



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 03:10 PM UTC

PDB ID : 5WVK / pdb_00005wvk
EMDB ID : EMD-6694
Title : Yeast proteasome-ADP-AlFx
Authors : Ding, Z.; Cong, Y.
Deposited on : 2016-12-25
Resolution : 4.20 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:

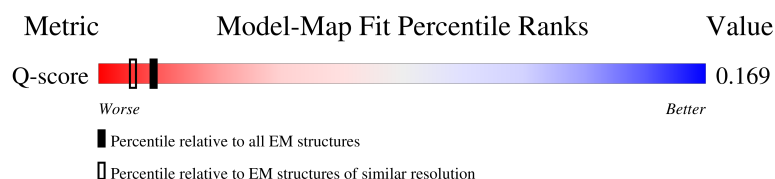
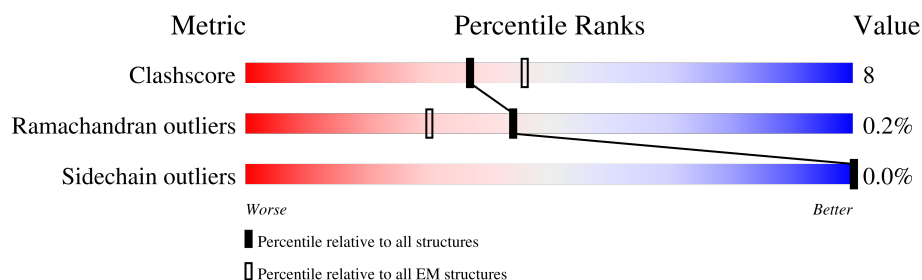
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.20 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	5410 (3.70 - 4.70)

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	1	215	
1	b	215	
2	2	261	
2	i	261	

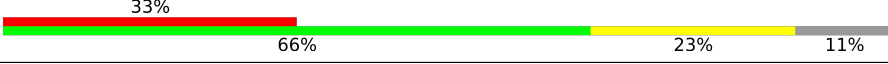
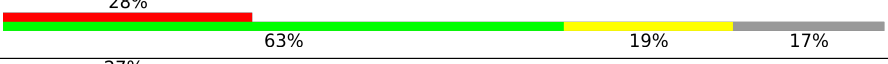
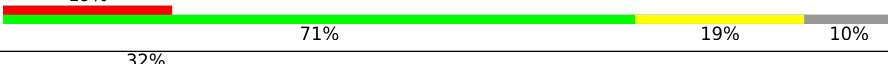
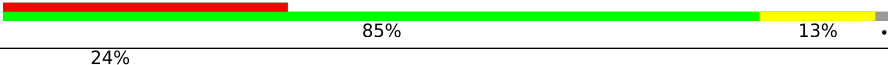
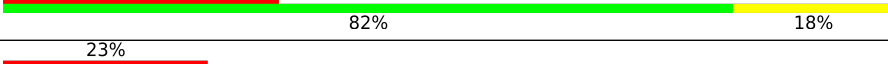
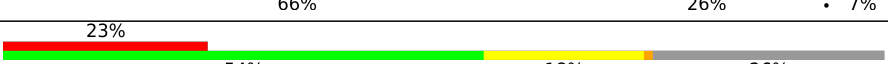
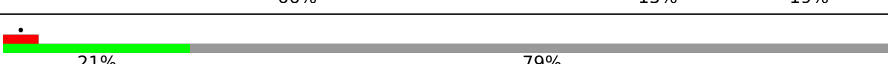
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Mol	Chain	Length	Quality of chain
3	3	205	
3	h	205	
4	4	198	
4	g	198	
5	5	287	
5	f	287	
6	6	241	
6	e	241	
7	7	266	
7	a	266	
8	A	252	
8	c	252	
9	B	250	
9	j	250	
10	C	258	
10	d	258	
11	D	254	
11	n	254	
12	E	260	
12	m	260	
13	F	234	
13	l	234	
14	G	288	
14	k	288	
15	H	467	

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Mol	Chain	Length	Quality of chain
16	I	437	
17	J	405	
18	K	428	
19	L	437	
20	M	434	
21	N	945	
22	O	393	
23	P	445	
24	Q	434	
25	R	429	
26	S	523	
27	T	274	
28	U	338	
29	V	306	
30	W	268	
31	X	156	
32	Y	89	
33	Z	993	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 105261 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 Proteasome subunit beta type-1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	223	Total	C	N	O	S	0	0
			1692	1067	294	324	7		
2	i	223	Total	C	N	O	S	0	0
			1692	1067	294	324	7		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	198	Total	C	N	O	S	0	0
			1585	1005	269	305	6		
4	g	198	Total	C	N	O	S	0	0
			1585	1005	269	305	6		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	233	Total	C	N	O	S	0	0
			1824	1154	312	351	7		
7	a	233	Total	C	N	O	S	0	0
			1824	1154	312	351	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	243	Total	C	N	O	S	0	0
			1921	1221	322	370	8		
8	c	243	Total	C	N	O	S	0	0
			1921	1221	322	370	8		

- Molecule 9 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		
9	j	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		

- Molecule 10 is a protein called Proteasome subunit alpha type-3.

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

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

- Molecule 11 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	241	Total	C	N	O	S	0	0
			1890	1181	331	374	4		
11	n	241	Total	C	N	O	S	0	0
			1890	1181	331	374	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		
12	m	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		

- Molecule 13 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		
13	l	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		

- Molecule 14 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	244	Total	C	N	O	S	0	0
			1896	1205	330	357	4		
14	k	244	Total	C	N	O	S	0	0
			1896	1205	330	357	4		

- Molecule 15 is a protein called 26S protease regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	359	Total	C	N	O	S	0	0
			2792	1755	499	523	15		

- Molecule 16 is a protein called 26S protease regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	362	Total	C	N	O	S	0	0
			2822	1773	471	563	15		

- Molecule 17 is a protein called 26S protease regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	373	Total	C	N	O	S	0	0
			2928	1837	527	547	17		

- Molecule 18 is a protein called 26S protease regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	381	Total	C	N	O	S	0	0
			3019	1898	530	581	10		

- Molecule 19 is a protein called 26S protease subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	361	Total	C	N	O	S	0	0
			2853	1798	507	536	12		

- Molecule 20 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	367	Total	C	N	O	S	0	0
			2866	1799	503	553	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	849	Total	C	N	O	S	0	0
			6562	4174	1099	1261	28		

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	387	Total	C	N	O	S	0	0
			3182	2047	520	606	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	432	Total	C	N	O	S	0	0
			3545	2260	592	684	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	431	Total	C	N	O	S	0	0
			3471	2205	574	676	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	400	Total	C	N	O	S	0	0
			3218	2051	527	630	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	353	Total	C	N	O	S	0	0
			2893	1857	482	541	13		

- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	272	Total	C	N	O	S	0	0
			2235	1432	355	441	7		

- Molecule 28 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	255	Total	C	N	O	S	0	0
			2061	1312	352	391	6		

- Molecule 29 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	284	Total	C	N	O	S	0	0
			2236	1405	381	436	14		

- Molecule 30 is a protein called 26S proteasome regulatory subunit RPN10.

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

- Molecule 31 is a protein called 26S proteasome regulatory subunit RPN13.

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

- Molecule 32 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y	19	Total	C	N	O	0	0
			168	101	30	37		

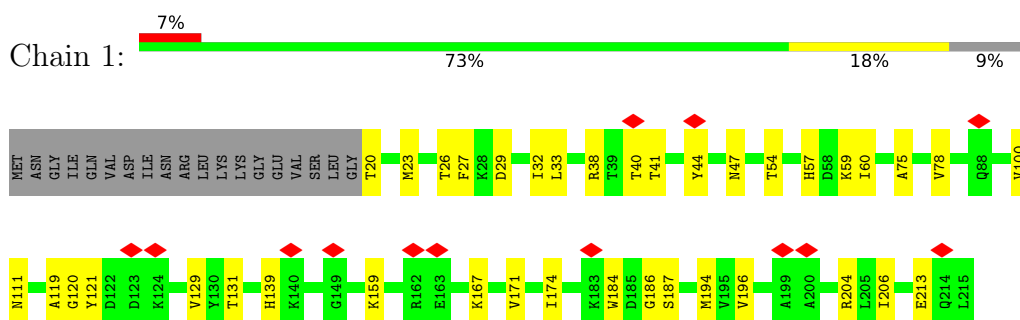
- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	813	Total	C	N	O	S	0	0
			6290	3995	1029	1237	29		

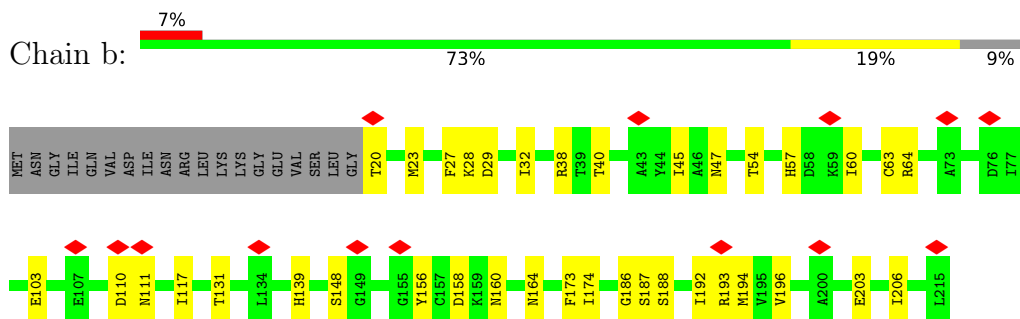
3 Residue-property plots

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.

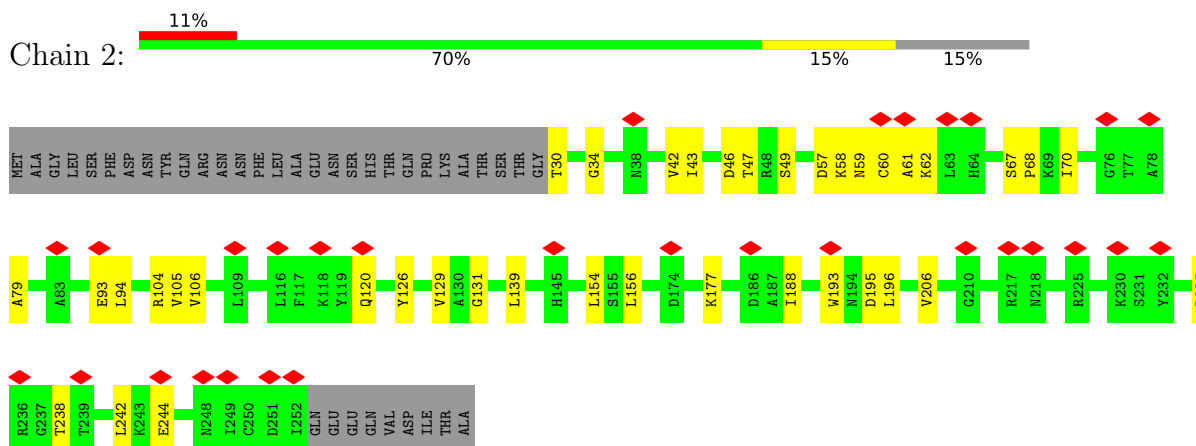
- Molecule 1: Proteasome subunit beta type-1



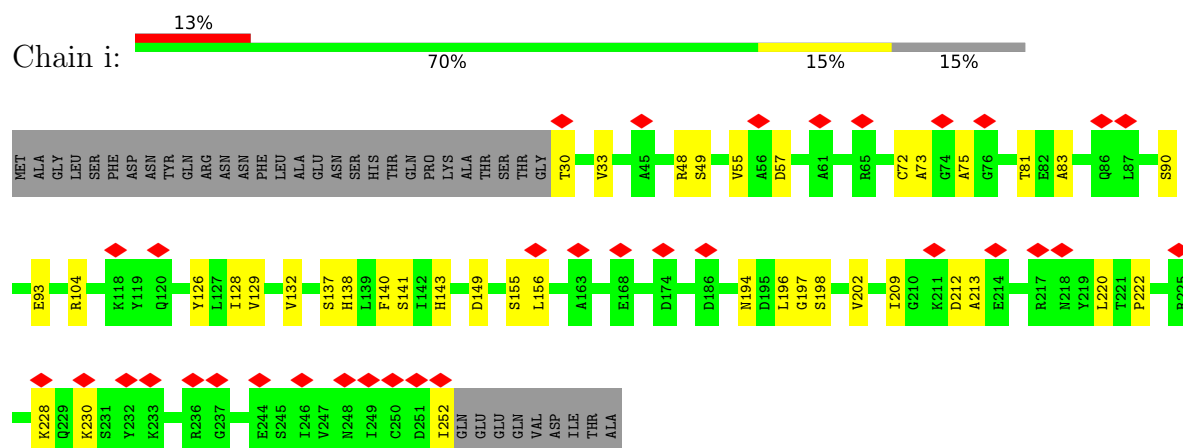
- Molecule 1: Proteasome subunit beta type-1



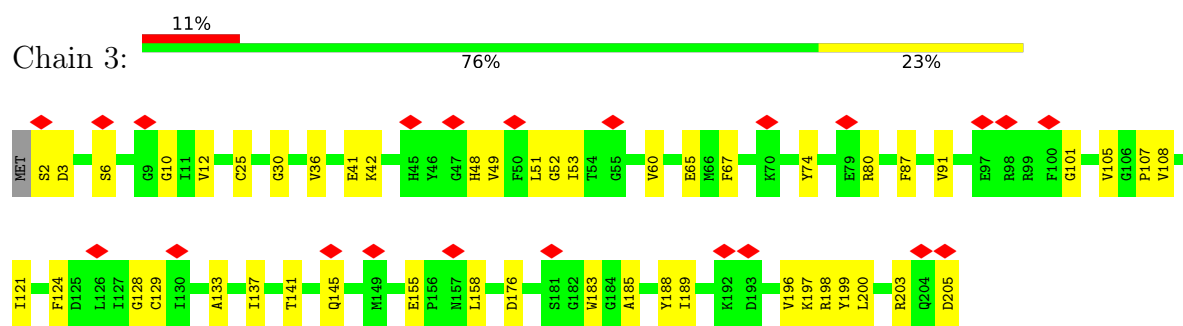
- Molecule 2: Proteasome subunit beta type-2



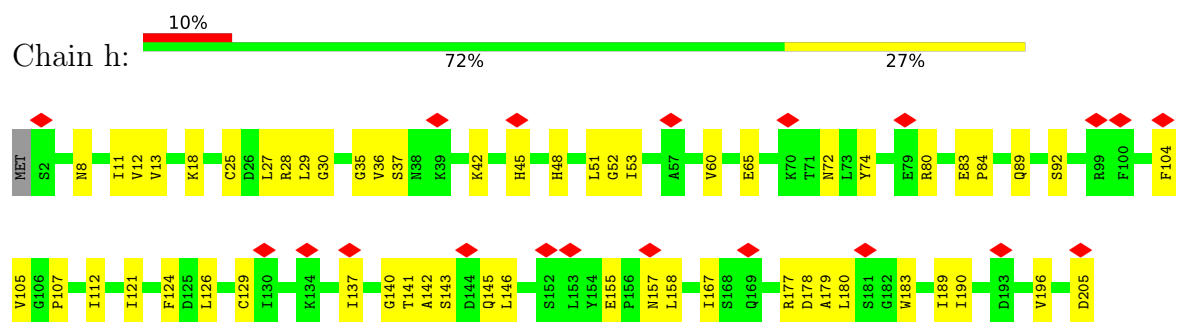
- Molecule 2: Proteasome subunit beta type-2



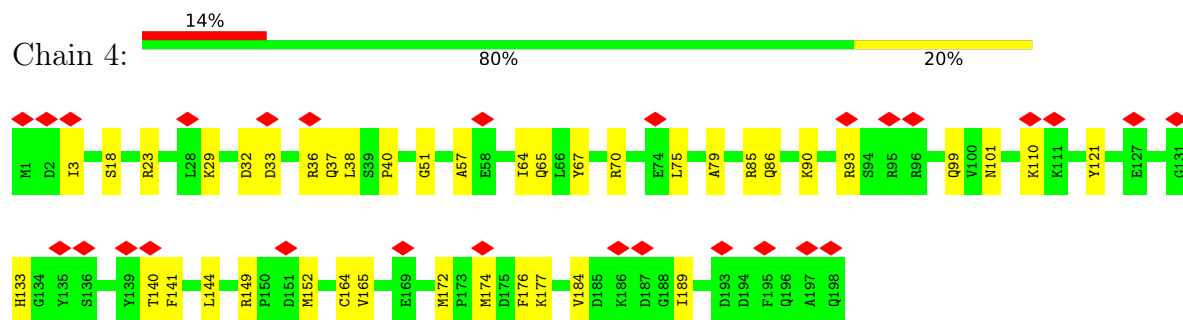
- Molecule 3: Proteasome subunit beta type-3



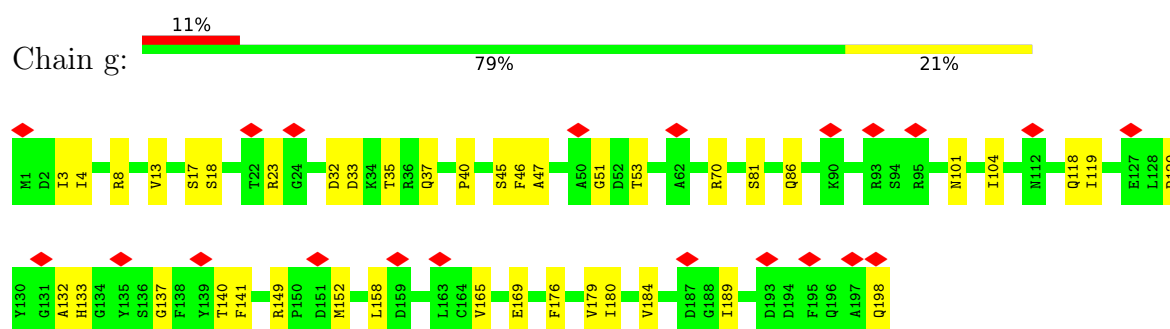
- Molecule 3: Proteasome subunit beta type-3



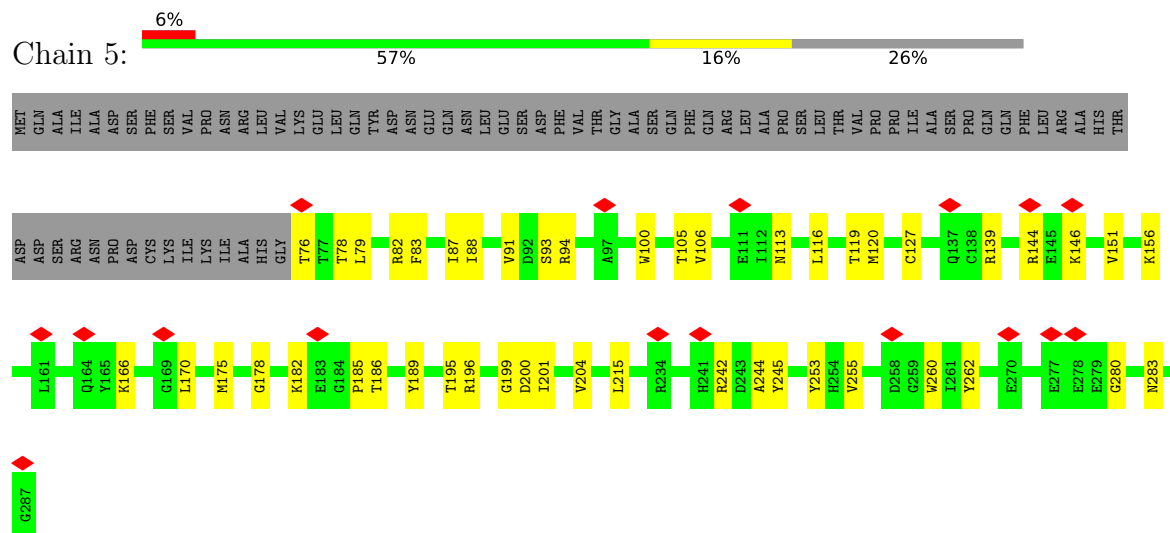
- Molecule 4: Proteasome subunit beta type-4



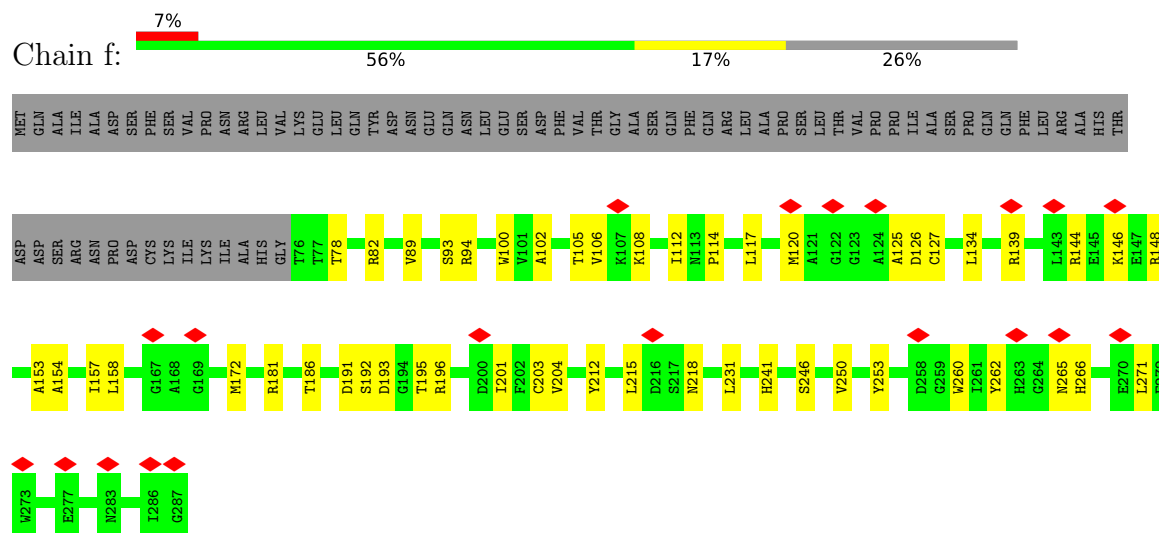
- Molecule 4: Proteasome subunit beta type-4



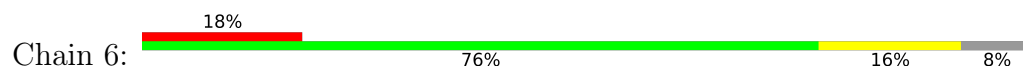
• Molecule 5: Proteasome subunit beta type-5

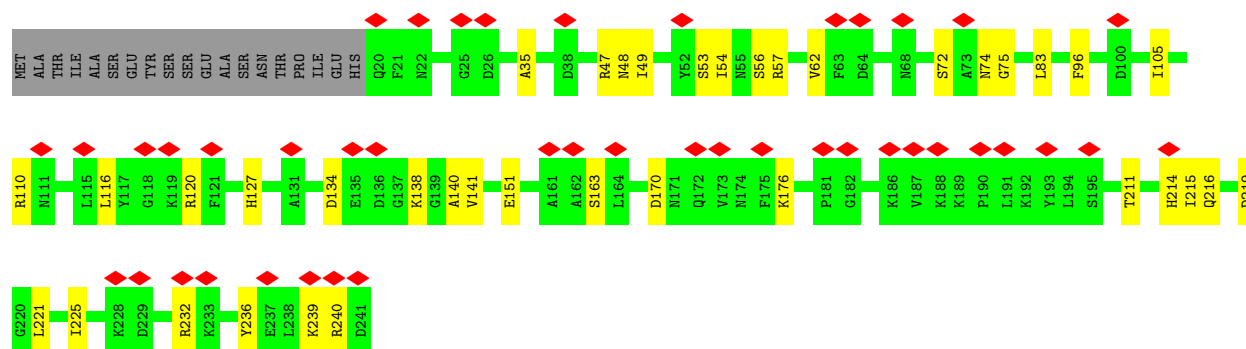


• Molecule 5: Proteasome subunit beta type-5

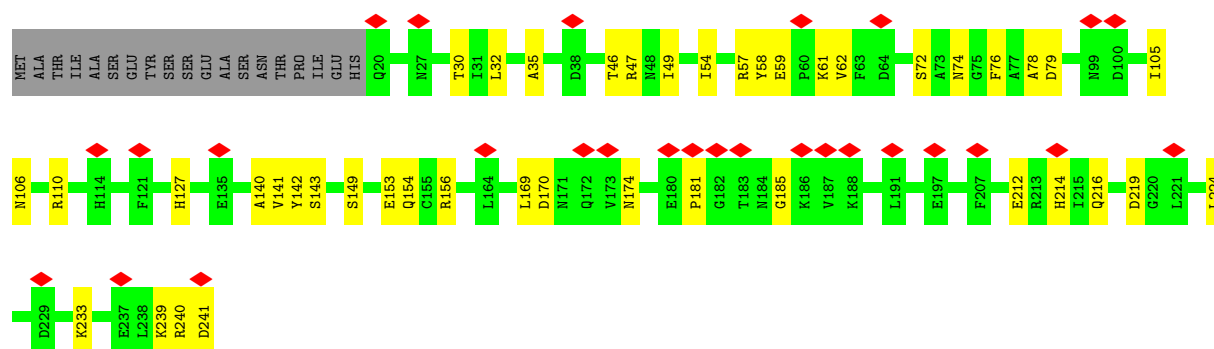


• Molecule 6: Proteasome subunit beta type-6

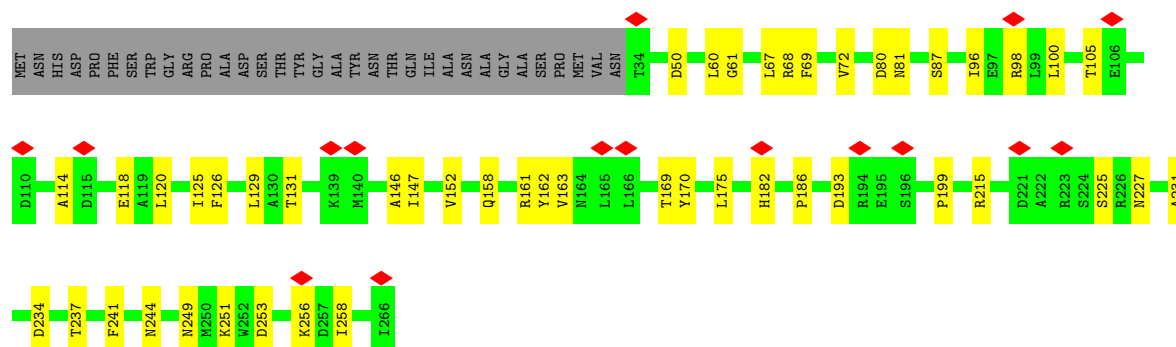




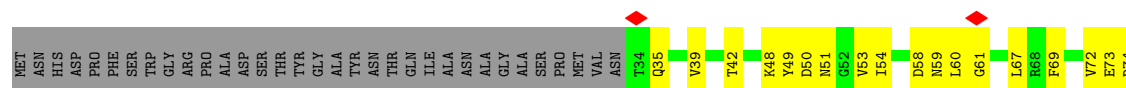
• Molecule 6: Proteasome subunit beta type-6

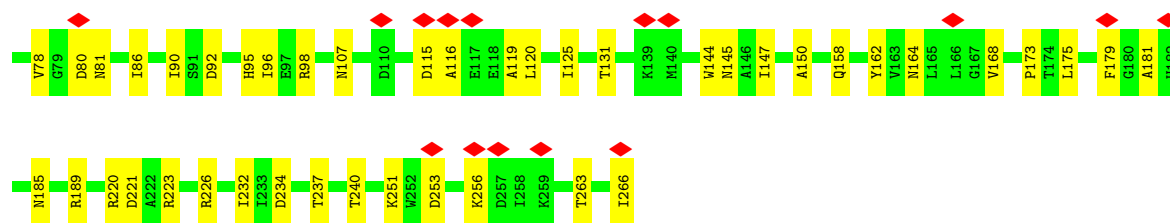


• Molecule 7: Proteasome subunit beta type-7

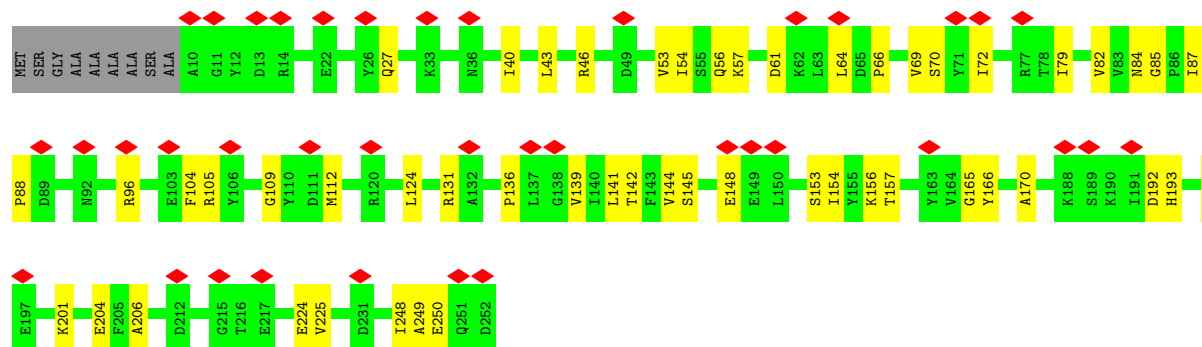
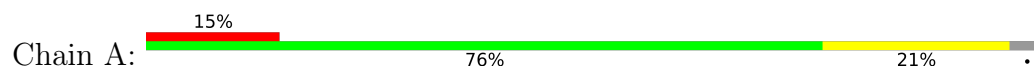


• Molecule 7: Proteasome subunit beta type-7

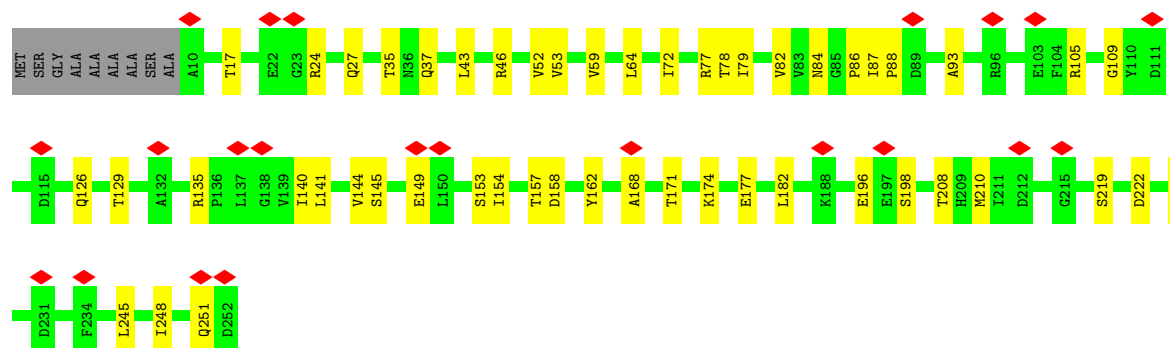
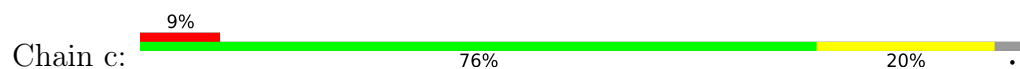




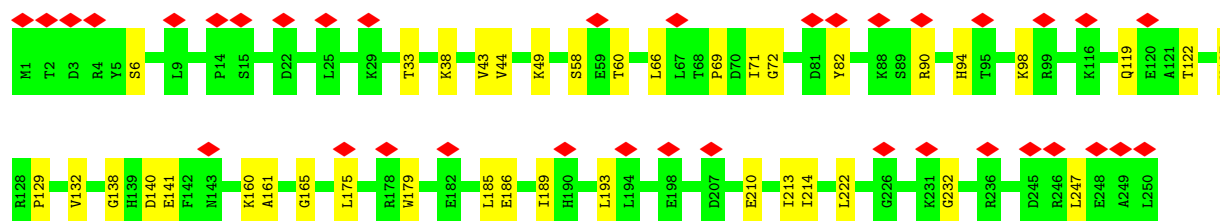
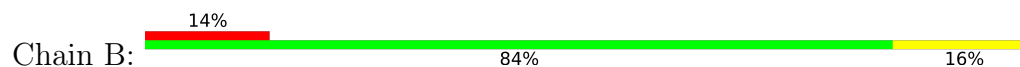
• Molecule 8: Proteasome subunit alpha type-1



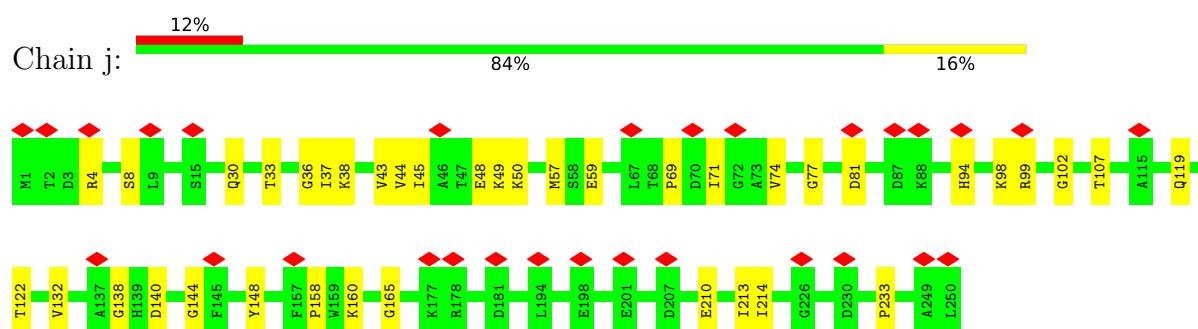
• Molecule 8: Proteasome subunit alpha type-1



