



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:53 PM UTC

PDB ID : 5VFS / pdb_00005vfs
EMDB ID : EMD-8666
Title : Nucleotide-Driven Triple-State Remodeling of the AAA-ATPase Channel in the Activated Human 26S Proteasome
Authors : Zhu, Y.; Wang, W.L.; Yu, D.; Ouyang, Q.; Lu, Y.; Mao, Y.
Deposited on : 2017-04-09
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

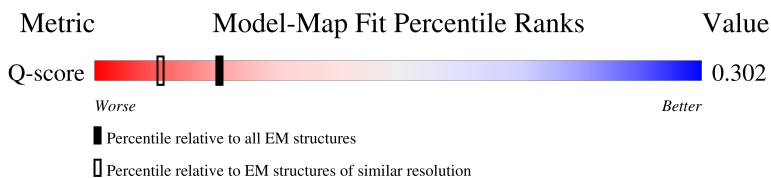
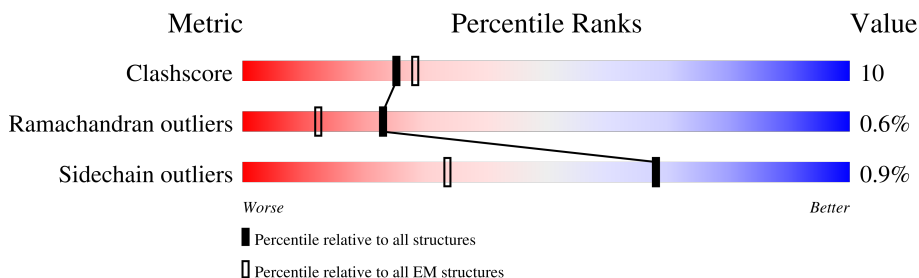
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	G	240	14% 82% 17% .
1	g	240	29% 82% 17% .
2	H	232	14% 85% 15%
2	h	232	29% 85% 14% .

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Mol	Chain	Length	Quality of chain
3	I	250	
3	i	250	
4	J	243	
4	j	243	
5	K	234	
5	k	234	
6	L	238	
6	l	238	
7	M	245	
7	m	245	
8	N	191	
8	n	191	
9	O	220	
9	o	220	
10	P	204	
10	p	204	
11	Q	199	
11	q	199	
12	R	201	
12	r	201	
13	S	213	
13	s	213	
14	T	215	
14	t	215	
15	U	911	

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Mol	Chain	Length	Quality of chain
16	V	480	
17	W	456	
18	X	380	
19	Y	378	
20	Z	286	
21	a	373	
22	b	191	
23	c	309	
24	d	257	
25	e	70	
26	B	369	
27	A	433	
28	E	403	
29	F	439	
30	C	389	
31	D	418	
32	f	848	

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 101431 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		
1	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		
2	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		
3	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

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

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

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

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 8 is a protein called Proteasome subunit beta type-6.

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

- Molecule 9 is a protein called Proteasome subunit beta type-7.

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

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

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

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

- Molecule 11 is a protein called Proteasome subunit beta type-2.

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

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

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

- Molecule 13 is a protein called Proteasome subunit beta type-1.

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

- Molecule 14 is a protein called Proteasome subunit beta type-4.

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

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	806	Total	C	N	O	S	0	0
			6287	3990	1075	1178	44		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

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

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

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

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Z	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 25 is a protein called Sem1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	359	Total	C	N	O	S	0	0
			2720	1708	465	535	12		

- Molecule 27 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A	380	Total	C	N	O	S	0	0
			2894	1818	515	543	18		

- Molecule 28 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	E	375	Total	C	N	O	S	0	0
			2860	1796	512	536	16		

- Molecule 29 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	F	376	Total	C	N	O	S	0	0
			2858	1802	496	545	15		

- Molecule 30 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	C	358	Total	C	N	O	S	0	0
			2820	1780	506	518	16		

- Molecule 31 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	D	380	Total	C	N	O	S	0	0
			3039	1923	524	579	13		

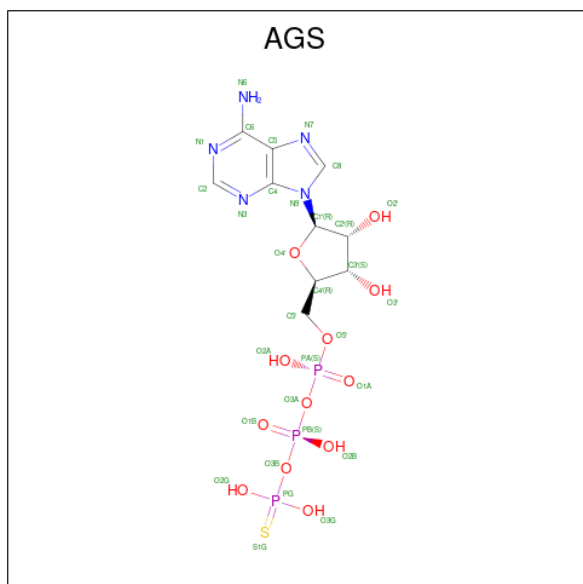
- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	689	Total	C	N	O	S	0	0
			5319	3343	904	1037	35		

- Molecule 33 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 34 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



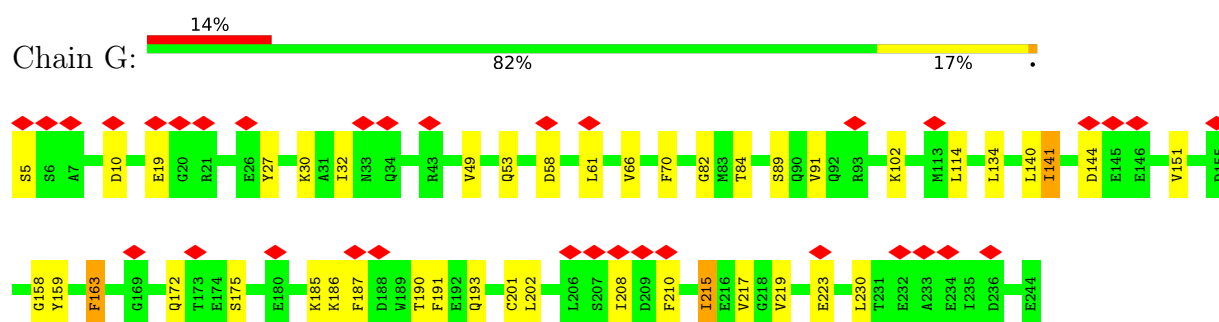
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Mol	Chain	Residues	Atoms						AltConf
34	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
34	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
34	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
34	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
34	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

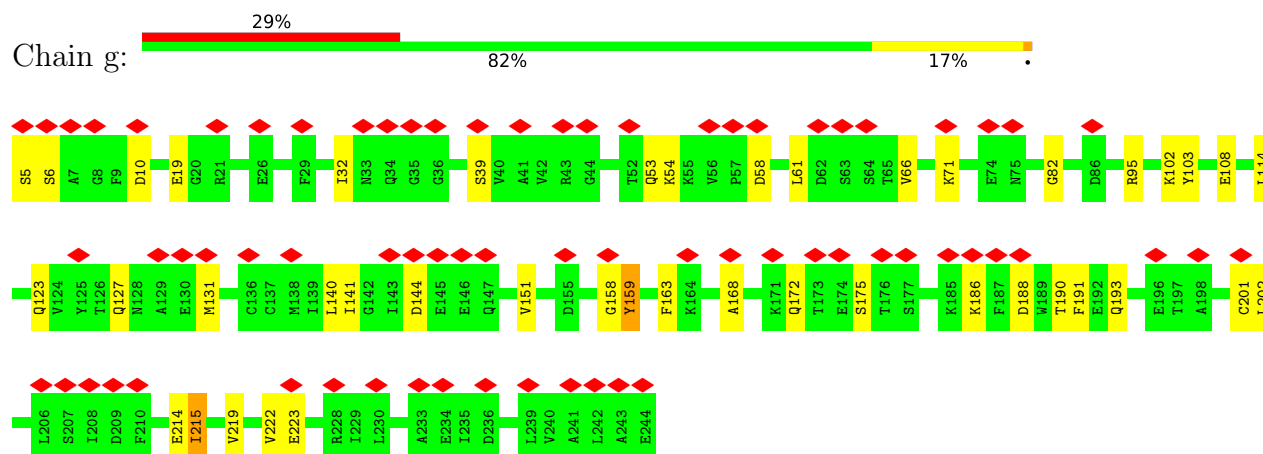
3 Residue-property plots

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

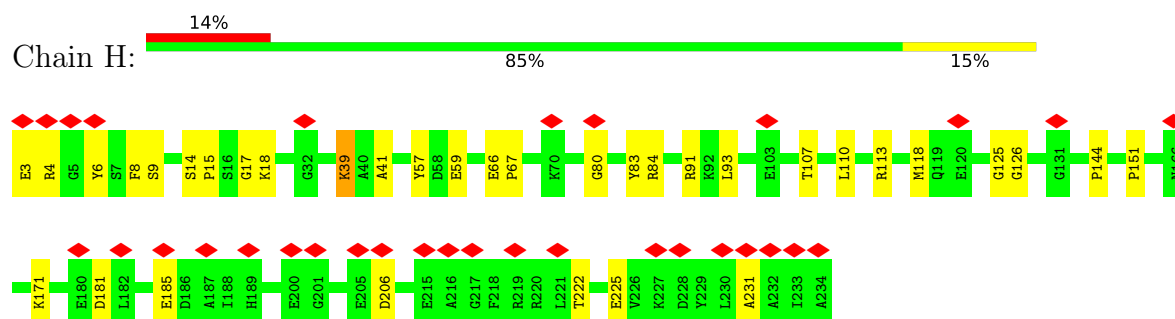
• Molecule 1: Proteasome subunit alpha type-6



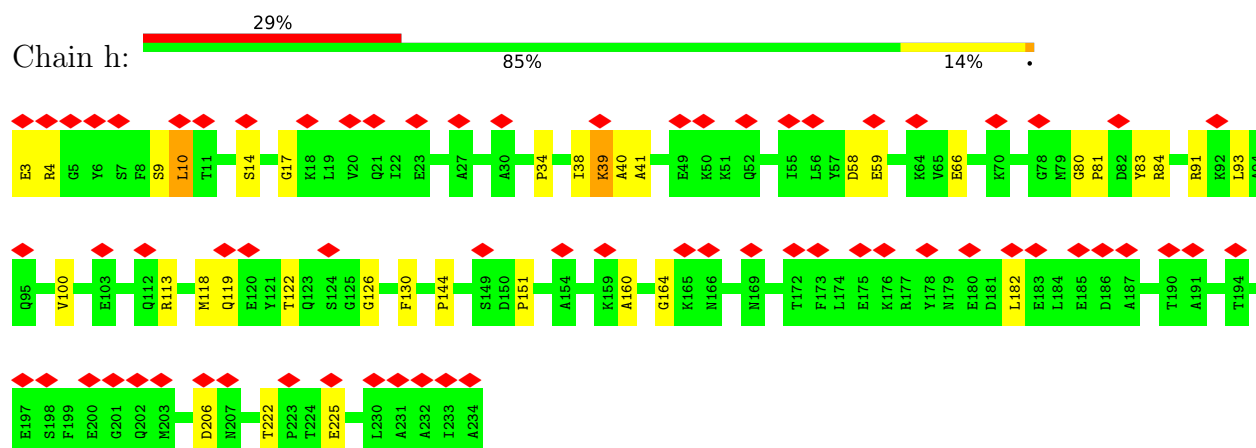
• Molecule 1: Proteasome subunit alpha type-6



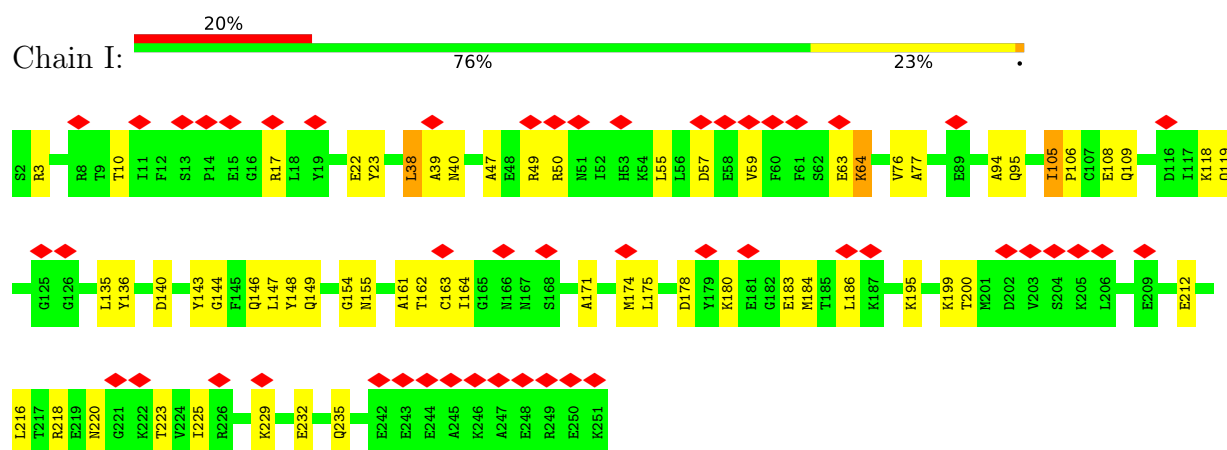
• Molecule 2: Proteasome subunit alpha type-2



