



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 09:38 PM UTC

PDB ID : 9BV2 / pdb_00009bv2
EMDB ID : EMD-44929
Title : M2B Midnolin-Proteasome (translocating)
Authors : Gao, J.; Yip, M.C.J.; Shao, S.
Deposited on : 2024-05-19
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

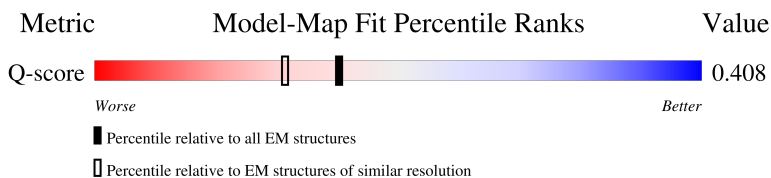
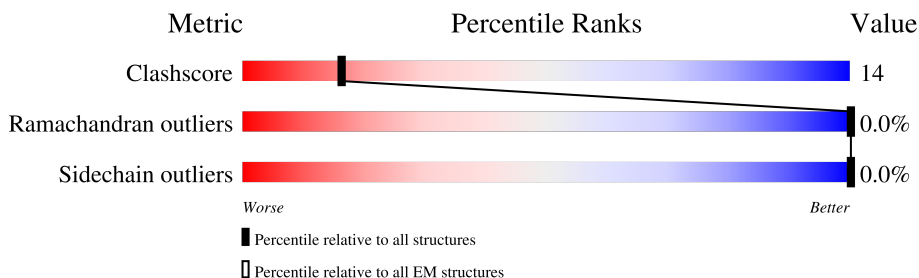
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 Å.

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



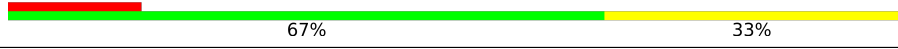
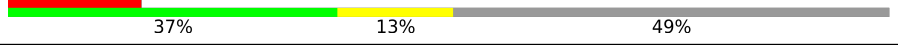
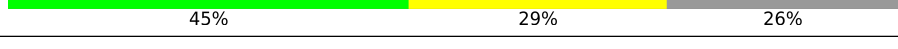
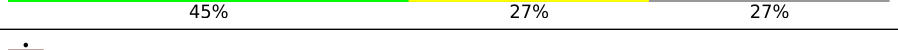
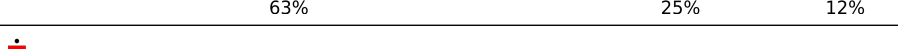
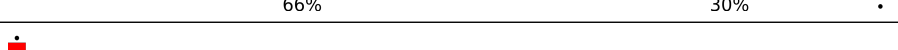
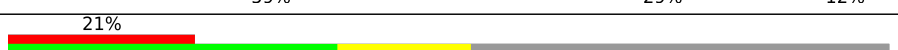
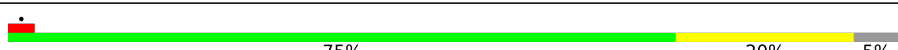
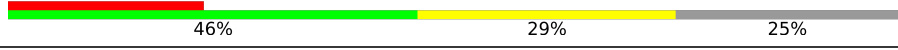
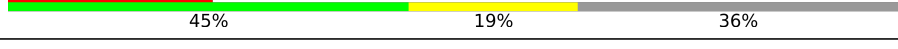
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	U	953	
2	V	534	
3	W	456	
4	X	422	

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Mol	Chain	Length	Quality of chain
5	Y	389	
6	Z	324	
7	a	376	
8	b	377	
9	c	310	
10	d	350	
11	e	70	
12	A	433	
13	B	440	
14	C	406	
15	D	418	
16	E	389	
17	F	439	
18	G	246	
19	H	234	
20	I	261	
21	J	248	
22	K	241	
23	L	263	
24	M	255	
25	N	239	
25	n	239	
26	O	277	
26	o	277	
27	P	205	

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Mol	Chain	Length	Quality of chain
27	p	205	
28	Q	201	
28	q	201	
29	R	263	
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 36 unique types of molecules in this entry. The entry contains 88606 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	852	Total	C	N	O	S	0	0
			6640	4215	1128	1252	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	430	Total	C	N	O	S	0	0
			3510	2224	601	662	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	316	Total	C	N	O	S	0	0
			2518	1598	440	467	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	386	Total	C	N	O	S	0	0
			3037	1916	514	592	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	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E	341	Total	C	N	O	S	0	0
			2706	1699	484	507	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F	231	Total	C	N	O	S	0	0
			1812	1152	311	337	12		

- 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	249	Total	C	N	O	S	0	0
			1963	1242	336	375	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	244	Total	C	N	O	S	0	0
			1916	1212	325	368	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	819	Total	C	N	O	S	0	0
			6351	4019	1073	1215	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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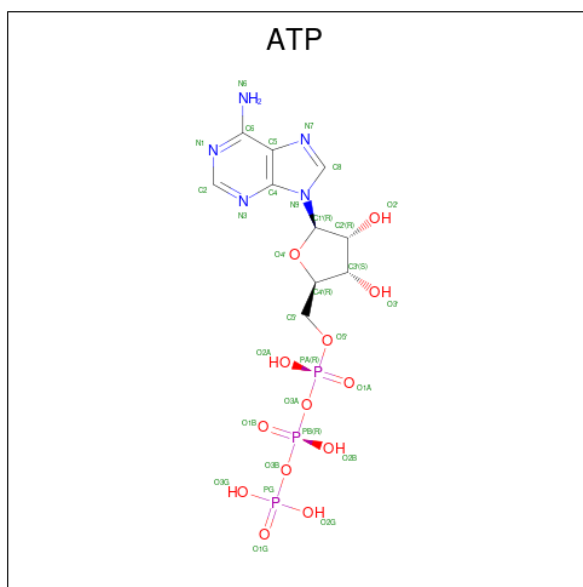
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Chain	Residue	Modelled	Actual	Comment	Reference
y	457	ALA	VAL	conflict	UNP Q504T8

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

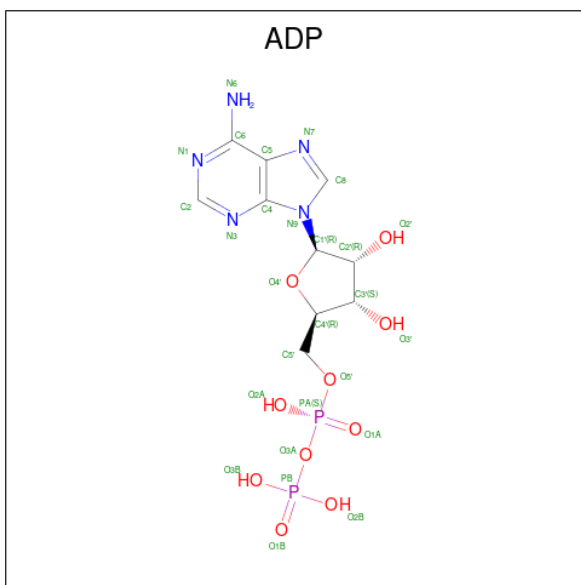
Mol	Chain	Residues	Atoms		AltConf
34	c	1	Total	Zn	0
			1	1	

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

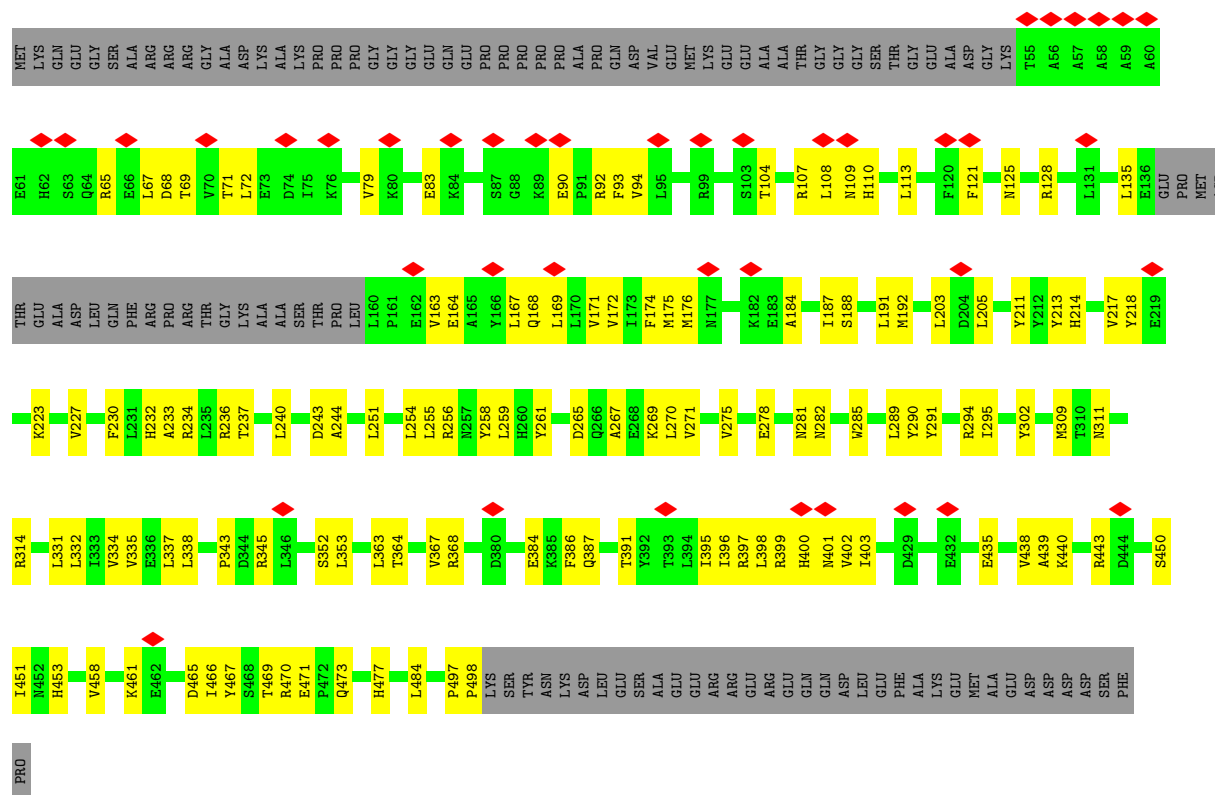


Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

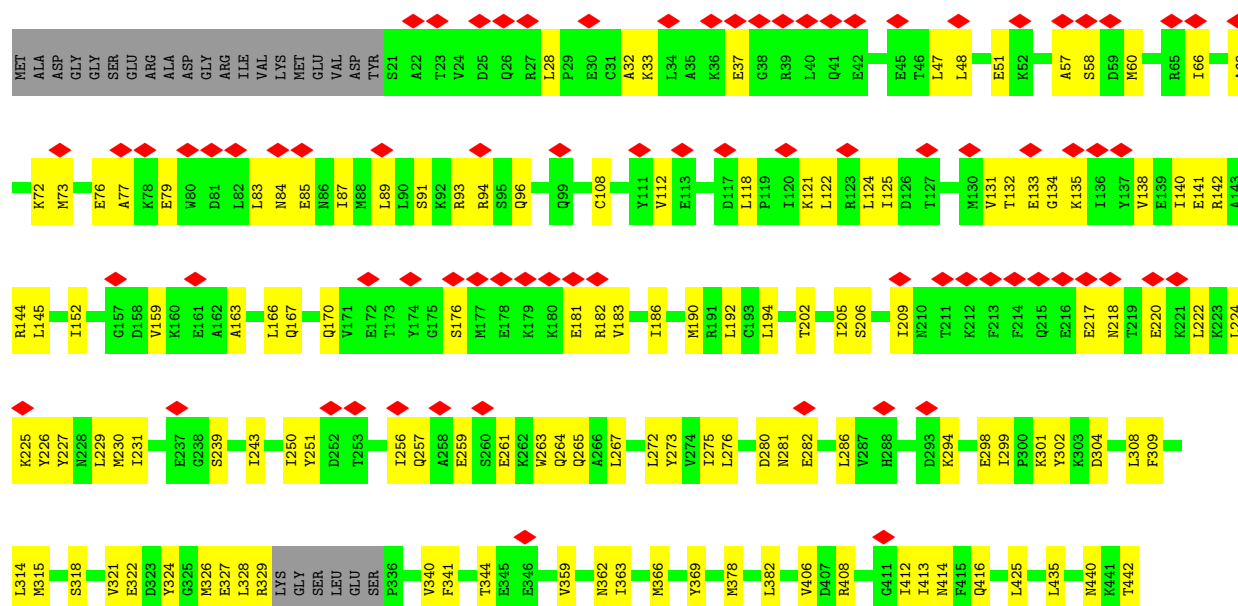
- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

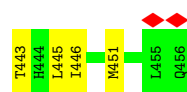


Mol	Chain	Residues	Atoms					AltConf
36	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

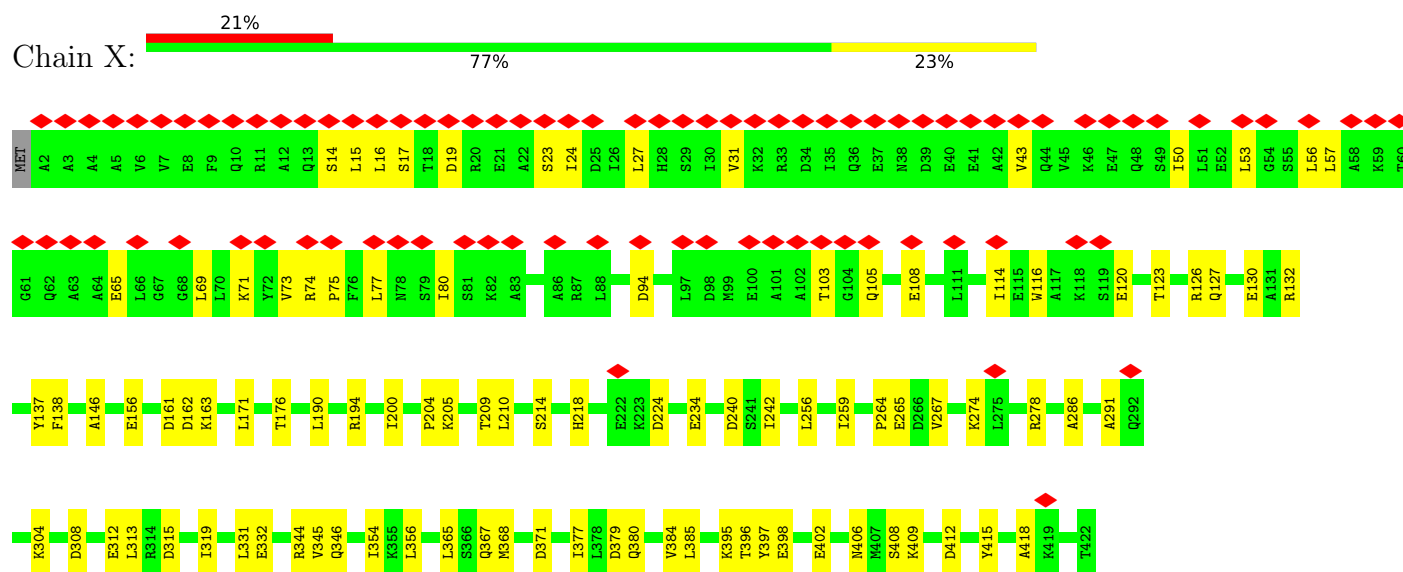


- Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

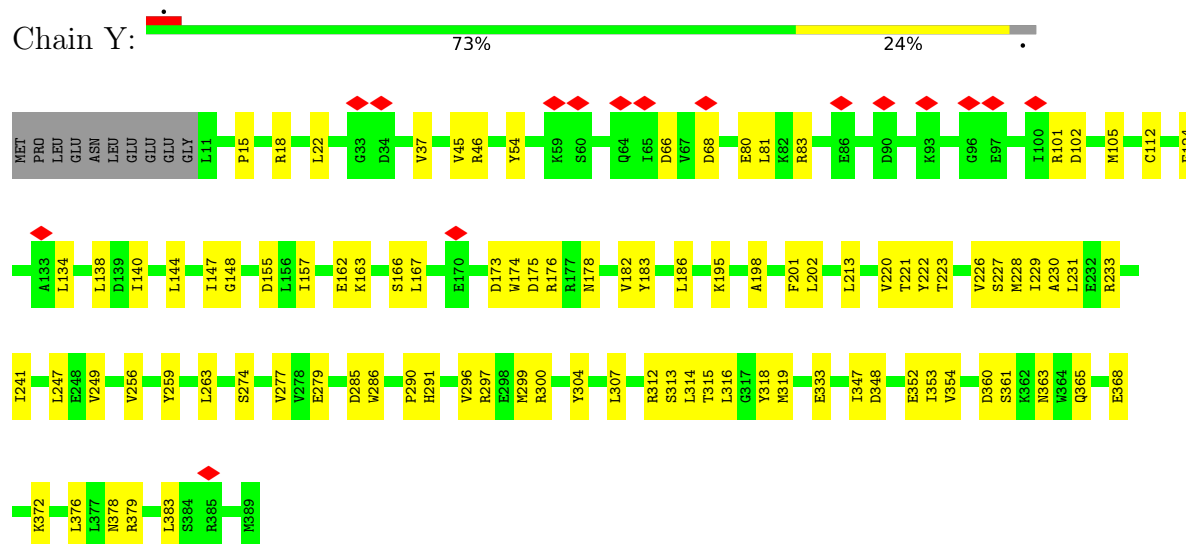




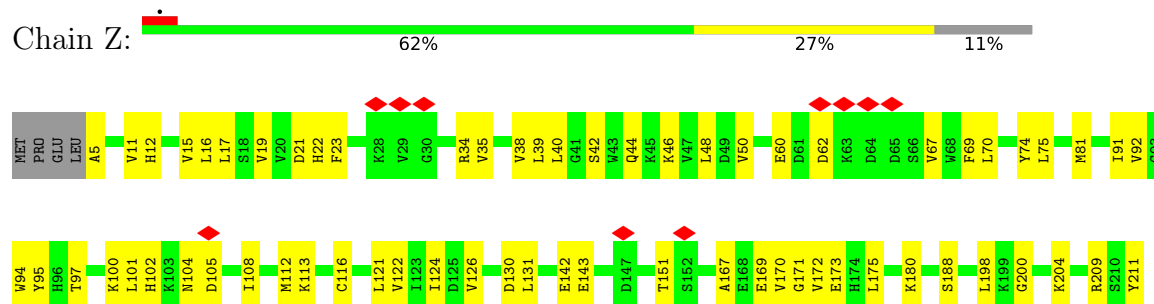
- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11



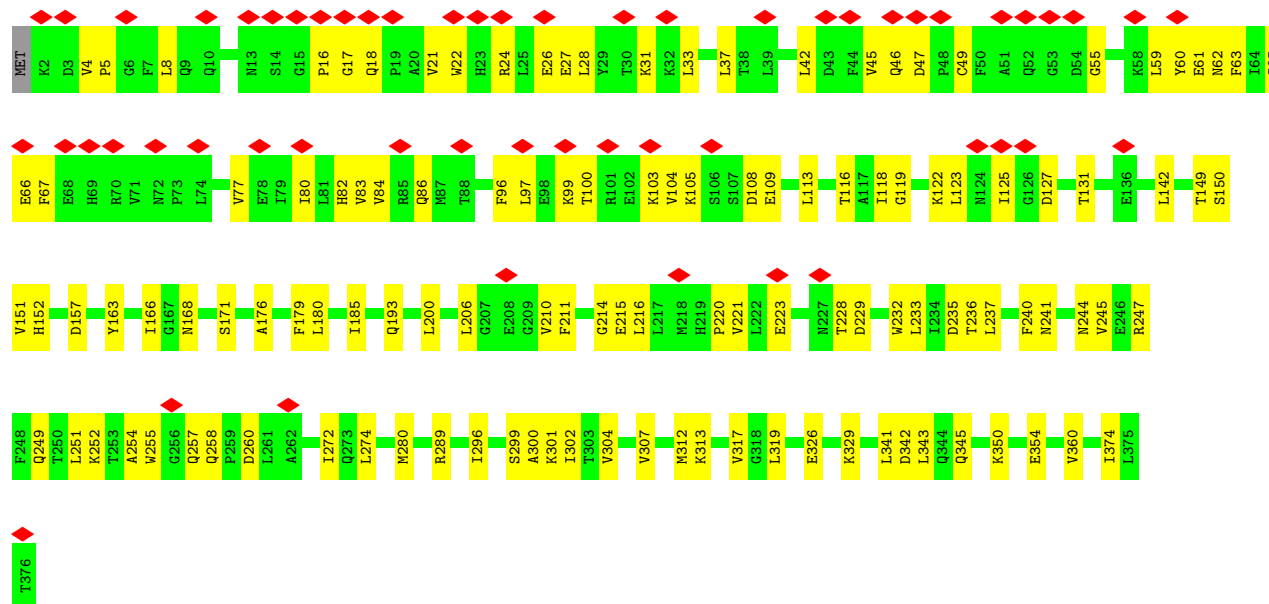
- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6



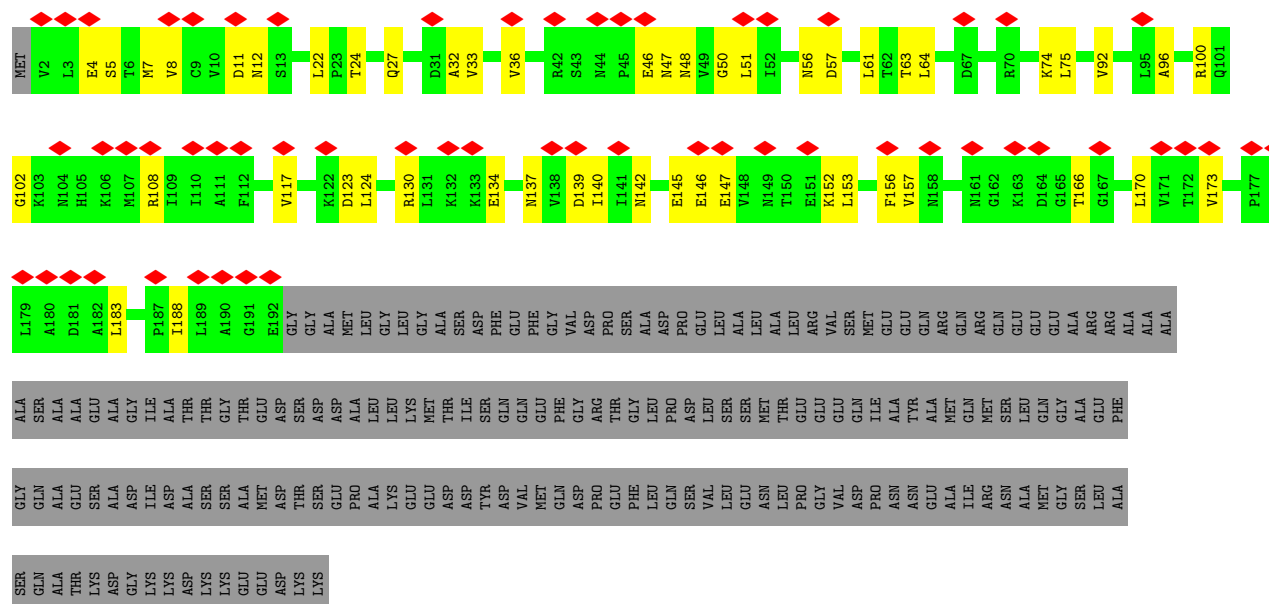
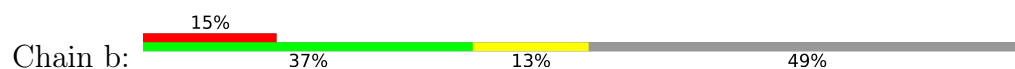
- Molecule 6: 26S proteasome non-ATPase regulatory subunit 7



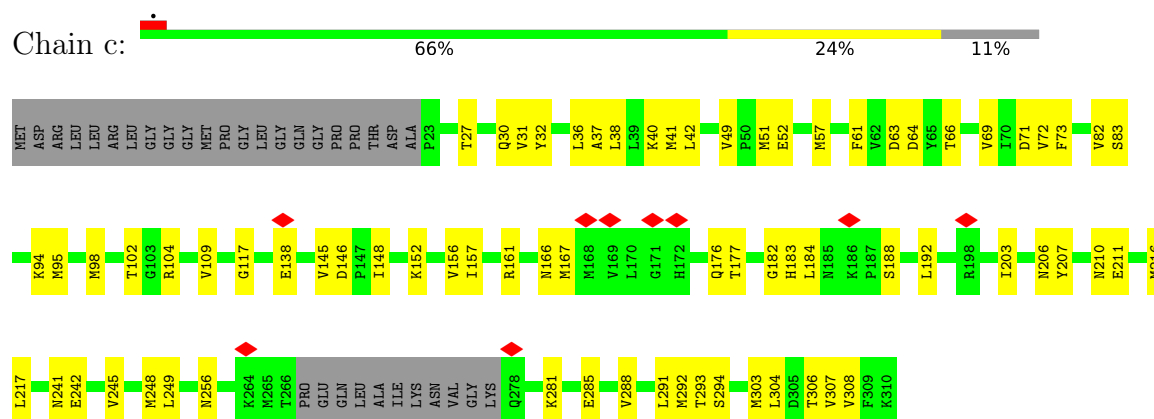
- Molecule 7: 26S proteasome non-ATPase regulatory subunit 13



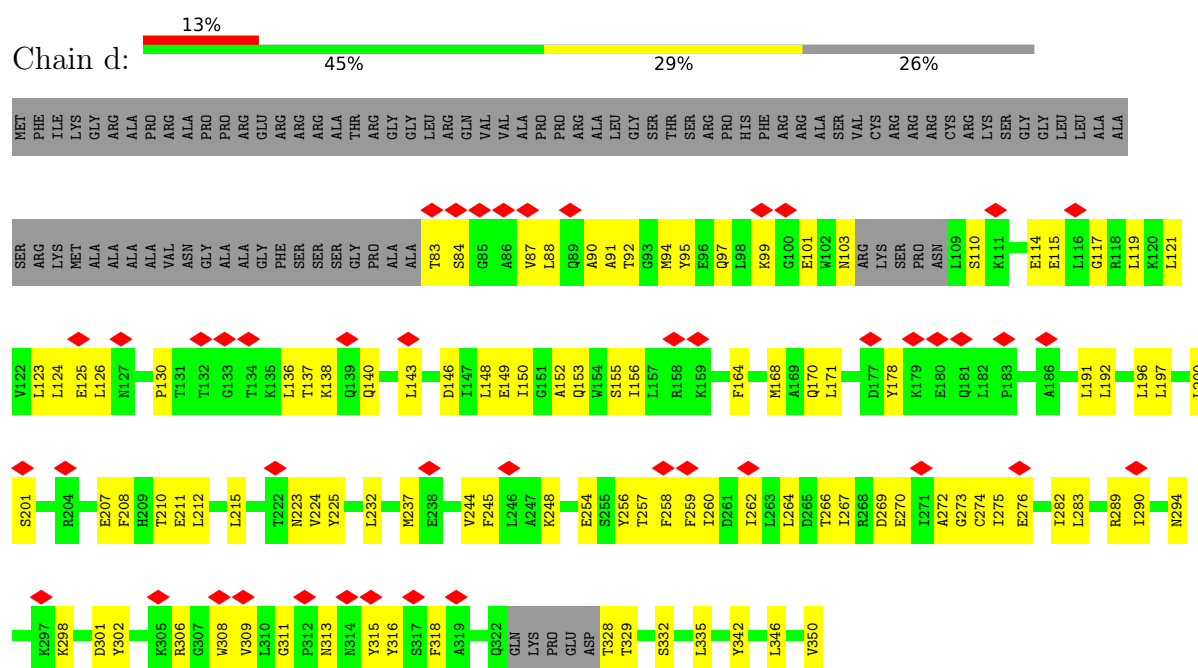
- Molecule 8: 26S proteasome non-ATPase regulatory subunit 4



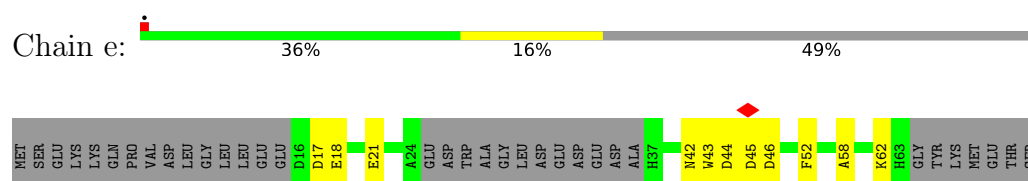
- Molecule 9: 26S proteasome non-ATPase regulatory subunit 14



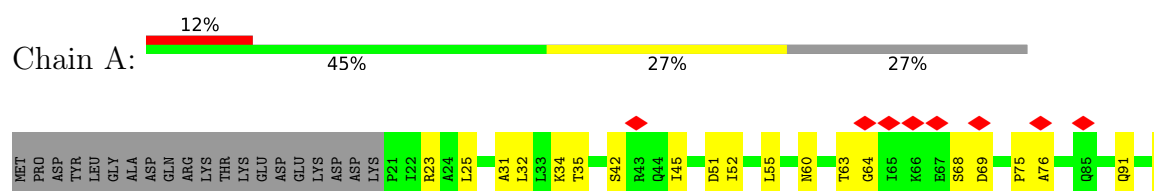
- Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

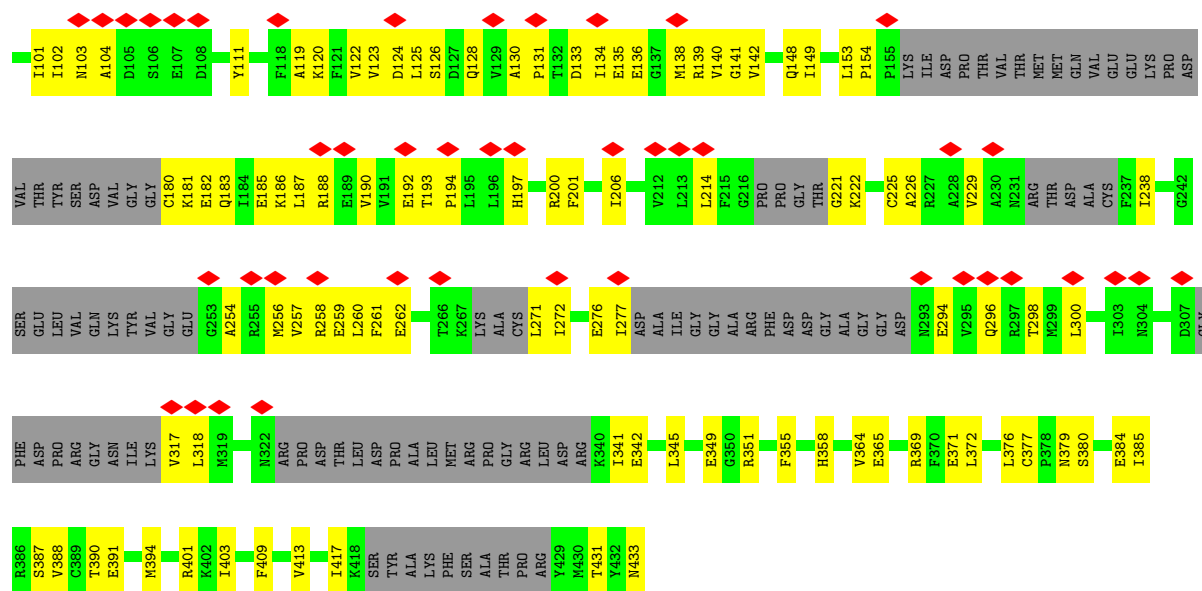


- Molecule 11: 26S proteasome complex subunit SEM1

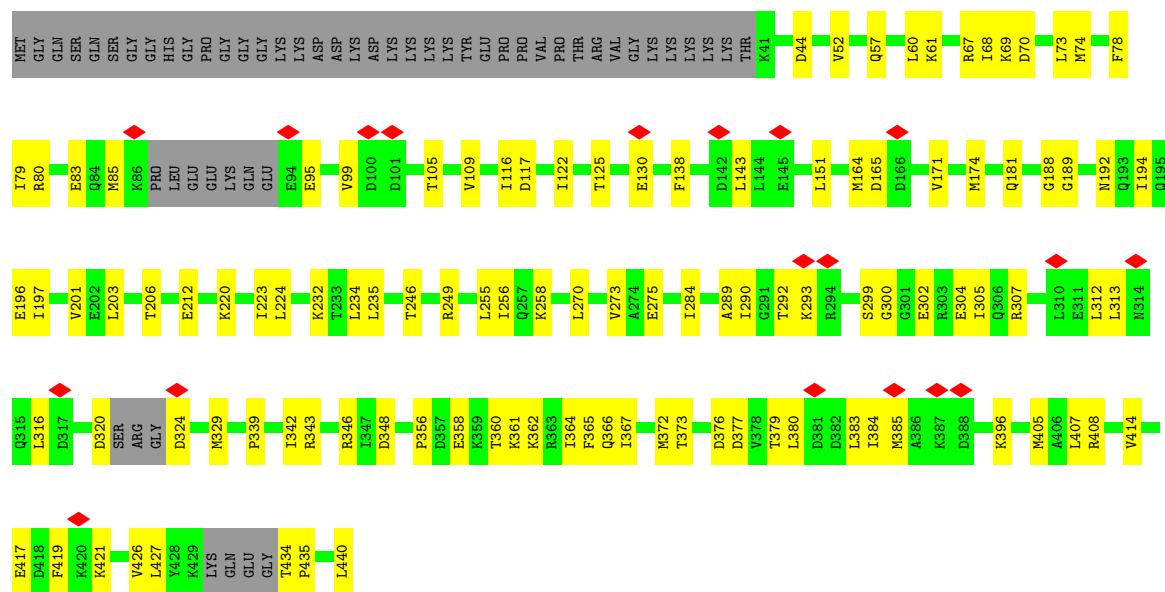


- Molecule 12: 26S proteasome regulatory subunit 7

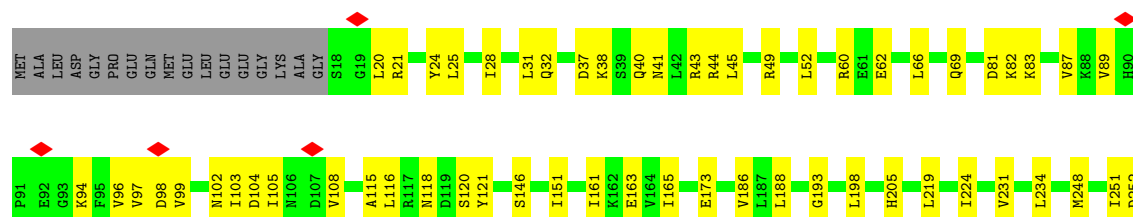


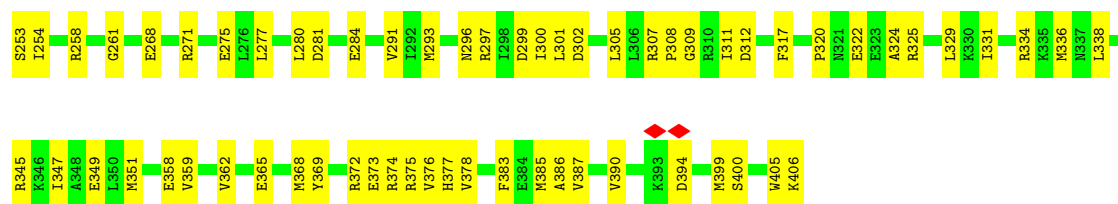


• Molecule 13: 26S proteasome regulatory subunit 4

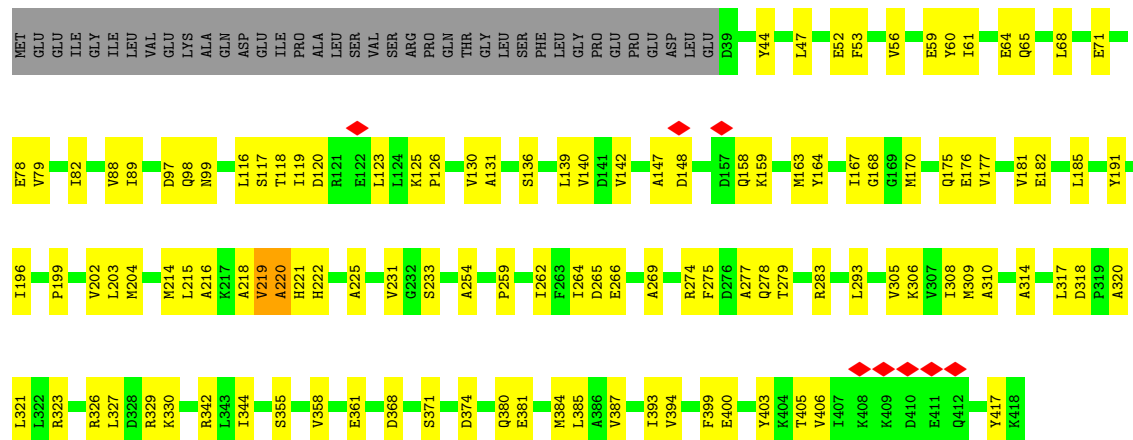


• Molecule 14: 26S protease regulatory subunit 8

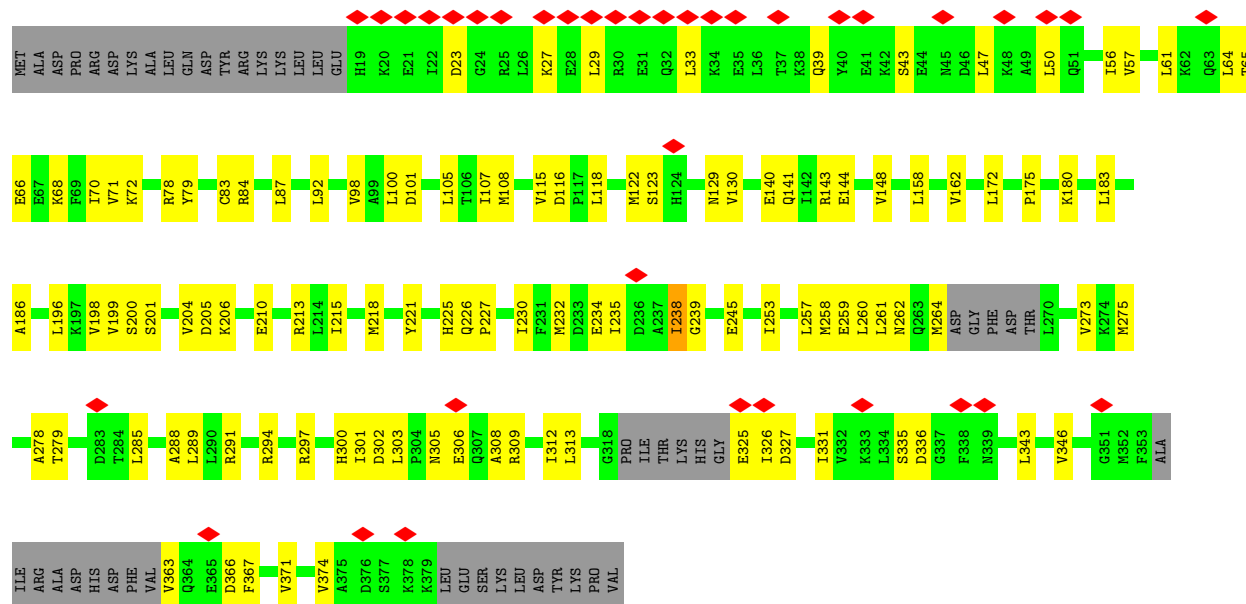




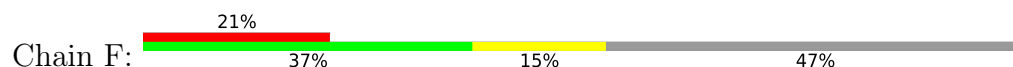
• Molecule 15: 26S proteasome regulatory subunit 6B

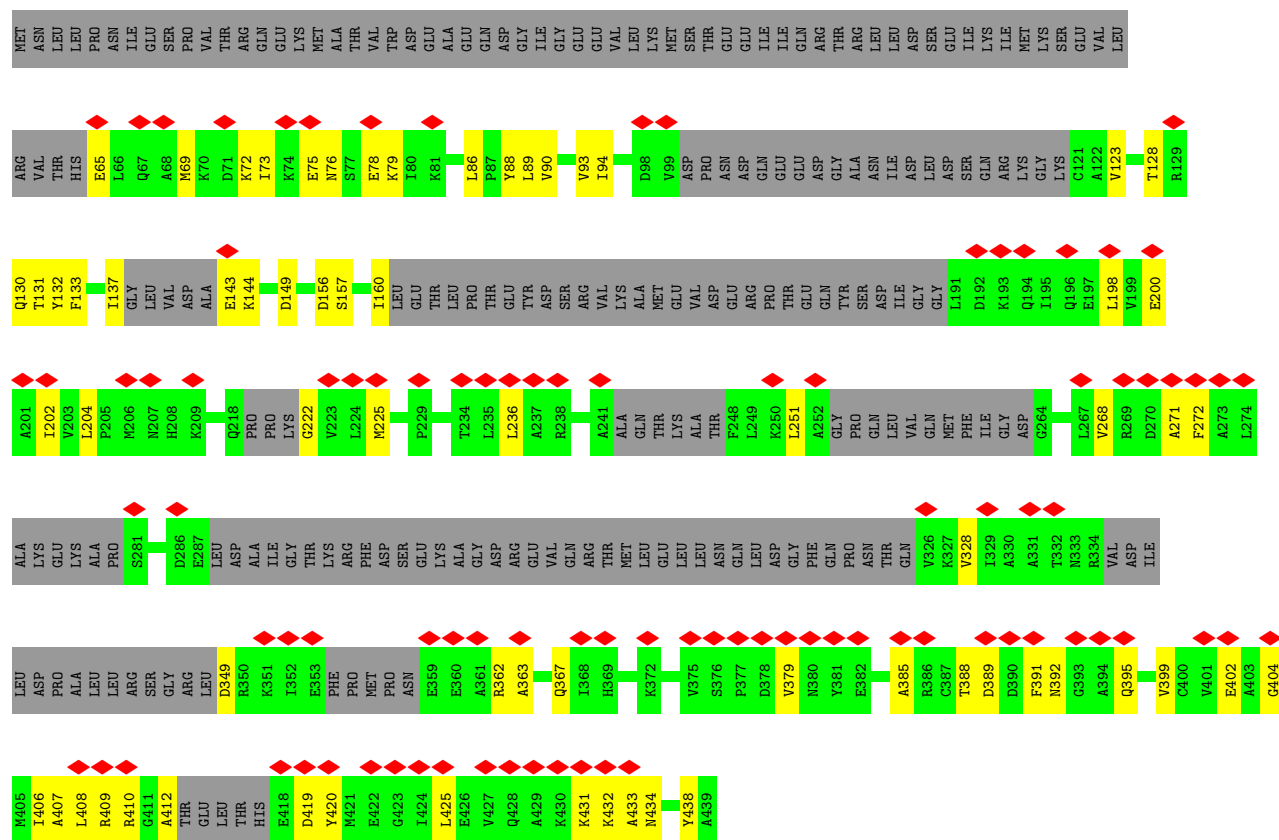


• Molecule 16: 26S protease regulatory subunit 10B

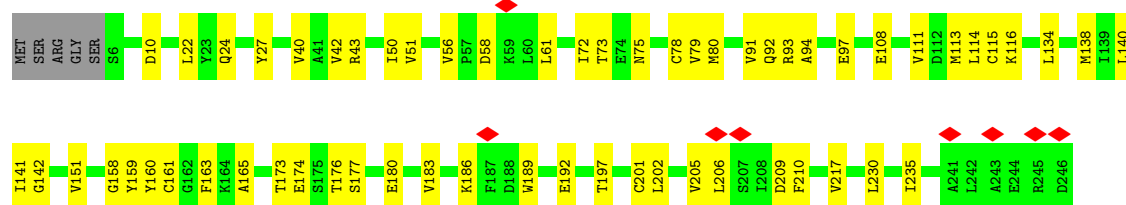


• Molecule 17: 26S proteasome regulatory subunit 6A

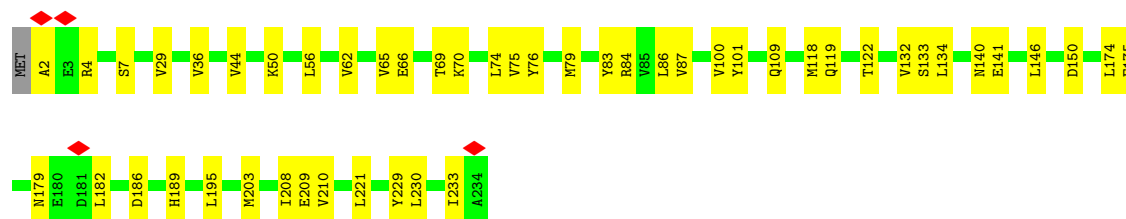
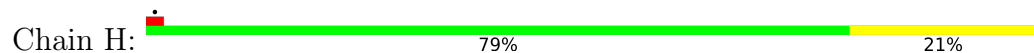