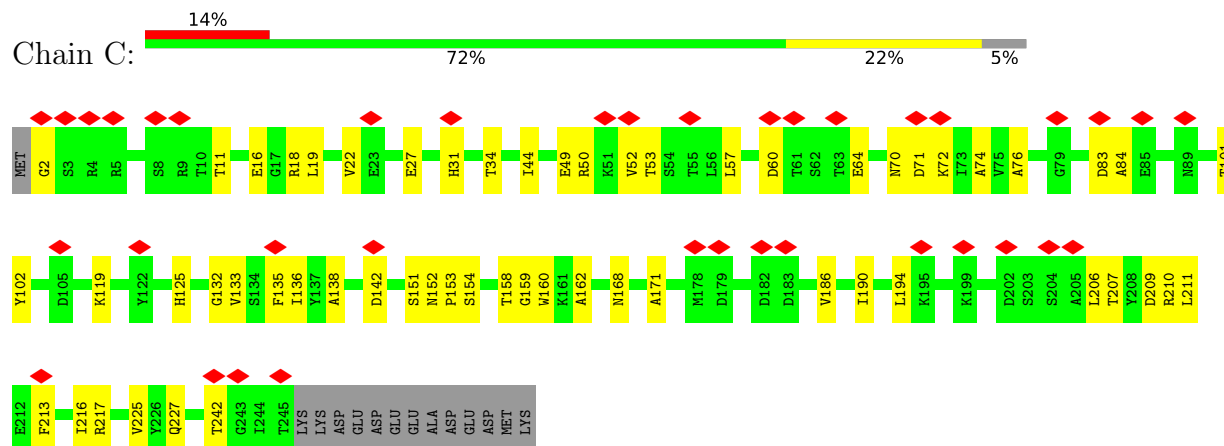
• Molecule 9: Proteasome subunit alpha type-2



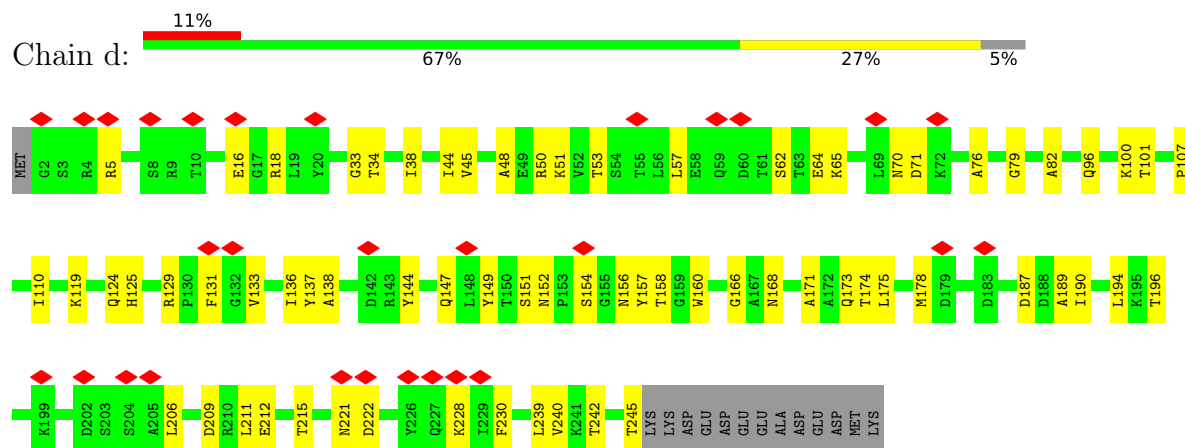
• Molecule 9: Proteasome subunit alpha type-2



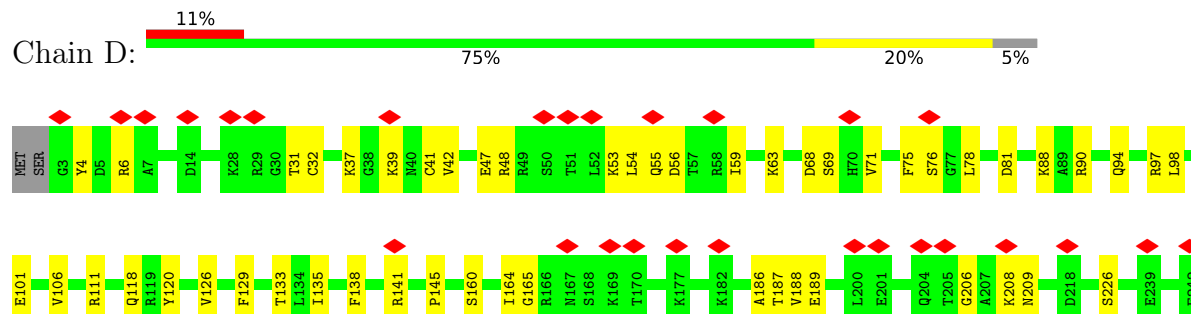
• Molecule 10: Proteasome subunit alpha type-3

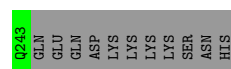


• Molecule 10: Proteasome subunit alpha type-3



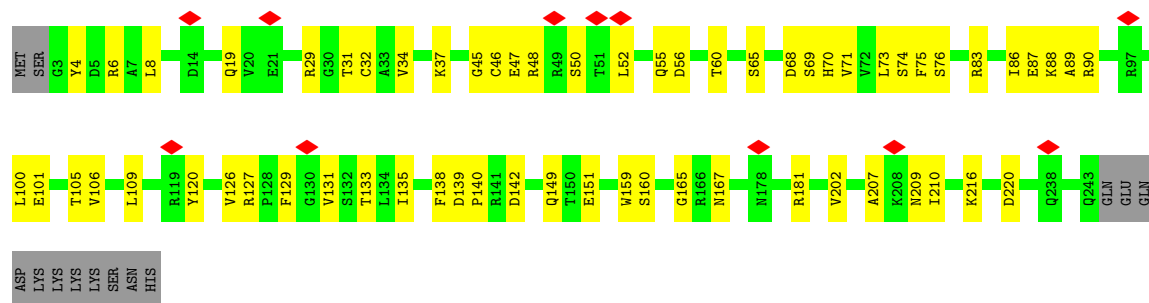
• Molecule 11: Proteasome subunit alpha type-4





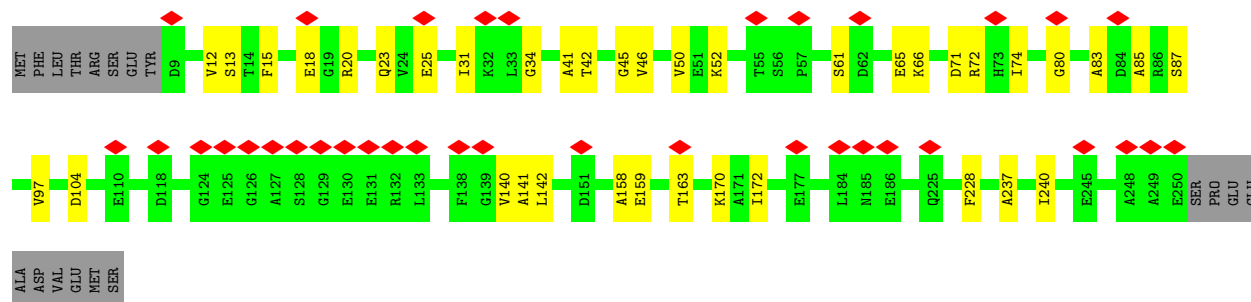
• Molecule 11: Proteasome subunit alpha type-4

Chain n:  70% 24% 5%



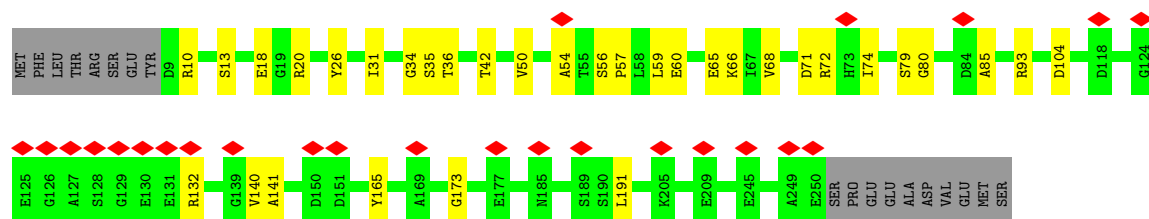
• Molecule 12: Proteasome subunit alpha type-5

Chain E:  14% 78% 15% 7%



• Molecule 12: Proteasome subunit alpha type-5

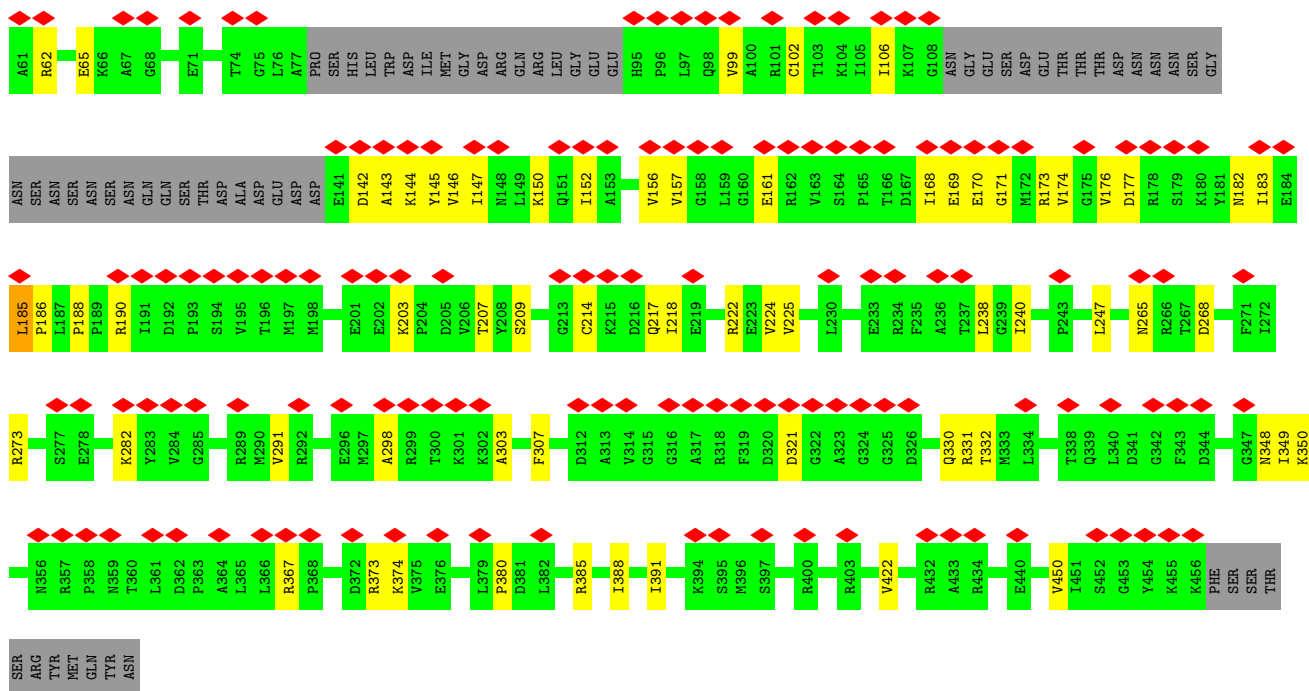
Chain m:  10% 80% 13% 7%



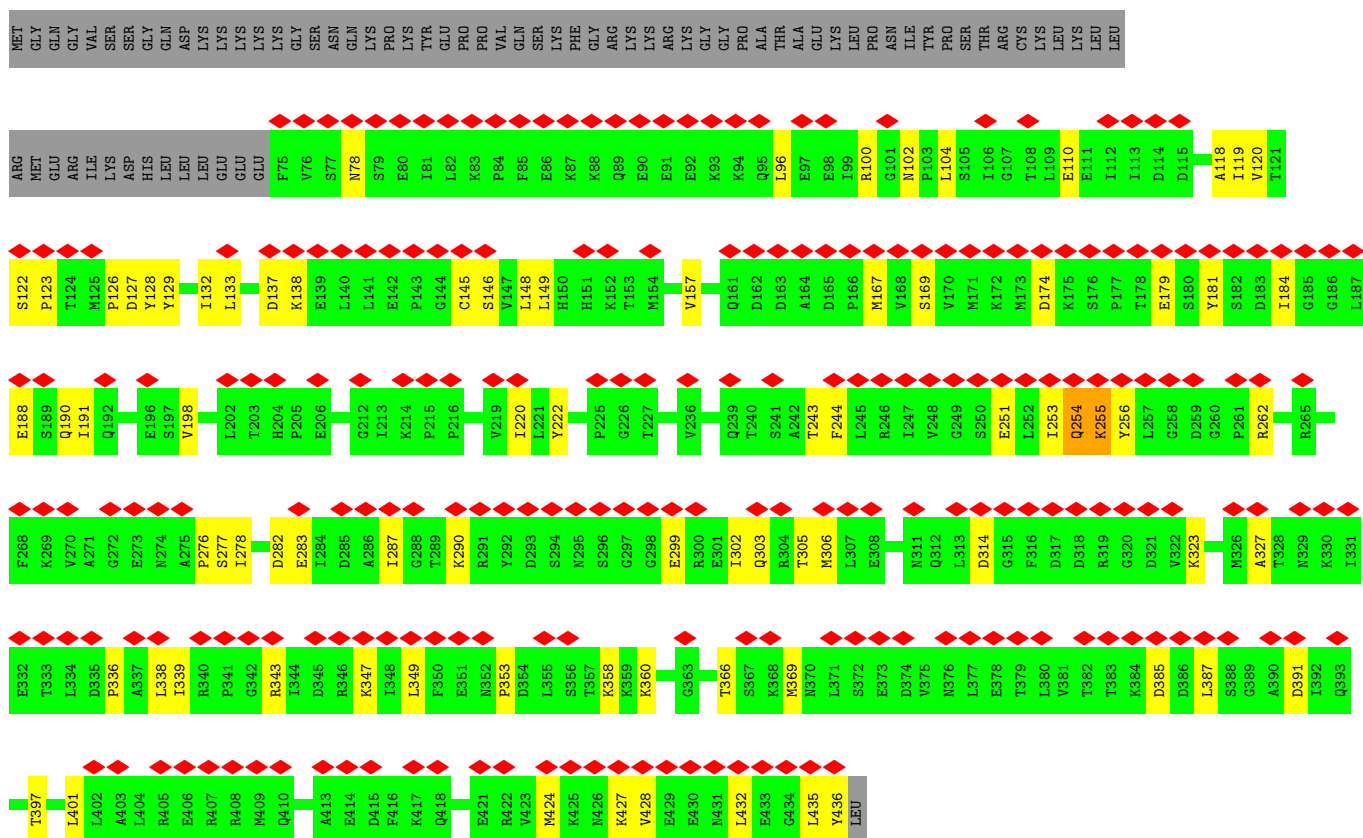
• Molecule 13: Proteasome subunit alpha type-6

Chain F:  15% 82% 17%

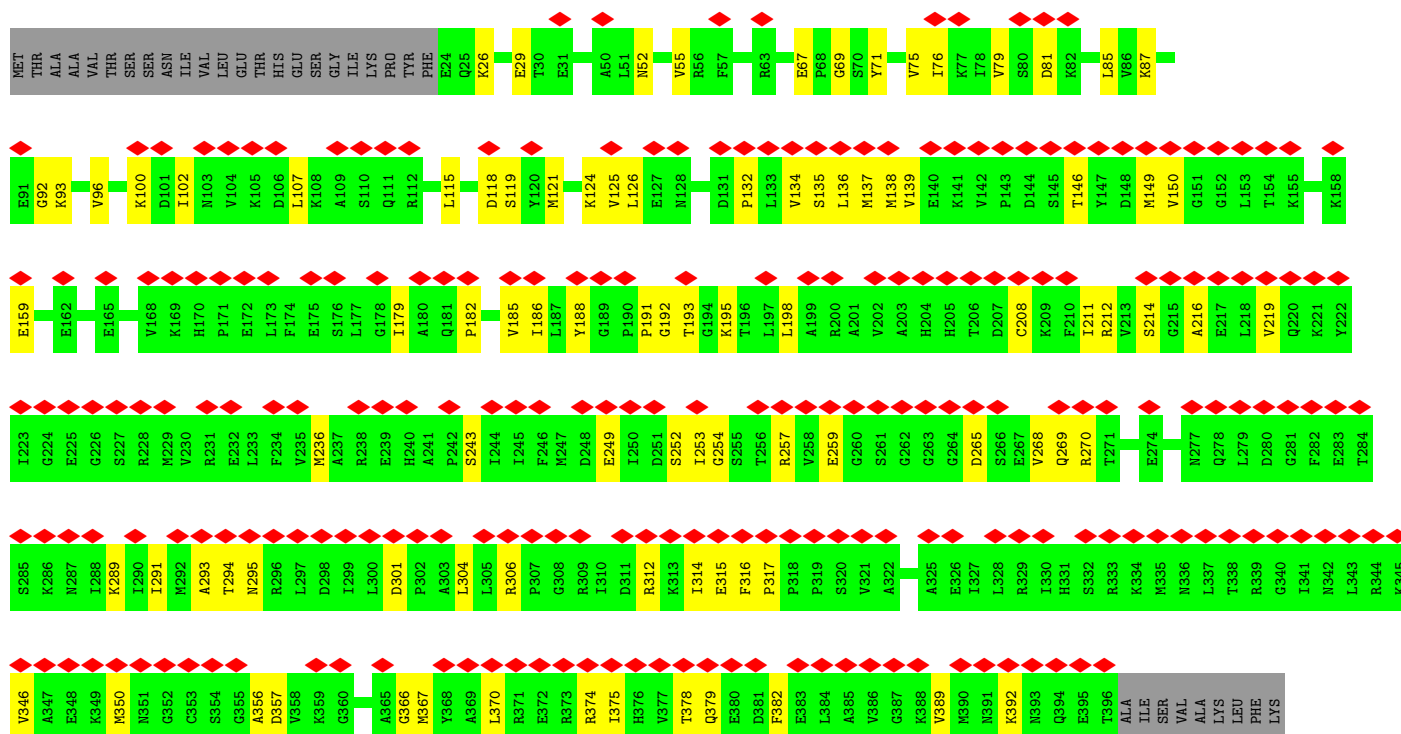




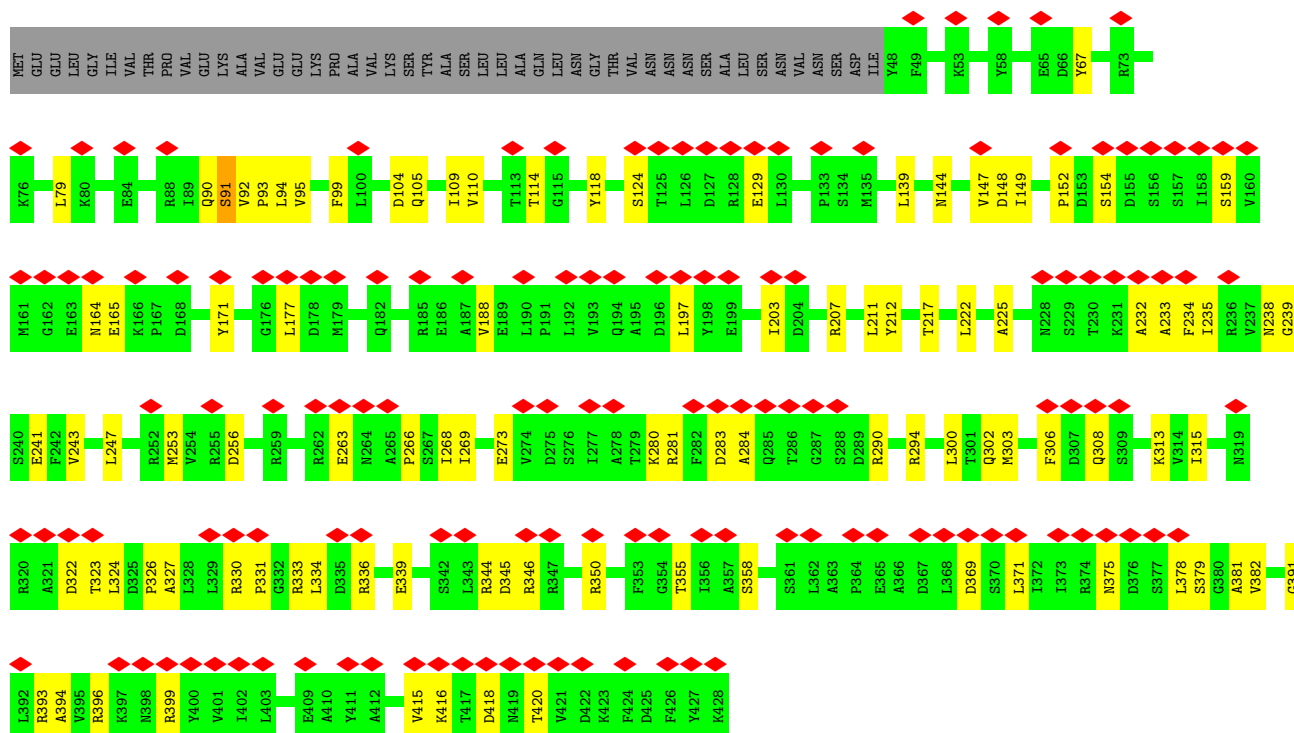
- Molecule 16: 26S protease regulatory subunit 4 homolog



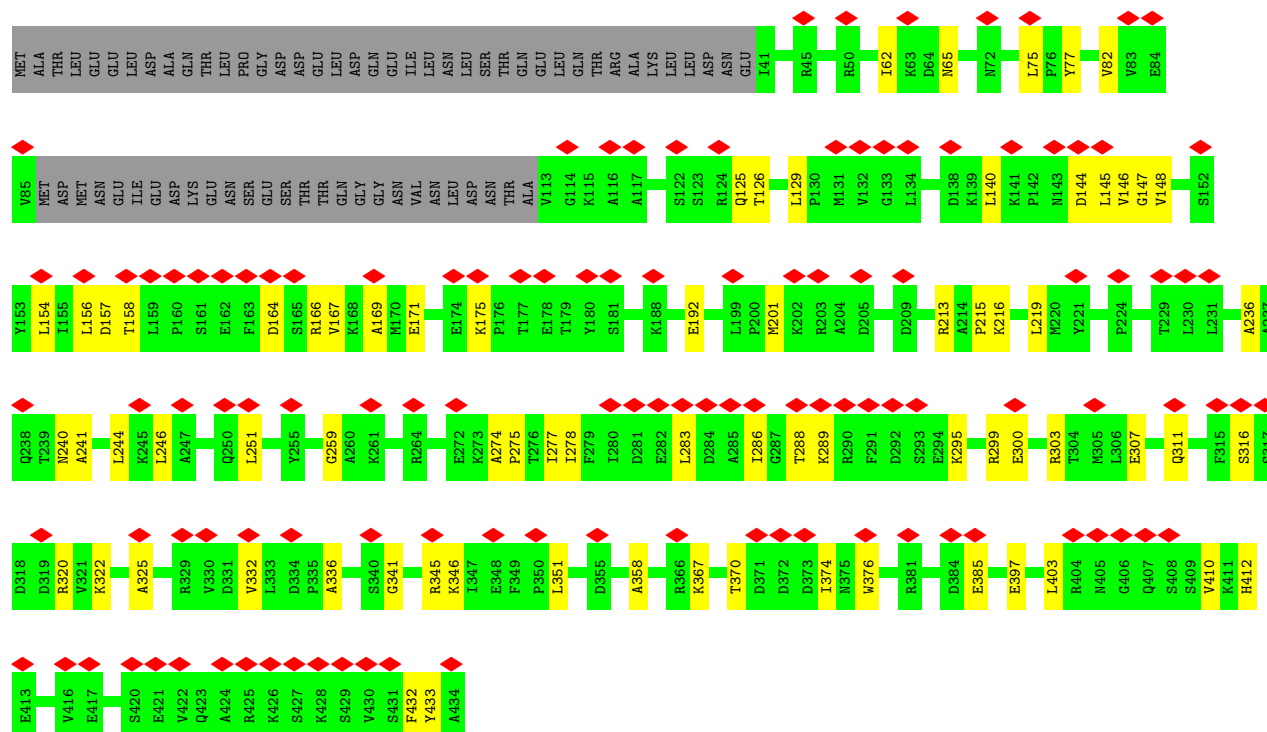
- Molecule 17: 26S protease regulatory subunit 8 homolog



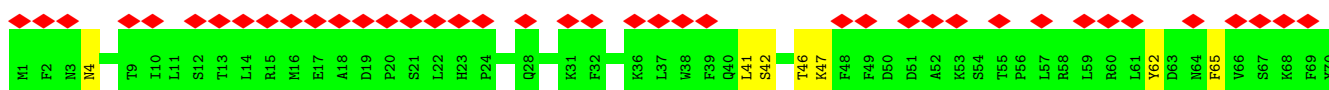
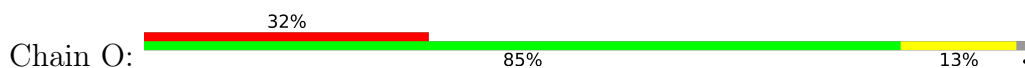
• Molecule 18: 26S protease regulatory subunit 6B homolog

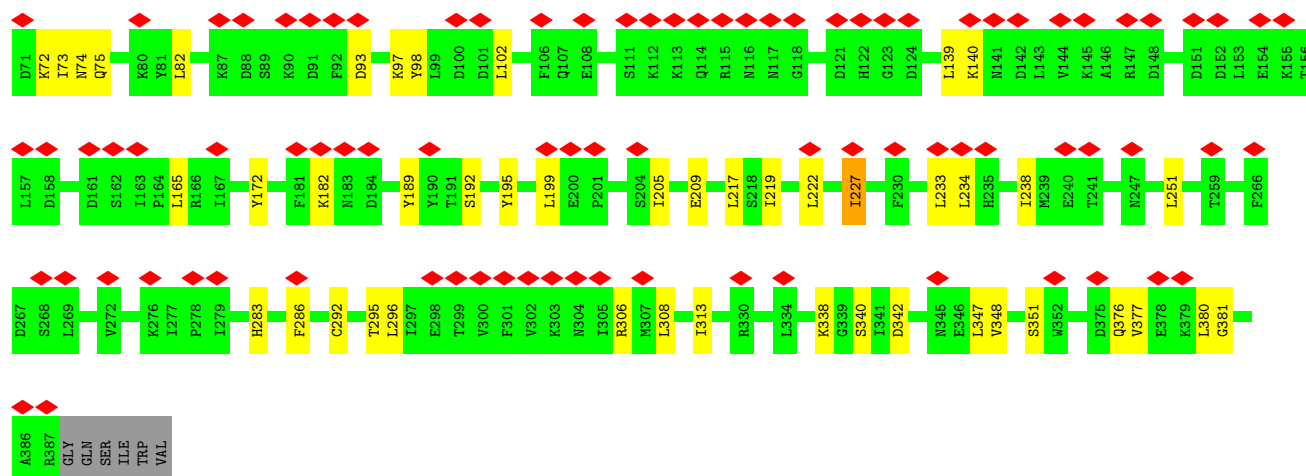


Chain L:

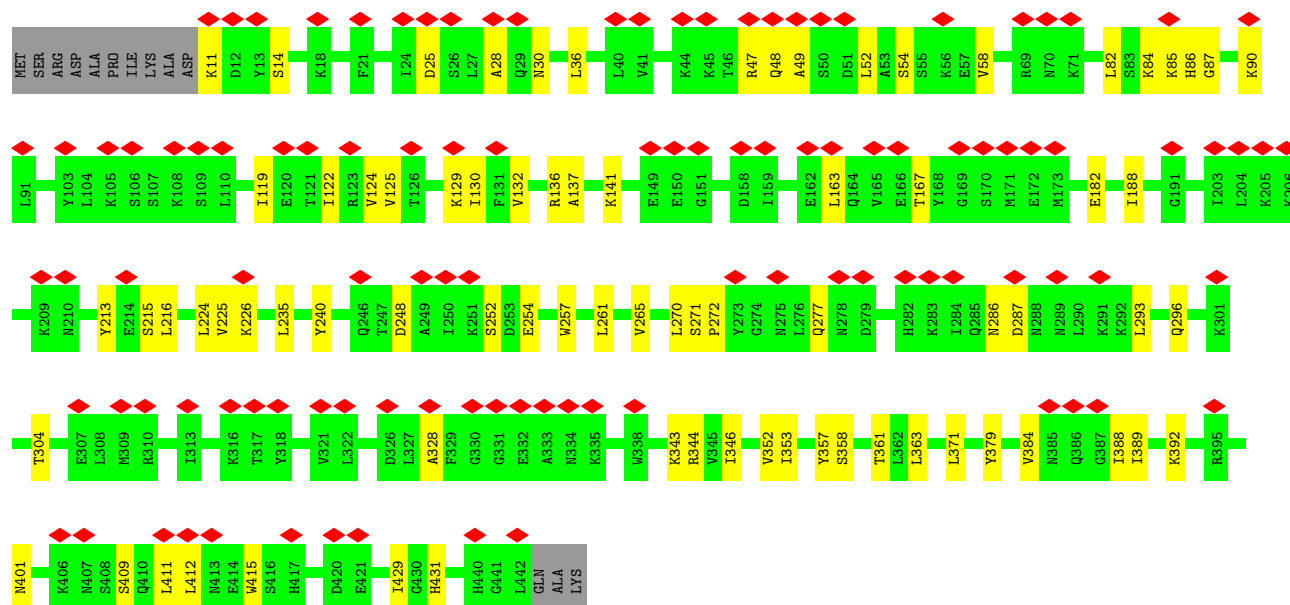
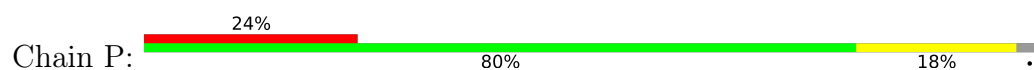


Chain N: 19% 71% 19% 10%

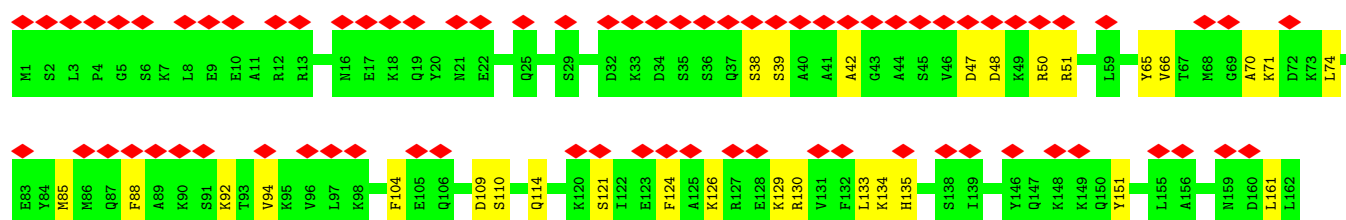
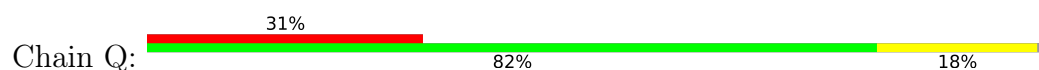


