184:VAL:HG21	15:D:73:LEU:HD12	2.00	0.44
8:b:153:LEU:HD23	8:b:170:LEU:CD1	2.47	0.44
16:E:223:ARG:NH2	16:E:268:ASP:HA	2.33	0.44
17:F:184:GLN:OE1	17:F:184:GLN:HA	2.17	0.44
20:I:17:ARG:NH2	20:I:22:GLU:OE1	2.51	0.44
25:n:74:ARG:O	25:n:74:ARG:HG2	2.18	0.44
1:U:2:ILE:C	1:U:3:THR:HG1	2.22	0.44
1:U:198:LEU:HB3	1:U:223:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:213:PHE:C	1:U:248:ILE:HD11	2.42	0.44
1:U:613:ASP:OD1	1:U:616:ARG:NH2	2.46	0.44
6:Z:249:PHE:CD2	10:d:330:ILE:HD13	2.53	0.44
9:c:52:GLU:HB2	9:c:82:VAL:HG13	1.99	0.44
12:A:24:ALA:C	13:B:410:ARG:HH22	2.25	0.44
17:F:256:LEU:HD23	17:F:268:VAL:HG22	1.98	0.44
20:I:140:ASP:OD2	20:I:146:GLN:NE2	2.42	0.44
21:J:122:ASN:OD1	21:J:122:ASN:O	2.36	0.44
22:K:121:LEU:HD23	22:K:160:GLY:HA3	2.00	0.44
25:N:161:ILE:HG22	25:N:166:SER:OG	2.17	0.44
27:P:87:LEU:O	27:P:91:VAL:HG23	2.17	0.44
27:P:179:ALA:HA	29:r:85:ILE:HD11	1.99	0.44
28:Q:23:SER:HB3	28:Q:28:MET:HE2	1.98	0.44
30:S:40:ILE:HD12	30:S:137:ILE:HD12	1.99	0.44
32:f:397:LYS:O	32:f:400:TYR:O	2.34	0.44
32:f:836:GLU:O	32:f:836:GLU:HG3	2.17	0.44
1:U:408:LEU:HD21	1:U:426:TYR:CG	2.52	0.44
1:U:673:GLU:HB3	1:U:674:PRO:HD3	2.00	0.44
1:U:693:LEU:HD13	1:U:746:ILE:HD13	2.00	0.44
2:V:176:MET:HE3	2:V:217:VAL:CG1	2.47	0.44
7:a:63:PHE:O	7:a:67:PHE:HB2	2.17	0.44
8:b:3:LEU:HD12	8:b:44:ASN:HD21	1.82	0.44
13:B:107:MET:HE3	13:B:160:ILE:HG13	1.99	0.44
14:C:37:ASP:OD1	14:C:37:ASP:C	2.60	0.44
16:E:40:TYR:OH	17:F:72:LYS:HD2	2.17	0.44
22:K:49:ALA:HB2	22:K:217:LEU:CD1	2.48	0.44
23:L:66:VAL:HG12	23:L:67:ASP:N	2.31	0.44
28:Q:44:LEU:HD23	28:Q:45:LEU:N	2.32	0.44
28:Q:135:GLY:CA	28:Q:167:LEU:HD11	2.46	0.44
29:R:207:GLU:HA	29:R:207:GLU:OE1	2.16	0.44
30:S:91:THR:HG21	31:T:142:TYR:CZ	2.53	0.44
30:S:99:ARG:HG3	30:S:123:ILE:HD11	2.00	0.44
32:f:106:LEU:O	32:f:126:ILE:HD11	2.18	0.44
32:f:237:VAL:HG13	32:f:245:ASN:OD1	2.18	0.44
32:f:466:LEU:HD22	32:f:481:SER:HA	1.99	0.44
32:f:740:ARG:O	32:f:744:MET:HG3	2.16	0.44
1:U:243:LEU:HB2	1:U:903:PHE:HE2	1.82	0.44
4:X:68:GLY:O	4:X:72:TYR:CD2	2.70	0.44
12:A:274:PHE:CD2	12:A:319:MET:HE2	2.53	0.44
13:B:256:ILE:HD12	13:B:305:ILE:HG12	2.00	0.44
30:S:103:TYR:CD1	30:S:111:MET:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:S:219:ASP:O	30:S:220:ALA:HB3	2.17	0.44
25:n:55:THR:HA	25:n:60:ILE:HA	2.00	0.44
25:n:114:ALA:HA	25:n:134:ILE:HD13	2.00	0.44
28:q:35:MET:HG3	28:q:45:LEU:HD22	2.00	0.44
30:s:181:VAL:CG2	30:s:194:LEU:HD22	2.48	0.44
32:f:157:GLU:OE1	32:f:160:ARG:NH1	2.50	0.44
1:U:885:MET:O	1:U:888:GLN:N	2.49	0.44
2:V:364:THR:HA	2:V:367:VAL:HG12	1.99	0.44
3:W:286:LEU:O	3:W:290:ILE:HG12	2.18	0.44
4:X:384:VAL:CG1	4:X:385:LEU:N	2.80	0.44
7:a:353:LEU:O	7:a:354:GLU:C	2.59	0.44
8:b:176:GLY:N	8:b:177:PRO:HD3	2.33	0.44
10:d:153:GLN:NE2	10:d:191:LEU:HD21	2.31	0.44
12:A:363:SER:O	12:A:363:SER:OG	2.36	0.44
21:J:39:ASP:OD1	21:J:213:ARG:NH2	2.48	0.44
28:Q:164:LEU:HD12	28:Q:194:ILE:HG21	1.98	0.44
32:f:263:PRO:HB3	32:f:891:THR:HG22	1.99	0.44
32:f:275:MET:HA	32:f:278:VAL:HG22	1.98	0.44
32:f:438:ASP:HB3	32:f:477:MET:SD	2.58	0.44
32:f:759:LEU:O	32:f:763:ARG:HG2	2.17	0.44
1:U:31:VAL:HG22	1:U:38:ILE:HD13	2.00	0.44
1:U:155:LEU:CD2	1:U:188:MET:HE1	2.45	0.44
1:U:609:ASP:OD2	1:U:614:VAL:HG11	2.18	0.44
6:Z:67:VAL:HG13	6:Z:67:VAL:O	2.17	0.44
7:a:247:ARG:NH2	7:a:251:LEU:HD21	2.32	0.44
9:c:127:ILE:CG2	9:c:162:LEU:HD21	2.48	0.44
10:d:110:SER:O	10:d:113:GLY:N	2.50	0.44
13:B:144:LEU:HD22	13:B:150:VAL:CG1	2.48	0.44
27:P:10:ALA:HB1	27:P:146:MET:CE	2.48	0.44
28:Q:169:LYS:O	28:Q:169:LYS:HD3	2.18	0.44
30:S:56:ARG:HD2	30:S:63:ILE:HG23	2.00	0.44
26:o:60:ASP:OD1	26:o:60:ASP:C	2.60	0.44
28:q:190:ASP:OD1	28:q:190:ASP:O	2.36	0.44
31:t:171:ASP:OD1	31:t:171:ASP:C	2.60	0.44
32:f:699:VAL:O	32:f:700:SER:OG	2.36	0.44
3:W:436:MET:O	3:W:439:VAL:HG12	2.18	0.44
4:X:160:MET:HE2	4:X:160:MET:HB3	1.95	0.44
4:X:177:TYR:CD2	4:X:185:LYS:HB3	2.52	0.44
5:Y:155:ASP:OD1	5:Y:155:ASP:N	2.51	0.44
9:c:259:VAL:HG22	9:c:263:ASP:OD2	2.16	0.44
10:d:148:LEU:HD21	10:d:170:GLN:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:62:GLU:OE2	15:D:116:LEU:HD12	2.18	0.44
16:E:154:THR:HG23	16:E:156:PRO:HD2	1.98	0.44
20:I:8:ARG:O	20:I:11:ILE:HG22	2.18	0.44
30:S:52:ALA:HB1	30:S:223:ILE:HD13	2.00	0.44
31:T:144:ARG:NH2	31:T:149:ASN:OD1	2.51	0.44
29:r:71:VAL:HB	29:r:238:VAL:HG22	2.00	0.44
30:s:132:TYR:HB3	30:s:134:VAL:HG12	2.00	0.44
31:t:217:CYS:O	31:t:220:VAL:HG12	2.18	0.44
32:f:290:VAL:HA	32:f:890:VAL:HG11	2.00	0.44
1:U:13:ASP:OD1	1:U:44:LYS:NZ	2.51	0.44
2:V:243:ASP:OD2	2:V:246:GLY:N	2.51	0.44
2:V:396:ILE:C	2:V:398:LEU:N	2.75	0.44
3:W:329:ARG:HH22	3:W:351:TRP:CB	2.29	0.44
5:Y:233:ARG:NH2	5:Y:264:TYR:O	2.50	0.44
5:Y:347:ILE:HG22	5:Y:348:ASP:N	2.33	0.44
7:a:228:THR:HG22	7:a:229:ASP:H	1.81	0.44
12:A:246:VAL:HG23	12:A:280:ILE:CD1	2.47	0.44
14:C:66:LEU:HD22	15:D:82:ILE:HD13	1.99	0.44
14:C:127:LEU:HD13	15:D:102:ILE:HD11	2.00	0.44
16:E:40:TYR:OH	17:F:73:ILE:CA	2.66	0.44
16:E:178:THR:OG1	16:E:301:ILE:HG21	2.17	0.44
16:E:193:CYS:HG	16:E:228:CYS:N	2.15	0.44
17:F:407:ALA:O	17:F:412:ALA:HB3	2.17	0.44
19:H:19:LEU:O	19:H:22:ILE:HG22	2.18	0.44
21:J:183:THR:CG2	21:J:186:LEU:HD23	2.48	0.44
28:Q:141:SER:HB3	29:r:197:VAL:HG23	1.99	0.44
30:S:169:ALA:O	30:S:173:LEU:HD13	2.18	0.44
26:o:206:ILE:HG23	26:o:213:GLY:O	2.18	0.44
27:p:178:ASP:OD1	27:p:178:ASP:C	2.60	0.44
29:r:63:LEU:HD23	29:r:63:LEU:C	2.43	0.44
29:r:152:MET:O	29:r:152:MET:HG2	2.18	0.44
29:r:233:VAL:O	29:r:234:ASN:C	2.61	0.44
32:f:447:ALA:O	32:f:451:VAL:HG23	2.16	0.44
1:U:520:MET:HE2	1:U:520:MET:HA	2.00	0.43
2:V:451:ILE:CG2	10:d:279:TYR:H	2.31	0.43
4:X:123:THR:O	4:X:127:GLN:HG2	2.18	0.43
6:Z:67:VAL:HG21	8:b:91:ARG:CB	2.48	0.43
8:b:33:VAL:HA	8:b:36:VAL:HG12	2.00	0.43
15:D:58:GLU:O	15:D:62:LYS:HG2	2.18	0.43
17:F:195:ILE:O	17:F:199:VAL:HG23	2.17	0.43
23:L:84:LEU:HD21	23:L:128:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:50:VAL:HG23	24:M:67:LEU:HD21	1.99	0.43
25:N:208:ILE:HG22	25:N:210:LEU:HD13	1.99	0.43
26:O:233:THR:HG22	26:O:234:VAL:N	2.33	0.43
27:P:45:MET:HB3	27:P:71:LEU:HD13	1.99	0.43
30:S:141:LEU:HD11	30:S:227:THR:C	2.43	0.43
32:f:799:VAL:HG12	32:f:803:PHE:CE2	2.53	0.43
1:U:877:LEU:C	1:U:878:LEU:HD22	2.44	0.43
2:V:113:LEU:HD23	2:V:135:LEU:HD21	1.98	0.43
2:V:168:GLN:CG	2:V:191:LEU:HD21	2.47	0.43
2:V:313:LEU:HD13	2:V:328:VAL:CG1	2.48	0.43
3:W:435:LEU:HD21	7:a:356:TRP:HH2	1.84	0.43
6:Z:19:VAL:HG21	6:Z:124:ILE:CD1	2.47	0.43
8:b:143:PHE:O	8:b:143:PHE:CD2	2.71	0.43
15:D:272:THR:O	15:D:273:LYS:C	2.61	0.43
15:D:351:LYS:HE2	16:E:162:VAL:HG21	1.99	0.43
25:N:192:ASN:O	25:N:196:LEU:HD13	2.18	0.43
26:O:210:LEU:CD2	30:s:63:ILE:HD11	2.48	0.43
28:Q:119:ASP:C	28:Q:119:ASP:OD1	2.59	0.43
29:R:164:ASP:OD1	29:R:164:ASP:N	2.50	0.43
31:t:137:LEU:CD1	31:t:157:ILE:HD11	2.48	0.43
1:U:517:GLY:HA3	1:U:551:GLY:HA2	2.00	0.43
4:X:256:LEU:HD13	4:X:319:ILE:HG13	2.01	0.43
5:Y:128:TYR:HB2	5:Y:140:ILE:HG21	2.00	0.43
6:Z:90:ARG:O	6:Z:92:VAL:HG13	2.17	0.43
6:Z:166:GLU:OE2	9:c:46:ARG:NH2	2.51	0.43
9:c:206:ASN:OD1	9:c:207:TYR:N	2.51	0.43
10:d:150:ILE:HA	10:d:153:GLN:HG2	2.01	0.43
14:C:276:LEU:HD23	14:C:276:LEU:C	2.44	0.43
20:I:216:LEU:C	20:I:216:LEU:HD23	2.44	0.43
24:M:220:LEU:HD12	24:M:221:THR:HG23	2.00	0.43
27:P:71:LEU:HD21	27:P:75:GLU:OE2	2.18	0.43
28:Q:14:LEU:CD2	28:Q:160:LEU:HD13	2.48	0.43
28:Q:162:LYS:HA	28:Q:165:GLU:CD	2.43	0.43
30:S:202:LEU:O	30:S:206:VAL:HG13	2.18	0.43
32:f:470:VAL:O	32:f:471:LEU:HB2	2.19	0.43
1:U:351:MET:SD	1:U:818:GLU:N	2.91	0.43
1:U:829:SER:O	1:U:830:THR:C	2.60	0.43
3:W:112:VAL:HG21	3:W:128:LEU:CD1	2.48	0.43
4:X:365:LEU:HD22	4:X:385:LEU:HD11	2.00	0.43
7:a:311:VAL:O	7:a:315:LEU:HD13	2.19	0.43
8:b:104:ASN:O	8:b:105:HIS:ND1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:124:LEU:HG	8:b:156:PHE:HE1	1.82	0.43
12:A:339:ARG:HG3	12:A:339:ARG:O	2.18	0.43
14:C:137:LEU:HG	14:C:137:LEU:O	2.18	0.43
15:D:344:ILE:HD12	37:D:501:ADP:C6	2.53	0.43
22:K:12:VAL:HG21	22:K:123:PHE:HB3	1.99	0.43
22:K:48:LEU:O	22:K:217:LEU:HD12	2.18	0.43
24:M:75:GLY:HA3	24:M:225:HIS:CD2	2.54	0.43
31:T:202:GLN:HG2	31:T:202:GLN:O	2.18	0.43
25:n:46:VAL:HG12	25:n:47:VAL:N	2.33	0.43
32:f:370:MET:SD	32:f:370:MET:N	2.90	0.43
1:U:420:LEU:HD21	1:U:460:TYR:CE2	2.53	0.43
1:U:443:LEU:HD13	1:U:477:GLY:HA3	2.00	0.43
1:U:803:LYS:O	1:U:893:THR:N	2.38	0.43
1:U:892:LEU:HD23	1:U:906:LEU:HB3	2.00	0.43
2:V:376:ASN:OD1	2:V:399:ARG:NH2	2.52	0.43
3:W:264:GLN:HG2	3:W:268:LYS:HE3	2.00	0.43
4:X:31:VAL:HG11	4:X:72:TYR:HE1	1.83	0.43
7:a:77:VAL:HA	7:a:80:ILE:HD12	2.00	0.43
8:b:109:ILE:HD13	8:b:136:VAL:CG1	2.49	0.43
10:d:153:GLN:O	10:d:157:LEU:HD13	2.17	0.43
10:d:257:THR:O	10:d:258:PHE:HB3	2.18	0.43
12:A:369:ARG:NH2	22:K:206:MET:O	2.52	0.43
13:B:306:GLN:O	13:B:310:LEU:HD13	2.18	0.43
15:D:394:VAL:HG11	15:D:399:PHE:HE1	1.82	0.43
17:F:221:LYS:HD2	17:F:320:PHE:CE1	2.53	0.43
23:L:193:ARG:NH1	23:L:237:GLU:OE2	2.51	0.43
26:O:244:ARG:NE	26:O:246:ARG:HE	2.16	0.43
27:P:168:SER:HB3	27:P:200:LEU:HD21	1.99	0.43
28:Q:35:MET:SD	28:Q:43:LEU:HD21	2.59	0.43
29:R:142:LEU:HD23	29:R:173:VAL:HG21	1.99	0.43
25:n:63:ARG:HD2	26:o:182:GLU:OE2	2.17	0.43
29:r:97:ASN:OD1	29:r:98:PRO:HD2	2.19	0.43
32:f:137:ARG:CG	32:f:165:GLU:HG3	2.48	0.43
1:U:343:ILE:HD13	1:U:930:ALA:HA	2.01	0.43
3:W:308:LEU:HD12	3:W:324:TYR:HE2	1.83	0.43
3:W:329:ARG:NH2	3:W:351:TRP:HE3	2.17	0.43
3:W:425:LEU:HD12	6:Z:252:LYS:HG3	2.00	0.43
7:a:174:LYS:O	7:a:178:ARG:HG3	2.18	0.43
7:a:224:SER:C	7:a:225:LEU:HD12	2.44	0.43
8:b:142:ASN:ND2	8:b:146:GLU:OE1	2.51	0.43
9:c:31:VAL:O	9:c:31:VAL:HG13	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:220:VAL:HG21	15:D:287:ARG:HD3	2.01	0.43
15:D:172:ILE:HD12	15:D:172:ILE:H	1.84	0.43
18:G:10:ASP:OD1	18:G:27:TYR:CE2	2.72	0.43
20:I:18:LEU:HD12	20:I:18:LEU:N	2.34	0.43
22:K:78:MET:HG3	22:K:85:ALA:HB1	2.00	0.43
27:P:94:LEU:C	27:P:94:LEU:HD23	2.44	0.43
26:o:202:ILE:HG21	26:o:216:ILE:HG13	2.01	0.43
28:q:19:ARG:HG2	28:q:177:THR:OG1	2.18	0.43
31:t:257:ALA:O	31:t:260:ILE:HG22	2.19	0.43
32:f:695:ALA:O	32:f:699:VAL:HG22	2.19	0.43
32:f:836:GLU:OE2	33:y:410:ARG:NH2	2.44	0.43
1:U:691:SER:OG	1:U:713:TYR:OH	2.34	0.43
2:V:231:LEU:O	2:V:250:LEU:HD12	2.18	0.43
4:X:345:VAL:HG12	4:X:346:GLN:N	2.32	0.43
5:Y:67:VAL:HG12	5:Y:71:ASN:OD1	2.19	0.43
6:Z:11:VAL:HG12	6:Z:12:HIS:N	2.33	0.43
6:Z:151:THR:HG23	7:a:148:VAL:HG21	2.01	0.43
6:Z:171:GLY:O	6:Z:175:LEU:HD13	2.18	0.43
17:F:251:LEU:HD22	17:F:285:ILE:HG12	2.01	0.43
19:H:141:GLU:OE2	27:P:115:LYS:NZ	2.50	0.43
22:K:117:SER:O	22:K:121:LEU:HG	2.18	0.43
27:P:138:VAL:HG22	27:P:147:TYR:CE1	2.54	0.43
30:S:56:ARG:O	30:S:70:LYS:NZ	2.39	0.43
30:S:200:MET:CE	30:S:225:ILE:HD11	2.48	0.43
25:n:119:GLU:OE1	25:n:119:GLU:HA	2.19	0.43
32:f:399:LEU:O	32:f:400:TYR:HD1	2.02	0.43
1:U:894:MET:SD	1:U:906:LEU:HD21	2.59	0.43
2:V:398:LEU:O	2:V:399:ARG:C	2.62	0.43
3:W:451:MET:HG3	6:Z:100:LYS:HD2	2.00	0.43
4:X:349:HIS:NE2	4:X:353:LEU:HD11	2.33	0.43
5:Y:308:LEU:O	5:Y:358:ARG:NH2	2.52	0.43
7:a:240:PHE:CE1	7:a:272:ILE:HB	2.54	0.43
9:c:285:GLU:HA	9:c:288:VAL:HG12	2.00	0.43
15:D:170:MET:HG2	15:D:170:MET:O	2.18	0.43
15:D:267:ILE:HG13	15:D:271:ALA:HB3	2.01	0.43
18:G:163:PHE:CD2	18:G:166:THR:HB	2.53	0.43
19:H:17:GLY:HA3	20:I:27:ALA:HB2	2.01	0.43
19:H:210:VAL:HG12	19:H:226:VAL:HG22	2.01	0.43
21:J:188:ILE:O	21:J:192:ILE:CD1	2.67	0.43
24:M:28:MET:HA	24:M:31:VAL:HG12	2.01	0.43
29:r:94:ILE:HD11	29:r:104:MET:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:s:175:PRO:O	30:s:178:ASP:OD1	2.37	0.43
32:f:147:SER:OG	32:f:149:GLU:HG3	2.19	0.43
32:f:315:GLU:HA	32:f:318:THR:HG22	2.01	0.43
32:f:551:LYS:O	32:f:551:LYS:HG2	2.19	0.43
1:U:115:ASN:HA	1:U:118:LEU:HD13	2.00	0.43
7:a:185:ILE:HG22	7:a:193:GLN:NE2	2.34	0.43
10:d:318:PHE:O	10:d:318:PHE:CG	2.72	0.43
13:B:51:LEU:HD23	13:B:51:LEU:H	1.82	0.43
16:E:149:ILE:HG12	16:E:153:LEU:HD23	2.01	0.43
16:E:169:GLY:HA3	16:E:275:MET:O	2.18	0.43
16:E:308:ALA:O	16:E:312:ILE:HG12	2.18	0.43
22:K:82:ILE:H	22:K:82:ILE:HD12	1.83	0.43
24:M:177:ILE:CG2	24:M:182:MET:HE1	2.48	0.43
26:O:195:LYS:HD2	26:O:220:VAL:HG21	2.00	0.43
32:f:349:TYR:CE1	32:f:763:ARG:HD2	2.53	0.43
6:Z:88:ARG:HD3	6:Z:88:ARG:N	2.33	0.43
7:a:128:LEU:HA	7:a:131:THR:HG22	2.01	0.43
12:A:297:ARG:HD3	17:F:257:VAL:HG21	2.01	0.43
17:F:188:ILE:HD13	17:F:191:LEU:HD11	2.01	0.43
17:F:263:ASP:OD1	17:F:266:LYS:NZ	2.46	0.43
18:G:170:VAL:HG23	18:G:171:LYS:HG2	2.01	0.43
19:H:101:TYR:O	19:H:103:GLU:N	2.49	0.43
24:M:94:GLU:OE1	24:M:94:GLU:HA	2.19	0.43
30:S:148:ALA:HB2	30:S:160:ARG:NH2	2.34	0.43
28:q:139:THR:CG2	28:q:167:LEU:HD11	2.47	0.43
29:r:71:VAL:HB	29:r:238:VAL:CG2	2.49	0.43
29:r:142:LEU:HD12	29:r:145:MET:HE2	2.01	0.43
29:r:142:LEU:HD22	29:r:160:ILE:HD11	2.00	0.43
31:t:162:ASP:N	31:t:162:ASP:OD1	2.51	0.43
32:f:834:ASP:OD1	32:f:836:GLU:N	2.50	0.43
1:U:199:ARG:CZ	1:U:223:LEU:HD23	2.49	0.42
2:V:451:ILE:HG22	10:d:279:TYR:H	1.84	0.42
3:W:335:SER:N	3:W:336:PRO:HD3	2.34	0.42
7:a:11:SER:OG	7:a:22:TRP:CZ2	2.70	0.42
7:a:254:ALA:O	7:a:257:GLN:HG2	2.19	0.42
9:c:29:GLU:OE2	9:c:139:ARG:NH2	2.50	0.42
10:d:200:LEU:HD11	10:d:233:GLU:HG2	1.99	0.42
13:B:292:THR:HG22	13:B:293:LYS:N	2.33	0.42
16:E:209:GLY:N	16:E:259:GLU:OE2	2.52	0.42
16:E:233:ASP:OD1	16:E:234:GLU:N	2.39	0.42
20:I:118:LYS:O	20:I:122:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:N:184:GLU:O	25:N:188:GLN:HG2	2.19	0.42
27:P:123:SER:C	27:P:124:LEU:HD12	2.44	0.42
31:T:82:ARG:NE	25:n:199:GLU:OE2	2.51	0.42
25:n:43:ASP:O	25:n:43:ASP:OD1	2.37	0.42
30:s:62:SER:O	30:s:63:ILE:C	2.62	0.42
32:f:423:ASP:OD1	32:f:424:GLY:N	2.50	0.42
32:f:685:THR:HG23	32:f:686:LEU:N	2.34	0.42
1:U:545:LEU:HB3	1:U:577:ILE:HG21	2.00	0.42
1:U:637:VAL:HG13	1:U:652:ALA:HB1	2.01	0.42
1:U:800:VAL:HG12	1:U:801:GLN:H	1.84	0.42
1:U:834:SER:HB3	13:B:66:GLU:OE1	2.18	0.42
2:V:404:LYS:O	2:V:407:VAL:HG12	2.19	0.42
2:V:493:ALA:HB3	6:Z:275:LEU:CD1	2.49	0.42
5:Y:282:MET:HE1	5:Y:295:TYR:CD1	2.54	0.42
6:Z:22:HIS:CE1	6:Z:35:VAL:HB	2.54	0.42
7:a:109:GLU:OE2	7:a:149:THR:HG21	2.18	0.42
7:a:210:VAL:HG23	7:a:210:VAL:O	2.18	0.42
8:b:147:GLU:HG2	8:b:148:VAL:HG23	2.00	0.42
12:A:134:ILE:HG23	12:A:135:GLU:N	2.34	0.42
13:B:174:MET:SD	13:B:270:LEU:HD13	2.59	0.42
14:C:213:ARG:O	14:C:213:ARG:CG	2.67	0.42
15:D:393:ILE:HG22	15:D:394:VAL:N	2.33	0.42
16:E:132:TYR:OH	16:E:142:ILE:HG21	2.19	0.42
20:I:220:ASN:O	20:I:220:ASN:CG	2.61	0.42
29:R:117:LEU:HD12	29:R:120:ARG:HD3	2.01	0.42
29:R:233:VAL:O	29:R:234:ASN:C	2.62	0.42
26:o:77:ILE:HG13	26:o:77:ILE:O	2.19	0.42
27:p:155:GLU:HB2	27:p:156:PRO:CD	2.49	0.42
1:U:894:MET:CE	1:U:902:PRO:HD3	2.50	0.42
2:V:497:PRO:HG2	2:V:498:PRO:CD	2.45	0.42
4:X:53:LEU:CD2	4:X:69:LEU:HD21	2.50	0.42
9:c:57:MET:HE1	9:c:143:VAL:HG21	2.01	0.42
10:d:208:PHE:CZ	10:d:212:LEU:HD11	2.54	0.42
10:d:257:THR:C	10:d:259:PHE:H	2.27	0.42
13:B:305:ILE:HD13	14:C:271:ARG:NH2	2.34	0.42
14:C:320:PRO:CB	14:C:324:ALA:HB3	2.50	0.42
15:D:176:GLU:OE1	15:D:329:ARG:NH2	2.51	0.42
15:D:265:ASP:O	15:D:310:ALA:HB3	2.19	0.42
15:D:360:LEU:HD21	15:D:399:PHE:CE2	2.55	0.42
18:G:13:ILE:HG23	18:G:14:THR:HG23	2.01	0.42
18:G:143:ILE:HD13	18:G:149:PRO:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:J:40:ILE:HD11	21:J:210:VAL:HG13	2.01	0.42
24:M:71:ASP:HA	31:T:121:LEU:HD21	2.01	0.42
30:S:132:TYR:HB3	30:S:134:VAL:HG12	2.01	0.42
31:T:187:GLY:HA3	31:T:221:LEU:HD21	2.01	0.42
28:q:139:THR:O	28:q:143:LEU:HD13	2.18	0.42
31:t:160:TYR:CE1	31:t:237:VAL:HG22	2.54	0.42
1:U:792:ASN:OD1	1:U:794:ASP:OD1	2.38	0.42
3:W:89:LEU:O	3:W:93:ARG:HG3	2.20	0.42
5:Y:315:THR:HG23	5:Y:318:TYR:H	1.84	0.42
6:Z:62:ASP:N	6:Z:62:ASP:OD1	2.53	0.42
6:Z:156:GLU:OE1	6:Z:156:GLU:HA	2.19	0.42
7:a:79:ILE:O	7:a:83:VAL:HG23	2.19	0.42
7:a:84:VAL:HG21	7:a:97:LEU:HD21	2.02	0.42
7:a:311:VAL:HG12	7:a:315:LEU:HD13	2.01	0.42
8:b:179:LEU:O	8:b:183:LEU:HD23	2.20	0.42
10:d:310:LEU:HB3	10:d:312:PRO:HD3	2.01	0.42
12:A:56:LEU:HD11	13:B:49:LEU:HD11	2.02	0.42
13:B:127:VAL:O	13:B:127:VAL:HG22	2.19	0.42
13:B:374:LEU:HD12	13:B:414:VAL:CG2	2.49	0.42
15:D:384:MET:HA	15:D:387:VAL:HG22	2.01	0.42
17:F:62:VAL:O	17:F:66:LEU:HD23	2.19	0.42
17:F:95:GLU:OE2	17:F:97:LEU:HD11	2.19	0.42
18:G:60:LEU:HD21	24:M:177:ILE:CG2	2.50	0.42
22:K:68:VAL:HG21	22:K:89:ILE:HD12	2.01	0.42
24:M:46:VAL:CG1	24:M:149:LEU:HD12	2.49	0.42
24:M:47:VAL:HG21	24:M:190:ILE:HG23	2.01	0.42
24:M:217:VAL:HG13	24:M:217:VAL:O	2.19	0.42
31:T:108:LEU:HD13	31:T:155:MET:HE1	2.00	0.42
32:f:206:ASP:OD1	32:f:232:TYR:OH	2.29	0.42
32:f:466:LEU:O	32:f:470:VAL:HG23	2.20	0.42
3:W:169:LEU:HB3	3:W:171:VAL:HG13	2.00	0.42
3:W:259:GLU:O	3:W:263:TRP:CD1	2.72	0.42
8:b:110:ILE:HG22	8:b:139:ASP:HB2	2.01	0.42
12:A:90:GLU:O	12:A:91:GLN:C	2.63	0.42
14:C:335:LYS:O	15:D:195:GLY:HA3	2.20	0.42
14:C:362:VAL:HG22	14:C:390:VAL:CG2	2.40	0.42
16:E:49:ALA:HB2	17:F:136:VAL:HG11	2.00	0.42
16:E:125:GLU:O	16:E:195:PHE:O	2.37	0.42
17:F:288:LEU:O	17:F:291:ILE:HG22	2.19	0.42
19:H:182:LEU:HD11	19:H:186:ASP:HB3	2.01	0.42
24:M:91:ILE:HD13	24:M:119:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:181:GLN:O	24:M:185:MET:HG3	2.20	0.42
25:N:48:LEU:CD1	25:N:213:ILE:HD12	2.49	0.42
1:U:11:LEU:HD23	1:U:14:GLU:OE2	2.19	0.42
1:U:140:ARG:NH1	1:U:144:ASP:OD2	2.53	0.42
1:U:346:ASN:O	1:U:348:THR:N	2.52	0.42
4:X:244:SER:OG	4:X:245:PRO:HD2	2.19	0.42
7:a:137:ASP:O	7:a:140:GLU:HG3	2.19	0.42
9:c:57:MET:HE1	9:c:143:VAL:CG2	2.50	0.42
10:d:301:ASP:O	10:d:302:TYR:HB2	2.19	0.42
12:A:63:THR:HA	32:f:681:TYR:OH	2.20	0.42
12:A:184:ILE:HD11	12:A:225:CYS:SG	2.60	0.42
14:C:338:LEU:HD23	14:C:378:VAL:CG2	2.49	0.42
15:D:210:CYS:SG	15:D:335:LEU:HD23	2.60	0.42
15:D:345:PHE:HB3	15:D:360:LEU:HD13	2.01	0.42
18:G:51:VAL:CG2	18:G:215:ILE:HD11	2.49	0.42
23:L:125:ARG:NH1	23:L:126:ARG:O	2.52	0.42
24:M:31:VAL:HG23	24:M:79:ALA:O	2.19	0.42
24:M:50:VAL:CG1	24:M:66:ARG:HE	2.33	0.42
28:Q:45:LEU:O	28:Q:102:LEU:HA	2.20	0.42
28:Q:161:ARG:O	28:Q:165:GLU:OE1	2.37	0.42
25:n:82:SER:O	25:n:86:THR:HG23	2.20	0.42
29:r:77:SER:O	29:r:78:ARG:HB3	2.18	0.42
32:f:298:LEU:HD22	32:f:303:VAL:CG1	2.50	0.42
3:W:89:LEU:HD23	3:W:90:LEU:N	2.34	0.42
3:W:241:LEU:HD11	3:W:286:LEU:HD12	2.01	0.42
3:W:297:GLU:HB3	3:W:299:ILE:HG23	2.01	0.42
4:X:371:ASP:OD1	5:Y:233:ARG:NH1	2.53	0.42
5:Y:68:ASP:OD1	5:Y:69:LEU:N	2.51	0.42
5:Y:224:VAL:O	5:Y:228:MET:HG3	2.20	0.42
6:Z:133:LEU:HD22	6:Z:162:ILE:CG1	2.49	0.42
7:a:149:THR:HG22	7:a:150:SER:H	1.84	0.42
7:a:252:LYS:HA	7:a:255:TRP:NE1	2.35	0.42
14:C:373:GLU:O	14:C:374:ARG:C	2.63	0.42
16:E:165:ILE:O	16:E:166:PRO:C	2.63	0.42
16:E:330:ALA:HA	16:E:333:LYS:HE2	2.00	0.42
19:H:44:VAL:CG1	19:H:146:LEU:HD12	2.49	0.42
20:I:12:PHE:HE1	20:I:18:LEU:HD11	1.85	0.42
21:J:42:VAL:CG2	21:J:208:LEU:HD12	2.49	0.42
21:J:43:LEU:HD22	21:J:72:ALA:CB	2.49	0.42
29:R:96:ILE:HG23	29:R:119:ALA:HB2	2.01	0.42
29:r:231:GLY:O	29:r:251:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:182:GLU:N	32:f:183:PRO:HD2	2.34	0.42
3:W:374:THR:HG22	3:W:376:LYS:H	1.84	0.42
4:X:412:ASP:OD1	5:Y:379:ARG:NH2	2.53	0.42
5:Y:291:HIS:HE1	11:e:39:TRP:CZ2	2.38	0.42
8:b:108:ARG:C	8:b:109:ILE:HD12	2.44	0.42
9:c:130:GLN:HG3	9:c:162:LEU:HD13	2.02	0.42
9:c:182:GLY:HA2	9:c:204:THR:HG21	2.01	0.42
13:B:164:MET:HG2	13:B:164:MET:O	2.19	0.42
16:E:154:THR:CG2	16:E:156:PRO:HD3	2.50	0.42
16:E:229:ILE:CD1	16:E:274:LYS:HD2	2.50	0.42
19:H:76:TYR:HB3	19:H:83:TYR:CD1	2.55	0.42
25:N:40:VAL:O	25:N:46:VAL:HG23	2.19	0.42
25:N:213:ILE:HG12	25:N:218:VAL:HG22	2.01	0.42
31:T:256:ILE:HD11	26:o:185:PHE:O	2.19	0.42
29:r:198:MET:O	29:r:202:TYR:HB3	2.19	0.42
32:f:45:LEU:HD13	32:f:49:ASP:OD2	2.19	0.42
32:f:400:TYR:CD1	32:f:407:MET:HE3	2.55	0.42
32:f:590:PHE:CE2	32:f:652:VAL:HG21	2.55	0.42
32:f:852:VAL:HG13	32:f:853:VAL:N	2.34	0.42
1:U:108:TYR:CD2	1:U:134:VAL:HG21	2.55	0.42
2:V:218:TYR:HD2	2:V:227:VAL:CG2	2.33	0.42
2:V:254:LEU:CD2	2:V:270:LEU:HD11	2.45	0.42
2:V:410:ILE:HD12	2:V:426:LEU:HD21	2.02	0.42
5:Y:80:GLU:O	5:Y:84:LEU:HD23	2.20	0.42
7:a:151:VAL:HG13	7:a:152:HIS:N	2.35	0.42
7:a:180:LEU:CD1	7:a:221:VAL:HG21	2.47	0.42
8:b:149:ASN:O	8:b:153:LEU:HD13	2.20	0.42
9:c:153:GLY:HA3	15:D:81:ARG:NH2	2.35	0.42
10:d:283:LEU:HD21	10:d:286:GLU:HB2	2.01	0.42
10:d:311:GLY:N	10:d:312:PRO:CD	2.83	0.42
12:A:186:LYS:O	12:A:190:VAL:HG12	2.20	0.42
13:B:251:VAL:HG11	14:C:275:GLU:OE1	2.20	0.42
14:C:325:ARG:CZ	14:C:351:MET:O	2.68	0.42
16:E:148:VAL:O	16:E:274:LYS:HE2	2.20	0.42