• Molecule 18: Proteasome subunit alpha type-6

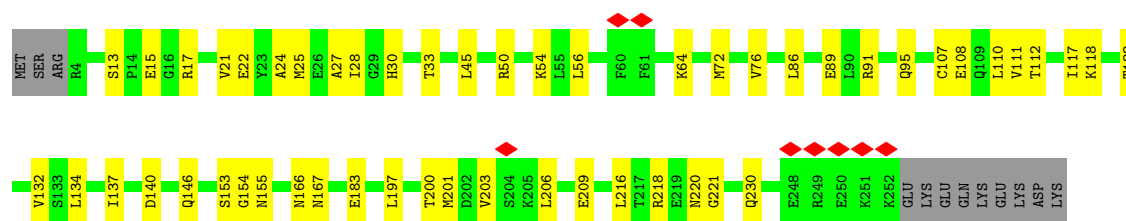


• Molecule 19: Proteasome subunit alpha type-2

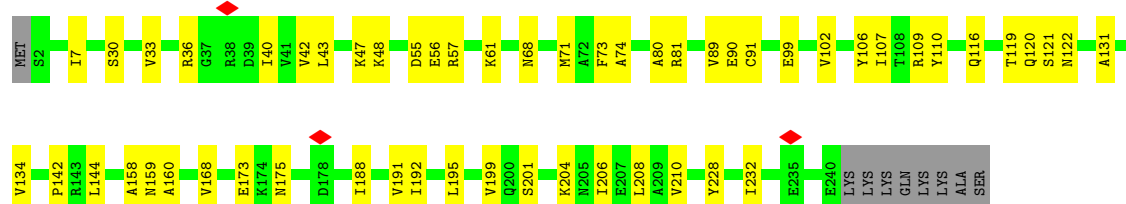


• Molecule 20: Proteasome subunit alpha type-4

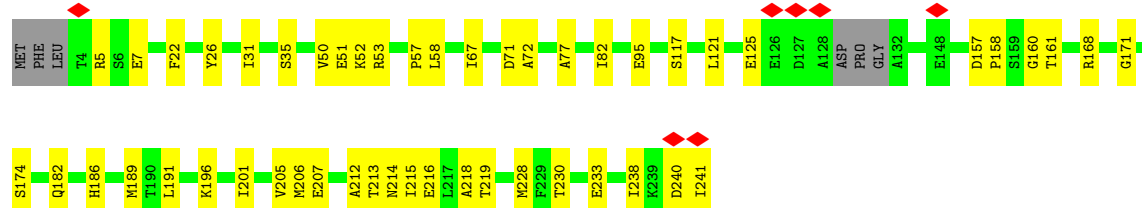
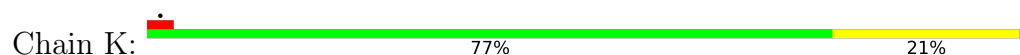




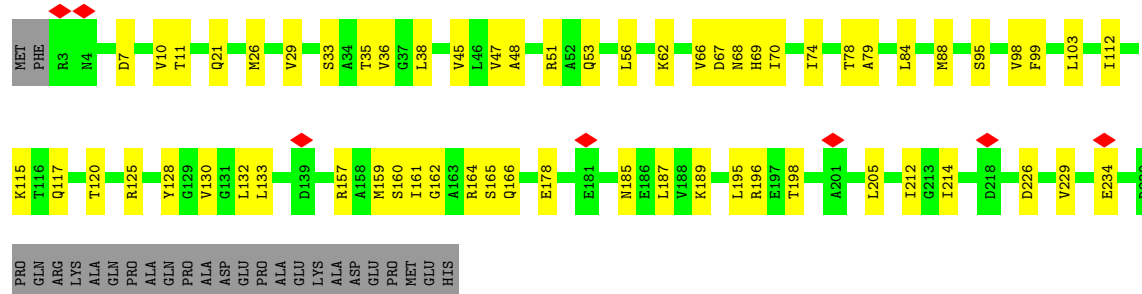
• Molecule 21: Proteasome subunit alpha type-7



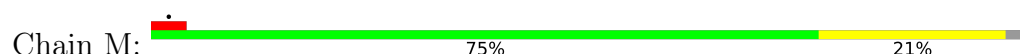
• Molecule 22: Proteasome subunit alpha type-5

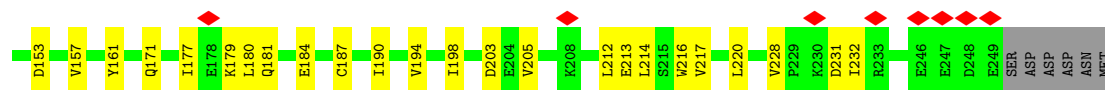


• Molecule 23: Proteasome subunit alpha type-1

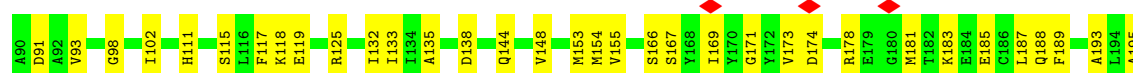
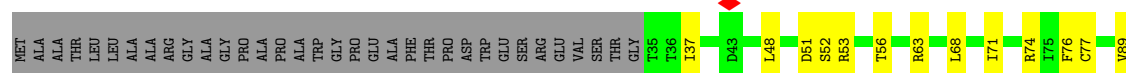


• Molecule 24: Proteasome subunit alpha type-3

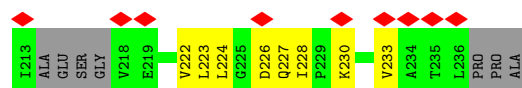
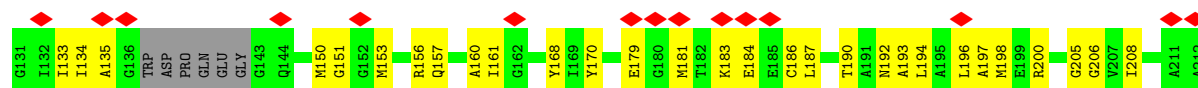
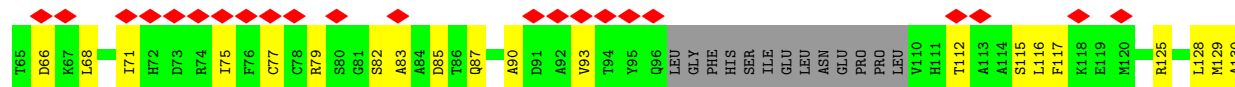
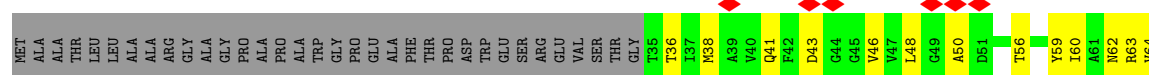




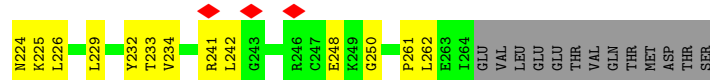
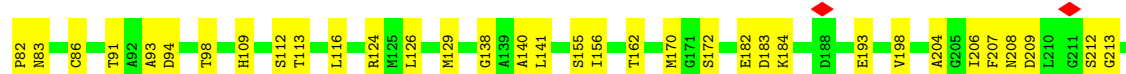
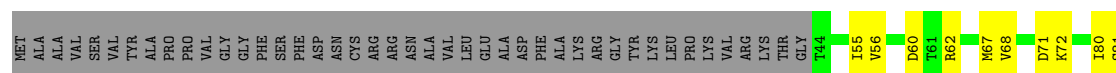
• Molecule 25: Proteasome subunit beta type-6

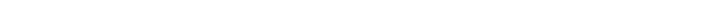


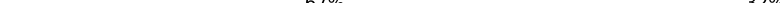
• Molecule 25: Proteasome subunit beta type-6

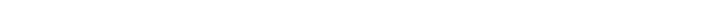


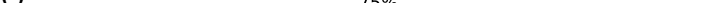
• Molecule 26: Proteasome subunit beta type-7

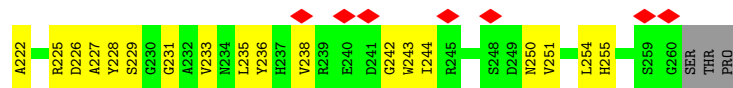


Chain o: 

Chain P:  67% 32%

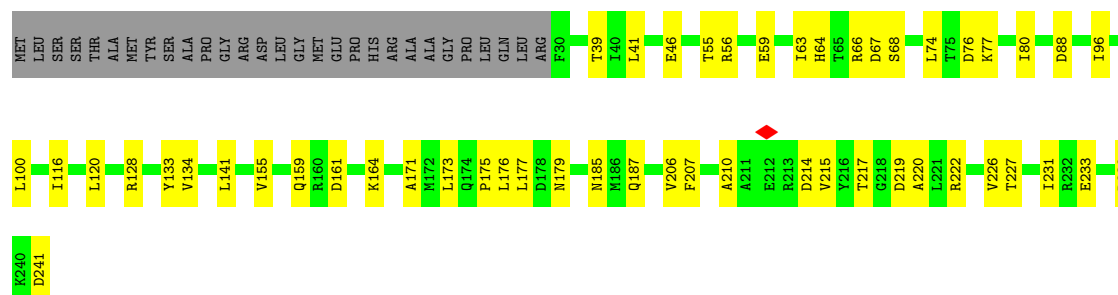
Chain p:  33% 59% 21% 20%

Chain Q:  75% 23%



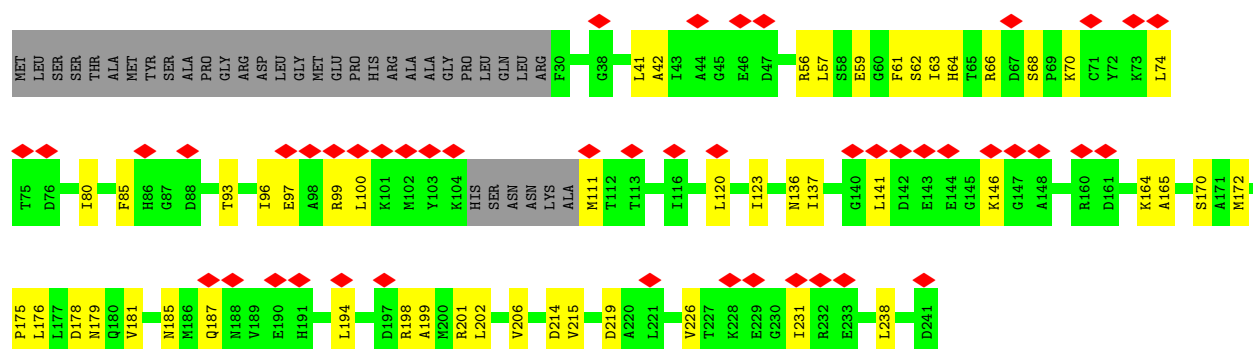
• Molecule 30: Proteasome subunit beta type-1

Chain S: 67% 21% 12%



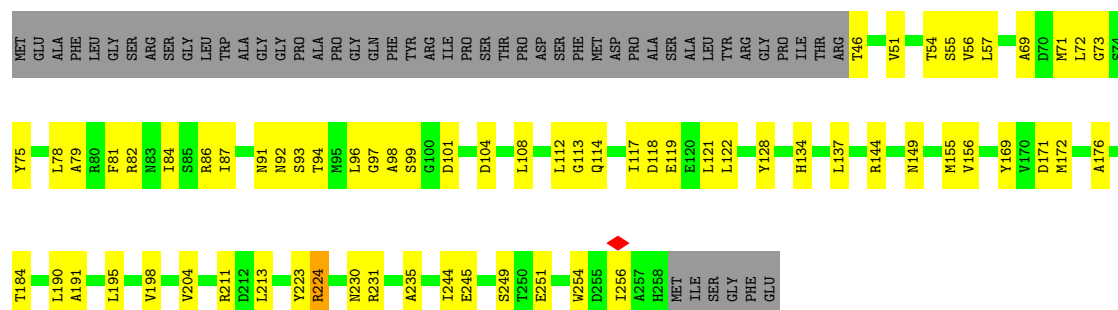
• Molecule 30: Proteasome subunit beta type-1

Chain s: 20% 65% 21% 15%



• Molecule 31: Proteasome subunit beta type-4

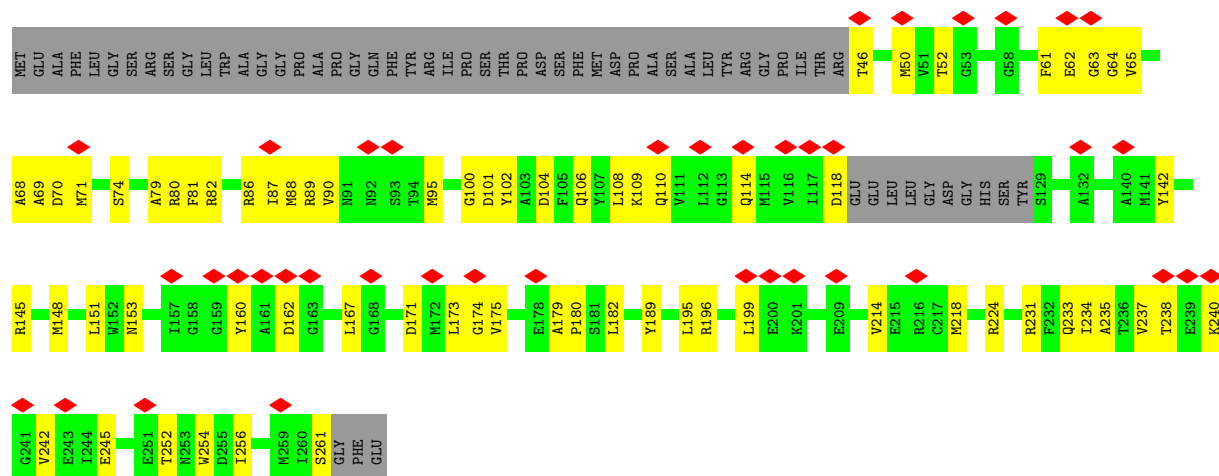
Chain T: 55% 25% 19%



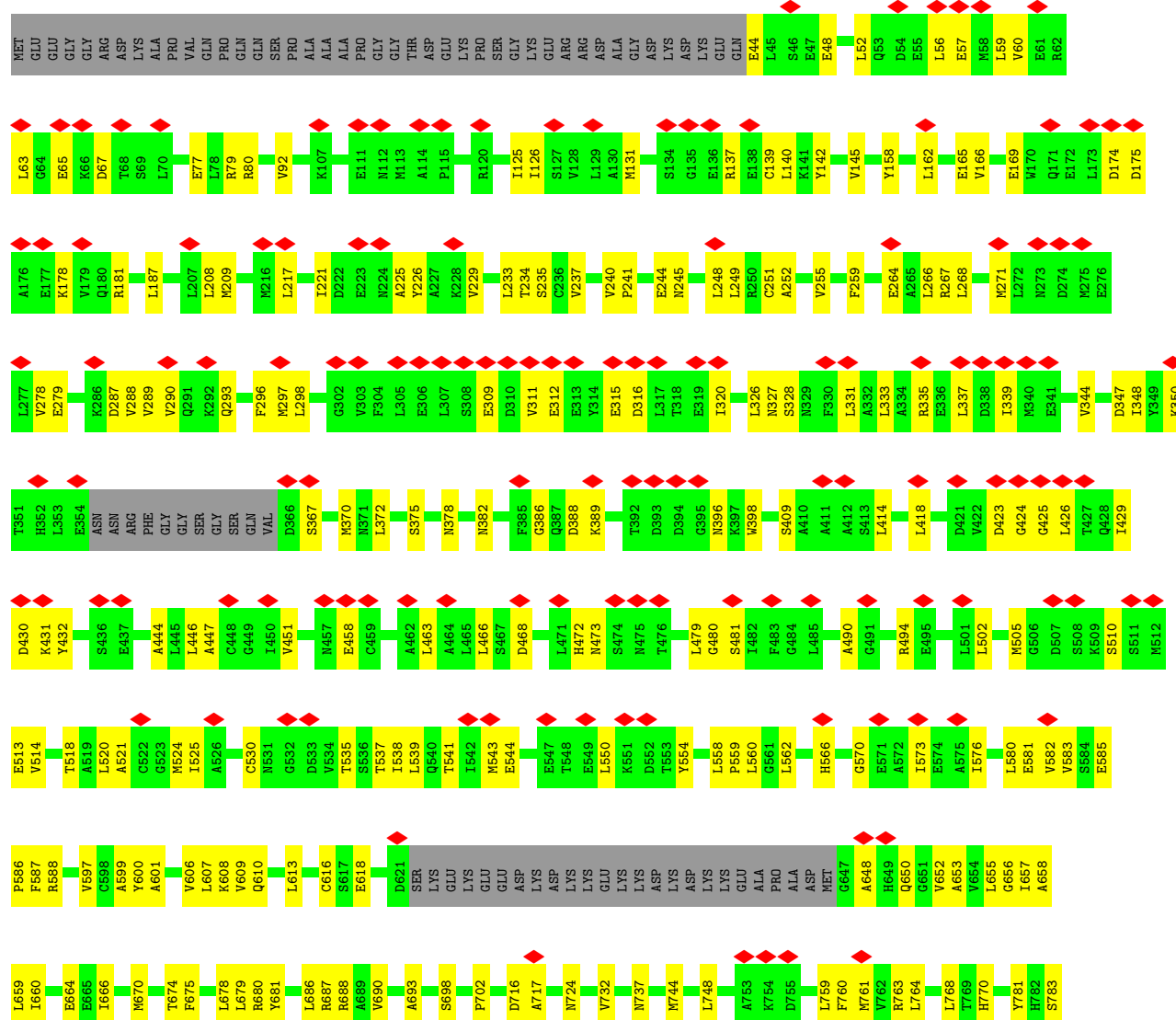
• Molecule 31: Proteasome subunit beta type-4

Chain t: 15% 52% 26% 22%





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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87326	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	1.528	Depositor
Minimum map value	-0.907	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.25	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: ATP, ZN, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	U	0.13	0/6755	0.29	0/9135
2	V	0.14	0/3499	0.33	0/4722
3	W	0.17	0/3556	0.38	0/4781
4	X	0.11	0/3373	0.27	0/4548
5	Y	0.13	0/3181	0.29	0/4285
6	Z	0.13	0/2333	0.30	0/3162
7	a	0.14	0/3070	0.34	0/4155
8	b	0.11	0/1479	0.30	0/2003
9	c	0.14	0/2225	0.33	0/3005
10	d	0.17	0/2141	0.40	0/2891
11	e	0.10	0/322	0.25	0/436
12	A	0.12	0/2548	0.33	0/3423
13	B	0.13	0/3080	0.32	0/4153
14	C	0.14	0/3112	0.32	0/4182
15	D	0.20	0/3090	0.42	1/4168 (0.0%)
16	E	0.17	0/2742	0.37	0/3685
17	F	0.12	0/1823	0.34	0/2433
18	G	0.13	0/1919	0.29	0/2593
19	H	0.14	0/1857	0.27	0/2514
20	I	0.13	0/1993	0.29	0/2683
21	J	0.14	0/1913	0.29	0/2581
22	K	0.12	0/1830	0.30	0/2468
23	L	0.12	0/1902	0.29	0/2569
24	M	0.12	0/1951	0.29	0/2627
25	N	0.14	0/1513	0.32	0/2047
25	n	0.13	0/1352	0.31	0/1822
26	O	0.13	0/1694	0.30	0/2293
26	o	0.14	0/1331	0.35	0/1791
27	P	0.14	0/1620	0.32	0/2184
27	p	0.15	0/1282	0.37	0/1722
28	Q	0.14	0/1611	0.29	0/2180
28	q	0.16	0/1405	0.36	1/1899 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	R	0.12	0/1580	0.29	0/2134
29	r	0.12	0/1460	0.32	0/1972
30	S	0.11	0/1673	0.27	0/2254
30	s	0.12	0/1625	0.31	0/2188
31	T	0.12	0/1698	0.31	0/2299
31	t	0.13	0/1639	0.34	0/2217
32	f	0.13	0/6458	0.30	0/8743
33	y	0.11	0/272	0.28	0/357
All	All	0.14	0/89907	0.32	2/121304 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
31	T	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	q	97	PRO	CA-N-CD	-5.77	103.93	112.00
15	D	219	VAL	N-CA-C	-5.76	101.27	109.51