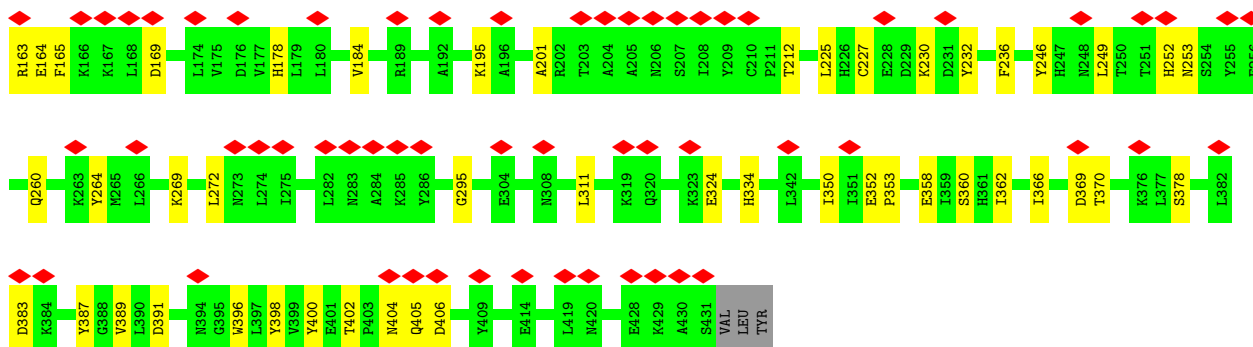


- Molecule 23: 26S proteasome regulatory subunit RPN5

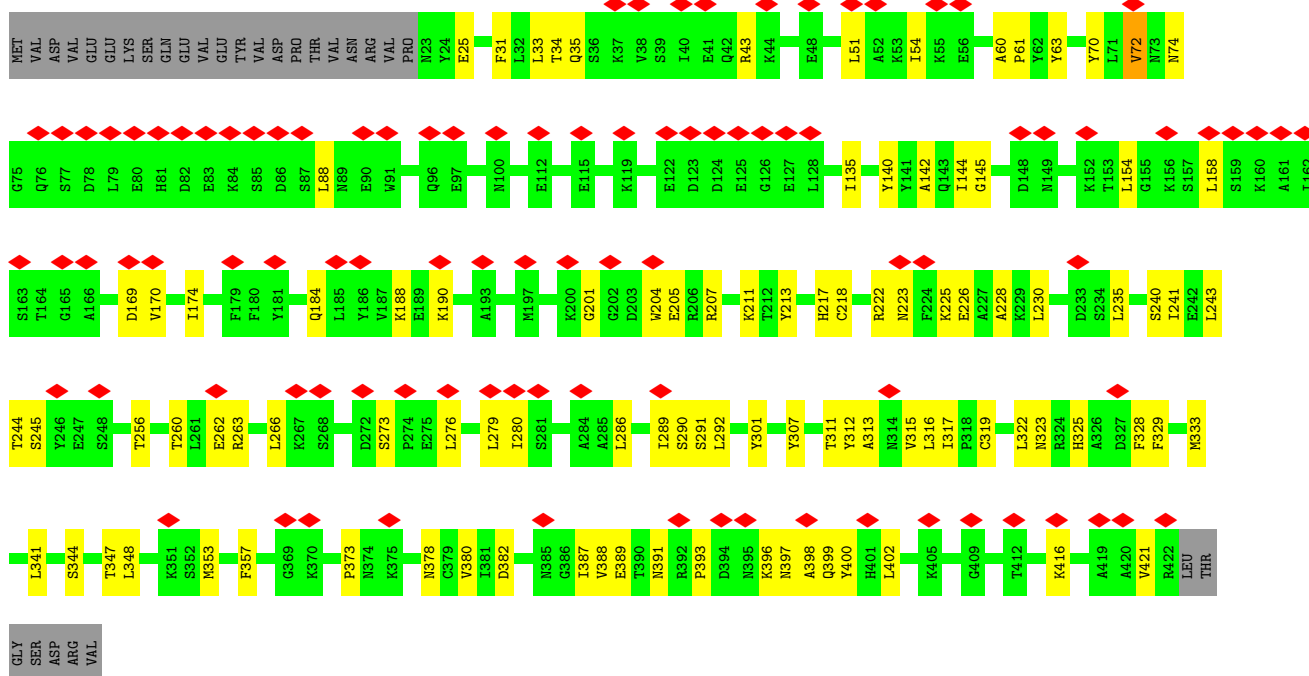


- Molecule 24: 26S proteasome regulatory subunit RPN6

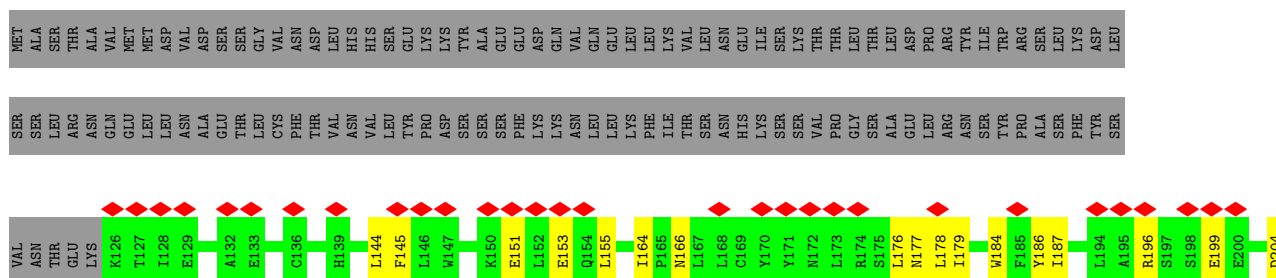




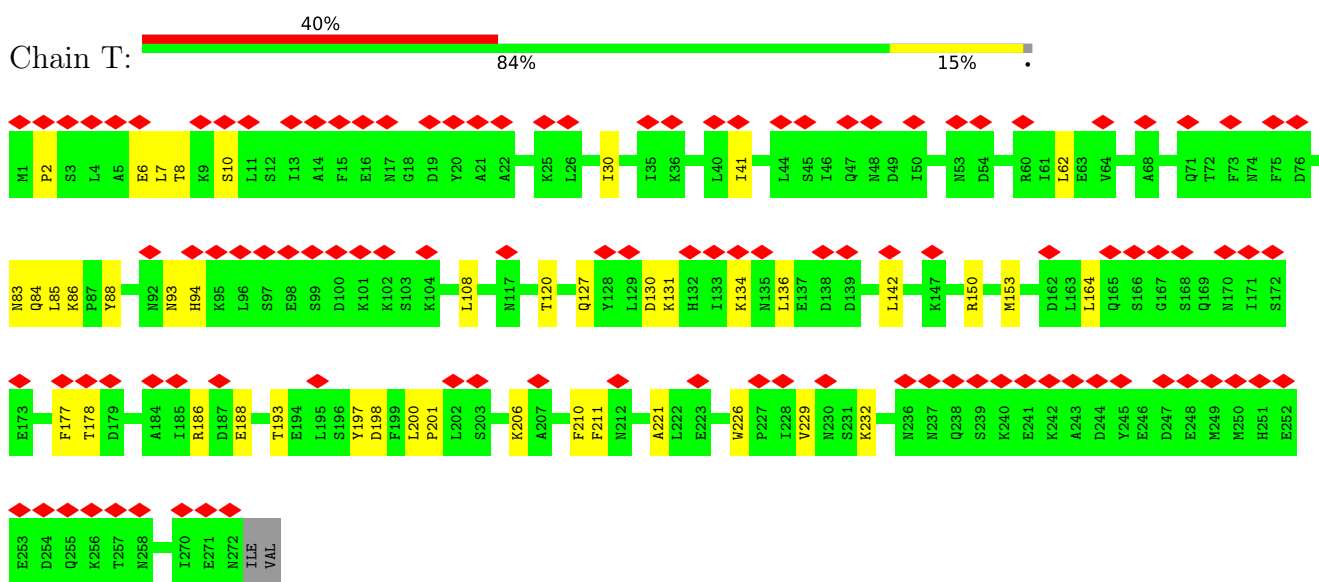
• Molecule 25: 26S proteasome regulatory subunit RPN7



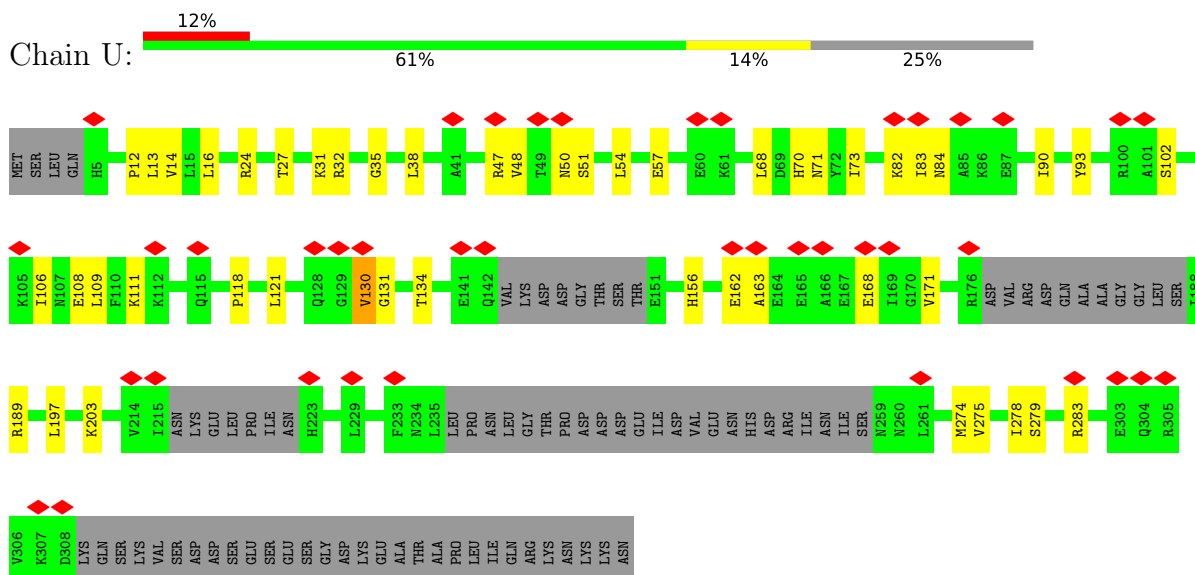
• Molecule 26: 26S proteasome regulatory subunit RPN3



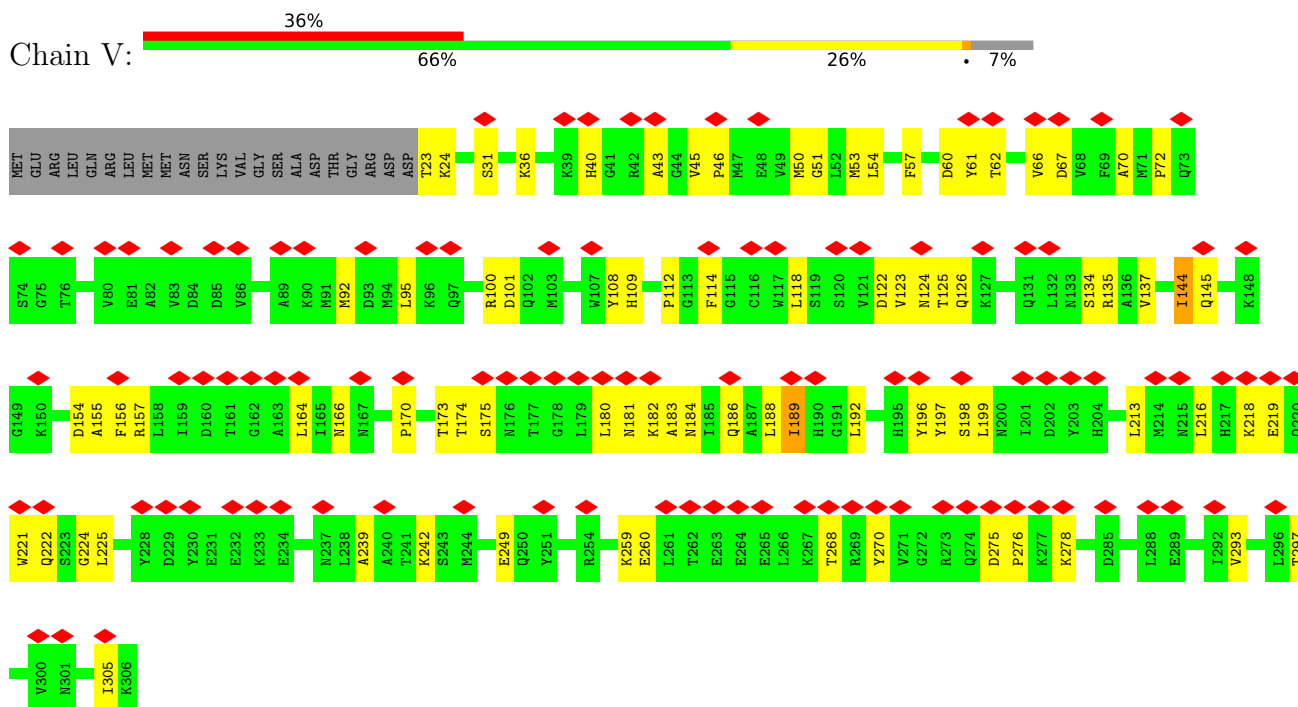
- Molecule 27: 26S proteasome regulatory subunit RPN12



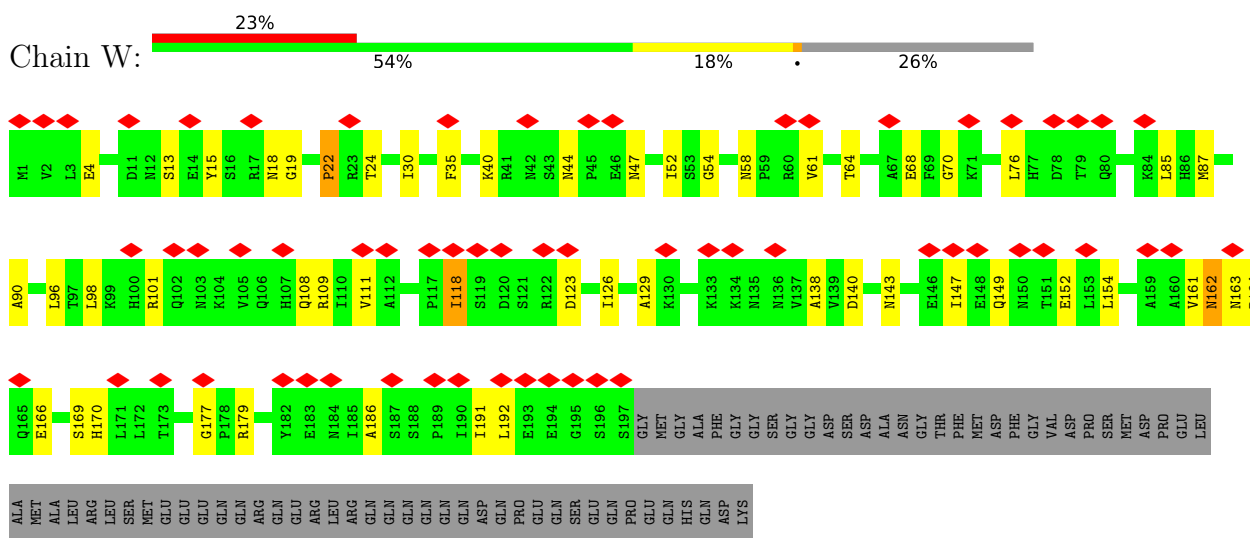
- Molecule 28: 26S proteasome regulatory subunit RPN8



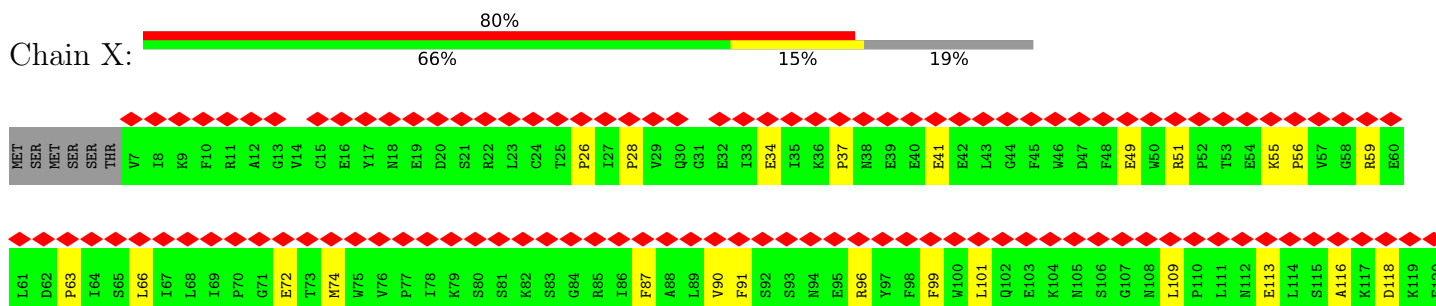
• Molecule 29: Ubiquitin carboxyl-terminal hydrolase RPN11

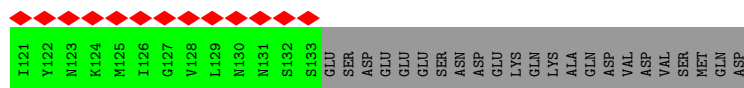


• Molecule 30: 26S proteasome regulatory subunit RPN10

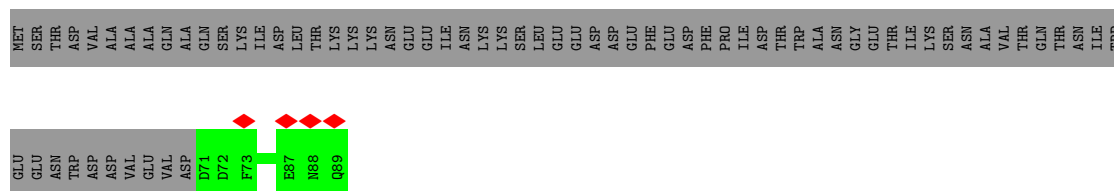


• Molecule 31: 26S proteasome regulatory subunit RPN13

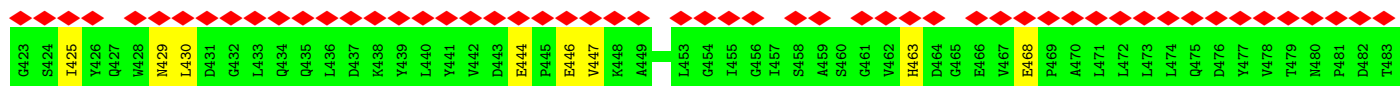
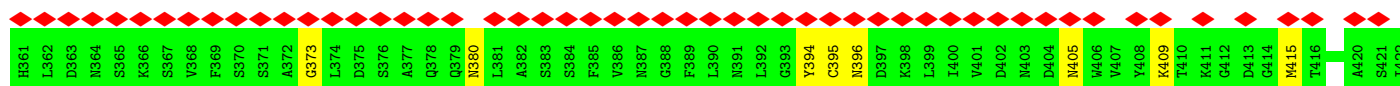
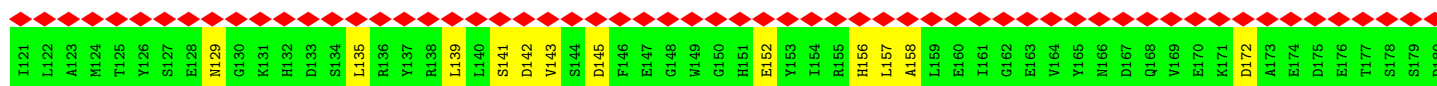
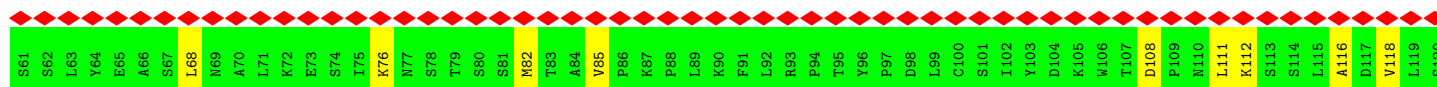
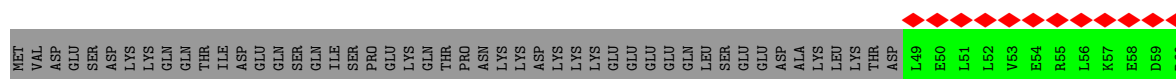
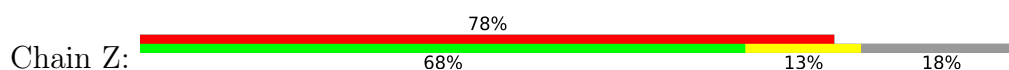




• Molecule 32: 26S proteasome complex subunit SEM1



• Molecule 33: 26S proteasome regulatory subunit RPN1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	178576	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 ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.666	Depositor
Minimum map value	-0.738	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.543	Depositor
Map size (Å)	474.47998, 474.47998, 474.47998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.318, 1.318, 1.318	Depositor

5 Model quality

5.1 Standard geometry

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	1	0.06	0/1541	0.22	0/2087
1	b	0.06	0/1541	0.21	0/2087
2	2	0.06	0/1723	0.20	0/2337
2	i	0.06	0/1723	0.20	0/2337
3	3	0.07	0/1611	0.26	0/2174
3	h	0.07	0/1611	0.25	0/2174
4	4	0.07	0/1613	0.22	0/2173
4	g	0.07	0/1613	0.22	0/2173
5	5	0.06	0/1681	0.21	0/2274
5	f	0.07	0/1681	0.23	0/2274
6	6	0.07	0/1795	0.23	0/2420
6	e	0.07	0/1795	0.22	0/2420
7	7	0.07	0/1855	0.23	0/2514
7	a	0.07	0/1855	0.24	0/2514
8	A	0.07	0/1959	0.23	0/2652
8	c	0.07	0/1959	0.22	0/2652
9	B	0.07	0/1952	0.22	0/2642
9	j	0.08	0/1952	0.22	0/2642
10	C	0.07	0/1934	0.26	0/2618
10	d	0.08	0/1934	0.25	0/2618
11	D	0.07	0/1919	0.24	0/2598
11	n	0.07	0/1919	0.24	0/2598
12	E	0.06	0/1886	0.23	0/2541
12	m	0.06	0/1886	0.20	0/2541
13	F	0.07	0/1823	0.25	0/2463
13	l	0.07	0/1823	0.24	0/2463
14	G	0.07	0/1936	0.21	0/2614
14	k	0.07	0/1936	0.22	0/2614
15	H	0.09	0/2831	0.30	0/3808
16	I	0.22	1/2860 (0.0%)	0.29	0/3856
17	J	0.08	0/2964	0.27	0/3981
18	K	0.12	0/3062	0.31	0/4132
19	L	0.08	0/2896	0.25	0/3895
20	M	0.23	2/2903 (0.1%)	0.27	0/3909

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
21	N	0.11	1/6670 (0.0%)	0.26	0/9023
22	O	0.09	0/3243	0.28	0/4374
23	P	0.07	0/3599	0.23	0/4854
24	Q	0.07	0/3527	0.24	0/4748
25	R	0.07	0/3272	0.24	0/4412
26	S	0.08	0/2945	0.28	0/3976
27	T	0.07	0/2279	0.24	0/3077
28	U	0.07	0/2087	0.21	0/2811
29	V	0.11	0/2271	0.41	0/3064
30	W	0.12	0/1557	0.31	0/2111
31	X	0.13	0/1058	0.30	0/1432
32	Y	0.06	0/169	0.18	0/223
33	Z	0.11	1/6404 (0.0%)	0.26	0/8686
All	All	0.10	5/107053 (0.0%)	0.25	0/144586

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
15	H	0	1
16	I	0	1
29	V	0	3
30	W	0	1
33	Z	0	1
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	I	102	ASN	C-N	10.78	1.59	1.33
20	M	274	ALA	C-N	8.80	1.54	1.33
20	M	75	LEU	C-N	7.65	1.51	1.33
21	N	217	MET	C-N	6.13	1.48	1.33
33	Z	468	GLU	C-N	5.78	1.47	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	H	185	LEU	Peptide
16	I	254	GLN	Peptide
29	V	222	GLN	Peptide
29	V	268	THR	Peptide
29	V	61	TYR	Peptide
30	W	162	ASN	Peptide
33	Z	255	LEU	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	1	1512	0	1478	28	0
1	b	1512	0	1478	28	0
2	2	1692	0	1696	28	0
2	i	1692	0	1696	26	0
3	3	1581	0	1571	34	0
3	h	1581	0	1571	42	0
4	4	1585	0	1590	28	0
4	g	1585	0	1590	30	0
5	5	1644	0	1592	34	0
5	f	1644	0	1592	34	0
6	6	1757	0	1708	29	0
6	e	1757	0	1708	30	0
7	7	1824	0	1829	32	0
7	a	1824	0	1829	45	0
8	A	1921	0	1910	34	0
8	c	1921	0	1910	33	0
9	B	1915	0	1929	25	0
9	j	1915	0	1929	30	0
10	C	1904	0	1901	39	0
10	d	1904	0	1901	46	0
11	D	1890	0	1900	41	0
11	n	1890	0	1900	42	0
12	E	1861	0	1836	26	0
12	m	1861	0	1836	23	0
13	F	1795	0	1797	29	0
13	l	1795	0	1797	24	0
14	G	1896	0	1886	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	k	1896	0	1886	22	0
15	H	2792	0	2879	43	0
16	I	2822	0	2870	56	0
17	J	2928	0	3057	65	0
18	K	3019	0	3084	76	0
19	L	2853	0	2926	53	0
20	M	2866	0	2938	48	0
21	N	6562	0	6625	112	0
22	O	3182	0	3207	30	0
23	P	3545	0	3629	52	0
24	Q	3471	0	3495	48	0
25	R	3218	0	3216	66	0
26	S	2893	0	2937	50	0
27	T	2235	0	2207	29	0
28	U	2061	0	2116	35	0
29	V	2236	0	2242	58	0
30	W	1534	0	1542	30	0
31	X	1032	0	1017	14	0
32	Y	168	0	153	0	0
33	Z	6290	0	6236	74	0
All	All	105261	0	105622	1595	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 8.