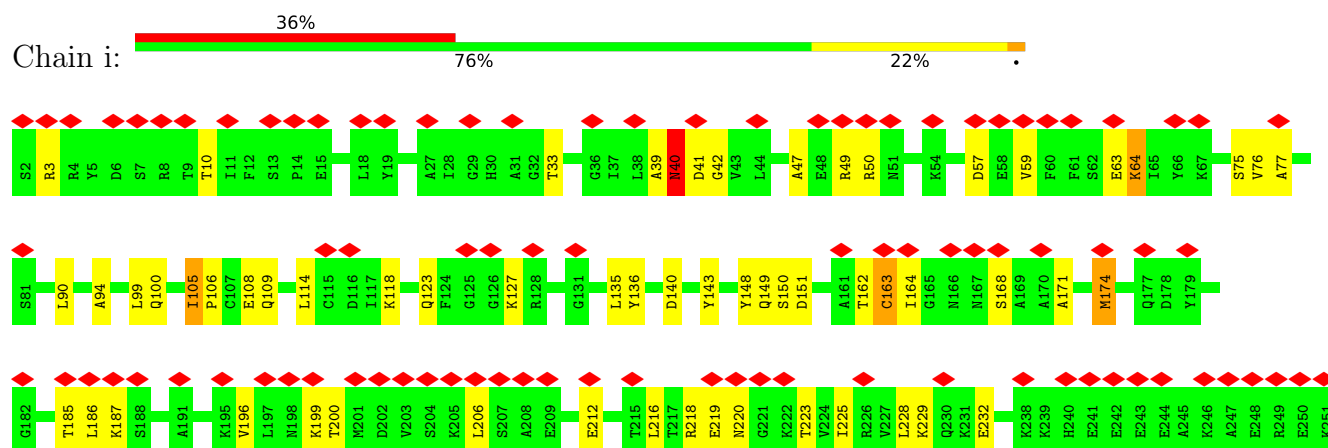
- Molecule 2: Proteasome subunit alpha type-2



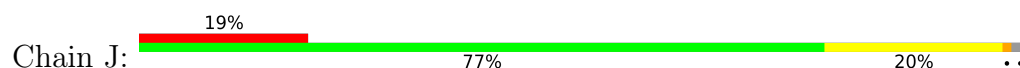
- Molecule 3: Proteasome subunit alpha type-4

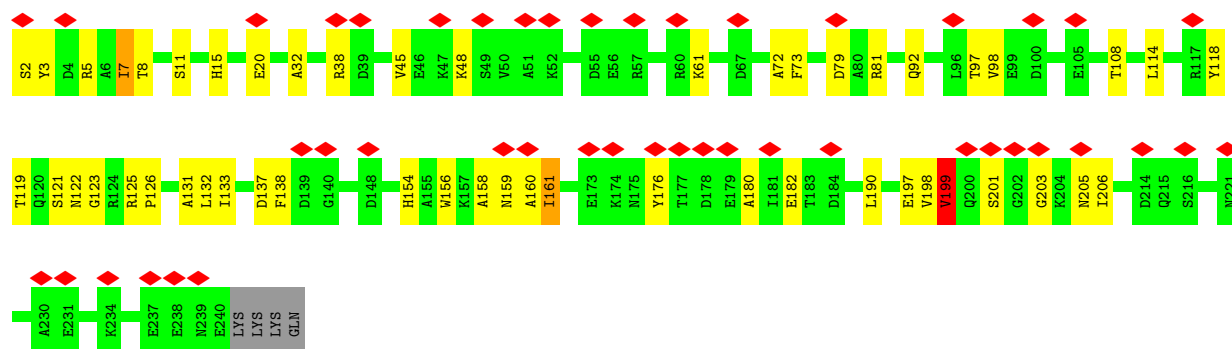


- Molecule 3: Proteasome subunit alpha type-4

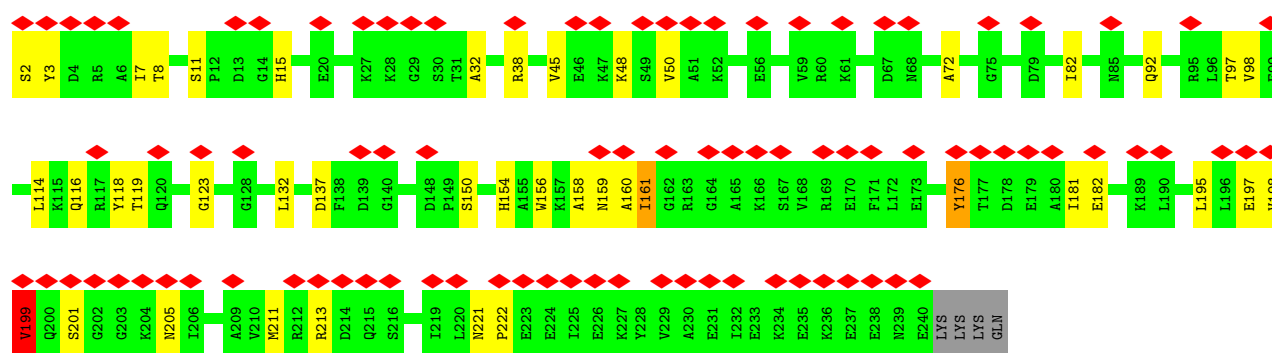
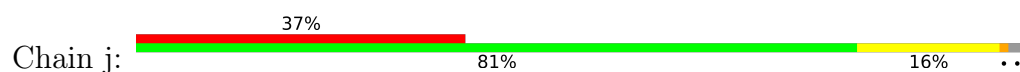


- Molecule 4: Proteasome subunit alpha type-7

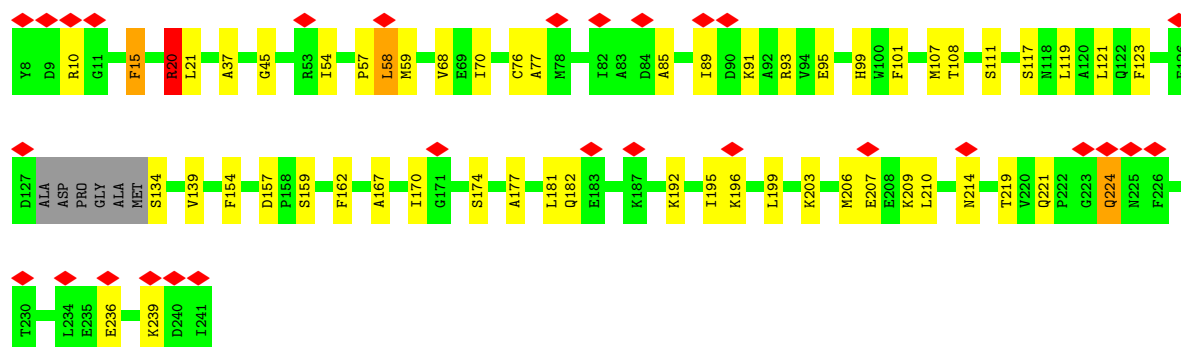
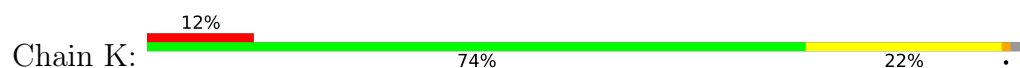




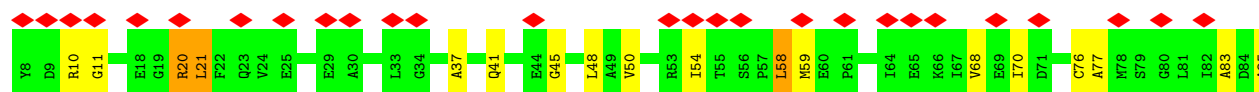
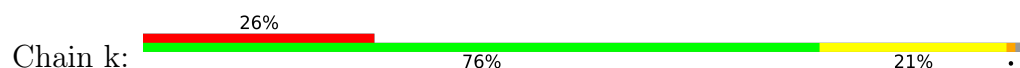
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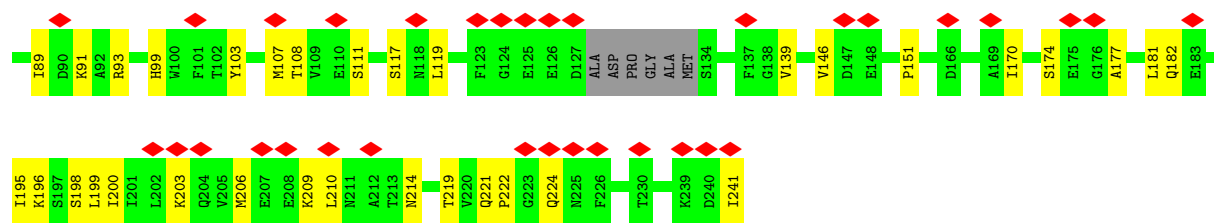


• Molecule 5: Proteasome subunit alpha type-5

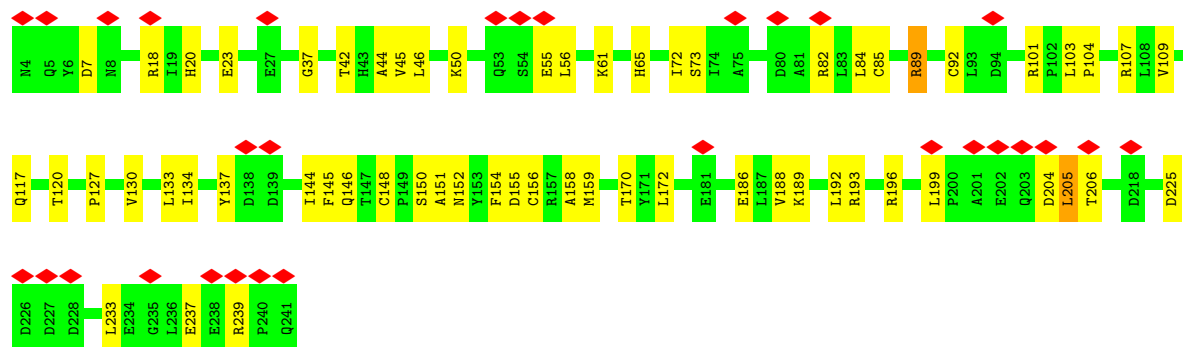
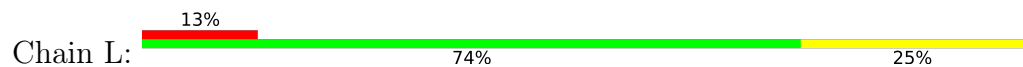


• Molecule 5: Proteasome subunit alpha type-5

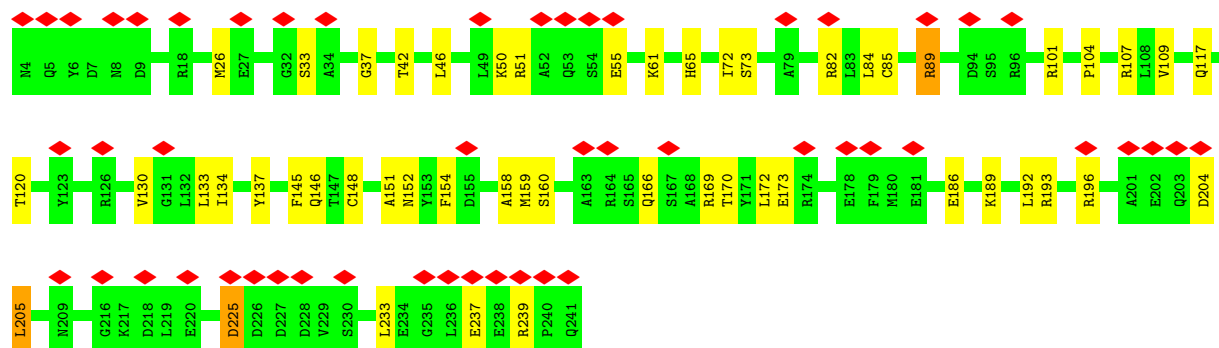
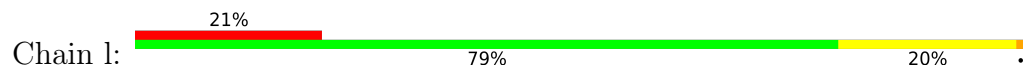




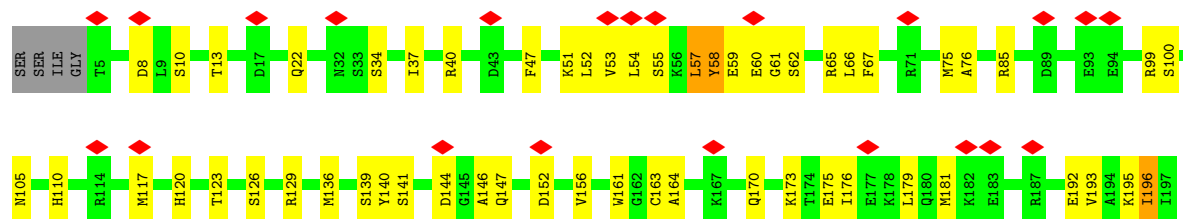
• Molecule 6: Proteasome subunit alpha type-1



• Molecule 6: Proteasome subunit alpha type-1

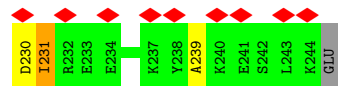
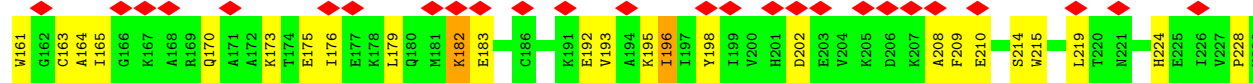
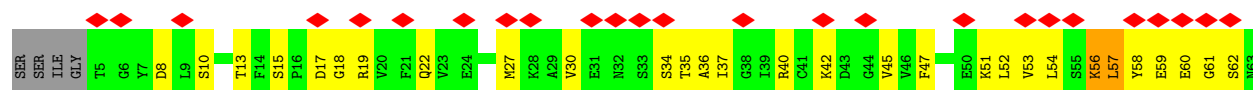