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	T	224	ARG	Sidechain

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	6640	0	6697	184	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	3434	0	3503	114	0
3	W	3510	0	3633	131	0
4	X	3327	0	3423	79	0
5	Y	3123	0	3130	72	0
6	Z	2290	0	2320	92	0
7	a	3012	0	3029	98	0
8	b	1459	0	1499	39	0
9	c	2184	0	2191	88	0
10	d	2099	0	2127	91	0
11	e	314	0	247	10	0
12	A	2518	0	2588	107	0
13	B	3037	0	3101	102	0
14	C	3071	0	3193	105	0
15	D	3040	0	3076	118	0
16	E	2706	0	2779	106	0
17	F	1812	0	1882	67	0
18	G	1885	0	1889	55	0
19	H	1818	0	1811	38	0
20	I	1963	0	1987	41	0
21	J	1887	0	1905	50	0
22	K	1804	0	1789	43	0
23	L	1868	0	1858	58	0
24	M	1916	0	1890	49	0
25	N	1487	0	1452	55	0
25	n	1336	0	1324	64	0
26	O	1667	0	1689	56	0
26	o	1315	0	1321	39	0
27	P	1591	0	1609	61	0
27	p	1264	0	1255	42	0
28	Q	1578	0	1580	43	0
28	q	1380	0	1399	50	0
29	R	1549	0	1512	51	0
29	r	1432	0	1384	45	0
30	S	1643	0	1640	49	0
30	s	1597	0	1597	47	0
31	T	1665	0	1638	63	0
31	t	1609	0	1597	70	0
32	f	6351	0	6362	196	0
33	y	273	0	309	8	0
34	c	1	0	0	0	0
35	A	31	0	12	4	0
35	B	31	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	C	31	0	12	1	0
35	D	31	0	12	2	0
36	E	27	0	12	1	0
All	All	88606	0	89275	2529	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 (2529) 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)
28:Q:5:ILE:HD11	28:Q:143:LEU:HD11	1.44	0.98
12:A:63:THR:O	32:f:681:TYR:OH	1.82	0.98
17:F:438:TYR:OH	23:L:62:LYS:NZ	1.98	0.97
6:Z:39:LEU:HD11	6:Z:95:TYR:HB3	1.50	0.94
27:p:58:THR:OG1	28:q:121:LEU:O	1.88	0.91
3:W:359:VAL:HG13	3:W:382:LEU:HD21	1.50	0.91
14:C:60:ARG:NH2	15:D:71:GLU:OE2	2.03	0.91
17:F:438:TYR:HH	23:L:33:SER:HG	1.13	0.90
28:q:44:LEU:HD11	28:q:102:LEU:HD12	1.54	0.90
15:D:274:ARG:NE	15:D:318:ASP:OD2	2.06	0.89
26:O:250:GLY:O	30:s:187:GLN:NE2	2.06	0.88
25:n:59:TYR:OH	26:o:178:MET:SD	2.32	0.88
35:C:501:ATP:O3G	15:D:326:ARG:NH2	2.06	0.88
6:Z:235:ASN:OD1	7:a:289:ARG:NH1	2.07	0.87
20:I:140:ASP:OD2	20:I:146:GLN:NE2	2.07	0.86
27:p:178:ASP:OD2	27:p:181:SER:OG	1.94	0.86
29:r:233:VAL:HG21	29:r:254:LEU:HD12	1.57	0.86
31:t:160:TYR:OH	31:t:237:VAL:O	1.93	0.86
27:P:34:MET:O	29:r:225:ARG:NH1	2.08	0.85
14:C:41:ASN:OD1	14:C:44:ARG:NH1	2.09	0.85
29:r:60:THR:N	29:r:229:SER:HG	1.74	0.85
1:U:609:ASP:OD1	1:U:610:VAL:N	2.10	0.84
2:V:440:LYS:NZ	10:d:237:MET:O	2.09	0.84
3:W:225:LYS:O	3:W:229:LEU:HD12	1.77	0.84
25:n:48:LEU:HD11	25:n:135:ALA:HB3	1.59	0.84
32:f:618:GLU:O	32:f:650:GLN:NE2	2.11	0.84
23:L:33:SER:OG	23:L:62:LYS:NZ	2.09	0.84
32:f:799:VAL:HG21	32:f:821:LEU:HD12	1.58	0.84
16:E:245:GLU:OE2	19:H:2:ALA:N	2.10	0.84
10:d:207:GLU:O	10:d:210:THR:OG1	1.96	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:405:MET:SD	13:B:408:ARG:NH1	2.51	0.83
27:P:58:THR:OG1	28:Q:121:LEU:O	1.96	0.83
15:D:368:ASP:OD2	15:D:403:TYR:OH	1.97	0.83
26:O:241:ARG:NH2	27:P:152:SER:O	2.13	0.82
25:n:48:LEU:HD11	25:n:135:ALA:CB	2.10	0.82
6:Z:188:SER:OG	7:a:374:ILE:O	1.98	0.82
7:a:83:VAL:O	7:a:86:GLN:NE2	2.12	0.82
1:U:568:GLU:OE2	1:U:572:ARG:NH2	2.13	0.81
32:f:573:ILE:HG21	32:f:599:ALA:HB2	1.59	0.81
21:J:109:ARG:NH2	29:R:129:ASN:OD1	2.13	0.81
10:d:254:GLU:O	10:d:257:THR:OG1	1.97	0.81
15:D:176:GLU:OE1	15:D:329:ARG:NH2	2.14	0.81
26:O:68:VAL:HG11	27:P:144:GLU:OE2	1.80	0.81
29:R:86:ALA:O	30:S:164:LYS:NZ	2.14	0.81
31:t:63:GLY:O	31:t:238:THR:OG1	1.99	0.81
3:W:451:MET:HE2	6:Z:101:LEU:HD12	1.63	0.80
4:X:234:GLU:OE2	15:D:342:ARG:NH2	2.14	0.80
32:f:505:MET:HE2	32:f:541:THR:HG21	1.64	0.80
4:X:398:GLU:OE2	5:Y:365:GLN:NE2	2.14	0.80
1:U:27:LEU:O	1:U:31:VAL:HG23	1.82	0.80
29:R:60:THR:N	29:R:228:TYR:O	2.14	0.80
12:A:64:GLY:O	32:f:680:ARG:NH2	2.15	0.80
17:F:128:THR:OG1	17:F:130:GLN:OE1	1.99	0.80
27:P:67:LEU:HD11	27:P:91:VAL:HG22	1.63	0.80
3:W:280:ASP:OD1	3:W:281:ASN:N	2.15	0.80
22:K:117:SER:OG	22:K:160:GLY:O	1.99	0.79
25:n:38:MET:HE3	25:n:190:THR:HG23	1.64	0.79
2:V:345:ARG:NH2	11:e:46:ASP:OD2	2.15	0.79
14:C:373:GLU:OE1	14:C:375:ARG:NH1	2.16	0.79
14:C:293:MET:CE	14:C:311:ILE:HD11	2.12	0.79
32:f:77:GLU:OE2	32:f:80:ARG:NH2	2.16	0.79
12:A:390:THR:HG22	12:A:394:MET:HE1	1.64	0.79
9:c:292:MET:HE2	10:d:346:LEU:HD11	1.64	0.79
29:R:225:ARG:NE	28:q:144:ASP:OD2	2.16	0.79
12:A:187:LEU:HD23	12:A:229:VAL:HG21	1.65	0.79
14:C:362:VAL:HG22	14:C:390:VAL:HG21	1.64	0.79
6:Z:21:ASP:OD2	9:c:104:ARG:NH2	2.15	0.78
31:T:230:ASN:OD1	31:T:249:SER:OG	2.00	0.78
3:W:304:ASP:OD2	3:W:324:TYR:OH	2.00	0.78
31:T:171:ASP:OD1	31:T:172:MET:N	2.15	0.78
4:X:379:ASP:OD1	5:Y:313:SER:OG	2.02	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:4:GLU:N	8:b:47:ASN:OD1	2.17	0.78
5:Y:22:LEU:HD12	5:Y:37:VAL:HG23	1.64	0.78
13:B:320:ASP:OD1	13:B:324:ASP:N	2.16	0.78
3:W:408:ARG:NH1	4:X:346:GLN:OE1	2.17	0.78
7:a:317:VAL:HG13	7:a:319:LEU:HD13	1.64	0.78
32:f:237:VAL:O	32:f:245:ASN:ND2	2.17	0.78
11:e:42:ASN:OD1	11:e:43:TRP:N	2.17	0.78
15:D:148:ASP:OD2	16:E:78:ARG:NE	2.17	0.78
32:f:79:ARG:HG3	32:f:125:ILE:HD11	1.66	0.78
32:f:573:ILE:HD13	32:f:599:ALA:CB	2.14	0.77
19:H:175:GLU:OE1	20:I:54:LYS:NZ	2.15	0.77
31:t:95:MET:HE2	31:t:237:VAL:HG12	1.67	0.77
32:f:175:ASP:OD1	32:f:178:LYS:NZ	2.17	0.77
32:f:573:ILE:HD13	32:f:599:ALA:HB3	1.65	0.77
10:d:223:ASN:OD1	10:d:224:VAL:N	2.17	0.77
1:U:70:HIS:O	2:V:236:ARG:NH1	2.17	0.77
3:W:51:GLU:OE1	3:W:93:ARG:NH1	2.18	0.77
4:X:16:LEU:HD12	4:X:56:LEU:HG	1.67	0.77
22:K:196:LYS:NZ	22:K:240:ASP:O	2.18	0.77
15:D:277:ALA:O	15:D:279:THR:HG22	1.85	0.77
5:Y:46:ARG:NH2	5:Y:66:ASP:OD2	2.18	0.77
22:K:125:GLU:OE2	23:L:125:ARG:NH1	2.18	0.77
32:f:888:LEU:HB3	32:f:901:ARG:HB2	1.65	0.77
1:U:21:GLU:OE1	1:U:21:GLU:N	2.18	0.77
21:J:73:PHE:CZ	21:J:80:ALA:HB2	2.19	0.77
13:B:68:ILE:HG23	32:f:670:MET:CE	2.16	0.76
25:N:199:GLU:OE2	31:t:82:ARG:NH1	2.17	0.76
15:D:321:LEU:HD23	15:D:321:LEU:O	1.85	0.76
1:U:140:ARG:NH1	1:U:144:ASP:OD2	2.19	0.76
1:U:40:GLU:OE2	2:V:269:LYS:NZ	2.15	0.76
4:X:94:ASP:OD1	4:X:132:ARG:NH2	2.19	0.76
26:O:67:MET:HE1	30:s:61:PHE:HE1	1.51	0.76
1:U:246:TYR:OH	1:U:324:LYS:NZ	2.17	0.76
12:A:377:CYS:SG	12:A:380:SER:OG	2.41	0.76
29:R:87:SER:HG	30:S:164:LYS:HZ1	1.32	0.75
12:A:52:ILE:HD12	13:B:68:ILE:HG22	1.67	0.75
14:C:281:ASP:OD2	14:C:307:ARG:NH2	2.19	0.75
31:T:55:SER:OG	31:T:184:THR:O	2.03	0.75
4:X:367:GLN:NE2	4:X:371:ASP:OD2	2.19	0.75
32:f:458:GLU:OE2	33:y:402:LYS:NZ	2.19	0.75
12:A:181:LYS:NZ	12:A:349:GLU:OE2	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:J:228:TYR:O	21:J:232:ILE:HD12	1.86	0.75
26:O:98:THR:HG23	26:O:129:MET:CE	2.16	0.75
26:O:224:ASN:OD1	26:O:225:LYS:N	2.19	0.75
1:U:490:ARG:NH2	1:U:492:ASP:OD2	2.20	0.75
1:U:560:MET:SD	1:U:593:SER:OG	2.42	0.75
2:V:213:TYR:O	2:V:217:VAL:HG13	1.86	0.75
17:F:438:TYR:HH	23:L:62:LYS:NZ	1.85	0.75
18:G:158:GLY:O	19:H:84:ARG:NH2	2.20	0.75
1:U:404:ALA:O	1:U:407:SER:OG	2.04	0.74
6:Z:38:VAL:HG11	6:Z:91:ILE:HD12	1.69	0.74
6:Z:274:ASN:OD1	9:c:281:LYS:NZ	2.19	0.74
17:F:251:LEU:HD13	17:F:271:ALA:HB2	1.67	0.74
23:L:164:ARG:O	23:L:198:THR:OG1	2.06	0.74
3:W:72:LYS:NZ	3:W:76:GLU:OE2	2.16	0.74
4:X:218:HIS:ND1	4:X:224:ASP:OD2	2.20	0.74
30:s:85:PHE:CZ	31:t:173:LEU:HD21	2.22	0.74
29:R:103:THR:O	29:R:158:THR:OG1	2.02	0.74
1:U:321:GLN:OE1	1:U:324:LYS:NZ	2.19	0.74
27:P:2:SER:N	27:P:5:SER:HG	1.86	0.74
30:S:41:LEU:HD11	30:S:177:LEU:HD11	1.68	0.74
5:Y:174:TRP:O	5:Y:178:ASN:ND2	2.21	0.74
2:V:368:ARG:NH2	11:e:46:ASP:OD1	2.21	0.74
10:d:201:SER:HB3	10:d:262:ILE:HG23	1.70	0.74
10:d:146:ASP:O	10:d:150:ILE:HD12	1.88	0.73
14:C:406:LYS:OXT	20:I:64:LYS:NZ	2.18	0.73
29:R:87:SER:OG	30:S:164:LYS:NZ	2.17	0.73
29:R:94:ILE:HD11	29:R:104:MET:HE3	1.70	0.73
3:W:294:LYS:NZ	3:W:298:GLU:OE2	2.19	0.73
1:U:596:ASN:ND2	15:D:52:GLU:OE1	2.19	0.73
2:V:465:ASP:OD1	5:Y:363:ASN:ND2	2.22	0.73
21:J:159:ASN:OD1	21:J:160:ALA:N	2.21	0.73
1:U:437:TYR:HD1	1:U:472:ILE:HG21	1.53	0.73
7:a:185:ILE:O	7:a:193:GLN:NE2	2.21	0.73
29:r:220:TYR:OH	29:r:255:HIS:ND1	2.22	0.73
2:V:311:ASN:OD1	2:V:314:ARG:NH2	2.21	0.73
19:H:74:LEU:HD21	19:H:134:LEU:HD22	1.70	0.73
9:c:71:ASP:OD1	9:c:72:VAL:N	2.20	0.73
16:E:196:LEU:HD21	16:E:218:MET:HG3	1.70	0.73
3:W:445:LEU:HD22	6:Z:226:ILE:HD11	1.70	0.72
23:L:88:MET:HE2	23:L:112:ILE:HD13	1.71	0.72
1:U:19:LEU:HD13	10:d:124:LEU:HD13	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:153:LEU:HD23	12:A:154:PRO:O	1.89	0.72
18:G:113:MET:HE3	26:O:113:THR:HG22	1.72	0.72
31:T:57:LEU:HD11	31:T:191:ALA:HB1	1.72	0.72
16:E:366:ASP:OD1	16:E:367:PHE:N	2.22	0.72
18:G:205:VAL:HG13	18:G:206:LEU:HD12	1.71	0.72
16:E:196:LEU:HD23	16:E:230:ILE:HD12	1.72	0.72
16:E:302:ASP:OD1	16:E:303:LEU:N	2.22	0.72
8:b:24:THR:OG1	8:b:27:GLN:OE1	2.07	0.72
2:V:121:PHE:O	2:V:128:ARG:NH1	2.22	0.72
15:D:130:VAL:HG12	15:D:142:VAL:HG12	1.72	0.72
31:t:50:MET:O	31:t:52:THR:HG23	1.88	0.72
13:B:289:ALA:O	14:C:271:ARG:NH1	2.23	0.72
18:G:50:ILE:HG23	18:G:141:ILE:HD13	1.70	0.72
2:V:334:VAL:O	2:V:338:LEU:HD23	1.90	0.72
13:B:197:ILE:O	13:B:201:VAL:HG22	1.90	0.72
31:T:223:TYR:O	25:n:60:ILE:HD11	1.90	0.71
24:M:137:MET:HE2	24:M:149:LEU:HD11	1.72	0.71
28:q:61:GLN:NE2	28:q:65:GLN:OE1	2.23	0.71
1:U:206:MET:HE1	1:U:232:ILE:HD11	1.71	0.71
29:R:87:SER:HG	30:S:164:LYS:NZ	1.87	0.71
6:Z:172:VAL:HG23	9:c:217:LEU:HD13	1.73	0.71
25:n:125:ARG:NH1	25:n:151:GLY:O	2.24	0.71
22:K:218:ALA:HB2	22:K:228:MET:HE1	1.73	0.71
18:G:217:VAL:HG21	18:G:235:ILE:HD13	1.73	0.71
23:L:196:ARG:HG2	23:L:205:LEU:HD13	1.72	0.71
1:U:631:GLU:N	1:U:631:GLU:OE1	2.22	0.71
14:C:293:MET:HE3	14:C:311:ILE:HD11	1.71	0.71
25:N:51:ASP:OD1	25:N:52:SER:N	2.22	0.71
27:p:135:ASP:OD1	27:p:136:PHE:N	2.24	0.70
32:f:479:LEU:HD23	32:f:816:TYR:OH	1.91	0.70
30:S:46:GLU:OE1	30:S:46:GLU:N	2.24	0.70
1:U:811:PHE:O	1:U:883:ARG:NH1	2.23	0.70
24:M:40:ILE:HD13	24:M:194:VAL:HG22	1.73	0.70
3:W:340:VAL:HG12	3:W:340:VAL:O	1.91	0.70
9:c:27:THR:HG22	9:c:177:THR:HA	1.74	0.70
2:V:309:MET:HE3	2:V:331:LEU:HG	1.71	0.70
4:X:397:TYR:CE1	6:Z:258:VAL:HG11	2.26	0.70
14:C:37:ASP:OD1	14:C:38:LYS:N	2.24	0.70
7:a:214:GLY:N	7:a:241:ASN:OD1	2.25	0.70
15:D:202:VAL:HG23	15:D:329:ARG:HB2	1.73	0.70
26:o:204:ALA:O	26:o:208:ASN:ND2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:303:MET:HE3	10:d:335:LEU:HD22	1.72	0.70
7:a:360:VAL:HG22	9:c:308:VAL:HG13	1.72	0.70
16:E:200:SER:OG	16:E:234:GLU:O	2.09	0.70
22:K:31:ILE:HD11	22:K:158:PRO:CG	2.22	0.70
15:D:119:ILE:O	15:D:119:ILE:HG22	1.92	0.70
23:L:164:ARG:NH1	23:L:198:THR:O	2.24	0.70
32:f:409:SER:OG	32:f:815:HIS:NE2	2.25	0.69
7:a:326:GLU:O	7:a:329:LYS:NZ	2.24	0.69
32:f:378:ASN:OD1	32:f:382:ASN:ND2	2.24	0.69
29:r:226:ASP:O	29:r:229:SER:N	2.24	0.69
4:X:240:ASP:OD1	4:X:278:ARG:NH2	2.24	0.69
6:Z:74:TYR:OH	9:c:102:THR:OG1	2.10	0.69
13:B:383:LEU:HD11	13:B:419:PHE:HB3	1.74	0.69
18:G:186:LYS:O	18:G:189:TRP:NE1	2.26	0.69
28:Q:18:ASP:OD1	28:Q:19:ARG:N	2.26	0.69
31:T:224:ARG:CZ	26:o:178:MET:HE2	2.23	0.69
3:W:206:SER:OG	3:W:230:MET:SD	2.45	0.69
15:D:185:LEU:HD23	15:D:225:ALA:HB2	1.73	0.69
7:a:96:PHE:O	7:a:100:THR:HG23	1.93	0.69
16:E:313:LEU:CD1	16:E:343:LEU:HD13	2.23	0.69
24:M:216:TRP:CZ3	24:M:228:VAL:HG22	2.27	0.69
3:W:186:ILE:HG21	3:W:209:ILE:HD11	1.75	0.69
27:P:178:ASP:OD2	27:P:181:SER:OG	2.05	0.68
12:A:254:ALA:HA	12:A:298:THR:HG22	1.75	0.68
32:f:783:SER:HB2	32:f:787:LEU:HD12	1.73	0.68
2:V:94:VAL:HG21	2:V:205:LEU:HD13	1.75	0.68
3:W:414:ASN:OD1	3:W:416:GLN:N	2.26	0.68
21:J:33:VAL:HG22	21:J:160:ALA:HB2	1.75	0.68
21:J:188:ILE:O	21:J:192:ILE:HD12	1.94	0.68
33:y:403:ARG:HH12	33:y:404:LEU:HD23	1.58	0.68
12:A:222:LYS:N	35:A:501:ATP:O1B	2.26	0.68
26:O:183:ASP:OD2	26:O:184:LYS:NZ	2.26	0.68
3:W:446:ILE:HD11	6:Z:211:TYR:CE1	2.29	0.68
27:p:155:GLU:OE1	27:p:155:GLU:N	2.27	0.68
5:Y:285:ASP:OD1	5:Y:286:TRP:N	2.25	0.68
16:E:239:GLY:HA2	16:E:257:LEU:HD13	1.74	0.68
28:Q:58:GLU:OE1	28:Q:62:LYS:NZ	2.21	0.68
5:Y:316:LEU:HD12	5:Y:352:GLU:OE1	1.94	0.68
30:S:187:GLN:NE2	26:o:251:THR:O	2.27	0.68
30:s:226:VAL:HG22	30:s:231:ILE:CD1	2.24	0.68
15:D:97:ASP:OD1	15:D:98:GLN:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:o:129:MET:SD	26:o:132:ARG:NH2	2.67	0.68
28:q:24:ASN:OD1	28:q:25:ILE:N	2.25	0.68
2:V:168:GLN:HG3	2:V:191:LEU:HD21	1.76	0.68
2:V:113:LEU:HD21	2:V:171:VAL:HA	1.76	0.68
3:W:132:THR:O	3:W:142:ARG:NH1	2.27	0.68
23:L:195:LEU:HD22	23:L:205:LEU:HD21	1.75	0.68
28:Q:169:LYS:O	28:q:27:GLN:NE2	2.27	0.68
29:R:239:ARG:NH2	29:R:241:ASP:OD2	2.27	0.68
20:I:209:GLU:OE1	20:I:230:GLN:NE2	2.27	0.67
26:O:71:ASP:OD1	26:O:72:LYS:N	2.26	0.67
3:W:446:ILE:HD11	6:Z:211:TYR:CZ	2.29	0.67
12:A:101:ILE:HD11	12:A:136:GLU:HA	1.77	0.67
8:b:145:GLU:OE1	8:b:145:GLU:N	2.28	0.67
21:J:191:VAL:HG11	21:J:208:LEU:HD21	1.76	0.67
25:N:173:VAL:HG23	25:N:189:PHE:HZ	1.59	0.67
27:P:24:ALA:HB2	27:P:42:ILE:HD11	1.75	0.67
4:X:65:GLU:OE1	4:X:65:GLU:N	2.28	0.67
9:c:166:ASN:OD1	9:c:167:MET:N	2.27	0.67
22:K:31:ILE:HD11	22:K:158:PRO:HG3	1.77	0.67
7:a:16:PRO:O	7:a:18:GLN:OE1	2.12	0.67
14:C:399:MET:CE	20:I:56:LEU:HD11	2.25	0.67
1:U:2:ILE:O	1:U:3:THR:OG1	2.12	0.67
2:V:243:ASP:OD1	2:V:244:ALA:N	2.27	0.67
4:X:332:GLU:HG3	4:X:368:MET:HE3	1.76	0.67
12:A:34:LYS:NZ	14:C:173:GLU:OE1	2.26	0.67
7:a:142:LEU:HD21	7:a:152:HIS:CD2	2.29	0.67
9:c:307:VAL:HG21	10:d:332:SER:HB2	1.75	0.67
16:E:309:ARG:NH1	16:E:335:SER:O	2.27	0.67
26:O:109:HIS:O	26:O:113:THR:HG23	1.95	0.67
31:T:119:GLU:OE2	31:T:128:TYR:N	2.28	0.67
25:n:71:ILE:HD11	25:n:77:CYS:HB3	1.77	0.67
6:Z:243:GLN:OE1	10:d:328:THR:OG1	2.12	0.67
12:A:153:LEU:HD11	13:B:122:ILE:HD11	1.76	0.67
26:O:206:ILE:HD12	26:O:213:GLY:O	1.94	0.67
27:P:59:ASP:OD2	27:P:104:TYR:N	2.25	0.67
32:f:463:LEU:HD22	32:f:494:ARG:HH21	1.59	0.67
4:X:137:TYR:HB3	4:X:146:ALA:HB2	1.77	0.67
5:Y:183:TYR:CE1	5:Y:213:LEU:HD11	2.29	0.67
16:E:158:LEU:O	16:E:162:VAL:HG23	1.94	0.67
9:c:307:VAL:O	9:c:307:VAL:HG12	1.94	0.67
10:d:197:LEU:HD22	10:d:256:TYR:HD2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:347:ILE:HG22	14:C:351:MET:HE2	1.77	0.67
31:T:117:ILE:O	31:T:121:LEU:HD23	1.95	0.67
17:F:222:GLY:O	17:F:349:ASP:N	2.28	0.66
25:N:185:GLU:OE1	25:N:188:GLN:NE2	2.28	0.66
18:G:113:MET:CE	26:O:113:THR:HG22	2.25	0.66
27:p:178:ASP:OD1	27:p:179:ALA:N	2.28	0.66
31:t:108:LEU:HD21	31:t:151:LEU:HD13	1.77	0.66
2:V:168:GLN:HE22	2:V:187:ILE:HD11	1.59	0.66
12:A:135:GLU:OE2	12:A:138:MET:N	2.27	0.66
12:A:139:ARG:HB3	12:A:153:LEU:HD22	1.77	0.66
12:A:238:ILE:HD13	12:A:271:LEU:O	1.95	0.66
30:s:219:ASP:O	30:s:238:LEU:N	2.29	0.66
24:M:9:ASP:O	24:M:23:GLN:NE2	2.28	0.66
31:t:171:ASP:OD1	31:t:174:GLY:N	2.28	0.66
32:f:409:SER:O	32:f:819:TYR:OH	2.12	0.66
2:V:259:LEU:HD21	2:V:295:ILE:HD11	1.76	0.66
30:s:56:ARG:NE	30:s:219:ASP:OD2	2.27	0.66
1:U:391:GLU:OE1	1:U:391:GLU:N	2.29	0.66
12:A:206:ILE:HD12	17:F:404:GLY:HA3	1.77	0.66
12:A:372:LEU:HD11	22:K:207:GLU:OE1	1.94	0.66
16:E:71:VAL:HG21	16:E:100:LEU:HD11	1.77	0.66
16:E:205:ASP:OD1	16:E:206:LYS:N	2.29	0.66
16:E:264:MET:HE3	16:E:294:ARG:HB3	1.76	0.66
8:b:123:ASP:OD1	8:b:124:LEU:N	2.29	0.66
12:A:413:VAL:HG13	12:A:417:ILE:HD13	1.77	0.66
18:G:51:VAL:HG13	18:G:202:LEU:HD11	1.78	0.66
1:U:446:LEU:HD21	1:U:457:ILE:HD11	1.76	0.66
3:W:108:CYS:O	3:W:112:VAL:HG23	1.95	0.66
3:W:133:GLU:OE1	3:W:133:GLU:N	2.28	0.66
9:c:292:MET:CE	10:d:346:LEU:HD11	2.25	0.66
26:O:172:SER:OG	26:O:209:ASP:OD1	2.10	0.66
31:T:54:THR:O	31:T:99:SER:OG	2.10	0.66
21:J:55:ASP:OD1	21:J:56:GLU:N	2.28	0.66
30:s:164:LYS:NZ	30:s:165:ALA:O	2.29	0.66
17:F:75:GLU:OE2	17:F:76:ASN:ND2	2.28	0.66
32:f:447:ALA:O	32:f:451:VAL:HG23	1.94	0.66
1:U:456:ASP:OD1	1:U:457:ILE:N	2.28	0.65
6:Z:175:LEU:HD11	9:c:38:LEU:HD23	1.79	0.65
7:a:109:GLU:HB3	7:a:151:VAL:HG11	1.77	0.65
14:C:81:ASP:OD1	14:C:82:LYS:N	2.29	0.65
22:K:238:ILE:HA	22:K:241:ILE:HG23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:n:46:VAL:HG11	25:n:135:ALA:HB1	1.78	0.65
29:r:142:LEU:HD22	29:r:173:VAL:HG21	1.78	0.65
32:f:287:ASP:OD2	32:f:901:ARG:NH2	2.29	0.65
19:H:229:TYR:O	19:H:233:ILE:HD12	1.95	0.65
10:d:171:LEU:HD13	10:d:191:LEU:HD21	1.79	0.65
24:M:153:ASP:OD1	24:M:157:VAL:HG22	1.96	0.65
29:R:66:LYS:O	29:R:202:TYR:OH	2.11	0.65
31:t:69:ALA:HB3	31:t:87:ILE:HD11	1.77	0.65
6:Z:255:ASP:O	6:Z:258:VAL:HG12	1.95	0.65
9:c:145:VAL:HG12	9:c:157:ILE:HG12	1.78	0.65
6:Z:35:VAL:HG22	6:Z:97:THR:OG1	1.96	0.65
1:U:613:ASP:OD1	1:U:616:ARG:NH2	2.29	0.65
3:W:435:LEU:HD11	6:Z:237:LEU:HD23	1.79	0.65
16:E:215:ILE:HD13	16:E:260:LEU:HB2	1.78	0.65
25:N:148:VAL:HG23	25:N:148:VAL:O	1.96	0.65
26:O:242:LEU:O	30:s:201:ARG:NH2	2.29	0.65
28:Q:108:ASP:OD1	28:Q:109:GLU:N	2.30	0.65
30:S:100:LEU:HD11	30:S:116:ILE:HD11	1.78	0.65
32:f:264:GLU:OE1	32:f:264:GLU:N	2.30	0.65
3:W:326:MET:SD	3:W:327:GLU:N	2.70	0.65
13:B:356:PRO:O	13:B:361:LYS:NZ	2.22	0.65
7:a:236:THR:HG22	7:a:251:LEU:HD13	1.77	0.65
12:A:371:GLU:N	12:A:371:GLU:OE1	2.28	0.65
16:E:238:ILE:HG22	16:E:238:ILE:O	1.97	0.65
18:G:114:LEU:HD22	18:G:140:LEU:HD21	1.78	0.65
18:G:138:MET:CE	18:G:140:LEU:HD11	2.27	0.65
32:f:386:GLY:HA2	32:f:418:LEU:HD23	1.77	0.65
1:U:798:PRO:O	1:U:880:ASN:ND2	2.30	0.65
1:U:697:GLN:O	1:U:698:GLN:NE2	2.30	0.64
9:c:177:THR:HG23	9:c:177:THR:O	1.96	0.64
21:J:89:VAL:HG22	28:Q:66:LEU:HD21	1.79	0.64
32:f:479:LEU:HD21	32:f:513:GLU:HB3	1.78	0.64
2:V:343:PRO:O	11:e:43:TRP:NE1	2.30	0.64
5:Y:228:MET:HE1	5:Y:259:TYR:CZ	2.33	0.64
6:Z:74:TYR:OH	9:c:98:MET:O	2.13	0.64
13:B:78:PHE:HB2	32:f:613:LEU:HD21	1.78	0.64
14:C:362:VAL:CG2	14:C:390:VAL:HG21	2.28	0.64
32:f:535:THR:O	32:f:539:LEU:HD23	1.97	0.64
1:U:437:TYR:CD1	1:U:472:ILE:HG21	2.32	0.64
1:U:603:LEU:HB3	15:D:60:TYR:CD1	2.32	0.64
9:c:57:MET:HE3	9:c:69:VAL:HG21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:477:HIS:ND1	10:d:342:TYR:OH	2.29	0.64
12:A:55:LEU:CD2	13:B:73:LEU:HD22	2.27	0.64
16:E:325:GLU:OE1	16:E:325:GLU:N	2.30	0.64
31:T:78:LEU:HD13	25:n:168:TYR:CZ	2.32	0.64
28:q:119:ASP:OD1	28:q:120:TYR:N	2.30	0.64
9:c:117:GLY:N	9:c:146:ASP:OD1	2.31	0.64
16:E:148:VAL:HG21	16:E:297:ARG:HG3	1.79	0.64
25:N:169:ILE:HG21	25:N:197:ALA:HB2	1.78	0.64
12:A:201:PHE:HZ	17:F:408:LEU:HD22	1.63	0.64
14:C:161:ILE:CD1	14:C:186:VAL:HG11	2.28	0.64
30:S:59:GLU:OE2	30:S:64:HIS:ND1	2.30	0.64
31:t:95:MET:HE1	31:t:235:ALA:O	1.98	0.64
3:W:112:VAL:HG22	3:W:124:LEU:CD2	2.28	0.64
6:Z:104:ASN:O	6:Z:108:ILE:HD12	1.98	0.64
12:A:433:ASN:H	22:K:82:ILE:HD11	1.62	0.64
13:B:249:ARG:NH1	14:C:284:GLU:OE2	2.30	0.64
29:r:60:THR:N	29:r:229:SER:OG	2.31	0.64
2:V:458:VAL:HG23	2:V:458:VAL:O	1.98	0.64
9:c:303:MET:CE	10:d:335:LEU:HD22	2.28	0.63
14:C:254:ILE:O	14:C:254:ILE:HG23	1.98	0.63
28:Q:170:ARG:NE	29:r:199:ASP:OD2	2.25	0.63
32:f:463:LEU:HD22	32:f:494:ARG:NH2	2.13	0.63
1:U:532:MET:HE1	1:U:555:VAL:HG21	1.78	0.63
4:X:43:VAL:HG21	4:X:77:LEU:HD12	1.80	0.63
12:A:180:CYS:SG	35:A:501:ATP:N6	2.71	0.63
27:P:37:THR:HG22	27:P:37:THR:O	1.97	0.63
1:U:161:ASP:OD1	1:U:162:VAL:N	2.30	0.63
25:N:169:ILE:CG2	25:N:197:ALA:HB2	2.27	0.63
14:C:280:LEU:HD21	14:C:291:VAL:HG21	1.79	0.63
25:n:117:PHE:CD2	25:n:134:ILE:HD11	2.32	0.63
17:F:86:LEU:O	17:F:88:TYR:N	2.31	0.63
13:B:95:GLU:O	13:B:99:VAL:HG23	1.98	0.63
1:U:49:TYR:CE1	1:U:61:ALA:HB2	2.33	0.63
3:W:440:ASN:O	3:W:443:THR:HG22	1.98	0.63
14:C:372:ARG:NH1	15:D:175:GLN:OE1	2.32	0.63
21:J:199:VAL:HG21	21:J:206:ILE:HD11	1.80	0.63
30:S:179:ASN:ND2	27:p:173:ASN:OD1	2.31	0.63
1:U:563:ALA:O	1:U:567:ILE:HD12	1.99	0.63
3:W:451:MET:HE2	6:Z:101:LEU:CD1	2.29	0.63
6:Z:67:VAL:HG23	8:b:92:VAL:HG23	1.81	0.63
22:K:230:THR:OG1	22:K:233:GLU:OE1	2.07	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:s:194:LEU:HD21	30:s:199:ALA:HB2	1.81	0.63
29:R:63:LEU:HD13	29:R:198:MET:SD	2.39	0.62
31:T:137:LEU:HD11	31:T:155:MET:HE1	1.80	0.62
31:t:245:GLU:OE1	31:t:245:GLU:N	2.32	0.62
32:f:208:LEU:HD13	32:f:217:LEU:HB2	1.80	0.62
16:E:50:LEU:HD22	17:F:79:LYS:HE3	1.80	0.62
17:F:392:ASN:N	17:F:395:GLN:OE1	2.32	0.62
1:U:517:GLY:HA2	1:U:555:VAL:HG23	1.79	0.62
1:U:641:SER:OG	1:U:675:MET:SD	2.45	0.62
5:Y:22:LEU:CD1	5:Y:37:VAL:HG23	2.29	0.62
6:Z:142:GLU:OE2	6:Z:143:GLU:N	2.32	0.62
10:d:272:ALA:O	10:d:276:GLU:OE1	2.18	0.62
24:M:190:ILE:O	24:M:194:VAL:HG23	1.99	0.62
30:S:96:ILE:O	30:S:100:LEU:HD23	1.99	0.62
7:a:77:VAL:HG12	7:a:113:LEU:HD22	1.81	0.62
15:D:219:VAL:O	15:D:220:ALA:HB3	2.00	0.62
31:T:91:ASN:OD1	31:T:94:THR:N	2.32	0.62
27:P:12:MET:HG3	27:P:138:VAL:HG12	1.82	0.62
30:S:67:ASP:O	30:S:68:SER:OG	2.15	0.62
31:T:224:ARG:NH2	26:o:178:MET:HE2	2.15	0.62
32:f:333:LEU:O	32:f:333:LEU:HD23	1.99	0.62
10:d:272:ALA:O	10:d:275:ILE:N	2.33	0.62
12:A:125:LEU:N	12:A:148:GLN:OE1	2.33	0.62
25:N:117:PHE:CE1	25:N:132:ILE:HD13	2.35	0.62
25:N:155:VAL:HG21	31:T:81:PHE:CD2	2.35	0.62
2:V:90:GLU:O	2:V:92:ARG:N	2.33	0.62
14:C:161:ILE:HD11	14:C:186:VAL:HG11	1.82	0.62
32:f:520:LEU:HD23	32:f:560:LEU:HD22	1.82	0.62
4:X:105:GLN:NE2	4:X:108:GLU:OE2	2.32	0.62
9:c:51:MET:HE1	17:F:156:ASP:OD2	2.00	0.62
28:Q:172:ILE:HD11	28:q:22:ALA:HB2	1.81	0.62
32:f:520:LEU:CD2	32:f:560:LEU:HD22	2.30	0.62
2:V:256:ARG:NH2	11:e:21:GLU:OE2	2.33	0.61
7:a:232:TRP:CZ2	7:a:254:ALA:HB3	2.34	0.61
22:K:58:LEU:HD23	22:K:58:LEU:O	2.00	0.61
26:O:60:ASP:HB2	26:O:206:ILE:HD11	1.82	0.61
1:U:357:LYS:NZ	1:U:389:ASN:OD1	2.24	0.61
11:e:17:ASP:OD1	11:e:18:GLU:N	2.33	0.61
30:s:93:THR:O	30:s:97:GLU:OE1	2.17	0.61
4:X:371:ASP:OD1	5:Y:233:ARG:NH1	2.34	0.61
17:F:395:GLN:O	17:F:399:VAL:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:n:117:PHE:HD2	25:n:134:ILE:HD11	1.65	0.61
8:b:51:LEU:HD11	8:b:75:LEU:HD12	1.81	0.61
27:P:176:ASP:OD2	30:s:185:ASN:ND2	2.33	0.61
5:Y:105:MET:HE3	5:Y:105:MET:O	2.00	0.61
29:R:200:ARG:HG3	28:q:142:ILE:HD12	1.82	0.61
32:f:234:THR:O	32:f:237:VAL:HG12	2.00	0.61
12:A:130:ALA:HB3	12:A:133:ASP:CG	2.26	0.61
18:G:40:VAL:HG23	18:G:202:LEU:HD21	1.83	0.61
21:J:73:PHE:CE2	21:J:80:ALA:HB2	2.35	0.61
23:L:26:MET:O	23:L:29:VAL:HG12	2.01	0.61
29:R:219:ILE:O	29:R:223:THR:HG23	2.00	0.61
6:Z:121:LEU:HD23	6:Z:122:VAL:N	2.16	0.61
6:Z:173:GLU:OE2	6:Z:180:LYS:NZ	2.34	0.61
12:A:23:ARG:NH2	32:f:44:GLU:O	2.33	0.61
15:D:314:ALA:HA	15:D:317:LEU:HD13	1.81	0.61
22:K:171:GLY:O	22:K:174:SER:OG	2.14	0.61
3:W:163:ALA:HA	3:W:192:LEU:HD23	1.82	0.61
7:a:258:GLN:OE1	7:a:260:ASP:N	2.33	0.61
24:M:10:LEU:O	24:M:11:SER:OG	2.15	0.61
5:Y:360:ASP:OD1	5:Y:361:SER:N	2.32	0.61
6:Z:40:LEU:CD2	6:Z:91:ILE:HD13	2.30	0.61
7:a:84:VAL:HG21	7:a:97:LEU:HD11	1.83	0.61
12:A:221:GLY:N	35:A:501:ATP:O2B	2.34	0.61
1:U:5:ALA:O	1:U:9:ILE:HD12	1.99	0.61
10:d:148:LEU:HD21	10:d:170:GLN:HB2	1.83	0.61
13:B:305:ILE:HG13	14:C:224:ILE:HD11	1.82	0.61
31:T:251:GLU:OE1	31:T:251:GLU:N	2.33	0.61
25:n:38:MET:HE1	25:n:193:ALA:HB3	1.82	0.61
18:G:80:MET:HE1	18:G:138:MET:HB2	1.83	0.60
26:O:262:LEU:HD23	27:P:195:ILE:HD12	1.82	0.60
4:X:69:LEU:O	4:X:73:VAL:HG22	2.00	0.60
6:Z:17:LEU:HD21	9:c:217:LEU:CD2	2.31	0.60
25:N:155:VAL:HG21	31:T:81:PHE:CE2	2.36	0.60
32:f:502:LEU:HD22	32:f:537:THR:HG21	1.83	0.60
15:D:380:GLN:HG2	15:D:384:MET:HE2	1.83	0.60
29:r:189:SER:OG	29:r:226:ASP:OD2	2.11	0.60
32:f:648:ALA:O	32:f:652:VAL:HG23	2.02	0.60
7:a:180:LEU:HD13	7:a:221:VAL:HG21	1.83	0.60
5:Y:134:LEU:O	5:Y:138:LEU:HD23	2.02	0.60
32:f:543:MET:HE1	32:f:583:VAL:HG22	1.83	0.60
32:f:656:GLY:O	32:f:660:ILE:HD12	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:363:LEU:HD21	2:V:398:LEU:CD2	2.31	0.60
13:B:68:ILE:HG23	32:f:670:MET:HE3	1.84	0.60
29:r:203:SER:H	29:r:206:LEU:HD11	1.65	0.60
31:t:252:THR:OG1	31:t:254:TRP:NE1	2.31	0.60
32:f:65:GLU:OE1	32:f:67:ASP:N	2.34	0.60
2:V:251:LEU:HD11	2:V:270:LEU:HD21	1.82	0.60
2:V:466:ILE:O	2:V:466:ILE:HG23	2.00	0.60
3:W:328:LEU:HD22	3:W:328:LEU:N	2.16	0.60
29:r:103:THR:OG1	29:r:159:MET:N	2.35	0.60
3:W:298:GLU:OE1	3:W:298:GLU:N	2.34	0.60
6:Z:23:PHE:CE2	6:Z:126:VAL:HG21	2.35	0.60
7:a:42:LEU:O	7:a:45:VAL:HG12	2.01	0.60
14:C:21:ARG:O	14:C:25:LEU:HD23	2.02	0.60
18:G:10:ASP:OD2	18:G:27:TYR:OH	2.13	0.60
18:G:134:LEU:O	18:G:134:LEU:HD12	2.02	0.60
5:Y:297:ARG:NH1	11:e:45:ASP:OD1	2.35	0.60
8:b:117:VAL:O	8:b:152:LYS:NZ	2.32	0.60
12:A:294:GLU:O	12:A:298:THR:HG23	2.02	0.60
28:q:12:TYR:HB2	28:q:182:ILE:HD11	1.83	0.60
4:X:265:GLU:N	4:X:265:GLU:OE1	2.34	0.60
15:D:381:GLU:HA	15:D:384:MET:HE3	1.82	0.60
10:d:171:LEU:HD13	10:d:191:LEU:CD2	2.32	0.59
16:E:172:LEU:HD11	16:E:183:LEU:HD23	1.84	0.59
16:E:180:LYS:CG	16:E:301:ILE:HD11	2.32	0.59
18:G:189:TRP:CH2	18:G:197:THR:HG21	2.36	0.59
31:T:87:ILE:HG21	31:T:235:ALA:HB2	1.84	0.59
27:p:67:LEU:HD21	27:p:87:LEU:HD21	1.82	0.59
32:f:344:VAL:O	32:f:348:ILE:HD12	2.02	0.59
22:K:7:GLU:N	22:K:7:GLU:OE1	2.35	0.59
1:U:550:VAL:O	1:U:554:LEU:HD23	2.02	0.59
2:V:65:ARG:O	2:V:69:THR:HG23	2.02	0.59
9:c:27:THR:N	9:c:176:GLN:O	2.34	0.59
2:V:314:ARG:NE	5:Y:378:ASN:OD1	2.36	0.59
10:d:121:LEU:O	10:d:125:GLU:OE1	2.21	0.59
6:Z:213:GLU:OE1	7:a:350:LYS:NZ	2.35	0.59
8:b:32:ALA:HB1	8:b:183:LEU:CD1	2.32	0.59
14:C:62:GLU:OE2	15:D:117:SER:N	2.35	0.59
10:d:192:LEU:HD13	10:d:215:LEU:HD21	1.85	0.59
25:N:37:ILE:CD1	25:N:133:ILE:HD12	2.32	0.59
25:n:161:ILE:HD11	25:n:170:TYR:CD1	2.37	0.59
29:r:63:LEU:HD11	29:r:198:MET:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:s:176:LEU:HD23	30:s:206:VAL:HG12	1.84	0.59
32:f:378:ASN:O	32:f:382:ASN:ND2	2.36	0.59
10:d:148:LEU:HD21	10:d:170:GLN:CB	2.33	0.59
20:I:17:ARG:NH2	20:I:22:GLU:OE1	2.36	0.59
28:Q:170:ARG:NH1	28:q:27:GLN:O	2.36	0.59
4:X:256:LEU:HD22	4:X:319:ILE:HG13	1.85	0.59
15:D:387:VAL:CG2	16:E:162:VAL:HG21	2.33	0.59
29:r:233:VAL:HG21	29:r:254:LEU:CD1	2.31	0.59
3:W:33:LYS:O	3:W:37:GLU:OE1	2.21	0.59
32:f:466:LEU:HD11	32:f:481:SER:HA	1.85	0.59
19:H:189:HIS:ND1	19:H:233:ILE:HD11	2.18	0.59
28:Q:35:MET:HE1	28:Q:45:LEU:HD11	1.85	0.59
1:U:263:SER:O	1:U:267:ASN:ND2	2.36	0.58
3:W:328:LEU:CD2	3:W:341:PHE:HA	2.33	0.58
7:a:142:LEU:HD21	7:a:152:HIS:HD2	1.67	0.58
15:D:225:ALA:HB1	15:D:259:PRO:O	2.03	0.58
25:N:98:GLY:O	25:N:102:ILE:HD12	2.03	0.58
28:Q:190:ASP:OD1	28:Q:191:LEU:N	2.36	0.58
29:r:250:ASN:OD1	29:r:251:VAL:N	2.36	0.58
6:Z:39:LEU:HD23	6:Z:50:VAL:HG11	1.85	0.58
30:S:56:ARG:NH1	30:S:215:VAL:O	2.33	0.58
26:o:165:LEU:HD12	26:o:168:VAL:HG12	1.86	0.58
30:s:178:ASP:OD1	30:s:179:ASN:N	2.36	0.58
15:D:202:VAL:HG13	15:D:308:ILE:HG23	1.85	0.58
21:J:40:ILE:HD11	21:J:210:VAL:CG1	2.34	0.58
25:n:228:ILE:O	25:n:230:LYS:NZ	2.36	0.58
13:B:313:LEU:O	13:B:346:ARG:NH1	2.36	0.58
24:M:102:ASN:HA	25:N:119:GLU:OE2	2.04	0.58
2:V:192:MET:HE2	2:V:230:PHE:HE2	1.68	0.58
16:E:140:GLU:O	16:E:144:GLU:OE1	2.21	0.58
32:f:174:ASP:O	32:f:181:ARG:NH2	2.36	0.58
32:f:882:LEU:HD11	32:f:900:LEU:HD21	1.84	0.58
6:Z:23:PHE:CD2	6:Z:126:VAL:HG21	2.38	0.58
13:B:220:LYS:N	13:B:348:ASP:OD2	2.36	0.58
14:C:104:ASP:OD1	14:C:105:ILE:N	2.36	0.58
25:N:222:VAL:HG23	25:N:224:LEU:HD21	1.86	0.58
31:t:106:GLN:O	31:t:110:GLN:OE1	2.20	0.58
4:X:259:ILE:HD11	4:X:291:ALA:HB2	1.84	0.58
28:q:56:PHE:HZ	28:q:98:TYR:HB3	1.69	0.58
1:U:520:MET:CB	1:U:555:VAL:HG22	2.33	0.58
14:C:251:ILE:HG23	14:C:301:LEU:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:J:192:ILE:HD11	21:J:208:LEU:HD11	1.85	0.58
29:r:61:THR:N	29:r:76:ASP:OD2	2.36	0.58
3:W:220:GLU:O	3:W:224:LEU:HD13	2.04	0.58
7:a:103:LYS:O	7:a:105:LYS:NZ	2.36	0.58
26:O:206:ILE:HD13	26:O:212:SER:HB3	1.86	0.58
27:P:194:LYS:HE2	27:P:194:LYS:HA	1.86	0.58
29:r:156:MET:N	29:r:175:SER:OG	2.36	0.58
5:Y:105:MET:HE1	5:Y:124:PHE:HE1	1.67	0.57
5:Y:222:TYR:OH	5:Y:285:ASP:OD2	2.15	0.57
16:E:180:LYS:HG3	16:E:301:ILE:HD11	1.84	0.57
18:G:93:ARG:NH1	18:G:97:GLU:OE2	2.37	0.57
20:I:153:SER:OG	20:I:155:ASN:OD1	2.21	0.57
28:q:8:GLN:NE2	28:q:113:PRO:O	2.37	0.57
31:t:101:ASP:N	31:t:153:ASN:OD1	2.36	0.57
32:f:698:SER:O	32:f:732:VAL:HG23	2.03	0.57
15:D:219:VAL:O	15:D:220:ALA:CB	2.53	0.57
15:D:64:GLU:O	15:D:68:LEU:HD23	2.04	0.57
15:D:326:ARG:C	15:D:327:LEU:HD22	2.29	0.57
17:F:363:ALA:O	17:F:367:GLN:OE1	2.22	0.57
22:K:218:ALA:HB2	22:K:228:MET:CE	2.34	0.57
30:s:96:ILE:O	30:s:100:LEU:HD23	2.04	0.57
14:C:386:ALA:O	14:C:390:VAL:HG22	2.05	0.57
18:G:50:ILE:HG23	18:G:141:ILE:HG21	1.87	0.57
28:Q:44:LEU:HD23	28:Q:45:LEU:N	2.19	0.57
31:t:71:MET:SD	31:t:231:ARG:HB3	2.45	0.57
1:U:658:ILE:HG23	1:U:763:VAL:HG11	1.85	0.57
5:Y:182:VAL:O	5:Y:186:LEU:HD23	2.05	0.57
8:b:61:LEU:O	8:b:74:LYS:NZ	2.24	0.57
9:c:156:VAL:HG13	9:c:156:VAL:O	2.05	0.57
14:C:376:VAL:O	14:C:376:VAL:HG12	2.04	0.57
14:C:399:MET:HE1	20:I:56:LEU:HD11	1.87	0.57
21:J:36:ARG:NE	21:J:142:PRO:O	2.38	0.57
31:T:96:LEU:HD11	31:T:155:MET:SD	2.44	0.57
32:f:48:GLU:OE1	32:f:48:GLU:N	2.38	0.57
32:f:554:TYR:OH	32:f:814:SER:OG	2.03	0.57
3:W:231:ILE:HG23	3:W:243:ILE:HG23	1.86	0.57
16:E:98:VAL:HG13	16:E:107:ILE:HG23	1.85	0.57
30:S:239:ARG:NH2	30:S:241:ASP:OD1	2.37	0.57
2:V:176:MET:SD	2:V:217:VAL:HG12	2.44	0.57
14:C:188:LEU:HD22	14:C:317:PHE:HE2	1.70	0.57
15:D:309:MET:HE1	15:D:321:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:179:LYS:C	24:M:180:LEU:HD12	2.29	0.57
7:a:28:LEU:HD22	7:a:37:LEU:HB3	1.86	0.57
18:G:116:LYS:NZ	26:O:112:SER:OG	2.35	0.57
29:r:117:LEU:O	29:r:121:GLN:OE1	2.22	0.57
32:f:309:GLU:OE1	32:f:309:GLU:N	2.37	0.57
2:V:211:TYR:OH	2:V:234:ARG:NE	2.38	0.57
3:W:57:ALA:O	3:W:58:SER:OG	2.19	0.57
3:W:445:LEU:HD22	6:Z:226:ILE:CD1	2.33	0.57
5:Y:315:THR:HG23	5:Y:318:TYR:H	1.69	0.57
9:c:167:MET:HA	9:c:167:MET:HE3	1.86	0.57
12:A:131:PRO:HA	12:A:134:ILE:HD12	1.86	0.57
13:B:342:ILE:O	13:B:342:ILE:HG22	2.03	0.57
31:T:137:LEU:HD21	31:T:155:MET:HE3	1.85	0.57
13:B:69:LYS:O	13:B:73:LEU:HD23	2.04	0.57
27:p:12:MET:HB2	27:p:138:VAL:HG12	1.86	0.57
10:d:207:GLU:O	10:d:211:GLU:OE1	2.23	0.56
29:R:100:LEU:C	29:R:101:LEU:HD12	2.30	0.56
2:V:469:THR:HG22	2:V:470:ARG:H	1.69	0.56
6:Z:22:HIS:ND1	6:Z:95:TYR:OH	2.33	0.56
13:B:192:ASN:O	13:B:196:GLU:OE1	2.23	0.56
13:B:302:GLU:OE1	13:B:302:GLU:N	2.38	0.56
19:H:4:ARG:O	19:H:7:SER:OG	2.14	0.56
28:Q:99:HIS:ND1	28:Q:99:HIS:O	2.38	0.56
30:S:96:ILE:HD11	30:S:120:LEU:HD11	1.88	0.56
1:U:19:LEU:CD1	10:d:124:LEU:HD13	2.34	0.56
1:U:32:ASN:O	2:V:232:HIS:ND1	2.38	0.56
1:U:899:ARG:NH1	1:U:920:ASP:OD2	2.38	0.56
4:X:312:GLU:OE1	4:X:312:GLU:N	2.38	0.56
7:a:37:LEU:HD21	7:a:67:PHE:CZ	2.40	0.56
7:a:108:ASP:OD1	7:a:109:GLU:N	2.38	0.56
7:a:210:VAL:HG23	7:a:210:VAL:O	2.06	0.56
9:c:210:ASN:OD1	9:c:211:GLU:N	2.38	0.56
17:F:425:LEU:HD21	23:L:166:GLN:NE2	2.20	0.56
21:J:195:LEU:O	21:J:199:VAL:HG22	2.05	0.56
21:J:201:SER:OG	21:J:204:LYS:N	2.37	0.56
25:N:138:ASP:OD2	25:N:144:GLN:NE2	2.38	0.56
25:n:41:GLN:OE1	25:n:156:ARG:NH2	2.38	0.56
27:p:36:THR:HG21	28:q:127:ALA:HB2	1.88	0.56
30:s:57:LEU:HD13	30:s:68:SER:OG	2.05	0.56
32:f:490:ALA:HB2	32:f:524:MET:HE1	1.86	0.56
32:f:530:CYS:SG	32:f:566:HIS:ND1	2.75	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:367:VAL:HG23	2:V:402:VAL:HG22	1.86	0.56
3:W:443:THR:HG21	6:Z:204:LYS:HD2	1.86	0.56
17:F:272:PHE:CE1	17:F:328:VAL:HG12	2.41	0.56
23:L:35:THR:HG22	23:L:48:ALA:HB1	1.87	0.56
27:P:138:VAL:HG11	27:P:146:MET:HB3	1.87	0.56
28:q:25:ILE:HG23	28:q:26:VAL:HG23	1.87	0.56
1:U:151:ILE:HD11	1:U:179:TYR:HD1	1.71	0.56
1:U:568:GLU:OE1	1:U:601:ARG:NH2	2.38	0.56
1:U:894:MET:N	1:U:894:MET:SD	2.78	0.56
2:V:281:ASN:OD1	2:V:282:ASN:N	2.39	0.56
19:H:182:LEU:HD11	19:H:186:ASP:OD2	2.05	0.56
12:A:388:VAL:HG21	12:A:417:ILE:HD11	1.88	0.56
15:D:309:MET:HE2	15:D:327:LEU:HD11	1.86	0.56
16:E:306:GLU:OE2	16:E:309:ARG:NH2	2.39	0.56
20:I:89:GLU:OE2	20:I:117:ILE:HG21	2.06	0.56
32:f:573:ILE:HA	32:f:576:ILE:HG22	1.86	0.56
1:U:891:VAL:O	1:U:891:VAL:HG13	2.05	0.56
3:W:272:LEU:HD22	3:W:340:VAL:HG21	1.86	0.56
4:X:53:LEU:HD22	4:X:69:LEU:HD21	1.86	0.56
13:B:292:THR:HG21	14:C:261:GLY:HA3	1.87	0.56
27:P:149:MET:HE2	30:s:175:PRO:HB2	1.88	0.56
12:A:238:ILE:HG21	12:A:272:ILE:HG23	1.86	0.56
15:D:358:VAL:HG21	15:D:399:PHE:CE2	2.41	0.56
19:H:69:THR:HG22	19:H:70:LYS:H	1.70	0.56
23:L:178:GLU:OE1	23:L:178:GLU:N	2.39	0.56
24:M:70:VAL:HG23	24:M:70:VAL:O	2.05	0.56
28:q:161:ARG:NE	28:q:165:GLU:OE2	2.39	0.56
29:r:103:THR:HG21	29:r:159:MET:HE3	1.88	0.56
3:W:60:MET:HE2	16:E:326:ILE:HG23	1.88	0.56
3:W:301:LYS:HE3	3:W:324:TYR:CD1	2.41	0.56
3:W:369:TYR:CD2	7:a:312:MET:HE1	2.41	0.56
13:B:44:ASP:N	13:B:246:THR:OG1	2.38	0.56
18:G:73:THR:OG1	18:G:108:GLU:OE2	2.14	0.56
20:I:118:LYS:O	20:I:122:THR:HG23	2.05	0.56
29:R:250:ASN:OD1	29:R:251:VAL:N	2.39	0.56
30:s:214:ASP:OD1	30:s:215:VAL:N	2.39	0.56
3:W:28:LEU:CD2	3:W:47:LEU:HD11	2.36	0.56
4:X:114:ILE:HD13	4:X:130:GLU:OE1	2.06	0.56
7:a:149:THR:HG22	7:a:150:SER:N	2.21	0.56
15:D:326:ARG:O	15:D:327:LEU:HD22	2.06	0.56
20:I:167:ASN:ND2	20:I:200:THR:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:J:99:GLU:OE1	29:R:179:ARG:NH2	2.36	0.56
30:s:41:LEU:HD12	30:s:42:ALA:H	1.69	0.56
32:f:327:ASN:OD1	32:f:328:SER:N	2.39	0.56
2:V:113:LEU:HD23	2:V:135:LEU:HD21	1.88	0.55
6:Z:167:ALA:HB1	9:c:42:LEU:HD23	1.87	0.55
7:a:211:PHE:CD2	7:a:319:LEU:HD21	2.41	0.55
7:a:214:GLY:O	7:a:215:GLU:HB3	2.05	0.55
16:E:61:LEU:HD11	16:E:72:LYS:HB2	1.86	0.55
20:I:95:GLN:HG3	27:P:73:LEU:HD22	1.87	0.55
28:Q:154:GLU:O	28:Q:158:GLU:OE1	2.24	0.55
31:T:51:VAL:HG22	31:T:75:TYR:HB2	1.88	0.55
31:t:50:MET:HA	31:t:50:MET:HE3	1.87	0.55
15:D:231:VAL:HG11	16:E:259:GLU:OE1	2.06	0.55
28:Q:154:GLU:OE1	28:Q:154:GLU:N	2.40	0.55
26:o:245:TYR:O	26:o:249:LYS:NZ	2.28	0.55
1:U:588:MET:HE2	1:U:588:MET:HA	1.87	0.55
1:U:658:ILE:HD11	1:U:767:THR:HG21	1.87	0.55
10:d:335:LEU:HD23	10:d:335:LEU:C	2.31	0.55
16:E:141:GLN:OE1	16:E:141:GLN:N	2.37	0.55
22:K:35:SER:OG	22:K:51:GLU:O	2.08	0.55
25:n:170:TYR:OH	31:t:80:ARG:NE	2.39	0.55
28:q:161:ARG:O	28:q:165:GLU:OE1	2.24	0.55
2:V:278:GLU:OE1	2:V:278:GLU:N	2.39	0.55
2:V:391:THR:O	2:V:395:ILE:N	2.38	0.55
16:E:98:VAL:CG1	16:E:107:ILE:HG23	2.35	0.55
31:T:69:ALA:HB3	31:T:87:ILE:HD11	1.88	0.55
31:t:87:ILE:HG21	31:t:235:ALA:CB	2.36	0.55
3:W:118:LEU:HD12	3:W:152:ILE:CG2	2.36	0.55
7:a:163:TYR:HA	7:a:166:ILE:HG22	1.88	0.55
32:f:761:MET:HA	32:f:761:MET:HE3	1.87	0.55
1:U:37:GLU:HA	2:V:269:LYS:HZ3	1.71	0.55
22:K:5:ARG:NH1	22:K:26:TYR:OH	2.39	0.55
23:L:84:LEU:HD12	23:L:130:VAL:HG21	1.89	0.55
28:q:38:MET:HE2	28:q:38:MET:HA	1.89	0.55
4:X:398:GLU:O	4:X:402:GLU:OE1	2.24	0.55
8:b:140:ILE:HG21	8:b:153:LEU:HG	1.88	0.55
10:d:232:LEU:HD13	10:d:244:VAL:HG23	1.89	0.55
24:M:214:LEU:HB2	24:M:228:VAL:HG21	1.89	0.55
25:n:71:ILE:HD12	25:n:75:ILE:HG22	1.89	0.55
27:p:155:GLU:HG3	27:p:158:MET:HE3	1.89	0.55
16:E:122:MET:SD	16:E:198:VAL:HG22	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Q:38:MET:HE1	28:Q:60:ILE:HG22	1.87	0.55
29:R:233:VAL:HG21	29:R:254:LEU:HD12	1.87	0.55
31:T:114:GLN:O	31:T:118:ASP:OD1	2.25	0.55
31:T:169:TYR:CG	31:T:169:TYR:O	2.59	0.55
1:U:327:LYS:O	1:U:330:SER:OG	2.24	0.55
3:W:94:ARG:O	3:W:96:GLN:N	2.39	0.55
3:W:451:MET:HE3	6:Z:100:LYS:HA	1.88	0.55
7:a:296:ILE:HG21	7:a:307:VAL:HG13	1.87	0.55
9:c:38:LEU:HD22	9:c:207:TYR:HE2	1.71	0.55
26:O:261:PRO:HA	27:P:194:LYS:HZ1	1.72	0.55
29:R:170:LEU:HD22	29:R:185:PHE:HD2	1.72	0.55
2:V:176:MET:CG	2:V:217:VAL:HG12	2.37	0.55
3:W:190:MET:HE1	3:W:206:SER:HA	1.89	0.55
6:Z:143:GLU:O	6:Z:151:THR:OG1	2.25	0.55
7:a:119:GLY:O	7:a:123:LEU:HD23	2.06	0.55
13:B:396:LYS:NZ	35:B:501:ATP:O3'	2.38	0.55
17:F:93:VAL:O	17:F:93:VAL:HG12	2.06	0.55
23:L:88:MET:CE	23:L:132:LEU:HD13	2.37	0.55
25:n:38:MET:HE2	25:n:194:LEU:HG	1.89	0.55
25:n:157:GLN:NE2	25:n:160:ALA:HB2	2.22	0.55
26:o:59:ALA:HB3	26:o:77:ILE:HD11	1.87	0.55
2:V:164:GLU:OE1	2:V:164:GLU:N	2.40	0.54
18:G:138:MET:HE2	18:G:140:LEU:HD11	1.89	0.54
23:L:33:SER:HG	23:L:62:LYS:NZ	2.03	0.54
25:n:93:VAL:HG11	25:n:117:PHE:CE1	2.42	0.54
1:U:632:GLN:O	1:U:635:SER:OG	2.24	0.54
1:U:740:GLY:O	1:U:743:ASN:ND2	2.40	0.54
2:V:484:LEU:HD23	6:Z:267:ARG:HH21	1.71	0.54
13:B:143:LEU:O	13:B:143:LEU:HD23	2.07	0.54
14:C:105:ILE:HA	14:C:108:VAL:HG22	1.88	0.54
16:E:92:LEU:HD11	16:E:107:ILE:HG21	1.89	0.54
23:L:162:GLY:O	23:L:165:SER:OG	2.20	0.54
32:f:244:GLU:O	32:f:248:LEU:HD23	2.08	0.54
32:f:388:ASP:OD1	32:f:389:LYS:N	2.40	0.54
10:d:123:LEU:O	10:d:126:LEU:C	2.50	0.54
16:E:210:GLU:OE2	16:E:213:ARG:NE	2.37	0.54
30:s:57:LEU:HD11	30:s:70:LYS:NZ	2.22	0.54
7:a:280:MET:HE2	7:a:280:MET:N	2.22	0.54
12:A:130:ALA:HB3	12:A:133:ASP:OD1	2.08	0.54
26:o:246:ARG:HD3	27:p:158:MET:HE1	1.90	0.54
16:E:39:GLN:NE2	17:F:76:ASN:OD1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E:363:VAL:N	16:E:366:ASP:OD2	2.40	0.54
25:N:37:ILE:HD12	25:N:133:ILE:HD12	1.89	0.54
27:P:67:LEU:CD1	27:P:91:VAL:HG22	2.35	0.54
32:f:472:HIS:CE1	32:f:514:VAL:HG11	2.42	0.54
5:Y:105:MET:HE1	5:Y:124:PHE:CE1	2.42	0.54
10:d:201:SER:CB	10:d:262:ILE:HG23	2.36	0.54
18:G:50:ILE:CG2	18:G:141:ILE:HG21	2.38	0.54
20:I:203:VAL:HG13	20:I:203:VAL:O	2.08	0.54
28:Q:164:LEU:HD12	28:Q:178:PHE:CE1	2.43	0.54
25:n:129:MET:HE1	25:n:150:MET:HE2	1.89	0.54
26:o:206:ILE:HG22	26:o:207:PHE:HD1	1.72	0.54
27:p:13:ALA:HB2	27:p:22:ILE:CD1	2.38	0.54
2:V:259:LEU:HD21	2:V:295:ILE:CD1	2.37	0.54
4:X:163:LYS:HB2	4:X:200:ILE:HD13	1.90	0.54
12:A:140:VAL:HB	12:A:149:ILE:HG21	1.90	0.54
22:K:50:VAL:CG1	22:K:67:ILE:HD11	2.37	0.54
22:K:50:VAL:HG13	22:K:67:ILE:HD11	1.90	0.54
24:M:50:VAL:CG2	24:M:67:LEU:HD11	2.38	0.54
28:q:138:LEU:H	28:q:138:LEU:HD12	1.73	0.54
29:r:142:LEU:HD22	29:r:173:VAL:CG2	2.37	0.54
31:t:173:LEU:O	31:t:173:LEU:HD23	2.07	0.54
32:f:327:ASN:O	32:f:331:LEU:HD23	2.08	0.54
9:c:183:HIS:O	9:c:184:LEU:HB2	2.07	0.54
29:R:94:ILE:HD13	29:R:115:GLU:OE1	2.07	0.54
7:a:235:ASP:OD2	7:a:251:LEU:HD11	2.08	0.54
10:d:164:PHE:CG	10:d:168:MET:HE1	2.42	0.54
13:B:405:MET:HE2	13:B:421:LYS:HG2	1.90	0.54
1:U:835:ILE:HG21	32:f:241:PRO:HG3	1.89	0.54
3:W:84:ASN:OD1	3:W:85:GLU:N	2.41	0.54
14:C:24:TYR:O	14:C:28:ILE:HG12	2.07	0.54
14:C:115:ALA:C	14:C:116:LEU:HD12	2.33	0.54
14:C:365:GLU:OE2	15:D:329:ARG:NH1	2.41	0.54
15:D:181:VAL:HG21	15:D:308:ILE:HD11	1.90	0.54
16:E:71:VAL:CG2	16:E:100:LEU:HD11	2.37	0.54
18:G:180:GLU:HA	18:G:183:VAL:HG12	1.90	0.54
18:G:72:ILE:HD11	18:G:78:CYS:SG	2.49	0.53
31:T:144:ARG:NH2	31:T:149:ASN:OD1	2.41	0.53
32:f:716:ASP:OD1	32:f:717:ALA:N	2.41	0.53
1:U:527:GLN:NE2	1:U:531:ASP:OD2	2.41	0.53
3:W:170:GLN:OE1	3:W:170:GLN:HA	2.08	0.53
4:X:385:LEU:HD23	4:X:385:LEU:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:n:161:ILE:HD11	25:n:170:TYR:CE1	2.43	0.53
1:U:503:GLN:O	1:U:535:TYR:OH	2.27	0.53
3:W:118:LEU:HD13	3:W:121:LYS:HE2	1.89	0.53
4:X:365:LEU:HD22	4:X:385:LEU:HD11	1.90	0.53
6:Z:263:ALA:HB1	9:c:288:VAL:HG23	1.91	0.53
13:B:361:LYS:HB2	13:B:384:ILE:HG23	1.91	0.53
18:G:43:ARG:NH1	18:G:163:PHE:O	2.41	0.53
27:P:24:ALA:CB	27:P:42:ILE:HD11	2.38	0.53
28:q:147:TYR:CE1	28:q:151:ILE:HG21	2.44	0.53
1:U:524:LYS:O	1:U:524:LYS:HG2	2.08	0.53
3:W:259:GLU:OE1	3:W:261:GLU:N	2.42	0.53
4:X:24:ILE:HG13	4:X:56:LEU:HD13	1.90	0.53
5:Y:112:CYS:SG	5:Y:147:ILE:HD11	2.48	0.53
13:B:255:LEU:HD12	13:B:290:ILE:HD11	1.91	0.53
14:C:40:GLN:HA	14:C:40:GLN:OE1	2.09	0.53
15:D:293:LEU:HD21	15:D:320:ALA:HB3	1.90	0.53
16:E:309:ARG:HG3	16:E:343:LEU:HD11	1.91	0.53
22:K:191:LEU:HD21	22:K:219:THR:OG1	2.07	0.53
30:s:226:VAL:HG22	30:s:231:ILE:HD13	1.89	0.53
1:U:141:CYS:SG	14:C:20:LEU:HD12	2.49	0.53
1:U:151:ILE:HD11	1:U:179:TYR:CD1	2.43	0.53
1:U:330:SER:OG	1:U:332:GLU:OE1	2.23	0.53
5:Y:162:GLU:OE2	5:Y:166:SER:OG	2.25	0.53
5:Y:221:THR:HG22	5:Y:256:VAL:HG21	1.91	0.53
10:d:91:ALA:HA	10:d:94:MET:SD	2.48	0.53
13:B:79:ILE:O	13:B:83:GLU:OE1	2.26	0.53
17:F:198:LEU:HD21	17:F:202:ILE:HD12	1.91	0.53
25:N:48:LEU:HD21	25:N:135:ALA:HB3	1.91	0.53
30:S:66:ARG:NH2	26:o:207:PHE:O	2.42	0.53
29:r:104:MET:HE1	29:r:112:SER:OG	2.09	0.53
3:W:118:LEU:HD12	3:W:152:ILE:HG23	1.89	0.53
4:X:380:GLN:HG2	5:Y:314:LEU:HD12	1.90	0.53
7:a:180:LEU:HD12	7:a:200:LEU:HD11	1.91	0.53
12:A:95:VAL:HG11	13:B:122:ILE:HD12	1.91	0.53
25:N:174:ASP:CG	25:n:200:ARG:HE	2.17	0.53
2:V:184:ALA:O	2:V:187:ILE:HG22	2.09	0.53
2:V:443:ARG:HH12	10:d:274:CYS:HA	1.74	0.53