All (1595) 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)
29:V:180:LEU:HD23	29:V:181:ASN:H	1.40	0.86
18:K:90:GLN:O	18:K:93:PRO:HD2	1.75	0.85
17:J:121:MET:SD	29:V:181:ASN:ND2	2.54	0.80
3:3:107:PRO:HD2	3:3:124:PHE:HB2	1.65	0.79
21:N:176:GLN:HE22	21:N:181:GLU:HB2	1.50	0.76
9:B:49:LYS:HE3	9:B:210:GLU:HB2	1.69	0.74
2:2:106:VAL:HB	7:a:263:THR:HG22	1.70	0.74
9:B:33:THR:HA	9:B:165:GLY:HA3	1.70	0.74
19:L:204:PRO:HG3	19:L:320:GLN:HE21	1.52	0.73
16:I:385:ASP:HB2	16:I:424:MET:HG3	1.70	0.73
24:Q:249:LEU:HB3	24:Q:252:HIS:HB2	1.70	0.73
5:5:100:TRP:HD1	3:h:145:GLN:HE21	1.37	0.72
11:D:37:LYS:HE3	11:D:160:SER:HA	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:34:GLY:HA3	12:m:80:GLY:HA2	1.71	0.72
19:L:213:LYS:HD2	19:L:214:PRO:HD2	1.70	0.72
16:I:100:ARG:NH1	16:I:157:VAL:O	2.22	0.71
29:V:173:THR:HG22	29:V:174:THR:HG22	1.72	0.71
13:l:129:GLY:HA2	13:l:149:PRO:HB3	1.72	0.71
17:J:79:VAL:HG12	17:J:81:ASP:H	1.55	0.71
19:L:171:THR:HB	19:L:245:PHE:HB3	1.72	0.70
22:O:296:LEU:HB3	22:O:306:ARG:HG3	1.74	0.70
7:a:60:LEU:HD21	7:a:67:LEU:HD22	1.72	0.70
13:l:132:LEU:HB2	13:l:147:PHE:HB3	1.74	0.70
20:M:289:LYS:HB2	20:M:295:LYS:HE2	1.73	0.70
9:j:49:LYS:HE3	9:j:210:GLU:HB2	1.73	0.70
15:H:161:GLU:HA	15:H:183:ILE:HD13	1.74	0.69
25:R:382:ASP:HB2	25:R:387:ILE:H	1.56	0.69
7:a:42:THR:OG1	7:a:74:ARG:NH2	2.25	0.69
17:J:96:VAL:HB	17:J:121:MET:HA	1.75	0.69
20:M:358:ALA:HB1	20:M:376:TRP:HB2	1.74	0.69
5:f:112:ILE:O	5:f:139:ARG:NH1	2.25	0.68
12:m:85:ALA:HB2	12:m:140:VAL:HG21	1.75	0.68
6:e:143:SER:HB2	6:e:156:ARG:HG2	1.74	0.68
3:h:141:THR:HG21	3:h:180:LEU:HD12	1.76	0.68
13:F:7:ASP:OD2	13:F:21:GLN:NE2	2.25	0.68
25:R:380:VAL:HB	25:R:389:GLU:HB3	1.75	0.68
20:M:241:ALA:HA	20:M:275:PRO:HB2	1.76	0.68
30:W:15:TYR:O	30:W:18:ASN:ND2	2.26	0.68
24:Q:246:TYR:HB3	24:Q:253:ASN:HD22	1.57	0.67
23:P:48:GLN:HG3	23:P:49:ALA:H	1.60	0.67
8:A:131:ARG:HG2	9:B:127:VAL:HG12	1.76	0.67
3:3:124:PHE:HB3	3:3:128:GLY:HA2	1.76	0.67
19:L:249:SER:HA	20:M:303:ARG:HD2	1.75	0.67
19:L:318:LEU:HB3	19:L:321:THR:HB	1.74	0.67
9:B:6:SER:HB2	11:D:4:TYR:HD1	1.59	0.67
13:F:81:ALA:HB2	13:F:130:VAL:HG21	1.75	0.67
11:n:48:ARG:HB3	11:n:209:ASN:HB3	1.77	0.67
15:H:147:ILE:HD11	15:H:157:VAL:HG23	1.75	0.67
4:g:149:ARG:H	4:g:152:MET:HE2	1.60	0.67
5:f:120:MET:HG3	5:f:127:CYS:HB2	1.77	0.66
23:P:304:THR:HA	23:P:352:VAL:HG11	1.76	0.66
33:Z:116:ALA:HB3	33:Z:141:SER:HB2	1.77	0.66
6:e:35:ALA:O	6:e:154:GLN:NE2	2.28	0.66
13:l:81:ALA:HB2	13:l:130:VAL:HG21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:596:LEU:O	21:N:632:LYS:NZ	2.28	0.66
1:1:33:LEU:HD11	1:1:119:ALA:HB3	1.76	0.66
7:a:181:ALA:O	7:a:185:ASN:ND2	2.28	0.66
10:C:16:GLU:OE1	10:C:18:ARG:NH2	2.29	0.66
21:N:190:LEU:HD22	21:N:207:LEU:HD23	1.76	0.66
25:R:201:GLY:HA3	25:R:207:ARG:HE	1.60	0.66
29:V:164:LEU:O	29:V:166:ASN:ND2	2.28	0.66
15:H:150:LYS:HE3	15:H:152:ILE:HB	1.77	0.66
17:J:67:GLU:HG2	17:J:69:GLY:H	1.60	0.66
7:7:186:PRO:HG3	2:i:194:ASN:HD22	1.59	0.66
18:K:207:ARG:HD2	18:K:308:GLN:HA	1.77	0.66
29:V:184:ASN:HB2	29:V:188:LEU:HD21	1.77	0.66
10:d:48:ALA:HB3	10:d:212:GLU:HB2	1.78	0.66
21:N:60:MET:SD	21:N:88:ARG:NH2	2.68	0.66
3:3:10:GLY:HA3	3:3:42:LYS:HE2	1.79	0.65
25:R:325:HIS:HB3	25:R:328:PHE:HB2	1.78	0.65
15:H:177:ASP:O	15:H:190:ARG:NH2	2.28	0.65
29:V:218:LYS:HG3	29:V:219:GLU:H	1.61	0.65
21:N:416:GLY:HA3	21:N:453:ALA:HB1	1.79	0.65
27:T:200:LEU:HD12	27:T:201:PRO:HD2	1.78	0.65
12:E:12:VAL:HG12	12:E:23:GLN:HG3	1.78	0.65
9:j:119:GLN:HE21	10:d:82:ALA:HB3	1.61	0.65
6:6:163:SER:HB2	3:h:145:GLN:HG3	1.79	0.65
9:B:119:GLN:NE2	10:C:83:ASP:OD1	2.30	0.65
8:c:72:ILE:HG12	8:c:82:VAL:HG22	1.78	0.65
30:W:68:GLU:HG2	30:W:70:GLY:H	1.60	0.65
9:B:222:LEU:HD13	9:B:232:GLY:HA2	1.78	0.65
29:V:24:LYS:NZ	29:V:198:SER:O	2.29	0.65
4:g:184:VAL:HG22	4:g:189:ILE:HG12	1.77	0.65
6:e:219:ASP:HA	6:e:240:ARG:HG2	1.79	0.65
11:D:78:LEU:HD22	16:I:436:TYR:HD2	1.61	0.65
13:l:50:LYS:HE3	13:l:212:SER:HB2	1.79	0.64
7:7:161:ARG:HD3	7:7:169:THR:HB	1.79	0.64
21:N:728:LYS:HB3	21:N:751:LEU:HB3	1.79	0.64
24:Q:151:TYR:HB2	24:Q:184:VAL:HG13	1.78	0.64
1:1:41:THR:OG1	1:1:44:TYR:O	2.15	0.64
5:5:106:VAL:HG13	6:6:151:GLU:HG3	1.78	0.64
6:6:219:ASP:HA	6:6:240:ARG:HG2	1.78	0.64
15:H:225:VAL:HA	15:H:350:LYS:HE3	1.79	0.64
1:b:40:THR:HG22	1:b:45:ILE:HG12	1.78	0.64
29:V:197:TYR:HE2	29:V:199:LEU:HB3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:137:TYR:HB2	10:d:149:TYR:HB2	1.80	0.64
31:X:37:PRO:HG2	31:X:41:GLU:HG2	1.78	0.64
15:H:102:CYS:HB2	15:H:146:VAL:HG13	1.79	0.64
6:e:170:ASP:HA	6:e:174:ASN:HB2	1.80	0.63
21:N:150:LEU:HD21	21:N:173:LYS:HG3	1.79	0.63
4:4:184:VAL:HG22	4:4:189:ILE:HG12	1.81	0.63
19:L:150:ILE:O	29:V:145:GLN:NE2	2.32	0.63
22:O:219:ILE:HA	22:O:222:LEU:HD13	1.80	0.63
9:B:66:LEU:HD21	9:B:69:PRO:HG3	1.80	0.63
9:j:71:ILE:HG12	9:j:138:GLY:HA3	1.81	0.63
1:b:47:ASN:HD22	2:i:149:ASP:HB3	1.63	0.63
6:e:54:ILE:HB	7:a:189:ARG:HH12	1.62	0.63
13:F:207:THR:OG1	13:F:210:ASN:ND2	2.29	0.63
16:I:254:GLN:O	16:I:256:TYR:N	2.31	0.63
17:J:193:THR:OG1	17:J:195:LYS:NZ	2.31	0.63
17:J:252:SER:HB3	17:J:295:ASN:H	1.63	0.63
22:O:338:LYS:HB2	22:O:351:SER:HB3	1.80	0.63
22:O:340:SER:HB2	23:P:358:SER:HB2	1.81	0.63
25:R:135:ILE:HG21	25:R:169:ASP:HB3	1.78	0.63
8:A:72:ILE:HG12	8:A:82:VAL:HG22	1.81	0.63
28:U:24:ARG:HE	29:V:66:VAL:HG13	1.64	0.63
29:V:112:PRO:HA	29:V:144:ILE:HG21	1.81	0.63
33:Z:241:THR:HG22	33:Z:243:GLN:H	1.64	0.63
2:i:132:VAL:HG11	2:i:209:ILE:HA	1.79	0.63
3:h:28:ARG:NH2	3:h:205:ASP:OXT	2.31	0.63
13:l:7:ASP:O	13:l:21:GLN:NE2	2.32	0.63
3:3:205:ASP:HA	5:f:241:HIS:HA	1.81	0.63
15:H:303:ALA:H	15:H:348:ASN:HB3	1.64	0.63
21:N:8:PRO:HB3	27:T:84:GLN:HA	1.81	0.63
23:P:11:LYS:N	23:P:14:SER:HG	1.97	0.62
2:2:193:TRP:O	6:e:57:ARG:NH2	2.30	0.62
7:7:131:THR:HG21	13:F:98:VAL:HG22	1.81	0.62
23:P:384:VAL:HG12	24:Q:352:GLU:HG3	1.80	0.62
31:X:109:LEU:N	31:X:118:ASP:OD2	2.31	0.62
25:R:218:CYS:HB3	25:R:223:ASN:HB2	1.80	0.62
25:R:348:LEU:HB2	25:R:388:VAL:HB	1.82	0.62
28:U:279:SER:HB2	29:V:242:LYS:HE2	1.81	0.62
7:a:58:ASP:O	7:a:74:ARG:NH2	2.32	0.62
10:d:70:ASN:OD1	10:d:71:ASP:N	2.32	0.62
17:J:257:ARG:NE	17:J:259:GLU:OE2	2.30	0.62
24:Q:92:LYS:HA	24:Q:129:LYS:HE2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:175:LYS:HE2	20:M:240:ASN:HB3	1.82	0.62
21:N:268:GLN:NE2	21:N:490:LEU:O	2.33	0.62
8:c:219:SER:H	8:c:222:ASP:HB2	1.65	0.62
11:n:32:CYS:HA	11:n:165:GLY:HA3	1.80	0.62
12:m:13:SER:HB2	13:l:126:ARG:HB3	1.82	0.62
33:Z:429:ASN:OD1	33:Z:430:LEU:N	2.33	0.62
10:C:70:ASN:OD1	10:C:71:ASP:N	2.33	0.62
19:L:101:ILE:HD11	29:V:43:ALA:HA	1.82	0.62
20:M:244:LEU:HD23	20:M:278:ILE:HG12	1.81	0.62
4:4:3:ILE:HB	4:4:18:SER:HB3	1.82	0.61
5:f:82:ARG:HH11	5:f:186:THR:HA	1.62	0.61
13:l:11:VAL:HA	14:k:130:ARG:HD3	1.82	0.61
29:V:137:VAL:HG12	29:V:157:ARG:HD2	1.82	0.61
16:I:78:ASN:ND2	33:Z:622:HIS:O	2.33	0.61
21:N:562:THR:OG1	21:N:597:ARG:NH1	2.32	0.61
26:S:199:GLU:O	27:T:93:ASN:ND2	2.32	0.61
30:W:98:LEU:O	30:W:101:ARG:NH1	2.34	0.61
13:F:13:PHE:H	14:G:23:GLN:HE22	1.47	0.61
33:Z:796:LEU:HD13	33:Z:815:MET:HG2	1.81	0.61
7:a:61:GLY:N	7:a:69:PHE:O	2.30	0.61
12:E:85:ALA:HB2	12:E:140:VAL:HG21	1.81	0.61
23:P:392:LYS:HB3	23:P:401:ASN:H	1.63	0.61
24:Q:378:SER:HB2	25:R:344:SER:HB2	1.81	0.61
18:K:344:ARG:HH21	18:K:379:SER:HA	1.64	0.61
17:J:208:CYS:HB3	17:J:243:SER:HA	1.83	0.61
22:O:189:TYR:HE2	22:O:227:ILE:HB	1.65	0.61
25:R:240:SER:HB2	25:R:244:THR:HG22	1.83	0.61
10:C:76:ALA:HB3	10:C:136:ILE:HB	1.81	0.61
20:M:215:PRO:O	20:M:322:LYS:NZ	2.32	0.61
5:f:146:LYS:NZ	12:m:65:GLU:OE1	2.33	0.61
18:K:118:TYR:HB3	18:K:144:ASN:HD21	1.66	0.61
33:Z:112:LYS:HD3	33:Z:202:ARG:HE	1.66	0.61
1:1:32:ILE:HG12	1:1:196:VAL:HA	1.82	0.60
16:I:179:GLU:OE1	16:I:360:LYS:NZ	2.33	0.60
5:5:113:ASN:OD1	5:5:116:LEU:N	2.33	0.60
12:E:50:VAL:HG21	12:E:66:LYS:HB2	1.82	0.60
19:L:220:LEU:HB3	19:L:349:ILE:HD11	1.82	0.60
22:O:74:ASN:OD1	22:O:75:GLN:N	2.34	0.60
30:W:129:ALA:HB1	30:W:161:VAL:HB	1.82	0.60
6:e:153:GLU:HG3	6:e:156:ARG:HH21	1.66	0.60
8:A:40:ILE:O	8:A:84:ASN:ND2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:173:PHE:HE2	19:L:176:GLY:HA2	1.66	0.60
25:R:61:PRO:HB3	25:R:145:GLY:HA2	1.82	0.60
21:N:781:ALA:O	21:N:873:ARG:NH1	2.33	0.60
25:R:228:ALA:HB2	25:R:256:THR:HG22	1.82	0.60
10:d:16:GLU:O	11:n:29:ARG:NH2	2.34	0.60
23:P:248:ASP:HA	23:P:252:SER:HB3	1.84	0.60
11:n:73:LEU:HD11	11:n:133:THR:HB	1.83	0.60
15:H:291:VAL:HG21	15:H:332:THR:HG23	1.84	0.60
10:C:158:THR:OG1	10:C:160:TRP:NE1	2.35	0.60
8:c:168:ALA:HB1	8:c:182:LEU:HD13	1.83	0.60
21:N:875:LEU:HD23	21:N:878:GLN:HG2	1.83	0.60
33:Z:347:ASN:HB3	33:Z:353:VAL:HG23	1.83	0.60
17:J:55:VAL:HG22	18:K:79:LEU:HD13	1.83	0.60
21:N:192:LEU:O	21:N:196:THR:OG1	2.19	0.60
22:O:42:SER:H	22:O:47:LYS:HD3	1.66	0.60
11:D:56:ASP:HB3	11:D:59:ILE:HG12	1.83	0.60
16:I:184:ILE:HD11	16:I:191:ILE:HD11	1.84	0.60
25:R:382:ASP:HA	26:S:399:TYR:HB2	1.83	0.60
33:Z:574:TYR:HB2	33:Z:581:VAL:HG22	1.83	0.60
4:4:177:LYS:NZ	4:g:169:GLU:O	2.34	0.59
33:Z:516:THR:HA	33:Z:523:ALA:HB3	1.84	0.59
1:b:20:THR:N	1:b:148:SER:HG	2.00	0.59
9:B:185:LEU:HD21	9:B:213:ILE:HD13	1.83	0.59
11:D:48:ARG:HH11	11:D:53:LYS:HE3	1.67	0.59
10:d:173:GLN:HG2	11:n:52:LEU:HD13	1.83	0.59
1:1:57:HIS:HB3	1:1:60:ILE:HB	1.83	0.59
14:G:65:VAL:HG12	14:G:67:ILE:H	1.67	0.59
25:R:313:ALA:HA	25:R:317:ILE:HD12	1.83	0.59
26:S:352:VAL:HG22	26:S:387:VAL:HG22	1.83	0.59
2:2:238:THR:HA	6:e:185:GLY:HA2	1.85	0.59
5:5:93:SER:HB2	5:5:105:THR:HA	1.83	0.59
12:E:18:GLU:OE1	12:E:20:ARG:NH2	2.35	0.59
16:I:287:ILE:HG13	16:I:302:ILE:HG23	1.85	0.59
18:K:238:ASN:HB3	18:K:241:GLU:HG3	1.85	0.59
1:1:38:ARG:NH1	1:1:186:GLY:O	2.35	0.59
6:6:49:ILE:HD11	6:6:216:GLN:HE21	1.66	0.59
21:N:222:TYR:H	21:N:894:ARG:HH21	1.50	0.59
27:T:131:LYS:HB3	27:T:134:LYS:HB3	1.85	0.59
5:f:93:SER:O	5:f:106:VAL:N	2.34	0.59
28:U:108:GLU:OE1	30:W:58:ASN:ND2	2.33	0.59
9:B:49:LYS:HD3	9:B:58:SER:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:k:224:THR:HB	14:k:227:LEU:HB2	1.84	0.58
15:H:207:THR:OG1	15:H:265:ASN:ND2	2.36	0.58
17:J:367:MET:HG3	18:K:336:ARG:HH21	1.68	0.58
21:N:757:THR:H	21:N:900:ASN:HB2	1.68	0.58
7:a:86:ILE:HG12	7:a:147:ILE:HG12	1.85	0.58
10:C:160:TRP:HE3	11:D:54:LEU:HD12	1.68	0.58
11:D:187:THR:HG22	11:D:189:GLU:H	1.68	0.58
19:L:287:GLY:HA2	19:L:305:LEU:HD11	1.84	0.58
22:O:41:LEU:HB3	22:O:82:LEU:HD23	1.84	0.58
14:G:86:ARG:O	14:G:90:ASN:ND2	2.36	0.58
10:d:152:ASN:OD1	10:d:156:ASN:N	2.36	0.58
26:S:322:LEU:HB3	26:S:383:LEU:HD13	1.85	0.58
33:Z:537:THR:O	33:Z:577:GLN:NE2	2.37	0.58
1:1:20:THR:N	1:1:187:SER:O	2.36	0.58
2:i:83:ALA:HB1	9:j:99:ARG:HH22	1.69	0.58
14:k:72:ARG:NH1	14:k:226:GLY:O	2.37	0.58
25:R:273:SER:HB3	25:R:276:LEU:HB2	1.84	0.58
17:J:52:ASN:ND2	21:N:611:LYS:O	2.36	0.58
5:f:250:VAL:HB	5:f:266:HIS:HB2	1.84	0.58
9:B:71:ILE:HG12	9:B:138:GLY:HA3	1.85	0.58
12:m:50:VAL:HG21	12:m:66:LYS:HB2	1.86	0.58
19:L:218:VAL:HA	19:L:345:ARG:HB2	1.84	0.58
30:W:13:SER:HB2	30:W:85:LEU:HD13	1.84	0.58
1:1:27:PHE:HE2	1:1:32:ILE:HG13	1.67	0.58
1:b:57:HIS:HB3	1:b:60:ILE:HB	1.86	0.58
15:H:168:ILE:HD12	15:H:174:VAL:HG11	1.84	0.58
18:K:378:LEU:HD22	18:K:382:VAL:HG11	1.86	0.58
23:P:265:VAL:HG11	23:P:296:GLN:HB3	1.85	0.58
8:c:196:GLU:HG3	8:c:198:SER:H	1.69	0.58
7:7:98:ARG:HD2	14:G:101:LYS:HA	1.86	0.57
15:H:145:TYR:HD2	15:H:169:GLU:HB2	1.68	0.57
19:L:228:LYS:NZ	19:L:282:GLU:OE2	2.37	0.57
6:e:46:THR:OG1	6:e:219:ASP:O	2.22	0.57
10:d:76:ALA:HB3	10:d:136:ILE:HB	1.86	0.57
10:C:19:LEU:HD23	10:C:22:VAL:HG23	1.86	0.57
10:d:152:ASN:ND2	10:d:154:SER:OG	2.37	0.57
12:m:54:ALA:HA	12:m:59:LEU:HD13	1.86	0.57
29:V:259:LYS:NZ	29:V:260:GLU:OE2	2.38	0.57
12:E:159:GLU:OE1	12:E:163:THR:OG1	2.22	0.57
26:S:395:ILE:HG12	26:S:410:LYS:HD3	1.87	0.57
3:h:28:ARG:NH1	3:h:179:ALA:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:126:GLN:NE2	9:j:81:ASP:OD1	2.37	0.57
15:H:282:LYS:NZ	16:I:303:GLN:OE1	2.35	0.57
4:4:64:ILE:HG23	4:4:75:LEU:HD12	1.86	0.57
7:a:50:ASP:O	7:a:158:GLN:NE2	2.38	0.57
25:R:223:ASN:HB3	25:R:226:GLU:HB3	1.85	0.57
20:M:164:ASP:OD2	20:M:166:ARG:NH2	2.37	0.57
3:3:6:SER:HA	3:3:141:THR:HG21	1.87	0.57
10:d:206:LEU:HD21	10:d:211:LEU:HD21	1.87	0.57
26:S:282:ILE:HA	26:S:382:ARG:HH12	1.70	0.57
26:S:431:VAL:HG12	26:S:432:ILE:HG23	1.87	0.57
30:W:162:ASN:ND2	30:W:169:SER:O	2.38	0.57
33:Z:797:THR:OG1	33:Z:833:GLN:NE2	2.38	0.57
2:2:49:SER:HB3	2:2:57:ASP:HB3	1.86	0.57
9:j:119:GLN:OE1	9:j:122:THR:OG1	2.22	0.57
10:d:38:ILE:HB	10:d:45:VAL:HB	1.87	0.57
20:M:77:TYR:HB3	20:M:148:VAL:H	1.70	0.57
23:P:54:SER:HA	23:P:58:VAL:HB	1.86	0.57
30:W:98:LEU:HD13	30:W:108:GLN:HB3	1.87	0.57
1:b:103:GLU:OE2	7:a:98:ARG:NH1	2.35	0.56
20:M:246:LEU:HD21	20:M:251:LEU:HD21	1.86	0.56
21:N:207:LEU:HB3	21:N:228:VAL:HG13	1.87	0.56
1:1:131:THR:HG21	7:7:68:ARG:HH21	1.70	0.56
23:P:90:LYS:HG3	23:P:129:LYS:HB3	1.87	0.56
3:h:12:VAL:HG11	3:h:52:GLY:HA3	1.87	0.56
8:A:249:ALA:HB1	23:P:85:LYS:HA	1.87	0.56
10:d:50:ARG:NH1	10:d:209:ASP:O	2.38	0.56
12:m:132:ARG:NH1	13:l:128:TYR:OH	2.38	0.56
16:I:353:PRO:O	16:I:358:LYS:NZ	2.39	0.56
22:O:182:LYS:NZ	23:P:287:ASP:OD2	2.31	0.56
25:R:378:ASN:HB3	25:R:391:ASN:HB3	1.88	0.56
26:S:382:ARG:HG2	27:T:153:MET:HE1	1.87	0.56
13:F:132:LEU:HB2	13:F:147:PHE:HB3	1.86	0.56
21:N:63:LEU:HD22	21:N:88:ARG:HD2	1.88	0.56
10:d:48:ALA:HB1	10:d:65:LYS:HD2	1.88	0.56
16:I:282:ASP:HA	16:I:327:ALA:HB3	1.86	0.56
25:R:396:LYS:HB3	25:R:400:TYR:HB2	1.87	0.56
4:4:37:GLN:HE21	4:4:40:PRO:HA	1.71	0.56
14:G:41:LYS:HE3	14:G:147:HIS:HA	1.88	0.56
22:O:165:LEU:HD12	22:O:199:LEU:HD21	1.86	0.56
23:P:411:LEU:HD12	23:P:415:TRP:HB2	1.86	0.56
28:U:130:VAL:HG22	28:U:131:GLY:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:82:MET:HE2	33:Z:85:VAL:HA	1.87	0.56
1:1:59:LYS:HB3	1:1:121:TYR:HB3	1.86	0.56
6:6:74:ASN:OD1	6:6:75:GLY:N	2.37	0.56
6:6:170:ASP:OD2	3:h:177:ARG:NH2	2.38	0.56
18:K:177:LEU:HD13	18:K:222:LEU:HD22	1.85	0.56
23:P:388:ILE:HG22	23:P:389:ILE:HG23	1.87	0.56
31:X:87:PHE:HB2	31:X:99:PHE:HB2	1.87	0.56
33:Z:68:LEU:HD22	33:Z:118:VAL:HG21	1.86	0.56
5:5:76:THR:N	5:5:245:TYR:O	2.39	0.56
8:A:82:VAL:HB	8:A:142:THR:HB	1.87	0.56
10:d:16:GLU:OE1	10:d:18:ARG:NH2	2.39	0.56
11:n:70:HIS:ND1	11:n:138:PHE:O	2.39	0.56
3:3:145:GLN:HE21	5:f:100:TRP:HD1	1.52	0.56
23:P:409:SER:HB3	23:P:412:LEU:HD12	1.87	0.56
2:2:46:ASP:HB2	2:2:188:ILE:HD11	1.88	0.56
29:V:23:THR:N	29:V:60:ASP:OD1	2.38	0.56
7:7:96:ILE:HD13	7:7:147:ILE:HD11	1.88	0.55
6:e:46:THR:HB	6:e:59:GLU:H	1.71	0.55
10:C:11:THR:OG1	11:D:6:ARG:NH2	2.40	0.55
13:l:40:SER:HB3	13:l:180:ILE:HA	1.89	0.55
14:k:68:GLN:HG3	14:k:89:VAL:HG21	1.87	0.55
16:I:145:CYS:SG	16:I:146:SER:N	2.79	0.55
23:P:36:LEU:HD22	23:P:82:LEU:HD21	1.89	0.55
24:Q:65:TYR:HD2	24:Q:74:LEU:HD13	1.71	0.55
27:T:221:ALA:HB1	27:T:226:TRP:HB2	1.89	0.55
3:h:11:ILE:HG22	3:h:140:GLY:HA3	1.87	0.55
8:A:46:ARG:HH11	8:A:153:SER:HA	1.71	0.55
17:J:150:VAL:HG21	17:J:198:LEU:HB3	1.88	0.55
18:K:114:THR:HG22	19:L:125:PRO:HG3	1.88	0.55
28:U:16:LEU:HD13	29:V:31:SER:HB2	1.87	0.55
2:i:93:GLU:OE2	9:j:98:LYS:NZ	2.39	0.55
4:g:8:ARG:HG3	4:g:13:VAL:HG22	1.87	0.55
18:K:396:ARG:NE	19:L:195:GLU:OE1	2.38	0.55
25:R:325:HIS:HB2	25:R:329:PHE:CE2	2.41	0.55
9:B:38:LYS:HG3	9:B:43:VAL:HG22	1.88	0.55
18:K:371:LEU:O	18:K:375:ASN:ND2	2.37	0.55
19:L:108:VAL:HA	19:L:119:VAL:HG12	1.89	0.55
23:P:261:LEU:HD21	23:P:293:LEU:HD13	1.88	0.55
10:C:207:THR:OG1	10:C:209:ASP:OD1	2.22	0.55
11:D:208:LYS:HG2	11:D:226:SER:HB2	1.89	0.55
19:L:361:PHE:O	19:L:365:THR:OG1	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:232:ILE:HB	7:a:240:THR:HB	1.87	0.55
19:L:313:ASP:OD2	19:L:342:ARG:NH2	2.37	0.55
1:b:78:VAL:HG22	1:b:100:VAL:HG12	1.88	0.55
3:h:51:LEU:HD11	3:h:107:PRO:HB3	1.89	0.55
11:n:181:ARG:NH1	12:m:57:PRO:O	2.36	0.55
23:P:47:ARG:HH22	23:P:54:SER:HB3	1.72	0.55
33:Z:769:ASN:OD1	33:Z:770:GLU:N	2.40	0.55
2:2:93:GLU:OE1	9:B:98:LYS:NZ	2.40	0.55
4:4:86:GLN:HG2	10:C:101:THR:HG22	1.89	0.55
9:B:122:THR:HA	9:B:129:PRO:HG3	1.89	0.55
7:7:100:LEU:HD21	7:7:129:LEU:HD11	1.89	0.55
17:J:29:GLU:HG2	26:S:224:LYS:HZ1	1.72	0.55
23:P:412:LEU:HD13	29:V:239:ALA:HB2	1.88	0.55
25:R:280:ILE:HG12	25:R:290:SER:HB2	1.89	0.55
28:U:48:VAL:HG22	28:U:90:ILE:HD11	1.87	0.55
4:4:149:ARG:HB2	4:4:152:MET:HG3	1.89	0.55
3:h:155:GLU:HB3	3:h:158:LEU:HD21	1.89	0.55
4:g:23:ARG:NH2	5:f:193:ASP:OD2	2.35	0.55
6:e:74:ASN:N	6:e:127:HIS:O	2.36	0.55
25:R:240:SER:HB3	25:R:243:LEU:HB2	1.89	0.55
25:R:348:LEU:N	25:R:388:VAL:O	2.40	0.55
33:Z:373:GLY:O	33:Z:380:ASN:ND2	2.40	0.55
6:6:56:SER:HB2	7:7:170:TYR:HB2	1.88	0.54
4:g:18:SER:HB2	4:g:176:PHE:HB2	1.89	0.54
14:k:80:GLY:HA3	14:k:134:VAL:HG12	1.88	0.54
16:I:283:GLU:OE2	17:J:306:ARG:NH1	2.39	0.54
18:K:91:SER:HB2	18:K:93:PRO:HD3	1.89	0.54
29:V:293:VAL:O	29:V:297:THR:OG1	2.20	0.54
30:W:22:PRO:HG3	30:W:177:GLY:H	1.72	0.54
5:5:78:THR:HA	5:5:91:VAL:HG12	1.88	0.54
10:d:221:ASN:OD1	10:d:222:ASP:N	2.40	0.54
18:K:94:LEU:HD22	18:K:147:VAL:HG21	1.88	0.54
18:K:129:GLU:OE2	29:V:270:TYR:OH	2.25	0.54
22:O:4:ASN:HB2	22:O:46:THR:HG21	1.88	0.54
22:O:308:LEU:HB3	22:O:348:VAL:HB	1.90	0.54
24:Q:178:HIS:HB2	24:Q:201:ALA:HB2	1.89	0.54
27:T:7:LEU:HB3	27:T:30:ILE:HG12	1.89	0.54
33:Z:463:HIS:HB2	33:Z:500:SER:HB2	1.89	0.54
2:i:30:THR:N	2:i:197:GLY:O	2.40	0.54
5:f:89:VAL:HG21	5:f:117:LEU:HD11	1.89	0.54
9:j:119:GLN:OE1	10:d:129:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:k:120:VAL:HG21	14:k:151:LEU:HD21	1.88	0.54
25:R:60:ALA:HA	25:R:63:TYR:HB3	1.89	0.54
7:7:87:SER:HB3	7:7:146:ALA:HB3	1.87	0.54
4:g:118:GLN:NE2	4:g:132:ALA:O	2.40	0.54
7:a:48:LYS:HG2	7:a:53:VAL:HG12	1.88	0.54
11:D:47:GLU:O	11:D:63:LYS:NZ	2.37	0.54
12:E:34:GLY:HA3	12:E:80:GLY:HA2	1.90	0.54
15:H:203:LYS:HE2	15:H:268:ASP:HB3	1.88	0.54
15:H:298:ALA:HB1	15:H:349:ILE:HD12	1.90	0.54
26:S:281:ALA:O	26:S:382:ARG:NH1	2.41	0.54
33:Z:317:GLN:HG3	33:Z:872:VAL:HG21	1.89	0.54
4:4:23:ARG:HE	5:5:195:THR:HG21	1.72	0.54
3:h:107:PRO:HD2	3:h:124:PHE:HB2	1.90	0.54
17:J:87:LYS:HA	17:J:93:LYS:HA	1.89	0.54
29:V:92:MET:HA	29:V:95:LEU:HD13	1.89	0.54
15:H:373:ARG:NH1	20:M:397:GLU:OE2	2.40	0.54
18:K:273:GLU:HB2	19:L:306:MET:HE3	1.90	0.54
26:S:227:ASN:HB2	26:S:263:ASP:HB2	1.89	0.54
29:V:54:LEU:HD12	29:V:67:ASP:HB3	1.90	0.54
4:g:4:ILE:HG13	4:g:47:ALA:HB2	1.89	0.54
6:e:35:ALA:HB2	6:e:141:VAL:HG23	1.90	0.54
10:C:53:THR:HG21	10:C:57:LEU:HD22	1.90	0.54
8:c:135:ARG:HD3	14:k:13:SER:HA	1.89	0.54
19:L:187:THR:HA	19:L:190:ILE:HB	1.90	0.54
21:N:707:ASN:OD1	21:N:711:ARG:NE	2.41	0.54
24:Q:51:ARG:HD3	24:Q:88:PHE:HB2	1.90	0.54
6:6:170:ASP:O	6:6:176:LYS:N	2.37	0.54
4:g:35:THR:HA	4:g:45:SER:HA	1.89	0.54
7:a:39:VAL:HG12	7:a:90:ILE:HD12	1.90	0.54
11:D:39:LYS:HD2	11:D:186:ALA:HB2	1.89	0.54
10:d:168:ASN:HB3	10:d:171:ALA:HB3	1.89	0.54
12:m:18:GLU:OE1	12:m:20:ARG:NH2	2.40	0.54
12:m:71:ASP:OD1	12:m:72:ARG:N	2.41	0.54
19:L:357:ARG:NH2	19:L:383:SER:O	2.41	0.54
21:N:9:LEU:HB3	21:N:28:ILE:HG12	1.90	0.54
21:N:518:ALA:HB1	21:N:550:GLY:HA3	1.89	0.54
3:3:74:TYR:OH	3:3:80:ARG:NH2	2.41	0.53
6:6:47:ARG:NH1	6:6:215:ILE:O	2.40	0.53
7:7:152:VAL:HG22	7:7:158:GLN:HG3	1.91	0.53
11:n:8:LEU:O	11:n:19:GLN:NE2	2.41	0.53
21:N:589:ILE:HA	21:N:624:ALA:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:U:14:VAL:HG21	28:U:48:VAL:HG12	1.90	0.53
18:K:207:ARG:NH2	18:K:302:GLN:O	2.40	0.53
20:M:213:ARG:NH1	20:M:316:SER:O	2.42	0.53
21:N:709:GLY:HA3	21:N:713:VAL:HG22	1.90	0.53
22:O:192:SER:HB2	22:O:217:LEU:HD23	1.89	0.53
23:P:270:LEU:HA	23:P:344:ARG:HG3	1.89	0.53
26:S:457:PRO:HB2	28:U:274:MET:HG3	1.89	0.53
15:H:247:LEU:HB3	15:H:374:LYS:HG2	1.90	0.53
5:5:116:LEU:HG	5:5:178:GLY:HA3	1.91	0.53
7:a:67:LEU:HD21	7:a:223:ARG:HG2	1.91	0.53
13:F:123:TYR:N	14:G:128:SER:O	2.37	0.53
15:H:380:PRO:O	15:H:385:ARG:NH1	2.41	0.53
19:L:179:THR:OG1	19:L:181:ASP:OD1	2.25	0.53
21:N:286:LEU:HA	21:N:289:ILE:HD12	1.91	0.53
22:O:93:ASP:O	22:O:97:LYS:NZ	2.30	0.53
29:V:134:SER:O	29:V:157:ARG:NH2	2.41	0.53
33:Z:342:LEU:HB2	33:Z:345:GLU:HG3	1.89	0.53
4:4:141:PHE:HD1	4:4:144:LEU:HD12	1.72	0.53
6:6:57:ARG:HH12	7:7:193:ASP:HA	1.72	0.53
3:3:101:GLY:O	4:4:93:ARG:NE	2.38	0.53
5:5:83:PHE:HE1	5:5:88:ILE:HG12	1.73	0.53
5:5:146:LYS:NZ	12:E:65:GLU:OE1	2.34	0.53
7:7:256:LYS:HG2	1:b:206:ILE:HG21	1.91	0.53
3:h:11:ILE:HG21	3:h:142:ALA:HB3	1.91	0.53
9:B:119:GLN:HE22	10:C:83:ASP:HA	1.73	0.53
21:N:775:CYS:HB2	21:N:882:ILE:HG23	1.89	0.53
21:N:875:LEU:HD12	21:N:876:PRO:HD2	1.90	0.53
31:X:72:GLU:HG3	31:X:91:PHE:HD1	1.73	0.53
1:b:23:MET:HE2	1:b:174:ILE:HG12	1.90	0.53
11:n:75:PHE:HB3	11:n:133:THR:HG22	1.90	0.53
20:M:288:THR:HG23	20:M:332:VAL:HG21	1.90	0.53
21:N:344:THR:HG22	21:N:375:HIS:HA	1.90	0.53
33:Z:139:LEU:HD22	33:Z:200:THR:HA	1.91	0.53
33:Z:158:ALA:HA	33:Z:203:LEU:HD11	1.90	0.53
2:2:47:THR:OG1	2:2:59:ASN:OD1	2.18	0.53
4:4:36:ARG:HG3	4:4:57:ALA:HB1	1.91	0.53
4:4:79:ALA:HB1	10:C:102:TYR:HD1	1.74	0.53
14:G:136:THR:HB	14:G:151:LEU:HB3	1.90	0.53
4:4:29:LYS:HD2	5:5:199:GLY:HA2	1.90	0.53
10:C:162:ALA:H	11:D:54:LEU:HD13	1.74	0.53
13:F:67:ASP:OD1	13:F:68:GLU:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:26:LYS:HA	17:J:29:GLU:HB2	1.90	0.53
17:J:375:ILE:HD11	25:R:205:GLU:HG3	1.91	0.53
19:L:216:LYS:NZ	19:L:312:MET:O	2.42	0.53
28:U:32:ARG:NH2	28:U:102:SER:OG	2.42	0.53
2:2:30:THR:OG1	2:2:62:LYS:NZ	2.41	0.53
3:3:189:ILE:HB	3:3:196:VAL:HB	1.91	0.53
5:5:82:ARG:NH2	5:5:200:ASP:OD1	2.42	0.53
4:g:47:ALA:HB3	4:g:101:ASN:HB2	1.91	0.53
11:D:68:ASP:OD1	11:D:69:SER:N	2.41	0.53
8:c:158:ASP:OD1	8:c:162:TYR:N	2.40	0.53
16:I:120:VAL:HG11	16:I:149:LEU:HD21	1.91	0.53
21:N:770:LYS:HD2	21:N:917:ILE:HD12	1.90	0.53
22:O:342:ASP:HB3	22:O:347:LEU:HB2	1.91	0.53
4:4:65:GLN:OE1	11:D:97:ARG:NH2	2.42	0.52
9:B:66:LEU:O	9:B:90:ARG:NH2	2.41	0.52
10:C:168:ASN:HB3	10:C:171:ALA:HB3	1.91	0.52
8:c:245:LEU:HD23	8:c:248:ILE:HD11	1.90	0.52
10:d:62:SER:OG	10:d:64:GLU:OE2	2.27	0.52
10:d:119:LYS:HG2	10:d:131:PHE:HB2	1.90	0.52
27:T:62:LEU:HD12	27:T:88:TYR:HE2	1.74	0.52
3:3:12:VAL:HB	3:3:108:VAL:HG21	1.91	0.52
5:f:218:ASN:HB3	5:f:231:LEU:HD13	1.89	0.52
20:M:192:GLU:OE1	20:M:345:ARG:NH2	2.42	0.52
30:W:30:ILE:HG12	30:W:76:LEU:HD13	1.89	0.52
8:A:144:VAL:HG12	8:A:154:ILE:HG12	1.91	0.52
14:G:36:THR:OG1	14:G:165:THR:O	2.23	0.52
13:l:67:ASP:OD2	13:l:102:LYS:NZ	2.42	0.52
23:P:286:ASN:OD1	23:P:287:ASP:N	2.42	0.52
5:f:153:ALA:HB1	11:n:100:LEU:HD22	1.92	0.52
20:M:144:ASP:OD1	20:M:145:LEU:N	2.43	0.52
21:N:211:PHE:HD1	21:N:225:LEU:HD22	1.75	0.52
26:S:145:PHE:HE1	26:S:186:TYR:HB2	1.75	0.52
33:Z:304:PRO:HA	33:Z:307:HIS:HD2	1.74	0.52
33:Z:868:ASN:OD1	33:Z:874:ASN:ND2	2.42	0.52
1:b:63:CYS:HB2	1:b:117:ILE:HB	1.90	0.52
8:A:57:LYS:NZ	8:A:66:PRO:O	2.42	0.52
11:n:159:TRP:HZ3	12:m:56:SER:HB3	1.73	0.52
13:l:67:ASP:OD1	13:l:68:GLU:N	2.42	0.52
23:P:86:HIS:ND1	23:P:87:GLY:O	2.42	0.52
24:Q:104:PHE:HB3	24:Q:114:GLN:HE21	1.73	0.52
1:1:204:ARG:NH2	7:a:266:ILE:OXT	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:104:PHE:HD1	3:h:126:LEU:HD22	1.75	0.52
8:A:105:ARG:HA	8:A:109:GLY:H	1.74	0.52
16:I:188:GLU:HA	16:I:191:ILE:HD12	1.90	0.52
17:J:136:LEU:HD22	17:J:214:SER:HB2	1.91	0.52
18:K:104:ASP:OD1	18:K:105:GLN:N	2.41	0.52
21:N:556:ALA:HB2	21:N:590:ALA:HB1	1.92	0.52
33:Z:257:PRO:HB2	33:Z:259:PRO:HD2	1.91	0.52
14:G:36:THR:HA	14:G:166:GLY:HA3	1.92	0.52
14:G:109:ILE:HG21	14:G:147:HIS:HB2	1.90	0.52
16:I:387:LEU:HB3	16:I:391:ASP:HB2	1.91	0.52
18:K:92:VAL:N	18:K:93:PRO:CD	2.73	0.52
18:K:232:ALA:HA	18:K:266:PRO:HB2	1.92	0.52
24:Q:163:ARG:NH1	24:Q:164:GLU:OE2	2.42	0.52
30:W:19:GLY:O	30:W:24:THR:HA	2.09	0.52
4:g:18:SER:HA	4:g:179:VAL:HA	1.90	0.52
17:J:370:LEU:HD11	18:K:197:LEU:HD13	1.92	0.52
20:M:251:LEU:HD13	20:M:286:ILE:HD13	1.91	0.52
26:S:435:LYS:O	26:S:444:GLU:N	2.41	0.52
29:V:188:LEU:HD12	29:V:189:ILE:N	2.24	0.52
1:l:23:MET:HE2	1:l:174:ILE:HG12	1.92	0.52
10:C:132:GLY:HA2	10:C:153:PRO:HG3	1.91	0.52
1:b:117:ILE:HG12	1:b:131:THR:HG22	1.91	0.52
6:e:49:ILE:HG22	6:e:54:ILE:HA	1.92	0.52
13:F:54:ASP:OD1	13:F:55:GLU:N	2.43	0.52
8:c:59:VAL:HG13	8:c:64:LEU:HD12	1.92	0.52
18:K:350:ARG:HH21	24:Q:236:PHE:HE2	1.57	0.52
23:P:235:LEU:HB2	23:P:272:PRO:HD2	1.92	0.52
10:C:152:ASN:ND2	10:C:154:SER:OG	2.43	0.51
10:C:186:VAL:HG21	10:C:217:ARG:HG2	1.92	0.51
8:c:84:ASN:ND2	8:c:171:THR:O	2.43	0.51
22:O:72:LYS:HG2	22:O:73:ILE:HG13	1.92	0.51
26:S:259:TYR:HB3	26:S:261:HIS:CE1	2.46	0.51
28:U:70:HIS:HA	28:U:73:ILE:HD12	1.92	0.51
28:U:283:ARG:NH1	29:V:249:GLU:OE1	2.42	0.51
33:Z:129:ASN:O	33:Z:156:HIS:NE2	2.42	0.51
2:2:244:GLU:HG2	3:3:198:ARG:HG2	1.93	0.51
6:6:49:ILE:HG22	6:6:54:ILE:HA	1.93	0.51
1:b:20:THR:N	1:b:188:SER:HG	2.09	0.51
16:I:299:GLU:HG3	17:J:270:ARG:HH12	1.75	0.51
23:P:125:VAL:HA	23:P:136:ARG:HG3	1.92	0.51
33:Z:172:ASP:HB3	33:Z:193:PHE:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:202:VAL:HB	2:i:220:LEU:HB3	1.92	0.51
3:h:74:TYR:OH	3:h:80:ARG:NH2	2.42	0.51
8:c:93:ALA:HB1	8:c:141:LEU:HD21	1.91	0.51
12:m:35:SER:O	12:m:79:SER:OG	2.27	0.51
15:H:422:VAL:HG22	15:H:450:VAL:HG21	1.92	0.51
1:b:20:THR:HB	1:b:148:SER:H	1.76	0.51
10:C:72:LYS:HG2	10:C:225:VAL:HB	1.93	0.51
16:I:282:ASP:OD1	16:I:283:GLU:N	2.44	0.51
25:R:393:PRO:HB2	25:R:396:LYS:HB2	1.92	0.51
3:3:203:ARG:NH1	3:3:205:ASP:OD1	2.43	0.51
7:a:162:TYR:HB2	7:a:175:LEU:HD13	1.92	0.51
10:C:125:HIS:HB3	11:D:126:VAL:HG12	1.93	0.51
13:F:164:ARG:HE	13:F:202:ARG:HG3	1.75	0.51
16:I:287:ILE:HD11	16:I:305:THR:HB	1.92	0.51
3:3:145:GLN:HE21	5:f:100:TRP:CD1	2.28	0.51
6:6:74:ASN:HB3	6:6:127:HIS:HB3	1.92	0.51
7:7:50:ASP:HB2	7:7:199:PRO:HA	1.93	0.51
8:c:37:GLN:NE2	14:k:19:GLY:O	2.43	0.51
11:n:68:ASP:OD1	11:n:69:SER:N	2.42	0.51
18:K:171:TYR:HA	18:K:225:ALA:HB1	1.91	0.51
26:S:280:ASN:HB2	26:S:289:ALA:HB2	1.91	0.51
27:T:83:ASN:HA	27:T:86:LYS:HE2	1.92	0.51
33:Z:142:ASP:HB3	33:Z:202:ARG:HD2	1.91	0.51
11:D:76:SER:HB3	11:D:164:ILE:HG13	1.93	0.51
8:c:27:GLN:NE2	14:k:13:SER:O	2.44	0.51
13:l:67:ASP:HB3	13:l:70:MET:HB3	1.93	0.51
17:J:346:VAL:HG12	17:J:350:MET:HE3	1.93	0.51
18:K:154:SER:HB3	18:K:256:ASP:HB3	1.92	0.51
26:S:164:ILE:O	26:S:166:ASN:N	2.40	0.51
26:S:176:LEU:HD23	26:S:177:ASN:HB2	1.93	0.51
33:Z:333:GLY:HA2	33:Z:339:PHE:HE2	1.74	0.51
2:2:60:CYS:SG	2:2:61:ALA:N	2.84	0.51
8:A:54:ILE:HG12	8:A:225:VAL:HG22	1.93	0.51
9:B:161:ALA:HB1	9:B:175:LEU:HD23	1.93	0.51
15:H:142:ASP:OD1	15:H:143:ALA:N	2.44	0.51
21:N:626:GLY:HA2	21:N:663:ILE:HD11	1.92	0.51
24:Q:47:ASP:OD1	24:Q:48:ASP:N	2.43	0.51
24:Q:389:VAL:HG23	24:Q:398:TYR:HB2	1.92	0.51
29:V:57:PHE:HB2	29:V:62:THR:O	2.11	0.51
1:1:167:LYS:HE3	1:1:196:VAL:HG11	1.93	0.51
5:f:93:SER:HB2	5:f:105:THR:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:f:266:HIS:HB3	5:f:271:LEU:HD11	1.93	0.51
24:Q:212:THR:HB	24:Q:249:LEU:HD21	1.92	0.51
6:6:170:ASP:HB3	6:6:176:LYS:HB2	1.92	0.51
10:C:190:ILE:HG12	10:C:213:PHE:HZ	1.76	0.51
12:E:71:ASP:OD1	12:E:72:ARG:N	2.41	0.51
8:c:144:VAL:HG12	8:c:154:ILE:HG12	1.92	0.51
10:d:194:LEU:HD13	10:d:239:LEU:HD23	1.92	0.51
22:O:308:LEU:HD11	22:O:313:ILE:HB	1.93	0.51
33:Z:108:ASP:HB3	33:Z:111:LEU:HB2	1.93	0.51
1:1:78:VAL:HG22	1:1:100:VAL:HG12	1.92	0.50
2:2:235:PRO:HG3	6:e:181:PRO:HD3	1.93	0.50
5:5:87:ILE:HB	5:5:255:VAL:HB	1.93	0.50
10:d:34:THR:HA	10:d:166:GLY:HA3	1.92	0.50
18:K:99:PHE:HA	18:K:110:VAL:HG12	1.93	0.50
24:Q:66:VAL:HA	24:Q:71:LYS:HB3	1.92	0.50
25:R:174:ILE:HD13	25:R:190:LYS:HB3	1.93	0.50
26:S:425:ARG:NH1	27:T:188:GLU:OE2	2.38	0.50
29:V:154:ASP:OD1	29:V:155:ALA:N	2.43	0.50
8:A:79:ILE:HA	8:A:145:SER:HB2	1.92	0.50
14:G:80:GLY:HA3	14:G:134:VAL:HG12	1.92	0.50
23:P:119:ILE:HG23	23:P:125:VAL:HG11	1.94	0.50
24:Q:161:LEU:HB3	24:Q:165:PHE:HE2	1.76	0.50
33:Z:595:MET:HE2	33:Z:737:ALA:HB3	1.93	0.50
2:2:177:LYS:HE3	2:2:206:VAL:HG11	1.94	0.50
7:7:251:LYS:HE3	7:7:253:ASP:HB2	1.92	0.50
1:b:196:VAL:HB	1:b:203:GLU:HB3	1.93	0.50
6:e:32:LEU:HD11	6:e:169:LEU:HD11	1.94	0.50
7:a:78:VAL:HG12	7:a:120:LEU:HD13	1.93	0.50
13:F:39:ARG:NH1	13:F:142:ALA:O	2.44	0.50
19:L:289:ARG:HE	19:L:335:PRO:HD3	1.76	0.50
20:M:219:LEU:HD22	20:M:346:LYS:HG2	1.94	0.50
23:P:125:VAL:O	23:P:136:ARG:NE	2.44	0.50
24:Q:269:LYS:HZ2	24:Q:272:LEU:HD23	1.77	0.50
29:V:45:VAL:HB	29:V:46:PRO:HD3	1.93	0.50
29:V:183:ALA:HB3	29:V:188:LEU:HD11	1.93	0.50
33:Z:76:LYS:NZ	33:Z:145:ASP:OD1	2.41	0.50
33:Z:358:TYR:HE1	33:Z:962:ARG:HB3	1.75	0.50
12:E:42:THR:OG1	12:E:45:GLY:O	2.26	0.50
11:n:65:SER:O	11:n:73:LEU:N	2.44	0.50
17:J:252:SER:HA	17:J:257:ARG:HG3	1.93	0.50
24:Q:227:CYS:HB3	24:Q:334:HIS:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:W:52:ILE:HG22	30:W:61:VAL:HG13	1.93	0.50
2:2:105:VAL:HG13	2:2:129:VAL:HG12	1.93	0.50
12:E:52:LYS:NZ	12:E:61:SER:O	2.43	0.50
19:L:364:HIS:CD2	19:L:392:ARG:HE	2.28	0.50
26:S:243:ASN:O	27:T:127:GLN:NE2	2.44	0.50
33:Z:211:PHE:HD1	33:Z:216:GLY:HA3	1.76	0.50
33:Z:359:LYS:HE2	33:Z:395:CYS:HB2	1.93	0.50
5:5:260:TRP:HZ3	5:5:262:TYR:HB2	1.77	0.50
4:g:32:ASP:OD1	4:g:33:ASP:N	2.45	0.50
5:f:201:ILE:HD11	5:f:215:LEU:HD13	1.94	0.50
9:j:45:ILE:HD12	9:j:74:VAL:HB	1.92	0.50
18:K:152:PRO:HG3	18:K:263:GLU:HG3	1.92	0.50
18:K:207:ARG:NH1	18:K:303:MET:O	2.44	0.50
18:K:211:LEU:HD13	18:K:315:ILE:HG23	1.93	0.50
19:L:149:ASP:HB3	19:L:154:THR:H	1.77	0.50
22:O:172:TYR:O	22:O:195:TYR:OH	2.29	0.50
29:V:95:LEU:HD12	29:V:100:ARG:HH21	1.77	0.50
5:5:196:ARG:NH2	11:D:101:GLU:OE2	2.31	0.50
1:b:27:PHE:HE2	1:b:32:ILE:HG13	1.76	0.50
8:A:156:LYS:NZ	8:A:170:ALA:O	2.45	0.50
8:c:126:GLN:HE22	9:j:81:ASP:HA	1.76	0.50
11:n:207:ALA:HA	11:n:210:ILE:HD12	1.92	0.50
17:J:139:VAL:HG22	17:J:211:ILE:HG12	1.94	0.50
27:T:136:LEU:HD12	27:T:142:LEU:HB3	1.93	0.50
33:Z:405:ASN:HB3	33:Z:409:LYS:HE3	1.93	0.50
2:2:70:ILE:HG12	2:2:131:GLY:HA3	1.94	0.50
4:4:32:ASP:OD1	4:4:33:ASP:N	2.44	0.50
2:i:72:CYS:SG	2:i:73:ALA:N	2.85	0.50
7:a:60:LEU:O	7:a:74:ARG:NH1	2.41	0.50
14:G:194:LYS:HG2	14:G:239:ALA:HA	1.93	0.50
11:n:83:ARG:HA	11:n:86:ILE:HB	1.94	0.50
15:H:238:LEU:HD22	20:M:403:LEU:HD11	1.92	0.50
16:I:397:THR:HG23	17:J:179:ILE:HD11	1.94	0.50
25:R:312:TYR:HA	25:R:316:LEU:HD12	1.93	0.50
30:W:4:GLU:OE2	30:W:40:LYS:NZ	2.45	0.50
6:6:214:HIS:HE1	6:6:216:GLN:HB2	1.77	0.50
13:l:39:ARG:NH1	13:l:40:SER:O	2.45	0.50
18:K:148:ASP:OD1	18:K:149:ILE:N	2.45	0.50
20:M:129:LEU:HD22	20:M:154:LEU:HA	1.93	0.50
21:N:87:ASP:OD1	21:N:88:ARG:N	2.40	0.50
21:N:735:MET:HE3	21:N:745:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:48:HIS:HE1	3:h:84:PRO:HD3	1.77	0.49
9:j:140:ASP:OD1	9:j:144:GLY:N	2.45	0.49
17:J:252:SER:H	17:J:294:THR:HA	1.76	0.49
18:K:93:PRO:O	18:K:94:LEU:HD23	2.12	0.49
18:K:331:PRO:HA	18:K:334:LEU:O	2.12	0.49
24:Q:42:ALA:HB2	24:Q:51:ARG:HH21	1.77	0.49
30:W:109:ARG:HA	30:W:138:ALA:HB3	1.93	0.49
33:Z:596:THR:HA	33:Z:599:ILE:HD12	1.93	0.49
10:C:74:ALA:HB3	10:C:216:ILE:HD11	1.94	0.49
11:D:37:LYS:HA	11:D:42:VAL:HA	1.94	0.49
11:D:37:LYS:HB3	11:D:42:VAL:HG23	1.93	0.49
9:j:69:PRO:HB3	9:j:233:PRO:HB3	1.94	0.49
10:d:215:THR:H	10:d:230:PHE:HE2	1.59	0.49
14:k:32:GLU:OE2	14:k:169:ARG:NH2	2.45	0.49
17:J:102:ILE:HD13	17:J:125:VAL:HG23	1.94	0.49
17:J:219:VAL:HG21	17:J:268:VAL:HB	1.94	0.49
17:J:356:ALA:HB3	18:K:330:ARG:HD3	1.94	0.49
22:O:283:HIS:HA	22:O:286:PHE:HD2	1.78	0.49
29:V:114:PHE:H	29:V:118:LEU:HG	1.77	0.49
33:Z:322:GLU:HG2	33:Z:499:GLY:HA2	1.94	0.49
11:D:68:ASP:HB3	11:D:71:VAL:HB	1.93	0.49
14:G:68:GLN:N	14:G:76:CYS:O	2.44	0.49
28:U:38:LEU:HB2	28:U:50:ASN:HB3	1.94	0.49
28:U:121:LEU:HD11	28:U:134:THR:HB	1.94	0.49
31:X:90:VAL:HA	31:X:96:ARG:HG2	1.93	0.49
1:1:40:THR:HG21	1:1:187:SER:HA	1.94	0.49
1:1:184:TRP:NE1	1:b:158:ASP:OD2	2.41	0.49
4:4:86:GLN:HE21	4:4:90:LYS:HE3	1.77	0.49
1:b:139:HIS:CE1	7:a:72:VAL:HG22	2.48	0.49
4:g:165:VAL:HG13	4:g:176:PHE:HZ	1.76	0.49
6:e:110:ARG:HG2	12:m:104:ASP:HB2	1.95	0.49
7:a:131:THR:HG21	13:l:98:VAL:HG22	1.93	0.49
11:D:81:ASP:HB3	11:D:129:PHE:HD1	1.78	0.49
12:E:13:SER:HA	13:F:126:ARG:HD3	1.94	0.49
11:n:50:SER:HA	11:n:55:GLN:HE22	1.77	0.49
19:L:375:ASP:H	19:L:412:PRO:HB3	1.77	0.49
26:S:228:GLU:HG2	26:S:232:MET:HE2	1.94	0.49
33:Z:208:VAL:HG11	33:Z:235:GLN:HG3	1.95	0.49
4:4:101:ASN:HB3	4:4:133:HIS:CD2	2.47	0.49
4:4:165:VAL:HG13	4:4:176:PHE:HZ	1.77	0.49
6:6:105:ILE:HD13	6:6:140:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:214:HIS:CE1	6:6:216:GLN:HB2	2.47	0.49
3:h:29:LEU:HD23	3:h:37:SER:HB3	1.93	0.49
3:h:121:ILE:HD12	3:h:137:ILE:HG12	1.94	0.49
6:e:212:GLU:OE2	6:e:239:LYS:NZ	2.43	0.49
10:C:50:ARG:NH2	10:C:64:GLU:HB2	2.28	0.49
12:m:71:ASP:HB3	12:m:74:ILE:HB	1.94	0.49
25:R:25:GLU:OE2	25:R:245:SER:OG	2.30	0.49
28:U:13:LEU:HD11	29:V:36:LYS:HD2	1.94	0.49
4:g:3:ILE:HB	4:g:18:SER:HB3	1.95	0.49
10:d:33:GLY:HA2	10:d:51:LYS:HE2	1.94	0.49
17:J:212:ARG:HH22	18:K:306:PHE:HE1	1.60	0.49
18:K:283:ASP:OD1	18:K:284:ALA:N	2.44	0.49
21:N:83:LEU:HD21	21:N:136:ILE:HD11	1.95	0.49
24:Q:195:LYS:HG2	24:Q:225:LEU:HD13	1.94	0.49
30:W:44:ASN:O	30:W:47:ASN:ND2	2.45	0.49
11:D:88:LYS:NZ	11:D:120:TYR:OH	2.45	0.49
15:H:240:ILE:HA	20:M:367:LYS:HE2	1.94	0.49
16:I:290:LYS:HD3	16:I:306:MET:HE1	1.94	0.49
18:K:350:ARG:NH1	18:K:369:ASP:OD1	2.44	0.49
23:P:361:THR:HG22	23:P:363:LEU:H	1.78	0.49
24:Q:387:TYR:HB3	24:Q:400:TYR:HD2	1.78	0.49
26:S:314:ASN:HD22	26:S:337:ASN:HD21	1.59	0.49
28:U:106:ILE:HA	28:U:109:LEU:HD13	1.95	0.49
28:U:111:LYS:HG2	28:U:118:PRO:HG2	1.93	0.49
33:Z:501:LYS:NZ	33:Z:538:CYS:O	2.45	0.49
2:2:79:ALA:HB2	3:3:129:CYS:HB2	1.94	0.49
3:3:12:VAL:HG11	3:3:52:GLY:HA3	1.94	0.49
4:g:17:SER:O	4:g:180:ILE:N	2.46	0.49
14:G:108:PRO:HB2	14:G:110:PRO:HD2	1.93	0.49
8:c:46:ARG:HH11	8:c:153:SER:HA	1.78	0.49
11:n:88:LYS:NZ	11:n:120:TYR:OH	2.44	0.49
17:J:259:GLU:HG3	18:K:280:LYS:HD2	1.94	0.49
22:O:98:TYR:HB2	22:O:102:LEU:HD13	1.94	0.49
2:i:90:SER:HB2	9:j:94:HIS:HB3	1.95	0.49
13:F:226:ASP:OD1	13:F:227:GLY:N	2.45	0.49
17:J:75:VAL:HG21	17:J:107:LEU:HD22	1.94	0.49
20:M:295:LYS:O	20:M:299:ARG:N	2.45	0.49
21:N:17:GLN:HE21	21:N:19:SER:HB2	1.78	0.49
21:N:327:LEU:HD11	29:V:170:PRO:HG2	1.95	0.49
21:N:742:TRP:CD2	21:N:743:PHE:HD2	2.31	0.49
29:V:170:PRO:O	29:V:175:SER:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:38:ARG:NH1	1:b:186:GLY:O	2.45	0.49
3:h:11:ILE:HD12	3:h:146:LEU:HD11	1.95	0.49
3:h:89:GLN:OE1	3:h:92:SER:OG	2.30	0.49
21:N:369:ALA:HB1	21:N:406:TYR:HD2	1.77	0.49
22:O:205:ILE:HG13	22:O:209:GLU:HB2	1.95	0.49
26:S:151:GLU:HG2	26:S:153:GLU:H	1.77	0.49
28:U:50:ASN:OD1	28:U:51:SER:N	2.46	0.49
31:X:26:PRO:HG2	31:X:28:PRO:HD3	1.94	0.49
3:h:189:ILE:HB	3:h:196:VAL:HB	1.94	0.48
21:N:163:LEU:HB3	21:N:209:LYS:HE3	1.95	0.48
25:R:380:VAL:HA	26:S:398:THR:HG21	1.94	0.48
25:R:396:LYS:NZ	26:S:450:ASN:O	2.46	0.48
5:f:203:CYS:HB2	5:f:212:TYR:CZ	2.48	0.48
8:A:53:VAL:HG21	8:A:82:VAL:HG21	1.95	0.48
10:C:159:GLY:O	11:D:55:GLN:NE2	2.46	0.48
11:D:32:CYS:N	11:D:47:GLU:OE2	2.44	0.48
12:E:71:ASP:HB3	12:E:74:ILE:HB	1.94	0.48
9:j:48:GLU:HG2	9:j:50:LYS:H	1.78	0.48
16:I:254:GLN:NE2	16:I:255:LYS:HD2	2.28	0.48
19:L:248:ALA:HA	19:L:251:ILE:HD12	1.94	0.48
20:M:62:ILE:HD12	20:M:65:ASN:HB2	1.94	0.48
20:M:82:VAL:HG21	20:M:140:LEU:HD22	1.95	0.48
21:N:765:ASP:OD1	21:N:766:GLN:N	2.46	0.48
33:Z:534:PHE:O	33:Z:537:THR:OG1	2.30	0.48
33:Z:813:PHE:HD1	33:Z:850:LEU:HB3	1.78	0.48
1:1:54:THR:HG21	1:1:75:ALA:HB1	1.93	0.48
3:h:11:ILE:HD13	3:h:142:ALA:HB3	1.95	0.48
5:f:148:ARG:HH22	5:f:181:ARG:HH21	1.61	0.48
10:C:135:PHE:N	10:C:151:SER:OG	2.42	0.48
11:D:94:GLN:OE1	11:D:97:ARG:NH2	2.46	0.48
10:d:137:TYR:HE2	10:d:151:SER:HB3	1.78	0.48
21:N:893:VAL:HG23	21:N:894:ARG:H	1.78	0.48
27:T:6:GLU:HG2	27:T:8:THR:H	1.77	0.48
30:W:143:ASN:HD21	30:W:149:GLN:HB2	1.77	0.48
33:Z:415:MET:HE2	33:Z:447:VAL:HG22	1.96	0.48
1:1:206:ILE:HG21	7:a:256:LYS:HG2	1.96	0.48
7:7:231:ALA:HA	7:7:241:PHE:HA	1.95	0.48
5:f:134:LEU:HD22	5:f:158:LEU:HB2	1.94	0.48
7:a:96:ILE:HD13	7:a:147:ILE:HD11	1.95	0.48
13:F:80:ASP:HB3	13:F:128:TYR:HB3	1.96	0.48
12:m:10:ARG:NH1	12:m:26:TYR:OH	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:243:THR:N	16:I:276:PRO:O	2.41	0.48
18:K:345:ASP:OD1	18:K:346:ARG:N	2.41	0.48
23:P:343:LYS:HG2	23:P:379:TYR:HE1	1.79	0.48
3:3:176:ASP:OD1	3:3:203:ARG:NE	2.34	0.48
6:6:211:THR:HG21	6:6:239:LYS:HB3	1.94	0.48
2:i:49:SER:HB3	2:i:57:ASP:HB3	1.95	0.48
16:I:427:LYS:HG2	16:I:428:VAL:HG23	1.95	0.48
17:J:71:TYR:N	17:J:115:LEU:O	2.46	0.48
6:6:62:VAL:HG22	6:6:72:SER:HB2	1.95	0.48
7:7:258:ILE:O	1:b:193:ARG:NH1	2.46	0.48
9:j:119:GLN:O	9:j:122:THR:OG1	2.30	0.48
11:n:46:CYS:SG	11:n:74:SER:OG	2.66	0.48
22:O:380:LEU:HD21	28:U:189:ARG:HH22	1.79	0.48
26:S:433:GLU:O	26:S:446:THR:OG1	2.28	0.48
28:U:71:ASN:ND2	30:W:64:THR:OG1	2.46	0.48
29:V:188:LEU:HD13	29:V:192:LEU:HD11	1.96	0.48
5:5:144:ARG:HB3	11:D:111:ARG:HH12	1.79	0.48
6:6:96:PHE:HB3	13:F:89:ARG:NH1	2.27	0.48
4:g:37:GLN:HE21	4:g:40:PRO:HA	1.78	0.48
5:f:102:ALA:O	6:e:156:ARG:NH1	2.47	0.48
5:f:172:MET:H	5:f:192:SER:HB3	1.79	0.48
14:G:114:ASP:OD1	14:G:157:TYR:OH	2.31	0.48
17:J:132:PRO:HB3	17:J:236:MET:HE1	1.94	0.48
18:K:300:LEU:HD22	18:K:327:ALA:HB3	1.95	0.48
29:V:53:MET:HE1	29:V:137:VAL:HG23	1.96	0.48
5:5:156:LYS:NZ	11:D:98:LEU:O	2.43	0.48
7:7:50:ASP:O	7:7:158:GLN:NE2	2.45	0.48
6:e:105:ILE:HG12	6:e:140:ALA:HB3	1.95	0.48
10:d:44:ILE:HG21	10:d:138:ALA:HB1	1.96	0.48
10:d:53:THR:HG23	10:d:57:LEU:HD23	1.94	0.48
14:k:108:PRO:HB2	14:k:110:PRO:HD2	1.95	0.48
17:J:192:GLY:HA3	18:K:330:ARG:HD2	1.96	0.48
18:K:188:VAL:HG22	18:K:313:LYS:HG2	1.96	0.48
