



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:54 AM UTC

PDB ID : 7QYB / pdb_00007qyb
EMDB ID : EMD-14211
Title : Proteasome-ZFAND5 Complex Z-C state
Authors : Zhu, Y.; Lu, Y.
Deposited on : 2022-01-27
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

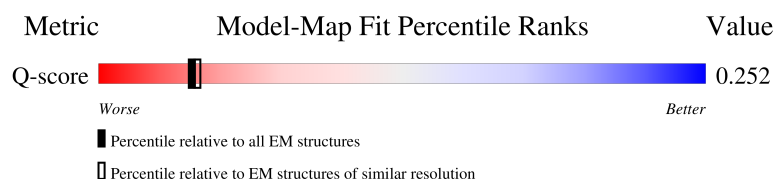
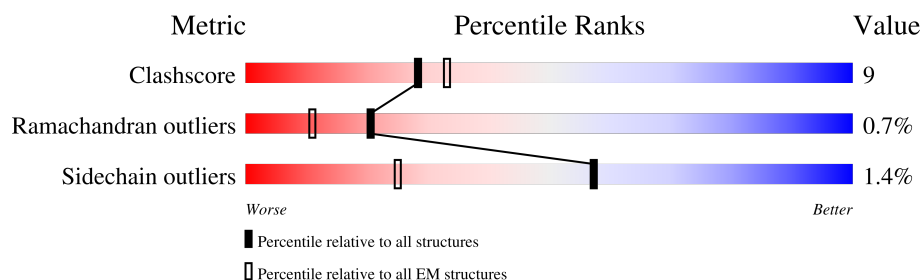
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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

Mol	Chain	Length	Quality of chain
1	U	953	
2	V	533	
3	W	456	
4	X	422	

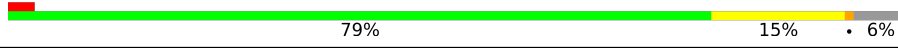
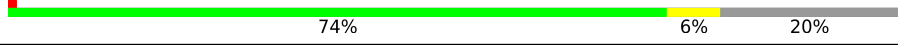
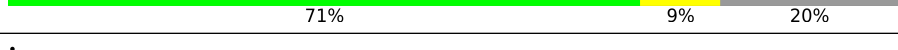
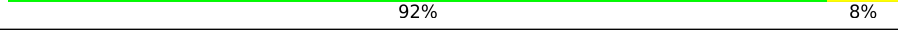
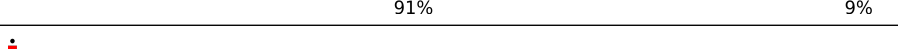
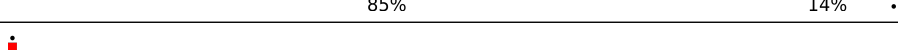
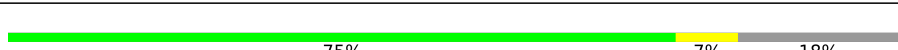
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Mol	Chain	Length	Quality of chain
5	Y	389	
6	Z	324	
7	a	376	
8	b	377	
9	c	309	
10	d	349	
11	e	70	
12	f	908	
13	A	433	
14	B	440	
15	C	398	
16	D	418	
17	E	403	
18	F	439	
19	G	245	
19	g	245	
20	H	233	
20	h	233	
21	I	260	
21	i	260	
22	J	247	
22	j	247	
23	K	240	
23	k	240	
24	L	268	

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Mol	Chain	Length	Quality of chain
24	l	268	
25	M	254	
25	m	254	
26	N	238	
26	n	238	
27	O	276	
27	o	276	
28	P	204	
28	p	204	
29	Q	201	
29	q	201	
30	R	262	
30	r	262	
31	S	240	
31	s	240	
32	T	263	
32	t	263	

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 105037 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	872	Total	C	N	O	S	0	0
			6828	4328	1157	1298	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	480	Total	C	N	O	S	0	0
			3852	2444	684	710	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	380	Total	C	N	O	S	0	0
			3009	1918	509	570	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	286	Total	C	N	O	S	0	0
			2276	1454	390	427	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	e	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	889	Total	C	N	O	S	0	0
			6866	4315	1174	1331	46		

- Molecule 13 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	413	Total	C	N	O	S	0	0
			3229	2034	566	611	18		

- Molecule 14 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	411	Total	C	N	O	S	0	0
			3207	2022	548	622	15		

- Molecule 15 is a protein called Isoform 2 of 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	396	Total	C	N	O	S	0	0
			3105	1954	558	576	17		

- Molecule 16 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		

- Molecule 17 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	389	Total	C	N	O	S	0	0
			3097	1947	552	581	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	395	Total	C	N	O	S	0	0
			3098	1951	533	596	18		

- Molecule 19 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	239	Total	C	N	O	S	0	0
			1820	1157	304	346	13		
19	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 20 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	H	230	Total	C	N	O	S	0	0
			1692	1073	285	329	5		
20	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 21 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	I	248	Total	C	N	O	S	0	0
			1895	1195	324	368	8		
21	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 22 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 23 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	K	228	Total	C	N	O	S	0	0
			1729	1086	284	349	10		
23	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 24 is a protein called Isoform Long of Proteasome subunit alpha type-1.

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

- Molecule 25 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 26 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		
26	n	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 27 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
27	o	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 28 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	P	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		
28	p	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 29 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
29	q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 30 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
30	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 31 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
31	s	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

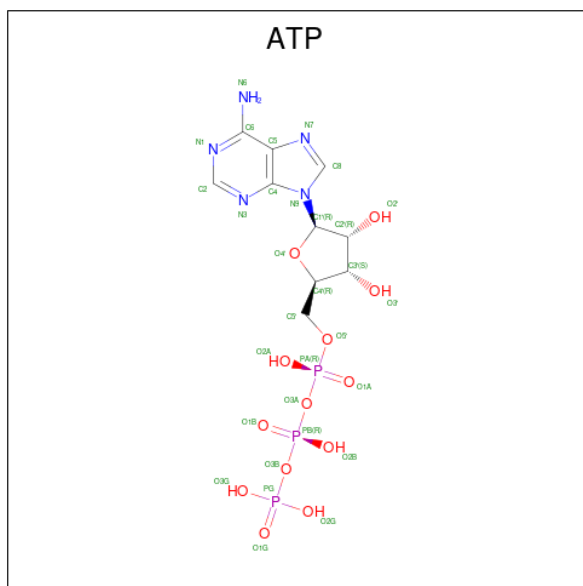
- Molecule 32 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
32	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 33 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



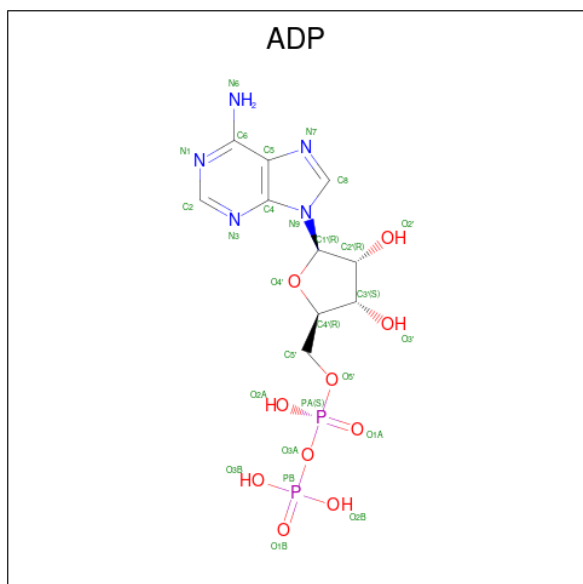
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Mol	Chain	Residues	Atoms					AltConf
34	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
35	A	1	Total	Mg	0
			1	1	
35	B	1	Total	Mg	0
			1	1	
35	C	1	Total	Mg	0
			1	1	
35	D	1	Total	Mg	0
			1	1	
35	F	1	Total	Mg	0
			1	1	

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

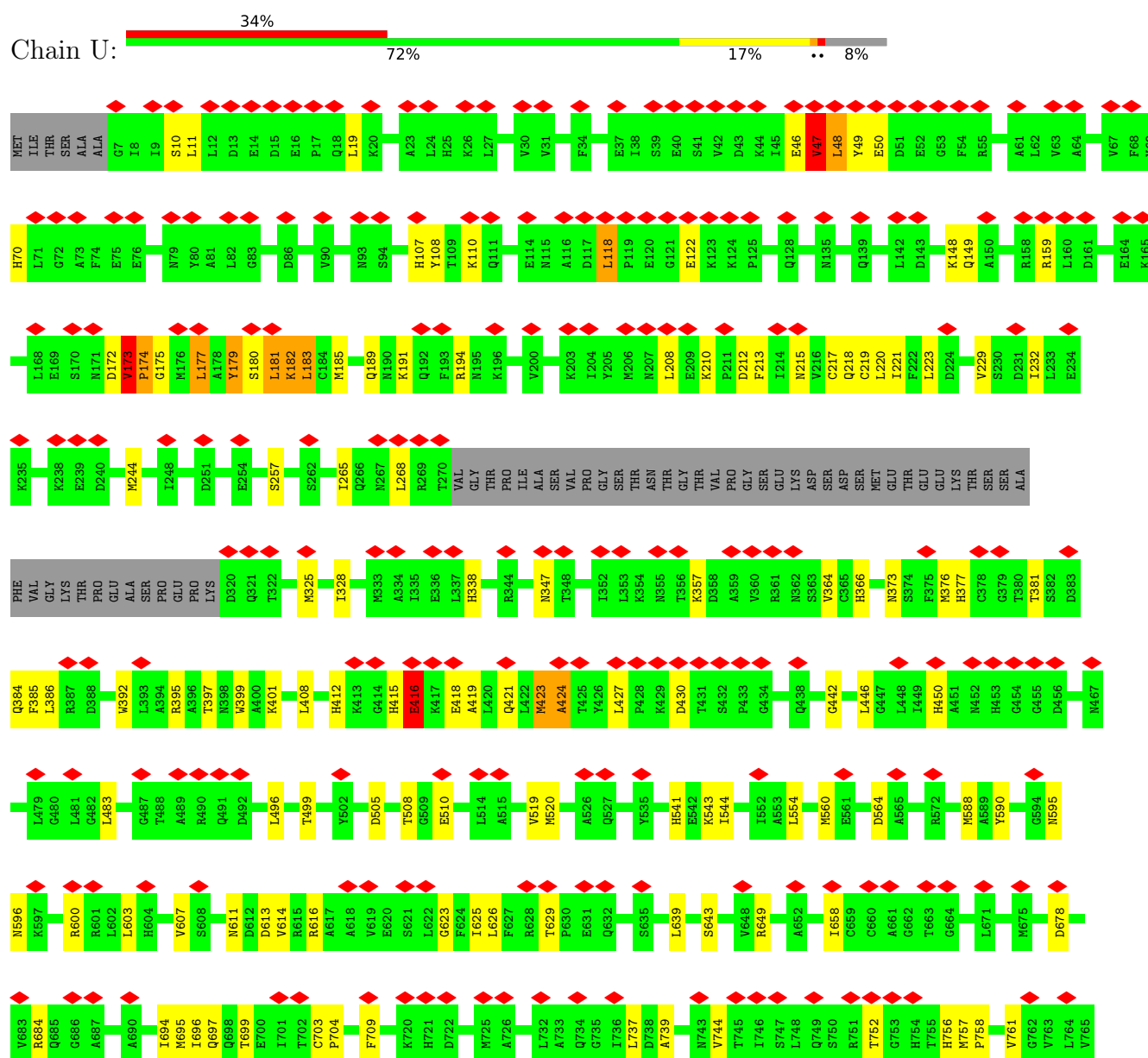


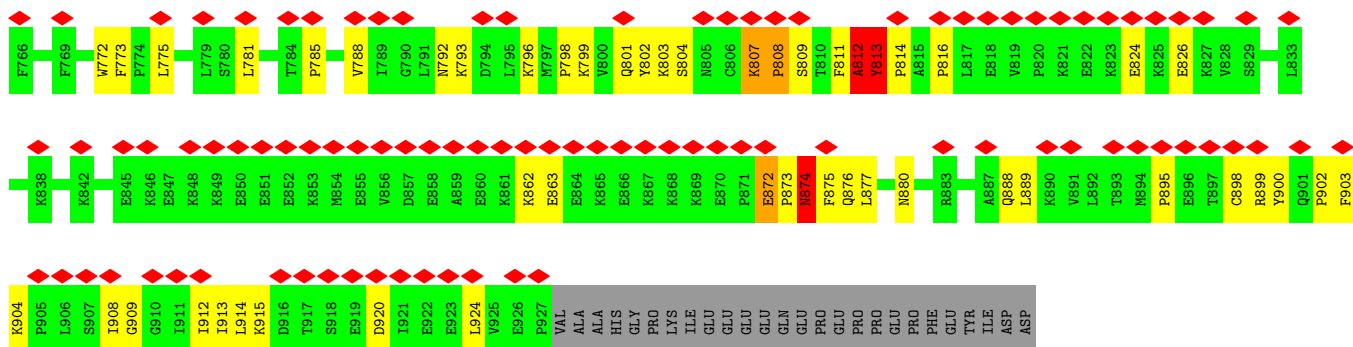
Mol	Chain	Residues	Atoms					AltConf
36	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots [i](#)

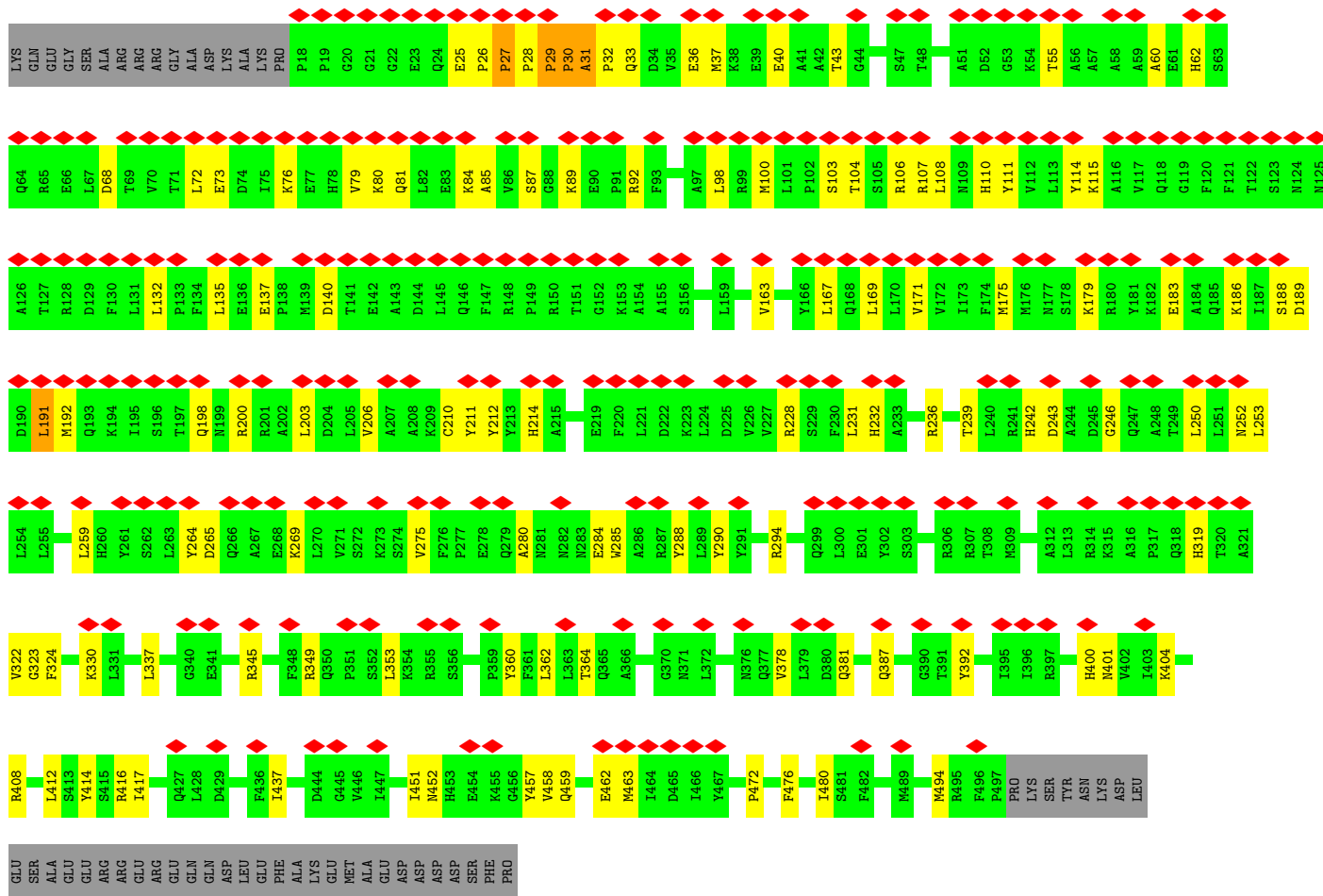
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

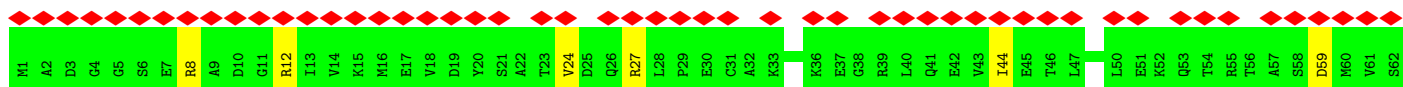
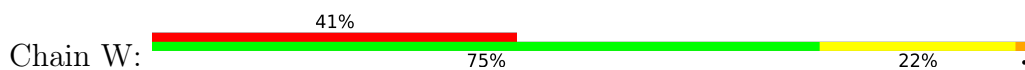


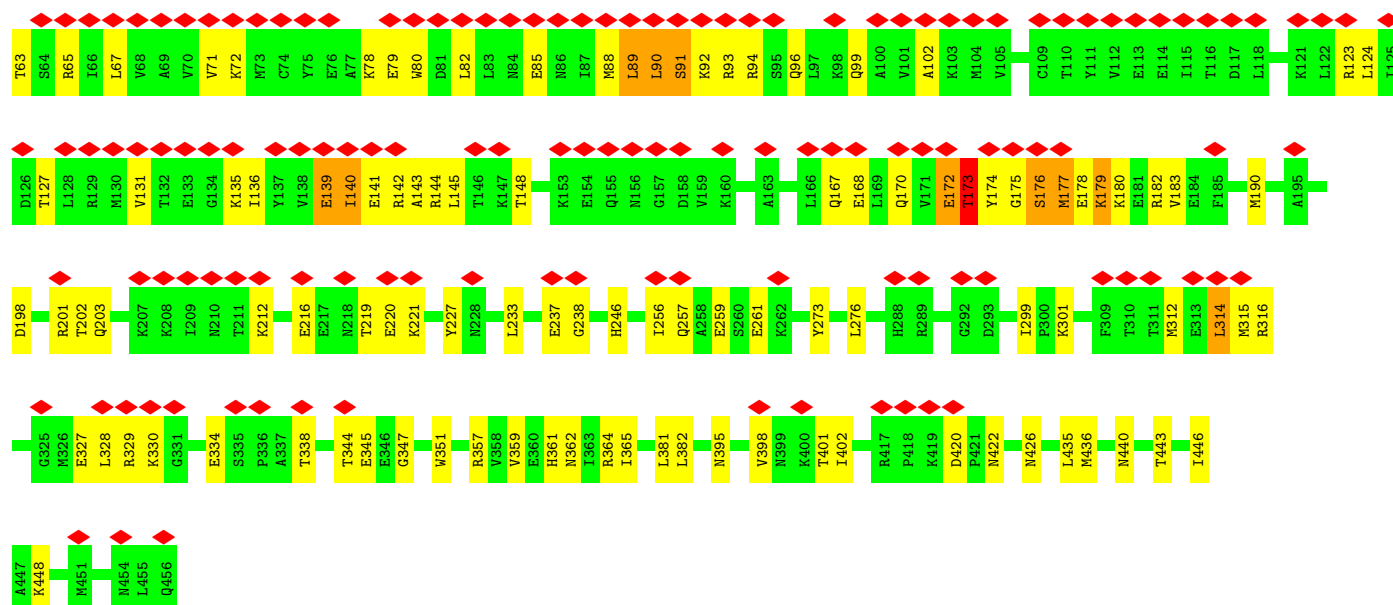


• Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

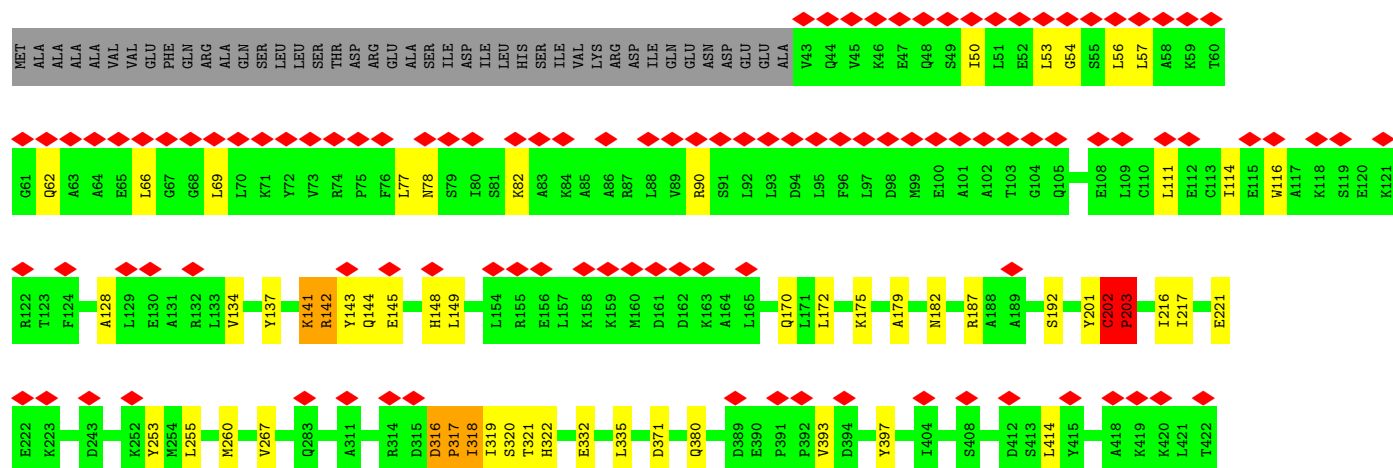
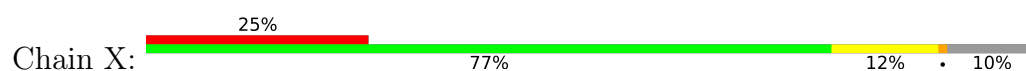


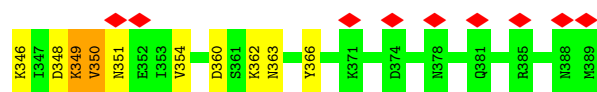
• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12



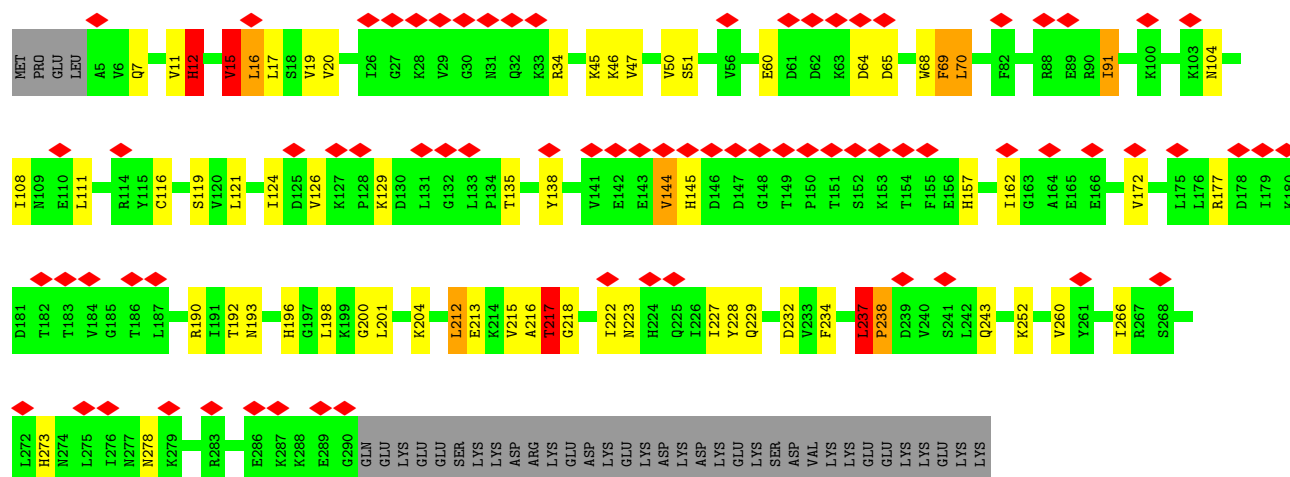


- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

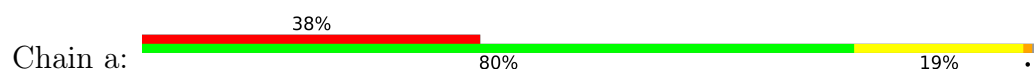




• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

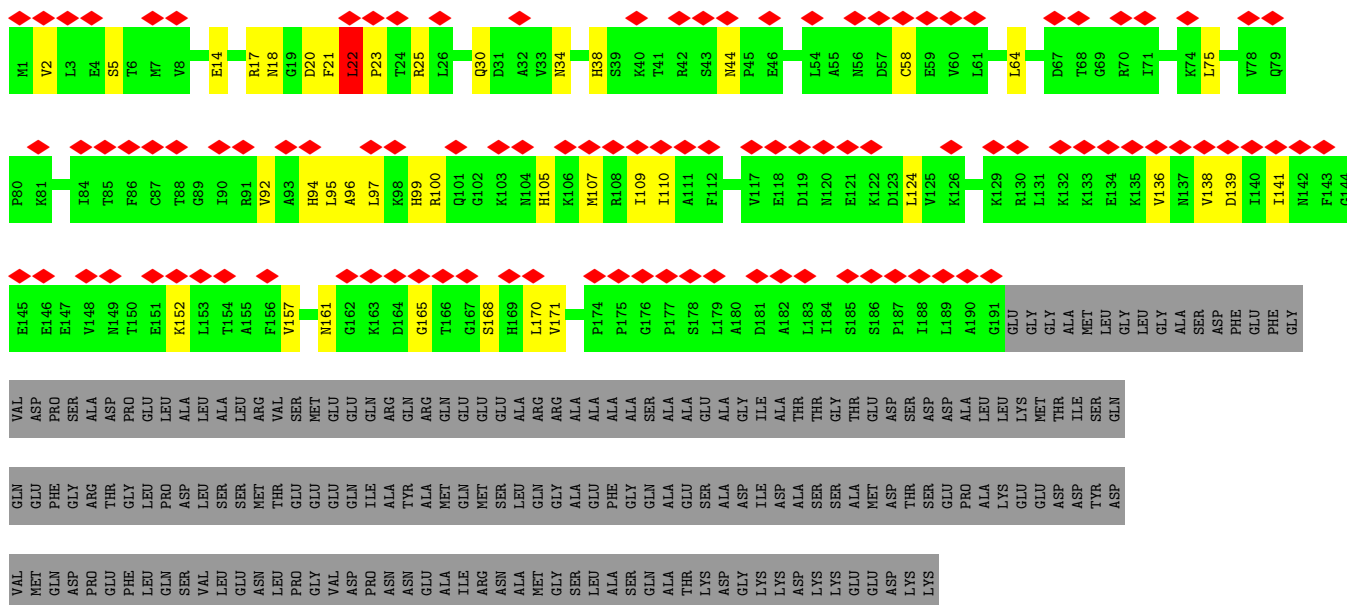


• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

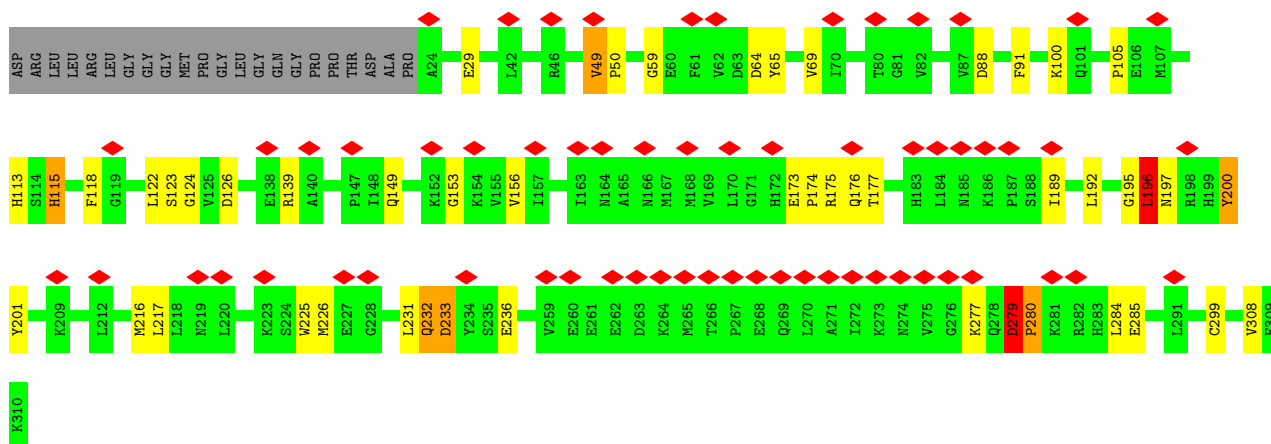
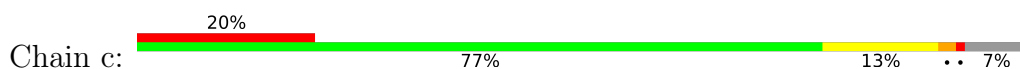


• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

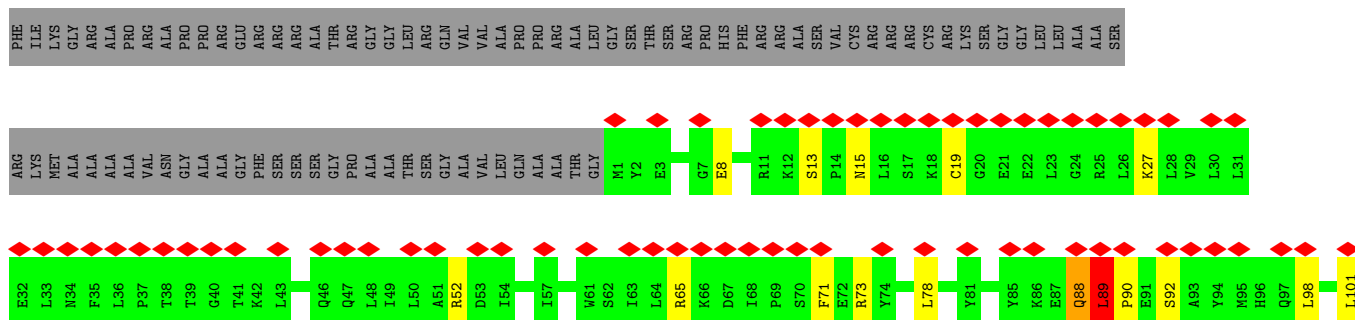
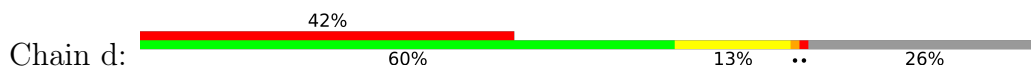


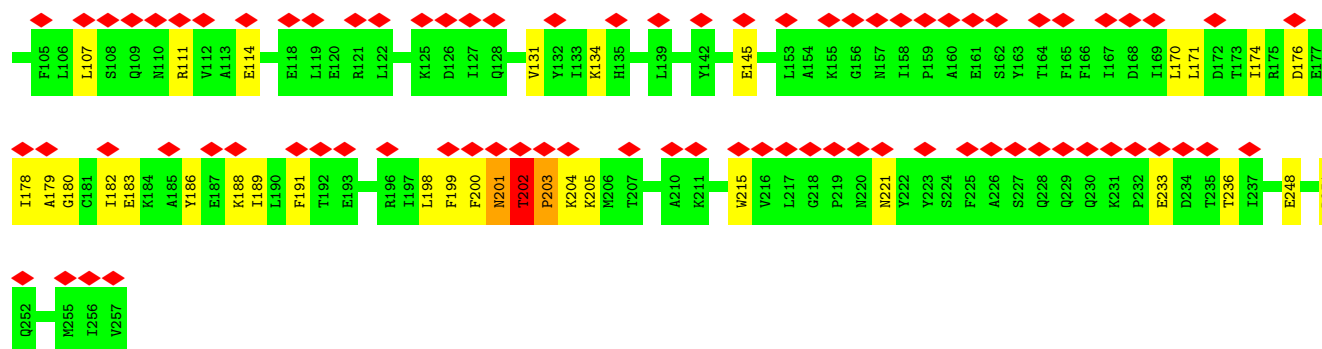


- Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

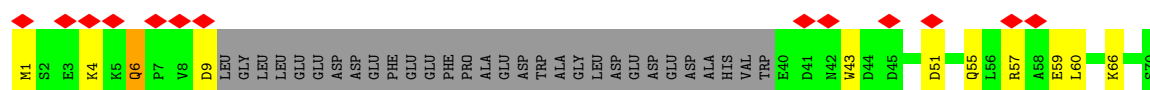
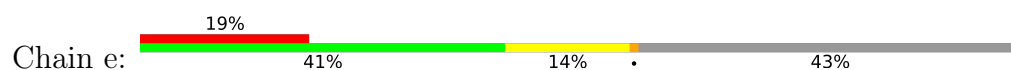


- Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

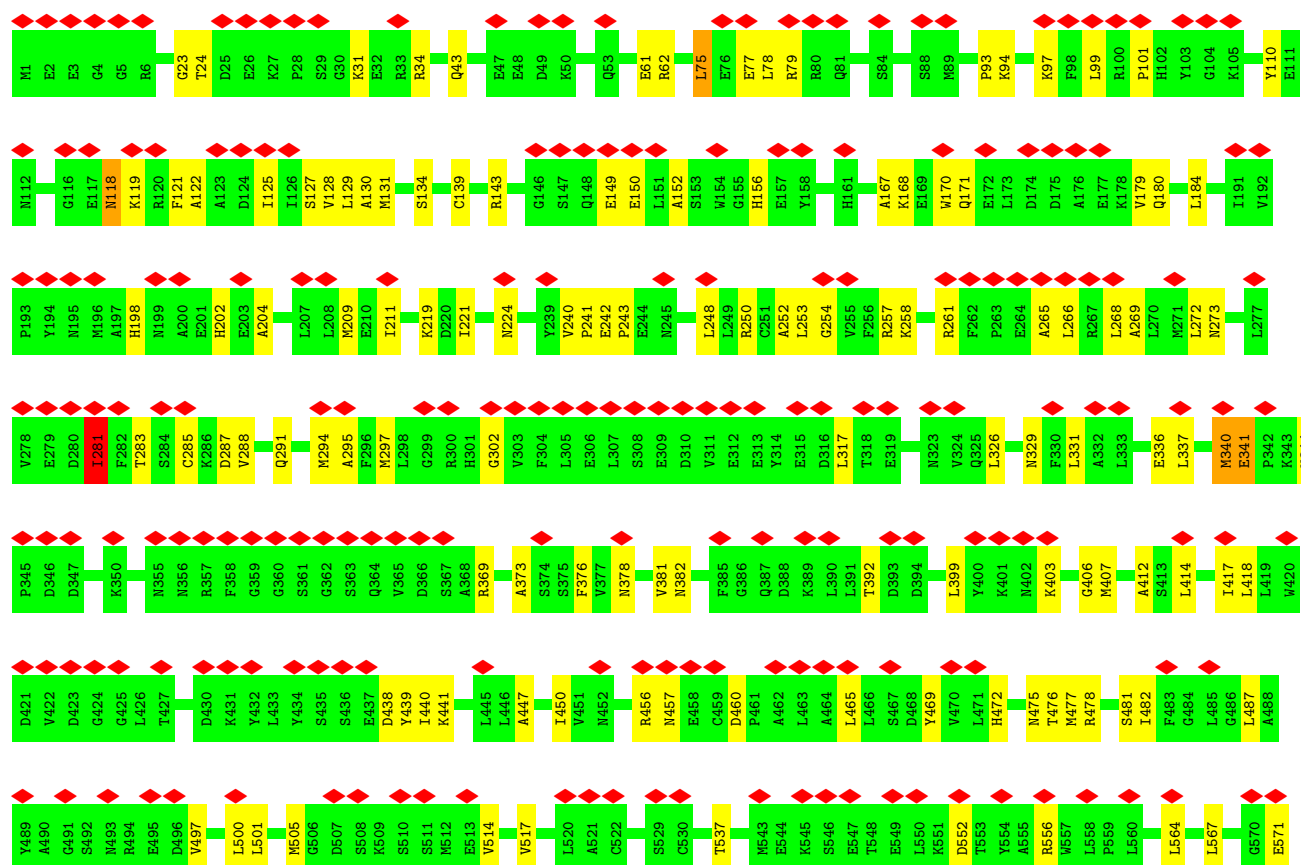


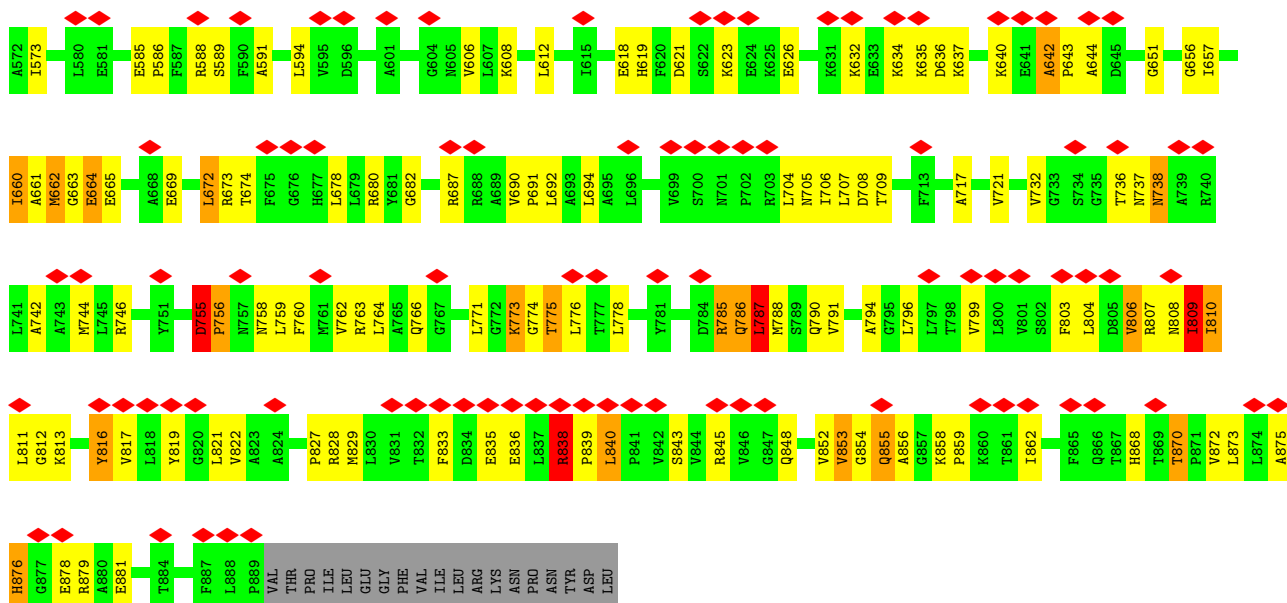


- Molecule 11: 26S proteasome complex subunit SEM1

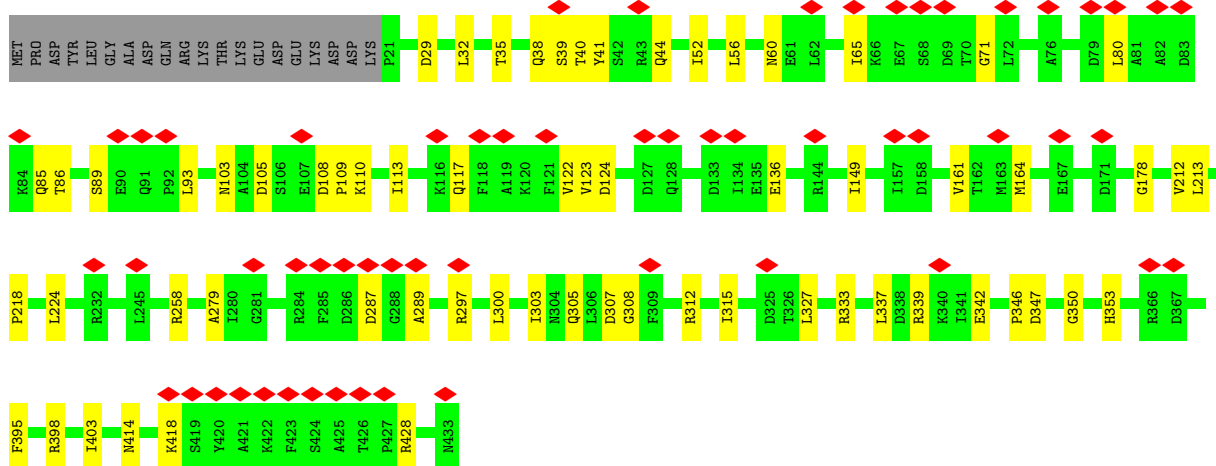
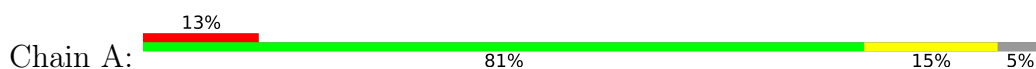