• Molecule 7: Proteasome subunit alpha type-3

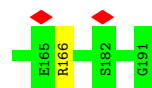
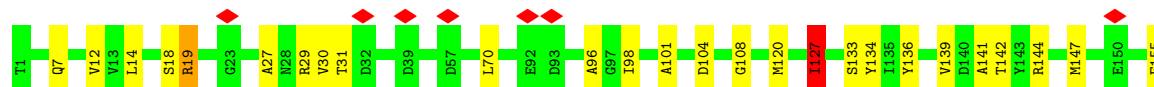
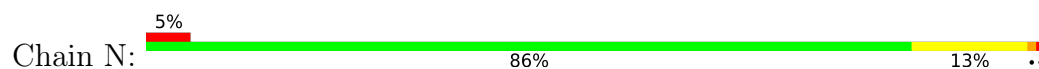




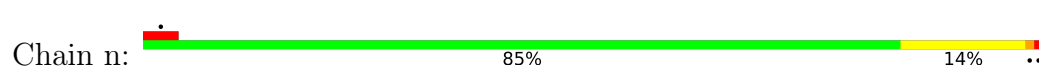
• Molecule 7: Proteasome subunit alpha type-3



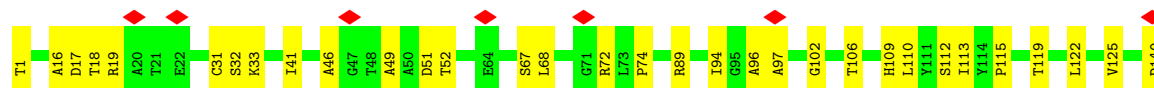
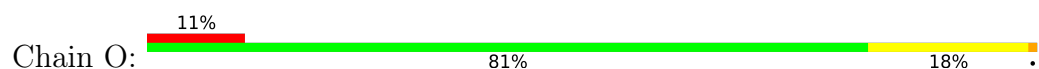
• Molecule 8: Proteasome subunit beta type-6

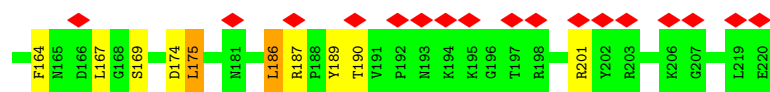


• Molecule 8: Proteasome subunit beta type-6

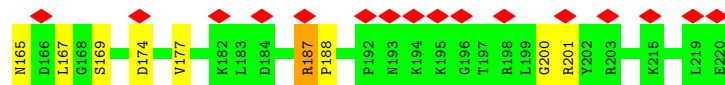
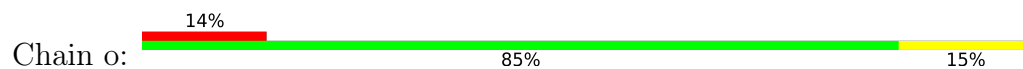


• Molecule 9: Proteasome subunit beta type-7

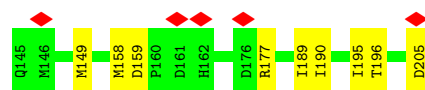
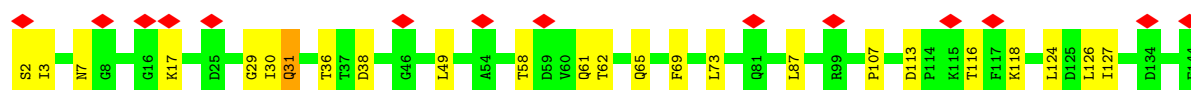
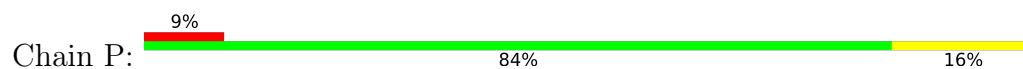




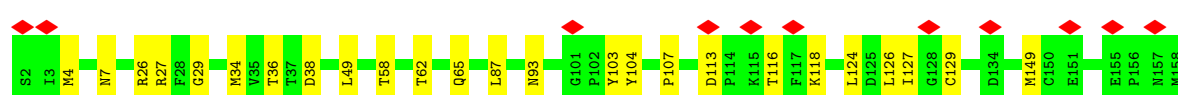
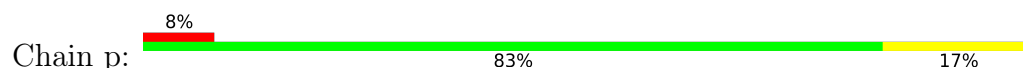
- Molecule 9: Proteasome subunit beta type-7



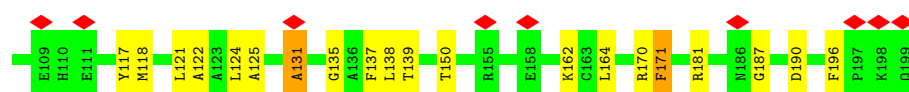
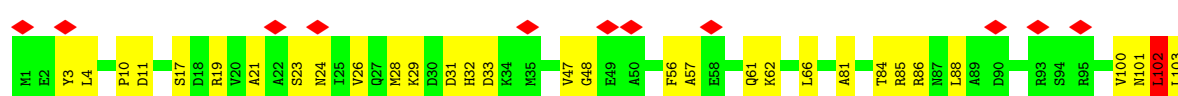
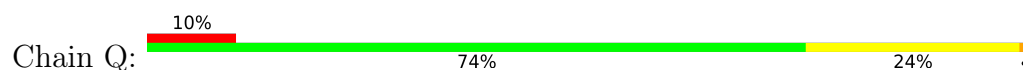
- Molecule 10: Proteasome subunit beta type-3



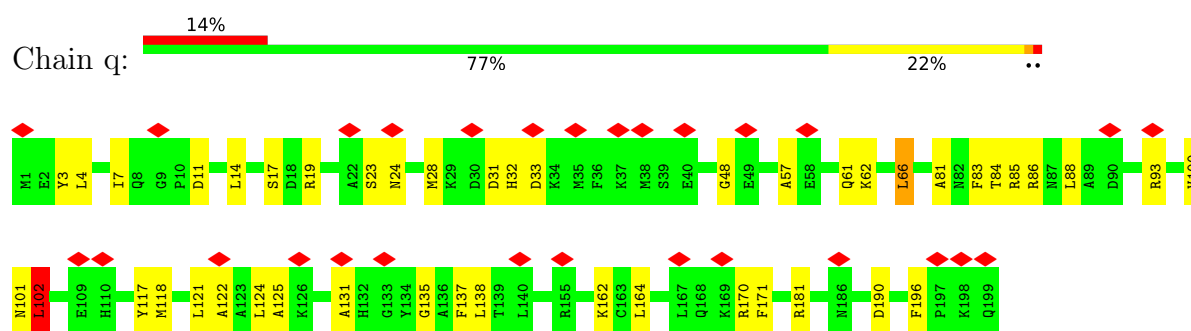
- Molecule 10: Proteasome subunit beta type-3



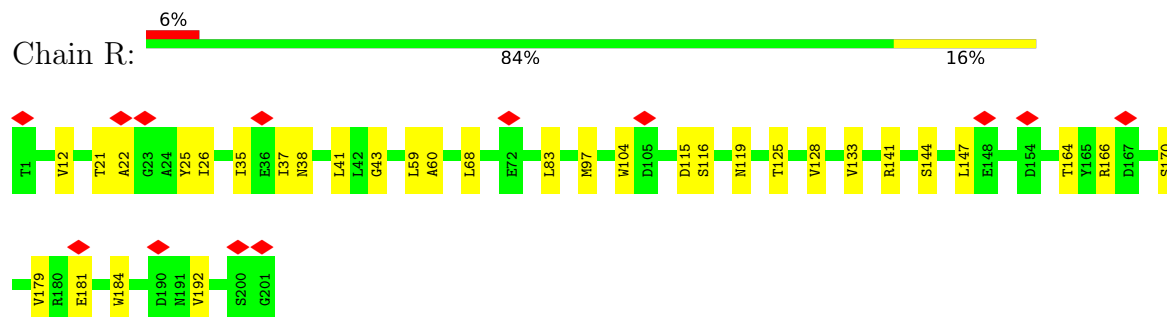
- Molecule 11: Proteasome subunit beta type-2



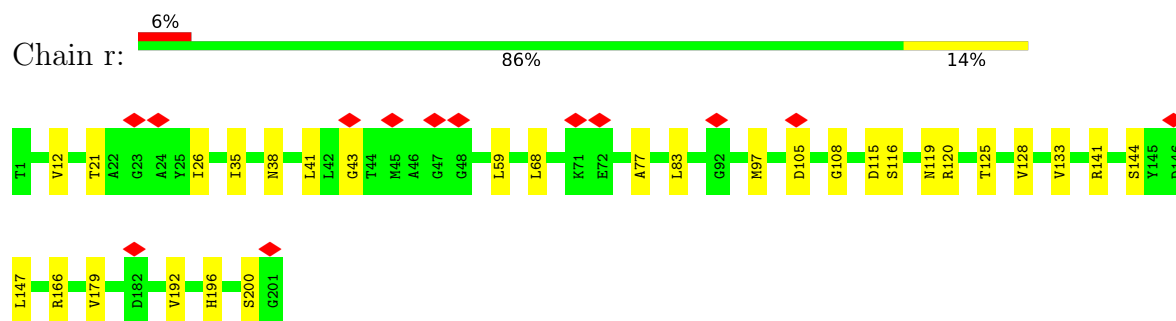
- Molecule 11: Proteasome subunit beta type-2



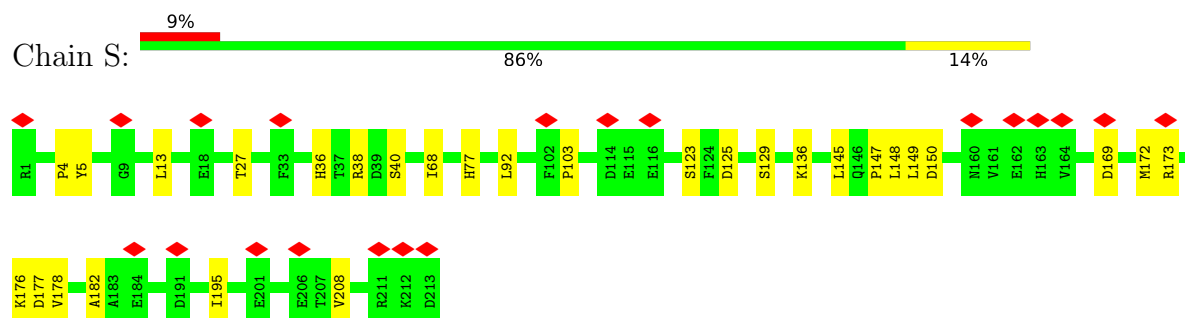
- Molecule 12: Proteasome subunit beta type-5



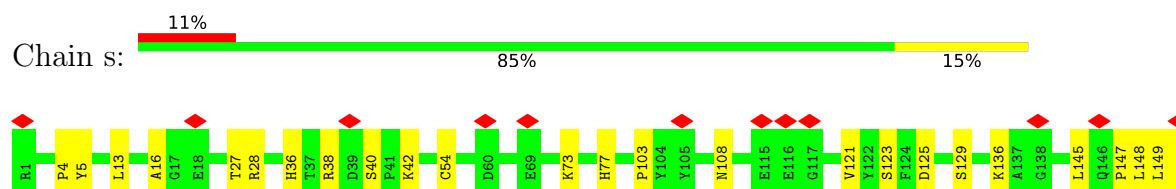
- Molecule 12: Proteasome subunit beta type-5



- Molecule 13: Proteasome subunit beta type-1

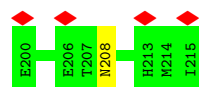
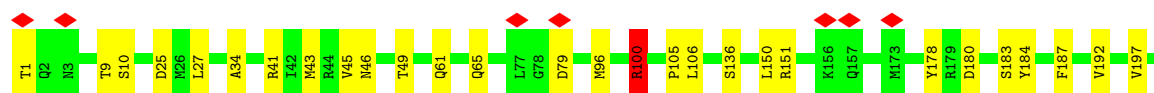
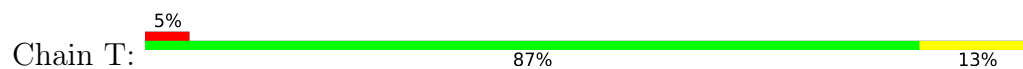


- Molecule 13: Proteasome subunit beta type-1

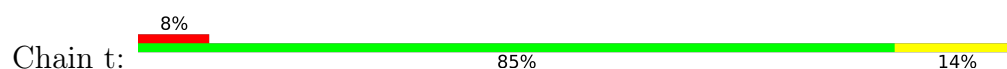




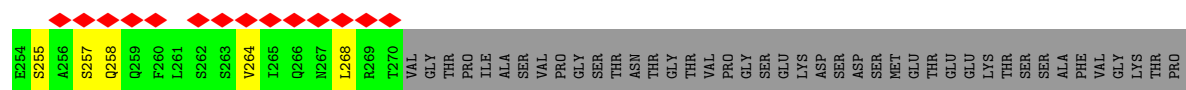
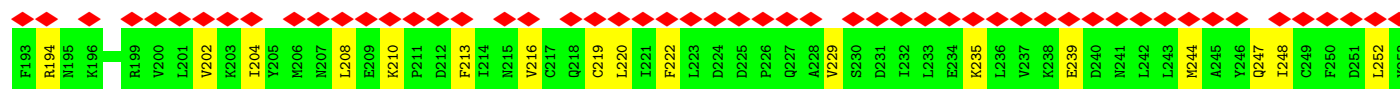
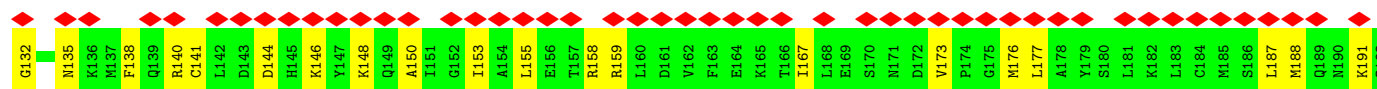
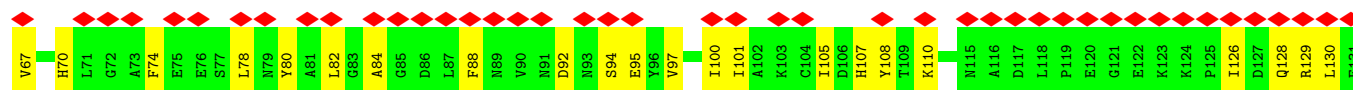
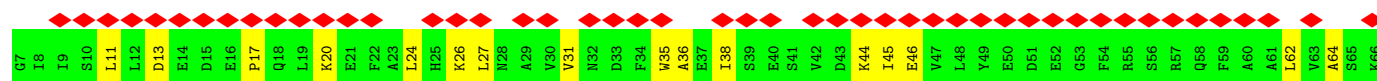
• Molecule 14: Proteasome subunit beta type-4

