



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:43 AM UTC

PDB ID : 7QO6 / pdb_00007qo6
EMDB ID : EMD-14085
Title : 26S proteasome Rpt1-RK -Ubp6-UbVS complex in the s2 state
Authors : Hung, K.Y.S.; Klumpe, S.; Eisele, M.R.; Elsassner, S.; Geng, T.T.; Cheng, T.C.; Joshi, T.; Rudack, T.; Sakata, E.; Finley, D.
Deposited on : 2021-12-23
Resolution : 6.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

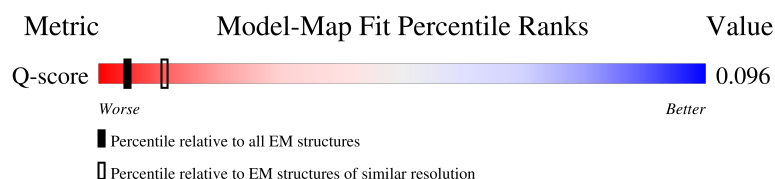
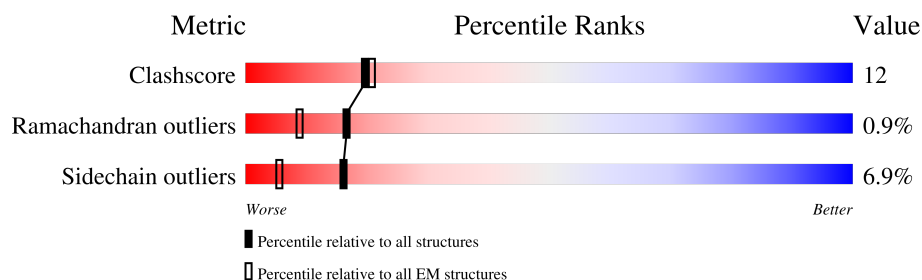
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

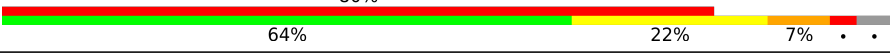
The reported resolution of this entry is 6.30 Å.

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	550 (5.80 - 6.80)

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

Mol	Chain	Length	Quality of chain
1	A	252	 15% 63% 23% 7% . .
1	a	252	 80% 64% 22% 7% . .
2	B	250	 23% 63% 27% 9%
2	b	250	 90% 64% 26% 9%

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Mol	Chain	Length	Quality of chain
3	C	258	
3	c	258	
4	D	254	
4	d	254	
5	E	260	
5	e	260	
6	F	234	
6	f	234	
7	G	288	
7	g	288	
8	l	215	
8	h	215	
9	2	261	
9	i	261	
10	3	205	
10	j	205	
11	4	198	
11	k	198	
12	5	287	
12	l	287	
13	6	241	
13	m	241	
14	7	266	
14	n	266	
15	W	268	

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Mol	Chain	Length	Quality of chain
16	V	306	
17	T	274	
18	X	156	
19	Y	89	
20	Z	993	
21	N	945	
22	S	523	
23	P	445	
24	Q	434	
25	R	429	
26	U	338	
27	O	393	
28	H	467	
29	I	437	
30	K	428	
31	L	437	
32	M	434	
33	J	405	
34	8	499	
35	9	76	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	GLZ	9	76	-	-	X	-
36	ATP	H	501	-	-	X	-
36	ATP	I	501	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	ATP	L	501	-	-	X	-
36	ATP	M	501	-	-	X	-
38	ADP	J	501	-	-	X	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 112930 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 BJ4_G0020160.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	242	Total	C	N	O	S	0	0
			1912	1217	321	366	8		
1	A	242	Total	C	N	O	S	0	0
			1912	1217	321	366	8		

- Molecule 2 is a protein called HLJ1_G0039880.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	249	Total	C	N	O	S	0	0
			1907	1214	314	376	3		
2	B	249	Total	C	N	O	S	0	0
			1907	1214	314	376	3		

- Molecule 3 is a protein called BJ4_G0021480.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		
3	C	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

- Molecule 4 is a protein called HLJ1_G0048980.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	236	Total	C	N	O	S	0	0
			1850	1158	323	365	4		
4	D	236	Total	C	N	O	S	0	0
			1850	1158	323	365	4		

- Molecule 5 is a protein called EM14S01-3B_G0035190.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	249	Total	C	N	O	S	0	0
			1925	1204	324	390	7		
5	E	249	Total	C	N	O	S	0	0
			1925	1204	324	390	7		

- Molecule 6 is a protein called BJ4_G0043800.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		
6	F	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		

- Molecule 7 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	242	Total	C	N	O	S	0	0
			1885	1199	328	354	4		
7	G	242	Total	C	N	O	S	0	0
			1885	1199	328	354	4		

- Molecule 8 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		
8	1	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		

- Molecule 9 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		
9	2	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		

- Molecule 10 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	3	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

- Molecule 11 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		
11	4	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
12	5	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		

- Molecule 13 is a protein called HLJ1_G0013750.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
13	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

- Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		
14	7	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		

- Molecule 15 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	197	Total	C	N	O	S	0	0
			1534	962	269	300	3		

- Molecule 16 is a protein called 26S proteasome regulatory subunit RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	289	Total	C	N	O	S	0	0
			2274	1425	389	446	14		

- Molecule 17 is a protein called EM14S01-3B_G0050020.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	266	Total	C	N	O	S	0	0
			2192	1405	349	432	6		

- Molecule 18 is a protein called HLJ1_G0030700.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	127	Total	C	N	O	S	0	0
			1032	664	169	195	4		

- Molecule 19 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Y	89	Total	C	N	O	S	0	0
			731	447	119	164	1		

- Molecule 20 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Z	906	Total	C	N	O	S	0	0
			7005	4416	1150	1409	30		

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	832	Total	C	N	O	S	0	0
			6418	4078	1077	1238	25		

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	475	Total	C	N	O	S	0	0
			3894	2488	653	738	15		

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	440	Total	C	N	O	S	0	0
			3608	2297	604	697	10		

- Molecule 24 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	434	Total	C	N	O	S	0	0
			3499	2225	577	681	16		

- Molecule 25 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	405	Total	C	N	O	S	0	0
			3258	2077	535	636	10		

- Molecule 26 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	290	Total	C	N	O	S	0	0
			2306	1454	392	453	7		

- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	O	388	Total	C	N	O	S	0	0
			3186	2051	519	608	8		

- Molecule 28 is a protein called 26S proteasome regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	H	391	Total	C	N	O	S	0	0
			3064	1927	551	569	17		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ARG	SER	variant	UNP A0A6A5PV22
H	166	LYS	THR	variant	UNP A0A6A5PV22

- Molecule 29 is a protein called 26S proteasome regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	I	384	Total	C	N	O	S	0	0
			3015	1895	507	596	17		

- Molecule 30 is a protein called 26S proteasome regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	K	394	Total	C	N	O	S	0	0
			3113	1951	548	604	10		

- Molecule 31 is a protein called 26S proteasome subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L	388	Total	C	N	O	S	0	0
			3082	1942	548	580	12		

- Molecule 32 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	M	421	Total	C	N	O	S	0	0
			3285	2043	573	656	13		

- Molecule 33 is a protein called 26S proteasome regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	J	405	Total	C	N	O	S	0	0
			3171	1995	565	593	18		

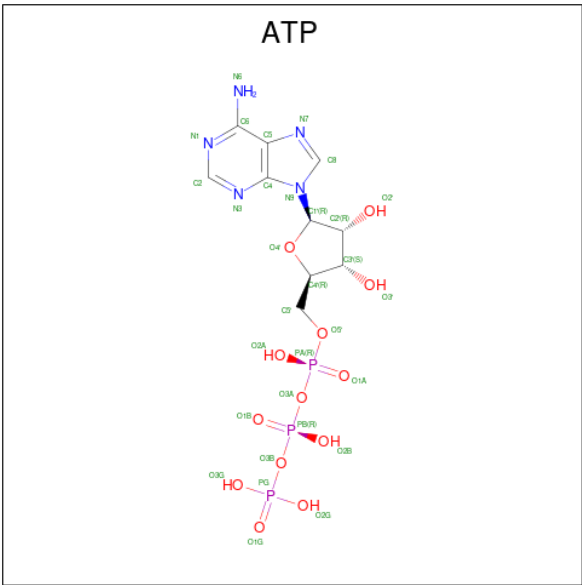
- Molecule 34 is a protein called Ubiquitin carboxyl-terminal hydrolase.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	372	Total	C	N	O	S	0	0
			3034	1918	521	583	12		

- Molecule 35 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	76	Total	C	N	O	S	0	0
			601	378	105	117	1		

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

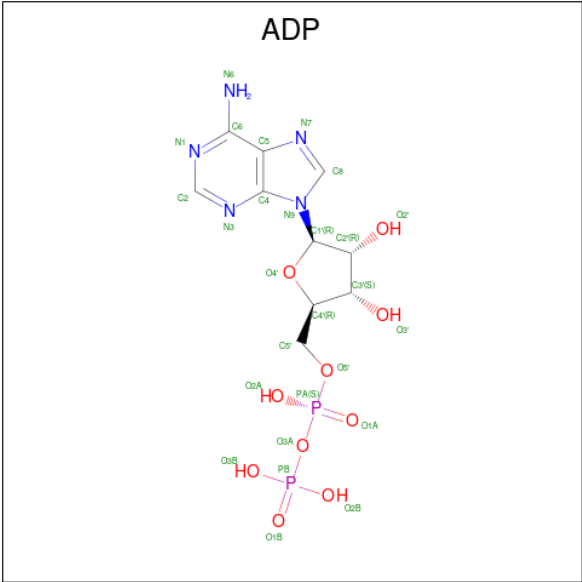


Mol	Chain	Residues	Atoms					AltConf
36	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	M	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	H	1	Total	Mg	0
			1	1	
37	I	1	Total	Mg	0
			1	1	
37	K	1	Total	Mg	0
			1	1	
37	L	1	Total	Mg	0
			1	1	
37	M	1	Total	Mg	0
			1	1	
37	J	1	Total	Mg	0
			1	1	

- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

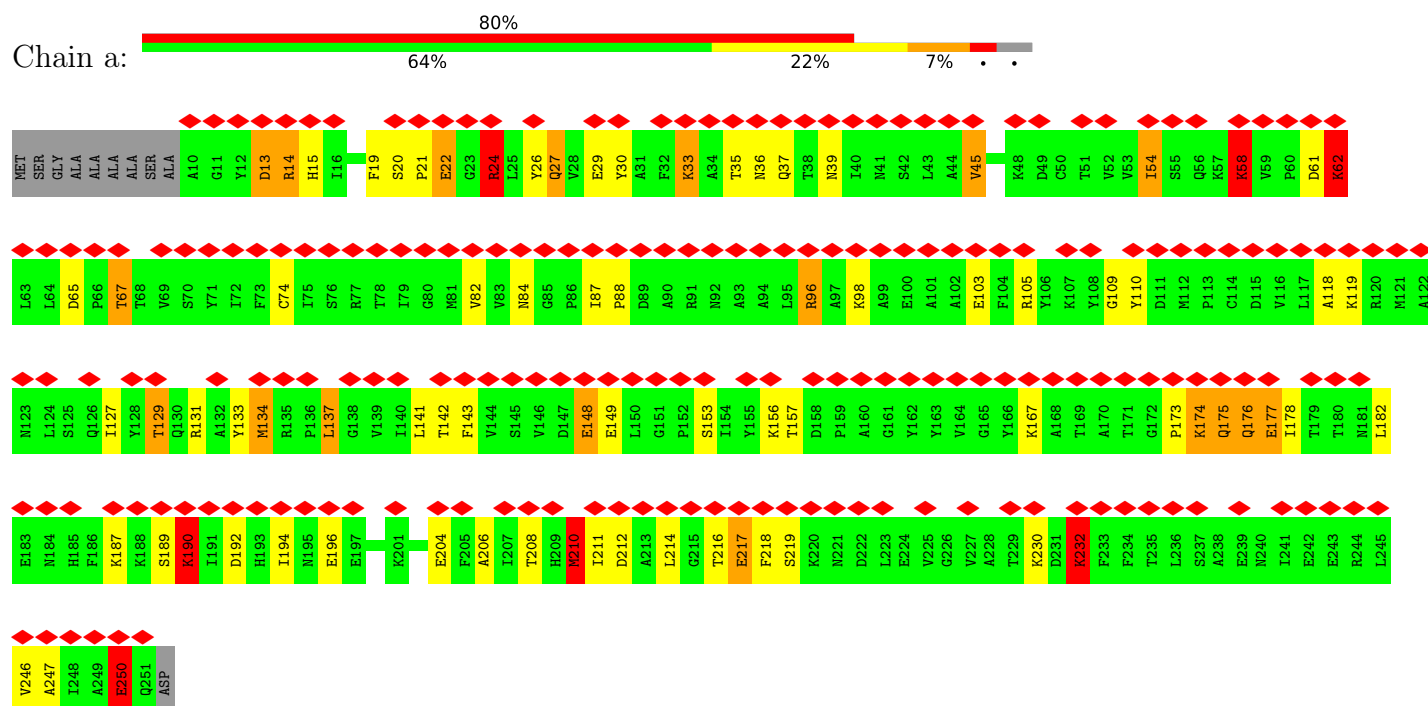


Mol	Chain	Residues	Atoms					AltConf
38	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

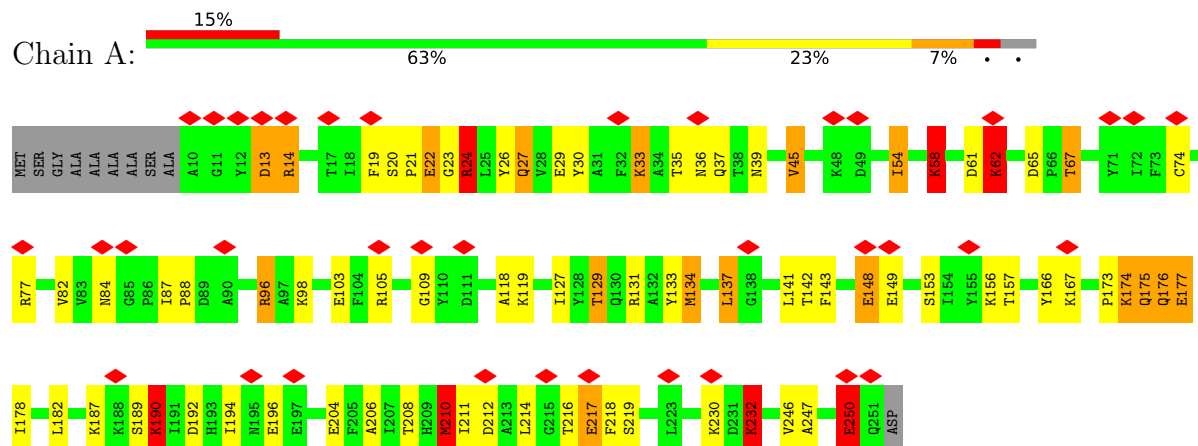
3 Residue-property plots

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

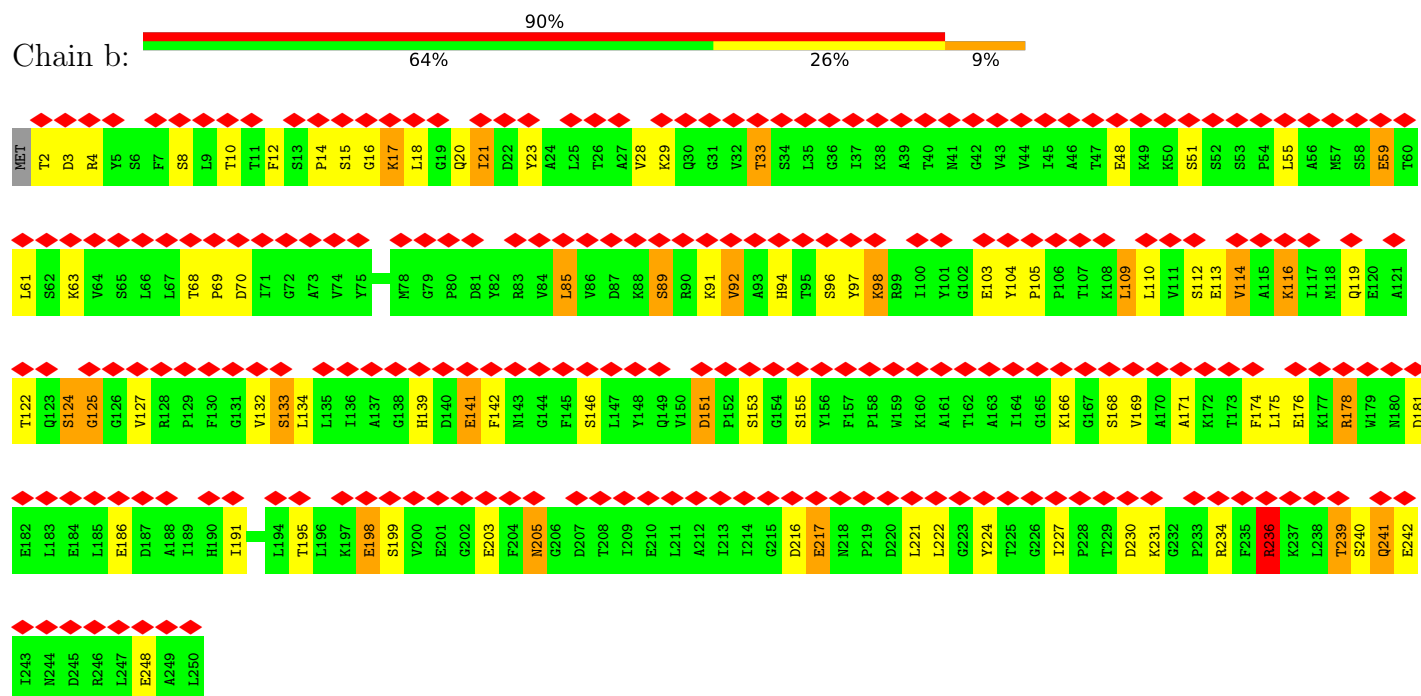
• Molecule 1: BJ4_G0020160.mRNA.1.CDS.1



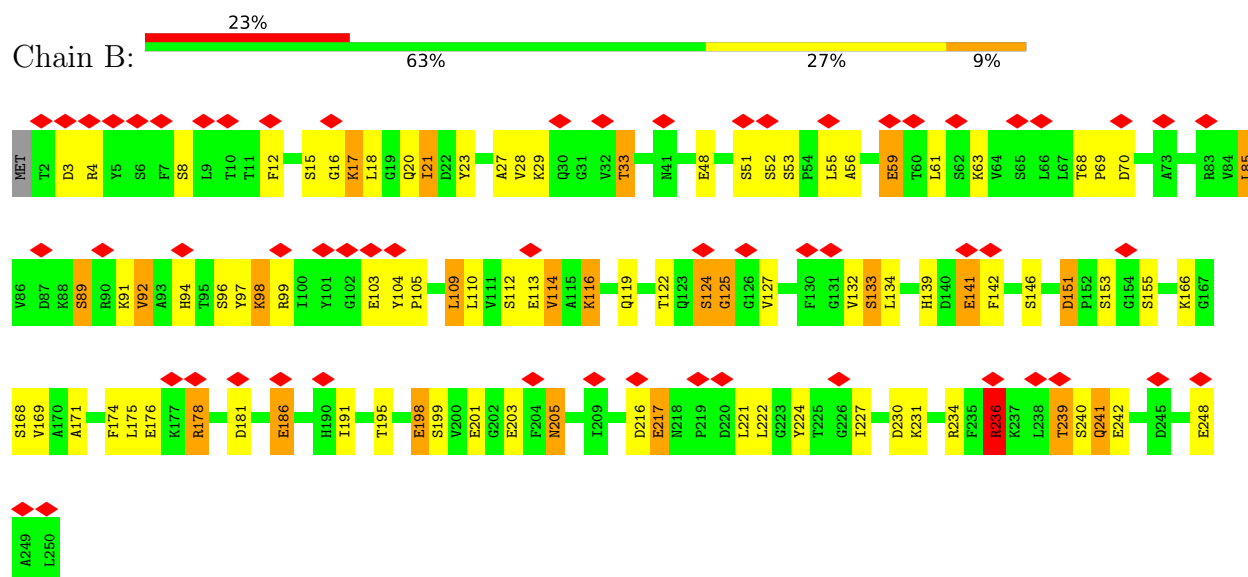
• Molecule 1: BJ4_G0020160.mRNA.1.CDS.1



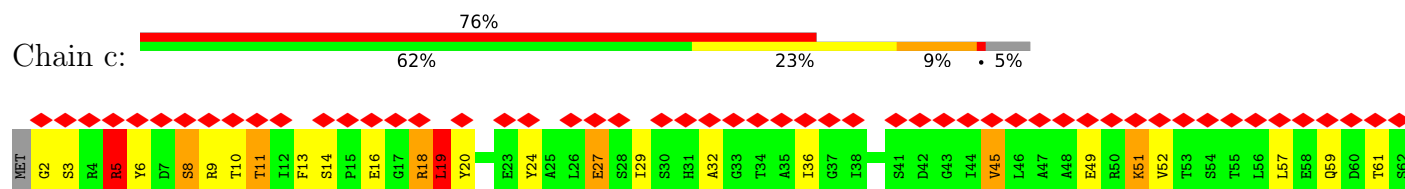
• Molecule 2: HLJ1_G0039880.mRNA.1.CDS.1

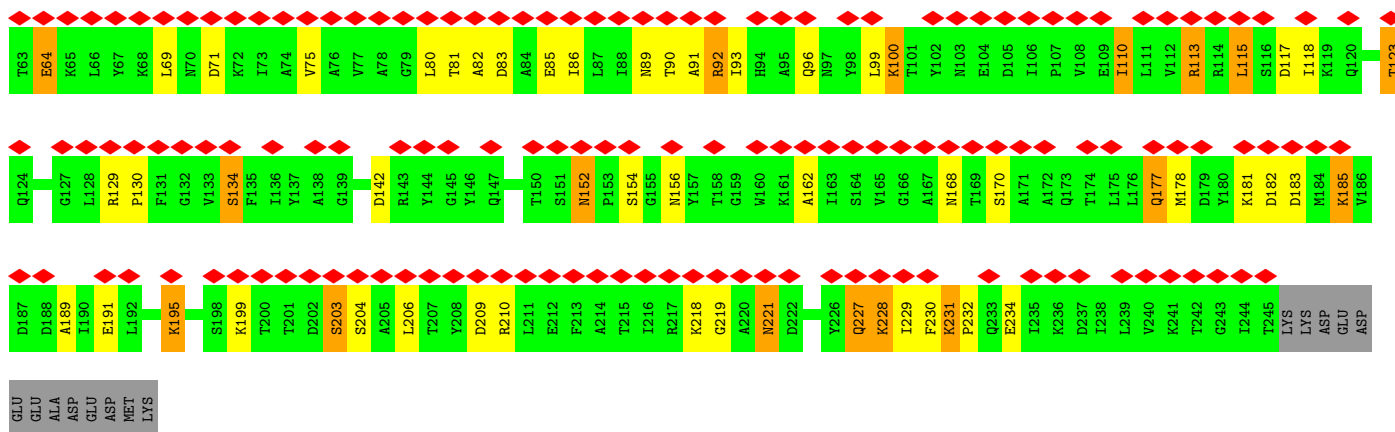


• Molecule 2: HLJ1_G0039880.mRNA.1.CDS.1

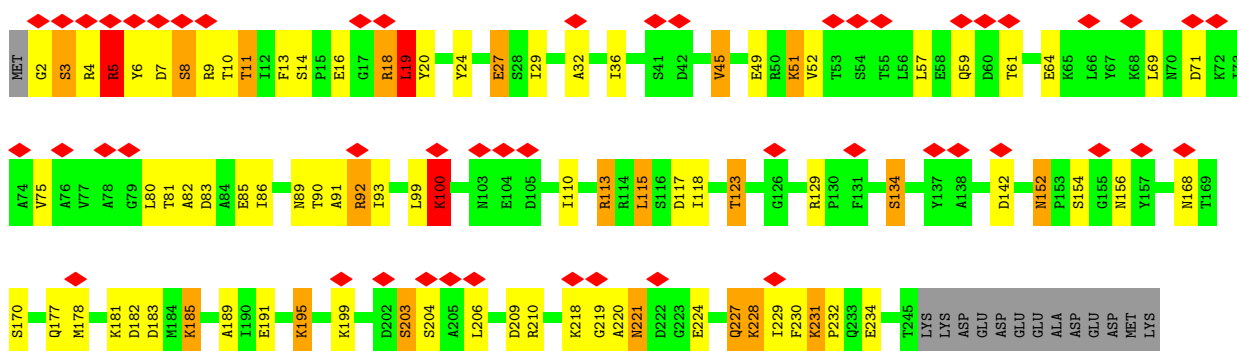


• Molecule 3: BJ4_G0021480.mRNA.1.CDS.1

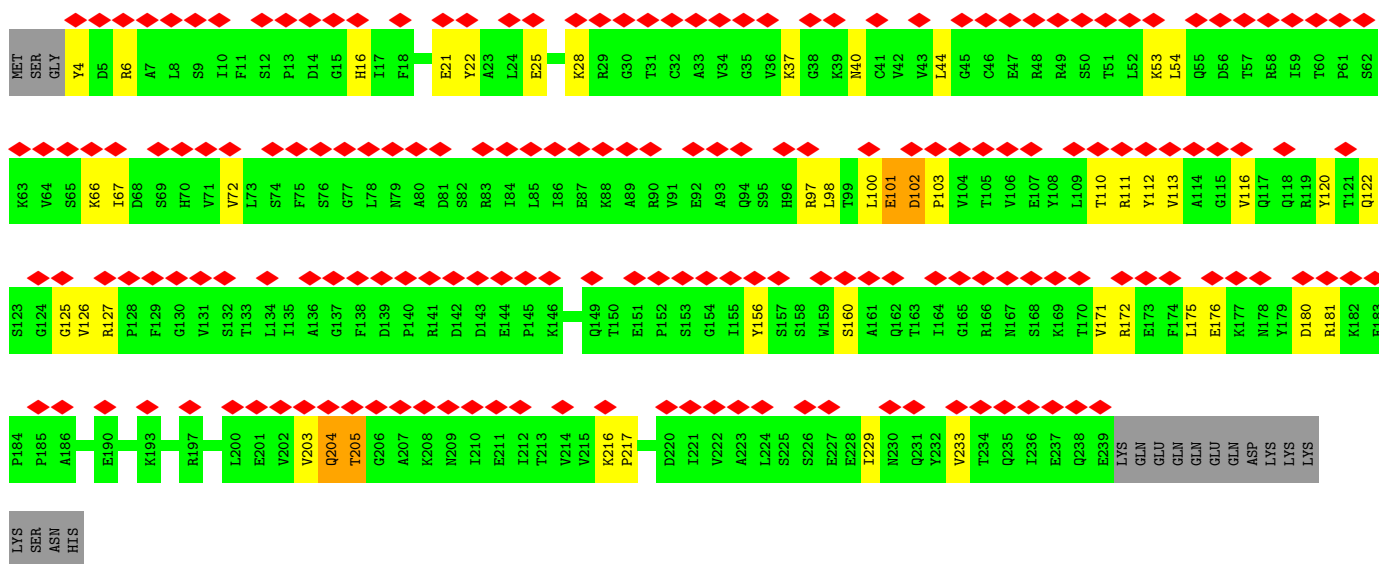
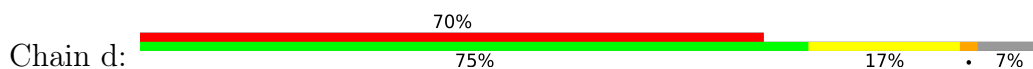




• Molecule 3: BJ4_G0021480.mRNA.1.CDS.1

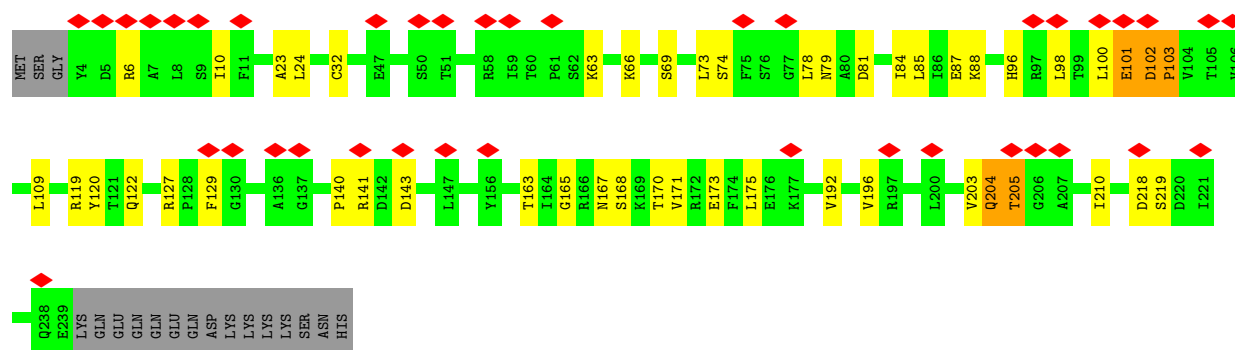


• Molecule 4: HLJ1_G0048980.mRNA.1.CDS.1



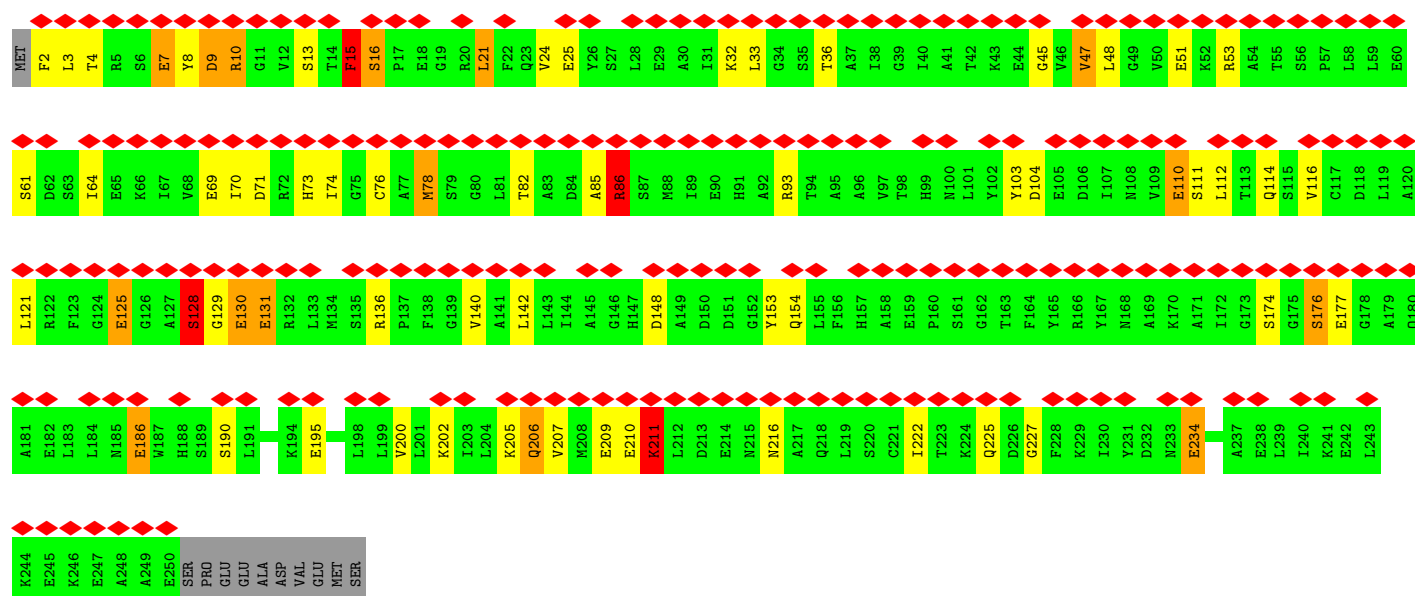
• Molecule 4: HLJ1_G0048980.mRNA.1.CDS.1

Chain D: 15% 74% 17% 7%



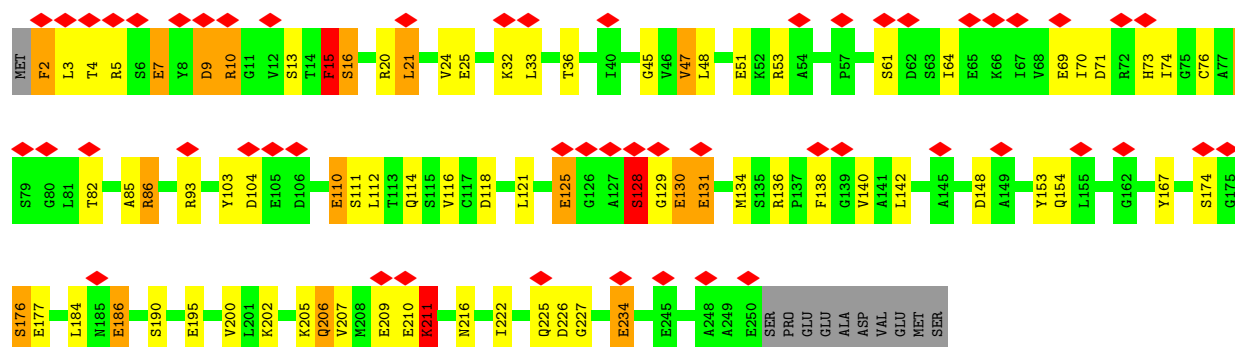
• Molecule 5: EM14S01-3B_G0035190.mRNA.1.CDS.1

Chain e: 83% 68% 20% 6%

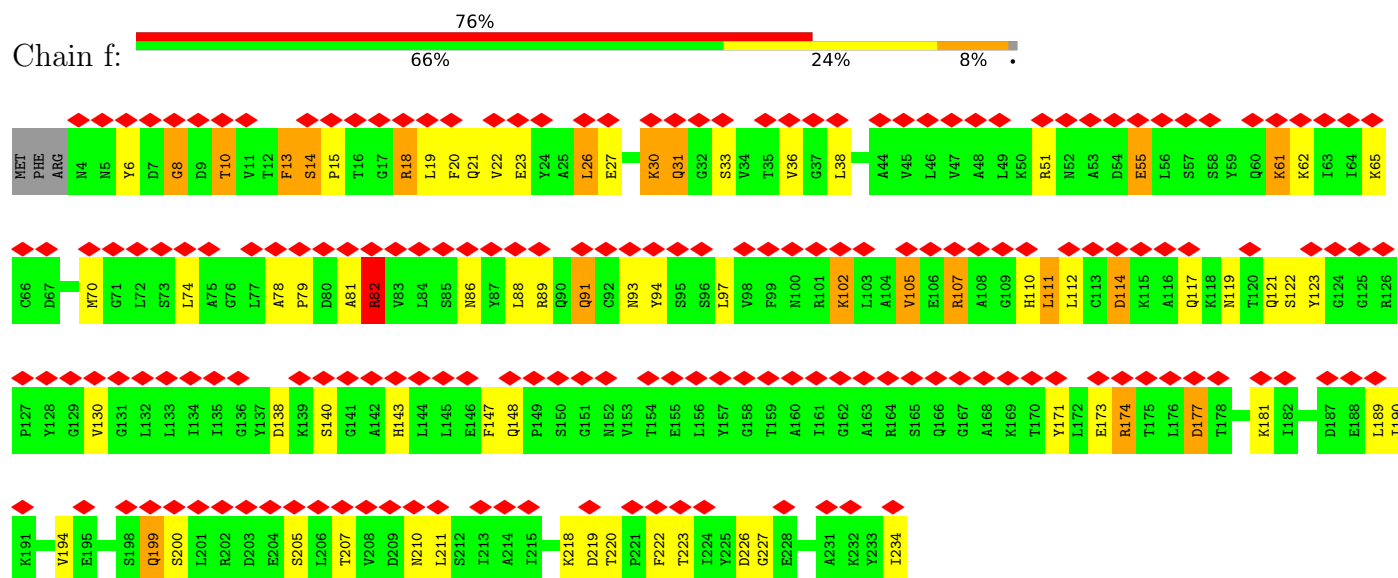


• Molecule 5: EM14S01-3B_G0035190.mRNA.1.CDS.1

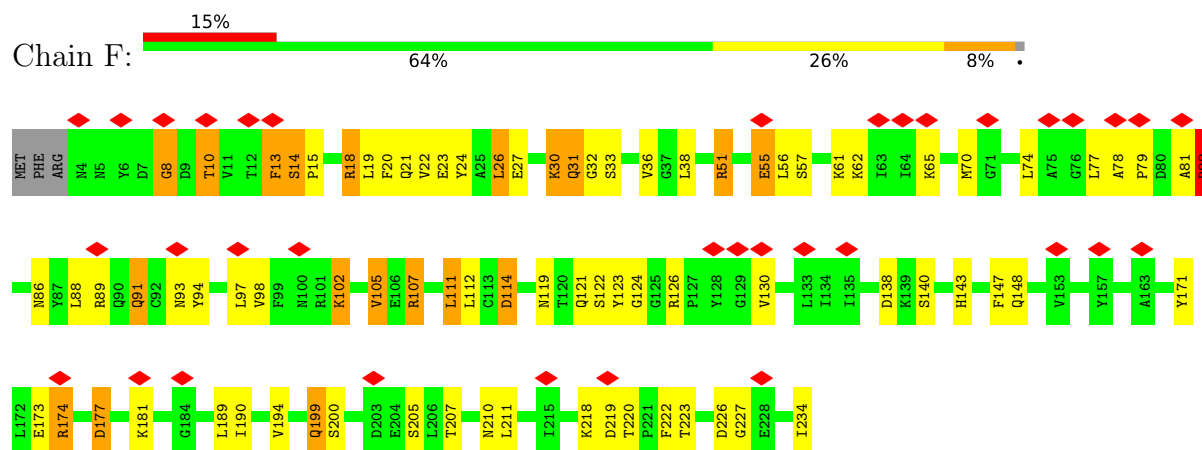
Chain E: 20% 65% 23% 7%



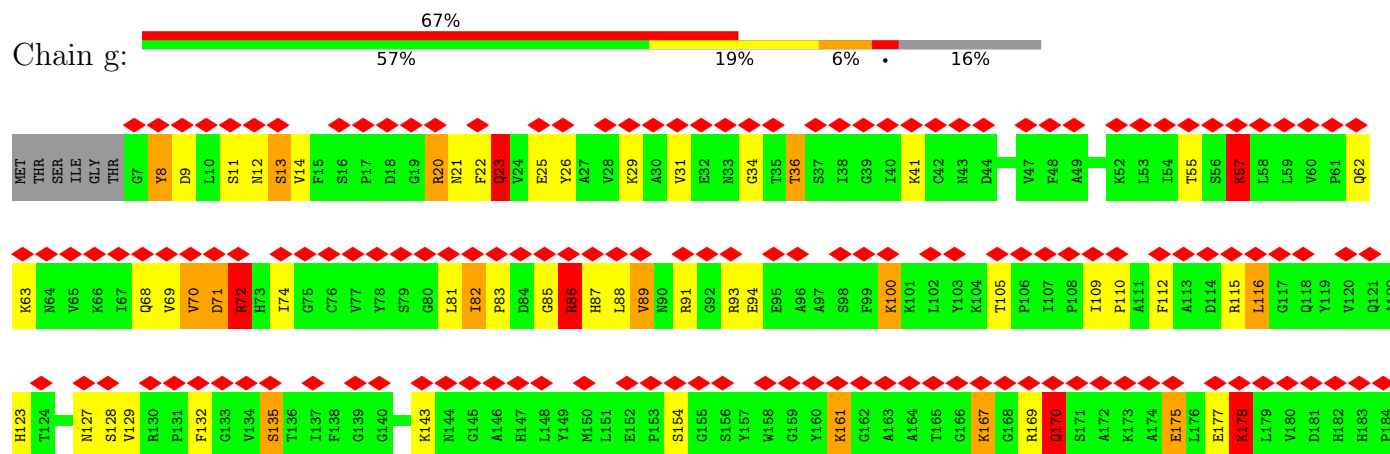
Chain f:



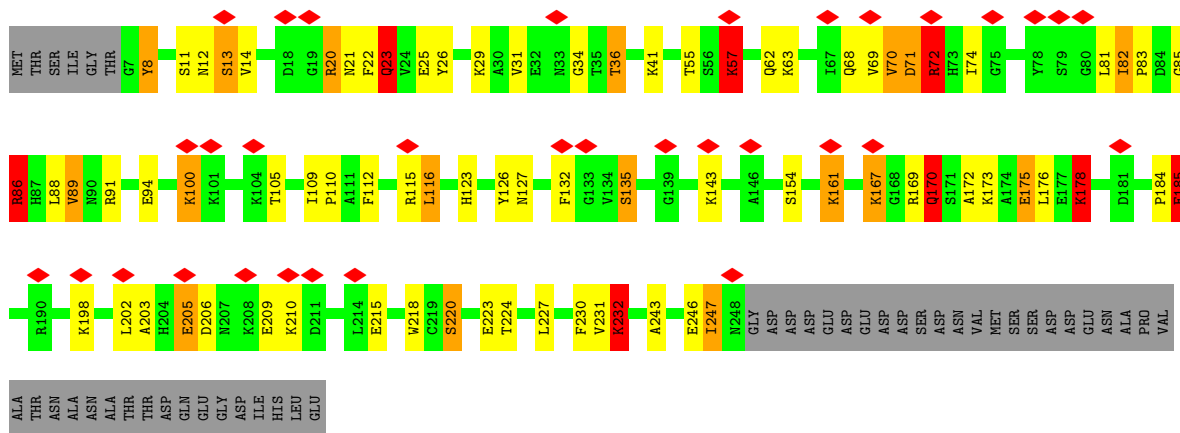
Chain F:



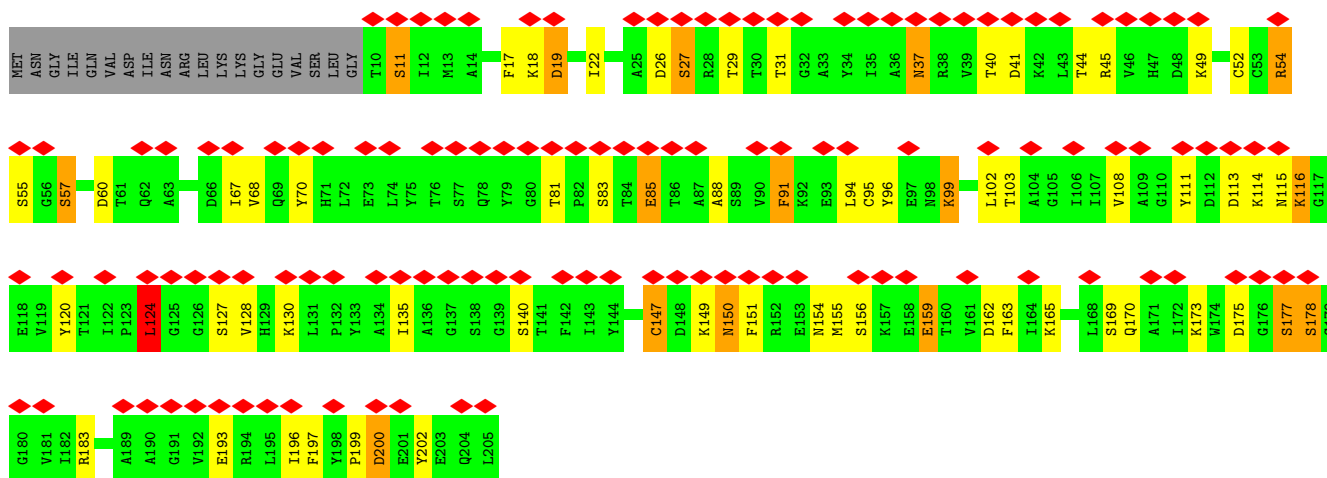
Chain g:



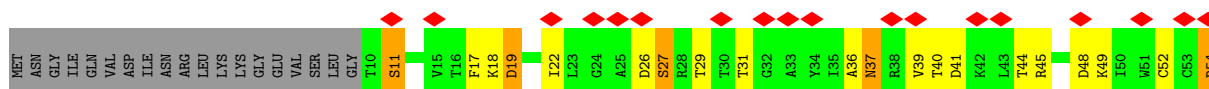
- Molecule 7: Probable proteasome subunit alpha type-7

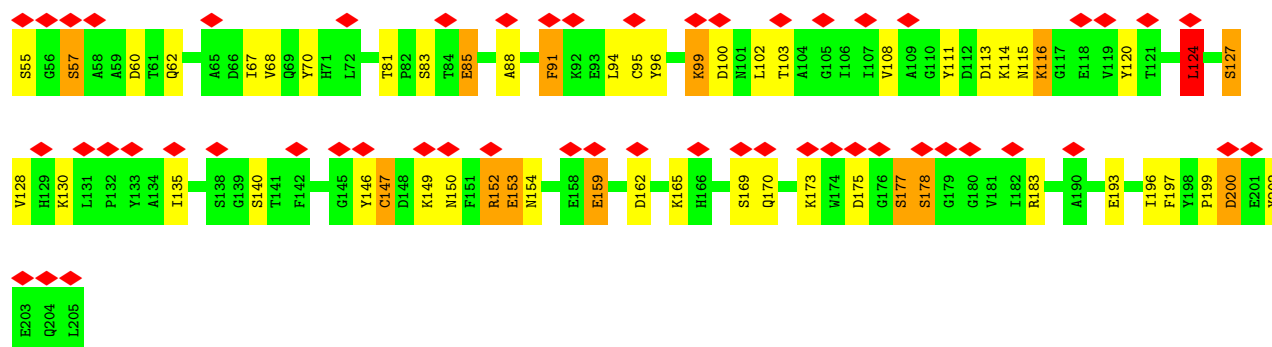


- Molecule 8: Proteasome subunit beta type-1

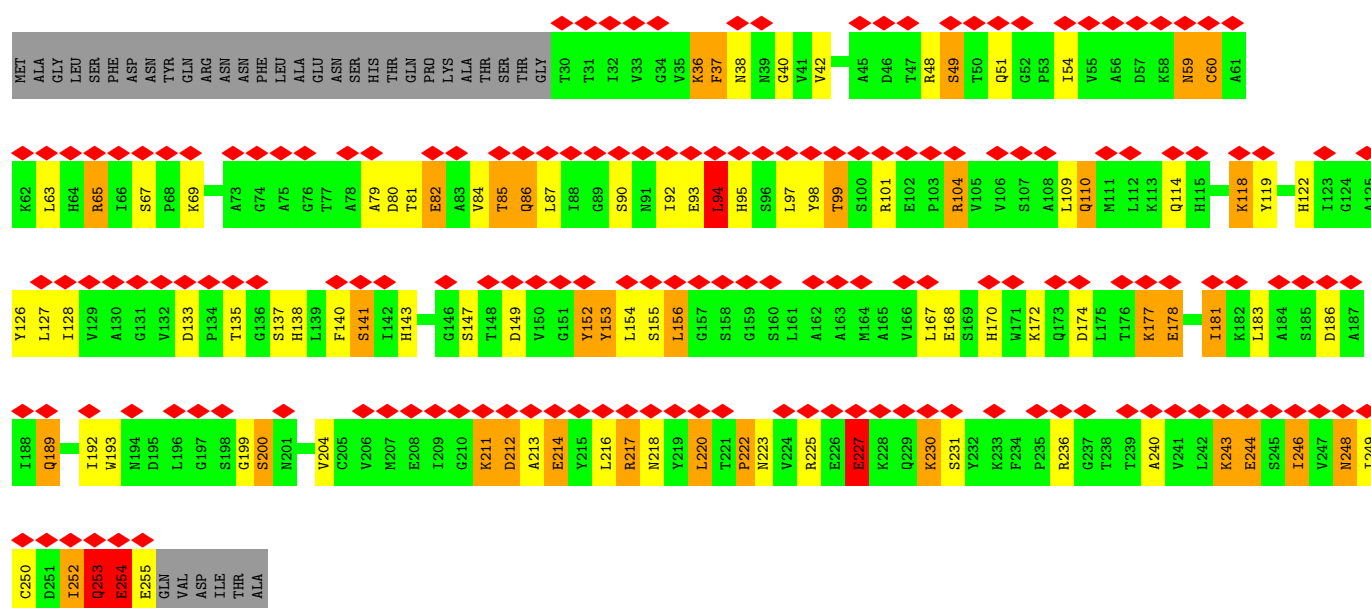


- Molecule 8: Proteasome subunit beta type-1

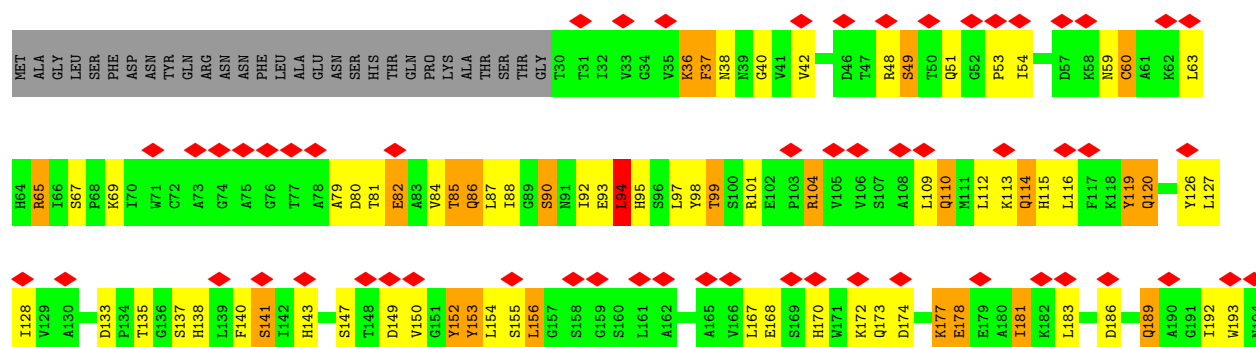


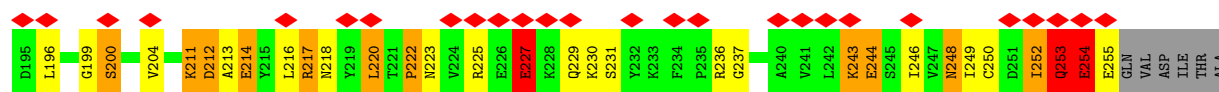


• Molecule 9: Proteasome endopeptidase complex

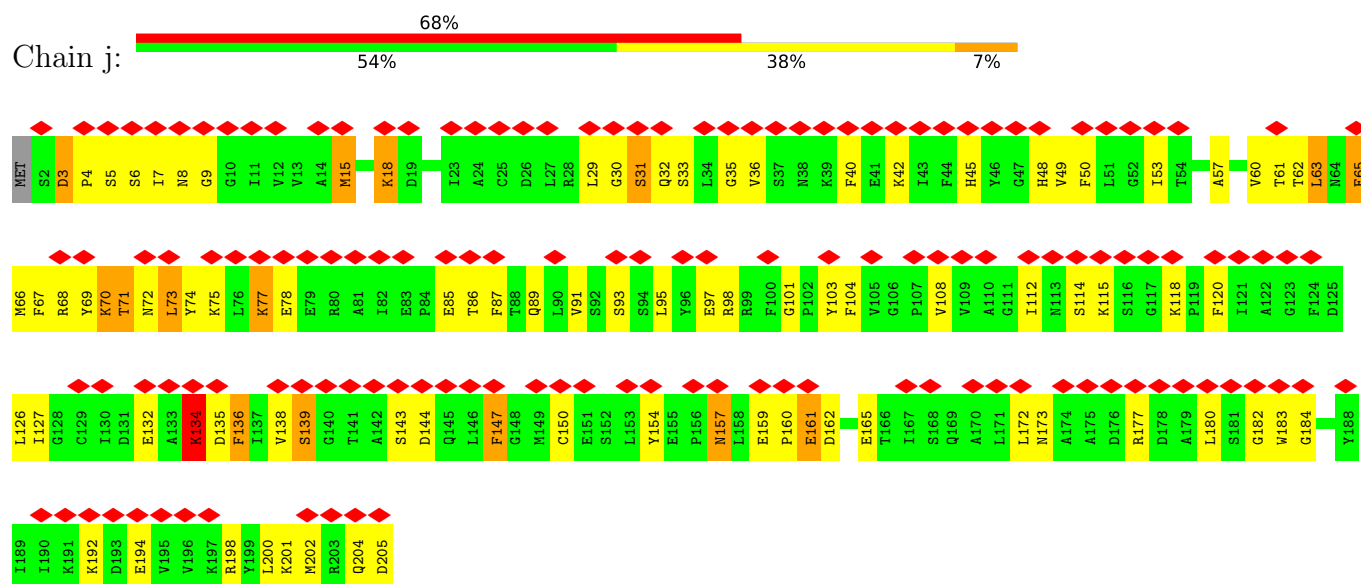


• Molecule 9: Proteasome endopeptidase complex

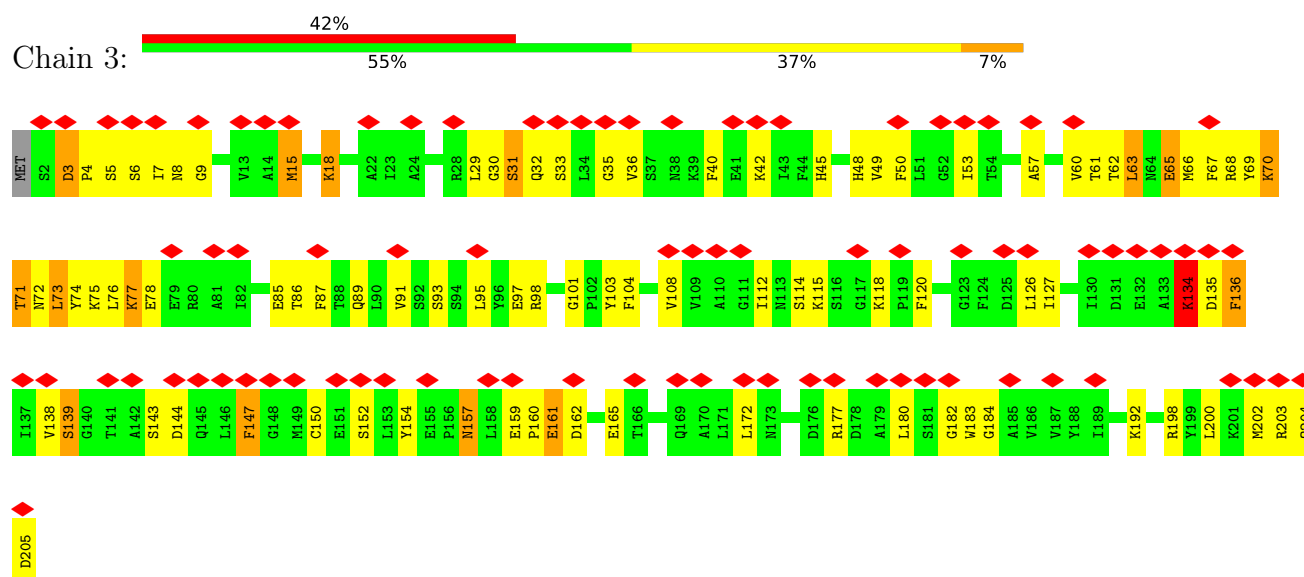




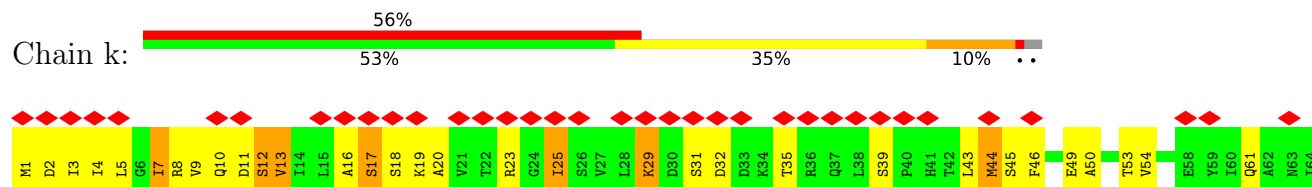
• Molecule 10: Proteasome endopeptidase complex