- Molecule 12: 26S proteasome non-ATPase regulatory subunit 2

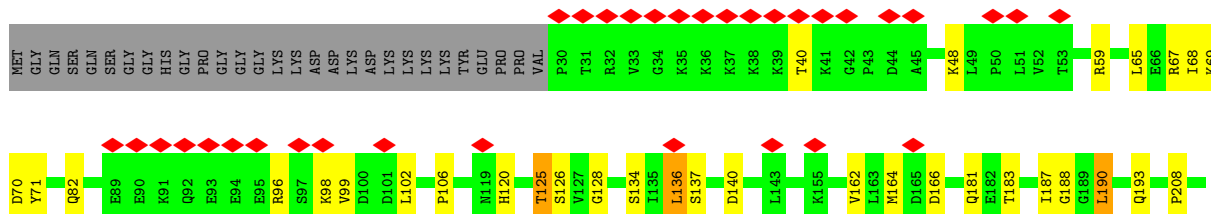
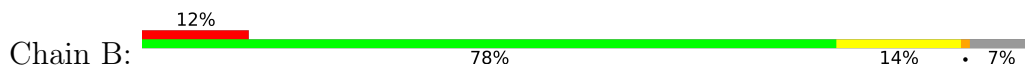


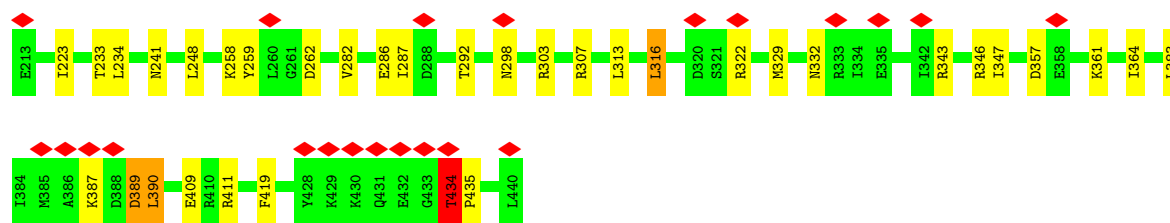


• Molecule 13: 26S protease regulatory subunit 7

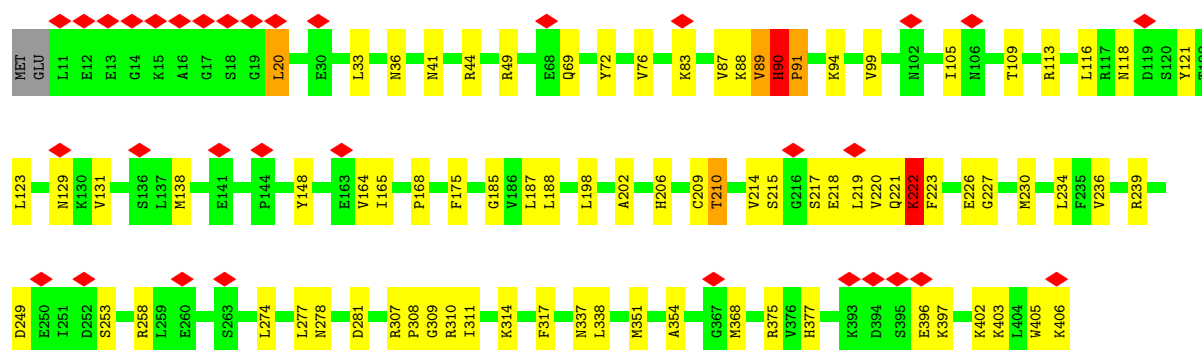
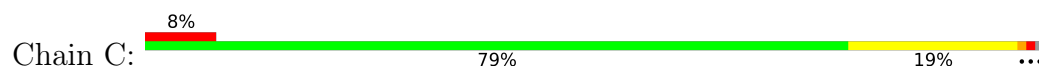


• Molecule 14: 26S protease regulatory subunit 4

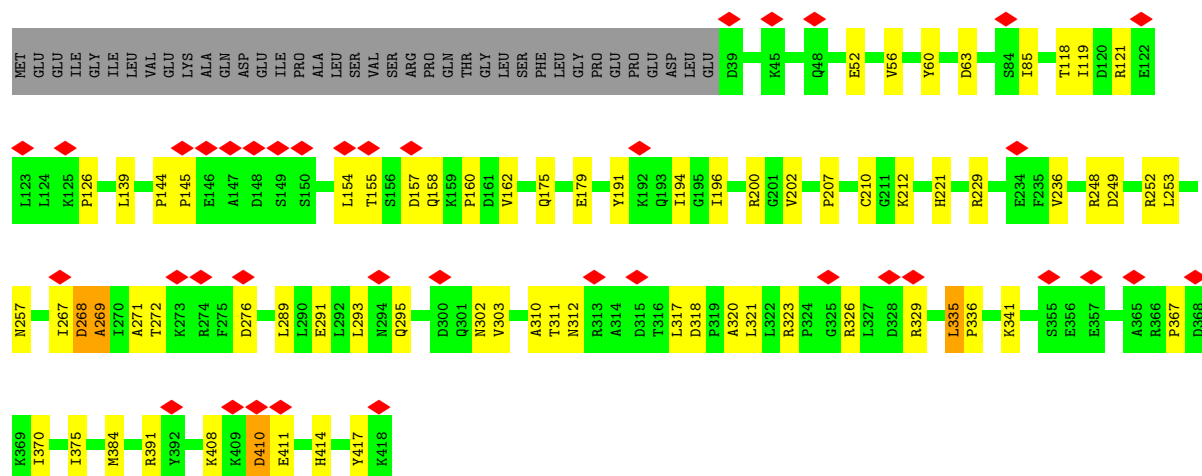
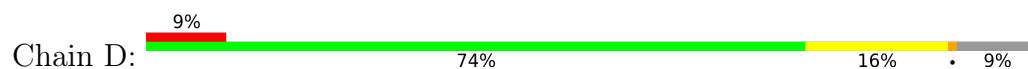




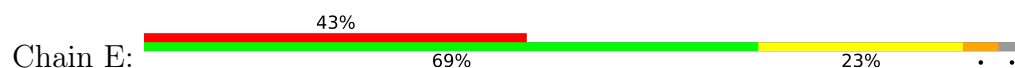
- Molecule 15: Isoform 2 of 26S proteasome regulatory subunit 8

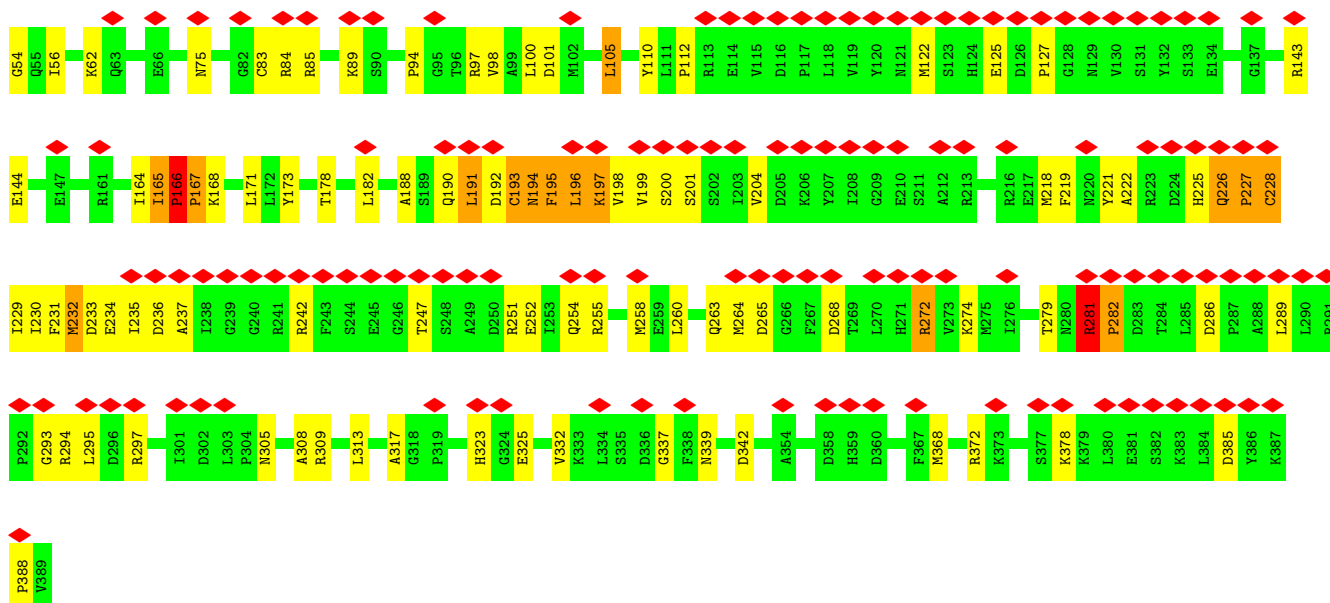


- Molecule 16: 26S protease regulatory subunit 6B



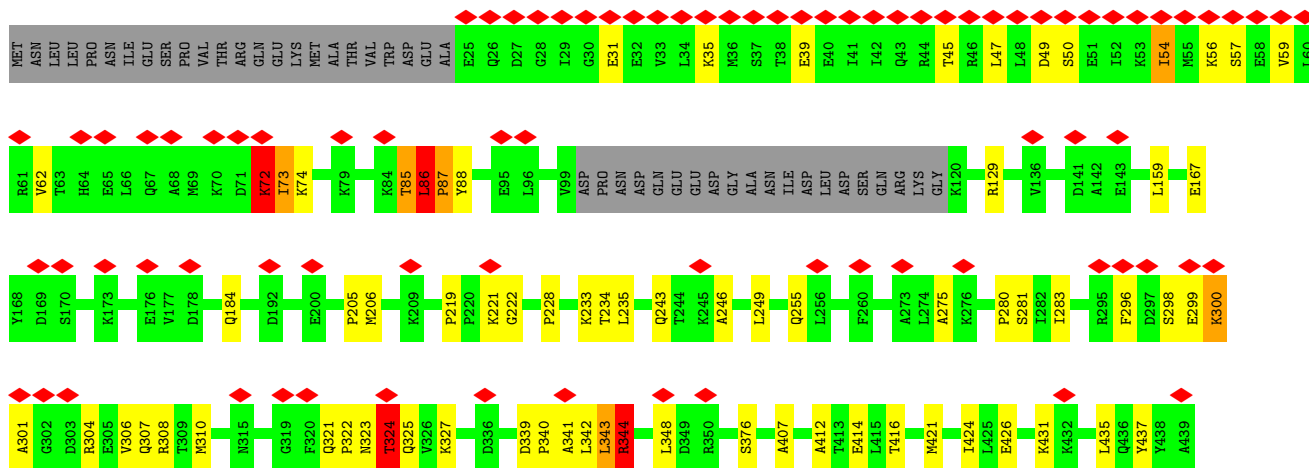
- Molecule 17: 26S proteasome regulatory subunit 10B





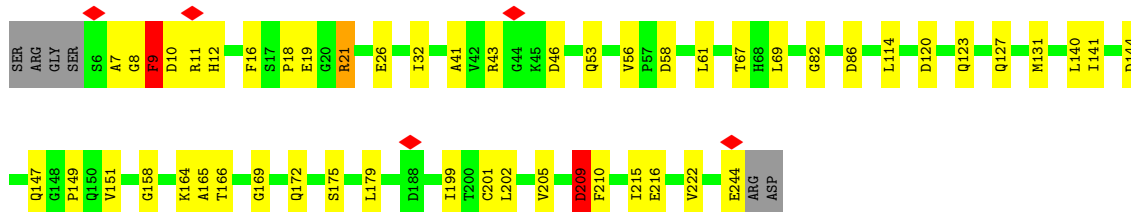
- Molecule 18: 26S protease regulatory subunit 6A

Chain F: 19% 73% 15% 10%



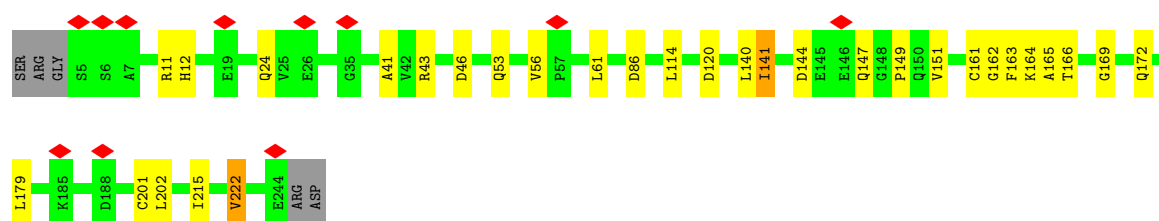
- Molecule 19: Proteasome subunit alpha type-6

Chain G: 76% 20%



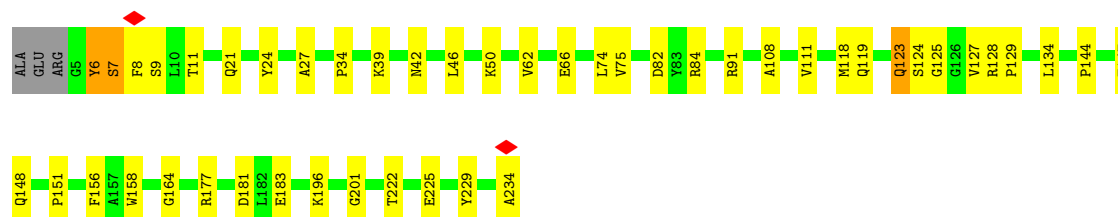
- Molecule 19: Proteasome subunit alpha type-6

Chain g: 

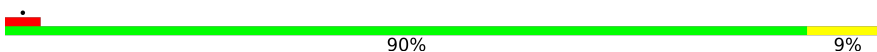


- Molecule 20: Proteasome subunit alpha type-2

Chain H: 



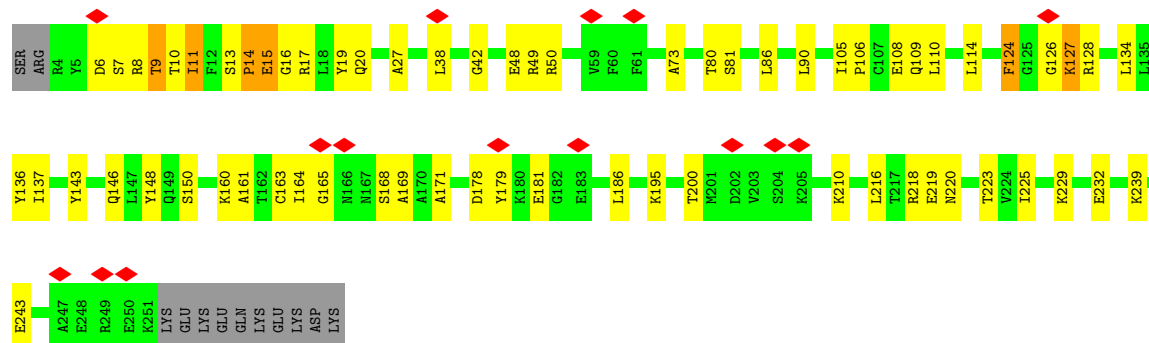
- Molecule 20: Proteasome subunit alpha type-2

Chain h: 



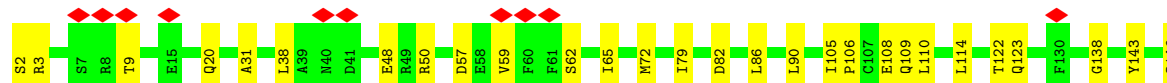
- Molecule 21: Proteasome subunit alpha type-4

Chain I: 

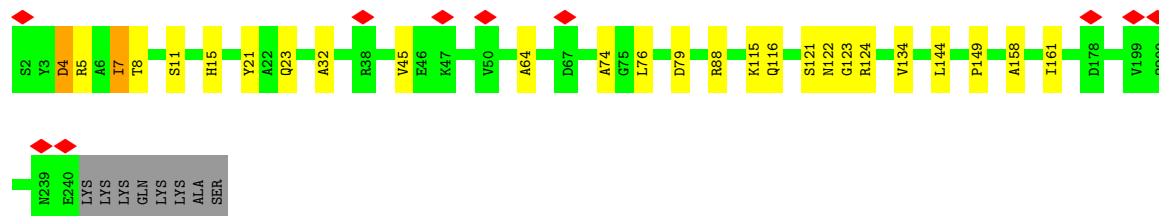
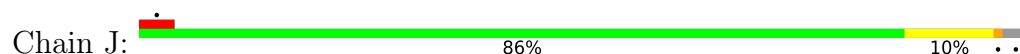


- Molecule 21: Proteasome subunit alpha type-4

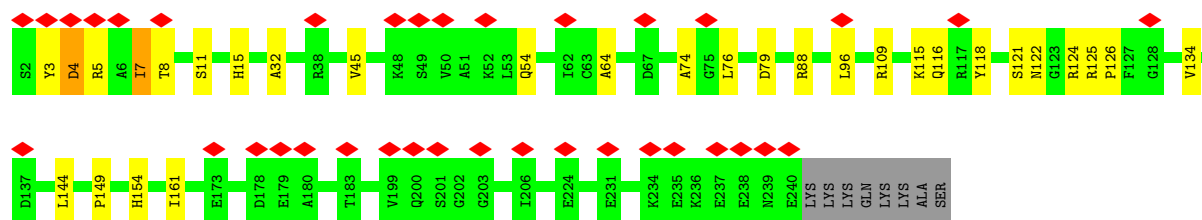
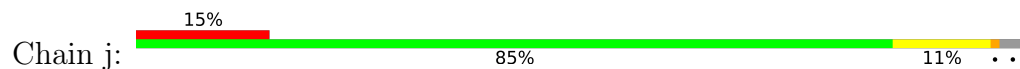
Chain i: 



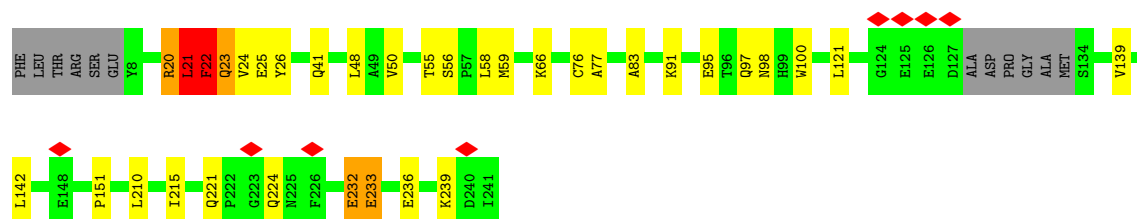
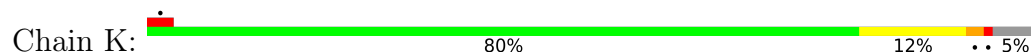
- Molecule 22: Proteasome subunit alpha type-7



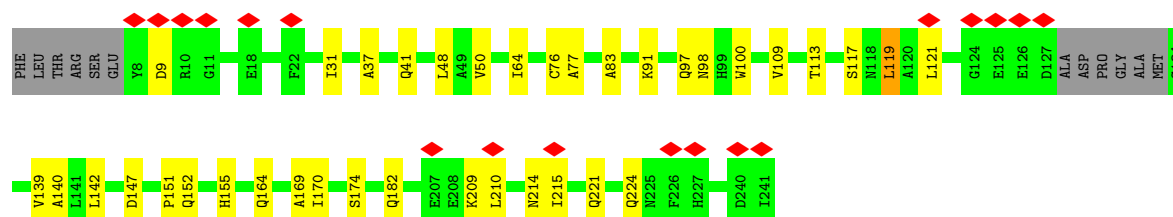
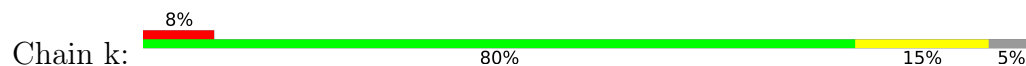
- Molecule 22: Proteasome subunit alpha type-7

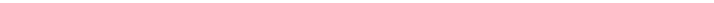


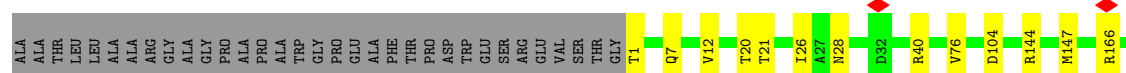
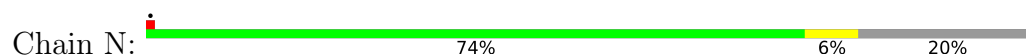
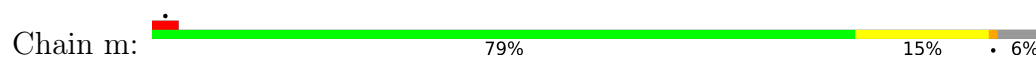
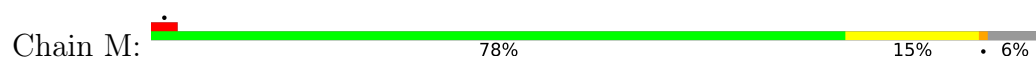
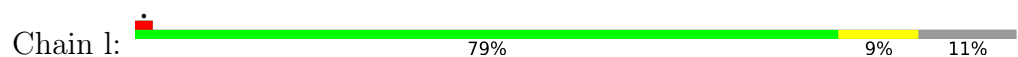
- Molecule 23: Proteasome subunit alpha type-5

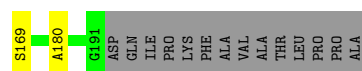


- Molecule 23: Proteasome subunit alpha type-5



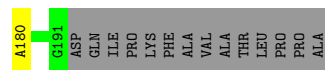
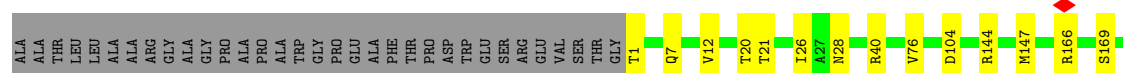
- Chain L:  81% 7% 11%





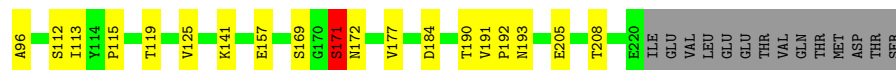
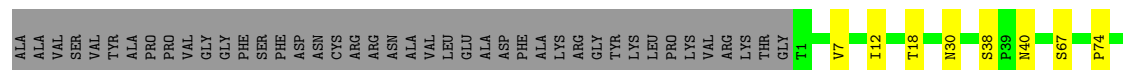
• Molecule 26: Proteasome subunit beta type-6

Chain n: 74% 6% 20%



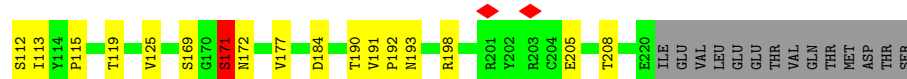
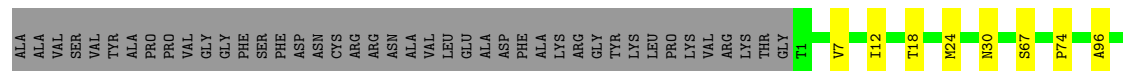
• Molecule 27: Proteasome subunit beta type-7

Chain O: 70% 9% 20%



• Molecule 27: Proteasome subunit beta type-7

Chain o: 71% 9% 20%



• Molecule 28: Proteasome subunit beta type-3

Chain P: 92% 8%

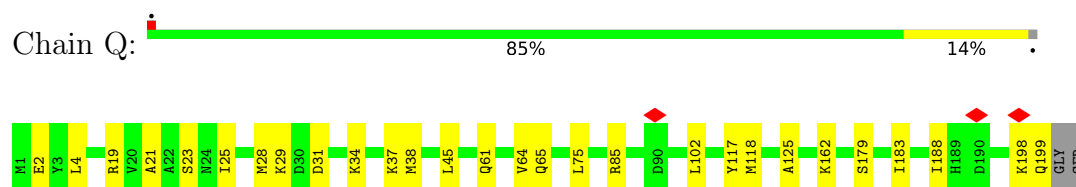


• Molecule 28: Proteasome subunit beta type-3

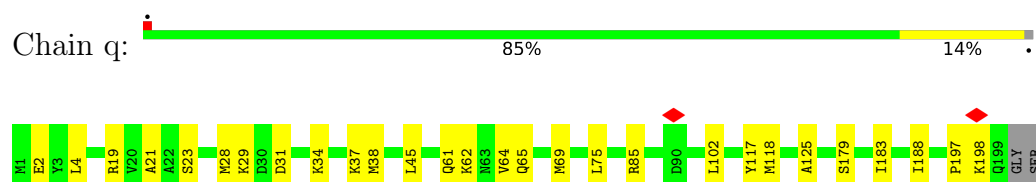
Chain p: 91% 9%



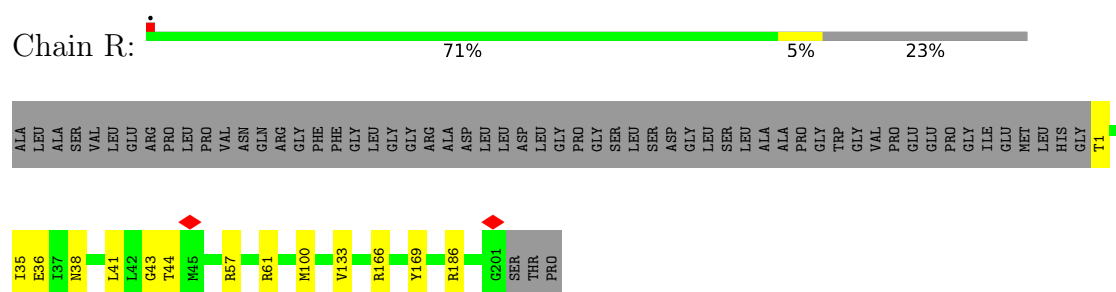
- Molecule 29: Proteasome subunit beta type-2



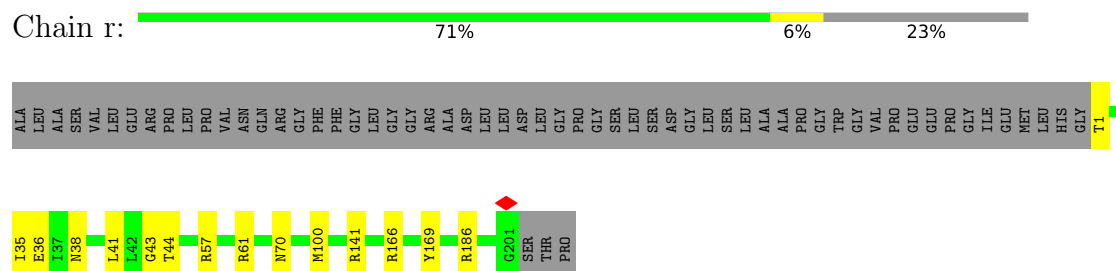
- Molecule 29: Proteasome subunit beta type-2



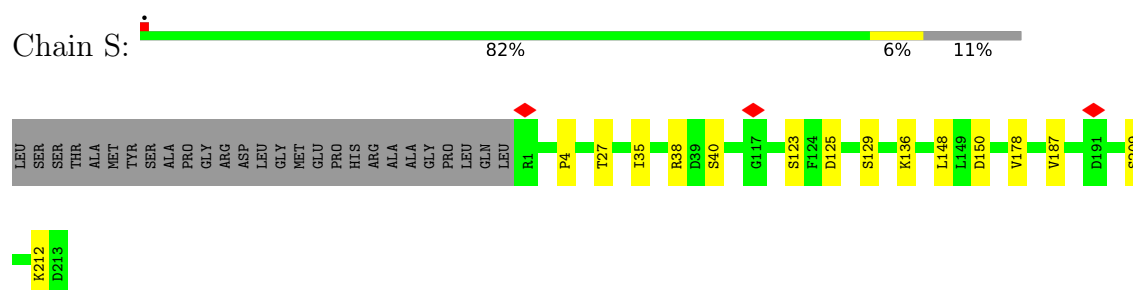
- Molecule 30: Proteasome subunit beta type-5



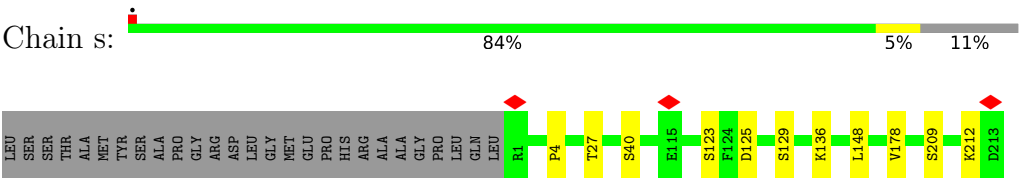
- Molecule 30: Proteasome subunit beta type-5



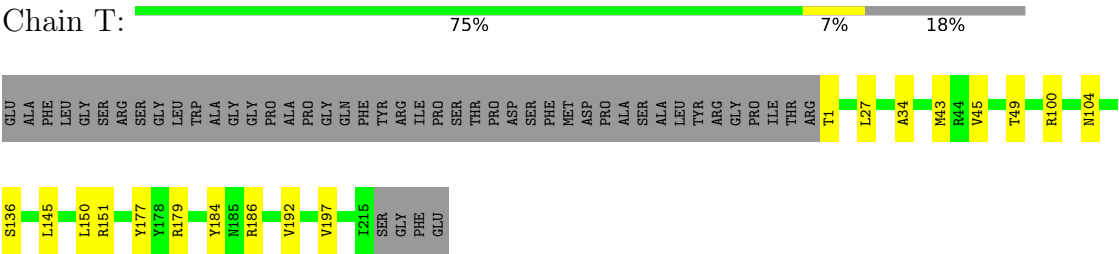
- Molecule 31: Proteasome subunit beta type-1



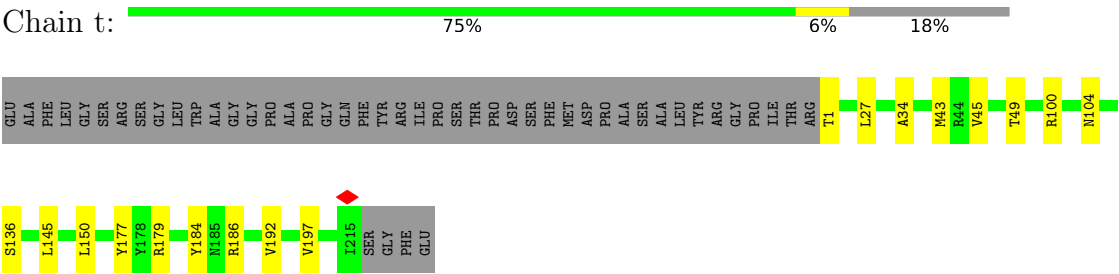
- Molecule 31: Proteasome subunit beta type-1



• Molecule 32: Proteasome subunit beta type-4



• Molecule 32: Proteasome subunit beta type-4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59461	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 ($e^-/\text{\AA}^2$)	46.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.117	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0337	Depositor
Map size ($\text{\AA}$)	438.4, 438.4, 438.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.37, 1.37, 1.37	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	U	0.25	0/6945	0.71	17/9382 (0.2%)
2	V	0.26	0/3929	0.71	4/5309 (0.1%)
3	W	0.24	0/3751	0.65	3/5042 (0.1%)
4	X	0.21	0/3053	0.66	4/4115 (0.1%)
5	Y	0.24	0/3173	0.66	2/4273 (0.0%)
6	Z	0.24	0/2318	0.82	12/3142 (0.4%)
7	a	0.24	0/3053	0.65	2/4133 (0.0%)
8	b	0.22	0/1478	0.70	2/2001 (0.1%)
9	c	0.25	0/2302	0.80	5/3110 (0.2%)
10	d	0.25	0/2162	0.72	8/2919 (0.3%)
11	e	0.24	0/338	0.67	0/450
12	f	0.30	0/6980	0.87	15/9433 (0.2%)
13	A	0.22	0/3283	0.59	0/4433
14	B	0.27	0/3254	0.69	3/4388 (0.1%)
15	C	0.24	0/3146	0.65	2/4226 (0.0%)
16	D	0.26	0/3090	0.68	5/4168 (0.1%)
17	E	0.27	0/3145	0.98	13/4233 (0.3%)
18	F	0.22	0/3137	0.63	5/4223 (0.1%)
19	G	0.26	0/1853	0.62	3/2515 (0.1%)
19	g	0.19	0/1859	0.52	0/2523
20	H	0.22	0/1727	0.53	0/2350
20	h	0.18	0/1743	0.44	0/2372
21	I	0.24	0/1925	0.62	2/2606 (0.1%)
21	i	0.18	0/1942	0.54	0/2628
22	J	0.18	0/1728	0.52	2/2358 (0.1%)
22	j	0.19	0/1728	0.53	2/2358 (0.1%)
23	K	0.23	0/1755	0.62	4/2375 (0.2%)
23	k	0.19	0/1747	0.47	0/2364
24	L	0.27	0/1885	0.53	1/2552 (0.0%)
24	l	0.27	0/1885	0.53	1/2552 (0.0%)
25	M	0.20	0/1891	0.59	2/2552 (0.1%)
25	m	0.20	0/1891	0.59	2/2552 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	N	0.18	0/1454	0.49	0/1967
26	n	0.18	0/1454	0.49	0/1967
27	O	0.19	0/1670	0.48	1/2265 (0.0%)
27	o	0.19	0/1670	0.48	1/2265 (0.0%)
28	P	0.17	0/1614	0.40	0/2177
28	p	0.17	0/1614	0.40	0/2177
29	Q	0.18	0/1603	0.47	0/2174
29	q	0.18	0/1603	0.47	0/2174
30	R	0.16	0/1579	0.37	0/2134
30	r	0.16	0/1579	0.37	0/2134
31	S	0.17	0/1671	0.42	0/2253
31	s	0.17	0/1671	0.42	0/2253
32	T	0.18	0/1700	0.43	0/2305
32	t	0.18	0/1700	0.43	0/2305
All	All	0.23	0/106678	0.64	123/144187 (0.1%)

There are no bond length outliers.

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	E	165	ILE	CA-C-N	25.38	146.53	120.38
17	E	165	ILE	C-N-CA	25.38	146.53	120.38
12	f	755	ASP	CA-C-N	14.88	138.45	119.84
12	f	755	ASP	C-N-CA	14.88	138.45	119.84
12	f	774	GLY	N-CA-C	-14.36	97.61	114.69
17	E	166	PRO	N-CA-C	13.42	127.07	110.70
6	Z	217	THR	N-CA-C	-13.13	97.02	111.07
4	X	203	PRO	N-CA-C	-12.59	95.34	110.70
5	Y	175	ASP	N-CA-C	-11.25	100.27	114.56
8	b	22	LEU	CA-C-N	10.90	130.31	118.97
8	b	22	LEU	C-N-CA	10.90	130.31	118.97
1	U	173	VAL	CA-C-N	10.70	133.21	119.84
1	U	173	VAL	C-N-CA	10.70	133.21	119.84
25	m	230	ASP	N-CA-C	-10.63	99.69	111.28
4	X	202	CYS	CA-C-N	10.60	131.30	120.38
4	X	202	CYS	C-N-CA	10.60	131.30	120.38
25	M	230	ASP	N-CA-C	-10.55	99.78	111.28
17	E	281	ARG	CA-C-N	10.37	132.80	119.84
17	E	281	ARG	C-N-CA	10.37	132.80	119.84
1	U	874	ASN	N-CA-C	-9.73	100.33	112.88
1	U	809	SER	N-CA-C	9.72	120.72	108.19
23	K	233	GLU	N-CA-C	-9.66	100.60	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	c	279	ASP	CA-C-N	8.69	130.70	119.84
9	c	279	ASP	C-N-CA	8.69	130.70	119.84
3	W	173	THR	N-CA-C	-8.66	101.75	111.71
4	X	317	PRO	N-CA-C	-8.54	101.26	113.47
5	Y	65	ILE	N-CA-C	8.50	123.55	112.76
6	Z	216	ALA	N-CA-C	-8.46	101.28	111.69
6	Z	237	LEU	CA-C-N	7.92	129.74	119.84
6	Z	237	LEU	C-N-CA	7.92	129.74	119.84
25	M	7	TYR	N-CA-C	-7.84	103.62	113.02
1	U	807	LYS	O-C-N	7.74	125.61	120.27
17	E	228	CYS	CA-C-N	-7.71	112.61	123.10
17	E	228	CYS	C-N-CA	-7.71	112.61	123.10
12	f	341	GLU	N-CA-C	7.60	122.15	108.55
10	d	89	LEU	CA-C-N	7.49	128.07	120.14
10	d	89	LEU	C-N-CA	7.49	128.07	120.14
12	f	773	LYS	N-CA-C	7.34	118.87	108.00
18	F	344	ARG	N-CA-C	7.32	126.39	110.80
15	C	397	LYS	CA-C-N	7.20	135.29	121.54
15	C	397	LYS	C-N-CA	7.20	135.29	121.54
10	d	202	THR	CA-C-N	7.18	128.81	119.84
10	d	202	THR	C-N-CA	7.18	128.81	119.84
12	f	341	GLU	CA-C-N	-7.08	110.99	119.84
12	f	341	GLU	C-N-CA	-7.08	110.99	119.84
27	o	171	SER	N-CA-C	7.07	125.86	110.80
27	O	171	SER	N-CA-C	7.03	125.77	110.80
6	Z	144	VAL	N-CA-C	-6.97	103.73	110.42
1	U	416	GLU	N-CA-C	6.78	119.29	111.02
23	K	21	LEU	CA-C-N	6.76	134.46	121.54
23	K	21	LEU	C-N-CA	6.76	134.46	121.54
6	Z	15	VAL	N-CA-C	6.76	116.91	110.42
18	F	86	LEU	CA-C-N	6.68	128.19	119.84
18	F	86	LEU	C-N-CA	6.68	128.19	119.84
1	U	872	GLU	CA-C-N	6.65	128.16	119.84
1	U	872	GLU	C-N-CA	6.65	128.16	119.84
19	G	9	PHE	CA-C-N	-6.58	112.99	122.67
19	G	9	PHE	C-N-CA	-6.58	112.99	122.67
21	I	13	SER	CA-C-N	6.54	128.01	119.84
21	I	13	SER	C-N-CA	6.54	128.01	119.84
25	m	7	TYR	N-CA-C	-6.50	105.33	113.20
10	d	236	THR	CA-C-N	6.36	126.54	120.43
10	d	236	THR	C-N-CA	6.36	126.54	120.43
9	c	279	ASP	N-CA-C	6.35	123.85	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	29	PRO	CA-C-N	6.32	127.74	119.84
2	V	29	PRO	C-N-CA	6.32	127.74	119.84
16	D	236	VAL	N-CA-C	-6.23	106.36	111.91
16	D	410	ASP	N-CA-C	-6.15	106.38	114.31
1	U	172	ASP	O-C-N	6.14	130.34	123.40
14	B	137	SER	N-CA-C	6.13	123.87	110.80
22	J	4	ASP	CA-C-N	6.00	132.99	121.54
22	J	4	ASP	C-N-CA	6.00	132.99	121.54
22	j	4	ASP	CA-C-N	5.99	132.98	121.54
22	j	4	ASP	C-N-CA	5.99	132.98	121.54
1	U	796	LYS	CA-C-N	-5.99	111.41	122.06
1	U	796	LYS	C-N-CA	-5.99	111.41	122.06
17	E	251	ARG	CA-C-O	-5.95	112.00	120.51
9	c	200	TYR	CA-C-N	5.94	132.89	121.54
9	c	200	TYR	C-N-CA	5.94	132.89	121.54
16	D	268	ASP	N-CA-C	-5.88	105.95	113.01
7	a	214	GLY	CA-C-N	5.85	132.72	121.54
7	a	214	GLY	C-N-CA	5.85	132.72	121.54
2	V	191	LEU	N-CA-C	-5.85	105.96	112.57
12	f	868	HIS	CA-C-N	5.69	132.42	121.54
12	f	868	HIS	C-N-CA	5.69	132.42	121.54
1	U	813	TYR	N-CA-C	5.66	122.32	109.81
18	F	72	LYS	CA-C-N	5.66	132.16	121.97
18	F	72	LYS	C-N-CA	5.66	132.16	121.97
6	Z	70	LEU	N-CA-C	-5.63	99.35	108.52
6	Z	64	ASP	CA-C-N	5.58	132.20	121.54
6	Z	64	ASP	C-N-CA	5.58	132.20	121.54
24	L	118	ILE	CA-CB-CG1	5.56	119.84	110.40
24	l	118	ILE	CA-CB-CG1	5.55	119.84	110.40
23	K	22	PHE	N-CA-CB	5.46	119.71	110.49
17	E	225	HIS	CA-C-N	5.41	135.00	121.80
17	E	225	HIS	C-N-CA	5.41	135.00	121.80
6	Z	12	HIS	CA-C-N	-5.40	113.34	120.96
6	Z	12	HIS	C-N-CA	-5.40	113.34	120.96
1	U	223	LEU	CA-C-N	5.37	131.80	121.54
1	U	223	LEU	C-N-CA	5.37	131.80	121.54
6	Z	69	PHE	N-CA-C	5.33	117.12	108.26
12	f	737	ASN	N-CA-C	-5.29	104.14	111.28
2	V	27	PRO	N-CA-C	5.29	117.15	110.70
16	D	269	ALA	CA-C-N	-5.26	115.80	122.43
16	D	269	ALA	C-N-CA	-5.26	115.80	122.43
1	U	812	ALA	N-CA-C	5.25	121.99	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	f	254	GLY	N-CA-C	5.21	118.54	112.50
14	B	164	MET	CA-C-N	5.21	131.48	121.54
14	B	164	MET	C-N-CA	5.21	131.48	121.54
17	E	165	ILE	C-N-CD	-5.20	103.69	125.00
10	d	198	LEU	CA-C-N	5.19	131.46	121.54
10	d	198	LEU	C-N-CA	5.19	131.46	121.54
12	f	619	HIS	CA-C-N	5.19	131.45	121.54
12	f	619	HIS	C-N-CA	5.19	131.45	121.54
17	E	2	ALA	CB-CA-C	-5.17	110.60	116.54
12	f	858	LYS	CA-C-N	-5.15	113.40	119.84
12	f	858	LYS	C-N-CA	-5.15	113.40	119.84
19	G	209	ASP	N-CA-C	-5.11	104.19	111.24
3	W	44	ILE	CA-C-N	5.05	131.19	121.54
3	W	44	ILE	C-N-CA	5.05	131.19	121.54
17	E	272	ARG	CA-CB-CG	5.05	124.20	114.10
1	U	424	ALA	N-CA-C	-5.02	105.93	111.71
1	U	182	LYS	N-CA-C	-5.01	105.51	110.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	6828	0	6884	154	0
2	V	3852	0	3893	120	0
3	W	3703	0	3822	125	0
4	X	3009	0	3112	64	0
5	Y	3115	0	3118	118	0
6	Z	2276	0	2307	104	0
7	a	2995	0	3012	51	0
8	b	1458	0	1505	43	0
9	c	2260	0	2276	52	0
10	d	2116	0	2146	33	0
11	e	334	0	294	27	0
12	f	6866	0	6866	277	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	A	3229	0	3260	55	0
14	B	3207	0	3278	53	0
15	C	3105	0	3218	76	0
16	D	3040	0	3075	64	0
17	E	3097	0	3174	145	0
18	F	3098	0	3186	117	0
19	G	1820	0	1791	67	0
19	g	1826	0	1796	29	0
20	H	1692	0	1586	53	0
20	h	1708	0	1594	13	0
21	I	1895	0	1833	56	0
21	i	1912	0	1851	28	0
22	J	1704	0	1517	18	0
22	j	1704	0	1517	24	0
23	K	1729	0	1680	41	0
23	k	1722	0	1673	24	0
24	L	1850	0	1822	11	0
24	l	1850	0	1822	16	0
25	M	1856	0	1814	38	0
25	m	1856	0	1814	36	0
26	N	1430	0	1398	8	0
26	n	1430	0	1398	8	0
27	O	1643	0	1644	21	0
27	o	1643	0	1644	20	0
28	P	1585	0	1598	10	0
28	p	1585	0	1598	12	0
29	Q	1570	0	1547	18	0
29	q	1570	0	1547	17	0
30	R	1548	0	1499	10	0
30	r	1548	0	1499	11	0
31	S	1641	0	1618	11	0
31	s	1641	0	1618	6	0
32	T	1667	0	1628	14	0
32	t	1667	0	1628	11	0
33	c	1	0	0	0	0
34	A	31	0	12	1	0
34	B	31	0	12	2	0
34	C	31	0	12	2	0
34	F	31	0	12	1	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	D	1	0	0	0	0
35	F	1	0	0	0	0
36	D	27	0	12	0	0
All	All	105037	0	104460	1986	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 9.