27:P:6:TYR:O	27:P:30:ILE:O	2.37	0.42
27:P:52:GLY:O	27:P:53:LEU:C	2.63	0.42
27:p:138:VAL:HG11	27:p:146:MET:HG3	2.01	0.42
28:q:14:LEU:HD12	28:q:181:ARG:O	2.20	0.42
32:f:437:GLU:OE1	32:f:437:GLU:N	2.53	0.42
32:f:461:PRO:HA	33:y:395:LEU:HD13	2.02	0.42
32:f:549:GLU:O	32:f:549:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:722:SER:O	32:f:723:TYR:C	2.62	0.42
32:f:836:GLU:OE2	33:y:410:ARG:NH1	2.51	0.42
1:U:35:TRP:CG	1:U:70:HIS:HB3	2.55	0.42
1:U:521:LEU:C	1:U:521:LEU:HD23	2.45	0.42
3:W:171:VAL:HG21	3:W:186:ILE:HG13	2.02	0.42
4:X:314:ARG:O	4:X:315:ASP:CG	2.63	0.42
4:X:365:LEU:HD22	4:X:385:LEU:CD1	2.50	0.42
12:A:432:TYR:OH	21:J:15:HIS:HA	2.20	0.42
15:D:69:LYS:O	15:D:73:LEU:HD23	2.20	0.42
15:D:354:LEU:HB3	15:D:358:VAL:HG11	2.02	0.42
15:D:384:MET:HE2	15:D:384:MET:N	2.35	0.42
16:E:198:VAL:HB	16:E:232:MET:HA	2.02	0.42
17:F:219:PRO:O	17:F:220:PRO:C	2.62	0.42
24:M:21:VAL:O	24:M:21:VAL:HG23	2.20	0.42
25:N:115:SER:O	25:N:119:GLU:HG2	2.20	0.42
27:P:37:THR:O	27:P:37:THR:CG2	2.67	0.42
26:o:164:LYS:O	26:o:165:LEU:HD23	2.20	0.42
27:p:53:LEU:HB2	27:p:60:VAL:HG13	2.02	0.42
28:q:38:MET:HB3	28:q:64:VAL:HG11	2.00	0.42
28:q:161:ARG:O	28:q:165:GLU:HG3	2.20	0.42
28:q:180:VAL:HG13	28:q:191:LEU:HB2	2.02	0.42
29:r:94:ILE:N	29:r:102:GLY:O	2.53	0.42
32:f:105:LYS:O	32:f:109:ILE:HG12	2.20	0.42
32:f:429:ILE:HG21	32:f:448:CYS:SG	2.59	0.42
1:U:628:ARG:NH2	1:U:755:THR:OG1	2.53	0.41
1:U:832:VAL:O	1:U:832:VAL:HG13	2.20	0.41
1:U:835:ILE:HG13	32:f:607:LEU:CD2	2.50	0.41
2:V:320:THR:OG1	11:e:18:GLU:OE2	2.37	0.41
5:Y:113:ARG:HG2	5:Y:113:ARG:HH11	1.85	0.41
7:a:217:LEU:H	7:a:217:LEU:HD12	1.85	0.41
12:A:96:ALA:HB1	12:A:113:ILE:HB	2.02	0.41
13:B:197:ILE:HD11	13:B:224:LEU:HD11	2.02	0.41
15:D:258:ALA:CB	15:D:259:PRO:CD	2.97	0.41
17:F:182:THR:HA	17:F:242:ALA:HB1	2.02	0.41
17:F:192:ASP:HA	17:F:195:ILE:HG22	2.02	0.41
20:I:45:LEU:HD22	20:I:75:SER:HB2	2.01	0.41
24:M:51:GLU:O	24:M:51:GLU:HG3	2.20	0.41
24:M:196:LYS:O	24:M:200:ILE:HG12	2.20	0.41
25:N:117:PHE:CE1	25:N:132:ILE:HD13	2.55	0.41
26:O:153:LEU:HD21	26:O:168:VAL:HG22	2.00	0.41
30:s:221:LEU:HG	30:s:221:LEU:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:t:89:ARG:O	31:t:90:VAL:C	2.63	0.41
32:f:308:SER:OG	32:f:309:GLU:N	2.52	0.41
32:f:386:GLY:HA2	32:f:418:LEU:HD13	2.01	0.41
32:f:679:LEU:CD1	32:f:690:VAL:HG11	2.50	0.41
2:V:128:ARG:O	2:V:132:LEU:HD23	2.21	0.41
2:V:309:MET:HE1	2:V:331:LEU:CB	2.50	0.41
2:V:309:MET:HE1	2:V:331:LEU:CD2	2.48	0.41
3:W:115:ILE:CG2	3:W:116:THR:N	2.83	0.41
3:W:446:ILE:HG23	6:Z:211:TYR:CD1	2.55	0.41
23:L:65:HIS:ND1	23:L:66:VAL:O	2.53	0.41
25:N:171:GLY:HA3	25:n:168:TYR:O	2.20	0.41
27:P:10:ALA:HB1	27:P:146:MET:HE2	2.02	0.41
25:n:60:ILE:O	25:n:60:ILE:HG13	2.20	0.41
32:f:110:TYR:OH	32:f:145:VAL:HG21	2.20	0.41
32:f:140:LEU:HD11	32:f:169:GLU:HG3	2.02	0.41
32:f:270:LEU:HD12	32:f:278:VAL:HG11	2.02	0.41
32:f:783:SER:HB2	32:f:787:LEU:HD12	2.02	0.41
32:f:834:ASP:HB3	32:f:840:LEU:HD11	2.02	0.41
32:f:869:THR:O	32:f:869:THR:HG23	2.20	0.41
1:U:243:LEU:HD22	1:U:913:ILE:CG2	2.49	0.41
1:U:498:LYS:NZ	1:U:531:ASP:OD2	2.39	0.41
2:V:131:LEU:CD2	2:V:171:VAL:HG21	2.50	0.41
5:Y:25:LEU:CD2	5:Y:37:VAL:HG21	2.50	0.41
6:Z:151:THR:HG21	7:a:148:VAL:HG21	2.02	0.41
8:b:87:CYS:O	8:b:91:ARG:HG2	2.21	0.41
12:A:190:VAL:HG11	12:A:212:VAL:CG2	2.50	0.41
13:B:223:ILE:O	13:B:223:ILE:HG23	2.21	0.41
13:B:329:MET:CE	13:B:347:ILE:HD11	2.51	0.41
14:C:82:LYS:O	14:C:83:LYS:CG	2.67	0.41
15:D:353:ASN:N	16:E:160:GLN:O	2.49	0.41
16:E:60:VAL:C	16:E:61:LEU:HD12	2.45	0.41
17:F:389:ASP:O	17:F:390:ASP:HB3	2.21	0.41
19:H:173:PHE:HB2	19:H:197:GLU:OE1	2.20	0.41
20:I:174:MET:HE3	20:I:174:MET:HB2	1.97	0.41
25:N:48:LEU:HD21	25:N:135:ALA:HB3	2.02	0.41
25:N:155:VAL:HG11	31:T:81:PHE:CE2	2.55	0.41
26:O:142:VAL:HG13	26:O:168:VAL:CG2	2.49	0.41
28:q:4:LEU:HD13	28:q:45:LEU:CB	2.51	0.41
31:t:55:SER:OG	31:t:221:LEU:HD13	2.20	0.41
32:f:102:HIS:O	32:f:106:LEU:HD23	2.20	0.41
32:f:445:LEU:HD21	32:f:469:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:405:THR:O	1:U:445:ALA:HB2	2.20	0.41
2:V:214:HIS:O	2:V:217:VAL:HG22	2.20	0.41
3:W:23:THR:HA	3:W:26:GLN:HG3	2.01	0.41
3:W:407:ASP:O	3:W:411:GLY:N	2.52	0.41
7:a:216:LEU:HD23	7:a:216:LEU:O	2.21	0.41
12:A:196:LEU:O	12:A:197:HIS:ND1	2.53	0.41
15:D:345:PHE:CD2	15:D:364:VAL:HG12	2.55	0.41
16:E:294:ARG:NE	16:E:296:ASP:OD2	2.53	0.41
18:G:180:GLU:O	18:G:184:LYS:HG3	2.21	0.41
27:P:159:ASP:O	27:P:160:PRO:C	2.63	0.41
29:R:227:ALA:CB	27:p:180:VAL:HG12	2.51	0.41
30:S:174:GLN:NE2	30:S:178:ASP:OD1	2.53	0.41
31:T:50:MET:HA	31:T:50:MET:HE3	2.03	0.41
31:T:72:LEU:HD11	31:T:79:ALA:HB1	2.02	0.41
25:n:52:SER:O	25:n:65:THR:OG1	2.31	0.41
32:f:524:MET:O	32:f:527:VAL:HG23	2.20	0.41
3:W:305:LEU:HD22	3:W:328:LEU:HD11	2.03	0.41
3:W:426:ASN:O	3:W:430:GLN:HG2	2.20	0.41
4:X:30:ILE:HG21	4:X:49:SER:OG	2.20	0.41
4:X:161:ASP:O	4:X:162:ASP:CG	2.63	0.41
5:Y:282:MET:HE3	5:Y:292:TYR:HA	2.02	0.41
7:a:115:LYS:HA	7:a:118:ILE:HG12	2.02	0.41
7:a:216:LEU:HD23	7:a:216:LEU:C	2.46	0.41
13:B:440:LEU:HD11	21:J:30:SER:N	2.34	0.41
13:B:440:LEU:N	21:J:77:THR:OG1	2.53	0.41
17:F:244:THR:HG21	17:F:282:ILE:CD1	2.50	0.41
19:H:124:SER:HB3	19:H:127:VAL:HG22	2.02	0.41
19:H:200:GLU:OE1	19:H:200:GLU:N	2.47	0.41
25:N:198:MET:SD	25:N:208:ILE:CG1	3.08	0.41
26:O:142:VAL:HG13	26:O:168:VAL:HG21	2.03	0.41
26:O:229:LEU:HD12	26:O:229:LEU:N	2.36	0.41
28:Q:141:SER:OG	29:r:193:TYR:HB3	2.21	0.41
30:S:134:VAL:HG13	30:S:134:VAL:O	2.21	0.41
31:T:57:LEU:HD21	31:T:217:CYS:HB3	2.03	0.41
29:r:114:TRP:CE3	29:r:145:MET:HE3	2.55	0.41
32:f:192:VAL:HB	32:f:193:PRO:HD3	2.02	0.41
32:f:211:ILE:O	32:f:211:ILE:HG22	2.19	0.41
32:f:726:ILE:HD12	32:f:726:ILE:H	1.86	0.41
1:U:828:VAL:O	1:U:828:VAL:HG13	2.19	0.41
2:V:203:LEU:O	2:V:203:LEU:HD23	2.21	0.41
3:W:67:LEU:HD12	3:W:100:ALA:HB1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:217:LEU:HD21	7:a:238:TYR:HA	2.03	0.41
8:b:59:GLU:OE1	8:b:61:LEU:HD23	2.21	0.41
14:C:402:LYS:HG2	20:I:51:ASN:OD1	2.19	0.41
18:G:113:MET:SD	26:O:113:THR:HA	2.60	0.41
21:J:183:THR:OG1	21:J:184:ASP:N	2.52	0.41
25:N:200:ARG:O	31:t:78:LEU:HD12	2.20	0.41
26:O:252:THR:HG21	27:P:168:SER:HB3	2.01	0.41
31:T:211:ARG:O	31:T:215:GLU:HG3	2.21	0.41
25:n:169:ILE:HG21	25:n:193:ALA:O	2.19	0.41
28:q:4:LEU:HD21	28:q:47:VAL:CG1	2.50	0.41
32:f:337:LEU:HD11	32:f:873:LEU:CD1	2.50	0.41
1:U:352:ILE:HG13	1:U:353:LEU:N	2.36	0.41
3:W:44:ILE:O	3:W:48:LEU:HG	2.21	0.41
3:W:106:GLN:O	3:W:110:THR:HG23	2.21	0.41
3:W:276:LEU:HD21	3:W:341:PHE:HZ	1.84	0.41
5:Y:202:LEU:HD11	5:Y:231:LEU:HD11	2.02	0.41
7:a:80:ILE:O	7:a:84:VAL:HG23	2.20	0.41
7:a:179:PHE:HD2	7:a:180:LEU:HD22	1.86	0.41
9:c:237:HIS:CG	9:c:298:GLN:OE1	2.74	0.41
10:d:334:GLU:O	10:d:338:GLN:HG3	2.20	0.41
12:A:101:ILE:O	12:A:101:ILE:CG2	2.66	0.41
21:J:99:GLU:O	21:J:100:ASP:OD1	2.39	0.41
21:J:155:ALA:N	22:K:63:SER:OG	2.49	0.41
29:R:195:TYR:OH	28:q:170:ARG:NE	2.54	0.41
31:T:211:ARG:NH1	31:T:245:GLU:OE1	2.54	0.41
25:n:64:VAL:HG23	25:n:64:VAL:O	2.19	0.41
30:s:75:THR:HG22	30:s:76:ASP:N	2.36	0.41
32:f:560:LEU:HA	32:f:594:LEU:HD21	2.01	0.41
32:f:593:THR:HG22	32:f:652:VAL:HG12	2.02	0.41
32:f:597:VAL:HG11	32:f:656:GLY:HA3	2.02	0.41
1:U:64:ALA:HA	1:U:67:VAL:HG12	2.03	0.41
1:U:364:VAL:CG2	9:c:177:THR:HG21	2.50	0.41
1:U:505:ASP:OD1	1:U:505:ASP:N	2.51	0.41
1:U:554:LEU:CD2	1:U:764:LEU:HD23	2.51	0.41
2:V:101:LEU:HD23	2:V:101:LEU:C	2.46	0.41
2:V:451:ILE:HG22	10:d:278:ALA:HB1	2.03	0.41
6:Z:161:GLU:HG2	6:Z:162:ILE:N	2.36	0.41
7:a:179:PHE:CD2	7:a:180:LEU:HD22	2.56	0.41
7:a:206:LEU:HD11	7:a:261:LEU:HD23	2.03	0.41
9:c:196:LEU:O	9:c:200:TYR:O	2.39	0.41
9:c:285:GLU:O	9:c:288:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:241:TYR:O	10:d:244:VAL:HG12	2.21	0.41
10:d:283:LEU:HD23	10:d:283:LEU:H	1.85	0.41
13:B:70:ASP:OD1	13:B:70:ASP:C	2.63	0.41
14:C:256:SER:O	14:C:257:SER:C	2.64	0.41
18:G:123:GLN:OE1	19:H:85:VAL:HG21	2.21	0.41
19:H:68:ILE:HD12	19:H:74:LEU:HB2	2.02	0.41
20:I:6:ASP:OD1	20:I:6:ASP:C	2.64	0.41
27:P:164:PHE:HB2	27:P:189:ILE:CD1	2.51	0.41
27:p:11:VAL:HG22	27:p:54:ALA:HB2	2.02	0.41
32:f:300:ARG:CZ	32:f:782:HIS:HB3	2.51	0.41
1:U:345:ASN:O	1:U:743:ASN:OD1	2.39	0.41
1:U:496:LEU:HD23	1:U:496:LEU:C	2.46	0.41
1:U:521:LEU:CD1	1:U:761:VAL:HG21	2.51	0.41
2:V:235:LEU:O	2:V:239:THR:HG22	2.21	0.41
2:V:374:LYS:O	2:V:377:GLN:HG3	2.21	0.41
2:V:391:THR:O	2:V:395:ILE:N	2.47	0.41
3:W:161:GLU:OE1	3:W:164:SER:HB2	2.21	0.41
7:a:101:ARG:CZ	7:a:101:ARG:HB3	2.51	0.41
7:a:240:PHE:CE1	7:a:248:PHE:CD1	3.09	0.41
9:c:77:GLN:OE1	9:c:77:GLN:HA	2.19	0.41
10:d:144:ALA:HA	10:d:147:ILE:HG22	2.03	0.41
10:d:208:PHE:CE2	10:d:212:LEU:HD11	2.56	0.41
10:d:232:LEU:CD1	10:d:244:VAL:HG23	2.49	0.41
10:d:254:GLU:O	10:d:257:THR:OG1	2.37	0.41
14:C:280:LEU:CD2	14:C:291:VAL:HG21	2.51	0.41
15:D:392:TYR:HE1	16:E:156:PRO:HB2	1.86	0.41
17:F:84:LYS:O	17:F:84:LYS:CG	2.69	0.41
17:F:169:ASP:OD2	17:F:266:LYS:NZ	2.43	0.41
18:G:60:LEU:HD23	24:M:163:GLY:C	2.45	0.41
19:H:46:LEU:HD11	19:H:137:CYS:SG	2.60	0.41
19:H:74:LEU:CD2	19:H:83:TYR:HE1	2.33	0.41
21:J:185:ASP:O	21:J:189:LYS:HD3	2.21	0.41
23:L:36:VAL:O	23:L:36:VAL:HG23	2.20	0.41
23:L:185:ASN:O	23:L:189:LYS:HG2	2.21	0.41
25:N:38:MET:HE2	25:N:40:VAL:CG2	2.51	0.41
26:O:49:VAL:HG13	26:O:56:VAL:HG12	2.03	0.41
30:S:198:ARG:O	30:S:202:LEU:HG	2.21	0.41
31:T:124:ASP:OD1	31:T:124:ASP:C	2.64	0.41
25:n:82:SER:OG	25:n:85:ASP:HB2	2.21	0.41
29:r:209:GLU:OE1	29:r:209:GLU:HA	2.21	0.41
30:s:127:ARG:O	30:s:128:ARG:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:170:TRP:CD2	32:f:211:ILE:HG23	2.55	0.41
32:f:399:LEU:O	32:f:400:TYR:CD1	2.74	0.41
32:f:472:HIS:ND1	32:f:473:ASN:N	2.69	0.41
32:f:759:LEU:HA	32:f:762:VAL:HG22	2.02	0.41
32:f:816:TYR:CD1	32:f:816:TYR:C	2.99	0.41
1:U:360:VAL:HG21	1:U:369:THR:CG2	2.48	0.41
1:U:903:PHE:HB2	1:U:913:ILE:O	2.21	0.41
2:V:171:VAL:HG12	2:V:175:MET:SD	2.61	0.41
10:d:110:SER:O	10:d:111:LYS:C	2.64	0.41
12:A:304:ASN:ND2	17:F:252:ALA:HB1	2.37	0.41
35:C:501:ATP:HO2'	15:D:326:ARG:HH21	1.62	0.41
17:F:244:THR:O	17:F:244:THR:CG2	2.69	0.41
17:F:437:TYR:OH	22:K:25:GLU:OE2	2.30	0.41
21:J:155:ALA:HB3	22:K:63:SER:OG	2.20	0.41
23:L:47:VAL:HG12	23:L:195:LEU:HD12	1.99	0.41
24:M:70:VAL:HG11	24:M:92:ALA:HB1	2.02	0.41
28:Q:91:CYS:O	28:Q:97:PRO:HA	2.21	0.41
29:r:186:SER:OG	29:r:194:ALA:HB3	2.21	0.41
32:f:366:ASP:N	32:f:370:MET:SD	2.94	0.41
1:U:141:CYS:HB2	14:C:20:LEU:HD12	2.02	0.40
1:U:364:VAL:HG23	9:c:177:THR:HG21	2.03	0.40
2:V:132:LEU:N	2:V:133:PRO:HD2	2.36	0.40
4:X:44:GLN:O	4:X:47:GLU:HG2	2.21	0.40
4:X:234:GLU:OE1	15:D:338:ARG:NH1	2.54	0.40
5:Y:348:ASP:C	5:Y:348:ASP:OD1	2.64	0.40
7:a:96:PHE:HA	7:a:99:LYS:HG2	2.03	0.40
7:a:232:TRP:CH2	7:a:255:TRP:HB3	2.56	0.40
12:A:355:PHE:CE1	12:A:385:ILE:HG12	2.56	0.40
15:D:131:ALA:HB2	15:D:143:LEU:HD21	2.02	0.40
15:D:384:MET:HA	15:D:384:MET:HE2	2.03	0.40
17:F:366:MET:SD	17:F:384:LEU:HB3	2.62	0.40
18:G:73:THR:HG23	18:G:75:ASN:H	1.87	0.40
26:O:80:ILE:HD11	26:O:86:CYS:SG	2.61	0.40
26:O:262:LEU:HD13	27:P:48:ARG:NH1	2.36	0.40
30:S:64:HIS:HE1	31:T:177:TYR:HD2	1.69	0.40
30:S:89:CYS:SG	30:S:134:VAL:HG23	2.61	0.40
31:t:256:ILE:HA	31:t:259:MET:HB3	2.02	0.40
1:U:443:LEU:HD11	1:U:464:GLN:HE21	1.84	0.40
2:V:175:MET:HE1	2:V:187:ILE:HD13	2.03	0.40
3:W:134:GLY:O	3:W:135:LYS:HG3	2.21	0.40
3:W:198:ASP:OD2	3:W:201:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:16:LEU:HD12	4:X:56:LEU:HG	2.03	0.40
4:X:76:PHE:CG	4:X:77:LEU:N	2.89	0.40
5:Y:338:ILE:HD11	5:Y:345:CYS:SG	2.61	0.40
10:d:123:LEU:HA	10:d:126:LEU:HB2	2.03	0.40
10:d:148:LEU:HD21	10:d:170:GLN:HB3	2.03	0.40
10:d:315:TYR:O	10:d:316:TYR:HB2	2.21	0.40
13:B:116:ILE:O	13:B:120:HIS:O	2.39	0.40
13:B:229:GLY:O	13:B:391:SER:HB3	2.21	0.40
13:B:361:LYS:HD3	13:B:390:LEU:HB2	2.03	0.40
16:E:179:GLY:O	16:E:180:LYS:C	2.64	0.40
19:H:34:PRO:HD2	19:H:49:GLU:CD	2.46	0.40
20:I:4:ARG:NE	20:I:4:ARG:O	2.54	0.40
20:I:72:MET:SD	20:I:107:CYS:HA	2.62	0.40
20:I:86:LEU:HD22	20:I:114:LEU:HD11	2.02	0.40
21:J:166:LYS:HG3	21:J:167:SER:N	2.37	0.40
25:N:150:MET:HE3	25:N:150:MET:HB3	1.97	0.40
27:P:22:ILE:O	27:P:22:ILE:HG23	2.21	0.40
27:P:28:PHE:O	27:P:29:GLY:C	2.64	0.40
31:T:55:SER:HA	31:T:184:THR:O	2.22	0.40
27:p:58:THR:HG23	27:p:59:ASP:N	2.36	0.40
1:U:32:ASN:O	1:U:32:ASN:OD1	2.40	0.40
1:U:155:LEU:HD22	1:U:188:MET:CE	2.49	0.40
2:V:131:LEU:HD23	2:V:171:VAL:HG11	2.03	0.40
2:V:160:LEU:HD12	2:V:160:LEU:N	2.37	0.40
2:V:418:SER:HA	2:V:457:TYR:HA	2.04	0.40
2:V:438:VAL:O	2:V:442:ILE:HG12	2.22	0.40
2:V:454:GLU:OE2	10:d:281:LYS:O	2.40	0.40
7:a:18:GLN:CD	7:a:22:TRP:NE1	2.79	0.40
12:A:80:LEU:O	12:A:81:ALA:HB3	2.21	0.40
12:A:111:TYR:CE2	12:A:125:LEU:HD21	2.57	0.40
13:B:174:MET:HB2	13:B:249:ARG:O	2.21	0.40
15:D:180:ALA:CB	15:D:202:VAL:HG11	2.51	0.40
23:L:66:VAL:O	23:L:67:ASP:C	2.64	0.40
23:L:103:LEU:HD23	23:L:108:LEU:HB2	2.03	0.40
23:L:206:THR:HG22	23:L:207:THR:N	2.37	0.40
25:N:35:THR:OG1	25:N:67:LYS:NZ	2.45	0.40
28:Q:170:ARG:NH1	28:q:27:GLN:O	2.55	0.40
29:R:74:ALA:CB	29:R:219:ILE:HD12	2.46	0.40
30:s:178:ASP:OD1	30:s:178:ASP:C	2.64	0.40
31:t:84:ILE:HG13	31:t:84:ILE:O	2.21	0.40
32:f:544:GLU:OE1	32:f:544:GLU:O	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:254:GLU:OE2	1:U:751:ARG:NH2	2.54	0.40
1:U:501:LEU:O	1:U:503:GLN:N	2.50	0.40
1:U:825:LYS:HB2	13:B:85:MET:CE	2.51	0.40
2:V:214:HIS:HA	2:V:217:VAL:HG22	2.03	0.40
2:V:283:ASN:ND2	11:e:17:ASP:HB3	2.35	0.40
2:V:337:LEU:HB3	2:V:398:LEU:HD11	2.03	0.40
2:V:433:ASP:O	2:V:437:ILE:HG12	2.21	0.40
8:b:176:GLY:N	8:b:177:PRO:CD	2.84	0.40
9:c:249:LEU:HD23	9:c:249:LEU:C	2.46	0.40
10:d:153:GLN:HE22	10:d:191:LEU:CD2	2.30	0.40
14:C:38:LYS:HD2	15:D:58:GLU:OE1	2.21	0.40
16:E:216:ARG:HA	16:E:219:PHE:CE2	2.56	0.40
17:F:252:ALA:O	17:F:254:PRO:HD2	2.21	0.40
19:H:203:MET:SD	19:H:208:ILE:HD12	2.62	0.40
21:J:4:ASP:OD2	21:J:21:TYR:CE2	2.74	0.40
26:O:210:LEU:HD11	30:s:58:SER:CB	2.51	0.40
28:Q:23:SER:CB	28:Q:28:MET:HE2	2.51	0.40
27:p:136:PHE:CG	27:p:150:CYS:SG	3.09	0.40
28:q:13:VAL:O	28:q:15:VAL:HG13	2.20	0.40
30:s:136:ASN:HB3	30:s:152:PHE:CD2	2.56	0.40
31:t:94:THR:HG21	31:t:133:ILE:CD1	2.51	0.40
32:f:577:LEU:HD12	32:f:577:LEU:C	2.46	0.40
1:U:9:ILE:HD12	1:U:9:ILE:H	1.87	0.40
2:V:171:VAL:O	2:V:175:MET:SD	2.80	0.40
3:W:153:LYS:HB3	3:W:162:ALA:HB2	2.04	0.40
3:W:316:ARG:NH2	3:W:383:ASP:OD1	2.44	0.40
4:X:217:ILE:O	4:X:221:GLU:HG3	2.22	0.40
4:X:318:ILE:HD12	4:X:318:ILE:H	1.86	0.40
7:a:7:PHE:HZ	7:a:59:LEU:HD12	1.86	0.40
7:a:254:ALA:O	7:a:256:GLY:N	2.54	0.40
10:d:308:TRP:O	10:d:309:VAL:C	2.64	0.40
11:e:48:VAL:HG13	11:e:48:VAL:O	2.22	0.40
12:A:412:ALA:O	12:A:416:VAL:HG23	2.22	0.40
13:B:125:THR:O	13:B:125:THR:CG2	2.68	0.40
16:E:152:PRO:HD3	16:E:274:LYS:CE	2.51	0.40
16:E:219:PHE:CD1	16:E:219:PHE:C	2.99	0.40
16:E:261:LEU:O	16:E:261:LEU:HD23	2.21	0.40
17:F:233:LYS:HG2	35:F:501:ATP:O1B	2.21	0.40
17:F:250:LYS:O	17:F:250:LYS:HG3	2.22	0.40
18:G:65:THR:HG21	24:M:160:GLY:HA3	2.03	0.40
19:H:139:TRP:CD1	19:H:139:TRP:O	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:I:45:LEU:HD11	20:I:137:ILE:CG2	2.51	0.40
21:J:73:PHE:CE2	21:J:80:ALA:HB2	2.55	0.40
22:K:68:VAL:CG2	22:K:89:ILE:HD12	2.52	0.40
22:K:155:HIS:O	22:K:162:PHE:HA	2.22	0.40
26:O:55:ILE:HG22	26:O:56:VAL:N	2.37	0.40
26:O:72:LYS:HD3	30:s:212:GLU:OE2	2.22	0.40
28:Q:27:GLN:O	28:Q:27:GLN:CG	2.69	0.40
29:R:133:ILE:O	29:R:133:ILE:HG23	2.21	0.40
30:S:96:ILE:HD11	30:S:120:LEU:CD1	2.51	0.40
26:o:191:GLU:OE2	26:o:195:LYS:HD2	2.22	0.40
29:r:97:ASN:O	29:r:98:PRO:C	2.64	0.40
32:f:402:ASN:ND2	32:f:410:ALA:HB2	2.35	0.40
32:f:456:ARG:NH1	32:f:492:SER:HB3	2.37	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	U	848/953 (89%)	790 (93%)	58 (7%)	0	100	100
2	V	417/534 (78%)	386 (93%)	31 (7%)	0	100	100
3	W	430/456 (94%)	393 (91%)	36 (8%)	1 (0%)	44	74
4	X	419/422 (99%)	395 (94%)	24 (6%)	0	100	100
5	Y	377/389 (97%)	365 (97%)	12 (3%)	0	100	100
6	Z	285/324 (88%)	276 (97%)	9 (3%)	0	100	100
7	a	373/376 (99%)	337 (90%)	36 (10%)	0	100	100
8	b	189/377 (50%)	174 (92%)	15 (8%)	0	100	100
9	c	273/310 (88%)	250 (92%)	23 (8%)	0	100	100
10	d	252/350 (72%)	220 (87%)	31 (12%)	1 (0%)	30	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	e	32/70 (46%)	31 (97%)	1 (3%)	0	100	100
12	A	401/433 (93%)	348 (87%)	51 (13%)	2 (0%)	25	58
13	B	384/440 (87%)	350 (91%)	34 (9%)	0	100	100
14	C	387/406 (95%)	359 (93%)	28 (7%)	0	100	100
15	D	369/418 (88%)	336 (91%)	32 (9%)	1 (0%)	37	68
16	E	297/389 (76%)	245 (82%)	52 (18%)	0	100	100
17	F	361/439 (82%)	310 (86%)	51 (14%)	0	100	100
18	G	239/246 (97%)	222 (93%)	17 (7%)	0	100	100
19	H	231/234 (99%)	222 (96%)	9 (4%)	0	100	100
20	I	256/261 (98%)	247 (96%)	9 (4%)	0	100	100
21	J	237/248 (96%)	226 (95%)	11 (5%)	0	100	100
22	K	231/241 (96%)	213 (92%)	18 (8%)	0	100	100
23	L	235/263 (89%)	215 (92%)	20 (8%)	0	100	100
24	M	243/255 (95%)	230 (95%)	13 (5%)	0	100	100
25	N	196/239 (82%)	178 (91%)	18 (9%)	0	100	100
25	n	171/239 (72%)	163 (95%)	8 (5%)	0	100	100
26	O	219/277 (79%)	208 (95%)	11 (5%)	0	100	100
26	o	166/277 (60%)	161 (97%)	5 (3%)	0	100	100
27	P	202/205 (98%)	183 (91%)	19 (9%)	0	100	100
27	p	152/205 (74%)	134 (88%)	18 (12%)	0	100	100
28	Q	195/201 (97%)	187 (96%)	8 (4%)	0	100	100
28	q	163/201 (81%)	150 (92%)	13 (8%)	0	100	100
29	R	197/263 (75%)	181 (92%)	16 (8%)	0	100	100
29	r	181/263 (69%)	163 (90%)	18 (10%)	0	100	100
30	S	210/241 (87%)	199 (95%)	11 (5%)	0	100	100
30	s	202/241 (84%)	188 (93%)	14 (7%)	0	100	100
31	T	211/264 (80%)	200 (95%)	11 (5%)	0	100	100
31	t	202/264 (76%)	181 (90%)	21 (10%)	0	100	100
32	f	822/908 (90%)	755 (92%)	66 (8%)	1 (0%)	48	79
33	y	29/505 (6%)	28 (97%)	1 (3%)	0	100	100
All	All	11284/13627 (83%)	10399 (92%)	879 (8%)	6 (0%)	50	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	W	345	GLU
32	f	393	ASP
15	D	258	ALA
12	A	65	ILE
12	A	399	ALA
10	d	312	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	729/816 (89%)	729 (100%)	0	100	100
2	V	371/460 (81%)	370 (100%)	1 (0%)	91	95
3	W	399/416 (96%)	399 (100%)	0	100	100
4	X	361/362 (100%)	361 (100%)	0	100	100
5	Y	335/344 (97%)	335 (100%)	0	100	100
6	Z	258/295 (88%)	258 (100%)	0	100	100
7	a	335/336 (100%)	335 (100%)	0	100	100
8	b	167/312 (54%)	167 (100%)	0	100	100
9	c	244/268 (91%)	244 (100%)	0	100	100
10	d	227/294 (77%)	227 (100%)	0	100	100
11	e	34/63 (54%)	34 (100%)	0	100	100
12	A	348/372 (94%)	346 (99%)	2 (1%)	84	91
13	B	344/385 (89%)	344 (100%)	0	100	100
14	C	340/352 (97%)	340 (100%)	0	100	100
15	D	327/366 (89%)	327 (100%)	0	100	100
16	E	272/341 (80%)	272 (100%)	0	100	100
17	F	314/379 (83%)	314 (100%)	0	100	100
18	G	206/210 (98%)	206 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	H	190/191 (100%)	190 (100%)	0	100	100
20	I	218/221 (99%)	218 (100%)	0	100	100
21	J	203/211 (96%)	203 (100%)	0	100	100
22	K	198/203 (98%)	198 (100%)	0	100	100
23	L	203/224 (91%)	203 (100%)	0	100	100
24	M	202/212 (95%)	202 (100%)	0	100	100
25	N	154/181 (85%)	154 (100%)	0	100	100
25	n	138/181 (76%)	138 (100%)	0	100	100
26	O	182/228 (80%)	182 (100%)	0	100	100
26	o	139/228 (61%)	139 (100%)	0	100	100
27	P	173/174 (99%)	173 (100%)	0	100	100
27	p	136/174 (78%)	136 (100%)	0	100	100
28	Q	168/171 (98%)	168 (100%)	0	100	100
28	q	148/171 (86%)	148 (100%)	0	100	100
29	R	155/202 (77%)	155 (100%)	0	100	100
29	r	142/202 (70%)	142 (100%)	0	100	100
30	S	177/199 (89%)	177 (100%)	0	100	100
30	s	172/199 (86%)	172 (100%)	0	100	100
31	T	176/215 (82%)	176 (100%)	0	100	100
31	t	171/215 (80%)	171 (100%)	0	100	100
32	f	699/763 (92%)	698 (100%)	1 (0%)	92	97
33	y	29/403 (7%)	29 (100%)	0	100	100
All	All	9784/11539 (85%)	9780 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	V	319	HIS
12	A	114	ASN
12	A	400	ARG
32	f	199	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	139	GLN
1	U	192	GLN
1	U	345	ASN
1	U	464	GLN
1	U	801	GLN
2	V	424	GLN
3	W	170	GLN
4	X	78	ASN
5	Y	31	HIS
5	Y	178	ASN
5	Y	363	ASN
6	Z	196	HIS
6	Z	225	GLN
8	b	76	HIS
8	b	104	ASN
9	c	92	GLN
9	c	256	ASN
10	d	209	HIS
12	A	44	GLN
12	A	94	GLN
12	A	414	ASN
13	B	131	HIS
13	B	195	GLN
13	B	207	HIS
14	C	241	HIS
15	D	49	GLN
15	D	286	GLN
15	D	294	ASN
15	D	304	ASN
16	E	86	GLN
16	E	190	GLN
19	H	63	HIS
19	H	95	GLN
19	H	166	ASN
19	H	169	ASN
19	H	179	ASN
20	I	102	GLN
22	K	114	GLN
22	K	227	HIS
23	L	60	GLN
23	L	190	HIS
25	N	41	GLN
26	O	78	HIS