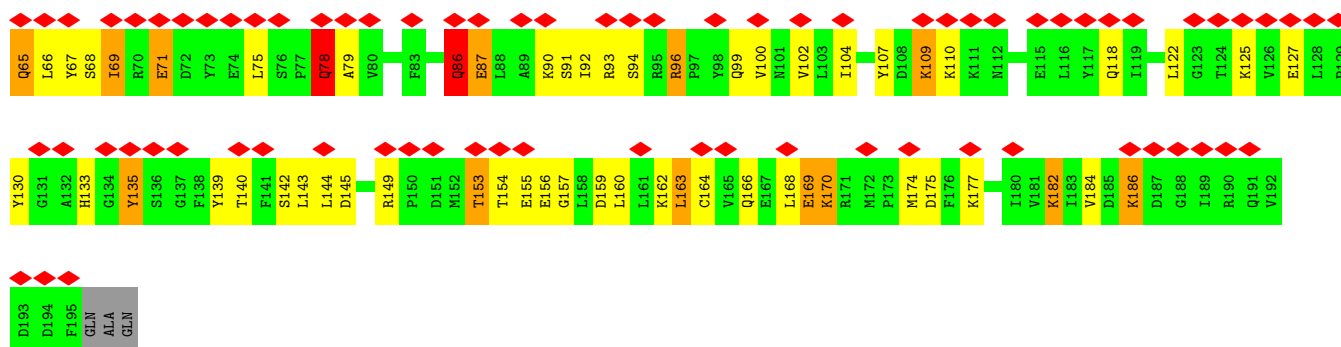


• Molecule 10: Proteasome endopeptidase complex

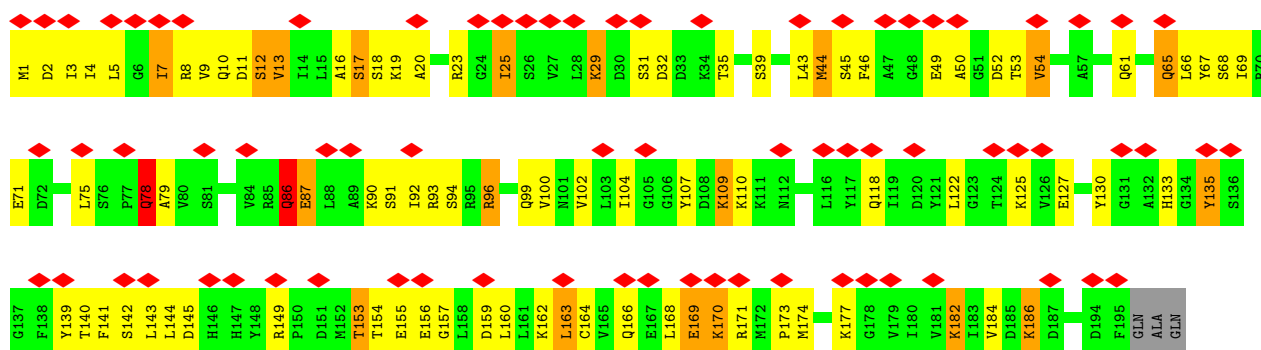


• Molecule 11: Proteasome subunit beta

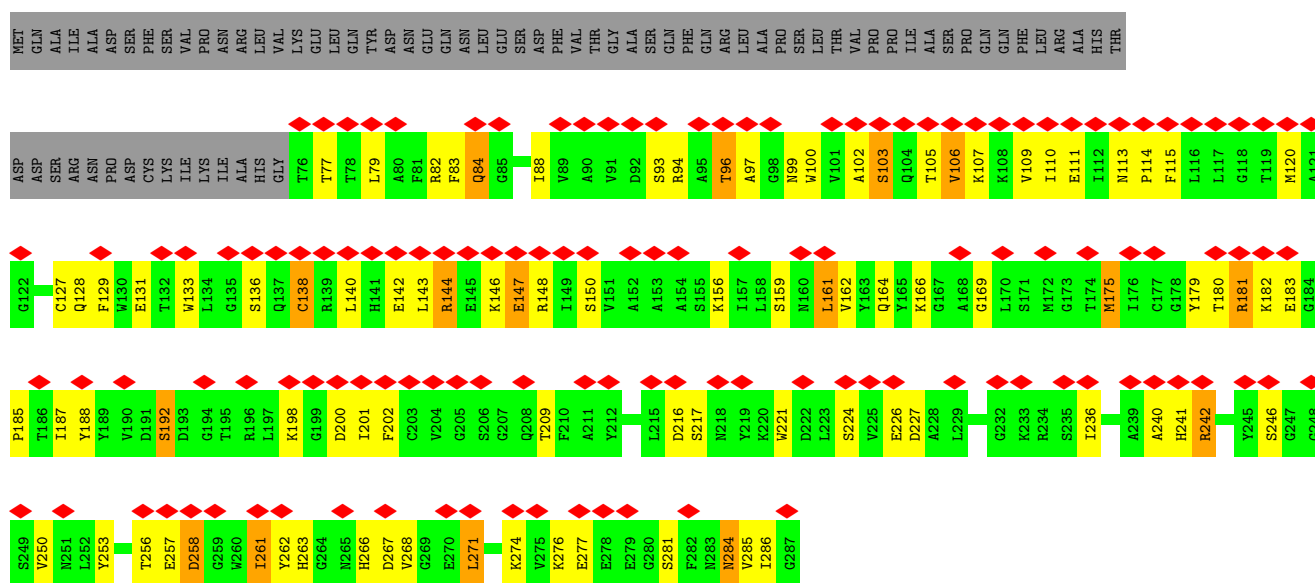




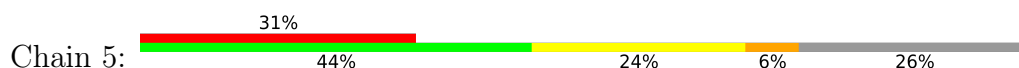
• Molecule 11: Proteasome subunit beta

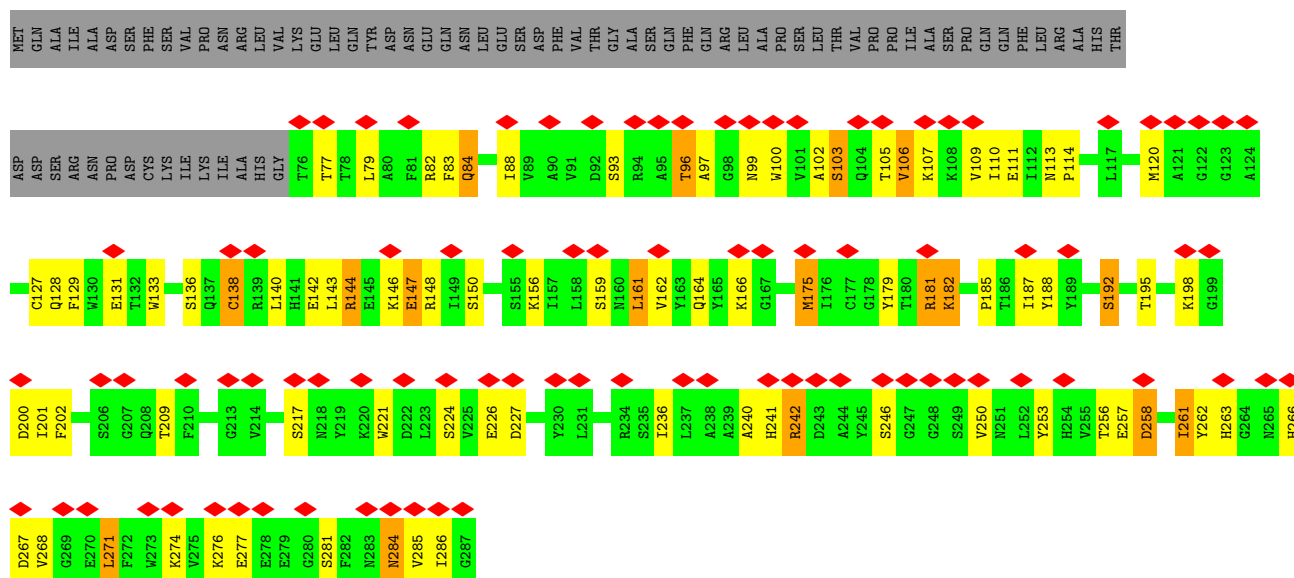


• Molecule 12: Proteasome subunit beta type-5

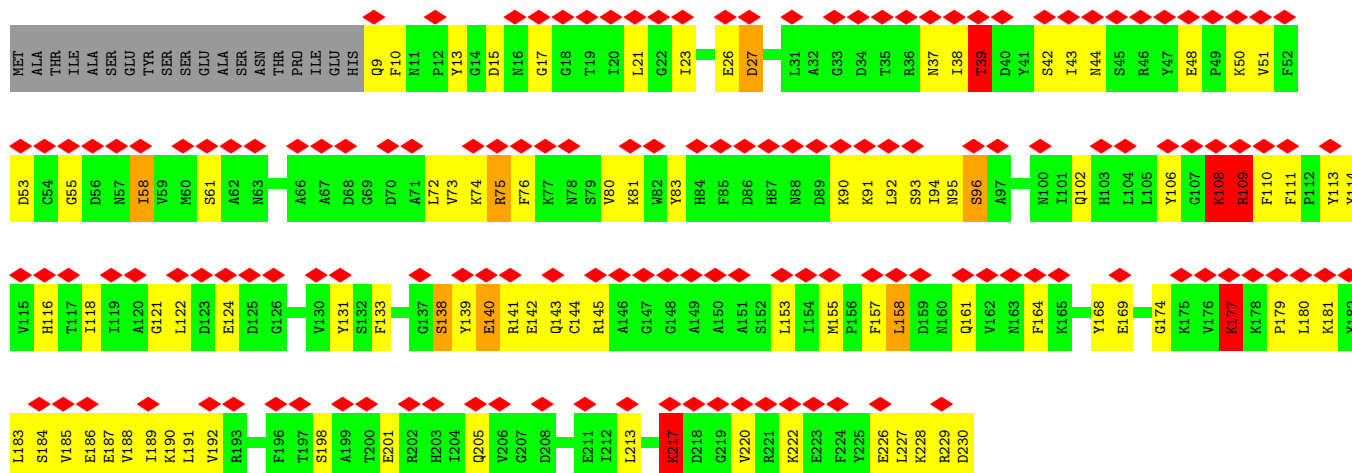


• Molecule 12: Proteasome subunit beta type-5

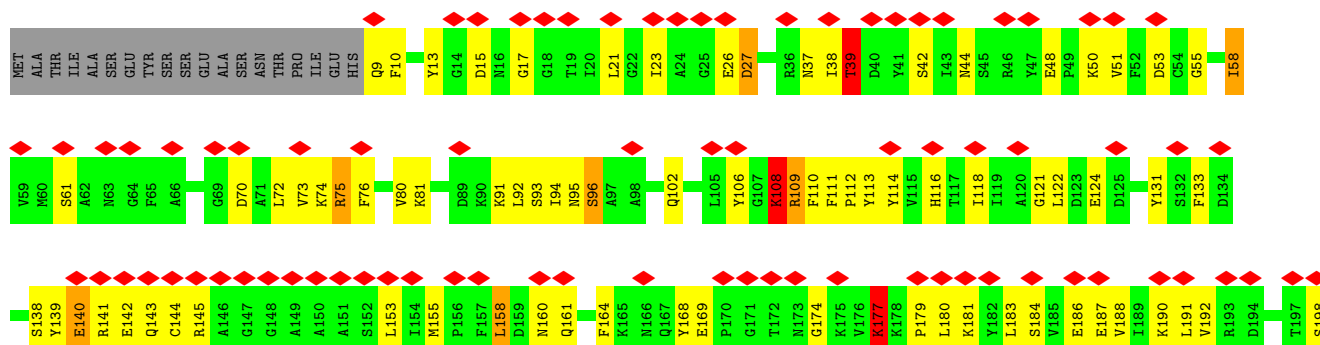
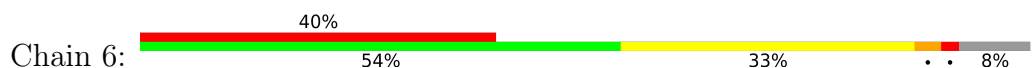


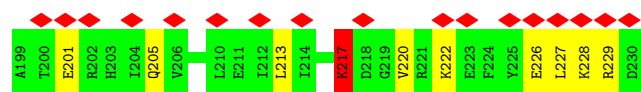


• Molecule 13: HLJ1_G0013750.mRNA.1.CDS.1

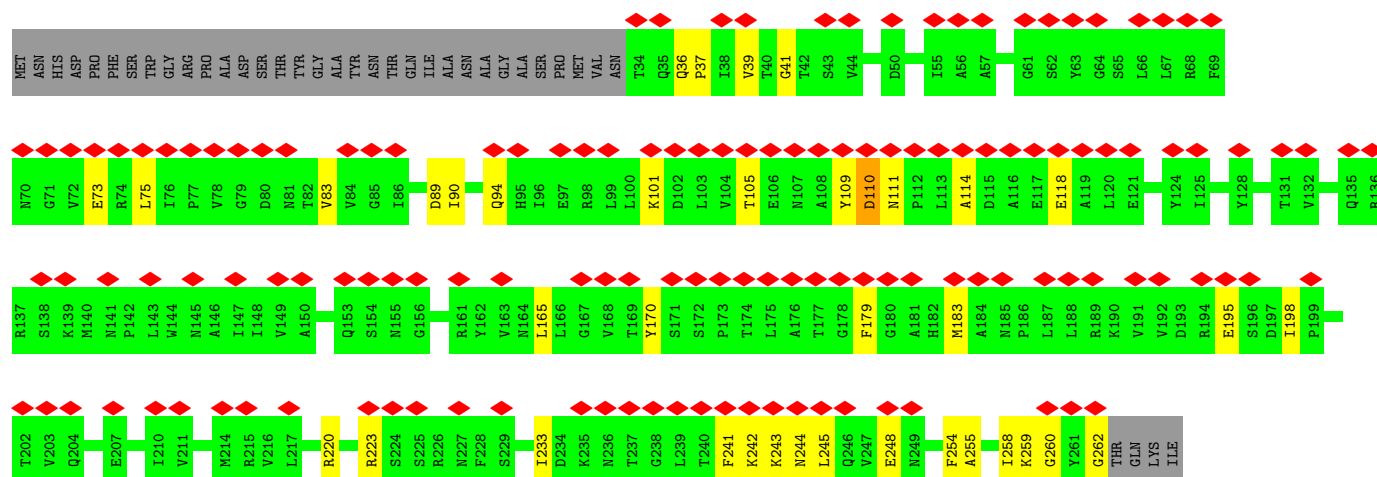
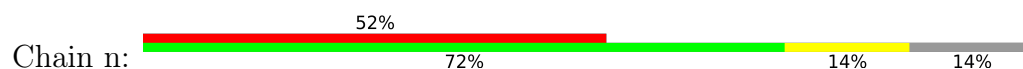


• Molecule 13: HLJ1_G0013750.mRNA.1.CDS.1

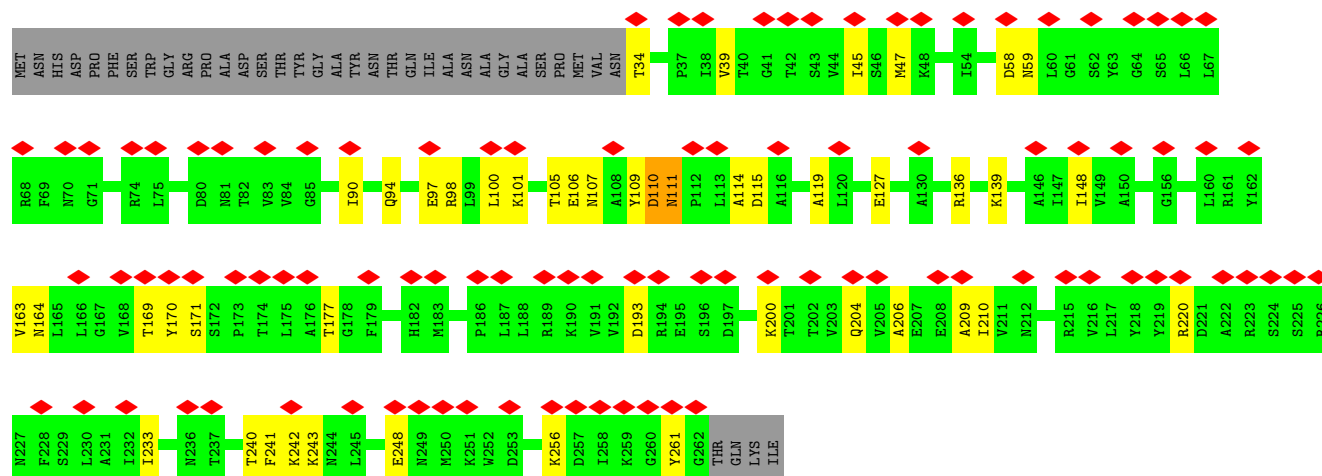




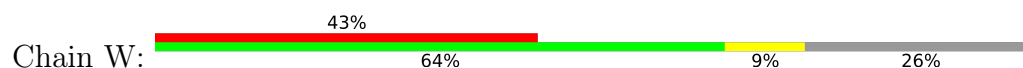
• Molecule 14: Proteasome subunit beta type-7

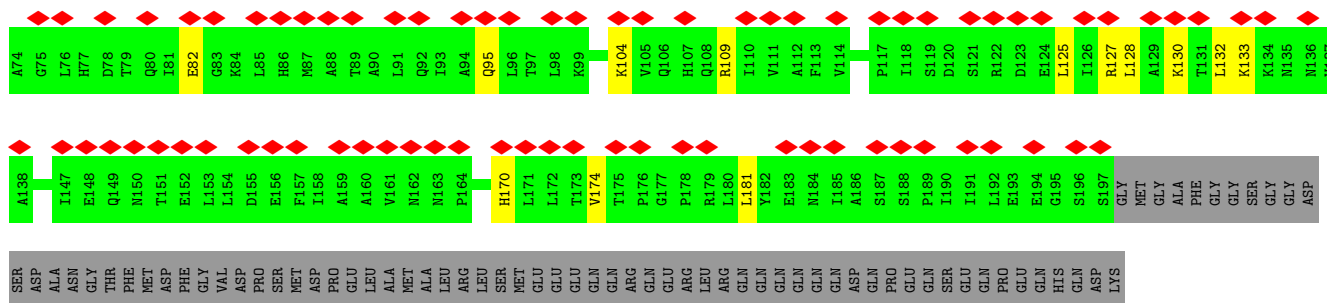


• Molecule 14: Proteasome subunit beta type-7

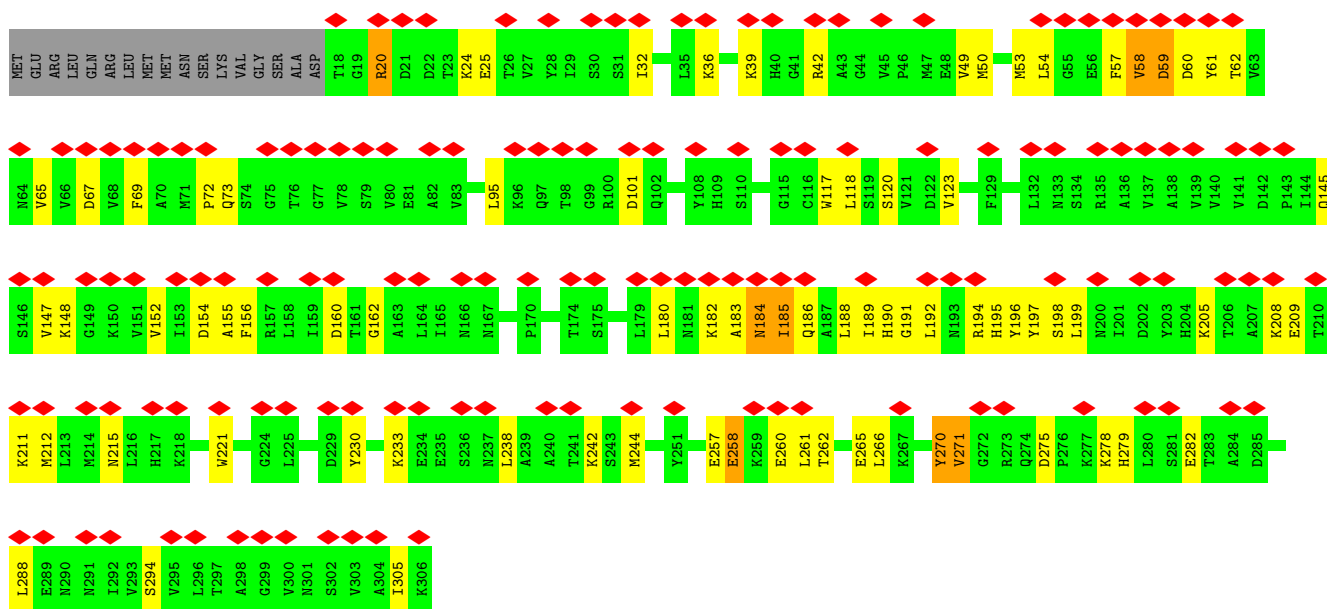


• Molecule 15: 26S proteasome regulatory subunit RPN10

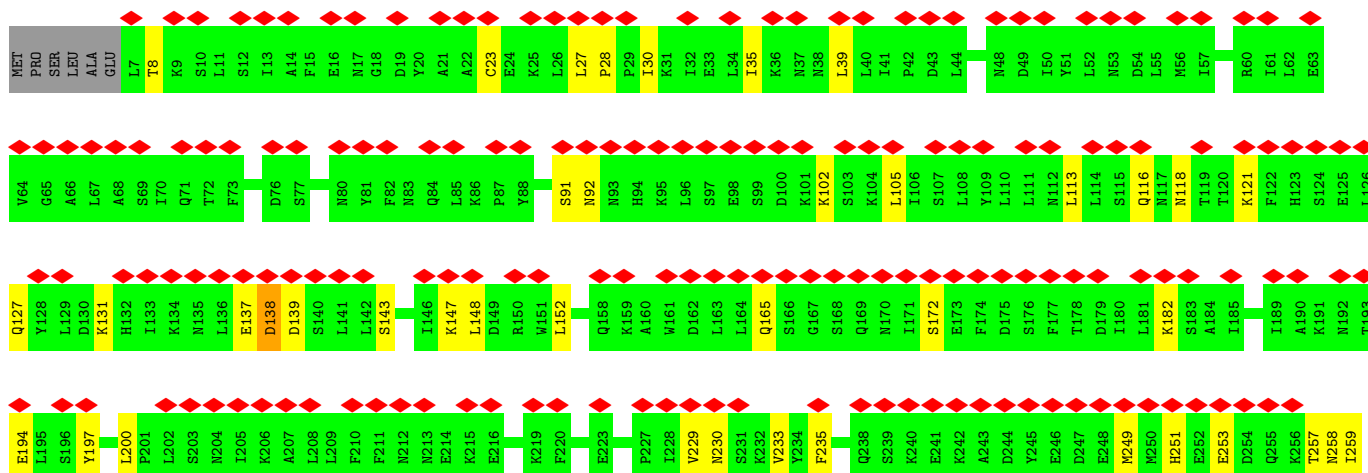
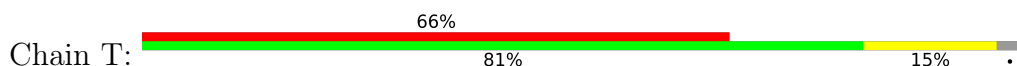


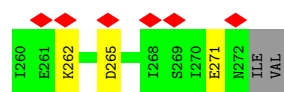


• Molecule 16: 26S proteasome regulatory subunit RPN11

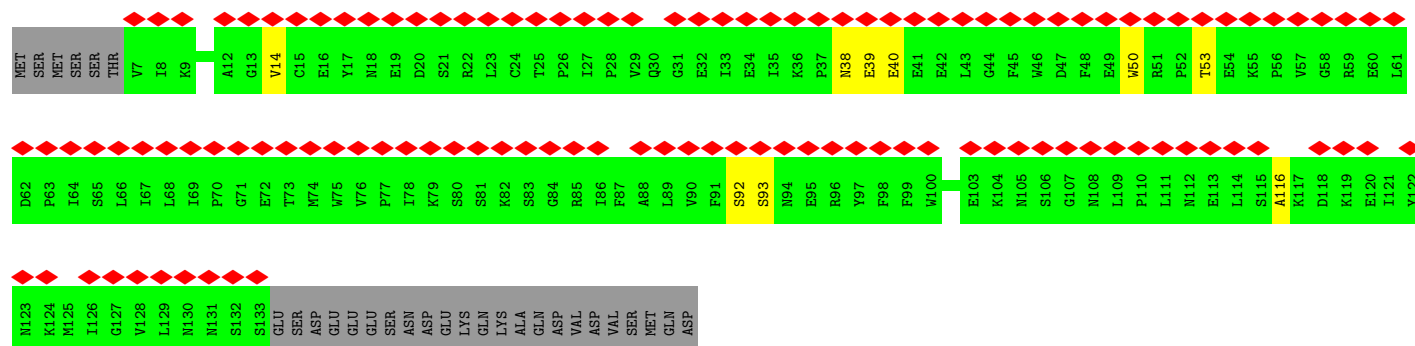
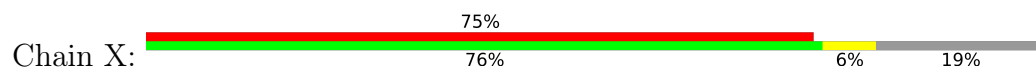


• Molecule 17: EM14S01-3B_G0050020.mRNA.1.CDS.1

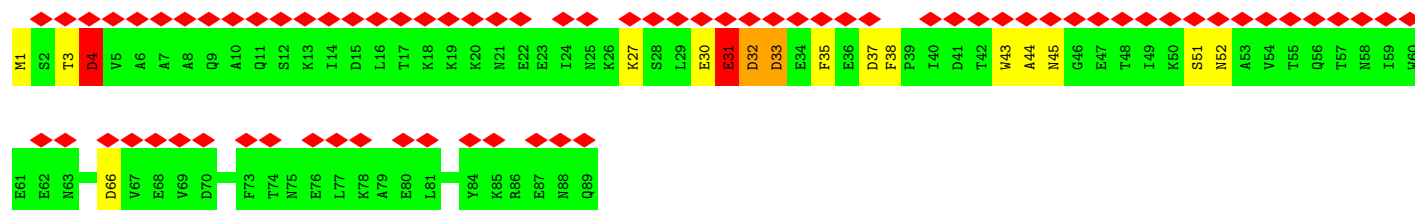
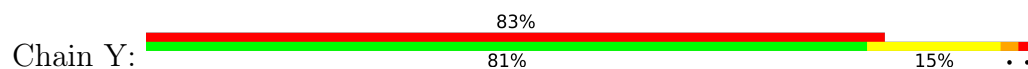




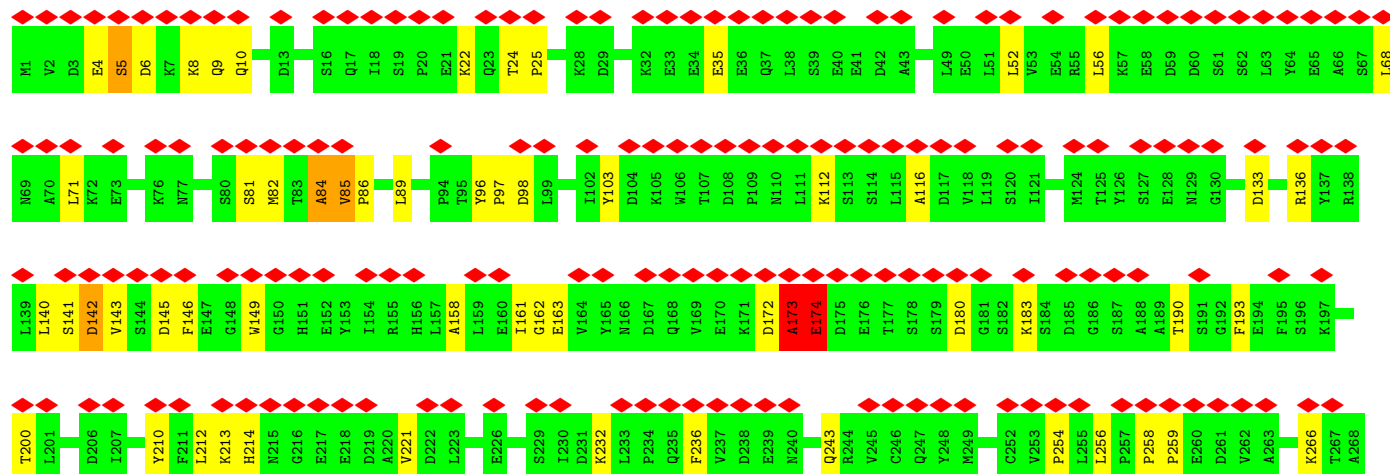
• Molecule 18: HLJ1_G0030700.mRNA.1.CDS.1

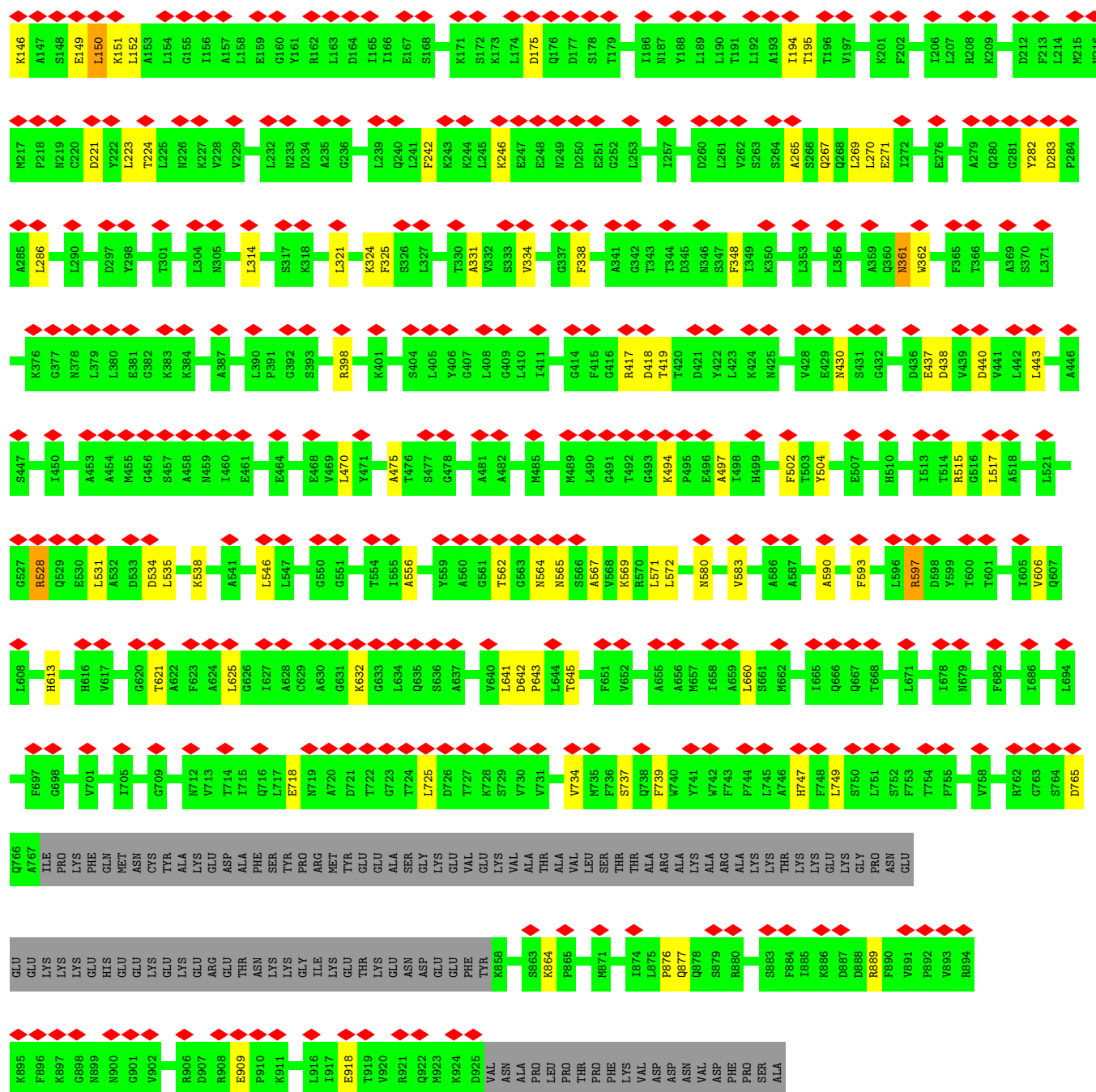


• Molecule 19: 26S proteasome complex subunit SEM1

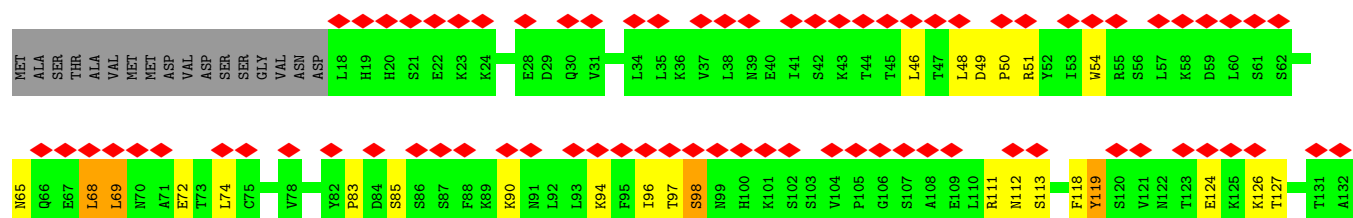
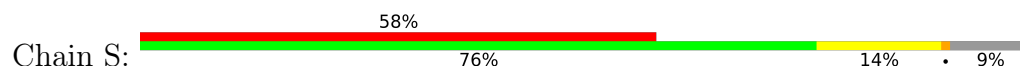


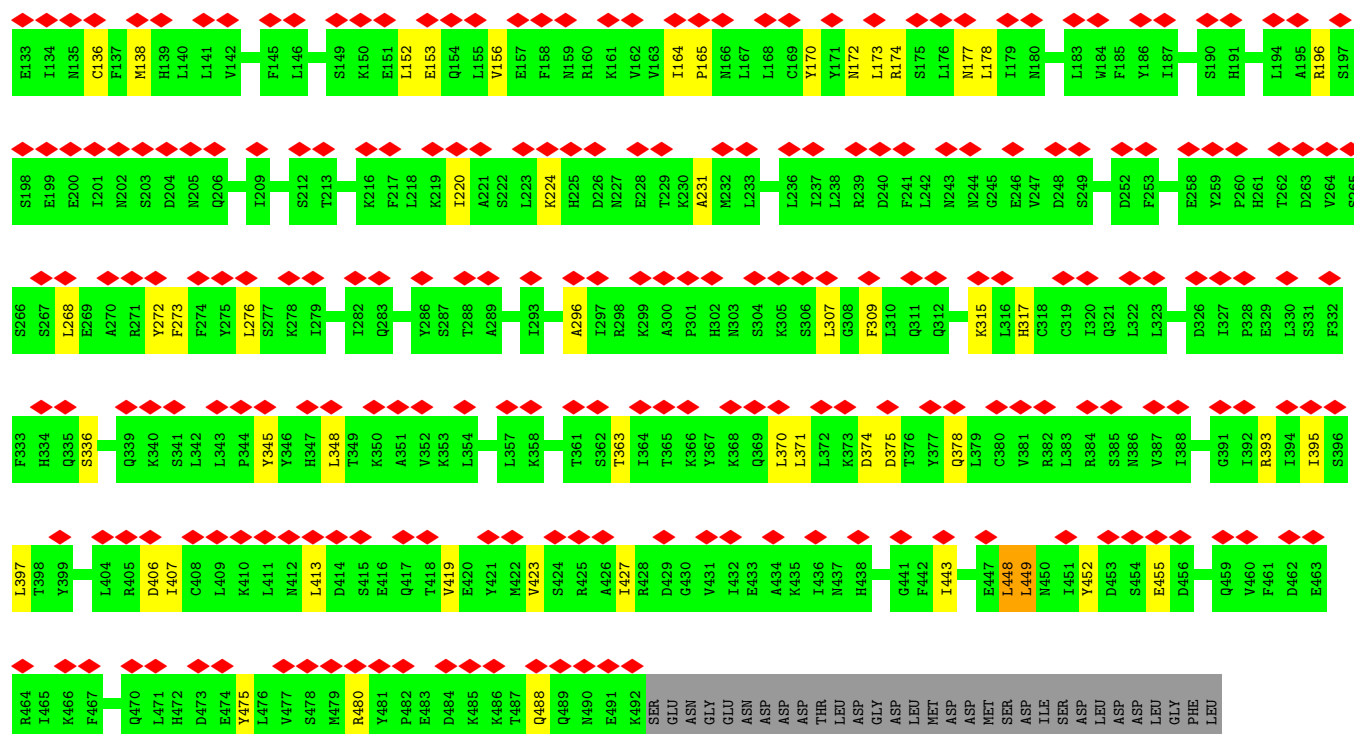
• Molecule 20: 26S proteasome regulatory subunit RPN1

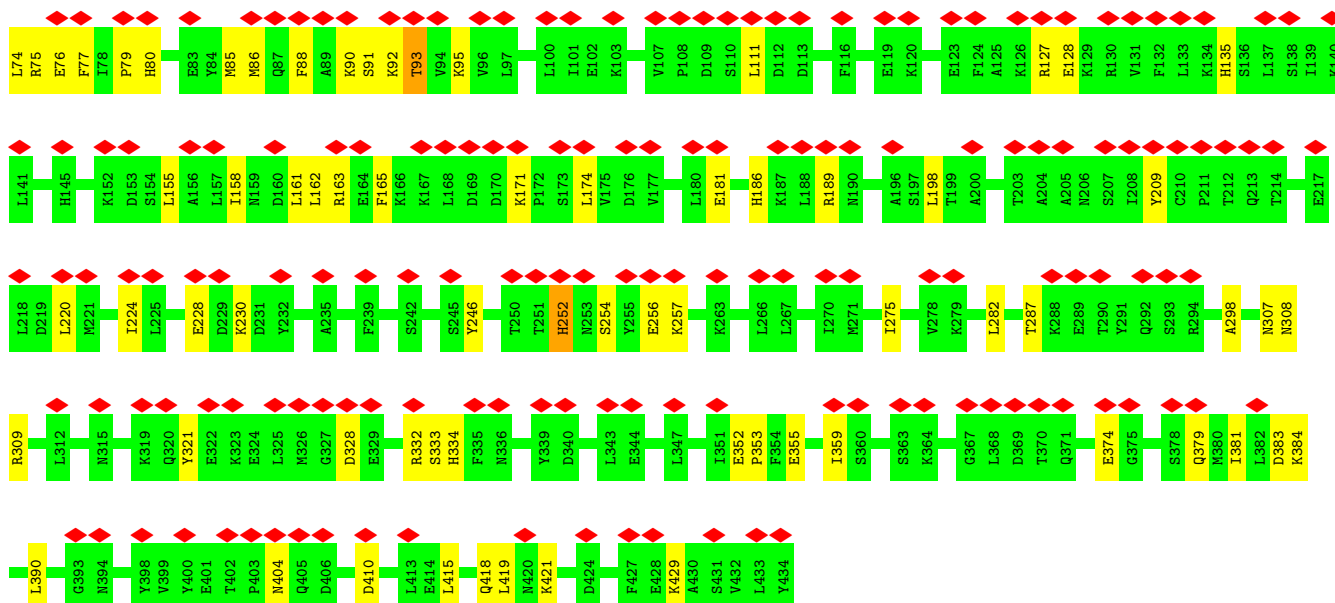




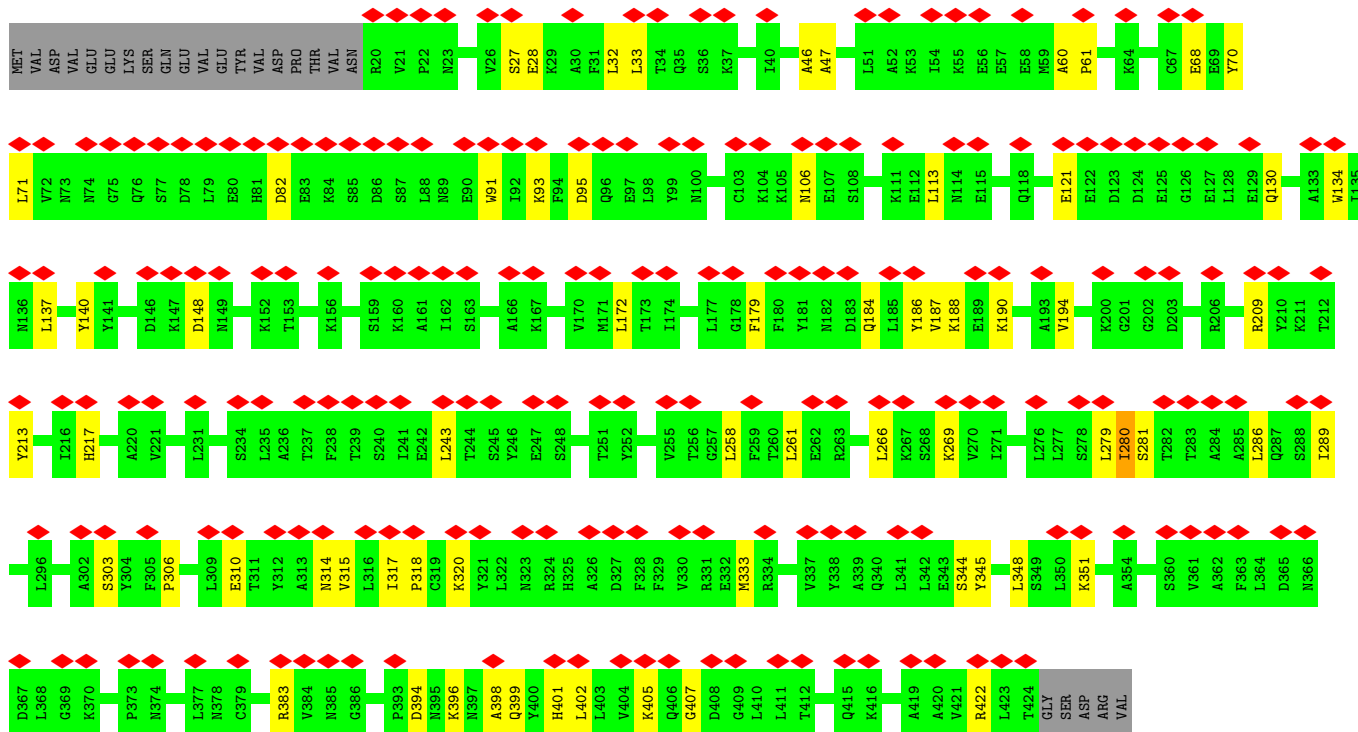
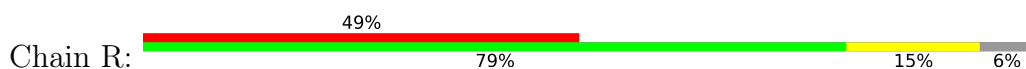
• Molecule 22: 26S proteasome regulatory subunit RPN3



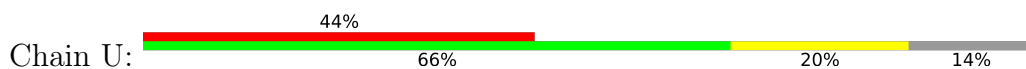


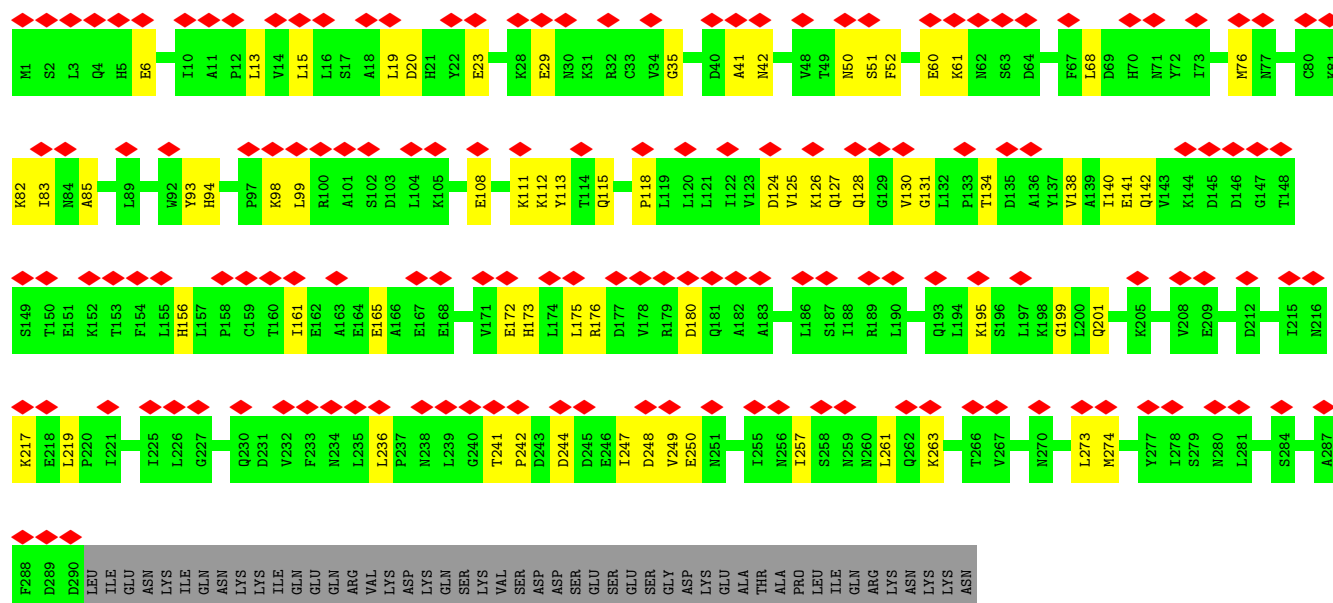


• Molecule 25: 26S proteasome regulatory subunit RPN7

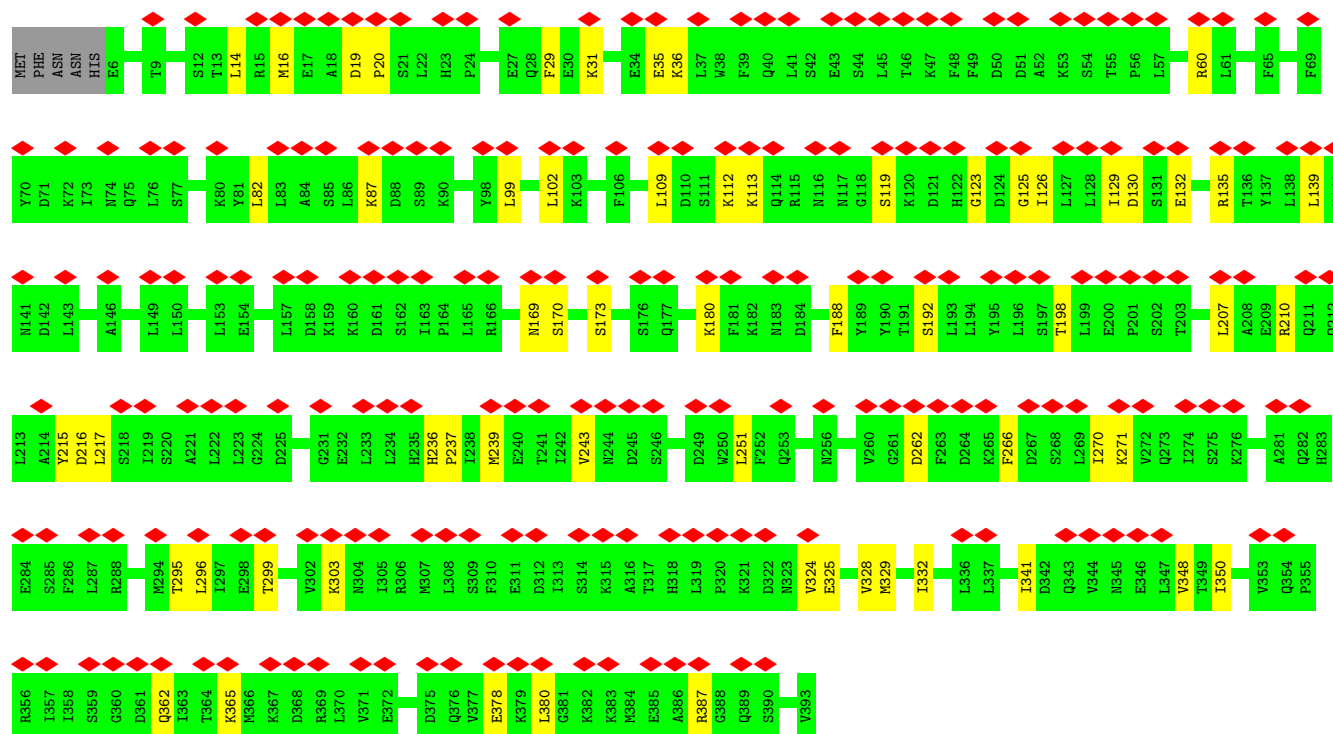
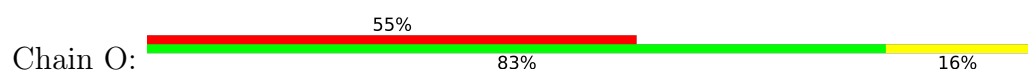


• Molecule 26: 26S proteasome regulatory subunit RPN8





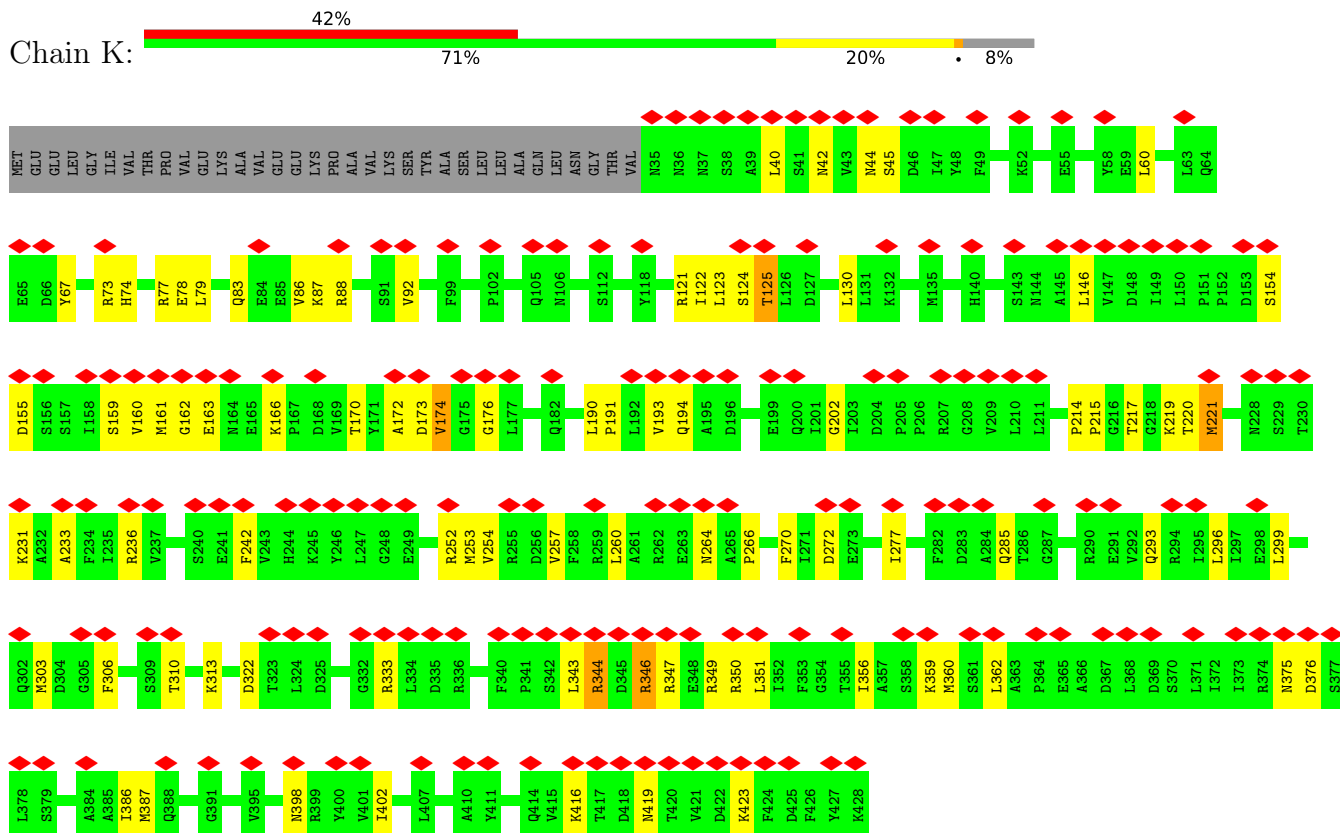
• Molecule 27: 26S proteasome regulatory subunit RPN9



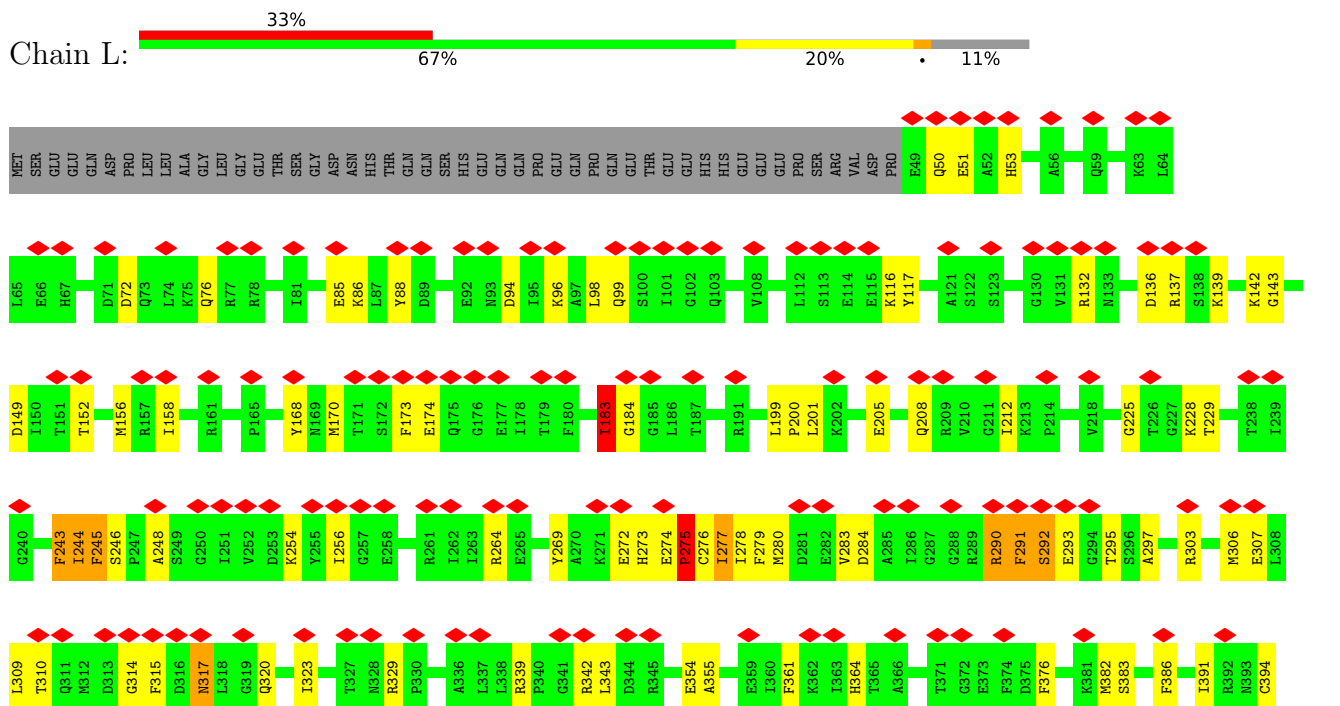
• Molecule 28: 26S proteasome regulatory subunit 7 homolog

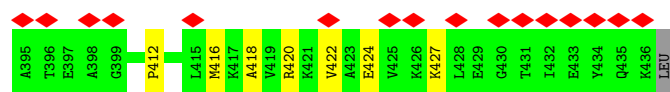


- Chain K:

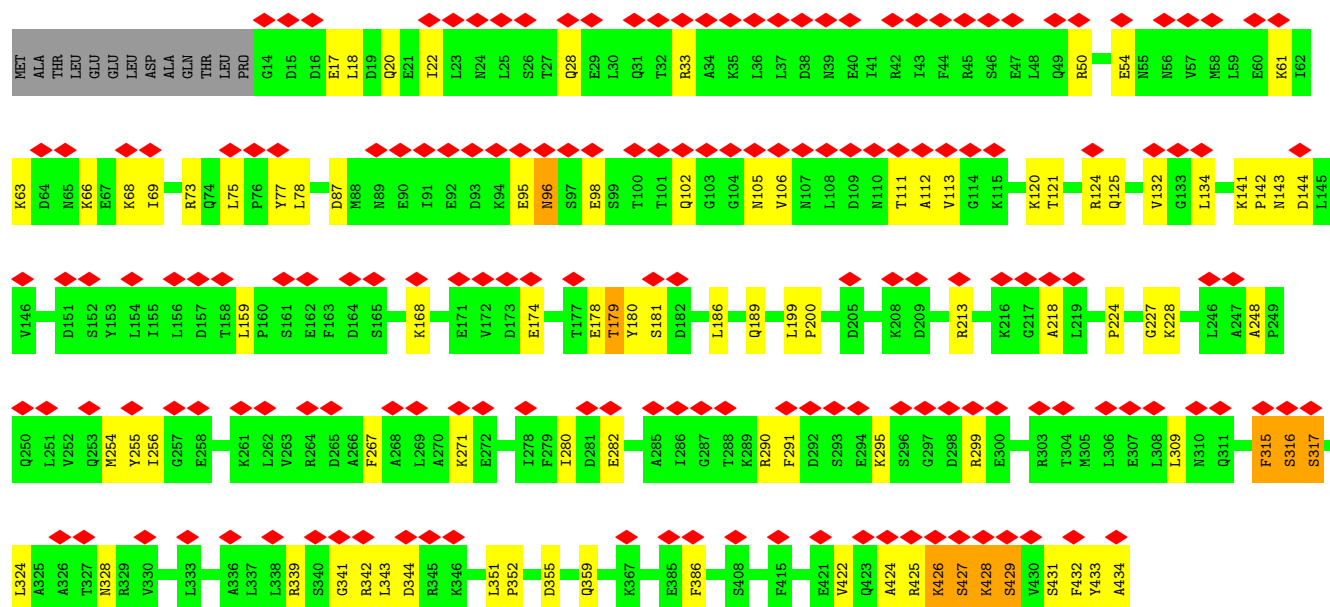
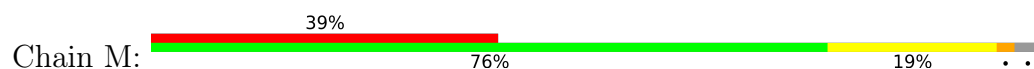


- Chain L:

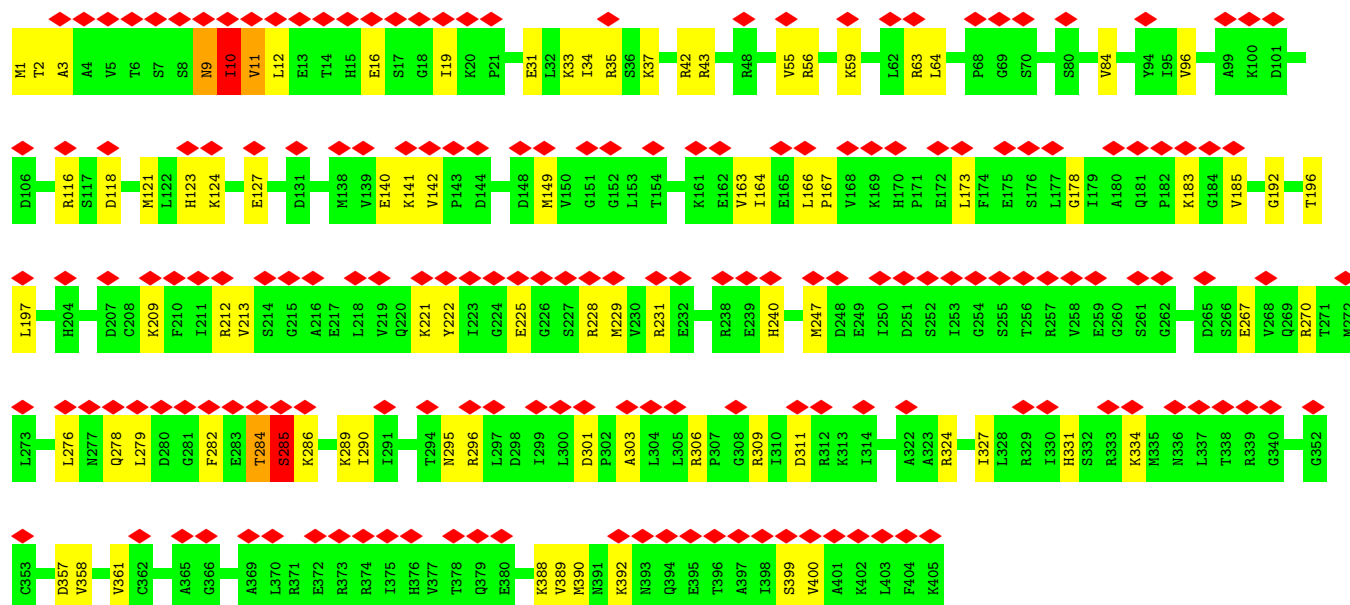
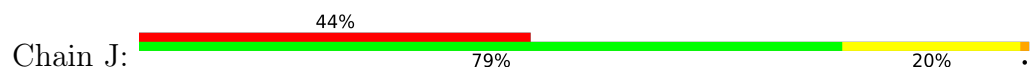




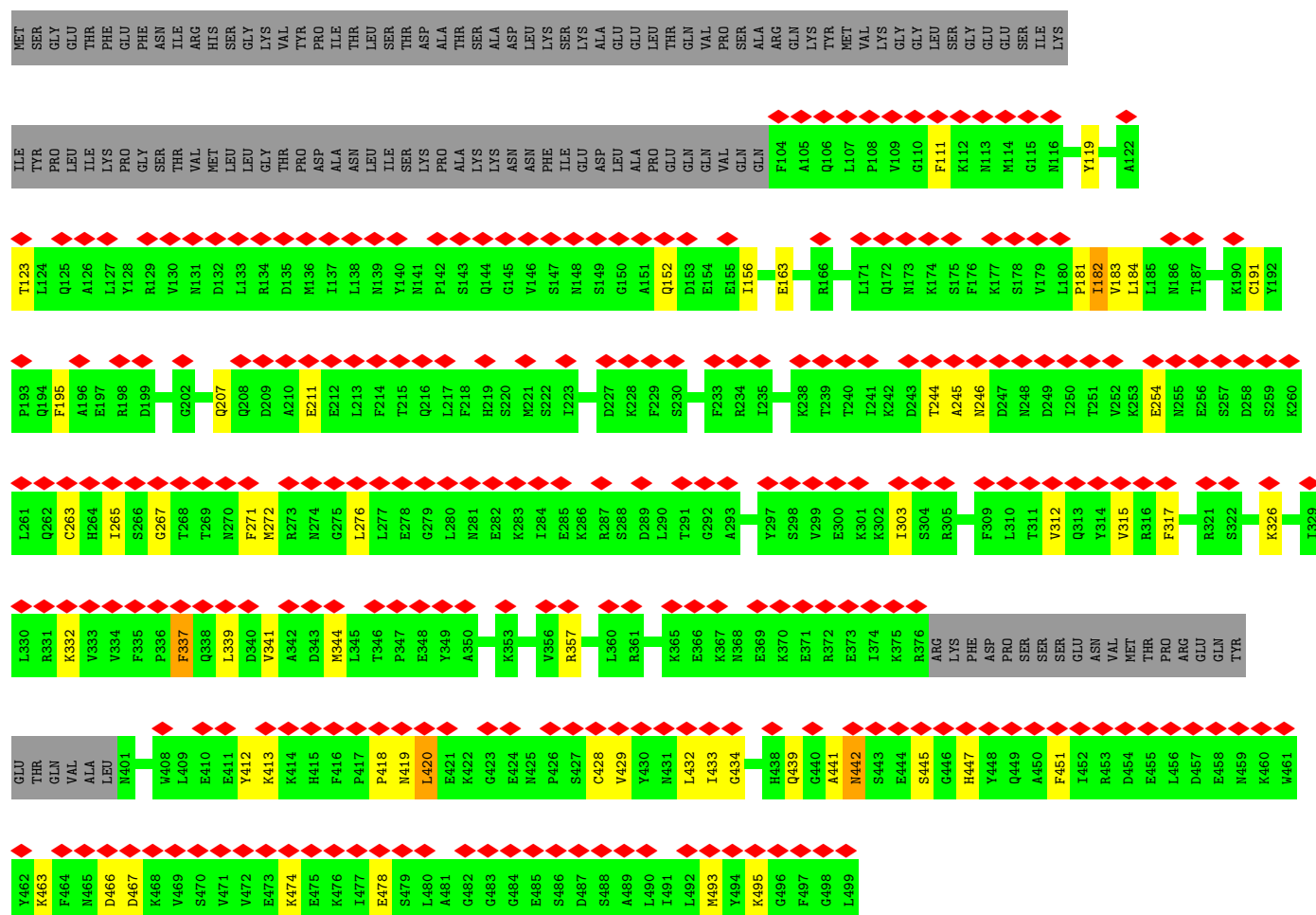
• Molecule 32: 26S proteasome regulatory subunit 6A