All (1986) 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)
17:E:164:ILE:CG1	17:E:166:PRO:HG2	1.39	1.52
8:b:22:LEU:HB3	8:b:23:PRO:CD	1.32	1.46
13:A:123:VAL:HA	18:F:86:LEU:CD1	1.42	1.46
12:f:281:ILE:HD11	12:f:285:CYS:SG	1.56	1.43
4:X:143:TYR:OH	5:Y:252:SER:CA	1.64	1.43
12:f:281:ILE:CD1	12:f:285:CYS:SG	2.07	1.41
5:Y:293:ARG:NE	11:e:57:ARG:CG	1.84	1.39
20:H:6:TYR:OH	21:I:6:ASP:CB	1.68	1.39
12:f:755:ASP:CB	12:f:756:PRO:HD3	1.35	1.37
2:V:188:SER:O	2:V:192:MET:CG	1.73	1.37
6:Z:234:PHE:O	6:Z:237:LEU:CD2	1.71	1.36
1:U:423:MET:SD	1:U:446:LEU:CD1	2.14	1.36
27:O:171:SER:OG	27:O:192:PRO:HD2	1.24	1.35
4:X:143:TYR:OH	5:Y:252:SER:CB	1.73	1.34
12:f:785:ARG:HH22	12:f:790:GLN:N	1.20	1.34
12:f:838:ARG:HB3	12:f:839:PRO:CD	1.48	1.34
5:Y:293:ARG:NE	11:e:57:ARG:HG3	1.01	1.32
17:E:196:LEU:O	17:E:197:LYS:HG3	1.19	1.32
13:A:123:VAL:CA	18:F:86:LEU:HD11	1.58	1.31
15:C:221:GLN:OE1	15:C:227:GLY:HA2	1.21	1.31
1:U:804:SER:HB3	1:U:874:ASN:O	1.19	1.31
8:b:22:LEU:HD12	18:F:49:ASP:OD2	1.26	1.29
12:f:810:ILE:CG2	12:f:855:GLN:OE1	1.79	1.29
19:G:12:HIS:NE2	25:M:7:TYR:HE1	1.30	1.29
1:U:347:ASN:CB	1:U:813:TYR:OH	1.80	1.28
27:o:171:SER:OG	27:o:192:PRO:HD2	1.27	1.27
14:B:434:THR:CB	14:B:435:PRO:HD3	1.65	1.26
8:b:22:LEU:CB	8:b:23:PRO:CD	2.13	1.25
17:E:165:ILE:N	17:E:166:PRO:HD2	1.21	1.24
17:E:164:ILE:HG13	17:E:166:PRO:CG	1.66	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:316:ASP:OD1	4:X:320:SER:HB3	1.36	1.22
16:D:336:PRO:HG3	16:D:370:ILE:O	1.07	1.22
5:Y:279:GLU:OE2	5:Y:292:TYR:HB2	1.40	1.21
1:U:423:MET:CE	1:U:442:GLY:O	1.89	1.20
5:Y:293:ARG:HE	11:e:57:ARG:CG	1.47	1.20
18:F:324:THR:HG22	18:F:327:LYS:CE	1.72	1.20
12:f:809:ILE:HD11	12:f:855:GLN:NE2	1.55	1.19
6:Z:234:PHE:O	6:Z:237:LEU:HD21	1.04	1.19
1:U:423:MET:HE1	1:U:442:GLY:O	1.06	1.18
13:A:123:VAL:C	18:F:86:LEU:HD11	1.68	1.18
12:f:785:ARG:NH2	12:f:790:GLN:H	1.42	1.18
18:F:86:LEU:HB3	18:F:87:PRO:HD3	1.22	1.18
1:U:347:ASN:HB3	1:U:813:TYR:CZ	1.78	1.17
8:b:22:LEU:CB	8:b:23:PRO:HD3	1.70	1.17
4:X:316:ASP:OD1	4:X:320:SER:CB	1.92	1.16
12:f:755:ASP:CB	12:f:756:PRO:CD	2.22	1.16
19:G:12:HIS:CD2	25:M:7:TYR:CE1	2.34	1.16
2:V:31:ALA:HB3	2:V:32:PRO:HD3	1.23	1.16
12:f:657:ILE:O	12:f:661:ALA:HB3	1.44	1.16
14:B:434:THR:HB	14:B:435:PRO:CD	1.73	1.15
18:F:435:LEU:CD2	23:K:20:ARG:HD3	1.76	1.15
12:f:764:LEU:CD1	12:f:775:THR:HG22	1.76	1.15
16:D:336:PRO:CG	16:D:370:ILE:O	1.94	1.15
1:U:423:MET:SD	1:U:446:LEU:HD11	1.86	1.14
17:E:235:ILE:CG2	17:E:279:THR:HB	1.78	1.14
19:G:12:HIS:NE2	25:M:7:TYR:CE1	2.14	1.14
2:V:188:SER:O	2:V:192:MET:HG2	0.95	1.12
12:f:755:ASP:CG	12:f:756:PRO:HD3	1.73	1.13
12:f:755:ASP:CG	12:f:756:PRO:CD	2.22	1.12
2:V:417:ILE:CD1	5:Y:349:LYS:HG2	1.79	1.12
19:G:12:HIS:CD2	25:M:7:TYR:HE1	1.66	1.12
4:X:316:ASP:OD1	4:X:320:SER:CA	1.96	1.12
3:W:435:LEU:HD13	6:Z:237:LEU:HB2	1.26	1.12
17:E:165:ILE:N	17:E:166:PRO:CD	2.13	1.11
12:f:838:ARG:CB	12:f:839:PRO:CD	2.27	1.11
3:W:426:ASN:OD1	9:c:233:ASP:OD1	1.67	1.11
5:Y:293:ARG:CZ	11:e:57:ARG:HG3	1.70	1.11
12:f:810:ILE:HG21	12:f:855:GLN:HA	1.30	1.11
1:U:423:MET:CE	1:U:446:LEU:HD12	1.82	1.10
12:f:809:ILE:CD1	12:f:855:GLN:HE22	1.64	1.10
16:D:335:LEU:HB3	16:D:336:PRO:CD	1.82	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:836:GLU:HB2	12:f:840:LEU:HD11	1.33	1.10
2:V:188:SER:C	2:V:192:MET:HG2	1.76	1.09
8:b:22:LEU:CD1	18:F:49:ASP:OD2	2.01	1.09
16:D:207:PRO:HG2	16:D:335:LEU:HD21	1.25	1.09
17:E:196:LEU:O	17:E:197:LYS:CG	2.00	1.09
14:B:434:THR:CB	14:B:435:PRO:CD	2.29	1.08
3:W:435:LEU:HD13	6:Z:237:LEU:CB	1.83	1.08
4:X:143:TYR:OH	5:Y:252:SER:HA	1.49	1.08
5:Y:174:TRP:CZ2	15:C:377:HIS:CD2	2.41	1.08
6:Z:237:LEU:CD2	6:Z:238:PRO:HD2	1.84	1.08
12:f:281:ILE:HD13	12:f:285:CYS:SG	1.84	1.08
4:X:143:TYR:OH	5:Y:252:SER:HB2	1.34	1.08
20:H:11:THR:OG1	21:I:127:LYS:HA	1.54	1.07
1:U:807:LYS:HB2	1:U:808:PRO:HD3	1.31	1.07
19:g:46:ASP:O	19:g:222:VAL:HG23	1.54	1.07
20:H:6:TYR:OH	21:I:6:ASP:HB2	1.55	1.07
20:H:6:TYR:OH	21:I:6:ASP:CG	1.96	1.06
8:b:22:LEU:HD11	18:F:45:THR:CG2	1.84	1.06
16:D:335:LEU:HB3	16:D:336:PRO:HD3	1.37	1.06
12:f:838:ARG:CB	12:f:839:PRO:HD2	1.83	1.05
1:U:347:ASN:HB3	1:U:813:TYR:OH	0.89	1.05
12:f:785:ARG:NH2	12:f:790:GLN:CA	2.20	1.05
12:f:250:ARG:HH12	12:f:281:ILE:HG12	1.18	1.04
12:f:250:ARG:NH2	12:f:281:ILE:HG21	1.71	1.04
18:F:324:THR:HA	18:F:327:LYS:HE3	1.39	1.04
18:F:435:LEU:HD23	23:K:20:ARG:HD3	1.37	1.04
12:f:755:ASP:OD1	12:f:756:PRO:HD2	1.55	1.04
12:f:810:ILE:HG23	12:f:855:GLN:OE1	1.57	1.04
12:f:785:ARG:NH2	12:f:790:GLN:N	2.00	1.03
17:E:235:ILE:HG22	17:E:279:THR:HB	1.05	1.03
19:g:12:HIS:NE2	25:m:7:TYR:CD1	2.26	1.03
27:O:171:SER:OG	27:O:192:PRO:CD	2.05	1.03
17:E:164:ILE:CG1	17:E:166:PRO:CG	2.32	1.03
18:F:324:THR:CG2	18:F:327:LYS:NZ	2.22	1.03
15:C:221:GLN:OE1	15:C:227:GLY:CA	2.07	1.03
1:U:424:ALA:O	1:U:427:LEU:HD11	1.59	1.02
18:F:341:ALA:HA	18:F:344:ARG:HD3	1.37	1.02
18:F:340:PRO:O	18:F:344:ARG:HG3	1.60	1.02
1:U:47:VAL:HG12	1:U:48:LEU:N	1.75	1.01
2:V:417:ILE:HD12	5:Y:349:LYS:HG2	1.02	1.01
3:W:435:LEU:CD1	6:Z:237:LEU:HG	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:755:ASP:HB2	12:f:756:PRO:HD3	1.02	1.01
3:W:435:LEU:HD11	6:Z:237:LEU:HD23	1.42	1.01
17:E:1:MET:SD	17:E:1:MET:N	2.31	1.01
1:U:148:LYS:HE3	1:U:179:TYR:CE2	1.97	1.00
1:U:174:PRO:HB3	1:U:208:LEU:HD11	1.44	1.00
12:f:785:ARG:HH22	12:f:790:GLN:CA	1.74	1.00
1:U:424:ALA:O	1:U:427:LEU:CD1	2.10	1.00
25:M:229:LYS:NZ	25:M:229:LYS:HA	1.76	1.00
4:X:318:ILE:O	4:X:318:ILE:HG22	1.60	0.99
12:f:810:ILE:HG21	12:f:855:GLN:OE1	1.62	0.99
25:m:229:LYS:HA	25:m:229:LYS:NZ	1.78	0.99
13:A:123:VAL:HA	18:F:86:LEU:HD11	1.11	0.99
19:G:19:GLU:HA	20:H:27:ALA:CB	1.93	0.99
20:H:6:TYR:OH	21:I:6:ASP:HB3	1.60	0.99
11:e:6:GLN:HE21	11:e:6:GLN:H	1.09	0.99
27:o:171:SER:OG	27:o:192:PRO:CD	2.10	0.99
3:W:435:LEU:CD1	6:Z:237:LEU:CG	2.41	0.98
2:V:417:ILE:HD12	5:Y:349:LYS:CG	1.93	0.98
3:W:435:LEU:HD12	6:Z:237:LEU:HG	1.45	0.98
12:f:809:ILE:HD11	12:f:855:GLN:HE22	1.07	0.98
23:K:23:GLN:HA	23:K:23:GLN:HE21	1.24	0.98
9:c:115:HIS:HD2	9:c:118:PHE:HZ	1.09	0.97
16:D:335:LEU:CB	16:D:336:PRO:CD	2.41	0.97
9:c:115:HIS:HD2	9:c:118:PHE:CZ	1.81	0.97
13:A:123:VAL:CA	18:F:86:LEU:CD1	2.26	0.97
18:F:324:THR:HG23	18:F:327:LYS:NZ	1.78	0.97
12:f:764:LEU:HD12	12:f:775:THR:HG22	1.44	0.97
5:Y:233:ARG:N	5:Y:234:PRO:HD2	1.78	0.97
5:Y:293:ARG:CZ	11:e:57:ARG:CG	2.30	0.96
12:f:567:LEU:HD22	12:f:773:LYS:CE	1.94	0.96
17:E:198:VAL:HG11	17:E:232:MET:SD	2.05	0.96
12:f:250:ARG:NH1	12:f:281:ILE:HG12	1.81	0.96
19:G:12:HIS:CE1	25:M:7:TYR:HE1	1.84	0.96
20:H:11:THR:OG1	21:I:127:LYS:CA	2.13	0.95
1:U:423:MET:CE	1:U:446:LEU:CD1	2.42	0.95
5:Y:231:LEU:HB2	5:Y:234:PRO:HG2	1.48	0.95
4:X:371:ASP:OD1	5:Y:233:ARG:NH1	1.99	0.95
6:Z:237:LEU:HB2	6:Z:238:PRO:HD3	1.45	0.95
27:O:171:SER:HG	27:O:192:PRO:HD2	1.29	0.95
9:c:50:PRO:HG2	17:E:53:VAL:CG1	1.95	0.95
17:E:235:ILE:HG22	17:E:279:THR:CB	1.95	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:341:ALA:HA	18:F:344:ARG:CD	1.96	0.94
19:g:46:ASP:CB	19:g:222:VAL:HG21	1.97	0.94
4:X:143:TYR:CZ	5:Y:252:SER:HB2	2.02	0.94
4:X:216:ILE:HD12	4:X:318:ILE:HD13	1.49	0.94
19:g:12:HIS:NE2	25:m:7:TYR:HD1	1.65	0.94
2:V:414:TYR:HE1	5:Y:349:LYS:NZ	1.65	0.94
12:f:785:ARG:CZ	12:f:790:GLN:HB2	1.97	0.94
1:U:804:SER:CB	1:U:874:ASN:O	2.15	0.94
13:A:123:VAL:HA	18:F:86:LEU:HD12	1.46	0.94
2:V:189:ASP:HA	2:V:192:MET:HB2	1.49	0.93
6:Z:237:LEU:HB2	6:Z:238:PRO:CD	1.95	0.93
12:f:785:ARG:HH21	12:f:791:VAL:N	1.67	0.93
1:U:423:MET:HE3	1:U:446:LEU:HD12	1.48	0.93
3:W:141:GLU:O	3:W:172:GLU:OE2	1.85	0.93
4:X:316:ASP:OD1	4:X:320:SER:N	2.02	0.92
17:E:281:ARG:HH11	17:E:281:ARG:HG3	1.34	0.92
12:f:567:LEU:HD22	12:f:773:LYS:HE3	1.50	0.92
12:f:810:ILE:HD13	12:f:853:VAL:O	1.68	0.92
17:E:281:ARG:N	17:E:282:PRO:HD2	1.82	0.92
5:Y:174:TRP:HZ3	15:C:337:ASN:O	1.52	0.92
12:f:281:ILE:HD11	12:f:285:CYS:HG	1.29	0.92
12:f:756:PRO:HG2	12:f:758:ASN:O	1.68	0.92
12:f:785:ARG:NH2	12:f:790:GLN:HB2	1.85	0.92
12:f:810:ILE:CD1	12:f:853:VAL:O	2.17	0.92
4:X:143:TYR:OH	5:Y:252:SER:N	2.02	0.91
1:U:873:PRO:O	1:U:876:GLN:NE2	2.03	0.91
12:f:764:LEU:CD1	12:f:775:THR:CG2	2.48	0.91
4:X:253:TYR:HE1	4:X:318:ILE:HB	1.35	0.91
5:Y:233:ARG:H	5:Y:234:PRO:HD2	1.33	0.91
17:E:235:ILE:CG2	17:E:279:THR:CB	2.49	0.91
18:F:435:LEU:HD21	23:K:20:ARG:HD3	1.51	0.91
1:U:423:MET:SD	1:U:446:LEU:HD13	2.09	0.90
17:E:127:PRO:HB3	17:E:193:CYS:SG	2.11	0.90
12:f:809:ILE:CG1	12:f:855:GLN:HE22	1.84	0.90
18:F:324:THR:CG2	18:F:327:LYS:CE	2.50	0.90
2:V:188:SER:O	2:V:192:MET:CB	2.18	0.90
3:W:142:ARG:HH22	3:W:178:GLU:HB2	1.37	0.90
12:f:764:LEU:HD23	12:f:764:LEU:O	1.70	0.90
18:F:324:THR:HG22	18:F:327:LYS:CD	2.00	0.90
12:f:755:ASP:HB2	12:f:756:PRO:CD	1.96	0.90
20:H:6:TYR:OH	21:I:6:ASP:OD2	1.87	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:174:TRP:CD1	5:Y:177:ARG:HD3	2.07	0.90
17:E:165:ILE:H	17:E:166:PRO:HD2	1.19	0.90
17:E:164:ILE:CD1	17:E:166:PRO:CG	2.50	0.90
20:H:11:THR:O	21:I:127:LYS:O	1.90	0.90
17:E:164:ILE:CD1	17:E:166:PRO:HG2	2.00	0.90
10:d:88:GLN:NE2	10:d:88:GLN:HA	1.87	0.89
14:B:434:THR:HB	14:B:435:PRO:HD3	0.91	0.89
2:V:31:ALA:HB3	2:V:32:PRO:CD	2.01	0.89
5:Y:293:ARG:NE	11:e:57:ARG:CB	2.34	0.89
3:W:435:LEU:CD1	6:Z:238:PRO:HD3	2.03	0.89
12:f:810:ILE:CG2	12:f:855:GLN:HA	2.01	0.89
12:f:567:LEU:CD2	12:f:773:LYS:HE3	2.02	0.89
9:c:115:HIS:CD2	9:c:118:PHE:CZ	2.61	0.89
12:f:755:ASP:CG	12:f:756:PRO:HD2	1.91	0.89
12:f:760:PHE:HE2	12:f:855:GLN:HE21	1.19	0.88
19:g:46:ASP:CB	19:g:222:VAL:CG2	2.51	0.88
8:b:22:LEU:HD11	18:F:45:THR:HG23	1.54	0.88
6:Z:234:PHE:O	6:Z:237:LEU:CD1	2.21	0.88
6:Z:237:LEU:HD23	6:Z:238:PRO:CD	2.04	0.87
8:b:22:LEU:CD1	18:F:45:THR:CG2	2.52	0.87
15:C:90:HIS:HB3	15:C:91:PRO:HD3	1.54	0.87
12:f:838:ARG:HB3	12:f:839:PRO:HD2	0.87	0.87
18:F:437:TYR:CE2	23:K:21:LEU:CD2	2.57	0.87
16:D:268:ASP:OD1	16:D:311:THR:CB	2.23	0.86
6:Z:234:PHE:O	6:Z:237:LEU:HD11	1.74	0.86
9:c:115:HIS:CD2	9:c:118:PHE:HZ	1.93	0.86
12:f:785:ARG:NH2	12:f:790:GLN:C	2.34	0.86
19:g:46:ASP:O	19:g:222:VAL:CG2	2.24	0.86
2:V:31:ALA:CB	2:V:32:PRO:HD3	2.06	0.86
3:W:426:ASN:OD1	9:c:233:ASP:CG	2.19	0.86
9:c:196:LEU:HA	9:c:200:TYR:CZ	2.10	0.86
23:K:21:LEU:H	23:K:21:LEU:HD22	1.37	0.86
8:b:22:LEU:CB	8:b:23:PRO:HD2	2.02	0.85
12:f:760:PHE:CE2	12:f:809:ILE:HD11	2.10	0.85
17:E:235:ILE:CG2	17:E:279:THR:CG2	2.54	0.85
12:f:785:ARG:NH2	12:f:790:GLN:CB	2.38	0.85
3:W:426:ASN:CG	9:c:233:ASP:OD2	2.20	0.85
5:Y:174:TRP:CD1	5:Y:177:ARG:CD	2.59	0.85
2:V:28:PRO:HB2	2:V:29:PRO:HD3	1.58	0.85
1:U:173:VAL:HG12	1:U:175:GLY:H	1.42	0.84
5:Y:174:TRP:NE1	5:Y:177:ARG:HD2	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:764:LEU:HD11	12:f:775:THR:CG2	2.06	0.84
6:Z:237:LEU:HD22	6:Z:238:PRO:HD2	1.57	0.84
4:X:143:TYR:CZ	5:Y:252:SER:CB	2.59	0.84
17:E:281:ARG:H	17:E:282:PRO:HD2	1.41	0.84
3:W:178:GLU:H	3:W:182:ARG:HB2	1.43	0.84
27:o:171:SER:HG	27:o:192:PRO:HD2	1.42	0.83
17:E:164:ILE:HD11	17:E:166:PRO:HG3	1.59	0.83
2:V:26:PRO:O	2:V:30:PRO:CG	2.27	0.83
17:E:188:ALA:HA	17:E:192:ASP:CB	2.08	0.83
2:V:26:PRO:O	2:V:30:PRO:CD	2.25	0.83
18:F:324:THR:HG22	18:F:327:LYS:HE3	1.59	0.83
6:Z:11:VAL:HB	6:Z:162:ILE:HD13	1.61	0.83
17:E:236:ASP:HB2	17:E:282:PRO:HG3	1.59	0.83
18:F:86:LEU:HB3	18:F:87:PRO:CD	2.07	0.83
19:g:12:HIS:NE2	25:m:7:TYR:CE1	2.47	0.83
12:f:836:GLU:CB	12:f:840:LEU:HD11	2.08	0.83
9:c:50:PRO:HG2	17:E:53:VAL:HG11	1.58	0.83
1:U:416:GLU:OE2	1:U:450:HIS:CD2	2.32	0.83
6:Z:228:TYR:HD2	7:a:341:LEU:HD21	1.43	0.82
17:E:198:VAL:HB	17:E:232:MET:HA	1.59	0.82
12:f:809:ILE:CD1	12:f:855:GLN:NE2	2.33	0.82
16:D:268:ASP:OD1	16:D:311:THR:HG22	1.79	0.82
5:Y:174:TRP:CH2	15:C:377:HIS:HA	2.15	0.82
6:Z:234:PHE:O	6:Z:237:LEU:CG	2.28	0.82
1:U:415:HIS:HE2	1:U:418:GLU:CD	1.86	0.81
9:c:279:ASP:HB3	9:c:280:PRO:CD	2.10	0.81
17:E:164:ILE:C	17:E:166:PRO:HD2	2.06	0.81
18:F:324:THR:CG2	18:F:327:LYS:HZ2	1.91	0.81
5:Y:293:ARG:CD	11:e:57:ARG:HB2	2.11	0.81
6:Z:237:LEU:CB	6:Z:238:PRO:CD	2.56	0.81
4:X:318:ILE:O	4:X:318:ILE:CG2	2.29	0.81
2:V:414:TYR:HE1	5:Y:349:LYS:HZ1	0.83	0.81
12:f:838:ARG:HD2	12:f:838:ARG:C	2.06	0.81
1:U:807:LYS:CB	1:U:808:PRO:HD3	2.06	0.80
12:f:642:ALA:N	12:f:643:PRO:HD2	1.95	0.80
6:Z:16:LEU:HD23	6:Z:17:LEU:H	1.46	0.80
18:F:324:THR:HG22	18:F:327:LYS:HD2	1.63	0.80
6:Z:237:LEU:HD23	6:Z:238:PRO:HD2	1.58	0.80
12:f:785:ARG:HH21	12:f:790:GLN:C	1.89	0.80
5:Y:293:ARG:HD3	11:e:57:ARG:HB2	1.62	0.80
3:W:142:ARG:NH2	3:W:178:GLU:HB2	1.95	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:237:LEU:CD2	6:Z:238:PRO:CD	2.59	0.80
12:f:662:MET:SD	13:A:65:ILE:HG21	2.20	0.80
18:F:437:TYR:CE2	23:K:21:LEU:HD22	2.17	0.79
1:U:180:SER:O	1:U:183:LEU:HB2	1.81	0.79
17:E:242:ARG:O	17:E:281:ARG:NH2	2.15	0.79
1:U:415:HIS:ND1	1:U:419:ALA:N	2.29	0.79
1:U:423:MET:HE1	1:U:442:GLY:C	2.04	0.79
5:Y:174:TRP:CE2	15:C:377:HIS:CD2	2.71	0.79
12:f:810:ILE:HD13	12:f:854:GLY:O	1.82	0.79
4:X:253:TYR:CE1	4:X:318:ILE:HB	2.18	0.79
6:Z:237:LEU:HD13	6:Z:237:LEU:H	1.45	0.79
18:F:324:THR:HG23	18:F:327:LYS:HZ1	1.48	0.79
17:E:164:ILE:HG13	17:E:166:PRO:HG2	0.81	0.79
19:G:12:HIS:CD2	25:M:7:TYR:CD1	2.72	0.78
2:V:29:PRO:HD2	2:V:30:PRO:HD2	1.65	0.78
17:E:164:ILE:HD11	17:E:166:PRO:CG	2.13	0.78
10:d:200:PHE:HB3	10:d:203:PRO:HG3	1.64	0.78
18:F:300:LYS:O	18:F:300:LYS:HE3	1.84	0.78
1:U:47:VAL:HG12	1:U:48:LEU:H	1.45	0.77
3:W:435:LEU:HD11	6:Z:237:LEU:CD2	2.14	0.77
4:X:143:TYR:CZ	5:Y:252:SER:HA	2.19	0.77
8:b:22:LEU:CD1	18:F:45:THR:HG22	2.13	0.77
19:g:12:HIS:CE1	25:m:7:TYR:HE1	2.02	0.77
5:Y:174:TRP:HE1	5:Y:177:ARG:HD2	1.50	0.77
20:H:6:TYR:HH	21:I:6:ASP:CG	1.82	0.77
12:f:337:LEU:HD23	12:f:341:GLU:OE1	1.85	0.77
16:D:268:ASP:OD2	16:D:312:ASN:N	2.17	0.77
17:E:236:ASP:CB	17:E:282:PRO:HG3	2.14	0.77
25:m:229:LYS:HD2	25:m:235:ALA:H	1.49	0.77
2:V:29:PRO:CD	2:V:30:PRO:HD2	2.15	0.77
12:f:838:ARG:HB3	12:f:839:PRO:HD3	1.66	0.77
3:W:142:ARG:HH22	3:W:178:GLU:CB	1.98	0.77
19:g:12:HIS:CE1	25:m:7:TYR:CE1	2.73	0.77
3:W:435:LEU:CD1	6:Z:237:LEU:HB2	2.11	0.76
4:X:316:ASP:OD1	4:X:320:SER:C	2.27	0.76
5:Y:233:ARG:N	5:Y:234:PRO:CD	2.48	0.76
17:E:222:ALA:HB1	17:E:228:CYS:SG	2.25	0.76
11:e:6:GLN:H	11:e:6:GLN:NE2	1.82	0.76
3:W:178:GLU:H	3:W:182:ARG:CB	1.97	0.76
16:D:335:LEU:CB	16:D:336:PRO:HD2	2.14	0.76
6:Z:16:LEU:CD2	6:Z:17:LEU:H	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:324:THR:CA	18:F:327:LYS:HE3	2.15	0.76
18:F:435:LEU:HD23	23:K:20:ARG:CD	2.13	0.76
12:f:773:LYS:HA	12:f:775:THR:HG23	1.67	0.76
5:Y:174:TRP:NE1	5:Y:177:ARG:CD	2.49	0.75
18:F:324:THR:HG22	18:F:327:LYS:NZ	1.91	0.75
25:M:229:LYS:O	25:M:229:LYS:HD3	1.85	0.75
17:E:198:VAL:HG11	17:E:232:MET:CE	2.16	0.75
17:E:194:ASN:CB	17:E:229:ILE:H	1.98	0.75
1:U:47:VAL:CG1	1:U:48:LEU:N	2.48	0.75
12:f:567:LEU:HD22	12:f:773:LYS:HE2	1.69	0.74
25:M:229:LYS:HA	25:M:229:LYS:CE	2.10	0.74
19:g:12:HIS:CD2	25:m:7:TYR:HD1	2.05	0.74
18:F:205:PRO:HB3	18:F:324:THR:CB	2.17	0.74
2:V:28:PRO:CB	2:V:29:PRO:HD3	2.17	0.74
17:E:235:ILE:HG23	17:E:236:ASP:H	1.52	0.74
5:Y:279:GLU:CD	5:Y:292:TYR:HB2	2.13	0.74
17:E:194:ASN:CG	17:E:229:ILE:H	1.96	0.74
12:f:785:ARG:NH2	12:f:791:VAL:N	2.35	0.73
12:f:828:ARG:CZ	12:f:843:SER:OG	2.37	0.73
14:B:434:THR:OG1	14:B:435:PRO:CD	2.35	0.73
16:D:210:CYS:SG	16:D:335:LEU:HD22	2.29	0.73
25:m:229:LYS:HA	25:m:229:LYS:CE	2.15	0.73
18:F:324:THR:HA	18:F:327:LYS:CE	2.16	0.73
4:X:137:TYR:HB3	4:X:142:ARG:HB2	1.69	0.73
2:V:25:GLU:O	2:V:28:PRO:HD2	1.88	0.73
3:W:435:LEU:HD11	6:Z:238:PRO:HD3	1.69	0.73
16:D:268:ASP:OD1	16:D:311:THR:CG2	2.36	0.73
8:b:22:LEU:HB3	8:b:23:PRO:HD3	0.74	0.73
12:f:657:ILE:O	12:f:661:ALA:CB	2.29	0.73
12:f:855:GLN:OE1	12:f:855:GLN:HA	1.88	0.73
2:V:189:ASP:CA	2:V:192:MET:HB2	2.19	0.72
4:X:316:ASP:OD1	4:X:321:THR:N	2.21	0.72
13:A:29:ASP:HA	13:A:32:LEU:HD23	1.70	0.72
19:G:11:ARG:HB3	25:M:7:TYR:OH	1.88	0.72
3:W:89:LEU:HD22	3:W:90:LEU:HD13	1.72	0.72
5:Y:289:ALA:HB3	5:Y:290:PRO:HD3	1.72	0.72
1:U:903:PHE:HB2	1:U:915:LYS:HB2	1.71	0.72
18:F:435:LEU:CD2	23:K:20:ARG:CD	2.63	0.72
20:H:123:GLN:HA	20:H:123:GLN:OE1	1.88	0.72
3:W:178:GLU:O	3:W:180:LYS:N	2.23	0.72
12:f:810:ILE:CD1	12:f:853:VAL:C	2.62	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:140:ILE:HG13	3:W:143:ALA:HB2	1.71	0.72
3:W:435:LEU:HD13	6:Z:237:LEU:CG	2.16	0.72
12:f:642:ALA:H	12:f:643:PRO:CD	2.03	0.72
12:f:836:GLU:H	12:f:840:LEU:HD21	1.52	0.72
4:X:142:ARG:HG3	4:X:145:GLU:CD	2.15	0.72
6:Z:234:PHE:C	6:Z:237:LEU:HD21	2.10	0.72
12:f:810:ILE:HD13	12:f:853:VAL:C	2.14	0.72
17:E:281:ARG:HG3	17:E:281:ARG:NH1	2.02	0.72
6:Z:237:LEU:HD22	6:Z:237:LEU:H	1.54	0.71
9:c:196:LEU:HA	9:c:200:TYR:CE2	2.25	0.71
16:D:268:ASP:OD1	16:D:311:THR:CA	2.38	0.71
18:F:324:THR:HG23	18:F:327:LYS:HZ2	1.51	0.71
25:m:229:LYS:O	25:m:229:LYS:HD3	1.89	0.71
4:X:142:ARG:HG3	4:X:145:GLU:HG2	1.69	0.71
16:D:408:LYS:CE	16:D:410:ASP:OD1	2.37	0.71
23:K:22:PHE:O	23:K:26:TYR:N	2.23	0.71
3:W:142:ARG:HH22	3:W:178:GLU:CG	2.04	0.71
3:W:426:ASN:ND2	9:c:233:ASP:OD2	2.24	0.71
12:f:755:ASP:OD1	12:f:755:ASP:N	2.21	0.71
19:g:12:HIS:CD2	25:m:7:TYR:CD1	2.78	0.71
22:j:3:TYR:OH	23:k:9:ASP:HB2	1.91	0.71
3:W:175:GLY:O	3:W:176:SER:OG	2.09	0.71
10:d:201:ASN:N	10:d:201:ASN:OD1	2.23	0.71
17:E:235:ILE:HG23	17:E:279:THR:HG21	1.72	0.71
5:Y:174:TRP:HE1	5:Y:177:ARG:CD	2.03	0.71
10:d:202:THR:N	10:d:203:PRO:HD3	2.06	0.71
12:f:642:ALA:N	12:f:643:PRO:CD	2.52	0.71
1:U:47:VAL:O	1:U:49:TYR:N	2.24	0.71
3:W:140:ILE:C	3:W:140:ILE:HD12	2.16	0.71
6:Z:237:LEU:HD13	6:Z:237:LEU:N	2.05	0.71
12:f:838:ARG:HG3	12:f:839:PRO:HD3	1.73	0.71
17:E:198:VAL:CG1	17:E:232:MET:SD	2.79	0.71
17:E:235:ILE:HG23	17:E:279:THR:CG2	2.20	0.71
9:c:196:LEU:N	9:c:200:TYR:CE1	2.58	0.70
12:f:295:ALA:O	12:f:807:ARG:HD2	1.91	0.70
2:V:29:PRO:N	2:V:30:PRO:HD2	2.06	0.70
5:Y:293:ARG:CZ	11:e:57:ARG:CB	2.69	0.70
2:V:27:PRO:HA	2:V:30:PRO:HG2	1.71	0.70
19:G:9:PHE:HE2	20:H:24:TYR:HE2	1.40	0.70
5:Y:233:ARG:H	5:Y:234:PRO:CD	2.05	0.70
6:Z:237:LEU:HD22	6:Z:237:LEU:N	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:222:LYS:HG2	15:C:222:LYS:O	1.92	0.70
19:G:9:PHE:HD2	19:G:18:PRO:CG	2.03	0.70
3:W:88:MET:HB3	19:G:209:ASP:O	1.91	0.70
17:E:235:ILE:HG23	17:E:236:ASP:N	2.05	0.70
3:W:435:LEU:HD13	6:Z:238:PRO:HD3	1.73	0.70
5:Y:349:LYS:HE2	5:Y:349:LYS:HA	1.73	0.70
15:C:277:LEU:HG	15:C:310:ARG:HH12	1.57	0.70
17:E:52:SER:O	17:E:54:GLY:N	2.25	0.70
1:U:423:MET:SD	1:U:446:LEU:HD12	2.16	0.70
16:D:268:ASP:OD1	16:D:311:THR:HB	1.90	0.69
3:W:8:ARG:HB3	3:W:27:ARG:HD3	1.74	0.69
2:V:322:VAL:HG22	11:e:6:GLN:HG2	1.74	0.69
4:X:260:MET:HE1	4:X:322:HIS:HB3	1.74	0.69
22:j:3:TYR:OH	23:k:9:ASP:CB	2.41	0.69
1:U:699:THR:HG21	1:U:812:ALA:H	1.56	0.69
17:E:236:ASP:OD2	17:E:282:PRO:HG3	1.93	0.69
12:f:862:ILE:O	12:f:876:HIS:NE2	2.26	0.68
25:M:229:LYS:HA	25:M:229:LYS:HZ2	1.56	0.68
1:U:10:SER:HB2	10:d:73:ARG:HG3	1.75	0.68
5:Y:174:TRP:HD1	5:Y:177:ARG:HD3	1.58	0.68
19:G:12:HIS:CE1	25:M:7:TYR:CE1	2.72	0.68
12:f:838:ARG:CG	12:f:839:PRO:HD3	2.23	0.68
16:D:268:ASP:OD1	16:D:311:THR:HA	1.93	0.68
19:G:9:PHE:CD2	19:G:18:PRO:HD3	2.29	0.68
15:C:368:MET:HG2	16:D:329:ARG:HH22	1.59	0.68
12:f:828:ARG:NE	12:f:843:SER:OG	2.26	0.67
17:E:52:SER:C	17:E:54:GLY:H	2.01	0.67
12:f:642:ALA:H	12:f:643:PRO:HD2	1.56	0.67
12:f:764:LEU:HD12	12:f:775:THR:CG2	2.18	0.67
13:A:124:ASP:N	18:F:86:LEU:HD11	2.10	0.67
23:K:23:GLN:HA	23:K:23:GLN:NE2	2.01	0.67
6:Z:228:TYR:CD2	7:a:341:LEU:HD21	2.27	0.67
19:G:46:ASP:O	19:G:222:VAL:HG23	1.94	0.67
12:f:250:ARG:HH22	12:f:281:ILE:CG1	2.06	0.67
17:E:194:ASN:ND2	17:E:228:CYS:HA	2.09	0.67
3:W:91:SER:OG	3:W:96:GLN:OE1	2.10	0.67
14:B:434:THR:OG1	14:B:435:PRO:HD2	1.95	0.67
3:W:435:LEU:CD1	6:Z:237:LEU:CD2	2.72	0.67
4:X:142:ARG:HG3	4:X:145:GLU:CG	2.25	0.66
16:D:335:LEU:HB3	16:D:336:PRO:HD2	1.72	0.66
19:G:19:GLU:HA	20:H:27:ALA:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:268:ASP:CG	16:D:312:ASN:H	2.03	0.66
12:f:250:ARG:NH2	12:f:281:ILE:CG2	2.56	0.66
5:Y:65:ILE:O	5:Y:65:ILE:HD13	1.95	0.66
6:Z:12:HIS:HB2	6:Z:50:VAL:O	1.94	0.66
17:E:188:ALA:HA	17:E:192:ASP:CG	2.20	0.66
3:W:201:ARG:HH22	16:D:391:ARG:HA	1.61	0.66
1:U:415:HIS:NE2	1:U:418:GLU:OE1	2.28	0.66
3:W:172:GLU:HB2	3:W:182:ARG:NH2	2.09	0.66
12:f:660:ILE:HG13	12:f:660:ILE:O	1.95	0.66
25:m:229:LYS:HA	25:m:229:LYS:HZ3	1.61	0.66
12:f:810:ILE:HD11	12:f:853:VAL:O	1.96	0.65
17:E:236:ASP:HB2	17:E:282:PRO:CG	2.26	0.65
19:G:19:GLU:HA	20:H:27:ALA:HB1	1.77	0.65
6:Z:15:VAL:O	6:Z:19:VAL:HG23	1.97	0.65
12:f:760:PHE:CE2	12:f:855:GLN:NE2	2.64	0.65
3:W:177:MET:HA	3:W:182:ARG:HG2	1.78	0.65
12:f:61:GLU:OE2	12:f:62:ARG:NH1	2.30	0.65
19:g:12:HIS:HE2	25:m:7:TYR:HD1	1.36	0.65
12:f:809:ILE:CG1	12:f:855:GLN:NE2	2.59	0.65
9:c:196:LEU:HD22	9:c:196:LEU:C	2.19	0.65
13:A:122:VAL:HB	18:F:88:TYR:HB2	1.77	0.65
18:F:324:THR:CG2	18:F:327:LYS:HE3	2.23	0.65
12:f:760:PHE:CD2	12:f:809:ILE:CD1	2.79	0.65
19:g:46:ASP:CB	19:g:222:VAL:HG23	2.26	0.65
1:U:639:LEU:HD21	15:C:49:ARG:HD2	1.79	0.65
19:G:21:ARG:HD3	19:G:21:ARG:N	2.11	0.64
3:W:170:GLN:O	3:W:173:THR:OG1	2.10	0.64
17:E:188:ALA:HA	17:E:192:ASP:HB3	1.78	0.64
17:E:195:PHE:O	17:E:231:PHE:HB3	1.97	0.64
18:F:86:LEU:C	18:F:86:LEU:HD13	2.22	0.64
21:I:218:ARG:NH1	21:I:223:THR:OG1	2.31	0.64
4:X:216:ILE:HD12	4:X:318:ILE:CD1	2.26	0.64
12:f:755:ASP:OD1	12:f:756:PRO:CD	2.27	0.64
6:Z:16:LEU:CG	6:Z:17:LEU:H	2.11	0.64
3:W:145:LEU:HD11	3:W:172:GLU:HG2	1.77	0.64
3:W:435:LEU:CD1	6:Z:237:LEU:HD23	2.23	0.64
4:X:316:ASP:CG	4:X:320:SER:HB3	2.20	0.64
1:U:148:LYS:HE3	1:U:179:TYR:CZ	2.33	0.64
2:V:280:ALA:HB1	2:V:284:GLU:HB3	1.78	0.64
12:f:785:ARG:HH22	12:f:790:GLN:H	0.67	0.64
14:B:389:ASP:O	14:B:390:LEU:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:86:LEU:CB	18:F:87:PRO:HD3	2.07	0.64
2:V:37:MET:SD	2:V:92:ARG:NH1	2.71	0.64
3:W:178:GLU:O	3:W:179:LYS:C	2.41	0.64
3:W:299:ILE:HG22	3:W:301:LYS:H	1.63	0.64
17:E:195:PHE:CD1	17:E:231:PHE:HB2	2.33	0.63
6:Z:234:PHE:C	6:Z:237:LEU:HD11	2.24	0.63
3:W:175:GLY:O	3:W:176:SER:CB	2.47	0.63
3:W:329:ARG:HG3	3:W:330:LYS:HG2	1.80	0.63
12:f:721:VAL:HG11	14:B:208:PRO:HD2	1.80	0.63
4:X:141:LYS:HZ1	4:X:179:ALA:HB1	1.64	0.63
6:Z:69:PHE:HE2	8:b:95:LEU:HB3	1.63	0.63
13:A:86:THR:HG22	14:B:136:LEU:CD1	2.27	0.63
31:s:27:THR:HB	31:s:40:SER:H	1.63	0.63
4:X:255:LEU:HD22	4:X:267:VAL:HG13	1.80	0.63
1:U:694:ILE:HG23	1:U:695:MET:HG3	1.81	0.63
17:E:164:ILE:HG13	17:E:166:PRO:CD	2.27	0.63
16:D:335:LEU:HB2	16:D:336:PRO:HD2	1.80	0.63
31:S:27:THR:HB	31:S:40:SER:H	1.63	0.63
5:Y:360:ASP:H	5:Y:363:ASN:HB2	1.64	0.63
12:f:673:ARG:HH22	12:f:709:THR:HA	1.63	0.63
19:G:9:PHE:CD2	19:G:18:PRO:HG3	2.34	0.63
3:W:314:LEU:HD12	7:a:309:LEU:HD23	1.81	0.62
19:G:9:PHE:HE2	20:H:24:TYR:CE2	2.16	0.62
5:Y:174:TRP:HE3	15:C:338:LEU:O	1.82	0.62
9:c:113:HIS:CD2	9:c:115:HIS:CE1	2.87	0.62
1:U:874:ASN:N	1:U:874:ASN:OD1	2.31	0.62
12:f:773:LYS:C	12:f:775:THR:H	2.06	0.62
13:A:86:THR:HG22	14:B:136:LEU:HD12	1.80	0.62
15:C:69:GLN:HB3	15:C:118:ASN:HD21	1.63	0.62
16:D:207:PRO:HG2	16:D:335:LEU:CD2	2.15	0.62
18:F:324:THR:O	18:F:325:GLN:HG3	1.99	0.62
20:H:7:SER:OG	20:H:21:GLN:NE2	2.28	0.62
23:K:22:PHE:HA	23:K:25:GLU:HB3	1.81	0.62
1:U:108:TYR:OH	1:U:159:ARG:NH1	2.32	0.62
2:V:476:PHE:HB3	6:Z:260:VAL:HG21	1.81	0.62
3:W:142:ARG:HG2	3:W:145:LEU:HD12	1.82	0.62
12:f:125:ILE:HD13	12:f:129:LEU:HB2	1.80	0.62
5:Y:174:TRP:CD1	5:Y:177:ARG:HD2	2.30	0.62
10:d:188:LYS:HD2	10:d:221:ASN:HD21	1.65	0.62
12:f:125:ILE:HD11	12:f:128:VAL:HB	1.81	0.62
17:E:222:ALA:CB	17:E:228:CYS:SG	2.88	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:n:21:THR:HG22	26:n:26:ILE:HG13	1.81	0.62
3:W:141:GLU:C	3:W:172:GLU:OE2	2.42	0.61
12:f:810:ILE:HD12	12:f:812:GLY:N	2.14	0.61
1:U:148:LYS:HE3	1:U:179:TYR:HE2	1.59	0.61
17:E:196:LEU:HD13	17:E:230:ILE:HD13	1.81	0.61
17:E:127:PRO:CB	17:E:193:CYS:SG	2.87	0.61
17:E:196:LEU:CD1	17:E:230:ILE:HD13	2.30	0.61
2:V:322:VAL:O	11:e:6:GLN:HB2	2.01	0.61
3:W:362:ASN:HD22	3:W:365:ILE:HD11	1.66	0.61
5:Y:331:ASP:OD1	5:Y:349:LYS:NZ	2.34	0.61
12:f:738:ASN:ND2	12:f:738:ASN:H	1.98	0.61
17:E:286:ASP:HB3	17:E:289:LEU:HB2	1.81	0.61
8:b:157:VAL:HG21	8:b:170:LEU:HB2	1.82	0.61
25:M:229:LYS:HD2	25:M:235:ALA:H	1.66	0.61
25:m:214:SER:OG	25:m:224:HIS:NE2	2.32	0.61
5:Y:283:LYS:HE2	5:Y:292:TYR:HD2	1.63	0.61
19:G:46:ASP:O	19:G:222:VAL:CG2	2.48	0.61
25:M:214:SER:OG	25:M:224:HIS:NE2	2.32	0.61
26:N:21:THR:HG22	26:N:26:ILE:HG13	1.81	0.61
2:V:198:GLN:HE22	15:C:33:LEU:HD11	1.66	0.61
3:W:436:MET:HE3	9:c:226:MET:HB2	1.83	0.61
4:X:182:ASN:ND2	5:Y:248:GLU:OE2	2.33	0.61
15:C:198:LEU:HD11	34:C:501:ATP:H2'	1.82	0.61
12:f:642:ALA:C	12:f:644:ALA:H	2.09	0.61
1:U:182:LYS:O	1:U:185:MET:N	2.25	0.61
1:U:347:ASN:CA	1:U:813:TYR:OH	2.48	0.61
1:U:366:HIS:HE1	1:U:395:ARG:HD2	1.65	0.61
1:U:625:ILE:HG13	1:U:626:LEU:HG	1.83	0.61
3:W:273:TYR:HB2	3:W:276:LEU:HB2	1.83	0.61
5:Y:231:LEU:HD12	5:Y:234:PRO:O	2.01	0.61
2:V:414:TYR:CE1	5:Y:349:LYS:HE3	2.37	0.60
12:f:127:SER:HA	12:f:131:MET:HB2	1.82	0.60
12:f:618:GLU:HG2	14:B:82:GLN:OE1	2.01	0.60
18:F:205:PRO:HB3	18:F:324:THR:HB	1.82	0.60
19:G:9:PHE:HD2	19:G:18:PRO:HD3	1.65	0.60
7:a:286:ALA:HA	7:a:289:ARG:HB3	1.84	0.60
24:L:148:CYS:HG	24:L:150:SER:HG	1.48	0.60
12:f:704:LEU:HA	12:f:707:LEU:HB2	1.83	0.60
21:I:143:TYR:HB2	21:I:146:GLN:HE21	1.64	0.60
3:W:142:ARG:HH12	3:W:178:GLU:HG3	1.66	0.60
12:f:250:ARG:CZ	12:f:281:ILE:HG12	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:408:LYS:HE2	16:D:410:ASP:OD1	2.01	0.60
19:G:127:GLN:NE2	20:H:128:ARG:O	2.35	0.60
2:V:414:TYR:CD1	5:Y:349:LYS:HE3	2.36	0.60
8:b:22:LEU:CG	18:F:49:ASP:OD2	2.48	0.60
12:f:586:PRO:HA	12:f:589:SER:HB2	1.83	0.60
12:f:811:LEU:HD11	12:f:862:ILE:HB	1.84	0.60
17:E:234:GLU:HB2	17:E:237:ALA:HB3	1.84	0.60
19:G:9:PHE:HD2	19:G:18:PRO:CD	2.14	0.60
20:H:39:LYS:HE2	20:H:144:PRO:HG2	1.83	0.60
14:B:313:LEU:O	14:B:346:ARG:NH1	2.35	0.60
19:G:46:ASP:CB	19:G:222:VAL:HG21	2.31	0.60
12:f:99:LEU:HG	12:f:101:PRO:HD2	1.83	0.60
1:U:505:ASP:HB3	1:U:508:THR:HG22	1.83	0.60
2:V:100:MET:H	2:V:103:SER:HB2	1.67	0.60
5:Y:174:TRP:HH2	15:C:377:HIS:HA	1.62	0.59
12:f:872:VAL:HG21	12:f:881:GLU:H	1.67	0.59
19:G:123:GLN:NE2	20:H:82:ASP:OD1	2.35	0.59
9:c:174:PRO:O	9:c:176:GLN:NE2	2.36	0.59
17:E:260:LEU:HD22	17:E:264:MET:HE3	1.84	0.59
6:Z:212:LEU:HA	6:Z:215:VAL:HG12	1.85	0.59
9:c:196:LEU:CA	9:c:200:TYR:CZ	2.83	0.59
12:f:302:GLY:HA2	12:f:317:LEU:HD11	1.84	0.59
21:i:163:CYS:SG	21:i:164:ILE:N	2.75	0.59
9:c:50:PRO:CG	17:E:53:VAL:HG11	2.31	0.59
18:F:206:MET:HE3	18:F:246:ALA:HB2	1.85	0.59
9:c:29:GLU:HG3	9:c:65:TYR:HB2	1.85	0.59
21:I:219:GLU:OE2	21:I:220:ASN:ND2	2.36	0.59
3:W:401:THR:HG23	3:W:402:ILE:HD12	1.84	0.59
18:F:437:TYR:CE2	23:K:21:LEU:HD23	2.35	0.59
30:R:166:ARG:NH2	28:p:34:MET:O	2.35	0.59
4:X:143:TYR:CE2	5:Y:252:SER:HB2	2.38	0.59
15:C:164:VAL:HG13	15:C:165:ILE:HG13	1.85	0.59
21:I:10:THR:HG23	21:I:10:THR:O	2.01	0.59
21:I:17:ARG:O	21:I:19:TYR:CD1	2.56	0.59
1:U:194:ARG:HH11	1:U:218:GLN:HE21	1.50	0.59
8:b:161:ASN:HD21	8:b:168:SER:H	1.51	0.59
12:f:672:LEU:HD21	12:f:690:VAL:HG22	1.83	0.59
2:V:55:THR:OG1	15:C:36:ASN:ND2	2.35	0.59
5:Y:174:TRP:CZ3	15:C:337:ASN:O	2.44	0.59
7:a:35:HIS:NE2	8:b:14:GLU:O	2.36	0.59
17:E:337:GLY:O	17:E:378:LYS:NZ	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:27:PRO:N	2:V:28:PRO:CD	2.66	0.59
19:G:21:ARG:HH21	19:G:21:ARG:CG	2.14	0.59
27:o:171:SER:HB3	27:o:193:ASN:HB2	1.85	0.59
25:M:51:LYS:NZ	25:M:62:SER:O	2.36	0.58
2:V:137:GLU:HA	2:V:140:ASP:HB2	1.85	0.58
12:f:764:LEU:HD11	12:f:775:THR:HG22	1.67	0.58
2:V:79:VAL:HG13	2:V:81:GLN:H	1.68	0.58
9:c:233:ASP:HB3	9:c:236:GLU:OE1	2.02	0.58
15:C:113:ARG:NH2	15:C:129:ASN:O	2.36	0.58
16:D:212:LYS:NZ	16:D:311:THR:O	2.36	0.58
21:I:163:CYS:SG	21:I:164:ILE:N	2.75	0.58
25:m:52:LEU:HA	25:m:209:PHE:HA	1.85	0.58
2:V:452:ASN:HB3	2:V:457:TYR:HB2	1.84	0.58
17:E:29:LEU:HB3	18:F:62:VAL:HG11	1.85	0.58
29:q:117:TYR:HB3	29:q:125:ALA:HB3	1.86	0.58
12:f:785:ARG:NH1	12:f:790:GLN:HB2	2.18	0.58
25:M:52:LEU:HA	25:M:209:PHE:HA	1.85	0.58
4:X:143:TYR:HD2	4:X:144:GLN:HG2	1.68	0.58
23:K:221:GLN:HB2	23:K:224:GLN:HB3	1.85	0.58
20:h:39:LYS:HE2	20:h:144:PRO:HG2	1.86	0.58
12:f:198:HIS:O	12:f:202:HIS:N	2.36	0.58
16:D:272:THR:HB	16:D:317:LEU:HA	1.85	0.58
13:A:103:ASN:ND2	18:F:167:GLU:OE1	2.36	0.58
27:o:171:SER:OG	27:o:171:SER:O	2.19	0.58
2:V:26:PRO:O	2:V:30:PRO:HG2	2.04	0.58
3:W:190:MET:HB2	3:W:202:THR:HG23	1.86	0.58
5:Y:292:TYR:N	5:Y:292:TYR:HD1	2.01	0.58
10:d:78:LEU:HD13	10:d:98:LEU:HD21	1.86	0.58
13:A:428:ARG:NH2	22:J:23:GLN:O	2.37	0.58
23:K:23:GLN:HE21	23:K:23:GLN:CA	2.02	0.58
19:G:67:THR:HG23	19:G:216:GLU:HG2	1.85	0.57
29:Q:117:TYR:HB3	29:Q:125:ALA:HB3	1.86	0.57
2:V:414:TYR:CE1	5:Y:349:LYS:CE	2.88	0.57
9:c:64:ASP:O	9:c:139:ARG:NH2	2.35	0.57
9:c:189:ILE:HA	9:c:192:LEU:HG	1.86	0.57
12:f:738:ASN:H	12:f:738:ASN:HD22	1.52	0.57
18:F:300:LYS:HE3	18:F:300:LYS:C	2.29	0.57
1:U:600:ARG:HE	16:D:56:VAL:HG22	1.68	0.57
15:C:215:SER:HA	15:C:249:ASP:HB2	1.86	0.57
25:m:51:LYS:NZ	25:m:62:SER:O	2.36	0.57
25:m:229:LYS:HA	25:m:229:LYS:HZ2	1.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:170:GLN:NE2	4:X:192:SER:OG	2.38	0.57
20:H:6:TYR:CZ	21:I:6:ASP:HB3	2.38	0.57
2:V:414:TYR:CE1	5:Y:349:LYS:NZ	2.51	0.57
3:W:80:TRP:NE1	19:G:244:GLU:OE1	2.37	0.57
6:Z:16:LEU:HD23	6:Z:17:LEU:N	2.18	0.57
6:Z:16:LEU:HG	6:Z:17:LEU:N	2.20	0.57
12:f:810:ILE:O	12:f:878:GLU:HB2	2.04	0.57
17:E:1:MET:O	17:E:4:PRO:HD3	2.05	0.57
18:F:205:PRO:CB	18:F:324:THR:HG21	2.34	0.57
26:N:1:THR:N	26:N:169:SER:O	2.37	0.57
27:O:171:SER:OG	27:O:192:PRO:CG	2.53	0.57
31:S:150:ASP:OD2	28:p:177:ARG:NH2	2.38	0.57
1:U:596:ASN:ND2	16:D:52:GLU:OE1	2.37	0.57
1:U:788:VAL:HG12	1:U:909:GLY:HA2	1.87	0.57
3:W:92:LYS:HB3	3:W:94:ARG:HB3	1.87	0.57
6:Z:11:VAL:CB	6:Z:162:ILE:HD13	2.31	0.57
8:b:110:ILE:HG22	8:b:139:ASP:HB2	1.85	0.57
12:f:591:ALA:HA	12:f:594:LEU:HD23	1.87	0.57
12:f:838:ARG:CG	12:f:839:PRO:CD	2.82	0.57
21:i:218:ARG:NH1	21:i:223:THR:OG1	2.37	0.57
5:Y:202:LEU:HD21	5:Y:239:LYS:HB3	1.86	0.57
6:Z:212:LEU:HD13	7:a:350:LYS:HG2	1.87	0.57
15:C:375:ARG:HG2	15:C:377:HIS:H	1.69	0.57
13:A:80:LEU:O	13:A:85:GLN:NE2	2.38	0.57
16:D:175:GLN:NE2	16:D:179:GLU:OE2	2.37	0.57
12:f:150:GLU:O	12:f:156:HIS:ND1	2.37	0.57
12:f:469:TYR:O	12:f:472:HIS:ND1	2.32	0.57
12:f:760:PHE:CE2	12:f:809:ILE:CD1	2.87	0.57
2:V:228:ARG:O	2:V:232:HIS:ND1	2.38	0.56
7:a:74:LEU:HD23	7:a:110:ALA:HB2	1.88	0.56
12:f:764:LEU:HD11	12:f:775:THR:HG21	1.87	0.56
12:f:790:GLN:HG2	12:f:794:ALA:HB3	1.87	0.56
12:f:810:ILE:HD11	12:f:853:VAL:C	2.30	0.56
14:B:258:LYS:HD3	15:C:226:GLU:HG2	1.87	0.56
5:Y:283:LYS:HE2	5:Y:292:TYR:CD2	2.40	0.56
7:a:182:CYS:SG	7:a:183:VAL:N	2.77	0.56
19:G:9:PHE:CE2	20:H:24:TYR:HE2	2.20	0.56
32:t:145:LEU:HD22	32:t:179:ARG:HH11	1.69	0.56
2:V:68:ASP:O	2:V:72:LEU:N	2.38	0.56
2:V:163:VAL:HA	2:V:175:MET:HE2	1.86	0.56
2:V:416:ARG:NH1	5:Y:351:ASN:OD1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:301:ILE:HG13	5:Y:343:LEU:HD12	1.86	0.56
12:f:760:PHE:CD2	12:f:809:ILE:HD11	2.41	0.56
14:B:106:PRO:HB3	15:C:121:TYR:HB2	1.87	0.56
16:D:417:TYR:OH	19:G:21:ARG:HD2	2.05	0.56
25:M:163:CYS:SG	25:M:164:ALA:N	2.78	0.56
32:T:145:LEU:HD22	32:T:179:ARG:HH11	1.69	0.56
26:n:1:THR:N	26:n:169:SER:O	2.37	0.56
2:V:290:TYR:OH	2:V:294:ARG:NH2	2.37	0.56
3:W:316:ARG:HH12	3:W:381:LEU:HA	1.71	0.56
6:Z:16:LEU:HD23	6:Z:16:LEU:N	2.20	0.56
12:f:738:ASN:HD22	12:f:738:ASN:N	2.03	0.56
25:M:229:LYS:HD2	25:M:234:GLU:N	2.21	0.56
1:U:811:PHE:CE1	1:U:888:GLN:NE2	2.73	0.56
2:V:345:ARG:HH12	2:V:353:LEU:HD11	1.70	0.56
9:c:279:ASP:HB3	9:c:280:PRO:HD3	1.88	0.56
12:f:691:PRO:HA	12:f:694:LEU:HB2	1.87	0.56
21:I:124:PHE:O	22:J:123:GLY:O	2.22	0.56
12:f:766:GLN:CG	12:f:807:ARG:HH11	2.17	0.56
15:C:88:LYS:HB2	15:C:94:LYS:HG2	1.86	0.56
21:I:90:LEU:HD12	21:I:114:LEU:HD22	1.88	0.56
25:m:163:CYS:SG	25:m:164:ALA:N	2.78	0.56
3:W:91:SER:HB3	3:W:96:GLN:HE22	1.71	0.56
10:d:52:ARG:HH22	10:d:92:SER:HB3	1.71	0.56
12:f:77:GLU:OE1	12:f:79:ARG:NH1	2.39	0.56
12:f:552:ASP:HB3	12:f:556:ARG:HG3	1.88	0.56
17:E:75:ASN:ND2	18:F:129:ARG:O	2.39	0.56
25:m:47:PHE:HB2	25:m:214:SER:HB3	1.88	0.56
8:b:22:LEU:HG	18:F:49:ASP:OD1	2.06	0.56
14:B:125:THR:OG1	14:B:126:SER:N	2.38	0.56
22:j:74:ALA:HB2	22:j:161:ILE:HD13	1.88	0.56
1:U:798:PRO:O	1:U:880:ASN:ND2	2.34	0.56
1:U:189:GLN:NE2	1:U:595:ASN:OD1	2.39	0.56
3:W:448:LYS:HE2	6:Z:157:HIS:HB2	1.86	0.56
5:Y:349:LYS:HE2	5:Y:349:LYS:CA	2.36	0.56
7:a:273:GLN:HB3	7:a:310:LEU:HD11	1.88	0.56
19:G:165:ALA:HB1	19:G:179:LEU:HD13	1.88	0.56
2:V:85:ALA:O	2:V:89:LYS:NZ	2.39	0.55
6:Z:7:GLN:HB2	6:Z:46:LYS:HG2	1.87	0.55
17:E:236:ASP:HB2	17:E:282:PRO:HD3	1.87	0.55
20:H:42:ASN:ND2	20:H:183:GLU:OE1	2.39	0.55
24:L:189:LYS:HA	24:L:192:LEU:HG	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:k:76:CYS:SG	23:k:77:ALA:N	2.79	0.55
1:U:814:PRO:HB2	1:U:816:PRO:HD3	1.88	0.55
8:b:97:LEU:HD23	8:b:107:MET:HB3	1.87	0.55
12:f:378:ASN:O	12:f:382:ASN:ND2	2.39	0.55
12:f:378:ASN:HD21	12:f:392:THR:HG22	1.70	0.55
18:F:437:TYR:CZ	23:K:21:LEU:HD23	2.42	0.55
29:Q:198:LYS:H	29:q:198:LYS:H	1.52	0.55
24:l:134:ILE:HB	24:l:145:PHE:HB2	1.89	0.55
6:Z:16:LEU:CG	6:Z:17:LEU:N	2.68	0.55
7:a:284:ARG:HD3	7:a:288:HIS:H	1.71	0.55
12:f:250:ARG:HH22	12:f:281:ILE:HD13	1.71	0.55
5:Y:174:TRP:HZ2	15:C:377:HIS:CD2	2.19	0.55
12:f:816:TYR:HB3	12:f:821:LEU:HD13	1.88	0.55
17:E:50:LEU:O	17:E:51:GLN:HG3	2.07	0.55
22:J:74:ALA:HB2	22:J:161:ILE:HD13	1.88	0.55
19:g:165:ALA:HB1	19:g:179:LEU:HD13	1.89	0.55
24:l:189:LYS:HA	24:l:192:LEU:HG	1.89	0.55
12:f:836:GLU:N	12:f:840:LEU:HD21	2.22	0.55
1:U:257:SER:HB2	1:U:757:MET:HE3	1.87	0.55
1:U:376:MET:HA	1:U:739:ALA:HA	1.89	0.55
4:X:317:PRO:O	4:X:318:ILE:HG13	2.07	0.55
12:f:250:ARG:HH12	12:f:281:ILE:CG1	2.05	0.55
17:E:263:GLN:HA	17:E:268:ASP:HB3	1.88	0.55
4:X:316:ASP:CG	4:X:321:THR:H	2.15	0.55
5:Y:88:LEU:HG	5:Y:100:ILE:HG13	1.88	0.55
12:f:828:ARG:CD	12:f:843:SER:OG	2.54	0.55
13:A:212:VAL:HG22	13:A:339:ARG:HB3	1.87	0.55
25:M:47:PHE:HB2	25:M:214:SER:HB3	1.88	0.55
2:V:188:SER:O	2:V:192:MET:HB2	2.05	0.55
6:Z:237:LEU:CD1	6:Z:237:LEU:H	2.06	0.55
12:f:465:LEU:O	12:f:481:SER:OG	2.25	0.55
12:f:594:LEU:O	12:f:635:LYS:NZ	2.40	0.55
18:F:435:LEU:HD21	23:K:20:ARG:CD	2.33	0.55
27:O:190:THR:HG22	27:O:192:PRO:HD3	1.89	0.55
21:i:79:ILE:HG22	21:i:82:ASP:H	1.72	0.55
1:U:219:CYS:SG	1:U:220:LEU:N	2.79	0.55
1:U:373:ASN:HD22	1:U:385:PHE:HD2	1.55	0.55
2:V:252:ASN:HD21	2:V:288:TYR:HB2	1.71	0.55
5:Y:325:VAL:O	11:e:66:LYS:NZ	2.39	0.55
6:Z:217:THR:HG22	6:Z:218:GLY:N	2.22	0.55
17:E:165:ILE:H	17:E:166:PRO:CD	1.96	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:43:ARG:NH1	19:G:149:PRO:O	2.39	0.55
3:W:220:GLU:HG3	3:W:221:LYS:HG2	1.89	0.55
6:Z:69:PHE:CZ	8:b:96:ALA:HB2	2.41	0.55
6:Z:129:LYS:HE2	9:c:216:MET:HB3	1.89	0.55
8:b:141:ILE:HA	8:b:171:VAL:HB	1.88	0.55
5:Y:174:TRP:CZ2	15:C:377:HIS:CG	2.94	0.54
5:Y:314:LEU:O	5:Y:354:VAL:N	2.40	0.54
23:k:209:LYS:O	23:k:214:ASN:ND2	2.40	0.54
1:U:623:GLY:HA3	1:U:658:ILE:HG13	1.90	0.54
2:V:416:ARG:HA	2:V:459:GLN:HA	1.89	0.54
4:X:143:TYR:CE1	5:Y:252:SER:HA	2.41	0.54
8:b:22:LEU:HB2	8:b:23:PRO:HD2	1.88	0.54
12:f:663:GLY:O	12:f:664:GLU:HG3	2.06	0.54
14:B:234:LEU:HD11	34:B:501:ATP:H2'	1.89	0.54
17:E:52:SER:C	17:E:54:GLY:N	2.65	0.54
27:O:113:ILE:HG12	27:O:119:THR:HG22	1.89	0.54
21:i:219:GLU:OE2	21:i:220:ASN:ND2	2.40	0.54
12:f:291:GLN:HE21	12:f:879:ARG:HH21	1.56	0.54
17:E:200:SER:CB	17:E:234:GLU:O	2.55	0.54
27:o:190:THR:HG22	27:o:192:PRO:HD3	1.89	0.54
12:f:209:MET:HG3	12:f:211:ILE:H	1.72	0.54
20:H:125:GLY:C	20:H:127:VAL:H	2.15	0.54
21:i:31:ALA:O	21:i:167:ASN:ND2	2.40	0.54
1:U:47:VAL:C	1:U:49:TYR:N	2.64	0.54
6:Z:68:TRP:CG	6:Z:104:ASN:HD21	2.26	0.54
6:Z:237:LEU:CB	6:Z:238:PRO:HD2	2.38	0.54
12:f:680:ARG:HB2	12:f:763:ARG:HE	1.72	0.54
14:B:332:ASN:HB2	15:C:258:ARG:HH22	1.72	0.54
1:U:179:TYR:CD1	1:U:179:TYR:C	2.86	0.54
12:f:447:ALA:HA	12:f:450:ILE:HD12	1.90	0.54
6:Z:11:VAL:HB	6:Z:162:ILE:CD1	2.36	0.54
12:f:139:CYS:O	12:f:143:ARG:NH1	2.41	0.54
12:f:634:LYS:HD2	12:f:637:LYS:HD2	1.90	0.54
13:A:308:GLY:HA2	18:F:234:THR:HG21	1.90	0.54
15:C:396:GLU:O	15:C:402:LYS:NZ	2.41	0.54
16:D:384:MET:HE2	17:E:167:PRO:HG3	1.90	0.54
19:G:169:GLY:O	19:G:172:GLN:NE2	2.41	0.54
23:K:21:LEU:HD13	23:K:21:LEU:N	2.22	0.54
21:i:38:LEU:HD13	21:i:160:LYS:HA	1.88	0.54
2:V:29:PRO:HD2	2:V:30:PRO:CD	2.35	0.54
5:Y:174:TRP:HZ3	15:C:337:ASN:C	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:378:ASN:OD1	12:f:382:ASN:ND2	2.40	0.54
16:D:119:ILE:O	16:D:121:ARG:NH1	2.41	0.54
17:E:236:ASP:HB2	17:E:282:PRO:CD	2.37	0.54
18:F:324:THR:CG2	18:F:327:LYS:HZ1	2.12	0.54
24:l:196:ARG:HH21	24:l:239:ARG:HG3	1.73	0.54
10:d:19:CYS:SG	10:d:65:ARG:NH1	2.79	0.54
17:E:33:LEU:HD11	18:F:62:VAL:HG13	1.90	0.54
17:E:52:SER:OG	18:F:159:LEU:HD12	2.08	0.54
20:H:6:TYR:CZ	21:I:6:ASP:CB	2.84	0.54
1:U:347:ASN:CB	1:U:813:TYR:CZ	2.71	0.54
12:f:585:GLU:HG3	12:f:588:ARG:HE	1.73	0.54
12:f:673:ARG:NH1	12:f:708:ASP:OD2	2.41	0.54
17:E:199:VAL:O	17:E:234:GLU:HG3	2.08	0.54
2:V:400:HIS:HA	10:d:145:GLU:HG3	1.91	0.53
4:X:90:ARG:HH21	4:X:128:ALA:HB1	1.72	0.53
9:c:113:HIS:CD2	9:c:115:HIS:ND1	2.77	0.53
12:f:441:LYS:HB2	12:f:477:MET:HE1	1.88	0.53
13:A:224:LEU:HD11	34:A:501:ATP:H2'	1.91	0.53
16:D:210:CYS:SG	16:D:335:LEU:CD2	2.96	0.53
24:L:196:ARG:HH21	24:L:239:ARG:HG3	1.73	0.53
1:U:416:GLU:OE2	1:U:450:HIS:NE2	2.41	0.53
2:V:80:LYS:O	2:V:87:SER:N	2.41	0.53
4:X:332:GLU:HA	4:X:335:LEU:HB2	1.89	0.53
16:D:408:LYS:HD2	16:D:410:ASP:OD1	2.08	0.53
17:E:235:ILE:CG2	17:E:236:ASP:H	2.21	0.53
18:F:184:GLN:OE1	18:F:243:GLN:NE2	2.40	0.53
23:k:117:SER:HB3	24:l:82:ARG:HH22	1.73	0.53
25:m:99:ARG:NH2	25:m:105:ASN:OD1	2.42	0.53
3:W:145:LEU:HA	3:W:148:THR:HG22	1.90	0.53
24:l:155:ASP:HB3	25:m:62:SER:HB2	1.90	0.53
1:U:174:PRO:CB	1:U:208:LEU:HD11	2.30	0.53
1:U:415:HIS:NE2	1:U:418:GLU:CD	2.60	0.53
2:V:451:ILE:HG23	2:V:458:VAL:HG22	1.88	0.53
3:W:140:ILE:HG23	3:W:140:ILE:O	2.07	0.53
5:Y:292:TYR:N	5:Y:292:TYR:CD1	2.73	0.53
12:f:240:VAL:HG13	12:f:257:ARG:HE	1.74	0.53
12:f:828:ARG:HD2	12:f:843:SER:OG	2.07	0.53
13:A:342:GLU:OE2	18:F:431:LYS:NZ	2.41	0.53
15:C:99:VAL:HG12	15:C:123:LEU:HD12	1.89	0.53
34:C:501:ATP:O2B	16:D:323:ARG:NH1	2.41	0.53
18:F:205:PRO:CB	18:F:324:THR:HB	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:I:8:ARG:HD3	21:I:126:GLY:CA	2.39	0.53
26:N:40:ARG:NH1	26:N:180:ALA:O	2.41	0.53
1:U:483:LEU:HD11	1:U:781:LEU:HD11	1.91	0.53
3:W:183:VAL:HG21	3:W:212:LYS:HG2	1.90	0.53
3:W:426:ASN:OD1	9:c:233:ASP:OD2	2.22	0.53
4:X:141:LYS:NZ	4:X:179:ALA:HB1	2.22	0.53
12:f:758:ASN:HB2	12:f:809:ILE:HG21	1.90	0.53
12:f:813:LYS:NZ	12:f:819:TYR:OH	2.34	0.53
15:C:185:GLY:HA3	15:C:311:ILE:HA	1.90	0.53
17:E:83:CYS:HB2	17:E:89:LYS:HE2	1.91	0.53
17:E:97:ARG:NH2	17:E:112:PRO:O	2.42	0.53
17:E:235:ILE:HG23	17:E:279:THR:CB	2.38	0.53
17:E:236:ASP:CB	17:E:282:PRO:HD3	2.38	0.53
2:V:265:ASP:O	2:V:269:LYS:NZ	2.40	0.53
10:d:131:VAL:HA	10:d:134:LYS:HB3	1.91	0.53
12:f:202:HIS:ND1	12:f:242:GLU:OE2	2.41	0.53
12:f:250:ARG:HH22	12:f:281:ILE:CD1	2.22	0.53
19:G:46:ASP:CB	19:G:222:VAL:CG2	2.86	0.53
2:V:106:ARG:O	2:V:110:HIS:ND1	2.42	0.53
3:W:172:GLU:CB	3:W:182:ARG:CZ	2.87	0.53
7:a:8:LEU:HD11	7:a:26:GLU:HB3	1.90	0.53
12:f:250:ARG:CZ	12:f:281:ILE:HG21	2.36	0.53
15:C:72:TYR:HB2	15:C:116:LEU:HB3	1.91	0.53
19:G:53:GLN:HA	19:G:215:ILE:HA	1.89	0.53
24:l:186:GLU:HA	24:l:189:LYS:HG2	1.90	0.53
1:U:397:THR:OG1	1:U:401:LYS:NZ	2.42	0.53
1:U:799:LYS:NZ	1:U:924:LEU:O	2.42	0.53
7:a:70:ARG:O	8:b:17:ARG:NH1	2.40	0.53
18:F:219:PRO:HG2	18:F:324:THR:HG23	1.91	0.53
26:n:40:ARG:NH1	26:n:180:ALA:O	2.41	0.53
27:o:113:ILE:HG12	27:o:119:THR:HG22	1.90	0.53
1:U:811:PHE:CZ	1:U:888:GLN:NE2	2.77	0.53
3:W:177:MET:HB3	3:W:182:ARG:HG2	1.90	0.53
10:d:8:GLU:O	10:d:13:SER:OG	2.27	0.53
24:L:186:GLU:HA	24:L:189:LYS:HG2	1.90	0.53
12:f:221:ILE:HA	12:f:224:ASN:HB2	1.90	0.53
24:L:134:ILE:HB	24:L:145:PHE:HB2	1.89	0.53
1:U:217:CYS:HG	1:U:752:THR:HG1	1.57	0.52
25:M:99:ARG:NH2	25:M:105:ASN:OD1	2.42	0.52
1:U:399:TRP:HD1	9:c:176:GLN:HG2	1.75	0.52
2:V:252:ASN:ND2	2:V:284:GLU:OE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:220:GLU:O	3:W:257:GLN:NE2	2.42	0.52
6:Z:200:GLY:HA3	9:c:225:TRP:HE1	1.73	0.52
10:d:183:GLU:OE2	10:d:215:TRP:NE1	2.43	0.52
21:i:216:LEU:HD12	21:i:225:ILE:HG12	1.91	0.52
1:U:424:ALA:O	1:U:427:LEU:HD12	2.04	0.52
1:U:889:LEU:HD13	1:U:908:ILE:HG13	1.90	0.52
5:Y:65:ILE:C	5:Y:67:VAL:H	2.17	0.52
19:G:67:THR:HG22	19:G:69:LEU:H	1.74	0.52
32:T:27:LEU:HD22	32:T:184:TYR:HB2	1.91	0.52
19:g:201:CYS:SG	19:g:202:LEU:N	2.83	0.52
31:s:125:ASP:OD1	31:s:129:SER:N	2.42	0.52
6:Z:198:LEU:HG	6:Z:201:LEU:HD12	1.91	0.52
14:B:383:LEU:HD11	14:B:419:PHE:HB3	1.91	0.52
16:D:271:ALA:HA	16:D:289:LEU:HD21	1.90	0.52
17:E:272:ARG:O	17:E:274:LYS:NZ	2.42	0.52
2:V:179:LYS:HE3	2:V:214:HIS:HB2	1.92	0.52
2:V:200:ARG:NH1	2:V:242:HIS:O	2.42	0.52
2:V:212:TYR:HB3	11:e:4:LYS:HE2	1.91	0.52
3:W:145:LEU:CD1	3:W:172:GLU:HG2	2.38	0.52
10:d:111:ARG:HB3	10:d:114:GLU:HB2	1.90	0.52
13:A:213:LEU:HD12	13:A:337:LEU:HD13	1.91	0.52
20:h:34:PRO:HA	20:h:164:GLY:HA3	1.92	0.52
32:t:27:LEU:HD11	32:t:34:ALA:HB1	1.91	0.52
32:t:27:LEU:HD22	32:t:184:TYR:HB2	1.91	0.52
3:W:91:SER:HG	3:W:96:GLN:CD	2.13	0.52
5:Y:160:ASN:HA	5:Y:163:LYS:HB2	1.90	0.52
8:b:2:VAL:O	8:b:44:ASN:ND2	2.43	0.52
13:A:300:LEU:HD23	13:A:303:ILE:HD12	1.91	0.52
19:G:41:ALA:HB3	19:G:166:THR:HB	1.92	0.52
1:U:862:LYS:HD2	1:U:863:GLU:HB3	1.92	0.52
2:V:29:PRO:HB2	2:V:30:PRO:HD3	1.92	0.52
3:W:440:ASN:OD1	6:Z:204:LYS:NZ	2.42	0.52
12:f:571:GLU:HG3	12:f:573:ILE:H	1.73	0.52
16:D:253:LEU:O	16:D:257:ASN:ND2	2.43	0.52
27:O:7:VAL:HG22	27:O:12:ILE:HG12	1.91	0.52
1:U:697:GLN:NE2	1:U:744:VAL:O	2.43	0.52
3:W:12:ARG:HD2	3:W:24:VAL:HG22	1.91	0.52
3:W:347:GLY:O	3:W:351:TRP:N	2.43	0.52
5:Y:191:ILE:H	11:e:43:TRP:HZ3	1.58	0.52
17:E:171:LEU:HB2	17:E:295:LEU:HD22	1.92	0.52
17:E:309:ARG:NH1	17:E:332:VAL:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:T:192:VAL:HG12	32:T:197:VAL:HG22	1.92	0.52
21:i:57:ASP:HB3	21:i:59:VAL:HG13	1.92	0.52
1:U:11:LEU:HD22	1:U:19:LEU:HD11	1.92	0.52
3:W:90:LEU:N	3:W:90:LEU:CD1	2.73	0.52
7:a:23:HIS:HA	7:a:26:GLU:HG2	1.91	0.52
12:f:110:TYR:OH	12:f:118:ASN:ND2	2.43	0.52
12:f:336:GLU:O	12:f:341:GLU:HB2	2.10	0.52
15:C:187:LEU:HD23	15:C:314:LYS:HE3	1.92	0.52
16:D:336:PRO:O	16:D:341:LYS:HE2	2.10	0.52
23:K:48:LEU:HD21	23:K:77:ALA:HB2	1.91	0.52
29:Q:21:ALA:HB3	29:Q:29:LYS:HB3	1.92	0.52
27:o:7:VAL:HG22	27:o:12:ILE:HG12	1.91	0.52
14:B:98:LYS:O	14:B:102:LEU:N	2.43	0.52
14:B:181:GLN:O	14:B:241:ASN:ND2	2.43	0.52
16:D:336:PRO:HB2	16:D:341:LYS:HZ3	1.75	0.52
25:M:40:ARG:NH1	25:M:146:ALA:O	2.43	0.52
29:q:4:LEU:HD22	29:q:45:LEU:HD13	1.92	0.52
1:U:900:TYR:HB3	1:U:914:LEU:HD21	1.91	0.51
2:V:25:GLU:C	2:V:28:PRO:HD2	2.35	0.51
2:V:264:TYR:OH	10:d:114:GLU:OE1	2.27	0.51
2:V:349:ARG:HA	2:V:353:LEU:HD23	1.90	0.51
5:Y:13:LYS:HE3	5:Y:146:ARG:HD2	1.93	0.51
2:V:28:PRO:HB2	2:V:29:PRO:CD	2.34	0.51
12:f:810:ILE:HG22	12:f:856:ALA:N	2.25	0.51
17:E:232:MET:HG3	17:E:232:MET:O	2.07	0.51
17:E:236:ASP:CG	17:E:282:PRO:HG3	2.33	0.51
20:H:111:VAL:HG21	20:H:147:PHE:HD2	1.75	0.51
27:O:171:SER:HB3	27:O:193:ASN:HB2	1.91	0.51
31:S:125:ASP:OD1	31:S:129:SER:N	2.42	0.51
32:T:27:LEU:HD11	32:T:34:ALA:HB1	1.91	0.51
28:p:62:THR:OG1	29:q:85:ARG:NH2	2.41	0.51
29:q:183:ILE:HG12	29:q:188:ILE:HG13	1.92	0.51
3:W:170:GLN:CA	3:W:173:THR:OG1	2.59	0.51
18:F:31:GLU:OE1	18:F:35:LYS:NZ	2.43	0.51
23:K:97:GLN:HG3	30:R:61:ARG:HG2	1.92	0.51
23:k:41:GLN:NE2	23:k:151:PRO:O	2.44	0.51
3:W:90:LEU:N	3:W:90:LEU:HD12	2.26	0.51
14:B:389:ASP:O	14:B:390:LEU:CB	2.56	0.51
16:D:200:ARG:NH2	16:D:302:ASN:OD1	2.35	0.51
19:G:21:ARG:N	19:G:21:ARG:CD	2.73	0.51
19:G:21:ARG:HH21	19:G:21:ARG:HG3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:201:CYS:SG	19:G:202:LEU:N	2.83	0.51
29:Q:183:ILE:HG12	29:Q:188:ILE:HG13	1.92	0.51
23:k:48:LEU:HD21	23:k:77:ALA:HB2	1.92	0.51
29:q:21:ALA:HB3	29:q:29:LYS:HB3	1.92	0.51
32:t:192:VAL:HG12	32:t:197:VAL:HG22	1.92	0.51
3:W:91:SER:CB	3:W:96:GLN:HE22	2.22	0.51
5:Y:349:LYS:HA	5:Y:349:LYS:CE	2.27	0.51
6:Z:16:LEU:CD2	6:Z:16:LEU:N	2.73	0.51
6:Z:252:LYS:HE2	9:c:299:CYS:HB2	1.91	0.51
10:d:179:ALA:HA	10:d:182:ILE:HG22	1.91	0.51
12:f:812:GLY:HA3	12:f:853:VAL:HA	1.92	0.51
14:B:223:ILE:HG13	14:B:347:ILE:HG21	1.93	0.51
19:g:43:ARG:NH1	19:g:149:PRO:O	2.43	0.51
2:V:412:LEU:O	5:Y:346:LYS:NZ	2.42	0.51
8:b:22:LEU:HD12	18:F:45:THR:HG22	1.91	0.51
12:f:497:VAL:HA	12:f:500:LEU:HB2	1.91	0.51
17:E:84:ARG:O	17:E:85:ARG:NE	2.43	0.51
17:E:368:MET:HB3	17:E:372:ARG:HH12	1.76	0.51
19:G:21:ARG:CG	19:G:21:ARG:NH2	2.73	0.51
21:I:38:LEU:HG	21:I:160:LYS:HB3	1.92	0.51
30:r:1:THR:N	30:r:169:TYR:O	2.44	0.51
6:Z:223:ASN:HB3	6:Z:227:ILE:HB	1.91	0.51
17:E:194:ASN:HD21	17:E:228:CYS:HA	1.74	0.51
17:E:195:PHE:HD1	17:E:231:PHE:HB2	1.76	0.51
17:E:201:SER:O	17:E:204:VAL:HG22	2.10	0.51
18:F:437:TYR:HE2	23:K:21:LEU:HD22	1.69	0.51
29:Q:4:LEU:HD22	29:Q:45:LEU:HD13	1.92	0.51
31:S:148:LEU:HD23	31:S:178:VAL:HG12	1.93	0.51
31:s:148:LEU:HD23	31:s:178:VAL:HG12	1.93	0.51
2:V:167:LEU:HD12	2:V:169:LEU:H	1.76	0.51
3:W:259:GLU:HG3	3:W:261:GLU:H	1.75	0.51
12:f:810:ILE:HG22	12:f:855:GLN:OE1	2.00	0.51
13:A:297:ARG:HH12	18:F:306:VAL:HG21	1.75	0.51
17:E:178:THR:HB	17:E:182:LEU:HD13	1.93	0.51
32:t:1:THR:N	32:t:104:ASN:OD1	2.43	0.51
7:a:140:GLU:O	7:a:143:ASN:ND2	2.44	0.51
12:f:606:VAL:HG11	14:B:70:ASP:HB3	1.93	0.51
12:f:785:ARG:HH22	12:f:790:GLN:CB	2.14	0.51
18:F:205:PRO:CG	18:F:324:THR:HG21	2.41	0.51
25:m:40:ARG:NH1	25:m:146:ALA:O	2.43	0.51
1:U:265:ILE:HA	1:U:268:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:696:ILE:HG22	1:U:737:LEU:HA	1.93	0.51
3:W:172:GLU:CB	3:W:182:ARG:NH2	2.73	0.51
15:C:217:SER:OG	16:D:291:GLU:OE1	2.29	0.51
30:R:1:THR:N	30:R:169:TYR:O	2.44	0.51
1:U:418:GLU:HG3	1:U:421:GLN:HE21	1.75	0.50
3:W:90:LEU:HD12	3:W:90:LEU:H	1.76	0.50