6:Z:231:GLN:NE2	7:a:341:LEU:HD11	2.23	0.53
12:A:101:ILE:O	12:A:101:ILE:HG22	2.07	0.53
15:D:88:VAL:HG22	16:E:79:TYR:CD1	2.43	0.53
17:F:362:ARG:NE	17:F:391:PHE:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:H:179:ASN:OD1	19:H:182:LEU:HD13	2.08	0.53
24:M:216:TRP:HE1	24:M:220:LEU:HD11	1.73	0.53
26:o:209:ASP:OD1	26:o:210:LEU:N	2.42	0.53
2:V:469:THR:HG22	2:V:470:ARG:N	2.24	0.53
3:W:183:VAL:HG11	3:W:222:LEU:HD21	1.89	0.53
10:d:87:VAL:HG12	10:d:126:LEU:HD11	1.91	0.53
15:D:305:VAL:O	15:D:305:VAL:HG12	2.09	0.53
16:E:331:ILE:HD11	16:E:367:PHE:HB3	1.90	0.53
19:H:50:LYS:NZ	19:H:209:GLU:OE2	2.23	0.53
28:q:8:GLN:O	28:q:147:TYR:OH	2.25	0.53
1:U:99:THR:HG21	2:V:240:LEU:HD12	1.91	0.53
2:V:352:SER:C	2:V:353:LEU:HD12	2.34	0.53
5:Y:227:SER:HB3	5:Y:231:LEU:HD12	1.91	0.53
12:A:125:LEU:CD1	12:A:134:ILE:HG21	2.39	0.53
16:E:312:ILE:HG21	16:E:343:LEU:HD12	1.91	0.53
17:F:93:VAL:HG23	17:F:149:ASP:O	2.09	0.53
20:I:108:GLU:OE1	21:J:57:ARG:NH2	2.42	0.53
29:R:223:THR:HG22	29:R:229:SER:O	2.09	0.53
25:n:112:THR:O	25:n:116:LEU:HD23	2.09	0.53
1:U:640:LEU:HD21	15:D:60:TYR:OH	2.09	0.53
3:W:83:LEU:HD11	3:W:87:ILE:HD11	1.90	0.53
5:Y:15:PRO:HG3	5:Y:147:ILE:HD13	1.91	0.53
12:A:258:ARG:O	12:A:262:GLU:OE1	2.27	0.53
23:L:117:GLN:O	23:L:120:THR:OG1	2.20	0.53
29:R:199:ASP:OD1	28:q:169:LYS:NZ	2.42	0.53
1:U:321:GLN:CD	1:U:324:LYS:HZ1	2.14	0.52
4:X:395:LYS:HB2	9:c:242:GLU:OE2	2.09	0.52
7:a:4:VAL:HB	7:a:5:PRO:HD3	1.91	0.52
9:c:41:MET:HG3	9:c:72:VAL:HG11	1.90	0.52
9:c:41:MET:SD	9:c:72:VAL:HG11	2.50	0.52
12:A:51:ASP:O	12:A:55:LEU:HD13	2.10	0.52
15:D:269:ALA:HB2	16:E:258:MET:HE3	1.91	0.52
17:F:388:THR:HG23	17:F:389:ASP:N	2.25	0.52
19:H:44:VAL:CG1	19:H:146:LEU:HD12	2.40	0.52
30:s:85:PHE:CE1	31:t:173:LEU:HD11	2.44	0.52
31:t:68:ALA:HB1	31:t:218:MET:HE2	1.91	0.52
3:W:275:ILE:HG23	3:W:309:PHE:CE2	2.43	0.52
8:b:100:ARG:NH1	8:b:102:GLY:O	2.42	0.52
8:b:166:THR:HG22	8:b:166:THR:O	2.10	0.52
9:c:38:LEU:HD22	9:c:207:TYR:CE2	2.44	0.52
12:A:125:LEU:HD23	12:A:126:SER:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:H:86:LEU:HD12	19:H:132:VAL:HG21	1.91	0.52
24:M:187:CYS:HA	24:M:190:ILE:HG22	1.90	0.52
25:n:36:THR:HG21	25:n:197:ALA:CB	2.38	0.52
28:q:45:LEU:O	28:q:102:LEU:HD13	2.09	0.52
32:f:560:LEU:HD11	32:f:798:THR:HA	1.91	0.52
4:X:15:LEU:O	4:X:19:ASP:C	2.51	0.52
17:F:225:MET:HE1	17:F:236:LEU:HD23	1.89	0.52
25:n:194:LEU:HD13	25:n:208:ILE:HG23	1.91	0.52
27:p:180:VAL:HG23	27:p:180:VAL:O	2.09	0.52
31:t:95:MET:HE2	31:t:237:VAL:CG1	2.38	0.52
1:U:188:MET:HE1	1:U:194:ARG:N	2.24	0.52
3:W:443:THR:HG21	6:Z:204:LYS:CD	2.39	0.52
6:Z:209:ARG:HD2	7:a:354:GLU:OE1	2.10	0.52
12:A:124:ASP:HB2	17:F:86:LEU:HD13	1.91	0.52
14:C:400:SER:OG	19:H:150:ASP:OD2	2.14	0.52
15:D:381:GLU:OE2	15:D:405:THR:OG1	2.21	0.52
18:G:192:GLU:OE1	18:G:192:GLU:N	2.41	0.52
28:Q:153:ARG:NH2	28:Q:184:ASP:OD2	2.42	0.52
30:S:176:LEU:HD23	30:S:206:VAL:HG12	1.92	0.52
31:T:118:ASP:O	31:T:122:LEU:HD23	2.09	0.52
1:U:352:ILE:O	1:U:356:THR:HG23	2.09	0.52
4:X:402:GLU:HB2	9:c:249:LEU:HD11	1.92	0.52
8:b:46:GLU:OE1	8:b:46:GLU:N	2.42	0.52
8:b:63:THR:HG22	8:b:64:LEU:N	2.24	0.52
12:A:257:VAL:HG22	12:A:261:PHE:CZ	2.45	0.52
26:O:94:ASP:OD1	27:P:99:ARG:NE	2.37	0.52
27:P:67:LEU:HD11	27:P:91:VAL:CG2	2.34	0.52
30:S:141:LEU:HD11	30:S:227:THR:CA	2.39	0.52
32:f:874:LEU:HD12	32:f:874:LEU:O	2.09	0.52
18:G:50:ILE:CG2	18:G:141:ILE:HD13	2.37	0.52
21:J:71:MET:HE3	21:J:131:ALA:CB	2.40	0.52
31:T:169:TYR:CD1	31:T:184:THR:HG22	2.43	0.52
31:t:52:THR:O	31:t:74:SER:N	2.39	0.52
32:f:331:LEU:O	32:f:335:ARG:HG3	2.09	0.52
2:V:168:GLN:NE2	2:V:187:ILE:HD11	2.25	0.52
4:X:27:LEU:HD12	4:X:56:LEU:HD12	1.91	0.52
4:X:138:PHE:HD2	4:X:176:THR:HG22	1.73	0.52
9:c:303:MET:HA	9:c:306:THR:HG22	1.91	0.52
12:A:355:PHE:CE1	12:A:385:ILE:HG23	2.45	0.52
23:L:115:LYS:NZ	23:L:128:TYR:OH	2.35	0.52
28:Q:35:MET:SD	28:Q:43:LEU:HD21	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:888:LEU:N	32:f:901:ARG:O	2.43	0.52
1:U:176:MET:HE2	1:U:176:MET:HA	1.92	0.52
3:W:366:MET:HE1	3:W:378:MET:HG3	1.92	0.52
4:X:103:THR:HG23	4:X:105:GLN:H	1.73	0.52
4:X:286:ALA:HB1	4:X:313:LEU:HD21	1.92	0.52
7:a:304:VAL:HG23	7:a:304:VAL:O	2.09	0.52
14:C:345:ARG:O	14:C:349:GLU:OE1	2.27	0.52
16:E:226:GLN:HA	16:E:227:PRO:C	2.34	0.52
16:E:235:ILE:HG22	16:E:279:THR:HB	1.91	0.52
26:O:80:ILE:HD11	26:O:86:CYS:SG	2.49	0.52
26:O:229:LEU:HD22	26:O:232:TYR:CD1	2.45	0.52
29:r:243:TRP:O	29:r:244:ILE:HG23	2.09	0.52
32:f:803:PHE:O	32:f:806:VAL:HG23	2.09	0.52
2:V:466:ILE:HD11	2:V:471:GLU:OE1	2.09	0.52
12:A:193:THR:HB	12:A:194:PRO:HD3	1.92	0.52
17:F:419:ASP:OD1	17:F:420:TYR:N	2.43	0.52
20:I:91:ARG:HG2	27:P:76:LEU:HD23	1.92	0.52
26:O:83:ASN:HD22	26:O:116:LEU:HD12	1.75	0.52
30:s:99:ARG:CD	30:s:123:ILE:HD11	2.39	0.52
31:t:238:THR:HG22	31:t:240:LYS:NZ	2.25	0.52
10:d:115:GLU:O	10:d:119:LEU:HD23	2.10	0.52
15:D:216:ALA:O	15:D:219:VAL:O	2.26	0.52
23:L:66:VAL:HG12	23:L:67:ASP:H	1.74	0.52
30:s:85:PHE:CZ	31:t:173:LEU:HD11	2.45	0.52
32:f:367:SER:N	32:f:370:MET:SD	2.83	0.52
1:U:583:MET:N	1:U:583:MET:HE2	2.25	0.51
3:W:140:ILE:HD11	3:W:144:ARG:NH2	2.25	0.51
5:Y:304:TYR:OH	5:Y:333:GLU:OE1	2.19	0.51
7:a:342:ASP:OD1	7:a:343:LEU:N	2.41	0.51
12:A:317:VAL:C	12:A:318:LEU:HD12	2.35	0.51
12:A:351:ARG:NE	12:A:377:CYS:O	2.43	0.51
18:G:141:ILE:HG22	18:G:151:VAL:HG22	1.92	0.51
20:I:201:MET:HB3	20:I:203:VAL:HG12	1.91	0.51
6:Z:130:ASP:N	6:Z:130:ASP:OD1	2.43	0.51
6:Z:169:GLU:OE2	9:c:152:LYS:NZ	2.41	0.51
10:d:318:PHE:CG	10:d:318:PHE:O	2.62	0.51
14:C:40:GLN:OE1	14:C:43:ARG:NH2	2.44	0.51
20:I:112:THR:HG23	21:J:81:ARG:HD2	1.92	0.51
21:J:116:GLN:O	21:J:120:GLN:HG3	2.10	0.51
21:J:158:ALA:O	22:K:58:LEU:HD21	2.10	0.51
1:U:364:VAL:CG2	9:c:177:THR:HG21	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:399:TRP:CH2	1:U:472:ILE:HG23	2.45	0.51
1:U:532:MET:CB	1:U:552:ILE:HD11	2.40	0.51
2:V:363:LEU:HD21	2:V:398:LEU:HD21	1.91	0.51
3:W:144:ARG:NE	3:W:181:GLU:OE2	2.42	0.51
4:X:380:GLN:OE1	5:Y:315:THR:HG22	2.10	0.51
5:Y:229:ILE:HA	5:Y:299:MET:HE1	1.92	0.51
12:A:358:HIS:NE2	35:A:501:ATP:O2'	2.32	0.51
15:D:266:GLU:OE2	16:E:258:MET:O	2.29	0.51
16:E:264:MET:HE1	16:E:289:LEU:HD12	1.92	0.51
30:s:100:LEU:HD13	30:s:111:MET:HE3	1.92	0.51
1:U:792:ASN:ND2	1:U:922:GLU:OE2	2.44	0.51
9:c:32:TYR:CD1	9:c:66:THR:HG23	2.46	0.51
9:c:37:ALA:HB1	9:c:72:VAL:HG13	1.91	0.51
27:P:12:MET:CG	27:P:138:VAL:HG12	2.41	0.51
26:o:86:CYS:SG	26:o:87:CYS:N	2.83	0.51
32:f:573:ILE:HG21	32:f:599:ALA:CB	2.37	0.51
32:f:600:TYR:HD2	32:f:608:LYS:HD2	1.74	0.51
2:V:233:ALA:O	2:V:237:THR:HG23	2.11	0.51
3:W:412:ILE:HG22	3:W:412:ILE:O	2.10	0.51
13:B:130:GLU:N	13:B:130:GLU:OE1	2.43	0.51
26:O:229:LEU:HD22	26:O:232:TYR:HD1	1.75	0.51
28:q:44:LEU:CD1	28:q:102:LEU:HD12	2.35	0.51
31:t:88:MET:HG3	31:t:109:LYS:HD3	1.92	0.51
1:U:833:LEU:HD22	13:B:70:ASP:OD1	2.11	0.51
4:X:194:ARG:HG2	4:X:210:LEU:HD21	1.93	0.51
12:A:91:GLN:HG3	12:A:91:GLN:O	2.11	0.51
30:S:88:ASP:OD2	30:S:133:TYR:N	2.41	0.51
28:q:29:LYS:HE2	29:r:180:ILE:HD11	1.92	0.51
32:f:429:ILE:HD11	32:f:444:ALA:HA	1.93	0.51
3:W:328:LEU:HG	3:W:341:PHE:CG	2.45	0.51
5:Y:290:PRO:O	5:Y:291:HIS:ND1	2.44	0.51
7:a:123:LEU:HD22	7:a:131:THR:CG2	2.41	0.51
10:d:97:GLN:NE2	10:d:101:GLU:OE2	2.43	0.51
10:d:266:THR:O	10:d:270:GLU:OE1	2.29	0.51
12:A:372:LEU:O	12:A:376:LEU:HD23	2.11	0.51
22:K:121:LEU:HD22	23:L:79:ALA:HA	1.93	0.51
1:U:469:SER:O	1:U:474:ARG:NH1	2.43	0.51
1:U:788:VAL:HG13	1:U:788:VAL:O	2.11	0.51
9:c:109:VAL:HG23	9:c:109:VAL:O	2.11	0.51
12:A:433:ASN:O	22:K:53:ARG:NH2	2.40	0.51
29:r:231:GLY:O	29:r:251:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:68:ASP:O	2:V:72:LEU:HD23	2.11	0.51
3:W:60:MET:HE2	16:E:326:ILE:CG2	2.41	0.51
3:W:60:MET:N	3:W:60:MET:SD	2.82	0.51
16:E:47:LEU:HD22	17:F:79:LYS:NZ	2.26	0.51
25:N:56:THR:O	25:N:56:THR:HG22	2.11	0.51
25:N:155:VAL:HG23	25:N:155:VAL:O	2.10	0.51
32:f:597:VAL:HG11	32:f:656:GLY:HA3	1.91	0.51
2:V:113:LEU:HD11	2:V:171:VAL:HG22	1.93	0.51
15:D:117:SER:O	15:D:118:THR:OG1	2.25	0.51
16:E:221:TYR:CE1	16:E:225:HIS:NE2	2.78	0.51
16:E:264:MET:HG3	16:E:275:MET:SD	2.50	0.51
22:K:67:ILE:HD13	22:K:77:ALA:HA	1.93	0.51
25:N:91:ASP:OD2	26:O:124:ARG:NH2	2.44	0.51
31:t:62:GLU:N	31:t:62:GLU:OE1	2.43	0.51
33:y:389:ARG:NH1	33:y:389:ARG:HB2	2.26	0.51
1:U:114:GLU:O	1:U:118:LEU:HD13	2.10	0.50
2:V:108:LEU:HD13	2:V:174:PHE:HB2	1.94	0.50
7:a:60:TYR:O	7:a:61:GLU:C	2.54	0.50
25:N:71:ILE:HD11	25:N:77:CYS:SG	2.52	0.50
26:o:196:ASN:O	26:o:200:GLU:OE1	2.28	0.50
1:U:332:GLU:OE1	1:U:332:GLU:N	2.40	0.50
2:V:79:VAL:O	2:V:83:GLU:OE1	2.30	0.50
5:Y:155:ASP:OD1	5:Y:155:ASP:N	2.43	0.50
9:c:161:ARG:NH1	9:c:203:ILE:HD11	2.25	0.50
12:A:401:ARG:NH1	12:A:403:ILE:O	2.43	0.50
15:D:164:TYR:OH	15:D:182:GLU:OE1	2.18	0.50
16:E:273:VAL:HG13	16:E:273:VAL:O	2.11	0.50
22:K:230:THR:N	22:K:233:GLU:OE1	2.44	0.50
28:q:160:LEU:O	28:q:164:LEU:HD13	2.11	0.50
32:f:240:VAL:O	32:f:245:ASN:ND2	2.45	0.50
32:f:430:ASP:OD1	32:f:431:LYS:N	2.43	0.50
1:U:622:LEU:C	1:U:622:LEU:HD23	2.36	0.50
2:V:467:TYR:OH	4:X:397:TYR:OH	2.12	0.50
3:W:243:ILE:HG21	3:W:273:TYR:CE1	2.46	0.50
9:c:306:THR:HG23	9:c:307:VAL:HG23	1.93	0.50
10:d:110:SER:O	10:d:114:GLU:OE1	2.30	0.50
13:B:212:GLU:OE1	13:B:212:GLU:N	2.44	0.50
14:C:28:ILE:HD11	15:D:44:TYR:HB2	1.93	0.50
15:D:221:HIS:O	15:D:222:HIS:CG	2.65	0.50
19:H:74:LEU:HD22	19:H:83:TYR:HE1	1.76	0.50
19:H:109:GLN:NE2	27:P:78:GLU:OE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:290:TYR:OH	2:V:294:ARG:NH1	2.44	0.50
3:W:89:LEU:O	3:W:93:ARG:HG3	2.12	0.50
6:Z:167:ALA:HB1	9:c:42:LEU:CD2	2.41	0.50
8:b:56:ASN:OD1	8:b:57:ASP:N	2.44	0.50
13:B:74:MET:CE	32:f:609:VAL:HG13	2.42	0.50
15:D:279:THR:O	15:D:283:ARG:HG3	2.12	0.50
30:S:173:LEU:HD21	30:S:210:ALA:HB2	1.94	0.50
29:r:97:ASN:OD1	29:r:98:PRO:HD2	2.10	0.50
1:U:832:VAL:C	1:U:833:LEU:HD23	2.37	0.50
3:W:186:ILE:HD13	3:W:209:ILE:HD11	1.93	0.50
4:X:23:SER:OG	4:X:56:LEU:HD11	2.11	0.50
7:a:118:ILE:HB	7:a:122:LYS:HZ3	1.76	0.50
10:d:136:LEU:HD12	10:d:138:LYS:HD2	1.92	0.50
10:d:245:PHE:O	10:d:248:LYS:NZ	2.40	0.50
14:C:331:ILE:O	14:C:334:ARG:NH1	2.40	0.50
16:E:29:LEU:O	16:E:33:LEU:HD23	2.11	0.50
17:F:438:TYR:HH	23:L:62:LYS:HZ1	1.60	0.50
25:N:153:MET:HE1	31:T:51:VAL:CG1	2.41	0.50
5:Y:220:VAL:HG21	5:Y:249:VAL:HG21	1.93	0.50
10:d:311:GLY:O	10:d:313:ASN:N	2.44	0.50
15:D:167:ILE:HD11	15:D:170:MET:SD	2.52	0.50
28:Q:5:ILE:HD11	28:Q:143:LEU:CD1	2.30	0.50
31:t:61:PHE:O	31:t:64:GLY:N	2.45	0.50
1:U:345:ASN:O	1:U:743:ASN:ND2	2.44	0.50
3:W:326:MET:O	3:W:329:ARG:N	2.45	0.50
4:X:264:PRO:O	4:X:267:VAL:HG12	2.12	0.50
7:a:122:LYS:HA	7:a:125:ILE:HG22	1.94	0.50
7:a:228:THR:HG22	7:a:229:ASP:N	2.27	0.50
8:b:108:ARG:NH2	8:b:139:ASP:OD2	2.44	0.50
17:F:409:ARG:O	17:F:410:ARG:HB2	2.11	0.50
29:R:89:THR:OG1	30:S:161:ASP:OD1	2.29	0.50
25:n:66:ASP:O	25:n:79:ARG:NH2	2.45	0.50
27:p:187:VAL:O	27:p:198:ARG:N	2.44	0.50
32:f:764:LEU:O	32:f:768:LEU:HD23	2.12	0.50
7:a:236:THR:CG2	7:a:251:LEU:HD13	2.42	0.50
9:c:307:VAL:O	9:c:307:VAL:CG1	2.60	0.50
13:B:292:THR:HG22	13:B:293:LYS:N	2.27	0.50
13:B:434:THR:HG23	20:I:17:ARG:NH1	2.27	0.50
16:E:129:ASN:O	16:E:129:ASN:OD1	2.30	0.50
18:G:174:GLU:OE1	18:G:174:GLU:N	2.41	0.50
27:P:133:THR:HG21	27:P:137:VAL:HG13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Q:153:ARG:O	28:Q:157:VAL:HG23	2.12	0.50
31:T:96:LEU:HD11	31:T:155:MET:CG	2.42	0.50
32:f:425:GLY:O	32:f:429:ILE:HG22	2.11	0.50
32:f:793:VAL:O	32:f:797:LEU:HD23	2.12	0.50
3:W:48:LEU:HD11	3:W:93:ARG:NE	2.27	0.50
6:Z:17:LEU:HD21	9:c:217:LEU:HD21	1.92	0.50
7:a:274:LEU:HD21	7:a:319:LEU:CD2	2.42	0.50
12:A:192:GLU:N	12:A:192:GLU:OE1	2.44	0.50
15:D:266:GLU:OE2	16:E:258:MET:HG2	2.12	0.50
16:E:264:MET:HE1	16:E:289:LEU:CD1	2.41	0.50
20:I:45:LEU:HD11	20:I:137:ILE:CG2	2.42	0.50
21:J:40:ILE:HD11	21:J:210:VAL:HG13	1.94	0.50
30:S:173:LEU:HD13	30:S:207:PHE:HE1	1.76	0.50
29:r:238:VAL:HG23	29:r:238:VAL:O	2.12	0.50
32:f:266:LEU:HD22	32:f:297:MET:HE3	1.94	0.50
9:c:63:ASP:OD1	9:c:63:ASP:N	2.45	0.49
10:d:164:PHE:CD1	10:d:168:MET:HE1	2.47	0.49
10:d:350:VAL:O	10:d:350:VAL:HG13	2.11	0.49
15:D:381:GLU:O	15:D:385:LEU:HD13	2.12	0.49
16:E:199:VAL:HG23	16:E:199:VAL:O	2.11	0.49
23:L:10:VAL:HG22	23:L:10:VAL:O	2.12	0.49
28:Q:161:ARG:O	28:Q:165:GLU:OE1	2.29	0.49
29:R:60:THR:HG23	29:R:92:LYS:NZ	2.27	0.49
32:f:217:LEU:O	32:f:221:ILE:HG13	2.11	0.49
32:f:521:ALA:O	32:f:525:ILE:HG12	2.12	0.49
3:W:239:SER:O	3:W:243:ILE:HD12	2.11	0.49
3:W:294:LYS:NZ	3:W:294:LYS:O	2.21	0.49
4:X:43:VAL:HG22	4:X:80:ILE:HD11	1.94	0.49
5:Y:228:MET:HE1	5:Y:259:TYR:CE2	2.47	0.49
9:c:248:MET:HE1	9:c:291:LEU:HD12	1.93	0.49
10:d:313:ASN:O	10:d:315:TYR:N	2.41	0.49
15:D:98:GLN:O	15:D:99:ASN:OD1	2.30	0.49
18:G:72:ILE:HG21	18:G:114:LEU:HD11	1.93	0.49
24:M:140:SER:HA	24:M:217:VAL:HG11	1.93	0.49
25:N:222:VAL:HG23	25:N:224:LEU:CD2	2.42	0.49
28:Q:172:ILE:HD11	28:q:22:ALA:CB	2.42	0.49
30:s:165:ALA:O	30:s:170:SER:OG	2.28	0.49
1:U:653:ALA:HB2	1:U:675:MET:CE	2.42	0.49
3:W:176:SER:O	3:W:182:ARG:NH1	2.45	0.49
13:B:362:LYS:O	13:B:366:GLN:OE1	2.30	0.49
26:O:182:GLU:HA	26:O:182:GLU:OE2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:R:240:GLU:HA	29:R:240:GLU:OE2	2.12	0.49
27:p:34:MET:HE2	27:p:183:MET:HE2	1.92	0.49
29:r:72:ILE:CG1	29:r:235:LEU:HD11	2.42	0.49
4:X:315:ASP:C	4:X:315:ASP:OD1	2.55	0.49
7:a:313:LYS:O	7:a:317:VAL:HG12	2.12	0.49
8:b:130:ARG:O	8:b:134:GLU:OE1	2.31	0.49
10:d:223:ASN:OD1	10:d:225:TYR:N	2.44	0.49
15:D:88:VAL:HG22	16:E:79:TYR:HD1	1.76	0.49
16:E:201:SER:O	16:E:204:VAL:HG22	2.12	0.49
18:G:80:MET:HE2	18:G:91:VAL:HG23	1.94	0.49
20:I:197:LEU:HA	20:I:200:THR:HG22	1.94	0.49
20:I:220:ASN:CG	20:I:220:ASN:O	2.54	0.49
28:Q:140:LEU:HD21	29:r:225:ARG:CZ	2.42	0.49
30:S:159:GLN:NE2	30:S:161:ASP:OD2	2.45	0.49
31:t:261:SER:O	31:t:261:SER:OG	2.30	0.49
32:f:225:ALA:O	32:f:229:VAL:HG22	2.13	0.49
32:f:744:MET:O	32:f:748:LEU:HD23	2.12	0.49
32:f:893:ILE:O	32:f:893:ILE:HG22	2.11	0.49
1:U:529:ILE:HD11	1:U:555:VAL:HG11	1.94	0.49
1:U:701:ILE:HG21	1:U:810:THR:HG22	1.93	0.49
7:a:42:LEU:O	7:a:46:GLN:OE1	2.30	0.49
7:a:245:VAL:O	7:a:249:GLN:OE1	2.29	0.49
10:d:196:LEU:HB3	10:d:208:PHE:HE1	1.78	0.49
17:F:72:LYS:O	17:F:75:GLU:HG3	2.12	0.49
25:N:48:LEU:HD11	25:N:213:ILE:HD12	1.93	0.49
32:f:463:LEU:HD13	32:f:494:ARG:HH22	1.77	0.49
4:X:205:LYS:N	4:X:242:ILE:HD11	2.26	0.49
7:a:77:VAL:CG1	7:a:113:LEU:HD22	2.43	0.49
16:E:123:SER:HB3	16:E:196:LEU:HD13	1.93	0.49
19:H:66:GLU:OE2	19:H:83:TYR:OH	2.30	0.49
25:N:173:VAL:HG23	25:N:189:PHE:CZ	2.44	0.49
25:N:200:ARG:NH1	31:t:79:ALA:O	2.41	0.49
26:O:225:LYS:C	26:O:226:LEU:HD12	2.37	0.49
27:P:69:PHE:O	27:P:73:LEU:HD23	2.12	0.49
10:d:335:LEU:HD23	10:d:335:LEU:O	2.12	0.49
25:N:63:ARG:HE	31:t:256:ILE:HD11	1.77	0.49
25:N:118:LYS:HB2	25:N:154:MET:HE3	1.94	0.49
29:R:129:ASN:O	29:R:131:GLU:N	2.43	0.49
32:f:840:LEU:HD13	32:f:887:PHE:CE2	2.47	0.49
5:Y:279:GLU:HG3	5:Y:296:VAL:HG21	1.94	0.49
7:a:206:LEU:O	7:a:206:LEU:HD23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:139:ARG:CB	12:A:153:LEU:HD22	2.41	0.49
15:D:79:VAL:O	15:D:82:ILE:HG22	2.13	0.49
15:D:116:LEU:HB3	15:D:119:ILE:HD11	1.95	0.49
19:H:86:LEU:HD13	19:H:134:LEU:HD11	1.95	0.49
25:N:68:LEU:HD12	25:N:76:PHE:HD2	1.77	0.49
32:f:835:GLU:OE2	32:f:901:ARG:NH1	2.45	0.49
1:U:460:TYR:O	1:U:464:GLN:OE1	2.31	0.49
1:U:584:TYR:HH	1:U:768:GLN:CD	2.14	0.49
1:U:832:VAL:O	1:U:833:LEU:HD23	2.13	0.49
2:V:386:PHE:CE2	2:V:395:ILE:HD12	2.48	0.49
4:X:418:ALA:HB2	6:Z:276:ILE:HD12	1.94	0.49
7:a:104:VAL:O	7:a:104:VAL:HG13	2.12	0.49
14:C:258:ARG:NE	14:C:302:ASP:OD2	2.38	0.49
15:D:265:ASP:OD1	15:D:266:GLU:N	2.46	0.49
16:E:346:VAL:HG22	16:E:374:VAL:HG11	1.95	0.49
25:N:227:GLN:N	25:N:227:GLN:OE1	2.46	0.49
1:U:216:VAL:O	1:U:220:LEU:HD23	2.13	0.49
7:a:244:ASN:O	7:a:247:ARG:N	2.45	0.49
7:a:274:LEU:HD21	7:a:319:LEU:HD23	1.95	0.49
10:d:208:PHE:O	10:d:212:LEU:HD13	2.13	0.49
22:K:168:ARG:NH2	23:L:53:GLN:OE1	2.43	0.49
29:R:226:ASP:OD1	29:R:228:TYR:N	2.46	0.49
31:T:86:ARG:NH1	31:T:98:ALA:O	2.46	0.49
28:q:154:GLU:OE2	28:q:154:GLU:HA	2.12	0.49
29:r:93:VAL:HG21	29:r:236:TYR:CE2	2.48	0.49
29:r:204:TYR:O	29:r:206:LEU:HD12	2.12	0.49
32:f:446:LEU:HD21	32:f:480:GLY:HA2	1.95	0.49
3:W:112:VAL:HG22	3:W:124:LEU:HD21	1.93	0.48
10:d:282:ILE:HG22	10:d:318:PHE:HB2	1.95	0.48
15:D:130:VAL:HG11	15:D:139:LEU:HD11	1.95	0.48
15:D:309:MET:CE	15:D:327:LEU:HD21	2.43	0.48
23:L:45:VAL:HG22	23:L:214:ILE:HG13	1.95	0.48
23:L:66:VAL:HG12	23:L:67:ASP:N	2.27	0.48
30:S:214:ASP:OD1	30:S:215:VAL:N	2.45	0.48
31:T:169:TYR:CE1	31:T:184:THR:HG22	2.48	0.48
1:U:669:ILE:HD11	1:U:695:MET:CG	2.42	0.48
7:a:45:VAL:HG21	7:a:82:HIS:HB3	1.95	0.48
16:E:122:MET:HG2	16:E:196:LEU:HD12	1.95	0.48
16:E:130:VAL:HG23	16:E:186:ALA:HA	1.95	0.48
17:F:438:TYR:OH	23:L:33:SER:OG	2.02	0.48
32:f:271:MET:HE1	32:f:786:GLN:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:226:PRO:HA	1:U:229:VAL:HG12	1.95	0.48
1:U:233:LEU:HD22	1:U:325:MET:HE1	1.94	0.48
7:a:299:SER:O	7:a:300:ALA:C	2.55	0.48
7:a:312:MET:HA	7:a:312:MET:HE3	1.95	0.48
8:b:157:VAL:HG21	8:b:170:LEU:HB3	1.96	0.48
9:c:242:GLU:HA	9:c:242:GLU:OE1	2.14	0.48
10:d:302:TYR:HB3	10:d:306:ARG:NH2	2.28	0.48
16:E:300:HIS:CG	16:E:300:HIS:O	2.65	0.48
18:G:138:MET:HE3	18:G:140:LEU:HD11	1.93	0.48
22:K:125:GLU:OE1	22:K:125:GLU:N	2.44	0.48
32:f:783:SER:CB	32:f:787:LEU:HD12	2.42	0.48
1:U:148:LYS:O	1:U:149:GLN:HB3	2.12	0.48
12:A:201:PHE:CZ	17:F:408:LEU:HD22	2.45	0.48
14:C:252:ASP:OD2	14:C:297:ARG:NH1	2.46	0.48
15:D:266:GLU:N	15:D:310:ALA:O	2.46	0.48
26:O:155:SER:OG	26:O:170:MET:SD	2.71	0.48
1:U:609:ASP:OD2	1:U:614:VAL:HG11	2.13	0.48
6:Z:42:SER:OG	6:Z:44:GLN:NE2	2.46	0.48
7:a:62:ASN:O	7:a:66:GLU:OE1	2.30	0.48
9:c:31:VAL:HG23	9:c:31:VAL:O	2.14	0.48
9:c:82:VAL:O	9:c:83:SER:OG	2.29	0.48
13:B:44:ASP:H	13:B:246:THR:HG1	1.59	0.48
13:B:52:VAL:O	13:B:52:VAL:HG23	2.14	0.48
13:B:385:MET:HE1	21:J:199:VAL:O	2.12	0.48
16:E:261:LEU:HD11	16:E:288:ALA:CB	2.43	0.48
19:H:65:VAL:HG22	19:H:75:VAL:HB	1.96	0.48
20:I:13:SER:OG	20:I:15:GLU:OE1	2.25	0.48
24:M:198:ILE:HG21	24:M:212:LEU:CD1	2.43	0.48
25:n:198:MET:HE1	25:n:205:GLY:C	2.38	0.48
1:U:356:THR:O	1:U:360:VAL:HG23	2.13	0.48
3:W:326:MET:O	3:W:327:GLU:C	2.57	0.48
15:D:309:MET:HE1	15:D:327:LEU:HD21	1.95	0.48
16:E:312:ILE:CG2	16:E:343:LEU:HD12	2.43	0.48
18:G:113:MET:HE2	26:O:113:THR:HA	1.94	0.48
18:G:173:THR:OG1	18:G:174:GLU:OE1	2.30	0.48
23:L:66:VAL:O	23:L:67:ASP:C	2.56	0.48
25:n:93:VAL:HG21	25:n:117:PHE:HE1	1.79	0.48
28:q:139:THR:O	28:q:143:LEU:HD13	2.14	0.48
32:f:166:VAL:HG21	32:f:187:LEU:HD11	1.95	0.48
2:V:285:TRP:O	2:V:289:LEU:HD13	2.14	0.48
7:a:216:LEU:HD23	7:a:237:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:123:ASP:OD1	8:b:123:ASP:C	2.56	0.48
10:d:328:THR:HG23	10:d:329:THR:HG23	1.95	0.48
14:C:151:ILE:HG12	14:C:198:LEU:HD22	1.95	0.48
15:D:327:LEU:O	15:D:330:LYS:NZ	2.45	0.48
28:Q:164:LEU:HD12	28:Q:178:PHE:CZ	2.49	0.48
31:T:256:ILE:HD11	26:o:185:PHE:O	2.14	0.48
3:W:340:VAL:O	3:W:340:VAL:CG1	2.62	0.48
5:Y:101:ARG:NH1	5:Y:102:ASP:OD1	2.46	0.48
10:d:84:SER:O	10:d:88:LEU:HD13	2.12	0.48
14:C:296:ASN:C	14:C:296:ASN:HD22	2.19	0.48
15:D:371:SER:N	15:D:374:ASP:OD2	2.41	0.48
18:G:61:LEU:HD23	24:M:161:TYR:CE1	2.48	0.48
23:L:84:LEU:HD12	23:L:130:VAL:CG2	2.43	0.48
27:P:144:GLU:OE1	30:s:172:MET:SD	2.72	0.48
31:T:198:VAL:HG11	31:T:213:LEU:HD22	1.95	0.48
32:f:658:ALA:HB2	32:f:693:ALA:HB1	1.94	0.48
32:f:887:PHE:CB	32:f:900:LEU:HD22	2.44	0.48
1:U:235:LYS:O	1:U:239:GLU:OE1	2.32	0.48
1:U:520:MET:HB2	1:U:555:VAL:HG22	1.95	0.48
7:a:342:ASP:N	7:a:345:GLN:OE1	2.43	0.48
12:A:391:GLU:HA	12:A:394:MET:HE2	1.95	0.48
14:C:96:VAL:HG23	14:C:96:VAL:O	2.13	0.48
14:C:102:ASN:O	14:C:103:ILE:HD13	2.13	0.48
14:C:336:MET:HE1	15:D:196:ILE:HD11	1.95	0.48
15:D:167:ILE:HG23	15:D:167:ILE:O	2.14	0.48
20:I:76:VAL:HA	20:I:134:LEU:HD23	1.94	0.48
20:I:86:LEU:HD12	20:I:132:VAL:CG2	2.44	0.48
20:I:107:CYS:O	20:I:111:VAL:HG23	2.14	0.48
22:K:214:ASN:OD1	22:K:215:ILE:HG23	2.14	0.48
25:N:154:MET:HE2	25:N:154:MET:HA	1.94	0.48
27:P:147:TYR:O	27:P:151:GLU:HG3	2.13	0.48
31:T:108:LEU:O	31:T:112:LEU:HD23	2.14	0.48
26:o:118:ARG:N	26:o:121:THR:HG1	2.12	0.48
1:U:899:ARG:NH2	1:U:916:ASP:OD2	2.47	0.48
5:Y:45:VAL:HG11	5:Y:54:TYR:HD2	1.79	0.48
6:Z:34:ARG:NH2	6:Z:60:GLU:OE2	2.43	0.48
9:c:241:ASN:O	9:c:245:VAL:HG23	2.14	0.48
13:B:372:MET:SD	13:B:414:VAL:HG11	2.54	0.48
20:I:33:THR:OG1	20:I:166:ASN:O	2.32	0.48
21:J:40:ILE:HD11	21:J:210:VAL:HG11	1.95	0.48
25:N:91:ASP:C	25:N:91:ASP:OD1	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:O:262:LEU:HD13	27:P:48:ARG:NH1	2.28	0.48
28:Q:140:LEU:HD21	29:r:225:ARG:NE	2.29	0.48
27:p:149:MET:HE3	27:p:173:ASN:CB	2.43	0.48
31:t:104:ASP:O	31:t:108:LEU:HD23	2.13	0.48
32:f:326:LEU:C	32:f:326:LEU:HD23	2.39	0.48
3:W:159:VAL:O	3:W:159:VAL:HG22	2.14	0.47
4:X:116:TRP:NE1	4:X:120:GLU:OE1	2.47	0.47
4:X:409:LYS:HG3	9:c:256:ASN:ND2	2.29	0.47
10:d:258:PHE:O	10:d:262:ILE:HG22	2.13	0.47
17:F:379:VAL:HG11	17:F:420:TYR:CE2	2.49	0.47
18:G:165:ALA:O	19:H:56:LEU:HD23	2.15	0.47
24:M:38:ILE:HD13	24:M:198:ILE:HD13	1.95	0.47
24:M:179:LYS:O	24:M:180:LEU:HD12	2.14	0.47
24:M:216:TRP:CZ3	24:M:228:VAL:HG13	2.49	0.47
31:t:71:MET:HE3	31:t:233:GLN:CD	2.39	0.47
31:t:237:VAL:HB	31:t:242:VAL:HG23	1.96	0.47
32:f:296:PHE:CD1	32:f:320:ILE:HG23	2.48	0.47
2:V:450:SER:OG	2:V:451:ILE:N	2.48	0.47
4:X:204:PRO:C	4:X:242:ILE:HD11	2.39	0.47
7:a:18:GLN:HB3	7:a:21:VAL:HB	1.96	0.47
13:B:361:LYS:CB	13:B:384:ILE:HG23	2.44	0.47
18:G:176:THR:HG23	19:H:56:LEU:HD22	1.96	0.47
22:K:95:GLU:OE1	22:K:95:GLU:HA	2.13	0.47
23:L:196:ARG:CG	23:L:205:LEU:HD13	2.42	0.47
32:f:347:ASP:O	32:f:350:LYS:NZ	2.44	0.47
1:U:532:MET:HB2	1:U:552:ILE:HD11	1.95	0.47
3:W:69:ALA:O	3:W:73:MET:HG3	2.14	0.47
6:Z:283:ARG:HH11	6:Z:283:ARG:HG3	1.79	0.47
7:a:232:TRP:CE2	7:a:254:ALA:HB3	2.48	0.47
12:A:141:GLY:O	12:A:149:ILE:HG23	2.14	0.47
13:B:365:PHE:HB3	13:B:380:LEU:HD13	1.95	0.47
16:E:101:ASP:O	16:E:105:LEU:HD23	2.15	0.47
23:L:36:VAL:HG12	23:L:160:SER:CB	2.44	0.47
28:Q:1:MET:SD	28:Q:2:GLU:N	2.87	0.47
29:R:109:ALA:CB	30:S:155:VAL:HG23	2.44	0.47
30:s:56:ARG:O	30:s:57:LEU:HD12	2.14	0.47
32:f:520:LEU:O	32:f:524:MET:HG3	2.14	0.47
7:a:157:ASP:HB2	7:a:179:PHE:CE1	2.50	0.47
9:c:27:THR:HG23	9:c:27:THR:O	2.13	0.47
9:c:138:GLU:OE1	9:c:138:GLU:O	2.33	0.47
12:A:214:LEU:HD12	12:A:341:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:225:CYS:O	12:A:229:VAL:HG23	2.14	0.47
13:B:234:LEU:HD11	35:B:501:ATP:H2'	1.96	0.47
15:D:266:GLU:OE2	16:E:258:MET:CG	2.61	0.47
35:D:501:ATP:O3G	16:E:291:ARG:NH2	2.44	0.47
18:G:217:VAL:HG11	18:G:230:LEU:HD12	1.95	0.47
19:H:65:VAL:HG22	19:H:75:VAL:CG2	2.43	0.47
20:I:21:VAL:O	20:I:25:MET:HG3	2.14	0.47
25:N:174:ASP:OD1	25:n:200:ARG:NH2	2.39	0.47
27:P:133:THR:OG1	27:P:135:ASP:OD1	2.31	0.47
32:f:581:GLU:O	32:f:588:ARG:NH1	2.47	0.47
2:V:255:LEU:HD21	2:V:271:VAL:CG1	2.45	0.47
3:W:122:LEU:HA	3:W:125:ILE:HD12	1.96	0.47
4:X:14:SER:O	4:X:17:SER:OG	2.28	0.47
10:d:208:PHE:CZ	10:d:212:LEU:HD11	2.49	0.47
14:C:219:LEU:HD13	14:C:231:VAL:CG2	2.44	0.47
15:D:125:LYS:NZ	15:D:126:PRO:O	2.47	0.47
20:I:154:GLY:O	21:J:81:ARG:NH2	2.47	0.47
24:M:231:ASP:OD1	24:M:232:ILE:N	2.47	0.47
25:n:112:THR:O	25:n:115:SER:OG	2.28	0.47
27:p:132:VAL:O	27:p:132:VAL:HG13	2.14	0.47
1:U:520:MET:HB3	1:U:555:VAL:HG22	1.96	0.47
5:Y:202:LEU:HD11	5:Y:231:LEU:HD11	1.95	0.47
6:Z:198:LEU:HD21	9:c:308:VAL:HG21	1.96	0.47
12:A:417:ILE:HD12	12:A:417:ILE:H	1.79	0.47
14:C:118:ASN:OD1	14:C:118:ASN:O	2.33	0.47
14:C:277:LEU:CD2	14:C:305:LEU:HD23	2.44	0.47
15:D:56:VAL:O	15:D:59:GLU:HG3	2.15	0.47
17:F:143:GLU:OE1	17:F:143:GLU:N	2.46	0.47
21:J:73:PHE:CD1	21:J:74:ALA:N	2.83	0.47
22:K:71:ASP:OD1	22:K:72:ALA:N	2.41	0.47
22:K:214:ASN:OD1	22:K:214:ASN:C	2.57	0.47
26:O:193:GLU:HA	26:O:193:GLU:OE1	2.15	0.47
28:Q:38:MET:HE1	28:Q:60:ILE:CG2	2.45	0.47
29:R:62:THR:OG1	29:R:103:THR:HG21	2.15	0.47
30:s:74:LEU:HD11	30:s:80:ILE:HD13	1.97	0.47
1:U:26:LYS:O	1:U:30:VAL:HG22	2.14	0.47
1:U:242:LEU:HD13	1:U:246:TYR:HE2	1.80	0.47
1:U:586:VAL:HG11	1:U:602:LEU:HD21	1.97	0.47
4:X:190:LEU:HD21	4:X:214:SER:HA	1.97	0.47
7:a:47:ASP:O	7:a:49:CYS:N	2.46	0.47
14:C:52:LEU:HD11	15:D:65:GLN:HE21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:62:GLU:O	14:C:66:LEU:HD13	2.14	0.47
16:E:65:THR:O	16:E:68:LYS:N	2.45	0.47
16:E:371:VAL:HA	16:E:374:VAL:HG12	1.97	0.47
18:G:159:TYR:CZ	18:G:161:CYS:HB2	2.50	0.47
23:L:133:LEU:HD11	23:L:161:ILE:HG22	1.96	0.47
24:M:24:VAL:HG22	24:M:124:THR:OG1	2.14	0.47
26:O:140:ALA:HB1	26:O:170:MET:CE	2.45	0.47
29:R:212:TYR:CZ	29:R:246:VAL:HG21	2.49	0.47
32:f:784:ASP:CG	32:f:784:ASP:O	2.58	0.47
1:U:219:CYS:O	1:U:223:LEU:HD13	2.15	0.47
1:U:383:ASP:OD1	1:U:383:ASP:N	2.44	0.47
1:U:451:ALA:O	1:U:452:ASN:C	2.57	0.47
1:U:483:LEU:HD21	1:U:778:PHE:CZ	2.50	0.47
8:b:63:THR:HG22	8:b:64:LEU:H	1.80	0.47
13:B:380:LEU:O	13:B:384:ILE:HD12	2.15	0.47
16:E:56:ILE:HG12	17:F:132:TYR:CE1	2.50	0.47
25:N:178:ARG:O	25:N:181:MET:HG3	2.15	0.47
26:O:262:LEU:HD23	27:P:195:ILE:CD1	2.45	0.47
27:P:141:THR:HG22	27:P:142:CYS:N	2.29	0.47
27:P:173:ASN:ND2	30:s:179:ASN:HB2	2.30	0.47
26:o:246:ARG:HD3	27:p:158:MET:CE	2.45	0.47
2:V:443:ARG:HA	2:V:443:ARG:HE	1.80	0.47
3:W:166:LEU:HD23	3:W:192:LEU:HD22	1.97	0.47
3:W:328:LEU:HD11	3:W:341:PHE:CE1	2.49	0.47
3:W:412:ILE:O	3:W:413:ILE:C	2.58	0.47
7:a:80:ILE:O	7:a:84:VAL:HG23	2.15	0.47
13:B:358:GLU:OE1	13:B:358:GLU:N	2.48	0.47
13:B:373:THR:HG23	13:B:373:THR:O	2.14	0.47
14:C:320:PRO:CB	14:C:324:ALA:HB3	2.45	0.47
23:L:67:ASP:OD1	23:L:68:ASN:N	2.48	0.47
25:N:219:GLU:OE1	25:N:219:GLU:N	2.48	0.47
29:R:101:LEU:HD11	29:R:243:TRP:CG	2.49	0.47
3:W:141:GLU:O	3:W:145:LEU:HD23	2.15	0.47
3:W:451:MET:CE	6:Z:101:LEU:HD12	2.41	0.47
13:B:125:THR:O	13:B:125:THR:HG22	2.14	0.47
13:B:312:LEU:HD23	13:B:316:LEU:HD13	1.97	0.47
14:C:161:ILE:HG13	14:C:165:ILE:HD13	1.97	0.47
17:F:268:VAL:HG13	17:F:272:PHE:HE2	1.80	0.47
21:J:121:SER:OG	21:J:122:ASN:N	2.48	0.47
25:N:53:ARG:NE	25:N:205:GLY:O	2.46	0.47
25:N:183:LYS:O	25:N:187:LEU:HD13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:R:196:GLY:C	28:q:142:ILE:HD11	2.39	0.47
28:q:36:PHE:HD2	28:q:57:ALA:HB1	1.80	0.47
28:q:52:ASP:O	28:q:56:PHE:CD2	2.68	0.47
31:t:52:THR:HG22	31:t:100:GLY:C	2.40	0.47
1:U:529:ILE:HD11	1:U:555:VAL:CG1	2.45	0.46
4:X:408:SER:HA	5:Y:376:LEU:HD13	1.97	0.46
5:Y:307:LEU:HD23	5:Y:319:MET:SD	2.55	0.46
6:Z:70:LEU:HD13	6:Z:108:ILE:HG23	1.95	0.46
6:Z:102:HIS:N	6:Z:105:ASP:OD2	2.39	0.46
12:A:409:PHE:O	12:A:413:VAL:HG23	2.14	0.46
13:B:270:LEU:O	13:B:273:VAL:HG12	2.15	0.46
17:F:89:LEU:HD23	17:F:90:VAL:N	2.30	0.46
17:F:438:TYR:HB2	23:L:78:THR:HG23	1.98	0.46
21:J:191:VAL:CG1	21:J:208:LEU:HD21	2.44	0.46
22:K:22:PHE:O	22:K:26:TYR:HD2	1.98	0.46
30:S:219:ASP:O	30:S:220:ALA:HB3	2.14	0.46
31:T:69:ALA:CB	31:T:87:ILE:HD11	2.45	0.46
31:t:109:LYS:HE2	31:t:109:LYS:HA	1.96	0.46
32:f:337:LEU:O	32:f:339:ILE:HG23	2.14	0.46
1:U:198:LEU:HB3	1:U:223:LEU:HD11	1.97	0.46
1:U:492:ASP:OD1	1:U:493:VAL:N	2.46	0.46
6:Z:19:VAL:HG21	6:Z:124:ILE:CD1	2.45	0.46
8:b:8:VAL:O	8:b:8:VAL:HG13	2.15	0.46
12:A:42:SER:N	13:B:57:GLN:OE1	2.49	0.46
14:C:277:LEU:HD23	14:C:305:LEU:HD23	1.97	0.46
14:C:320:PRO:HB3	14:C:324:ALA:HB3	1.97	0.46
16:E:235:ILE:O	16:E:239:GLY:HA3	2.16	0.46
30:S:226:VAL:HG22	30:S:231:ILE:CD1	2.45	0.46
26:o:129:MET:HG2	26:o:132:ARG:HH21	1.79	0.46
3:W:121:LYS:HG2	3:W:125:ILE:HD11	1.97	0.46
3:W:301:LYS:HE2	3:W:326:MET:HG2	1.97	0.46
4:X:57:LEU:HD22	4:X:65:GLU:OE2	2.15	0.46
4:X:210:LEU:C	4:X:210:LEU:HD23	2.41	0.46
5:Y:241:ILE:O	5:Y:247:LEU:HD11	2.15	0.46
10:d:272:ALA:C	10:d:276:GLU:OE1	2.58	0.46
12:A:130:ALA:O	12:A:134:ILE:HG13	2.16	0.46
12:A:345:LEU:HD22	12:A:379:ASN:HA	1.97	0.46
13:B:426:VAL:HG13	13:B:427:LEU:N	2.31	0.46
14:C:369:TYR:HE2	14:C:385:MET:HB3	1.80	0.46
18:G:10:ASP:O	18:G:24:GLN:NE2	2.44	0.46
18:G:73:THR:HG23	18:G:75:ASN:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:O:60:ASP:CB	26:O:206:ILE:HD11	2.46	0.46
28:Q:42:ILE:HD11	28:Q:75:LEU:O	2.15	0.46
29:R:170:LEU:HD23	29:R:171:TYR:N	2.31	0.46
31:T:96:LEU:HD12	31:T:156:VAL:O	2.15	0.46
25:n:83:ALA:O	25:n:87:GLN:HG2	2.15	0.46
25:n:194:LEU:CD1	25:n:208:ILE:HG23	2.45	0.46
30:s:96:ILE:HD11	30:s:120:LEU:HD13	1.97	0.46
2:V:254:LEU:HD21	2:V:258:TYR:CE2	2.50	0.46
13:B:85:MET:HA	13:B:85:MET:HE2	1.97	0.46
15:D:163:MET:CE	15:D:221:HIS:CE1	2.98	0.46
21:J:43:LEU:HD11	21:J:134:VAL:HG22	1.97	0.46
23:L:212:ILE:HG22	23:L:214:ILE:HD11	1.97	0.46
25:n:56:THR:O	25:n:56:THR:HG23	2.15	0.46
1:U:39:SER:O	1:U:42:VAL:HG12	2.16	0.46
1:U:383:ASP:OD2	1:U:426:TYR:OH	2.25	0.46
2:V:435:GLU:OE2	2:V:453:HIS:ND1	2.49	0.46
3:W:275:ILE:HG23	3:W:309:PHE:CD2	2.50	0.46
5:Y:198:ALA:HB2	5:Y:226:VAL:HG12	1.97	0.46
15:D:78:GLU:HA	15:D:78:GLU:OE2	2.16	0.46
18:G:189:TRP:CZ3	18:G:197:THR:HG21	2.50	0.46
21:J:33:VAL:CG2	21:J:168:VAL:HG11	2.45	0.46
31:T:71:MET:HE1	31:T:231:ARG:HG2	1.98	0.46
26:o:50:VAL:HG13	26:o:151:PRO:HB2	1.97	0.46
32:f:289:VAL:HG21	32:f:835:GLU:CD	2.40	0.46
1:U:206:MET:HE1	1:U:232:ILE:CD1	2.43	0.46
3:W:77:ALA:O	3:W:79:GLU:OE1	2.33	0.46
13:B:79:ILE:O	13:B:80:ARG:C	2.58	0.46
21:J:42:VAL:CG2	21:J:208:LEU:HD22	2.46	0.46
23:L:157:ARG:N	24:M:60:GLU:OE1	2.48	0.46
24:M:198:ILE:HG21	24:M:212:LEU:HD13	1.97	0.46
26:O:98:THR:HG23	26:O:129:MET:HE3	1.95	0.46
31:T:82:ARG:NH2	25:n:233:VAL:HG13	2.31	0.46
31:t:64:GLY:HA2	31:t:160:TYR:OH	2.15	0.46
32:f:550:LEU:HD13	32:f:587:PHE:HB2	1.97	0.46
1:U:876:GLN:OE1	1:U:876:GLN:HA	2.15	0.46
2:V:67:LEU:O	2:V:71:THR:HG23	2.16	0.46
2:V:302:TYR:OH	2:V:397:ARG:NE	2.48	0.46
4:X:161:ASP:CG	4:X:162:ASP:H	2.24	0.46
13:B:197:ILE:HG21	13:B:235:LEU:HD11	1.97	0.46
16:E:262:ASN:C	16:E:262:ASN:HD22	2.23	0.46
17:F:432:LYS:O	17:F:433:ALA:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:184:GLU:OE1	24:M:184:GLU:N	2.48	0.46
31:T:51:VAL:HG22	31:T:75:TYR:CB	2.46	0.46
31:T:137:LEU:HD21	31:T:155:MET:CE	2.45	0.46
32:f:278:VAL:HG13	32:f:279:GLU:N	2.31	0.46
1:U:486:MET:HE3	1:U:757:MET:HE1	1.97	0.46
1:U:728:PHE:CE1	1:U:732:LEU:HD12	2.50	0.46
2:V:236:ARG:O	2:V:240:LEU:HD23	2.16	0.46
6:Z:67:VAL:HG23	8:b:92:VAL:CG2	2.45	0.46
8:b:4:GLU:OE2	8:b:108:ARG:HB2	2.16	0.46
8:b:108:ARG:HG2	8:b:137:ASN:HB2	1.98	0.46
12:A:101:ILE:HG23	12:A:111:TYR:CD1	2.50	0.46
14:C:45:LEU:HB3	15:D:61:ILE:HG21	1.98	0.46
14:C:146:SER:O	14:C:205:HIS:ND1	2.45	0.46
14:C:405:TRP:CH2	20:I:27:ALA:HB1	2.51	0.46
15:D:203:LEU:HB2	15:D:327:LEU:HD12	1.98	0.46
15:D:394:VAL:HG21	15:D:399:PHE:CE1	2.51	0.46
27:P:11:VAL:HG21	27:P:52:GLY:HA3	1.98	0.46
31:T:57:LEU:HD11	31:T:191:ALA:CB	2.44	0.46
9:c:249:LEU:HD23	9:c:249:LEU:C	2.41	0.46
12:A:125:LEU:HD11	12:A:134:ILE:HG21	1.96	0.46
12:A:142:VAL:HG12	12:A:149:ILE:HG12	1.98	0.46
12:A:183:GLN:NE2	12:A:342:GLU:OE1	2.49	0.46
15:D:318:ASP:OD1	15:D:320:ALA:N	2.35	0.46
19:H:79:MET:H	19:H:132:VAL:HG12	1.80	0.46
23:L:95:SER:HB2	23:L:103:LEU:HD13	1.97	0.46
24:M:21:VAL:HG23	24:M:24:VAL:HB	1.98	0.46
28:q:58:GLU:HA	28:q:58:GLU:OE2	2.15	0.46
32:f:472:HIS:HE1	32:f:514:VAL:HG11	1.81	0.46
32:f:888:LEU:O	32:f:901:ARG:HB2	2.15	0.46
1:U:542:GLU:OE1	1:U:542:GLU:N	2.37	0.46
1:U:586:VAL:CG1	1:U:602:LEU:HD21	2.46	0.46
3:W:135:LYS:HB2	3:W:138:VAL:HG22	1.98	0.46
4:X:224:ASP:OD1	4:X:224:ASP:N	2.43	0.46
4:X:365:LEU:HD22	4:X:385:LEU:CD1	2.46	0.46
12:A:25:LEU:HD11	13:B:407:LEU:HD21	1.97	0.46
14:C:251:ILE:O	14:C:254:ILE:C	2.59	0.46
15:D:119:ILE:O	15:D:119:ILE:CG2	2.63	0.46
27:P:158:MET:HE3	27:P:162:HIS:HB2	1.97	0.46
28:Q:14:LEU:HD21	28:Q:160:LEU:HD13	1.97	0.46
29:R:233:VAL:O	29:R:233:VAL:HG12	2.16	0.46
30:S:141:LEU:HD11	30:S:227:THR:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:r:226:ASP:O	29:r:228:TYR:N	2.48	0.46
3:W:186:ILE:HG21	3:W:209:ILE:CD1	2.44	0.45
3:W:425:LEU:HD12	6:Z:252:LYS:HG3	1.98	0.45
6:Z:5:ALA:O	6:Z:46:LYS:NZ	2.34	0.45
6:Z:81:MET:HE2	9:c:95:MET:SD	2.56	0.45
7:a:180:LEU:CD1	7:a:200:LEU:HD11	2.46	0.45
8:b:33:VAL:HG11	8:b:75:LEU:HD13	1.97	0.45
12:A:75:PRO:O	12:A:76:ALA:HB3	2.16	0.45
13:B:304:GLU:OE1	13:B:307:ARG:NH1	2.49	0.45
15:D:131:ALA:O	15:D:140:VAL:HG22	2.16	0.45
15:D:394:VAL:HG21	15:D:399:PHE:CZ	2.51	0.45
19:H:140:ASN:OD1	19:H:141:GLU:N	2.49	0.45
20:I:183:GLU:OE1	20:I:183:GLU:N	2.49	0.45
26:O:91:THR:N	26:O:138:GLY:O	2.45	0.45
27:p:15:LYS:NZ	27:p:134:ASP:O	2.32	0.45
27:p:153:LEU:HB3	27:p:166:THR:HG23	1.99	0.45
29:r:197:VAL:HG11	29:r:218:ALA:HA	1.98	0.45
32:f:52:LEU:O	32:f:56:LEU:HD23	2.15	0.45
32:f:426:LEU:HD22	33:y:395:LEU:CD1	2.46	0.45
32:f:679:LEU:HD12	32:f:687:ARG:HG2	1.98	0.45
1:U:517:GLY:HA3	1:U:551:GLY:HA2	1.97	0.45
1:U:554:LEU:HD11	1:U:761:VAL:HG13	1.98	0.45
2:V:203:LEU:O	2:V:203:LEU:HD23	2.17	0.45
6:Z:39:LEU:HD13	6:Z:94:TRP:C	2.41	0.45
6:Z:75:LEU:HD23	6:Z:75:LEU:C	2.40	0.45
6:Z:171:GLY:O	6:Z:175:LEU:HD13	2.16	0.45
9:c:51:MET:N	9:c:51:MET:SD	2.90	0.45
12:A:101:ILE:O	12:A:102:ILE:HG22	2.16	0.45
13:B:68:ILE:HG23	32:f:670:MET:HE1	1.97	0.45
17:F:86:LEU:O	17:F:86:LEU:HD23	2.16	0.45
22:K:182:GLN:HG2	23:L:56:LEU:HD23	1.99	0.45
30:S:39:THR:CG2	30:S:173:LEU:HD11	2.46	0.45
27:p:28:PHE:CE1	27:p:39:PHE:CE1	3.05	0.45
27:p:87:LEU:HD23	27:p:87:LEU:O	2.15	0.45
29:r:97:ASN:HB3	29:r:100:LEU:HG	1.97	0.45
32:f:267:ARG:HG3	32:f:297:MET:HE1	1.98	0.45
32:f:606:VAL:HG23	32:f:607:LEU:HD22	1.98	0.45
2:V:435:GLU:O	2:V:438:VAL:HG12	2.16	0.45
2:V:451:ILE:HD12	2:V:458:VAL:HG12	1.97	0.45
6:Z:70:LEU:HD11	6:Z:112:MET:HE1	1.98	0.45
11:e:44:ASP:OD1	11:e:44:ASP:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:125:LEU:HD21	12:A:128:GLN:CG	2.47	0.45
15:D:164:TYR:O	15:D:167:ILE:HG22	2.16	0.45
15:D:254:ALA:CB	15:D:262:ILE:HD11	2.47	0.45
16:E:198:VAL:HB	16:E:232:MET:HG2	1.98	0.45
17:F:385:ALA:O	17:F:388:THR:HG22	2.16	0.45
23:L:67:ASP:O	23:L:69:HIS:N	2.50	0.45
24:M:181:GLN:OE1	24:M:181:GLN:N	2.50	0.45
27:P:149:MET:HE1	30:s:176:LEU:HA	1.98	0.45
29:R:60:THR:HG23	29:R:92:LYS:HZ3	1.81	0.45
26:o:61:THR:OG1	26:o:215:ASN:HB3	2.17	0.45
32:f:140:LEU:HD21	32:f:162:LEU:HD12	1.97	0.45
32:f:423:ASP:OD1	32:f:424:GLY:N	2.46	0.45
2:V:125:ASN:O	2:V:128:ARG:NH1	2.49	0.45
4:X:396:THR:OG1	9:c:242:GLU:OE1	2.29	0.45
6:Z:39:LEU:HD11	6:Z:95:TYR:CB	2.36	0.45
9:c:188:SER:O	9:c:192:LEU:HD23	2.16	0.45
21:J:91:CYS:SG	21:J:107:ILE:HD13	2.56	0.45
25:N:171:GLY:O	25:n:196:LEU:HD23	2.17	0.45
28:q:86:ARG:HD3	28:q:90:ASP:OD2	2.17	0.45
1:U:545:LEU:HB3	1:U:577:ILE:HG21	1.97	0.45
3:W:32:ALA:HB2	3:W:73:MET:HE2	1.98	0.45
4:X:331:LEU:HD13	4:X:356:LEU:HD11	1.97	0.45
5:Y:80:GLU:OE1	5:Y:83:ARG:NH2	2.49	0.45
14:C:234:LEU:HD23	14:C:234:LEU:C	2.41	0.45
15:D:277:ALA:O	15:D:279:THR:N	2.49	0.45
16:E:305:ASN:O	16:E:306:GLU:C	2.60	0.45
19:H:100:VAL:HG12	19:H:101:TYR:CE1	2.51	0.45
22:K:157:ASP:OD1	22:K:161:THR:O	2.34	0.45
23:L:11:THR:HG22	23:L:11:THR:O	2.17	0.45
26:O:262:LEU:C	26:O:262:LEU:HD12	2.41	0.45
31:T:254:TRP:CZ2	25:n:206:GLY:HA2	2.52	0.45
25:n:38:MET:HA	25:n:133:ILE:HD13	1.98	0.45
1:U:471:ASP:OD1	1:U:472:ILE:N	2.49	0.45
2:V:214:HIS:O	2:V:217:VAL:HG22	2.16	0.45
2:V:398:LEU:O	2:V:401:ASN:N	2.50	0.45
3:W:445:LEU:CD2	6:Z:226:ILE:HD11	2.43	0.45
4:X:126:ARG:NH2	4:X:156:GLU:OE2	2.41	0.45
5:Y:174:TRP:CD1	5:Y:178:ASN:HD21	2.34	0.45
8:b:124:LEU:HG	8:b:156:PHE:HE1	1.82	0.45
24:M:203:ASP:OD1	24:M:205:VAL:HG22	2.16	0.45
31:T:224:ARG:NH1	25:n:63:ARG:HE	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:o:123:ASN:HD21	26:o:162:THR:HG23	1.81	0.45
31:t:70:ASP:OD1	31:t:70:ASP:N	2.50	0.45
1:U:173:VAL:O	1:U:177:LEU:HD23	2.17	0.45
1:U:257:SER:O	1:U:261:LEU:HD23	2.17	0.45
1:U:588:MET:HE2	1:U:588:MET:CA	2.46	0.45
1:U:879:ASP:OD1	1:U:879:ASP:N	2.48	0.45
3:W:359:VAL:O	3:W:363:ILE:HG12	2.16	0.45
10:d:260:ILE:O	10:d:264:LEU:HD13	2.17	0.45
10:d:283:LEU:HD13	10:d:315:TYR:CD1	2.52	0.45
12:A:123:VAL:HG13	12:A:148:GLN:HA	1.98	0.45
12:A:225:CYS:SG	12:A:226:ALA:N	2.90	0.45
13:B:116:ILE:HG22	13:B:117:ASP:N	2.31	0.45
14:C:299:ASP:OD1	14:C:300:ILE:HG23	2.17	0.45
15:D:381:GLU:OE2	15:D:406:VAL:HG23	2.17	0.45
16:E:43:SER:O	16:E:47:LEU:HD23	2.16	0.45
16:E:83:CYS:SG	16:E:87:LEU:HD12	2.57	0.45
16:E:98:VAL:HG11	16:E:107:ILE:HG12	1.99	0.45
25:N:222:VAL:CG2	25:N:224:LEU:HD21	2.47	0.45
30:S:176:LEU:HA	27:p:149:MET:HE1	1.98	0.45
31:T:87:ILE:HG21	31:T:235:ALA:CB	2.46	0.45
25:n:62:ASN:OD1	26:o:165:LEU:HD21	2.17	0.45
25:n:181:MET:HB3	25:n:186:CYS:SG	2.57	0.45
26:o:89:ALA:HB3	26:o:170:MET:CE	2.47	0.45
26:o:181:PHE:O	26:o:185:PHE:HB3	2.16	0.45
29:r:98:PRO:HA	29:r:243:TRP:CZ2	2.52	0.45
32:f:59:LEU:O	32:f:63:LEU:HD23	2.16	0.45
32:f:278:VAL:CG2	32:f:298:LEU:HD21	2.46	0.45
2:V:386:PHE:HE2	2:V:395:ILE:HD12	1.82	0.45
5:Y:174:TRP:CH2	14:C:377:HIS:CD2	3.04	0.45
6:Z:16:LEU:HB3	9:c:216:MET:HE3	1.98	0.45
7:a:113:LEU:O	7:a:116:THR:OG1	2.27	0.45
13:B:223:ILE:HG23	13:B:223:ILE:O	2.17	0.45
13:B:232:LYS:NZ	35:B:501:ATP:O1B	2.36	0.45
14:C:394:ASP:O	14:C:394:ASP:OD1	2.35	0.45
31:T:230:ASN:OD1	31:T:230:ASN:O	2.35	0.45
28:q:11:ASP:N	28:q:11:ASP:OD1	2.50	0.45
30:s:62:SER:HG	31:t:189:TYR:HE1	1.65	0.45
1:U:22:PHE:HB3	10:d:124:LEU:HD11	1.99	0.45
1:U:637:VAL:O	1:U:637:VAL:HG12	2.17	0.45
3:W:328:LEU:HG	3:W:341:PHE:HA	1.99	0.45
4:X:69:LEU:O	4:X:73:VAL:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:412:ASP:OD1	5:Y:379:ARG:NH2	2.49	0.45
5:Y:18:ARG:O	5:Y:22:LEU:HD23	2.17	0.45
5:Y:173:ASP:OD1	5:Y:176:ARG:HD3	2.17	0.45
5:Y:175:ASP:HA	5:Y:178:ASN:HD22	1.82	0.45
7:a:240:PHE:HA	7:a:272:ILE:HD13	1.98	0.45
14:C:268:GLU:O	14:C:271:ARG:HG2	2.16	0.45
16:E:204:VAL:HG12	16:E:253:ILE:CD1	2.47	0.45
16:E:285:LEU:HD13	16:E:289:LEU:HD23	1.99	0.45
24:M:171:GLN:OE1	24:M:171:GLN:HA	2.16	0.45
25:N:48:LEU:CD1	25:N:213:ILE:HD12	2.47	0.45
27:P:3:ILE:H	27:P:3:ILE:HD12	1.82	0.45
28:Q:14:LEU:HD11	28:Q:157:VAL:HG22	1.98	0.45
30:s:64:HIS:O	31:t:196:ARG:NH2	2.49	0.45
1:U:665:ASN:OD1	1:U:666:LYS:N	2.50	0.45
2:V:439:ALA:HB1	10:d:274:CYS:SG	2.57	0.45
4:X:53:LEU:CD2	4:X:69:LEU:HD21	2.47	0.45
4:X:304:LYS:NZ	4:X:308:ASP:OD2	2.50	0.45
9:c:49:VAL:HG21	9:c:148:ILE:HD11	1.99	0.45
17:F:268:VAL:HG13	17:F:272:PHE:CE2	2.52	0.45
18:G:209:ASP:OD1	18:G:210:PHE:N	2.45	0.45
27:P:12:MET:HB3	27:P:171:MET:HE1	1.99	0.45
29:R:96:ILE:HG23	29:R:119:ALA:HB2	1.99	0.45
27:p:142:CYS:C	27:p:146:MET:HE3	2.42	0.45
1:U:214:ILE:H	1:U:214:ILE:HD12	1.82	0.44
1:U:791:LEU:HD11	1:U:795:LEU:C	2.42	0.44
4:X:71:LYS:HA	4:X:74:ARG:HE	1.82	0.44
4:X:377:ILE:HG21	5:Y:312:ARG:HB2	1.98	0.44
7:a:168:ASN:OD1	7:a:171:SER:OG	2.34	0.44
10:d:149:GLU:O	10:d:153:GLN:NE2	2.49	0.44
17:F:407:ALA:HA	17:F:412:ALA:HB3	1.99	0.44
23:L:48:ALA:HB3	23:L:62:LYS:HG2	1.99	0.44
25:N:115:SER:O	25:N:119:GLU:HG3	2.17	0.44
31:T:224:ARG:CZ	26:o:182:GLU:OE2	2.65	0.44
30:s:57:LEU:HD11	30:s:70:LYS:HZ3	1.82	0.44
1:U:31:VAL:HG11	1:U:66:LYS:HB3	2.00	0.44
2:V:267:ALA:O	2:V:271:VAL:HG13	2.18	0.44
2:V:458:VAL:O	2:V:458:VAL:CG2	2.63	0.44
2:V:497:PRO:N	2:V:498:PRO:CD	2.80	0.44
6:Z:113:LYS:HA	6:Z:116:CYS:O	2.17	0.44
8:b:8:VAL:HG21	8:b:33:VAL:HG23	1.98	0.44
8:b:157:VAL:HG21	8:b:170:LEU:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:304:LEU:O	9:c:308:VAL:HG23	2.18	0.44
10:d:117:GLY:O	10:d:121:LEU:HD23	2.16	0.44
10:d:232:LEU:HD13	10:d:244:VAL:CG2	2.47	0.44
10:d:273:GLY:CA	10:d:276:GLU:OE1	2.64	0.44
12:A:68:SER:OG	13:B:165:ASP:OD2	2.35	0.44
12:A:384:GLU:O	12:A:387:SER:OG	2.29	0.44
13:B:379:THR:HG23	13:B:379:THR:O	2.18	0.44
14:C:83:LYS:O	14:C:99:VAL:HG12	2.17	0.44
15:D:53:PHE:O	15:D:56:VAL:HG12	2.18	0.44
17:F:156:ASP:OD1	17:F:157:SER:N	2.46	0.44
21:J:7:ILE:H	21:J:7:ILE:HD12	1.83	0.44
21:J:134:VAL:HG12	21:J:144:LEU:HD12	1.99	0.44
23:L:84:LEU:HD13	23:L:132:LEU:HD11	2.00	0.44
24:M:212:LEU:HG	24:M:214:LEU:CD1	2.47	0.44