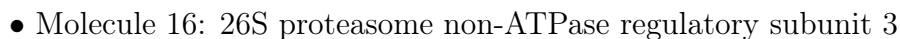


• Molecule 14: Proteasome subunit beta type-4

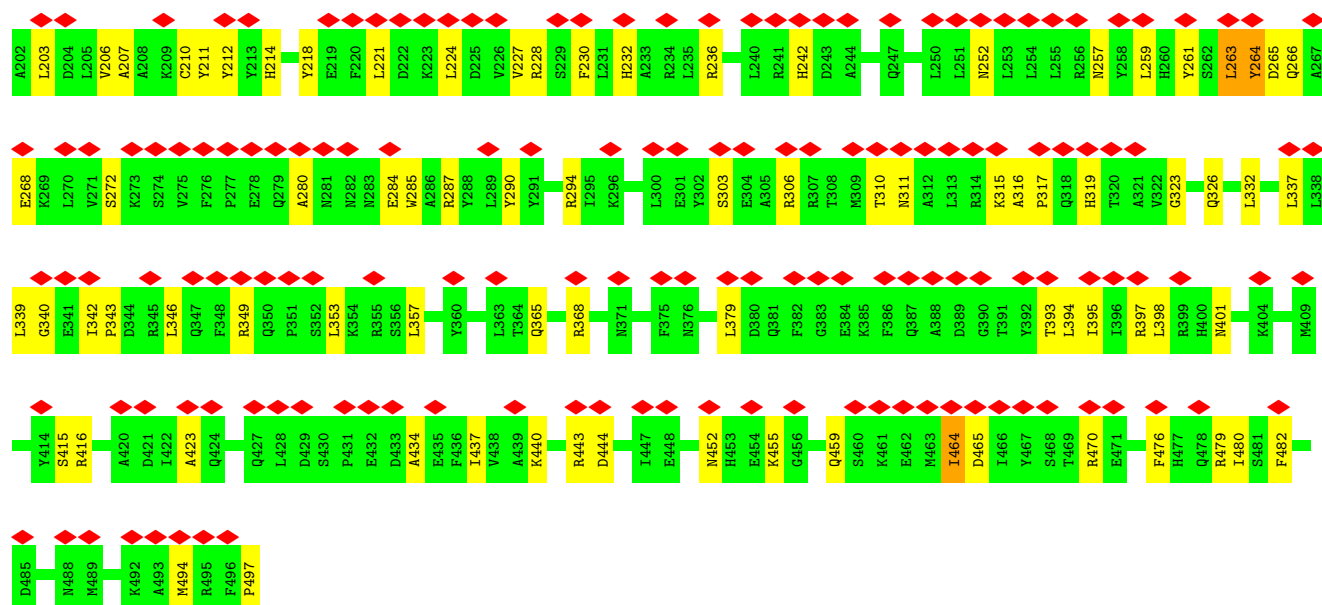


• Molecule 15: 26S proteasome non-ATPase regulatory subunit 1

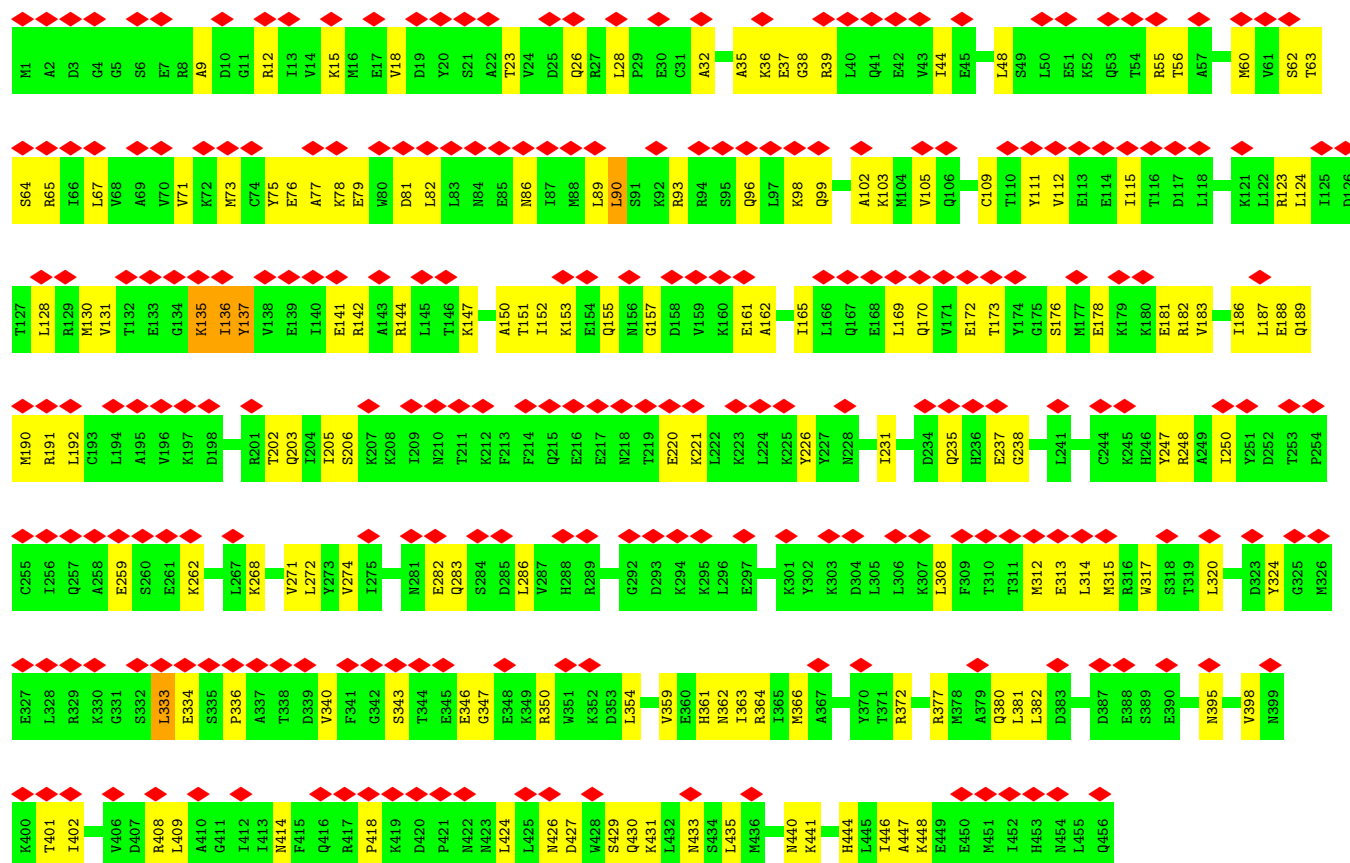




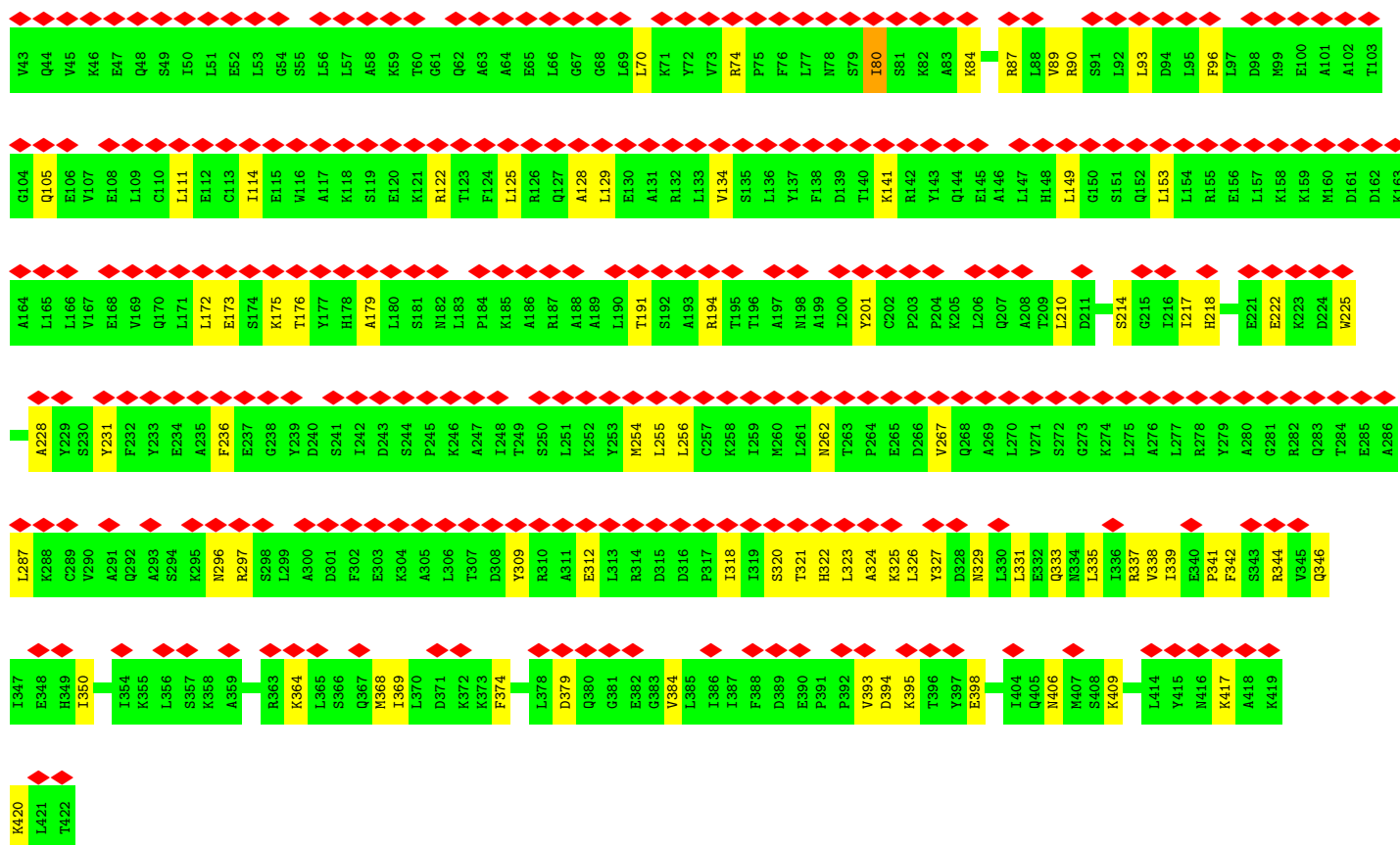
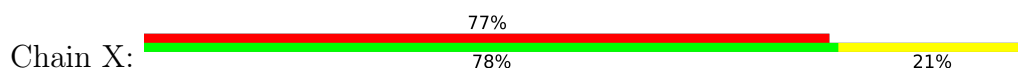
P18	P19	G20	G21	G22	E23	Q24	E25	P26	P27	P28	P29	P30	A31	P32	Q33	Q34	V35	E36	K37	K38	E39	E40	T43	G46	S47	T48	G49	E50	A51	D52	G53	K54	T55	A56	A57	A58	A59	A60	E61	H62	S63	Q64	R65	E66	L67	D68	T69	V70	T71	L72	E73	D74	I75	K76	E77	H78	V79		
K90	Q81	L82	E83	K84	A85	V86	S87	G88	K89	E90	P91	R92	F93	V94	L95	R96	A97	L98	R99	M100	L101	P102	S103	T104	S105	R106	R107	L108	M109	H110	Y111	V112	L113	Y114	K115	A116	V117	Q118	G119	F120	F121	T122	S123	N124	N125	A126	T127	R128	D129	F130	L131	L132	P133	F134	L135	R136	E137	P138	M139
D140	T141	E142	A143	D144	L145	Q146	F147	R148	P149	R150	T151	G152	K153	A154	P158	L159	L160	P161	E162	V163	E164	A165	V166	L167	Q168	L169	L170	V171	V172	I173	F174	M175	M176	M177	S178	K179	R180	Y181	K182	E183	A184	Q185	K186	L187	S188	D189	D190	L191	M192	Q193	K194	L195	S196	T197	Q198	M199	R200	R201	