8:b:21:PHE:HB2	8:b:25:ARG:HG2	1.92	0.50
8:b:30:GLN:HG3	8:b:75:LEU:HD13	1.91	0.50
10:d:8:GLU:HG3	10:d:15:ASN:HD21	1.76	0.50
15:C:281:ASP:OD2	15:C:307:ARG:NH2	2.44	0.50
24:l:157:ARG:HD2	24:l:176:MET:HE3	1.93	0.50
30:r:38:ASN:HD22	30:r:41:LEU:HD12	1.77	0.50
3:W:359:VAL:HG23	3:W:382:LEU:HD22	1.93	0.50
6:Z:237:LEU:CD2	6:Z:237:LEU:H	2.12	0.50
16:D:408:LYS:CD	16:D:410:ASP:OD1	2.60	0.50
19:G:56:VAL:HG13	19:G:61:LEU:HD22	1.93	0.50
20:h:66:GLU:OE2	20:h:91:ARG:NH2	2.44	0.50
3:W:123:ARG:HH12	3:W:127:THR:HB	1.77	0.50
12:f:810:ILE:HD12	12:f:812:GLY:H	1.77	0.50
17:E:98:VAL:HA	17:E:110:TYR:HA	1.92	0.50
17:E:200:SER:HB2	17:E:234:GLU:O	2.11	0.50
24:L:157:ARG:HD2	24:L:176:MET:HE3	1.93	0.50
32:T:1:THR:N	32:T:104:ASN:OD1	2.43	0.50
21:i:48:GLU:OE2	21:i:50:ARG:NH2	2.45	0.50
23:k:221:GLN:HB2	23:k:224:GLN:HB3	1.94	0.50
3:W:72:LYS:HD3	3:W:123:ARG:HA	1.93	0.50
3:W:172:GLU:HB2	3:W:182:ARG:CZ	2.42	0.50
5:Y:96:GLY:O	5:Y:130:LYS:NZ	2.44	0.50
12:f:94:LYS:HA	12:f:97:LYS:HB2	1.92	0.50
21:I:9:THR:HG23	21:I:20:GLN:HB2	1.93	0.50
21:i:143:TYR:HB2	21:i:146:GLN:HE21	1.77	0.50
22:j:4:ASP:N	22:j:4:ASP:OD1	2.44	0.50
1:U:423:MET:CE	1:U:442:GLY:C	2.72	0.50
12:f:764:LEU:O	12:f:764:LEU:CD2	2.52	0.50
17:E:101:ASP:HB3	17:E:105:LEU:H	1.77	0.50
19:G:158:GLY:O	20:H:84:ARG:NH2	2.44	0.50
28:P:126:LEU:HD12	28:P:127:ILE:HG23	1.93	0.50
28:p:126:LEU:HD12	28:p:127:ILE:HG23	1.94	0.50
31:s:209:SER:OG	31:s:212:LYS:NZ	2.44	0.50
6:Z:16:LEU:HG	6:Z:17:LEU:H	1.74	0.50
9:c:149:GLN:HB3	9:c:156:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:71:GLY:HA2	14:B:162:VAL:HG12	1.94	0.50
2:V:401:ASN:HA	2:V:404:LYS:HB2	1.94	0.50
5:Y:203:ASP:OD1	5:Y:203:ASP:N	2.43	0.50
5:Y:336:ARG:NH1	11:e:55:GLN:OE1	2.44	0.50
10:d:203:PRO:C	10:d:205:LYS:H	2.19	0.50
12:f:682:GLY:HA3	12:f:687:ARG:HH11	1.76	0.50
23:k:97:GLN:HG3	30:r:61:ARG:HG2	1.93	0.50
25:m:170:GLN:HA	25:m:173:LYS:HE2	1.93	0.50
9:c:122:LEU:HD12	9:c:126:ASP:HB3	1.94	0.50
12:f:796:LEU:HA	12:f:799:VAL:HG12	1.93	0.50
13:A:41:TYR:HA	13:A:44:GLN:HB3	1.94	0.50
15:C:215:SER:OG	15:C:218:GLU:OE1	2.27	0.50
15:C:218:GLU:O	15:C:221:GLN:NE2	2.45	0.50
18:F:376:SER:HB3	18:F:414:GLU:HG3	1.94	0.50
19:G:43:ARG:HH21	19:G:164:LYS:HG2	1.76	0.50
3:W:344:THR:OG1	3:W:345:GLU:OE1	2.30	0.50
7:a:33:LEU:HA	8:b:18:ASN:HB2	1.93	0.50
8:b:161:ASN:HB2	8:b:165:GLY:HA3	1.94	0.50
12:f:149:GLU:HG3	12:f:152:ALA:HB2	1.93	0.50
21:I:106:PRO:HD2	21:I:109:GLN:HE21	1.75	0.50
31:S:209:SER:OG	31:S:212:LYS:NZ	2.44	0.50
2:V:239:THR:HG23	2:V:243:ASP:HB2	1.93	0.49
12:f:250:ARG:NH2	12:f:281:ILE:HG12	2.26	0.49
12:f:269:ALA:O	12:f:273:ASN:N	2.41	0.49
18:F:437:TYR:CE2	23:K:20:ARG:HB2	2.47	0.49
25:M:170:GLN:HA	25:M:173:LYS:HE2	1.93	0.49
1:U:898:CYS:SG	1:U:899:ARG:N	2.86	0.49
3:W:203:GLN:HB3	3:W:233:LEU:HD21	1.94	0.49
4:X:141:LYS:CD	4:X:141:LYS:C	2.85	0.49
5:Y:293:ARG:CZ	11:e:57:ARG:HB3	2.42	0.49
12:f:252:ALA:O	12:f:257:ARG:NH1	2.45	0.49
12:f:482:ILE:HG22	12:f:501:LEU:HD22	1.94	0.49
12:f:612:LEU:HD21	12:f:636:ASP:HA	1.94	0.49
14:B:409:GLU:OE2	14:B:411:ARG:NH2	2.35	0.49
20:H:66:GLU:OE2	20:H:91:ARG:NH2	2.45	0.49
24:L:186:GLU:O	24:L:190:HIS:N	2.45	0.49
29:q:64:VAL:HG13	29:q:75:LEU:HD12	1.94	0.49
1:U:824:GLU:HB3	1:U:826:GLU:HB2	1.94	0.49
3:W:99:GLN:HA	3:W:102:ALA:HB3	1.94	0.49
7:a:120:ALA:O	7:a:124:ASN:ND2	2.45	0.49
9:c:100:LYS:HG2	9:c:105:PRO:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:154:LEU:HD11	16:D:229:ARG:HE	1.76	0.49
19:G:114:LEU:HD22	19:G:140:LEU:HD21	1.93	0.49
27:o:198:ARG:NH1	28:p:152:SER:O	2.45	0.49
1:U:107:HIS:HA	1:U:110:LYS:HE3	1.94	0.49
1:U:416:GLU:OE2	1:U:450:HIS:HD2	1.93	0.49
3:W:443:THR:HA	3:W:446:ILE:HG12	1.95	0.49
12:f:618:GLU:HG2	14:B:82:GLN:CD	2.38	0.49
1:U:678:ASP:O	1:U:684:ARG:NH1	2.40	0.49
4:X:172:LEU:HD12	4:X:175:LYS:HD3	1.94	0.49
9:c:196:LEU:N	9:c:200:TYR:CZ	2.79	0.49
12:f:487:LEU:HD11	12:f:804:LEU:HD12	1.95	0.49
18:F:86:LEU:CD1	18:F:86:LEU:C	2.86	0.49
19:G:86:ASP:OD1	25:M:120:HIS:NE2	2.45	0.49
20:H:11:THR:HG1	21:I:127:LYS:CA	2.25	0.49
23:K:98:ASN:OD1	30:R:61:ARG:NH2	2.41	0.49
26:N:166:ARG:HH22	32:t:177:TYR:HE1	1.58	0.49
29:Q:64:VAL:HG13	29:Q:75:LEU:HD12	1.94	0.49
23:k:121:LEU:HD13	24:l:79:ALA:HA	1.93	0.49
1:U:872:GLU:HB2	1:U:873:PRO:HD2	1.95	0.49
2:V:29:PRO:CD	2:V:30:PRO:CD	2.87	0.49
4:X:78:ASN:HA	4:X:82:LYS:HE3	1.95	0.49
6:Z:192:THR:HG22	7:a:375:LEU:HG	1.94	0.49
12:f:257:ARG:HG2	12:f:272:LEU:HD13	1.94	0.49
12:f:742:ALA:O	12:f:746:ARG:NE	2.40	0.49
17:E:166:PRO:O	17:E:293:GLY:HA2	2.12	0.49
26:N:76:VAL:HG23	26:N:104:ASP:HB2	1.94	0.49
23:k:37:ALA:HB2	23:k:50:VAL:HG23	1.93	0.49
5:Y:279:GLU:OE2	5:Y:292:TYR:CB	2.34	0.49
5:Y:279:GLU:OE1	5:Y:292:TYR:HA	2.12	0.49
9:c:196:LEU:HD23	9:c:200:TYR:CE2	2.48	0.49
10:d:191:PHE:HZ	10:d:202:THR:H	1.59	0.49
12:f:119:LYS:HA	12:f:122:ALA:HB3	1.94	0.49
16:D:249:ASP:OD1	16:D:252:ARG:NH2	2.44	0.49
17:E:127:PRO:CA	17:E:193:CYS:SG	3.01	0.49
20:H:222:THR:OG1	20:H:225:GLU:OE1	2.26	0.49
21:I:7:SER:OG	21:I:11:ILE:CD1	2.61	0.49
30:R:38:ASN:HD22	30:R:41:LEU:HD12	1.77	0.49
5:Y:102:ASP:HA	5:Y:105:MET:HG2	1.94	0.49
16:D:335:LEU:HD23	16:D:335:LEU:N	2.27	0.49
17:E:193:CYS:SG	17:E:194:ASN:N	2.85	0.49
20:h:139:TRP:HA	20:h:144:PRO:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:228:ARG:NH2	2:V:253:LEU:O	2.46	0.49
3:W:65:ARG:HG3	3:W:67:LEU:H	1.78	0.49
3:W:82:LEU:HA	3:W:85:GLU:HB2	1.95	0.49
5:Y:300:ARG:NH2	11:e:59:GLU:OE1	2.44	0.49
8:b:34:ASN:O	8:b:38:HIS:ND1	2.38	0.49
10:d:248:GLU:HA	10:d:251:ARG:HB3	1.95	0.49
12:f:785:ARG:NH2	12:f:791:VAL:H	2.10	0.49
17:E:194:ASN:CG	17:E:228:CYS:HA	2.37	0.49
23:K:41:GLN:NE2	23:K:151:PRO:O	2.45	0.49
19:g:120:ASP:OD1	20:h:84:ARG:NH1	2.44	0.49
19:g:169:GLY:O	19:g:172:GLN:NE2	2.44	0.49
28:p:189:ILE:HG23	28:p:196:THR:HB	1.94	0.49
1:U:554:LEU:HG	1:U:588:MET:HE1	1.94	0.49
5:Y:141:VAL:HG13	5:Y:160:ASN:HB2	1.95	0.49
8:b:100:ARG:NH1	8:b:105:HIS:O	2.46	0.49
12:f:337:LEU:CD2	12:f:341:GLU:OE1	2.60	0.49
12:f:773:LYS:HE2	12:f:776:LEU:CD1	2.43	0.49
15:C:307:ARG:HD2	15:C:309:GLY:H	1.76	0.49
18:F:341:ALA:HA	18:F:344:ARG:HD2	1.90	0.49
19:G:120:ASP:OD1	20:H:84:ARG:NH1	2.46	0.49
28:P:189:ILE:HG23	28:P:196:THR:HB	1.94	0.49
21:i:159:TRP:HA	22:j:54:GLN:HA	1.95	0.49
1:U:510:GLU:HG3	1:U:543:LYS:HB3	1.95	0.48
2:V:29:PRO:N	2:V:30:PRO:CD	2.75	0.48
2:V:163:VAL:HG22	2:V:175:MET:HG2	1.94	0.48
3:W:59:ASP:HB3	3:W:71:VAL:HG23	1.95	0.48
12:f:171:GLN:HG3	12:f:179:VAL:HG22	1.95	0.48
17:E:196:LEU:HD13	17:E:230:ILE:CD1	2.43	0.48
19:g:11:ARG:O	19:g:24:GLN:NE2	2.46	0.48
21:i:105:ILE:HD11	21:i:109:GLN:HG3	1.95	0.48
26:n:76:VAL:HG23	26:n:104:ASP:HB2	1.93	0.48
3:W:172:GLU:HB3	3:W:182:ARG:CZ	2.43	0.48
5:Y:179:ARG:HH11	5:Y:182:VAL:HG11	1.77	0.48
7:a:227:ASN:O	7:a:231:GLN:NE2	2.44	0.48
12:f:373:ALA:HB2	12:f:744:MET:HA	1.94	0.48
22:J:4:ASP:OD1	22:J:4:ASP:N	2.44	0.48
27:O:171:SER:OG	27:O:171:SER:O	2.18	0.48
1:U:47:VAL:C	1:U:49:TYR:H	2.22	0.48
13:A:113:ILE:HD11	13:A:149:ILE:HD11	1.96	0.48
17:E:196:LEU:C	17:E:197:LYS:HG3	2.21	0.48
31:S:123:SER:HB3	31:S:136:LYS:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:643:SER:HA	15:C:49:ARG:HH22	1.78	0.48
4:X:317:PRO:HD2	4:X:319:ILE:HG13	1.95	0.48
6:Z:237:LEU:CD2	6:Z:237:LEU:N	2.73	0.48
14:B:188:GLY:HA3	14:B:364:ILE:HD13	1.94	0.48
24:L:189:LYS:O	24:L:193:ARG:NH1	2.46	0.48
19:g:41:ALA:HB3	19:g:166:THR:HB	1.96	0.48
23:k:182:GLN:NE2	24:l:55:GLU:OE1	2.44	0.48
1:U:325:MET:HA	1:U:328:ILE:HG12	1.95	0.48
1:U:643:SER:O	1:U:649:ARG:NH1	2.46	0.48
2:V:33:GLN:NE2	2:V:84:LYS:O	2.46	0.48
3:W:216:GLU:HA	3:W:219:THR:HB	1.96	0.48
5:Y:238:GLU:HA	5:Y:242:LYS:HB2	1.96	0.48
6:Z:237:LEU:HD23	6:Z:238:PRO:HD3	1.88	0.48
7:a:70:ARG:HH21	8:b:17:ARG:HA	1.77	0.48
12:f:288:VAL:HA	12:f:291:GLN:HG2	1.94	0.48
12:f:708:ASP:OD1	12:f:785:ARG:HG3	2.14	0.48
12:f:833:PHE:HB2	12:f:840:LEU:HG	1.95	0.48
17:E:127:PRO:HA	17:E:193:CYS:SG	2.54	0.48
21:I:86:LEU:HD22	21:I:114:LEU:HD11	1.94	0.48
23:K:236:GLU:HA	23:K:239:LYS:HE3	1.95	0.48
32:T:177:TYR:HE1	26:n:166:ARG:HH22	1.61	0.48
1:U:47:VAL:O	1:U:48:LEU:C	2.54	0.48
1:U:208:LEU:HD23	1:U:210:LYS:H	1.78	0.48
8:b:5:SER:HB3	8:b:64:LEU:HD21	1.95	0.48
12:f:253:LEU:HD11	12:f:272:LEU:HB3	1.95	0.48
16:D:248:ARG:HG2	16:D:295:GLN:HE22	1.78	0.48
21:I:239:LYS:NZ	21:I:243:GLU:OE2	2.46	0.48
1:U:895:PRO:HG2	1:U:902:PRO:HD3	1.96	0.48
2:V:107:ARG:HA	2:V:110:HIS:HD1	1.78	0.48
9:c:50:PRO:HG2	17:E:53:VAL:HG13	1.89	0.48
9:c:173:GLU:HG3	9:c:175:ARG:HD2	1.95	0.48
13:A:178:GLY:HA3	13:A:353:HIS:HD2	1.77	0.48
16:D:367:PRO:HG2	20:H:201:GLY:HA2	1.95	0.48
20:H:181:ASP:OD1	20:H:181:ASP:N	2.47	0.48
19:g:43:ARG:HH21	19:g:164:LYS:HG2	1.79	0.48
1:U:807:LYS:CB	1:U:808:PRO:CD	2.88	0.48
5:Y:212:GLU:HG3	5:Y:213:LEU:HG	1.95	0.48
8:b:58:CYS:HB3	8:b:92:VAL:HG11	1.95	0.48
8:b:95:LEU:O	8:b:99:HIS:ND1	2.47	0.48
8:b:109:ILE:HB	8:b:138:VAL:HG22	1.96	0.48
15:C:219:LEU:HA	15:C:221:GLN:HE22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:I:7:SER:OG	21:I:11:ILE:HD11	2.13	0.48
24:l:42:THR:O	24:l:137:TYR:OH	2.29	0.48
12:f:243:PRO:HD2	12:f:257:ARG:HH22	1.79	0.48
18:F:50:SER:O	18:F:54:ILE:N	2.38	0.48
18:F:228:PRO:O	18:F:233:LYS:NZ	2.47	0.48
23:K:77:ALA:HB3	23:K:142:LEU:HB2	1.95	0.48
22:j:116:GLN:HE22	23:k:83:ALA:HB1	1.79	0.48
23:k:100:TRP:O	30:r:57:ARG:NH2	2.47	0.48
23:k:169:ALA:O	23:k:174:SER:OG	2.32	0.48
24:l:186:GLU:O	24:l:190:HIS:N	2.45	0.48
29:q:19:ARG:HH21	29:q:31:ASP:HB2	1.79	0.48
1:U:423:MET:CE	1:U:446:LEU:HD13	2.35	0.48
9:c:196:LEU:C	9:c:196:LEU:CD2	2.85	0.48
12:f:23:GLY:HA3	12:f:34:ARG:HH22	1.78	0.48
12:f:369:ARG:NH2	12:f:791:VAL:O	2.45	0.48
12:f:637:LYS:HE2	12:f:673:ARG:HB2	1.96	0.48
12:f:764:LEU:HD11	12:f:771:LEU:HD11	1.37	0.48
13:A:122:VAL:O	18:F:86:LEU:HD13	2.14	0.48
18:F:339:ASP:HB3	18:F:342:LEU:HD13	1.96	0.48
29:Q:19:ARG:HH21	29:Q:31:ASP:HB2	1.79	0.48
1:U:773:PHE:H	9:c:177:THR:HB	1.79	0.47
10:d:182:ILE:HD12	10:d:186:TYR:HD2	1.78	0.47
12:f:640:LYS:HD3	12:f:651:GLY:HA3	1.96	0.47
12:f:810:ILE:CD1	12:f:854:GLY:O	2.57	0.47
15:C:113:ARG:HD2	15:C:131:VAL:HG13	1.95	0.47
17:E:125:GLU:OE1	17:E:221:TYR:OH	2.31	0.47
17:E:193:CYS:O	17:E:194:ASN:C	2.57	0.47
17:E:235:ILE:CG2	17:E:236:ASP:N	2.73	0.47
20:H:119:GLN:NE2	21:I:81:SER:O	2.47	0.47
24:L:42:THR:O	24:L:137:TYR:OH	2.29	0.47
31:S:187:VAL:HG21	27:o:24:MET:HE3	1.96	0.47
29:q:38:MET:O	29:q:65:GLN:NE2	2.45	0.47
3:W:227:TYR:HB3	3:W:246:HIS:NE2	2.30	0.47
4:X:145:GLU:HA	4:X:148:HIS:HB2	1.95	0.47
5:Y:60:SER:OG	5:Y:61:LEU:N	2.47	0.47
5:Y:297:ARG:HH12	11:e:51:ASP:HB3	1.79	0.47
17:E:235:ILE:CG2	17:E:279:THR:HG22	2.42	0.47
20:H:11:THR:OG1	21:I:127:LYS:N	2.48	0.47
21:I:105:ILE:HD11	21:I:109:GLN:HG3	1.96	0.47
23:K:100:TRP:O	30:R:57:ARG:NH2	2.47	0.47
24:l:189:LYS:O	24:l:193:ARG:NH1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:m:66:LEU:HD13	25:m:214:SER:HB2	1.96	0.47
1:U:381:THR:HG22	1:U:412:HIS:HA	1.96	0.47
4:X:397:TYR:OH	5:Y:362:LYS:NZ	2.47	0.47
12:f:612:LEU:HA	12:f:632:LYS:HD2	1.96	0.47
13:A:279:ALA:HB1	14:B:307:ARG:HG3	1.95	0.47
15:C:83:LYS:H	15:C:105:ILE:HD11	1.79	0.47
21:I:42:GLY:HA3	21:I:186:LEU:HD21	1.96	0.47
21:I:105:ILE:HG12	21:I:110:LEU:HB2	1.96	0.47
22:J:7:ILE:HD12	22:J:8:THR:HG23	1.97	0.47
27:O:177:VAL:HB	27:O:184:ASP:HB2	1.95	0.47
31:s:123:SER:HB3	31:s:136:LYS:HG3	1.95	0.47
2:V:26:PRO:O	2:V:30:PRO:HD2	2.14	0.47
3:W:63:THR:HG21	3:W:71:VAL:H	1.78	0.47
5:Y:44:ALA:HA	5:Y:49:ASN:HD22	1.79	0.47
6:Z:237:LEU:CB	6:Z:238:PRO:HD3	2.26	0.47
12:f:168:LYS:HD3	12:f:204:ALA:HB1	1.97	0.47
13:A:35:THR:O	13:A:39:SER:OG	2.31	0.47
29:Q:25:ILE:HD11	30:R:133:VAL:HG11	1.96	0.47
21:i:105:ILE:HG12	21:i:110:LEU:HB2	1.96	0.47
2:V:28:PRO:CB	2:V:29:PRO:CD	2.90	0.47
6:Z:20:VAL:HG22	6:Z:126:VAL:HG23	1.96	0.47
12:f:93:PRO:HB2	12:f:97:LYS:HG3	1.97	0.47
12:f:202:HIS:CE1	12:f:241:PRO:HB2	2.50	0.47
15:C:236:VAL:HA	15:C:239:ARG:HD3	1.96	0.47
21:I:178:ASP:OD2	21:I:195:LYS:NZ	2.38	0.47
23:K:76:CYS:SG	23:K:77:ALA:N	2.87	0.47
25:M:66:LEU:HD13	25:M:214:SER:HB2	1.96	0.47
1:U:229:VAL:HA	1:U:232:ILE:HG12	1.96	0.47
3:W:167:GLN:HG3	3:W:168:GLU:HG3	1.97	0.47
12:f:283:THR:O	12:f:287:ASP:N	2.46	0.47
19:G:144:ASP:HB3	19:G:147:GLN:HB2	1.96	0.47
22:J:158:ALA:HB3	23:K:58:LEU:HD13	1.95	0.47
2:V:179:LYS:HD2	2:V:210:CYS:HB2	1.96	0.47
2:V:203:LEU:HA	2:V:206:VAL:HB	1.96	0.47
5:Y:50:MET:HE1	5:Y:67:VAL:HG13	1.97	0.47
5:Y:174:TRP:NE1	15:C:377:HIS:NE2	2.62	0.47
5:Y:174:TRP:CE3	15:C:337:ASN:OD1	2.68	0.47
7:a:360:VAL:HG22	9:c:308:VAL:HG13	1.95	0.47
10:d:89:LEU:CD1	10:d:90:PRO:HD2	2.45	0.47
12:f:469:TYR:OH	12:f:478:ARG:NH1	2.47	0.47
12:f:482:ILE:HD11	12:f:517:VAL:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:403:LYS:HG3	20:H:156:PHE:HE1	1.80	0.47
17:E:122:MET:HB2	17:E:218:MET:HG2	1.97	0.47
18:F:249:LEU:HD23	18:F:283:ILE:HG12	1.97	0.47
19:G:9:PHE:HD2	19:G:18:PRO:HG3	1.68	0.47
19:G:19:GLU:CA	20:H:27:ALA:HB1	2.42	0.47
20:H:196:LYS:NZ	20:H:234:ALA:O	2.41	0.47
21:I:229:LYS:N	21:I:232:GLU:OE2	2.47	0.47
23:K:91:LYS:HG2	23:K:95:GLU:HG2	1.96	0.47
29:Q:38:MET:O	29:Q:65:GLN:NE2	2.45	0.47
21:i:9:THR:HA	21:i:20:GLN:HG3	1.97	0.47
25:m:152:ASP:OD1	25:m:156:VAL:N	2.48	0.47
28:p:2:SER:OG	28:p:3:ILE:N	2.47	0.47
7:a:214:GLY:HA2	7:a:217:LEU:HD13	1.97	0.47
8:b:22:LEU:HG	18:F:49:ASP:CG	2.39	0.47
15:C:90:HIS:C	15:C:90:HIS:ND1	2.73	0.47
22:j:7:ILE:HD12	22:j:8:THR:HG23	1.96	0.47
27:o:205:GLU:HB2	27:o:208:THR:HB	1.97	0.47
6:Z:45:LYS:HB3	6:Z:47:VAL:HG12	1.95	0.47
7:a:75:SER:HA	7:a:78:GLU:HB2	1.97	0.47
15:C:307:ARG:HH21	15:C:310:ARG:HE	1.63	0.47
18:F:205:PRO:CB	18:F:324:THR:CB	2.91	0.47
23:K:55:THR:OG1	23:K:59:MET:SD	2.71	0.47
2:V:324:PHE:H	11:e:6:GLN:HB3	1.79	0.47
10:d:88:GLN:HA	10:d:88:GLN:HE21	1.73	0.47
12:f:773:LYS:CA	12:f:775:THR:HG23	2.43	0.47
12:f:827:PRO:HG2	12:f:848:GLN:HB3	1.96	0.47
15:C:406:LYS:HE2	21:I:80:THR:HG22	1.97	0.47
18:F:86:LEU:CB	18:F:87:PRO:CD	2.78	0.47
25:M:229:LYS:HA	25:M:229:LYS:HZ3	1.68	0.47
26:N:144:ARG:H	26:N:147:MET:HE3	1.80	0.47
27:o:177:VAL:HB	27:o:184:ASP:HB2	1.95	0.47
1:U:181:LEU:HD23	1:U:181:LEU:C	2.40	0.46
7:a:247:ARG:HH21	7:a:250:THR:HG23	1.80	0.46
13:A:56:LEU:HD11	14:B:48:LYS:HD3	1.97	0.46
17:E:252:GLU:HA	17:E:255:ARG:HE	1.80	0.46
23:K:232:GLU:CD	23:K:232:GLU:N	2.73	0.46
25:M:152:ASP:OD1	25:M:156:VAL:N	2.48	0.46
19:g:144:ASP:HB3	19:g:147:GLN:HB2	1.97	0.46
3:W:170:GLN:C	3:W:173:THR:OG1	2.58	0.46
6:Z:192:THR:O	6:Z:196:HIS:ND1	2.47	0.46
17:E:281:ARG:NH1	17:E:281:ARG:CG	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:199:ILE:HD12	19:G:210:PHE:HZ	1.80	0.46
20:H:225:GLU:O	20:H:229:TYR:N	2.49	0.46
28:P:2:SER:OG	28:P:3:ILE:N	2.47	0.46
26:n:20:THR:HB	26:n:28:ASN:HB3	1.97	0.46
28:p:190:ILE:HG22	28:p:195:ILE:HG23	1.97	0.46
31:s:4:PRO:O	32:t:100:ARG:NH2	2.46	0.46
1:U:801:GLN:HB3	1:U:877:LEU:HD22	1.97	0.46
13:A:218:PRO:HB2	14:B:343:ARG:HD3	1.95	0.46
13:A:339:ARG:NH1	18:F:426:GLU:OE2	2.48	0.46
14:B:287:ILE:HG12	14:B:329:MET:HB3	1.97	0.46
19:g:163:PHE:HB3	20:h:57:TYR:HA	1.98	0.46
22:j:109:ARG:NH2	30:r:70:ASN:OD1	2.48	0.46
26:n:144:ARG:H	26:n:147:MET:HE3	1.80	0.46
3:W:435:LEU:HD11	6:Z:238:PRO:CD	2.43	0.46
7:a:150:SER:OG	7:a:154:ARG:NH1	2.48	0.46
9:c:232:GLN:O	9:c:232:GLN:HG3	2.15	0.46
26:N:20:THR:HB	26:N:28:ASN:HB3	1.97	0.46
31:S:4:PRO:O	32:T:100:ARG:NH2	2.47	0.46
1:U:519:VAL:HG23	1:U:520:MET:HG2	1.97	0.46
2:V:188:SER:C	2:V:192:MET:CG	2.59	0.46
3:W:422:ASN:O	3:W:426:ASN:N	2.48	0.46
7:a:27:GLU:OE1	7:a:31:LYS:NZ	2.47	0.46
7:a:321:LYS:O	7:a:334:THR:OG1	2.34	0.46
12:f:505:MET:HE3	12:f:537:THR:HG22	1.98	0.46
17:E:192:ASP:O	17:E:193:CYS:HB3	2.14	0.46
17:E:305:ASN:HB3	17:E:308:ALA:H	1.80	0.46
21:I:14:PRO:HA	22:J:21:TYR:CE2	2.50	0.46
1:U:416:GLU:OE2	1:U:416:GLU:HA	2.15	0.46
2:V:110:HIS:HD2	2:V:114:TYR:HE2	1.63	0.46
21:I:165:GLY:O	21:I:168:SER:N	2.46	0.46
22:J:134:VAL:HG22	22:J:144:LEU:HB2	1.98	0.46
1:U:695:MET:HE1	1:U:709:PHE:HD2	1.81	0.46
2:V:26:PRO:O	2:V:29:PRO:HD2	2.16	0.46
5:Y:233:ARG:HD3	5:Y:233:ARG:HA	1.57	0.46
7:a:50:PHE:O	7:a:86:GLN:NE2	2.49	0.46
10:d:203:PRO:O	10:d:205:LYS:N	2.48	0.46
13:A:307:ASP:OD2	13:A:333:ARG:NH2	2.49	0.46
17:E:194:ASN:CG	17:E:229:ILE:N	2.69	0.46
18:F:222:GLY:HA3	18:F:348:LEU:HA	1.96	0.46
18:F:321:GLN:NE2	18:F:323:ASN:HD21	2.13	0.46
19:G:209:ASP:N	19:G:209:ASP:OD1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:699:THR:HG21	1:U:812:ALA:HA	1.98	0.46
2:V:183:GLU:HA	2:V:186:LYS:HB3	1.98	0.46
4:X:54:GLY:HA2	4:X:57:LEU:HD12	1.98	0.46
5:Y:81:LEU:HD22	5:Y:107:LYS:HG2	1.98	0.46
9:c:49:VAL:HG23	9:c:50:PRO:HD3	1.96	0.46
9:c:233:ASP:CB	9:c:236:GLU:OE1	2.63	0.46
9:c:279:ASP:CB	9:c:280:PRO:CD	2.79	0.46
13:A:89:SER:HA	13:A:93:LEU:HD23	1.98	0.46
13:A:103:ASN:HA	13:A:136:GLU:HG2	1.97	0.46
14:B:67:ARG:NH2	14:B:71:TYR:OH	2.49	0.46
14:B:248:LEU:HD12	14:B:282:VAL:HG22	1.98	0.46
16:D:320:ALA:O	16:D:326:ARG:NH2	2.49	0.46
29:Q:199:GLN:H	29:q:197:PRO:HA	1.80	0.46
2:V:480:ILE:HD11	6:Z:260:VAL:HA	1.98	0.46
5:Y:293:ARG:CD	11:e:57:ARG:CB	2.82	0.46
6:Z:237:LEU:CD1	6:Z:237:LEU:N	2.73	0.46
7:a:19:PRO:HA	7:a:23:HIS:HD2	1.81	0.46
10:d:71:PHE:HZ	10:d:101:LEU:HB3	1.80	0.46
13:A:117:GLN:HE22	14:B:128:GLY:HA3	1.80	0.46
14:B:233:THR:OG1	34:B:501:ATP:O2B	2.32	0.46
15:C:222:LYS:HD3	15:C:223:PHE:CE1	2.51	0.46
1:U:607:VAL:HG11	16:D:63:ASP:HB3	1.97	0.46
3:W:170:GLN:HA	3:W:173:THR:OG1	2.16	0.46
4:X:202:CYS:HA	4:X:203:PRO:HD3	1.66	0.46
6:Z:124:ILE:HG22	6:Z:135:THR:HG22	1.98	0.46
13:A:395:PHE:HA	13:A:398:ARG:HD2	1.98	0.46
14:B:120:HIS:HA	14:B:134:SER:HA	1.98	0.46
17:E:198:VAL:HB	17:E:232:MET:CA	2.38	0.46
18:F:86:LEU:HD13	18:F:86:LEU:O	2.16	0.46
32:T:136:SER:HB2	32:T:150:LEU:HD13	1.98	0.46
21:i:2:SER:OG	21:i:3:ARG:N	2.46	0.46
21:i:86:LEU:HD22	21:i:114:LEU:HD11	1.97	0.46
4:X:137:TYR:HB3	4:X:142:ARG:CB	2.42	0.45
6:Z:177:ARG:NH2	9:c:153:GLY:O	2.49	0.45
12:f:785:ARG:HD3	12:f:785:ARG:HA	1.40	0.45
15:C:138:MET:HE3	15:C:234:LEU:HD13	1.97	0.45
17:E:254:GLN:HB3	17:E:258:MET:HE2	1.97	0.45
21:i:108:GLU:OE2	21:i:146:GLN:NE2	2.49	0.45
22:j:32:ALA:HB3	22:j:161:ILE:HD11	1.98	0.45
1:U:173:VAL:HA	1:U:174:PRO:HD3	1.55	0.45
12:f:828:ARG:NE	12:f:843:SER:HG	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:72:LYS:O	18:F:74:LYS:N	2.48	0.45
19:G:32:ILE:HA	19:G:82:GLY:HA2	1.97	0.45
21:I:49:ARG:HB2	21:I:210:LYS:HA	1.99	0.45
27:O:205:GLU:HB2	27:O:208:THR:HB	1.97	0.45
31:S:35:ILE:O	32:T:151:ARG:NH2	2.38	0.45
1:U:772:TRP:HD1	1:U:775:LEU:HG	1.82	0.45
5:Y:184:GLN:HB3	5:Y:197:ALA:HA	1.99	0.45
12:f:810:ILE:HD13	12:f:854:GLY:C	2.39	0.45
19:g:141:ILE:HG22	19:g:151:VAL:HG22	1.98	0.45
22:j:32:ALA:HB2	22:j:45:VAL:HG23	1.98	0.45
1:U:180:SER:HA	1:U:183:LEU:HD12	1.98	0.45
1:U:802:TYR:HB3	1:U:895:PRO:HB3	1.98	0.45
3:W:172:GLU:C	3:W:175:GLY:H	2.24	0.45
12:f:24:THR:HG23	12:f:31:LYS:HG3	1.97	0.45
17:E:339:ASN:HB3	17:E:342:ASP:HB2	1.98	0.45
18:F:205:PRO:HB3	18:F:324:THR:HG21	1.98	0.45
1:U:603:LEU:HD21	16:D:60:TYR:HB2	1.99	0.45
3:W:139:GLU:HA	3:W:139:GLU:OE1	2.16	0.45
12:f:626:GLU:OE1	12:f:665:GLU:HB3	2.16	0.45
12:f:778:LEU:HA	12:f:803:PHE:HB3	1.99	0.45
18:F:205:PRO:HB3	18:F:324:THR:CG2	2.46	0.45
20:H:34:PRO:HA	20:H:164:GLY:HA3	1.99	0.45
22:J:32:ALA:HB3	22:J:161:ILE:HD11	1.98	0.45
28:P:135:ASP:OD1	28:P:135:ASP:N	2.48	0.45
21:i:90:LEU:HD12	21:i:114:LEU:HD22	1.99	0.45
7:a:119:GLY:HA2	7:a:122:LYS:HB3	1.98	0.45
12:f:75:LEU:HD12	12:f:78:LEU:HD13	1.99	0.45
13:A:105:ASP:HB2	13:A:110:LYS:HB2	1.98	0.45
16:D:207:PRO:CG	16:D:335:LEU:HD21	2.18	0.45
27:O:112:SER:HB3	27:O:125:VAL:HG11	1.99	0.45
21:i:62:SER:OG	21:i:65:ILE:O	2.32	0.45
27:o:169:SER:C	27:o:171:SER:H	2.25	0.45
3:W:174:TYR:HA	17:E:143:ARG:HD2	1.99	0.45
4:X:57:LEU:HD13	4:X:66:LEU:HA	1.99	0.45
6:Z:229:GLN:HG3	7:a:338:PRO:HB2	1.99	0.45
12:f:184:LEU:HG	14:B:59:ARG:HB2	1.98	0.45
12:f:717:ALA:HB1	12:f:760:PHE:HB2	1.97	0.45
21:I:8:ARG:HD3	21:I:126:GLY:HA3	1.98	0.45
25:M:168:ALA:HB1	25:M:171:ALA:HB3	1.99	0.45
31:S:35:ILE:HB	32:T:151:ARG:HH12	1.81	0.45
25:m:37:ILE:HD11	25:m:193:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:m:168:ALA:HB1	25:m:171:ALA:HB3	1.99	0.45
28:p:28:PHE:HB2	28:p:39:PHE:HB2	1.99	0.45
5:Y:47:ASP:OD1	5:Y:113:ARG:NE	2.38	0.45
6:Z:12:HIS:ND1	6:Z:51:SER:HA	2.32	0.45
12:f:564:LEU:HD22	12:f:776:LEU:HG	1.99	0.45
16:D:202:VAL:HA	16:D:329:ARG:HB2	1.98	0.45
17:E:190:GLN:O	17:E:191:LEU:C	2.60	0.45
25:M:41:CYS:HB3	25:M:189:ILE:HG13	1.98	0.45
6:Z:198:LEU:HD22	7:a:364:GLU:HB2	1.99	0.45
17:E:53:VAL:O	17:E:53:VAL:HG12	2.17	0.45
17:E:62:LYS:HA	17:E:94:PRO:HB3	1.98	0.45
21:I:216:LEU:HD12	21:I:225:ILE:HG12	1.98	0.45
30:R:36:GLU:OE2	30:R:186:ARG:NH2	2.50	0.45
22:j:134:VAL:HG22	22:j:144:LEU:HB2	1.98	0.45
1:U:357:LYS:HE3	1:U:392:TRP:CD2	2.52	0.45
1:U:756:HIS:HB3	1:U:758:PRO:HD2	1.99	0.45
17:E:235:ILE:HG21	17:E:279:THR:HG22	1.98	0.45
29:Q:37:LYS:O	29:Q:61:GLN:NE2	2.46	0.45
25:m:76:ALA:HB3	25:m:136:MET:HB2	1.99	0.45
12:f:759:LEU:H	12:f:809:ILE:HB	1.82	0.44
17:E:56:ILE:HB	17:E:100:LEU:HB2	1.98	0.44
17:E:194:ASN:HB2	17:E:229:ILE:H	1.79	0.44
28:P:62:THR:OG1	29:Q:85:ARG:NH2	2.48	0.44
25:m:41:CYS:HB3	25:m:189:ILE:HG13	1.98	0.44
27:o:112:SER:HB3	27:o:125:VAL:HG11	1.99	0.44
30:r:36:GLU:OE2	30:r:186:ARG:NH2	2.50	0.44
1:U:118:LEU:HD13	1:U:122:GLU:HG3	1.98	0.44
1:U:699:THR:HG21	1:U:812:ALA:N	2.28	0.44
4:X:414:LEU:HD11	6:Z:273:HIS:CE1	2.53	0.44
10:d:176:ASP:O	10:d:180:GLY:N	2.48	0.44
23:K:22:PHE:CA	23:K:25:GLU:HB3	2.46	0.44
23:K:121:LEU:HD13	24:L:79:ALA:HA	1.98	0.44
28:P:190:ILE:HG22	28:P:195:ILE:HG23	1.97	0.44
19:g:53:GLN:HA	19:g:215:ILE:HA	1.99	0.44
1:U:811:PHE:HE1	1:U:888:GLN:HE22	1.66	0.44
2:V:323:GLY:HA2	11:e:9:ASP:HB2	1.98	0.44
3:W:178:GLU:H	3:W:182:ARG:HB3	1.81	0.44
4:X:134:VAL:HB	4:X:149:LEU:HD23	1.97	0.44
6:Z:190:ARG:HA	6:Z:193:ASN:HD22	1.82	0.44
12:f:403:LYS:HG3	12:f:406:GLY:H	1.82	0.44
12:f:417:ILE:HG22	12:f:418:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:346:PRO:HB3	13:A:350:GLY:HA3	1.99	0.44
14:B:190:LEU:HD13	14:B:193:GLN:HB2	1.99	0.44
17:E:385:ASP:OD1	17:E:385:ASP:N	2.50	0.44
19:G:10:ASP:OD1	19:G:10:ASP:N	2.50	0.44
22:J:115:LYS:HD3	22:J:149:PRO:HA	1.99	0.44
32:t:136:SER:HB2	32:t:150:LEU:HD13	1.98	0.44
2:V:37:MET:HE2	2:V:115:LYS:HE2	2.00	0.44
4:X:380:GLN:HB3	5:Y:315:THR:HG22	1.98	0.44
5:Y:174:TRP:NE1	5:Y:177:ARG:HD3	2.25	0.44
7:a:168:ASN:OD1	7:a:171:SER:OG	2.33	0.44
12:f:167:ALA:HA	12:f:170:TRP:HD1	1.82	0.44
12:f:732:VAL:O	12:f:736:THR:OG1	2.36	0.44
18:F:339:ASP:O	18:F:343:LEU:HD21	2.17	0.44
20:H:6:TYR:CE1	21:I:6:ASP:HB3	2.52	0.44
20:h:222:THR:OG1	20:h:225:GLU:OE1	2.29	0.44
22:j:115:LYS:HD3	22:j:149:PRO:HA	1.99	0.44
2:V:243:ASP:OD1	2:V:246:GLY:N	2.50	0.44
6:Z:243:GLN:NE2	10:d:233:GLU:OE2	2.50	0.44
9:c:277:LYS:NZ	16:D:118:THR:O	2.51	0.44
12:f:171:GLN:HE21	12:f:179:VAL:HA	1.83	0.44
17:E:196:LEU:C	17:E:197:LYS:CG	2.86	0.44
27:O:169:SER:C	27:O:171:SER:H	2.26	0.44
4:X:53:LEU:HD23	4:X:56:LEU:HD12	2.00	0.44
4:X:201:TYR:HD1	20:H:177:ARG:HA	1.82	0.44
5:Y:144:LEU:HB3	5:Y:160:ASN:HD22	1.83	0.44
6:Z:70:LEU:HD23	6:Z:70:LEU:HA	1.78	0.44
13:A:161:VAL:HA	13:A:164:MET:HG2	2.00	0.44
19:G:12:HIS:CG	25:M:7:TYR:CE1	2.98	0.44
29:Q:2:GLU:HG3	29:Q:34:LYS:HE2	1.99	0.44
28:p:36:THR:OG1	28:p:38:ASP:OD1	2.33	0.44
3:W:139:GLU:C	3:W:139:GLU:CD	2.86	0.44
12:f:810:ILE:HD11	12:f:853:VAL:CA	2.48	0.44
18:F:321:GLN:HE21	18:F:323:ASN:ND2	2.15	0.44
22:J:32:ALA:HB2	22:J:45:VAL:HG23	1.98	0.44
25:M:76:ALA:HB3	25:M:136:MET:HB2	1.99	0.44
29:Q:23:SER:HB2	29:Q:28:MET:HE2	2.00	0.44
27:o:171:SER:OG	27:o:192:PRO:CG	2.64	0.44
1:U:416:GLU:CD	1:U:450:HIS:HD2	2.26	0.44
5:Y:174:TRP:CE3	15:C:338:LEU:O	2.68	0.44
12:f:130:ALA:O	12:f:134:SER:N	2.49	0.44
12:f:336:GLU:O	12:f:341:GLU:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:656:GLY:O	12:f:660:ILE:CG2	2.66	0.44
13:A:124:ASP:HB2	18:F:86:LEU:HG	2.00	0.44
18:F:205:PRO:CB	18:F:324:THR:CG2	2.95	0.44
25:M:37:ILE:HD11	25:M:193:VAL:HG13	1.99	0.44
20:h:192:ILE:O	20:h:196:LYS:N	2.46	0.44
32:t:45:VAL:HB	32:t:49:THR:HG23	2.00	0.44
1:U:496:LEU:HA	1:U:499:THR:HG22	2.00	0.44
3:W:136:ILE:HG22	3:W:143:ALA:HB3	1.98	0.44
9:c:231:LEU:C	9:c:233:ASP:N	2.72	0.44
12:f:43:GLN:HG3	12:f:121:PHE:HB2	2.00	0.44
17:E:194:ASN:HD22	17:E:229:ILE:HG12	1.82	0.44
19:G:141:ILE:HG22	19:G:151:VAL:HG22	1.99	0.44
21:I:48:GLU:OE2	21:I:50:ARG:NH2	2.50	0.44
22:j:11:SER:OG	22:j:15:HIS:N	2.51	0.44
27:o:96:ALA:H	27:o:115:PRO:HB3	1.82	0.44
27:o:171:SER:HB2	27:o:193:ASN:OD1	2.18	0.44
29:q:23:SER:HB2	29:q:28:MET:HE2	2.00	0.44
1:U:900:TYR:OH	1:U:920:ASP:O	2.36	0.43
5:Y:349:LYS:HA	5:Y:349:LYS:HD3	1.71	0.43
7:a:122:LYS:HD3	7:a:130:VAL:HG13	1.99	0.43
7:a:252:LYS:HA	7:a:255:TRP:HD1	1.82	0.43
8:b:34:ASN:HB3	18:F:56:LYS:HZ2	1.83	0.43
13:A:258:ARG:HG2	13:A:305:GLN:HE22	1.83	0.43
17:E:144:GLU:O	17:E:297:ARG:NH2	2.51	0.43
17:E:232:MET:HE2	17:E:232:MET:HB2	1.76	0.43
27:O:38:SER:OG	27:O:40:ASN:OD1	2.32	0.43
23:k:91:LYS:HE3	23:k:119:LEU:HD22	2.00	0.43
1:U:19:LEU:HB2	10:d:27:LYS:HZ3	1.84	0.43
1:U:46:GLU:O	1:U:50:GLU:HG2	2.18	0.43
4:X:50:ILE:HG23	4:X:69:LEU:HD11	2.00	0.43
6:Z:70:LEU:HD12	6:Z:111:LEU:HD22	2.00	0.43
7:a:145:LEU:HD12	7:a:148:VAL:HG23	1.99	0.43
17:E:194:ASN:ND2	17:E:229:ILE:N	2.66	0.43
18:F:300:LYS:HA	18:F:300:LYS:HD2	1.79	0.43
20:H:11:THR:OG1	21:I:126:GLY:C	2.61	0.43
23:k:155:HIS:CE1	23:k:170:ILE:HG21	2.53	0.43
27:o:67:SER:HB3	27:o:74:PRO:HG3	2.00	0.43
1:U:70:HIS:HA	2:V:236:ARG:HH22	1.83	0.43
2:V:132:LEU:HD23	2:V:135:LEU:HD12	1.99	0.43
2:V:337:LEU:HD11	2:V:364:THR:HB	2.00	0.43
6:Z:116:CYS:O	6:Z:119:SER:OG	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:787:LEU:HB3	12:f:788:MET:H	1.52	0.43
14:B:357:ASP:O	14:B:361:LYS:NZ	2.45	0.43
15:C:148:TYR:HB2	15:C:206:HIS:CD2	2.53	0.43
16:D:194:ILE:HD12	16:D:196:ILE:HD11	2.00	0.43
28:P:28:PHE:HB2	28:P:39:PHE:HB2	1.99	0.43
21:i:105:ILE:HA	21:i:106:PRO:HD3	1.84	0.43
29:q:2:GLU:HG3	29:q:34:LYS:HE2	1.99	0.43
3:W:178:GLU:C	3:W:180:LYS:N	2.76	0.43
3:W:237:GLU:HG2	3:W:238:GLY:H	1.83	0.43
3:W:446:ILE:HA	6:Z:227:ILE:HD11	1.99	0.43
4:X:57:LEU:HD23	4:X:62:GLN:HE21	1.82	0.43
9:c:88:ASP:HB3	9:c:91:PHE:HB3	1.99	0.43
12:f:810:ILE:CG2	12:f:855:GLN:CD	2.80	0.43
14:B:303:ARG:O	14:B:307:ARG:N	2.49	0.43
16:D:144:PRO:HA	16:D:145:PRO:HD3	1.91	0.43
17:E:198:VAL:HG21	17:E:232:MET:HE2	2.00	0.43
20:H:7:SER:O	20:H:9:SER:N	2.51	0.43
25:m:144:ASP:O	25:m:147:GLN:NE2	2.52	0.43
2:V:28:PRO:CD	2:V:29:PRO:HD3	2.48	0.43
3:W:334:GLU:OE2	3:W:338:THR:OG1	2.36	0.43
5:Y:179:ARG:HD3	5:Y:179:ARG:HA	1.69	0.43
6:Z:228:TYR:O	6:Z:232:ASP:N	2.50	0.43
7:a:77:VAL:HA	7:a:80:ILE:HG22	2.01	0.43
12:f:438:ASP:HA	12:f:477:MET:HE2	2.00	0.43
19:G:175:SER:HA	19:G:205:VAL:HG21	2.01	0.43
27:O:18:THR:HB	27:O:30:ASN:HA	2.00	0.43
22:j:121:SER:HB3	22:j:124:ARG:HD3	2.00	0.43
28:p:135:ASP:OD1	28:p:135:ASP:N	2.48	0.43
1:U:177:LEU:HD13	1:U:177:LEU:N	2.32	0.43
1:U:554:LEU:HD11	1:U:761:VAL:HG13	2.00	0.43
2:V:322:VAL:CG2	11:e:6:GLN:HG2	2.46	0.43
3:W:361:HIS:HA	3:W:364:ARG:HH11	1.84	0.43
7:a:138:VAL:O	7:a:142:LEU:N	2.52	0.43
10:d:171:LEU:HD23	10:d:174:ILE:HD12	2.01	0.43
12:f:253:LEU:HA	12:f:257:ARG:HD3	2.01	0.43
12:f:621:ASP:O	12:f:623:LYS:N	2.51	0.43
12:f:852:VAL:O	12:f:854:GLY:N	2.34	0.43
18:F:235:LEU:HG	34:F:501:ATP:H2'	2.00	0.43
32:T:43:MET:HE3	32:T:45:VAL:HG22	2.00	0.43
1:U:213:PHE:HE1	1:U:244:MET:HB2	1.83	0.43
1:U:699:THR:CG2	1:U:812:ALA:HA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:70:LEU:HD11	6:Z:108:ILE:HG23	2.00	0.43
10:d:89:LEU:HD12	10:d:90:PRO:HD2	2.00	0.43
12:f:692:LEU:HD22	14:B:40:THR:HB	1.99	0.43
12:f:836:GLU:HB2	12:f:840:LEU:CD1	2.24	0.43
14:B:187:ILE:HG22	14:B:234:LEU:HD13	2.00	0.43
20:H:50:LYS:NZ	20:H:62:VAL:O	2.40	0.43
20:H:125:GLY:C	20:H:127:VAL:N	2.76	0.43
22:J:11:SER:OG	22:J:15:HIS:N	2.51	0.43
31:S:38:ARG:HH12	32:T:151:ARG:HD3	1.84	0.43
24:l:41:LYS:NZ	24:l:180:MET:O	2.42	0.43
12:f:705:ASN:OD1	12:f:706:ILE:N	2.48	0.43
15:C:198:LEU:O	15:C:202:ALA:N	2.44	0.43
18:F:221:LYS:HD3	18:F:322:PRO:HA	2.01	0.43
21:I:108:GLU:OE2	21:I:146:GLN:NE2	2.51	0.43
28:P:58:THR:O	29:Q:85:ARG:NH2	2.52	0.43
32:T:45:VAL:HB	32:T:49:THR:HG23	2.01	0.43
19:g:56:VAL:HG13	19:g:61:LEU:HD22	2.00	0.43
19:g:114:LEU:HD22	19:g:140:LEU:HD21	2.00	0.43
21:i:180:LYS:HE2	21:i:183:GLU:HG2	2.01	0.43
27:o:18:THR:HB	27:o:30:ASN:HA	2.00	0.43
3:W:89:LEU:HA	19:G:209:ASP:OD2	2.18	0.43
4:X:187:ARG:NH2	4:X:221:GLU:OE2	2.52	0.43
9:c:59:GLY:HA3	9:c:69:VAL:HA	2.00	0.43
12:f:399:LEU:HD11	12:f:440:ILE:HG12	2.00	0.43
13:A:124:ASP:HB2	18:F:86:LEU:CD2	2.49	0.43
18:F:35:LYS:HE2	18:F:39:GLU:HG2	2.01	0.43
21:I:171:ALA:HB2	21:I:200:THR:HG21	2.00	0.43
32:T:184:TYR:CE2	32:T:186:ARG:HB3	2.54	0.43
23:k:152:GLN:OE1	23:k:164:GLN:NE2	2.52	0.43
1:U:792:ASN:HB3	1:U:914:LEU:HB3	2.01	0.43
3:W:312:MET:HG2	3:W:315:MET:H	1.84	0.43
5:Y:291:HIS:O	5:Y:295:TYR:N	2.43	0.43
6:Z:34:ARG:NH1	6:Z:60:GLU:OE1	2.52	0.43
8:b:18:ASN:OD1	8:b:18:ASN:N	2.49	0.43
10:d:203:PRO:C	10:d:205:LYS:N	2.76	0.43
15:C:230:MET:O	15:C:234:LEU:N	2.52	0.43
18:F:307:GLN:HA	18:F:310:MET:HB3	2.01	0.43
18:F:407:ALA:HB1	18:F:412:ALA:HB3	2.01	0.43
21:I:179:TYR:OH	21:I:181:GLU:OE1	2.30	0.43
29:Q:162:LYS:O	30:r:141:ARG:NH2	2.52	0.43
20:h:108:ALA:HA	20:h:147:PHE:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:l:46:LEU:HD13	24:l:73:SER:HB2	2.01	0.43
1:U:423:MET:HE1	1:U:446:LEU:CD1	2.41	0.42
2:V:108:LEU:HA	2:V:111:TYR:HD2	1.84	0.42
5:Y:279:GLU:CD	5:Y:292:TYR:CB	2.88	0.42
12:f:608:LYS:HB3	12:f:608:LYS:HE3	1.84	0.42
12:f:762:VAL:HG13	12:f:806:VAL:HG13	2.01	0.42
12:f:822:VAL:HG12	12:f:852:VAL:HG21	1.99	0.42
15:C:209:CYS:SG	15:C:210:THR:N	2.92	0.42
17:E:40:TYR:HA	18:F:73:ILE:HD12	2.00	0.42
20:H:74:LEU:HD21	20:H:134:LEU:HD22	2.00	0.42
27:O:96:ALA:H	27:O:115:PRO:HB3	1.82	0.42
27:O:141:LYS:NZ	27:O:157:GLU:OE2	2.43	0.42
28:P:107:PRO:HG2	28:P:124:LEU:HB2	2.01	0.42
19:g:86:ASP:OD1	25:m:120:HIS:NE2	2.52	0.42
25:m:108:LEU:HD11	25:m:137:LEU:HB3	2.01	0.42
32:t:43:MET:HE3	32:t:45:VAL:HG22	2.00	0.42
1:U:212:ASP:H	1:U:215:ASN:HD21	1.65	0.42
2:V:29:PRO:CB	2:V:30:PRO:CD	2.97	0.42
7:a:9:GLN:HE22	7:a:23:HIS:CE1	2.37	0.42
12:f:240:VAL:O	12:f:257:ARG:NH2	2.36	0.42
12:f:412:ALA:HA	12:f:447:ALA:HB2	2.01	0.42
12:f:809:ILE:HD11	12:f:855:GLN:HE21	1.69	0.42
13:A:287:ASP:OD2	14:B:298:ASN:ND2	2.39	0.42
14:B:316:LEU:HD22	14:B:322:ARG:HH12	1.84	0.42
15:C:405:TRP:HH2	21:I:27:ALA:HB1	1.83	0.42
12:f:180:GLN:HE22	12:f:835:GLU:HB3	1.85	0.42
13:A:108:ASP:OD2	13:A:110:LYS:NZ	2.53	0.42
17:E:198:VAL:O	17:E:233:ASP:O	2.37	0.42
18:F:324:THR:CB	18:F:327:LYS:HE3	2.49	0.42
20:H:46:LEU:HD13	20:H:75:VAL:HG13	2.01	0.42
21:I:165:GLY:O	21:I:169:ALA:N	2.53	0.42
22:J:64:ALA:O	22:J:88:ARG:NH1	2.53	0.42
30:r:35:ILE:N	30:r:43:GLY:O	2.52	0.42
2:V:378:VAL:HA	2:V:381:GLN:HB3	2.01	0.42
4:X:77:LEU:HD22	4:X:116:TRP:HH2	1.84	0.42
6:Z:16:LEU:CD2	6:Z:16:LEU:H	2.32	0.42
6:Z:213:GLU:O	6:Z:217:THR:HB	2.19	0.42
12:f:460:ASP:OD1	12:f:460:ASP:N	2.52	0.42
12:f:665:GLU:HG2	12:f:669:GLU:HG3	2.01	0.42
12:f:674:THR:O	12:f:678:LEU:N	2.51	0.42
14:B:136:LEU:HD13	14:B:136:LEU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:90:HIS:CB	15:C:91:PRO:HD3	2.34	0.42
17:E:190:GLN:O	17:E:192:ASP:N	2.52	0.42
21:I:136:TYR:HB2	21:I:148:TYR:HB2	2.00	0.42
22:J:7:ILE:H	22:J:7:ILE:HG13	1.58	0.42
24:L:46:LEU:HD13	24:L:73:SER:HB2	2.01	0.42
25:M:144:ASP:O	25:M:147:GLN:NE2	2.52	0.42
27:O:67:SER:HB3	27:O:74:PRO:HG3	2.00	0.42
21:i:122:THR:HB	22:j:125:ARG:HH12	1.83	0.42
3:W:140:ILE:HD12	3:W:140:ILE:O	2.19	0.42
12:f:265:ALA:HB3	12:f:268:LEU:HB2	2.02	0.42
12:f:870:THR:O	12:f:870:THR:OG1	2.27	0.42
13:A:289:ALA:HB1	18:F:296:PHE:HB3	2.02	0.42
13:A:414:ASN:HA	13:A:418:LYS:HB2	2.01	0.42
17:E:191:LEU:HB3	17:E:192:ASP:H	1.62	0.42
17:E:313:LEU:O	17:E:317:ALA:N	2.45	0.42
18:F:304:ARG:O	18:F:308:ARG:NH1	2.52	0.42
22:J:7:ILE:HD11	22:J:122:ASN:HA	2.01	0.42
30:R:35:ILE:N	30:R:43:GLY:O	2.52	0.42
22:j:76:LEU:HD12	22:j:79:ASP:H	1.85	0.42
23:k:210:LEU:HD11	23:k:215:ILE:HG12	2.01	0.42
29:q:37:LYS:O	29:q:61:GLN:NE2	2.46	0.42
2:V:36:GLU:HG3	2:V:76:LYS:HG2	2.02	0.42
2:V:171:VAL:O	2:V:175:MET:N	2.42	0.42
2:V:319:HIS:HE1	11:e:1:MET:HB3	1.83	0.42
5:Y:71:ASN:HA	5:Y:74:LYS:HG2	2.01	0.42
5:Y:283:LYS:HD3	5:Y:288:PHE:HZ	1.85	0.42
18:F:324:THR:O	18:F:325:GLN:CG	2.67	0.42
22:j:7:ILE:HD11	22:j:122:ASN:HA	2.01	0.42
25:m:160:TYR:HD2	25:m:163:CYS:HB2	1.85	0.42
1:U:803:LYS:HB2	1:U:875:PHE:HA	2.00	0.42
2:V:231:LEU:HD11	2:V:250:LEU:HD22	2.02	0.42
2:V:494:MET:HG2	6:Z:278:ASN:HD22	1.83	0.42
3:W:93:ARG:HE	3:W:135:LYS:H	1.68	0.42
6:Z:91:ILE:H	6:Z:91:ILE:HG13	1.52	0.42
6:Z:228:TYR:CD2	7:a:341:LEU:CD2	3.00	0.42
6:Z:234:PHE:HA	6:Z:237:LEU:HD11	2.00	0.42
7:a:100:THR:HA	7:a:103:LYS:HE2	2.02	0.42
12:f:294:MET:HE1	12:f:456:ARG:HG2	2.02	0.42
19:G:9:PHE:CD2	19:G:18:PRO:CG	2.89	0.42
22:J:121:SER:HB3	22:J:124:ARG:HD3	2.01	0.42
21:i:123:GLN:NE2	22:j:79:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:i:238:LYS:HA	21:i:241:GLU:HB2	2.00	0.42
32:t:184:TYR:CE2	32:t:186:ARG:HB3	2.54	0.42
3:W:395:ASN:HA	3:W:398:VAL:HG22	2.02	0.42
7:a:55:GLY:HA2	7:a:58:LYS:HG2	2.00	0.42
13:A:347:ASP:OD1	13:A:347:ASP:N	2.51	0.42
19:G:19:GLU:O	20:H:27:ALA:HB1	2.20	0.42
23:K:210:LEU:HD11	23:K:215:ILE:HG12	2.01	0.42
23:k:31:ILE:HD13	23:k:140:ALA:HB2	2.02	0.42
1:U:386:LEU:HD22	1:U:408:LEU:HD13	2.02	0.42
1:U:541:HIS:HB2	1:U:544:ILE:HG22	2.02	0.42
2:V:98:LEU:HD23	2:V:104:THR:HA	2.02	0.42
2:V:324:PHE:N	11:e:6:GLN:HB3	2.34	0.42
3:W:435:LEU:CD1	6:Z:237:LEU:CB	2.61	0.42
5:Y:178:ASN:ND2	5:Y:212:GLU:OE1	2.53	0.42
5:Y:276:ALA:HB1	11:e:60:LEU:HD13	2.01	0.42
12:f:250:ARG:NH2	12:f:281:ILE:CG1	2.76	0.42
15:C:217:SER:OG	16:D:248:ARG:NH2	2.53	0.42
15:C:274:LEU:O	15:C:278:ASN:ND2	2.53	0.42
20:H:148:GLN:OE1	20:H:158:TRP:NE1	2.52	0.42
22:j:64:ALA:O	22:j:88:ARG:NH1	2.53	0.42
23:k:77:ALA:HB3	23:k:142:LEU:HB2	2.02	0.42
2:V:211:TYR:HA	2:V:214:HIS:HB3	2.02	0.42
3:W:124:LEU:HA	3:W:127:THR:HG22	2.01	0.42
12:f:261:ARG:HG2	12:f:266:LEU:HD13	2.02	0.42
12:f:618:GLU:HG2	14:B:82:GLN:NE2	2.35	0.42
12:f:663:GLY:C	12:f:664:GLU:HG3	2.45	0.42
15:C:83:LYS:HB3	15:C:99:VAL:HG22	2.01	0.42
17:E:173:TYR:HB2	17:E:388:PRO:HB2	2.02	0.42
30:R:44:THR:HG21	30:R:100:MET:HE3	2.02	0.42
21:i:72:MET:HG2	21:i:138:GLY:HA3	2.01	0.42
1:U:338:HIS:HE1	1:U:785:PRO:HB3	1.85	0.41
1:U:611:ASN:HB3	1:U:614:VAL:HG12	2.01	0.41
2:V:60:ALA:HB3	2:V:62:HIS:CD2	2.54	0.41
3:W:91:SER:OG	3:W:96:GLN:CD	2.60	0.41
3:W:91:SER:OG	3:W:96:GLN:NE2	2.53	0.41
8:b:124:LEU:HD21	8:b:152:LYS:HB3	2.02	0.41
14:B:65:LEU:HD23	14:B:68:ILE:HD12	2.02	0.41
15:C:168:PRO:HG3	15:C:175:PHE:HE2	1.84	0.41
16:D:414:HIS:CE1	19:G:26:GLU:HB2	2.55	0.41
1:U:179:TYR:CD1	1:U:179:TYR:O	2.73	0.41
1:U:811:PHE:HE1	1:U:888:GLN:NE2	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:174:TRP:CZ3	15:C:337:ASN:C	2.96	0.41
12:f:873:LEU:HG	12:f:875:ALA:H	1.84	0.41
16:D:318:ASP:HB3	16:D:321:LEU:HD23	2.03	0.41
18:F:343:LEU:H	18:F:343:LEU:HG	1.63	0.41
21:I:73:ALA:HB3	21:I:137:ILE:HD11	2.02	0.41
2:V:40:GLU:HA	2:V:43:THR:HB	2.02	0.41
4:X:317:PRO:C	4:X:318:ILE:HG13	2.44	0.41
7:a:247:ARG:HH12	7:a:251:LEU:HD13	1.84	0.41
12:f:93:PRO:HB2	12:f:97:LYS:HE3	2.00	0.41
12:f:250:ARG:HH22	12:f:281:ILE:CB	2.33	0.41
12:f:407:MET:HE3	12:f:439:TYR:HB2	2.03	0.41
12:f:760:PHE:HE2	12:f:855:GLN:NE2	1.97	0.41
13:A:258:ARG:NH2	18:F:255:GLN:HA	2.35	0.41
15:C:307:ARG:HA	15:C:308:PRO:HD3	1.91	0.41
18:F:421:MET:HA	18:F:424:ILE:HD12	2.02	0.41
19:G:16:PHE:HE2	20:H:129:PRO:HD2	1.85	0.41
23:K:56:SER:HB3	23:K:59:MET:HB2	2.01	0.41
20:h:148:GLN:OE1	20:h:158:TRP:NE1	2.54	0.41
22:j:88:ARG:NH1	29:q:69:MET:O	2.54	0.41
1:U:772:TRP:CD1	1:U:775:LEU:HG	2.56	0.41
5:Y:348:ASP:C	5:Y:349:LYS:HE2	2.46	0.41
8:b:20:ASP:CG	8:b:25:ARG:HH21	2.28	0.41
12:f:478:ARG:HG3	12:f:514:VAL:HG11	2.01	0.41
13:A:38:GLN:NE2	13:A:40:THR:OG1	2.53	0.41
13:A:56:LEU:O	13:A:60:ASN:ND2	2.53	0.41
15:C:41:ASN:OD1	15:C:44:ARG:NH1	2.49	0.41
15:C:188:LEU:HB3	15:C:317:PHE:HE2	1.86	0.41
16:D:139:LEU:HD23	16:D:139:LEU:HA	1.87	0.41
17:E:235:ILE:HG21	17:E:279:THR:CG2	2.46	0.41
18:F:86:LEU:N	18:F:87:PRO:CD	2.83	0.41
18:F:275:ALA:O	18:F:281:SER:OG	2.38	0.41
20:H:108:ALA:HA	20:H:147:PHE:HE2	1.85	0.41
20:H:118:MET:HE2	20:H:151:PRO:HA	2.02	0.41
23:K:50:VAL:HG21	23:K:66:LYS:HB3	2.01	0.41
27:O:171:SER:OG	27:O:192:PRO:HG2	2.18	0.41
20:h:6:TYR:HE2	20:h:126:GLY:HA3	1.85	0.41
21:i:229:LYS:N	21:i:232:GLU:OE2	2.53	0.41
22:j:154:HIS:HE1	23:k:64:ILE:HG13	1.86	0.41
1:U:564:ASP:OD1	1:U:590:TYR:OH	2.38	0.41
1:U:792:ASN:OD1	1:U:793:LYS:N	2.50	0.41
2:V:280:ALA:HB3	2:V:285:TRP:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:330:LYS:HG3	2:V:360:TYR:CE2	2.56	0.41
3:W:198:ASP:O	3:W:202:THR:OG1	2.31	0.41
9:c:123:SER:OG	9:c:124:GLY:N	2.53	0.41
12:f:381:VAL:HA	12:f:755:ASP:O	2.19	0.41
12:f:787:LEU:HD13	12:f:787:LEU:HA	1.81	0.41
17:E:219:PHE:HA	17:E:222:ALA:HB3	2.03	0.41
19:G:58:ASP:HB3	19:G:61:LEU:HB2	2.02	0.41
1:U:889:LEU:HB3	1:U:908:ILE:HA	2.01	0.41
7:a:81:LEU:HA	7:a:84:VAL:HG12	2.02	0.41
15:C:351:MET:HB3	15:C:354:ALA:HB2	2.03	0.41
16:D:417:TYR:CZ	19:G:21:ARG:HD2	2.55	0.41
19:G:9:PHE:CD2	19:G:18:PRO:CD	2.96	0.41
23:K:21:LEU:HG	23:K:24:VAL:HG23	2.03	0.41
25:M:108:LEU:HD11	25:M:137:LEU:HB3	2.01	0.41
29:Q:19:ARG:HH11	29:Q:179:SER:HB3	1.86	0.41
20:h:111:VAL:HG21	20:h:147:PHE:HD2	1.84	0.41
23:k:98:ASN:OD1	30:r:61:ARG:NH2	2.49	0.41
25:m:34:SER:OG	25:m:65:ARG:NH2	2.43	0.41
1:U:173:VAL:HG12	1:U:175:GLY:N	2.22	0.41
1:U:872:GLU:HB2	1:U:873:PRO:CD	2.50	0.41
2:V:188:SER:HB2	2:V:192:MET:HE3	2.02	0.41
2:V:259:LEU:HD21	2:V:294:ARG:HH11	1.86	0.41
3:W:131:VAL:HG12	3:W:144:ARG:HE	1.86	0.41
6:Z:215:VAL:HG22	6:Z:222:ILE:HG13	2.03	0.41
12:f:340:MET:O	12:f:340:MET:SD	2.79	0.41
12:f:828:ARG:HG2	12:f:845:ARG:C	2.44	0.41
21:I:134:LEU:N	21:I:150:SER:OG	2.49	0.41
22:J:76:LEU:HD12	22:J:79:ASP:H	1.85	0.41
26:N:7:GLN:HA	26:N:12:VAL:HA	2.03	0.41
25:m:40:ARG:HE	25:m:161:TRP:HD1	1.68	0.41
26:n:7:GLN:HA	26:n:12:VAL:HA	2.03	0.41
1:U:191:LYS:HE3	1:U:560:MET:HG3	2.02	0.41
1:U:613:ASP:HA	1:U:616:ARG:HE	1.86	0.41
1:U:904:LYS:HD3	1:U:912:ILE:HG22	2.03	0.41
2:V:401:ASN:HD21	2:V:408:ARG:HH12	1.68	0.41
3:W:170:GLN:C	3:W:173:THR:HG1	2.18	0.41
5:Y:65:ILE:C	5:Y:67:VAL:N	2.78	0.41
6:Z:228:TYR:HD2	7:a:341:LEU:CD2	2.23	0.41
12:f:373:ALA:HA	12:f:376:PHE:HD2	1.86	0.41
12:f:810:ILE:HD11	12:f:853:VAL:HA	2.02	0.41
13:A:312:ARG:HB2	13:A:315:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:293:LEU:HD21	16:D:321:LEU:HD22	2.03	0.41
17:E:195:PHE:HD1	17:E:195:PHE:HA	1.66	0.41
27:O:171:SER:HB2	27:O:193:ASN:OD1	2.21	0.41
24:l:148:CYS:SG	24:l:150:SER:OG	2.67	0.41
1:U:47:VAL:O	1:U:50:GLU:N	2.47	0.41
2:V:462:GLU:HG2	2:V:463:MET:H	1.86	0.41
2:V:472:PRO:HB3	5:Y:366:TYR:CE1	2.56	0.41
4:X:111:LEU:HD23	4:X:114:ILE:HD12	2.03	0.41
6:Z:172:VAL:HG13	9:c:217:LEU:HD21	2.02	0.41
7:a:112:ILE:H	7:a:112:ILE:HG13	1.58	0.41
7:a:254:ALA:O	7:a:258:GLN:NE2	2.53	0.41
12:f:721:VAL:HG21	14:B:208:PRO:HG2	2.02	0.41
12:f:829:MET:H	12:f:845:ARG:HB3	1.86	0.41
13:A:122:VAL:O	18:F:86:LEU:O	2.39	0.41
14:B:140:ASP:OD1	14:B:140:ASP:N	2.54	0.41
18:F:246:ALA:HB1	18:F:280:PRO:HB2	2.03	0.41
18:F:321:GLN:NE2	18:F:323:ASN:ND2	2.69	0.41
21:I:38:LEU:HD12	21:I:161:ALA:HB2	2.03	0.41
23:K:21:LEU:HD23	23:K:24:VAL:HB	2.03	0.41
23:K:23:GLN:NE2	23:K:23:GLN:CA	2.74	0.41
25:M:160:TYR:HD2	25:M:163:CYS:HB2	1.85	0.41
25:m:74:GLY:HA3	25:m:224:HIS:CE1	2.56	0.41
27:o:172:ASN:HD22	27:o:191:VAL:HG22	1.86	0.41
1:U:149:GLN:NE2	15:C:20:LEU:O	2.50	0.41
1:U:221:ILE:H	1:U:221:ILE:HG13	1.72	0.41
1:U:377:HIS:CE1	1:U:384:GLN:HE22	2.39	0.41
2:V:29:PRO:HB2	2:V:30:PRO:CD	2.50	0.41
3:W:177:MET:H	3:W:177:MET:HG3	1.51	0.41
4:X:57:LEU:HB3	4:X:66:LEU:HB2	2.02	0.41
4:X:141:LYS:C	4:X:141:LYS:HD3	2.46	0.41
8:b:94:HIS:CD2	8:b:136:VAL:HG21	2.56	0.41
12:f:642:ALA:C	12:f:644:ALA:N	2.79	0.41
17:E:279:THR:HG23	17:E:282:PRO:HG2	2.02	0.41
20:H:11:THR:OG1	21:I:127:LYS:C	2.63	0.41
21:I:127:LYS:HB2	21:I:128:ARG:H	1.69	0.41
25:M:6:GLY:C	25:M:8:ASP:H	2.29	0.41
21:i:206:LEU:HD22	21:i:237:ILE:HG12	2.03	0.41
22:j:96:LEU:HD12	29:q:62:LYS:HB2	2.03	0.41
30:r:44:THR:HG21	30:r:100:MET:HE3	2.02	0.41
2:V:28:PRO:N	2:V:29:PRO:CD	2.84	0.40
3:W:276:LEU:HA	3:W:357:ARG:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:316:ASP:CG	4:X:321:THR:N	2.76	0.40
10:d:107:LEU:HD22	10:d:170:LEU:HD11	2.01	0.40
12:f:326:LEU:HD22	12:f:329:ASN:HB2	2.02	0.40
12:f:414:LEU:HD23	12:f:417:ILE:HD12	2.03	0.40
14:B:286:GLU:HG2	15:C:274:LEU:HD12	2.03	0.40
15:C:76:VAL:HA	15:C:87:VAL:HG22	2.04	0.40
15:C:214:VAL:HG21	15:C:234:LEU:HD21	2.02	0.40
16:D:162:VAL:O	16:D:221:HIS:ND1	2.54	0.40
17:E:15:LYS:HA	18:F:47:LEU:HD22	2.03	0.40
17:E:168:LYS:NZ	17:E:265:ASP:OD2	2.37	0.40
17:E:289:LEU:HD12	17:E:294:ARG:HD3	2.03	0.40
29:q:19:ARG:HH11	29:q:179:SER:HB3	1.86	0.40
1:U:427:LEU:HB2	1:U:430:ASP:HB2	2.03	0.40
1:U:813:TYR:O	1:U:813:TYR:CG	2.73	0.40
2:V:73:GLU:HA	2:V:76:LYS:HB3	2.04	0.40
3:W:420:ASP:OD1	3:W:420:ASP:N	2.54	0.40
7:a:121:LEU:HA	7:a:124:ASN:HD22	1.86	0.40
12:f:180:GLN:HB3	12:f:219:LYS:NZ	2.36	0.40
12:f:248:LEU:HD12	12:f:250:ARG:HD3	2.02	0.40
15:C:307:ARG:NH2	15:C:310:ARG:HE	2.20	0.40
16:D:276:ASP:OD1	16:D:276:ASP:N	2.46	0.40
19:G:131:MET:HE3	25:M:124:LEU:HD13	2.02	0.40
21:I:14:PRO:HB2	21:I:15:GLU:CD	2.46	0.40
28:P:34:MET:O	30:r:166:ARG:NH2	2.55	0.40
29:Q:102:LEU:HB2	29:Q:118:MET:HB3	2.03	0.40
22:j:118:TYR:HD1	22:j:124:ARG:HH21	1.69	0.40
28:p:107:PRO:HG2	28:p:124:LEU:HB2	2.01	0.40
29:q:102:LEU:HB2	29:q:118:MET:HB3	2.04	0.40
2:V:72:LEU:O	2:V:76:LYS:N	2.47	0.40
3:W:177:MET:CA	3:W:182:ARG:HG2	2.47	0.40
4:X:141:LYS:HD3	4:X:141:LYS:HA	1.84	0.40
6:Z:68:TRP:HH2	6:Z:111:LEU:HD13	1.86	0.40
7:a:148:VAL:HG12	7:a:150:SER:H	1.85	0.40
7:a:252:LYS:HD2	7:a:255:TRP:CD1	2.57	0.40
15:C:187:LEU:HB2	15:C:311:ILE:HG21	2.02	0.40
15:C:368:MET:HE1	16:D:191:TYR:HE1	1.87	0.40
17:E:226:GLN:HB2	17:E:227:PRO:CD	2.52	0.40
17:E:323:HIS:HB2	17:E:325:GLU:HB2	2.03	0.40
19:G:210:PHE:CE1	19:G:215:ILE:HG12	2.56	0.40
19:g:161:CYS:SG	19:g:162:GLY:N	2.95	0.40
20:h:118:MET:HE2	20:h:151:PRO:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:j:125:ARG:HA	22:j:126:PRO:HD3	1.97	0.40
24:l:37:GLY:HA2	24:l:46:LEU:HA	2.03	0.40
1:U:703:CYS:HA	1:U:704:PRO:HD3	1.85	0.40
2:V:189:ASP:C	2:V:192:MET:HB2	2.47	0.40
2:V:228:ARG:HA	2:V:228:ARG:HD3	1.91	0.40
2:V:387:GLN:HG2	2:V:392:TYR:CE1	2.57	0.40
3:W:78:LYS:HG3	3:W:79:GLU:HG3	2.02	0.40
8:b:30:GLN:NE2	18:F:57:SER:OG	2.54	0.40
10:d:176:ASP:HA	10:d:179:ALA:HB3	2.03	0.40
13:A:52:ILE:HD13	14:B:69:LYS:HA	2.04	0.40
14:B:96:ARG:HA	14:B:99:VAL:HB	2.03	0.40
15:C:406:LYS:HE2	15:C:406:LYS:HB3	1.87	0.40
17:E:226:GLN:O	17:E:227:PRO:C	2.62	0.40
25:M:74:GLY:HA3	25:M:224:HIS:CE1	2.56	0.40
21:i:165:GLY:O	21:i:168:SER:N	2.54	0.40
3:W:327:GLU:HG3	3:W:328:LEU:HD12	2.04	0.40
6:Z:121:LEU:HD11	6:Z:138:TYR:HD2	1.87	0.40
7:a:9:GLN:HE22	7:a:23:HIS:HE1	1.68	0.40
7:a:15:GLY:HA2	7:a:16:PRO:HD3	1.90	0.40
12:f:31:LYS:HE2	12:f:31:LYS:HB3	1.92	0.40
12:f:258:LYS:HG2	12:f:297:MET:HG3	2.04	0.40
12:f:331:LEU:HD12	12:f:813:LYS:HE2	2.03	0.40
13:A:327:LEU:HD13	13:A:327:LEU:HA	1.85	0.40
14:B:259:TYR:HB2	14:B:262:ASP:HB2	2.04	0.40
16:D:212:LYS:HE2	16:D:310:ALA:HB1	2.04	0.40
22:J:116:GLN:HE22	23:K:83:ALA:HB1	1.85	0.40
25:M:40:ARG:HE	25:M:161:TRP:HD1	1.68	0.40
27:O:172:ASN:HD22	27:O:191:VAL:HG22	1.86	0.40
23:k:109:VAL:HG23	23:k:147:ASP:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	868/953 (91%)	782 (90%)	78 (9%)	8 (1%)	14	49
2	V	478/533 (90%)	413 (86%)	63 (13%)	2 (0%)	30	65
3	W	454/456 (100%)	409 (90%)	41 (9%)	4 (1%)	14	49
4	X	378/422 (90%)	355 (94%)	21 (6%)	2 (0%)	24	61
5	Y	376/389 (97%)	332 (88%)	41 (11%)	3 (1%)	16	52
6	Z	284/324 (88%)	243 (86%)	37 (13%)	4 (1%)	9	39
7	a	371/376 (99%)	334 (90%)	34 (9%)	3 (1%)	16	52
8	b	189/377 (50%)	164 (87%)	24 (13%)	1 (0%)	24	61
9	c	285/309 (92%)	246 (86%)	32 (11%)	7 (2%)	4	29
10	d	255/349 (73%)	214 (84%)	38 (15%)	3 (1%)	10	42
11	e	36/70 (51%)	29 (81%)	7 (19%)	0	100	100
12	f	887/908 (98%)	707 (80%)	164 (18%)	16 (2%)	6	35
13	A	411/433 (95%)	364 (89%)	46 (11%)	1 (0%)	43	76
14	B	409/440 (93%)	349 (85%)	57 (14%)	3 (1%)	18	55
15	C	394/398 (99%)	353 (90%)	36 (9%)	5 (1%)	9	41
16	D	378/418 (90%)	321 (85%)	53 (14%)	4 (1%)	11	44
17	E	387/403 (96%)	323 (84%)	54 (14%)	10 (3%)	4	28
18	F	391/439 (89%)	336 (86%)	47 (12%)	8 (2%)	6	33
19	G	237/245 (97%)	209 (88%)	25 (10%)	3 (1%)	9	41
19	g	238/245 (97%)	222 (93%)	16 (7%)	0	100	100
20	H	228/233 (98%)	215 (94%)	10 (4%)	3 (1%)	9	41
20	h	230/233 (99%)	222 (96%)	8 (4%)	0	100	100
21	I	246/260 (95%)	217 (88%)	26 (11%)	3 (1%)	10	42
21	i	248/260 (95%)	223 (90%)	25 (10%)	0	100	100
22	J	237/247 (96%)	216 (91%)	20 (8%)	1 (0%)	30	65
22	j	237/247 (96%)	216 (91%)	20 (8%)	1 (0%)	30	65
23	K	224/240 (93%)	208 (93%)	14 (6%)	2 (1%)	14	49
23	k	224/240 (93%)	210 (94%)	14 (6%)	0	100	100
24	L	236/268 (88%)	226 (96%)	10 (4%)	0	100	100
24	l	236/268 (88%)	226 (96%)	10 (4%)	0	100	100
25	M	238/254 (94%)	220 (92%)	18 (8%)	0	100	100
25	m	238/254 (94%)	219 (92%)	19 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	N	189/238 (79%)	180 (95%)	9 (5%)	0	100	100
26	n	189/238 (79%)	180 (95%)	9 (5%)	0	100	100
27	O	218/276 (79%)	207 (95%)	10 (5%)	1 (0%)	24	61
27	o	218/276 (79%)	207 (95%)	10 (5%)	1 (0%)	24	61
28	P	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
28	p	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
29	Q	197/201 (98%)	186 (94%)	11 (6%)	0	100	100
29	q	197/201 (98%)	186 (94%)	11 (6%)	0	100	100
30	R	199/262 (76%)	193 (97%)	6 (3%)	0	100	100
30	r	199/262 (76%)	193 (97%)	6 (3%)	0	100	100
31	S	211/240 (88%)	205 (97%)	6 (3%)	0	100	100
31	s	211/240 (88%)	205 (97%)	6 (3%)	0	100	100
32	T	213/263 (81%)	202 (95%)	11 (5%)	0	100	100
32	t	213/263 (81%)	202 (95%)	11 (5%)	0	100	100
All	All	13386/14859 (90%)	12057 (90%)	1230 (9%)	99 (1%)	20	55