25:N:148:VAL:O	25:N:148:VAL:CG2	2.64	0.44
26:O:93:ALA:HB3	27:P:127:ILE:HD12	1.98	0.44
31:T:96:LEU:HD12	31:T:97:GLY:H	1.82	0.44
28:q:3:TYR:N	28:q:18:ASP:OD1	2.48	0.44
30:s:99:ARG:HD3	30:s:123:ILE:HD11	2.00	0.44
32:f:616:CYS:SG	32:f:653:ALA:HB3	2.57	0.44
1:U:583:MET:HE2	1:U:583:MET:CA	2.48	0.44
2:V:92:ARG:O	2:V:93:PHE:HB2	2.17	0.44
3:W:282:GLU:O	3:W:286:LEU:HD23	2.17	0.44
9:c:73:PHE:HE1	9:c:95:MET:HG2	1.83	0.44
12:A:32:LEU:C	12:A:32:LEU:HD23	2.42	0.44
13:B:299:SER:OG	13:B:300:GLY:N	2.50	0.44
14:C:37:ASP:OD1	14:C:37:ASP:C	2.60	0.44
14:C:253:SER:OG	14:C:254:ILE:N	2.48	0.44
16:E:234:GLU:N	16:E:278:ALA:O	2.51	0.44
19:H:75:VAL:HG22	19:H:76:TYR:N	2.32	0.44
24:M:214:LEU:CB	24:M:228:VAL:HG21	2.47	0.44
25:n:128:LEU:HD21	25:n:130:ALA:HB3	2.00	0.44
32:f:137:ARG:NE	32:f:169:GLU:OE2	2.50	0.44
32:f:221:ILE:HG23	32:f:225:ALA:HB3	1.99	0.44
32:f:688:ARG:O	32:f:724:ASN:ND2	2.50	0.44
32:f:838:ARG:NH1	32:f:839:PRO:O	2.51	0.44
1:U:398:ASN:HA	1:U:437:TYR:CE2	2.52	0.44
1:U:639:LEU:O	14:C:49:ARG:NH2	2.50	0.44
2:V:337:LEU:HD22	2:V:367:VAL:HG11	2.00	0.44
10:d:192:LEU:O	10:d:196:LEU:HG	2.18	0.44
10:d:200:LEU:CD2	10:d:208:PHE:CE1	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:273:GLY:HA2	10:d:276:GLU:OE1	2.18	0.44
14:C:69:GLN:HB2	14:C:118:ASN:ND2	2.33	0.44
14:C:336:MET:HG2	14:C:338:LEU:HD22	2.00	0.44
14:C:358:GLU:O	14:C:362:VAL:HG23	2.17	0.44
23:L:38:LEU:HD11	23:L:187:LEU:HG	2.00	0.44
23:L:98:VAL:HG13	23:L:99:PHE:N	2.32	0.44
25:N:221:GLN:OE1	25:N:221:GLN:N	2.50	0.44
26:O:156:ILE:HG12	26:O:162:THR:HG22	1.98	0.44
26:O:248:GLU:OE1	26:O:248:GLU:N	2.50	0.44
29:R:142:LEU:HD23	29:R:173:VAL:HG21	2.00	0.44
31:T:54:THR:OG1	31:T:55:SER:N	2.51	0.44
25:n:222:VAL:HB	25:n:224:LEU:HD11	1.98	0.44
32:f:370:MET:SD	32:f:370:MET:N	2.90	0.44
1:U:639:LEU:HD12	14:C:49:ARG:HH21	1.82	0.44
3:W:308:LEU:O	3:W:315:MET:HE1	2.18	0.44
4:X:396:THR:HA	9:c:242:GLU:OE1	2.18	0.44
7:a:17:GLY:O	7:a:22:TRP:CZ3	2.71	0.44
7:a:228:THR:HG22	7:a:229:ASP:OD1	2.16	0.44
8:b:7:MET:SD	8:b:50:GLY:C	3.00	0.44
10:d:309:VAL:HG22	10:d:309:VAL:O	2.17	0.44
13:B:74:MET:HE1	32:f:609:VAL:HG13	1.99	0.44
13:B:434:THR:N	13:B:435:PRO:HD2	2.33	0.44
18:G:115:CYS:SG	18:G:160:TYR:HB2	2.58	0.44
19:H:75:VAL:HG22	19:H:76:TYR:H	1.82	0.44
26:O:126:LEU:HD22	26:O:141:LEU:CD1	2.47	0.44
28:Q:6:GLY:O	28:Q:7:ILE:HD13	2.18	0.44
29:R:170:LEU:HD22	29:R:185:PHE:CD2	2.53	0.44
29:r:60:THR:O	29:r:60:THR:HG22	2.18	0.44
29:r:206:LEU:CD2	29:r:214:LEU:HD12	2.46	0.44
2:V:94:VAL:CG2	2:V:205:LEU:HD13	2.45	0.44
3:W:406:VAL:HG22	3:W:413:ILE:HG12	2.00	0.44
8:b:11:ASP:OD1	8:b:12:ASN:N	2.50	0.44
10:d:95:TYR:HD2	10:d:143:LEU:HD11	1.83	0.44
12:A:120:LYS:HB2	17:F:90:VAL:CG2	2.48	0.44
12:A:431:THR:O	12:A:431:THR:HG22	2.18	0.44
14:C:368:MET:HE3	15:D:199:PRO:HG3	2.00	0.44
15:D:231:VAL:HG12	15:D:233:SER:H	1.82	0.44
15:D:277:ALA:O	15:D:278:GLN:C	2.60	0.44
16:E:327:ASP:N	16:E:327:ASP:OD1	2.49	0.44
18:G:113:MET:CE	26:O:113:THR:HA	2.47	0.44
19:H:195:LEU:CD1	19:H:208:ILE:HD11	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:I:30:HIS:O	20:I:50:ARG:NH1	2.51	0.44
21:J:173:GLU:OE2	22:K:57:PRO:HD2	2.18	0.44
22:K:212:ALA:H	22:K:238:ILE:HD13	1.83	0.44
24:M:38:ILE:HD13	24:M:198:ILE:CD1	2.47	0.44
24:M:121:HIS:HA	24:M:124:THR:HG22	1.99	0.44
27:P:12:MET:HE3	27:P:14:MET:HE2	1.99	0.44
26:o:60:ASP:OD2	26:o:206:ILE:HG13	2.18	0.44
26:o:157:TYR:HB3	26:o:158:PRO:HD2	1.99	0.44
31:t:114:GLN:NE2	31:t:118:ASP:OD1	2.51	0.44
32:f:290:VAL:HA	32:f:890:VAL:HG11	2.00	0.44
32:f:582:VAL:HG22	32:f:582:VAL:O	2.18	0.44
32:f:659:LEU:HD13	32:f:797:LEU:HD21	2.00	0.44
1:U:242:LEU:HD13	1:U:246:TYR:CE2	2.53	0.44
1:U:682:TYR:CD2	9:c:184:LEU:CD2	3.01	0.44
1:U:806:CYS:SG	1:U:807:LYS:N	2.91	0.44
2:V:398:LEU:O	2:V:399:ARG:C	2.59	0.44
7:a:220:PRO:HA	7:a:223:GLU:OE1	2.18	0.44
15:D:158:GLN:O	15:D:159:LYS:C	2.60	0.44
16:E:64:LEU:O	16:E:65:THR:C	2.61	0.44
16:E:66:GLU:OE1	16:E:66:GLU:N	2.49	0.44
16:E:115:VAL:O	16:E:115:VAL:HG13	2.18	0.44
17:F:200:GLU:HG2	17:F:204:LEU:HD12	1.99	0.44
17:F:402:GLU:OE2	17:F:409:ARG:NH2	2.51	0.44
23:L:74:ILE:HG22	23:L:132:LEU:CD2	2.48	0.44
26:O:233:THR:HG22	26:O:234:VAL:N	2.32	0.44
30:S:74:LEU:HD21	30:S:80:ILE:CG2	2.47	0.44
25:n:36:THR:HG21	25:n:197:ALA:HB3	1.98	0.44
1:U:360:VAL:HG21	1:U:369:THR:HG21	2.00	0.44
2:V:400:HIS:O	2:V:403:ILE:HG22	2.17	0.44
5:Y:201:PHE:HB3	5:Y:223:THR:HG23	2.00	0.44
7:a:176:ALA:HB3	7:a:200:LEU:HD21	1.99	0.44
13:B:256:ILE:O	13:B:256:ILE:HG13	2.17	0.44
15:D:266:GLU:OE1	16:E:262:ASN:HB2	2.17	0.44
16:E:57:VAL:HG22	17:F:131:THR:O	2.17	0.44
23:L:67:ASP:O	23:L:70:ILE:N	2.46	0.44
24:M:216:TRP:NE1	24:M:220:LEU:HD11	2.32	0.44
27:P:94:LEU:CD2	27:P:95:LEU:HD22	2.48	0.44
31:T:92:ASN:OD1	31:T:93:SER:N	2.51	0.44
27:p:13:ALA:HB2	27:p:22:ILE:HD12	1.98	0.44
27:p:149:MET:HE3	27:p:173:ASN:HB2	2.00	0.44
29:r:226:ASP:O	29:r:227:ALA:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:311:VAL:HG22	32:f:312:GLU:N	2.33	0.44
1:U:393:LEU:HD23	1:U:393:LEU:C	2.43	0.44
6:Z:69:PHE:CD2	6:Z:69:PHE:O	2.71	0.44
7:a:59:LEU:O	7:a:63:PHE:CD2	2.71	0.44
8:b:173:VAL:HG23	8:b:173:VAL:O	2.18	0.44
10:d:269:ASP:O	10:d:272:ALA:HB3	2.18	0.44
14:C:336:MET:CE	15:D:196:ILE:HD11	2.48	0.44
17:F:72:LYS:HA	17:F:75:GLU:HG3	1.99	0.44
19:H:210:VAL:CG1	19:H:221:LEU:HD12	2.48	0.44
24:M:37:ALA:C	24:M:38:ILE:HD12	2.43	0.44
29:R:110:ASP:OD2	30:S:128:ARG:NH2	2.49	0.44
31:T:211:ARG:NH2	31:T:245:GLU:OE1	2.51	0.44
1:U:13:ASP:C	1:U:13:ASP:OD1	2.61	0.43
7:a:127:ASP:O	7:a:131:THR:HG23	2.17	0.43
7:a:149:THR:HG22	7:a:150:SER:H	1.83	0.43
12:A:355:PHE:CD1	12:A:385:ILE:HG23	2.53	0.43
13:B:224:LEU:N	13:B:224:LEU:HD12	2.33	0.43
13:B:417:GLU:OE1	13:B:417:GLU:N	2.41	0.43
14:C:322:GLU:HA	14:C:325:ARG:HB2	1.99	0.43
15:D:177:VAL:O	15:D:181:VAL:HG22	2.18	0.43
16:E:175:PRO:O	16:E:180:LYS:NZ	2.51	0.43
16:E:313:LEU:HD12	16:E:343:LEU:HD13	1.97	0.43
17:F:86:LEU:HD23	17:F:86:LEU:C	2.43	0.43
19:H:69:THR:HG22	19:H:70:LYS:N	2.32	0.43
21:J:116:GLN:HA	21:J:119:THR:HG22	2.00	0.43
21:J:175:ASN:OD1	21:J:175:ASN:O	2.35	0.43
24:M:38:ILE:HG21	24:M:177:ILE:HD11	2.00	0.43
25:N:74:ARG:O	25:N:213:ILE:HD13	2.17	0.43
27:P:182:GLY:O	27:P:183:MET:HE2	2.18	0.43
30:S:39:THR:HG21	30:S:173:LEU:HD11	1.99	0.43
30:s:178:ASP:OD1	30:s:178:ASP:C	2.60	0.43
31:t:68:ALA:CB	31:t:218:MET:HE2	2.48	0.43
32:f:251:CYS:O	32:f:255:VAL:HG23	2.18	0.43
1:U:86:ASP:N	1:U:86:ASP:OD1	2.51	0.43
2:V:218:TYR:HD2	2:V:227:VAL:HG13	1.83	0.43
2:V:473:GLN:HG2	6:Z:257:MET:HE2	2.00	0.43
3:W:435:LEU:HD23	3:W:435:LEU:C	2.43	0.43
3:W:442:THR:HG21	6:Z:230:LEU:HD21	2.00	0.43
5:Y:81:LEU:HD23	5:Y:81:LEU:C	2.43	0.43
6:Z:17:LEU:HD21	9:c:217:LEU:HD23	1.98	0.43
12:A:122:VAL:HG23	17:F:86:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:153:LEU:HD11	13:B:122:ILE:CD1	2.46	0.43
13:B:188:GLY:CA	13:B:367:ILE:HD12	2.48	0.43
13:B:290:ILE:O	13:B:290:ILE:HG13	2.17	0.43
17:F:137:ILE:O	17:F:160:ILE:N	2.50	0.43
20:I:45:LEU:CD1	20:I:137:ILE:HD13	2.48	0.43
30:S:56:ARG:NH2	30:S:217:THR:O	2.50	0.43
28:q:13:VAL:O	28:q:15:VAL:HG13	2.18	0.43
32:f:558:LEU:HB2	32:f:559:PRO:HD3	2.01	0.43
32:f:850:VAL:O	32:f:850:VAL:HG12	2.18	0.43
1:U:364:VAL:HG23	9:c:177:THR:HG21	1.99	0.43
2:V:251:LEU:CD1	2:V:270:LEU:HD21	2.48	0.43
3:W:446:ILE:HD11	6:Z:211:TYR:CD1	2.53	0.43
5:Y:140:ILE:O	5:Y:144:LEU:HD23	2.18	0.43
7:a:142:LEU:HD23	7:a:142:LEU:O	2.18	0.43
7:a:301:LYS:O	7:a:302:ILE:HG23	2.18	0.43
8:b:33:VAL:HA	8:b:36:VAL:HG12	1.99	0.43
9:c:30:GLN:NE2	9:c:206:ASN:HB2	2.33	0.43
9:c:64:ASP:OD1	9:c:64:ASP:N	2.51	0.43
13:B:275:GLU:HA	13:B:275:GLU:OE2	2.18	0.43
15:D:168:GLY:HA3	15:D:344:ILE:HD13	1.99	0.43
15:D:266:GLU:CG	16:E:258:MET:HG2	2.48	0.43
23:L:47:VAL:HG12	23:L:212:ILE:HD12	1.99	0.43
23:L:195:LEU:O	23:L:198:THR:HG22	2.18	0.43
27:p:28:PHE:O	27:p:28:PHE:CD2	2.71	0.43
32:f:426:LEU:HD11	33:y:392:VAL:HG13	1.99	0.43
32:f:543:MET:CE	32:f:583:VAL:HG22	2.47	0.43
32:f:759:LEU:O	32:f:763:ARG:HG2	2.17	0.43
1:U:22:PHE:CG	10:d:124:LEU:HD11	2.53	0.43
1:U:919:GLU:OE1	1:U:919:GLU:N	2.51	0.43
3:W:227:TYR:O	3:W:231:ILE:HG13	2.18	0.43
3:W:328:LEU:HD23	3:W:341:PHE:HA	1.99	0.43
5:Y:148:GLY:O	5:Y:157:ILE:HD11	2.17	0.43
6:Z:242:LEU:HD23	6:Z:244:GLU:OE2	2.18	0.43
14:C:373:GLU:O	14:C:374:ARG:C	2.62	0.43
16:E:257:LEU:HD11	16:E:289:LEU:HD22	2.01	0.43
16:E:366:ASP:OD1	16:E:366:ASP:C	2.61	0.43
17:F:144:LYS:HD2	17:F:144:LYS:O	2.18	0.43
18:G:201:CYS:O	18:G:205:VAL:HG12	2.17	0.43
19:H:119:GLN:HA	19:H:122:THR:HG22	2.01	0.43
29:R:63:LEU:HD12	29:R:63:LEU:C	2.44	0.43
25:n:153:MET:SD	31:t:102:TYR:HB3	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:n:226:ASP:OD1	25:n:227:GLN:N	2.52	0.43
31:t:175:VAL:HG23	31:t:175:VAL:O	2.18	0.43
32:f:315:GLU:OE1	32:f:315:GLU:N	2.42	0.43
32:f:656:GLY:O	32:f:657:ILE:C	2.61	0.43
32:f:660:ILE:HD12	32:f:660:ILE:H	1.84	0.43
32:f:819:TYR:O	32:f:822:VAL:HG13	2.17	0.43
2:V:109:ASN:OD1	2:V:110:HIS:N	2.50	0.43
2:V:192:MET:HE2	2:V:230:PHE:CE2	2.50	0.43
2:V:470:ARG:O	2:V:470:ARG:HG2	2.18	0.43
5:Y:368:GLU:OE2	5:Y:372:LYS:NZ	2.41	0.43
6:Z:170:VAL:HG23	9:c:152:LYS:HA	2.00	0.43
7:a:55:GLY:O	7:a:59:LEU:HD13	2.17	0.43
12:A:187:LEU:HA	12:A:190:VAL:HG12	2.00	0.43
12:A:256:MET:O	12:A:260:LEU:HD23	2.18	0.43
13:B:60:LEU:HD21	32:f:235:SER:HB2	2.00	0.43
13:B:440:LEU:CD2	21:J:73:PHE:CE2	3.02	0.43
13:B:440:LEU:HD12	21:J:30:SER:H	1.82	0.43
24:M:104:GLY:O	25:N:111:HIS:NE2	2.52	0.43
24:M:213:GLU:C	24:M:214:LEU:HD12	2.44	0.43
29:R:61:THR:HG1	29:R:229:SER:CB	2.29	0.43
25:n:90:ALA:O	25:n:93:VAL:HG22	2.19	0.43
26:o:140:ALA:HB1	26:o:170:MET:SD	2.58	0.43
27:p:105:THR:HG23	27:p:105:THR:O	2.18	0.43
32:f:887:PHE:CD2	32:f:900:LEU:HB3	2.53	0.43
1:U:689:ILE:O	1:U:693:LEU:HD23	2.18	0.43
2:V:265:ASP:O	2:V:269:LYS:HG2	2.19	0.43
2:V:291:TYR:O	2:V:295:ILE:HG12	2.17	0.43
3:W:341:PHE:CD2	3:W:344:THR:HG21	2.53	0.43
6:Z:11:VAL:HG12	6:Z:12:HIS:N	2.33	0.43
6:Z:266:ILE:HD12	9:c:248:MET:HE3	2.01	0.43
8:b:142:ASN:ND2	8:b:146:GLU:OE1	2.52	0.43
8:b:147:GLU:OE1	8:b:147:GLU:N	2.42	0.43
10:d:164:PHE:CD2	10:d:168:MET:HE1	2.54	0.43
10:d:259:PHE:HA	10:d:262:ILE:HG22	2.00	0.43
12:A:69:ASP:N	12:A:69:ASP:OD1	2.50	0.43
12:A:197:HIS:CE1	12:A:200:ARG:HB3	2.53	0.43
13:B:360:THR:O	13:B:364:ILE:HG12	2.19	0.43
13:B:434:THR:N	13:B:435:PRO:CD	2.81	0.43
14:C:368:MET:HE3	15:D:199:PRO:CG	2.48	0.43
17:F:406:ILE:O	17:F:409:ARG:O	2.36	0.43
28:Q:38:MET:HE3	28:Q:44:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:T:57:LEU:HD12	31:T:195:LEU:HD11	2.01	0.43
29:r:93:VAL:HG21	29:r:236:TYR:CZ	2.53	0.43
31:t:65:VAL:N	31:t:160:TYR:OH	2.51	0.43
32:f:426:LEU:HD22	33:y:395:LEU:HD11	2.01	0.43
32:f:479:LEU:HD12	32:f:514:VAL:HG22	2.00	0.43
1:U:99:THR:HG21	2:V:240:LEU:CD1	2.48	0.43
2:V:223:LYS:O	2:V:261:TYR:OH	2.36	0.43
5:Y:183:TYR:CD1	5:Y:213:LEU:HD11	2.54	0.43
8:b:153:LEU:HB3	8:b:170:LEU:HD22	2.01	0.43
10:d:245:PHE:CE1	10:d:267:ILE:HG21	2.54	0.43
15:D:214:MET:HE1	35:D:501:ATP:C4	2.53	0.43
19:H:203:MET:SD	19:H:230:LEU:HD21	2.58	0.43
27:P:49:LEU:CD2	27:P:87:LEU:HD22	2.48	0.43
28:Q:27:GLN:O	28:q:170:ARG:NH1	2.43	0.43
29:R:78:ARG:CZ	29:R:230:GLY:HA3	2.49	0.43
29:R:146:VAL:HG21	29:R:156:MET:SD	2.58	0.43
31:T:101:ASP:HB3	31:T:104:ASP:OD2	2.18	0.43
27:p:142:CYS:O	27:p:146:MET:HE3	2.18	0.43
27:p:171:MET:O	27:p:175:VAL:HG13	2.18	0.43
28:q:19:ARG:HE	28:q:177:THR:HB	1.84	0.43
28:q:167:LEU:HD23	28:q:178:PHE:CZ	2.54	0.43
31:t:89:ARG:O	31:t:90:VAL:C	2.62	0.43
32:f:505:MET:HE2	32:f:541:THR:CG2	2.41	0.43
32:f:655:LEU:HD21	32:f:800:LEU:HB3	2.00	0.43
32:f:760:PHE:O	32:f:764:LEU:HD23	2.19	0.43
1:U:638:SER:HB3	1:U:671:LEU:HD11	1.99	0.43
4:X:16:LEU:HD12	4:X:56:LEU:CG	2.44	0.43
4:X:345:VAL:HG12	4:X:346:GLN:N	2.34	0.43
12:A:32:LEU:HD22	32:f:92:VAL:HA	2.01	0.43
12:A:364:VAL:HG22	12:A:365:GLU:N	2.34	0.43
12:A:369:ARG:NH2	22:K:206:MET:O	2.49	0.43
14:C:307:ARG:HD2	14:C:308:PRO:O	2.19	0.43
16:E:180:LYS:N	36:E:401:ADP:O2B	2.41	0.43
23:L:195:LEU:HD22	23:L:205:LEU:CD2	2.44	0.43
25:N:173:VAL:O	25:N:174:ASP:C	2.62	0.43
27:P:123:SER:C	27:P:124:LEU:HD12	2.44	0.43
31:t:195:LEU:O	31:t:199:LEU:HD23	2.19	0.43
32:f:473:ASN:OD1	33:y:381:ARG:NH2	2.46	0.43
32:f:656:GLY:O	32:f:659:LEU:N	2.51	0.43
2:V:167:LEU:O	2:V:171:VAL:HG23	2.19	0.43
13:B:164:MET:SD	13:B:164:MET:N	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:296:ASN:O	14:C:296:ASN:ND2	2.51	0.43
16:E:140:GLU:O	16:E:143:ARG:HB3	2.18	0.43
18:G:42:VAL:HG22	18:G:165:ALA:HB1	2.01	0.43
18:G:111:VAL:HG21	18:G:142:GLY:HA3	2.00	0.43
23:L:7:ASP:O	23:L:21:GLN:NE2	2.46	0.43
23:L:84:LEU:O	23:L:88:MET:HG3	2.19	0.43
26:O:91:THR:HG21	26:O:94:ASP:OD2	2.19	0.43
28:q:96:THR:O	28:q:98:TYR:CD2	2.72	0.43
29:r:204:TYR:O	29:r:205:ASP:OD1	2.36	0.43
29:r:233:VAL:O	29:r:233:VAL:HG12	2.18	0.43
31:t:87:ILE:O	31:t:88:MET:HE2	2.19	0.43
31:t:160:TYR:HH	31:t:237:VAL:C	2.10	0.43
1:U:54:PHE:O	1:U:55:ARG:HB2	2.17	0.43
1:U:353:LEU:HD21	1:U:373:ASN:HB2	2.01	0.43
1:U:682:TYR:CE2	9:c:184:LEU:HD22	2.54	0.43
6:Z:94:TRP:CZ3	6:Z:108:ILE:HG21	2.54	0.43
10:d:136:LEU:O	10:d:137:THR:OG1	2.27	0.43
12:A:206:ILE:HD12	17:F:404:GLY:CA	2.46	0.43
14:C:275:GLU:OE1	14:C:275:GLU:HA	2.19	0.43
15:D:89:ILE:CD1	16:E:70:ILE:HG23	2.49	0.43
15:D:355:SER:HA	15:D:393:ILE:HD11	2.00	0.43
17:F:75:GLU:O	17:F:78:GLU:HG3	2.19	0.43
21:J:102:VAL:HG23	21:J:106:TYR:CD1	2.53	0.43
22:K:57:PRO:O	22:K:58:LEU:HB3	2.19	0.43
31:T:73:GLY:HA3	31:T:84:ILE:HD11	2.00	0.43
25:n:125:ARG:NE	31:t:46:THR:OG1	2.52	0.43
30:s:181:VAL:CG1	30:s:194:LEU:HD22	2.49	0.43
31:t:87:ILE:HG21	31:t:235:ALA:HB2	2.01	0.43
32:f:372:LEU:O	32:f:375:SER:OG	2.33	0.43
1:U:621:SER:O	1:U:625:ILE:HG12	2.19	0.42
2:V:395:ILE:O	2:V:398:LEU:HB3	2.19	0.42
3:W:47:LEU:HD12	3:W:66:ILE:HG13	2.01	0.42
3:W:91:SER:CB	3:W:131:VAL:HG23	2.49	0.42
3:W:134:GLY:O	3:W:135:LYS:HG3	2.19	0.42
3:W:326:MET:SD	3:W:326:MET:C	3.02	0.42
5:Y:300:ARG:NH1	5:Y:333:GLU:OE2	2.43	0.42
6:Z:15:VAL:O	6:Z:19:VAL:HG23	2.19	0.42
6:Z:131:LEU:HD22	6:Z:200:GLY:HA2	2.00	0.42
12:A:125:LEU:HD22	12:A:134:ILE:HD13	2.00	0.42
12:A:197:HIS:ND1	12:A:200:ARG:HB3	2.34	0.42
15:D:275:PHE:CE2	15:D:277:ALA:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:F:431:LYS:O	17:F:432:LYS:HG2	2.19	0.42
18:G:94:ALA:HB1	18:G:114:LEU:HD21	2.01	0.42
25:N:63:ARG:NE	31:t:256:ILE:HD11	2.34	0.42
31:T:190:LEU:HD11	26:o:175:LEU:HD12	2.01	0.42
25:n:153:MET:HE1	31:t:81:PHE:CE2	2.54	0.42
32:f:544:GLU:O	32:f:544:GLU:CD	2.62	0.42
3:W:318:SER:O	3:W:322:GLU:HG2	2.19	0.42
7:a:254:ALA:O	7:a:257:GLN:HG2	2.19	0.42
8:b:7:MET:HE3	8:b:96:ALA:CB	2.49	0.42
10:d:83:THR:OG1	10:d:84:SER:N	2.52	0.42
10:d:289:ARG:HH12	10:d:290:ILE:HD11	1.84	0.42
14:C:248:MET:HB3	14:C:293:MET:HG2	2.01	0.42
14:C:377:HIS:O	14:C:378:VAL:HG23	2.18	0.42
17:F:123:VAL:HG22	17:F:133:PHE:HD1	1.82	0.42
20:I:45:LEU:HD11	20:I:137:ILE:HG23	2.00	0.42
21:J:33:VAL:HG21	21:J:168:VAL:HG11	2.00	0.42
28:q:56:PHE:CZ	28:q:98:TYR:HB3	2.50	0.42
1:U:870:GLU:OE1	1:U:870:GLU:N	2.52	0.42
2:V:353:LEU:HD12	2:V:353:LEU:N	2.34	0.42
2:V:440:LYS:O	2:V:443:ARG:HB2	2.19	0.42
3:W:261:GLU:HA	3:W:264:GLN:HG2	2.00	0.42
3:W:318:SER:O	3:W:321:VAL:HG22	2.19	0.42
3:W:341:PHE:HD2	3:W:344:THR:HB	1.85	0.42
4:X:74:ARG:N	4:X:75:PRO:CD	2.83	0.42
4:X:274:LYS:CD	4:X:274:LYS:N	2.83	0.42
5:Y:347:ILE:HG22	5:Y:348:ASP:N	2.33	0.42
7:a:28:LEU:HG	7:a:33:LEU:HD12	2.00	0.42
7:a:63:PHE:O	7:a:67:PHE:HB3	2.19	0.42
9:c:61:PHE:CZ	9:c:109:VAL:HG12	2.55	0.42
13:B:181:GLN:HG2	13:B:181:GLN:O	2.20	0.42
14:C:309:GLY:N	14:C:312:ASP:OD1	2.52	0.42
16:E:23:ASP:O	16:E:27:LYS:HG2	2.20	0.42
21:J:33:VAL:HG22	21:J:160:ALA:CB	2.46	0.42
23:L:159:MET:SD	23:L:160:SER:N	2.91	0.42
28:q:13:VAL:O	28:q:13:VAL:HG12	2.19	0.42
31:t:238:THR:HG22	31:t:240:LYS:HZ2	1.84	0.42
32:f:209:MET:CE	32:f:233:LEU:HD23	2.49	0.42
32:f:585:GLU:HG3	32:f:586:PRO:HD3	2.01	0.42
32:f:905:ASN:OD1	32:f:906:TYR:N	2.52	0.42
1:U:199:ARG:CZ	1:U:223:LEU:HD23	2.50	0.42
1:U:505:ASP:N	1:U:505:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:409:LYS:HE3	9:c:256:ASN:HD22	1.84	0.42
7:a:99:LYS:O	7:a:103:LYS:HG3	2.19	0.42
9:c:36:LEU:HD11	9:c:40:LYS:HE3	2.02	0.42
13:B:408:ARG:NH2	14:C:163:GLU:OE1	2.52	0.42
15:D:202:VAL:HG23	15:D:329:ARG:CB	2.44	0.42
15:D:399:PHE:O	15:D:400:GLU:C	2.61	0.42
15:D:417:TYR:OH	18:G:22:LEU:N	2.48	0.42
17:F:406:ILE:HG21	17:F:419:ASP:HB2	2.00	0.42
19:H:79:MET:N	19:H:132:VAL:HG12	2.33	0.42
20:I:72:MET:HE2	20:I:107:CYS:HB2	2.01	0.42
26:O:67:MET:HE1	30:s:61:PHE:CE1	2.41	0.42
27:P:70:ARG:HH22	27:P:94:LEU:HA	1.85	0.42
27:P:136:PHE:CB	27:P:150:CYS:HG	2.31	0.42
30:S:215:VAL:HG21	26:o:67:MET:HE3	2.00	0.42
25:n:64:VAL:HG23	25:n:64:VAL:O	2.19	0.42
26:o:233:THR:HG22	26:o:234:VAL:N	2.35	0.42
32:f:131:MET:SD	32:f:158:TYR:HA	2.59	0.42
32:f:287:ASP:OD1	32:f:288:VAL:N	2.53	0.42
32:f:597:VAL:HG11	32:f:656:GLY:CA	2.49	0.42
1:U:336:GLU:OE1	1:U:336:GLU:HA	2.18	0.42
1:U:740:GLY:HA3	1:U:744:VAL:HG22	2.00	0.42
3:W:186:ILE:HG23	3:W:205:ILE:CG2	2.50	0.42
3:W:257:GLN:HE22	3:W:263:TRP:CD1	2.37	0.42
3:W:257:GLN:HE22	3:W:263:TRP:CG	2.35	0.42
4:X:344:ARG:HG2	4:X:384:VAL:HG13	2.01	0.42
8:b:22:LEU:HD12	8:b:22:LEU:O	2.19	0.42
9:c:52:GLU:HB2	9:c:82:VAL:HG13	2.01	0.42
9:c:206:ASN:OD1	9:c:207:TYR:N	2.53	0.42
13:B:188:GLY:HA3	13:B:367:ILE:HD12	2.00	0.42
18:G:56:VAL:O	18:G:58:ASP:N	2.48	0.42
21:J:47:LYS:O	21:J:48:LYS:HB3	2.20	0.42
25:N:169:ILE:HG21	25:N:193:ALA:O	2.20	0.42
28:Q:49:GLU:O	28:Q:53:THR:HG23	2.19	0.42
30:S:134:VAL:HG13	30:S:134:VAL:O	2.19	0.42
30:s:194:LEU:CD2	30:s:199:ALA:HB2	2.49	0.42
31:t:70:ASP:O	31:t:86:ARG:NH1	2.53	0.42
32:f:293:GLN:HG2	32:f:890:VAL:HB	2.02	0.42
1:U:603:LEU:HG	1:U:622:LEU:HD12	2.01	0.42
1:U:800:VAL:HG12	1:U:801:GLN:N	2.35	0.42
2:V:384:GLU:HA	2:V:387:GLN:OE1	2.20	0.42
2:V:443:ARG:HA	2:V:443:ARG:NE	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:299:ILE:HG23	3:W:302:TYR:H	1.84	0.42
9:c:49:VAL:CG2	9:c:148:ILE:HD11	2.49	0.42
10:d:156:ILE:HG22	10:d:164:PHE:CE1	2.54	0.42
12:A:276:GLU:O	12:A:277:ILE:C	2.62	0.42
13:B:109:VAL:HG22	13:B:151:LEU:HD23	2.02	0.42
14:C:87:VAL:HG21	14:C:116:LEU:HD21	2.01	0.42
15:D:139:LEU:HD23	15:D:139:LEU:O	2.20	0.42
16:E:238:ILE:O	16:E:238:ILE:CG2	2.67	0.42
19:H:84:ARG:HA	19:H:87:VAL:HG12	2.02	0.42
20:I:72:MET:SD	20:I:110:LEU:HD23	2.59	0.42
22:K:186:HIS:O	22:K:189:MET:HE3	2.20	0.42
24:M:51:GLU:O	24:M:51:GLU:CD	2.62	0.42
24:M:101:SER:O	25:N:119:GLU:OE2	2.37	0.42
29:R:85:ILE:HD12	27:p:177:ARG:O	2.20	0.42
29:r:205:ASP:OD1	29:r:205:ASP:C	2.62	0.42
1:U:583:MET:HE2	1:U:583:MET:HA	2.01	0.42
2:V:71:THR:HG22	2:V:107:ARG:NE	2.35	0.42
3:W:79:GLU:HB2	3:W:83:LEU:HB2	2.00	0.42
3:W:167:GLN:HG3	3:W:167:GLN:O	2.20	0.42
3:W:250:ILE:O	3:W:256:ILE:HG21	2.19	0.42
4:X:171:LEU:HD21	4:X:209:THR:HG22	2.00	0.42
4:X:415:TYR:HE1	5:Y:383:LEU:HB2	1.85	0.42
5:Y:353:ILE:HG22	5:Y:354:VAL:N	2.35	0.42
9:c:293:THR:HG23	9:c:294:SER:N	2.35	0.42
13:B:105:THR:HG23	14:C:98:ASP:OD2	2.20	0.42
26:O:98:THR:HG23	26:O:129:MET:HE1	2.00	0.42
27:P:141:THR:HG22	27:P:142:CYS:H	1.84	0.42
29:R:103:THR:HG22	29:R:104:MET:N	2.34	0.42
30:S:171:ALA:O	27:p:145:GLN:NE2	2.52	0.42
31:T:134:HIS:NE2	31:T:176:ALA:HB1	2.35	0.42
29:r:238:VAL:HG12	29:r:242:GLY:O	2.19	0.42
30:s:198:ARG:O	30:s:202:LEU:HD13	2.20	0.42
31:t:142:TYR:HA	31:t:145:ARG:HG2	2.02	0.42
32:f:781:TYR:HB3	32:f:785:ARG:HA	2.02	0.42
1:U:521:LEU:C	1:U:521:LEU:HD23	2.45	0.42
2:V:332:LEU:HA	2:V:335:VAL:HG12	2.01	0.42
4:X:31:VAL:HG22	4:X:50:ILE:HG13	2.01	0.42
5:Y:68:ASP:N	5:Y:68:ASP:OD1	2.51	0.42
7:a:27:GLU:OE1	7:a:31:LYS:NZ	2.43	0.42
10:d:99:LYS:O	10:d:103:ASN:N	2.53	0.42
10:d:294:ASN:HB2	10:d:298:LYS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:393:ILE:O	15:D:393:ILE:HG23	2.19	0.42
17:F:65:GLU:OE1	17:F:65:GLU:N	2.53	0.42
22:K:52:LYS:NZ	22:K:216:GLU:OE2	2.42	0.42
24:M:194:VAL:O	24:M:198:ILE:HG12	2.19	0.42
28:Q:184:ASP:OD1	28:Q:185:LYS:N	2.49	0.42
29:R:77:SER:OG	29:R:232:ALA:N	2.53	0.42
1:U:599:ILE:HG22	1:U:603:LEU:HD12	2.01	0.42
2:V:79:VAL:HG13	2:V:163:VAL:HG22	2.01	0.42
7:a:17:GLY:O	7:a:22:TRP:HZ3	2.03	0.42
10:d:316:TYR:O	10:d:318:PHE:N	2.53	0.42
12:A:124:ASP:O	12:A:125:LEU:HB3	2.19	0.42
13:B:67:ARG:NH1	32:f:664:GLU:OE1	2.53	0.42
14:C:118:ASN:C	14:C:120:SER:H	2.27	0.42
14:C:296:ASN:C	14:C:296:ASN:ND2	2.77	0.42
14:C:375:ARG:HE	14:C:377:HIS:HB2	1.84	0.42
19:H:29:VAL:HG11	19:H:133:SER:OG	2.20	0.42
26:O:204:ALA:O	26:O:208:ASN:ND2	2.35	0.42
27:P:45:MET:HB3	27:P:71:LEU:HD13	2.01	0.42
25:n:43:ASP:N	25:n:43:ASP:OD1	2.53	0.42
25:n:184:GLU:HA	25:n:184:GLU:OE2	2.20	0.42
31:t:88:MET:CG	31:t:109:LYS:HZ2	2.33	0.42
32:f:139:CYS:HB3	32:f:165:GLU:OE1	2.20	0.42
1:U:524:LYS:HE3	1:U:562:GLU:HB3	2.01	0.42
2:V:163:VAL:O	2:V:167:LEU:HD23	2.20	0.42
2:V:169:LEU:HA	2:V:172:VAL:HG12	2.01	0.42
5:Y:228:MET:SD	5:Y:263:LEU:HD23	2.60	0.42
10:d:88:LEU:HD23	10:d:140:GLN:HG3	2.01	0.42
16:E:116:ASP:OD1	16:E:118:LEU:N	2.47	0.42
17:F:94:ILE:O	17:F:123:VAL:O	2.38	0.42
21:J:71:MET:HE3	21:J:131:ALA:HB1	2.01	0.42
30:S:63:ILE:HG23	30:S:64:HIS:N	2.35	0.42
30:S:185:ASN:OD1	27:p:173:ASN:ND2	2.52	0.42
31:T:204:VAL:HG13	31:T:204:VAL:O	2.20	0.42
32:f:675:PHE:HB3	32:f:690:VAL:HG13	2.02	0.42
1:U:128:GLN:OE1	1:U:128:GLN:N	2.50	0.41
1:U:232:ILE:O	1:U:236:LEU:HD23	2.20	0.41
1:U:373:ASN:OD1	1:U:377:HIS:ND1	2.43	0.41
1:U:673:GLU:HB2	1:U:674:PRO:HD3	2.01	0.41
3:W:261:GLU:O	3:W:265:GLN:HG2	2.20	0.41
4:X:123:THR:O	4:X:127:GLN:HG2	2.20	0.41
5:Y:274:SER:HA	5:Y:277:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:28:LEU:HD23	7:a:28:LEU:C	2.45	0.41
11:e:58:ALA:O	11:e:62:LYS:HE2	2.20	0.41
12:A:186:LYS:O	12:A:186:LYS:HD3	2.20	0.41
13:B:85:MET:HE2	13:B:85:MET:CA	2.50	0.41
13:B:171:VAL:HA	13:B:174:MET:HG2	2.02	0.41
15:D:147:ALA:O	15:D:148:ASP:HB3	2.20	0.41
21:J:68:ASN:OD1	21:J:68:ASN:N	2.53	0.41
25:N:89:VAL:O	25:N:93:VAL:HG23	2.20	0.41
26:O:56:VAL:HG13	26:O:198:VAL:HG21	2.02	0.41
27:P:28:PHE:O	27:P:28:PHE:CG	2.72	0.41
27:P:159:ASP:OD1	27:P:159:ASP:N	2.53	0.41
30:S:222:ARG:NH1	30:S:233:GLU:OE2	2.53	0.41
28:q:116:TYR:HB3	28:q:124:LEU:HD11	2.02	0.41
29:r:222:ALA:O	29:r:226:ASP:HB3	2.19	0.41
32:f:145:VAL:HG13	32:f:145:VAL:O	2.19	0.41
32:f:237:VAL:HG21	32:f:249:LEU:HG	2.01	0.41
1:U:532:MET:HB3	1:U:552:ILE:HD11	2.01	0.41
3:W:366:MET:HE1	3:W:378:MET:CG	2.50	0.41
4:X:354:ILE:HG23	4:X:356:LEU:HG	2.02	0.41
6:Z:44:GLN:OE1	6:Z:44:GLN:N	2.53	0.41
6:Z:211:TYR:CZ	6:Z:215:VAL:HG21	2.55	0.41
7:a:149:THR:CG2	7:a:150:SER:N	2.83	0.41
14:C:31:LEU:HB3	15:D:47:LEU:CD2	2.49	0.41
18:G:50:ILE:HD12	18:G:79:VAL:HB	2.02	0.41
20:I:72:MET:HE3	20:I:72:MET:HB2	1.88	0.41
24:M:41:ARG:NE	24:M:147:ALA:O	2.53	0.41
26:O:62:ARG:CB	26:O:213:GLY:HA2	2.50	0.41
27:P:12:MET:HE1	27:P:170:ALA:HB3	2.02	0.41
28:Q:160:LEU:C	28:Q:160:LEU:HD23	2.45	0.41
25:n:226:ASP:O	25:n:230:LYS:NZ	2.51	0.41
26:o:183:ASP:C	26:o:184:LYS:HD3	2.45	0.41
27:p:186:ILE:O	27:p:186:ILE:HG23	2.20	0.41
28:q:8:GLN:HB3	28:q:128:PRO:HA	2.02	0.41
29:r:142:LEU:HD23	29:r:142:LEU:C	2.45	0.41
31:t:167:LEU:HG	31:t:182:LEU:HD12	2.02	0.41
32:f:538:ILE:HB	32:f:562:LEU:HD21	2.01	0.41
1:U:464:GLN:HA	1:U:467:ASN:OD1	2.20	0.41
6:Z:40:LEU:HD22	6:Z:91:ILE:HD13	2.01	0.41
6:Z:81:MET:CE	9:c:94:LYS:HZ1	2.32	0.41
10:d:276:GLU:OE2	10:d:308:TRP:CZ2	2.74	0.41
12:A:384:GLU:O	12:A:388:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:339:PRO:O	13:B:343:ARG:N	2.53	0.41
13:B:376:ASP:OD1	13:B:377:ASP:N	2.53	0.41
14:C:32:GLN:OE1	15:D:47:LEU:HD11	2.19	0.41
21:J:175:ASN:O	21:J:175:ASN:CG	2.64	0.41
26:O:140:ALA:HB1	26:O:170:MET:HE3	2.01	0.41
30:S:175:PRO:CB	27:p:149:MET:HE2	2.51	0.41
25:n:93:VAL:HG11	25:n:117:PHE:HE1	1.83	0.41
28:q:15:VAL:HG21	28:q:43:LEU:HD23	2.03	0.41
32:f:137:ARG:CZ	32:f:140:LEU:HB2	2.51	0.41
1:U:202:VAL:HG23	1:U:216:VAL:HG13	2.01	0.41
1:U:596:ASN:OD1	15:D:56:VAL:HG11	2.20	0.41
3:W:276:LEU:HD11	3:W:340:VAL:HG22	2.02	0.41
5:Y:300:ARG:O	5:Y:304:TYR:CD2	2.73	0.41
6:Z:175:LEU:HD22	9:c:217:LEU:HD11	2.02	0.41
7:a:233:LEU:O	7:a:236:THR:OG1	2.32	0.41
9:c:27:THR:O	9:c:182:GLY:HA3	2.20	0.41
12:A:119:ALA:HB2	17:F:128:THR:HG22	2.02	0.41
15:D:120:ASP:O	15:D:123:LEU:N	2.52	0.41
17:F:433:ALA:O	17:F:434:ASN:C	2.61	0.41
18:G:202:LEU:O	18:G:206:LEU:HD13	2.19	0.41
20:I:218:ARG:NH1	20:I:221:GLY:O	2.53	0.41
24:M:24:VAL:O	24:M:28:MET:HG3	2.20	0.41
26:O:207:PHE:O	30:s:66:ARG:NH2	2.53	0.41
27:P:177:ARG:HG2	30:s:175:PRO:HG3	2.02	0.41
29:R:176:GLU:OE1	29:R:176:GLU:N	2.52	0.41
25:n:179:GLU:OE1	25:n:179:GLU:HA	2.20	0.41
32:f:126:ILE:HG21	32:f:142:TYR:CD2	2.55	0.41
32:f:550:LEU:C	32:f:550:LEU:HD12	2.46	0.41
1:U:636:VAL:CG2	15:D:53:PHE:HZ	2.34	0.41
2:V:443:ARG:HH12	10:d:274:CYS:CA	2.33	0.41
2:V:461:LYS:C	2:V:461:LYS:HD3	2.45	0.41
7:a:63:PHE:O	7:a:67:PHE:CB	2.68	0.41
12:A:182:GLU:HA	12:A:185:GLU:HB2	2.02	0.41
14:C:368:MET:HE1	15:D:191:TYR:CE1	2.55	0.41
16:E:336:ASP:O	16:E:336:ASP:CG	2.64	0.41
27:P:11:VAL:HG23	27:P:24:ALA:HB2	2.02	0.41
28:Q:182:ILE:HG12	28:Q:191:LEU:HD13	2.02	0.41
30:S:74:LEU:HD21	30:S:80:ILE:HG21	2.02	0.41
31:T:56:VAL:HG23	31:T:99:SER:HB2	2.02	0.41
31:T:78:LEU:HD13	25:n:168:TYR:CE1	2.55	0.41
25:n:82:SER:OG	25:n:85:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:o:123:ASN:OD1	26:o:156:ILE:HD11	2.20	0.41
27:p:6:TYR:O	27:p:7:ASN:ND2	2.53	0.41
32:f:266:LEU:HD22	32:f:297:MET:CE	2.50	0.41
32:f:514:VAL:O	32:f:518:THR:HG22	2.20	0.41
32:f:887:PHE:HB3	32:f:900:LEU:HD22	2.01	0.41
1:U:51:ASP:O	1:U:57:ARG:NH2	2.54	0.41
1:U:646:PRO:HB2	1:U:682:TYR:CE1	2.56	0.41
2:V:104:THR:O	2:V:108:LEU:HG	2.20	0.41
3:W:112:VAL:HG22	3:W:124:LEU:HD23	1.98	0.41
3:W:259:GLU:O	3:W:263:TRP:CD1	2.74	0.41
3:W:304:ASP:CG	3:W:324:TYR:OH	2.63	0.41
6:Z:48:LEU:HD11	6:Z:92:VAL:HG11	2.03	0.41
7:a:8:LEU:HD22	7:a:26:GLU:HB3	2.03	0.41
7:a:61:GLU:O	7:a:65:SER:CB	2.69	0.41
10:d:301:ASP:O	10:d:302:TYR:HB2	2.21	0.41
12:A:60:ASN:HA	12:A:63:THR:HG23	2.02	0.41
13:B:189:GLY:HA3	13:B:360:THR:HG23	2.02	0.41
14:C:329:LEU:CD2	14:C:359:VAL:HG13	2.51	0.41
14:C:383:PHE:O	14:C:387:VAL:HG23	2.21	0.41
15:D:305:VAL:O	15:D:306:LYS:C	2.64	0.41
16:E:235:ILE:HG23	16:E:285:LEU:HD21	2.02	0.41
24:M:148:GLN:HE21	24:M:148:GLN:HB2	1.57	0.41
27:P:199:THR:O	27:P:200:LEU:C	2.64	0.41
29:R:78:ARG:HD3	29:R:85:ILE:HG12	2.03	0.41
29:R:115:GLU:OE2	29:R:158:THR:OG1	2.39	0.41
30:S:171:ALA:HB3	27:p:144:GLU:OE1	2.21	0.41
25:n:50:ALA:CB	25:n:68:LEU:HD21	2.50	0.41
25:n:192:ASN:O	25:n:196:LEU:HD13	2.21	0.41
26:o:189:MET:HE2	26:o:189:MET:HB2	1.98	0.41
30:s:63:ILE:HG23	30:s:63:ILE:O	2.20	0.41
31:t:52:THR:HG22	31:t:101:ASP:N	2.34	0.41
31:t:65:VAL:HG12	31:t:237:VAL:HG13	2.03	0.41
31:t:214:VAL:O	31:t:218:MET:HG2	2.21	0.41
32:f:233:LEU:HD22	32:f:248:LEU:HD12	2.03	0.41
32:f:315:GLU:HG2	32:f:316:ASP:N	2.36	0.41
32:f:580:LEU:O	32:f:583:VAL:HG23	2.20	0.41
32:f:686:LEU:H	32:f:686:LEU:HD23	1.85	0.41
1:U:32:ASN:OD1	1:U:32:ASN:N	2.53	0.41
3:W:446:ILE:HD11	6:Z:211:TYR:CE2	2.55	0.41
5:Y:138:LEU:HD22	5:Y:167:LEU:HD23	2.03	0.41
6:Z:62:ASP:OD1	6:Z:62:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:31:ALA:O	12:A:35:THR:HG23	2.20	0.41
13:B:68:ILE:HD11	32:f:666:ILE:HD11	2.02	0.41
15:D:262:ILE:HG22	15:D:264:ILE:HG13	2.02	0.41
19:H:86:LEU:CD1	19:H:118:MET:HE2	2.51	0.41
20:I:45:LEU:HD12	20:I:137:ILE:HD13	2.02	0.41
24:M:38:ILE:CG2	24:M:177:ILE:HD11	2.50	0.41
24:M:115:ARG:O	24:M:118:MET:HB2	2.21	0.41
25:N:125:ARG:NH2	31:T:46:THR:HG23	2.36	0.41
26:O:206:ILE:HD12	26:O:213:GLY:C	2.44	0.41
31:T:72:LEU:HD11	31:T:79:ALA:HA	2.01	0.41
31:T:244:ILE:O	31:T:244:ILE:HG13	2.20	0.41
31:t:87:ILE:HG21	31:t:235:ALA:HB3	2.02	0.41
31:t:160:TYR:CZ	31:t:238:THR:HA	2.56	0.41
31:t:179:ALA:HB1	31:t:180:PRO:CD	2.51	0.41
32:f:472:HIS:NE2	32:f:510:SER:OG	2.44	0.41
1:U:586:VAL:HG11	1:U:602:LEU:CD2	2.51	0.41
1:U:895:PRO:C	1:U:896:GLU:HG3	2.46	0.41
5:Y:163:LYS:O	5:Y:167:LEU:HD13	2.20	0.41
9:c:183:HIS:O	9:c:184:LEU:CB	2.69	0.41
12:A:103:ASN:O	12:A:104:ALA:HB3	2.21	0.41
12:A:130:ALA:O	12:A:133:ASP:OD1	2.39	0.41
12:A:188:ARG:HA	12:A:192:GLU:OE1	2.21	0.41
13:B:203:LEU:HA	13:B:206:THR:HG22	2.03	0.41
16:E:180:LYS:HG2	16:E:301:ILE:HD11	2.01	0.41
16:E:300:HIS:O	16:E:300:HIS:ND1	2.54	0.41
19:H:62:VAL:O	19:H:62:VAL:HG13	2.20	0.41
25:N:166:SER:O	25:N:167:SER:C	2.63	0.41
26:O:262:LEU:HD21	27:P:193:ASP:HA	2.02	0.41
30:S:76:ASP:OD1	30:S:77:LYS:N	2.53	0.41
30:S:226:VAL:HG13	30:S:231:ILE:CD1	2.51	0.41
25:n:183:LYS:O	25:n:187:LEU:HD13	2.20	0.41
25:n:223:LEU:C	25:n:224:LEU:HD12	2.46	0.41
26:o:97:MET:SD	27:p:96:TYR:CD1	3.14	0.41
28:q:48:GLY:N	28:q:53:THR:HG21	2.36	0.41
29:r:222:ALA:O	29:r:226:ASP:CB	2.69	0.41
31:t:160:TYR:HE1	31:t:237:VAL:HG13	1.86	0.41
31:t:162:ASP:OD1	31:t:162:ASP:N	2.53	0.41
32:f:570:GLY:HA2	32:f:600:TYR:CE1	2.56	0.41
1:U:188:MET:HE2	1:U:193:PHE:CD2	2.56	0.41
1:U:757:MET:HA	1:U:760:VAL:HG12	2.01	0.41
2:V:477:HIS:HD1	10:d:342:TYR:HH	1.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:186:ILE:CD1	3:W:209:ILE:HD11	2.51	0.41
3:W:194:LEU:HD21	3:W:202:THR:HG21	2.03	0.41
3:W:314:LEU:HD12	3:W:314:LEU:O	2.20	0.41
3:W:359:VAL:CG1	3:W:382:LEU:HD21	2.36	0.41
4:X:406:ASN:HA	4:X:409:LYS:HE2	2.03	0.41
5:Y:195:LYS:HE2	5:Y:195:LYS:HB2	1.91	0.41
6:Z:260:VAL:HG13	9:c:292:MET:HE3	2.02	0.41
7:a:24:ARG:O	7:a:27:GLU:HG3	2.21	0.41
10:d:207:GLU:O	10:d:208:PHE:C	2.64	0.41
12:A:45:ILE:HD12	13:B:61:LYS:NZ	2.36	0.41
12:A:296:GLN:O	12:A:300:LEU:HD13	2.20	0.41
13:B:74:MET:HE1	32:f:610:GLN:N	2.36	0.41
13:B:109:VAL:HB	14:C:94:LYS:HG3	2.03	0.41
13:B:224:LEU:HD21	13:B:235:LEU:HD23	2.01	0.41
14:C:66:LEU:O	15:D:136:SER:OG	2.25	0.41
14:C:97:VAL:HB	14:C:121:TYR:O	2.21	0.41
14:C:193:GLY:CA	15:D:323:ARG:HD2	2.51	0.41
14:C:198:LEU:C	14:C:198:LEU:HD23	2.46	0.41
15:D:204:MET:HE2	15:D:308:ILE:HG22	2.03	0.41
15:D:309:MET:CE	15:D:327:LEU:HD11	2.50	0.41
16:E:327:ASP:O	16:E:331:ILE:HD12	2.20	0.41
20:I:24:ALA:O	20:I:28:ILE:HG12	2.20	0.41
20:I:206:LEU:O	20:I:206:LEU:HD23	2.21	0.41
20:I:216:LEU:C	20:I:216:LEU:HD23	2.46	0.41
21:J:61:LYS:NZ	21:J:73:PHE:O	2.51	0.41
23:L:33:SER:HB3	23:L:51:ARG:HE	1.85	0.41
26:O:55:ILE:HG22	26:O:56:VAL:N	2.36	0.41
28:Q:15:VAL:HG21	28:Q:45:LEU:HD12	2.03	0.41
28:Q:154:GLU:O	28:Q:157:VAL:N	2.54	0.41
30:S:55:THR:O	30:S:55:THR:HG22	2.21	0.41
30:S:175:PRO:HB2	27:p:149:MET:HE2	2.03	0.41
31:T:113:GLY:O	31:T:117:ILE:HG13	2.19	0.41
25:n:208:ILE:HD12	25:n:228:ILE:HG12	2.03	0.41
27:p:27:ARG:NH1	27:p:180:VAL:HB	2.36	0.41
30:s:141:LEU:HD23	30:s:146:LYS:O	2.21	0.41
32:f:226:TYR:OH	32:f:259:PHE:HD2	2.04	0.41
32:f:803:PHE:HZ	32:f:818:LEU:HD11	1.86	0.41
32:f:830:LEU:HD11	32:f:894:LEU:CD2	2.50	0.41
1:U:556:MET:SD	1:U:563:ALA:HB2	2.60	0.41
2:V:254:LEU:CD2	2:V:270:LEU:HD13	2.51	0.41
2:V:275:VAL:O	2:V:275:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:364:THR:HA	2:V:367:VAL:HG12	2.02	0.41
3:W:226:TYR:OH	3:W:230:MET:HE2	2.21	0.41
7:a:252:LYS:HA	7:a:255:TRP:NE1	2.36	0.41
7:a:312:MET:HE3	7:a:312:MET:CA	2.51	0.41
8:b:5:SER:HA	8:b:48:ASN:OD1	2.20	0.41
10:d:90:ALA:O	10:d:94:MET:CE	2.69	0.41
12:A:125:LEU:HD13	12:A:134:ILE:HG21	2.03	0.41
15:D:116:LEU:O	15:D:119:ILE:HD13	2.20	0.41
16:E:308:ALA:O	16:E:312:ILE:HG13	2.21	0.41
17:F:89:LEU:HD23	17:F:90:VAL:O	2.20	0.41
25:N:181:MET:CE	25:N:185:GLU:HG3	2.51	0.41
26:O:182:GLU:OE1	31:t:224:ARG:NH1	2.54	0.41
27:P:111:GLY:C	27:P:112:LEU:HD22	2.46	0.41
25:n:93:VAL:HG11	25:n:117:PHE:CD1	2.56	0.41
26:o:51:TYR:CE1	26:o:56:VAL:HG23	2.56	0.41
30:s:59:GLU:O	30:s:59:GLU:HG2	2.20	0.41
32:f:418:LEU:HD13	32:f:425:GLY:HA2	2.03	0.41
32:f:505:MET:HG3	32:f:518:THR:HG23	2.03	0.41
3:W:217:GLU:OE1	3:W:217:GLU:N	2.37	0.40
3:W:251:TYR:CE1	3:W:267:LEU:HD13	2.56	0.40
5:Y:279:GLU:OE1	11:e:52:PHE:HB3	2.22	0.40
6:Z:142:GLU:OE2	6:Z:151:THR:OG1	2.39	0.40
7:a:185:ILE:H	7:a:185:ILE:HD12	1.86	0.40
9:c:41:MET:CG	9:c:72:VAL:HG11	2.51	0.40
10:d:152:ALA:O	10:d:155:SER:OG	2.31	0.40
13:B:99:VAL:HG13	13:B:138:PHE:CE1	2.56	0.40
13:B:284:ILE:HD12	13:B:329:MET:SD	2.61	0.40
13:B:342:ILE:O	13:B:342:ILE:CG2	2.69	0.40
16:E:366:ASP:OD1	16:E:367:PHE:CD1	2.74	0.40
17:F:69:MET:O	17:F:73:ILE:HG12	2.21	0.40
21:J:90:GLU:HG3	21:J:110:TYR:CE1	2.57	0.40
22:K:213:THR:O	22:K:214:ASN:CG	2.65	0.40
25:N:195:ALA:HB2	25:N:228:ILE:HG13	2.04	0.40
27:P:3:ILE:HG21	27:P:104:TYR:CD2	2.56	0.40
28:Q:35:MET:CE	28:Q:45:LEU:HD21	2.50	0.40
30:S:141:LEU:HD11	30:S:227:THR:C	2.46	0.40
25:n:125:ARG:HE	31:t:46:THR:HG23	1.87	0.40
26:o:102:ILE:HG13	26:o:126:LEU:HD23	2.03	0.40
28:q:85:ARG:HD3	28:q:124:LEU:HB2	2.02	0.40
32:f:570:GLY:O	32:f:573:ILE:HG12	2.21	0.40
32:f:674:THR:O	32:f:678:LEU:HD13	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:61:ALA:HB3	1:U:84:ALA:HA	2.04	0.40
1:U:242:LEU:HD12	1:U:243:LEU:N	2.35	0.40
1:U:587:ALA:HB2	1:U:621:SER:CB	2.51	0.40
1:U:676:THR:HG21	1:U:712:LEU:HD21	2.02	0.40
1:U:719:ASP:HB3	1:U:722:ASP:HB2	2.03	0.40
5:Y:259:TYR:HB2	5:Y:274:SER:HB3	2.02	0.40
8:b:188:ILE:H	8:b:188:ILE:HD12	1.86	0.40
13:B:99:VAL:HG13	13:B:138:PHE:CD1	2.56	0.40
13:B:258:LYS:HA	14:C:224:ILE:HG23	2.03	0.40
15:D:342:ARG:NH1	15:D:361:GLU:OE1	2.54	0.40
16:E:84:ARG:NE	16:E:108:MET:O	2.54	0.40
19:H:36:VAL:HG13	19:H:174:LEU:HD11	2.02	0.40
23:L:185:ASN:O	23:L:189:LYS:HG2	2.21	0.40
23:L:234:GLU:HA	23:L:234:GLU:OE1	2.21	0.40
24:M:87:SER:O	24:M:91:ILE:HG12	2.21	0.40
26:O:81:SER:O	26:O:82:PRO:C	2.64	0.40
27:P:158:MET:HE3	27:P:159:ASP:OD1	2.21	0.40
28:Q:140:LEU:HD23	28:Q:140:LEU:O	2.21	0.40
30:S:171:ALA:HB1	27:p:145:GLN:HE21	1.86	0.40
32:f:396:ASN:N	32:f:432:TYR:OH	2.54	0.40
32:f:539:LEU:O	32:f:543:MET:HG2	2.22	0.40
2:V:175:MET:SD	2:V:187:ILE:HD13	2.61	0.40
5:Y:195:LYS:HA	5:Y:230:ALA:HB1	2.03	0.40
9:c:285:GLU:O	9:c:288:VAL:HG12	2.21	0.40
10:d:92:THR:HG23	10:d:140:GLN:HE22	1.86	0.40
10:d:130:PRO:HG2	10:d:178:TYR:CZ	2.57	0.40
14:C:89:VAL:O	14:C:89:VAL:HG23	2.21	0.40
17:F:268:VAL:O	17:F:272:PHE:HD2	2.04	0.40
18:G:92:GLN:HG3	24:M:118:MET:CE	2.52	0.40
18:G:217:VAL:CG1	18:G:230:LEU:HD12	2.51	0.40
23:L:226:ASP:O	23:L:229:VAL:HG22	2.21	0.40
24:M:216:TRP:CE3	24:M:228:VAL:HG22	2.57	0.40
26:o:254:VAL:HG22	27:p:164:PHE:HZ	1.86	0.40
32:f:702:PRO:HA	32:f:732:VAL:HG22	2.03	0.40
1:U:894:MET:HE2	1:U:902:PRO:HD3	2.03	0.40
2:V:188:SER:HG	2:V:214:HIS:CE1	2.39	0.40
3:W:362:ASN:O	3:W:366:MET:HG3	2.21	0.40
6:Z:121:LEU:HD23	6:Z:121:LEU:C	2.46	0.40
10:d:272:ALA:O	10:d:273:GLY:C	2.64	0.40
13:B:194:ILE:HA	13:B:197:ILE:HG22	2.03	0.40
15:D:64:GLU:HG2	15:D:68:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:215:LEU:O	15:D:218:ALA:HB3	2.22	0.40
18:G:177:SER:O	18:G:180:GLU:HG2	2.21	0.40
22:K:201:ILE:O	22:K:205:VAL:HG22	2.21	0.40
29:R:94:ILE:HD12	29:R:94:ILE:H	1.86	0.40
31:T:55:SER:HA	31:T:184:THR:O	2.21	0.40
31:T:223:TYR:HB3	31:T:224:ARG:HD2	2.04	0.40
28:q:4:LEU:HD13	28:q:45:LEU:HB3	2.03	0.40
30:s:136:ASN:O	30:s:137:ILE:HD13	2.21	0.40
31:t:148:MET:N	31:t:148:MET:SD	2.94	0.40
32:f:252:ALA:HB3	32:f:268:LEU:HD13	2.02	0.40
32:f:271:MET:HE1	32:f:786:GLN:C	2.46	0.40
32:f:468:ASP:OD2	33:y:391:LYS:NZ	2.43	0.40
32:f:601:ALA:HB2	32:f:659:LEU:HD21	2.03	0.40
32:f:828:ARG:HG3	32:f:828:ARG:O	2.21	0.40
32:f:884:THR:HG22	32:f:885:GLU:N	2.37	0.40
1:U:140:ARG:NH2	1:U:141:CYS:SG	2.94	0.40
2:V:396:ILE:C	2:V:398:LEU:N	2.79	0.40
3:W:217:GLU:HG2	3:W:218:ASN:N	2.36	0.40
3:W:220:GLU:O	3:W:224:LEU:CD1	2.69	0.40
3:W:243:ILE:HG21	3:W:273:TYR:CZ	2.57	0.40
4:X:204:PRO:HB2	4:X:242:ILE:HD11	2.03	0.40
5:Y:226:VAL:HA	5:Y:229:ILE:HG22	2.03	0.40
6:Z:19:VAL:HG13	6:Z:95:TYR:CE2	2.56	0.40
6:Z:22:HIS:CE1	6:Z:35:VAL:HB	2.56	0.40
7:a:100:THR:O	7:a:104:VAL:HG12	2.21	0.40
12:A:123:VAL:HG12	12:A:125:LEU:N	2.37	0.40
12:A:259:GLU:HA	12:A:262:GLU:OE1	2.22	0.40
17:F:434:ASN:ND2	23:L:51:ARG:NH1	2.70	0.40
21:J:158:ALA:H	22:K:58:LEU:HD21	1.86	0.40
22:K:71:ASP:CG	22:K:72:ALA:H	2.29	0.40
27:P:149:MET:CE	30:s:175:PRO:HB2	2.52	0.40
27:P:183:MET:HE2	27:P:183:MET:HA	2.04	0.40
29:R:195:TYR:HE2	28:q:170:ARG:NE	2.20	0.40
31:t:234:ILE:HG22	31:t:235:ALA:N	2.37	0.40
32:f:57:GLU:HA	32:f:60:VAL:HG12	2.04	0.40
32:f:375:SER:HB3	32:f:398:TRP:HE1	1.87	0.40
32:f:414:LEU:HD23	32:f:429:ILE:HD13	2.03	0.40
32:f:737:ASN:OD1	32:f:770:HIS:ND1	2.54	0.40
32:f:795:GLY:O	32:f:798:THR:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	814/953 (85%)	754 (93%)	60 (7%)	0	100	100
2	V	417/534 (78%)	389 (93%)	28 (7%)	0	100	100
3	W	426/456 (93%)	392 (92%)	34 (8%)	0	100	100
4	X	419/422 (99%)	391 (93%)	28 (7%)	0	100	100
5	Y	377/389 (97%)	361 (96%)	16 (4%)	0	100	100
6	Z	285/324 (88%)	274 (96%)	11 (4%)	0	100	100
7	a	373/376 (99%)	343 (92%)	30 (8%)	0	100	100
8	b	189/377 (50%)	172 (91%)	17 (9%)	0	100	100
9	c	273/310 (88%)	253 (93%)	20 (7%)	0	100	100
10	d	252/350 (72%)	215 (85%)	37 (15%)	0	100	100
11	e	32/70 (46%)	31 (97%)	1 (3%)	0	100	100
12	A	296/433 (68%)	258 (87%)	38 (13%)	0	100	100
13	B	378/440 (86%)	346 (92%)	32 (8%)	0	100	100
14	C	387/406 (95%)	354 (92%)	33 (8%)	0	100	100
15	D	378/418 (90%)	336 (89%)	41 (11%)	1 (0%)	36	65
16	E	333/389 (86%)	303 (91%)	29 (9%)	1 (0%)	36	65
17	F	207/439 (47%)	183 (88%)	24 (12%)	0	100	100
18	G	239/246 (97%)	226 (95%)	13 (5%)	0	100	100
19	H	231/234 (99%)	218 (94%)	13 (6%)	0	100	100
20	I	247/261 (95%)	240 (97%)	7 (3%)	0	100	100
21	J	237/248 (96%)	223 (94%)	14 (6%)	0	100	100
22	K	231/241 (96%)	213 (92%)	18 (8%)	0	100	100
23	L	235/263 (89%)	220 (94%)	15 (6%)	0	100	100
24	M	242/255 (95%)	234 (97%)	8 (3%)	0	100	100
25	N	196/239 (82%)	180 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	n	171/239 (72%)	164 (96%)	7 (4%)	0	100	100
26	O	219/277 (79%)	210 (96%)	9 (4%)	0	100	100
26	o	166/277 (60%)	155 (93%)	11 (7%)	0	100	100
27	P	202/205 (98%)	186 (92%)	16 (8%)	0	100	100
27	p	152/205 (74%)	139 (91%)	13 (9%)	0	100	100
28	Q	195/201 (97%)	186 (95%)	9 (5%)	0	100	100
28	q	163/201 (81%)	152 (93%)	11 (7%)	0	100	100
29	R	197/263 (75%)	187 (95%)	10 (5%)	0	100	100
29	r	181/263 (69%)	165 (91%)	16 (9%)	0	100	100
30	S	210/241 (87%)	198 (94%)	12 (6%)	0	100	100
30	s	202/241 (84%)	191 (95%)	11 (5%)	0	100	100
31	T	211/264 (80%)	200 (95%)	11 (5%)	0	100	100
31	t	202/264 (76%)	183 (91%)	19 (9%)	0	100	100
32	f	811/908 (89%)	746 (92%)	65 (8%)	0	100	100
33	y	29/505 (6%)	29 (100%)	0	0	100	100
All	All	11005/13627 (81%)	10200 (93%)	803 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	D	220	ALA
16	E	238	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	708/816 (87%)	708 (100%)	0	100	100
2	V	371/460 (81%)	371 (100%)	0	100	100
3	W	396/416 (95%)	396 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	X	361/362 (100%)	361 (100%)	0	100	100
5	Y	188/344 (55%)	188 (100%)	0	100	100
6	Z	67/295 (23%)	67 (100%)	0	100	100
7	a	284/336 (84%)	284 (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	233/372 (63%)	233 (100%)	0	100	100
13	B	249/385 (65%)	249 (100%)	0	100	100
14	C	260/352 (74%)	260 (100%)	0	100	100
15	D	320/366 (87%)	320 (100%)	0	100	100
16	E	170/341 (50%)	170 (100%)	0	100	100
17	F	196/379 (52%)	196 (100%)	0	100	100
18	G	206/210 (98%)	206 (100%)	0	100	100
19	H	190/191 (100%)	190 (100%)	0	100	100
20	I	209/221 (95%)	209 (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	121/212 (57%)	120 (99%)	1 (1%)	73	77
25	N	140/181 (77%)	140 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	693/763 (91%)	693 (100%)	0	100	100
33	y	29/403 (7%)	29 (100%)	0	100	100
All	All	8744/11539 (76%)	8743 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	M	148	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	259	GLN
1	U	345	ASN
1	U	384	GLN
1	U	452	ASN
1	U	596	ASN
2	V	168	GLN
2	V	350	GLN
2	V	376	ASN
3	W	99	GLN
3	W	246	HIS
3	W	380	GLN
3	W	416	GLN
4	X	78	ASN
4	X	207	GLN
4	X	333	GLN
5	Y	178	ASN
7	a	72	ASN
9	c	131	GLN
9	c	240	HIS
9	c	256	ASN
12	A	150	HIS
13	B	82	GLN
14	C	46	GLN