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Mol	Chain	Res	Type
28	Q	71	ASN
28	Q	186	ASN
28	Q	189	HIS
30	S	185	ASN
30	S	191	HIS
26	o	196	ASN
27	p	173	ASN
28	q	55	GLN
29	r	88	GLN
29	r	144	ASN
30	s	136	ASN
30	s	191	HIS
32	f	180	GLN
32	f	402	ASN
32	f	738	ASN
32	f	808	ASN
32	f	876	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 5 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	$\#\|Z\|>2$
35	ATP	A	501	36	28,33,33	0.82	0	34,52,52	0.95	1 (2%)
37	ADP	E	401	-	24,29,29	0.89	0	29,45,45	1.27	2 (6%)
37	ADP	D	501	-	24,29,29	0.85	0	29,45,45	1.31	2 (6%)
35	ATP	F	501	-	28,33,33	0.83	1 (3%)	34,52,52	0.92	2 (5%)
35	ATP	C	501	36	28,33,33	0.72	0	34,52,52	0.97	2 (5%)
35	ATP	B	501	36	28,33,33	0.77	0	34,52,52	0.92	3 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ATP	A	501	36	-	6/18/38/38	0/3/3/3
37	ADP	E	401	-	-	2/12/32/32	0/3/3/3
37	ADP	D	501	-	-	2/12/32/32	0/3/3/3
35	ATP	F	501	-	-	8/18/38/38	0/3/3/3
35	ATP	C	501	36	-	5/18/38/38	0/3/3/3
35	ATP	B	501	36	-	7/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	F	501	ATP	PA-O3A	-2.16	1.57	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	D	501	ADP	N3-C2-N1	-4.21	122.95	128.67
37	E	401	ADP	N3-C2-N1	-4.09	123.13	128.67
37	E	401	ADP	C4-C5-N7	-2.52	106.67	109.34
35	C	501	ATP	C5-C6-N6	2.35	123.90	120.31
35	B	501	ATP	C5-C6-N6	2.34	123.87	120.31
35	A	501	ATP	C5-C6-N6	2.30	123.82	120.31
35	F	501	ATP	C5-C6-N6	2.29	123.80	120.31
35	B	501	ATP	O3'-C3'-C2'	-2.26	104.56	111.82
37	D	501	ADP	C4-C5-N7	-2.26	106.95	109.34
35	C	501	ATP	O2'-C2'-C3'	-2.15	104.93	111.82
35	B	501	ATP	O3'-C3'-C4'	-2.08	105.12	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	F	501	ATP	O3'-C3'-C2'	-2.03	105.30	111.82