All (99) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	48	LEU
3	W	91	SER
3	W	176	SER
3	W	179	LYS
4	X	203	PRO
6	Z	238	PRO
8	b	22	LEU
9	c	196	LEU
9	c	279	ASP
9	c	280	PRO
9	c	285	GLU
12	f	281	ILE
12	f	756	PRO
12	f	838	ARG
12	f	853	VAL
14	B	434	THR
15	C	91	PRO
16	D	335	LEU

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Mol	Chain	Res	Type
17	E	53	VAL
17	E	194	ASN
17	E	282	PRO
18	F	73	ILE
18	F	85	THR
18	F	344	ARG
19	G	7	ALA
19	G	8	GLY
20	H	7	SER
22	J	5	ARG
23	K	22	PHE
22	j	5	ARG
1	U	47	VAL
1	U	183	LEU
1	U	808	PRO
4	X	318	ILE
5	Y	350	VAL
6	Z	145	HIS
6	Z	237	LEU
7	a	69	HIS
7	a	187	ASP
9	c	195	GLY
10	d	203	PRO
10	d	204	LYS
12	f	786	GLN
14	B	390	LEU
15	C	89	VAL
18	F	86	LEU
19	G	9	PHE
20	H	8	PHE
20	H	124	SER
21	I	16	GLY
21	I	124	PHE
23	K	21	LEU
10	d	199	PHE
12	f	118	ASN
12	f	476	THR
12	f	664	GLU
12	f	738	ASN
12	f	816	TYR
12	f	859	PRO
14	B	166	ASP