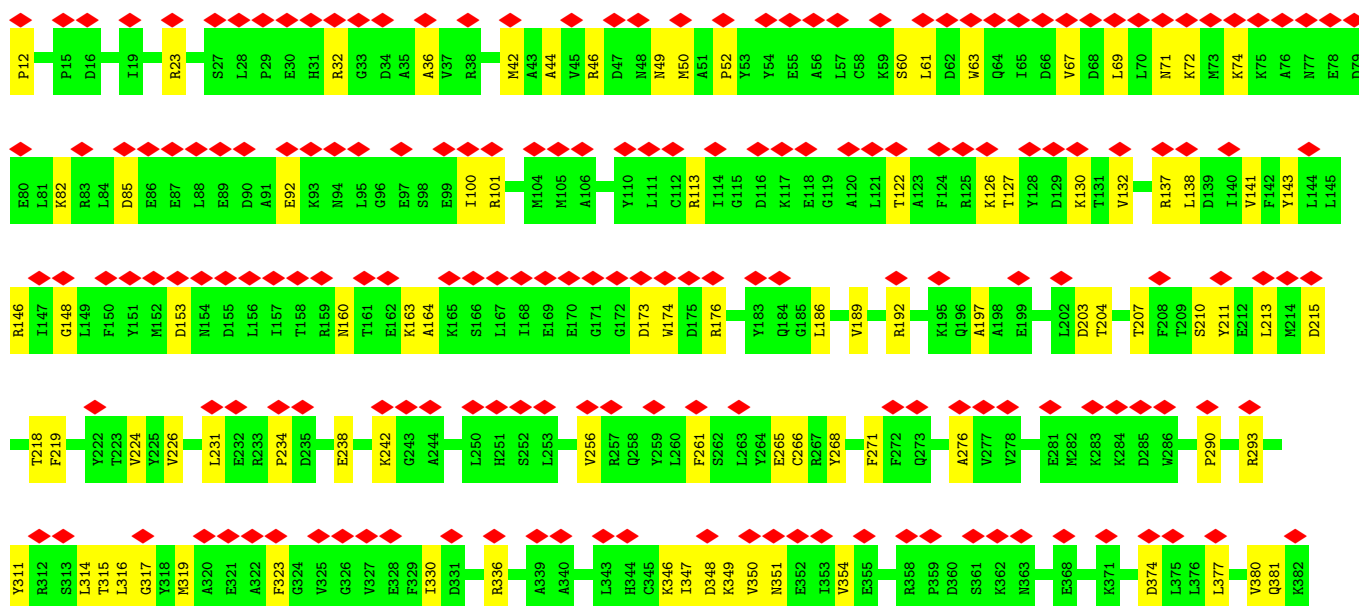
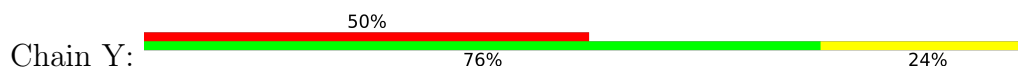
- Molecule 17: 26S proteasome non-ATPase regulatory subunit 12

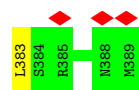


- Molecule 18: 26S proteasome non-ATPase regulatory subunit 11

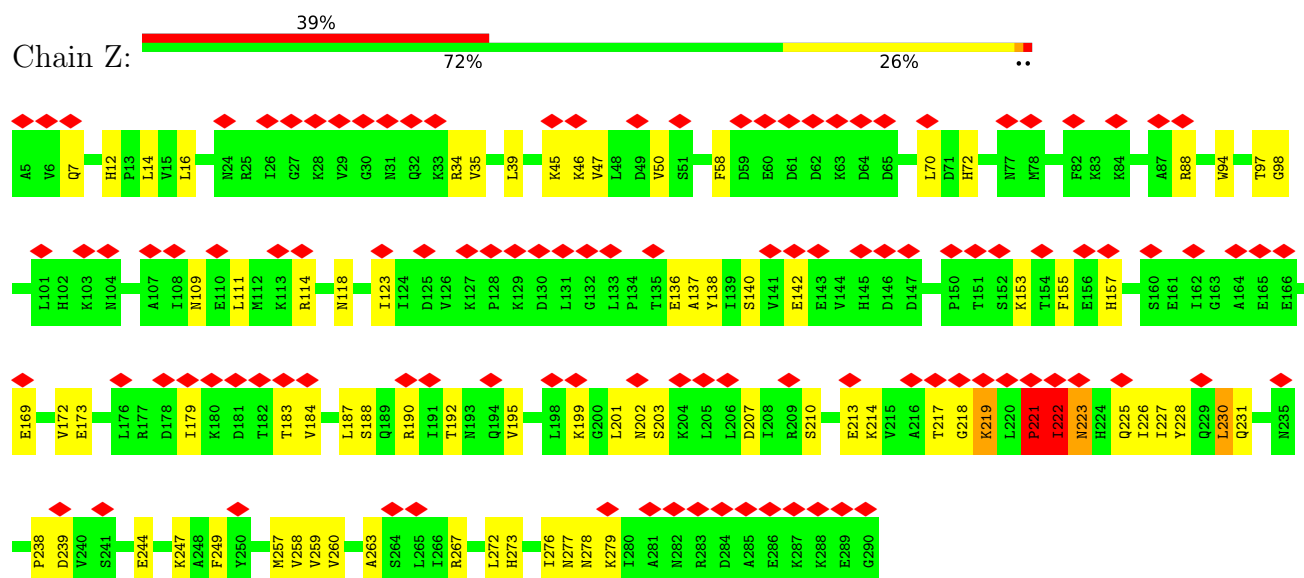


• Molecule 19: 26S proteasome non-ATPase regulatory subunit 6

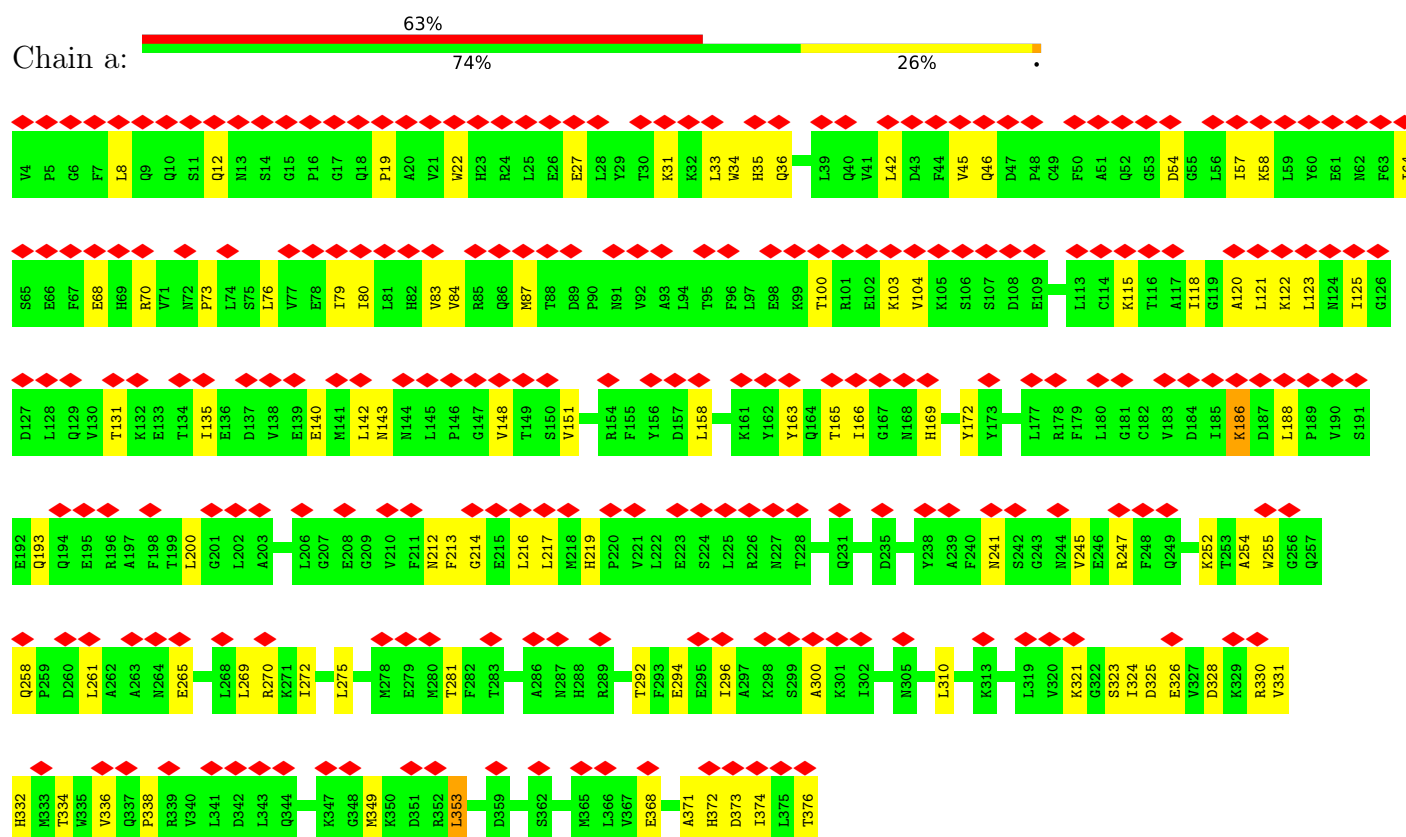




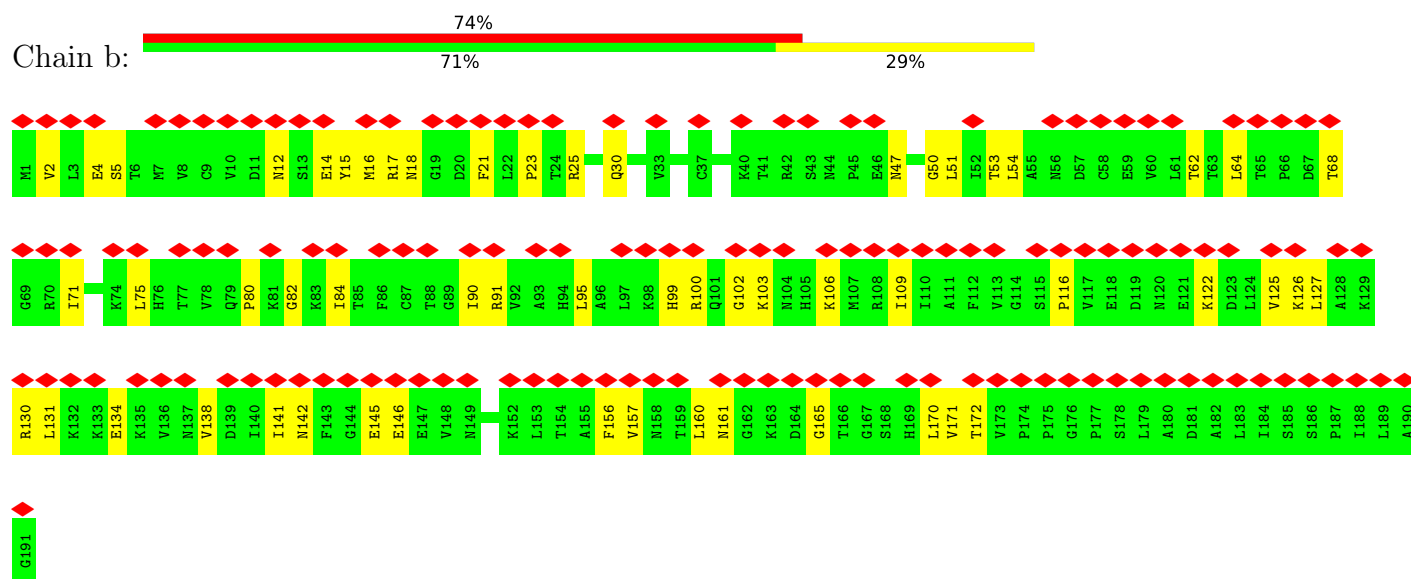
- Molecule 20: 26S proteasome non-ATPase regulatory subunit 7



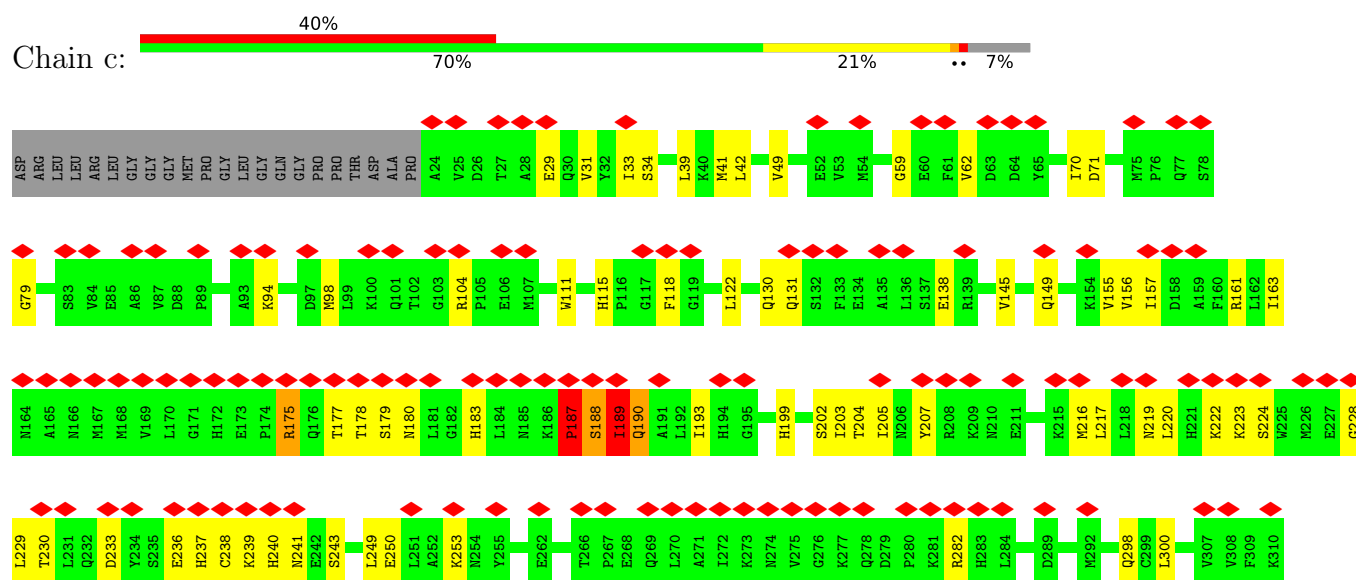
- Molecule 21: 26S proteasome non-ATPase regulatory subunit 13