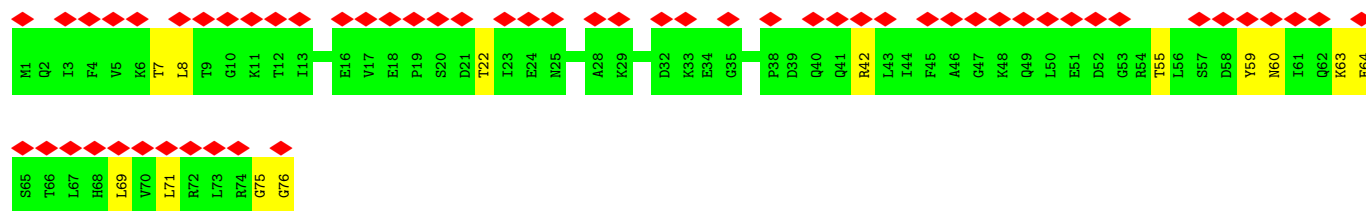
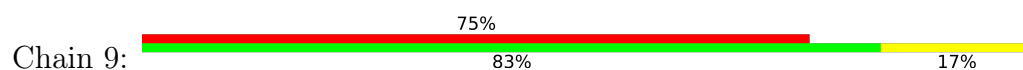
• Molecule 33: 26S proteasome regulatory subunit 8 homolog



• Molecule 34: Ubiquitin carboxyl-terminal hydrolase



• Molecule 35: Polyubiquitin-B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74842	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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	26.593	Depositor
Minimum map value	-21.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.913	Depositor
Recommended contour level	5.2	Depositor
Map size (Å)	529.92, 529.92, 529.92	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	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, GLZ, MG, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/1950	0.94	14/2641 (0.5%)
1	a	0.40	0/1950	0.94	14/2641 (0.5%)
2	B	0.39	0/1944	0.71	4/2632 (0.2%)
2	b	0.39	0/1944	0.71	4/2632 (0.2%)
3	C	0.43	0/1934	0.92	10/2618 (0.4%)
3	c	0.43	0/1934	0.92	10/2618 (0.4%)
4	D	0.45	0/1879	0.63	0/2546
4	d	0.25	0/1879	0.62	0/2546
5	E	0.39	0/1952	0.77	5/2630 (0.2%)
5	e	0.39	0/1952	0.77	5/2630 (0.2%)
6	F	0.41	0/1800	0.82	3/2433 (0.1%)
6	f	0.41	0/1800	0.82	3/2433 (0.1%)
7	G	0.56	1/1925 (0.1%)	0.91	14/2599 (0.5%)
7	g	0.56	1/1925 (0.1%)	0.91	14/2599 (0.5%)
8	1	0.42	0/1541	0.81	2/2087 (0.1%)
8	h	0.58	0/1541	0.94	7/2087 (0.3%)
9	2	0.64	2/1750 (0.1%)	1.00	13/2373 (0.5%)
9	i	0.47	0/1750	0.92	7/2373 (0.3%)
10	3	0.45	0/1611	0.86	4/2174 (0.2%)
10	j	0.45	0/1611	0.86	4/2174 (0.2%)
11	4	0.52	0/1589	0.92	6/2142 (0.3%)
11	k	0.52	0/1589	0.92	6/2142 (0.3%)
12	5	0.47	0/1681	1.02	6/2274 (0.3%)
12	l	0.47	0/1681	1.02	6/2274 (0.3%)
13	6	0.41	0/1795	0.86	9/2420 (0.4%)
13	m	0.41	0/1795	0.86	9/2420 (0.4%)
14	7	0.40	0/1821	0.61	0/2470
14	n	0.28	0/1821	0.57	0/2470
15	W	0.57	5/1557 (0.3%)	0.75	5/2111 (0.2%)
16	V	0.36	0/2309	0.65	4/3115 (0.1%)
17	T	0.24	0/2235	0.56	0/3017
18	X	0.19	0/1058	0.63	2/1432 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	Y	0.24	0/741	0.74	2/1000 (0.2%)
20	Z	0.31	2/7122 (0.0%)	0.68	7/9645 (0.1%)
21	N	0.31	0/6521	0.51	2/8824 (0.0%)
22	S	0.29	0/3966	0.57	0/5355
23	P	0.31	0/3663	0.51	0/4940
24	Q	0.28	0/3556	0.57	1/4787 (0.0%)
25	R	0.29	0/3313	0.53	0/4469
26	U	0.48	1/2340 (0.0%)	0.66	5/3168 (0.2%)
27	O	0.28	0/3247	0.53	0/4380
28	H	0.37	0/3113	0.64	2/4187 (0.0%)
29	I	0.56	4/3054 (0.1%)	0.82	10/4111 (0.2%)
30	K	0.44	2/3156 (0.1%)	0.75	10/4261 (0.2%)
31	L	0.62	3/3128 (0.1%)	0.88	17/4204 (0.4%)
32	M	0.38	0/3323	0.65	1/4478 (0.0%)
33	J	0.39	1/3212 (0.0%)	0.66	3/4316 (0.1%)
34	8	0.44	5/3089 (0.2%)	0.68	7/4144 (0.2%)
35	9	0.26	0/603	0.57	0/811
All	All	0.41	27/114650 (0.0%)	0.74	257/154833 (0.2%)

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
4	d	0	1
5	E	0	1
5	e	0	1
6	F	0	3
6	f	0	3
7	G	0	1
7	g	0	1
8	h	0	1
9	2	0	7
9	i	0	6
10	3	0	1
10	j	0	1
11	4	0	1
11	k	0	1
13	6	0	1
13	m	0	1
16	V	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
17	T	0	3
19	Y	0	1
20	Z	0	2
21	N	0	1
22	S	0	3
24	Q	0	2
25	R	0	1
27	O	0	1
28	H	0	8
29	I	0	6
30	K	0	2
31	L	0	6
32	M	0	4
33	J	0	4
34	8	0	2
All	All	0	78

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	82	ILE	CA-CB	-10.87	1.48	1.54
7	G	82	ILE	CA-CB	-10.83	1.48	1.54
9	2	114	GLN	C-N	-10.08	1.21	1.33
15	W	25	ARG	CA-C	-7.83	1.42	1.52
29	I	86	GLU	C-N	-6.98	1.24	1.34
30	K	221	MET	CA-C	-6.62	1.44	1.52
34	8	182	ILE	CA-C	-6.60	1.44	1.52
20	Z	747	ALA	CA-C	-6.51	1.44	1.52
26	U	98	LYS	CA-C	-6.51	1.45	1.53
34	8	182	ILE	CA-CB	6.46	1.63	1.54
30	K	173	ASP	N-CA	-6.35	1.38	1.46
20	Z	743	ILE	C-N	-6.32	1.25	1.34
31	L	183	ILE	CA-C	-6.26	1.46	1.52
15	W	25	ARG	CD-NE	6.24	1.54	1.46
29	I	86	GLU	CA-CB	5.99	1.61	1.53
15	W	23	ARG	CA-C	5.96	1.60	1.52
15	W	20	ASP	N-CA	5.87	1.54	1.45
33	J	357	ASP	C-N	5.83	1.40	1.34
31	L	184	GLY	N-CA	-5.63	1.39	1.46
15	W	25	ARG	NE-CZ	5.59	1.39	1.33
34	8	181	PRO	N-CA	-5.57	1.40	1.47
34	8	271	PHE	N-CA	-5.47	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	273	HIS	ND1-CE1	5.35	1.38	1.32
9	2	120	GLN	C-N	5.29	1.40	1.33
34	8	181	PRO	CA-CB	-5.26	1.46	1.53
29	I	273	GLU	CA-C	-5.17	1.46	1.52
29	I	231	LEU	N-CA	-5.01	1.39	1.46

All (257) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	19	LEU	CB-CG-CD1	19.12	168.05	110.70
3	C	19	LEU	CB-CG-CD1	19.12	168.05	110.70
12	5	144	ARG	CG-CD-NE	-17.21	74.14	112.00
12	l	144	ARG	CG-CD-NE	-17.20	74.16	112.00
12	l	161	LEU	CB-CG-CD1	14.89	155.36	110.70
12	5	161	LEU	CB-CG-CD1	14.88	155.36	110.70
11	k	163	LEU	CA-CB-CG	12.00	158.29	116.30
11	4	163	LEU	CA-CB-CG	11.99	158.26	116.30
30	K	220	THR	CA-C-N	11.91	136.24	120.28
30	K	220	THR	C-N-CA	11.91	136.24	120.28
12	l	161	LEU	CB-CG-CD2	-11.80	75.29	110.70
12	5	161	LEU	CB-CG-CD2	-11.80	75.28	110.70
12	l	161	LEU	CD1-CG-CD2	-11.68	85.09	110.80
12	5	161	LEU	CD1-CG-CD2	-11.68	85.10	110.80
3	c	19	LEU	CD1-CG-CD2	-11.36	85.81	110.80
3	C	19	LEU	CD1-CG-CD2	-11.36	85.81	110.80
1	A	210	MET	CB-CG-SD	10.87	145.30	112.70
1	a	210	MET	CB-CG-SD	10.86	145.27	112.70
30	K	219	LYS	O-C-N	-10.48	111.19	122.09
5	E	33	LEU	CA-CB-CG	9.82	150.66	116.30
5	e	33	LEU	CA-CB-CG	9.81	150.65	116.30
3	C	100	LYS	CG-CD-CE	9.80	133.83	111.30
3	c	100	LYS	CG-CD-CE	9.78	133.79	111.30
3	C	19	LEU	CB-CG-CD2	-9.48	82.27	110.70
3	c	19	LEU	CB-CG-CD2	-9.48	82.27	110.70
1	A	232	LYS	CA-CB-CG	9.33	132.76	114.10
1	a	232	LYS	CA-CB-CG	9.31	132.73	114.10
6	F	102	LYS	CD-CE-NZ	9.12	141.09	111.90
6	f	102	LYS	CD-CE-NZ	9.11	141.06	111.90
30	K	221	MET	CA-C-N	-8.70	105.90	120.68
30	K	221	MET	C-N-CA	-8.70	105.90	120.68
31	L	315	PHE	CA-CB-CG	-8.65	105.15	113.80
7	g	57	LYS	CD-CE-NZ	-8.55	84.53	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	ARG	CG-CD-NE	-8.55	93.19	112.00
7	G	57	LYS	CD-CE-NZ	-8.55	84.55	111.90
1	a	24	ARG	CG-CD-NE	-8.53	93.23	112.00
26	U	94	HIS	CA-CB-CG	8.36	122.16	113.80
31	L	277	ILE	N-CA-C	-8.33	95.37	107.78
9	i	118	LYS	CA-CB-CG	8.31	130.73	114.10
34	8	272	MET	O-C-N	8.31	131.62	122.15
8	h	156	SER	CA-C-N	8.29	131.22	120.44
8	h	156	SER	C-N-CA	8.29	131.22	120.44
31	L	275	PRO	CA-N-CD	-8.11	100.65	112.00
20	Z	173	ALA	CA-C-N	8.09	136.99	121.54
20	Z	173	ALA	C-N-CA	8.09	136.99	121.54
7	G	86	ARG	CG-CD-NE	-8.08	94.23	112.00
31	L	183	ILE	CA-C-N	8.06	128.22	122.33
31	L	183	ILE	C-N-CA	8.06	128.22	122.33
7	g	86	ARG	CG-CD-NE	-8.06	94.26	112.00
5	e	3	LEU	CA-CB-CG	8.04	144.45	116.30
29	I	81	ILE	N-CA-C	-8.03	103.36	111.88
5	E	3	LEU	CA-CB-CG	8.03	144.39	116.30
31	L	228	LYS	O-C-N	-7.71	113.94	122.12
7	G	185	GLU	CA-CB-CG	7.69	129.48	114.10
7	g	185	GLU	CA-CB-CG	7.69	129.48	114.10
12	5	144	ARG	CB-CG-CD	7.66	128.92	111.30
12	l	144	ARG	CB-CG-CD	7.65	128.90	111.30
30	K	221	MET	O-C-N	7.63	130.21	122.12
20	Z	376	SER	N-CA-C	7.61	119.81	110.91
30	K	220	THR	N-CA-CB	7.57	122.02	110.28
30	K	221	MET	N-CA-C	-7.44	103.17	111.28
7	g	115	ARG	NE-CZ-NH2	-7.43	112.51	119.20
7	G	115	ARG	NE-CZ-NH2	-7.42	112.53	119.20
10	3	134	LYS	CG-CD-CE	7.30	128.09	111.30
10	j	134	LYS	CG-CD-CE	7.30	128.09	111.30
13	6	109	ARG	CB-CG-CD	7.28	128.04	111.30
9	2	243	LYS	CD-CE-NZ	7.28	135.18	111.90
9	i	243	LYS	CD-CE-NZ	7.27	135.16	111.90
13	m	109	ARG	CB-CG-CD	7.25	127.98	111.30
20	Z	174	GLU	N-CA-C	7.18	126.08	110.80
8	1	173	LYS	CD-CE-NZ	7.05	134.46	111.90
8	h	173	LYS	CD-CE-NZ	7.05	134.45	111.90
8	h	156	SER	O-C-N	-7.00	114.81	122.79
7	g	167	LYS	CD-CE-NZ	6.99	134.28	111.90
7	G	57	LYS	CG-CD-CE	6.99	127.38	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	57	LYS	CG-CD-CE	6.98	127.35	111.30
7	G	167	LYS	CD-CE-NZ	6.98	134.24	111.90
15	W	21	PHE	CA-C-N	6.95	128.53	119.84
15	W	21	PHE	C-N-CA	6.95	128.53	119.84
1	A	187	LYS	CD-CE-NZ	6.88	133.90	111.90
1	a	187	LYS	CD-CE-NZ	6.86	133.84	111.90
31	L	314	GLY	CA-C-N	6.82	129.98	120.29
31	L	314	GLY	C-N-CA	6.82	129.98	120.29
28	H	466	TYR	N-CA-C	6.75	125.19	110.80
1	A	96	ARG	CB-CG-CD	6.74	126.80	111.30
3	C	185	LYS	CB-CG-CD	6.74	126.80	111.30
3	c	185	LYS	CB-CG-CD	6.73	126.78	111.30
31	L	274	GLU	CA-C-O	-6.72	113.43	119.75
1	a	96	ARG	CB-CG-CD	6.72	126.75	111.30
8	h	124	LEU	CA-CB-CG	6.64	139.55	116.30
8	1	124	LEU	CA-CB-CG	6.63	139.52	116.30
9	2	115	HIS	CG-CD2-NE2	6.62	113.82	107.20
18	X	53	THR	N-CA-C	-6.61	105.85	114.04
1	A	98	LYS	CD-CE-NZ	6.58	132.97	111.90
1	a	98	LYS	CD-CE-NZ	6.58	132.95	111.90
19	Y	32	ASP	N-CA-C	6.58	124.81	110.80
1	a	190	LYS	CB-CG-CD	6.57	126.40	111.30
1	A	190	LYS	CB-CG-CD	6.55	126.38	111.30
1	a	58	LYS	CB-CG-CD	6.50	126.24	111.30
1	A	58	LYS	CB-CG-CD	6.49	126.23	111.30
26	U	99	LEU	O-C-N	-6.45	115.84	123.06
1	A	98	LYS	CG-CD-CE	6.37	125.94	111.30
1	a	98	LYS	CG-CD-CE	6.36	125.93	111.30
20	Z	143	VAL	N-CA-C	-6.35	105.64	111.67
31	L	276	CYS	CA-C-O	-6.34	114.76	121.99
30	K	220	THR	CB-CA-C	-6.34	98.50	110.67
1	A	232	LYS	CD-CE-NZ	6.30	132.07	111.90
1	a	232	LYS	CD-CE-NZ	6.30	132.06	111.90
28	H	466	TYR	CB-CA-C	-6.29	97.90	110.42
24	Q	252	HIS	N-CA-C	-6.22	107.53	114.62
1	a	62	LYS	CD-CE-NZ	6.19	131.72	111.90
1	A	62	LYS	CD-CE-NZ	6.19	131.72	111.90
3	c	5	ARG	CB-CG-CD	6.15	125.44	111.30
2	b	116	LYS	CD-CE-NZ	6.15	131.57	111.90
21	N	597	ARG	CG-CD-NE	6.15	125.52	112.00
2	B	116	LYS	CD-CE-NZ	6.15	131.57	111.90
3	C	5	ARG	CB-CG-CD	6.14	125.43	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	170	LYS	CD-CE-NZ	6.14	131.54	111.90
11	4	170	LYS	CD-CE-NZ	6.12	131.48	111.90
9	2	120	GLN	CA-C-N	6.12	130.82	120.91
9	2	120	GLN	C-N-CA	6.12	130.82	120.91
6	F	82	ARG	CB-CG-CD	6.08	125.28	111.30
6	f	82	ARG	CB-CG-CD	6.08	125.27	111.30
31	L	274	GLU	N-CA-C	6.08	118.23	109.48
10	3	42	LYS	CD-CE-NZ	6.06	131.29	111.90
10	j	42	LYS	CD-CE-NZ	6.05	131.27	111.90
11	4	86	GLN	CA-CB-CG	6.05	126.21	114.10
29	I	82	LEU	CA-C-N	6.05	136.57	121.80
29	I	82	LEU	C-N-CA	6.05	136.57	121.80
11	k	86	GLN	CA-CB-CG	6.04	126.18	114.10
8	h	156	SER	N-CA-C	-6.03	102.57	110.53
10	j	18	LYS	CA-CB-CG	-6.03	102.03	114.10
10	3	18	LYS	CA-CB-CG	-6.01	102.08	114.10
21	N	128	ILE	N-CA-C	-6.01	107.64	113.53
19	Y	4	ASP	N-CA-C	-6.00	98.01	110.80
10	j	65	GLU	CA-CB-CG	6.00	126.10	114.10
3	c	5	ARG	CA-CB-CG	5.98	126.06	114.10
1	a	58	LYS	CA-CB-CG	5.98	126.06	114.10
1	A	58	LYS	CA-CB-CG	5.98	126.06	114.10
3	C	5	ARG	CA-CB-CG	5.98	126.05	114.10
9	i	94	LEU	CB-CG-CD1	5.97	128.62	110.70
10	3	65	GLU	CA-CB-CG	5.97	126.05	114.10
9	2	94	LEU	CB-CG-CD1	5.97	128.61	110.70
29	I	85	PHE	N-CA-C	-5.92	104.59	112.94
9	i	118	LYS	CD-CE-NZ	5.89	130.74	111.90
20	Z	174	GLU	N-CA-CB	-5.88	100.55	110.49
31	L	229	THR	CA-CB-CG2	-5.87	100.52	110.50
18	X	116	ALA	N-CA-C	-5.85	107.95	114.62
34	8	418	PRO	CA-C-N	5.82	132.66	121.54
34	8	418	PRO	C-N-CA	5.82	132.66	121.54
13	6	177	LYS	CB-CG-CD	5.73	124.49	111.30
9	2	116	LEU	CA-C-N	5.72	130.27	120.72
9	2	116	LEU	C-N-CA	5.72	130.27	120.72
13	m	177	LYS	CB-CG-CD	5.71	124.43	111.30
7	g	232	LYS	CD-CE-NZ	-5.68	93.71	111.90
7	G	232	LYS	CD-CE-NZ	-5.68	93.73	111.90
7	G	72	ARG	CG-CD-NE	-5.66	99.54	112.00
20	Z	498	ALA	N-CA-C	-5.66	98.75	110.80
3	c	19	LEU	CA-CB-CG	5.65	136.08	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	185	GLU	CB-CG-CD	5.65	122.20	112.60
12	5	144	ARG	CB-CA-C	-5.65	102.19	110.95
3	C	19	LEU	CA-CB-CG	5.64	136.06	116.30
9	2	227	GLU	CA-CB-CG	5.64	125.39	114.10
3	c	185	LYS	CG-CD-CE	-5.64	98.33	111.30
7	g	185	GLU	CB-CG-CD	5.63	122.18	112.60
12	l	144	ARG	CB-CA-C	-5.63	102.22	110.95
32	M	428	LYS	CA-C-O	-5.63	112.46	120.51
7	g	72	ARG	CG-CD-NE	-5.63	99.61	112.00
9	i	227	GLU	CA-CB-CG	5.63	125.36	114.10
3	C	185	LYS	CG-CD-CE	-5.63	98.35	111.30
8	h	150	ASN	CA-CB-CG	-5.58	107.02	112.60
13	m	217	LYS	CB-CG-CD	5.58	124.14	111.30
15	W	24	THR	CA-C-N	5.58	128.03	120.38
15	W	24	THR	C-N-CA	5.58	128.03	120.38
13	6	217	LYS	CB-CG-CD	5.58	124.14	111.30
16	V	20	ARG	CB-CG-CD	5.56	124.09	111.30
11	k	86	GLN	CB-CG-CD	5.55	122.03	112.60
11	4	86	GLN	CB-CG-CD	5.55	122.03	112.60
26	U	94	HIS	CG-CD2-NE2	5.54	112.75	107.20
7	G	23	GLN	CA-CB-CG	5.50	125.09	114.10
29	I	125	MET	N-CA-C	-5.49	97.67	109.81
26	U	94	HIS	CE1-NE2-CD2	-5.48	103.52	109.00
7	g	23	GLN	CA-CB-CG	5.46	125.03	114.10
29	I	55	CYS	CA-C-N	5.46	131.38	122.65
29	I	55	CYS	C-N-CA	5.46	131.38	122.65
29	I	83	LYS	CA-C-O	-5.46	112.68	120.16
34	8	181	PRO	CA-C-N	5.45	131.77	121.97
34	8	181	PRO	C-N-CA	5.45	131.77	121.97
29	I	83	LYS	O-C-N	5.44	127.58	121.32
9	i	104	ARG	CB-CG-CD	5.43	123.78	111.30
9	2	104	ARG	CB-CG-CD	5.42	123.78	111.30
16	V	185	ILE	CA-C-N	5.42	131.90	121.54
16	V	185	ILE	C-N-CA	5.42	131.90	121.54
7	G	170	GLN	CA-CB-CG	5.42	124.94	114.10
7	g	170	GLN	CA-CB-CG	5.40	124.91	114.10
15	W	21	PHE	N-CA-CB	5.39	119.96	110.37
33	J	285	SER	N-CA-C	5.36	122.22	110.80
13	m	177	LYS	CG-CD-CE	5.34	123.58	111.30
33	J	284	THR	CA-C-N	5.33	131.73	121.54
33	J	284	THR	C-N-CA	5.33	131.73	121.54
13	6	177	LYS	CG-CD-CE	5.33	123.55	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	173	ASP	N-CA-C	-5.30	103.44	111.56
13	m	108	LYS	CG-CD-CE	5.30	123.49	111.30
13	m	109	ARG	NE-CZ-NH2	-5.30	114.43	119.20
7	G	8	TYR	CA-CB-CG	-5.30	104.36	113.90
7	g	8	TYR	CA-CB-CG	-5.30	104.37	113.90
13	6	108	LYS	CG-CD-CE	5.29	123.48	111.30
9	i	253	GLN	N-CA-C	5.29	118.10	109.59
9	2	253	GLN	N-CA-C	5.28	118.09	109.59
2	B	236	ARG	NE-CZ-NH2	5.28	123.95	119.20
3	C	92	ARG	NE-CZ-NH1	-5.28	116.22	121.50
9	2	119	TYR	CA-C-N	5.28	131.62	121.54
9	2	119	TYR	C-N-CA	5.28	131.62	121.54
31	L	272	GLU	N-CA-C	-5.28	106.69	113.23
13	6	228	LYS	CG-CD-CE	5.26	123.39	111.30
7	G	81	LEU	CB-CG-CD2	-5.25	94.93	110.70
7	g	81	LEU	CB-CG-CD2	-5.25	94.94	110.70
13	6	109	ARG	NE-CZ-NH2	-5.25	114.48	119.20
2	b	236	ARG	NE-CZ-NH2	5.24	123.92	119.20
13	m	228	LYS	CG-CD-CE	5.24	123.36	111.30
3	c	92	ARG	NE-CZ-NH1	-5.24	116.26	121.50
31	L	320	GLN	O-C-N	-5.22	116.04	122.20
34	8	183	VAL	N-CA-C	5.21	115.93	110.62
26	U	94	HIS	O-C-N	-5.20	117.11	123.19
13	6	180	LEU	CD1-CG-CD2	-5.19	99.38	110.80
29	I	125	MET	C-N-CD	-5.19	103.71	125.00
13	m	180	LEU	CD1-CG-CD2	-5.18	99.41	110.80
34	8	272	MET	CG-SD-CE	-5.17	89.53	100.90
9	2	115	HIS	CE1-NE2-CD2	-5.15	103.85	109.00
1	a	190	LYS	CD-CE-NZ	5.13	128.32	111.90
1	A	190	LYS	CD-CE-NZ	5.13	128.32	111.90
1	a	250	GLU	CA-CB-CG	5.11	124.32	114.10
1	A	250	GLU	CA-CB-CG	5.11	124.32	114.10
5	e	15	PHE	CA-C-N	5.10	130.88	121.70
5	e	15	PHE	C-N-CA	5.10	130.88	121.70
2	B	59	GLU	CB-CG-CD	5.09	121.25	112.60
5	E	15	PHE	CA-C-N	5.09	130.85	121.70
5	E	15	PHE	C-N-CA	5.09	130.85	121.70
5	E	86	ARG	NE-CZ-NH2	5.09	123.78	119.20
6	F	199	GLN	CB-CG-CD	5.08	121.24	112.60
6	f	199	GLN	CB-CG-CD	5.08	121.24	112.60
13	m	109	ARG	CG-CD-NE	-5.08	100.83	112.00
16	V	58	VAL	N-CA-C	-5.08	98.78	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	109	ARG	CG-CD-NE	-5.07	100.84	112.00
5	e	86	ARG	NE-CZ-NH2	5.07	123.76	119.20
2	b	59	GLU	CB-CG-CD	5.05	121.19	112.60
2	B	91	LYS	CG-CD-CE	-5.05	99.69	111.30
7	G	178	LYS	CD-CE-NZ	5.04	128.04	111.90
7	g	178	LYS	CD-CE-NZ	5.04	128.03	111.90
11	k	78	GLN	CA-CB-CG	5.04	124.18	114.10
11	k	163	LEU	CB-CG-CD2	5.04	125.81	110.70
11	4	163	LEU	CB-CG-CD2	5.03	125.80	110.70
2	b	91	LYS	CG-CD-CE	-5.03	99.74	111.30
11	4	78	GLN	CA-CB-CG	5.02	124.14	114.10
31	L	317	ASN	OD1-CG-ND2	5.02	127.62	122.60
31	L	245	PHE	N-CA-C	-5.02	100.09	108.07
31	L	229	THR	N-CA-CB	5.01	118.02	110.30

There are no chirality outliers.

All (78) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	2	119	TYR	Sidechain
9	2	152	TYR	Peptide
9	2	222	PRO	Peptide
9	2	252	ILE	Peptide
9	2	253	GLN	Peptide
9	2	254	GLU	Peptide
9	2	59	ASN	Peptide
10	3	31	SER	Peptide
11	4	1	MET	Peptide
13	6	39	THR	Peptide
34	8	337	PHE	Peptide
34	8	441	ALA	Peptide
5	E	15	PHE	Peptide
6	F	13	PHE	Peptide
6	F	18	ARG	Peptide
6	F	8	GLY	Peptide
7	G	70	VAL	Peptide
28	H	151	GLN	Peptide
28	H	205	ASP	Peptide
28	H	312	ASP	Peptide
28	H	313	ALA	Peptide
28	H	371	ILE	Peptide
28	H	465	GLN	Peptide

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Mol	Chain	Res	Type	Group
28	H	90	ARG	Peptide
28	H	94	GLU	Peptide
29	I	101	GLY	Peptide
29	I	104	LEU	Peptide
29	I	134	SER	Peptide
29	I	182	SER	Peptide
29	I	344	ILE	Peptide
29	I	429	GLU	Peptide
33	J	10	ILE	Peptide
33	J	286	LYS	Peptide
33	J	399	SER	Peptide
33	J	9	ASN	Peptide
30	K	125	THR	Peptide
30	K	174	VAL	Peptide
31	L	243	PHE	Peptide
31	L	244	ILE	Peptide
31	L	290	ARG	Peptide
31	L	292	SER	Peptide
31	L	343	LEU	Peptide
31	L	376	PHE	Peptide
32	M	105	ASN	Peptide
32	M	290	ARG	Peptide
32	M	315	PHE	Peptide
32	M	426	LYS	Peptide
21	N	528	ARG	Peptide
27	O	119	SER	Peptide
24	Q	161	LEU	Peptide
24	Q	67	THR	Peptide
25	R	70	TYR	Peptide
22	S	124	GLU	Peptide
22	S	127	THR	Peptide
22	S	448	LEU	Peptide
17	T	172	SER	Peptide
17	T	251	HIS	Peptide
17	T	91	SER	Peptide
16	V	270	TYR	Peptide
19	Y	31	GLU	Peptide
20	Z	173	ALA	Peptide
20	Z	84	ALA	Peptide
4	d	16	HIS	Peptide
5	e	15	PHE	Peptide
6	f	13	PHE	Peptide

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Mol	Chain	Res	Type	Group
6	f	18	ARG	Peptide
6	f	8	GLY	Peptide
7	g	70	VAL	Peptide
8	h	151	PHE	Sidechain
9	i	152	TYR	Peptide
9	i	222	PRO	Peptide
9	i	252	ILE	Peptide
9	i	253	GLN	Peptide
9	i	254	GLU	Peptide
9	i	59	ASN	Peptide
10	j	31	SER	Peptide
11	k	1	MET	Peptide
13	m	39	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1912	0	1906	74	0
1	a	1912	0	1906	66	0
2	B	1907	0	1917	67	0
2	b	1907	0	1917	68	0
3	C	1904	0	1901	72	0
3	c	1904	0	1901	65	0
4	D	1850	0	1862	59	0
4	d	1850	0	1862	42	0
5	E	1925	0	1896	63	0
5	e	1925	0	1896	54	0
6	F	1773	0	1775	62	0
6	f	1773	0	1775	62	0
7	G	1885	0	1876	80	0
7	g	1885	0	1876	89	0
8	1	1512	0	1478	63	0
8	h	1512	0	1478	61	0
9	2	1719	0	1716	96	0
9	i	1719	0	1716	85	0
10	3	1581	0	1571	83	0
10	j	1581	0	1571	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	4	1561	0	1569	67	0
11	k	1561	0	1569	67	0
12	5	1644	0	1592	66	0
12	l	1644	0	1592	80	0
13	6	1757	0	1708	69	0
13	m	1757	0	1708	74	0
14	7	1790	0	1790	41	0
14	n	1790	0	1790	47	0
15	W	1534	0	1542	16	0
16	V	2274	0	2273	81	0
17	T	2192	0	2161	25	0
18	X	1032	0	1017	3	0
19	Y	731	0	675	16	0
20	Z	7005	0	6932	161	0
21	N	6418	0	6487	90	0
22	S	3894	0	3938	67	0
23	P	3608	0	3694	39	0
24	Q	3499	0	3524	52	0
25	R	3258	0	3263	56	0
26	U	2306	0	2331	58	0
27	O	3186	0	3213	43	0
28	H	3064	0	3141	112	0
29	I	3015	0	3084	132	0
30	K	3113	0	3168	83	0
31	L	3082	0	3157	80	0
32	M	3285	0	3320	102	0
33	J	3171	0	3311	88	0
34	8	3034	0	3005	48	0
35	9	601	0	629	12	0
36	H	31	0	12	32	0
36	I	31	0	11	20	0
36	K	31	0	12	7	0
36	L	31	0	12	10	0
36	M	31	0	11	15	0
37	H	1	0	0	0	0
37	I	1	0	0	0	0
37	J	1	0	0	0	0
37	K	1	0	0	0	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
38	J	27	0	11	14	0
All	All	112930	0	113048	2815	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 12.