21:N:761:ILE:HG13	21:N:904:VAL:HG22	1.95	0.48
26:S:144:LEU:HD21	26:S:155:LEU:HD11	1.95	0.48
26:S:184:TRP:HA	26:S:187:ILE:HD12	1.96	0.48
28:U:82:LYS:HG3	29:V:72:PRO:HB3	1.94	0.48
29:V:182:LYS:HG3	29:V:186:GLN:HE21	1.78	0.48
31:X:101:LEU:HD11	31:X:116:ALA:HB3	1.95	0.48
33:Z:602:LEU:HD21	33:Z:620:LEU:HD11	1.96	0.48
6:6:48:ASN:HB3	6:6:56:SER:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:215:ILE:HB	2:i:196:LEU:HB3	1.96	0.48
2:i:220:LEU:HG	2:i:222:PRO:HD3	1.94	0.48
12:E:31:ILE:HD13	12:E:141:ALA:HB2	1.96	0.48
12:E:142:LEU:HB2	12:E:158:ALA:HB3	1.95	0.48
10:d:152:ASN:HD21	10:d:156:ASN:HB2	1.79	0.48
10:d:158:THR:OG1	10:d:160:TRP:NE1	2.47	0.48
11:n:4:TYR:CZ	11:n:6:ARG:HB2	2.48	0.48
15:H:209:SER:HA	15:H:391:ILE:HG21	1.96	0.48
18:K:324:LEU:HD12	18:K:324:LEU:O	2.13	0.48
18:K:418:ASP:OD1	18:K:420:THR:OG1	2.29	0.48
21:N:259:PHE:HE2	21:N:904:VAL:HG11	1.79	0.48
21:N:685:VAL:HG13	21:N:691:GLN:HG3	1.95	0.48
21:N:868:VAL:HG22	21:N:870:ASN:H	1.78	0.48
1:1:47:ASN:HA	7:a:220:ARG:HH12	1.79	0.48
3:3:185:ALA:HB3	3:3:200:LEU:HD12	1.96	0.48
14:G:68:GLN:HB3	14:G:89:VAL:HG11	1.96	0.48
9:j:57:MET:HG2	9:j:59:GLU:H	1.79	0.48
18:K:91:SER:C	18:K:93:PRO:HD2	2.39	0.48
21:N:495:PRO:HA	21:N:498:ILE:HD12	1.96	0.48
21:N:627:ILE:HG23	21:N:733:LEU:HD13	1.96	0.48
22:O:139:LEU:HG	22:O:140:LYS:H	1.79	0.48
33:Z:142:ASP:OD1	33:Z:143:VAL:N	2.47	0.48
3:h:143:SER:HA	3:h:146:LEU:HD12	1.95	0.47
10:C:119:LYS:NZ	10:C:133:VAL:O	2.44	0.47
12:E:13:SER:HB2	13:F:126:ARG:HB3	1.96	0.47
17:J:186:ILE:HG23	17:J:293:ALA:HA	1.96	0.47
23:P:122:ILE:HG22	23:P:124:VAL:H	1.79	0.47
33:Z:821:GLY:HA3	33:Z:862:MET:HB2	1.95	0.47
5:5:242:ARG:HH12	4:g:141:PHE:HB3	1.79	0.47
8:A:61:ASP:HB3	8:A:64:LEU:HG	1.95	0.47
10:d:187:ASP:HA	10:d:190:ILE:HD12	1.94	0.47
11:n:149:GLN:NE2	11:n:151:GLU:OE2	2.47	0.47
17:J:26:LYS:NZ	21:N:104:LYS:O	2.43	0.47
18:K:233:ALA:O	18:K:268:ILE:N	2.43	0.47
23:P:271:SER:OG	23:P:277:GLN:NE2	2.47	0.47
24:Q:135:HIS:ND1	24:Q:169:ASP:OD2	2.47	0.47
24:Q:227:CYS:HB3	24:Q:334:HIS:HE1	1.78	0.47
26:S:226:ASP:OD1	26:S:229:THR:OG1	2.28	0.47
27:T:193:THR:HA	27:T:197:TYR:HD2	1.79	0.47
33:Z:234:PRO:HB3	33:Z:268:ALA:HA	1.96	0.47
5:5:139:ARG:HD3	12:E:97:VAL:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:106:VAL:HG13	11:D:135:ILE:HG22	1.96	0.47
8:c:79:ILE:HA	8:c:145:SER:HB2	1.95	0.47
19:L:129:VAL:HG11	19:L:148:LEU:HD22	1.96	0.47
21:N:742:TRP:CE3	21:N:743:PHE:HB2	2.49	0.47
25:R:398:ALA:O	25:R:402:LEU:HB2	2.14	0.47
31:X:63:PRO:HG2	31:X:66:LEU:HB2	1.96	0.47
33:Z:255:LEU:HG	33:Z:257:PRO:O	2.15	0.47
5:f:196:ARG:NH2	11:n:101:GLU:OE2	2.46	0.47
8:c:105:ARG:HA	8:c:109:GLY:H	1.80	0.47
21:N:154:LEU:HB3	21:N:189:LEU:HD21	1.96	0.47
25:R:396:LYS:HZ1	26:S:451:ILE:HA	1.79	0.47
3:h:13:VAL:HG23	3:h:167:ILE:HD11	1.96	0.47
4:g:70:ARG:NH2	11:n:87:GLU:OE2	2.46	0.47
8:A:27:GLN:NE2	14:G:13:SER:O	2.47	0.47
9:B:44:VAL:HG23	9:B:213:ILE:HG22	1.96	0.47
21:N:178:SER:O	21:N:179:THR:OG1	2.29	0.47
21:N:312:GLY:HA3	21:N:787:MET:HE1	1.95	0.47
22:O:233:LEU:HD11	22:O:238:ILE:HG21	1.97	0.47
22:O:234:LEU:HB2	22:O:251:LEU:HD21	1.97	0.47
23:P:225:VAL:HG11	23:P:328:ALA:HB1	1.96	0.47
24:Q:47:ASP:HB3	24:Q:50:ARG:HG2	1.96	0.47
29:V:95:LEU:HB3	29:V:101:ASP:HA	1.97	0.47
1:b:54:THR:OG1	1:b:64:ARG:NE	2.47	0.47
10:d:174:THR:HG22	10:d:178:MET:HE3	1.96	0.47
21:N:376:LYS:HA	21:N:411:ILE:HG12	1.97	0.47
22:O:376:GLN:O	22:O:381:GLY:N	2.38	0.47
26:S:196:ARG:NH1	26:S:204:ASP:OD1	2.47	0.47
2:2:242:LEU:HB3	3:3:199:TYR:HB2	1.97	0.47
6:e:76:PHE:HD2	6:e:79:ASP:H	1.63	0.47
7:a:48:LYS:HD3	7:a:173:PRO:HA	1.96	0.47
18:K:207:ARG:HD3	18:K:333:ARG:HD2	1.96	0.47
21:N:313:LEU:HB3	21:N:703:GLN:HE21	1.80	0.47
21:N:373:VAL:HG23	21:N:410:LEU:HD13	1.96	0.47
23:P:188:ILE:HG21	23:P:226:LYS:HB3	1.97	0.47
24:Q:260:GLN:NE2	24:Q:264:TYR:OH	2.48	0.47
24:Q:405:GLN:HG2	24:Q:406:ASP:O	2.14	0.47
30:W:177:GLY:O	30:W:179:ARG:N	2.47	0.47
31:X:34:GLU:N	31:X:49:GLU:O	2.43	0.47
7:a:92:ASP:HB2	7:a:145:ASN:HD21	1.80	0.47
13:F:43:HIS:CD2	13:F:217:GLY:HA3	2.49	0.47
15:H:58:ASP:O	15:H:62:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:278:ILE:HG12	16:I:323:LYS:HB2	1.96	0.47
17:J:76:ILE:HD11	17:J:87:LYS:HB2	1.96	0.47
21:N:378:ASN:HD21	21:N:381:GLU:HB2	1.80	0.47
24:Q:404:ASN:O	25:R:397:ASN:ND2	2.44	0.47
30:W:87:MET:HB2	30:W:118:ILE:HD12	1.96	0.47
4:4:140:THR:HG22	4:4:164:CYS:HB3	1.97	0.47
5:5:280:GLY:O	5:5:283:ASN:ND2	2.47	0.47
10:C:44:ILE:HG21	10:C:138:ALA:HB1	1.97	0.47
15:H:99:VAL:HG11	16:I:127:ASP:HB2	1.97	0.47
20:M:432:PHE:HD2	20:M:433:TYR:HD1	1.61	0.47
23:P:124:VAL:HG22	23:P:129:LYS:HG3	1.97	0.47
25:R:51:LEU:HD12	25:R:54:ILE:HD11	1.97	0.47
16:I:118:ALA:HB2	16:I:132:ILE:HD11	1.96	0.47
16:I:366:THR:HA	16:I:369:MET:HB3	1.96	0.47
21:N:416:GLY:O	21:N:420:THR:N	2.45	0.47
21:N:716:GLN:HE22	21:N:900:ASN:HD21	1.63	0.47
33:Z:528:LEU:HD22	33:Z:883:THR:HG23	1.96	0.47
3:h:25:CYS:HB2	3:h:42:LYS:HE2	1.97	0.46
8:A:70:SER:OG	8:A:224:GLU:OE2	2.31	0.46
8:A:136:PRO:HD2	14:G:15:PHE:HE2	1.80	0.46
10:C:50:ARG:HH21	10:C:64:GLU:HB2	1.79	0.46
12:E:41:ALA:HA	12:E:46:VAL:HG22	1.98	0.46
8:c:24:ARG:HH12	9:j:30:GLN:HB3	1.81	0.46
10:d:240:VAL:HG22	10:d:245:THR:HG22	1.97	0.46
16:I:432:LEU:HD12	16:I:432:LEU:O	2.15	0.46
21:N:533:ASP:OD1	21:N:559:TYR:OH	2.33	0.46
25:R:280:ILE:HA	25:R:286:LEU:HD12	1.97	0.46
29:V:95:LEU:HG	29:V:100:ARG:HE	1.80	0.46
4:g:158:LEU:HD22	4:g:198:GLN:HB3	1.97	0.46
7:a:54:ILE:HG12	7:a:232:ILE:HG12	1.97	0.46
11:D:118:GLN:NE2	12:E:87:SER:OG	2.47	0.46
10:d:125:HIS:HB3	11:n:126:VAL:HG12	1.97	0.46
18:K:235:ILE:HB	18:K:269:ILE:HA	1.97	0.46
19:L:123:SER:HA	20:M:125:GLN:HA	1.97	0.46
20:M:351:LEU:HD13	20:M:385:GLU:HB3	1.97	0.46
21:N:473:ASP:OD1	21:N:504:TYR:OH	2.30	0.46
33:Z:208:VAL:HG13	33:Z:236:PHE:HA	1.98	0.46
33:Z:788:PRO:HB3	33:Z:826:ARG:HD2	1.97	0.46
3:3:30:GLY:HA2	3:3:36:VAL:HG23	1.97	0.46
5:5:94:ARG:NH1	5:5:244:ALA:O	2.48	0.46
5:f:78:THR:OG1	5:f:204:VAL:O	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:135:ARG:HB3	14:k:13:SER:HB2	1.97	0.46
9:j:37:ILE:N	9:j:44:VAL:O	2.45	0.46
16:I:222:TYR:HD2	16:I:349:LEU:HA	1.80	0.46
6:e:30:THR:HA	6:e:74:ASN:ND2	2.30	0.46
14:k:69:VAL:HG22	14:k:228:HIS:HD2	1.81	0.46
15:H:65:GLU:HB3	16:I:133:LEU:HD22	1.96	0.46
29:V:224:GLY:O	29:V:225:LEU:HD12	2.14	0.46
31:X:74:MET:HB2	31:X:90:VAL:HB	1.97	0.46
2:2:42:VAL:HG22	2:2:206:VAL:HG13	1.96	0.46
7:7:105:THR:HG23	14:G:71:ASP:HA	1.97	0.46
11:n:167:ASN:HD22	11:n:202:VAL:HG13	1.80	0.46
17:J:76:ILE:HD12	17:J:85:LEU:HG	1.97	0.46
17:J:135:SER:C	17:J:137:MET:H	2.23	0.46
21:N:362:TRP:HA	21:N:365:PHE:HB3	1.97	0.46
21:N:581:ASP:HB3	21:N:616:HIS:CG	2.51	0.46
23:P:392:LYS:HD2	23:P:401:ASN:HB2	1.98	0.46
21:N:52:ASP:O	21:N:58:ARG:NH2	2.42	0.46
21:N:185:ILE:HA	21:N:188:TYR:HD2	1.81	0.46
25:R:222:ARG:HG2	25:R:325:HIS:NE2	2.31	0.46
26:S:436:ILE:HG12	26:S:443:ILE:HG12	1.98	0.46
9:j:33:THR:HA	9:j:165:GLY:HA3	1.96	0.46
14:k:41:LYS:HE3	14:k:147:HIS:HA	1.97	0.46
16:I:126:PRO:HB2	16:I:128:TYR:CZ	2.51	0.46
24:Q:109:ASP:OD1	24:Q:110:SER:N	2.49	0.46
4:4:51:GLY:HA3	5:5:166:LYS:HE2	1.98	0.46
1:b:40:THR:HG21	1:b:187:SER:HA	1.97	0.46
1:b:83:GLU:HB3	8:c:105:ARG:HH21	1.80	0.46
8:A:104:PHE:HB2	8:A:112:MET:HE3	1.98	0.46
8:A:250:GLU:HA	23:P:84:LYS:HE2	1.98	0.46
16:I:137:ASP:OD1	16:I:138:LYS:N	2.49	0.46
19:L:105:ILE:HD12	20:M:126:THR:HG22	1.96	0.46
20:M:77:TYR:CE1	20:M:156:LEU:HB2	2.51	0.46
20:M:307:GLU:OE2	20:M:311:GLN:NE2	2.35	0.46
21:N:256:GLN:HE22	21:N:893:VAL:HG21	1.81	0.46
24:Q:383:ASP:OD1	25:R:263:ARG:NH1	2.38	0.46
25:R:34:THR:HG22	25:R:35:GLN:HG2	1.98	0.46
25:R:396:LYS:O	25:R:399:GLN:HG2	2.16	0.46
26:S:435:LYS:HD3	27:T:198:ASP:HB2	1.98	0.46
2:2:126:TYR:HB3	2:2:156:LEU:HD13	1.98	0.46
5:5:253:TYR:HE1	5:5:262:TYR:HD1	1.63	0.46
6:6:221:LEU:HB3	6:6:236:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:114:ALA:HA	7:7:118:GLU:O	2.15	0.46
7:7:120:LEU:HB3	7:7:125:ILE:HD11	1.98	0.46
7:a:120:LEU:HB3	7:a:125:ILE:HD11	1.98	0.46
16:I:220:ILE:HD12	16:I:347:LYS:HG2	1.97	0.46
17:J:379:GLN:HA	17:J:382:PHE:HD2	1.81	0.46
21:N:182:ASN:ND2	21:N:185:ILE:HD12	2.31	0.46
21:N:475:ALA:HB1	29:V:60:ASP:HB2	1.98	0.46
28:U:14:VAL:HG13	28:U:51:SER:HB3	1.98	0.46
29:V:126:GLN:HB2	29:V:156:PHE:HE1	1.81	0.46
2:2:42:VAL:HG13	2:2:206:VAL:HG22	1.98	0.46
2:i:129:VAL:N	2:i:140:PHE:O	2.46	0.46
11:n:106:VAL:HG13	11:n:135:ILE:HG22	1.97	0.46
16:I:181:TYR:HB3	16:I:191:ILE:HD13	1.97	0.46
18:K:67:TYR:CE1	21:N:572:LEU:HB3	2.51	0.46
19:L:225:GLY:HA3	20:M:336:ALA:HA	1.99	0.46
33:Z:571:GLY:HA2	33:Z:574:TYR:HE2	1.81	0.46
2:i:48:ARG:HH21	2:i:55:VAL:HG21	1.80	0.45
2:i:212:ASP:OD1	2:i:213:ALA:N	2.49	0.45
13:F:77:LEU:HD23	20:M:433:TYR:HB3	1.97	0.45
8:c:77:ARG:HG3	8:c:78:THR:HG23	1.98	0.45
10:d:144:TYR:HB2	10:d:147:GLN:HE21	1.81	0.45
14:k:95:GLU:HB3	14:k:115:ARG:HD3	1.98	0.45
17:J:389:VAL:HA	17:J:392:LYS:HE3	1.98	0.45
18:K:124:SER:O	29:V:278:LYS:NZ	2.30	0.45
20:M:283:LEU:HB2	20:M:325:ALA:HB1	1.98	0.45
22:O:292:CYS:O	22:O:295:THR:OG1	2.30	0.45
24:Q:94:VAL:HG11	24:Q:133:LEU:HD12	1.98	0.45
29:V:122:ASP:OD1	29:V:125:THR:OG1	2.22	0.45
29:V:135:ARG:HA	29:V:157:ARG:HH21	1.80	0.45
3:h:12:VAL:HG22	3:h:25:CYS:HB3	1.98	0.45
3:h:30:GLY:HA2	3:h:36:VAL:HG23	1.98	0.45
5:f:108:LYS:HA	5:f:120:MET:HE2	1.98	0.45
19:L:297:ALA:O	20:M:299:ARG:NH1	2.48	0.45
24:Q:48:ASP:HA	24:Q:51:ARG:NH1	2.31	0.45
27:T:201:PRO:HA	27:T:232:LYS:HA	1.98	0.45
33:Z:272:TYR:O	33:Z:276:ASN:N	2.49	0.45
5:5:116:LEU:HD21	5:5:151:VAL:HG22	1.97	0.45
4:g:101:ASN:HB3	4:g:133:HIS:CG	2.51	0.45
14:G:70:VAL:HB	14:G:74:ILE:HB	1.98	0.45
18:K:91:SER:C	18:K:93:PRO:CD	2.90	0.45
19:L:219:LEU:HB2	19:L:343:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:259:GLY:N	20:M:300:GLU:OE2	2.49	0.45
21:N:413:ALA:HA	21:N:453:ALA:HA	1.97	0.45
21:N:713:VAL:HG12	21:N:755:PRO:HA	1.99	0.45
25:R:347:THR:HA	25:R:389:GLU:HA	1.97	0.45
7:7:227:ASN:HB3	7:7:244:ASN:HA	1.99	0.45
4:g:101:ASN:HB3	4:g:133:HIS:CD2	2.52	0.45
6:e:76:PHE:HE2	6:e:78:ALA:HB3	1.81	0.45
10:C:2:GLY:HA3	13:F:123:TYR:CZ	2.51	0.45
8:c:86:PRO:HB2	8:c:88:PRO:HD2	1.98	0.45
16:I:123:PRO:HG3	17:J:92:GLY:HA3	1.98	0.45
17:J:26:LYS:HZ3	21:N:107:GLU:HB3	1.80	0.45
18:K:322:ASP:CG	18:K:323:THR:H	2.24	0.45
20:M:62:ILE:HA	20:M:65:ASN:HB2	1.97	0.45
24:Q:38:SER:OG	24:Q:39:SER:N	2.48	0.45
6:6:225:ILE:HD12	6:6:232:ARG:HH21	1.81	0.45
2:i:48:ARG:NH1	2:i:198:SER:O	2.50	0.45
4:g:70:ARG:HA	11:n:90:ARG:NH1	2.32	0.45
7:a:53:VAL:HG21	7:a:150:ALA:HB1	1.98	0.45
9:B:186:GLU:HA	9:B:189:ILE:HD12	1.98	0.45
16:I:122:SER:HB2	16:I:123:PRO:HD2	1.99	0.45
16:I:174:ASP:HB3	16:I:244:PHE:HB3	1.99	0.45
18:K:164:ASN:HB3	18:K:234:PHE:HB3	1.98	0.45
20:M:157:ASP:OD1	20:M:158:THR:N	2.49	0.45
23:P:270:LEU:O	23:P:344:ARG:NE	2.42	0.45
27:T:108:LEU:HB3	27:T:177:PHE:HE2	1.82	0.45
31:X:113:GLU:HB2	31:X:118:ASP:OD1	2.16	0.45
33:Z:152:GLU:O	33:Z:156:HIS:N	2.50	0.45
4:4:38:LEU:HD22	4:4:64:ILE:HB	1.98	0.45
3:h:178:ASP:OD1	3:h:179:ALA:N	2.49	0.45
10:d:5:ARG:HD3	14:k:10:LEU:HD13	1.99	0.45
15:H:176:VAL:HG12	15:H:188:PRO:HA	1.99	0.45
15:H:190:ARG:HH21	15:H:331:ARG:HH12	1.65	0.45
33:Z:770:GLU:OE2	33:Z:773:ARG:NH1	2.49	0.45
6:e:62:VAL:HG22	6:e:72:SER:HB2	1.98	0.45
9:B:82:TYR:HB2	9:B:132:VAL:HG21	1.98	0.45
13:l:12:THR:HA	14:k:23:GLN:HE22	1.81	0.45
13:l:217:GLY:N	13:l:220:THR:O	2.43	0.45
18:K:394:ALA:O	18:K:399:ARG:N	2.50	0.45
25:R:279:LEU:HG	25:R:286:LEU:HD11	1.97	0.45
25:R:319:CYS:HB2	25:R:322:LEU:HB2	1.98	0.45
25:R:373:PRO:HB3	26:S:394:ILE:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:238:ASP:OD1	33:Z:239:GLU:N	2.48	0.45
33:Z:394:TYR:CE2	33:Z:396:ASN:HB2	2.51	0.45
3:h:45:HIS:O	3:h:45:HIS:ND1	2.50	0.45
5:f:191:ASP:OD1	5:f:195:THR:N	2.48	0.45
12:E:52:LYS:HZ2	12:E:61:SER:HB2	1.82	0.45
8:c:174:LYS:HD3	8:c:177:GLU:HG3	1.98	0.45
16:I:401:LEU:HD21	17:J:312:ARG:HE	1.82	0.45
21:N:405:LEU:HD13	21:N:446:ALA:HB2	1.97	0.45
23:P:137:ALA:HB2	23:P:167:THR:HG21	1.99	0.45
33:Z:827:LEU:HD23	33:Z:831:LEU:HB2	1.98	0.45
2:2:57:ASP:OD1	2:2:58:LYS:N	2.50	0.45
5:5:82:ARG:HH11	5:5:186:THR:HA	1.82	0.45
6:6:35:ALA:HB2	6:6:141:VAL:HG23	1.98	0.45
6:6:83:LEU:HD11	6:6:116:LEU:HD21	1.98	0.45
10:d:194:LEU:HD12	10:d:242:THR:HG21	1.99	0.45
19:L:351:LEU:HD22	19:L:385:GLY:HA3	1.99	0.45
21:N:510:HIS:CE1	21:N:512:ASN:HB2	2.52	0.45
23:P:254:GLU:HA	23:P:257:TRP:HB3	1.98	0.45
26:S:230:LYS:HD3	26:S:261:HIS:HE1	1.82	0.45
28:U:57:GLU:HG2	30:W:96:LEU:HD22	1.98	0.45
1:1:139:HIS:CE1	7:7:72:VAL:HG22	2.52	0.45
2:i:104:ARG:NH2	8:c:149:GLU:OE2	2.50	0.45
3:h:80:ARG:HH12	3:h:83:GLU:HG2	1.81	0.45
8:A:192:ASP:OD1	8:A:193:HIS:N	2.50	0.45
13:F:50:LYS:HE2	13:F:61:LYS:HA	1.99	0.45
8:c:52:VAL:HG22	8:c:227:VAL:HG22	1.99	0.45
15:H:385:ARG:HA	15:H:388:ILE:HD12	1.99	0.45
17:J:124:LYS:HE3	17:J:126:LEU:HD21	1.99	0.45
21:N:711:ARG:HH11	21:N:784:TYR:HB2	1.82	0.45
25:R:380:VAL:N	25:R:389:GLU:O	2.43	0.45
3:3:41:GLU:OE2	3:3:188:TYR:OH	2.30	0.44
2:i:132:VAL:HG22	2:i:137:SER:HB3	1.98	0.44
11:D:32:CYS:HA	11:D:165:GLY:HA3	1.99	0.44
9:j:8:SER:OG	9:j:122:THR:O	2.23	0.44
14:k:103:TYR:C	14:k:105:THR:H	2.25	0.44
21:N:510:HIS:HE1	21:N:512:ASN:HB2	1.82	0.44
21:N:528:ARG:HB3	21:N:531:LEU:HB2	1.99	0.44
33:Z:282:ILE:HG21	33:Z:975:SER:HB2	1.98	0.44
5:5:100:TRP:CD1	3:h:145:GLN:HE21	2.25	0.44
7:7:162:TYR:HB2	7:7:175:LEU:HD13	1.99	0.44
20:M:82:VAL:HG23	20:M:146:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:277:ILE:HG23	20:M:322:LYS:HB2	1.99	0.44
24:Q:85:MET:HG3	24:Q:126:LYS:HE2	1.99	0.44
27:T:206:LYS:HG3	27:T:211:PHE:HB2	1.99	0.44
29:V:51:GLY:HA3	29:V:108:TYR:CZ	2.52	0.44
33:Z:328:ASP:O	33:Z:332:ASN:ND2	2.50	0.44
4:4:110:LYS:NZ	10:C:142:ASP:OD2	2.43	0.44
14:G:70:VAL:HG21	14:G:112:PHE:CZ	2.53	0.44
13:l:95:SER:O	13:l:101:ARG:N	2.35	0.44
17:J:357:ASP:OD1	18:K:330:ARG:HG3	2.17	0.44
18:K:243:VAL:HG21	19:L:303:ARG:HD2	2.00	0.44
21:N:349:ILE:HA	21:N:356:LEU:HD11	1.98	0.44
24:Q:369:ASP:OD1	24:Q:370:THR:N	2.50	0.44
29:V:197:TYR:CE2	29:V:199:LEU:HB3	2.49	0.44
33:Z:624:LEU:HB3	33:Z:764:LEU:HD11	1.99	0.44
2:2:94:LEU:HD21	9:B:94:HIS:CE1	2.52	0.44
2:i:228:LYS:HG2	2:i:230:LYS:H	1.82	0.44
7:a:72:VAL:HG11	7:a:90:ILE:HD13	1.99	0.44
8:A:85:GLY:HA3	8:A:139:VAL:HG12	1.99	0.44
11:D:4:TYR:OH	11:D:6:ARG:NE	2.47	0.44
13:F:14:SER:OG	13:F:18:ARG:O	2.33	0.44
11:n:89:ALA:HB1	11:n:109:LEU:HD11	2.00	0.44
18:K:90:GLN:HA	18:K:94:LEU:HD21	1.99	0.44
18:K:212:TYR:HD2	18:K:339:GLU:HG3	1.81	0.44
21:N:75:TYR:HB2	21:N:104:LYS:HE2	1.98	0.44
23:P:28:ALA:C	23:P:30:ASN:H	2.25	0.44
25:R:211:LYS:HG2	25:R:230:LEU:HD13	1.99	0.44
29:V:40:HIS:CG	29:V:70:ALA:HB2	2.53	0.44
1:1:213:GLU:OE1	7:a:226:ARG:NH1	2.49	0.44
1:b:192:ILE:HG22	1:b:194:MET:HG3	1.99	0.44
14:G:73:HIS:CD2	14:G:74:ILE:HG13	2.52	0.44
17:J:182:PRO:O	17:J:289:LYS:NZ	2.50	0.44
17:J:366:GLY:HA3	18:K:203:ILE:HD13	1.99	0.44
21:N:340:HIS:HB2	21:N:374:ILE:HG12	1.99	0.44
25:R:280:ILE:HB	25:R:289:ILE:HD11	1.98	0.44
26:S:176:LEU:C	26:S:178:LEU:H	2.25	0.44
26:S:427:ILE:HD11	26:S:434:ALA:HB3	1.99	0.44
27:T:93:ASN:CG	27:T:94:HIS:H	2.25	0.44
4:4:99:GLN:HG3	4:4:121:TYR:HB2	1.99	0.44
8:A:196:GLU:HG2	8:A:201:LYS:HB2	1.99	0.44
8:c:141:LEU:HB2	8:c:157:THR:HB	1.99	0.44
15:H:99:VAL:HG12	15:H:173:ARG:HH22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:188:TYR:HB2	17:J:315:GLU:HA	1.99	0.44
21:N:923:MET:HE1	31:X:55:LYS:HB3	2.00	0.44
29:V:180:LEU:CD2	29:V:181:ASN:H	2.20	0.44
31:X:56:PRO:HB2	31:X:59:ARG:HB2	1.99	0.44
33:Z:790:MET:HE1	33:Z:829:GLN:HG2	2.00	0.44
2:2:67:SER:HB2	2:2:68:PRO:HD2	2.00	0.44
3:3:185:ALA:O	3:3:200:LEU:N	2.50	0.44
3:h:89:GLN:HG2	9:j:102:GLY:HA3	2.00	0.44
6:e:214:HIS:NE2	6:e:216:GLN:HB2	2.32	0.44
13:F:89:ARG:O	13:F:93:ASN:ND2	2.48	0.44
13:F:110:HIS:HE1	14:G:90:ASN:HD21	1.66	0.44
11:n:181:ARG:HH22	12:m:60:GLU:HA	1.82	0.44
15:H:273:ARG:HG3	15:H:307:PHE:HD2	1.82	0.44
16:I:167:MET:HB3	16:I:262:ARG:HH12	1.82	0.44
17:J:146:THR:HG23	17:J:149:MET:H	1.82	0.44
20:M:201:MET:HE1	20:M:320:ARG:HG2	1.99	0.44
21:N:504:TYR:HD2	21:N:517:LEU:HD11	1.82	0.44
23:P:353:ILE:HG23	23:P:357:TYR:HB2	1.98	0.44
28:U:12:PRO:HD2	28:U:163:ALA:HB2	2.00	0.44
30:W:166:GLU:HA	30:W:170:HIS:CE1	2.53	0.44
4:4:172:MET:HG2	4:4:174:MET:H	1.81	0.44
9:B:160:LYS:HD3	9:B:179:TRP:CZ2	2.53	0.44
10:C:18:ARG:HG2	16:I:435:LEU:HD21	1.99	0.44
16:I:96:LEU:O	16:I:100:ARG:HG2	2.18	0.44
20:M:370:THR:HG22	20:M:410:VAL:HB	2.00	0.44
21:N:28:ILE:O	21:N:32:VAL:HG23	2.17	0.44
25:R:43:ARG:HH11	25:R:88:LEU:HD22	1.83	0.44
26:S:234:ILE:HG13	26:S:257:LEU:HD13	1.99	0.44
2:2:139:LEU:HG	2:2:154:LEU:HD12	2.00	0.44
3:3:155:GLU:HB3	3:3:158:LEU:HD11	1.99	0.44
6:e:106:ASN:OD1	6:e:142:TYR:OH	2.33	0.44
10:d:79:GLY:HA3	10:d:133:VAL:HG13	2.00	0.44
11:n:34:VAL:O	11:n:45:GLY:N	2.51	0.44
13:l:187:ASP:OD1	13:l:188:GLU:N	2.50	0.44
15:H:367:ARG:NH1	20:M:171:GLU:OE1	2.42	0.44
16:I:387:LEU:HD13	16:I:391:ASP:HB3	2.00	0.44
29:V:50:MET:HA	29:V:109:HIS:HA	2.00	0.44
29:V:188:LEU:HD12	29:V:189:ILE:H	1.82	0.44
29:V:192:LEU:HD13	29:V:196:TYR:HB2	2.00	0.44
30:W:54:GLY:HA3	30:W:90:ALA:HB2	2.00	0.44
33:Z:135:LEU:HD23	33:Z:157:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:111:ASN:O	2:2:120:GLN:NE2	2.51	0.43
2:2:195:ASP:OD1	2:2:196:LEU:N	2.50	0.43
6:6:110:ARG:HG3	12:E:104:ASP:HB2	1.99	0.43
17:J:100:LYS:HD3	21:N:690:HIS:CE1	2.52	0.43
18:K:247:LEU:HD22	18:K:294:ARG:NE	2.33	0.43
19:L:112:LEU:HB2	19:L:118:ILE:HG13	1.99	0.43
19:L:200:PRO:HB3	19:L:207:PHE:HE2	1.83	0.43
28:U:35:GLY:HA3	28:U:93:TYR:CZ	2.53	0.43
1:1:171:VAL:HA	1:1:194:MET:HE1	1.99	0.43
7:7:61:GLY:N	7:7:69:PHE:O	2.51	0.43
4:g:81:SER:HB2	4:g:119:ILE:HD11	1.99	0.43
5:f:265:ASN:OD1	5:f:266:HIS:N	2.51	0.43
7:a:35:GLN:O	7:a:144:TRP:NE1	2.46	0.43
14:G:48:PHE:HE1	14:G:137:ILE:HG22	1.83	0.43
13:l:74:LEU:HD22	13:l:81:ALA:HB3	2.01	0.43
19:L:259:SER:HB2	19:L:303:ARG:HE	1.83	0.43
21:N:55:PHE:CZ	21:N:57:ASP:HB2	2.53	0.43
21:N:603:PRO:HG3	21:N:634:LEU:HD21	2.00	0.43
21:N:875:LEU:HG	21:N:877:GLN:H	1.82	0.43
25:R:225:LYS:HB2	25:R:260:THR:HG23	2.00	0.43
7:7:234:ASP:OD2	7:7:237:THR:N	2.42	0.43
1:b:20:THR:N	1:b:148:SER:OG	2.51	0.43
2:i:252:ILE:HG21	10:d:228:LYS:HD3	1.99	0.43
10:C:206:LEU:HD21	10:C:211:LEU:HD13	2.00	0.43
14:G:231:VAL:HG12	14:G:236:LEU:HB2	1.99	0.43
9:j:36:GLY:HA2	9:j:45:ILE:HA	2.00	0.43
25:R:34:THR:HG23	25:R:70:TYR:CG	2.54	0.43
30:W:123:ASP:HA	30:W:126:ILE:HD12	1.99	0.43
5:5:182:LYS:HB3	11:D:141:ARG:HH11	1.84	0.43
6:6:134:ASP:OD1	6:6:138:LYS:N	2.38	0.43
10:d:124:GLN:NE2	11:n:127:ARG:O	2.50	0.43
17:J:316:PHE:CD1	17:J:317:PRO:HD2	2.53	0.43
24:Q:391:ASP:HB3	24:Q:396:TRP:H	1.83	0.43
25:R:204:TRP:HH2	25:R:235:LEU:H	1.64	0.43
26:S:352:VAL:HG13	26:S:387:VAL:HA	2.00	0.43
1:b:160:ASN:HB3	1:b:173:PHE:HE1	1.84	0.43
2:i:128:ILE:HA	2:i:141:SER:HA	2.00	0.43
3:h:65:GLU:HB3	10:d:100:LYS:HG3	1.99	0.43
5:f:154:ALA:HA	5:f:157:ILE:HD12	2.00	0.43
12:E:20:ARG:NE	12:E:25:GLU:OE2	2.40	0.43
9:j:44:VAL:HG22	9:j:213:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:243:THR:H	16:I:277:SER:HA	1.84	0.43
16:I:314:ASP:OD1	16:I:343:ARG:NE	2.52	0.43
19:L:298:ASP:HA	20:M:299:ARG:HH12	1.83	0.43
23:P:213:TYR:HD2	23:P:216:LEU:H	1.66	0.43
23:P:431:HIS:HD2	28:U:156:HIS:HB2	1.83	0.43
24:Q:311:LEU:HD12	24:Q:366:ILE:HG23	2.01	0.43
26:S:384:ARG:HD2	27:T:150:ARG:HD2	2.01	0.43
33:Z:309:GLN:OE1	33:Z:982:ILE:N	2.50	0.43
5:5:201:ILE:HD11	5:5:215:LEU:HD13	2.01	0.43
3:h:124:PHE:HA	3:h:129:CYS:O	2.19	0.43
10:C:50:ARG:O	10:C:210:ARG:NE	2.43	0.43
12:m:68:VAL:HB	12:m:93:ARG:NH2	2.33	0.43
17:J:75:VAL:HG11	17:J:107:LEU:HB3	2.00	0.43
17:J:134:VAL:HG13	17:J:138:MET:HB2	2.00	0.43
17:J:191:PRO:HA	17:J:254:GLY:HA3	2.01	0.43
18:K:91:SER:OG	18:K:93:PRO:HD2	2.19	0.43
19:L:254:LYS:NZ	19:L:300:GLU:OE2	2.35	0.43
21:N:223:LEU:HD11	21:N:897:LYS:HE2	2.01	0.43
23:P:346:ILE:HD13	23:P:371:LEU:HD11	1.99	0.43
3:3:51:LEU:HD22	3:3:87:PHE:HZ	1.84	0.43
5:5:79:LEU:HD13	5:5:215:LEU:HD11	2.01	0.43
10:C:18:ARG:NH1	16:I:432:LEU:HD11	2.34	0.43
10:d:175:LEU:HD12	10:d:196:THR:HG23	1.99	0.43
19:L:327:THR:HG21	19:L:333:LEU:HD11	2.01	0.43
21:N:380:LEU:HD23	21:N:924:LYS:HE2	2.01	0.43
23:P:224:LEU:HD13	23:P:240:TYR:CG	2.54	0.43
25:R:140:TYR:O	25:R:144:ILE:HG12	2.19	0.43
25:R:291:SER:HB3	25:R:307:TYR:CG	2.54	0.43
33:Z:617:ILE:HG23	33:Z:618:GLN:H	1.84	0.43
3:3:121:ILE:HD12	3:3:137:ILE:HG12	2.00	0.43
3:3:183:TRP:HE1	3:3:205:ASP:C	2.23	0.43
5:5:120:MET:HG2	5:5:127:CYS:HB3	2.01	0.43
4:g:149:ARG:HB2	4:g:152:MET:HG3	2.01	0.43
7:a:179:PHE:HZ	7:a:220:ARG:HB2	1.81	0.43
12:E:237:ALA:HA	12:E:240:ILE:HD12	2.01	0.43
16:I:104:LEU:HD13	16:I:148:LEU:HD23	2.00	0.43
16:I:110:GLU:HB3	16:I:119:ILE:HB	2.01	0.43
18:K:159:SER:HB2	18:K:253:MET:HG3	2.00	0.43
18:K:217:THR:HG22	18:K:381:ALA:HB3	2.00	0.43
19:L:175:GLN:HG2	19:L:240:GLY:HA2	2.00	0.43
19:L:197:ILE:HG12	19:L:322:LYS:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:72:VAL:HG12	25:R:72:VAL:O	2.19	0.43
33:Z:228:GLU:HA	33:Z:264:PHE:HZ	1.84	0.43
7:7:80:ASP:OD1	7:7:81:ASN:N	2.51	0.43
4:g:8:ARG:N	4:g:129:PRO:O	2.49	0.43
11:D:138:PHE:HE1	11:D:145:PRO:HB3	1.84	0.43
16:I:120:VAL:HB	16:I:149:LEU:HD11	1.99	0.43
16:I:336:PRO:HA	16:I:339:ILE:HD12	2.00	0.43
18:K:355:THR:O	18:K:358:SER:OG	2.31	0.43
20:M:236:ALA:HB2	20:M:277:ILE:HD12	2.00	0.43
25:R:301:TYR:HE2	25:R:341:LEU:HD22	1.84	0.43
29:V:216:LEU:HG	29:V:221:TRP:HH2	1.84	0.43
30:W:152:GLU:HG3	30:W:154:LEU:H	1.84	0.43
33:Z:263:ALA:HA	33:Z:266:LYS:HD3	2.00	0.43
4:g:51:GLY:HA3	5:f:193:ASP:HB3	2.01	0.43
5:f:94:ARG:HB3	5:f:246:SER:O	2.19	0.43
8:A:156:LYS:HB3	8:A:166:TYR:CE2	2.54	0.43
9:B:140:ASP:OD1	9:B:141:GLU:N	2.51	0.43
14:G:103:TYR:C	14:G:105:THR:H	2.27	0.43
12:m:31:ILE:HD13	12:m:141:ALA:HB2	2.00	0.43
15:H:214:CYS:HB3	15:H:217:GLN:OE1	2.19	0.43
17:J:374:ARG:HH12	17:J:378:THR:HG23	1.83	0.43
23:P:429:ILE:HD11	28:U:203:LYS:HD2	1.99	0.43
25:R:262:GLU:O	25:R:266:LEU:HG	2.18	0.43
29:V:51:GLY:N	29:V:108:TYR:O	2.52	0.43
1:b:28:LYS:HB2	1:b:164:ASN:HB3	2.01	0.42
6:e:47:ARG:NH1	6:e:241:ASP:H	2.17	0.42
15:H:321:ASP:HB3	15:H:330:GLN:HE21	1.84	0.42
21:N:366:THR:HG23	21:N:747:HIS:CE1	2.54	0.42
23:P:213:TYR:HE2	23:P:215:SER:HB3	1.84	0.42
24:Q:387:TYR:CE2	24:Q:402:THR:HG23	2.54	0.42
26:S:435:LYS:N	26:S:444:GLU:O	2.39	0.42
33:Z:804:ASP:OD1	33:Z:805:LEU:N	2.52	0.42
8:A:43:LEU:HD11	8:A:206:ALA:HB1	2.01	0.42
11:D:41:CYS:HB2	11:D:188:VAL:HG12	2.01	0.42
9:j:148:TYR:CE1	9:j:158:PRO:HB3	2.54	0.42
11:n:139:ASP:HB2	11:n:142:ASP:HB3	2.01	0.42
17:J:185:VAL:HG12	17:J:291:ILE:HD12	2.01	0.42
21:N:293:LEU:HB2	21:N:294:PRO:HD3	2.01	0.42
24:Q:65:TYR:O	24:Q:70:ALA:N	2.49	0.42
24:Q:121:SER:HA	24:Q:124:PHE:HD2	1.84	0.42
25:R:61:PRO:HG3	25:R:142:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:T:164:LEU:HB3	27:T:178:THR:HG23	2.01	0.42
30:W:35:PHE:HZ	30:W:186:ALA:HB2	1.84	0.42
1:1:60:ILE:HA	1:1:120:GLY:HA2	2.01	0.42
7:a:162:TYR:CE2	7:a:164:ASN:HB3	2.53	0.42
8:A:165:GLY:H	9:B:60:THR:HB	1.84	0.42
12:m:165:TYR:CE1	13:l:60:GLN:HB2	2.55	0.42
13:l:105:VAL:HG13	13:l:134:ILE:HG22	2.02	0.42
16:I:306:MET:HG3	16:I:338:LEU:HD22	2.02	0.42
19:L:288:GLY:HA2	19:L:332:THR:O	2.19	0.42
21:N:668:THR:HG22	21:N:675:VAL:HG11	2.01	0.42
21:N:884:PHE:HZ	21:N:890:PHE:HB2	1.84	0.42
22:O:62:TYR:HA	22:O:65:PHE:CD2	2.54	0.42
3:h:27:LEU:HB2	3:h:183:TRP:O	2.18	0.42
8:A:69:VAL:HG22	14:G:158:TRP:CD1	2.55	0.42
12:E:15:PHE:CE2	13:F:126:ARG:HB2	2.55	0.42
13:F:67:ASP:HB3	13:F:70:MET:HB3	2.00	0.42
11:n:31:THR:O	11:n:76:SER:OG	2.35	0.42
14:k:91:ARG:HH22	14:k:123:HIS:CE1	2.37	0.42
18:K:92:VAL:HG12	18:K:92:VAL:O	2.18	0.42
21:N:912:GLU:O	21:N:914:VAL:N	2.49	0.42
23:P:136:ARG:HE	23:P:163:LEU:HD22	1.85	0.42
25:R:311:THR:O	25:R:315:VAL:HB	2.19	0.42
29:V:275:ASP:HB3	29:V:276:PRO:HD3	2.01	0.42
1:b:110:ASP:OD1	1:b:111:ASN:N	2.52	0.42
10:d:157:TYR:HE1	11:n:83:ARG:HH22	1.68	0.42
13:l:50:LYS:HB3	13:l:59:TYR:HB3	2.01	0.42
18:K:91:SER:CB	18:K:93:PRO:CD	2.98	0.42
21:N:9:LEU:HD21	27:T:41:ILE:HD13	2.01	0.42
21:N:375:HIS:CD2	21:N:385:VAL:HG21	2.54	0.42
25:R:353:MET:HA	25:R:357:PHE:CD2	2.54	0.42
27:T:229:VAL:HG23	27:T:232:LYS:HB2	2.01	0.42
5:5:170:LEU:HD23	6:6:120:ARG:HH21	1.84	0.42
7:7:126:PHE:CZ	7:7:163:VAL:HB	2.55	0.42
5:f:253:TYR:HE1	5:f:262:TYR:HD1	1.68	0.42
17:J:195:LYS:HE3	17:J:253:ILE:HB	2.02	0.42
18:K:391:GLY:HA3	19:L:212:ILE:HG21	2.01	0.42
21:N:681:ASN:HA	21:N:684:SER:HB2	2.01	0.42
25:R:31:PHE:HZ	25:R:323:ASN:HD22	1.67	0.42
1:1:103:GLU:HG3	14:G:102:LEU:HD23	2.01	0.42
3:3:176:ASP:O	3:3:203:ARG:NH2	2.53	0.42
3:h:18:LYS:HB2	3:h:157:ASN:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:59:ASN:OD1	7:a:73:GLU:HA	2.20	0.42
10:C:194:LEU:HD12	10:C:242:THR:HG21	2.02	0.42
10:C:216:ILE:HG12	10:C:227:GLN:HG2	2.02	0.42
8:c:17:THR:OG1	8:c:129:THR:O	2.30	0.42
10:d:45:VAL:HG21	10:d:189:ALA:HB3	2.01	0.42
16:I:169:SER:HB3	16:I:251:GLU:HB3	2.00	0.42
19:L:352:PRO:HD2	19:L:385:GLY:HA2	2.00	0.42
30:W:191:ILE:HG22	30:W:192:LEU:HG	2.00	0.42
2:i:75:ALA:H	2:i:81:THR:HG21	1.85	0.42
8:A:156:LYS:HB3	8:A:166:TYR:HE2	1.83	0.42
11:D:41:CYS:SG	11:D:42:VAL:N	2.93	0.42
11:D:206:GLY:HA2	11:D:209:ASN:HB2	2.02	0.42
13:F:157:TYR:CE2	14:G:60:VAL:HG22	2.55	0.42
15:H:156:VAL:HB	15:H:182:ASN:ND2	2.35	0.42
19:L:215:PRO:O	19:L:322:LYS:NZ	2.47	0.42
22:O:377:VAL:HG21	28:U:197:LEU:HD22	2.02	0.42
24:Q:358:GLU:HG2	24:Q:360:SER:H	1.85	0.42
26:S:145:PHE:CE1	26:S:186:TYR:HB2	2.53	0.42
26:S:283:GLN:HA	27:T:120:THR:HG23	2.02	0.42
1:l:103:GLU:OE2	7:7:98:ARG:NH1	2.51	0.42
5:5:87:ILE:HD11	5:5:185:PRO:HB2	2.01	0.42
7:7:215:ARG:HH12	7:7:249:ASN:HD22	1.68	0.42
3:h:35:GLY:HA3	3:h:183:TRP:HH2	1.84	0.42
10:C:84:ALA:HB2	10:C:133:VAL:HG11	2.02	0.42
12:E:72:ARG:O	12:E:228:PHE:N	2.49	0.42
9:j:148:TYR:HE1	9:j:158:PRO:HB3	1.84	0.42
14:k:36:THR:HA	14:k:166:GLY:HA3	2.02	0.42
21:N:371:LEU:HD23	21:N:374:ILE:HD12	2.01	0.42
22:O:42:SER:HB3	22:O:47:LYS:HB2	2.02	0.42
25:R:416:LYS:HA	26:S:298:ARG:HD3	2.01	0.42
33:Z:444:GLU:HG2	33:Z:446:GLU:H	1.85	0.42
2:i:143:HIS:NE2	2:i:149:ASP:OD2	2.47	0.42
7:a:164:ASN:HD21	7:a:168:VAL:HB	1.85	0.42
13:F:50:LYS:HG2	13:F:62:LYS:HG2	2.02	0.42
11:n:216:LYS:HB2	11:n:220:ASP:HB3	2.01	0.42
15:H:176:VAL:HG13	15:H:177:ASP:H	1.84	0.42
17:J:126:LEU:HD13	18:K:109:ILE:HD11	2.02	0.42
17:J:159:GLU:HB3	17:J:314:ILE:HG12	2.01	0.42
18:K:415:VAL:HG13	18:K:416:LYS:HG3	2.01	0.42
20:M:216:LYS:HB2	20:M:341:GLY:HA2	2.02	0.42
21:N:510:HIS:HB3	21:N:513:ILE:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:292:LEU:HD13	25:R:333:MET:HE1	2.02	0.42
8:c:208:THR:HG23	8:c:251:GLN:HE22	1.85	0.41
14:k:54:ILE:HG12	14:k:59:LEU:HD22	2.01	0.41
18:K:238:ASN:OD1	18:K:239:GLY:N	2.53	0.41
20:M:147:GLY:HA3	20:M:157:ASP:O	2.20	0.41
21:N:743:PHE:HB3	21:N:744:PRO:HD2	2.01	0.41
25:R:154:LEU:HD11	25:R:170:VAL:HG13	2.01	0.41
28:U:83:ILE:HG22	28:U:84:ASN:ND2	2.35	0.41
2:i:126:TYR:HB3	2:i:156:LEU:HD13	2.02	0.41
7:a:49:TYR:CE1	7:a:54:ILE:HG13	2.55	0.41
9:j:4:ARG:CZ	13:l:123:TYR:HB3	2.50	0.41
9:j:38:LYS:HE3	9:j:160:LYS:HA	2.01	0.41
11:n:37:LYS:HD3	11:n:160:SER:HA	2.02	0.41
14:k:68:GLN:OE1	14:k:93:ARG:NH2	2.52	0.41
17:J:214:SER:OG	17:J:249:GLU:OE2	2.28	0.41
27:T:94:HIS:NE2	27:T:130:ASP:OD2	2.52	0.41
28:U:54:LEU:HD13	28:U:68:LEU:HD11	2.01	0.41
28:U:275:VAL:HA	28:U:278:ILE:HD12	2.01	0.41
30:W:111:VAL:HA	30:W:140:ASP:HB2	2.02	0.41
33:Z:813:PHE:HE2	33:Z:888:LEU:HD11	1.84	0.41
33:Z:972:SER:OG	33:Z:982:ILE:O	2.32	0.41
3:3:53:ILE:HG22	3:3:60:VAL:HG22	2.02	0.41
7:7:60:LEU:HD21	7:7:67:LEU:HD22	2.02	0.41
4:g:86:GLN:HG3	10:d:101:THR:HG23	2.01	0.41
5:f:126:ASP:HB3	5:f:172:MET:HB3	2.01	0.41
5:f:144:ARG:HA	12:m:93:ARG:NH1	2.34	0.41
9:j:77:GLY:HA3	9:j:132:VAL:HG23	2.02	0.41
9:j:107:THR:HG22	9:j:148:TYR:CE2	2.56	0.41
15:H:224:VAL:HG23	15:H:225:VAL:HG23	2.02	0.41
15:H:330:GLN:HE21	20:M:169:ALA:HB2	1.86	0.41
21:N:21:LYS:HA	21:N:24:ALA:HB3	2.03	0.41
3:h:8:ASN:ND2	3:h:30:GLY:O	2.37	0.41
4:g:104:ILE:HD12	4:g:119:ILE:HD12	2.02	0.41
6:e:224:LEU:HG	6:e:233:LYS:HG2	2.01	0.41
18:K:164:ASN:OD1	18:K:165:GLU:N	2.53	0.41
19:L:354:GLU:HG3	19:L:357:ARG:NH2	2.35	0.41
21:N:171:LYS:HB2	21:N:213:PHE:HE1	1.85	0.41
33:Z:395:CYS:HA	33:Z:425:ILE:HG23	2.02	0.41
1:1:159:LYS:HG2	1:b:156:TYR:CE1	2.55	0.41
2:i:33:VAL:HG12	2:i:155:SER:HB2	2.03	0.41
7:a:50:ASP:OD1	7:a:51:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:141:LEU:O	8:A:157:THR:N	2.53	0.41
8:c:53:VAL:HG21	8:c:82:VAL:HG21	2.03	0.41
15:H:218:ILE:O	15:H:222:ARG:HG3	2.21	0.41
21:N:141:ILE:HG13	21:N:165:ILE:HG21	2.01	0.41
21:N:176:GLN:HG3	21:N:182:ASN:HB2	2.02	0.41
21:N:444:HIS:CE1	21:N:480:ALA:HB2	2.56	0.41
23:P:47:ARG:HD3	23:P:52:LEU:HG	2.03	0.41
30:W:163:ASN:HB2	30:W:164:PRO:HD3	2.02	0.41
2:2:57:ASP:CG	3:3:133:ALA:HB2	2.46	0.41
7:a:107:ASN:ND2	7:a:119:ALA:O	2.54	0.41
8:c:43:LEU:HD21	8:c:210:MET:HB2	2.03	0.41
11:n:73:LEU:HD23	11:n:86:ILE:HG12	2.02	0.41
11:n:129:PHE:HB3	11:n:131:VAL:HG12	2.01	0.41
16:I:198:VAL:HA	16:I:323:LYS:NZ	2.36	0.41
24:Q:161:LEU:HB3	24:Q:165:PHE:CE2	2.54	0.41
25:R:158:LEU:HD13	25:R:170:VAL:HG11	2.02	0.41
25:R:184:GLN:HB3	25:R:217:HIS:CE1	2.56	0.41
29:V:123:VAL:HG13	29:V:124:ASN:N	2.34	0.41
30:W:4:GLU:CD	30:W:109:ARG:HE	2.28	0.41
2:2:104:ARG:NH2	8:A:148:GLU:OE2	2.53	0.41
3:3:65:GLU:OE2	4:4:85:ARG:NH2	2.53	0.41
3:h:183:TRP:HE1	3:h:205:ASP:C	2.29	0.41
5:f:125:ALA:HB2	6:e:149:SER:HB2	2.02	0.41
7:a:251:LYS:HE3	7:a:253:ASP:HB2	2.02	0.41
11:D:31:THR:O	11:D:76:SER:OG	2.25	0.41
13:F:45:VAL:HG11	13:F:190:ILE:HA	2.03	0.41
16:I:119:ILE:HG13	16:I:129:TYR:HD1	1.86	0.41
17:J:216:ALA:O	18:K:294:ARG:NH2	2.54	0.41
23:P:130:ILE:HG23	23:P:132:VAL:H	1.85	0.41
23:P:384:VAL:HG11	24:Q:353:PRO:HA	2.02	0.41
26:S:246:GLU:HG2	26:S:248:ASP:H	1.86	0.41
28:U:27:THR:HG23	28:U:31:LYS:HB2	2.03	0.41
3:3:188:TYR:HE1	3:3:197:LYS:HG3	1.86	0.41
4:4:67:TYR:CE2	4:4:75:LEU:HD21	2.56	0.41
3:h:72:ASN:ND2	10:d:96:GLN:OE1	2.45	0.41
7:a:115:ASP:OD1	7:a:116:ALA:N	2.50	0.41
12:E:170:LYS:HE3	12:E:172:ILE:HG22	2.03	0.41
9:j:43:VAL:HB	9:j:214:ILE:HD13	2.02	0.41
21:N:606:VAL:HB	21:N:621:THR:HB	2.03	0.41
21:N:893:VAL:HG23	21:N:894:ARG:N	2.36	0.41
23:P:141:LYS:HE3	23:P:182:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:U:47:ARG:HH12	28:U:162:GLU:HB2	1.85	0.41
33:Z:394:TYR:HE2	33:Z:396:ASN:HB2	1.85	0.41
2:i:138:HIS:HB3	2:i:140:PHE:CE2	2.56	0.41
3:h:28:ARG:HG3	3:h:183:TRP:CE3	2.56	0.41
6:e:46:THR:HB	6:e:58:TYR:HA	2.03	0.41
7:a:234:ASP:OD2	7:a:237:THR:N	2.42	0.41
8:A:96:ARG:HE	8:A:124:LEU:HD13	1.85	0.41
8:A:204:GLU:HG2	8:A:248:ILE:HB	2.01	0.41
9:B:72:GLY:H	9:B:214:ILE:HD11	1.86	0.41
11:D:75:PHE:HB3	11:D:133:THR:HG22	2.02	0.41
8:c:35:THR:HG21	8:c:140:ILE:HG13	2.02	0.41
11:n:47:GLU:HA	11:n:210:ILE:HA	2.03	0.41
12:m:42:THR:HG22	12:m:191:LEU:HD13	2.02	0.41
15:H:106:ILE:HA	15:H:144:LYS:HE3	2.03	0.41
15:H:170:GLU:HG2	15:H:171:GLY:O	2.21	0.41
17:J:118:ASP:OD1	17:J:119:SER:N	2.47	0.41
17:J:265:ASP:O	17:J:269:GLN:HG3	2.21	0.41
17:J:301:ASP:HB3	17:J:304:LEU:HG	2.02	0.41
19:L:196:VAL:HG23	19:L:197:ILE:HG13	2.03	0.41
19:L:244:ILE:HB	19:L:278:ILE:HG13	2.02	0.41
21:N:324:LYS:HB2	21:N:328:PHE:HB2	2.03	0.41
21:N:870:ASN:OD1	21:N:871:MET:HG3	2.21	0.41
24:Q:350:ILE:HD13	24:Q:362:ILE:HG23	2.03	0.41
25:R:188:LYS:HB2	25:R:213:TYR:HE2	1.86	0.41
26:S:184:TRP:CZ3	26:S:236:LEU:HD22	2.55	0.41
27:T:2:PRO:HA	27:T:10:SER:HB3	2.02	0.41
28:U:163:ALA:HB3	28:U:168:GLU:HG3	2.03	0.41
3:3:12:VAL:HG22	3:3:25:CYS:HB3	2.03	0.41
3:3:48:HIS:CD2	3:3:49:VAL:HG23	2.56	0.41
5:5:119:THR:OG1	5:5:175:MET:N	2.54	0.41
6:6:53:SER:HB2	7:7:182:HIS:CE1	2.56	0.41
3:h:53:ILE:HG22	3:h:60:VAL:HG22	2.03	0.41
4:g:46:PHE:HB2	4:g:53:THR:HB	2.03	0.41
18:K:91:SER:CB	18:K:93:PRO:HD3	2.51	0.41
21:N:710:GLY:O	21:N:712:ASN:ND2	2.53	0.41
25:R:33:LEU:HB3	25:R:74:ASN:ND2	2.35	0.41
26:S:227:ASN:O	26:S:261:HIS:ND1	2.54	0.41
26:S:259:TYR:CD1	26:S:260:PRO:HD2	2.56	0.41
27:T:186:ARG:NH2	27:T:210:PHE:O	2.54	0.41
28:U:108:GLU:HA	28:U:111:LYS:HD2	2.02	0.41
31:X:34:GLU:OE2	31:X:51:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:230:ILE:HG22	33:Z:264:PHE:HD1	1.86	0.41
7:a:95:HIS:HA	7:a:98:ARG:HE	1.87	0.40
10:C:27:GLU:OE2	10:C:31:HIS:NE2	2.53	0.40
10:C:34:THR:O	10:C:49:GLU:N	2.53	0.40
13:F:37:GLY:HA2	13:F:45:VAL:O	2.21	0.40
18:K:281:ARG:NH1	18:K:290:ARG:HA	2.36	0.40
19:L:300:GLU:HB2	20:M:299:ARG:NH2	2.35	0.40
19:L:336:ALA:HA	19:L:339:ARG:CZ	2.51	0.40
21:N:352:ASN:HB3	21:N:355:TRP:CE3	2.55	0.40
21:N:742:TRP:CE2	21:N:743:PHE:HD2	2.39	0.40
24:Q:230:LYS:HA	24:Q:232:TYR:CE2	2.57	0.40
26:S:214:MET:HG3	26:S:233:LEU:HD23	2.03	0.40
26:S:400:LYS:O	26:S:444:GLU:HA	2.20	0.40
1:1:26:THR:HG23	1:1:129:VAL:HG23	2.02	0.40
2:2:34:GLY:HA2	2:2:43:ILE:HA	2.03	0.40
7:a:49:TYR:HE1	7:a:54:ILE:HG13	1.86	0.40
7:a:80:ASP:OD1	7:a:81:ASN:N	2.54	0.40
8:A:87:ILE:N	8:A:88:PRO:HD2	2.35	0.40
10:d:50:ARG:NH2	10:d:62:SER:O	2.47	0.40
11:n:68:ASP:HB3	11:n:71:VAL:HB	2.03	0.40
16:I:190:GLN:NE2	16:I:349:LEU:O	2.53	0.40
18:K:243:VAL:HG23	19:L:257:GLY:HA2	2.03	0.40
4:4:70:ARG:HA	11:D:90:ARG:HH11	1.85	0.40
5:5:189:TYR:CE1	5:5:204:VAL:HG21	2.57	0.40
7:7:60:LEU:HD12	7:7:225:SER:HB3	2.03	0.40
1:b:27:PHE:HE1	1:b:29:ASP:HB2	1.86	0.40
6:e:59:GLU:O	6:e:61:LYS:N	2.54	0.40
8:A:141:LEU:HB2	8:A:157:THR:HB	2.02	0.40
9:B:193:LEU:HD13	9:B:247:LEU:HD23	2.02	0.40
11:n:56:ASP:O	11:n:60:THR:OG1	2.30	0.40
15:H:156:VAL:HB	15:H:182:ASN:HD21	1.87	0.40
15:H:185:LEU:N	15:H:186:PRO:HD3	2.37	0.40
21:N:259:PHE:CE2	21:N:904:VAL:HG11	2.56	0.40
24:Q:130:ARG:O	24:Q:134:LYS:HB3	2.21	0.40
24:Q:391:ASP:OD1	25:R:347:THR:OG1	2.28	0.40
27:T:85:LEU:HD23	27:T:88:TYR:HD2	1.87	0.40
27:T:186:ARG:HD3	27:T:211:PHE:HE1	1.87	0.40
1:1:27:PHE:HE1	1:1:29:ASP:HB2	1.86	0.40
3:3:2:SER:OG	3:3:3:ASP:N	2.51	0.40
3:h:112:ILE:HD12	3:h:190:ILE:HG22	2.02	0.40
4:g:137:GLY:HA2	4:g:140:THR:OG1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:40:ILE:HG23	8:A:56:GLN:HB2	2.02	0.40
8:c:87:ILE:N	8:c:88:PRO:HD2	2.37	0.40
11:n:105:THR:HG22	11:n:140:PRO:HD2	2.02	0.40
11:n:159:TRP:CZ3	12:m:56:SER:HB3	2.56	0.40
13:l:201:LEU:HD11	13:l:206:LEU:HG	2.03	0.40
15:H:176:VAL:HG13	15:H:177:ASP:N	2.36	0.40
16:I:253:ILE:HD11	16:I:287:ILE:HB	2.02	0.40
18:K:95:VAL:HG23	18:K:139:LEU:HB2	2.02	0.40
20:M:374:ILE:HA	20:M:412:HIS:ND1	2.36	0.40
23:P:54:SER:O	23:P:58:VAL:N	2.54	0.40
24:Q:295:GLY:N	24:Q:324:GLU:OE1	2.50	0.40
28:U:171:VAL:HG13	29:V:213:LEU:HD13	2.03	0.40
30:W:161:VAL:HG13	30:W:162:ASN:N	2.36	0.40
33:Z:517:ASP:HB2	33:Z:521:GLU:OE1	2.21	0.40
3:3:67:PHE:CZ	3:3:91:VAL:HG13	2.57	0.40
4:4:70:ARG:HA	11:D:90:ARG:NH1	2.36	0.40
5:f:114:PRO:HA	5:f:260:TRP:NE1	2.36	0.40
7:a:179:PHE:CE2	7:a:221:ASP:HB2	2.56	0.40
11:D:118:GLN:NE2	12:E:83:ALA:O	2.55	0.40
10:d:107:PRO:HD2	10:d:110:ILE:HD12	2.03	0.40
12:m:36:THR:HA	12:m:173:GLY:HA3	2.03	0.40
18:K:393:ARG:HA	18:K:396:ARG:HD3	2.03	0.40
18:K:394:ALA:HB1	18:K:399:ARG:HB2	2.03	0.40
33:Z:225:LEU:HD12	33:Z:256:LEU:HD12	2.04	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	1	194/215 (90%)	186 (96%)	8 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	194/215 (90%)	185 (95%)	9 (5%)	0	100	100
2	2	221/261 (85%)	208 (94%)	13 (6%)	0	100	100
2	i	221/261 (85%)	209 (95%)	12 (5%)	0	100	100
3	3	202/205 (98%)	192 (95%)	9 (4%)	1 (0%)	24	62
3	h	202/205 (98%)	192 (95%)	9 (4%)	1 (0%)	24	62
4	4	196/198 (99%)	183 (93%)	13 (7%)	0	100	100
4	g	196/198 (99%)	186 (95%)	10 (5%)	0	100	100
5	5	210/287 (73%)	198 (94%)	12 (6%)	0	100	100
5	f	210/287 (73%)	198 (94%)	12 (6%)	0	100	100
6	6	220/241 (91%)	211 (96%)	9 (4%)	0	100	100
6	e	220/241 (91%)	206 (94%)	14 (6%)	0	100	100
7	7	231/266 (87%)	220 (95%)	11 (5%)	0	100	100
7	a	231/266 (87%)	218 (94%)	13 (6%)	0	100	100
8	A	241/252 (96%)	230 (95%)	11 (5%)	0	100	100
8	c	241/252 (96%)	229 (95%)	12 (5%)	0	100	100
9	B	248/250 (99%)	237 (96%)	11 (4%)	0	100	100
9	j	248/250 (99%)	235 (95%)	13 (5%)	0	100	100
10	C	242/258 (94%)	224 (93%)	16 (7%)	2 (1%)	16	52
10	d	242/258 (94%)	228 (94%)	14 (6%)	0	100	100
11	D	239/254 (94%)	230 (96%)	9 (4%)	0	100	100
11	n	239/254 (94%)	224 (94%)	15 (6%)	0	100	100
12	E	240/260 (92%)	230 (96%)	10 (4%)	0	100	100
12	m	240/260 (92%)	231 (96%)	9 (4%)	0	100	100
13	F	231/234 (99%)	220 (95%)	11 (5%)	0	100	100
13	l	231/234 (99%)	221 (96%)	10 (4%)	0	100	100
14	G	242/288 (84%)	235 (97%)	7 (3%)	0	100	100
14	k	242/288 (84%)	232 (96%)	10 (4%)	0	100	100
15	H	353/467 (76%)	321 (91%)	32 (9%)	0	100	100
16	I	360/437 (82%)	334 (93%)	25 (7%)	1 (0%)	36	71
17	J	371/405 (92%)	351 (95%)	20 (5%)	0	100	100
18	K	379/428 (89%)	345 (91%)	33 (9%)	1 (0%)	36	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	L	359/437 (82%)	334 (93%)	25 (7%)	0	100	100
20	M	363/434 (84%)	343 (94%)	19 (5%)	1 (0%)	36	71
21	N	843/945 (89%)	796 (94%)	43 (5%)	4 (0%)	24	62
22	O	385/393 (98%)	339 (88%)	45 (12%)	1 (0%)	36	71
23	P	430/445 (97%)	387 (90%)	42 (10%)	1 (0%)	43	77
24	Q	429/434 (99%)	400 (93%)	29 (7%)	0	100	100
25	R	398/429 (93%)	366 (92%)	29 (7%)	3 (1%)	16	52
26	S	351/523 (67%)	320 (91%)	30 (8%)	1 (0%)	36	71
27	T	270/274 (98%)	244 (90%)	26 (10%)	0	100	100
28	U	245/338 (72%)	237 (97%)	7 (3%)	1 (0%)	30	66
29	V	282/306 (92%)	242 (86%)	37 (13%)	3 (1%)	11	45
30	W	195/268 (73%)	170 (87%)	22 (11%)	3 (2%)	8	38
31	X	125/156 (80%)	100 (80%)	25 (20%)	0	100	100
32	Y	17/89 (19%)	17 (100%)	0	0	100	100
33	Z	807/993 (81%)	736 (91%)	71 (9%)	0	100	100
All	All	13276/15139 (88%)	12380 (93%)	872 (7%)	24 (0%)	44	77