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Mol	Chain	Res	Type
14	C	118	ASN
14	C	124	HIS
14	C	377	HIS
15	D	173	GLN
15	D	294	ASN
15	D	302	ASN
15	D	312	ASN
15	D	376	ASN
17	F	196	GLN
18	G	12	HIS
19	H	102	GLN
19	H	109	GLN
20	I	84	ASN
21	J	154	HIS
24	M	148	GLN
26	O	78	HIS
27	P	33	GLN
28	Q	55	GLN
29	R	210	GLN
30	S	105	HIS
31	T	153	ASN
31	T	192	GLN
31	T	253	ASN
26	o	123	ASN
26	o	196	ASN
28	q	101	ASN
29	r	88	GLN
30	s	191	HIS
32	f	291	GLN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	-	32,33,33	0.27	0	48,52,52	0.67	1 (2%)
36	ADP	E	401	-	28,29,29	1.39	4 (14%)	43,45,45	1.87	11 (25%)
35	ATP	C	501	-	32,33,33	0.38	0	48,52,52	0.71	0
35	ATP	D	501	-	32,33,33	0.34	0	48,52,52	0.69	0
35	ATP	B	501	-	32,33,33	0.41	0	48,52,52	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ATP	A	501	-	-	6/22/38/38	0/3/3/3
36	ADP	E	401	-	-	2/16/32/32	0/3/3/3
35	ATP	C	501	-	-	7/22/38/38	0/3/3/3
35	ATP	D	501	-	-	5/22/38/38	0/3/3/3
35	ATP	B	501	-	-	1/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	E	401	ADP	C5-C4	4.52	1.47	1.39
36	E	401	ADP	C5-C6	2.64	1.48	1.41
36	E	401	ADP	C5-N7	-2.37	1.34	1.39
36	E	401	ADP	C8-N7	2.35	1.36	1.31