All (2815) 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)
20:Z:916:LEU:HD12	29:I:54:ARG:O	1.29	1.28
29:I:393:GLN:HE22	36:I:501:ATP:C4'	1.49	1.26
20:Z:916:LEU:CD1	29:I:54:ARG:O	1.84	1.24
20:Z:916:LEU:HD11	29:I:54:ARG:N	1.57	1.19
1:A:14:ARG:NE	7:G:8:TYR:OH	1.76	1.19
36:L:501:ATP:O3B	32:M:339:ARG:NH1	1.77	1.16
29:I:393:GLN:NE2	36:I:501:ATP:C4'	2.09	1.15
32:M:228:LYS:HG2	36:M:501:ATP:PB	1.87	1.14
36:H:501:ATP:PA	29:I:340:ARG:HH22	1.71	1.13
32:M:228:LYS:HG2	36:M:501:ATP:O1B	1.51	1.10
8:h:155:MET:HE2	8:h:159:GLU:OE1	1.49	1.10
33:J:197:LEU:HD11	38:J:501:ADP:H2'	1.32	1.09
36:K:501:ATP:H5'1	31:L:339:ARG:HH22	0.92	1.09
2:b:104:TYR:OH	9:i:93:GLU:OE2	1.73	1.03
36:L:501:ATP:PG	32:M:339:ARG:NH1	2.31	1.03
36:K:501:ATP:H5'1	31:L:339:ARG:NH2	1.71	1.03
7:G:170:GLN:NE2	31:L:382:MET:O	1.92	1.02
12:5:181:ARG:N	12:5:257:GLU:OE2	1.92	1.02
12:l:181:ARG:N	12:l:257:GLU:OE2	1.92	1.01
30:K:215:PRO:O	36:K:501:ATP:O1B	1.76	1.01
36:K:501:ATP:C5'	31:L:339:ARG:HH22	1.75	1.00
29:I:230:THR:OG1	36:I:501:ATP:O2B	1.78	1.00
10:3:71:THR:OG1	10:3:75:LYS:NZ	1.96	0.98
9:2:69:LYS:NZ	9:2:211:LYS:O	1.97	0.98
10:j:71:THR:OG1	10:j:75:LYS:NZ	1.96	0.98
1:A:14:ARG:HE	7:G:8:TYR:HH	1.01	0.98
29:I:393:GLN:HE22	36:I:501:ATP:C5'	1.77	0.97
4:d:204:GLN:O	4:d:205:THR:OG1	1.83	0.96
9:i:69:LYS:NZ	9:i:211:LYS:O	1.97	0.96
1:A:148:GLU:N	1:A:148:GLU:OE2	1.99	0.96
5:E:121:LEU:HD22	6:F:79:PRO:HB3	1.47	0.96
28:H:258:LEU:HD21	36:H:501:ATP:H2'	1.46	0.96
1:a:148:GLU:N	1:a:148:GLU:OE2	1.99	0.94
20:Z:952:SER:OG	20:Z:969:GLU:OE2	1.82	0.94
20:Z:773:ARG:NH2	20:Z:938:GLN:OE1	2.02	0.92
1:a:14:ARG:NE	7:g:8:TYR:OH	2.02	0.92
7:g:230:PHE:HB2	7:g:232:LYS:HZ1	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:135:TYR:OH	11:k:174:MET:SD	2.28	0.91
9:i:49:SER:OG	9:i:60:CYS:SG	2.28	0.91
5:E:32:LYS:NZ	5:E:176:SER:OG	2.04	0.91
4:D:204:GLN:O	4:D:205:THR:OG1	1.88	0.91
9:2:49:SER:OG	9:2:60:CYS:SG	2.28	0.91
11:4:135:TYR:OH	11:4:174:MET:SD	2.29	0.90
5:e:32:LYS:NZ	5:e:176:SER:OG	2.04	0.90
5:e:15:PHE:HA	5:e:16:SER:HB2	1.54	0.89
5:E:15:PHE:HA	5:E:16:SER:HB2	1.53	0.88
33:J:196:THR:HB	38:J:501:ADP:O1A	1.73	0.88
7:G:230:PHE:HB2	7:G:232:LYS:HZ1	1.38	0.88
8:h:155:MET:CE	8:h:159:GLU:OE1	2.22	0.87
8:h:26:ASP:OD2	8:h:178:SER:OG	1.92	0.87
9:2:214:GLU:OE1	9:2:214:GLU:N	2.08	0.87
28:H:258:LEU:CD2	36:H:501:ATP:H2'	2.03	0.87
32:M:186:LEU:HD11	36:M:501:ATP:N6	1.89	0.87
20:Z:408:TYR:OH	20:Z:443:ASP:OD2	1.91	0.86
36:L:501:ATP:O3G	32:M:339:ARG:NH1	2.09	0.86
9:i:214:GLU:N	9:i:214:GLU:OE1	2.08	0.86
29:I:74:GLU:OE2	29:I:78:ASN:ND2	2.09	0.86
8:1:26:ASP:OD2	8:1:178:SER:OG	1.92	0.86
2:b:33:THR:OG1	2:b:48:GLU:OE2	1.95	0.84
9:i:48:ARG:HB2	9:i:199:GLY:O	1.76	0.84
14:n:242:LYS:NZ	14:n:245:LEU:HD21	1.92	0.84
9:2:48:ARG:HB2	9:2:199:GLY:O	1.76	0.84
2:b:141:GLU:N	2:b:141:GLU:OE2	2.11	0.83
32:M:228:LYS:CG	36:M:501:ATP:O1B	2.27	0.83
2:B:33:THR:OG1	2:B:48:GLU:OE2	1.95	0.83
12:l:113:ASN:OD1	12:l:114:PRO:HD2	1.79	0.82
2:B:141:GLU:N	2:B:141:GLU:OE2	2.11	0.82
6:F:13:PHE:HA	6:F:14:SER:HB2	1.61	0.82
11:4:96:ARG:NH2	12:5:166:LYS:O	2.10	0.82
7:G:205:GLU:N	7:G:205:GLU:OE2	2.12	0.82
7:g:205:GLU:N	7:g:205:GLU:OE2	2.12	0.82
4:d:67:ILE:O	11:k:69:ILE:HD11	1.79	0.82
6:f:13:PHE:HA	6:f:14:SER:HB2	1.61	0.82
29:I:226:GLY:N	36:I:501:ATP:O1G	2.14	0.81
33:J:197:LEU:HD11	38:J:501:ADP:C2'	2.10	0.81
11:4:143:LEU:HD11	11:4:163:LEU:HD13	1.62	0.81
13:6:75:ARG:NH2	13:6:113:TYR:OH	2.14	0.81
20:Z:916:LEU:CD1	29:I:54:ARG:C	2.52	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:5:113:ASN:OD1	12:5:114:PRO:HD2	1.79	0.81
33:J:197:LEU:CD1	38:J:501:ADP:H2'	2.11	0.80
11:k:143:LEU:HD11	11:k:163:LEU:HD13	1.62	0.80
3:c:177:GLN:HE21	4:d:53:LYS:HB2	1.46	0.80
9:i:119:TYR:O	9:i:122:HIS:ND1	2.14	0.80
10:j:101:GLY:O	11:k:93:ARG:NH1	2.14	0.80
5:E:154:GLN:OE1	5:E:154:GLN:N	2.15	0.80
13:m:75:ARG:NH2	13:m:113:TYR:OH	2.14	0.80
1:a:65:ASP:OD1	1:a:67:THR:OG1	1.99	0.80
16:V:58:VAL:O	16:V:59:ASP:O	2.00	0.80
14:n:242:LYS:HZ3	14:n:245:LEU:HD21	1.46	0.80
1:A:65:ASP:OD1	1:A:67:THR:OG1	1.99	0.79
29:I:393:GLN:NE2	36:I:501:ATP:C5'	2.42	0.79
11:k:49:GLU:OE1	12:l:166:LYS:NZ	2.15	0.79
32:M:186:LEU:CD1	36:M:501:ATP:N6	2.46	0.79
5:e:154:GLN:N	5:e:154:GLN:OE1	2.15	0.78
32:M:228:LYS:HG2	36:M:501:ATP:O2B	1.82	0.78
20:Z:308:LYS:O	20:Z:309:GLN:O	2.02	0.78
32:M:341:GLY:N	32:M:344:ASP:OD1	2.16	0.78
5:E:5:ARG:NH1	28:H:357:ARG:HE	1.82	0.78
25:R:172:LEU:HB3	25:R:213:TYR:CE2	2.19	0.77
3:C:18:ARG:HH21	29:I:433:GLU:CD	1.93	0.77
20:Z:490:ILE:HD12	20:Z:526:ALA:HA	1.66	0.77
12:l:102:ALA:O	13:m:145:ARG:NH1	2.18	0.76
11:4:156:GLU:O	11:4:159:ASP:OD2	2.03	0.76
7:G:218:TRP:CH2	7:G:224:THR:HG23	2.21	0.76
8:1:103:THR:HG23	8:1:124:LEU:HD12	1.68	0.76
36:H:501:ATP:C5'	29:I:340:ARG:NH2	2.49	0.76
4:D:203:VAL:O	4:D:204:GLN:O	2.03	0.76
36:H:501:ATP:O1A	29:I:340:ARG:NH2	2.19	0.76
7:g:218:TRP:CH2	7:g:224:THR:HG23	2.21	0.76
8:h:103:THR:HG23	8:h:124:LEU:HD12	1.68	0.76
1:A:134:MET:HE1	7:G:126:TYR:CE1	2.21	0.76
7:G:230:PHE:HB2	7:G:232:LYS:NZ	2.01	0.76
13:6:142:GLU:OE1	13:6:145:ARG:NH2	2.19	0.76
11:k:156:GLU:O	11:k:159:ASP:OD2	2.03	0.75
10:3:71:THR:HG1	10:3:75:LYS:HZ1	1.34	0.75
6:f:30:LYS:HE2	6:f:30:LYS:HA	1.69	0.75
7:g:230:PHE:HB2	7:g:232:LYS:NZ	2.01	0.75
4:d:98:LEU:O	12:l:156:LYS:NZ	2.20	0.74
5:E:47:VAL:CG1	5:E:200:VAL:HG21	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:L:501:ATP:O3B	32:M:339:ARG:CZ	2.35	0.74
4:d:6:ARG:HA	5:e:125:GLU:OE1	1.87	0.74
22:S:136:CYS:SG	22:S:170:TYR:OH	2.44	0.74
8:h:170:GLN:NE2	8:l:149:LYS:HB2	2.03	0.74
32:M:186:LEU:HD11	36:M:501:ATP:HN61	1.49	0.74
6:F:30:LYS:HE2	6:F:30:LYS:HA	1.69	0.74
24:Q:67:THR:H	24:Q:68:MET:HB2	1.53	0.74
18:X:92:SER:O	18:X:93:SER:OG	2.05	0.74
5:e:47:VAL:CG1	5:e:200:VAL:HG21	2.17	0.74
7:g:72:ARG:NH2	14:n:105:THR:OG1	2.21	0.73
7:g:218:TRP:CH2	7:g:223:GLU:HB2	2.24	0.73
7:G:218:TRP:CH2	7:G:223:GLU:HB2	2.24	0.73
16:V:186:GLN:O	16:V:190:HIS:CD2	2.41	0.73
29:I:179:GLU:CD	29:I:231:LEU:HD11	2.13	0.73
31:L:116:LYS:HA	31:L:116:LYS:HE3	1.71	0.73
2:B:104:TYR:OH	9:2:93:GLU:OE2	2.05	0.73
32:M:95:GLU:O	32:M:96:ASN:O	2.07	0.73
24:Q:404:ASN:ND2	25:R:394:ASP:O	2.22	0.73
28:H:258:LEU:HD13	36:H:501:ATP:H3'	1.70	0.73
6:F:8:GLY:O	6:F:21:GLN:NE2	2.22	0.72
1:a:61:ASP:OD2	1:a:62:LYS:N	2.23	0.72
36:L:501:ATP:PB	32:M:339:ARG:HH22	2.11	0.72
11:4:3:ILE:N	11:4:18:SER:OG	2.22	0.72
11:k:3:ILE:N	11:k:18:SER:OG	2.23	0.72
14:7:109:TYR:O	14:7:110:ASP:O	2.08	0.72
20:Z:161:ILE:HG23	20:Z:210:TYR:HE2	1.54	0.72
14:n:220:ARG:HD3	9:2:168:GLU:OE2	1.89	0.72
1:A:61:ASP:OD2	1:A:62:LYS:N	2.23	0.72
11:4:86:GLN:HA	11:4:86:GLN:HE21	1.55	0.72
13:6:48:GLU:OE1	14:7:171:SER:N	2.23	0.71
36:H:501:ATP:O5'	29:I:340:ARG:NH2	2.23	0.71
29:I:101:GLY:C	29:I:102:ASN:O	2.33	0.71
8:1:146:TYR:O	8:1:150:ASN:OD1	2.09	0.71
28:H:256:LYS:N	36:H:501:ATP:O1B	2.22	0.71
11:k:86:GLN:HA	11:k:86:GLN:HE21	1.55	0.71
7:g:20:ARG:HA	7:g:20:ARG:HE	1.56	0.71
1:A:119:LYS:NZ	9:2:98:TYR:O	2.22	0.71
29:I:125:MET:HB3	29:I:126:PRO:HD3	1.72	0.71
6:f:8:GLY:O	6:f:21:GLN:NE2	2.23	0.70
13:m:142:GLU:OE1	13:m:145:ARG:NH2	2.19	0.70
30:K:343:LEU:HD23	30:K:343:LEU:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:L:501:ATP:PG	32:M:339:ARG:HH12	2.03	0.70
20:Z:140:LEU:HD11	20:Z:200:THR:HG22	1.72	0.70
31:L:329:ARG:HB3	32:M:291:PHE:HE2	1.57	0.70
8:h:150:ASN:O	8:h:163:PHE:CZ	2.45	0.70
11:k:67:TYR:CD2	11:k:75:LEU:HD11	2.27	0.70
5:e:9:ASP:OD1	5:e:10:ARG:NH1	2.25	0.70
8:h:170:GLN:HE22	8:1:149:LYS:HB2	1.56	0.70
7:G:112:PHE:CE2	7:G:116:LEU:HD12	2.26	0.70
1:A:175:GLN:OE1	1:A:176:GLN:N	2.24	0.70
5:E:20:ARG:HH22	32:M:431:SER:HA	1.56	0.70
20:Z:700:GLU:N	20:Z:700:GLU:OE2	2.24	0.70
1:a:175:GLN:OE1	1:a:176:GLN:N	2.24	0.70
4:d:203:VAL:O	4:d:204:GLN:O	2.09	0.70
9:2:236:ARG:NH2	10:3:162:ASP:OD1	2.24	0.70
28:H:90:ARG:O	28:H:92:GLY:N	2.22	0.69
30:K:343:LEU:O	30:K:344:ARG:O	2.10	0.69
26:U:115:GLN:OE1	26:U:115:GLN:N	2.25	0.69
9:i:153:TYR:CE1	9:i:167:LEU:HB3	2.27	0.69
11:4:67:TYR:CD2	11:4:75:LEU:HD11	2.27	0.69
1:a:119:LYS:NZ	9:i:98:TYR:O	2.24	0.69
7:G:20:ARG:HA	7:G:20:ARG:HE	1.57	0.69
9:2:153:TYR:CE1	9:2:167:LEU:HB3	2.27	0.69
21:N:642:ASP:O	21:N:645:THR:OG1	2.09	0.69
31:L:51:GLU:HG3	31:L:53:HIS:H	1.57	0.69
33:J:306:ARG:HG3	33:J:309:ARG:HG3	1.74	0.69
9:i:126:TYR:HB3	9:i:156:LEU:HD13	1.75	0.69
5:E:121:LEU:CD2	6:F:79:PRO:HB3	2.22	0.69
20:Z:556:ILE:HD12	20:Z:559:LYS:HB2	1.75	0.69
7:g:112:PHE:CE2	7:g:116:LEU:HD12	2.26	0.69
36:H:501:ATP:H5'1	29:I:340:ARG:HH21	1.57	0.69
32:M:224:PRO:HB3	36:M:501:ATP:O3G	1.93	0.69
5:E:9:ASP:OD1	5:E:10:ARG:NH1	2.25	0.69
21:N:569:LYS:HG3	30:K:67:TYR:OH	1.92	0.69
6:F:111:LEU:O	6:F:114:ASP:OD1	2.11	0.68
20:Z:161:ILE:HG23	20:Z:210:TYR:CE2	2.28	0.68
20:Z:269:TYR:HA	20:Z:284:LEU:HD23	1.75	0.68
2:b:14:PRO:HA	3:c:24:TYR:CD1	2.28	0.68
13:m:145:ARG:HH11	13:m:155:MET:HE1	1.58	0.68
28:H:258:LEU:HD22	36:H:501:ATP:N9	2.08	0.68
11:k:160:LEU:HD12	11:k:163:LEU:HD12	1.75	0.68
21:N:87:ASP:OD1	21:N:88:ARG:NH1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ASP:N	1:A:13:ASP:OD1	2.26	0.68
8:1:152:ARG:NH2	8:1:159:GLU:OE1	2.27	0.68
32:M:227:GLY:HA2	36:M:501:ATP:O3A	1.94	0.68
6:f:111:LEU:O	6:f:114:ASP:OD1	2.11	0.68
28:H:420:ARG:NE	36:H:501:ATP:H1'	2.09	0.68
9:i:199:GLY:O	9:i:200:SER:OG	2.12	0.68
3:C:152:ASN:N	3:C:152:ASN:OD1	2.25	0.68
4:D:79:ASN:ND2	29:I:436:TYR:O	2.27	0.68
29:I:179:GLU:OE1	29:I:231:LEU:CD1	2.41	0.68
5:e:8:TYR:CE2	6:f:8:GLY:HA2	2.27	0.68
12:l:103:SER:OG	13:m:145:ARG:NH2	2.27	0.68
9:2:126:TYR:HB3	9:2:156:LEU:HD13	1.75	0.68
10:j:71:THR:HG1	10:j:75:LYS:HZ2	1.41	0.67
16:V:160:ASP:OD1	16:V:162:GLY:N	2.27	0.67
26:U:172:GLU:O	26:U:176:ARG:NH1	2.27	0.67
31:L:174:GLU:N	31:L:174:GLU:OE2	2.27	0.67
1:a:131:ARG:HB2	1:a:134:MET:HG2	1.76	0.67
29:I:173:MET:SD	33:J:231:ARG:NH2	2.65	0.67
1:a:58:LYS:HD2	1:a:58:LYS:C	2.19	0.67
20:Z:916:LEU:HD11	29:I:54:ARG:CA	2.24	0.67
36:H:501:ATP:H5'1	29:I:340:ARG:NH2	2.10	0.67
36:H:501:ATP:O3A	29:I:340:ARG:NH1	2.24	0.67
6:F:55:GLU:OE1	6:F:55:GLU:N	2.28	0.67
12:5:102:ALA:O	13:6:145:ARG:NH1	2.27	0.67
16:V:205:LYS:HZ2	16:V:209:GLU:HB3	1.59	0.67
20:Z:916:LEU:HD11	29:I:54:ARG:C	2.19	0.67
29:I:225:PRO:CA	36:I:501:ATP:O1G	2.42	0.67
31:L:132:ARG:NH2	32:M:111:THR:OG1	2.27	0.67
3:c:51:LYS:HB2	3:c:51:LYS:NZ	2.09	0.67
6:f:55:GLU:OE1	6:f:55:GLU:N	2.28	0.67
3:C:20:TYR:HB3	3:C:24:TYR:CE2	2.30	0.67
28:H:420:ARG:CD	36:H:501:ATP:H1'	2.25	0.67
3:c:96:GLN:HE22	10:j:73:LEU:HG	1.60	0.67
11:4:160:LEU:HD12	11:4:163:LEU:HD12	1.75	0.67
30:K:122:ILE:HG23	30:K:146:LEU:HD22	1.74	0.67
1:A:58:LYS:HD2	1:A:58:LYS:C	2.19	0.67
3:C:9:ARG:NH2	4:D:10:ILE:CD1	2.57	0.67
9:2:199:GLY:O	9:2:200:SER:OG	2.12	0.67
2:b:224:TYR:CZ	9:i:65:ARG:NH1	2.63	0.67
1:a:13:ASP:N	1:a:13:ASP:OD1	2.26	0.66
4:d:111:ARG:HG3	5:e:86:ARG:NH2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:14:PRO:HA	3:c:24:TYR:CE1	2.30	0.66
3:c:20:TYR:HB3	3:c:24:TYR:CE2	2.30	0.66
3:C:18:ARG:NH2	29:I:433:GLU:CD	2.52	0.66
17:T:165:GLN:OE1	17:T:182:LYS:NZ	2.28	0.66
1:A:131:ARG:HB2	1:A:134:MET:HG2	1.76	0.66
3:C:51:LYS:HB2	3:C:51:LYS:NZ	2.09	0.66
13:6:145:ARG:HH11	13:6:155:MET:HE1	1.58	0.66
20:Z:68:LEU:HD13	20:Z:98:ASP:OD1	1.95	0.66
9:i:249:ILE:HD12	10:j:48:HIS:HA	1.76	0.66
5:E:5:ARG:HH12	28:H:357:ARG:HE	1.41	0.66
27:O:14:LEU:HD21	27:O:60:ARG:HG2	1.76	0.66
3:C:18:ARG:NH2	29:I:433:GLU:OE2	2.29	0.66
28:H:258:LEU:CD2	36:H:501:ATP:C4	2.79	0.66
34:8:419:ASN:O	34:8:420:LEU:HG	1.96	0.66
1:a:14:ARG:HE	7:g:8:TYR:HH	1.42	0.66
11:k:92:ILE:HD11	11:k:122:LEU:HA	1.77	0.66
34:8:357:ARG:HD3	34:8:428:CYS:HB2	1.77	0.66
8:h:68:VAL:HG21	8:h:91:PHE:CD1	2.31	0.66
8:1:68:VAL:HG21	8:1:91:PHE:CD1	2.31	0.66
28:H:255:GLY:HA3	36:H:501:ATP:N7	2.11	0.66
34:8:111:PHE:O	34:8:466:ASP:O	2.14	0.66
9:i:38:ASN:ND2	9:i:174:ASP:OD1	2.29	0.66
2:B:195:THR:HA	2:B:198:GLU:OE2	1.95	0.66
9:2:38:ASN:ND2	9:2:174:ASP:OD1	2.29	0.66
11:4:92:ILE:HD11	11:4:122:LEU:HA	1.77	0.66
36:H:501:ATP:PA	29:I:340:ARG:NH2	2.57	0.66
3:c:152:ASN:N	3:c:152:ASN:OD1	2.26	0.65
7:G:185:GLU:OE1	7:G:185:GLU:C	2.39	0.65
21:N:282:TYR:CD2	21:N:283:ASP:N	2.64	0.65
11:k:78:GLN:OE1	11:k:79:ALA:N	2.29	0.65
14:n:262:GLY:HA3	9:2:140:PHE:HE1	1.60	0.65
13:6:13:TYR:OH	13:6:112:PRO:O	2.13	0.65
20:Z:140:LEU:CD1	20:Z:200:THR:HG22	2.25	0.65
2:b:195:THR:HA	2:b:198:GLU:OE2	1.95	0.65
7:G:71:ASP:C	7:G:72:ARG:HE	2.04	0.65
11:4:78:GLN:OE1	11:4:79:ALA:N	2.29	0.65
12:5:258:ASP:N	12:5:258:ASP:OD2	2.28	0.65
36:L:501:ATP:PG	32:M:339:ARG:CZ	2.85	0.65
7:g:71:ASP:C	7:g:72:ARG:HE	2.04	0.65
32:M:120:LYS:HD2	32:M:124:ARG:HH22	1.62	0.65
3:c:71:ASP:OD1	3:c:71:ASP:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:J:56:ARG:HH11	33:J:59:LYS:HZ3	1.44	0.65
5:E:5:ARG:NH1	28:H:357:ARG:NE	2.45	0.65
10:3:85:GLU:O	10:3:89:GLN:OE1	2.15	0.65
15:W:130:LYS:HB2	15:W:133:LYS:HE3	1.79	0.65
3:c:92:ARG:HH12	10:j:77:LYS:HG2	1.61	0.65
7:g:185:GLU:C	7:g:185:GLU:OE1	2.39	0.65
28:H:456:LYS:HZ2	28:H:457:PHE:HE2	1.45	0.65
6:F:77:LEU:HD22	32:M:433:TYR:CE2	2.32	0.65
29:I:234:LYS:HZ3	33:J:278:GLN:HB3	1.62	0.65
12:l:258:ASP:OD2	12:l:258:ASP:N	2.28	0.64
3:C:71:ASP:OD1	3:C:71:ASP:O	2.15	0.64
28:H:258:LEU:CD2	36:H:501:ATP:C2'	2.75	0.64
12:l:181:ARG:H	12:l:181:ARG:HD3	1.63	0.64
6:F:226:ASP:OD1	6:F:227:GLY:N	2.31	0.64
16:V:192:LEU:HA	16:V:196:TYR:CZ	2.32	0.64
21:N:265:ALA:HB1	21:N:269:LEU:HD23	1.79	0.64
3:C:219:GLY:C	9:2:255:GLU:HG2	2.23	0.64
5:e:121:LEU:HD22	6:f:79:PRO:HB3	1.78	0.64
8:h:120:TYR:CE1	8:h:130:LYS:HG3	2.33	0.64
7:G:218:TRP:CZ2	7:G:224:THR:HG23	2.33	0.64
5:E:13:SER:HA	5:E:21:LEU:HD21	1.80	0.64
12:5:79:LEU:HA	12:5:175:MET:HE1	1.80	0.64
29:I:102:ASN:O	29:I:103:PRO:C	2.40	0.64
29:I:179:GLU:OE1	29:I:231:LEU:HD11	1.97	0.64
4:d:100:LEU:O	4:d:101:GLU:O	2.14	0.64
7:G:71:ASP:O	7:G:72:ARG:NE	2.31	0.63
10:3:98:ARG:HG3	10:3:103:TYR:CE2	2.33	0.63
5:e:114:GLN:CG	6:f:82:ARG:HH12	2.12	0.63
6:f:226:ASP:OD1	6:f:227:GLY:N	2.31	0.63
7:g:218:TRP:CZ2	7:g:224:THR:HG23	2.33	0.63
9:i:79:ALA:HA	9:i:82:GLU:OE2	1.98	0.63
28:H:465:GLN:OE1	28:H:465:GLN:N	2.32	0.63
6:f:22:VAL:O	6:f:26:LEU:HD12	1.98	0.63
10:j:85:GLU:O	10:j:89:GLN:OE1	2.15	0.63
30:K:236:ARG:HH22	31:L:310:THR:CG2	2.10	0.63
12:l:169:GLY:O	13:m:109:ARG:NH2	2.30	0.63
13:6:133:PHE:CD2	13:6:139:TYR:HB3	2.34	0.63
1:A:77:ARG:NH1	8:1:48:ASP:OD2	2.31	0.63
2:B:28:VAL:HG11	2:B:133:SER:OG	1.99	0.63
12:5:181:ARG:H	12:5:181:ARG:HD3	1.63	0.63
16:V:154:ASP:OD1	16:V:155:ALA:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:365:SER:O	20:Z:366:LYS:HG2	1.98	0.63
20:Z:925:VAL:O	20:Z:926:ASN:O	2.17	0.63
2:b:94:HIS:ND1	9:i:94:LEU:HD22	2.14	0.63
5:e:234:GLU:H	5:e:234:GLU:CD	2.06	0.63
12:l:79:LEU:HA	12:l:175:MET:HE1	1.80	0.63
6:F:22:VAL:O	6:F:26:LEU:HD12	1.98	0.63
13:6:177:LYS:HE2	13:6:177:LYS:HA	1.80	0.63
20:Z:442:VAL:O	20:Z:443:ASP:O	2.16	0.63
2:b:28:VAL:HG11	2:b:133:SER:OG	1.99	0.63
7:g:71:ASP:O	7:g:72:ARG:NE	2.31	0.63
9:2:153:TYR:OH	9:2:168:GLU:HG3	1.99	0.63
28:H:156:VAL:HG21	32:M:77:TYR:CZ	2.34	0.63
28:H:208:TYR:CD2	28:H:266:ARG:HB2	2.33	0.63
7:G:72:ARG:CZ	14:7:105:THR:HG23	2.29	0.62
31:L:244:ILE:HG22	31:L:245:PHE:N	2.14	0.62
5:E:234:GLU:H	5:E:234:GLU:CD	2.06	0.62
8:1:152:ARG:HH22	8:1:159:GLU:CD	2.08	0.62
12:5:103:SER:HB3	12:5:106:VAL:HG22	1.81	0.62
36:L:501:ATP:O3B	32:M:339:ARG:NH2	2.33	0.62
8:h:54:ARG:NH2	14:7:261:TYR:HE1	1.96	0.62
13:m:133:PHE:CD2	13:m:139:TYR:HB3	2.33	0.62
2:B:29:LYS:NZ	2:B:168:SER:OG	2.28	0.62
16:V:25:GLU:OE1	16:V:62:THR:N	2.31	0.62
34:8:445:SER:OG	35:9:75:GLY:O	2.13	0.62
8:h:155:MET:SD	8:h:159:GLU:OE1	2.58	0.62
19:Y:33:ASP:OD2	19:Y:35:PHE:N	2.32	0.62
20:Z:909:ARG:HB2	20:Z:926:ASN:ND2	2.14	0.62
5:e:114:GLN:HG2	6:f:82:ARG:HH22	1.63	0.62
4:D:85:LEU:HD21	4:D:129:PHE:CE2	2.35	0.62
8:1:120:TYR:CE1	8:1:130:LYS:HG3	2.33	0.62
13:6:51:VAL:HG12	13:6:213:LEU:HD12	1.81	0.62
21:N:569:LYS:CG	30:K:67:TYR:OH	2.48	0.62
28:H:258:LEU:HD22	36:H:501:ATP:C2'	2.28	0.62
36:H:501:ATP:PB	29:I:340:ARG:HH12	2.20	0.62
12:5:84:GLN:HA	12:5:84:GLN:HE21	1.65	0.62
5:e:13:SER:HA	5:e:21:LEU:HD21	1.80	0.62
5:e:128:SER:O	5:e:130:GLU:N	2.32	0.62
10:j:98:ARG:HG3	10:j:103:TYR:CE2	2.33	0.62
12:l:242:ARG:NH1	11:4:141:PHE:HB3	2.13	0.62
7:G:36:THR:HG21	7:G:203:ALA:HB1	1.82	0.62
11:4:54:VAL:HG21	12:5:195:THR:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:4:GLU:O	20:Z:5:SER:O	2.16	0.62
27:O:328:VAL:HG11	27:O:341:ILE:HD11	1.79	0.62
30:K:121:ARG:NH1	33:J:64:LEU:O	2.33	0.62
6:f:121:GLN:NE2	7:g:132:PHE:HE1	1.98	0.62
9:i:153:TYR:OH	9:i:168:GLU:HG3	1.99	0.62
13:m:177:LYS:HE2	13:m:177:LYS:HA	1.80	0.62
30:K:77:ARG:NH2	30:K:78:GLU:OE2	2.33	0.62
31:L:244:ILE:HG22	31:L:245:PHE:H	1.65	0.62
32:M:18:LEU:HG	32:M:20:GLN:H	1.65	0.62
33:J:276:LEU:HD12	33:J:279:LEU:HD22	1.81	0.62
7:G:202:LEU:HA	7:G:205:GLU:OE1	2.00	0.61
10:3:71:THR:HG1	10:3:75:LYS:NZ	1.89	0.61
20:Z:212:LEU:HD22	20:Z:221:VAL:HA	1.82	0.61
20:Z:387:ASN:ND2	20:Z:400:ILE:HG21	2.15	0.61
28:H:464:MET:O	28:H:465:GLN:O	2.17	0.61
9:2:79:ALA:HA	9:2:82:GLU:OE2	1.98	0.61
13:6:213:LEU:CD2	13:6:222:LYS:HG3	2.30	0.61
3:c:86:ILE:O	3:c:89:ASN:OD1	2.19	0.61
6:f:15:PRO:HA	7:g:26:TYR:CD1	2.35	0.61
10:j:71:THR:HG1	10:j:75:LYS:NZ	1.94	0.61
11:k:78:GLN:OE1	11:k:78:GLN:C	2.44	0.61
13:m:213:LEU:CD2	13:m:222:LYS:HG3	2.30	0.61
13:6:191:LEU:HD12	13:6:192:VAL:N	2.15	0.61
20:Z:8:LYS:HD3	20:Z:10:GLN:H	1.65	0.61
22:S:51:ARG:HE	22:S:178:LEU:HD22	1.64	0.61
30:K:236:ARG:HH22	31:L:310:THR:HG22	1.65	0.61
22:S:448:LEU:O	22:S:449:LEU:HB2	2.00	0.61
25:R:279:LEU:HG	25:R:279:LEU:O	2.00	0.61
8:h:193:GLU:OE1	8:h:193:GLU:N	2.33	0.61
1:A:134:MET:HE2	1:A:134:MET:HA	1.83	0.61
5:E:128:SER:O	5:E:130:GLU:N	2.32	0.61
13:6:95:ASN:OD1	13:6:96:SER:N	2.33	0.61
33:J:197:LEU:HG	38:J:501:ADP:O1A	2.01	0.61
7:g:202:LEU:HA	7:g:205:GLU:OE1	2.00	0.61
13:m:191:LEU:HD12	13:m:192:VAL:N	2.15	0.61
8:1:193:GLU:N	8:1:193:GLU:OE1	2.33	0.61
2:b:85:LEU:HD21	2:b:134:LEU:HD11	1.82	0.61
5:e:78:MET:HA	5:e:142:LEU:HD13	1.83	0.61
7:g:36:THR:HG21	7:g:203:ALA:HB1	1.82	0.61
12:l:103:SER:HB3	12:l:106:VAL:HG22	1.81	0.61
16:V:156:PHE:CD1	16:V:196:TYR:CE2	2.89	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:U:124:ASP:OD1	26:U:127:GLN:N	2.33	0.61
12:l:84:GLN:HA	12:l:84:GLN:HE21	1.65	0.61
3:C:86:ILE:O	3:C:89:ASN:OD1	2.19	0.61
34:8:207:GLN:OE1	35:9:76:GLZ:N	2.32	0.61
1:a:134:MET:HE2	1:a:134:MET:HA	1.83	0.61
13:m:51:VAL:HG12	13:m:213:LEU:HD12	1.81	0.61
13:m:95:ASN:OD1	13:m:96:SER:N	2.33	0.61
36:K:501:ATP:O1G	31:L:342:ARG:NH2	2.32	0.61
7:g:72:ARG:NH1	14:n:105:THR:OG1	2.34	0.61
8:h:135:ILE:HG22	8:h:140:SER:HB2	1.82	0.60
5:E:78:MET:HA	5:E:142:LEU:HD13	1.83	0.60
23:P:171:MET:HE2	23:P:176:LYS:HG2	1.83	0.60
26:U:257:ILE:O	26:U:261:LEU:HD13	2.01	0.60
13:m:15:ASP:OD2	13:m:17:GLY:N	2.34	0.60
4:D:6:ARG:HA	5:E:125:GLU:OE1	2.01	0.60
17:T:197:TYR:CE2	17:T:200:LEU:HG	2.36	0.60
32:M:124:ARG:NE	32:M:124:ARG:HA	2.15	0.60
33:J:196:THR:HB	38:J:501:ADP:PA	2.41	0.60
9:2:199:GLY:O	9:2:200:SER:CB	2.49	0.60
10:j:68:ARG:O	10:j:72:ASN:OD1	2.20	0.60
12:5:109:VAL:HG11	12:5:253:TYR:CE2	2.37	0.60
13:6:15:ASP:OD2	13:6:17:GLY:N	2.34	0.60
36:I:501:ATP:O3G	33:J:306:ARG:NH2	2.34	0.60
2:B:85:LEU:HD21	2:B:134:LEU:HD11	1.82	0.60
4:D:98:LEU:O	12:5:156:LYS:NZ	2.25	0.60
32:M:121:THR:O	32:M:124:ARG:NH1	2.34	0.60
5:e:8:TYR:HE2	6:f:8:GLY:HA2	1.67	0.60
6:f:110:HIS:CG	7:g:86:ARG:HH22	2.20	0.60
9:i:199:GLY:O	9:i:200:SER:CB	2.49	0.60
28:H:311:ILE:C	28:H:313:ALA:O	2.45	0.60
32:M:228:LYS:CG	36:M:501:ATP:O2B	2.50	0.60
3:c:13:PHE:HD1	4:d:22:TYR:HB2	1.67	0.60
5:e:114:GLN:NE2	6:f:82:ARG:HH12	2.00	0.60
28:H:258:LEU:HD23	36:H:501:ATP:C4	2.37	0.60
28:H:311:ILE:HD11	28:H:353:PHE:CD1	2.36	0.60
6:f:110:HIS:CG	7:g:86:ARG:NH2	2.70	0.60
8:h:150:ASN:O	8:h:163:PHE:HZ	1.84	0.60
8:l:135:ILE:HG22	8:l:140:SER:HB2	1.82	0.60
13:m:122:LEU:CB	13:m:217:LYS:HZ3	2.15	0.60
11:4:78:GLN:OE1	11:4:78:GLN:C	2.44	0.60
32:M:178:GLU:O	32:M:179:THR:O	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:137:LEU:HD23	1:a:137:LEU:H	1.65	0.59
11:4:49:GLU:HB2	11:4:99:GLN:HB2	1.84	0.59
4:d:4:TYR:CE2	4:d:125:GLY:HA2	2.37	0.59
8:h:103:THR:CG2	8:h:124:LEU:HD12	2.32	0.59
1:A:137:LEU:HD23	1:A:137:LEU:H	1.65	0.59
3:C:4:ARG:HH12	6:F:124:GLY:CA	2.15	0.59
3:C:14:SER:HB3	3:C:20:TYR:CE2	2.37	0.59
7:G:175:GLU:OE1	7:G:178:LYS:HE2	2.02	0.59
8:1:103:THR:CG2	8:1:124:LEU:HD12	2.32	0.59
20:Z:497:PHE:O	20:Z:498:ALA:CB	2.50	0.59
21:N:149:GLU:O	21:N:151:LYS:N	2.35	0.59
12:l:109:VAL:HG11	12:l:253:TYR:CE2	2.37	0.59
10:3:62:THR:HA	10:3:65:GLU:OE1	2.02	0.59
2:b:29:LYS:NZ	2:b:168:SER:OG	2.28	0.59
9:i:177:LYS:HZ3	9:i:181:ILE:HD12	1.67	0.59
11:k:8:ARG:NH1	11:k:127:GLU:OE1	2.35	0.59
5:E:234:GLU:OE2	5:E:234:GLU:N	2.31	0.59
11:4:8:ARG:NH1	11:4:127:GLU:OE1	2.35	0.59
13:6:58:ILE:HG23	13:6:94:ILE:HD13	1.85	0.59
36:I:501:ATP:O3G	33:J:306:ARG:CZ	2.50	0.59
3:c:14:SER:HB3	3:c:20:TYR:CE2	2.37	0.59
7:g:175:GLU:OE1	7:g:178:LYS:HE2	2.02	0.59
16:V:215:ASN:ND2	26:U:130:VAL:O	2.36	0.59
29:I:393:GLN:CD	36:I:501:ATP:C4'	2.74	0.59
10:j:173:ASN:ND2	13:6:160:ASN:HB2	2.17	0.59
11:k:169:GLU:OE1	11:k:169:GLU:HA	2.01	0.59
6:F:70:MET:HE2	6:F:88:LEU:HD21	1.84	0.59
10:3:68:ARG:O	10:3:72:ASN:OD1	2.20	0.59
11:4:169:GLU:OE1	11:4:169:GLU:HA	2.01	0.59
26:U:60:GLU:N	26:U:60:GLU:OE2	2.35	0.59
4:D:119:ARG:CZ	4:D:120:TYR:HE1	2.15	0.59
5:e:234:GLU:OE2	5:e:234:GLU:N	2.31	0.59
20:Z:463:HIS:NE2	20:Z:497:PHE:O	2.35	0.59
20:Z:916:LEU:CD1	29:I:54:ARG:N	2.50	0.59
22:S:96:ILE:O	22:S:97:THR:OG1	2.18	0.59
9:i:236:ARG:HE	10:j:161:GLU:HB2	1.68	0.59
11:k:170:LYS:HA	11:4:177:LYS:HZ1	1.68	0.59
7:G:184:PRO:O	23:P:3:ARG:NH2	2.35	0.59
20:Z:556:ILE:HD11	20:Z:562:TRP:CE3	2.38	0.58
6:F:10:THR:O	6:F:10:THR:OG1	2.18	0.58
27:O:82:LEU:HD22	27:O:102:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:M:426:LYS:O	32:M:427:SER:O	2.22	0.58
8:h:170:GLN:NE2	8:1:149:LYS:HD3	2.18	0.58
10:j:62:THR:HA	10:j:65:GLU:OE1	2.02	0.58
8:1:153:GLU:HA	8:1:153:GLU:OE2	2.02	0.58
20:Z:386:VAL:HG13	20:Z:837:TYR:CG	2.39	0.58
3:c:19:LEU:HD11	3:c:123:THR:HG22	1.86	0.58
12:l:82:ARG:HD3	12:l:200:ASP:OD2	2.03	0.58
2:B:68:THR:HB	2:B:104:TYR:CD1	2.38	0.58
5:E:2:PHE:CZ	29:I:332:GLU:OE1	2.57	0.58
7:G:170:GLN:NE2	31:L:382:MET:C	2.61	0.58
9:2:177:LYS:NZ	9:2:181:ILE:HD12	2.18	0.58
14:7:248:GLU:N	14:7:248:GLU:OE2	2.36	0.58
23:P:130:ILE:O	23:P:132:VAL:N	2.35	0.58
3:C:218:LYS:HG3	3:C:218:LYS:O	2.04	0.58
34:8:317:PHE:CE2	35:9:8:LEU:HD22	2.38	0.58
6:f:70:MET:HE2	6:f:88:LEU:HD21	1.84	0.58
6:f:93:ASN:OD1	13:m:81:LYS:HE3	2.03	0.58
8:1:37:ASN:OD1	9:2:150:VAL:O	2.21	0.58
12:5:82:ARG:HD3	12:5:200:ASP:OD2	2.03	0.58
16:V:184:ASN:O	16:V:188:LEU:HB2	2.03	0.58
20:Z:141:SER:O	20:Z:142:ASP:O	2.22	0.58
24:Q:67:THR:HB	24:Q:68:MET:HA	1.85	0.58
31:L:72:ASP:O	31:L:76:GLN:HG3	2.04	0.58
9:i:177:LYS:NZ	9:i:181:ILE:HD12	2.18	0.58
10:j:180:LEU:HD12	12:5:99:ASN:HD21	1.68	0.58
1:A:54:ILE:HD11	1:A:206:ALA:HB1	1.85	0.58
1:A:134:MET:HE1	7:G:126:TYR:CZ	2.39	0.58
5:E:118:ASP:OD1	6:F:82:ARG:NH2	2.37	0.58
20:Z:463:HIS:CD2	20:Z:497:PHE:O	2.57	0.58
1:a:45:VAL:HG21	1:a:194:ILE:HD12	1.86	0.58
7:g:70:VAL:HG21	7:g:112:PHE:CE1	2.39	0.58
7:G:230:PHE:CB	7:G:232:LYS:HZ1	2.15	0.58
8:1:27:SER:HB3	8:1:40:THR:O	2.04	0.58
2:b:68:THR:HB	2:b:104:TYR:CD1	2.38	0.58
7:g:72:ARG:CZ	14:n:105:THR:OG1	2.52	0.58
11:k:49:GLU:HB2	11:k:99:GLN:HB2	1.84	0.58
13:m:58:ILE:HG23	13:m:94:ILE:HD13	1.85	0.58
13:m:190:LYS:O	9:2:229:GLN:OE1	2.22	0.58
1:A:174:LYS:HE3	1:A:214:LEU:HD22	1.85	0.58
7:G:70:VAL:HG21	7:G:112:PHE:CE1	2.39	0.58
13:6:122:LEU:CB	13:6:217:LYS:HZ3	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:7:58:ASP:OD2	14:7:59:ASN:N	2.37	0.58
31:L:170:MET:CB	31:L:244:ILE:HG23	2.34	0.58
3:c:177:GLN:NE2	4:d:53:LYS:HB2	2.17	0.58
3:c:218:LYS:HG3	3:c:218:LYS:O	2.04	0.58
3:C:9:ARG:NH2	4:D:10:ILE:HD11	2.19	0.58
8:1:165:LYS:HD2	8:1:197:PHE:CD2	2.39	0.58
22:S:452:TYR:CE2	25:R:396:LYS:HD3	2.39	0.58
3:c:96:GLN:HB3	10:j:69:TYR:CD1	2.39	0.57
8:h:27:SER:HB3	8:h:40:THR:O	2.04	0.57
8:1:96:TYR:O	8:1:99:LYS:HD3	2.04	0.57
20:Z:790:MET:HA	20:Z:790:MET:HE2	1.85	0.57
28:H:282:LYS:HZ3	30:K:285:GLN:HB2	1.68	0.57
11:k:2:ASP:HB2	11:k:18:SER:OG	2.05	0.57
6:F:30:LYS:HA	6:F:30:LYS:CE	2.35	0.57
20:Z:24:THR:HB	20:Z:25:PRO:CD	2.34	0.57
28:H:420:ARG:NH1	36:H:501:ATP:C8	2.70	0.57
29:I:199:GLU:OE1	29:I:239:GLN:NE2	2.38	0.57
12:l:142:GLU:OE2	12:l:147:GLU:C	2.48	0.57
10:3:135:ASP:OD2	10:3:154:TYR:CE2	2.58	0.57
19:Y:3:THR:O	19:Y:4:ASP:OD1	2.22	0.57
19:Y:31:GLU:OE2	22:S:196:ARG:NH2	2.38	0.57
34:8:211:GLU:OE2	35:9:42:ARG:NH2	2.37	0.57
5:e:7:GLU:OE1	5:e:7:GLU:HA	2.04	0.57
7:g:74:ILE:HD13	7:g:112:PHE:HD1	1.69	0.57
8:h:165:LYS:HD2	8:h:197:PHE:CD2	2.39	0.57
5:E:7:GLU:OE1	5:E:7:GLU:HA	2.04	0.57
11:4:11:ASP:OD2	11:4:12:SER:OG	2.21	0.57
15:W:125:LEU:HD23	15:W:128:LEU:HD12	1.87	0.57
17:T:197:TYR:CZ	17:T:200:LEU:HG	2.40	0.57
25:R:121:GLU:OE1	25:R:130:GLN:NE2	2.38	0.57
8:h:113:ASP:OD1	8:h:114:LYS:N	2.38	0.57
8:h:149:LYS:HB2	8:1:170:GLN:NE2	2.20	0.57
1:A:45:VAL:HG21	1:A:194:ILE:HD12	1.86	0.57
3:C:19:LEU:HD11	3:C:123:THR:HG22	1.86	0.57
5:E:51:GLU:HG2	5:E:216:ASN:O	2.04	0.57
3:C:219:GLY:O	9:2:255:GLU:HG2	2.03	0.57
22:S:455:GLU:OE1	26:U:248:ASP:HB3	2.05	0.57
1:a:54:ILE:HD11	1:a:206:ALA:HB1	1.85	0.57
2:b:124:SER:O	2:b:127:VAL:HG22	2.05	0.57
6:f:30:LYS:HA	6:f:30:LYS:CE	2.35	0.57
5:E:118:ASP:CG	6:F:82:ARG:NH2	2.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:177:ASP:OD1	6:F:177:ASP:N	2.38	0.57
7:G:74:ILE:HD13	7:G:112:PHE:HD1	1.69	0.57
20:Z:68:LEU:HD22	20:Z:71:LEU:HD22	1.85	0.57
9:2:193:TRP:N	9:2:193:TRP:CD1	2.72	0.57
11:4:2:ASP:HB2	11:4:18:SER:OG	2.05	0.57
19:Y:51:SER:O	19:Y:52:ASN:ND2	2.38	0.57
20:Z:161:ILE:CG2	20:Z:210:TYR:HE2	2.18	0.57
20:Z:376:SER:O	20:Z:377:ALA:HB2	2.05	0.57
20:Z:382:ALA:O	20:Z:386:VAL:HG23	2.05	0.57
9:i:69:LYS:HZ3	9:i:212:ASP:HA	1.70	0.56
2:B:124:SER:O	2:B:127:VAL:HG22	2.05	0.56
12:5:142:GLU:OE2	12:5:147:GLU:C	2.48	0.56
16:V:24:LYS:HD3	16:V:199:LEU:HD23	1.86	0.56
16:V:275:ASP:O	16:V:279:HIS:CD2	2.58	0.56
22:S:452:TYR:CZ	26:U:249:VAL:HG13	2.40	0.56
25:R:113:LEU:HD11	25:R:137:LEU:HD21	1.87	0.56
4:d:25:GLU:HA	4:d:28:LYS:HG2	1.85	0.56
21:N:194:ILE:HG22	21:N:597:ARG:NH2	2.20	0.56
29:I:225:PRO:HA	36:I:501:ATP:O1G	2.05	0.56
1:a:217:GLU:C	1:a:217:GLU:CD	2.73	0.56
8:h:96:TYR:O	8:h:99:LYS:HD3	2.04	0.56
9:i:193:TRP:N	9:i:193:TRP:CD1	2.72	0.56
13:6:188:VAL:O	13:6:191:LEU:HG	2.05	0.56
20:Z:443:ASP:O	20:Z:444:GLU:O	2.23	0.56
20:Z:773:ARG:HH22	20:Z:938:GLN:CD	2.13	0.56
30:K:221:MET:N	36:K:501:ATP:O1A	2.38	0.56
34:8:317:PHE:CE2	35:9:8:LEU:CD2	2.88	0.56
1:a:174:LYS:HE3	1:a:214:LEU:HD22	1.85	0.56
6:f:173:GLU:OE1	7:g:57:LYS:HB3	2.06	0.56
11:k:170:LYS:HA	11:4:177:LYS:NZ	2.20	0.56
4:d:156:TYR:HE1	5:e:86:ARG:HD2	1.69	0.56
13:m:188:VAL:O	13:m:191:LEU:HG	2.05	0.56
14:n:248:GLU:N	14:n:248:GLU:OE2	2.39	0.56
7:G:68:GLN:HE22	7:G:86:ARG:HH21	1.53	0.56
8:1:85:GLU:C	8:1:85:GLU:CD	2.74	0.56
21:N:504:TYR:HD2	21:N:517:LEU:HD11	1.71	0.56
27:O:266:PHE:O	27:O:270:ILE:HG12	2.05	0.56
32:M:124:ARG:HA	32:M:124:ARG:CZ	2.36	0.56
32:M:425:ARG:HG2	32:M:426:LYS:O	2.06	0.56
33:J:192:GLY:H	38:J:501:ADP:PB	2.28	0.56
5:e:51:GLU:HG2	5:e:216:ASN:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:135:ASP:OD2	10:j:154:TYR:CE2	2.58	0.56
1:A:217:GLU:C	1:A:217:GLU:CD	2.73	0.56
16:V:197:TYR:CE2	16:V:199:LEU:HD21	2.40	0.56
1:a:62:LYS:NZ	7:g:177:GLU:HG2	2.20	0.56
5:e:114:GLN:CD	6:f:82:ARG:HH12	2.14	0.56
12:l:99:ASN:HD21	10:3:180:LEU:HD12	1.70	0.56
8:1:113:ASP:OD1	8:1:114:LYS:N	2.38	0.56
25:R:172:LEU:HD13	25:R:213:TYR:CE2	2.41	0.56
9:i:153:TYR:HE1	9:i:167:LEU:HB3	1.71	0.56
29:I:409:MET:HE3	33:J:173:LEU:HD22	1.88	0.56
25:R:172:LEU:HD22	25:R:213:TYR:HD2	1.71	0.56
25:R:279:LEU:O	25:R:280:ILE:O	2.24	0.56
3:C:8:SER:OG	3:C:10:THR:HG23	2.06	0.55
6:F:15:PRO:HA	7:G:26:TYR:CD1	2.41	0.55
9:2:153:TYR:HE1	9:2:167:LEU:HB3	1.71	0.55
20:Z:556:ILE:HD11	20:Z:562:TRP:HE3	1.71	0.55
21:N:282:TYR:CE2	21:N:286:LEU:HB2	2.41	0.55
5:e:114:GLN:CG	6:f:82:ARG:NH1	2.69	0.55
9:i:99:THR:OG1	9:i:101:ARG:HB3	2.06	0.55
10:j:35:GLY:HA3	10:j:183:TRP:CH2	2.42	0.55
16:V:258:GLU:CG	16:V:270:TYR:HB2	2.36	0.55
28:H:211:VAL:HG23	28:H:262:ALA:HB2	1.87	0.55
33:J:1:MET:O	33:J:2:THR:OG1	2.22	0.55
25:R:172:LEU:HD13	25:R:213:TYR:HE2	1.72	0.55
26:U:85:ALA:HB1	31:L:96:LYS:HD3	1.87	0.55
8:h:85:GLU:CD	8:h:85:GLU:C	2.74	0.55
3:C:92:ARG:HD3	10:3:76:LEU:HD13	1.87	0.55
8:1:135:ILE:CG2	8:1:140:SER:HB2	2.36	0.55
9:2:99:THR:OG1	9:2:101:ARG:HB3	2.06	0.55
9:2:110:GLN:OE1	9:2:110:GLN:C	2.50	0.55
11:4:107:TYR:CD1	11:4:109:LYS:HD3	2.42	0.55
15:W:82:GLU:OE1	15:W:82:GLU:N	2.39	0.55
16:V:24:LYS:HB3	16:V:199:LEU:HD23	1.89	0.55
29:I:102:ASN:HB3	29:I:103:PRO:CD	2.36	0.55
6:f:10:THR:O	6:f:10:THR:OG1	2.18	0.55
10:j:3:ASP:OD2	10:j:3:ASP:C	2.49	0.55
5:E:206:GLN:OE1	5:E:207:VAL:HG13	2.07	0.55
10:3:3:ASP:C	10:3:3:ASP:OD2	2.49	0.55
10:3:182:GLY:O	10:3:202:MET:CE	2.55	0.55
11:4:49:GLU:OE1	12:5:166:LYS:NZ	2.33	0.55
17:T:257:THR:O	17:T:262:LYS:HE3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:P:361:THR:HG23	23:P:364:ARG:H	1.71	0.55
32:M:17:GLU:HG3	32:M:33:ARG:HD2	1.87	0.55
8:h:135:ILE:CG2	8:h:140:SER:HB2	2.36	0.55
9:i:110:GLN:C	9:i:110:GLN:OE1	2.50	0.55
12:5:284:ASN:C	12:5:284:ASN:OD1	2.50	0.55
13:6:70:ASP:OD1	14:7:169:THR:OG1	2.25	0.55
1:a:196:GLU:HA	1:a:196:GLU:OE2	2.07	0.55
9:i:192:ILE:HB	9:i:193:TRP:CD1	2.42	0.55
14:n:41:GLY:O	14:n:223:ARG:NH2	2.40	0.55
11:4:23:ARG:NH1	11:4:50:ALA:HA	2.22	0.55
28:H:252:PRO:HA	28:H:256:LYS:HZ2	1.71	0.55
2:b:18:LEU:HD11	3:c:129:ARG:NH2	2.21	0.55
9:i:192:ILE:HB	9:i:193:TRP:HD1	1.72	0.55
11:k:107:TYR:CD1	11:k:109:LYS:HD3	2.42	0.55
13:m:39:THR:OG1	13:m:44:ASN:ND2	2.37	0.55
24:Q:275:ILE:HD13	24:Q:307:ASN:HB2	1.88	0.55
29:I:393:GLN:NE2	36:I:501:ATP:O4'	2.39	0.55
30:K:346:ARG:HE	30:K:349:ARG:HH22	1.54	0.55
9:i:133:ASP:OD1	9:i:138:HIS:NE2	2.40	0.55
1:A:21:PRO:HA	2:B:23:TYR:HD1	1.72	0.55
3:C:221:ASN:N	3:C:221:ASN:OD1	2.40	0.55
5:E:15:PHE:HB3	6:F:24:TYR:HB3	1.87	0.55
29:I:433:GLU:CD	29:I:437:LEU:H	2.14	0.55
30:K:346:ARG:HE	30:K:349:ARG:NH2	2.04	0.55
31:L:142:LYS:HD3	31:L:143:GLY:N	2.22	0.55
4:d:101:GLU:O	4:d:102:ASP:HB2	2.07	0.55
5:e:206:GLN:OE1	5:e:207:VAL:HG13	2.07	0.55
11:k:3:ILE:HD12	11:k:168:LEU:HD13	1.89	0.55
11:k:96:ARG:NH2	12:l:166:LYS:O	2.35	0.55
13:m:145:ARG:NH1	13:m:155:MET:HE1	2.22	0.55
14:n:258:ILE:CG2	9:2:152:TYR:HE2	2.20	0.55
7:G:13:SER:OG	7:G:127:ASN:OD1	2.20	0.55
9:2:192:ILE:HB	9:2:193:TRP:HD1	1.72	0.55
20:Z:174:GLU:HB3	20:Z:183:LYS:HA	1.88	0.55
28:H:190:ARG:HA	28:H:190:ARG:CZ	2.37	0.55
31:L:225:GLY:HA2	32:M:339:ARG:NH2	2.22	0.55
10:j:182:GLY:O	10:j:202:MET:CE	2.55	0.54
5:E:93:ARG:HD3	12:5:143:LEU:HD13	1.88	0.54
9:2:192:ILE:HB	9:2:193:TRP:CD1	2.42	0.54
10:3:101:GLY:O	11:4:93:ARG:NH1	2.40	0.54
11:4:130:TYR:OH	11:4:145:ASP:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:398:ARG:HG2	21:N:438:ASP:HA	1.88	0.54
25:R:209:ARG:NH2	25:R:213:TYR:OH	2.40	0.54
29:I:234:LYS:NZ	33:J:278:GLN:HB3	2.21	0.54
34:8:413:LYS:HD3	34:8:413:LYS:N	2.22	0.54
10:j:45:HIS:HB3	10:j:50:PHE:CD2	2.42	0.54
13:m:55:GLY:O	13:m:58:ILE:HG13	2.07	0.54
6:F:105:VAL:HG21	6:F:143:HIS:HB2	1.90	0.54
10:3:35:GLY:HA3	10:3:183:TRP:CH2	2.42	0.54
16:V:32:ILE:HD11	26:U:20:ASP:HB2	1.88	0.54
32:M:228:LYS:CG	36:M:501:ATP:PB	2.79	0.54
3:c:221:ASN:N	3:c:221:ASN:OD1	2.40	0.54
7:g:72:ARG:CZ	14:n:105:THR:HG23	2.37	0.54
11:k:4:ILE:HA	11:k:16:ALA:O	2.08	0.54
5:E:148:ASP:OD2	5:E:154:GLN:NE2	2.40	0.54
12:5:143:LEU:O	12:5:146:LYS:NZ	2.34	0.54
13:6:55:GLY:O	13:6:58:ILE:HG13	2.07	0.54
13:6:164:PHE:CE2	13:6:181:LYS:HG3	2.43	0.54
9:i:48:ARG:CB	9:i:199:GLY:O	2.54	0.54
12:l:143:LEU:O	12:l:146:LYS:NZ	2.34	0.54
7:G:218:TRP:CH2	7:G:223:GLU:CB	2.91	0.54
12:5:110:ILE:HD11	12:5:120:MET:HB2	1.89	0.54
22:S:94:LYS:HD3	22:S:98:SER:OG	2.08	0.54
31:L:170:MET:HB3	31:L:244:ILE:HG23	1.89	0.54
34:8:337:PHE:O	34:8:432:LEU:HD11	2.07	0.54
7:g:68:GLN:HE22	7:g:86:ARG:HH21	1.53	0.54
9:2:236:ARG:HA	10:3:165:GLU:OE2	2.07	0.54
10:3:45:HIS:HB3	10:3:50:PHE:CD2	2.43	0.54
15:W:127:ARG:HA	15:W:130:LYS:HG2	1.89	0.54
20:Z:574:TYR:HB3	20:Z:581:VAL:HG22	1.89	0.54
22:S:452:TYR:CD2	22:S:452:TYR:O	2.60	0.54
9:i:95:HIS:HA	9:i:98:TYR:HD2	1.73	0.54
9:i:253:GLN:HB3	9:i:254:GLU:O	2.07	0.54
10:j:67:PHE:O	10:j:71:THR:HG22	2.08	0.54
11:k:3:ILE:O	11:k:17:SER:HA	2.07	0.54
9:2:95:HIS:HA	9:2:98:TYR:HD2	1.72	0.54
32:M:316:SER:O	32:M:317:SER:OG	2.21	0.54
6:f:107:ARG:CZ	14:n:109:TYR:O	2.56	0.54
11:k:23:ARG:NH1	11:k:50:ALA:HA	2.22	0.54
13:m:164:PHE:CE2	13:m:181:LYS:HG3	2.42	0.54
16:V:257:GLU:O	16:V:258:GLU:HB2	2.08	0.54
3:c:8:SER:OG	3:c:10:THR:HG23	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:152:ASN:OD1	3:c:156:ASN:O	2.26	0.54
11:k:130:TYR:OH	11:k:145:ASP:HB3	2.07	0.54
13:m:48:GLU:OE1	14:n:170:TYR:HA	2.08	0.54
1:A:196:GLU:HA	1:A:196:GLU:OE2	2.07	0.54
6:F:121:GLN:NE2	7:G:132:PHE:HE1	2.06	0.54
21:N:143:LYS:HB3	33:J:19:ILE:HD12	1.88	0.54
25:R:33:LEU:HD13	25:R:47:ALA:HB2	1.90	0.54
25:R:68:GLU:O	25:R:71:LEU:CD2	2.56	0.54
32:M:428:LYS:O	32:M:429:SER:HB3	2.08	0.54
6:f:105:VAL:HG21	6:f:143:HIS:HB2	1.90	0.54
4:D:73:LEU:HD23	4:D:74:SER:N	2.22	0.54
11:4:3:ILE:O	11:4:17:SER:HA	2.07	0.54
23:P:84:LYS:HE3	23:P:84:LYS:HA	1.90	0.54
4:d:67:ILE:O	11:k:69:ILE:CD1	2.52	0.54
7:g:218:TRP:CH2	7:g:223:GLU:CB	2.91	0.54
8:h:149:LYS:HB2	8:1:170:GLN:HE22	1.72	0.54
12:l:284:ASN:C	12:l:284:ASN:OD1	2.50	0.54
3:C:152:ASN:OD1	3:C:156:ASN:O	2.26	0.54
6:F:77:LEU:HB3	32:M:433:TYR:HE2	1.73	0.54
20:Z:81:SER:O	20:Z:82:MET:HE2	2.07	0.54
28:H:459:SER:HA	28:H:462:ARG:HB2	1.90	0.54
12:l:113:ASN:OD1	12:l:114:PRO:CD	2.55	0.53
17:T:127:GLN:O	17:T:131:LYS:NZ	2.41	0.53
25:R:172:LEU:HD22	25:R:213:TYR:CD2	2.43	0.53
5:e:148:ASP:OD2	5:e:154:GLN:NE2	2.40	0.53
10:j:173:ASN:HD22	13:6:160:ASN:HB2	1.74	0.53
24:Q:67:THR:H	24:Q:68:MET:CB	2.19	0.53
7:g:13:SER:OG	7:g:127:ASN:OD1	2.20	0.53
9:i:104:ARG:NH1	9:i:135:THR:OG1	2.41	0.53
11:4:3:ILE:HD12	11:4:168:LEU:HD13	1.88	0.53
11:4:96:ARG:HH22	12:5:166:LYS:C	2.12	0.53
33:J:270:ARG:HG2	33:J:270:ARG:HH11	1.73	0.53
12:l:253:TYR:CE1	12:l:262:TYR:CD1	2.97	0.53
5:E:45:GLY:HA2	5:E:153:TYR:CE2	2.43	0.53
9:2:104:ARG:NH1	9:2:135:THR:OG1	2.41	0.53
9:2:253:GLN:HB3	9:2:254:GLU:O	2.07	0.53
16:V:257:GLU:OE1	16:V:270:TYR:CE1	2.61	0.53
20:Z:387:ASN:HD21	20:Z:400:ILE:HG21	1.72	0.53
24:Q:73:LYS:HG3	24:Q:77:PHE:CE2	2.43	0.53
8:h:135:ILE:HG22	8:h:140:SER:CB	2.39	0.53
10:j:8:ASN:HD21	10:j:57:ALA:CA	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:125:GLU:HA	5:E:125:GLU:OE2	2.09	0.53
10:3:172:LEU:HD11	10:3:200:LEU:HD13	1.91	0.53
12:5:103:SER:OG	13:6:145:ARG:NH2	2.41	0.53
16:V:147:VAL:O	30:K:88:ARG:NH2	2.42	0.53
17:T:253:GLU:N	17:T:253:GLU:OE2	2.39	0.53
26:U:257:ILE:HG22	26:U:261:LEU:HD13	1.90	0.53
28:H:203:LYS:HE3	28:H:268:ASP:HA	1.91	0.53
28:H:291:VAL:HG12	28:H:339:GLN:NE2	2.24	0.53
28:H:308:PHE:HB3	28:H:311:ILE:HD13	1.91	0.53
5:e:45:GLY:HA2	5:e:153:TYR:CE2	2.43	0.53
7:g:36:THR:HG21	7:g:203:ALA:CB	2.38	0.53
9:i:236:ARG:HE	10:j:161:GLU:CB	2.20	0.53
11:4:4:ILE:HA	11:4:16:ALA:O	2.08	0.53
17:T:35:ILE:O	17:T:39:LEU:HD23	2.09	0.53
31:L:290:ARG:O	31:L:290:ARG:HD2	2.09	0.53
32:M:17:GLU:CG	32:M:33:ARG:HD2	2.38	0.53
6:f:121:GLN:HE22	7:g:132:PHE:HE1	1.56	0.53
8:h:196:ILE:C	8:h:197:PHE:HD1	2.17	0.53
12:l:110:ILE:HD11	12:l:120:MET:HB2	1.89	0.53
8:1:135:ILE:HG22	8:1:140:SER:CB	2.39	0.53
9:2:249:ILE:HD12	10:3:48:HIS:HA	1.89	0.53
10:3:67:PHE:O	10:3:71:THR:HG22	2.08	0.53
10:3:69:TYR:O	10:3:73:LEU:HD12	2.09	0.53
12:5:188:TYR:HE1	12:5:198:LYS:HD3	1.74	0.53
17:T:8:THR:HA	17:T:30:ILE:HD12	1.91	0.53
24:Q:75:ARG:O	24:Q:79:PRO:HD2	2.09	0.53
29:I:225:PRO:CB	36:I:501:ATP:O1G	2.57	0.53
2:b:119:GLN:O	2:b:122:THR:OG1	2.25	0.53
4:d:40:ASN:O	4:d:216:LYS:HD2	2.08	0.53
10:j:172:LEU:HD11	10:j:200:LEU:HD13	1.91	0.53
4:D:122:GLN:NE2	5:E:136:ARG:NH1	2.57	0.53
10:3:8:ASN:HD21	10:3:57:ALA:CA	2.21	0.53
24:Q:275:ILE:HD13	24:Q:307:ASN:CB	2.39	0.53
27:O:324:VAL:O	27:O:328:VAL:HG23	2.09	0.53
29:I:101:GLY:HA3	29:I:102:ASN:O	2.08	0.53
34:8:315:VAL:HG13	34:8:317:PHE:CE1	2.43	0.53
1:a:167:LYS:HE3	1:a:192:ASP:CB	2.39	0.53
2:b:2:THR:HA	7:g:128:SER:HB3	1.91	0.53
11:k:142:SER:HA	12:5:242:ARG:HH12	1.74	0.53
7:G:36:THR:HG21	7:G:203:ALA:CB	2.39	0.53
7:G:161:LYS:NZ	23:P:2:SER:HB3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:3:120:PHE:HA	10:3:134:LYS:NZ	2.24	0.53
16:V:145:GLN:O	16:V:148:LYS:NZ	2.41	0.53
20:Z:399:LEU:H	20:Z:399:LEU:HD12	1.72	0.53
1:A:26:TYR:O	1:A:29:GLU:HB2	2.09	0.52
2:B:20:GLN:HA	2:B:23:TYR:HD2	1.74	0.52
2:B:109:LEU:HD12	10:3:78:GLU:OE2	2.09	0.52
5:E:76:CYS:SG	5:E:142:LEU:HD12	2.50	0.52
10:3:159:GLU:OE1	10:3:159:GLU:HA	2.09	0.52
12:5:253:TYR:CE1	12:5:262:TYR:CD1	2.97	0.52
20:Z:266:LYS:HZ3	20:Z:290:GLU:CD	2.17	0.52
30:K:344:ARG:O	30:K:349:ARG:NH1	2.42	0.52
33:J:276:LEU:HD22	33:J:290:ILE:HD12	1.91	0.52
1:a:26:TYR:O	1:a:29:GLU:HB2	2.09	0.52
7:g:71:ASP:OD2	7:g:72:ARG:NH2	2.41	0.52
10:j:69:TYR:O	10:j:73:LEU:HD12	2.09	0.52
11:k:11:ASP:OD2	11:k:12:SER:OG	2.21	0.52
3:C:7:ASP:OD2	4:D:6:ARG:HD3	2.09	0.52
5:E:186:GLU:HA	5:E:186:GLU:OE1	2.07	0.52
6:F:121:GLN:HE22	7:G:132:PHE:HE1	1.57	0.52
8:1:17:PHE:CE1	8:1:22:ILE:HG13	2.45	0.52
8:1:196:ILE:C	8:1:197:PHE:HD1	2.17	0.52
9:2:133:ASP:OD1	9:2:138:HIS:NE2	2.40	0.52
36:K:501:ATP:PG	31:L:342:ARG:HH22	2.31	0.52
9:i:236:ARG:NH2	10:j:162:ASP:OD1	2.42	0.52
10:j:138:VAL:HG22	10:j:147:PHE:CE1	2.44	0.52
2:B:119:GLN:O	2:B:122:THR:OG1	2.25	0.52
13:6:145:ARG:NH1	13:6:155:MET:HE1	2.22	0.52
20:Z:471:LEU:HD12	20:Z:505:VAL:CG2	2.40	0.52
2:b:113:GLU:HA	2:b:116:LYS:NZ	2.25	0.52
6:f:177:ASP:OD1	6:f:177:ASP:N	2.38	0.52
13:m:157:PHE:CE2	10:3:152:SER:HB3	2.44	0.52
9:2:170:HIS:HB3	9:2:183:LEU:HD11	1.91	0.52
5:e:114:GLN:HG2	6:f:82:ARG:NH2	2.23	0.52
5:e:186:GLU:OE1	5:e:186:GLU:HA	2.07	0.52
10:j:159:GLU:OE1	10:j:159:GLU:HA	2.09	0.52
12:l:188:TYR:HE1	12:l:198:LYS:HD3	1.74	0.52
13:m:201:GLU:OE2	9:2:225:ARG:HD2	2.08	0.52
2:B:224:TYR:CZ	9:2:65:ARG:NH1	2.77	0.52
7:G:170:GLN:HA	7:G:170:GLN:HE21	1.74	0.52
20:Z:875:LYS:HG3	20:Z:877:THR:H	1.74	0.52
6:f:102:LYS:HE3	6:f:138:ASP:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:6:38:ILE:CD1	13:6:205:GLN:HG2	2.40	0.52
17:T:143:SER:HB3	17:T:147:LYS:HE2	1.92	0.52
20:Z:611:THR:HG23	20:Z:612:GLY:N	2.24	0.52
5:e:76:CYS:SG	5:e:142:LEU:HD12	2.50	0.52
8:h:175:ASP:OD1	8:h:177:SER:N	2.40	0.52
1:A:21:PRO:HA	2:B:23:TYR:CD1	2.44	0.52
1:A:54:ILE:HD11	1:A:206:ALA:CB	2.40	0.52
1:A:167:LYS:HE3	1:A:192:ASP:CB	2.39	0.52
3:C:113:ARG:O	3:C:117:ASP:OD2	2.28	0.52
6:F:102:LYS:HE3	6:F:138:ASP:HA	1.91	0.52
8:1:62:GLN:HB3	9:2:113:LYS:NZ	2.24	0.52
20:Z:351:PRO:C	20:Z:354:PRO:HD2	2.35	0.52
22:S:164:ILE:HB	22:S:165:PRO:HD3	1.91	0.52
23:P:171:MET:HE3	23:P:175:GLU:HB3	1.91	0.52
27:O:236:HIS:ND1	27:O:237:PRO:HD2	2.25	0.52
28:H:104:LYS:HA	32:M:168:LYS:HE3	1.92	0.52
28:H:314:VAL:O	28:H:314:VAL:HG13	2.09	0.52
29:I:265:ARG:HB3	29:I:265:ARG:CZ	2.39	0.52
31:L:284:ASP:O	32:M:299:ARG:NH2	2.42	0.52
32:M:432:PHE:CE2	32:M:433:TYR:HE1	2.28	0.52
33:J:9:ASN:O	33:J:10:ILE:C	2.52	0.52
33:J:197:LEU:CD1	38:J:501:ADP:C4	2.92	0.52
8:h:115:ASN:O	8:h:116:LYS:CG	2.58	0.52
9:i:86:GLN:HA	9:i:86:GLN:OE1	2.10	0.52
9:i:189:GLN:O	9:i:192:ILE:N	2.43	0.52
13:m:158:LEU:HD11	13:m:191:LEU:HD13	1.92	0.52
1:A:29:GLU:OE1	30:K:419:ASN:HB3	2.09	0.52
2:B:21:ILE:HG21	2:B:153:SER:HA	1.92	0.52
4:D:204:GLN:O	4:D:205:THR:CB	2.55	0.52
6:F:77:LEU:HD22	32:M:433:TYR:CZ	2.44	0.52
13:6:37:ASN:OD1	13:6:50:LYS:NZ	2.40	0.52
22:S:68:LEU:O	22:S:69:LEU:O	2.28	0.52
24:Q:88:PHE:CZ	24:Q:90:LYS:HD3	2.45	0.52
28:H:331:ARG:NE	28:H:331:ARG:HA	2.24	0.52
34:8:419:ASN:O	34:8:420:LEU:CG	2.58	0.52
1:a:210:MET:SD	1:a:214:LEU:HD11	2.50	0.52
2:b:20:GLN:HA	2:b:23:TYR:HD2	1.74	0.52
3:c:27:GLU:OE1	3:c:27:GLU:HA	2.10	0.52
14:n:109:TYR:O	14:n:110:ASP:CB	2.56	0.52
20:Z:272:TYR:CE2	20:Z:284:LEU:HD22	2.44	0.52
10:j:120:PHE:HA	10:j:134:LYS:NZ	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:107:TYR:HD1	11:k:109:LYS:HD3	1.74	0.52
12:l:242:ARG:CZ	11:4:141:PHE:HB3	2.40	0.52
14:n:262:GLY:HA3	9:2:140:PHE:CE1	2.42	0.52
3:C:13:PHE:HE1	4:D:23:ALA:HB2	1.75	0.52
9:2:86:GLN:OE1	9:2:86:GLN:HA	2.10	0.52
14:7:47:MET:HE1	14:7:209:ALA:HB3	1.90	0.52
16:V:238:LEU:HD11	16:V:242:LYS:HE3	1.92	0.52
31:L:293:GLU:OE2	32:M:295:LYS:HD2	2.09	0.52
32:M:213:ARG:NH1	32:M:344:ASP:OD2	2.36	0.52
33:J:324:ARG:HG3	33:J:358:VAL:HG11	1.92	0.52
33:J:327:ILE:HG22	33:J:331:HIS:CE1	2.45	0.52
8:h:17:PHE:CE1	8:h:22:ILE:HG13	2.45	0.51
2:B:113:GLU:HA	2:B:116:LYS:NZ	2.25	0.51
4:D:122:GLN:OE1	5:E:134:MET:HA	2.09	0.51
9:2:155:SER:O	9:2:156:LEU:HD23	2.11	0.51
18:X:14:VAL:HG13	18:X:50:TRP:CE2	2.45	0.51
20:Z:163:GLU:OE1	20:Z:180:ASP:HB2	2.10	0.51
21:N:613:HIS:O	33:J:59:LYS:NZ	2.43	0.51
29:I:217:LYS:HZ1	29:I:322:VAL:C	2.18	0.51
30:K:160:VAL:HG22	30:K:162:GLY:H	1.75	0.51
34:8:337:PHE:O	34:8:432:LEU:CD1	2.57	0.51
1:a:54:ILE:HD11	1:a:206:ALA:CB	2.40	0.51
2:b:119:GLN:NE2	3:c:83:ASP:OD1	2.43	0.51
6:f:78:ALA:HB3	6:f:79:PRO:HD3	1.92	0.51
9:i:155:SER:O	9:i:156:LEU:HD23	2.11	0.51
1:A:246:VAL:O	1:A:250:GLU:OE2	2.28	0.51
8:1:115:ASN:O	8:1:116:LYS:CG	2.58	0.51
9:2:189:GLN:O	9:2:192:ILE:N	2.43	0.51
13:6:164:PHE:CE2	13:6:181:LYS:CG	2.94	0.51
14:7:106:GLU:HA	14:7:109:TYR:CE1	2.44	0.51
21:N:632:LYS:HZ2	21:N:877:GLN:HG2	1.75	0.51
29:I:62:MET:HE3	29:I:66:LYS:HE2	1.91	0.51
30:K:252:ARG:HH21	30:K:253:MET:HE2	1.75	0.51
4:d:112:TYR:O	4:d:116:VAL:HG23	2.10	0.51
13:m:38:ILE:CD1	13:m:205:GLN:HG2	2.40	0.51
2:B:97:TYR:CD2	2:B:105:PRO:HA	2.45	0.51
5:E:103:TYR:HB3	13:6:96:SER:OG	2.10	0.51
7:G:206:ASP:HA	31:L:420:ARG:HD3	1.91	0.51
20:Z:145:ASP:HA	20:Z:149:TRP:HE1	1.75	0.51
21:N:25:LEU:HB2	21:N:60:MET:HE3	1.91	0.51
22:S:315:LYS:HE3	22:S:345:TYR:HE1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:142:PHE:HE1	10:j:115:LYS:HD2	1.74	0.51
1:A:210:MET:SD	1:A:214:LEU:HD11	2.49	0.51
2:B:52:SER:O	30:K:423:LYS:HE3	2.10	0.51
10:3:138:VAL:HG22	10:3:147:PHE:CE1	2.44	0.51
16:V:191:GLY:HA2	16:V:195:HIS:ND1	2.25	0.51
20:Z:365:SER:O	20:Z:366:LYS:CG	2.58	0.51
21:N:282:TYR:CE2	21:N:286:LEU:CB	2.93	0.51
26:U:29:GLU:HA	26:U:29:GLU:OE2	2.10	0.51
31:L:424:GLU:HA	31:L:427:LYS:HD2	1.91	0.51
32:M:69:ILE:O	32:M:73:ARG:HG2	2.11	0.51
32:M:77:TYR:HD2	32:M:78:LEU:O	1.93	0.51
2:b:241:GLN:HA	2:b:241:GLN:OE1	2.10	0.51
1:A:134:MET:CE	7:G:126:TYR:CE1	2.92	0.51
9:2:69:LYS:HZ3	9:2:212:ASP:HA	1.75	0.51
11:4:107:TYR:HD1	11:4:109:LYS:HD3	1.74	0.51
13:6:158:LEU:HD11	13:6:191:LEU:HD13	1.92	0.51
16:V:120:SER:O	16:V:123:VAL:HG12	2.10	0.51
28:H:313:ALA:O	28:H:314:VAL:C	2.52	0.51
28:H:313:ALA:O	28:H:314:VAL:O	2.28	0.51
29:I:184:ILE:HD12	29:I:191:ILE:CD1	2.40	0.51
33:J:311:ASP:N	33:J:311:ASP:OD1	2.42	0.51
34:8:207:GLN:OE1	35:9:76:GLZ:CA	2.59	0.51
1:a:246:VAL:O	1:a:250:GLU:OE2	2.28	0.51
2:b:2:THR:CA	7:g:128:SER:HB3	2.41	0.51
2:b:21:ILE:HG21	2:b:153:SER:HA	1.92	0.51
3:c:113:ARG:O	3:c:117:ASP:OD2	2.28	0.51
4:d:204:GLN:O	4:d:205:THR:CB	2.58	0.51
7:g:170:GLN:HE21	7:g:170:GLN:HA	1.74	0.51
10:j:160:PRO:HB2	10:j:161:GLU:OE2	2.11	0.51
3:C:5:ARG:HB3	3:C:6:TYR:CD1	2.46	0.51
3:C:13:PHE:CE2	4:D:127:ARG:HD2	2.46	0.51
3:C:27:GLU:HA	3:C:27:GLU:OE1	2.10	0.51
3:C:71:ASP:C	3:C:227:GLN:NE2	2.69	0.51
13:6:168:TYR:CD1	13:6:174:GLY:HA2	2.45	0.51
16:V:183:ALA:O	16:V:184:ASN:O	2.27	0.51
23:P:364:ARG:NH2	27:O:325:GLU:OE2	2.44	0.51
28:H:466:TYR:N	28:H:466:TYR:CD1	2.79	0.51
30:K:356:ILE:HD12	30:K:359:LYS:HD3	1.93	0.51
34:8:263:CYS:SG	34:8:276:LEU:N	2.84	0.51
2:b:97:TYR:CD2	2:b:105:PRO:HA	2.45	0.51
4:d:4:TYR:CZ	4:d:6:ARG:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:P:396:PRO:O	23:P:397:ALA:HB3	2.10	0.51
1:a:82:VAL:HB	1:a:142:THR:OG1	2.11	0.51
9:i:170:HIS:HB3	9:i:183:LEU:HD11	1.91	0.51
12:5:84:GLN:HA	12:5:84:GLN:NE2	2.26	0.51
12:5:162:VAL:HG11	12:5:192:SER:HA	1.93	0.51
14:7:47:MET:CE	14:7:206:ALA:HA	2.40	0.51
15:W:130:LYS:CB	15:W:133:LYS:HE3	2.41	0.51
20:Z:146:PHE:HA	29:I:409:MET:HG2	1.91	0.51
20:Z:512:ILE:O	20:Z:513:ALA:HB3	2.11	0.51
20:Z:938:GLN:O	20:Z:939:ALA:HB3	2.11	0.51
21:N:534:ASP:OD1	21:N:535:LEU:N	2.44	0.51
24:Q:127:ARG:NE	24:Q:128:GLU:OE2	2.44	0.51
31:L:117:TYR:OH	31:L:137:ARG:HD3	2.11	0.51
32:M:355:ASP:OD1	32:M:355:ASP:N	2.44	0.51
2:b:4:ARG:HH12	6:f:123:TYR:HD2	1.59	0.51
3:c:5:ARG:HB3	3:c:6:TYR:CD1	2.46	0.51
9:i:178:GLU:OE2	9:i:178:GLU:HA	2.11	0.51
11:k:159:ASP:OD2	11:k:160:LEU:N	2.44	0.51
13:m:168:TYR:CD1	13:m:174:GLY:HA2	2.45	0.51
1:A:29:GLU:OE1	30:K:419:ASN:CG	2.54	0.51
2:B:4:ARG:NH2	6:F:123:TYR:O	2.44	0.51
21:N:146:LYS:HE2	33:J:16:GLU:OE1	2.10	0.51
25:R:310:GLU:O	25:R:314:ASN:ND2	2.44	0.51
30:K:170:THR:HG23	30:K:172:ALA:H	1.75	0.51
34:8:439:GLN:OE1	34:8:447:HIS:O	2.29	0.51
3:c:13:PHE:HE2	4:d:127:ARG:CZ	2.24	0.51
5:e:125:GLU:HA	5:e:125:GLU:OE2	2.09	0.51
9:i:236:ARG:HH21	10:j:161:GLU:HB2	1.76	0.51
12:l:84:GLN:HA	12:l:84:GLN:NE2	2.26	0.51
3:C:57:LEU:HD23	3:C:59:GLN:HE21	1.76	0.51
9:2:178:GLU:HA	9:2:178:GLU:OE2	2.11	0.51
13:6:145:ARG:HD3	13:6:155:MET:HE1	1.93	0.51
21:N:144:CYS:HB3	21:N:152:LEU:HB2	1.93	0.51
22:S:85:SER:HB3	22:S:138:MET:HE1	1.93	0.51
6:f:10:THR:HA	6:f:19:LEU:HD21	1.93	0.50
10:j:49:VAL:HG11	10:j:87:PHE:CD2	2.47	0.50
13:m:145:ARG:HD3	13:m:155:MET:HE1	1.93	0.50
6:F:10:THR:HA	6:F:19:LEU:HD21	1.93	0.50
9:2:110:GLN:OE1	9:2:110:GLN:O	2.29	0.50
20:Z:84:ALA:O	20:Z:86:PRO:HD2	2.11	0.50
20:Z:161:ILE:HG22	20:Z:162:GLY:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:H:195:VAL:HG23	28:H:290:MET:HE1	1.93	0.50
30:K:202:GLY:O	33:J:334:LYS:HE3	2.10	0.50
2:b:151:ASP:OD1	2:b:155:SER:O	2.29	0.50
3:c:71:ASP:C	3:c:227:GLN:NE2	2.69	0.50
7:g:170:GLN:HA	7:g:170:GLN:NE2	2.27	0.50
12:l:162:VAL:HG11	12:l:192:SER:HA	1.93	0.50
13:m:164:PHE:CE2	13:m:181:LYS:CG	2.94	0.50
1:A:82:VAL:HB	1:A:142:THR:OG1	2.11	0.50
2:B:151:ASP:OD1	2:B:155:SER:O	2.29	0.50
6:F:55:GLU:OE1	6:F:55:GLU:CA	2.59	0.50
21:N:149:GLU:C	21:N:151:LYS:H	2.20	0.50
6:f:55:GLU:OE1	6:f:55:GLU:CA	2.59	0.50
3:C:4:ARG:HH12	6:F:124:GLY:N	2.09	0.50
3:C:100:LYS:HD3	10:3:65:GLU:HG3	1.93	0.50
4:D:96:HIS:CE1	4:D:102:ASP:O	2.64	0.50
7:G:70:VAL:HG23	7:G:74:ILE:HB	1.93	0.50
10:3:9:GLY:HA3	10:3:180:LEU:HB3	1.92	0.50
11:4:159:ASP:OD2	11:4:160:LEU:N	2.44	0.50
17:T:271:GLU:O	30:K:73:ARG:NH1	2.44	0.50
20:Z:377:ALA:HB3	20:Z:379:GLN:CD	2.36	0.50
20:Z:743:ILE:HG23	20:Z:754:LYS:HE3	1.94	0.50
22:S:315:LYS:NZ	22:S:374:ASP:OD2	2.39	0.50
31:L:245:PHE:O	31:L:246:SER:OG	2.27	0.50
3:c:57:LEU:HD23	3:c:59:GLN:HE21	1.76	0.50
10:j:29:LEU:HD22	10:j:40:PHE:CD2	2.46	0.50
13:m:133:PHE:CD2	13:m:139:TYR:CB	2.94	0.50
1:A:29:GLU:OE1	30:K:419:ASN:ND2	2.44	0.50
4:D:101:GLU:OE1	4:D:101:GLU:HA	2.10	0.50
7:G:112:PHE:CE2	7:G:116:LEU:CD1	2.95	0.50
20:Z:773:ARG:HH22	20:Z:938:GLN:HB2	1.76	0.50
29:I:116:ASP:H	29:I:138:LYS:HZ3	1.58	0.50
3:c:32:ALA:HA	3:c:51:LYS:CE	2.42	0.50
4:d:97:ARG:NH1	11:k:65:GLN:HE22	2.09	0.50
10:j:205:ASP:OD2	12:5:246:SER:O	2.30	0.50
11:k:65:GLN:O	11:k:66:LEU:C	2.55	0.50
6:F:51:ARG:NH2	32:M:434:ALA:O	2.44	0.50
9:2:37:PHE:CE2	9:2:177:LYS:HA	2.47	0.50
11:4:65:GLN:O	11:4:68:SER:N	2.44	0.50
13:6:133:PHE:CD2	13:6:139:TYR:CB	2.94	0.50
29:I:101:GLY:H	29:I:104:LEU:HD21	1.76	0.50
32:M:422:VAL:HG23	32:M:422:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:150:ASN:O	8:h:163:PHE:CE1	2.64	0.50
9:i:110:GLN:OE1	9:i:110:GLN:O	2.29	0.50
11:k:87:GLU:HA	11:k:87:GLU:OE2	2.10	0.50
11:k:143:LEU:HD21	11:k:164:CYS:HA	1.94	0.50
6:F:107:ARG:NH2	14:7:107:ASN:O	2.45	0.50
10:3:97:GLU:OE1	10:3:97:GLU:HA	2.12	0.50
10:3:204:GLN:O	10:3:205:ASP:C	2.55	0.50
28:H:256:LYS:NZ	36:H:501:ATP:PG	2.85	0.50
29:I:433:GLU:OE1	29:I:437:LEU:HB2	2.11	0.50
30:K:386:ILE:HB	30:K:387:MET:HE2	1.92	0.50
2:b:205:ASN:N	2:b:205:ASN:OD1	2.45	0.50
8:h:26:ASP:OD1	8:h:26:ASP:N	2.44	0.50
9:i:59:ASN:O	10:j:132:GLU:OE2	2.29	0.50
9:i:168:GLU:OE2	14:7:220:ARG:NE	2.41	0.50
10:j:97:GLU:OE1	10:j:97:GLU:HA	2.12	0.50
11:k:65:GLN:O	11:k:68:SER:N	2.44	0.50
13:m:37:ASN:CG	13:m:50:LYS:NZ	2.70	0.50
14:n:255:ALA:HB2	8:l:39:VAL:CG1	2.41	0.50
3:C:9:ARG:NH2	4:D:10:ILE:HD12	2.26	0.50
4:D:170:THR:HA	4:D:173:GLU:OE1	2.12	0.50
7:G:170:GLN:NE2	7:G:170:GLN:HA	2.27	0.50
27:O:239:MET:O	27:O:243:VAL:HG13	2.11	0.50
36:H:501:ATP:C5'	29:I:340:ARG:HH21	2.19	0.50
29:I:124:THR:O	29:I:125:MET:HB2	2.12	0.50
7:g:70:VAL:HG23	7:g:74:ILE:HB	1.93	0.50
14:n:36:GLN:NE2	14:n:37:PRO:O	2.45	0.50
10:3:49:VAL:HG11	10:3:87:PHE:CD2	2.47	0.50
22:S:170:TYR:CE2	22:S:172:ASN:OD1	2.65	0.50
29:I:302:ILE:HG13	29:I:303:GLN:N	2.27	0.50
10:j:66:MET:HG3	10:j:70:LYS:NZ	2.27	0.50
1:A:22:GLU:CD	1:A:22:GLU:N	2.70	0.50
6:F:78:ALA:HB3	6:F:79:PRO:HD3	1.92	0.50
9:2:236:ARG:HH21	10:3:161:GLU:HB2	1.77	0.50
10:3:29:LEU:HD22	10:3:40:PHE:CD2	2.46	0.50
10:3:182:GLY:O	10:3:202:MET:HE2	2.12	0.50
25:R:213:TYR:HE1	25:R:243:LEU:HG	1.77	0.50
1:a:110:TYR:OH	9:i:101:ARG:NH2	2.45	0.49
12:l:83:PHE:CE1	12:l:88:ILE:HG12	2.47	0.49
13:m:37:ASN:OD1	13:m:50:LYS:NZ	2.40	0.49
4:D:120:TYR:CE2	4:D:129:PHE:CZ	2.99	0.49
29:I:401:LEU:HD22	29:I:422:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:I:433:GLU:OE2	29:I:436:TYR:HA	2.12	0.49
34:8:265:ILE:HG22	34:8:267:GLY:H	1.77	0.49
1:a:210:MET:HG2	1:a:218:PHE:CE1	2.47	0.49
7:g:112:PHE:CE2	7:g:116:LEU:CD1	2.95	0.49
9:i:37:PHE:CE2	9:i:177:LYS:HA	2.47	0.49
2:B:85:LEU:O	2:B:89:SER:OG	2.30	0.49
2:B:241:GLN:OE1	2:B:241:GLN:HA	2.10	0.49
20:Z:784:SER:O	20:Z:790:MET:HE1	2.12	0.49
1:a:246:VAL:HG12	1:a:250:GLU:OE2	2.13	0.49
4:d:21:GLU:O	4:d:25:GLU:OE2	2.30	0.49
4:d:122:GLN:HA	5:e:136:ARG:CZ	2.42	0.49
5:e:69:GLU:O	5:e:93:ARG:NE	2.39	0.49
7:g:74:ILE:HD13	7:g:112:PHE:CD1	2.47	0.49
10:j:9:GLY:HA3	10:j:180:LEU:HB3	1.92	0.49
1:A:210:MET:HG2	1:A:218:PHE:CE1	2.47	0.49
1:A:246:VAL:HG12	1:A:250:GLU:OE2	2.12	0.49
3:C:82:ALA:HA	3:C:85:GLU:OE2	2.12	0.49
5:E:114:GLN:CG	6:F:82:ARG:HH12	2.25	0.49
7:G:74:ILE:HD13	7:G:112:PHE:CD1	2.47	0.49
10:3:160:PRO:HB2	10:3:161:GLU:OE2	2.11	0.49
11:4:65:GLN:O	11:4:66:LEU:C	2.55	0.49
14:7:47:MET:HE1	14:7:206:ALA:HA	1.94	0.49
20:Z:443:ASP:O	20:Z:444:GLU:C	2.55	0.49
24:Q:88:PHE:HD2	24:Q:93:THR:HG1	1.58	0.49
29:I:152:LYS:O	29:I:153:THR:C	2.54	0.49
3:C:231:LYS:HD3	3:C:232:PRO:HD2	1.94	0.49
4:D:78:LEU:HD13	4:D:81:ASP:OD2	2.13	0.49
4:D:163:THR:HG23	4:D:168:SER:HB2	1.93	0.49
9:2:249:ILE:HD13	10:3:50:PHE:HE2	1.76	0.49
10:3:8:ASN:HD21	10:3:57:ALA:HB2	1.77	0.49
12:5:83:PHE:CE1	12:5:88:ILE:HG12	2.47	0.49
21:N:29:ASN:HA	21:N:67:LYS:HE2	1.94	0.49
23:P:69:ARG:HH12	23:P:109:SER:HB3	1.78	0.49
24:Q:252:HIS:N	24:Q:252:HIS:ND1	2.60	0.49
26:U:244:ASP:HA	26:U:247:ILE:HD12	1.94	0.49
32:M:179:THR:C	32:M:181:SER:H	2.20	0.49
1:a:22:GLU:CD	1:a:22:GLU:N	2.70	0.49
3:c:11:THR:O	4:d:127:ARG:HD2	2.12	0.49
3:c:231:LYS:HD3	3:c:232:PRO:HD2	1.94	0.49
10:j:204:GLN:O	10:j:205:ASP:C	2.55	0.49
11:4:143:LEU:HD21	11:4:164:CYS:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:5:113:ASN:OD1	12:5:114:PRO:CD	2.55	0.49
12:5:179:TYR:CD2	12:5:257:GLU:N	2.80	0.49
14:7:97:GLU:HA	14:7:100:LEU:HD12	1.94	0.49
16:V:42:ARG:HH21	31:L:152:THR:HG22	1.78	0.49
23:P:378:THR:O	23:P:381:SER:OG	2.25	0.49
29:I:226:GLY:CA	36:I:501:ATP:O1B	2.61	0.49
29:I:290:LYS:HE3	33:J:267:GLU:HA	1.95	0.49
30:K:146:LEU:C	30:K:146:LEU:HD23	2.37	0.49
30:K:159:SER:OG	30:K:160:VAL:N	2.46	0.49
2:b:98:LYS:HE2	2:b:104:TYR:CE2	2.48	0.49
2:b:178:ARG:HG3	2:b:191:ILE:HG23	1.94	0.49
10:j:8:ASN:HD21	10:j:57:ALA:HB2	1.77	0.49
13:m:153:LEU:HD12	10:3:144:ASP:OD1	2.13	0.49
13:m:229:ARG:NH1	9:2:193:TRP:HZ3	2.10	0.49
3:C:92:ARG:HH12	10:3:77:LYS:HG2	1.77	0.49
4:D:85:LEU:HD21	4:D:129:PHE:CD2	2.47	0.49
13:6:48:GLU:OE1	14:7:170:TYR:HA	2.12	0.49
18:X:38:ASN:O	18:X:40:GLU:N	2.46	0.49
21:N:338:PHE:CZ	21:N:749:LEU:HD23	2.48	0.49
31:L:412:PRO:O	31:L:416:MET:HG2	2.13	0.49
32:M:186:LEU:HD12	36:M:501:ATP:N6	2.26	0.49
9:i:109:LEU:HD22	9:i:140:PHE:CG	2.48	0.49
11:k:139:TYR:HE1	12:5:209:THR:HG22	1.77	0.49
2:B:178:ARG:HG3	2:B:191:ILE:HG23	1.94	0.49
13:6:37:ASN:CG	13:6:50:LYS:NZ	2.70	0.49
16:V:212:MET:HE3	26:U:127:GLN:HE21	1.77	0.49
25:R:269:LYS:HD3	25:R:269:LYS:N	2.27	0.49
28:H:456:LYS:O	28:H:456:LYS:HD3	2.13	0.49
29:I:422:ARG:HA	29:I:425:LYS:HD2	1.94	0.49
11:k:153:THR:HG23	11:k:156:GLU:OE1	2.12	0.49
11:k:175:ASP:OD2	11:4:173:PRO:HA	2.12	0.49
2:B:205:ASN:N	2:B:205:ASN:OD1	2.45	0.49
8:1:26:ASP:OD1	8:1:26:ASP:N	2.44	0.49
8:1:135:ILE:CG2	8:1:140:SER:CB	2.91	0.49
9:2:48:ARG:CB	9:2:199:GLY:O	2.54	0.49
9:2:109:LEU:HD22	9:2:140:PHE:CG	2.48	0.49
11:4:43:LEU:HD21	11:4:182:LYS:HD3	1.94	0.49
11:4:153:THR:HG23	11:4:156:GLU:OE1	2.12	0.49
16:V:53:MET:HE3	16:V:65:VAL:HG21	1.95	0.49
24:Q:162:LEU:HB3	24:Q:163:ARG:NH2	2.27	0.49
26:U:108:GLU:OE2	26:U:111:LYS:HD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:85:LEU:O	2:b:89:SER:OG	2.30	0.49
2:b:94:HIS:ND1	9:i:94:LEU:CD2	2.76	0.49
2:b:151:ASP:OD1	2:b:151:ASP:N	2.44	0.49
7:g:205:GLU:N	7:g:205:GLU:CD	2.71	0.49
12:l:179:TYR:CD2	12:l:257:GLU:N	2.80	0.49
3:C:32:ALA:HA	3:C:51:LYS:CE	2.42	0.49
6:F:32:GLY:HA2	32:M:434:ALA:OXT	2.13	0.49
11:4:87:GLU:HA	11:4:87:GLU:OE2	2.11	0.49
11:4:160:LEU:HD12	11:4:163:LEU:CD1	2.43	0.49
20:Z:863:THR:O	20:Z:863:THR:HG22	2.12	0.49
21:N:271:GLU:OE2	21:N:417:ARG:NH2	2.46	0.49
21:N:334:VAL:HG22	21:N:747:HIS:CE1	2.47	0.49
32:M:77:TYR:OH	32:M:159:LEU:HD11	2.13	0.49
33:J:389:VAL:HA	33:J:392:LYS:HE2	1.95	0.49
34:8:326:LYS:O	34:8:442:ASN:HB3	2.13	0.49
2:b:174:PHE:CE1	2:b:198:GLU:OE1	2.66	0.49
3:c:82:ALA:HA	3:c:85:GLU:OE2	2.12	0.49
11:k:20:ALA:HB2	11:k:177:LYS:HG3	1.94	0.49
12:l:250:VAL:HG13	12:l:268:VAL:HG22	1.95	0.49
7:G:22:PHE:HB3	7:G:26:TYR:CE2	2.48	0.49
10:3:66:MET:HG3	10:3:70:LYS:NZ	2.27	0.49
20:Z:308:LYS:O	20:Z:312:TYR:HB2	2.13	0.49
28:H:233:GLU:CD	34:8:357:ARG:NH2	2.71	0.49
28:H:331:ARG:HA	28:H:331:ARG:HE	1.77	0.49
34:8:493:MET:HA	34:8:493:MET:HE3	1.95	0.49
1:a:62:LYS:HZ2	7:g:177:GLU:HG2	1.76	0.48
4:d:229:ILE:O	4:d:233:VAL:HG23	2.13	0.48
6:f:27:GLU:O	6:f:31:GLN:HG3	2.13	0.48
7:g:230:PHE:CB	7:g:232:LYS:NZ	2.74	0.48
5:E:20:ARG:NH1	32:M:432:PHE:CE1	2.81	0.48
7:G:91:ARG:HA	7:G:94:GLU:OE1	2.13	0.48
11:4:86:GLN:HA	11:4:86:GLN:NE2	2.25	0.48
20:Z:24:THR:HB	20:Z:25:PRO:HD3	1.94	0.48
20:Z:471:LEU:HD13	20:Z:504:GLU:HB2	1.95	0.48
27:O:271:LYS:HA	27:O:271:LYS:HE3	1.95	0.48
34:8:244:THR:O	34:8:245:ALA:HB3	2.13	0.48
34:8:433:ILE:CG2	34:8:495:LYS:HD3	2.43	0.48
2:b:2:THR:C	7:g:128:SER:OG	2.56	0.48
2:b:139:HIS:HB3	2:b:234:ARG:HD2	1.95	0.48
4:d:111:ARG:HG3	5:e:86:ARG:HH22	1.77	0.48
6:f:20:PHE:HA	6:f:23:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:65:LYS:HD2	6:f:222:PHE:HD2	1.78	0.48
7:g:22:PHE:HB3	7:g:26:TYR:CE2	2.48	0.48
1:A:129:THR:O	1:A:129:THR:OG1	2.29	0.48
9:2:186:ASP:HA	9:2:189:GLN:HE21	1.78	0.48
23:P:290:LEU:HD23	23:P:291:LYS:HE2	1.96	0.48
25:R:261:LEU:HB2	25:R:266:LEU:HG	1.94	0.48
29:I:58:LYS:N	29:I:58:LYS:HD2	2.28	0.48
31:L:168:TYR:CE1	32:M:142:PRO:HD2	2.48	0.48
9:i:189:GLN:HE22	9:i:220:LEU:HD21	1.78	0.48
2:B:98:LYS:HE2	2:B:104:TYR:CE2	2.48	0.48
4:D:167:ASN:OD1	4:D:170:THR:HG23	2.14	0.48
13:6:39:THR:OG1	13:6:44:ASN:ND2	2.37	0.48
20:Z:133:ASP:HA	20:Z:136:ARG:HD2	1.96	0.48
20:Z:269:TYR:CE2	20:Z:293:MET:SD	3.06	0.48
21:N:94:LYS:HA	21:N:94:LYS:HE3	1.94	0.48
31:L:183:ILE:HG23	36:L:501:ATP:HN62	1.78	0.48
32:M:50:ARG:HG2	32:M:54:GLU:OE2	2.13	0.48
3:c:16:GLU:HB2	3:c:18:ARG:HB2	1.95	0.48
9:i:189:GLN:O	9:i:193:TRP:CD1	2.66	0.48
2:B:171:ALA:O	2:B:175:LEU:HD12	2.14	0.48
4:D:84:ILE:O	4:D:87:GLU:HG3	2.13	0.48
4:D:85:LEU:HA	4:D:88:LYS:HD2	1.95	0.48
6:F:27:GLU:O	6:F:31:GLN:HG3	2.13	0.48
7:G:230:PHE:CB	7:G:232:LYS:NZ	2.74	0.48
9:2:193:TRP:N	9:2:193:TRP:HD1	2.11	0.48
13:6:140:GLU:HA	13:6:140:GLU:OE2	2.13	0.48
14:7:110:ASP:O	14:7:111:ASN:CB	2.60	0.48
19:Y:43:TRP:O	19:Y:44:ALA:HB3	2.13	0.48
20:Z:875:LYS:HG3	20:Z:876:VAL:N	2.28	0.48
29:I:300:ARG:HD3	29:I:300:ARG:N	2.29	0.48
30:K:214:PRO:HG2	30:K:217:THR:HG23	1.95	0.48
30:K:260:LEU:O	30:K:264:ASN:ND2	2.47	0.48
32:M:179:THR:O	32:M:181:SER:N	2.45	0.48
33:J:16:GLU:OE1	33:J:16:GLU:HA	2.14	0.48
33:J:197:LEU:HD11	38:J:501:ADP:C1'	2.43	0.48
34:8:119:TYR:HE1	34:8:207:GLN:OE1	1.95	0.48
34:8:156:ILE:HG21	34:8:191:CYS:HB2	1.95	0.48
7:g:218:TRP:HD1	7:g:231:VAL:CG2	2.27	0.48
2:B:139:HIS:HB3	2:B:234:ARG:HD2	1.95	0.48
6:F:65:LYS:HD2	6:F:222:PHE:HD2	1.78	0.48
7:G:74:ILE:HG21	7:G:112:PHE:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:218:TRP:HD1	7:G:231:VAL:CG2	2.27	0.48
14:7:148:ILE:HD11	14:7:177:THR:HG23	1.95	0.48
20:Z:309:GLN:C	20:Z:311:ALA:N	2.70	0.48
23:P:394:ASN:ND2	24:Q:355:GLU:O	2.47	0.48
26:U:241:THR:OG1	26:U:242:PRO:HD2	2.13	0.48
28:H:256:LYS:HB2	36:H:501:ATP:O1B	2.14	0.48
7:g:91:ARG:HA	7:g:94:GLU:OE1	2.14	0.48
8:h:17:PHE:O	8:h:18:LYS:C	2.57	0.48
8:h:150:ASN:C	8:h:163:PHE:HZ	2.22	0.48
14:n:109:TYR:O	14:n:110:ASP:OD2	2.32	0.48
9:2:177:LYS:HZ3	9:2:181:ILE:HD12	1.78	0.48
20:Z:499:GLY:HA3	20:Z:861:THR:HG21	1.95	0.48
22:S:455:GLU:OE1	22:S:455:GLU:HA	2.13	0.48
29:I:268:PHE:C	29:I:319:ARG:HE	2.22	0.48
31:L:248:ALA:HB2	31:L:283:VAL:HA	1.94	0.48
33:J:197:LEU:HD12	38:J:501:ADP:C5	2.49	0.48
9:i:193:TRP:N	9:i:193:TRP:HD1	2.11	0.48
12:l:236:ILE:HG21	12:l:250:VAL:HG12	1.95	0.48
1:A:14:ARG:NE	7:G:8:TYR:HH	1.84	0.48
3:C:191:GLU:HG2	3:C:195:LYS:HD2	1.96	0.48
4:D:203:VAL:HG11	4:D:210:ILE:CD1	2.43	0.48
9:2:189:GLN:O	9:2:193:TRP:CD1	2.66	0.48
10:3:74:TYR:O	10:3:78:GLU:OE1	2.32	0.48
11:4:20:ALA:HB2	11:4:177:LYS:HG3	1.94	0.48
20:Z:442:VAL:O	20:Z:448:LYS:HE2	2.13	0.48
21:N:918:GLU:H	21:N:918:GLU:CD	2.22	0.48
29:I:101:GLY:CA	29:I:102:ASN:O	2.62	0.48
30:K:344:ARG:NH1	30:K:344:ARG:HB2	2.28	0.48
7:g:218:TRP:CE3	7:g:220:SER:HB3	2.49	0.48
11:k:43:LEU:HD21	11:k:182:LYS:HD3	1.94	0.48
12:l:113:ASN:ND2	12:l:138:CYS:SG	2.87	0.48
1:A:166:TYR:CD1	2:B:56:ALA:HA	2.48	0.48
2:B:69:PRO:HD2	2:B:104:TYR:CE1	2.49	0.48
8:1:60:ASP:OD1	8:1:102:LEU:HD22	2.13	0.48
12:5:175:MET:HE2	12:5:202:PHE:O	2.14	0.48
20:Z:52:LEU:O	20:Z:56:LEU:N	2.46	0.48
20:Z:556:ILE:CD1	20:Z:562:TRP:HE3	2.26	0.48
30:K:231:LYS:HA	30:K:231:LYS:HE3	1.96	0.48
30:K:322:ASP:OD2	31:L:290:ARG:NE	2.47	0.48
2:b:69:PRO:HD2	2:b:104:TYR:CE1	2.49	0.48
4:d:4:TYR:CD2	4:d:125:GLY:HA2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:37:LYS:HE2	4:d:160:SER:HA	1.96	0.48
12:l:129:PHE:CD2	13:m:106:TYR:CG	3.02	0.48
2:B:109:LEU:CD1	10:3:78:GLU:OE2	2.62	0.48
2:B:174:PHE:CE1	2:B:198:GLU:OE1	2.66	0.48
8:1:17:PHE:O	8:1:18:LYS:C	2.57	0.48
8:1:41:ASP:HB2	8:1:183:ARG:HH12	1.79	0.48
8:1:175:ASP:OD1	8:1:177:SER:N	2.40	0.48
16:V:270:TYR:O	16:V:271:VAL:C	2.56	0.48
26:U:180:ASP:OD2	26:U:195:LYS:NZ	2.47	0.48
33:J:183:LYS:HB3	33:J:276:LEU:HD23	1.96	0.48
1:a:19:PHE:HA	1:a:24:ARG:O	2.14	0.48
1:a:87:ILE:CG2	1:a:88:PRO:HD3	2.44	0.48
2:b:2:THR:N	7:g:128:SER:HB3	2.29	0.48
6:f:173:GLU:OE1	7:g:57:LYS:CB	2.62	0.48
1:A:175:GLN:OE1	1:A:175:GLN:C	2.57	0.48
3:C:16:GLU:HB2	3:C:18:ARG:HB2	1.95	0.48
16:V:221:TRP:CH2	26:U:199:GLY:HA2	2.48	0.48
17:T:259:ILE:HA	17:T:262:LYS:HD2	1.94	0.48
20:Z:68:LEU:HB3	20:Z:98:ASP:OD1	2.14	0.48
27:O:99:LEU:HD21	27:O:132:GLU:HG2	1.95	0.48
28:H:371:ILE:HG23	28:H:371:ILE:O	2.13	0.48
29:I:260:GLY:N	29:I:261:PRO:HD2	2.29	0.48
34:8:357:ARG:HD2	34:8:429:VAL:HG23	1.95	0.48
2:b:97:TYR:CE2	2:b:105:PRO:HA	2.49	0.47
3:c:162:ALA:HB3	4:d:54:LEU:HD13	1.95	0.47
8:h:44:THR:HG21	8:h:54:ARG:HE	1.79	0.47
8:h:60:ASP:OD1	8:h:102:LEU:HD22	2.13	0.47
8:h:135:ILE:CG2	8:h:140:SER:CB	2.91	0.47
9:i:186:ASP:HA	9:i:189:GLN:HE21	1.78	0.47
13:m:153:LEU:CD1	10:3:144:ASP:OD1	2.62	0.47
1:A:232:LYS:HE3	1:A:232:LYS:HB3	1.56	0.47
7:G:21:ASN:O	7:G:25:GLU:OE1	2.32	0.47
7:G:100:LYS:HZ2	14:7:101:LYS:HE3	1.78	0.47
14:7:98:ARG:O	14:7:101:LYS:HG3	2.14	0.47
16:V:258:GLU:HG3	16:V:270:TYR:HB2	1.96	0.47
21:N:889:ARG:NH1	21:N:909:GLU:OE2	2.46	0.47
28:H:464:MET:O	28:H:465:GLN:C	2.57	0.47
13:m:157:PHE:CE2	10:3:152:SER:CB	2.97	0.47
11:4:11:ASP:OD2	11:4:11:ASP:C	2.57	0.47
12:5:250:VAL:HG13	12:5:268:VAL:HG22	1.95	0.47
13:6:23:ILE:HD13	13:6:191:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:548:ASP:OD2	20:Z:549:ASN:N	2.47	0.47
20:Z:802:ASP:OD1	20:Z:849:ARG:NH2	2.38	0.47
21:N:282:TYR:HE2	21:N:286:LEU:HB2	1.80	0.47
21:N:569:LYS:HG3	30:K:67:TYR:CZ	2.48	0.47
23:P:254:GLU:HB3	23:P:258:LYS:HZ3	1.77	0.47
23:P:326:ASP:O	23:P:327:LEU:HB2	2.14	0.47
28:H:67:ALA:HA	29:I:74:GLU:OE2	2.14	0.47
32:M:98:GLU:OE2	32:M:113:VAL:N	2.47	0.47
3:c:191:GLU:HG2	3:c:195:LYS:HD2	1.96	0.47
9:i:36:LYS:HB2	9:i:152:TYR:O	2.13	0.47
11:k:86:GLN:HA	11:k:86:GLN:NE2	2.26	0.47
2:b:171:ALA:O	2:b:175:LEU:HD12	2.13	0.47
7:g:74:ILE:HG21	7:g:112:PHE:CD1	2.48	0.47
11:k:142:SER:HA	11:k:145:ASP:OD1	2.14	0.47
12:l:181:ARG:HD3	12:l:257:GLU:OE2	2.14	0.47
6:F:20:PHE:HA	6:F:23:GLU:OE2	2.13	0.47
7:G:205:GLU:N	7:G:205:GLU:CD	2.71	0.47
7:G:218:TRP:CD1	7:G:231:VAL:CG2	2.97	0.47
9:2:213:ALA:C	9:2:214:GLU:OE1	2.58	0.47
10:3:67:PHE:O	10:3:71:THR:CG2	2.62	0.47
16:V:73:GLN:CD	16:V:73:GLN:H	2.23	0.47
16:V:230:TYR:CD1	26:U:250:GLU:HG2	2.50	0.47
19:Y:30:GLU:O	19:Y:31:GLU:HB2	2.14	0.47
20:Z:35:GLU:O	20:Z:35:GLU:HG2	2.13	0.47
26:U:50:ASN:OD1	26:U:51:SER:N	2.48	0.47
27:O:329:MET:HA	27:O:332:ILE:HD12	1.96	0.47
31:L:280:MET:HE1	31:L:323:ILE:CG2	2.44	0.47
32:M:248:ALA:HB3	32:M:282:GLU:O	2.14	0.47
32:M:355:ASP:O	32:M:359:GLN:NE2	2.47	0.47
6:f:107:ARG:CD	14:n:110:ASP:OD2	2.62	0.47
10:j:182:GLY:O	10:j:202:MET:HE2	2.12	0.47
13:m:140:GLU:HA	13:m:140:GLU:OE2	2.13	0.47
1:A:19:PHE:HA	1:A:24:ARG:O	2.14	0.47
3:C:29:ILE:HD13	3:C:134:SER:OG	2.15	0.47
9:2:189:GLN:HE22	9:2:220:LEU:HD21	1.78	0.47
10:3:73:LEU:O	10:3:77:LYS:HD2	2.14	0.47
20:Z:309:GLN:O	20:Z:310:LEU:C	2.55	0.47
21:N:641:LEU:HD13	21:N:660:LEU:HG	1.97	0.47
25:R:179:PHE:CE1	25:R:187:VAL:HG21	2.49	0.47
32:M:228:LYS:N	36:M:501:ATP:O2B	2.34	0.47
33:J:388:LYS:O	33:J:392:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:10:THR:O	3:c:129:ARG:HD2	2.14	0.47
3:c:29:ILE:HD13	3:c:134:SER:OG	2.15	0.47
4:d:4:TYR:HE2	4:d:125:GLY:HA2	1.79	0.47
9:i:225:ARG:HD2	13:6:201:GLU:OE2	2.14	0.47
10:j:73:LEU:O	10:j:77:LYS:HD2	2.14	0.47
10:j:74:TYR:O	10:j:78:GLU:OE1	2.32	0.47
13:m:53:ASP:OD1	13:m:220:VAL:HG21	2.14	0.47
6:F:62:LYS:HA	6:F:74:LEU:HD21	1.97	0.47
7:G:218:TRP:CE3	7:G:220:SER:HB3	2.49	0.47
12:5:236:ILE:HG21	12:5:250:VAL:HG12	1.96	0.47
26:U:201:GLN:HG2	27:O:378:GLU:OE1	2.14	0.47
30:K:124:SER:O	30:K:125:THR:OG1	2.29	0.47
1:a:175:GLN:OE1	1:a:175:GLN:C	2.57	0.47
6:f:6:TYR:CE2	7:g:9:ASP:OD1	2.67	0.47
7:g:72:ARG:HH22	14:n:101:LYS:HZ2	1.63	0.47
8:h:49:LYS:HE3	8:h:111:TYR:O	2.15	0.47
9:i:254:GLU:O	9:i:255:GLU:HG3	2.15	0.47
10:j:67:PHE:O	10:j:71:THR:CG2	2.62	0.47
13:m:23:ILE:HD13	13:m:191:LEU:HD11	1.96	0.47
14:n:258:ILE:O	14:n:259:LYS:HD3	2.15	0.47
6:F:77:LEU:CD2	32:M:433:TYR:CE2	2.98	0.47
8:1:49:LYS:HE3	8:1:111:TYR:O	2.15	0.47
9:2:254:GLU:O	9:2:255:GLU:HG3	2.15	0.47
10:3:53:ILE:CG2	10:3:60:VAL:HG13	2.45	0.47
11:4:109:LYS:HE3	11:4:186:LYS:HA	1.97	0.47
11:4:142:SER:HA	11:4:145:ASP:OD1	2.14	0.47
13:6:226:GLU:OE1	13:6:227:LEU:O	2.32	0.47
14:7:114:ALA:O	14:7:119:ALA:HB2	2.14	0.47
15:W:130:LYS:CA	15:W:133:LYS:HE3	2.44	0.47
16:V:205:LYS:NZ	16:V:209:GLU:HB3	2.28	0.47
17:T:265:ASP:OD2	27:O:387:ARG:NH2	2.47	0.47
19:Y:3:THR:OG1	22:S:317:HIS:CD2	2.68	0.47
22:S:273:PHE:HB2	22:S:296:ALA:HB2	1.97	0.47
22:S:452:TYR:OH	26:U:249:VAL:HG13	2.15	0.47
23:P:266:TYR:CE2	23:P:328:ALA:HB2	2.50	0.47
24:Q:68:MET:HB3	24:Q:74:LEU:HD12	1.96	0.47
28:H:77:ALA:HB3	28:H:78:PRO:HD3	1.97	0.47
28:H:258:LEU:CD2	36:H:501:ATP:N9	2.74	0.47
29:I:95:GLN:HG2	29:I:95:GLN:O	2.14	0.47
29:I:262:ARG:HD2	29:I:262:ARG:N	2.29	0.47
31:L:245:PHE:CE1	31:L:279:PHE:CD1	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:L:291:PHE:O	31:L:293:GLU:OE2	2.33	0.47
33:J:31:GLU:HA	33:J:34:ILE:HD12	1.97	0.47
34:8:119:TYR:CE1	34:8:207:GLN:OE1	2.68	0.47
34:8:434:GLY:HA2	34:8:451:PHE:O	2.14	0.47
8:h:115:ASN:O	8:h:116:LYS:HG2	2.15	0.47
9:i:81:THR:O	9:i:85:THR:HG22	2.14	0.47
12:l:93:SER:O	12:l:106:VAL:HG23	2.15	0.47