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Mol	Chain	Res	Type
15	C	90	HIS
16	D	160	PRO
17	E	166	PRO
17	E	191	LEU
17	E	197	LYS
18	F	72	LYS
1	U	812	ALA
5	Y	66	ASP
6	Z	65	ASP
9	c	201	TYR
15	C	222	LYS
16	D	269	ALA
17	E	193	CYS
18	F	87	PRO
18	F	301	ALA
1	U	173	VAL
1	U	813	TYR
3	W	139	GLU
7	a	343	LEU
9	c	284	LEU
12	f	475	ASN
12	f	787	LEU
18	F	324	THR
27	O	171	SER
27	o	171	SER
5	Y	290	PRO
13	A	109	PRO
15	C	253	SER
17	E	227	PRO
21	I	14	PRO
1	U	174	PRO
12	f	642	ALA
12	f	809	ILE
12	f	817	VAL
2	V	30	PRO
2	V	31	ALA
17	E	167	PRO
16	D	126	PRO
17	E	226	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	748/816 (92%)	736 (98%)	12 (2%)	55	69
2	V	414/459 (90%)	410 (99%)	4 (1%)	68	76
3	W	416/416 (100%)	408 (98%)	8 (2%)	50	67
4	X	327/362 (90%)	321 (98%)	6 (2%)	51	67
5	Y	334/344 (97%)	326 (98%)	8 (2%)	43	63
6	Z	256/295 (87%)	247 (96%)	9 (4%)	32	54
7	a	333/336 (99%)	330 (99%)	3 (1%)	70	76
8	b	167/312 (54%)	166 (99%)	1 (1%)	78	80
9	c	252/267 (94%)	246 (98%)	6 (2%)	43	63
10	d	231/293 (79%)	225 (97%)	6 (3%)	40	61
11	e	38/63 (60%)	37 (97%)	1 (3%)	40	61
12	f	745/763 (98%)	723 (97%)	22 (3%)	36	57
13	A	348/372 (94%)	347 (100%)	1 (0%)	86	85
14	B	357/385 (93%)	348 (98%)	9 (2%)	42	62
15	C	340/346 (98%)	333 (98%)	7 (2%)	47	65
16	D	333/366 (91%)	325 (98%)	8 (2%)	43	63
17	E	341/353 (97%)	333 (98%)	8 (2%)	44	64
18	F	340/379 (90%)	331 (97%)	9 (3%)	40	61
19	G	192/209 (92%)	189 (98%)	3 (2%)	55	69
19	g	193/209 (92%)	191 (99%)	2 (1%)	68	76
20	H	163/190 (86%)	161 (99%)	2 (1%)	63	73
20	h	164/190 (86%)	164 (100%)	0	100	100
21	I	191/220 (87%)	187 (98%)	4 (2%)	47	65
21	i	193/220 (88%)	193 (100%)	0	100	100
22	J	152/210 (72%)	151 (99%)	1 (1%)	76	79
22	j	152/210 (72%)	151 (99%)	1 (1%)	76	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	K	187/202 (93%)	181 (97%)	6 (3%)	34	56
23	k	186/202 (92%)	183 (98%)	3 (2%)	55	69
24	L	198/229 (86%)	196 (99%)	2 (1%)	68	76
24	l	198/229 (86%)	197 (100%)	1 (0%)	81	82
25	M	192/211 (91%)	190 (99%)	2 (1%)	68	76
25	m	192/211 (91%)	190 (99%)	2 (1%)	68	76
26	N	148/180 (82%)	148 (100%)	0	100	100
26	n	148/180 (82%)	148 (100%)	0	100	100
27	O	177/227 (78%)	177 (100%)	0	100	100
27	o	177/227 (78%)	177 (100%)	0	100	100
28	P	172/173 (99%)	172 (100%)	0	100	100
28	p	172/173 (99%)	172 (100%)	0	100	100
29	Q	164/171 (96%)	164 (100%)	0	100	100
29	q	164/171 (96%)	164 (100%)	0	100	100
30	R	153/201 (76%)	153 (100%)	0	100	100
30	r	153/201 (76%)	153 (100%)	0	100	100
31	S	174/198 (88%)	174 (100%)	0	100	100
31	s	174/198 (88%)	174 (100%)	0	100	100
32	T	175/214 (82%)	175 (100%)	0	100	100
32	t	175/214 (82%)	175 (100%)	0	100	100
All	All	11199/12597 (89%)	11042 (99%)	157 (1%)	57	71