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	C	52	VAL
16	I	255	LYS
21	N	874	ILE
28	U	130	VAL
3	3	105	VAL
21	N	903	VAL
30	W	22	PRO
21	N	761	ILE
25	R	241	ILE
25	R	421	VAL
29	V	189	ILE
29	V	305	ILE
30	W	147	ILE
10	C	60	ASP
18	K	326	PRO
23	P	25	ASP
29	V	144	ILE

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Mol	Chain	Res	Type
3	h	105	VAL
20	M	167	VAL
25	R	72	VAL
26	S	179	ILE
21	N	904	VAL
22	O	227	ILE
30	W	118	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	162/178 (91%)	162 (100%)	0	100	100
1	b	162/178 (91%)	162 (100%)	0	100	100
2	2	182/214 (85%)	182 (100%)	0	100	100
2	i	182/214 (85%)	182 (100%)	0	100	100
3	3	172/173 (99%)	172 (100%)	0	100	100
3	h	172/173 (99%)	172 (100%)	0	100	100
4	4	175/175 (100%)	175 (100%)	0	100	100
4	g	175/175 (100%)	175 (100%)	0	100	100
5	5	169/235 (72%)	169 (100%)	0	100	100
5	f	169/235 (72%)	169 (100%)	0	100	100
6	6	185/201 (92%)	185 (100%)	0	100	100
6	e	185/201 (92%)	185 (100%)	0	100	100
7	7	199/224 (89%)	199 (100%)	0	100	100
7	a	199/224 (89%)	199 (100%)	0	100	100
8	A	207/210 (99%)	207 (100%)	0	100	100
8	c	207/210 (99%)	207 (100%)	0	100	100
9	B	209/209 (100%)	209 (100%)	0	100	100
9	j	209/209 (100%)	209 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	C	203/216 (94%)	203 (100%)	0	100	100
10	d	203/216 (94%)	203 (100%)	0	100	100
11	D	213/226 (94%)	213 (100%)	0	100	100
11	n	213/226 (94%)	213 (100%)	0	100	100
12	E	198/215 (92%)	198 (100%)	0	100	100
12	m	198/215 (92%)	198 (100%)	0	100	100
13	F	192/193 (100%)	192 (100%)	0	100	100
13	l	192/193 (100%)	192 (100%)	0	100	100
14	G	201/239 (84%)	201 (100%)	0	100	100
14	k	201/239 (84%)	201 (100%)	0	100	100
15	H	303/399 (76%)	303 (100%)	0	100	100
16	I	319/385 (83%)	319 (100%)	0	100	100
17	J	325/352 (92%)	325 (100%)	0	100	100
18	K	334/374 (89%)	333 (100%)	1 (0%)	86	84
19	L	308/377 (82%)	308 (100%)	0	100	100
20	M	315/375 (84%)	315 (100%)	0	100	100
21	N	713/797 (90%)	713 (100%)	0	100	100
22	O	363/368 (99%)	363 (100%)	0	100	100
23	P	405/415 (98%)	405 (100%)	0	100	100
24	Q	388/391 (99%)	388 (100%)	0	100	100
25	R	351/379 (93%)	351 (100%)	0	100	100
26	S	330/489 (68%)	330 (100%)	0	100	100
27	T	254/256 (99%)	254 (100%)	0	100	100
28	U	234/308 (76%)	234 (100%)	0	100	100
29	V	249/268 (93%)	249 (100%)	0	100	100
30	W	171/230 (74%)	171 (100%)	0	100	100
31	X	116/144 (81%)	116 (100%)	0	100	100
32	Y	18/81 (22%)	18 (100%)	0	100	100
33	Z	692/850 (81%)	692 (100%)	0	100	100
All	All	11522/13054 (88%)	11521 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
18	K	91	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (132) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	120	GLN
4	4	37	GLN
4	4	86	GLN
4	4	112	ASN
4	4	133	HIS
5	5	137	GLN
6	6	55	ASN
6	6	216	GLN
7	7	51	ASN
7	7	145	ASN
7	7	182	HIS
7	7	246	GLN
7	7	249	ASN
1	b	139	HIS
2	i	194	ASN
3	h	48	HIS
3	h	169	GLN
4	g	37	GLN
4	g	41	HIS
4	g	55	GLN
4	g	133	HIS
4	g	146	HIS
4	g	147	HIS
5	f	104	GLN
6	e	48	ASN
6	e	114	HIS
6	e	214	HIS
6	e	216	GLN
7	a	107	ASN
7	a	145	ASN
7	a	227	ASN
9	B	119	GLN
9	B	139	HIS
10	C	59	GLN
10	C	156	ASN
11	D	118	GLN
12	E	180	GLN
13	F	117	GLN