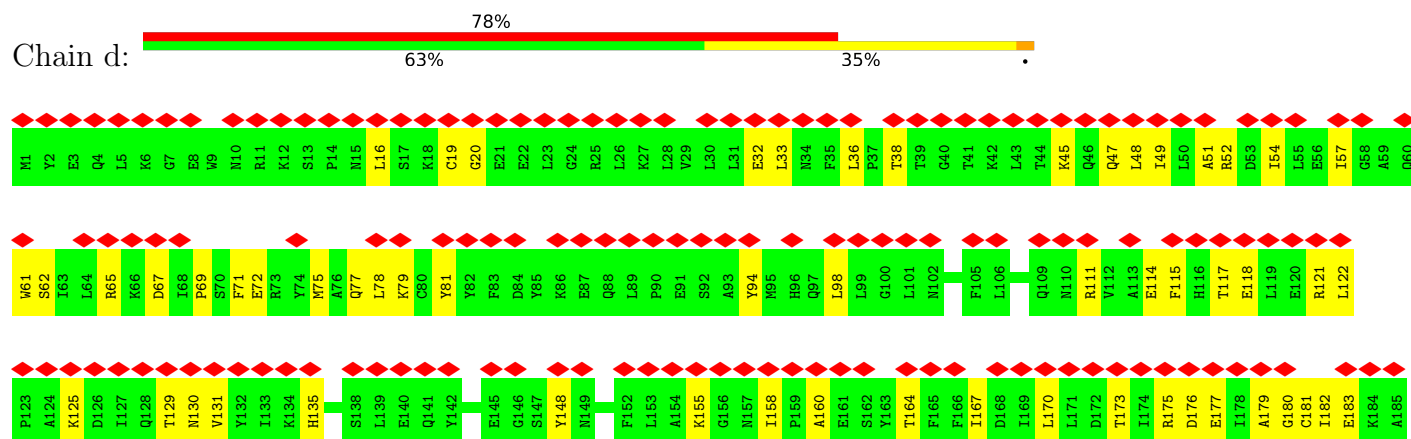
- Molecule 22: 26S proteasome non-ATPase regulatory subunit 4

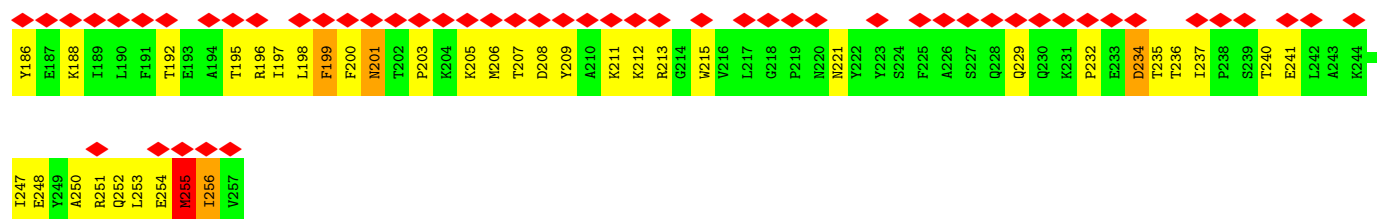


- Molecule 23: 26S proteasome non-ATPase regulatory subunit 14

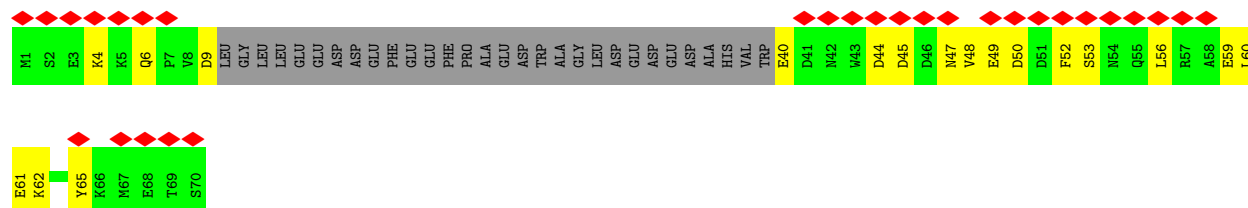
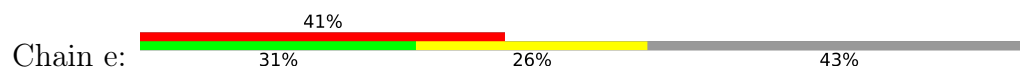


- Molecule 24: 26S proteasome non-ATPase regulatory subunit 8

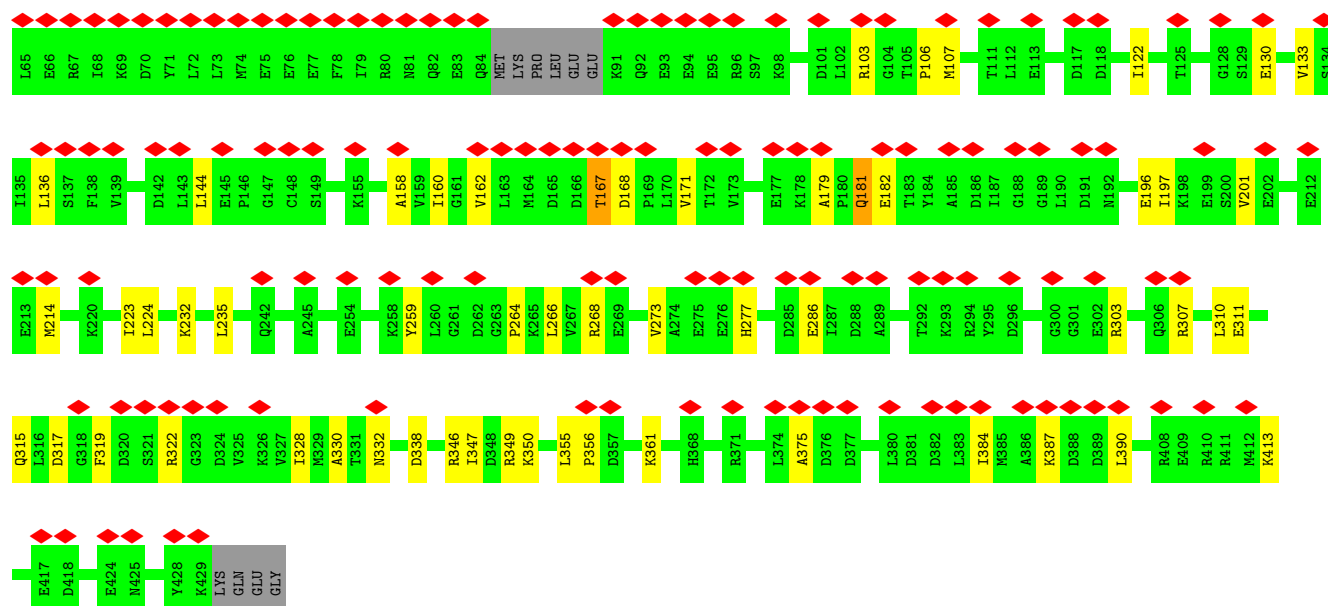
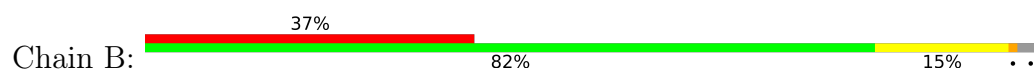




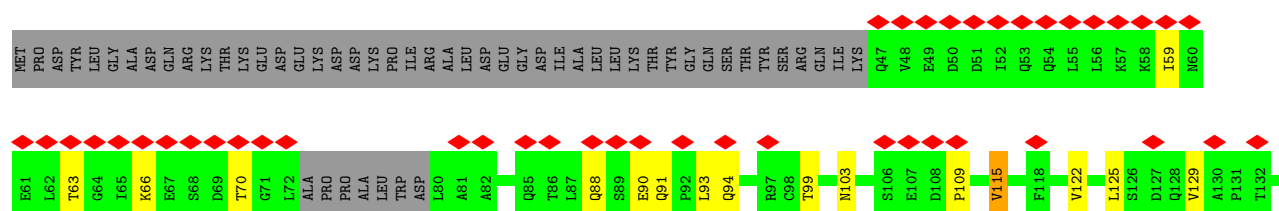
• Molecule 25: Sem1

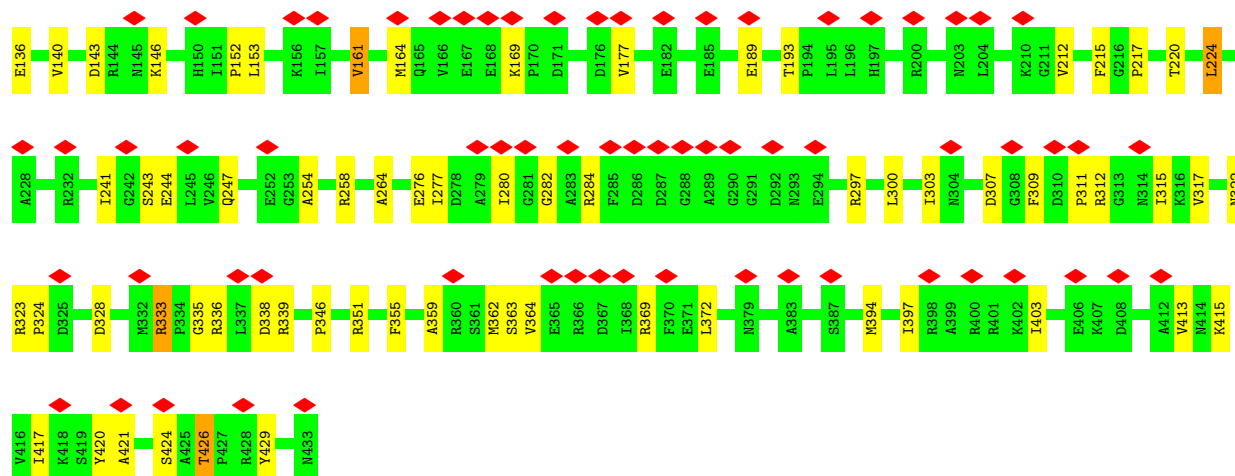


• Molecule 26: 26S proteasome regulatory subunit 4

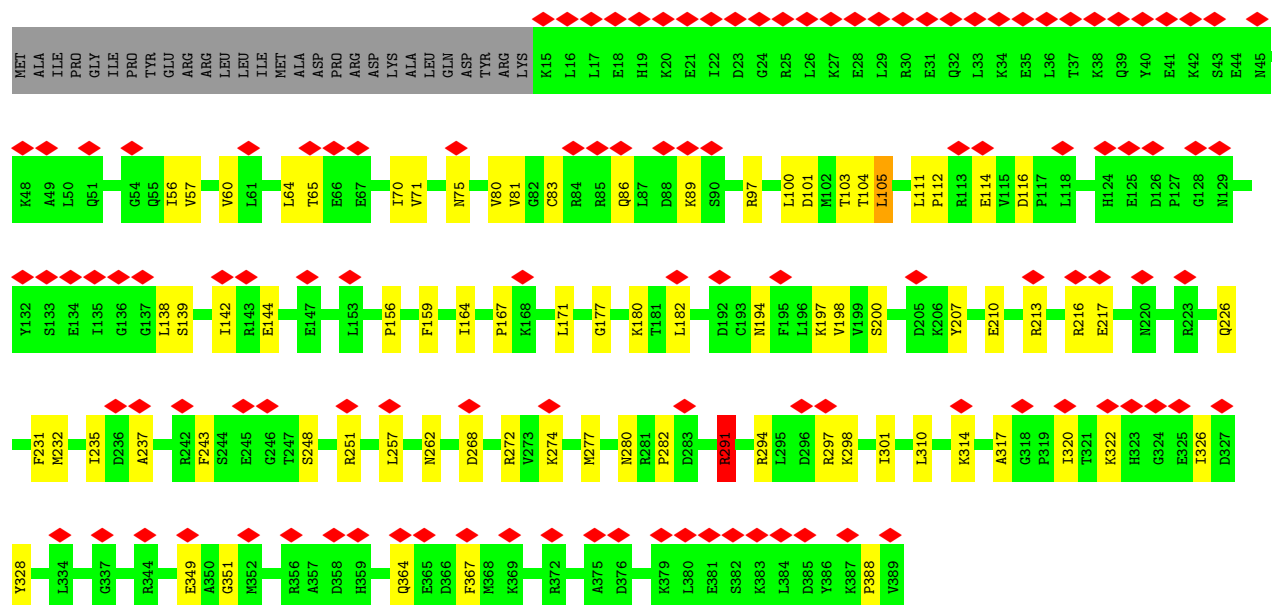
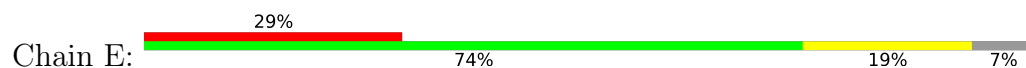


• Molecule 27: 26S proteasome regulatory subunit 7

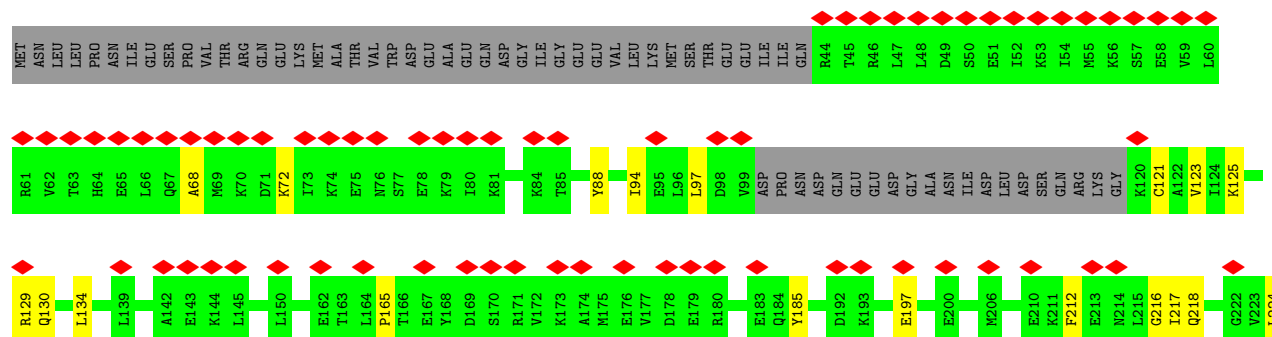
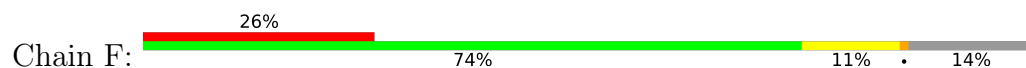