12:l:175:MET:HE2	12:l:202:PHE:O	2.14	0.47
14:n:165:LEU:HD23	14:n:165:LEU:H	1.80	0.47
2:B:99:ARG:NH2	9:2:90:SER:HB3	2.30	0.47
4:D:122:GLN:OE1	4:D:122:GLN:O	2.33	0.47
9:2:36:LYS:HB2	9:2:152:TYR:O	2.13	0.47
12:5:181:ARG:HD3	12:5:257:GLU:OE2	2.14	0.47
28:H:177:ASP:HB3	28:H:180:LYS:O	2.15	0.47
28:H:233:GLU:CD	34:8:357:ARG:HH21	2.23	0.47
28:H:282:LYS:NZ	30:K:285:GLN:HB2	2.30	0.47
29:I:279:VAL:HG13	29:I:279:VAL:O	2.14	0.47
31:L:50:GLN:H	31:L:50:GLN:CD	2.23	0.47
32:M:309:LEU:O	32:M:342:ARG:NH1	2.48	0.47
3:c:5:ARG:NE	3:c:5:ARG:HA	2.30	0.47
4:d:171:VAL:O	4:d:175:LEU:HG	2.15	0.47
7:g:21:ASN:O	7:g:25:GLU:OE1	2.32	0.47
9:i:214:GLU:N	9:i:214:GLU:CD	2.73	0.47
11:k:11:ASP:OD2	11:k:11:ASP:C	2.57	0.47
11:k:109:LYS:HE3	11:k:186:LYS:HA	1.97	0.47
2:B:97:TYR:CE2	2:B:105:PRO:HA	2.49	0.47
9:2:81:THR:O	9:2:85:THR:HG22	2.14	0.47
9:2:170:HIS:CG	9:2:183:LEU:HD11	2.50	0.47
10:3:165:GLU:OE1	10:3:165:GLU:HA	2.15	0.47
12:5:93:SER:O	12:5:106:VAL:HG23	2.15	0.47
13:6:122:LEU:HB2	13:6:217:LYS:HZ3	1.79	0.47
20:Z:81:SER:O	20:Z:82:MET:SD	2.73	0.47
20:Z:112:LYS:C	20:Z:112:LYS:HD3	2.40	0.47
20:Z:212:LEU:HD22	20:Z:221:VAL:CA	2.44	0.47
21:N:606:VAL:HG21	21:N:625:LEU:HD21	1.96	0.47
29:I:90:GLU:O	29:I:94:LYS:HD3	2.15	0.47
29:I:99:ILE:HD11	29:I:135:PHE:CE1	2.49	0.47
29:I:122:SER:OG	29:I:125:MET:O	2.29	0.47
30:K:79:LEU:HA	33:J:55:VAL:HG23	1.97	0.47
31:L:173:PHE:O	31:L:245:PHE:CE2	2.68	0.47
34:8:254:GLU:O	34:8:254:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:32:ALA:HA	3:c:51:LYS:HE3	1.97	0.47
7:g:218:TRP:CD1	7:g:231:VAL:CG2	2.98	0.47
8:h:41:ASP:HB2	8:h:183:ARG:HH12	1.79	0.47
13:m:122:LEU:HB2	13:m:217:LYS:HZ3	1.78	0.47
1:A:36:ASN:OD1	1:A:173:PRO:HA	2.15	0.47
8:1:115:ASN:O	8:1:116:LYS:HG2	2.15	0.47
9:2:186:ASP:HA	9:2:189:GLN:HG2	1.96	0.47
10:3:95:LEU:HB3	10:3:127:ILE:O	2.15	0.47
11:4:44:MET:HG3	11:4:104:ILE:HG12	1.97	0.47
12:5:113:ASN:ND2	12:5:138:CYS:SG	2.87	0.47
13:6:169:GLU:OE1	13:6:179:PRO:HD3	2.15	0.47
16:V:39:LYS:NZ	26:U:13:LEU:HD23	2.30	0.47
16:V:185:ILE:HG13	33:J:118:ASP:HB2	1.96	0.47
30:K:346:ARG:NE	30:K:349:ARG:HH22	2.12	0.47
31:L:170:MET:HB2	31:L:244:ILE:HG23	1.97	0.47
7:g:93:ARG:NH1	14:n:109:TYR:CD2	2.83	0.46
9:i:213:ALA:C	9:i:214:GLU:OE1	2.58	0.46
12:l:129:PHE:CD2	13:m:106:TYR:CD2	3.03	0.46
12:l:179:TYR:HD2	12:l:257:GLU:N	2.13	0.46
5:E:69:GLU:O	5:E:93:ARG:NE	2.39	0.46
7:G:71:ASP:OD2	7:G:72:ARG:NH2	2.41	0.46
10:3:73:LEU:C	10:3:77:LYS:HD2	2.40	0.46
12:5:179:TYR:HD2	12:5:257:GLU:N	2.13	0.46
16:V:36:LYS:HE2	26:U:13:LEU:HD11	1.96	0.46
16:V:198:SER:O	16:V:199:LEU:HD22	2.16	0.46
22:S:118:PHE:O	22:S:119:TYR:C	2.58	0.46
28:H:254:THR:HB	28:H:377:PHE:CE2	2.50	0.46
28:H:256:LYS:HZ1	36:H:501:ATP:PG	2.37	0.46
5:e:51:GLU:OE2	5:e:210:GLU:OE1	2.34	0.46
11:k:177:LYS:NZ	11:4:170:LYS:HA	2.30	0.46
13:m:188:VAL:HA	13:m:191:LEU:HG	1.97	0.46
13:m:213:LEU:HD23	13:m:222:LYS:HG3	1.97	0.46
13:m:226:GLU:OE1	13:m:227:LEU:O	2.32	0.46
3:C:9:ARG:HE	4:D:6:ARG:HH12	1.62	0.46
5:E:85:ALA:HB2	5:E:140:VAL:HG21	1.96	0.46
13:6:53:ASP:OD1	13:6:220:VAL:HG21	2.14	0.46
14:7:136:ARG:HA	14:7:139:LYS:HZ3	1.79	0.46
16:V:60:ASP:OD2	21:N:475:ALA:HB1	2.15	0.46
16:V:244:MET:HE2	24:Q:415:LEU:HD21	1.97	0.46
29:I:300:ARG:O	29:I:304:ARG:HG2	2.15	0.46
31:L:329:ARG:CB	32:M:291:PHE:HE2	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:10:ARG:HD3	5:e:10:ARG:HA	1.67	0.46
5:e:70:ILE:HD12	5:e:74:ILE:HG22	1.97	0.46
5:e:85:ALA:HB2	5:e:140:VAL:HG21	1.96	0.46
6:f:112:LEU:HG	6:f:147:PHE:CE1	2.51	0.46
9:i:170:HIS:CG	9:i:183:LEU:HD11	2.50	0.46
10:j:53:ILE:CG2	10:j:60:VAL:HG13	2.45	0.46
1:A:87:ILE:CG2	1:A:88:PRO:HD3	2.44	0.46
3:C:32:ALA:HA	3:C:51:LYS:HE3	1.97	0.46
5:E:10:ARG:HD3	5:E:10:ARG:HA	1.67	0.46
6:F:112:LEU:HG	6:F:147:PHE:CE1	2.50	0.46
7:G:11:SER:C	7:G:23:GLN:HG2	2.41	0.46
8:1:44:THR:HG21	8:1:54:ARG:HE	1.79	0.46
13:6:48:GLU:OE1	14:7:170:TYR:CA	2.63	0.46
16:V:25:GLU:OE1	16:V:61:TYR:C	2.58	0.46
19:Y:38:PHE:CZ	22:S:370:LEU:HD12	2.50	0.46
20:Z:871:HIS:CG	20:Z:871:HIS:O	2.68	0.46
30:K:154:SER:O	30:K:155:ASP:HB3	2.15	0.46
31:L:254:LYS:HD3	32:M:256:ILE:O	2.16	0.46
34:8:119:TYR:O	34:8:123:THR:HG23	2.15	0.46
1:a:14:ARG:HG2	7:g:8:TYR:OH	2.16	0.46
1:a:129:THR:O	1:a:129:THR:OG1	2.29	0.46
7:g:218:TRP:HH2	7:g:223:GLU:C	2.24	0.46
9:i:254:GLU:C	9:i:255:GLU:HG3	2.41	0.46
2:B:198:GLU:O	24:Q:209:TYR:CZ	2.68	0.46
8:1:57:SER:HB3	8:1:60:ASP:OD2	2.16	0.46
12:5:84:GLN:OE1	12:5:221:TRP:CD1	2.69	0.46
17:T:143:SER:CB	17:T:147:LYS:HE2	2.45	0.46
19:Y:27:LYS:NZ	22:S:307:LEU:HB3	2.30	0.46
20:Z:82:MET:HE1	20:Z:89:LEU:HD13	1.97	0.46
21:N:221:ASP:OD2	21:N:223:LEU:HB3	2.15	0.46
21:N:282:TYR:CZ	21:N:286:LEU:HD22	2.51	0.46
21:N:572:LEU:HD12	30:K:67:TYR:CD2	2.50	0.46
29:I:295:ASN:CG	32:M:295:LYS:O	2.59	0.46
30:K:161:MET:HG3	30:K:236:ARG:HB3	1.97	0.46
1:a:36:ASN:OD1	1:a:173:PRO:HA	2.15	0.46
5:e:110:GLU:OE1	5:e:111:SER:N	2.49	0.46
8:h:135:ILE:HD11	8:h:147:CYS:SG	2.56	0.46
10:j:120:PHE:HA	10:j:134:LYS:HZ3	1.79	0.46
10:j:165:GLU:OE1	10:j:165:GLU:HA	2.15	0.46
11:k:160:LEU:HD12	11:k:163:LEU:CD1	2.43	0.46
4:D:84:ILE:HG22	4:D:88:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:171:VAL:O	4:D:175:LEU:HG	2.15	0.46
5:E:70:ILE:HD12	5:E:74:ILE:HG22	1.97	0.46
5:E:110:GLU:OE1	5:E:111:SER:N	2.49	0.46
11:4:19:LYS:HB3	11:4:19:LYS:HE3	1.76	0.46
20:Z:232:LYS:O	20:Z:236:PHE:O	2.33	0.46
21:N:494:LYS:HE2	21:N:497:ALA:HB2	1.97	0.46
21:N:515:ARG:HG2	21:N:546:LEU:CD1	2.45	0.46
22:S:65:ASN:HA	22:S:72:GLU:OE2	2.16	0.46
22:S:126:LYS:O	33:J:3:ALA:CB	2.63	0.46
26:U:35:GLY:HA3	26:U:93:TYR:CE2	2.50	0.46
28:H:416:GLY:O	28:H:420:ARG:HD2	2.15	0.46
30:K:375:ASN:OD1	30:K:376:ASP:N	2.47	0.46
7:g:11:SER:C	7:g:23:GLN:HG2	2.41	0.46
10:j:53:ILE:HG21	10:j:60:VAL:HG13	1.98	0.46
10:j:73:LEU:C	10:j:77:LYS:HD2	2.40	0.46
14:n:262:GLY:CA	9:2:140:PHE:HE1	2.27	0.46
1:A:141:LEU:HB3	1:A:143:PHE:HE2	1.81	0.46
2:B:109:LEU:O	2:B:113:GLU:HG3	2.16	0.46
3:C:5:ARG:NE	3:C:5:ARG:HA	2.30	0.46
3:C:89:ASN:OD1	3:C:90:THR:N	2.49	0.46
3:C:219:GLY:HA3	9:2:255:GLU:OE1	2.16	0.46
5:E:184:LEU:HD23	6:F:56:LEU:HD11	1.96	0.46
8:1:127:SER:HB3	14:7:94:GLN:CD	2.41	0.46
8:1:165:LYS:HE3	8:1:202:TYR:HB3	1.98	0.46
9:2:254:GLU:C	9:2:255:GLU:HG3	2.41	0.46
20:Z:6:ASP:OD2	20:Z:22:LYS:NZ	2.48	0.46
20:Z:523:ALA:HB3	20:Z:562:TRP:CZ2	2.51	0.46
21:N:562:THR:CG2	21:N:564:ASN:OD1	2.64	0.46
25:R:213:TYR:CD1	25:R:243:LEU:HD21	2.51	0.46
25:R:306:PRO:O	25:R:310:GLU:HG2	2.16	0.46
31:L:309:LEU:HB3	31:L:342:ARG:HH12	1.80	0.46
9:i:186:ASP:HA	9:i:189:GLN:HG2	1.96	0.46
1:A:58:LYS:HD2	1:A:58:LYS:O	2.16	0.46
5:E:51:GLU:OE2	5:E:210:GLU:OE1	2.33	0.46
9:2:244:GLU:HB2	10:3:198:ARG:HG2	1.96	0.46
13:6:21:LEU:HD11	13:6:158:LEU:HD23	1.98	0.46
13:6:122:LEU:HB3	13:6:217:LYS:HZ3	1.81	0.46
13:6:188:VAL:HA	13:6:191:LEU:HG	1.97	0.46
14:7:39:VAL:HG23	14:7:90:ILE:HG12	1.98	0.46
20:Z:592:GLU:OE2	20:Z:597:SER:OG	2.34	0.46
21:N:739:PHE:CD1	21:N:739:PHE:C	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Q:298:ALA:HA	24:Q:321:TYR:CD1	2.51	0.46
24:Q:415:LEU:O	24:Q:419:LEU:HG	2.16	0.46
26:U:41:ALA:O	26:U:42:ASN:HB2	2.15	0.46
28:H:151:GLN:O	28:H:152:ILE:C	2.58	0.46
30:K:416:LYS:O	30:K:416:LYS:HG3	2.15	0.46
32:M:132:VAL:HG12	32:M:134:LEU:H	1.81	0.46
32:M:432:PHE:CE2	32:M:433:TYR:CE1	3.04	0.46
33:J:197:LEU:HD11	38:J:501:ADP:N9	2.31	0.46
3:c:89:ASN:OD1	3:c:90:THR:N	2.49	0.46
9:i:222:PRO:HB2	9:i:223:ASN:ND2	2.31	0.46
12:l:276:LYS:HD2	12:l:281:SER:O	2.16	0.46
13:m:122:LEU:HB3	13:m:217:LYS:HZ3	1.81	0.46
2:B:178:ARG:NE	2:B:178:ARG:HA	2.31	0.46
7:G:218:TRP:HH2	7:G:223:GLU:C	2.24	0.46
10:3:74:TYR:CD1	10:3:78:GLU:OE1	2.69	0.46
11:4:25:ILE:O	11:4:25:ILE:HG13	2.15	0.46
12:5:253:TYR:HE1	12:5:262:TYR:CD1	2.33	0.46
20:Z:56:LEU:O	20:Z:146:PHE:CE1	2.68	0.46
20:Z:85:VAL:HB	20:Z:86:PRO:HD3	1.97	0.46
24:Q:256:GLU:OE2	24:Q:256:GLU:HA	2.15	0.46
27:O:188:PHE:CE2	27:O:217:LEU:HD23	2.50	0.46
28:H:156:VAL:HG21	32:M:77:TYR:OH	2.15	0.46
30:K:387:MET:HE2	30:K:387:MET:N	2.30	0.46
31:L:354:GLU:HG2	31:L:355:ALA:N	2.31	0.46
4:d:120:TYR:CD2	4:d:126:VAL:HB	2.51	0.46
11:k:25:ILE:O	11:k:25:ILE:HG13	2.15	0.46
11:k:44:MET:HG3	11:k:104:ILE:HG12	1.97	0.46
12:l:84:GLN:OE1	12:l:221:TRP:CD1	2.69	0.46
14:n:109:TYR:O	14:n:110:ASP:HB2	2.15	0.46
4:D:120:TYR:CD2	4:D:129:PHE:CE2	3.04	0.46
8:1:135:ILE:HD11	8:1:147:CYS:SG	2.56	0.46
14:7:200:LYS:CD	14:7:200:LYS:N	2.78	0.46
21:N:590:ALA:HA	21:N:593:PHE:CD1	2.51	0.46
23:P:69:ARG:HH12	23:P:109:SER:CB	2.28	0.46
28:H:208:TYR:HA	28:H:262:ALA:HB1	1.97	0.46
29:I:102:ASN:HB3	29:I:103:PRO:HD2	1.98	0.46
31:L:85:GLU:OE1	31:L:86:LYS:HE2	2.16	0.46
32:M:199:LEU:N	32:M:200:PRO:HD2	2.31	0.46
33:J:116:ARG:HG3	33:J:123:HIS:HB2	1.98	0.46
3:c:5:ARG:HB3	3:c:6:TYR:HD1	1.81	0.46
3:c:69:LEU:HD11	3:c:75:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:199:LYS:HD3	3:c:199:LYS:N	2.31	0.46
6:f:211:LEU:HD22	6:f:234:ILE:HD11	1.98	0.46
8:h:57:SER:HB3	8:h:60:ASP:OD2	2.16	0.46
13:m:21:LEU:HD11	13:m:158:LEU:HD23	1.98	0.46
3:C:51:LYS:HB2	3:C:51:LYS:HZ3	1.81	0.46
5:E:222:ILE:HD12	5:E:227:GLY:C	2.41	0.46
16:V:288:LEU:HD13	26:U:261:LEU:HB2	1.97	0.46
20:Z:800:SER:C	20:Z:802:ASP:H	2.24	0.46
21:N:143:LYS:HA	21:N:146:LYS:HZ3	1.80	0.46
22:S:74:LEU:HD11	22:S:90:LYS:HD3	1.98	0.46
22:S:174:ARG:HA	22:S:177:ASN:ND2	2.31	0.46
23:P:291:LYS:HD3	23:P:291:LYS:N	2.30	0.46
1:a:133:TYR:CE2	2:b:3:ASP:OD1	2.69	0.45
7:g:93:ARG:HD3	14:n:109:TYR:CE1	2.51	0.45
10:j:74:TYR:CD1	10:j:78:GLU:OE1	2.69	0.45
12:l:179:TYR:CD1	12:l:185:PRO:HG3	2.51	0.45
13:m:26:GLU:OE1	13:m:183:LEU:HB2	2.16	0.45
6:F:91:GLN:OE1	6:F:111:LEU:HD12	2.16	0.45
9:2:69:LYS:HA	9:2:69:LYS:HD2	1.72	0.45
10:3:4:PRO:HA	10:3:7:ILE:HD12	1.98	0.45
12:5:179:TYR:CD1	12:5:185:PRO:HG3	2.51	0.45
14:7:163:VAL:HG22	14:7:164:ASN:N	2.30	0.45
16:V:49:VAL:HG12	16:V:50:MET:N	2.31	0.45
17:T:249:MET:HA	17:T:249:MET:HE3	1.98	0.45
21:N:151:LYS:HE3	30:K:42:ASN:O	2.16	0.45
26:U:82:LYS:HA	32:M:68:LYS:HZ1	1.81	0.45
28:H:64:LYS:HG3	28:H:65:GLU:N	2.31	0.45
33:J:197:LEU:HD12	38:J:501:ADP:C4	2.51	0.45
7:g:185:GLU:OE1	7:g:185:GLU:O	2.35	0.45
6:F:211:LEU:HD22	6:F:234:ILE:HD11	1.98	0.45
10:3:53:ILE:HG21	10:3:60:VAL:HG13	1.98	0.45
10:3:182:GLY:O	10:3:184:GLY:N	2.49	0.45
19:Y:37:ASP:OD2	19:Y:37:ASP:N	2.49	0.45
20:Z:172:ASP:O	20:Z:173:ALA:O	2.34	0.45
20:Z:254:PRO:HG3	29:I:62:MET:SD	2.56	0.45
20:Z:313:ILE:HD11	20:Z:897:HIS:HD2	1.80	0.45
20:Z:923:ILE:CG1	20:Z:924:LYS:H	2.29	0.45
22:S:452:TYR:CZ	25:R:396:LYS:HD3	2.52	0.45
27:O:341:ILE:HD13	27:O:348:VAL:HA	1.98	0.45
28:H:362:ASP:OD2	28:H:363:PRO:HD2	2.16	0.45
33:J:35:ARG:HD2	33:J:35:ARG:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:J:163:VAL:HG23	33:J:164:ILE:HG12	1.97	0.45
1:a:105:ARG:NH1	1:a:109:GLY:O	2.49	0.45
1:a:211:ILE:HG13	1:a:212:ASP:N	2.32	0.45
3:c:219:GLY:C	9:i:255:GLU:HG2	2.42	0.45
6:f:62:LYS:HA	6:f:74:LEU:HD21	1.97	0.45
9:i:93:GLU:O	9:i:97:LEU:HD13	2.16	0.45
10:j:63:LEU:O	10:j:67:PHE:HD2	1.98	0.45
10:j:95:LEU:HB3	10:j:127:ILE:O	2.15	0.45
11:k:29:LYS:HG3	11:k:32:ASP:HB2	1.99	0.45
12:l:253:TYR:HE1	12:l:262:TYR:CD1	2.33	0.45
13:m:169:GLU:OE1	13:m:179:PRO:HD3	2.15	0.45
1:A:211:ILE:HG13	1:A:212:ASP:N	2.32	0.45
9:2:227:GLU:CD	9:2:227:GLU:C	2.85	0.45
10:3:63:LEU:O	10:3:67:PHE:HD2	1.99	0.45
22:S:173:LEU:HG	22:S:174:ARG:H	1.81	0.45
24:Q:328:ASP:O	24:Q:332:ARG:NE	2.50	0.45
27:O:132:GLU:OE1	27:O:135:ARG:NH1	2.50	0.45
1:a:58:LYS:HD2	1:a:58:LYS:O	2.16	0.45
1:a:141:LEU:HB3	1:a:143:PHE:HE2	1.81	0.45
1:a:149:GLU:CD	1:a:149:GLU:N	2.75	0.45
2:b:68:THR:CG2	2:b:104:TYR:HD1	2.29	0.45
4:d:44:LEU:HD12	4:d:72:VAL:HG23	1.99	0.45
5:e:70:ILE:HD11	5:e:76:CYS:HB2	1.98	0.45
2:B:217:GLU:OE2	2:B:217:GLU:C	2.60	0.45
8:1:68:VAL:HG21	8:1:91:PHE:CE1	2.51	0.45
11:4:46:PHE:CE2	11:4:53:THR:HB	2.52	0.45
12:5:276:LYS:HD2	12:5:281:SER:O	2.16	0.45
20:Z:163:GLU:OE2	20:Z:174:GLU:HA	2.16	0.45
20:Z:911:LYS:HB3	29:I:181:TYR:CE1	2.52	0.45
22:S:348:LEU:HD23	22:S:363:THR:HG21	1.98	0.45
23:P:241:LEU:HB3	23:P:264:ILE:HG12	1.98	0.45
25:R:281:SER:HA	25:R:286:LEU:HD23	1.99	0.45
25:R:401:HIS:O	25:R:405:LYS:HG2	2.17	0.45
26:U:15:LEU:HD21	26:U:134:THR:CG2	2.47	0.45
29:I:428:VAL:HG12	29:I:428:VAL:O	2.16	0.45
30:K:350:ARG:HB3	30:K:350:ARG:HH11	1.82	0.45
31:L:170:MET:O	31:L:245:PHE:CD2	2.69	0.45
6:f:91:GLN:OE1	6:f:111:LEU:HD12	2.16	0.45
6:f:121:GLN:OE1	7:g:129:VAL:HB	2.17	0.45
7:g:85:GLY:O	7:g:89:VAL:HG12	2.16	0.45
12:l:133:TRP:O	12:l:136:SER:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:223:ARG:HG3	14:n:223:ARG:O	2.17	0.45
4:D:73:LEU:HD23	4:D:73:LEU:C	2.41	0.45
5:E:121:LEU:HD22	6:F:79:PRO:CB	2.32	0.45
10:3:204:GLN:O	10:3:205:ASP:O	2.34	0.45
13:6:26:GLU:OE1	13:6:183:LEU:HB2	2.17	0.45
14:7:240:THR:HG21	14:7:242:LYS:NZ	2.32	0.45
16:V:186:GLN:N	16:V:189:ILE:HG22	2.31	0.45
20:Z:958:ASN:C	20:Z:958:ASN:OD1	2.60	0.45
27:O:350:ILE:H	27:O:350:ILE:HD12	1.81	0.45
28:H:196:THR:O	28:H:200:VAL:HG23	2.16	0.45
29:I:225:PRO:C	36:I:501:ATP:O1G	2.59	0.45
29:I:258:GLY:O	29:I:262:ARG:HG2	2.16	0.45
30:K:87:LYS:HD3	30:K:87:LYS:N	2.31	0.45
34:8:317:PHE:CD2	35:9:71:LEU:HB2	2.51	0.45
2:b:217:GLU:OE2	2:b:217:GLU:C	2.60	0.45
9:i:227:GLU:C	9:i:227:GLU:CD	2.85	0.45
10:j:66:MET:CG	10:j:70:LYS:NZ	2.79	0.45
13:m:58:ILE:HG23	13:m:94:ILE:CD1	2.47	0.45
1:A:105:ARG:NH1	1:A:109:GLY:O	2.49	0.45
4:D:204:GLN:C	4:D:205:THR:HG23	2.42	0.45
9:2:214:GLU:N	9:2:214:GLU:CD	2.73	0.45
11:4:19:LYS:HE2	11:4:177:LYS:O	2.16	0.45
12:5:133:TRP:O	12:5:136:SER:HB2	2.17	0.45
12:5:266:HIS:CG	12:5:271:LEU:HD12	2.51	0.45
16:V:147:VAL:O	16:V:147:VAL:HG22	2.17	0.45
21:N:25:LEU:HB3	21:N:60:MET:HG2	1.99	0.45
22:S:452:TYR:O	22:S:452:TYR:CG	2.69	0.45
25:R:345:TYR:CB	25:R:348:LEU:HD11	2.47	0.45
26:U:165:GLU:H	26:U:165:GLU:CD	2.24	0.45
28:H:434:ARG:HA	28:H:434:ARG:NE	2.30	0.45
29:I:271:ALA:HB1	29:I:322:VAL:HG22	1.97	0.45
30:K:270:PHE:CE2	30:K:272:ASP:OD1	2.70	0.45
32:M:98:GLU:OE2	32:M:112:ALA:HB1	2.17	0.45
34:8:463:LYS:HD2	34:8:463:LYS:C	2.41	0.45
3:c:49:GLU:OE2	3:c:206:LEU:HD12	2.17	0.45
6:f:171:TYR:CD2	6:f:174:ARG:NH2	2.85	0.45
7:g:218:TRP:CZ3	7:g:223:GLU:HB2	2.52	0.45
10:j:182:GLY:O	10:j:184:GLY:N	2.49	0.45
10:j:204:GLN:O	10:j:205:ASP:O	2.34	0.45
12:l:266:HIS:CG	12:l:271:LEU:HD12	2.51	0.45
3:C:69:LEU:HD11	3:C:75:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:71:ASP:OD1	5:E:73:HIS:ND1	2.50	0.45
6:F:171:TYR:CD2	6:F:174:ARG:NH2	2.84	0.45
6:F:173:GLU:OE1	7:G:57:LYS:HB3	2.17	0.45
7:G:85:GLY:O	7:G:89:VAL:HG12	2.16	0.45
7:G:218:TRP:CZ3	7:G:223:GLU:HB2	2.52	0.45
16:V:25:GLU:OE2	16:V:57:PHE:HE1	2.00	0.45
21:N:556:ALA:HB2	21:N:590:ALA:HB1	1.98	0.45
22:S:393:ARG:HG2	22:S:393:ARG:HH11	1.81	0.45
26:U:111:LYS:HG2	26:U:118:PRO:HG2	1.97	0.45
28:H:396:MET:HE3	29:I:211:MET:HE3	1.97	0.45
29:I:58:LYS:HD2	29:I:58:LYS:H	1.82	0.45
2:b:109:LEU:O	2:b:113:GLU:HG3	2.16	0.45
8:h:68:VAL:HG21	8:h:91:PHE:CE1	2.51	0.45
13:m:188:VAL:HA	13:m:191:LEU:CD2	2.47	0.45
3:C:199:LYS:HD3	3:C:199:LYS:N	2.31	0.45
9:2:93:GLU:O	9:2:97:LEU:HD13	2.16	0.45
9:2:222:PRO:HB2	9:2:223:ASN:ND2	2.31	0.45
11:4:2:ASP:HB2	11:4:18:SER:CB	2.47	0.45
13:6:27:ASP:O	13:6:27:ASP:CG	2.60	0.45
21:N:282:TYR:CE2	21:N:286:LEU:HD22	2.52	0.45
22:S:48:LEU:HD12	22:S:48:LEU:H	1.81	0.45
22:S:315:LYS:HE3	22:S:345:TYR:CE1	2.52	0.45
28:H:88:ARG:NE	28:H:94:GLU:OE2	2.49	0.45
28:H:196:THR:HG22	28:H:290:MET:CE	2.47	0.45
29:I:85:PHE:HA	29:I:90:GLU:OE1	2.17	0.45
29:I:198:VAL:HA	29:I:323:LYS:HE3	1.99	0.45
2:b:124:SER:O	2:b:125:GLY:O	2.35	0.45
2:b:224:TYR:CE1	9:i:65:ARG:NH1	2.85	0.45
3:c:19:LEU:HD22	3:c:19:LEU:HA	1.54	0.45
6:f:78:ALA:N	6:f:79:PRO:CD	2.80	0.45
8:h:165:LYS:HD2	8:h:197:PHE:CE2	2.52	0.45
11:k:46:PHE:CE2	11:k:53:THR:HB	2.52	0.45
12:l:179:TYR:CE2	12:l:257:GLU:HB2	2.52	0.45
1:A:26:TYR:O	1:A:30:TYR:CD1	2.70	0.45
2:B:201:GLU:OE2	24:Q:209:TYR:OH	2.25	0.45
5:E:70:ILE:HD11	5:E:76:CYS:HB2	1.98	0.45
8:1:165:LYS:HD2	8:1:197:PHE:CE2	2.52	0.45
9:2:237:GLY:N	10:3:165:GLU:OE2	2.50	0.45
10:3:30:GLY:HA2	10:3:36:VAL:HG23	1.99	0.45
13:6:58:ILE:HG23	13:6:94:ILE:CD1	2.47	0.45
13:6:213:LEU:HD23	13:6:222:LYS:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:765:MET:HA	20:Z:770:GLU:HG2	1.99	0.45
20:Z:827:LEU:HD12	20:Z:828:ALA:N	2.32	0.45
22:S:315:LYS:HE2	22:S:374:ASP:CG	2.42	0.45
22:S:348:LEU:HD23	22:S:363:THR:CG2	2.46	0.45
25:R:134:TRP:HD1	25:R:137:LEU:HD12	1.82	0.45
25:R:186:TYR:HE1	25:R:190:LYS:HE2	1.82	0.45
2:b:239:THR:OG1	2:b:240:SER:N	2.50	0.45
7:g:69:VAL:HG22	7:g:70:VAL:O	2.17	0.45
7:g:88:LEU:HG	7:g:116:LEU:HD21	1.99	0.45
8:h:17:PHE:HE2	8:h:19:ASP:HB2	1.81	0.45
14:n:114:ALA:HA	14:n:118:GLU:HB2	1.99	0.45
6:F:78:ALA:N	6:F:79:PRO:CD	2.80	0.45
7:G:88:LEU:HG	7:G:116:LEU:HD21	1.99	0.45
16:V:95:LEU:HB2	16:V:101:ASP:HB3	1.99	0.45
16:V:215:ASN:ND2	26:U:131:GLY:O	2.50	0.45
16:V:261:LEU:H	16:V:261:LEU:HD23	1.82	0.45
20:Z:8:LYS:HD3	20:Z:9:GLN:N	2.32	0.45
20:Z:243:GLN:NE2	20:Z:921:GLU:OE2	2.50	0.45
21:N:535:LEU:HD12	21:N:538:LYS:HZ3	1.81	0.45
24:Q:282:LEU:HD23	24:Q:287:THR:HG21	1.99	0.45
26:U:61:LYS:CD	26:U:61:LYS:H	2.30	0.45
5:e:131:GLU:OE1	5:e:131:GLU:HA	2.17	0.44
5:e:222:ILE:HD12	5:e:227:GLY:C	2.41	0.44
10:j:172:LEU:HD11	10:j:200:LEU:CD1	2.47	0.44
11:k:2:ASP:HB2	11:k:18:SER:CB	2.47	0.44
1:A:149:GLU:CD	1:A:149:GLU:N	2.75	0.44
2:B:68:THR:CG2	2:B:104:TYR:HD1	2.29	0.44
3:C:5:ARG:HB3	3:C:6:TYR:HD1	1.80	0.44
4:D:24:LEU:HD23	4:D:24:LEU:C	2.42	0.44
6:F:86:ASN:OD1	6:F:89:ARG:NH2	2.50	0.44
7:G:72:ARG:NH1	14:7:105:THR:OG1	2.50	0.44
10:3:66:MET:CG	10:3:70:LYS:NZ	2.79	0.44
14:7:233:ILE:HD12	14:7:233:ILE:N	2.32	0.44
20:Z:462:VAL:HG13	20:Z:462:VAL:O	2.16	0.44
21:N:151:LYS:HG2	30:K:45:SER:HB2	1.99	0.44
21:N:430:ASN:HB2	21:N:443:LEU:HD13	1.99	0.44
22:S:113:SER:HG	22:S:119:TYR:HH	1.63	0.44
27:O:112:LYS:HD3	27:O:112:LYS:N	2.33	0.44
29:I:230:THR:CB	36:I:501:ATP:O2B	2.63	0.44
30:K:277:ILE:HG22	30:K:296:LEU:HD13	1.99	0.44
33:J:279:LEU:CD1	33:J:282:PHE:CE1	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:230:LYS:NZ	13:6:190:LYS:CB	2.80	0.44
10:j:30:GLY:HA2	10:j:36:VAL:HG23	1.99	0.44
11:k:19:LYS:HE2	11:k:177:LYS:O	2.16	0.44
13:m:27:ASP:CG	13:m:27:ASP:O	2.60	0.44
14:n:241:PHE:HE2	14:n:243:LYS:HD3	1.82	0.44
3:C:49:GLU:OE2	3:C:206:LEU:HD12	2.17	0.44
3:C:100:LYS:HD3	10:3:65:GLU:CG	2.48	0.44
4:D:120:TYR:HE2	4:D:129:PHE:CZ	2.35	0.44
5:E:9:ASP:OD1	5:E:9:ASP:C	2.60	0.44
9:2:80:ASP:O	9:2:84:VAL:HG22	2.18	0.44
10:3:172:LEU:HD11	10:3:200:LEU:CD1	2.47	0.44
11:4:153:THR:OG1	11:4:154:THR:N	2.50	0.44
17:T:23:CYS:O	17:T:27:LEU:HG	2.16	0.44
20:Z:780:MET:HE3	20:Z:792:VAL:HG21	1.99	0.44
20:Z:869:ASP:OD2	20:Z:878:LEU:HD12	2.17	0.44
21:N:135:SER:O	21:N:139:ARG:HD3	2.17	0.44
24:Q:158:ILE:HG21	24:Q:181:GLU:OE2	2.17	0.44
29:I:213:ILE:O	29:I:214:LYS:C	2.60	0.44
1:a:26:TYR:O	1:a:30:TYR:CD1	2.70	0.44
2:b:178:ARG:NE	2:b:178:ARG:HA	2.31	0.44
5:e:32:LYS:HD3	5:e:32:LYS:HA	1.79	0.44
7:g:82:ILE:HB	7:g:83:PRO:HD3	2.00	0.44
8:h:165:LYS:HE3	8:h:202:TYR:HB3	1.98	0.44
12:l:128:GLN:OE1	13:m:102:GLN:NE2	2.50	0.44
12:l:240:ALA:O	10:3:205:ASP:OD2	2.35	0.44
2:B:239:THR:OG1	2:B:240:SER:N	2.50	0.44
3:C:228:LYS:HE2	3:C:230:PHE:CE1	2.52	0.44
13:6:188:VAL:HA	13:6:191:LEU:CD2	2.47	0.44
15:W:130:LYS:HA	15:W:133:LYS:HE3	1.99	0.44
16:V:24:LYS:HB3	16:V:199:LEU:CD2	2.46	0.44
16:V:154:ASP:OD1	16:V:156:PHE:CE1	2.71	0.44
17:T:200:LEU:H	17:T:233:VAL:HG12	1.81	0.44
19:Y:33:ASP:OD2	19:Y:33:ASP:C	2.60	0.44
20:Z:266:LYS:NZ	20:Z:290:GLU:OE1	2.50	0.44
21:N:149:GLU:C	21:N:151:LYS:N	2.75	0.44
22:S:51:ARG:HE	22:S:178:LEU:CD2	2.29	0.44
23:P:84:LYS:O	23:P:85:LYS:C	2.60	0.44
28:H:225:VAL:HA	28:H:350:LYS:HD2	2.00	0.44
28:H:308:PHE:HB2	28:H:352:MET:O	2.17	0.44
29:I:117:HIS:HB3	29:I:129:TYR:CE1	2.52	0.44
1:a:133:TYR:CZ	2:b:3:ASP:OD1	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:71:ASP:OD1	5:e:73:HIS:ND1	2.50	0.44
8:h:88:ALA:CB	8:h:120:TYR:HD2	2.30	0.44
10:j:4:PRO:HA	10:j:7:ILE:HD12	1.98	0.44
12:l:188:TYR:CE1	12:l:198:LYS:HB2	2.52	0.44
8:1:88:ALA:CB	8:1:120:TYR:HD2	2.31	0.44
8:1:200:ASP:OD2	8:1:200:ASP:N	2.50	0.44
12:5:93:SER:HA	12:5:106:VAL:O	2.18	0.44
20:Z:258:PRO:HB2	20:Z:259:PRO:HD3	2.00	0.44
20:Z:509:LEU:O	20:Z:512:ILE:O	2.36	0.44
21:N:567:ALA:O	21:N:571:LEU:HG	2.18	0.44
22:S:406:ASP:OD1	25:R:383:ARG:CZ	2.66	0.44
24:Q:228:GLU:O	24:Q:230:LYS:HD3	2.18	0.44
26:U:6:GLU:H	26:U:6:GLU:CD	2.25	0.44
28:H:431:ILE:O	28:H:434:ARG:HD2	2.17	0.44
3:c:2:GLY:HA2	7:g:127:ASN:HB3	2.00	0.44
8:h:196:ILE:HG22	14:7:256:LYS:HE2	2.00	0.44
12:l:257:GLU:OE1	12:l:257:GLU:HA	2.18	0.44
2:B:124:SER:O	2:B:125:GLY:C	2.61	0.44
4:D:122:GLN:HE21	5:E:136:ARG:NH1	2.15	0.44
11:4:162:LYS:O	11:4:166:GLN:HG2	2.18	0.44
16:V:20:ARG:HD3	21:N:437:GLU:HG2	1.98	0.44
20:Z:376:SER:O	20:Z:377:ALA:CB	2.65	0.44
23:P:431:HIS:ND1	26:U:156:HIS:CD2	2.86	0.44
25:R:60:ALA:HB3	25:R:61:PRO:HD3	2.00	0.44
27:O:135:ARG:O	27:O:139:LEU:HG	2.18	0.44
27:O:192:SER:CB	27:O:217:LEU:HD21	2.47	0.44
29:I:419:ALA:HA	29:I:422:ARG:HH11	1.83	0.44
30:K:92:VAL:CG1	31:L:116:LYS:HE2	2.47	0.44
30:K:163:GLU:O	30:K:166:LYS:NZ	2.50	0.44
31:L:244:ILE:HD11	31:L:269:TYR:CE1	2.53	0.44
32:M:174:GLU:O	32:M:174:GLU:CD	2.60	0.44
33:J:306:ARG:HD3	33:J:309:ARG:CZ	2.47	0.44
1:a:35:THR:C	1:a:36:ASN:HD22	2.26	0.44
1:A:119:LYS:NZ	9:2:98:TYR:C	2.75	0.44
2:B:92:VAL:HG22	2:B:113:GLU:OE1	2.18	0.44
2:B:222:LEU:HD11	2:B:224:TYR:OH	2.18	0.44
7:G:184:PRO:O	23:P:3:ARG:CZ	2.65	0.44
12:5:82:ARG:HB2	12:5:200:ASP:OD2	2.18	0.44
13:6:75:ARG:CZ	13:6:113:TYR:OH	2.66	0.44
16:V:180:LEU:HD23	16:V:180:LEU:H	1.82	0.44
26:U:141:GLU:O	26:U:142:GLN:CD	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:H:276:GLY:O	28:H:314:VAL:HG12	2.18	0.44
28:H:328:GLU:H	28:H:328:GLU:CD	2.26	0.44
29:I:283:GLU:HA	29:I:283:GLU:OE2	2.17	0.44
31:L:264:ARG:HB2	31:L:307:GLU:OE1	2.17	0.44
33:J:33:LYS:HD3	33:J:37:LYS:NZ	2.33	0.44
33:J:121:MET:HA	33:J:121:MET:HE2	1.99	0.44
2:b:222:LEU:HD11	2:b:224:TYR:OH	2.18	0.44
6:f:61:LYS:HD2	6:f:61:LYS:HA	1.80	0.44
9:i:69:LYS:HD2	9:i:69:LYS:HA	1.72	0.44
11:k:49:GLU:CD	12:l:166:LYS:NZ	2.76	0.44
12:l:93:SER:HA	12:l:106:VAL:O	2.17	0.44
12:l:209:THR:HG22	11:4:139:TYR:HE1	1.81	0.44
2:B:142:PHE:HE1	10:3:115:LYS:HD2	1.82	0.44
2:B:221:LEU:HD11	2:B:236:ARG:HD3	2.00	0.44
5:E:131:GLU:OE1	5:E:131:GLU:HA	2.17	0.44
9:2:217:ARG:O	9:2:218:ASN:HB2	2.18	0.44
20:Z:510:LEU:HB2	20:Z:511:PRO:HD3	1.99	0.44
20:Z:784:SER:HB3	20:Z:792:VAL:HG11	1.99	0.44
28:H:196:THR:OG1	28:H:197:MET:HE2	2.18	0.44
29:I:125:MET:HB3	29:I:126:PRO:CD	2.44	0.44
32:M:75:LEU:N	32:M:75:LEU:HD23	2.33	0.44
33:J:361:VAL:CG2	33:J:389:VAL:HG21	2.48	0.44
2:b:20:GLN:HA	2:b:23:TYR:CD2	2.52	0.44
5:e:9:ASP:OD1	5:e:9:ASP:C	2.60	0.44
6:f:81:ALA:HB2	6:f:130:VAL:HG21	2.00	0.44
6:f:86:ASN:OD1	6:f:89:ARG:NH2	2.50	0.44
9:i:80:ASP:O	9:i:84:VAL:HG22	2.18	0.44
9:i:217:ARG:O	9:i:218:ASN:HB2	2.18	0.44
13:m:110:PHE:N	13:m:110:PHE:CD2	2.86	0.44
3:C:168:ASN:OD1	3:C:168:ASN:O	2.36	0.44
4:D:102:ASP:O	4:D:103:PRO:C	2.61	0.44
6:F:98:VAL:O	14:7:127:GLU:HG3	2.18	0.44
7:G:69:VAL:HG22	7:G:70:VAL:O	2.17	0.44
8:1:17:PHE:HE2	8:1:19:ASP:HB2	1.81	0.44
12:5:96:THR:OG1	12:5:97:ALA:N	2.51	0.44
12:5:179:TYR:CE2	12:5:257:GLU:HB2	2.52	0.44
12:5:188:TYR:CE1	12:5:198:LYS:HB2	2.52	0.44
13:6:229:ARG:HH12	14:7:193:ASP:CG	2.25	0.44
16:V:25:GLU:OE1	16:V:62:THR:C	2.61	0.44
16:V:188:LEU:H	16:V:188:LEU:HD12	1.83	0.44
16:V:230:TYR:CD2	23:P:412:LEU:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:632:LYS:HZ1	21:N:876:PRO:HD2	1.82	0.44
22:S:49:ASP:HB2	22:S:50:PRO:HD3	2.00	0.44
24:Q:198:LEU:HD23	24:Q:198:LEU:C	2.43	0.44
26:U:173:HIS:O	26:U:176:ARG:NH2	2.51	0.44
28:H:272:ILE:HD12	28:H:305:ILE:O	2.17	0.44
28:H:291:VAL:HB	28:H:335:GLU:HG2	2.00	0.44
29:I:133:LEU:HD22	29:I:155:SER:OG	2.17	0.44
29:I:248:VAL:HG12	29:I:250:SER:H	1.83	0.44
31:L:136:ASP:HB3	31:L:139:LYS:HG3	2.00	0.44
31:L:244:ILE:HG22	31:L:245:PHE:O	2.18	0.44
3:c:228:LYS:HE2	3:c:230:PHE:CE1	2.52	0.44
6:f:110:HIS:ND1	7:g:86:ARG:CZ	2.80	0.44
7:g:74:ILE:HG21	7:g:112:PHE:CE1	2.52	0.44
1:A:204:GLU:OE2	1:A:247:ALA:HB3	2.18	0.44
6:F:81:ALA:HB2	6:F:130:VAL:HG21	2.00	0.44
9:2:37:PHE:CE2	9:2:177:LYS:CA	3.01	0.44
11:4:29:LYS:HG3	11:4:32:ASP:HB2	1.99	0.44
14:7:111:ASN:O	14:7:115:ASP:HB3	2.18	0.44
16:V:205:LYS:HZ2	16:V:209:GLU:CB	2.29	0.44
16:V:258:GLU:OE2	16:V:270:TYR:O	2.36	0.44
22:S:220:ILE:O	22:S:224:LYS:HG2	2.18	0.44
24:Q:254:SER:HA	24:Q:257:LYS:HE2	1.99	0.44
25:R:93:LYS:NZ	25:R:95:ASP:OD1	2.51	0.44
27:O:16:MET:HA	27:O:16:MET:HE2	1.98	0.44
28:H:439:THR:O	28:H:442:ASP:OD1	2.36	0.44
30:K:214:PRO:HG2	30:K:217:THR:CG2	2.48	0.44
31:L:361:PHE:CE1	31:L:391:ILE:HD12	2.52	0.44
32:M:315:PHE:O	32:M:316:SER:O	2.35	0.44
2:b:221:LEU:HD11	2:b:236:ARG:HD3	2.00	0.43
3:c:71:ASP:O	3:c:71:ASP:CG	2.60	0.43
4:d:97:ARG:NH1	11:k:65:GLN:NE2	2.66	0.43
11:k:162:LYS:O	11:k:166:GLN:HG2	2.18	0.43
14:n:254:PHE:HB3	9:2:173:GLN:CD	2.43	0.43
2:B:124:SER:O	2:B:125:GLY:O	2.35	0.43
17:T:113:LEU:HD21	17:T:121:LYS:HE2	2.00	0.43
21:N:734:VAL:O	21:N:737:SER:OG	2.35	0.43
25:R:113:LEU:HD11	25:R:137:LEU:HD11	1.99	0.43
28:H:420:ARG:HD3	36:H:501:ATP:H1'	1.99	0.43
28:H:464:MET:N	28:H:464:MET:SD	2.90	0.43
31:L:132:ARG:CD	31:L:156:MET:HG2	2.48	0.43
33:J:222:TYR:OH	33:J:229:MET:HE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:143:PHE:CD2	1:a:143:PHE:N	2.87	0.43
3:c:110:ILE:HD13	11:k:71:GLU:OE1	2.18	0.43
4:d:101:GLU:O	4:d:102:ASP:CB	2.66	0.43
5:e:121:LEU:CD2	6:f:79:PRO:HB3	2.47	0.43
8:h:200:ASP:OD2	8:h:200:ASP:N	2.50	0.43
9:i:37:PHE:CE2	9:i:177:LYS:CA	3.01	0.43
12:l:246:SER:O	10:3:205:ASP:OD2	2.36	0.43
13:m:205:GLN:NE2	9:2:53:PRO:HB3	2.33	0.43
14:n:195:GLU:HG3	14:n:198:ILE:HD12	2.00	0.43
3:C:2:GLY:HA3	6:F:123:TYR:CE2	2.53	0.43
3:C:71:ASP:O	3:C:71:ASP:CG	2.60	0.43
8:1:62:GLN:HB3	9:2:113:LYS:HZ2	1.83	0.43
12:5:257:GLU:OE1	12:5:257:GLU:HA	2.18	0.43
15:W:95:GLN:NE2	15:W:132:LEU:HD23	2.34	0.43
20:Z:909:ARG:HB2	20:Z:926:ASN:HD22	1.82	0.43
22:S:480:ARG:HB2	33:J:43:ARG:HG3	2.00	0.43
25:R:351:LYS:HD2	25:R:351:LYS:C	2.43	0.43
26:U:52:PHE:CG	26:U:76:MET:HE2	2.53	0.43
28:H:87:ASP:OD2	28:H:87:ASP:N	2.50	0.43
28:H:191:ILE:O	28:H:191:ILE:HG13	2.18	0.43
29:I:230:THR:HB	36:I:501:ATP:O1A	2.17	0.43
30:K:83:GLN:O	30:K:86:VAL:HG12	2.19	0.43
30:K:362:LEU:HD23	30:K:402:ILE:HB	1.99	0.43
33:J:10:ILE:O	33:J:12:LEU:HD23	2.18	0.43
34:8:195:PHE:O	34:8:195:PHE:CD1	2.71	0.43
2:b:227:ILE:HG22	2:b:230:ASP:H	1.83	0.43
7:g:70:VAL:HG21	7:g:112:PHE:HE1	1.82	0.43
8:h:155:MET:HE1	8:h:163:PHE:CE1	2.53	0.43
8:1:18:LYS:HE2	8:1:154:ASN:HB3	2.01	0.43
11:4:9:VAL:O	11:4:11:ASP:N	2.52	0.43
20:Z:161:ILE:HG12	20:Z:210:TYR:CE2	2.52	0.43
20:Z:213:LYS:HE2	20:Z:256:LEU:HG	2.01	0.43
20:Z:498:ALA:O	20:Z:533:VAL:HA	2.17	0.43
20:Z:528:LEU:HD23	20:Z:569:ALA:HB2	2.01	0.43
21:N:502:PHE:CZ	21:N:538:LYS:HE2	2.54	0.43
21:N:565:ASN:OD1	30:K:60:LEU:HD12	2.18	0.43
22:S:488:GLN:CG	33:J:42:ARG:HH12	2.31	0.43
24:Q:155:LEU:HD12	24:Q:181:GLU:CD	2.43	0.43
25:R:113:LEU:HD21	25:R:137:LEU:CD2	2.47	0.43
26:U:83:ILE:O	31:L:99:GLN:NE2	2.52	0.43
26:U:85:ALA:O	31:L:96:LYS:CE	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:H:247:LEU:HG	28:H:249:TYR:CD1	2.53	0.43
28:H:258:LEU:CD1	36:H:501:ATP:H3'	2.45	0.43
33:J:9:ASN:O	33:J:10:ILE:O	2.36	0.43
1:a:15:HIS:HB3	3:c:6:TYR:OH	2.19	0.43
9:i:94:LEU:O	9:i:98:TYR:CD2	2.71	0.43
10:j:136:PHE:CD1	10:j:150:CYS:HB3	2.54	0.43
10:j:180:LEU:HG	12:5:99:ASN:OD1	2.18	0.43
11:k:153:THR:OG1	11:k:154:THR:N	2.50	0.43
12:l:82:ARG:HB2	12:l:200:ASP:OD2	2.18	0.43
12:l:96:THR:OG1	12:l:97:ALA:N	2.51	0.43
14:n:220:ARG:NH2	8:l:36:ALA:O	2.51	0.43
1:A:27:GLN:OE1	1:A:27:GLN:HA	2.18	0.43
4:D:63:LYS:N	4:D:63:LYS:HD3	2.32	0.43
5:E:32:LYS:HD3	5:E:32:LYS:HA	1.79	0.43
7:G:185:GLU:OE1	7:G:185:GLU:O	2.35	0.43
10:3:120:PHE:HA	10:3:134:LYS:HZ3	1.82	0.43
21:N:642:ASP:N	21:N:643:PRO:HD2	2.34	0.43
22:S:272:TYR:CE2	22:S:276:LEU:HD11	2.54	0.43
28:H:367:ARG:CZ	36:M:501:ATP:O1G	2.67	0.43
32:M:63:LYS:HA	32:M:66:LYS:HG2	2.00	0.43
32:M:186:LEU:CD1	36:M:501:ATP:HN62	2.27	0.43
1:a:33:LYS:CD	1:a:33:LYS:N	2.81	0.43
6:f:74:LEU:HD23	6:f:74:LEU:H	1.83	0.43
7:g:23:GLN:HA	7:g:23:GLN:OE1	2.19	0.43
9:i:135:THR:HG22	9:i:135:THR:O	2.18	0.43
1:A:87:ILE:HG22	1:A:88:PRO:HD3	2.01	0.43
2:B:20:GLN:HA	2:B:23:TYR:CD2	2.52	0.43
12:5:179:TYR:HD2	12:5:256:THR:C	2.27	0.43
13:6:13:TYR:CE2	13:6:114:TYR:CE1	3.06	0.43
14:7:204:GLN:OE1	14:7:204:GLN:N	2.47	0.43
16:V:54:LEU:HD12	16:V:54:LEU:N	2.33	0.43
16:V:67:ASP:N	16:V:67:ASP:OD1	2.50	0.43
20:Z:490:ILE:CD1	20:Z:526:ALA:HA	2.42	0.43
22:S:126:LYS:O	33:J:3:ALA:HB3	2.18	0.43
24:Q:352:GLU:HB3	24:Q:353:PRO:HD3	2.00	0.43
26:U:125:VAL:HG23	26:U:126:LYS:HD2	1.99	0.43
27:O:303:LYS:HA	27:O:303:LYS:HE3	1.99	0.43
28:H:202:GLU:CD	28:H:203:LYS:N	2.77	0.43
29:I:265:ARG:HB2	29:I:308:GLU:OE1	2.18	0.43
31:L:94:ASP:O	31:L:98:LEU:HG	2.18	0.43
33:J:149:MET:O	38:J:501:ADP:C2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:J:279:LEU:HD12	33:J:282:PHE:CE1	2.53	0.43
1:a:178:ILE:O	1:a:182:LEU:HG	2.19	0.43
1:a:189:SER:O	1:a:190:LYS:HB2	2.18	0.43
2:b:92:VAL:HG22	2:b:113:GLU:OE1	2.18	0.43
3:c:168:ASN:OD1	3:c:168:ASN:O	2.36	0.43
9:i:240:ALA:HB3	10:j:201:LYS:HB3	2.01	0.43
12:l:240:ALA:O	12:l:241:HIS:C	2.61	0.43
1:A:29:GLU:OE1	30:K:419:ASN:CB	2.67	0.43
4:D:66:LYS:HE3	4:D:66:LYS:HB2	1.91	0.43
4:D:218:ASP:O	4:D:219:SER:HB3	2.18	0.43
5:E:121:LEU:CD2	6:F:79:PRO:CB	2.94	0.43
7:G:109:ILE:HB	7:G:110:PRO:HD3	2.01	0.43
8:1:91:PHE:HD2	8:1:108:VAL:HG21	1.84	0.43
12:5:240:ALA:O	12:5:241:HIS:C	2.61	0.43
16:V:211:LYS:HD3	26:U:127:GLN:HB3	2.01	0.43
20:Z:133:ASP:OD1	20:Z:136:ARG:NH1	2.52	0.43
21:N:25:LEU:HD12	21:N:57:ASP:OD1	2.19	0.43
21:N:270:LEU:HD12	21:N:271:GLU:N	2.33	0.43
22:S:54:TRP:HZ3	22:S:178:LEU:HB2	1.84	0.43
22:S:406:ASP:OD1	25:R:383:ARG:NE	2.52	0.43
24:Q:381:ILE:HG21	25:R:344:SER:HA	2.00	0.43
24:Q:410:ASP:OD1	25:R:399:GLN:NE2	2.52	0.43
28:H:436:LYS:O	28:H:436:LYS:HG2	2.18	0.43
29:I:137:ASP:O	29:I:138:LYS:C	2.61	0.43
29:I:182:SER:H	29:I:184:ILE:HG12	1.83	0.43
29:I:269:LYS:CG	29:I:319:ARG:HH21	2.32	0.43
30:K:266:PRO:HB3	30:K:310:THR:HG23	1.99	0.43
34:8:357:ARG:HG2	34:8:357:ARG:HH11	1.84	0.43
35:9:63:LYS:O	35:9:64:GLU:HB2	2.18	0.43
7:g:31:VAL:HG11	7:g:135:SER:HB2	2.00	0.43
12:l:179:TYR:HD2	12:l:256:THR:C	2.27	0.43
14:n:179:PHE:CE2	14:n:183:MET:HG3	2.53	0.43
1:A:33:LYS:CD	1:A:33:LYS:N	2.81	0.43
2:B:103:GLU:OE2	2:B:104:TYR:N	2.52	0.43
2:B:103:GLU:OE2	2:B:104:TYR:O	2.37	0.43
4:D:140:PRO:O	4:D:141:ARG:HB2	2.18	0.43
7:G:74:ILE:HG21	7:G:112:PHE:CE1	2.52	0.43
8:1:100:ASP:OD2	14:7:34:THR:O	2.36	0.43
10:3:136:PHE:CD1	10:3:150:CYS:HB3	2.54	0.43
13:6:76:PHE:O	13:6:80:VAL:HG23	2.19	0.43
16:V:194:ARG:NH2	16:V:195:HIS:CE1	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:903:MET:O	20:Z:931:GLN:CD	2.62	0.43
21:N:175:ASP:OD2	21:N:175:ASP:N	2.52	0.43
23:P:130:ILE:O	23:P:131:PHE:C	2.60	0.43
23:P:419:VAL:O	23:P:423:LEU:HG	2.19	0.43
24:Q:308:ASN:O	24:Q:309:ARG:HB2	2.19	0.43
27:O:31:LYS:HD3	27:O:31:LYS:N	2.34	0.43
28:H:214:CYS:O	28:H:214:CYS:SG	2.77	0.43
29:I:266:GLN:O	29:I:267:ILE:C	2.62	0.43
29:I:393:GLN:OE1	36:I:501:ATP:C1'	2.66	0.43
30:K:40:LEU:C	30:K:44:ASN:OD1	2.62	0.43
30:K:306:PHE:CE2	30:K:313:LYS:HA	2.54	0.43
31:L:199:LEU:N	31:L:200:PRO:HD2	2.33	0.43
34:8:207:GLN:HB3	35:9:75:GLY:H	1.84	0.43
2:b:124:SER:O	2:b:125:GLY:C	2.61	0.43
3:c:45:VAL:CG2	3:c:189:ALA:HB1	2.49	0.43
5:e:70:ILE:HG21	5:e:112:LEU:HD21	2.00	0.43
12:l:99:ASN:OD1	10:3:180:LEU:HG	2.18	0.43
12:l:187:ILE:O	12:l:188:TYR:HD1	2.02	0.43
3:C:9:ARG:HH22	4:D:10:ILE:CD1	2.30	0.43
3:C:45:VAL:HG21	3:C:189:ALA:HB1	2.01	0.43
5:E:184:LEU:HD23	6:F:56:LEU:CD1	2.48	0.43
6:F:74:LEU:HD23	6:F:74:LEU:H	1.83	0.43
21:N:43:LEU:N	21:N:44:PRO:CD	2.82	0.43
21:N:470:LEU:HD11	21:N:504:TYR:CD2	2.54	0.43
23:P:23:LYS:O	23:P:27:LEU:HG	2.18	0.43
28:H:272:ILE:HD12	28:H:272:ILE:N	2.34	0.43
28:H:328:GLU:CD	28:H:328:GLU:N	2.77	0.43
29:I:394:ALA:HA	29:I:397:THR:OG1	2.18	0.43
30:K:346:ARG:HG2	30:K:346:ARG:HH11	1.83	0.43
34:8:111:PHE:O	34:8:467:ASP:OD1	2.36	0.43
34:8:245:ALA:O	34:8:246:ASN:HB2	2.18	0.43
13:m:76:PHE:O	13:m:80:VAL:HG23	2.19	0.43
1:A:35:THR:C	1:A:36:ASN:HD22	2.26	0.43
1:A:178:ILE:O	1:A:182:LEU:HG	2.19	0.43
2:B:53:SER:HA	30:K:423:LYS:HE3	1.99	0.43
3:C:69:LEU:HD11	3:C:75:VAL:CG1	2.49	0.43
7:G:82:ILE:HB	7:G:83:PRO:HD3	2.00	0.43
7:G:246:GLU:HA	7:G:246:GLU:OE2	2.19	0.43
11:4:118:GLN:HG3	11:4:133:HIS:CE1	2.54	0.43
22:S:111:ARG:O	22:S:112:ASN:C	2.61	0.43
24:Q:163:ARG:HG2	24:Q:163:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Q:220:LEU:HD13	24:Q:246:TYR:HE2	1.84	0.43
29:I:401:LEU:HD22	29:I:422:ARG:HH22	1.84	0.43
31:L:277:ILE:O	31:L:278:ILE:HD13	2.19	0.43
31:L:303:ARG:NH1	31:L:306:MET:HE1	2.34	0.43
34:8:412:TYR:HB3	34:8:413:LYS:HD3	2.00	0.43
34:8:433:ILE:HG22	34:8:495:LYS:NZ	2.34	0.43
1:a:27:GLN:OE1	1:a:27:GLN:HA	2.18	0.43
6:f:107:ARG:NH2	14:n:109:TYR:O	2.52	0.43
10:j:144:ASP:OD1	13:6:153:LEU:CD1	2.67	0.43
13:m:141:ARG:C	13:m:142:GLU:HG2	2.43	0.43
1:A:143:PHE:N	1:A:143:PHE:CD2	2.87	0.43
3:C:45:VAL:CG2	3:C:189:ALA:HB1	2.49	0.43
4:D:32:CYS:HA	4:D:165:GLY:HA3	2.01	0.43
5:E:13:SER:HB3	6:F:126:ARG:HD3	2.00	0.43
12:5:187:ILE:O	12:5:188:TYR:HD1	2.02	0.43
13:6:141:ARG:C	13:6:142:GLU:HG2	2.43	0.43
15:W:14:GLU:CD	15:W:14:GLU:N	2.77	0.43
17:T:27:LEU:N	17:T:28:PRO:HD2	2.34	0.43
19:Y:30:GLU:OE1	22:S:309:PHE:N	2.52	0.43
20:Z:700:GLU:HG2	20:Z:701:ILE:H	1.84	0.43
22:S:152:LEU:O	22:S:156:VAL:HB	2.19	0.43
25:R:280:ILE:O	25:R:280:ILE:HG13	2.19	0.43
27:O:19:ASP:OD2	27:O:20:PRO:HD2	2.18	0.43
28:H:90:ARG:CZ	29:I:99:ILE:HA	2.49	0.43
28:H:246:ILE:HA	28:H:373:ARG:O	2.18	0.43
28:H:444:LEU:HB2	28:H:445:LYS:NZ	2.34	0.43
29:I:184:ILE:HD12	29:I:191:ILE:HD11	2.01	0.43
30:K:303:MET:HE3	30:K:333:ARG:CG	2.48	0.43
30:K:343:LEU:HD23	30:K:343:LEU:C	2.43	0.43
1:a:204:GLU:OE2	1:a:247:ALA:HB3	2.18	0.42
3:c:64:GLU:H	3:c:64:GLU:HG2	1.61	0.42
4:d:172:ARG:O	4:d:176:GLU:OE2	2.37	0.42
6:f:110:HIS:CB	7:g:86:ARG:HH12	2.32	0.42
12:l:142:GLU:OE2	12:l:148:ARG:HA	2.19	0.42
2:B:227:ILE:HG22	2:B:230:ASP:H	1.83	0.42
4:D:203:VAL:HG11	4:D:210:ILE:HD13	2.01	0.42
9:2:94:LEU:O	9:2:98:TYR:CD2	2.71	0.42
11:4:35:THR:HG21	11:4:182:LYS:NZ	2.34	0.42
16:V:73:GLN:CD	16:V:73:GLN:N	2.77	0.42
20:Z:721:ASN:HB3	20:Z:767:TYR:CD1	2.54	0.42
20:Z:791:LYS:HB2	20:Z:874:ASN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:242:PHE:O	21:N:246:LYS:HG2	2.19	0.42
22:S:374:ASP:C	22:S:375:ASP:OD1	2.62	0.42
24:Q:24:GLU:CD	24:Q:73:LYS:HG2	2.43	0.42
24:Q:85:MET:HE1	24:Q:86:MET:SD	2.58	0.42
25:R:184:GLN:O	25:R:217:HIS:HE1	2.01	0.42
25:R:303:SER:C	25:R:306:PRO:HD2	2.44	0.42
32:M:125:GLN:OE1	32:M:125:GLN:N	2.51	0.42
33:J:221:LYS:O	33:J:221:LYS:HG2	2.19	0.42
1:a:36:ASN:O	1:a:39:ASN:ND2	2.53	0.42
4:d:180:ASP:OD2	4:d:181:ARG:N	2.52	0.42
6:f:38:LEU:CD1	6:f:189:LEU:HD12	2.49	0.42
7:g:246:GLU:OE2	7:g:246:GLU:HA	2.19	0.42
10:j:15:MET:HE2	10:j:154:TYR:HD1	1.84	0.42
12:l:129:PHE:HD2	13:m:106:TYR:CD2	2.37	0.42
13:m:13:TYR:CE2	13:m:114:TYR:CE1	3.06	0.42
14:n:39:VAL:O	14:n:89:ASP:HA	2.18	0.42
2:B:12:PHE:HA	2:B:18:LEU:HD23	2.01	0.42
2:B:186:GLU:OE1	24:Q:91:SER:HB3	2.20	0.42
6:F:38:LEU:CD1	6:F:189:LEU:HD12	2.49	0.42
13:6:110:PHE:CD2	13:6:110:PHE:N	2.86	0.42
16:V:117:TRP:CE3	16:V:118:LEU:O	2.71	0.42
16:V:260:GLU:O	16:V:266:LEU:HD11	2.19	0.42
22:S:423:VAL:O	22:S:427:ILE:HG12	2.19	0.42
24:Q:76:GLU:HG2	24:Q:80:HIS:CE1	2.54	0.42
24:Q:333:SER:HG	24:Q:334:HIS:CE1	2.37	0.42
24:Q:374:GLU:CD	24:Q:390:LEU:HD21	2.44	0.42
26:U:175:LEU:O	26:U:176:ARG:HD3	2.19	0.42
27:O:126:ILE:O	27:O:130:ASP:OD1	2.37	0.42
28:H:203:LYS:HD2	28:H:264:ALA:O	2.19	0.42
33:J:33:LYS:CD	33:J:37:LYS:NZ	2.82	0.42
34:8:451:PHE:CE2	34:8:463:LYS:HG2	2.54	0.42
7:g:34:GLY:O	7:g:167:LYS:HE3	2.19	0.42
8:h:91:PHE:HD2	8:h:108:VAL:HG21	1.84	0.42
11:k:9:VAL:O	11:k:11:ASP:N	2.52	0.42
13:m:91:LYS:HG2	13:m:92:LEU:N	2.34	0.42
14:n:258:ILE:CG2	9:2:152:TYR:CE2	3.00	0.42
1:A:133:TYR:CZ	2:B:3:ASP:OD1	2.73	0.42
4:D:69:SER:HB3	4:D:219:SER:OG	2.18	0.42
4:D:192:VAL:O	4:D:196:VAL:HG23	2.20	0.42
5:E:53:ARG:O	5:E:53:ARG:HG3	2.18	0.42
8:1:67:ILE:O	8:1:70:TYR:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:135:THR:O	9:2:135:THR:HG22	2.18	0.42
10:3:134:LYS:HD3	10:3:134:LYS:HA	1.79	0.42
12:5:142:GLU:OE2	12:5:148:ARG:HA	2.19	0.42
12:5:261:ILE:CG2	12:5:263:HIS:CE1	3.02	0.42
21:N:195:THR:HG22	21:N:597:ARG:NH1	2.34	0.42
24:Q:381:ILE:O	24:Q:384:LYS:HD3	2.19	0.42
25:R:71:LEU:HD22	25:R:71:LEU:H	1.84	0.42
25:R:407:GLY:HA2	26:U:263:LYS:NZ	2.35	0.42
27:O:125:GLY:O	27:O:129:ILE:HG12	2.19	0.42
27:O:180:LYS:NZ	27:O:216:ASP:O	2.52	0.42
28:H:211:VAL:HG23	28:H:262:ALA:CB	2.49	0.42
31:L:139:LYS:HE2	31:L:158:ILE:HD13	2.00	0.42
32:M:28:GLN:CD	32:M:28:GLN:N	2.78	0.42
32:M:267:PHE:O	32:M:271:LYS:HG3	2.20	0.42
33:J:361:VAL:HG22	33:J:389:VAL:HG21	2.01	0.42
2:b:12:PHE:HA	2:b:18:LEU:HD23	2.01	0.42
8:h:175:ASP:OD1	8:h:177:SER:OG	2.33	0.42
14:n:242:LYS:NZ	14:n:245:LEU:HD11	2.35	0.42
1:A:14:ARG:CD	7:G:8:TYR:OH	2.61	0.42
1:A:189:SER:O	1:A:190:LYS:HB2	2.18	0.42
5:E:210:GLU:O	5:E:211:LYS:HB3	2.19	0.42
6:F:51:ARG:HH12	32:M:431:SER:CB	2.32	0.42
7:G:31:VAL:HG11	7:G:135:SER:HB2	2.00	0.42
12:5:96:THR:HA	12:5:102:ALA:H	1.85	0.42
13:6:9:GLN:OE1	13:6:10:PHE:N	2.53	0.42
16:V:278:LYS:HG2	16:V:282:GLU:OE1	2.19	0.42
20:Z:142:ASP:OD1	20:Z:142:ASP:C	2.62	0.42
20:Z:161:ILE:CG2	20:Z:210:TYR:CE2	2.98	0.42
20:Z:766:HIS:HA	20:Z:799:PHE:HD1	1.83	0.42
20:Z:782:ILE:H	20:Z:782:ILE:HD12	1.84	0.42
24:Q:50:ARG:NH2	24:Q:88:PHE:CD1	2.88	0.42
24:Q:379:GLN:NE2	24:Q:383:ASP:OD2	2.51	0.42
27:O:109:LEU:HG	27:O:113:LYS:HG3	2.01	0.42
27:O:236:HIS:HD1	27:O:237:PRO:HD2	1.84	0.42
27:O:295:THR:O	27:O:299:THR:HG23	2.19	0.42
28:H:259:CYS:O	28:H:263:VAL:HG23	2.19	0.42
29:I:314:ASP:OD2	29:I:314:ASP:C	2.63	0.42
29:I:368:LYS:HE3	33:J:178:GLY:O	2.18	0.42
33:J:197:LEU:CD1	38:J:501:ADP:N9	2.82	0.42
35:9:7:THR:HG22	35:9:69:LEU:HD13	2.01	0.42
1:a:33:LYS:N	1:a:33:LYS:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:174:LYS:HG3	1:a:174:LYS:O	2.19	0.42
2:b:110:LEU:HA	2:b:113:GLU:HG3	2.02	0.42
2:b:230:ASP:OD2	2:b:230:ASP:N	2.53	0.42
8:h:196:ILE:O	8:h:197:PHE:HD1	2.03	0.42
11:k:96:ARG:HD2	11:k:96:ARG:HA	1.85	0.42
14:n:83:VAL:HG23	14:n:233:ILE:HD11	2.02	0.42
1:A:30:TYR:CD1	1:A:30:TYR:N	2.87	0.42
4:D:96:HIS:CD2	4:D:100:LEU:HD12	2.55	0.42
10:3:157:ASN:N	10:3:157:ASN:OD1	2.53	0.42
16:V:53:MET:SD	16:V:65:VAL:HG11	2.60	0.42
17:T:148:LEU:O	17:T:152:LEU:HG	2.19	0.42
20:Z:56:LEU:C	20:Z:146:PHE:CE1	2.97	0.42
20:Z:759:ARG:NH1	20:Z:789:GLN:OE1	2.53	0.42
21:N:271:GLU:OE2	21:N:417:ARG:CZ	2.67	0.42
23:P:168:TYR:HD1	30:K:398:ASN:ND2	2.18	0.42
24:Q:92:LYS:HA	24:Q:95:LYS:HE2	2.01	0.42
25:R:289:ILE:HD13	25:R:315:VAL:HG11	2.01	0.42
28:H:275:ILE:HB	28:H:278:GLU:HB2	2.01	0.42
29:I:219:VAL:HG12	29:I:220:ILE:N	2.34	0.42
29:I:268:PHE:HB2	29:I:319:ARG:CZ	2.49	0.42
32:M:189:GLN:CD	32:M:189:GLN:N	2.77	0.42
32:M:351:LEU:HG	32:M:352:PRO:HD2	2.01	0.42
33:J:225:GLU:OE2	33:J:228:ARG:HD2	2.20	0.42
34:8:152:GLN:H	34:8:152:GLN:CD	2.28	0.42
35:9:22:THR:HA	35:9:55:THR:HA	2.02	0.42
1:a:24:ARG:NH2	1:a:29:GLU:OE2	2.53	0.42
1:a:210:MET:SD	1:a:214:LEU:CD1	3.07	0.42
3:c:51:LYS:HB2	3:c:51:LYS:HZ3	1.80	0.42
6:f:110:HIS:HB3	7:g:86:ARG:HH12	1.84	0.42
7:g:100:LYS:NZ	14:n:101:LYS:NZ	2.67	0.42
8:h:67:ILE:O	8:h:70:TYR:HB3	2.19	0.42
9:i:189:GLN:NE2	9:i:220:LEU:HD21	2.35	0.42
9:i:246:ILE:HG13	10:j:194:GLU:OE2	2.20	0.42
11:k:7:ILE:HD11	11:k:157:GLY:HA2	2.01	0.42
11:k:118:GLN:HG3	11:k:133:HIS:CE1	2.54	0.42
1:A:174:LYS:O	1:A:174:LYS:HG3	2.19	0.42
1:A:210:MET:SD	1:A:214:LEU:CD1	3.07	0.42
4:D:143:ASP:OD1	4:D:143:ASP:N	2.52	0.42
9:2:248:ASN:HD22	9:2:248:ASN:N	2.18	0.42
14:7:47:MET:HE2	14:7:210:ILE:HG12	2.02	0.42
14:7:241:PHE:CE2	14:7:243:LYS:HD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:6:THR:HA	15:W:109:ARG:O	2.19	0.42
16:V:233:LYS:HE2	16:V:294:SER:HB2	2.02	0.42
20:Z:438:LYS:O	20:Z:442:VAL:HG22	2.20	0.42
21:N:515:ARG:CG	21:N:546:LEU:CD1	2.97	0.42
22:S:51:ARG:HH21	22:S:178:LEU:HD21	1.84	0.42
28:H:258:LEU:HD22	36:H:501:ATP:C8	2.54	0.42
30:K:193:VAL:O	30:K:194:GLN:HG3	2.20	0.42
31:L:295:THR:HG23	31:L:297:ALA:H	1.84	0.42
32:M:95:GLU:CD	32:M:95:GLU:N	2.78	0.42
33:J:124:LYS:NZ	33:J:127:GLU:OE1	2.52	0.42
2:b:103:GLU:OE2	2:b:104:TYR:N	2.52	0.42
3:c:69:LEU:HD11	3:c:75:VAL:CG1	2.49	0.42
3:c:218:LYS:O	3:c:218:LYS:CG	2.68	0.42
7:g:109:ILE:HB	7:g:110:PRO:HD3	2.01	0.42
11:k:130:TYR:CD2	11:k:144:LEU:HD13	2.55	0.42
12:l:94:ARG:HH11	12:l:94:ARG:HD3	1.73	0.42
12:l:128:GLN:OE1	13:m:138:SER:HA	2.20	0.42
13:m:9:GLN:OE1	13:m:10:PHE:N	2.53	0.42
4:D:102:ASP:O	4:D:103:PRO:O	2.37	0.42
5:E:47:VAL:HG11	5:E:200:VAL:HG21	2.01	0.42
5:E:70:ILE:HG21	5:E:112:LEU:HD21	2.00	0.42
7:G:23:GLN:HA	7:G:23:GLN:OE1	2.19	0.42
13:6:121:GLY:O	13:6:122:LEU:HD23	2.20	0.42
16:V:194:ARG:HB3	16:V:194:ARG:HH11	1.84	0.42
21:N:94:LYS:HA	21:N:94:LYS:CE	2.50	0.42
21:N:606:VAL:HB	21:N:621:THR:HG23	2.02	0.42
24:Q:359:ILE:HD13	24:Q:374:GLU:OE1	2.20	0.42
25:R:172:LEU:HD21	25:R:194:VAL:HG11	2.02	0.42
26:U:217:LYS:HD3	26:U:219:LEU:CD1	2.49	0.42
27:O:87:LYS:HD2	27:O:135:ARG:CZ	2.50	0.42
27:O:362:GLN:OE1	27:O:365:LYS:HD3	2.20	0.42
28:H:61:ALA:HA	28:H:64:LYS:HE3	2.01	0.42
28:H:310:GLU:OE2	29:I:311:ASN:ND2	2.53	0.42
28:H:428:MET:HA	28:H:431:ILE:HG12	2.00	0.42
29:I:222:TYR:CE2	29:I:349:LEU:HD13	2.54	0.42
32:M:179:THR:C	32:M:181:SER:N	2.77	0.42
32:M:282:GLU:OE2	32:M:328:ASN:ND2	2.53	0.42
1:a:87:ILE:N	1:a:88:PRO:HD2	2.35	0.42
2:b:17:LYS:HA	2:b:17:LYS:HD3	1.70	0.42
5:e:210:GLU:O	5:e:211:LYS:HB3	2.20	0.42
6:f:93:ASN:OD1	13:m:81:LYS:CE	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:108:VAL:CG2	10:j:139:SER:OG	2.68	0.42
12:l:140:LEU:HG	12:l:144:ARG:HH21	1.85	0.42
3:C:219:GLY:C	9:2:255:GLU:CD	2.88	0.42
7:G:11:SER:O	7:G:14:VAL:HG22	2.20	0.42
8:1:196:ILE:O	8:1:197:PHE:HD1	2.03	0.42
16:V:24:LYS:CG	16:V:199:LEU:HD23	2.50	0.42
16:V:148:LYS:HZ1	16:V:152:VAL:HG23	1.84	0.42
16:V:305:ILE:HG22	26:U:236:LEU:HD11	2.02	0.42
20:Z:743:ILE:HD11	20:Z:761:PHE:HB2	2.02	0.42
25:R:47:ALA:HB1	25:R:91:TRP:HB2	2.02	0.42
25:R:106:ASN:HA	25:R:140:TYR:OH	2.19	0.42
25:R:258:LEU:HD13	25:R:333:MET:HE2	2.00	0.42
26:U:60:GLU:N	26:U:60:GLU:CD	2.78	0.42
27:O:296:LEU:HD21	27:O:328:VAL:HG22	2.00	0.42
28:H:258:LEU:HD22	36:H:501:ATP:C1'	2.50	0.42
31:L:386:PHE:CE2	31:L:394:CYS:SG	3.13	0.42
31:L:420:ARG:HD2	31:L:420:ARG:C	2.44	0.42
3:c:9:ARG:HH22	5:e:10:ARG:NH1	2.17	0.42
8:h:37:ASN:HB3	8:h:40:THR:OG1	2.20	0.42
12:l:261:ILE:CG2	12:l:263:HIS:CE1	3.02	0.42
12:l:268:VAL:HB	10:3:203:ARG:NH2	2.34	0.42
14:n:179:PHE:CD2	14:n:183:MET:HG3	2.54	0.42
2:B:110:LEU:HA	2:B:113:GLU:HG3	2.02	0.42
4:D:141:ARG:CZ	12:5:182:LYS:CE	2.98	0.42
11:4:7:ILE:HD11	11:4:157:GLY:HA2	2.01	0.42
17:T:229:VAL:O	17:T:230:ASN:CG	2.62	0.42
20:Z:158:ALA:HA	20:Z:161:ILE:HB	2.01	0.42
20:Z:503:ASP:OD1	20:Z:504:GLU:N	2.53	0.42
21:N:430:ASN:CB	21:N:443:LEU:HD13	2.49	0.42
24:Q:95:LYS:HD3	24:Q:95:LYS:N	2.35	0.42
29:I:197:SER:O	29:I:323:LYS:NZ	2.46	0.42
29:I:433:GLU:OE1	29:I:437:LEU:CB	2.68	0.42
32:M:77:TYR:C	32:M:77:TYR:CD2	2.98	0.42
33:J:140:GLU:HG3	33:J:212:ARG:HH21	1.85	0.42
34:8:276:LEU:HD13	34:8:312:VAL:HG13	2.01	0.42
1:a:87:ILE:HG22	1:a:88:PRO:HD3	2.01	0.42
4:d:66:LYS:O	4:d:66:LYS:HG3	2.19	0.42
10:j:157:ASN:N	10:j:157:ASN:OD1	2.53	0.42
12:l:99:ASN:OD1	12:l:99:ASN:O	2.37	0.42
12:l:127:CYS:O	12:l:131:GLU:HG3	2.20	0.42
6:F:190:ILE:O	6:F:194:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:175:GLU:HA	7:G:178:LYS:HG3	2.02	0.42
9:2:189:GLN:NE2	9:2:220:LEU:HD21	2.35	0.42
12:5:140:LEU:HG	12:5:144:ARG:HH21	1.85	0.42
14:7:110:ASP:O	14:7:111:ASN:HB2	2.20	0.42
20:Z:318:LYS:HA	20:Z:321:PHE:CE1	2.55	0.42
20:Z:945:ILE:HG13	20:Z:958:ASN:CG	2.44	0.42
25:R:422:ARG:HE	26:U:273:LEU:HD21	1.84	0.42
26:U:61:LYS:CD	26:U:61:LYS:N	2.83	0.42
27:O:236:HIS:ND1	27:O:237:PRO:CD	2.83	0.42
28:H:192:ASP:N	28:H:193:PRO:HD2	2.35	0.42
28:H:255:GLY:CA	36:H:501:ATP:N7	2.81	0.42
29:I:338:LEU:C	29:I:338:LEU:HD23	2.45	0.42
30:K:347:ARG:O	30:K:351:LEU:HG	2.20	0.42
32:M:141:LYS:H	32:M:144:ASP:HB2	1.85	0.42
32:M:324:LEU:HD23	32:M:324:LEU:HA	1.91	0.42
34:8:303:ILE:HD12	34:8:344:MET:HB3	2.02	0.42
2:b:103:GLU:OE2	2:b:104:TYR:O	2.37	0.41
5:e:110:GLU:OE1	5:e:111:SER:CA	2.68	0.41
6:f:190:ILE:O	6:f:194:VAL:HG23	2.20	0.41
7:g:25:GLU:OE1	7:g:25:GLU:N	2.40	0.41
1:A:118:ALA:HA	1:A:143:PHE:CE1	2.55	0.41
3:C:4:ARG:HH12	6:F:124:GLY:HA2	1.83	0.41
3:C:231:LYS:HB2	3:C:234:GLU:OE1	2.20	0.41
17:T:127:GLN:HA	22:S:378:GLN:HE22	1.85	0.41
20:Z:563:VAL:HG12	20:Z:707:LYS:NZ	2.35	0.41
21:N:143:LYS:HB3	33:J:19:ILE:CD1	2.49	0.41
21:N:150:LEU:H	21:N:150:LEU:HD22	1.85	0.41
22:S:231:ALA:HB1	22:S:268:LEU:HD23	2.01	0.41
23:P:166:GLU:HG2	23:P:167:THR:N	2.35	0.41
25:R:27:SER:OG	25:R:320:LYS:NZ	2.44	0.41
30:K:254:VAL:O	30:K:257:VAL:HG12	2.20	0.41
1:a:30:TYR:N	1:a:30:TYR:HD1	2.18	0.41
9:i:230:LYS:NZ	13:6:190:LYS:HB2	2.35	0.41
1:A:87:ILE:N	1:A:88:PRO:HD2	2.35	0.41
9:2:212:ASP:O	9:2:214:GLU:OE1	2.37	0.41
12:5:99:ASN:OD1	12:5:99:ASN:O	2.37	0.41
15:W:50:GLY:HA2	15:W:72:ILE:HD11	2.02	0.41
16:V:182:LYS:HE2	16:V:183:ALA:C	2.44	0.41
17:T:137:GLU:O	17:T:138:ASP:O	2.38	0.41
21:N:470:LEU:HD11	21:N:504:TYR:CE2	2.55	0.41
22:S:475:TYR:CD1	22:S:475:TYR:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:P:130:ILE:C	23:P:132:VAL:N	2.77	0.41
23:P:319:GLU:HB3	23:P:320:PRO:HD3	2.00	0.41
26:U:112:LYS:HE3	26:U:113:TYR:CE1	2.55	0.41
27:O:29:PHE:CD1	27:O:29:PHE:N	2.87	0.41
27:O:170:SER:O	27:O:173:SER:OG	2.32	0.41
28:H:296:GLU:OE2	28:H:299:ARG:HD2	2.19	0.41
29:I:226:GLY:HA2	36:I:501:ATP:PB	2.60	0.41
29:I:234:LYS:HD3	33:J:278:GLN:HG2	2.00	0.41
33:J:185:VAL:HG23	33:J:185:VAL:O	2.21	0.41
34:8:474:LYS:O	34:8:478:GLU:OE2	2.37	0.41
2:b:94:HIS:HA	2:b:98:LYS:HB2	2.02	0.41
3:c:219:GLY:O	9:i:255:GLU:HG2	2.20	0.41
4:d:156:TYR:CE1	5:e:86:ARG:HD2	2.53	0.41
7:g:72:ARG:NH2	14:n:101:LYS:HZ2	2.17	0.41
10:j:134:LYS:HD3	10:j:134:LYS:HA	1.79	0.41
13:m:121:GLY:O	13:m:122:LEU:HD23	2.20	0.41
13:m:230:ASP:OD1	9:2:199:GLY:CA	2.68	0.41
1:A:30:TYR:N	1:A:30:TYR:HD1	2.18	0.41
3:C:91:ALA:HB2	3:C:115:LEU:HD21	2.01	0.41
7:G:34:GLY:O	7:G:167:LYS:HE3	2.19	0.41
8:1:11:SER:HB2	8:1:178:SER:OG	2.20	0.41
9:2:141:SER:HB3	9:2:154:LEU:HD13	2.03	0.41
10:3:108:VAL:CG2	10:3:139:SER:OG	2.68	0.41
16:V:262:THR:CG2	16:V:265:GLU:HG3	2.51	0.41
20:Z:471:LEU:HD12	20:Z:505:VAL:HG23	2.01	0.41
20:Z:727:GLU:OE1	20:Z:727:GLU:N	2.53	0.41
20:Z:864:MET:N	20:Z:864:MET:SD	2.94	0.41
20:Z:903:MET:O	20:Z:931:GLN:NE2	2.53	0.41
23:P:431:HIS:O	23:P:434:THR:OG1	2.34	0.41
28:H:81:LEU:HD23	28:H:81:LEU:C	2.44	0.41
28:H:243:PRO:O	28:H:350:LYS:HE2	2.21	0.41
30:K:123:LEU:HG	30:K:124:SER:O	2.21	0.41
30:K:163:GLU:OE1	30:K:233:ALA:HA	2.20	0.41
31:L:88:TYR:CE2	32:M:61:LYS:HB3	2.56	0.41
34:8:339:LEU:HD12	34:8:339:LEU:HA	1.94	0.41
3:c:45:VAL:HG21	3:c:189:ALA:HB1	2.01	0.41
8:h:170:GLN:HE22	8:1:149:LYS:CB	2.27	0.41
11:k:35:THR:HG21	11:k:182:LYS:NZ	2.34	0.41
11:k:100:VAL:HG12	11:k:102:VAL:HG13	2.02	0.41
2:B:17:LYS:HA	2:B:17:LYS:HD3	1.70	0.41
3:C:156:ASN:HD21	4:D:79:ASN:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:110:GLU:OE1	5:E:111:SER:CA	2.68	0.41
8:1:37:ASN:HB3	8:1:40:THR:OG1	2.20	0.41
11:4:8:ARG:NH1	11:4:127:GLU:CD	2.79	0.41
12:5:240:ALA:HA	12:5:246:SER:HB2	2.03	0.41
15:W:6:THR:O	15:W:49:VAL:HG13	2.20	0.41
15:W:109:ARG:HH22	15:W:170:HIS:CE1	2.38	0.41
16:V:211:LYS:HE2	26:U:127:GLN:O	2.20	0.41
17:T:116:GLN:OE1	17:T:118:ASN:HB2	2.20	0.41
22:S:54:TRP:CZ3	22:S:178:LEU:HB2	2.55	0.41
22:S:393:ARG:HH12	22:S:397:LEU:HB2	1.84	0.41
23:P:364:ARG:HA	23:P:367:GLU:OE2	2.21	0.41
23:P:400:VAL:O	23:P:400:VAL:HG13	2.21	0.41
28:H:165:PRO:HA	28:H:168:ILE:CD1	2.51	0.41
29:I:226:GLY:C	36:I:501:ATP:O1B	2.64	0.41
31:L:418:ALA:O	31:L:422:VAL:HG23	2.21	0.41
1:a:30:TYR:CD1	1:a:30:TYR:N	2.87	0.41
2:b:61:LEU:HD21	2:b:63:LYS:CE	2.50	0.41
3:c:231:LYS:HB2	3:c:234:GLU:OE1	2.20	0.41
9:i:212:ASP:O	9:i:214:GLU:OE1	2.37	0.41
9:i:236:ARG:HA	10:j:165:GLU:OE2	2.20	0.41
12:l:179:TYR:HE1	12:l:185:PRO:HD3	1.85	0.41
1:A:33:LYS:N	1:A:33:LYS:HD2	2.34	0.41
1:A:36:ASN:O	1:A:39:ASN:ND2	2.53	0.41
1:A:177:GLU:N	1:A:177:GLU:CD	2.79	0.41
3:C:7:ASP:OD2	4:D:6:ARG:CD	2.67	0.41
4:D:109:LEU:HD23	4:D:109:LEU:C	2.46	0.41
7:G:12:ASN:ND2	7:G:123:HIS:O	2.54	0.41
7:G:161:LYS:HZ3	23:P:2:SER:HB3	1.84	0.41
8:1:91:PHE:HD2	8:1:108:VAL:CG2	2.34	0.41
9:2:227:GLU:OE2	9:2:227:GLU:O	2.39	0.41
16:V:148:LYS:NZ	16:V:152:VAL:HG23	2.34	0.41
20:Z:210:TYR:CZ	20:Z:214:HIS:CE1	3.09	0.41
20:Z:548:ASP:OD2	20:Z:548:ASP:C	2.63	0.41
20:Z:790:MET:HE2	20:Z:790:MET:CA	2.49	0.41
21:N:267:GLN:O	21:N:270:LEU:HG	2.20	0.41
22:S:231:ALA:CB	22:S:268:LEU:HD23	2.50	0.41
22:S:407:ILE:HD11	22:S:443:ILE:HD11	2.02	0.41
22:S:488:GLN:OE1	33:J:42:ARG:NH2	2.45	0.41
24:Q:429:LYS:HB2	26:U:274:MET:SD	2.60	0.41
25:R:28:GLU:HA	25:R:320:LYS:CE	2.51	0.41
25:R:398:ALA:O	25:R:402:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:I:284:ILE:HG13	29:I:284:ILE:O	2.20	0.41
30:K:333:ARG:NH2	33:J:141:LYS:HD3	2.35	0.41
31:L:256:ILE:N	31:L:256:ILE:HD12	2.35	0.41
32:M:254:MET:SD	32:M:255:TYR:CE2	3.14	0.41
35:9:59:TYR:O	35:9:60:ASN:OD1	2.38	0.41
1:a:177:GLU:N	1:a:177:GLU:CD	2.79	0.41
4:d:4:TYR:OH	4:d:6:ARG:HB3	2.21	0.41
10:j:144:ASP:OD1	13:6:153:LEU:HD12	2.19	0.41
12:l:240:ALA:C	10:3:205:ASP:OD2	2.64	0.41
2:B:230:ASP:OD2	2:B:230:ASP:N	2.53	0.41
3:C:11:THR:O	4:D:127:ARG:HD3	2.21	0.41
4:D:119:ARG:CZ	4:D:120:TYR:CE1	3.01	0.41
5:E:110:GLU:C	5:E:110:GLU:CD	2.89	0.41
10:3:15:MET:HE2	10:3:154:TYR:HD1	1.84	0.41
11:4:130:TYR:CD2	11:4:144:LEU:HD13	2.55	0.41
13:6:131:TYR:CE2	13:6:141:ARG:HB2	2.55	0.41
14:7:45:ILE:HD11	14:7:210:ILE:HG23	2.02	0.41
15:W:61:VAL:HG21	26:U:68:LEU:O	2.20	0.41
15:W:104:LYS:N	15:W:104:LYS:HD3	2.36	0.41
16:V:69:PHE:CD1	16:V:69:PHE:C	2.98	0.41
20:Z:68:LEU:CD1	20:Z:98:ASP:OD1	2.66	0.41
20:Z:96:TYR:HB3	20:Z:97:PRO:HD3	2.03	0.41
20:Z:190:THR:HA	20:Z:193:PHE:CD2	2.56	0.41
20:Z:386:VAL:HG13	20:Z:837:TYR:CD2	2.56	0.41
20:Z:552:GLU:CD	20:Z:566:LEU:HD13	2.45	0.41
21:N:321:LEU:CD2	21:N:331:ALA:HB3	2.51	0.41
25:R:121:GLU:CD	25:R:130:GLN:HE22	2.26	0.41
28:H:80:HIS:NE2	29:I:91:GLU:OE2	2.54	0.41
29:I:248:VAL:HG13	33:J:270:ARG:HH22	1.86	0.41
33:J:84:VAL:HG22	33:J:96:VAL:O	2.20	0.41
1:a:33:LYS:HD2	1:a:33:LYS:HA	1.97	0.41
1:a:118:ALA:HA	1:a:143:PHE:CE1	2.56	0.41
2:b:12:PHE:CE1	3:c:130:PRO:HG2	2.56	0.41
5:e:53:ARG:O	5:e:53:ARG:HG3	2.18	0.41
7:g:175:GLU:HA	7:g:178:LYS:HG3	2.01	0.41
8:h:199:PRO:HA	8:h:202:TYR:CZ	2.56	0.41
11:k:8:ARG:NH1	11:k:127:GLU:CD	2.79	0.41
13:m:75:ARG:CZ	13:m:113:TYR:OH	2.66	0.41
4:D:122:GLN:HE21	5:E:138:PHE:HE2	1.69	0.41
5:E:225:GLN:H	5:E:225:GLN:CD	2.28	0.41
6:F:93:ASN:OD1	13:6:81:LYS:HE3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:17:PHE:CD1	8:1:22:ILE:HG13	2.56	0.41
13:6:108:LYS:HE3	13:6:111:PHE:HD2	1.86	0.41
13:6:122:LEU:HB2	13:6:217:LYS:NZ	2.36	0.41
16:V:197:TYR:CE2	16:V:199:LEU:CD2	3.02	0.41
20:Z:787:ASP:C	20:Z:787:ASP:OD1	2.63	0.41
20:Z:789:GLN:OE1	20:Z:874:ASN:ND2	2.53	0.41
22:S:46:LEU:O	22:S:50:PRO:HD2	2.21	0.41
23:P:123:ARG:HB2	23:P:123:ARG:HH11	1.85	0.41
23:P:254:GLU:HB3	23:P:258:LYS:NZ	2.36	0.41
23:P:281:ILE:HG12	23:P:304:THR:CG2	2.51	0.41
30:K:130:LEU:H	30:K:130:LEU:HD12	1.86	0.41
30:K:242:PHE:CE2	30:K:254:VAL:HA	2.56	0.41
31:L:205:GLU:OE2	31:L:208:GLN:HB2	2.21	0.41
32:M:141:LYS:C	32:M:143:ASN:H	2.29	0.41
32:M:218:ALA:N	32:M:343:LEU:HD22	2.36	0.41
33:J:389:VAL:HG23	33:J:390:MET:N	2.35	0.41
2:b:4:ARG:NH1	6:f:123:TYR:HD2	2.19	0.41
2:b:110:LEU:O	2:b:114:VAL:HG22	2.20	0.41
3:c:91:ALA:HB2	3:c:115:LEU:HD21	2.01	0.41
3:c:231:LYS:CD	3:c:232:PRO:HD2	2.50	0.41
5:e:103:TYR:HB3	13:m:96:SER:OG	2.21	0.41
6:f:207:THR:OG1	6:f:210:ASN:HB2	2.20	0.41
8:h:91:PHE:HD2	8:h:108:VAL:CG2	2.34	0.41
9:i:95:HIS:HA	9:i:98:TYR:CD2	2.56	0.41
9:i:244:GLU:HB2	10:j:198:ARG:HG2	2.03	0.41
12:l:250:VAL:HG22	12:l:266:HIS:O	2.21	0.41
1:A:23:GLY:O	2:B:27:ALA:HB2	2.21	0.41
2:B:61:LEU:HD21	2:B:63:LYS:CE	2.50	0.41
10:3:48:HIS:HE1	10:3:112:ILE:O	2.04	0.41
10:3:104:PHE:HA	10:3:126:LEU:HD23	2.02	0.41
13:6:91:LYS:HG2	13:6:92:LEU:N	2.34	0.41
14:7:105:THR:HG22	14:7:109:TYR:CZ	2.56	0.41
16:V:53:MET:CE	16:V:65:VAL:HG11	2.51	0.41
21:N:221:ASP:O	21:N:224:THR:HG22	2.21	0.41
21:N:418:ASP:OD2	21:N:419:THR:N	2.54	0.41
21:N:765:ASP:C	21:N:765:ASP:OD1	2.64	0.41
22:S:395:ILE:HG21	22:S:407:ILE:HG12	2.03	0.41
26:U:161:ILE:O	26:U:161:ILE:HG13	2.20	0.41
27:O:123:GLY:HA2	27:O:126:ILE:HD12	2.03	0.41
27:O:207:LEU:HD13	27:O:210:ARG:HH21	1.85	0.41
30:K:74:HIS:HB3	30:K:77:ARG:HH21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:L:243:PHE:CD1	31:L:245:PHE:CZ	3.09	0.41
2:b:178:ARG:HA	2:b:178:ARG:HE	1.86	0.41
4:d:110:THR:O	4:d:113:VAL:HG12	2.21	0.41
5:e:225:GLN:H	5:e:225:GLN:CD	2.28	0.41
6:f:117:GLN:HG3	7:g:87:HIS:HB2	2.03	0.41
7:g:218:TRP:HD1	7:g:231:VAL:HG23	1.85	0.41
9:i:141:SER:HB3	9:i:154:LEU:HD13	2.03	0.41
9:i:248:ASN:HD22	9:i:248:ASN:N	2.18	0.41
10:j:8:ASN:HD21	10:j:57:ALA:CB	2.34	0.41
10:j:104:PHE:HA	10:j:126:LEU:HD23	2.02	0.41
12:l:180:THR:OG1	12:l:183:GLU:HB3	2.21	0.41
13:m:43:ILE:HG12	9:2:196:LEU:HD21	2.03	0.41
14:n:73:GLU:OE2	14:n:75:LEU:HB2	2.21	0.41
14:n:243:LYS:HG3	14:n:244:ASN:CG	2.46	0.41
2:B:110:LEU:O	2:B:114:VAL:HG22	2.20	0.41
2:B:142:PHE:CE1	10:3:115:LYS:HD2	2.55	0.41
3:C:228:LYS:HG2	3:C:230:PHE:CE1	2.56	0.41
3:C:231:LYS:CD	3:C:232:PRO:HD2	2.50	0.41
4:D:66:LYS:HG3	4:D:66:LYS:O	2.21	0.41
5:E:167:TYR:CE2	6:F:57:SER:HB2	2.56	0.41
7:G:70:VAL:HG21	7:G:112:PHE:HE1	1.82	0.41
12:5:127:CYS:O	12:5:131:GLU:HG3	2.20	0.41
12:5:129:PHE:CD2	13:6:106:TYR:CD2	3.09	0.41
15:W:174:VAL:HG11	15:W:181:LEU:HD12	2.02	0.41
17:T:102:LYS:HA	17:T:105:LEU:HD12	2.03	0.41
19:Y:30:GLU:O	19:Y:31:GLU:O	2.39	0.41
20:Z:352:LYS:HD3	20:Z:352:LYS:C	2.46	0.41
20:Z:830:LEU:O	20:Z:834:LEU:HD13	2.21	0.41
21:N:324:LYS:HG3	21:N:325:PHE:CD1	2.56	0.41
21:N:580:ASN:OD1	21:N:583:VAL:HG23	2.21	0.41
25:R:32:LEU:HD22	25:R:46:ALA:HB3	2.03	0.41
30:K:299:LEU:HD23	30:K:299:LEU:C	2.45	0.41
31:L:201:LEU:HD23	31:L:201:LEU:C	2.45	0.41
31:L:383:SER:O	31:L:386:PHE:CE1	2.74	0.41
32:M:95:GLU:N	32:M:95:GLU:OE2	2.53	0.41
32:M:254:MET:SD	32:M:254:MET:C	3.04	0.41
33:J:142:VAL:HG11	33:J:212:ARG:HB2	2.03	0.41
34:8:341:VAL:HG13	34:8:344:MET:HE2	2.03	0.41
1:a:21:PRO:HA	2:b:23:TYR:HD1	1.86	0.41
1:a:232:LYS:HB3	1:a:232:LYS:HE3	1.56	0.41
3:c:96:GLN:OE1	10:j:73:LEU:HD11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:227:GLU:O	9:i:227:GLU:OE2	2.39	0.41
13:m:185:VAL:O	13:m:189:ILE:HG13	2.21	0.41
14:n:260:GLY:CA	8:l:41:ASP:HB3	2.50	0.41
1:A:24:ARG:NH2	1:A:29:GLU:OE2	2.53	0.41
7:G:173:LYS:HB2	31:L:382:MET:HE2	2.03	0.41
11:4:86:GLN:HE21	11:4:86:GLN:CA	2.31	0.41
12:5:250:VAL:HG22	12:5:266:HIS:O	2.21	0.41
20:Z:103:TYR:CE1	20:Z:116:ALA:HB2	2.56	0.41
21:N:361:ASN:ND2	21:N:362:TRP:CD1	2.89	0.41
22:S:69:LEU:O	22:S:72:GLU:OE1	2.38	0.41
24:Q:171:LYS:HE3	24:Q:174:LEU:HD21	2.03	0.41
25:R:148:ASP:OD2	25:R:148:ASP:N	2.54	0.41
25:R:188:LYS:HE3	25:R:217:HIS:NE2	2.36	0.41
26:U:19:LEU:O	26:U:23:GLU:HG2	2.21	0.41
28:H:297:MET:O	28:H:300:THR:OG1	2.37	0.41
29:I:234:LYS:NZ	29:I:246:ARG:NH1	2.69	0.41
29:I:433:GLU:OE1	29:I:437:LEU:N	2.49	0.41
30:K:190:LEU:N	30:K:191:PRO:HD2	2.35	0.41
30:K:346:ARG:HG2	30:K:346:ARG:NH1	2.36	0.41
31:L:50:GLN:NE2	32:M:22:ILE:HD12	2.36	0.41
31:L:317:ASN:HD22	31:L:317:ASN:HA	1.76	0.41
33:J:63:ARG:O	33:J:63:ARG:HD2	2.21	0.41
33:J:284:THR:O	33:J:285:SER:O	2.39	0.41
4:d:216:LYS:NZ	4:d:217:PRO:HD2	2.36	0.40
8:h:17:PHE:CD1	8:h:22:ILE:HG13	2.56	0.40
8:h:54:ARG:HH22	14:7:261:TYR:HE1	1.65	0.40
10:j:8:ASN:HD21	10:j:57:ALA:N	2.19	0.40
10:j:87:PHE:O	10:j:91:VAL:HG23	2.21	0.40
11:k:13:VAL:HG23	11:k:184:VAL:HB	2.03	0.40
2:B:94:HIS:HA	2:B:98:LYS:HB2	2.02	0.40
6:F:207:THR:OG1	6:F:210:ASN:HB2	2.21	0.40
7:G:243:ALA:O	7:G:247:ILE:HG22	2.21	0.40
9:2:40:GLY:HA2	9:2:137:SER:OG	2.21	0.40
20:Z:850:LEU:HD23	20:Z:850:LEU:O	2.22	0.40
21:N:528:ARG:O	21:N:531:LEU:N	2.54	0.40
24:Q:135:HIS:HB3	24:Q:165:PHE:CZ	2.56	0.40
24:Q:418:GLN:HA	24:Q:421:LYS:NZ	2.36	0.40
25:R:71:LEU:CD1	25:R:82:ASP:OD2	2.69	0.40
26:U:126:LYS:HB2	26:U:128:GLN:HG2	2.04	0.40
32:M:282:GLU:OE2	32:M:282:GLU:HA	2.21	0.40
33:J:164:ILE:HA	33:J:289:LYS:NZ	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:J:247:MET:HE2	33:J:247:MET:HA	2.02	0.40
33:J:295:ASN:O	33:J:296:ARG:HD3	2.22	0.40
3:c:203:SER:HB3	3:c:210:ARG:NH1	2.36	0.40
7:g:11:SER:O	7:g:14:VAL:HG22	2.20	0.40
7:g:12:ASN:ND2	7:g:123:HIS:O	2.54	0.40
8:h:115:ASN:O	8:h:116:LYS:CB	2.69	0.40
10:j:48:HIS:HE1	10:j:112:ILE:O	2.04	0.40
12:l:96:THR:HA	12:l:102:ALA:H	1.85	0.40
12:l:266:HIS:ND1	12:l:271:LEU:HD12	2.37	0.40
13:m:131:TYR:CE2	13:m:141:ARG:HB2	2.55	0.40
1:A:77:ARG:CZ	8:1:48:ASP:OD2	2.69	0.40
1:A:105:ARG:HH11	1:A:109:GLY:C	2.29	0.40
9:2:88:ILE:HD13	9:2:112:LEU:HG	2.02	0.40
9:2:249:ILE:HD13	10:3:50:PHE:CE2	2.56	0.40
10:3:71:THR:O	10:3:75:LYS:HD2	2.21	0.40
10:3:98:ARG:HG3	10:3:103:TYR:CZ	2.56	0.40
16:V:50:MET:HE3	16:V:72:PRO:O	2.21	0.40
16:V:148:LYS:O	30:K:88:ARG:NH2	2.53	0.40
19:Y:66:ASP:OD2	19:Y:66:ASP:N	2.52	0.40
21:N:64:ILE:HA	21:N:67:LYS:HD3	2.02	0.40
21:N:87:ASP:C	21:N:88:ARG:HG3	2.47	0.40
21:N:440:ASP:OD2	21:N:440:ASP:C	2.64	0.40
21:N:718:GLU:OE1	21:N:725:LEU:HA	2.22	0.40
22:S:413:LEU:HD13	22:S:419:VAL:HB	2.03	0.40
30:K:231:LYS:HA	30:K:231:LYS:CE	2.51	0.40
30:K:344:ARG:HH12	30:K:349:ARG:N	2.19	0.40
31:L:149:ASP:HB2	31:L:152:THR:OG1	2.22	0.40
33:J:166:LEU:N	33:J:167:PRO:HD2	2.37	0.40
33:J:209:LYS:HE2	33:J:240:HIS:CD2	2.56	0.40
33:J:301:ASP:OD1	33:J:303:ALA:N	2.39	0.40
5:e:110:GLU:C	5:e:110:GLU:CD	2.89	0.40
8:h:11:SER:HB2	8:h:178:SER:OG	2.20	0.40
13:m:108:LYS:HE3	13:m:111:PHE:HD2	1.86	0.40
13:m:230:ASP:CB	9:2:223:ASN:ND2	2.84	0.40
3:C:203:SER:HB3	3:C:210:ARG:NH1	2.36	0.40
7:G:41:LYS:HB3	7:G:161:LYS:O	2.21	0.40
10:3:87:PHE:O	10:3:91:VAL:HG23	2.21	0.40
10:3:127:ILE:O	10:3:127:ILE:HG22	2.22	0.40
11:4:13:VAL:HG23	11:4:184:VAL:HB	2.03	0.40
21:N:152:LEU:HD12	21:N:152:LEU:H	1.86	0.40
21:N:314:LEU:HD13	21:N:348:PHE:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:864:LYS:HD2	21:N:864:LYS:C	2.46	0.40
27:O:215:TYR:CD1	27:O:251:LEU:HD22	2.56	0.40
27:O:262:ASP:N	27:O:262:ASP:OD1	2.54	0.40
28:H:87:ASP:HA	28:H:90:ARG:HD3	2.04	0.40
28:H:144:LYS:HD3	28:H:156:VAL:CG1	2.50	0.40
28:H:247:LEU:HB3	28:H:374:LYS:HG2	2.03	0.40
28:H:425:GLU:OE2	29:I:345:ASP:O	2.40	0.40
29:I:269:LYS:HG2	29:I:319:ARG:HH21	1.86	0.40
31:L:51:GLU:HG3	31:L:53:HIS:N	2.30	0.40
32:M:280:ILE:HD12	32:M:280:ILE:N	2.36	0.40
32:M:352:PRO:HG2	32:M:386:PHE:O	2.21	0.40
34:8:163:GLU:HB2	34:8:184:LEU:HD13	2.03	0.40
34:8:332:LYS:HD3	34:8:332:LYS:N	2.36	0.40
1:a:87:ILE:N	1:a:88:PRO:CD	2.85	0.40
12:l:113:ASN:C	12:l:115:PHE:H	2.29	0.40
12:l:142:GLU:OE2	12:l:148:ARG:N	2.55	0.40
12:l:180:THR:C	12:l:257:GLU:OE2	2.62	0.40
12:l:216:ASP:CG	11:4:171:ARG:HH21	2.29	0.40
12:l:240:ALA:HA	12:l:246:SER:HB2	2.03	0.40
13:m:83:TYR:OH	13:m:90:LYS:HD2	2.22	0.40
14:n:90:ILE:O	14:n:94:GLN:HG2	2.21	0.40
2:B:4:ARG:HB2	3:C:3:SER:OG	2.21	0.40
2:B:18:LEU:HD11	3:C:129:ARG:NH2	2.36	0.40
3:C:219:GLY:C	9:2:255:GLU:CG	2.93	0.40
3:C:220:ALA:O	3:C:224:GLU:O	2.40	0.40
5:E:225:GLN:HG2	5:E:226:ASP:OD1	2.22	0.40
7:G:172:ALA:O	7:G:176:LEU:HG	2.21	0.40
11:4:52:ASP:OD2	11:4:99:GLN:N	2.48	0.40
11:4:100:VAL:HG12	11:4:102:VAL:HG13	2.02	0.40
17:T:194:GLU:HG2	17:T:235:PHE:HD1	1.87	0.40
20:Z:909:ARG:HH22	29:I:182:SER:CB	2.34	0.40
21:N:265:ALA:CB	21:N:269:LEU:HD23	2.48	0.40
24:Q:186:HIS:O	24:Q:189:ARG:CZ	2.69	0.40
24:Q:224:ILE:O	24:Q:228:GLU:HG2	2.21	0.40
27:O:35:GLU:O	27:O:36:LYS:HB2	2.21	0.40
27:O:380:LEU:C	27:O:380:LEU:HD23	2.47	0.40
28:H:296:GLU:OE2	28:H:296:GLU:HA	2.22	0.40
30:K:293:GLN:HB2	33:J:221:LYS:NZ	2.36	0.40
31:L:139:LYS:HE3	32:M:102:GLN:HA	2.03	0.40
31:L:364:HIS:CE1	36:L:501:ATP:H2	2.39	0.40
33:J:10:ILE:O	33:J:11:VAL:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:41:LYS:HB3	7:g:161:LYS:O	2.21	0.40
7:g:93:ARG:CD	14:n:109:TYR:CZ	3.04	0.40
9:i:40:GLY:HA2	9:i:137:SER:OG	2.21	0.40
10:j:71:THR:O	10:j:75:LYS:HD2	2.21	0.40
10:j:98:ARG:HG3	10:j:103:TYR:CZ	2.56	0.40
12:l:79:LEU:CA	12:l:175:MET:HE1	2.49	0.40
14:n:36:GLN:HB2	14:n:37:PRO:HD2	2.03	0.40
2:B:119:GLN:NE2	3:C:83:ASP:OD1	2.55	0.40
2:B:222:LEU:HD11	2:B:224:TYR:CZ	2.57	0.40
7:G:170:GLN:HE22	31:L:382:MET:HE3	1.86	0.40
8:1:199:PRO:HA	8:1:202:TYR:CZ	2.56	0.40
12:5:128:GLN:OE1	13:6:102:GLN:NE2	2.55	0.40
16:V:208:LYS:HB3	26:U:19:LEU:HD21	2.03	0.40
19:Y:1:MET:HA	22:S:336:SER:HB3	2.04	0.40
19:Y:3:THR:O	19:Y:4:ASP:CB	2.69	0.40
20:Z:717:THR:HG23	20:Z:718:ASP:N	2.36	0.40
20:Z:913:ILE:HG22	20:Z:913:ILE:O	2.21	0.40
21:N:31:VAL:HG23	21:N:31:VAL:O	2.21	0.40
22:S:371:LEU:O	22:S:375:ASP:N	2.55	0.40
23:P:89:LEU:O	23:P:91:LEU:N	2.54	0.40
23:P:266:TYR:CD2	23:P:328:ALA:HB2	2.56	0.40
25:R:317:ILE:HG13	25:R:318:PRO:HD3	2.03	0.40
26:U:138:VAL:HG13	26:U:140:ILE:HD11	2.03	0.40
27:O:169:ASN:OD1	27:O:198:THR:HG23	2.22	0.40
28:H:48:LYS:CD	29:I:57:LEU:HD11	2.52	0.40
29:I:131:SER:C	29:I:132:ILE:HG13	2.47	0.40
29:I:248:VAL:CG1	33:J:270:ARG:HH22	2.34	0.40
29:I:309:LEU:HD23	29:I:309:LEU:C	2.46	0.40
30:K:360:MET:CE	31:L:212:ILE:HG22	2.52	0.40
33:J:96:VAL:HG22	33:J:121:MET:CE	2.51	0.40
33:J:213:VAL:HG11	33:J:247:MET:CE	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	240/252 (95%)	236 (98%)	4 (2%)	0	100	100
1	a	240/252 (95%)	236 (98%)	4 (2%)	0	100	100
2	B	247/250 (99%)	238 (96%)	7 (3%)	2 (1%)	16	54
2	b	247/250 (99%)	238 (96%)	7 (3%)	2 (1%)	16	54
3	C	242/258 (94%)	237 (98%)	5 (2%)	0	100	100
3	c	242/258 (94%)	237 (98%)	5 (2%)	0	100	100
4	D	234/254 (92%)	224 (96%)	5 (2%)	5 (2%)	5	29
4	d	234/254 (92%)	224 (96%)	5 (2%)	5 (2%)	5	29
5	E	247/260 (95%)	238 (96%)	6 (2%)	3 (1%)	10	43
5	e	247/260 (95%)	238 (96%)	6 (2%)	3 (1%)	10	43
6	F	229/234 (98%)	219 (96%)	9 (4%)	1 (0%)	30	67
6	f	229/234 (98%)	219 (96%)	9 (4%)	1 (0%)	30	67
7	G	240/288 (83%)	235 (98%)	4 (2%)	1 (0%)	30	67
7	g	240/288 (83%)	235 (98%)	4 (2%)	1 (0%)	30	67
8	1	194/215 (90%)	187 (96%)	6 (3%)	1 (0%)	24	63
8	h	194/215 (90%)	187 (96%)	5 (3%)	2 (1%)	12	48
9	2	224/261 (86%)	210 (94%)	10 (4%)	4 (2%)	6	34
9	i	224/261 (86%)	211 (94%)	10 (4%)	3 (1%)	9	42
10	3	202/205 (98%)	183 (91%)	18 (9%)	1 (0%)	24	63
10	j	202/205 (98%)	183 (91%)	18 (9%)	1 (0%)	24	63
11	4	193/198 (98%)	187 (97%)	5 (3%)	1 (0%)	24	63
11	k	193/198 (98%)	187 (97%)	5 (3%)	1 (0%)	24	63
12	5	210/287 (73%)	198 (94%)	12 (6%)	0	100	100
12	l	210/287 (73%)	198 (94%)	12 (6%)	0	100	100
13	6	220/241 (91%)	207 (94%)	12 (6%)	1 (0%)	24	63
13	m	220/241 (91%)	207 (94%)	12 (6%)	1 (0%)	24	63
14	7	227/266 (85%)	215 (95%)	10 (4%)	2 (1%)	14	50
14	n	227/266 (85%)	214 (94%)	11 (5%)	2 (1%)	14	50
15	W	195/268 (73%)	182 (93%)	12 (6%)	1 (0%)	24	63
16	V	287/306 (94%)	264 (92%)	19 (7%)	4 (1%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	T	264/274 (96%)	247 (94%)	13 (5%)	4 (2%)	8	39
18	X	125/156 (80%)	116 (93%)	8 (6%)	1 (1%)	16	54
19	Y	87/89 (98%)	73 (84%)	9 (10%)	5 (6%)	1	13
20	Z	902/993 (91%)	822 (91%)	65 (7%)	15 (2%)	7	36
21	N	828/945 (88%)	800 (97%)	26 (3%)	2 (0%)	43	77
22	S	473/523 (90%)	439 (93%)	27 (6%)	7 (2%)	8	39
23	P	438/445 (98%)	419 (96%)	17 (4%)	2 (0%)	24	63
24	Q	432/434 (100%)	404 (94%)	27 (6%)	1 (0%)	43	77
25	R	403/429 (94%)	384 (95%)	18 (4%)	1 (0%)	43	77
26	U	288/338 (85%)	280 (97%)	8 (3%)	0	100	100
27	O	386/393 (98%)	373 (97%)	13 (3%)	0	100	100
28	H	387/467 (83%)	353 (91%)	27 (7%)	7 (2%)	6	34
29	I	382/437 (87%)	342 (90%)	29 (8%)	11 (3%)	3	23
30	K	392/428 (92%)	371 (95%)	18 (5%)	3 (1%)	16	54
31	L	386/437 (88%)	358 (93%)	25 (6%)	3 (1%)	16	54
32	M	419/434 (96%)	387 (92%)	22 (5%)	10 (2%)	4	27
33	J	403/405 (100%)	368 (91%)	31 (8%)	4 (1%)	12	48
34	8	368/499 (74%)	345 (94%)	20 (5%)	3 (1%)	16	54
35	9	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
All	All	14217/15714 (90%)	13424 (94%)	665 (5%)	128 (1%)	16	50