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	501	ATP	PB-O3B-PG-O3G
35	A	501	ATP	C5'-O5'-PA-O1A
35	B	501	ATP	C5'-O5'-PA-O1A
35	B	501	ATP	C5'-O5'-PA-O2A
35	B	501	ATP	C5'-O5'-PA-O3A
35	B	501	ATP	O4'-C4'-C5'-O5'
35	B	501	ATP	C3'-C4'-C5'-O5'
35	C	501	ATP	PB-O3B-PG-O3G
35	C	501	ATP	C5'-O5'-PA-O2A
35	F	501	ATP	PB-O3B-PG-O2G
35	F	501	ATP	C5'-O5'-PA-O1A
35	F	501	ATP	C5'-O5'-PA-O3A
37	E	401	ADP	PB-O3A-PA-O1A
35	A	501	ATP	PB-O3B-PG-O2G
37	D	501	ADP	C3'-C4'-C5'-O5'
37	D	501	ADP	O4'-C4'-C5'-O5'
35	A	501	ATP	C5'-O5'-PA-O3A
35	C	501	ATP	C5'-O5'-PA-O1A
35	F	501	ATP	C5'-O5'-PA-O2A
35	F	501	ATP	PB-O3B-PG-O1G
35	F	501	ATP	O4'-C4'-C5'-O5'
35	C	501	ATP	PA-O3A-PB-O1B
35	C	501	ATP	PA-O3A-PB-O2B
35	F	501	ATP	PG-O3B-PB-O1B
37	E	401	ADP	PB-O3A-PA-O2A
35	A	501	ATP	O4'-C4'-C5'-O5'
35	B	501	ATP	PA-O3A-PB-O1B
35	B	501	ATP	PA-O3A-PB-O2B
35	F	501	ATP	PG-O3B-PB-O2B
35	A	501	ATP	C3'-C4'-C5'-O5'