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	47	VAL
1	U	118	LEU
1	U	173	VAL
1	U	177	LEU
1	U	179	TYR
1	U	181	LEU
1	U	364	VAL
1	U	416	GLU
1	U	423	MET
1	U	629	THR

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Mol	Chain	Res	Type
1	U	874	ASN
1	U	913	ILE
2	V	191	LEU
2	V	275	VAL
2	V	362	LEU
2	V	437	ILE
3	W	89	LEU
3	W	90	LEU
3	W	140	ILE
3	W	172	GLU
3	W	173	THR
3	W	177	MET
3	W	256	ILE
3	W	314	LEU
4	X	141	LYS
4	X	142	ARG
4	X	202	CYS
4	X	217	ILE
4	X	316	ASP
4	X	393	VAL
5	Y	65	ILE
5	Y	81	LEU
5	Y	174	TRP
5	Y	175	ASP
5	Y	233	ARG
5	Y	292	TYR
5	Y	349	LYS
5	Y	350	VAL
6	Z	12	HIS
6	Z	15	VAL
6	Z	16	LEU
6	Z	91	ILE
6	Z	144	VAL
6	Z	212	LEU
6	Z	217	THR
6	Z	237	LEU
6	Z	266	ILE
7	a	112	ILE
7	a	145	LEU
7	a	341	LEU
8	b	22	LEU
9	c	49	VAL

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Mol	Chain	Res	Type
9	c	115	HIS
9	c	196	LEU
9	c	197	ASN
9	c	232	GLN
9	c	233	ASP
10	d	88	GLN
10	d	89	LEU
10	d	178	ILE
10	d	189	ILE
10	d	201	ASN
10	d	202	THR
11	e	6	GLN
12	f	75	LEU
12	f	281	ILE
12	f	340	MET
12	f	344	VAL
12	f	457	ASN
12	f	660	ILE
12	f	662	MET
12	f	672	LEU
12	f	755	ASP
12	f	775	THR
12	f	785	ARG
12	f	786	GLN
12	f	787	LEU
12	f	806	VAL
12	f	808	ASN
12	f	809	ILE
12	f	810	ILE
12	f	838	ARG
12	f	840	LEU
12	f	855	GLN
12	f	870	THR
12	f	876	HIS
13	A	403	ILE
14	B	125	THR
14	B	136	LEU
14	B	183	THR
14	B	190	LEU
14	B	292	THR
14	B	316	LEU
14	B	387	LYS

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Mol	Chain	Res	Type
14	B	389	ASP
14	B	434	THR
15	C	20	LEU
15	C	89	VAL
15	C	90	HIS
15	C	109	THR
15	C	210	THR
15	C	220	VAL
15	C	222	LYS
16	D	85	ILE
16	D	155	THR
16	D	157	ASP
16	D	158	GLN
16	D	267	ILE
16	D	303	VAL
16	D	375	ILE
16	D	411	GLU
17	E	1	MET
17	E	50	LEU
17	E	105	LEU
17	E	195	PHE
17	E	196	LEU
17	E	232	MET
17	E	247	THR
17	E	281	ARG
18	F	54	ILE
18	F	59	VAL
18	F	85	THR
18	F	298	SER
18	F	299	GLU
18	F	300	LYS
18	F	324	THR
18	F	343	LEU
18	F	416	THR
19	G	9	PHE
19	G	21	ARG
19	G	209	ASP
20	H	6	TYR
20	H	123	GLN
21	I	9	THR
21	I	11	ILE
21	I	15	GLU

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Mol	Chain	Res	Type
21	I	127	LYS
22	J	7	ILE
23	K	20	ARG
23	K	21	LEU
23	K	23	GLN
23	K	139	VAL
23	K	232	GLU
23	K	233	GLU
24	L	118	ILE
24	L	161	ILE
25	M	229	LYS
25	M	230	ASP
19	g	141	ILE
19	g	222	VAL
22	j	7	ILE
23	k	113	THR
23	k	119	LEU
23	k	139	VAL
24	l	118	ILE
25	m	229	LYS
25	m	230	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (191) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	18	GLN
1	U	70	HIS
1	U	89	ASN
1	U	111	GLN
1	U	218	GLN
1	U	241	ASN
1	U	267	ASN
1	U	338	HIS
1	U	345	ASN
1	U	377	HIS
1	U	421	GLN
1	U	491	GLN
1	U	596	ASN
1	U	768	GLN
1	U	888	GLN
2	V	62	HIS
2	V	168	GLN

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Mol	Chain	Res	Type
2	V	198	GLN
2	V	252	ASN
2	V	260	HIS
2	V	319	HIS
2	V	401	ASN
2	V	473	GLN
2	V	487	HIS
3	W	106	GLN
3	W	107	GLN
3	W	203	GLN
3	W	362	ASN
3	W	454	ASN
4	X	170	GLN
4	X	198	ASN
4	X	213	GLN
4	X	322	HIS
4	X	349	HIS
4	X	416	ASN
5	Y	31	HIS
5	Y	48	ASN
5	Y	49	ASN
5	Y	77	ASN
5	Y	136	HIS
5	Y	178	ASN
5	Y	273	GLN
5	Y	344	HIS
5	Y	365	GLN
5	Y	367	GLN
6	Z	32	GLN
6	Z	77	ASN
6	Z	109	ASN
6	Z	189	GLN
6	Z	193	ASN
6	Z	256	GLN
7	a	9	GLN
7	a	86	GLN
7	a	124	ASN
7	a	227	ASN
7	a	249	GLN
7	a	273	GLN
7	a	288	HIS
8	b	30	GLN

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Mol	Chain	Res	Type
8	b	161	ASN
9	c	92	GLN
9	c	115	HIS
9	c	130	GLN
9	c	149	GLN
9	c	185	ASN
9	c	214	GLN
9	c	237	HIS
9	c	254	ASN
9	c	274	ASN
9	c	283	HIS
10	d	15	ASN
10	d	46	GLN
10	d	88	GLN
10	d	96	HIS
10	d	149	ASN
10	d	221	ASN
11	e	6	GLN
12	f	14	GLN
12	f	43	GLN
12	f	112	ASN
12	f	118	ASN
12	f	213	GLN
12	f	291	GLN
12	f	378	ASN
12	f	382	ASN
12	f	396	ASN
12	f	457	ASN
12	f	531	ASN
12	f	565	ASN
12	f	619	HIS
12	f	738	ASN
12	f	747	GLN
12	f	752	HIS
12	f	757	ASN
12	f	766	GLN
12	f	815	HIS
13	A	38	GLN
13	A	54	GLN
13	A	60	ASN
13	A	94	GLN
13	A	203	ASN

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Mol	Chain	Res	Type
13	A	247	GLN
13	A	304	ASN
13	A	353	HIS
14	B	154	HIS
14	B	195	GLN
14	B	368	HIS
15	C	36	ASN
15	C	50	ASN
15	C	67	GLN
15	C	69	GLN
15	C	205	HIS
15	C	279	GLN
15	C	377	HIS
16	D	98	GLN
16	D	127	ASN
16	D	135	HIS
16	D	222	HIS
16	D	294	ASN
16	D	414	HIS
17	E	121	ASN
17	E	194	ASN
17	E	339	ASN
17	E	364	GLN
18	F	64	HIS
18	F	83	ASN
18	F	323	ASN
18	F	325	GLN
19	G	75	ASN
19	G	193	GLN
20	H	71	HIS
20	H	102	GLN
20	H	169	ASN
21	I	102	GLN
21	I	123	GLN
21	I	146	GLN
21	I	167	ASN
22	J	68	ASN
22	J	92	GLN
22	J	116	GLN
22	J	122	ASN
23	K	23	GLN
23	K	114	GLN

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Mol	Chain	Res	Type
23	K	155	HIS
23	K	164	GLN
23	K	214	ASN
24	L	20	HIS
24	L	117	GLN
25	M	180	GLN
27	O	62	ASN
27	O	172	ASN
28	P	18	ASN
29	Q	71	ASN
30	R	38	ASN
31	S	58	HIS
31	S	146	GLN
31	S	159	GLN
32	T	69	GLN
32	T	89	HIS
19	g	127	GLN
19	g	193	GLN
20	h	21	GLN
20	h	102	GLN
20	h	169	ASN
20	h	189	HIS
21	i	119	GLN
21	i	149	GLN
21	i	167	ASN
22	j	68	ASN
22	j	92	GLN
22	j	116	GLN
22	j	122	ASN
23	k	23	GLN
23	k	99	HIS
23	k	155	HIS
23	k	164	GLN
23	k	214	ASN
24	l	117	GLN
24	l	166	GLN
25	m	97	ASN
25	m	180	GLN
27	o	62	ASN
27	o	172	ASN
28	p	18	ASN
29	q	71	ASN

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Mol	Chain	Res	Type
30	r	38	ASN
30	r	85	ASN
31	s	146	GLN
31	s	159	GLN
32	t	69	GLN
32	t	89	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
34	ATP	C	501	35	32,33,33	1.31	4 (12%)	48,52,52	1.81	7 (14%)
34	ATP	B	501	35	32,33,33	1.32	4 (12%)	48,52,52	1.90	9 (18%)
34	ATP	F	501	35	32,33,33	1.35	5 (15%)	48,52,52	1.81	8 (16%)
36	ADP	D	501	35	28,29,29	1.37	4 (14%)	43,45,45	1.88	9 (20%)
34	ATP	A	501	35	32,33,33	1.32	4 (12%)	48,52,52	1.79	10 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	ATP	C	501	35	-	5/22/38/38	0/3/3/3
34	ATP	B	501	35	-	3/22/38/38	0/3/3/3
34	ATP	F	501	35	-	4/22/38/38	0/3/3/3
36	ADP	D	501	35	-	1/16/32/32	0/3/3/3
34	ATP	A	501	35	-	3/22/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	501	ATP	C5-C4	4.65	1.47	1.39
34	C	501	ATP	C5-C4	4.64	1.47	1.39
34	F	501	ATP	C5-C4	4.60	1.47	1.39
34	A	501	ATP	C5-C4	4.53	1.47	1.39
36	D	501	ADP	C5-C4	4.52	1.47	1.39
34	B	501	ATP	C5-N7	-2.62	1.34	1.39
34	A	501	ATP	C5-C6	2.61	1.48	1.41
36	D	501	ADP	C5-C6	2.60	1.48	1.41
34	C	501	ATP	C5-N7	-2.58	1.34	1.39
34	F	501	ATP	C5-C6	2.58	1.48	1.41
34	C	501	ATP	C5-C6	2.56	1.48	1.41
34	B	501	ATP	C5-C6	2.50	1.48	1.41
34	F	501	ATP	C5-N7	-2.45	1.34	1.39
34	A	501	ATP	C5-N7	-2.45	1.34	1.39
36	D	501	ADP	C5-N7	-2.42	1.34	1.39
36	D	501	ADP	C8-N7	2.19	1.35	1.31
34	A	501	ATP	C8-N7	2.17	1.35	1.31
34	C	501	ATP	C8-N7	2.14	1.35	1.31
34	F	501	ATP	C8-N7	2.09	1.35	1.31
34	B	501	ATP	C8-N7	2.05	1.35	1.31
34	F	501	ATP	C4-N9	-2.04	1.33	1.37

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	501	ATP	C5-C4-N3	-6.55	117.70	126.72
34	C	501	ATP	C5-C4-N3	-6.34	117.99	126.72
34	A	501	ATP	C5-C4-N3	-5.92	118.57	126.72
34	F	501	ATP	C5-C4-N3	-5.76	118.78	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	D	501	ADP	C5-C4-N3	-5.74	118.81	126.72
34	B	501	ATP	N3-C4-N9	5.40	136.35	127.17
34	C	501	ATP	N3-C4-N9	5.14	135.90	127.17
34	F	501	ATP	N3-C4-N9	4.80	135.32	127.17
34	A	501	ATP	N3-C4-N9	4.73	135.21	127.17
36	D	501	ADP	N3-C4-N9	4.68	135.12	127.17
34	B	501	ATP	C2-N3-C4	4.01	121.63	111.83
34	C	501	ATP	C2-N3-C4	3.94	121.45	111.83
34	A	501	ATP	C2-N3-C4	3.79	121.08	111.83
36	D	501	ADP	C2-N3-C4	3.71	120.89	111.83
34	F	501	ATP	C2-N3-C4	3.67	120.80	111.83
34	A	501	ATP	C4-C5-N7	-3.47	106.61	110.58
34	C	501	ATP	N3-C2-N1	-3.45	123.37	128.58
34	B	501	ATP	N3-C2-N1	-3.37	123.48	128.58
36	D	501	ADP	N3-C2-N1	-3.32	123.56	128.58
34	A	501	ATP	N3-C2-N1	-3.26	123.65	128.58
36	D	501	ADP	C4-C5-N7	-3.26	106.86	110.58
34	C	501	ATP	C4-C5-N7	-3.25	106.87	110.58
34	F	501	ATP	N3-C2-N1	-3.25	123.67	128.58
34	F	501	ATP	C4-C5-N7	-3.20	106.92	110.58
34	B	501	ATP	C4-C5-N7	-3.08	107.06	110.58
34	B	501	ATP	C3'-C2'-C1'	2.89	106.94	101.46
34	F	501	ATP	C4-N9-C8	2.89	108.77	105.74
36	D	501	ADP	C3'-C2'-C1'	2.83	106.81	101.46
36	D	501	ADP	C4-N9-C8	2.79	108.66	105.74
34	A	501	ATP	C4-N9-C8	2.70	108.57	105.74
34	F	501	ATP	C3'-C2'-C1'	2.67	106.52	101.46
34	A	501	ATP	C5-N7-C8	2.59	107.51	103.45
34	A	501	ATP	C3'-C2'-C1'	2.48	106.15	101.46
34	C	501	ATP	C5-N7-C8	2.47	107.33	103.45
36	D	501	ADP	C5-N7-C8	2.43	107.26	103.45
34	F	501	ATP	C5-N7-C8	2.39	107.21	103.45
34	B	501	ATP	C5-N7-C8	2.39	107.20	103.45
34	C	501	ATP	C4-N9-C8	2.34	108.19	105.74
34	B	501	ATP	C4-N9-C8	2.23	108.08	105.74
34	B	501	ATP	C1'-N9-C8	-2.13	122.36	127.09
34	A	501	ATP	C6-C5-N7	2.10	136.13	132.09
36	D	501	ADP	C6-C5-N7	2.02	135.99	132.09
34	A	501	ATP	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

All (16) torsion outliers are listed below:

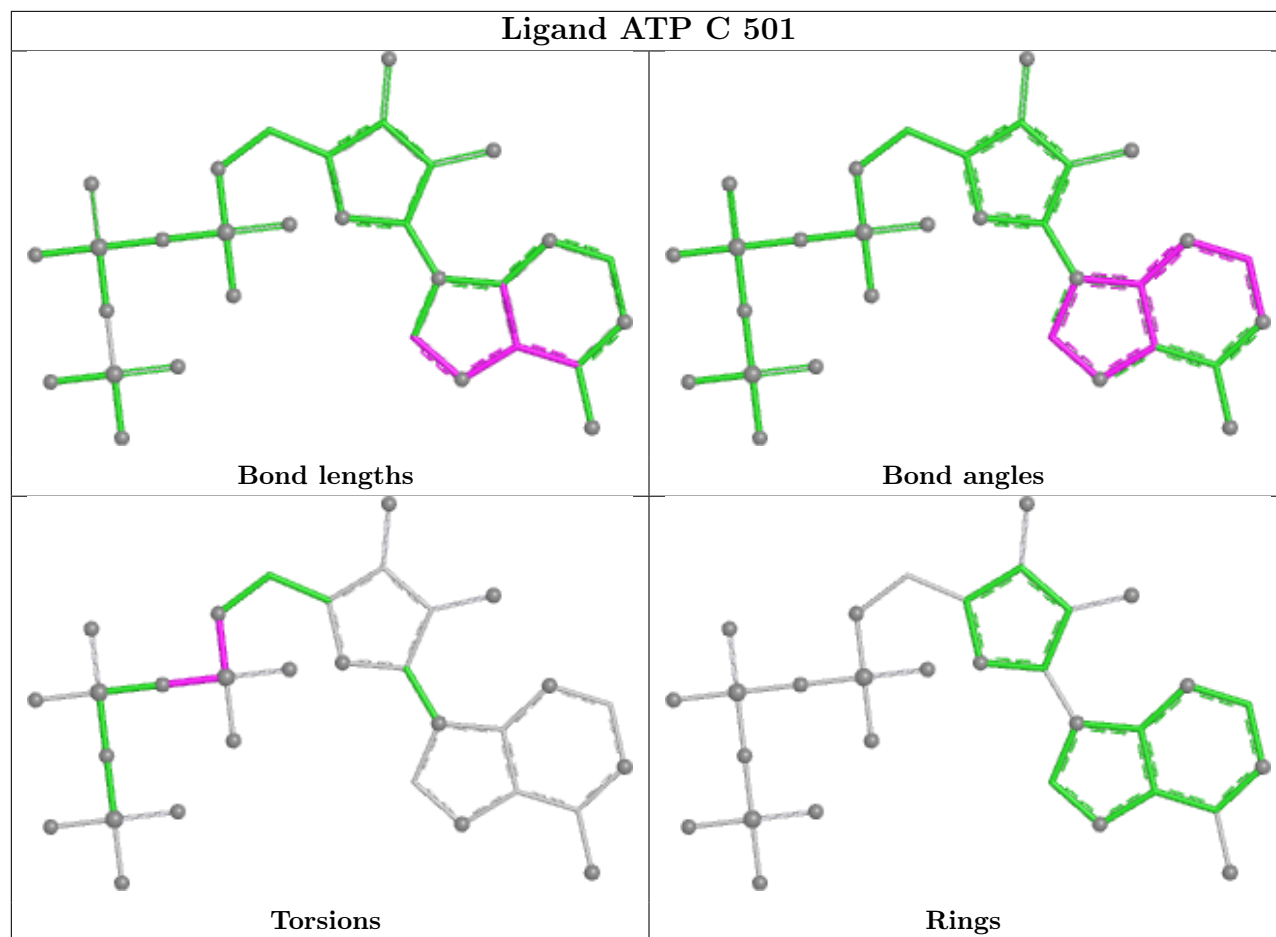
Mol	Chain	Res	Type	Atoms
34	A	501	ATP	C5'-O5'-PA-O1A
34	A	501	ATP	C5'-O5'-PA-O2A
34	A	501	ATP	C5'-O5'-PA-O3A
34	B	501	ATP	C5'-O5'-PA-O2A
34	B	501	ATP	C5'-O5'-PA-O3A
34	C	501	ATP	C5'-O5'-PA-O1A
34	C	501	ATP	C5'-O5'-PA-O2A
34	C	501	ATP	C5'-O5'-PA-O3A
34	F	501	ATP	C3'-C4'-C5'-O5'
34	F	501	ATP	O4'-C4'-C5'-O5'
34	C	501	ATP	PB-O3A-PA-O1A
34	F	501	ATP	PB-O3A-PA-O1A
34	C	501	ATP	PB-O3A-PA-O2A
34	F	501	ATP	PB-O3A-PA-O2A
36	D	501	ADP	O4'-C4'-C5'-O5'
34	B	501	ATP	PA-O3A-PB-O2B

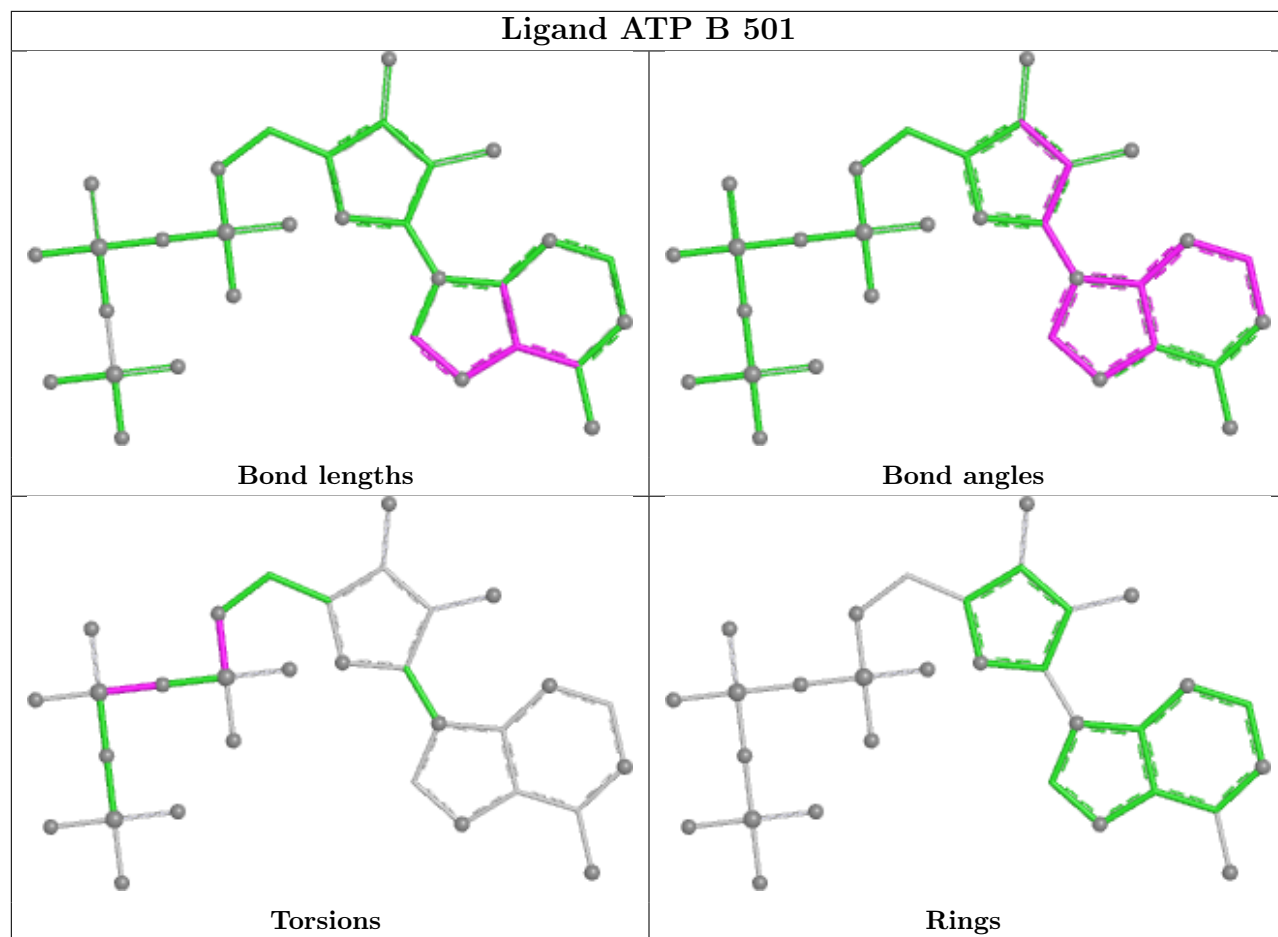
There are no ring outliers.