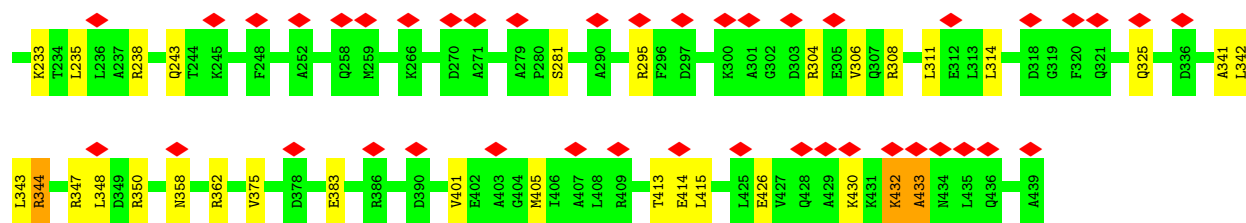


• Molecule 28: 26S proteasome regulatory subunit 10B



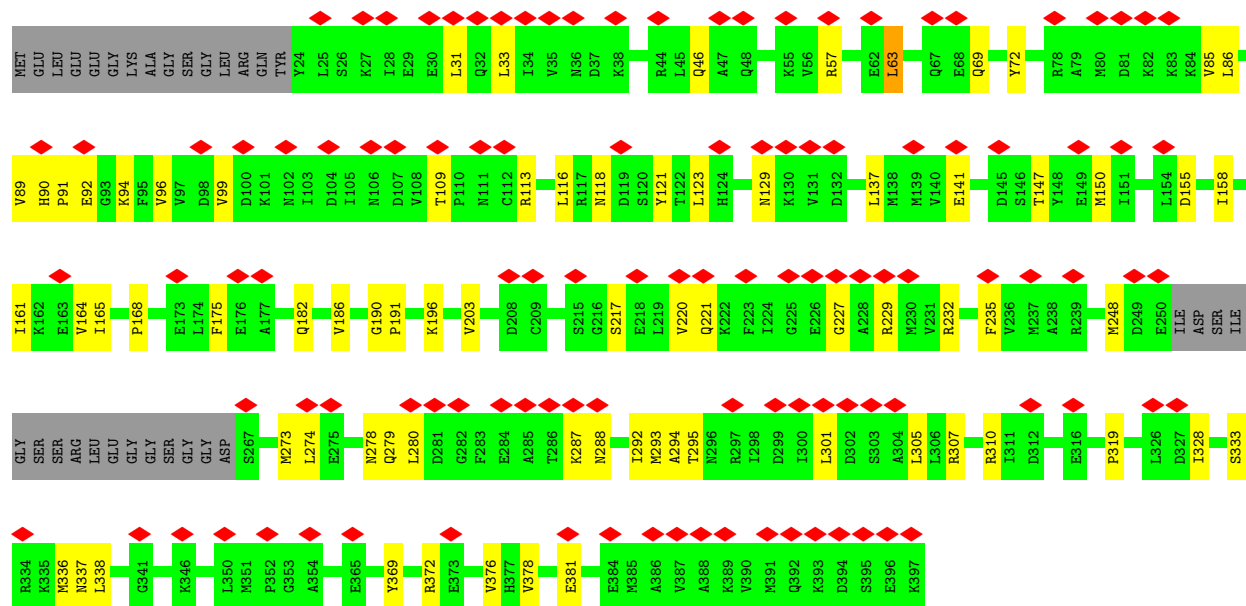
• Molecule 29: 26S proteasome regulatory subunit 6A





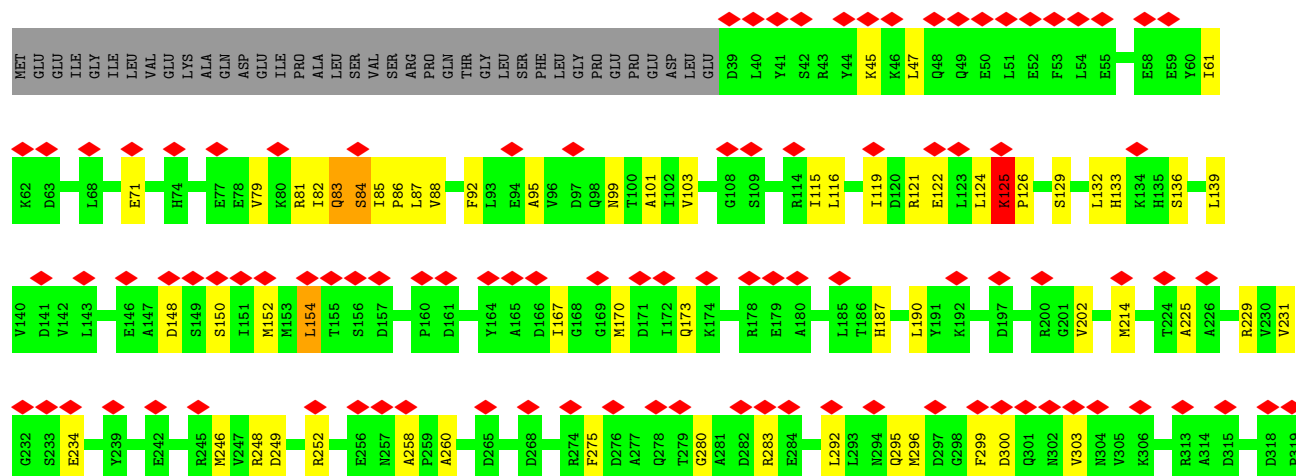
• Molecule 30: 26S proteasome regulatory subunit 8

Chain C: 29% 73% 19% 8%



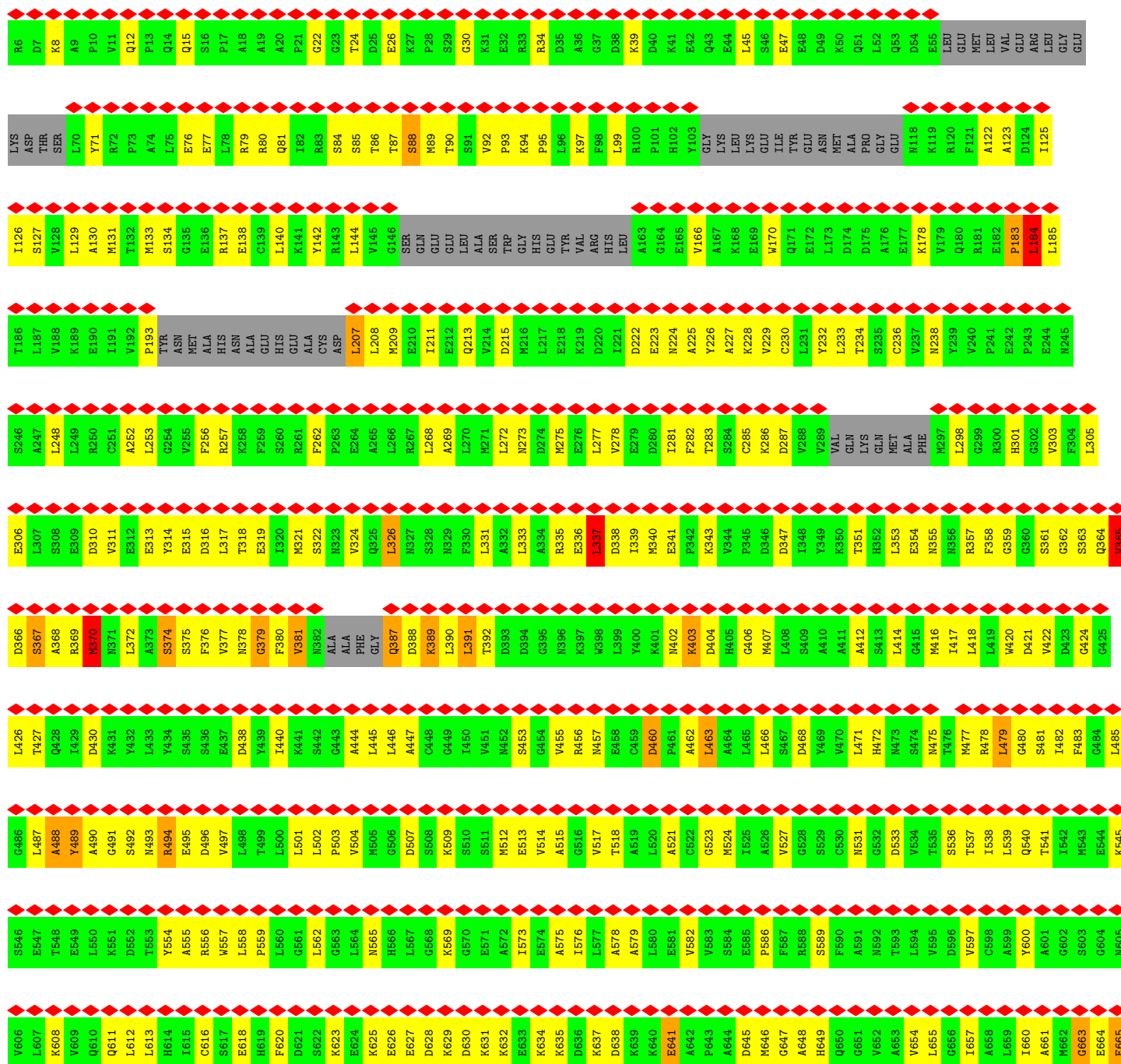
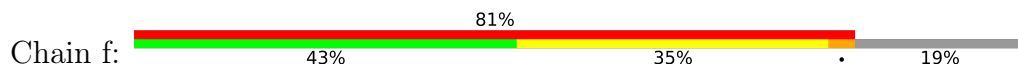
• Molecule 31: 26S proteasome regulatory subunit 6B

Chain D: 33% 70% 19% 9%





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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	230602	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.025	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.75, 0.75, 0.75	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	G	0.39	0/1859	0.91	4/2523 (0.2%)
1	g	0.37	0/1859	0.85	2/2523 (0.1%)
2	H	0.39	0/1743	0.82	2/2372 (0.1%)
2	h	0.36	0/1743	0.81	2/2372 (0.1%)
3	I	0.45	0/1942	1.05	7/2628 (0.3%)
3	i	0.46	0/1942	1.11	11/2628 (0.4%)
4	J	0.46	0/1728	1.04	11/2358 (0.5%)
4	j	0.44	0/1728	1.03	11/2358 (0.5%)
5	K	0.49	1/1747 (0.1%)	1.00	5/2364 (0.2%)
5	k	0.39	0/1747	0.96	3/2364 (0.1%)
6	L	0.43	0/1885	0.85	1/2552 (0.0%)
6	l	0.38	0/1885	0.85	3/2552 (0.1%)
7	M	0.44	0/1891	1.00	6/2552 (0.2%)
7	m	0.42	0/1891	0.99	11/2552 (0.4%)
8	N	0.39	0/1454	0.81	1/1967 (0.1%)
8	n	0.43	0/1454	0.88	5/1967 (0.3%)
9	O	0.38	0/1670	0.77	1/2265 (0.0%)
9	o	0.41	0/1670	0.79	1/2265 (0.0%)
10	P	0.38	0/1614	0.72	2/2177 (0.1%)
10	p	0.37	0/1614	0.66	0/2177
11	Q	0.48	0/1603	0.99	6/2174 (0.3%)
11	q	0.46	0/1603	0.97	5/2174 (0.2%)
12	R	0.39	0/1579	0.64	1/2134 (0.0%)
12	r	0.37	0/1579	0.62	1/2134 (0.0%)
13	S	0.39	0/1671	0.65	0/2253
13	s	0.38	0/1671	0.68	0/2253
14	T	0.40	0/1700	0.72	1/2305 (0.0%)
14	t	0.37	0/1700	0.71	2/2305 (0.1%)
15	U	0.27	0/6396	0.62	0/8646
16	V	0.35	0/3929	0.77	1/5309 (0.0%)
17	W	0.31	0/3751	0.76	5/5042 (0.1%)
18	X	0.27	0/3053	0.61	0/4115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	Y	0.31	0/3173	0.74	4/4273 (0.1%)
20	Z	0.32	0/2324	0.77	8/3150 (0.3%)
21	a	0.30	0/3053	0.71	2/4133 (0.0%)
22	b	0.28	0/1478	0.71	0/2001
23	c	0.35	0/2302	0.86	9/3110 (0.3%)
24	d	0.34	0/2162	0.89	13/2919 (0.4%)
25	e	0.30	0/338	0.84	0/450
26	B	0.31	0/2756	0.66	4/3727 (0.1%)
27	A	0.33	0/2940	0.66	2/3972 (0.1%)
28	E	0.31	0/2904	0.62	0/3924
29	F	0.32	0/2896	0.64	2/3912 (0.1%)
30	C	0.31	0/2857	0.64	0/3844
31	D	0.32	0/3089	0.74	7/4168 (0.2%)
32	f	0.33	1/5393 (0.0%)	0.87	19/7271 (0.3%)
All	All	0.36	2/102966 (0.0%)	0.80	181/139214 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	g	0	1
3	I	0	1
3	i	0	1
4	J	0	1
4	j	0	1
5	K	0	1
15	U	0	1
16	V	0	2
17	W	0	2
20	Z	0	3
21	a	0	1
22	b	0	1
23	c	0	3
24	d	0	1
26	B	0	3
27	A	0	2
28	E	0	1
29	F	0	2
31	D	0	5
All	All	0	33