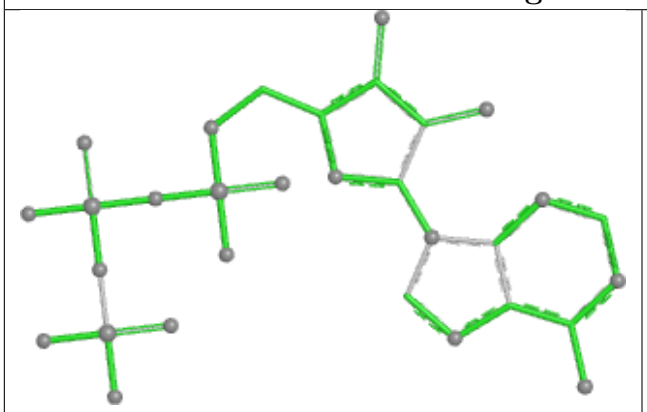
There are no ring outliers.

6 monomers are involved in 20 short contacts:

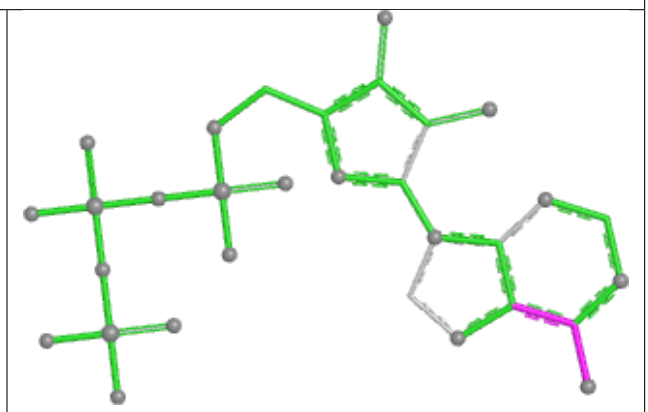
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	501	ATP	3	0
37	E	401	ADP	2	0
37	D	501	ADP	1	0
35	F	501	ATP	6	0
35	C	501	ATP	4	0
35	B	501	ATP	4	0

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 then 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.

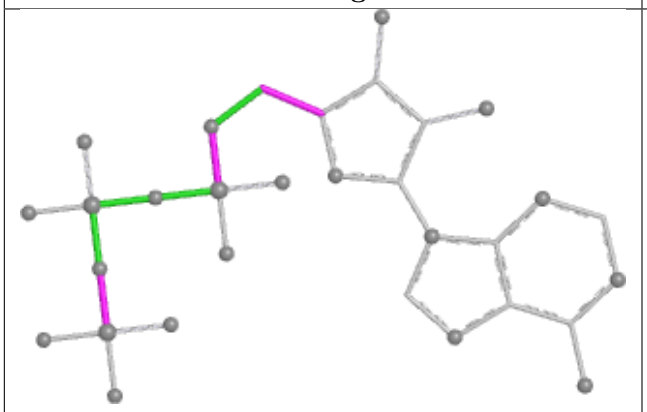
Ligand ATP A 501



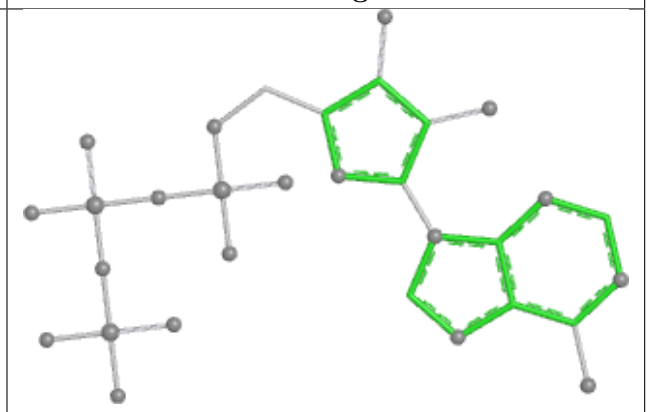
Bond lengths



Bond angles

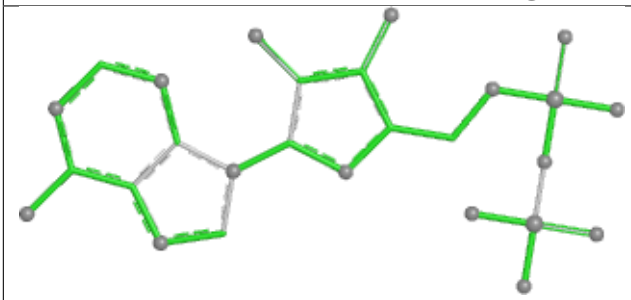


Torsions



Rings

Ligand ADP E 401



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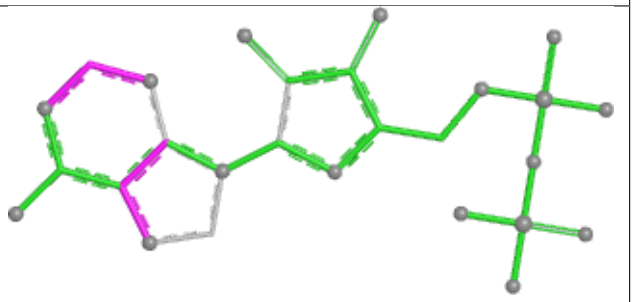
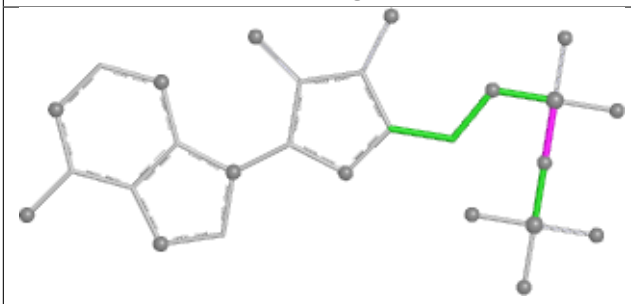


Bond angles



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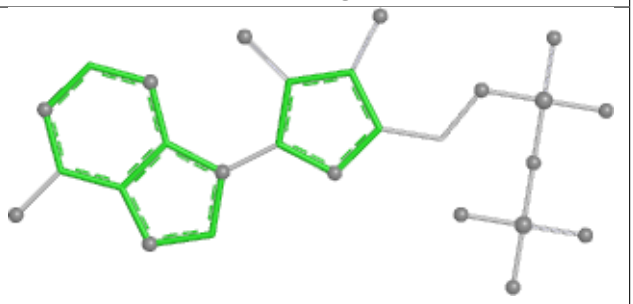
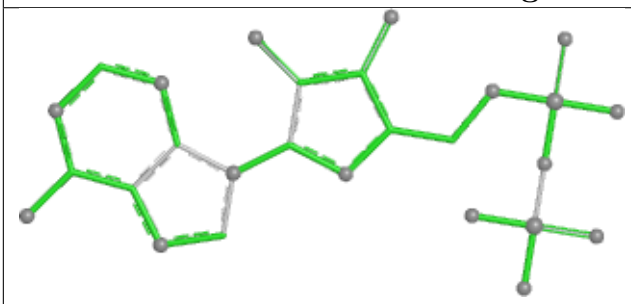
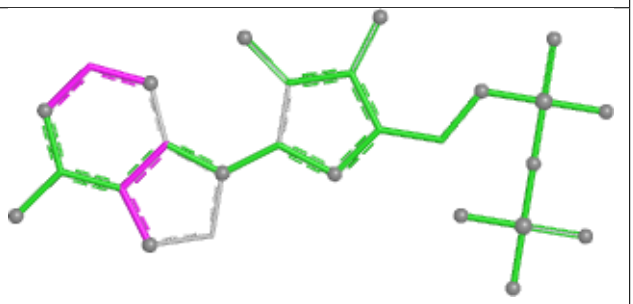