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	E	401	ADP	C5-C4-N3	-5.65	118.94	126.72
36	E	401	ADP	N3-C4-N9	4.47	134.76	127.17
36	E	401	ADP	C2-N3-C4	3.78	121.07	111.83
36	E	401	ADP	N3-C2-N1	-3.62	123.10	128.58
36	E	401	ADP	C4-C5-N7	-3.48	106.60	110.58
36	E	401	ADP	C4-N9-C8	2.84	108.72	105.74
36	E	401	ADP	C5-N7-C8	2.66	107.63	103.45
36	E	401	ADP	C3'-C2'-C1'	2.59	106.37	101.46
36	E	401	ADP	N9-C8-N7	-2.24	110.75	113.94
36	E	401	ADP	C6-C5-N7	2.19	136.30	132.09
36	E	401	ADP	C2-N1-C6	2.05	122.11	118.73
35	A	501	ATP	O3'-C3'-C4'	-2.02	105.29	111.08

There are no chirality outliers.

All (21) torsion outliers are listed below:

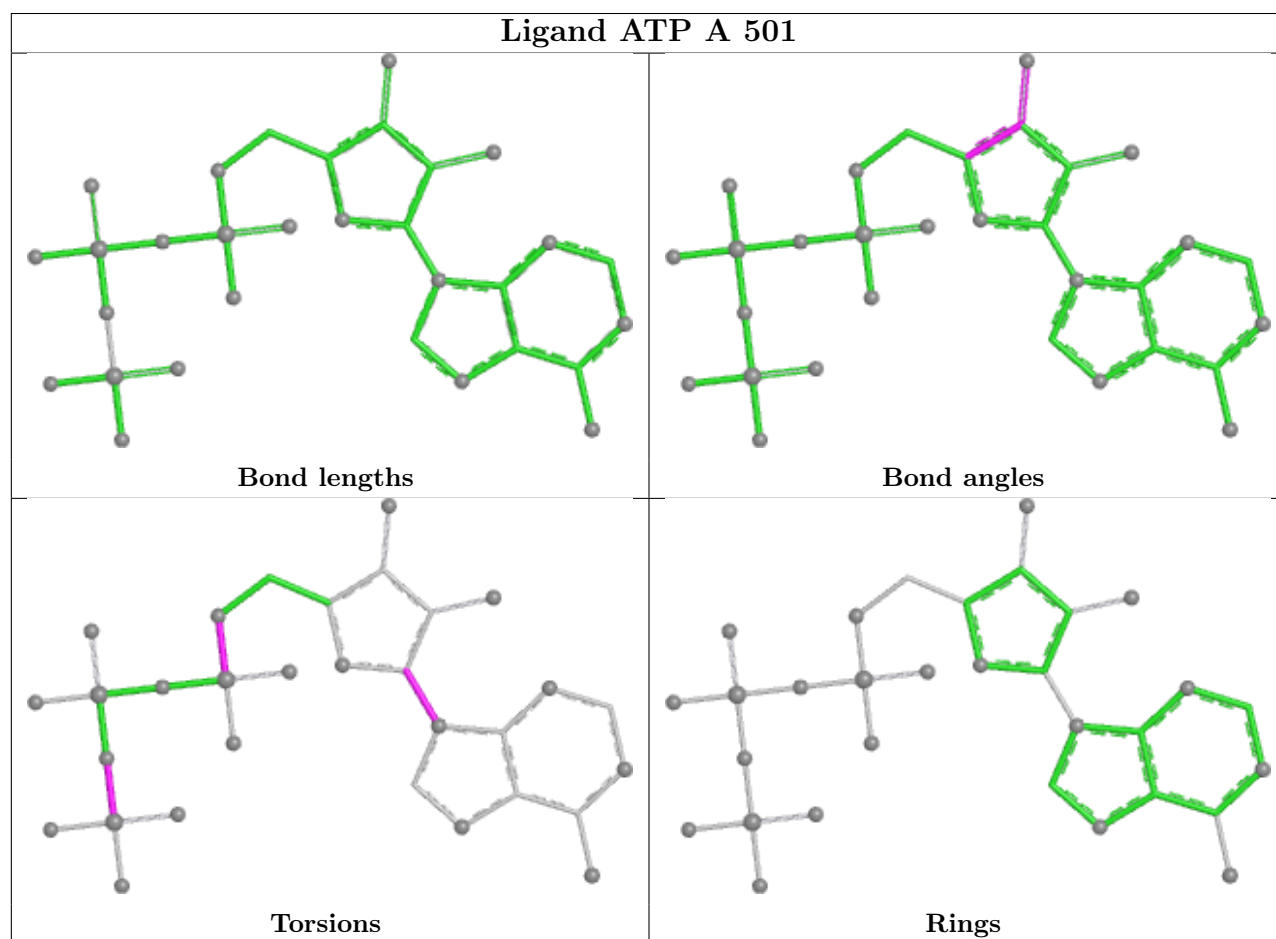
Mol	Chain	Res	Type	Atoms
35	A	501	ATP	PB-O3B-PG-O2G
35	A	501	ATP	PB-O3B-PG-O3G
35	A	501	ATP	C5'-O5'-PA-O2A
35	A	501	ATP	C5'-O5'-PA-O3A
35	C	501	ATP	C5'-O5'-PA-O2A
35	D	501	ATP	C5'-O5'-PA-O2A
36	E	401	ADP	PB-O3A-PA-O1A
35	C	501	ATP	C5'-O5'-PA-O1A
35	C	501	ATP	C5'-O5'-PA-O3A
35	D	501	ATP	C5'-O5'-PA-O1A
35	D	501	ATP	C5'-O5'-PA-O3A
35	B	501	ATP	PA-O3A-PB-O2B
35	C	501	ATP	PA-O3A-PB-O2B
35	A	501	ATP	C2'-C1'-N9-C4
35	A	501	ATP	C2'-C1'-N9-C8
35	C	501	ATP	PA-O3A-PB-O1B
35	D	501	ATP	PA-O3A-PB-O1B
36	E	401	ADP	PB-O3A-PA-O2A
35	C	501	ATP	PG-O3B-PB-O1B
35	D	501	ATP	PA-O3A-PB-O2B
35	C	501	ATP	PG-O3B-PB-O2B

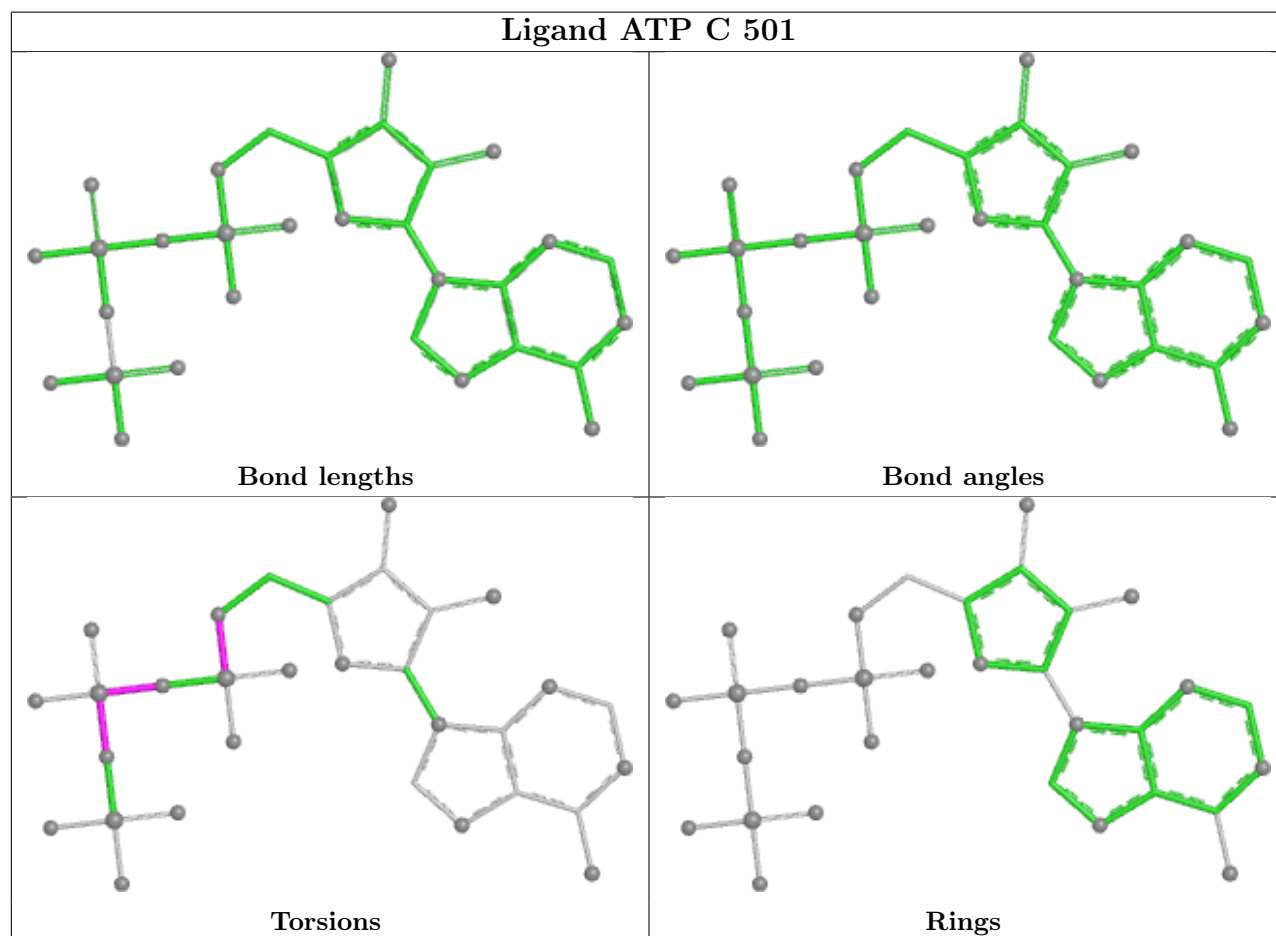
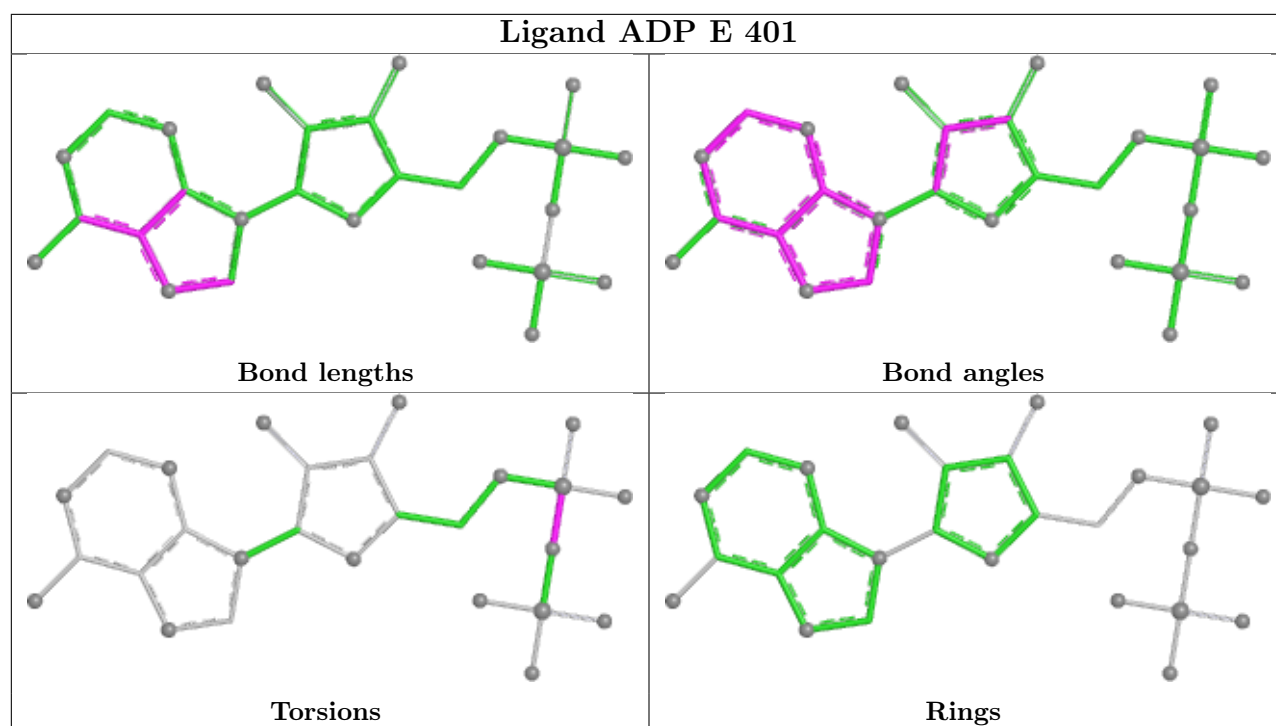
There are no ring outliers.