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Mol	Chain	Res	Type
13	F	210	ASN
14	G	23	GLN
14	G	90	ASN
14	G	147	HIS
8	c	84	ASN
8	c	92	ASN
8	c	126	GLN
8	c	209	HIS
10	d	120	GLN
10	d	173	GLN
11	n	55	GLN
11	n	122	GLN
11	n	149	GLN
11	n	167	ASN
11	n	209	ASN
12	m	91	HIS
12	m	147	HIS
13	l	60	GLN
13	l	148	GLN
14	k	23	GLN
14	k	147	HIS
14	k	183	HIS
14	k	228	HIS
15	H	182	ASN
15	H	265	ASN
15	H	330	GLN
15	H	413	ASN
16	I	78	ASN
16	I	254	GLN
18	K	144	ASN
18	K	302	GLN
19	L	133	ASN
19	L	273	HIS
19	L	320	GLN
19	L	364	HIS
20	M	74	GLN
20	M	240	ASN
20	M	364	HIS
21	N	17	GLN
21	N	240	GLN
21	N	256	GLN
21	N	329	HIS

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Mol	Chain	Res	Type
21	N	616	HIS
21	N	690	HIS
21	N	712	ASN
21	N	716	GLN
22	O	23	HIS
22	O	105	GLN
22	O	117	ASN
22	O	354	GLN
23	P	76	ASN
23	P	183	GLN
23	P	195	GLN
23	P	277	GLN
23	P	336	HIS
23	P	401	ASN
23	P	418	ASN
23	P	440	HIS
24	Q	87	GLN
24	Q	178	HIS
24	Q	186	HIS
24	Q	260	GLN
24	Q	334	HIS
25	R	81	HIS
25	R	143	GLN
25	R	184	GLN
25	R	208	ASN
25	R	323	ASN
25	R	376	GLN
25	R	401	HIS
26	S	314	ASN
27	T	127	GLN
27	T	132	HIS
28	U	71	ASN
28	U	84	ASN
28	U	156	HIS
28	U	270	ASN
29	V	97	GLN
29	V	111	HIS
29	V	126	GLN
29	V	172	GLN
29	V	184	ASN
29	V	204	HIS
29	V	290	ASN

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Mol	Chain	Res	Type
30	W	44	ASN
30	W	86	HIS
30	W	100	HIS
30	W	143	ASN
30	W	170	HIS
33	Z	132	HIS
33	Z	532	HIS
33	Z	810	ASN
33	Z	833	GLN
33	Z	897	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

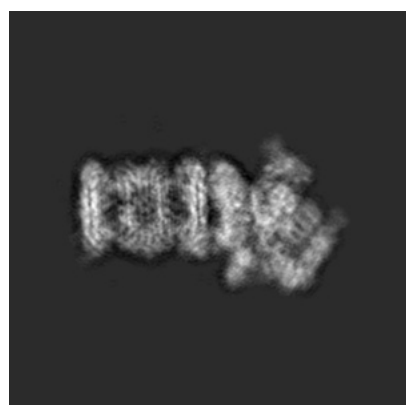
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6694. These allow visual inspection of the internal detail of the map and identification of artifacts.