Rings

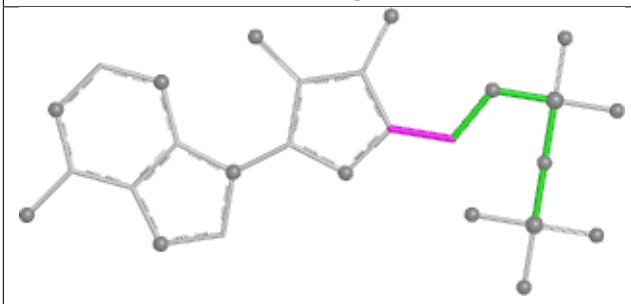
Ligand ADP D 501



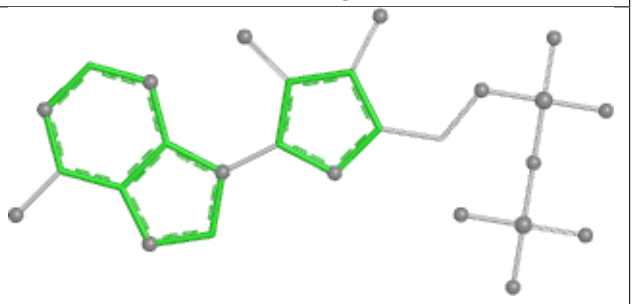
Bond lengths



Bond angles

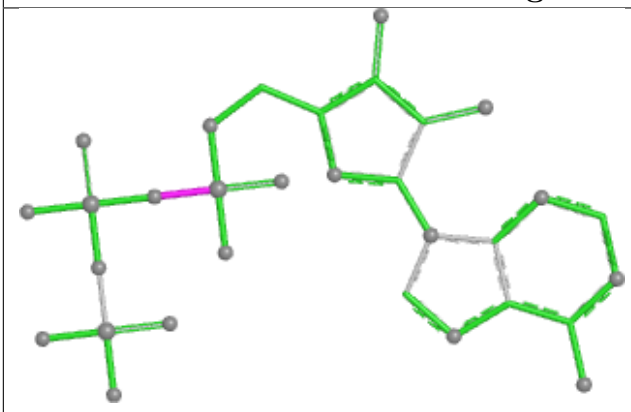


Torsions

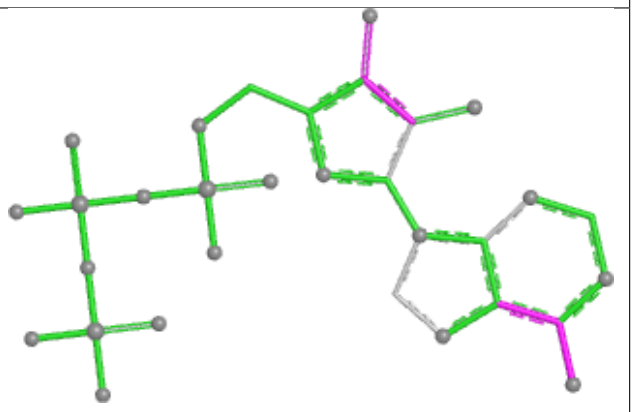


Rings

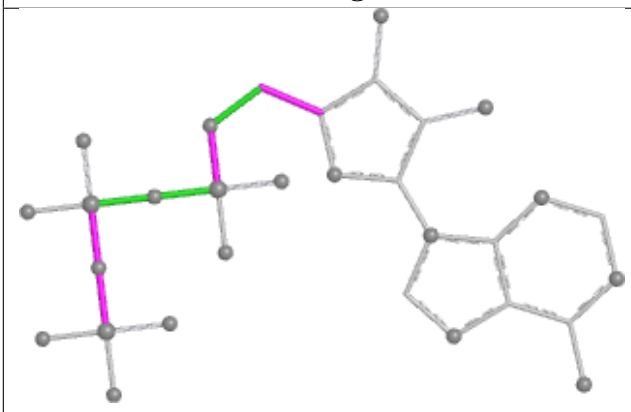
Ligand ATP F 501



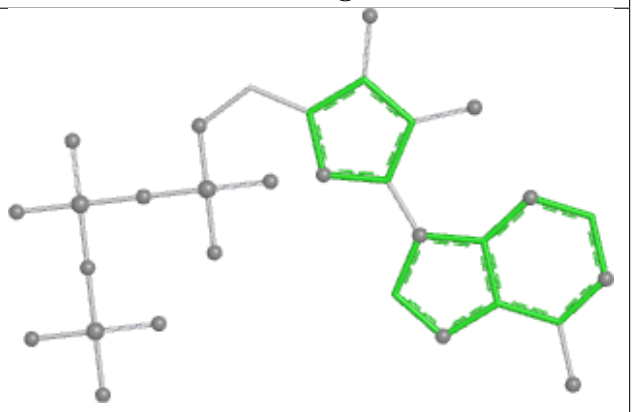
Bond lengths



Bond angles

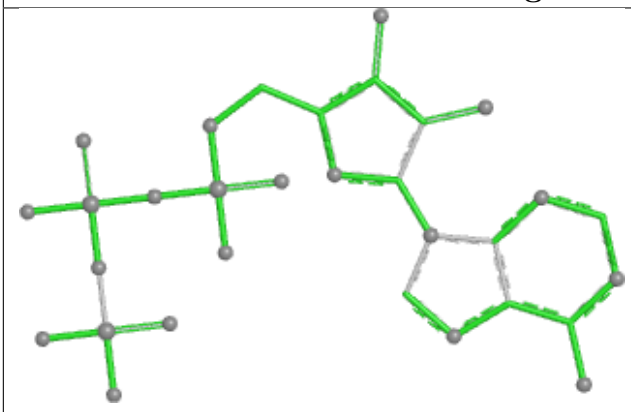


Torsions

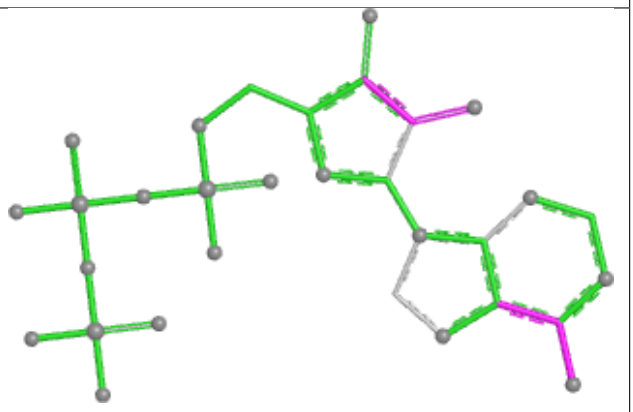


Rings

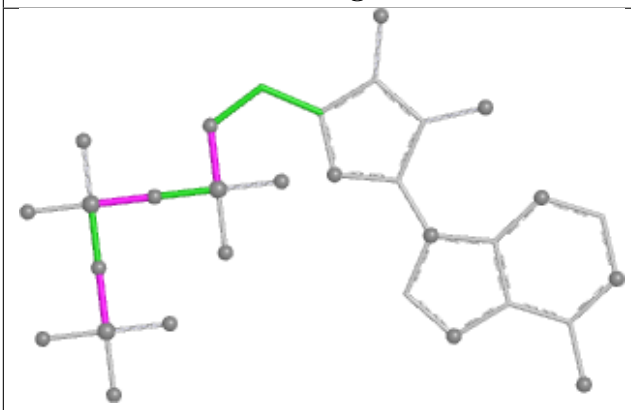
Ligand ATP C 501



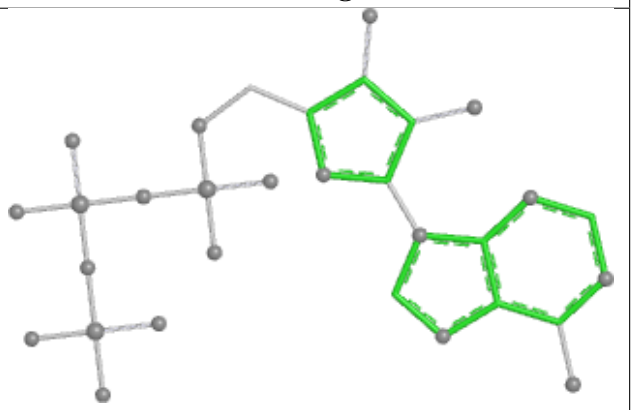
Bond lengths



Bond angles

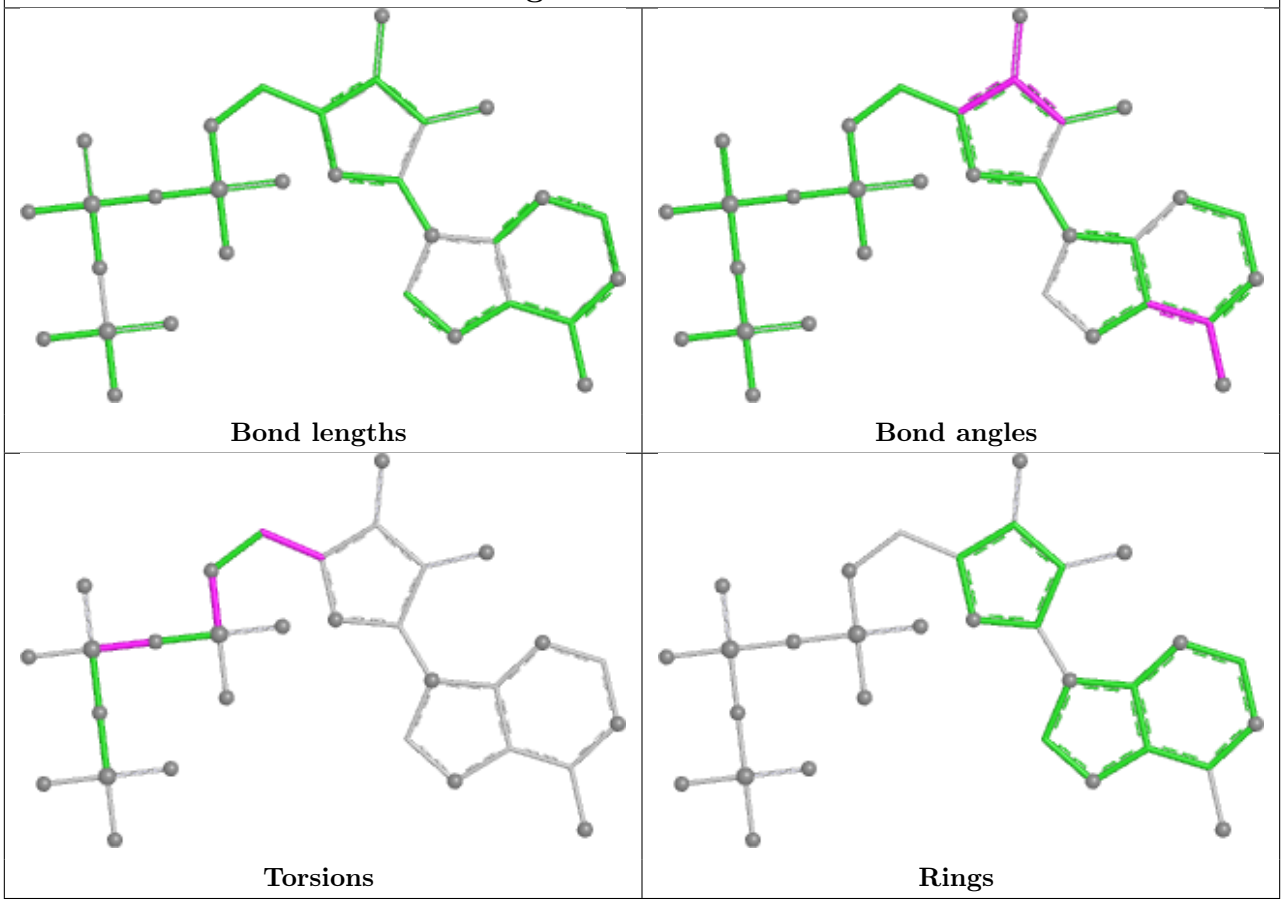


Torsions



Rings

Ligand ATP B 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.

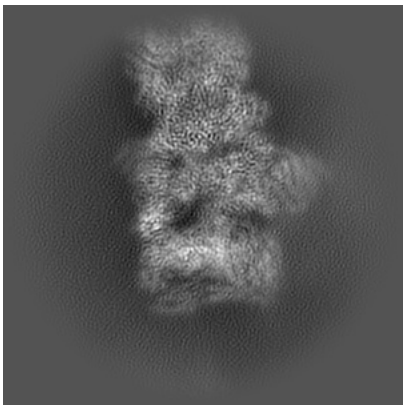
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44927. These allow visual inspection of the internal detail of the map and identification of artifacts.

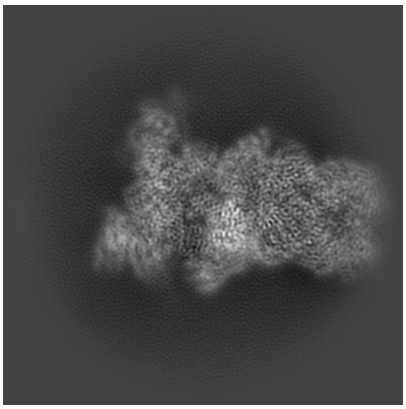
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

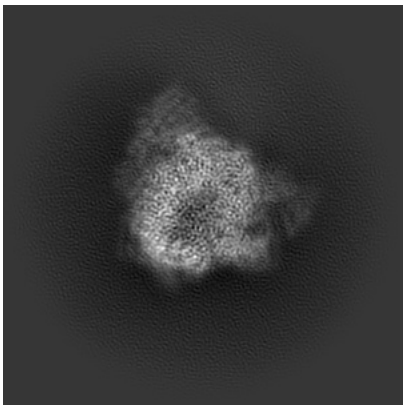
6.1.1 Primary map



X

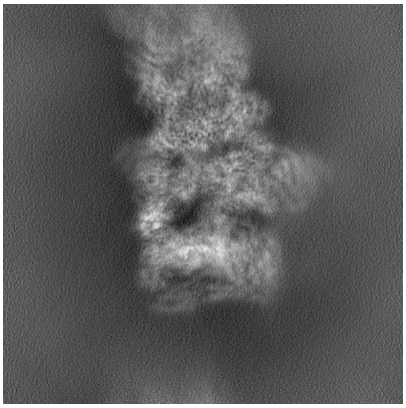


Y

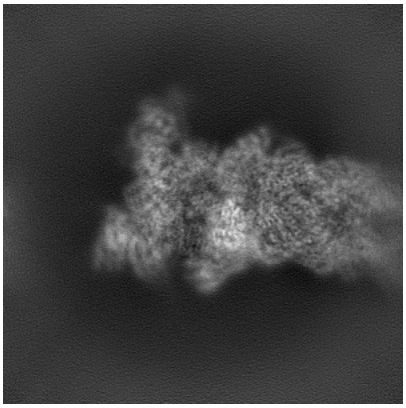


Z

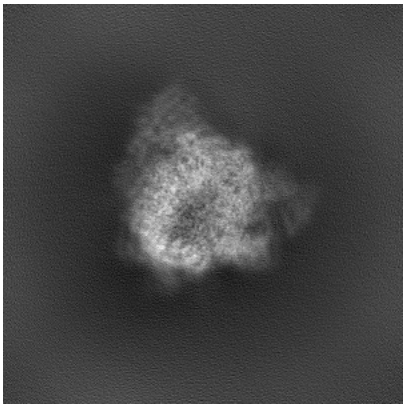
6.1.2 Raw map



X



Y

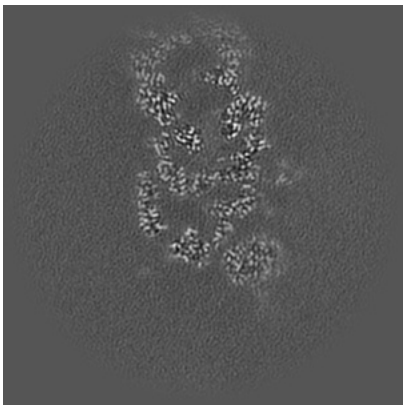


Z

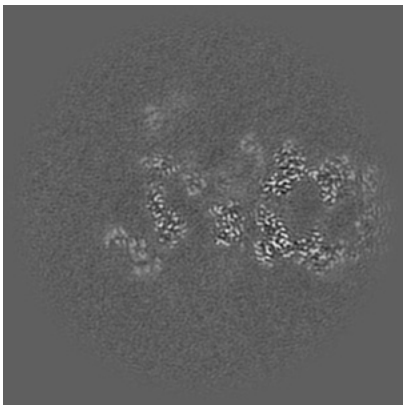
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