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	125	GLY
4	d	101	GLU
4	d	204	GLN
8	h	116	LYS
9	i	200	SER
14	n	110	ASP
2	B	125	GLY
4	D	204	GLN
8	1	116	LYS
9	2	200	SER
14	7	110	ASP

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Mol	Chain	Res	Type
16	V	59	ASP
16	V	184	ASN
16	V	271	VAL
17	T	138	ASP
18	X	39	GLU
19	Y	4	ASP
19	Y	32	ASP
20	Z	5	SER
20	Z	142	ASP
20	Z	174	GLU
20	Z	309	GLN
20	Z	366	LYS
20	Z	443	ASP
20	Z	444	GLU
20	Z	498	ALA
20	Z	926	ASN
21	N	150	LEU
22	S	69	LEU
22	S	98	SER
22	S	449	LEU
25	R	280	ILE
28	H	95	HIS
28	H	152	ILE
28	H	465	GLN
28	H	466	TYR
29	I	102	ASN
29	I	125	MET
29	I	213	ILE
30	K	344	ARG
31	L	275	PRO
31	L	292	SER
32	M	96	ASN
32	M	179	THR
32	M	316	SER
32	M	427	SER
32	M	429	SER
33	J	10	ILE
33	J	285	SER
34	8	182	ILE
4	d	205	THR
5	e	211	LYS
6	f	205	SER