4 monomers are involved in 6 short contacts:

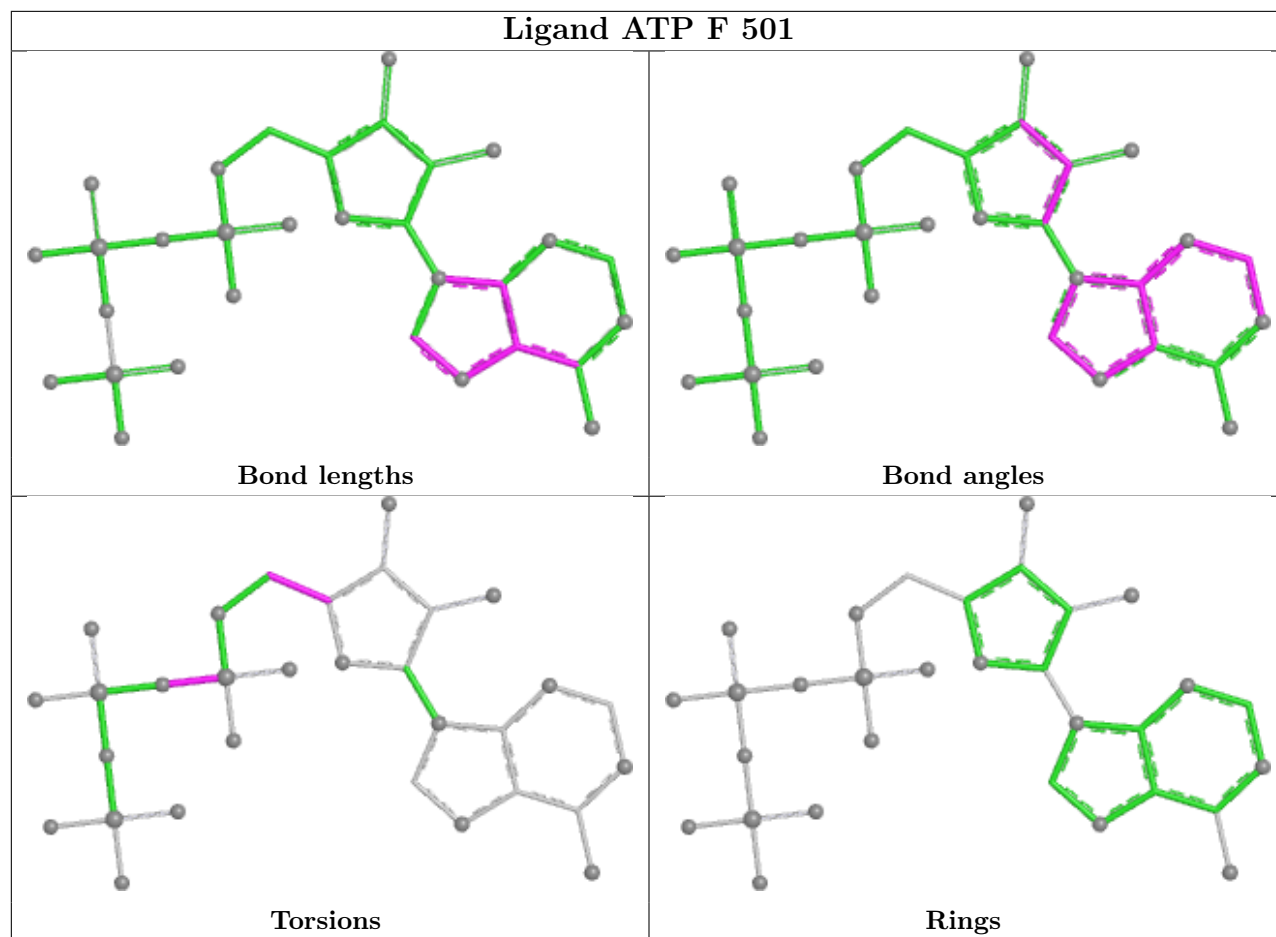
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	C	501	ATP	2	0
34	B	501	ATP	2	0
34	F	501	ATP	1	0
34	A	501	ATP	1	0

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

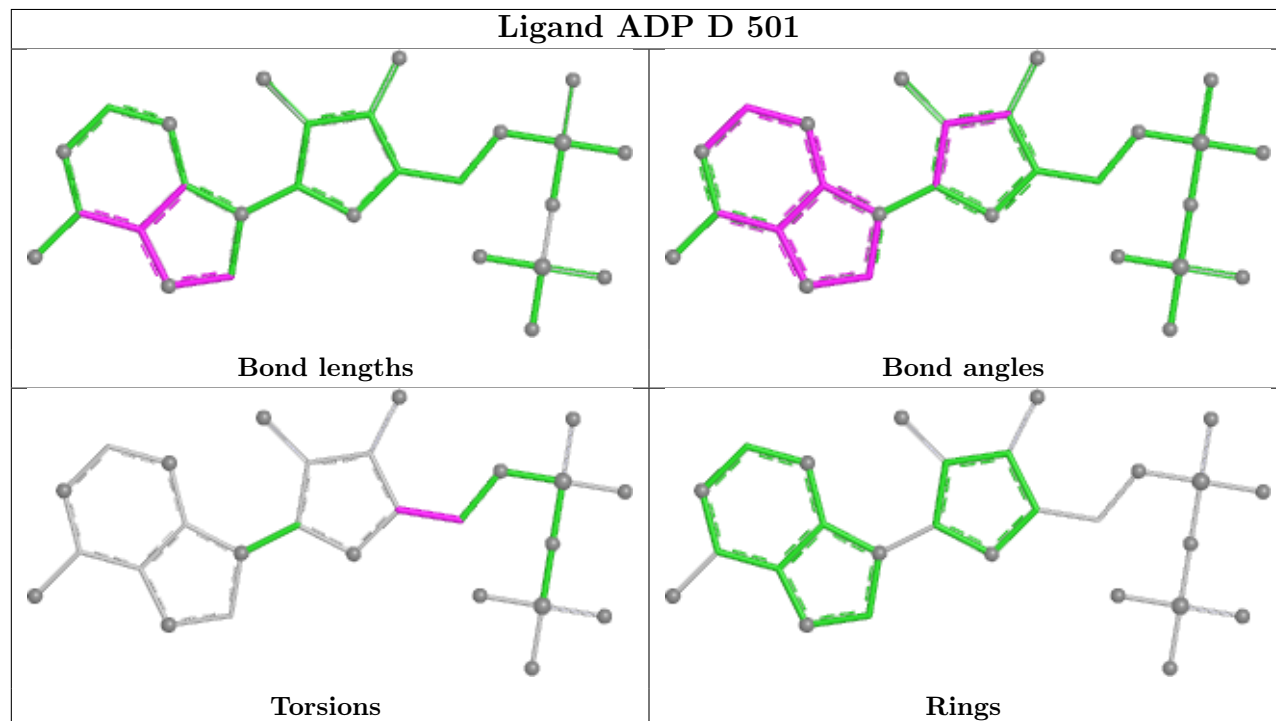


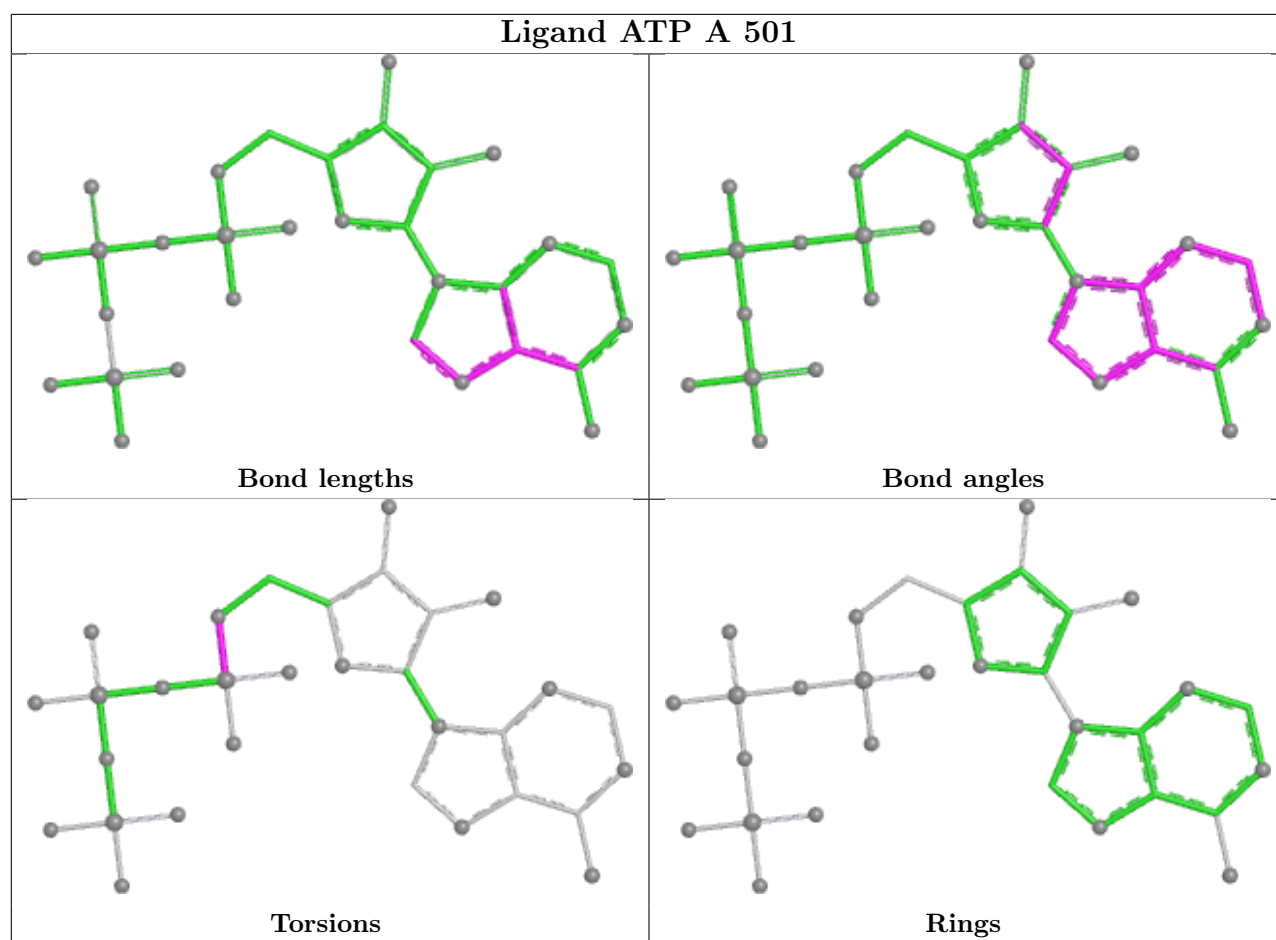


Ligand ATP F 501



Ligand ADP D 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

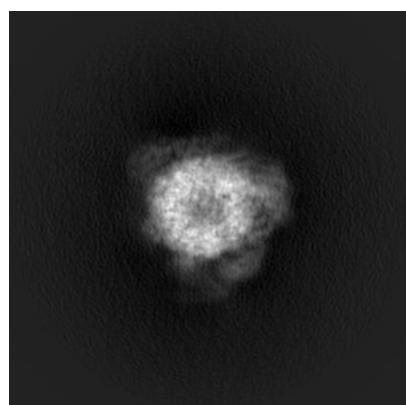
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14211. These allow visual inspection of the internal detail of the map and identification of artifacts.

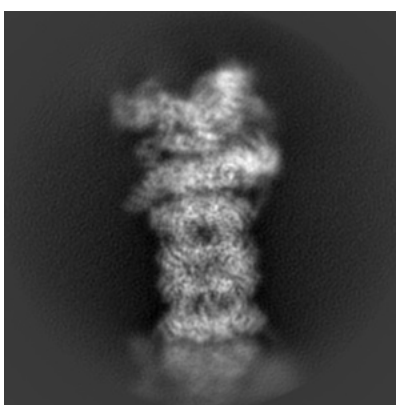
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

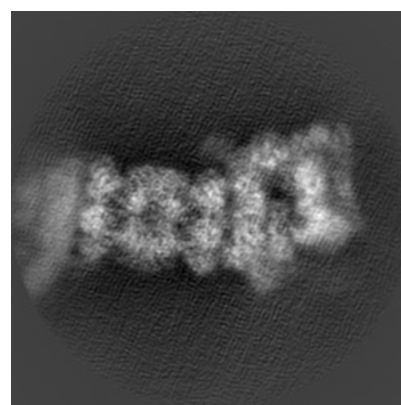
6.1.1 Primary map



X



Y

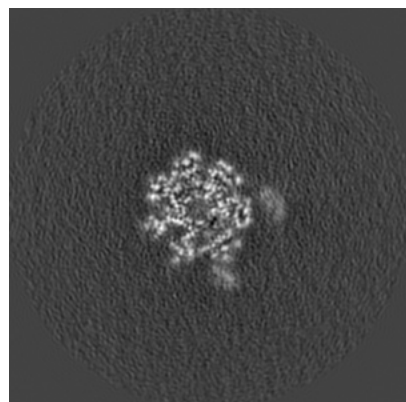


Z

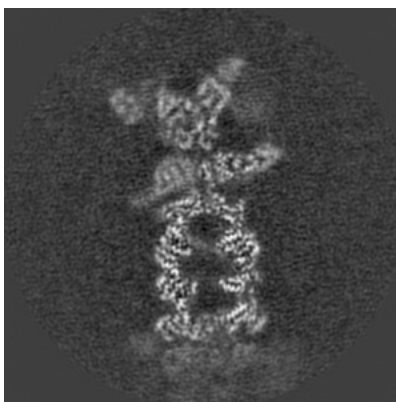
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

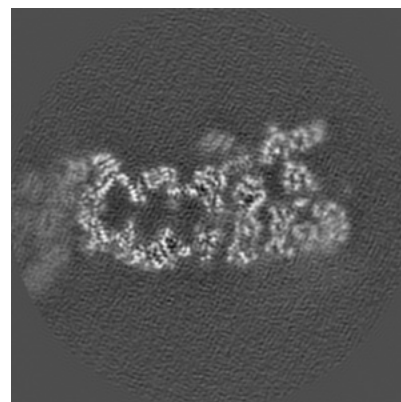
6.2.1 Primary map



X Index: 160



Y Index: 160

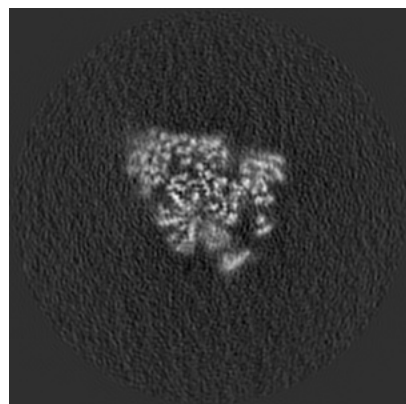


Z Index: 160

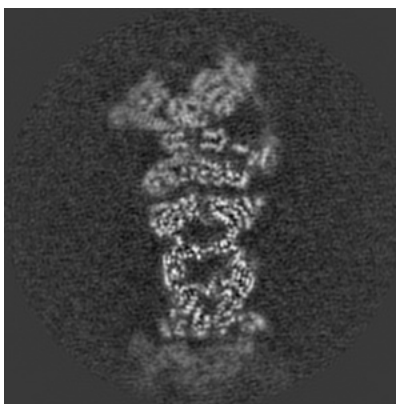
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

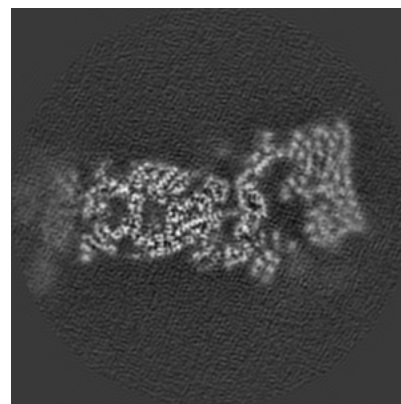
6.3.1 Primary map



X Index: 196



Y Index: 143

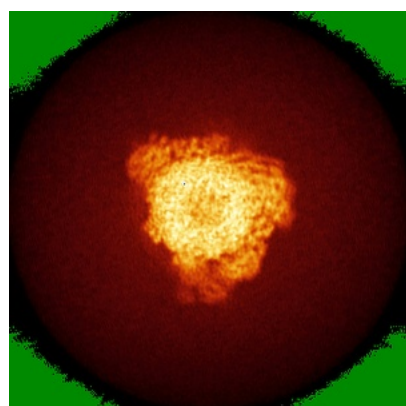


Z Index: 180

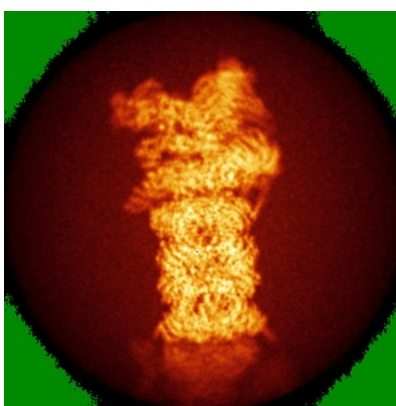
The images above show the largest variance slices of the map in three orthogonal directions.

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

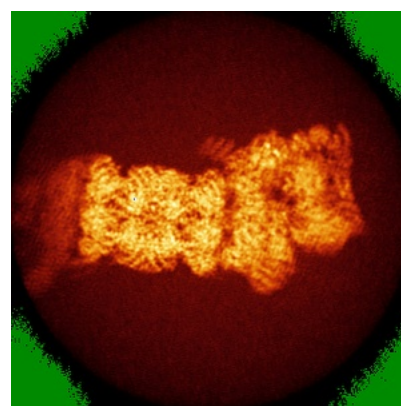
6.4.1 Primary map



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

This section was not generated.

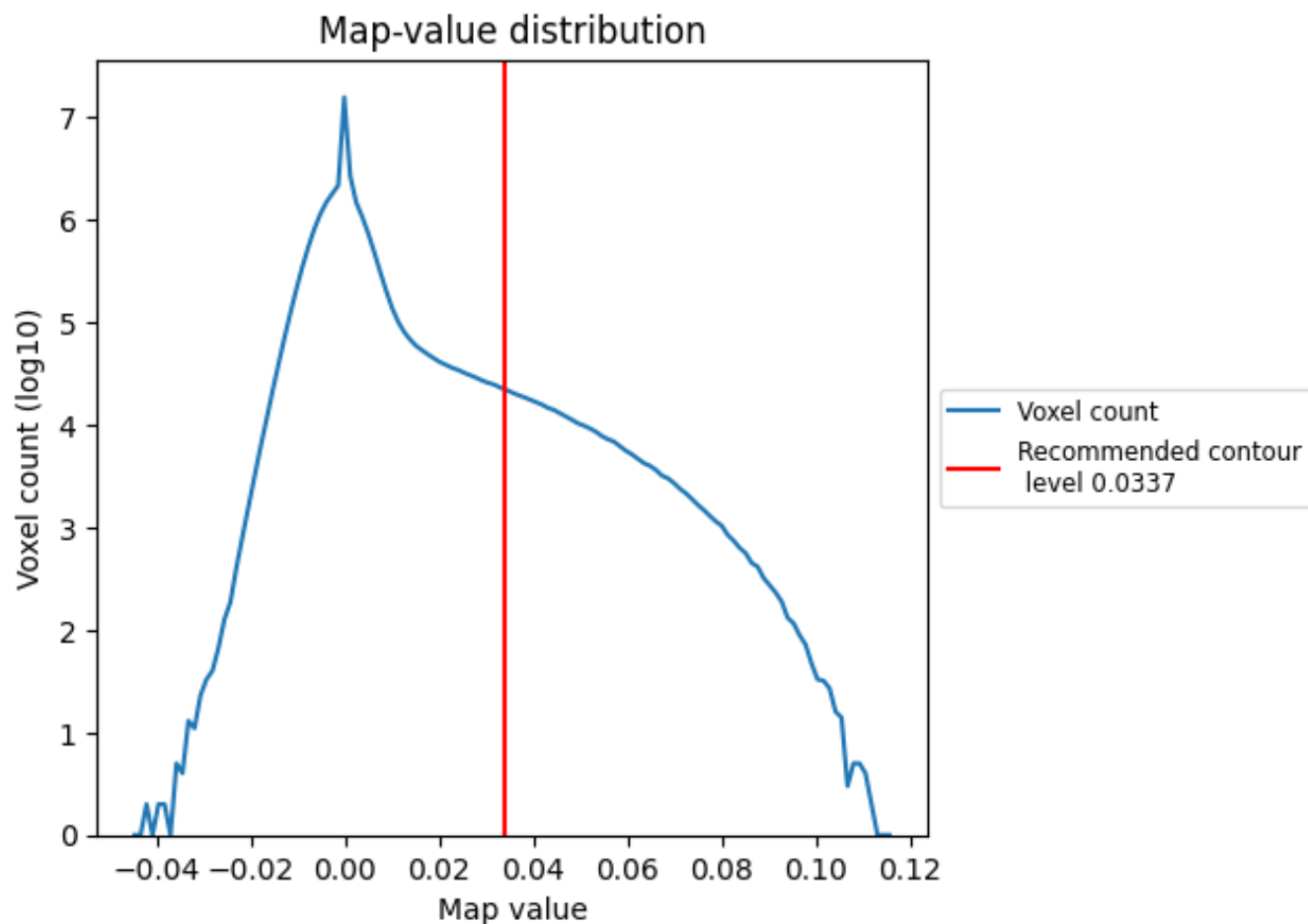
6.6 Mask visualisation

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

7 Map analysis [i](#)

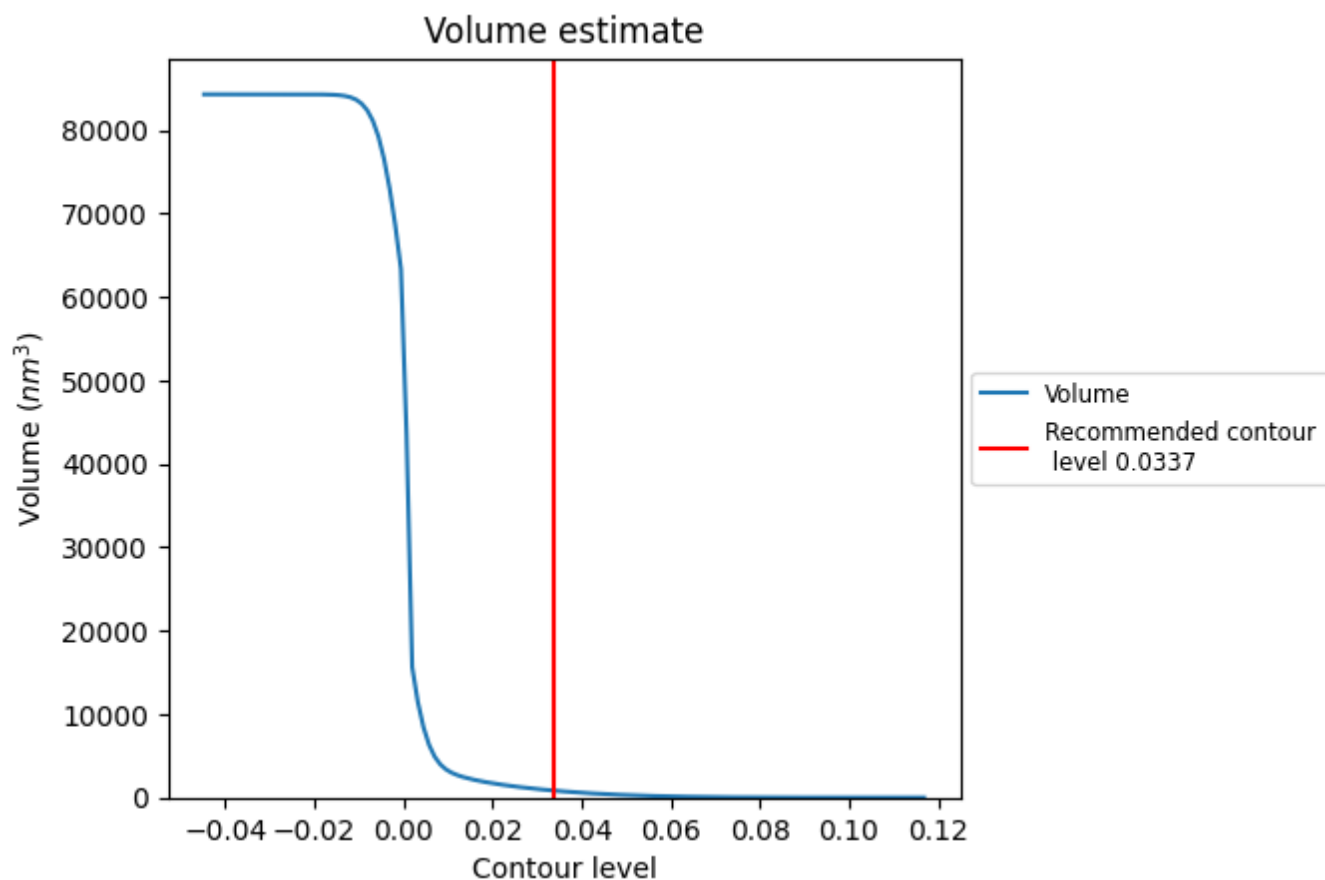
This section contains the results of statistical analysis of the map.

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.

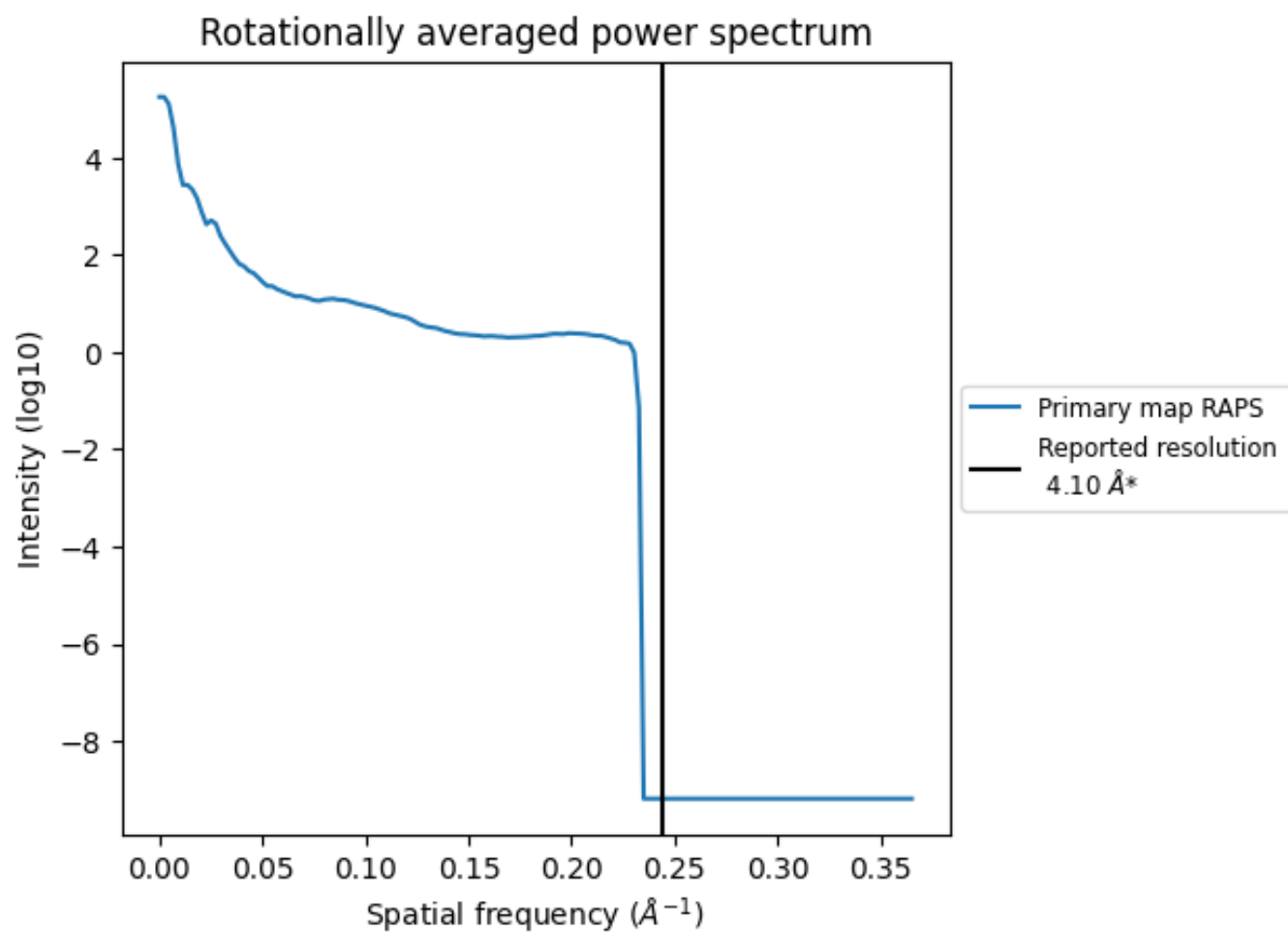
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 837 nm³; this corresponds to an approximate mass of 756 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 0.244 Å⁻¹

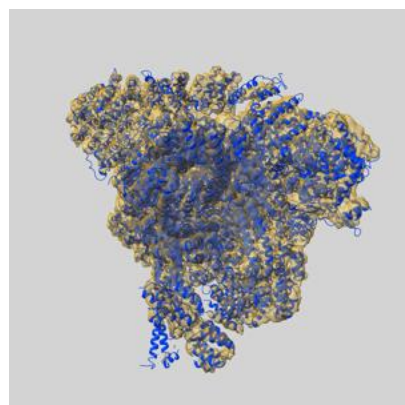
8 Fourier-Shell correlation

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

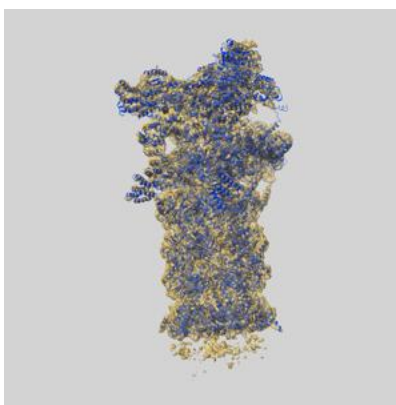
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14211 and PDB model 7QYB. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

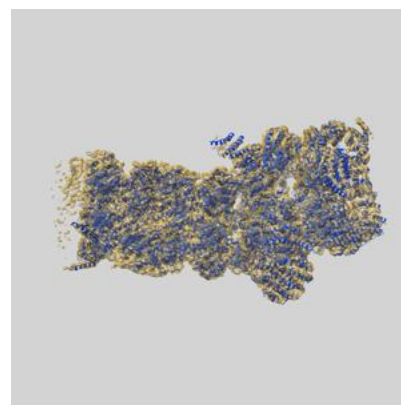
9.1 Map-model overlay [i](#)



X



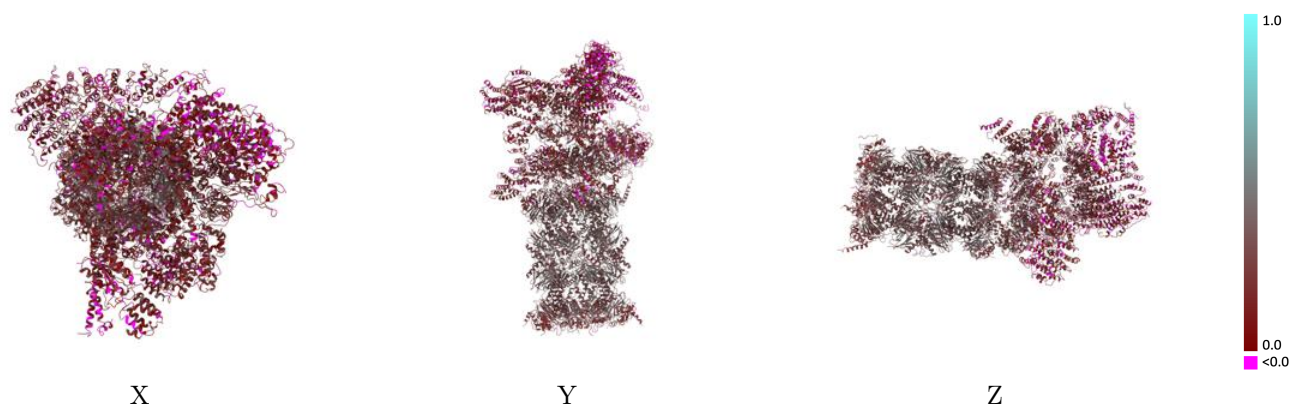
Y



Z

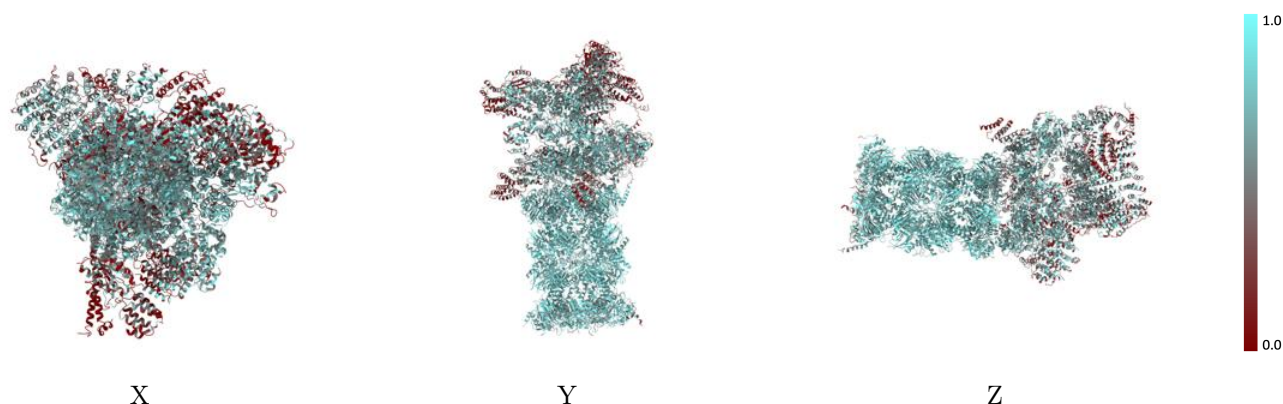
The images above show the 3D surface view of the map at the recommended contour level 0.0337 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



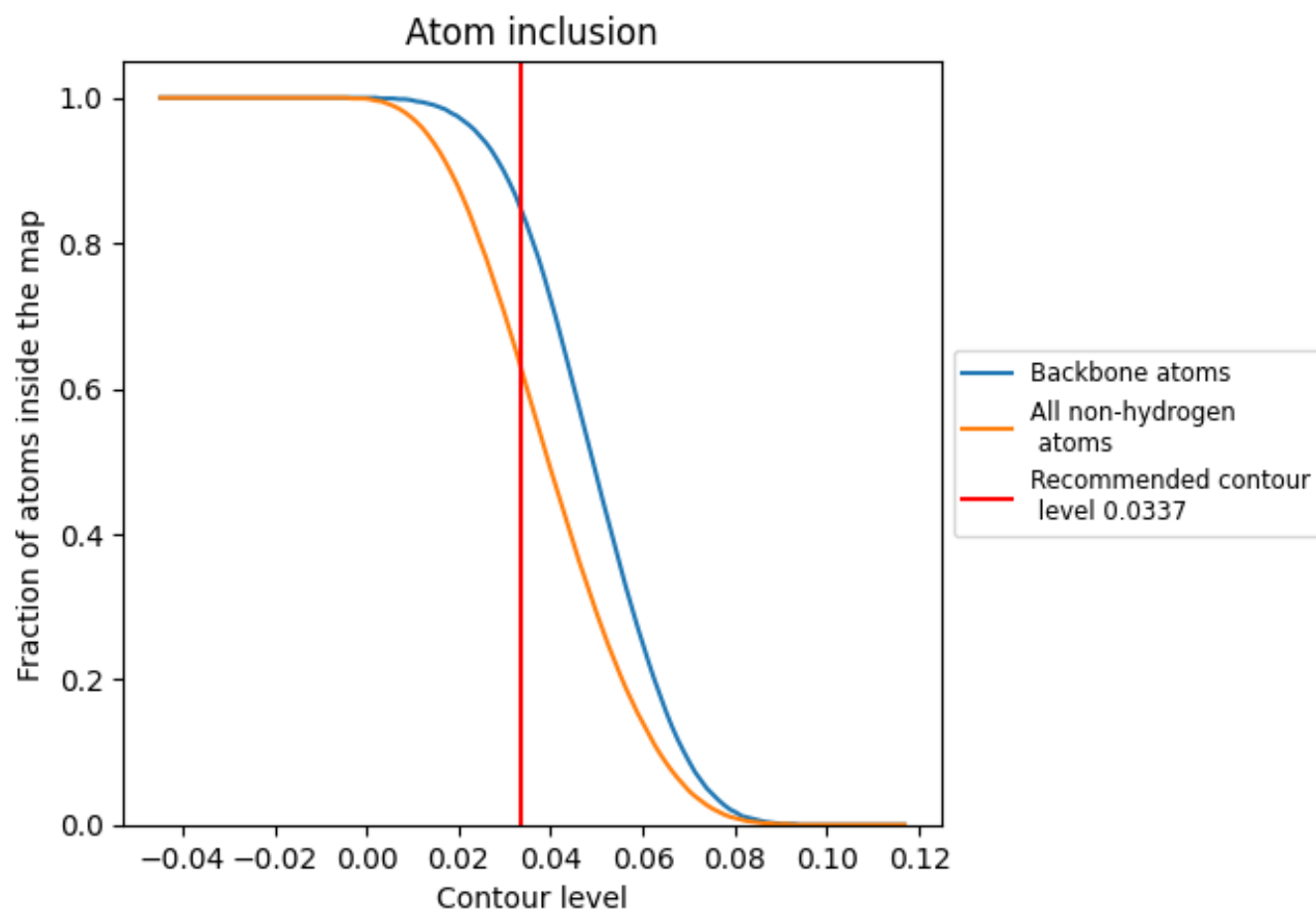
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0337).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 62% 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 (0.0337) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6250	 0.2520
A	 0.6340	 0.2650
B	 0.6170	 0.2700
C	 0.6530	 0.2820
D	 0.6330	 0.2600
E	 0.4120	 0.1550
F	 0.5660	 0.2320
G	 0.7440	 0.3140
H	 0.7590	 0.3370
I	 0.7170	 0.3180
J	 0.7540	 0.3340
K	 0.7340	 0.3320
L	 0.7760	 0.3470
M	 0.7380	 0.3150
N	 0.7930	 0.3520
O	 0.7890	 0.3540
P	 0.7890	 0.3590
Q	 0.7860	 0.3480
R	 0.8200	 0.3590
S	 0.7960	 0.3680
T	 0.7970	 0.3560
U	 0.4710	 0.1370
V	 0.3860	 0.1150
W	 0.4450	 0.1670
X	 0.5250	 0.2160
Y	 0.6590	 0.1970
Z	 0.5510	 0.2010
a	 0.4530	 0.1600
b	 0.3520	 0.1510
c	 0.5780	 0.2070
d	 0.3770	 0.1210
e	 0.5240	 0.1550
f	 0.5070	 0.1490
g	 0.7070	 0.3090
h	 0.7030	 0.3050



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Chain	Atom inclusion	Q-score
i	 0.6580	 0.2750
j	 0.6690	 0.2670
k	 0.6850	 0.2950
l	 0.7380	 0.3180
m	 0.7240	 0.2940
n	 0.7980	 0.3480
o	 0.7910	 0.3540
p	 0.7750	 0.3510
q	 0.7840	 0.3370
r	 0.8140	 0.3570
s	 0.7920	 0.3600
t	 0.7970	 0.3560