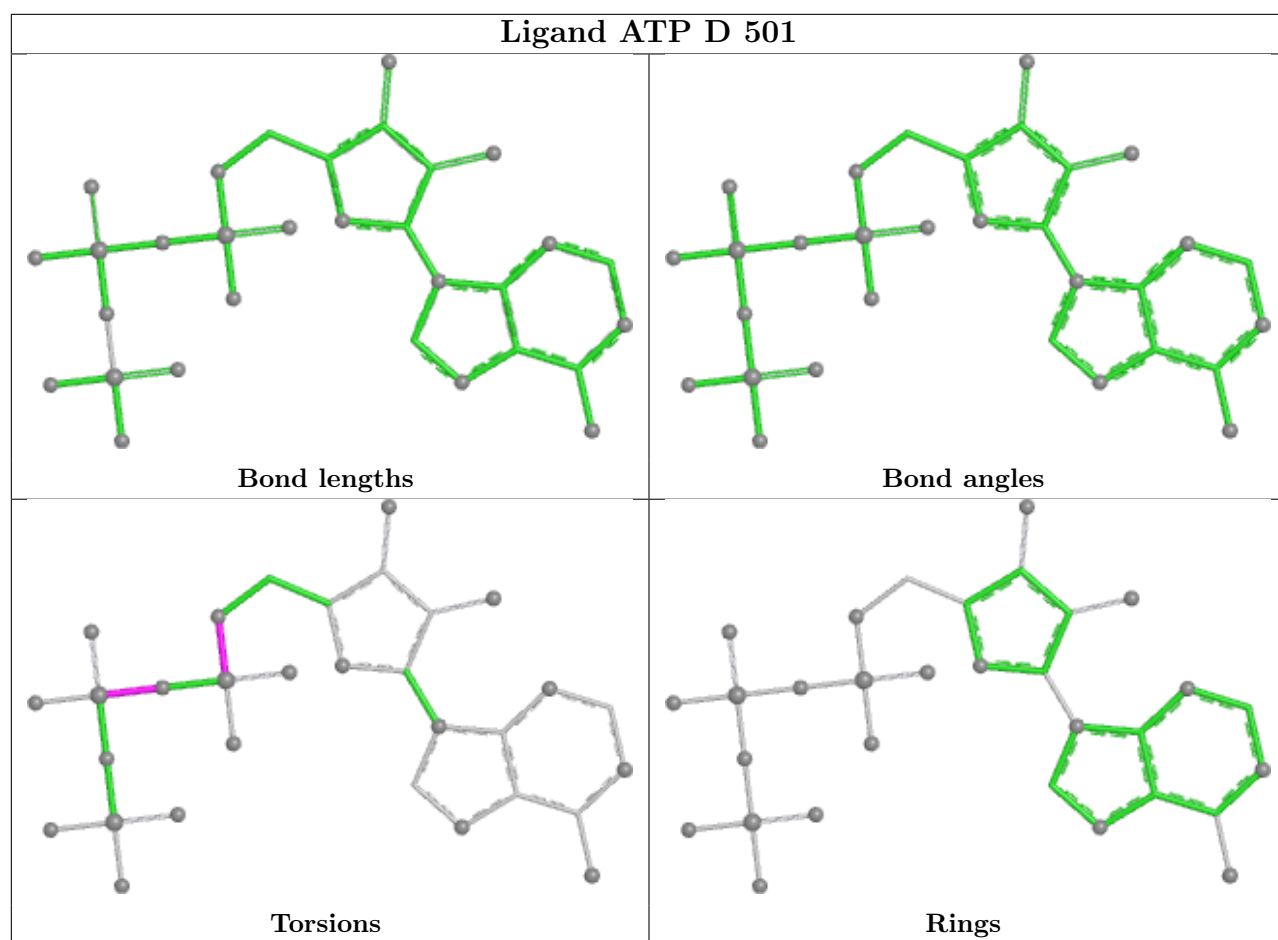
5 monomers are involved in 11 short contacts:

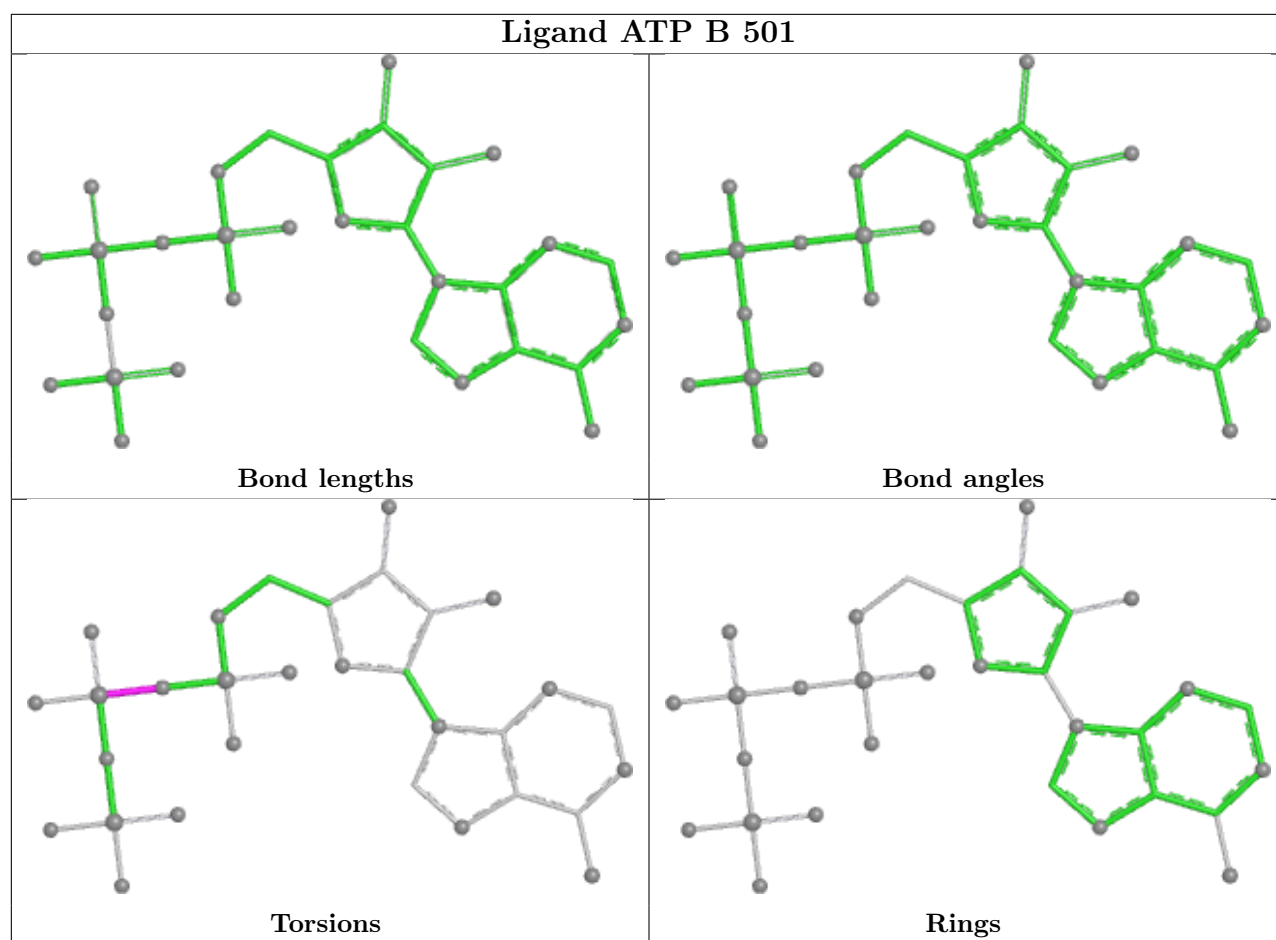
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	501	ATP	4	0
36	E	401	ADP	1	0
35	C	501	ATP	1	0
35	D	501	ATP	2	0
35	B	501	ATP	3	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

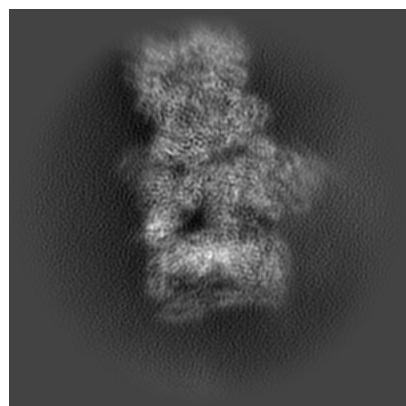
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44929. These allow visual inspection of the internal detail of the map and identification of artifacts.

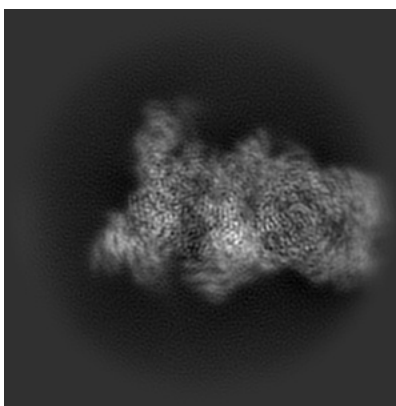
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

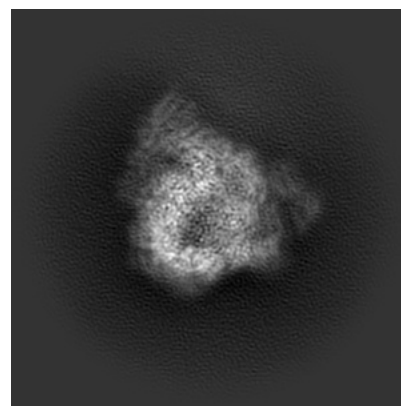
6.1.1 Primary map



X

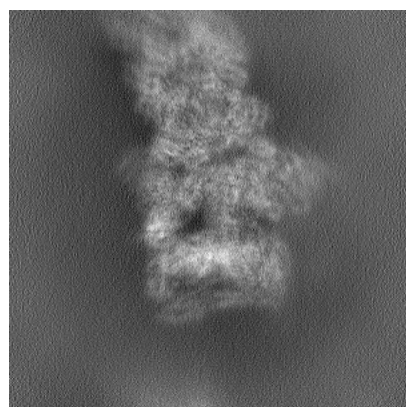


Y

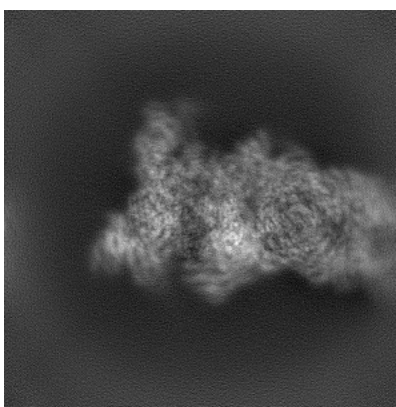


Z

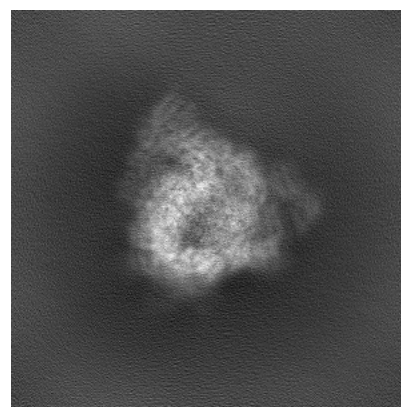
6.1.2 Raw map



X



Y

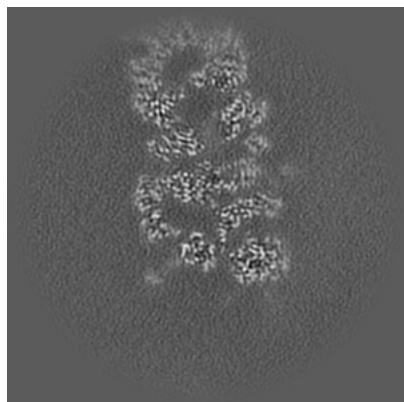


Z

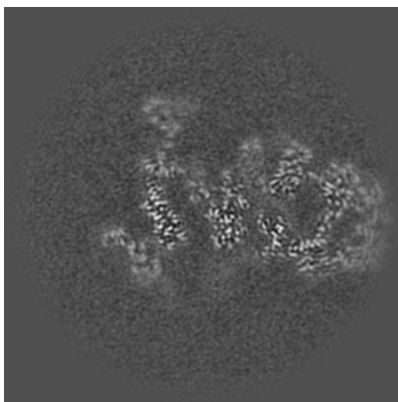
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

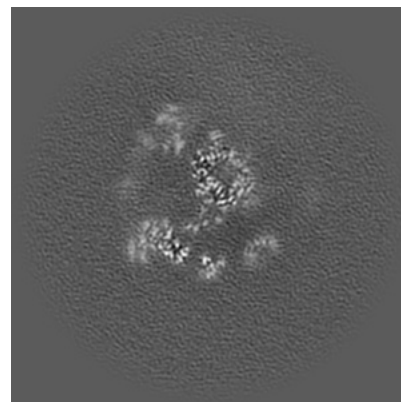
6.2.1 Primary map



X Index: 220

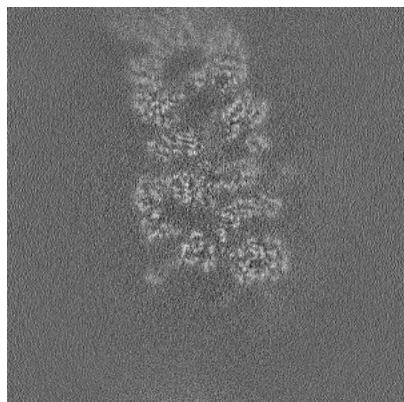


Y Index: 220

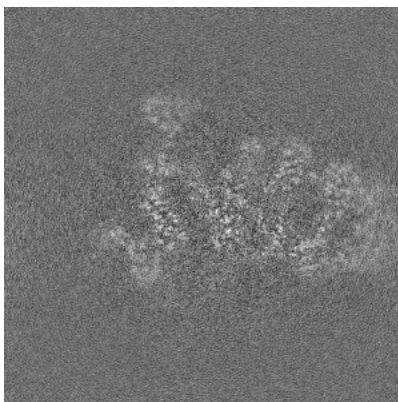


Z Index: 220

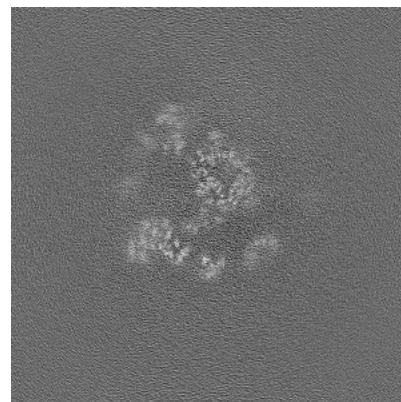
6.2.2 Raw map



X Index: 220



Y Index: 220

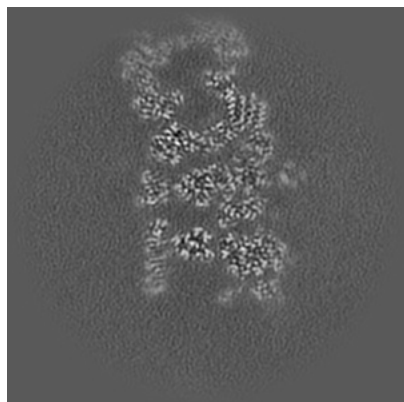


Z Index: 220

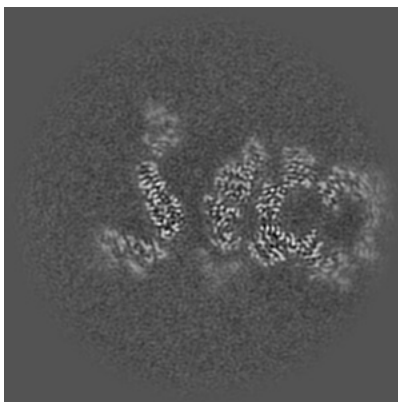
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

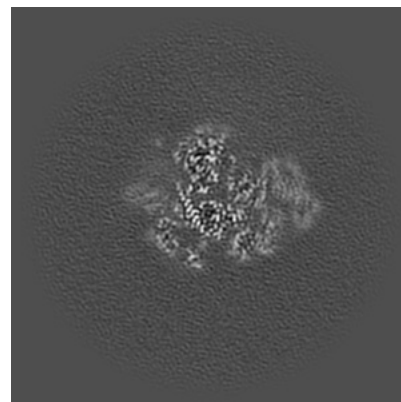
6.3.1 Primary map



X Index: 209

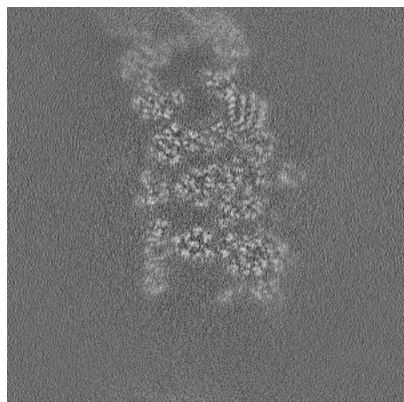


Y Index: 205

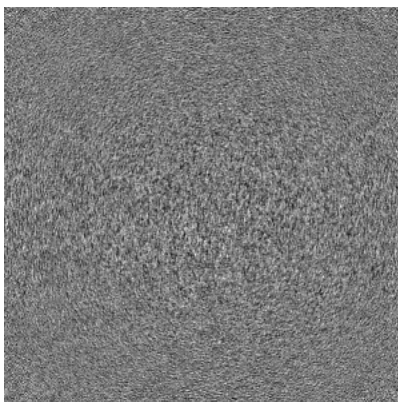


Z Index: 170

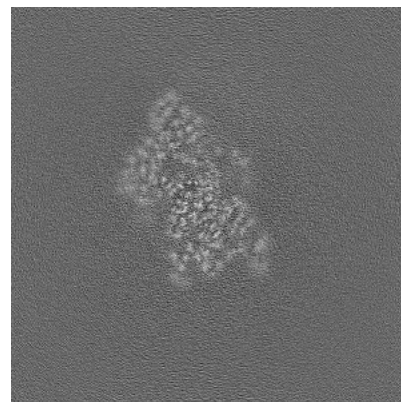
6.3.2 Raw map



X Index: 209



Y Index: 0

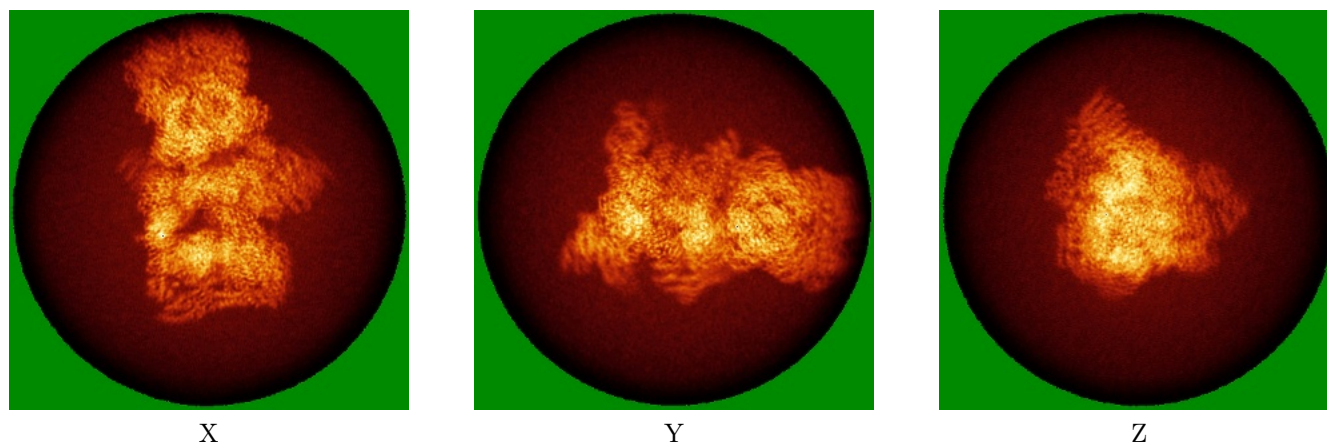


Z Index: 243

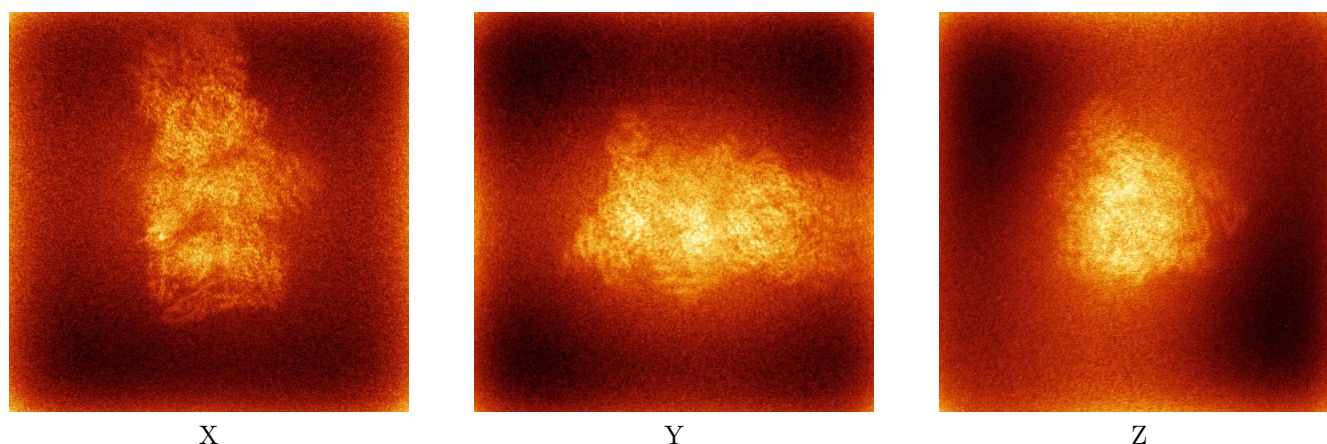
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

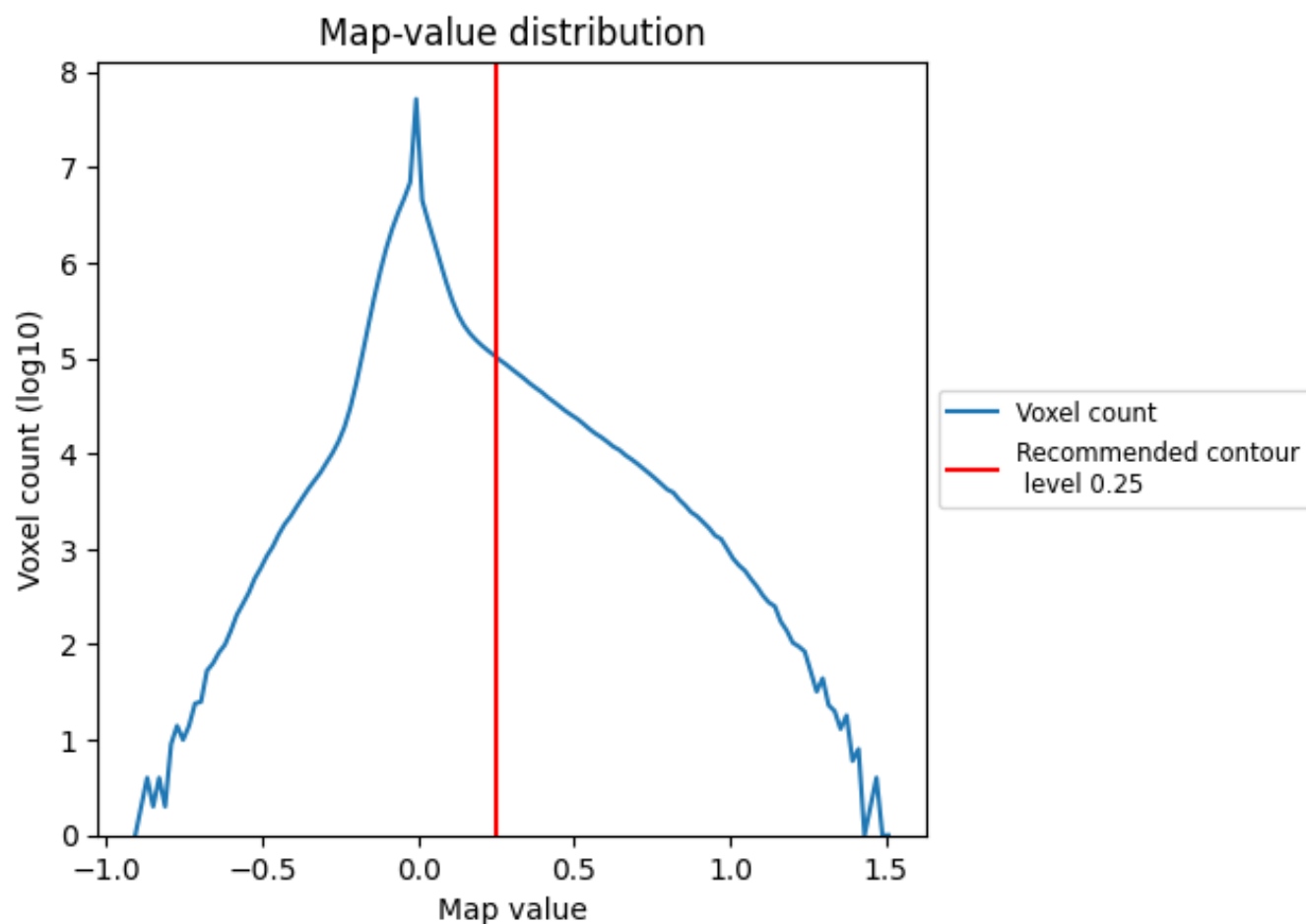
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

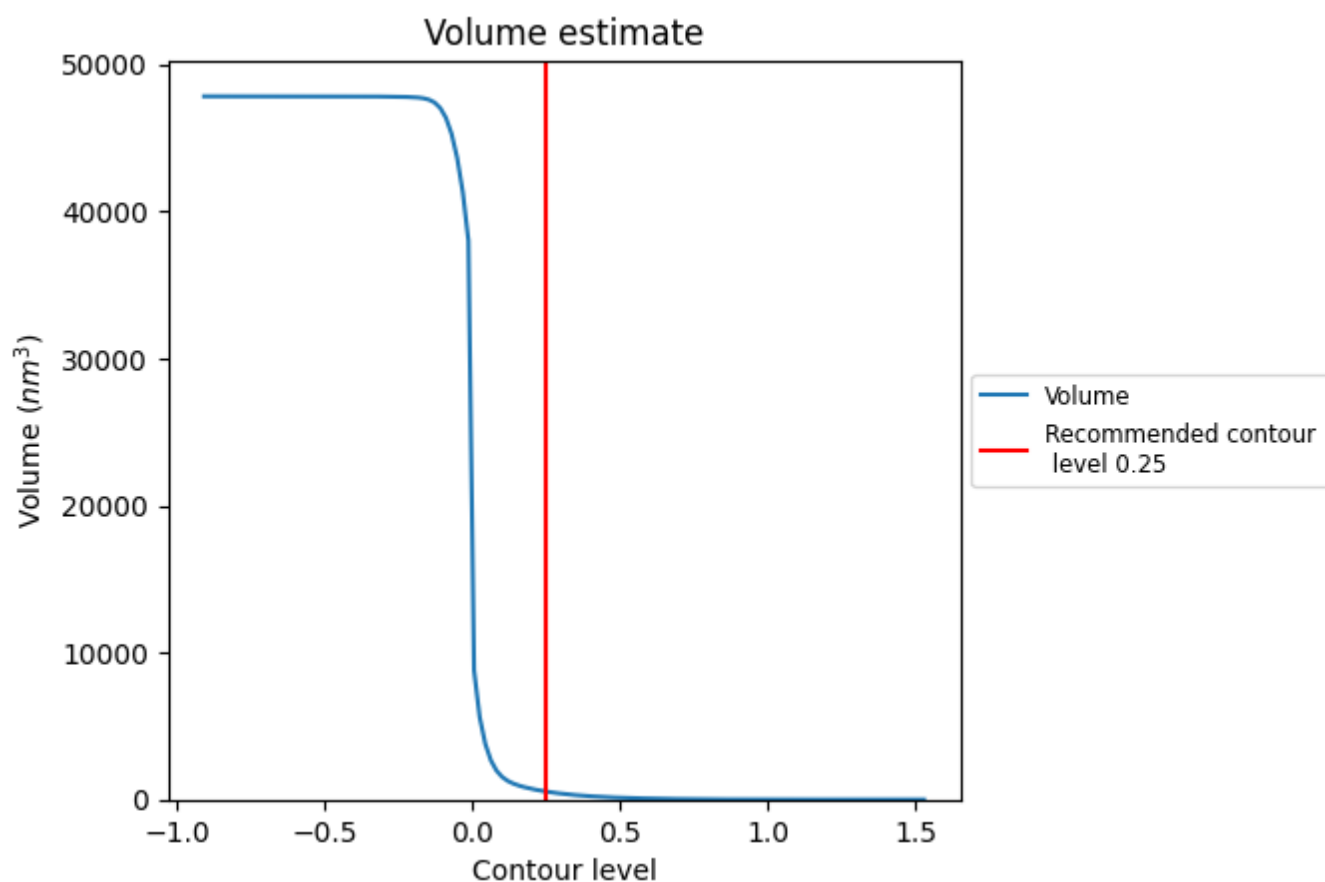
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

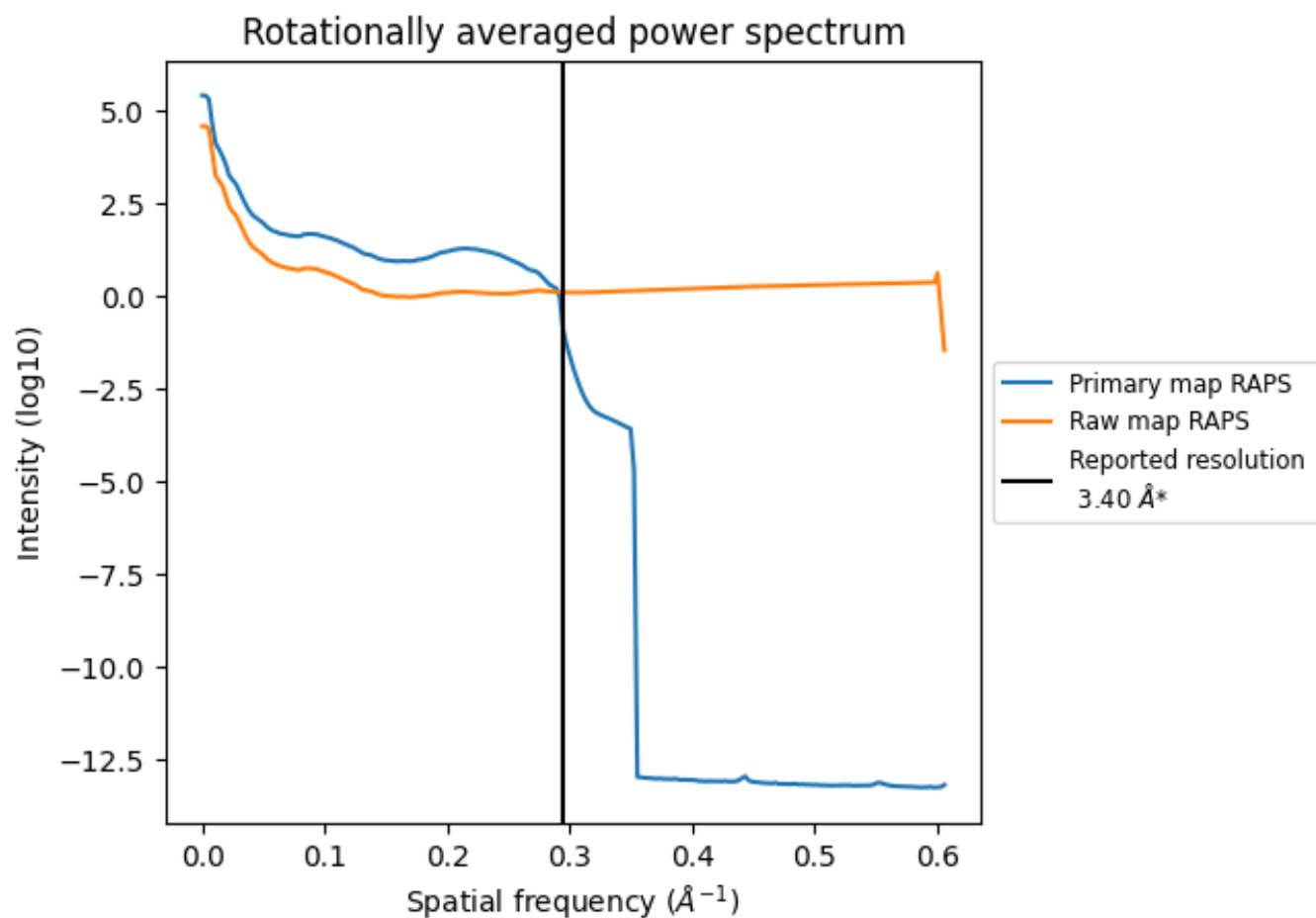
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 545 nm³; this corresponds to an approximate mass of 492 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

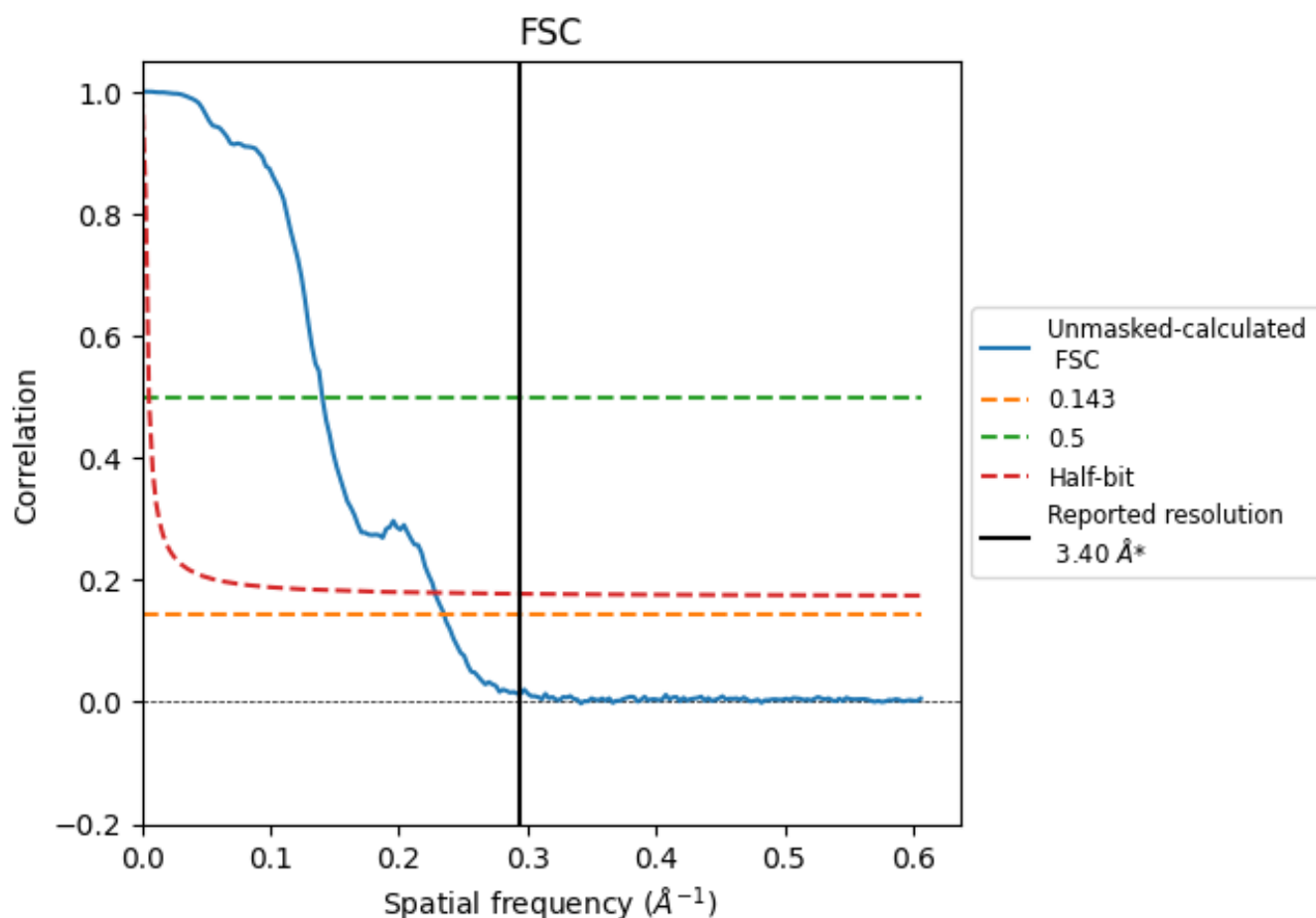


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

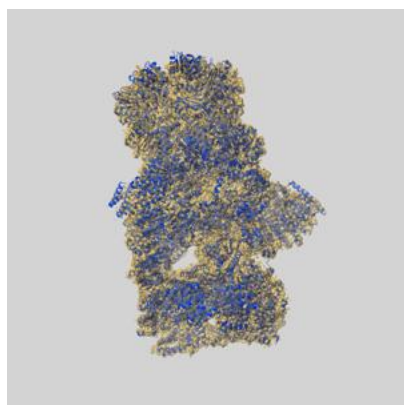
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.26	7.13	4.39

*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 4.26 differs from the reported value 3.4 by more than 10 %

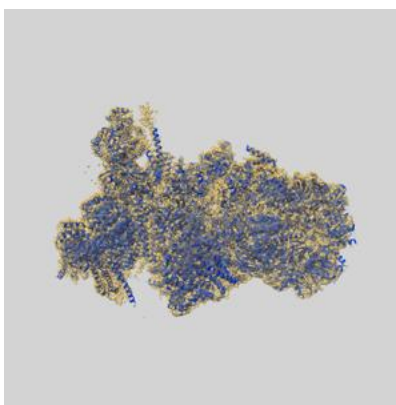
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44929 and PDB model 9BV2. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

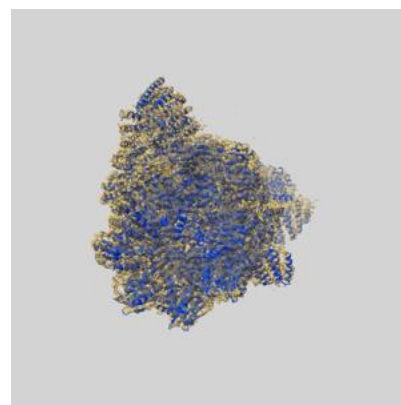
9.1 Map-model overlay [i](#)



X



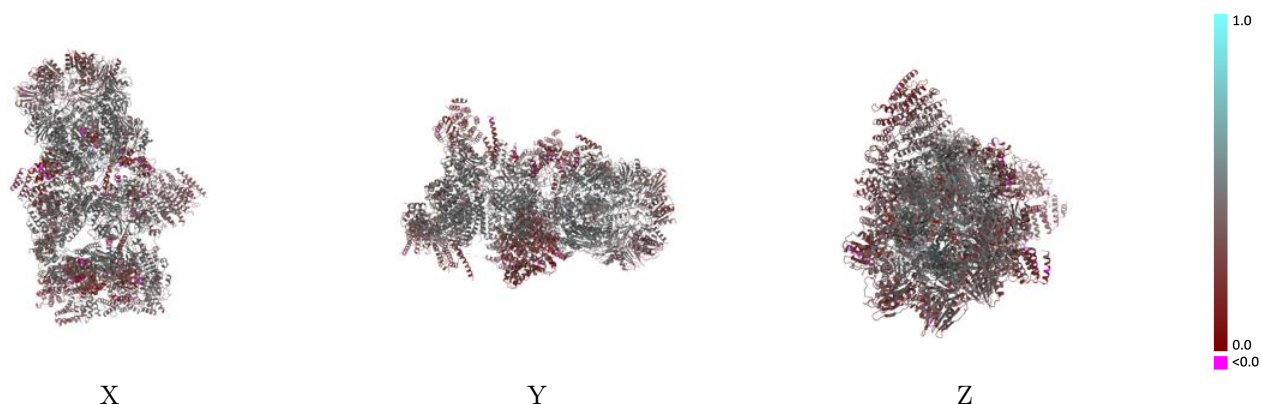
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

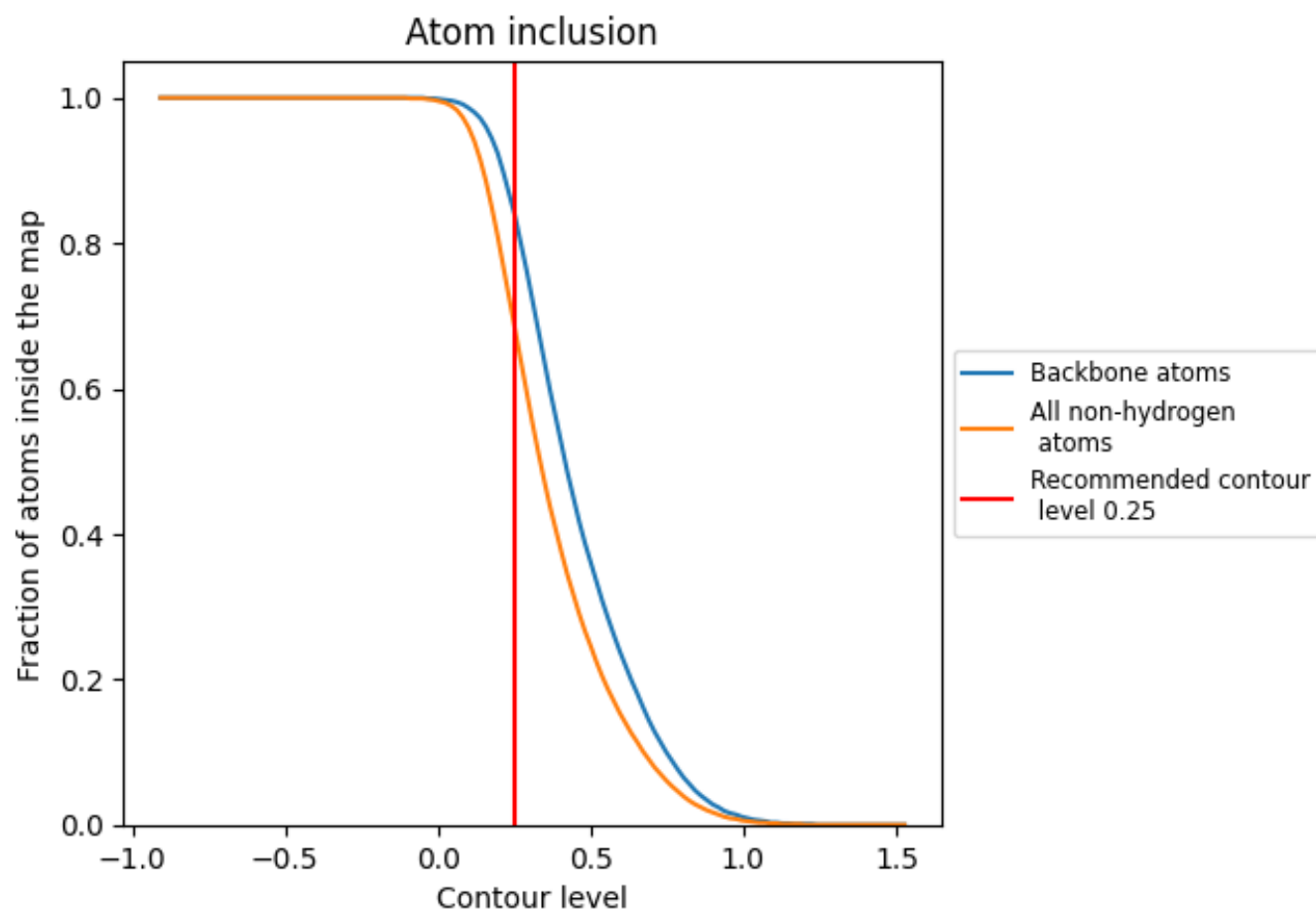


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 69% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6890	 0.4080
A	 0.6130	 0.3640
B	 0.7170	 0.4540
C	 0.7870	 0.4860
D	 0.7800	 0.4890
E	 0.6910	 0.4240
F	 0.4740	 0.2760
G	 0.7480	 0.4510
H	 0.8170	 0.5000
I	 0.7880	 0.4940
J	 0.7860	 0.4840
K	 0.7720	 0.4780
L	 0.7890	 0.4490
M	 0.7300	 0.4230
N	 0.7700	 0.4530
O	 0.7620	 0.4740
P	 0.7850	 0.4750
Q	 0.7670	 0.4670
R	 0.8100	 0.4590
S	 0.7790	 0.4550
T	 0.7730	 0.4340
U	 0.7630	 0.4310
V	 0.7040	 0.3890
W	 0.6160	 0.3470
X	 0.6430	 0.3880
Y	 0.7790	 0.4300
Z	 0.7620	 0.4550
a	 0.6470	 0.3340
b	 0.5130	 0.2890
c	 0.7530	 0.4680
d	 0.6200	 0.3010
e	 0.7610	 0.4480
f	 0.5860	 0.3090
n	 0.5370	 0.3750
o	 0.4950	 0.3490



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Chain	Atom inclusion	Q-score
p	 0.4610	 0.3570
q	 0.4730	 0.3400
r	 0.5150	 0.3360
s	 0.5570	 0.3610
t	 0.5790	 0.3830
y	 0.2470	 0.2550