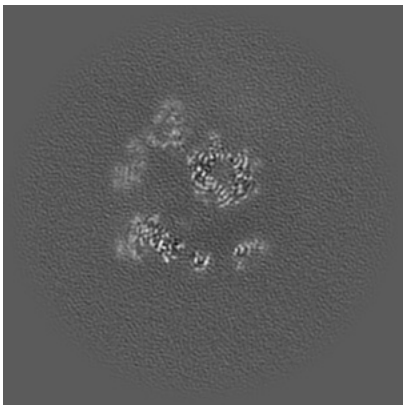
6.2.1 Primary map



X Index: 220

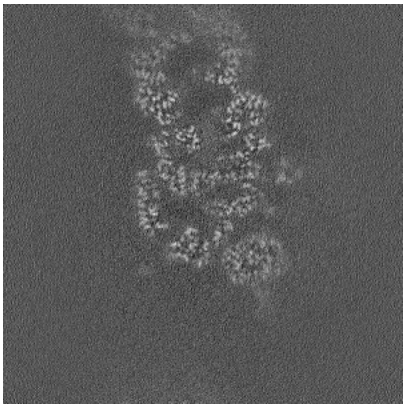


Y Index: 220

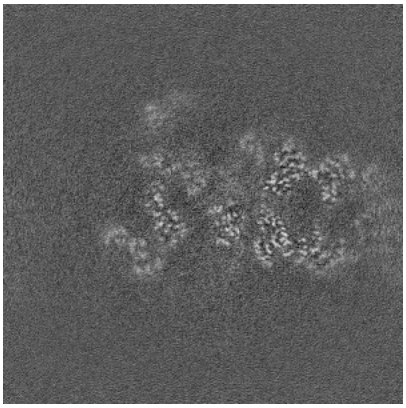


Z Index: 220

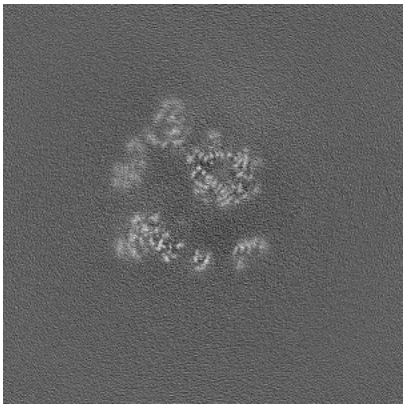
6.2.2 Raw map



X Index: 220



Y Index: 220

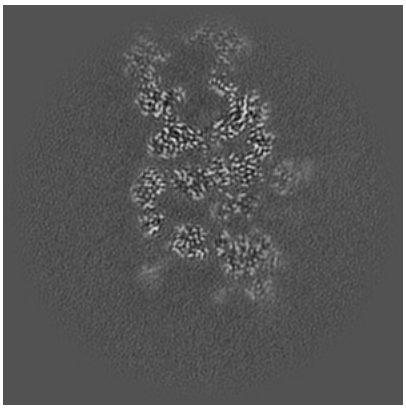


Z Index: 220

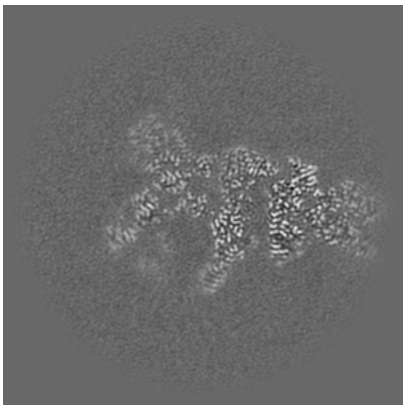
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

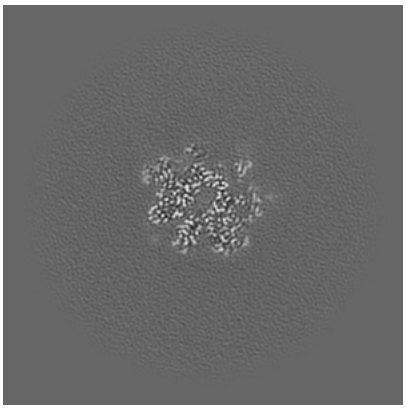
6.3.1 Primary map



X Index: 211

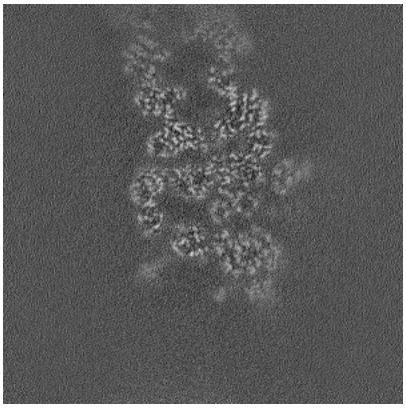


Y Index: 248

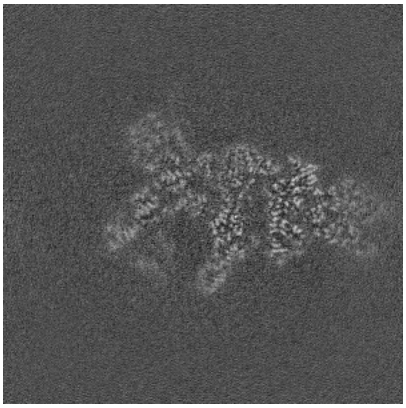


Z Index: 304

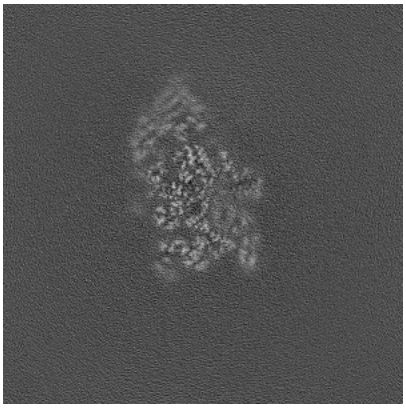
6.3.2 Raw map



X Index: 212



Y Index: 248

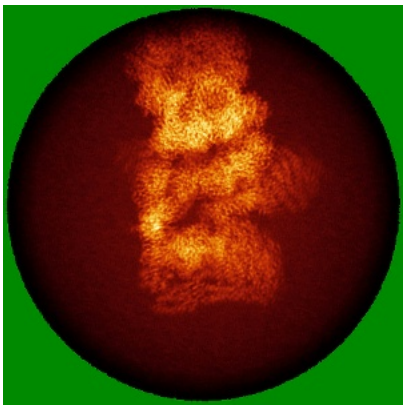


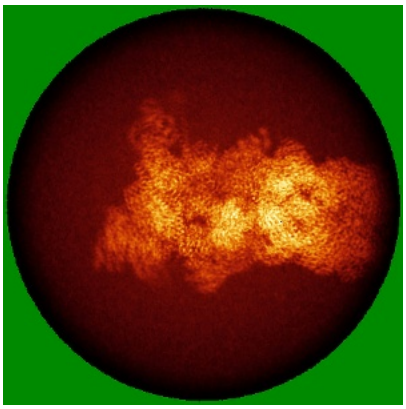
Z Index: 251

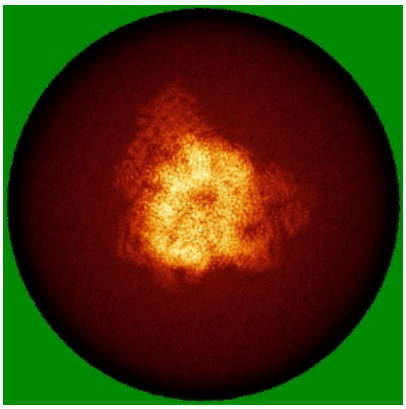
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

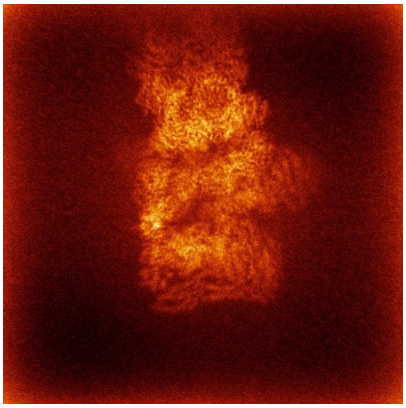
6.4.1 Primary map

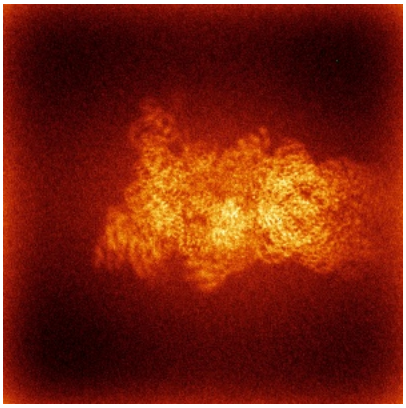

X

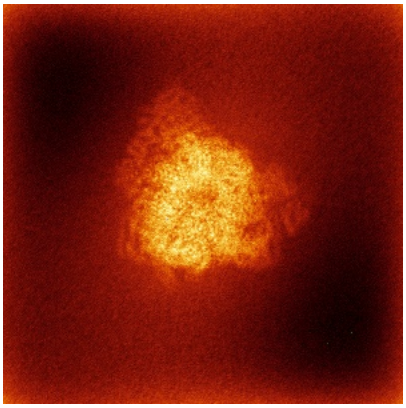

Y


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

X

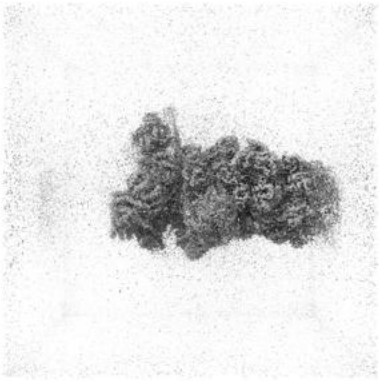
Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. 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

X



Y

Z

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.

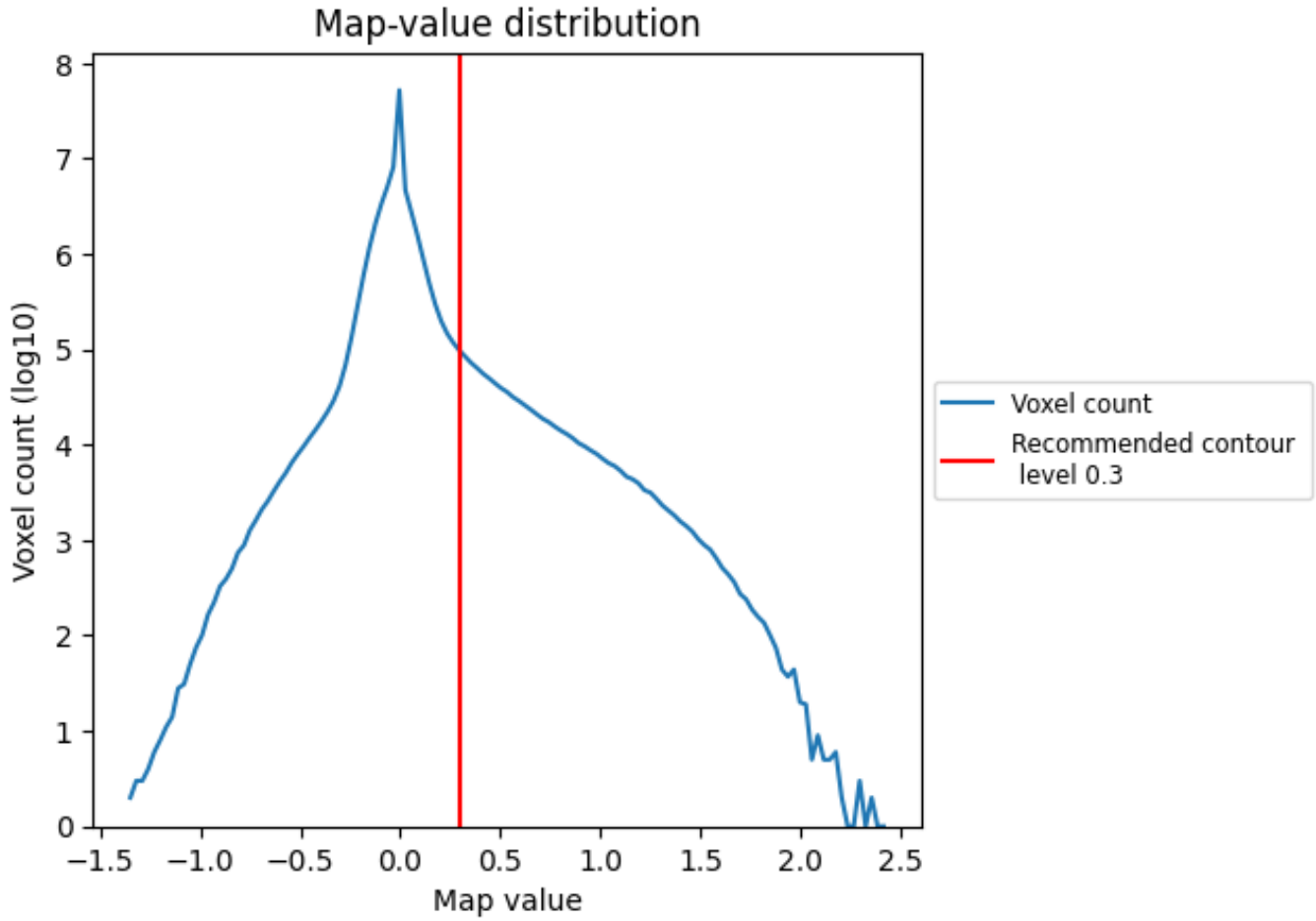
6.6 Mask visualisation (i)

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

7 Map analysis

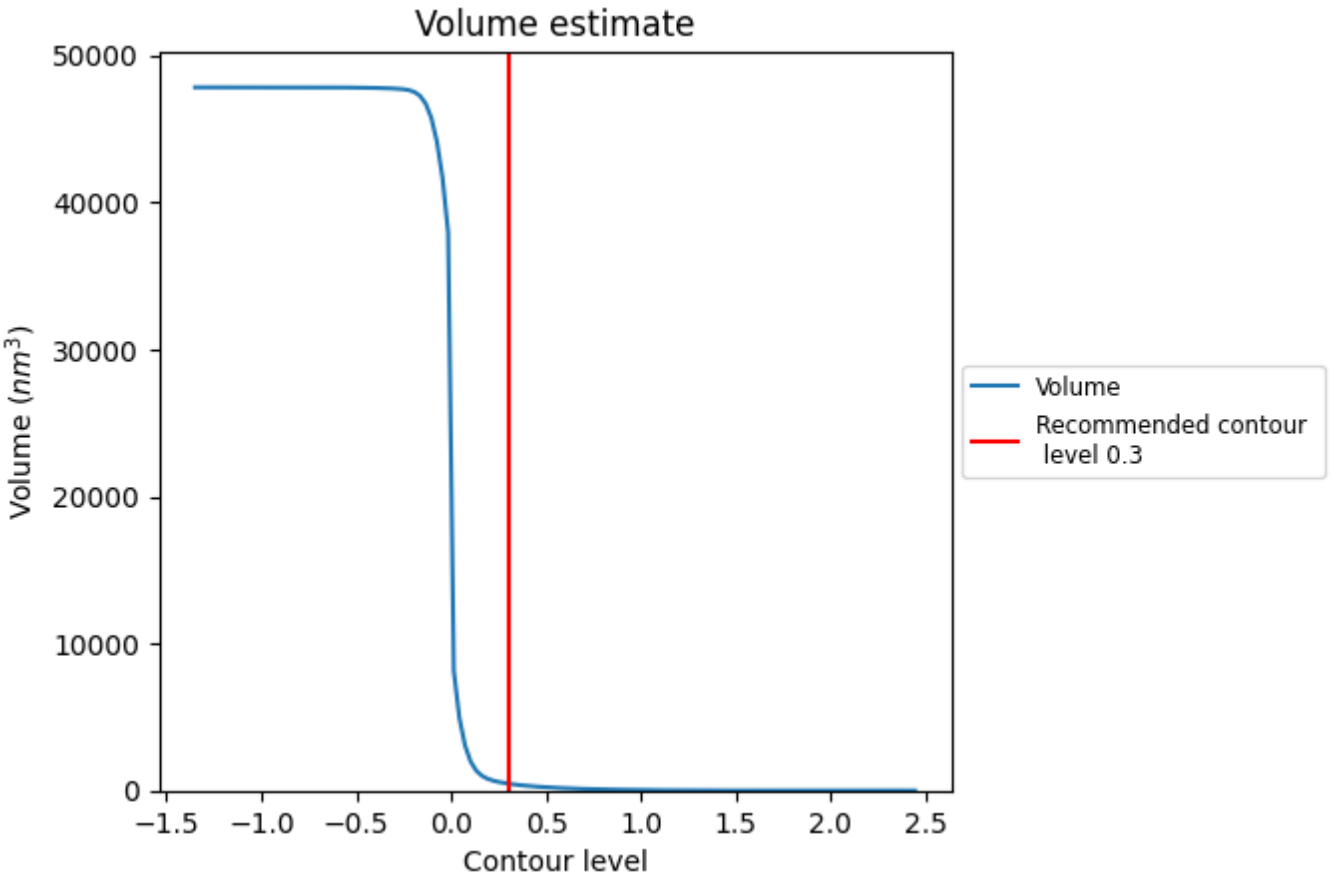
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