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Mol	Chain	Res	Type
7	g	71	ASP
4	D	102	ASP
4	D	103	PRO
4	D	205	THR
5	E	211	LYS
6	F	205	SER
7	G	71	ASP
17	T	92	ASN
19	Y	33	ASP
19	Y	45	ASN
20	Z	310	LEU
23	P	90	LYS
23	P	131	PHE
28	H	314	VAL
29	I	126	PRO
29	I	293	ASP
30	K	174	VAL
32	M	87	ASP
32	M	106	VAL
33	J	400	VAL
34	8	442	ASN
4	d	102	ASP
4	d	103	PRO
5	e	128	SER
9	i	153	TYR
5	E	128	SER
9	2	120	GLN
9	2	153	TYR
19	Y	31	GLU
20	Z	85	VAL
20	Z	802	ASP
21	N	361	ASN
22	S	68	LEU
22	S	119	TYR
24	Q	51	ARG
29	I	84	PRO
29	I	103	PRO
29	I	138	LYS
31	L	291	PHE
32	M	180	TYR
32	M	317	SER
34	8	420	LEU

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Mol	Chain	Res	Type
9	i	254	GLU
13	m	138	SER
4	D	101	GLU
9	2	254	GLU
13	6	138	SER
15	W	23	ARG
20	Z	173	ALA
20	Z	377	ALA
28	H	91	LEU
28	H	372	ASP
29	I	83	LYS
10	j	32	GLN
11	k	10	GLN
14	n	111	ASN
10	3	32	GLN
11	4	10	GLN
16	V	258	GLU
17	T	139	ASP
17	T	258	ASN
22	S	153	GLU
29	I	345	ASP
5	e	129	GLY
8	h	154	ASN
5	E	129	GLY
32	M	424	ALA
33	J	11	VAL
29	I	214	LYS
30	K	176	GLY
14	7	111	ASN
20	Z	612	GLY
22	S	83	PRO
2	b	16	GLY
2	B	16	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/210 (98%)	168 (82%)	38 (18%)	1	8
1	a	206/210 (98%)	168 (82%)	38 (18%)	1	8
2	B	208/209 (100%)	167 (80%)	41 (20%)	1	7
2	b	208/209 (100%)	167 (80%)	41 (20%)	1	7
3	C	203/216 (94%)	160 (79%)	43 (21%)	1	6
3	c	203/216 (94%)	160 (79%)	43 (21%)	1	6
4	D	209/226 (92%)	209 (100%)	0	100	100
4	d	209/226 (92%)	209 (100%)	0	100	100
5	E	205/215 (95%)	169 (82%)	36 (18%)	2	9
5	e	205/215 (95%)	169 (82%)	36 (18%)	2	9
6	F	190/193 (98%)	158 (83%)	32 (17%)	2	10
6	f	190/193 (98%)	158 (83%)	32 (17%)	2	10
7	G	200/239 (84%)	167 (84%)	33 (16%)	2	10
7	g	200/239 (84%)	167 (84%)	33 (16%)	2	10
8	1	162/178 (91%)	132 (82%)	30 (18%)	1	8
8	h	162/178 (91%)	134 (83%)	28 (17%)	2	9
9	2	185/214 (86%)	137 (74%)	48 (26%)	0	3
9	i	185/214 (86%)	136 (74%)	49 (26%)	0	3
10	3	172/173 (99%)	146 (85%)	26 (15%)	3	12
10	j	172/173 (99%)	146 (85%)	26 (15%)	3	12
11	4	173/175 (99%)	139 (80%)	34 (20%)	1	7
11	k	173/175 (99%)	139 (80%)	34 (20%)	1	7
12	5	169/235 (72%)	135 (80%)	34 (20%)	1	7
12	l	169/235 (72%)	135 (80%)	34 (20%)	1	7
13	6	185/201 (92%)	158 (85%)	27 (15%)	3	13
13	m	185/201 (92%)	158 (85%)	27 (15%)	3	13
14	7	195/224 (87%)	195 (100%)	0	100	100
14	n	195/224 (87%)	195 (100%)	0	100	100
15	W	171/230 (74%)	170 (99%)	1 (1%)	78	83
16	V	253/268 (94%)	253 (100%)	0	100	100
17	T	249/256 (97%)	249 (100%)	0	100	100
18	X	116/144 (81%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	Y	81/81 (100%)	81 (100%)	0	100	100
20	Z	773/850 (91%)	772 (100%)	1 (0%)	88	89
21	N	698/797 (88%)	698 (100%)	0	100	100
22	S	447/489 (91%)	447 (100%)	0	100	100
23	P	412/415 (99%)	412 (100%)	0	100	100
24	Q	391/391 (100%)	389 (100%)	2 (0%)	81	83
25	R	356/379 (94%)	356 (100%)	0	100	100
26	U	263/308 (85%)	263 (100%)	0	100	100
27	O	363/368 (99%)	363 (100%)	0	100	100
28	H	330/399 (83%)	328 (99%)	2 (1%)	78	83
29	I	341/385 (89%)	339 (99%)	2 (1%)	78	83
30	K	346/374 (92%)	345 (100%)	1 (0%)	86	85
31	L	332/377 (88%)	330 (99%)	2 (1%)	78	83
32	M	364/375 (97%)	364 (100%)	0	100	100
33	J	352/352 (100%)	352 (100%)	0	100	100
34	8	337/449 (75%)	337 (100%)	0	100	100
35	9	68/68 (100%)	68 (100%)	0	100	100
All	All	12367/13571 (91%)	11513 (93%)	854 (7%)	16	36

All (854) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	13	ASP
1	a	14	ARG
1	a	20	SER
1	a	22	GLU
1	a	24	ARG
1	a	27	GLN
1	a	33	LYS
1	a	37	GLN
1	a	45	VAL
1	a	54	ILE
1	a	58	LYS
1	a	62	LYS
1	a	67	THR
1	a	74	CYS

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Mol	Chain	Res	Type
1	a	84	ASN
1	a	96	ARG
1	a	103	GLU
1	a	127	ILE
1	a	129	THR
1	a	134	MET
1	a	137	LEU
1	a	148	GLU
1	a	153	SER
1	a	156	LYS
1	a	157	THR
1	a	174	LYS
1	a	175	GLN
1	a	176	GLN
1	a	177	GLU
1	a	190	LYS
1	a	208	THR
1	a	210	MET
1	a	216	THR
1	a	217	GLU
1	a	219	SER
1	a	230	LYS
1	a	232	LYS
1	a	250	GLU
2	b	8	SER
2	b	15	SER
2	b	17	LYS
2	b	21	ILE
2	b	33	THR
2	b	51	SER
2	b	55	LEU
2	b	59	GLU
2	b	70	ASP
2	b	85	LEU
2	b	89	SER
2	b	92	VAL
2	b	96	SER
2	b	98	LYS
2	b	109	LEU
2	b	112	SER
2	b	114	VAL
2	b	124	SER

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Mol	Chain	Res	Type
2	b	132	VAL
2	b	133	SER
2	b	141	GLU
2	b	146	SER
2	b	151	ASP
2	b	166	LYS
2	b	169	VAL
2	b	176	GLU
2	b	178	ARG
2	b	181	ASP
2	b	186	GLU
2	b	198	GLU
2	b	199	SER
2	b	203	GLU
2	b	205	ASN
2	b	216	ASP
2	b	217	GLU
2	b	231	LYS
2	b	236	ARG
2	b	239	THR
2	b	241	GLN
2	b	242	GLU
2	b	248	GLU
3	c	3	SER
3	c	5	ARG
3	c	8	SER
3	c	11	THR
3	c	18	ARG
3	c	19	LEU
3	c	27	GLU
3	c	36	ILE
3	c	45	VAL
3	c	51	LYS
3	c	52	VAL
3	c	61	THR
3	c	64	GLU
3	c	80	LEU
3	c	81	THR
3	c	93	ILE
3	c	99	LEU
3	c	100	LYS
3	c	110	ILE

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Mol	Chain	Res	Type
3	c	113	ARG
3	c	115	LEU
3	c	118	ILE
3	c	123	THR
3	c	134	SER
3	c	142	ASP
3	c	152	ASN
3	c	154	SER
3	c	170	SER
3	c	177	GLN
3	c	178	MET
3	c	181	LYS
3	c	182	ASP
3	c	183	ASP
3	c	185	LYS
3	c	195	LYS
3	c	203	SER
3	c	204	SER
3	c	209	ASP
3	c	221	ASN
3	c	227	GLN
3	c	228	LYS
3	c	229	ILE
3	c	231	LYS
5	e	2	PHE
5	e	4	THR
5	e	7	GLU
5	e	9	ASP
5	e	10	ARG
5	e	16	SER
5	e	21	LEU
5	e	24	VAL
5	e	25	GLU
5	e	36	THR
5	e	47	VAL
5	e	48	LEU
5	e	61	SER
5	e	64	ILE
5	e	78	MET
5	e	82	THR
5	e	86	ARG
5	e	104	ASP

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Mol	Chain	Res	Type
5	e	110	GLU
5	e	116	VAL
5	e	125	GLU
5	e	128	SER
5	e	130	GLU
5	e	131	GLU
5	e	174	SER
5	e	176	SER
5	e	177	GLU
5	e	186	GLU
5	e	190	SER
5	e	195	GLU
5	e	202	LYS
5	e	205	LYS
5	e	206	GLN
5	e	209	GLU
5	e	211	LYS
5	e	234	GLU
6	f	10	THR
6	f	14	SER
6	f	18	ARG
6	f	26	LEU
6	f	30	LYS
6	f	31	GLN
6	f	33	SER
6	f	36	VAL
6	f	51	ARG
6	f	55	GLU
6	f	61	LYS
6	f	82	ARG
6	f	91	GLN
6	f	94	TYR
6	f	97	LEU
6	f	105	VAL
6	f	107	ARG
6	f	111	LEU
6	f	114	ASP
6	f	119	ASN
6	f	122	SER
6	f	140	SER
6	f	148	GLN
6	f	174	ARG

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Mol	Chain	Res	Type
6	f	177	ASP
6	f	181	LYS
6	f	199	GLN
6	f	200	SER
6	f	218	LYS
6	f	219	ASP
6	f	220	THR
6	f	223	THR
7	g	13	SER
7	g	20	ARG
7	g	23	GLN
7	g	29	LYS
7	g	36	THR
7	g	55	THR
7	g	57	LYS
7	g	62	GLN
7	g	63	LYS
7	g	72	ARG
7	g	86	ARG
7	g	89	VAL
7	g	100	LYS
7	g	105	THR
7	g	116	LEU
7	g	135	SER
7	g	143	LYS
7	g	154	SER
7	g	161	LYS
7	g	169	ARG
7	g	170	GLN
7	g	175	GLU
7	g	178	LYS
7	g	185	GLU
7	g	198	LYS
7	g	205	GLU
7	g	209	GLU
7	g	210	LYS
7	g	215	GLU
7	g	220	SER
7	g	227	LEU
7	g	232	LYS
7	g	247	ILE
8	h	11	SER

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Mol	Chain	Res	Type
8	h	19	ASP
8	h	27	SER
8	h	29	THR
8	h	31	THR
8	h	37	ASN
8	h	45	ARG
8	h	52	CYS
8	h	54	ARG
8	h	55	SER
8	h	57	SER
8	h	81	THR
8	h	83	SER
8	h	85	GLU
8	h	91	PHE
8	h	94	LEU
8	h	95	CYS
8	h	99	LYS
8	h	124	LEU
8	h	127	SER
8	h	128	VAL
8	h	147	CYS
8	h	159	GLU
8	h	162	ASP
8	h	169	SER
8	h	177	SER
8	h	178	SER
8	h	200	ASP
9	i	36	LYS
9	i	37	PHE
9	i	42	VAL
9	i	49	SER
9	i	51	GLN
9	i	54	ILE
9	i	60	CYS
9	i	63	LEU
9	i	65	ARG
9	i	67	SER
9	i	82	GLU
9	i	85	THR
9	i	86	GLN
9	i	87	LEU
9	i	90	SER

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Mol	Chain	Res	Type
9	i	92	ILE
9	i	94	LEU
9	i	99	THR
9	i	110	GLN
9	i	114	GLN
9	i	118	LYS
9	i	127	LEU
9	i	128	ILE
9	i	141	SER
9	i	143	HIS
9	i	147	SER
9	i	149	ASP
9	i	156	LEU
9	i	172	LYS
9	i	177	LYS
9	i	178	GLU
9	i	181	ILE
9	i	189	GLN
9	i	204	VAL
9	i	211	LYS
9	i	212	ASP
9	i	214	GLU
9	i	216	LEU
9	i	217	ARG
9	i	220	LEU
9	i	227	GLU
9	i	230	LYS
9	i	231	SER
9	i	243	LYS
9	i	244	GLU
9	i	246	ILE
9	i	248	ASN
9	i	250	CYS
9	i	252	ILE
10	j	3	ASP
10	j	5	SER
10	j	6	SER
10	j	15	MET
10	j	18	LYS
10	j	31	SER
10	j	33	SER
10	j	61	THR

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Mol	Chain	Res	Type
10	j	63	LEU
10	j	70	LYS
10	j	71	THR
10	j	73	LEU
10	j	77	LYS
10	j	86	THR
10	j	93	SER
10	j	114	SER
10	j	118	LYS
10	j	134	LYS
10	j	136	PHE
10	j	139	SER
10	j	143	SER
10	j	147	PHE
10	j	157	ASN
10	j	161	GLU
10	j	177	ARG
10	j	192	LYS
11	k	5	LEU
11	k	7	ILE
11	k	12	SER
11	k	13	VAL
11	k	17	SER
11	k	25	ILE
11	k	29	LYS
11	k	31	SER
11	k	39	SER
11	k	44	MET
11	k	45	SER
11	k	54	VAL
11	k	61	GLN
11	k	65	GLN
11	k	69	ILE
11	k	71	GLU
11	k	78	GLN
11	k	86	GLN
11	k	87	GLU
11	k	90	LYS
11	k	91	SER
11	k	94	SER
11	k	96	ARG
11	k	109	LYS

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Mol	Chain	Res	Type
11	k	110	LYS
11	k	125	LYS
11	k	135	TYR
11	k	140	THR
11	k	149	ARG
11	k	153	THR
11	k	155	GLU
11	k	169	GLU
11	k	182	LYS
11	k	186	LYS
12	l	77	THR
12	l	84	GLN
12	l	96	THR
12	l	100	TRP
12	l	103	SER
12	l	105	THR
12	l	106	VAL
12	l	107	LYS
12	l	111	GLU
12	l	138	CYS
12	l	147	GLU
12	l	150	SER
12	l	159	SER
12	l	161	LEU
12	l	164	GLN
12	l	175	MET
12	l	181	ARG
12	l	182	LYS
12	l	192	SER
12	l	201	ILE
12	l	217	SER
12	l	224	SER
12	l	226	GLU
12	l	227	ASP
12	l	242	ARG
12	l	258	ASP
12	l	261	ILE
12	l	267	ASP
12	l	271	LEU
12	l	274	LYS
12	l	277	GLU
12	l	284	ASN

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Mol	Chain	Res	Type
12	l	285	VAL
12	l	286	ILE
13	m	27	ASP
13	m	39	THR
13	m	42	SER
13	m	58	ILE
13	m	61	SER
13	m	72	LEU
13	m	73	VAL
13	m	74	LYS
13	m	75	ARG
13	m	93	SER
13	m	96	SER
13	m	108	LYS
13	m	109	ARG
13	m	116	HIS
13	m	118	ILE
13	m	124	GLU
13	m	140	GLU
13	m	143	GLN
13	m	144	CYS
13	m	158	LEU
13	m	161	GLN
13	m	177	LYS
13	m	184	SER
13	m	186	GLU
13	m	187	GLU
13	m	198	SER
13	m	217	LYS
1	A	13	ASP
1	A	14	ARG
1	A	20	SER
1	A	22	GLU
1	A	24	ARG
1	A	27	GLN
1	A	33	LYS
1	A	37	GLN
1	A	45	VAL
1	A	54	ILE
1	A	58	LYS
1	A	62	LYS
1	A	67	THR

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Mol	Chain	Res	Type
1	A	74	CYS
1	A	84	ASN
1	A	96	ARG
1	A	103	GLU
1	A	127	ILE
1	A	129	THR
1	A	134	MET
1	A	137	LEU
1	A	148	GLU
1	A	153	SER
1	A	156	LYS
1	A	157	THR
1	A	174	LYS
1	A	175	GLN
1	A	176	GLN
1	A	177	GLU
1	A	190	LYS
1	A	208	THR
1	A	210	MET
1	A	216	THR
1	A	217	GLU
1	A	219	SER
1	A	230	LYS
1	A	232	LYS
1	A	250	GLU
2	B	8	SER
2	B	15	SER
2	B	17	LYS
2	B	21	ILE
2	B	33	THR
2	B	51	SER
2	B	55	LEU
2	B	59	GLU
2	B	70	ASP
2	B	85	LEU
2	B	89	SER
2	B	92	VAL
2	B	96	SER
2	B	98	LYS
2	B	109	LEU
2	B	112	SER
2	B	114	VAL

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Mol	Chain	Res	Type
2	B	124	SER
2	B	132	VAL
2	B	133	SER
2	B	141	GLU
2	B	146	SER
2	B	151	ASP
2	B	166	LYS
2	B	169	VAL
2	B	176	GLU
2	B	178	ARG
2	B	181	ASP
2	B	186	GLU
2	B	198	GLU
2	B	199	SER
2	B	203	GLU
2	B	205	ASN
2	B	216	ASP
2	B	217	GLU
2	B	231	LYS
2	B	236	ARG
2	B	239	THR
2	B	241	GLN
2	B	242	GLU
2	B	248	GLU
3	C	3	SER
3	C	5	ARG
3	C	8	SER
3	C	11	THR
3	C	18	ARG
3	C	19	LEU
3	C	27	GLU
3	C	36	ILE
3	C	45	VAL
3	C	51	LYS
3	C	52	VAL
3	C	61	THR
3	C	64	GLU
3	C	80	LEU
3	C	81	THR
3	C	93	ILE
3	C	99	LEU
3	C	100	LYS

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Mol	Chain	Res	Type
3	C	110	ILE
3	C	113	ARG
3	C	115	LEU
3	C	118	ILE
3	C	123	THR
3	C	134	SER
3	C	142	ASP
3	C	152	ASN
3	C	154	SER
3	C	170	SER
3	C	177	GLN
3	C	178	MET
3	C	181	LYS
3	C	182	ASP
3	C	183	ASP
3	C	185	LYS
3	C	195	LYS
3	C	203	SER
3	C	204	SER
3	C	209	ASP
3	C	221	ASN
3	C	227	GLN
3	C	228	LYS
3	C	229	ILE
3	C	231	LYS
5	E	2	PHE
5	E	4	THR
5	E	7	GLU
5	E	9	ASP
5	E	10	ARG
5	E	16	SER
5	E	21	LEU
5	E	24	VAL
5	E	25	GLU
5	E	36	THR
5	E	47	VAL
5	E	48	LEU
5	E	61	SER
5	E	64	ILE
5	E	78	MET
5	E	82	THR
5	E	86	ARG

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Mol	Chain	Res	Type
5	E	104	ASP
5	E	110	GLU
5	E	116	VAL
5	E	125	GLU
5	E	128	SER
5	E	130	GLU
5	E	131	GLU
5	E	174	SER
5	E	176	SER
5	E	177	GLU
5	E	186	GLU
5	E	190	SER
5	E	195	GLU
5	E	202	LYS
5	E	205	LYS
5	E	206	GLN
5	E	209	GLU
5	E	211	LYS
5	E	234	GLU
6	F	10	THR
6	F	14	SER
6	F	18	ARG
6	F	26	LEU
6	F	30	LYS
6	F	31	GLN
6	F	33	SER
6	F	36	VAL
6	F	51	ARG
6	F	55	GLU
6	F	61	LYS
6	F	82	ARG
6	F	91	GLN
6	F	94	TYR
6	F	97	LEU
6	F	105	VAL
6	F	107	ARG
6	F	111	LEU
6	F	114	ASP
6	F	119	ASN
6	F	122	SER
6	F	140	SER
6	F	148	GLN

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Mol	Chain	Res	Type
6	F	174	ARG
6	F	177	ASP
6	F	181	LYS
6	F	199	GLN
6	F	200	SER
6	F	218	LYS
6	F	219	ASP
6	F	220	THR
6	F	223	THR
7	G	13	SER
7	G	20	ARG
7	G	23	GLN
7	G	29	LYS
7	G	36	THR
7	G	55	THR
7	G	57	LYS
7	G	62	GLN
7	G	63	LYS
7	G	72	ARG
7	G	86	ARG
7	G	89	VAL
7	G	100	LYS
7	G	105	THR
7	G	116	LEU
7	G	135	SER
7	G	143	LYS
7	G	154	SER
7	G	161	LYS
7	G	169	ARG
7	G	170	GLN
7	G	175	GLU
7	G	178	LYS
7	G	185	GLU
7	G	198	LYS
7	G	205	GLU
7	G	209	GLU
7	G	210	LYS
7	G	215	GLU
7	G	220	SER
7	G	227	LEU
7	G	232	LYS
7	G	247	ILE

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Mol	Chain	Res	Type
8	1	11	SER
8	1	19	ASP
8	1	27	SER
8	1	29	THR
8	1	31	THR
8	1	37	ASN
8	1	45	ARG
8	1	52	CYS
8	1	54	ARG
8	1	55	SER
8	1	57	SER
8	1	81	THR
8	1	83	SER
8	1	85	GLU
8	1	91	PHE
8	1	94	LEU
8	1	95	CYS
8	1	99	LYS
8	1	124	LEU
8	1	127	SER
8	1	128	VAL
8	1	147	CYS
8	1	152	ARG
8	1	153	GLU
8	1	159	GLU
8	1	162	ASP
8	1	169	SER
8	1	177	SER
8	1	178	SER
8	1	200	ASP
9	2	36	LYS
9	2	37	PHE
9	2	42	VAL
9	2	49	SER
9	2	51	GLN
9	2	54	ILE
9	2	60	CYS
9	2	63	LEU
9	2	65	ARG
9	2	67	SER
9	2	82	GLU
9	2	85	THR

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Mol	Chain	Res	Type
9	2	86	GLN
9	2	87	LEU
9	2	90	SER
9	2	92	ILE
9	2	94	LEU
9	2	99	THR
9	2	110	GLN
9	2	114	GLN
9	2	127	LEU
9	2	128	ILE
9	2	141	SER
9	2	143	HIS
9	2	147	SER
9	2	149	ASP
9	2	156	LEU
9	2	172	LYS
9	2	177	LYS
9	2	178	GLU
9	2	181	ILE
9	2	189	GLN
9	2	204	VAL
9	2	211	LYS
9	2	212	ASP
9	2	214	GLU
9	2	216	LEU
9	2	217	ARG
9	2	220	LEU
9	2	227	GLU
9	2	230	LYS
9	2	231	SER
9	2	243	LYS
9	2	244	GLU
9	2	246	ILE
9	2	248	ASN
9	2	250	CYS
9	2	252	ILE
10	3	3	ASP
10	3	5	SER
10	3	6	SER
10	3	15	MET
10	3	18	LYS
10	3	31	SER

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Mol	Chain	Res	Type
10	3	33	SER
10	3	61	THR
10	3	63	LEU
10	3	70	LYS
10	3	71	THR
10	3	73	LEU
10	3	77	LYS
10	3	86	THR
10	3	93	SER
10	3	114	SER
10	3	118	LYS
10	3	134	LYS
10	3	136	PHE
10	3	139	SER
10	3	143	SER
10	3	147	PHE
10	3	157	ASN
10	3	161	GLU
10	3	177	ARG
10	3	192	LYS
11	4	5	LEU
11	4	7	ILE
11	4	12	SER
11	4	13	VAL
11	4	17	SER
11	4	25	ILE
11	4	29	LYS
11	4	31	SER
11	4	39	SER
11	4	44	MET
11	4	45	SER
11	4	54	VAL
11	4	61	GLN
11	4	65	GLN
11	4	69	ILE
11	4	71	GLU
11	4	78	GLN
11	4	86	GLN
11	4	87	GLU
11	4	90	LYS
11	4	91	SER
11	4	94	SER

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Mol	Chain	Res	Type
11	4	96	ARG
11	4	109	LYS
11	4	110	LYS
11	4	125	LYS
11	4	135	TYR
11	4	140	THR
11	4	149	ARG
11	4	153	THR
11	4	155	GLU
11	4	169	GLU
11	4	182	LYS
11	4	186	LYS
12	5	77	THR
12	5	84	GLN
12	5	96	THR
12	5	100	TRP
12	5	103	SER
12	5	105	THR
12	5	106	VAL
12	5	107	LYS
12	5	111	GLU
12	5	138	CYS
12	5	147	GLU
12	5	150	SER
12	5	159	SER
12	5	161	LEU
12	5	164	GLN
12	5	175	MET
12	5	181	ARG
12	5	182	LYS
12	5	192	SER
12	5	201	ILE
12	5	217	SER
12	5	224	SER
12	5	226	GLU
12	5	227	ASP
12	5	242	ARG
12	5	258	ASP
12	5	261	ILE
12	5	267	ASP
12	5	271	LEU
12	5	274	LYS

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Mol	Chain	Res	Type
12	5	277	GLU
12	5	284	ASN
12	5	285	VAL
12	5	286	ILE
13	6	27	ASP
13	6	39	THR
13	6	42	SER
13	6	58	ILE
13	6	61	SER
13	6	72	LEU
13	6	73	VAL
13	6	74	LYS
13	6	75	ARG
13	6	93	SER
13	6	96	SER
13	6	108	LYS
13	6	109	ARG
13	6	116	HIS
13	6	118	ILE
13	6	124	GLU
13	6	140	GLU
13	6	143	GLN
13	6	144	CYS
13	6	158	LEU
13	6	161	GLN
13	6	177	LYS
13	6	184	SER
13	6	186	GLU
13	6	187	GLU
13	6	198	SER
13	6	217	LYS
15	W	22	PRO
20	Z	949	ILE
24	Q	93	THR
24	Q	111	LEU
28	H	230	LEU
28	H	466	TYR
29	I	81	ILE
29	I	422	ARG
30	K	346	ARG
31	L	183	ILE
31	L	275	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (241) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	37	GLN
1	a	41	ASN
1	a	56	GLN
1	a	84	ASN
1	a	130	GLN
1	a	176	GLN
1	a	221	ASN
2	b	30	GLN
3	c	168	ASN
3	c	177	GLN
3	c	227	GLN
4	d	94	GLN
5	e	23	GLN
5	e	91	HIS
5	e	99	HIS
5	e	108	ASN
5	e	114	GLN
6	f	60	GLN
6	f	90	GLN
6	f	119	ASN
7	g	33	ASN
7	g	68	GLN
7	g	170	GLN
7	g	228	HIS
8	h	37	ASN
8	h	98	ASN
8	h	170	GLN
9	i	201	ASN
9	i	223	ASN
9	i	248	ASN
10	j	8	ASN
10	j	38	ASN
10	j	48	HIS
10	j	173	ASN
11	k	37	GLN
11	k	41	HIS
11	k	61	GLN
11	k	63	ASN
11	k	86	GLN
12	l	218	ASN
12	l	251	ASN

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Mol	Chain	Res	Type
13	m	11	ASN
13	m	84	HIS
13	m	102	GLN
13	m	143	GLN
13	m	161	GLN
13	m	166	ASN
13	m	205	GLN
1	A	15	HIS
1	A	37	GLN
1	A	41	ASN
1	A	56	GLN
1	A	84	ASN
1	A	176	GLN
1	A	221	ASN
2	B	30	GLN
3	C	168	ASN
3	C	177	GLN
3	C	227	GLN
4	D	79	ASN
4	D	96	HIS
4	D	209	ASN
5	E	91	HIS
5	E	99	HIS
5	E	108	ASN
5	E	114	GLN
6	F	60	GLN
6	F	69	HIS
6	F	90	GLN
6	F	119	ASN
7	G	33	ASN
7	G	68	GLN
7	G	170	GLN
7	G	228	HIS
8	1	37	ASN
8	1	98	ASN
8	1	129	HIS
9	2	201	ASN
9	2	223	ASN
9	2	248	ASN
10	3	8	ASN
10	3	48	HIS
10	3	173	ASN

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Mol	Chain	Res	Type
11	4	37	GLN
11	4	41	HIS
11	4	61	GLN
11	4	63	ASN
11	4	86	GLN
12	5	208	GLN
12	5	218	ASN
12	5	251	ASN
13	6	11	ASN
13	6	84	HIS
13	6	102	GLN
13	6	143	GLN
13	6	205	GLN
14	7	81	ASN
14	7	107	ASN
14	7	158	GLN
14	7	236	ASN
15	W	106	GLN
15	W	149	GLN
15	W	165	GLN
15	W	170	HIS
16	V	64	ASN
16	V	102	GLN
16	V	111	HIS
16	V	124	ASN
16	V	181	ASN
16	V	184	ASN
16	V	186	GLN
16	V	190	HIS
16	V	200	ASN
16	V	222	GLN
16	V	279	HIS
16	V	290	ASN
17	T	71	GLN
17	T	92	ASN
17	T	94	HIS
17	T	117	ASN
17	T	213	ASN
17	T	230	ASN
17	T	251	HIS
18	X	94	ASN
18	X	131	ASN

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Mol	Chain	Res	Type
19	Y	52	ASN
20	Z	23	GLN
20	Z	110	ASN
20	Z	214	HIS
20	Z	215	ASN
20	Z	243	GLN
20	Z	276	ASN
20	Z	327	GLN
20	Z	387	ASN
20	Z	593	HIS
20	Z	628	ASN
20	Z	771	HIS
20	Z	824	ASN
20	Z	829	GLN
20	Z	868	ASN
20	Z	874	ASN
20	Z	897	HIS
20	Z	905	ASN
20	Z	926	ASN
20	Z	931	GLN
20	Z	951	GLN
20	Z	959	HIS
21	N	233	ASN
21	N	340	HIS
21	N	346	ASN
21	N	499	HIS
21	N	509	GLN
21	N	613	HIS
21	N	616	HIS
21	N	654	GLN
21	N	691	GLN
21	N	738	GLN
21	N	747	HIS
21	N	877	GLN
22	S	20	HIS
22	S	154	GLN
22	S	159	ASN
22	S	312	GLN
22	S	412	ASN
22	S	458	GLN
23	P	29	GLN
23	P	33	ASN

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Mol	Chain	Res	Type
23	P	94	GLN
23	P	178	GLN
23	P	183	GLN
23	P	195	GLN
23	P	210	ASN
23	P	222	ASN
23	P	239	GLN
23	P	275	ASN
23	P	285	GLN
23	P	349	ASN
23	P	366	ASN
23	P	394	ASN
23	P	440	HIS
24	Q	54	GLN
24	Q	150	GLN
24	Q	178	HIS
24	Q	248	ASN
24	Q	292	GLN
24	Q	394	ASN
25	R	23	ASN
25	R	74	ASN
25	R	89	ASN
25	R	314	ASN
25	R	399	GLN
25	R	401	HIS
26	U	5	HIS
26	U	21	HIS
26	U	26	GLN
26	U	127	GLN
26	U	238	ASN
26	U	251	ASN
27	O	177	GLN
27	O	186	ASN
27	O	283	HIS
27	O	326	HIS
27	O	374	ASN
28	H	151	GLN
28	H	339	GLN
29	I	68	HIS
29	I	102	ASN
29	I	190	GLN
29	I	204	HIS

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Mol	Chain	Res	Type
29	I	238	ASN
29	I	426	ASN
30	K	36	ASN
30	K	90	GLN
30	K	180	GLN
30	K	228	ASN
30	K	264	ASN
31	L	59	GLN
31	L	99	GLN
31	L	175	GLN
31	L	317	ASN
32	M	53	HIS
32	M	107	ASN
32	M	240	ASN
32	M	328	ASN
32	M	423	GLN
33	J	123	HIS
33	J	170	HIS
33	J	204	HIS
33	J	331	HIS
33	J	376	HIS
34	8	139	ASN
34	8	159	GLN
34	8	186	ASN
34	8	208	GLN
34	8	264	HIS
34	8	274	ASN
34	8	338	GLN
34	8	415	HIS
34	8	425	ASN
35	9	2	GLN
35	9	49	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	GLZ	9	76	35	3,3,3	0.54	0	1,2,2	0.06	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	GLZ	9	76	35	-	0/0/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	9	76	GLZ	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
36	ATP	I	501	37	32,33,33	1.57	4 (12%)	48,52,52	2.52	21 (43%)
36	ATP	M	501	37	32,33,33	1.40	5 (15%)	48,52,52	2.38	15 (31%)
36	ATP	K	501	37	32,33,33	2.55	5 (15%)	48,52,52	2.46	16 (33%)
36	ATP	H	501	37	32,33,33	1.83	7 (21%)	48,52,52	2.29	21 (43%)
38	ADP	J	501	37	28,29,29	1.86	6 (21%)	43,45,45	2.95	20 (46%)
36	ATP	L	501	37	32,33,33	2.17	8 (25%)	48,52,52	1.51	4 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ATP	I	501	37	-	4/22/38/38	0/3/3/3
36	ATP	M	501	37	-	5/22/38/38	0/3/3/3
36	ATP	K	501	37	-	5/22/38/38	0/3/3/3
36	ATP	H	501	37	-	6/22/38/38	0/3/3/3
38	ADP	J	501	37	-	3/16/32/32	0/3/3/3
36	ATP	L	501	37	-	4/22/38/38	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	K	501	ATP	PA-O3A	8.14	1.68	1.59
36	K	501	ATP	PB-O3A	7.90	1.68	1.59
38	J	501	ADP	PA-O3A	6.25	1.66	1.59
36	L	501	ATP	PA-O3A	6.17	1.66	1.59
36	L	501	ATP	PB-O3A	5.97	1.65	1.59
36	H	501	ATP	PB-O3B	5.72	1.65	1.59
36	L	501	ATP	C5-N7	-5.01	1.29	1.39
36	K	501	ATP	PB-O3B	4.74	1.64	1.59
36	I	501	ATP	C5-C4	4.43	1.47	1.39
36	K	501	ATP	C5-C6	4.30	1.53	1.41
36	H	501	ATP	C5-C4	3.82	1.45	1.39
36	H	501	ATP	PA-O3A	3.71	1.63	1.59
36	H	501	ATP	PB-O3A	3.55	1.63	1.59
36	M	501	ATP	C4-N9	-3.43	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	L	501	ATP	C4-N9	-3.34	1.30	1.37
36	I	501	ATP	PB-O3B	3.22	1.63	1.59
38	J	501	ADP	C4-N9	-3.02	1.31	1.37
38	J	501	ADP	C5-C4	2.99	1.44	1.39
36	K	501	ATP	C5-C4	2.94	1.44	1.39
36	M	501	ATP	C5-C4	2.87	1.44	1.39
36	I	501	ATP	C5-C6	2.76	1.48	1.41
36	M	501	ATP	C8-N9	-2.68	1.33	1.37
38	J	501	ADP	C5'-C4'	-2.64	1.43	1.51
36	I	501	ATP	PA-O3A	2.64	1.62	1.59
36	L	501	ATP	C2-N1	2.63	1.38	1.33
36	H	501	ATP	C5-N7	-2.57	1.34	1.39
36	L	501	ATP	PB-O2B	-2.56	1.43	1.55
36	H	501	ATP	C8-N7	2.38	1.36	1.31
38	J	501	ADP	C8-N9	-2.37	1.33	1.37
36	M	501	ATP	PA-O3A	2.23	1.61	1.59
36	L	501	ATP	C6-N6	2.20	1.39	1.34
36	M	501	ATP	PB-O3B	2.12	1.61	1.59
36	L	501	ATP	PB-O3B	2.11	1.61	1.59
36	H	501	ATP	C5-C6	2.06	1.46	1.41
38	J	501	ADP	O4'-C4'	2.05	1.49	1.45