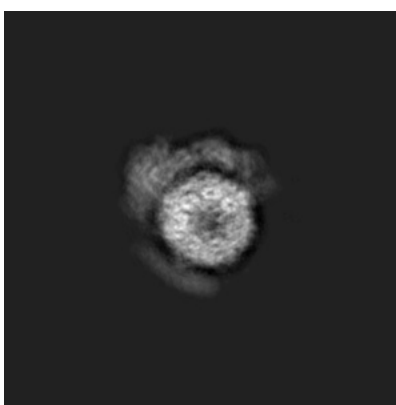
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

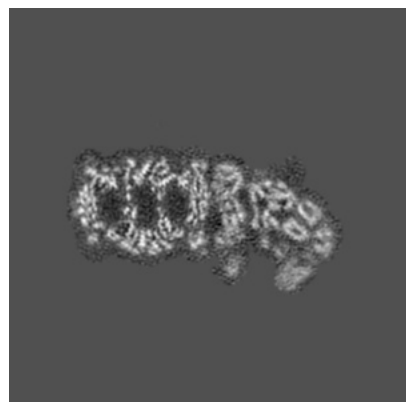


Z

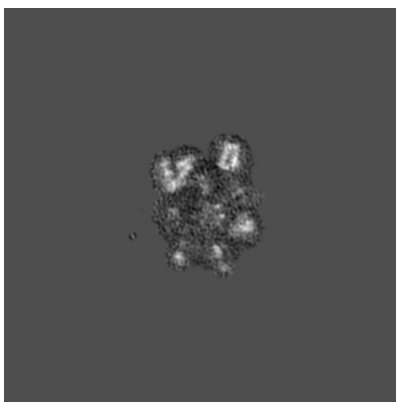
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

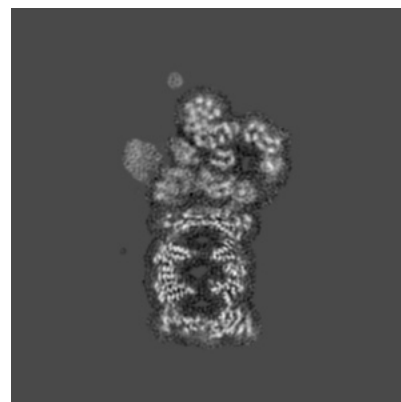
6.2.1 Primary map



X Index: 180



Y Index: 180

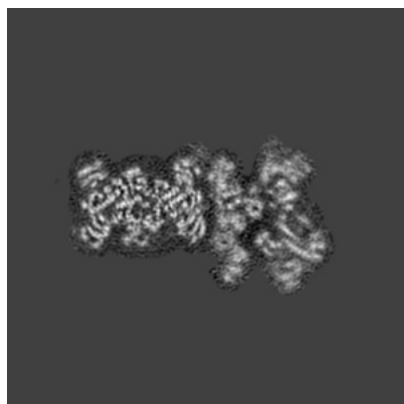


Z Index: 180

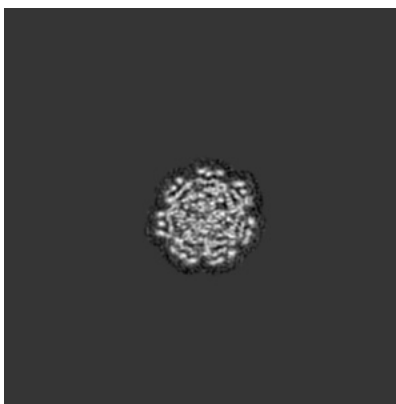
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

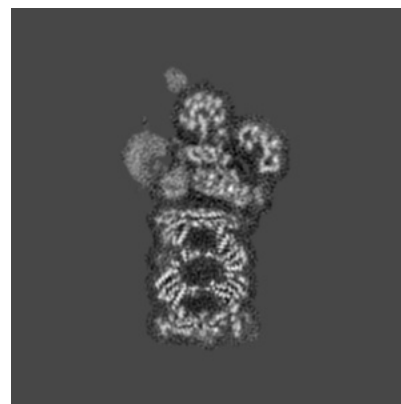
6.3.1 Primary map



X Index: 192



Y Index: 77

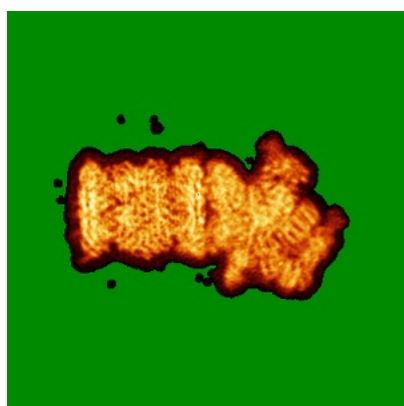


Z Index: 173

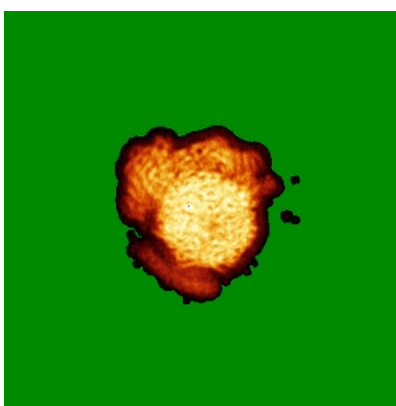
The images above show the largest variance slices of the map in three orthogonal directions.

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

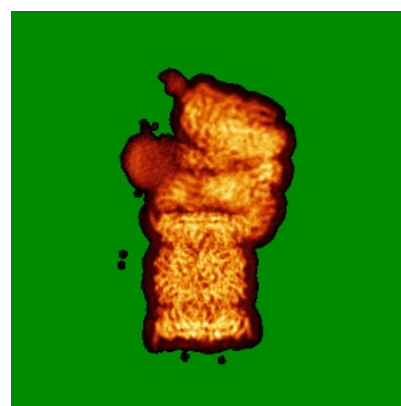
6.4.1 Primary map



X



Y

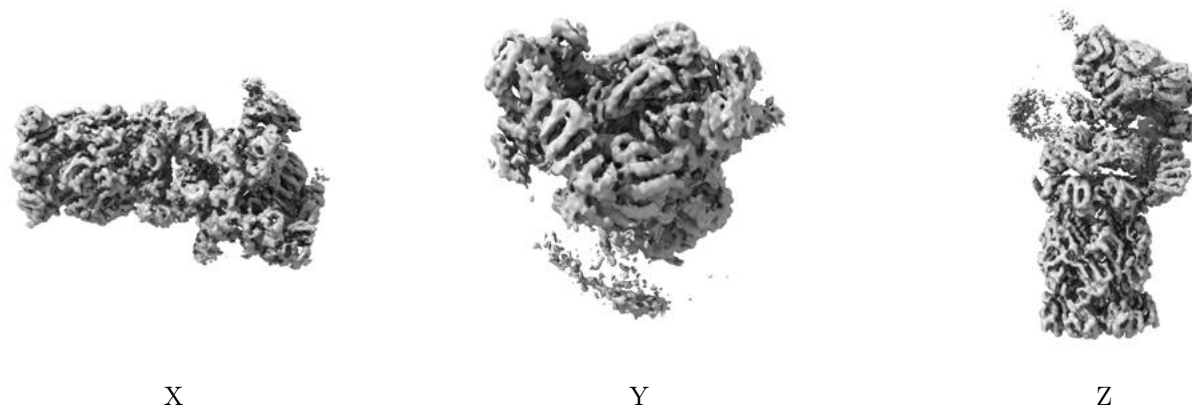


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.543. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

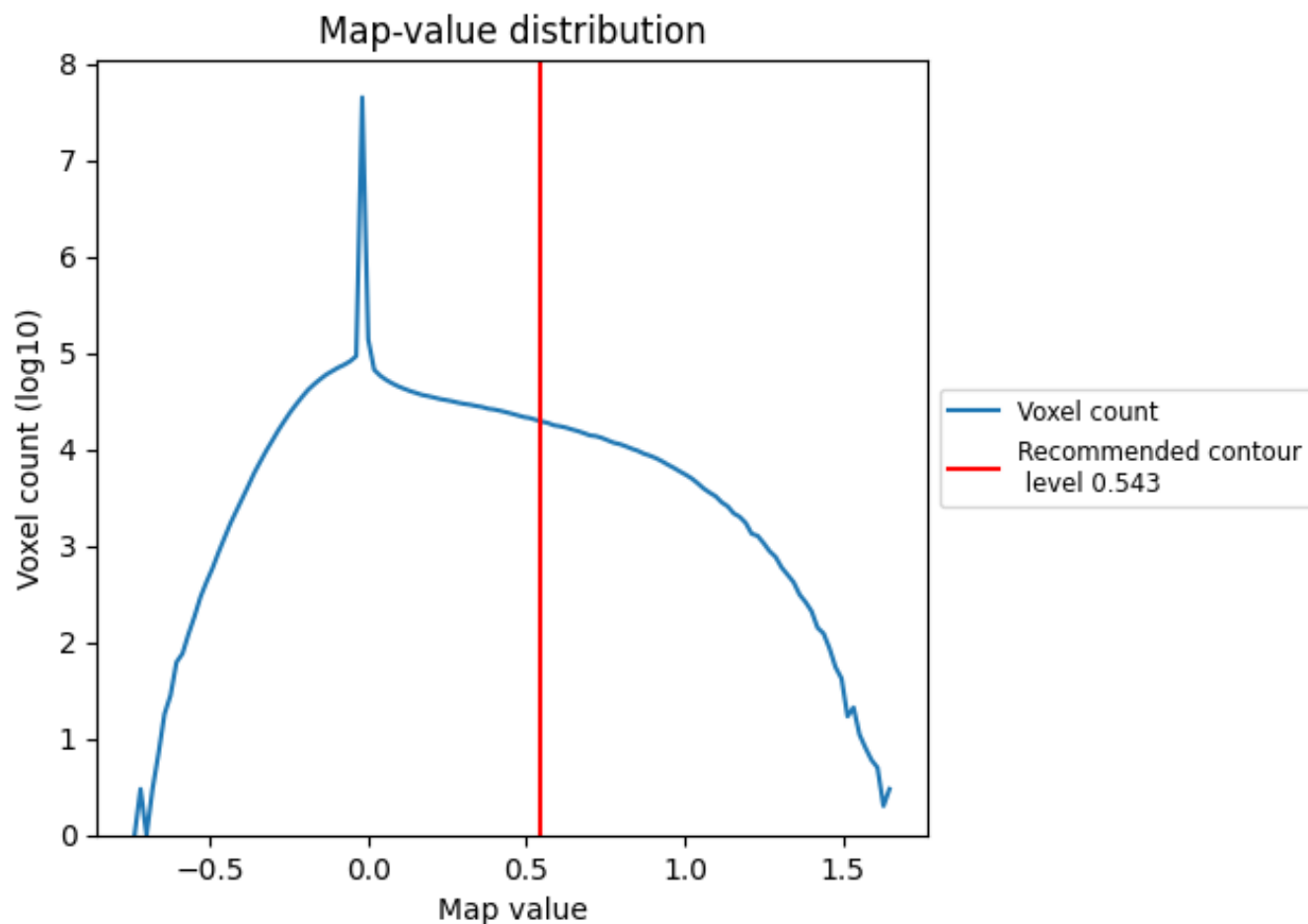
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

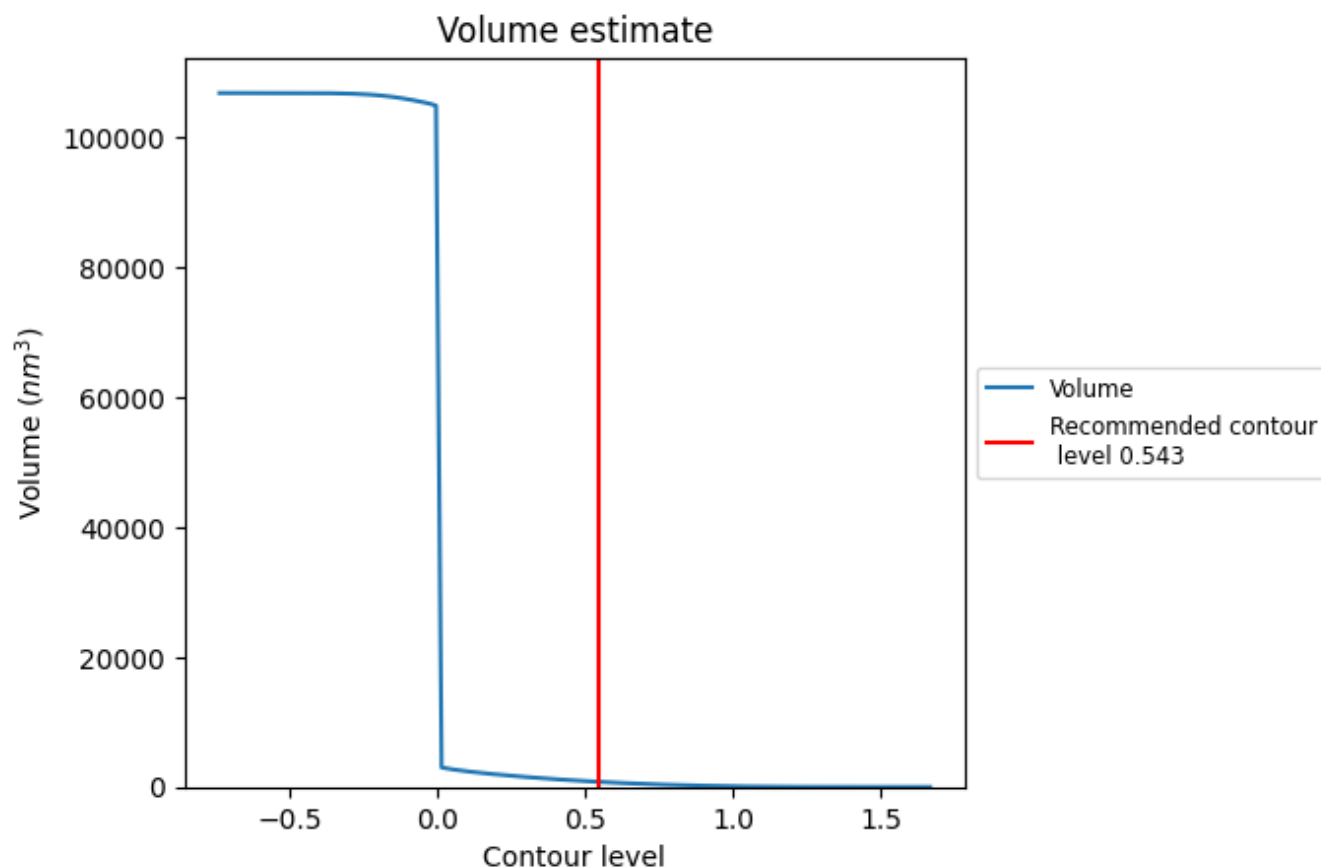
This section contains the results of statistical analysis of the map.

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.

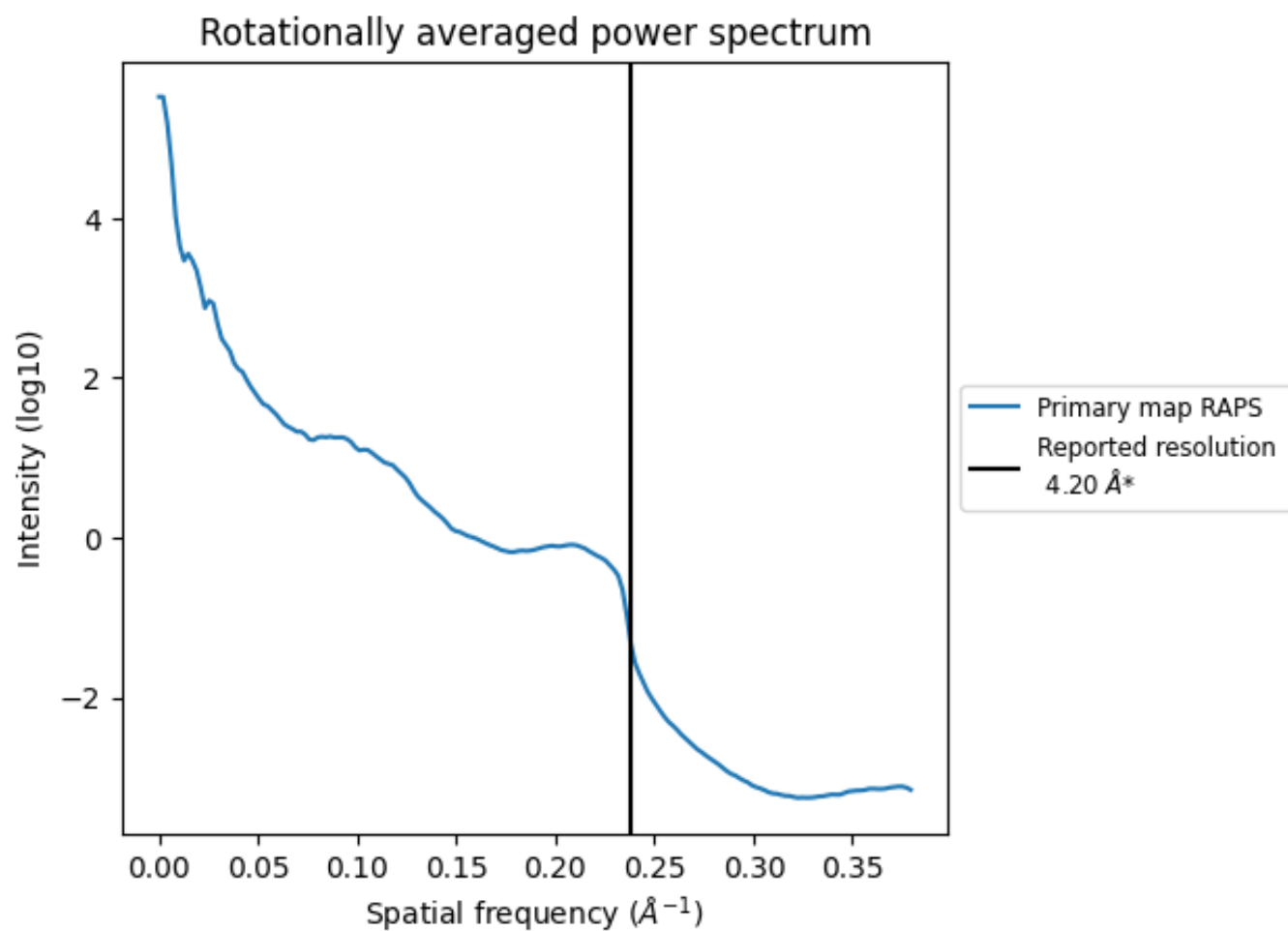
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 792 nm³; this corresponds to an approximate mass of 715 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 0.238 Å⁻¹

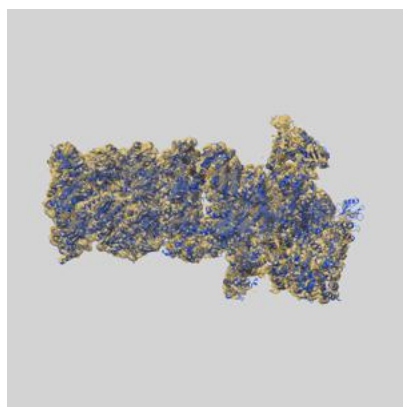
8 Fourier-Shell correlation

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

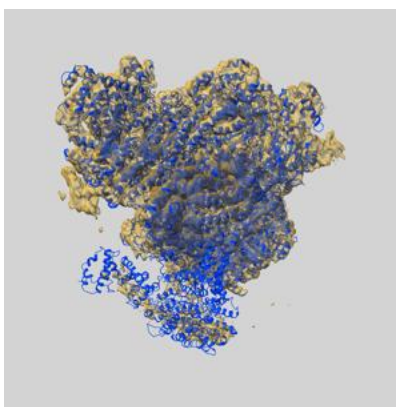
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6694 and PDB model 5WVK. Per-residue inclusion information can be found in section 3 on page 11.

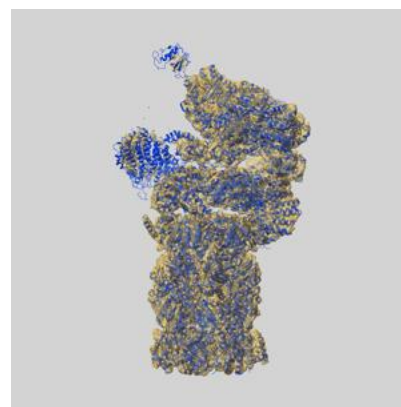
9.1 Map-model overlay [i](#)



X



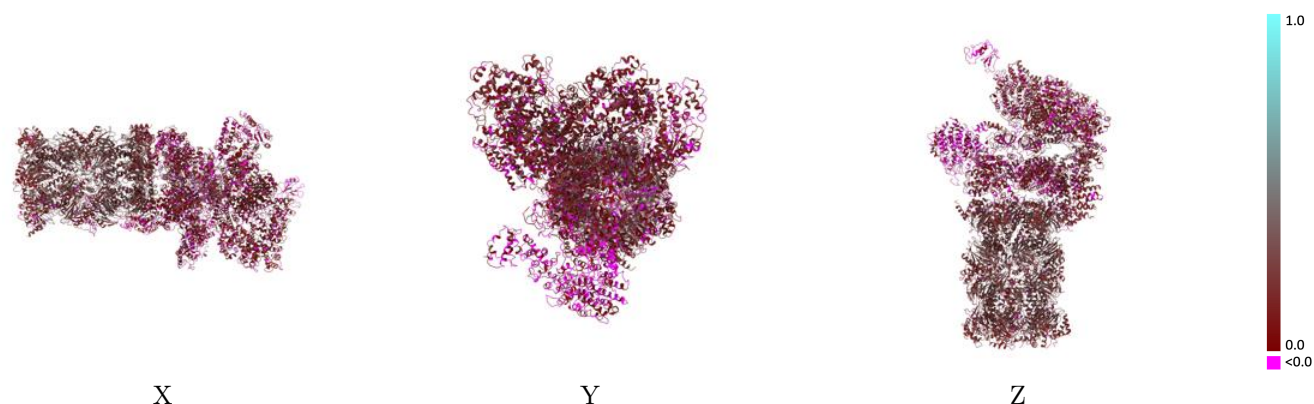
Y



Z

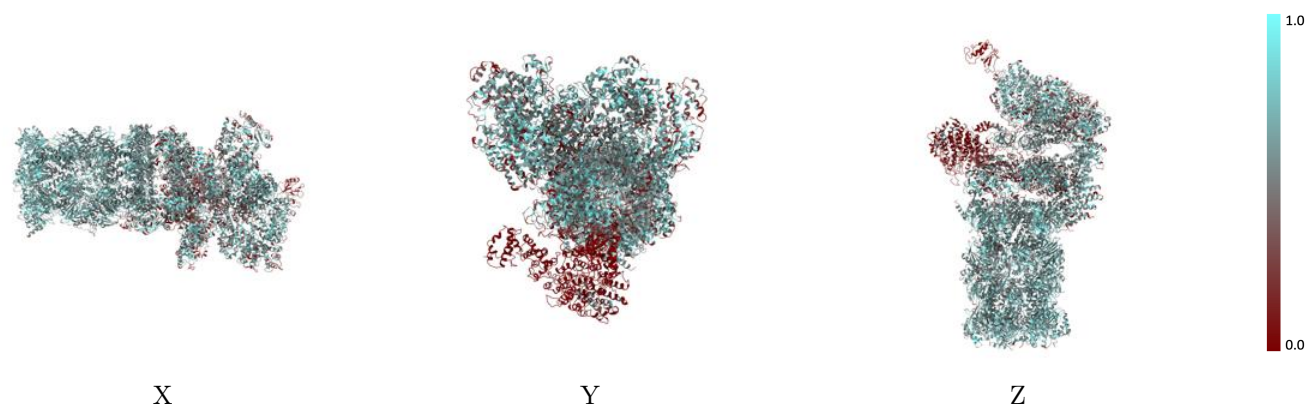
The images above show the 3D surface view of the map at the recommended contour level 0.543 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



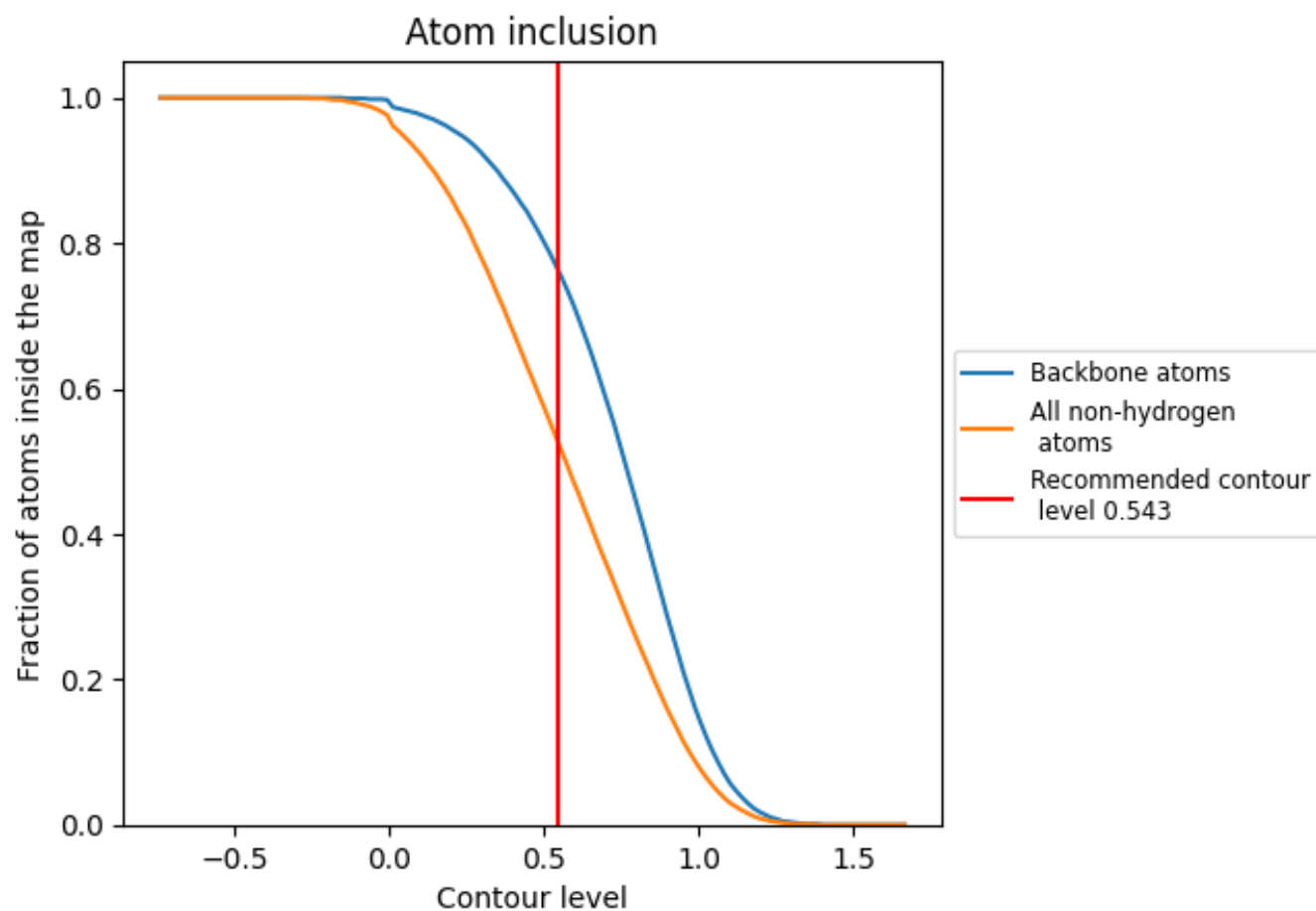
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.543).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.543) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5290	 0.1690
1	 0.6540	 0.2880
2	 0.6190	 0.2380
3	 0.6190	 0.2580
4	 0.6090	 0.2530
5	 0.6320	 0.2570
6	 0.5800	 0.2350
7	 0.6320	 0.2730
A	 0.6000	 0.2470
B	 0.5950	 0.2350
C	 0.5960	 0.2100
D	 0.6140	 0.2250
E	 0.6080	 0.2210
F	 0.6080	 0.2210
G	 0.6190	 0.2380
H	 0.4700	 0.1010
I	 0.2980	 0.1050
J	 0.3150	 0.1100
K	 0.4830	 0.1280
L	 0.4950	 0.1090
M	 0.5340	 0.1160
N	 0.5850	 0.1410
O	 0.5110	 0.1140
P	 0.5450	 0.1280
Q	 0.5450	 0.1160
R	 0.5780	 0.1210
S	 0.5380	 0.1170
T	 0.4650	 0.1310
U	 0.5920	 0.1770
V	 0.4650	 0.1180
W	 0.5480	 0.1080
X	 0.0210	 -0.0290
Y	 0.5520	 0.1430
Z	 0.0500	 0.0070
a	 0.6470	 0.2620



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Chain	Atom inclusion	Q-score
b	 0.6490	 0.2850
c	 0.6430	 0.2330
d	 0.6410	 0.2160
e	 0.6140	 0.2250
f	 0.6360	 0.2320
g	 0.6280	 0.2620
h	 0.6070	 0.2550
i	 0.5980	 0.2350
j	 0.6400	 0.2250
k	 0.6610	 0.2330
l	 0.6600	 0.2140
m	 0.6320	 0.2110
n	 0.6600	 0.2240