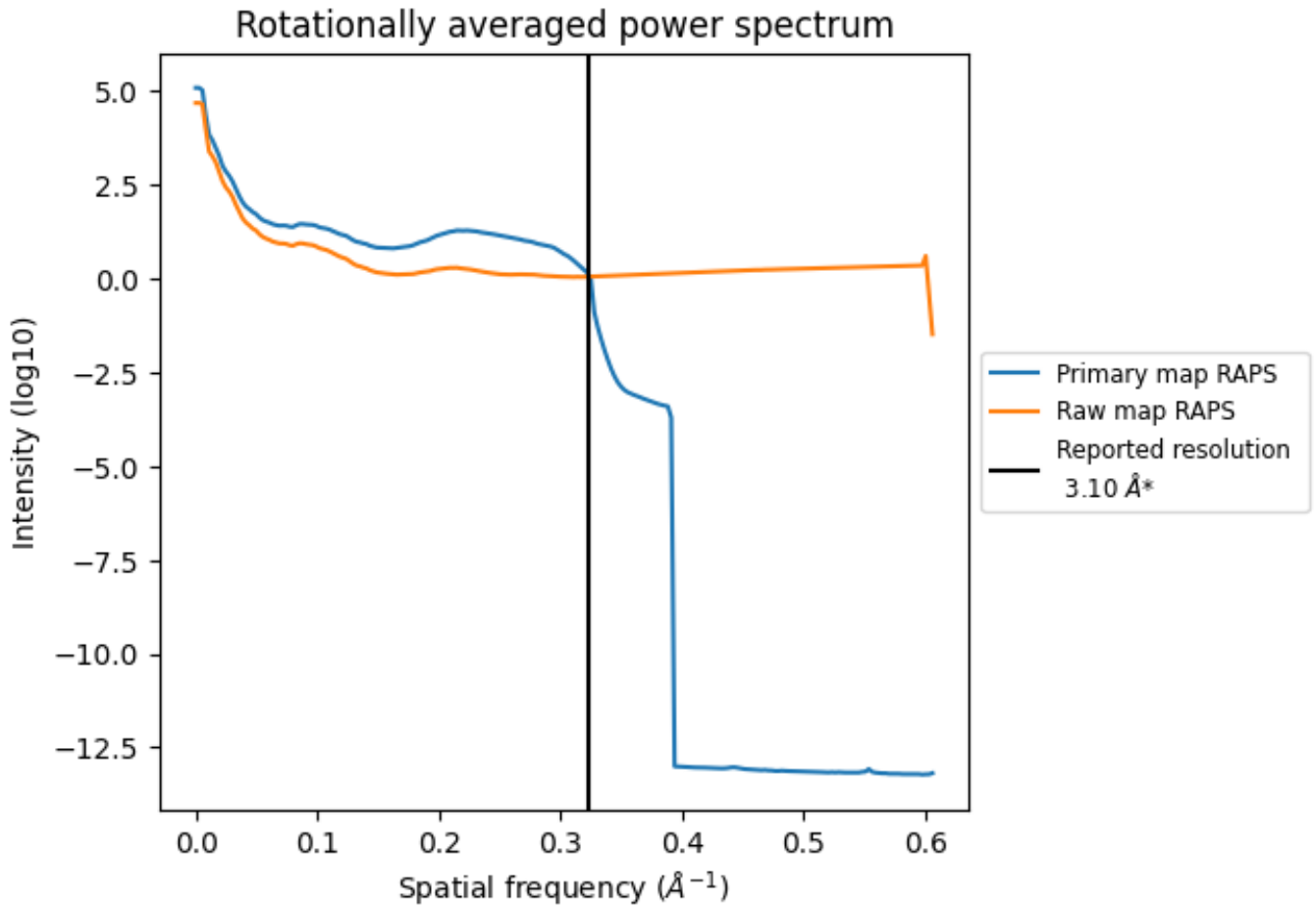
7.2 Volume estimate



The volume at the recommended contour level is 474 nm^3; this corresponds to an approximate mass of 428 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 (i)

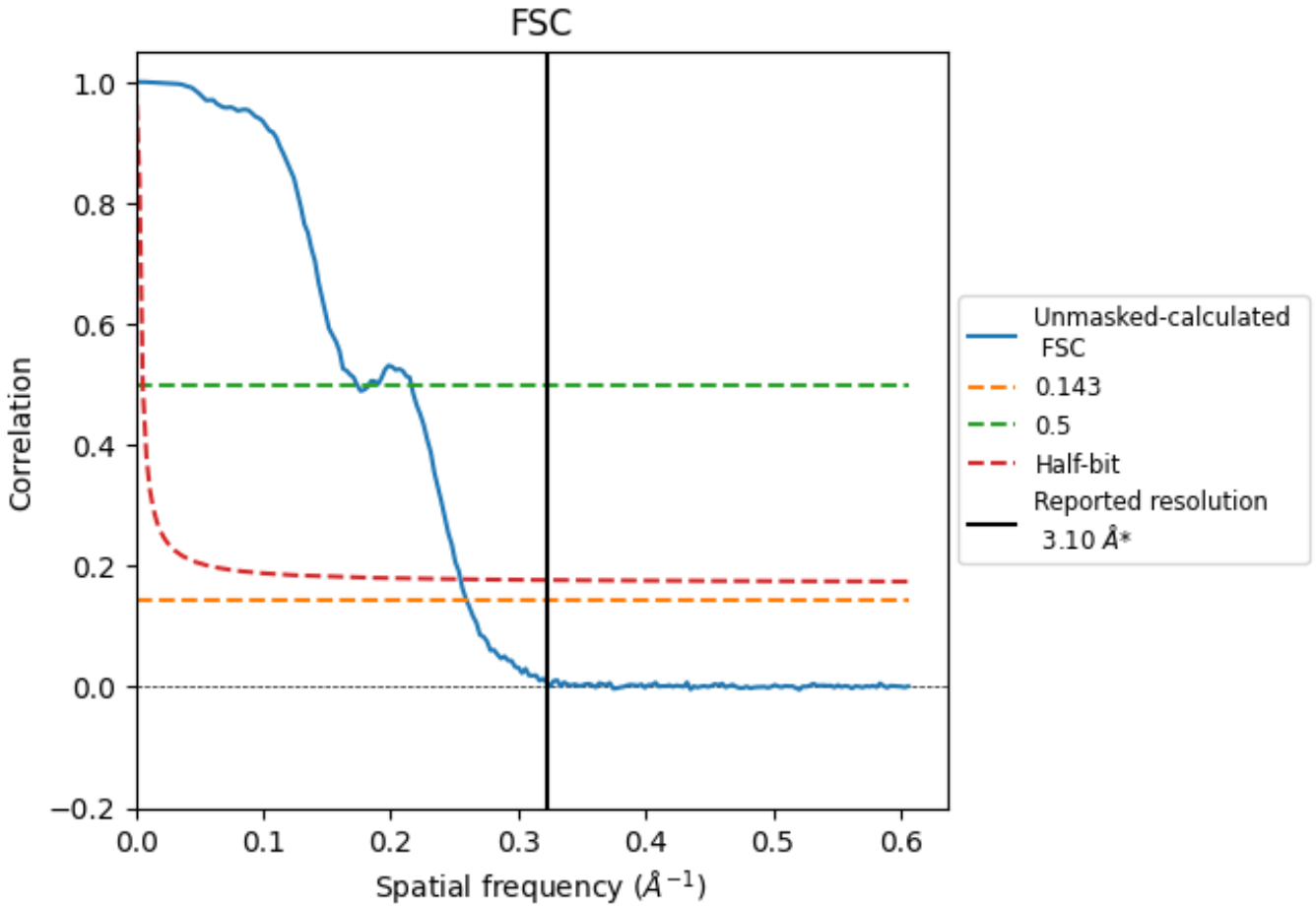


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8.2 Resolution estimates (i)

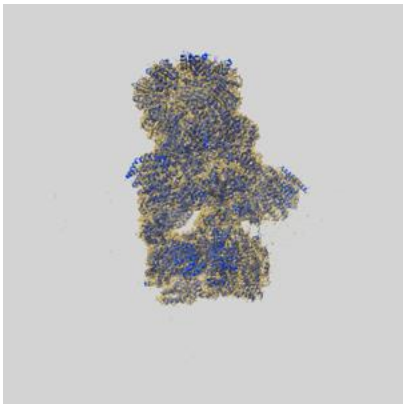
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.86	5.77	3.92

*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 3.86 differs from the reported value 3.1 by more than 10 %

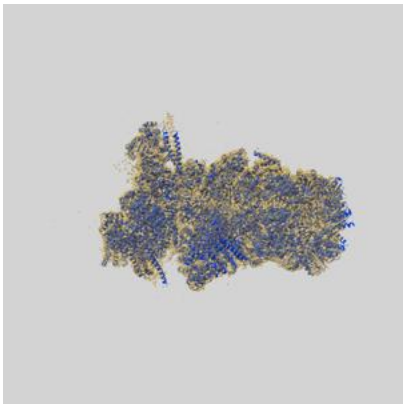
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44927 and PDB model 9BV1. Per-residue inclusion information can be found in section 3 on page 13.

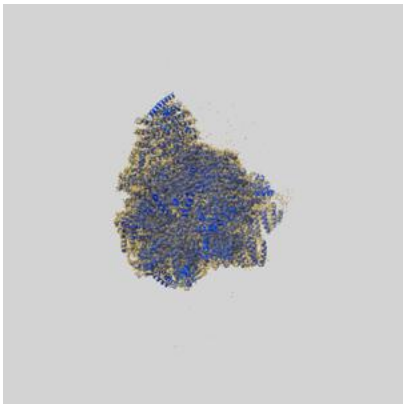
9.1 Map-model overlay



X



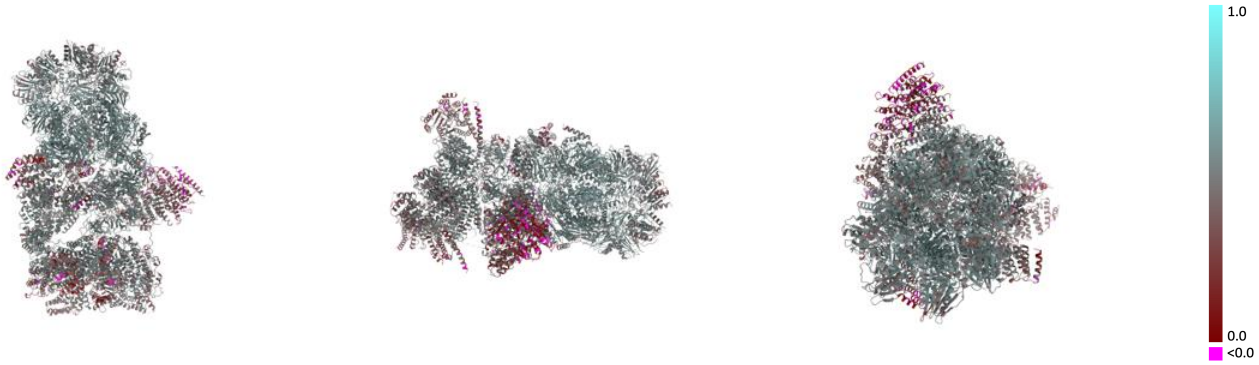
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

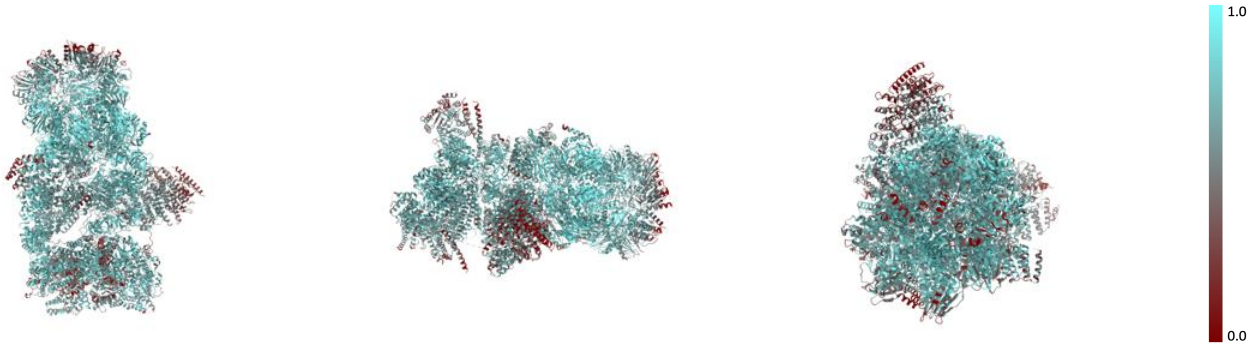
9.2 Q-score mapped to coordinate model



X Y Z

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.

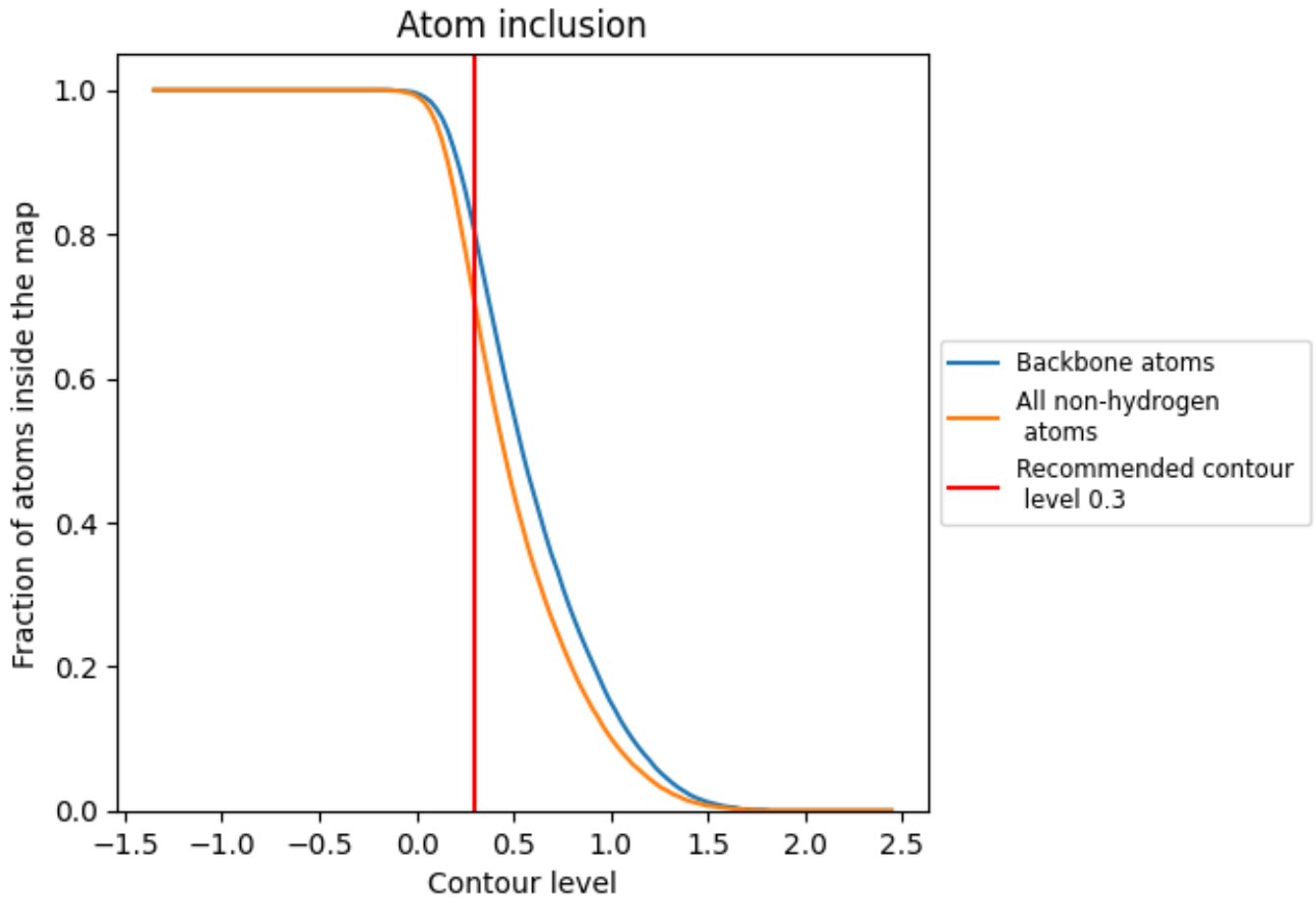
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 70% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7050	0.4710
A	0.7650	0.5060
B	0.7890	0.5220
C	0.8150	0.5360
D	0.7750	0.5150
E	0.5040	0.3490
F	0.7160	0.4900
G	0.8410	0.5490
H	0.8870	0.5770
I	0.8190	0.5470
J	0.8280	0.5350
K	0.8630	0.5530
L	0.8800	0.5570
M	0.8440	0.5460
N	0.8280	0.5470
O	0.8350	0.5510
P	0.8640	0.5600
Q	0.8240	0.5490
R	0.8380	0.5440
S	0.7890	0.5280
T	0.8100	0.5330
U	0.7030	0.4520
V	0.6760	0.4290
W	0.7000	0.4540
X	0.6360	0.4260
Y	0.7900	0.4940
Z	0.7890	0.5230
a	0.6410	0.4040
b	0.4960	0.3660
c	0.7510	0.5020
d	0.6250	0.3740
e	0.7840	0.5130
f	0.4250	0.2290
n	0.5840	0.4980
o	0.4550	0.4700

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
p	0.4310	0.4600
q	0.4840	0.4730
r	0.6180	0.5020
s	0.6480	0.5080
t	0.6450	0.5000
y	0.0390	0.0890