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	J	501	ADP	C4-N9-C8	8.82	115.00	105.74
36	M	501	ATP	C4-N9-C8	8.58	114.75	105.74
36	K	501	ATP	C5-C4-N3	-7.87	115.88	126.72
36	L	501	ATP	O2B-PB-O3A	6.13	123.83	107.27
36	I	501	ATP	C5-C4-N3	-5.96	118.52	126.72
36	I	501	ATP	N3-C4-N9	5.91	137.21	127.17
38	J	501	ADP	N3-C4-N9	5.84	137.10	127.17
38	J	501	ADP	N3-C2-N1	-5.81	119.79	128.58
36	H	501	ATP	C5-C4-N3	-5.77	118.77	126.72
38	J	501	ADP	C5'-C4'-C3'	5.53	135.12	115.21
36	K	501	ATP	N3-C4-N9	5.44	136.42	127.17
36	I	501	ATP	C4-N9-C8	5.06	111.05	105.74
36	M	501	ATP	N3-C2-N1	-4.99	121.02	128.58
36	H	501	ATP	N3-C2-N1	-4.99	121.03	128.58
36	K	501	ATP	C2-N1-C6	-4.90	110.68	118.73
36	M	501	ATP	N3-C4-N9	4.89	135.48	127.17
36	I	501	ATP	O5'-C5'-C4'	-4.87	92.40	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	H	501	ATP	C2-N3-C4	4.79	123.54	111.83
36	K	501	ATP	C5-C6-N6	-4.63	111.81	123.29
36	M	501	ATP	N9-C8-N7	-4.57	107.45	113.94
36	K	501	ATP	O2B-PB-O3A	4.53	119.52	107.27
38	J	501	ADP	N9-C8-N7	-4.49	107.56	113.94
36	H	501	ATP	N3-C4-N9	4.41	134.67	127.17
38	J	501	ADP	C5-C4-N9	-4.39	101.03	105.81
38	J	501	ADP	C2-N3-C4	4.29	122.30	111.83
36	K	501	ATP	C4-C5-N7	-4.28	105.68	110.58
36	H	501	ATP	O3A-PB-O1B	-4.22	98.02	110.70
36	I	501	ATP	O4'-C4'-C3'	4.17	113.44	105.15
36	L	501	ATP	O2B-PB-O3B	-4.16	96.02	107.27
36	I	501	ATP	C2-N3-C4	4.00	121.61	111.83
36	I	501	ATP	N3-C2-N1	-3.97	122.57	128.58
38	J	501	ADP	C3'-C2'-C1'	3.88	108.80	101.46
38	J	501	ADP	C5-C6-N6	-3.72	114.07	123.29
36	M	501	ATP	C2-N3-C4	3.72	120.92	111.83
36	K	501	ATP	C2-N3-C4	3.67	120.80	111.83
38	J	501	ADP	C6-C5-C4	-3.62	112.23	117.18
36	M	501	ATP	C6-C5-C4	-3.62	112.23	117.18
38	J	501	ADP	C5-C4-N3	-3.60	121.76	126.72
38	J	501	ADP	C2'-C1'-N9	3.50	122.00	113.30
36	M	501	ATP	C6-C5-N7	3.45	138.73	132.09
36	M	501	ATP	C5-C4-N9	-3.40	102.11	105.81
36	I	501	ATP	N9-C8-N7	-3.38	109.14	113.94
36	I	501	ATP	O4'-C4'-C5'	3.36	120.11	109.33
36	K	501	ATP	N6-C6-N1	3.28	125.68	118.38
36	I	501	ATP	C5-N7-C8	3.25	108.55	103.45
36	I	501	ATP	C4-C5-N7	-3.15	106.98	110.58
36	H	501	ATP	C6-C5-N7	3.15	138.16	132.09
36	H	501	ATP	C5-C6-N6	-3.14	115.50	123.29
36	M	501	ATP	C5-C4-N3	-3.13	122.41	126.72
36	H	501	ATP	O3A-PA-O1A	-3.10	101.37	110.70
36	K	501	ATP	O5'-C5'-C4'	3.03	119.31	108.99
36	K	501	ATP	O5'-PA-O1A	-3.00	97.05	108.94
36	M	501	ATP	C5-C6-N6	-2.91	116.08	123.29
36	I	501	ATP	O2A-PA-O3A	2.91	115.13	107.27
38	J	501	ADP	C6-C5-N7	2.87	137.62	132.09
36	H	501	ATP	O5'-C5'-C4'	2.81	118.57	108.99
36	K	501	ATP	C2'-C1'-N9	-2.73	106.53	113.30
36	I	501	ATP	O3'-C3'-C2'	2.72	120.54	111.82
36	K	501	ATP	C5-N7-C8	2.65	107.61	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	M	501	ATP	C4-N9-C1'	-2.64	120.45	126.63
36	I	501	ATP	C3'-C2'-C1'	2.61	106.41	101.46
36	M	501	ATP	C2'-C1'-N9	-2.50	107.10	113.30
36	H	501	ATP	C4-N9-C8	2.49	108.36	105.74
36	I	501	ATP	C1'-N9-C8	-2.48	121.59	127.09
36	M	501	ATP	O4'-C1'-C2'	2.45	111.85	106.62
36	K	501	ATP	C4-N9-C8	2.43	108.29	105.74
36	L	501	ATP	O3G-PG-O2G	2.41	116.83	107.80
36	I	501	ATP	O2B-PB-O3A	-2.39	100.80	107.27
36	I	501	ATP	O2B-PB-O3B	2.39	113.73	107.27
36	H	501	ATP	C4-C5-N7	-2.39	107.85	110.58
36	H	501	ATP	N9-C8-N7	-2.36	110.59	113.94
36	H	501	ATP	C6-C5-C4	-2.33	113.99	117.18
38	J	501	ADP	C4'-O4'-C1'	2.31	114.57	109.47
36	H	501	ATP	O2A-PA-O1A	2.29	123.10	112.44
36	H	501	ATP	C5-N7-C8	2.26	107.01	103.45
38	J	501	ADP	O5'-PA-O1A	-2.26	99.97	108.94
36	I	501	ATP	O2'-C2'-C3'	2.26	119.06	111.82
36	H	501	ATP	O5'-PA-O1A	-2.26	99.98	108.94
38	J	501	ADP	O3A-PA-O1A	2.20	117.31	110.70
36	K	501	ATP	N9-C8-N7	-2.19	110.83	113.94
36	K	501	ATP	O3G-PG-O2G	2.15	115.88	107.80
38	J	501	ADP	N6-C6-N1	2.14	123.13	118.38
38	J	501	ADP	O4'-C4'-C5'	-2.13	102.53	109.33
36	H	501	ATP	O2G-PG-O1G	2.11	119.07	110.83
36	K	501	ATP	O3B-PB-O1B	2.10	117.03	110.70
36	H	501	ATP	C4-N9-C1'	-2.10	121.71	126.63
36	L	501	ATP	C6-C5-C4	2.10	120.04	117.18
38	J	501	ADP	C1'-N9-C8	-2.10	122.44	127.09
36	H	501	ATP	C3'-C2'-C1'	2.10	105.43	101.46
38	J	501	ADP	C5-C6-N1	2.08	122.80	117.51
36	H	501	ATP	O2A-PA-O3A	2.06	112.85	107.27
36	I	501	ATP	C2'-C1'-N9	-2.04	108.23	113.30
36	M	501	ATP	C5-N7-C8	2.04	106.66	103.45
36	M	501	ATP	O2A-PA-O3A	2.04	112.78	107.27
36	I	501	ATP	O3G-PG-O2G	2.03	115.43	107.80
36	H	501	ATP	O2B-PB-O3B	2.03	112.76	107.27
36	I	501	ATP	N6-C6-N1	2.01	122.85	118.38

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	H	501	ATP	PB-O3B-PG-O3G
36	H	501	ATP	C5'-O5'-PA-O2A
36	H	501	ATP	C5'-O5'-PA-O3A
36	I	501	ATP	C5'-O5'-PA-O1A
36	I	501	ATP	C5'-O5'-PA-O2A
36	I	501	ATP	C5'-O5'-PA-O3A
36	K	501	ATP	PB-O3B-PG-O2G
36	K	501	ATP	PB-O3B-PG-O3G
36	L	501	ATP	C5'-O5'-PA-O2A
36	L	501	ATP	C5'-O5'-PA-O3A
36	M	501	ATP	PB-O3B-PG-O2G
36	M	501	ATP	C5'-O5'-PA-O2A
36	M	501	ATP	C5'-O5'-PA-O3A
36	I	501	ATP	O4'-C4'-C5'-O5'
36	H	501	ATP	PB-O3B-PG-O2G
38	J	501	ADP	O4'-C4'-C5'-O5'
36	H	501	ATP	PG-O3B-PB-O2B
36	K	501	ATP	PG-O3B-PB-O2B
36	L	501	ATP	O4'-C4'-C5'-O5'
36	M	501	ATP	PB-O3B-PG-O3G
38	J	501	ADP	PA-O3A-PB-O2B
38	J	501	ADP	PA-O3A-PB-O3B
36	H	501	ATP	PG-O3B-PB-O1B
36	K	501	ATP	PG-O3B-PB-O1B
36	K	501	ATP	PB-O3B-PG-O1G
36	M	501	ATP	PG-O3B-PB-O2B
36	L	501	ATP	C3'-C4'-C5'-O5'

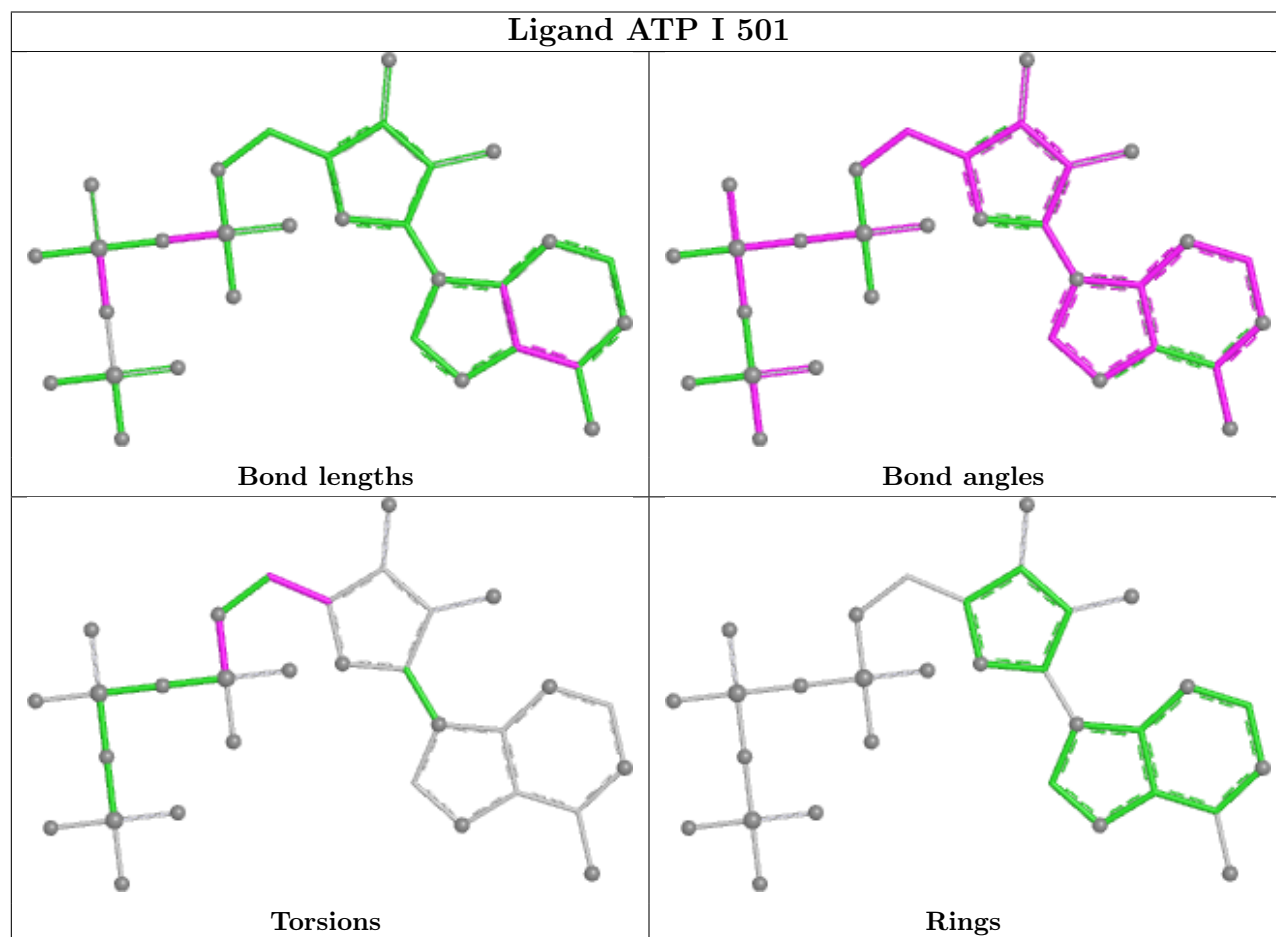
There are no ring outliers.

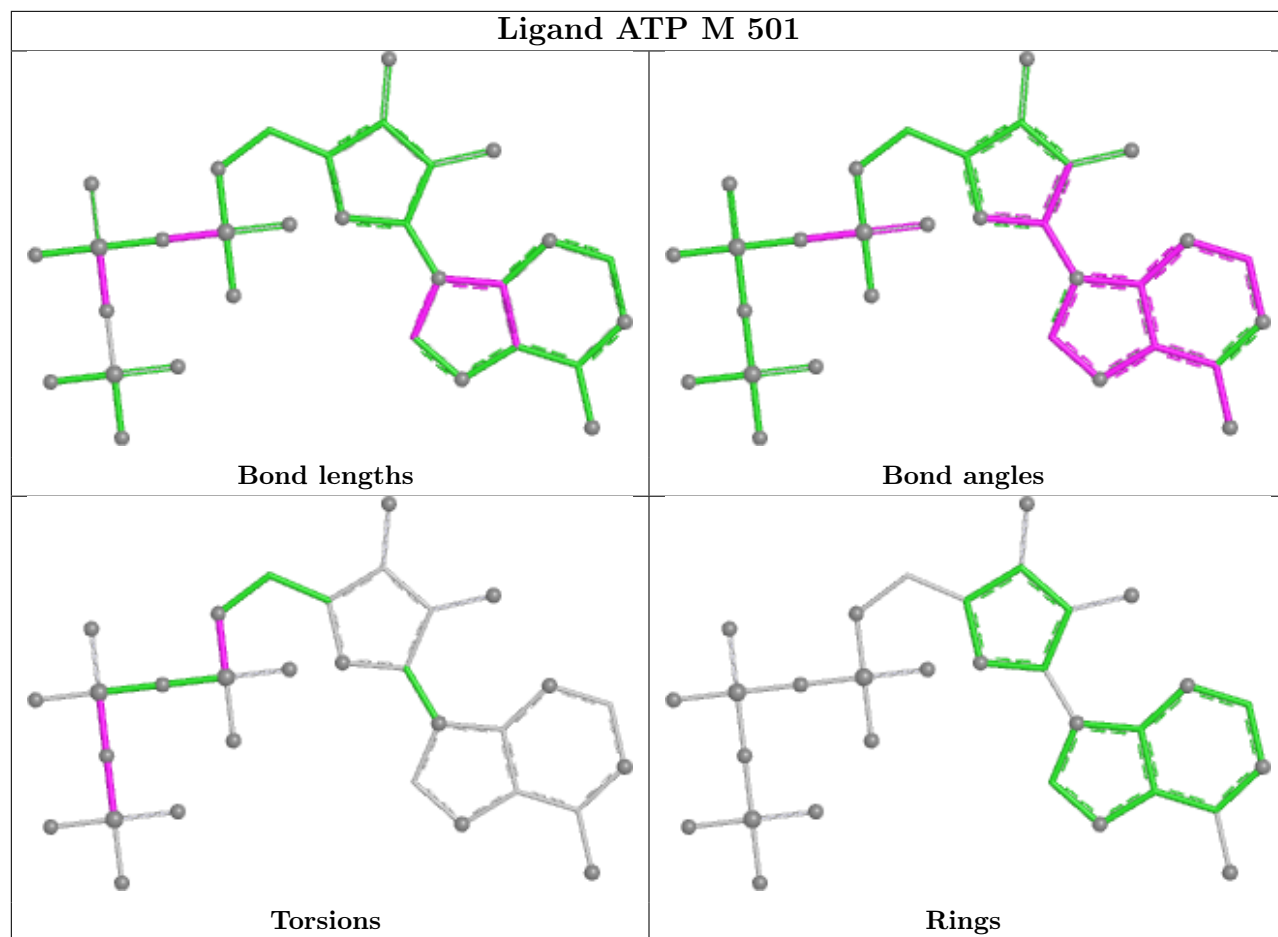
6 monomers are involved in 98 short contacts:

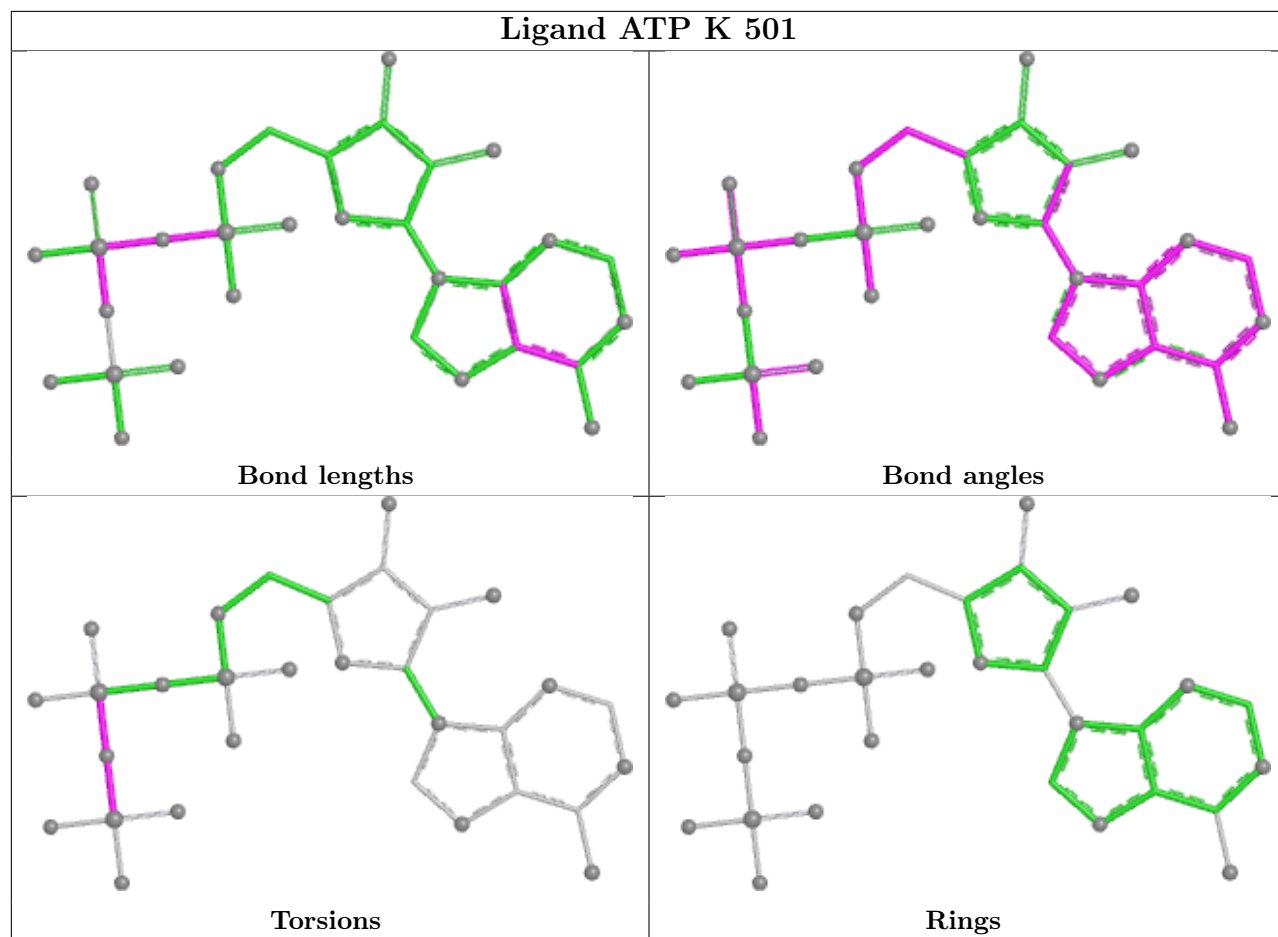
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	I	501	ATP	20	0
36	M	501	ATP	15	0
36	K	501	ATP	7	0
36	H	501	ATP	32	0
38	J	501	ADP	14	0
36	L	501	ATP	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

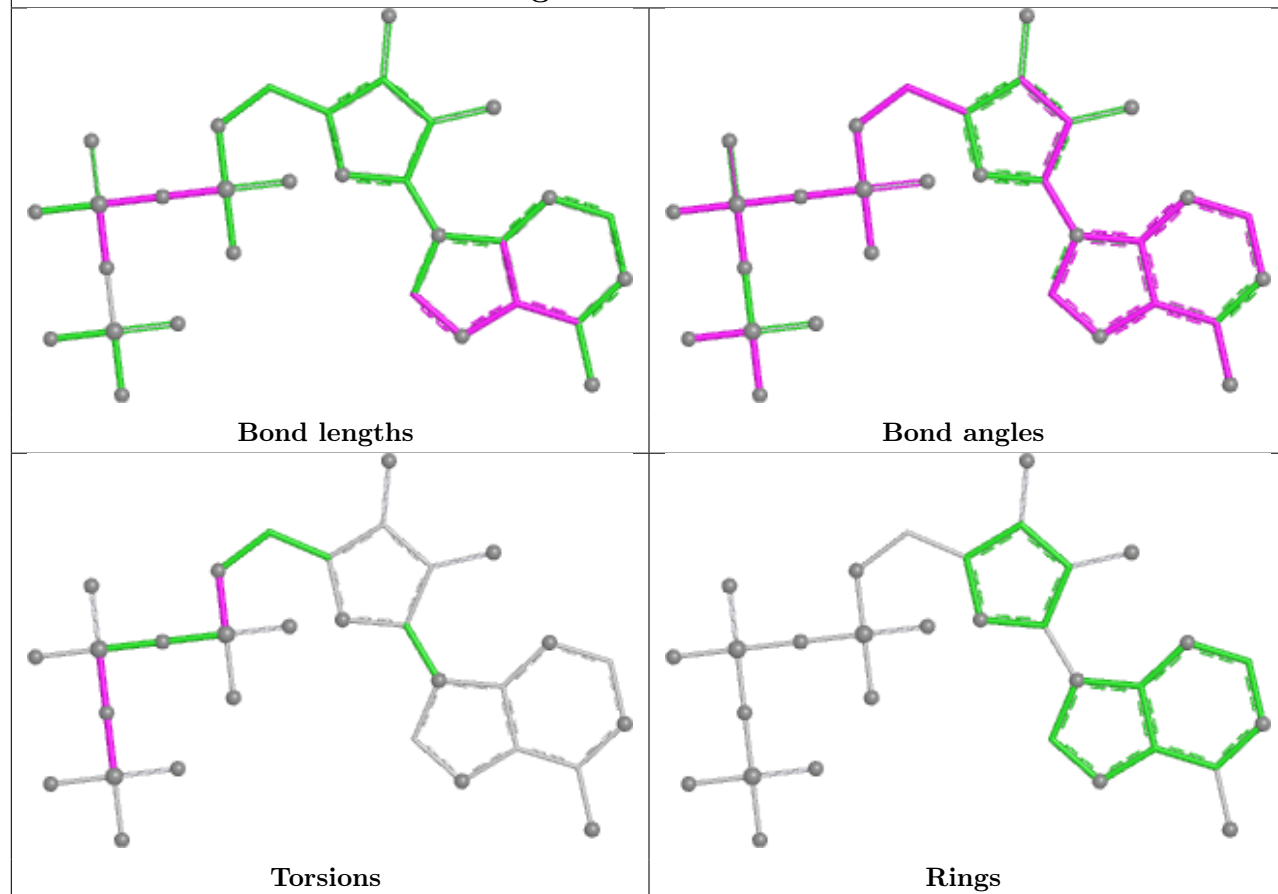
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



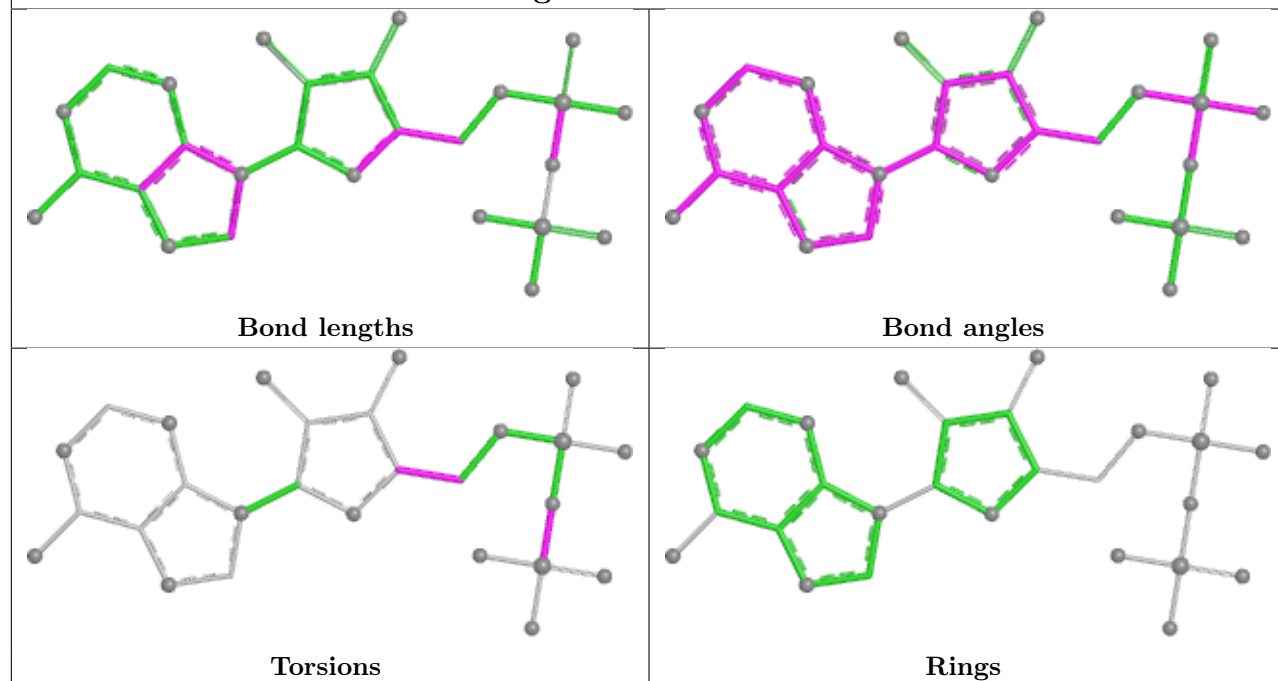


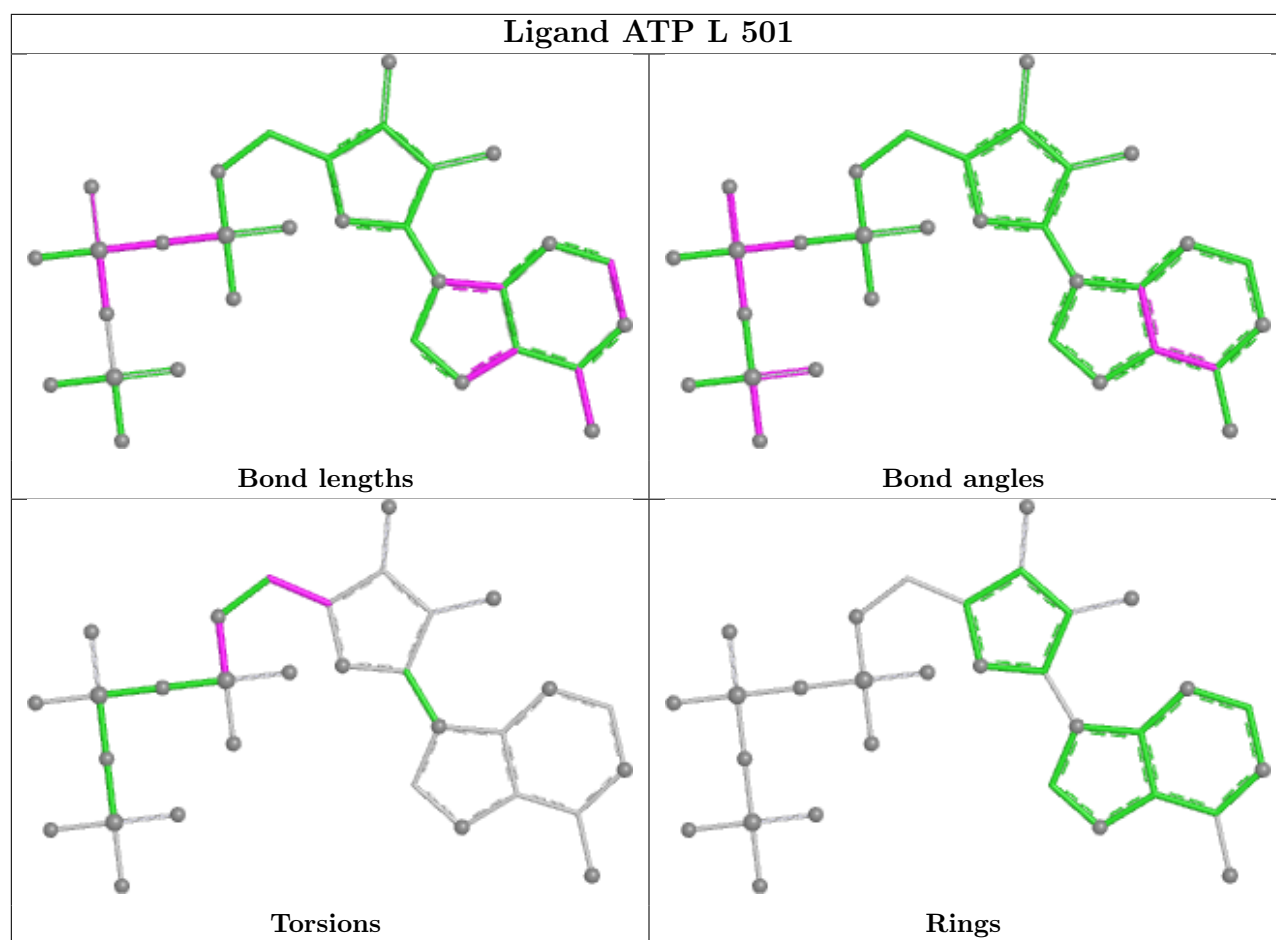


Ligand ATP H 501



Ligand ADP J 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

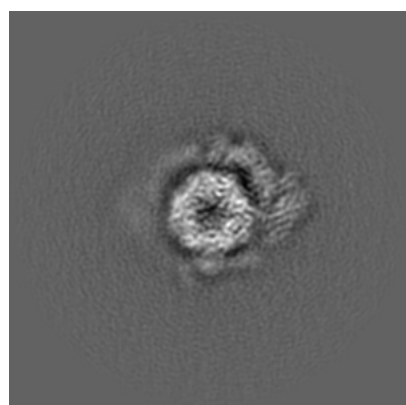
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14085. These allow visual inspection of the internal detail of the map and identification of artifacts.

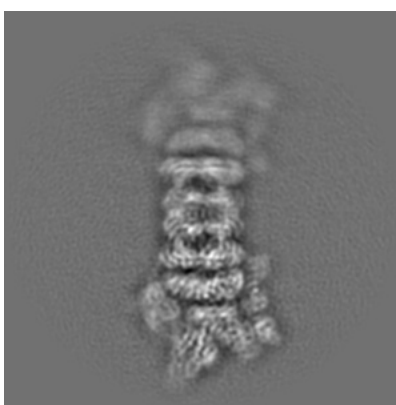
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

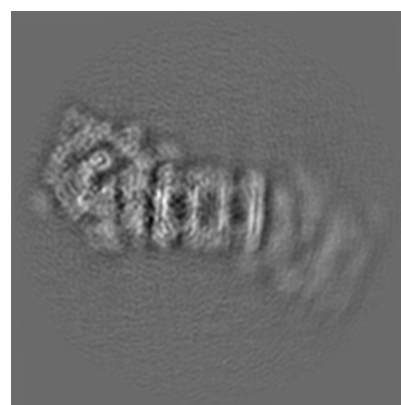
6.1.1 Primary map



X



Y

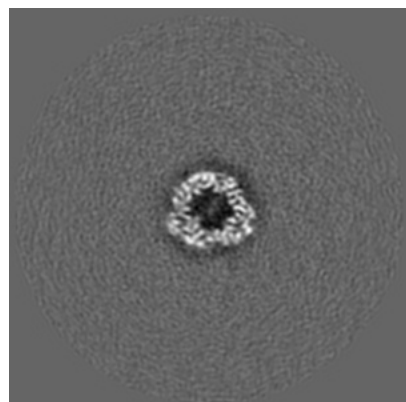


Z

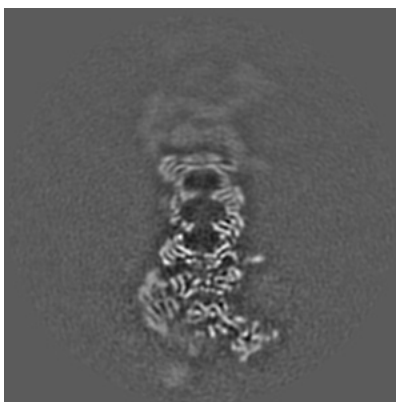
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

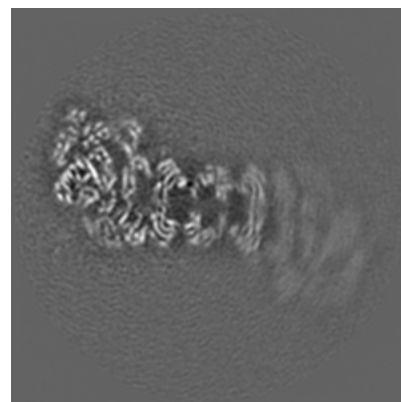
6.2.1 Primary map



X Index: 192



Y Index: 192

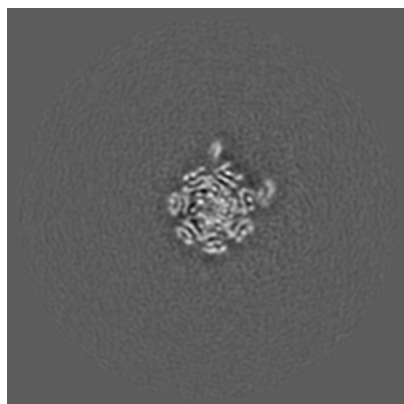


Z Index: 192

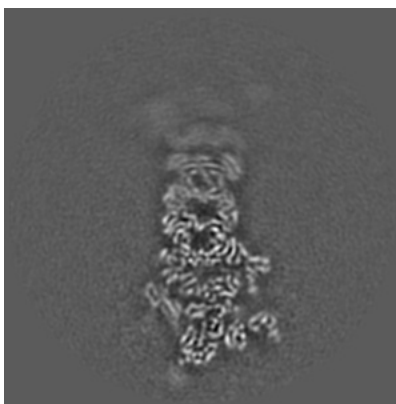
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

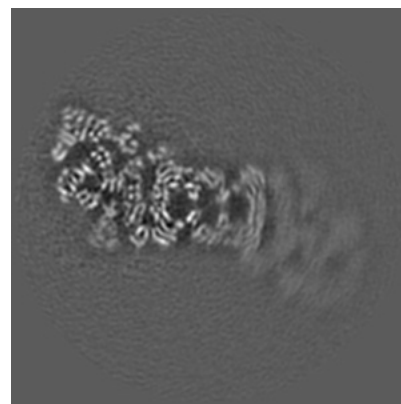
6.3.1 Primary map



X Index: 148



Y Index: 208

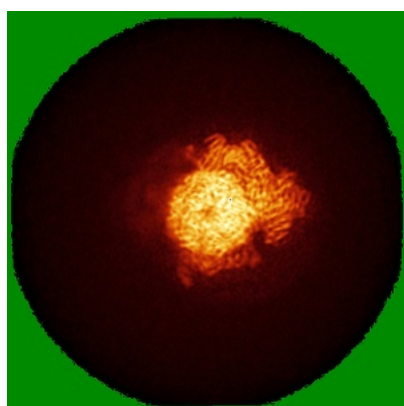


Z Index: 197

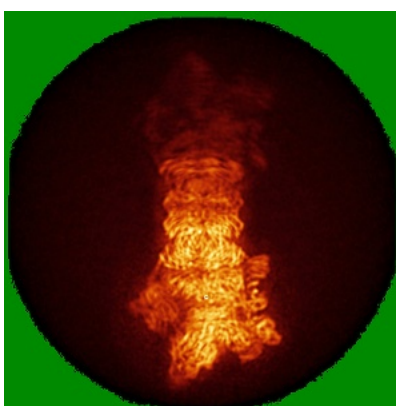
The images above show the largest variance slices of the map in three orthogonal directions.

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

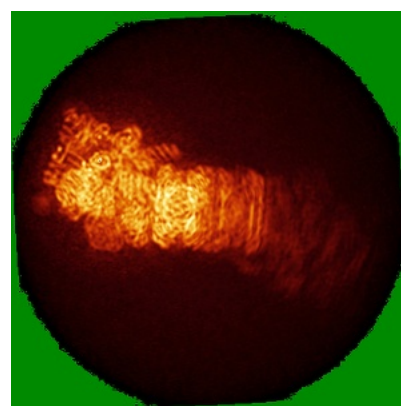
6.4.1 Primary map



X



Y

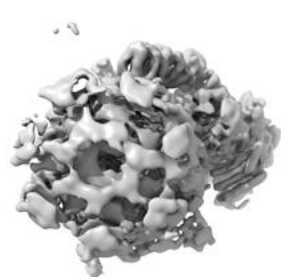


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

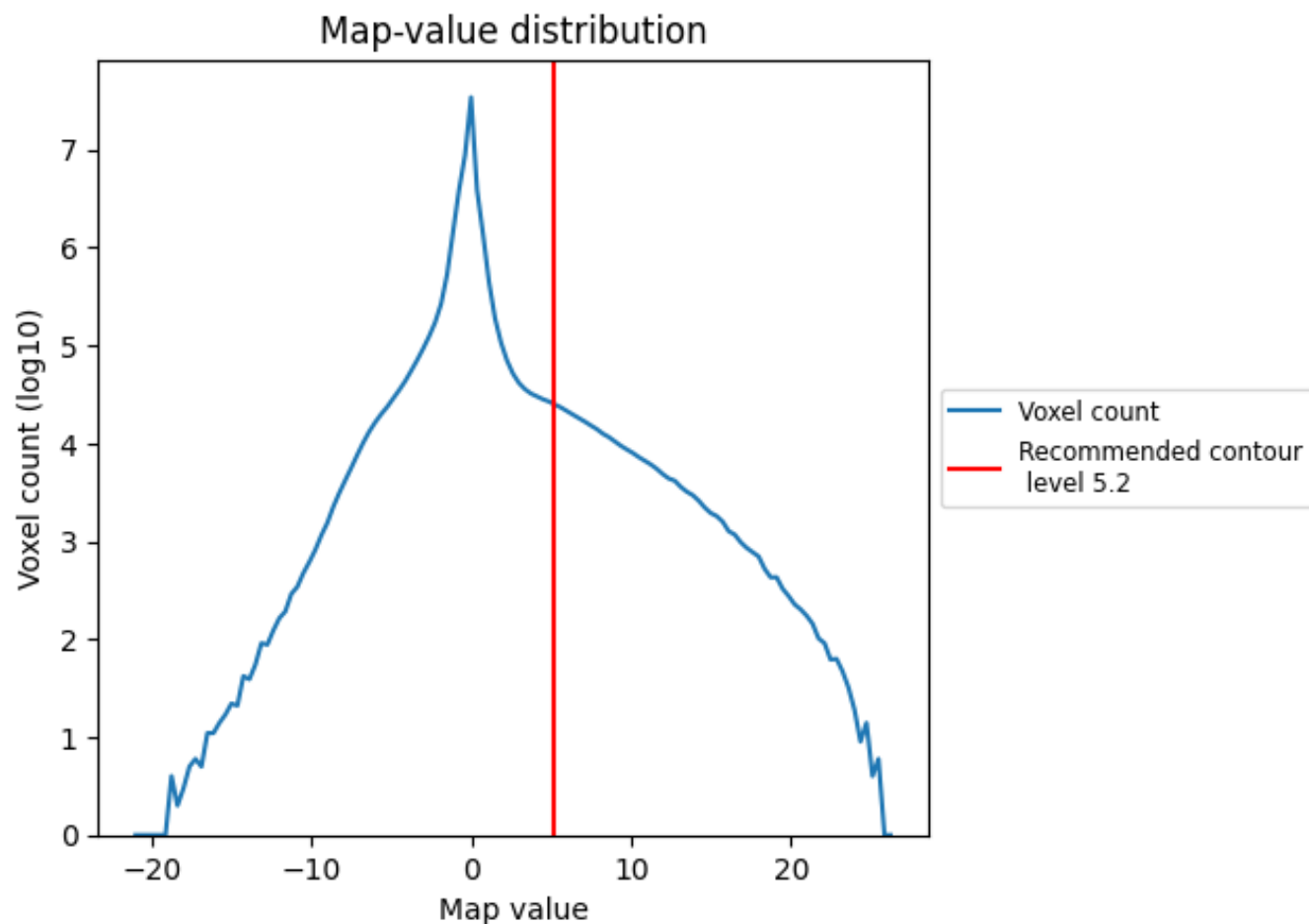
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

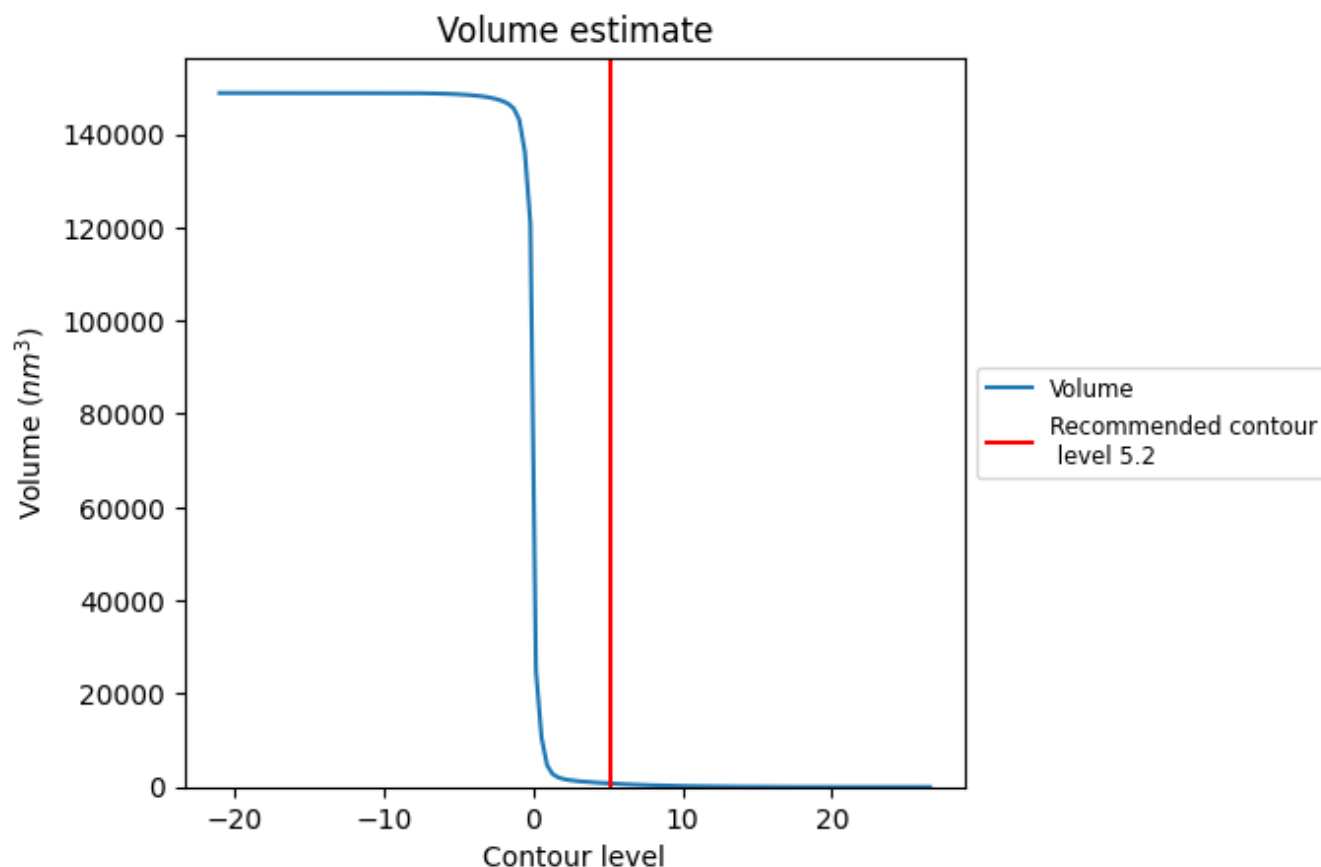
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

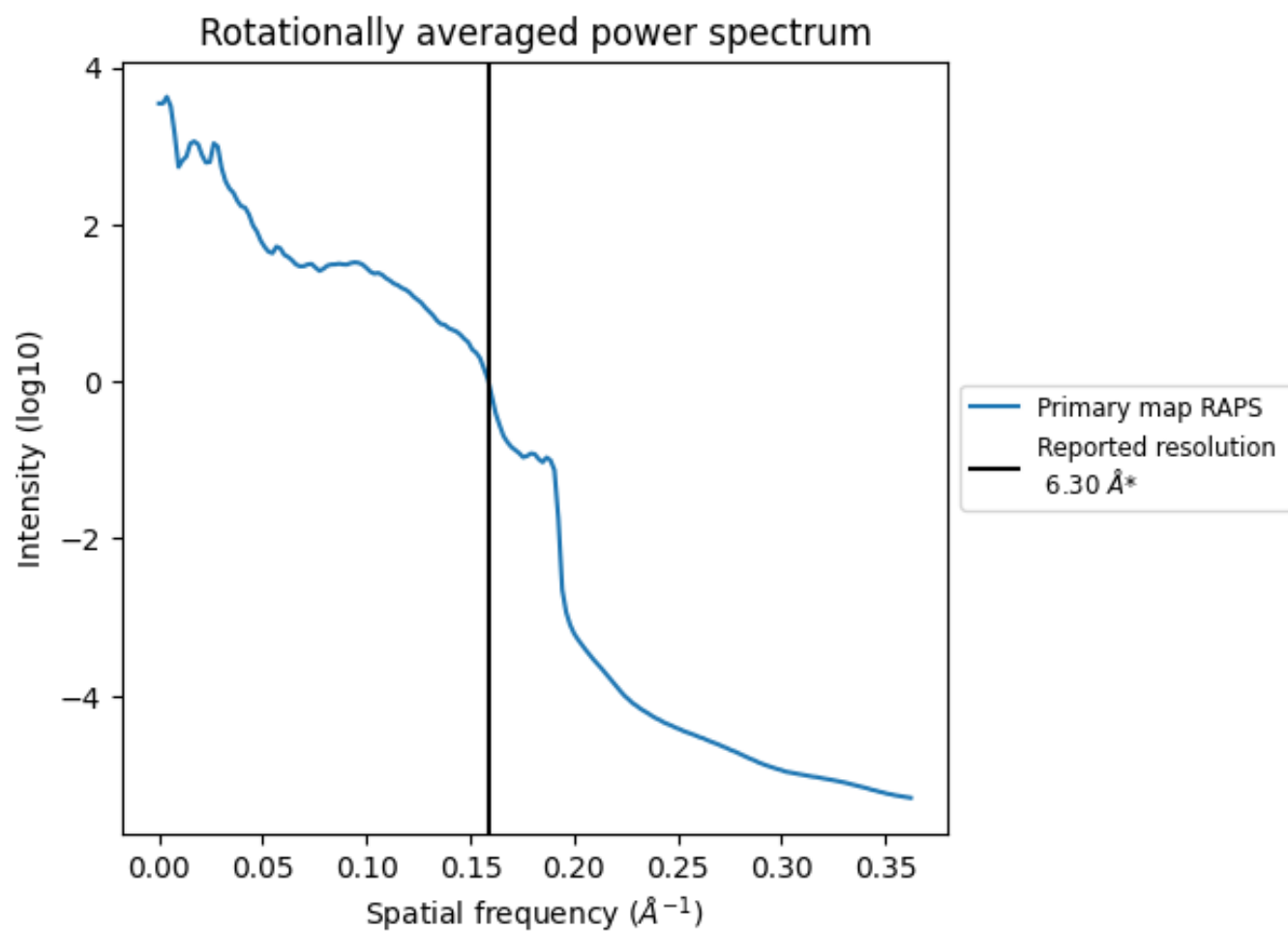
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 745 nm^3 ; this corresponds to an approximate mass of 673 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 0.159 Å⁻¹

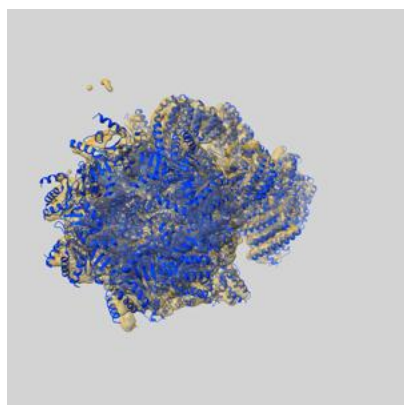
8 Fourier-Shell correlation

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

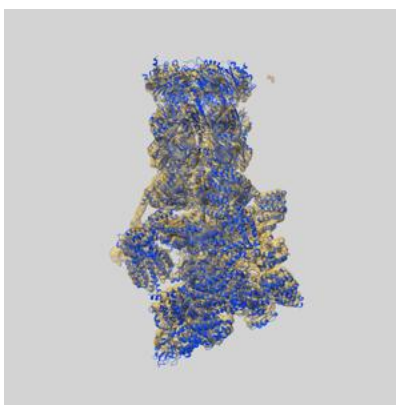
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14085 and PDB model 7QO6. Per-residue inclusion information can be found in section 3 on page 14.

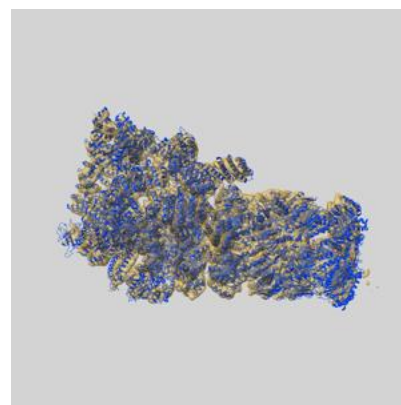
9.1 Map-model overlay [i](#)



X



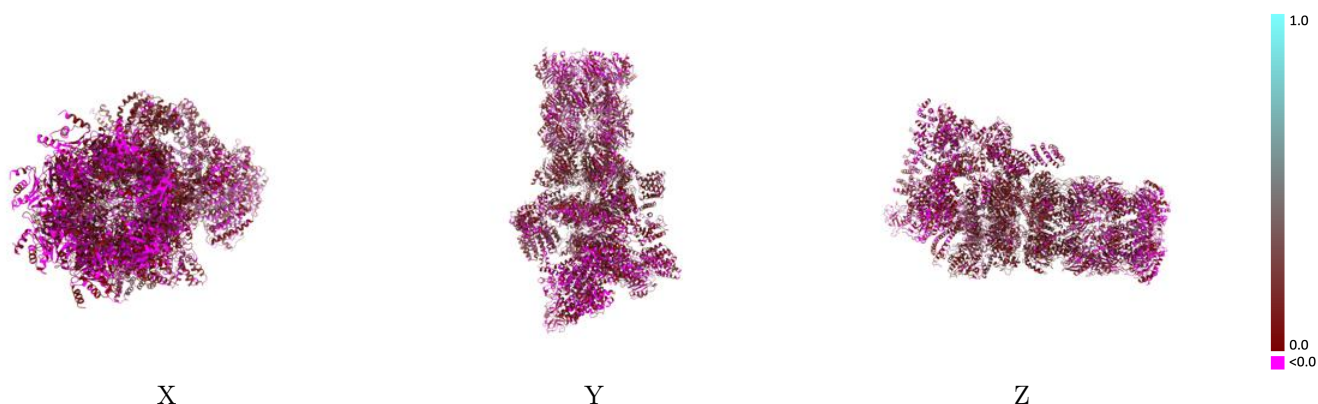
Y



Z

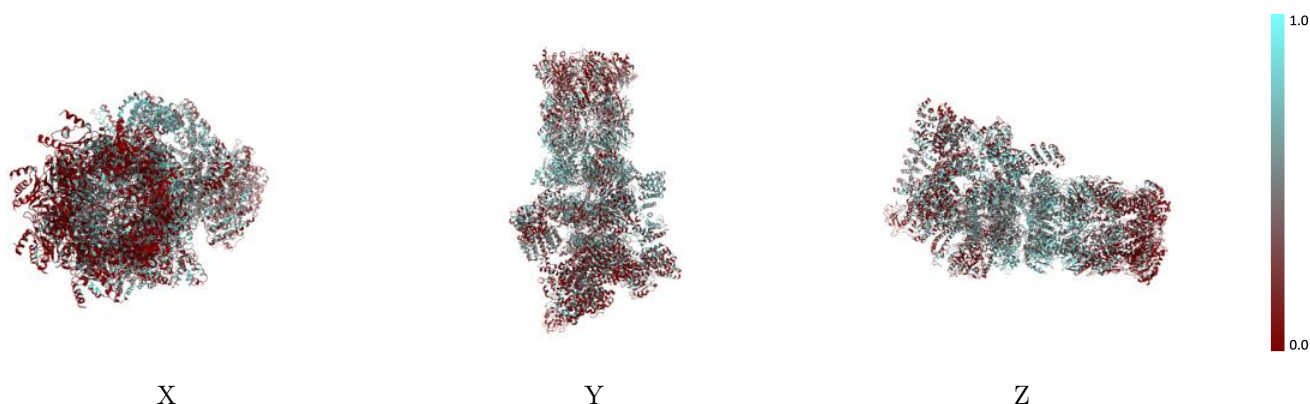
The images above show the 3D surface view of the map at the recommended contour level 5.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



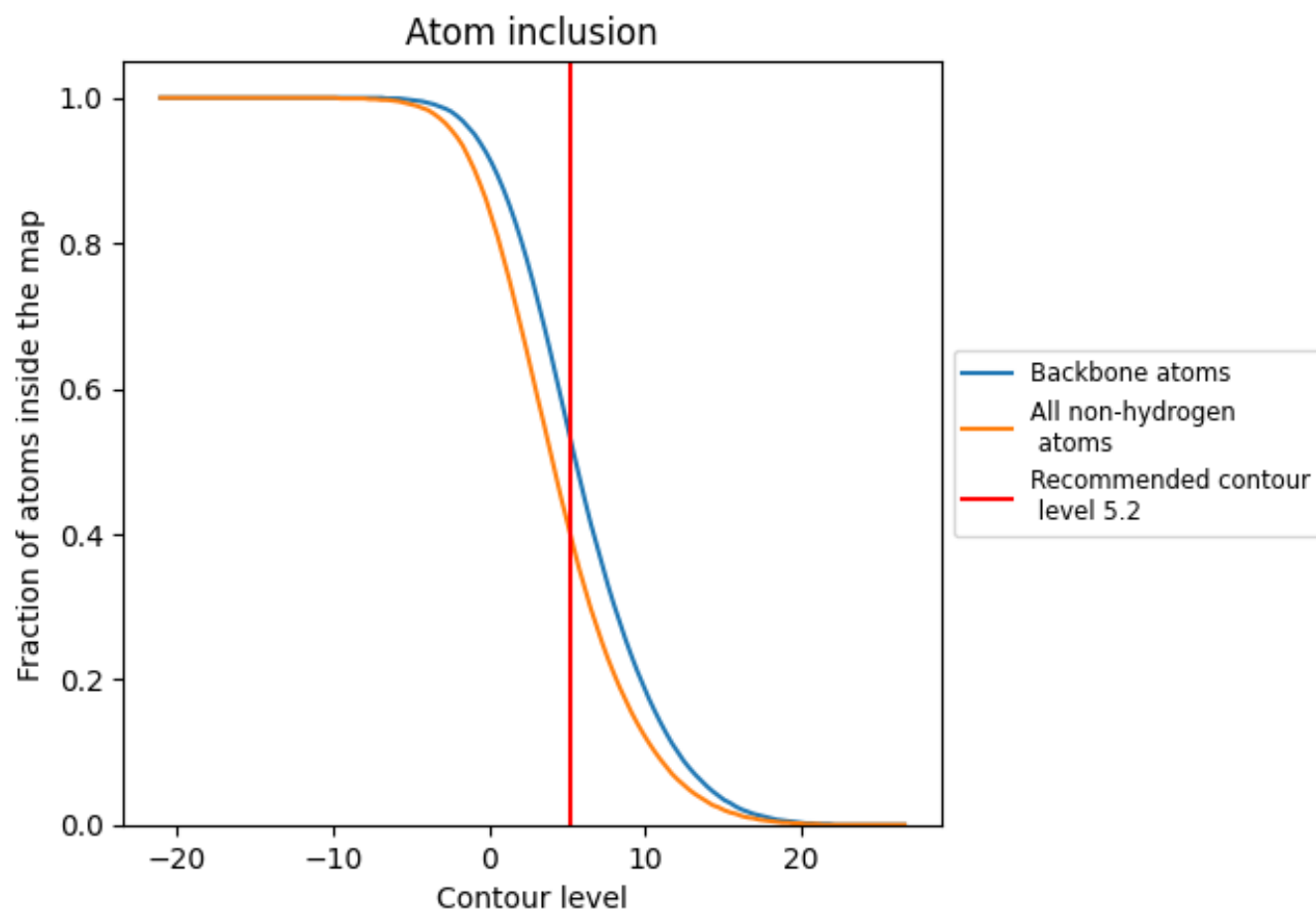
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 40% 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 (5.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3990	 0.0960
1	 0.5360	 0.1020
2	 0.4980	 0.1120
3	 0.4630	 0.0920
4	 0.5220	 0.0970
5	 0.5080	 0.1010
6	 0.4690	 0.0980
7	 0.4990	 0.1070
8	 0.2550	 0.1370
9	 0.2330	 0.1490
A	 0.5950	 0.1630
B	 0.5470	 0.1640
C	 0.5670	 0.1530
D	 0.6000	 0.1650
E	 0.5780	 0.1510
F	 0.6050	 0.1570
G	 0.6020	 0.1720
H	 0.4720	 0.1510
I	 0.4490	 0.1450
J	 0.4540	 0.1260
K	 0.4430	 0.1300
L	 0.4870	 0.1330
M	 0.4700	 0.1380
N	 0.4360	 0.0810
O	 0.4130	 0.0770
P	 0.5720	 0.1220
Q	 0.4490	 0.0970
R	 0.4240	 0.0760
S	 0.3240	 0.0270
T	 0.2800	 0.0620
U	 0.4290	 0.0920
V	 0.4310	 0.0920
W	 0.3920	 0.0590
X	 0.0920	 0.0550
Y	 0.1870	 0.0620



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Chain	Atom inclusion	Q-score
Z	 0.3130	 0.0990
a	 0.1620	 0.0110
b	 0.0930	 0.0010
c	 0.1800	 0.0020
d	 0.2110	 0.0180
e	 0.1510	 0.0110
f	 0.2080	 0.0090
g	 0.1770	 0.0150
h	 0.3560	 0.0760
i	 0.2460	 0.0720
j	 0.2860	 0.0880
k	 0.3790	 0.0880
l	 0.3350	 0.0850
m	 0.2930	 0.0750
n	 0.3460	 0.0880