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	15	PHE	C-N	-6.78	1.21	1.33
32	f	494	ARG	CA-C	5.20	1.59	1.52

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	30	ILE	N-CA-C	12.30	124.39	106.55
32	f	488	ALA	N-CA-C	10.54	122.85	111.36
3	I	105	ILE	N-CA-C	9.83	117.08	108.63
1	G	223	GLU	N-CA-C	-9.31	104.00	114.62
7	M	202	ASP	CA-C-N	9.21	139.14	121.54
7	M	202	ASP	C-N-CA	9.21	139.14	121.54
27	A	161	VAL	N-CA-C	-9.00	104.71	113.53
29	F	432	LYS	CA-C-N	8.87	137.66	121.70
29	F	432	LYS	C-N-CA	8.87	137.66	121.70
17	W	89	LEU	CA-CB-CG	8.56	146.28	116.30
3	i	105	ILE	N-CA-C	8.53	115.97	108.63
24	d	234	ASP	CA-C-N	8.51	137.01	121.70
24	d	234	ASP	C-N-CA	8.51	137.01	121.70
3	i	174	MET	CB-CG-SD	-8.39	87.54	112.70
31	D	124	LEU	CA-C-N	8.33	142.12	121.80
31	D	124	LEU	C-N-CA	8.33	142.12	121.80
5	K	58	LEU	CA-CB-CG	8.15	144.81	116.30
20	Z	222	ILE	CA-C-N	8.01	136.84	121.54
20	Z	222	ILE	C-N-CA	8.01	136.84	121.54
24	d	256	ILE	N-CA-C	7.94	125.86	109.34
5	k	58	LEU	CA-CB-CG	7.82	143.65	116.30
1	G	134	LEU	N-CA-C	7.28	120.11	111.02
1	g	223	GLU	N-CA-C	-7.27	106.34	114.62
7	M	196	ILE	CG1-CB-CG2	-7.21	89.06	110.70
3	I	39	ALA	CA-C-N	7.18	135.26	121.54
3	I	39	ALA	C-N-CA	7.18	135.26	121.54
20	Z	221	PRO	CA-C-N	7.14	134.83	121.97
20	Z	221	PRO	C-N-CA	7.14	134.83	121.97
32	f	493	ASN	N-CA-C	-7.00	95.88	110.80
31	D	83	GLN	CA-C-N	7.00	134.91	121.54
31	D	83	GLN	C-N-CA	7.00	134.91	121.54
32	f	472	HIS	CA-C-N	6.94	130.44	120.79
32	f	472	HIS	C-N-CA	6.94	130.44	120.79
32	f	493	ASN	CA-C-N	-6.88	111.13	120.82
32	f	493	ASN	C-N-CA	-6.88	111.13	120.82
23	c	155	VAL	CA-C-N	6.79	133.92	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	155	VAL	C-N-CA	6.79	133.92	121.70
26	B	167	THR	CA-C-N	6.77	133.88	121.70
26	B	167	THR	C-N-CA	6.77	133.88	121.70
11	Q	187	GLY	N-CA-C	6.77	118.25	111.21
5	K	20	ARG	CA-C-N	6.65	134.25	121.54
5	K	20	ARG	C-N-CA	6.65	134.25	121.54
23	c	187	PRO	N-CA-C	6.64	126.14	112.47
3	i	39	ALA	CA-C-N	6.64	134.22	121.54
3	i	39	ALA	C-N-CA	6.64	134.22	121.54
4	j	198	VAL	N-CA-C	-6.59	99.60	108.96
11	Q	102	LEU	CA-C-N	6.57	130.68	120.75
11	Q	102	LEU	C-N-CA	6.57	130.68	120.75
7	m	202	ASP	CA-C-N	6.50	133.96	121.54
7	m	202	ASP	C-N-CA	6.50	133.96	121.54
3	I	220	ASN	CA-C-N	-6.42	108.83	121.41
3	I	220	ASN	C-N-CA	-6.42	108.83	121.41
24	d	255	MET	CA-C-N	6.39	133.48	121.97
24	d	255	MET	C-N-CA	6.39	133.48	121.97
8	N	127	ILE	N-CA-CB	-6.38	103.86	111.90
7	m	176	ILE	N-CA-C	-6.37	104.29	110.72
32	f	492	SER	N-CA-C	-6.34	104.36	111.28
8	n	127	ILE	N-CA-CB	-6.30	103.97	111.90
5	k	20	ARG	CA-C-N	6.24	133.46	121.54
5	k	20	ARG	C-N-CA	6.24	133.46	121.54
11	q	102	LEU	CA-C-N	6.23	131.74	121.39
11	q	102	LEU	C-N-CA	6.23	131.74	121.39
4	J	198	VAL	N-CA-C	-6.20	100.16	108.96
7	m	196	ILE	CG1-CB-CG2	-6.19	92.14	110.70
32	f	663	GLY	N-CA-C	6.13	121.37	110.95
32	f	370	MET	N-CA-C	-6.10	104.71	111.36
32	f	324	VAL	CA-C-N	6.06	133.12	121.54
32	f	324	VAL	C-N-CA	6.06	133.12	121.54
23	c	187	PRO	CA-C-N	6.06	133.12	121.54
23	c	187	PRO	C-N-CA	6.06	133.12	121.54
24	d	32	GLU	CA-C-N	-6.05	114.27	121.90
24	d	32	GLU	C-N-CA	-6.05	114.27	121.90
10	P	31	GLN	N-CA-C	6.02	123.63	110.80
6	L	89	ARG	CA-CB-CG	6.00	126.10	114.10
12	r	166	ARG	CG-CD-NE	5.97	125.14	112.00
32	f	489	TYR	N-CA-C	5.97	118.49	109.23
3	i	220	ASN	CA-C-N	-5.96	109.72	121.41
3	i	220	ASN	C-N-CA	-5.96	109.72	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	j	50	VAL	CA-C-N	-5.96	112.95	122.66
4	j	50	VAL	C-N-CA	-5.96	112.95	122.66
7	m	182	LYS	N-CA-C	-5.94	104.16	111.40
11	Q	101	ASN	CA-C-N	-5.90	114.37	122.93
11	Q	101	ASN	C-N-CA	-5.90	114.37	122.93
11	q	101	ASN	CA-C-N	-5.89	112.55	122.92
11	q	101	ASN	C-N-CA	-5.89	112.55	122.92
2	h	39	LYS	CA-C-N	-5.89	112.62	122.92
2	h	39	LYS	C-N-CA	-5.89	112.62	122.92
24	d	253	LEU	CA-C-N	5.88	128.48	120.54
24	d	253	LEU	C-N-CA	5.88	128.48	120.54
24	d	198	LEU	CA-C-N	5.88	132.76	121.54
24	d	198	LEU	C-N-CA	5.88	132.76	121.54
6	l	89	ARG	CA-CB-CG	5.85	125.81	114.10
12	R	166	ARG	CG-CD-NE	5.84	124.86	112.00
4	J	198	VAL	CA-C-N	5.83	132.46	121.97
4	J	198	VAL	C-N-CA	5.83	132.46	121.97
23	c	189	ILE	N-CA-C	-5.83	97.22	109.34
7	m	231	ILE	CA-C-N	5.83	132.67	121.54
7	m	231	ILE	C-N-CA	5.83	132.67	121.54
32	f	365	VAL	N-CA-C	5.80	121.40	109.34
20	Z	218	GLY	CA-C-N	5.79	132.60	121.54
20	Z	218	GLY	C-N-CA	5.79	132.60	121.54
4	j	198	VAL	CA-C-N	5.78	132.38	121.97
4	j	198	VAL	C-N-CA	5.78	132.38	121.97
11	q	101	ASN	N-CA-C	5.77	118.27	110.88
5	K	224	GLN	N-CA-C	-5.76	98.53	110.80
16	V	27	PRO	N-CA-C	5.76	117.72	110.70
8	n	126	ALA	CA-C-N	5.75	130.84	123.13
8	n	126	ALA	C-N-CA	5.75	130.84	123.13
32	f	374	SER	CA-C-N	-5.69	112.65	120.28
32	f	374	SER	C-N-CA	-5.69	112.65	120.28
4	J	199	VAL	N-CA-C	5.68	121.15	109.34
8	n	92	GLU	N-CA-C	5.65	118.21	111.71
23	c	229	LEU	CA-C-N	5.65	132.32	121.54
23	c	229	LEU	C-N-CA	5.65	132.32	121.54
4	j	199	VAL	N-CA-C	5.64	121.08	109.34
4	j	8	THR	CA-C-N	5.60	131.66	122.64
4	j	8	THR	C-N-CA	5.60	131.66	122.64
32	f	379	GLY	CA-C-N	-5.59	113.55	122.66
32	f	379	GLY	C-N-CA	-5.59	113.55	122.66
4	J	203	GLY	N-CA-C	-5.59	107.28	115.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	231	ILE	CA-C-N	5.58	132.20	121.54
7	M	231	ILE	C-N-CA	5.58	132.20	121.54
19	Y	63	TRP	CA-C-N	5.58	129.19	120.82
19	Y	63	TRP	C-N-CA	5.58	129.19	120.82
11	Q	131	ALA	N-CA-C	5.58	116.74	108.60
26	B	319	PHE	CA-C-N	5.58	130.74	122.82
26	B	319	PHE	C-N-CA	5.58	130.74	122.82
17	W	135	LYS	CA-C-N	5.57	131.99	121.97
17	W	135	LYS	C-N-CA	5.57	131.99	121.97
3	I	77	ALA	N-CA-C	-5.57	99.19	108.32
3	I	38	LEU	CA-CB-CG	5.52	135.62	116.30
7	M	176	ILE	N-CA-C	-5.52	105.15	110.72
3	i	219	GLU	N-CA-C	-5.51	100.91	109.72
32	f	337	LEU	N-CA-C	5.50	122.51	110.80
3	i	163	CYS	CA-C-N	-5.49	112.08	121.97
3	i	163	CYS	C-N-CA	-5.49	112.08	121.97
3	i	39	ALA	N-CA-C	-5.49	99.37	108.75
2	H	39	LYS	CA-C-N	-5.47	113.84	122.76
2	H	39	LYS	C-N-CA	-5.47	113.84	122.76
4	J	197	GLU	CA-C-N	5.45	130.35	122.77
4	J	197	GLU	C-N-CA	5.45	130.35	122.77
4	j	176	TYR	CA-CB-CG	5.45	123.70	113.90
4	j	197	GLU	CA-C-N	5.44	130.33	122.77
4	j	197	GLU	C-N-CA	5.44	130.33	122.77
5	K	101	PHE	CA-CB-CG	-5.44	108.36	113.80
8	n	29	ARG	N-CA-C	-5.40	105.82	112.90
4	J	8	THR	CA-C-N	5.38	131.31	122.64
4	J	8	THR	C-N-CA	5.38	131.31	122.64
31	D	125	LYS	N-CA-C	5.33	121.60	109.81
14	t	179	ARG	CB-CA-C	-5.33	102.87	111.18
17	W	90	LEU	CA-C-N	5.32	131.71	121.54
17	W	90	LEU	C-N-CA	5.32	131.71	121.54
24	d	229	GLN	CA-C-N	5.28	131.63	121.54
24	d	229	GLN	C-N-CA	5.28	131.63	121.54
9	O	187	ARG	CA-CB-CG	5.26	124.62	114.10
14	t	179	ARG	CA-CB-CG	5.25	124.60	114.10
7	m	62	SER	CA-C-N	5.24	131.54	121.54
7	m	62	SER	C-N-CA	5.24	131.54	121.54
23	c	188	SER	N-CA-C	-5.20	99.72	110.80
1	G	159	TYR	CA-C-N	-5.18	112.78	121.39
1	G	159	TYR	C-N-CA	-5.18	112.78	121.39
14	T	100	ARG	CB-CG-CD	5.17	123.20	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	o	187	ARG	CG-CD-NE	5.16	123.36	112.00
19	Y	207	THR	CA-C-N	5.14	129.58	121.56
19	Y	207	THR	C-N-CA	5.14	129.58	121.56
3	i	127	LYS	N-CA-C	-5.14	102.59	110.14
6	l	225	ASP	CA-C-N	5.13	131.34	121.54
6	l	225	ASP	C-N-CA	5.13	131.34	121.54
27	A	426	THR	N-CA-C	5.13	118.68	110.73
21	a	186	LYS	CA-C-N	5.11	131.31	121.54
21	a	186	LYS	C-N-CA	5.11	131.31	121.54
20	Z	219	LYS	CA-C-N	5.07	134.16	121.80
20	Z	219	LYS	C-N-CA	5.07	134.16	121.80
7	m	183	GLU	CA-C-N	-5.07	116.01	123.00
7	m	183	GLU	C-N-CA	-5.07	116.01	123.00
1	g	159	TYR	CA-CB-CG	5.04	122.97	113.90
31	D	154	LEU	CA-C-N	5.04	131.17	121.54
31	D	154	LEU	C-N-CA	5.04	131.17	121.54
32	f	404	ASP	N-CA-C	5.02	117.14	111.02
4	J	138	PHE	CA-C-N	5.01	129.66	122.40
4	J	138	PHE	C-N-CA	5.01	129.66	122.40

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	A	311	PRO	Peptide
27	A	333	ARG	Sidechain
26	B	167	THR	Peptide
26	B	179	ALA	Peptide
26	B	355	LEU	Peptide
31	D	125	LYS	Peptide
31	D	150	SER	Peptide
31	D	258	ALA	Peptide
31	D	354	LEU	Peptide
31	D	84	SER	Peptide
28	E	291	ARG	Sidechain
29	F	343	LEU	Peptide
29	F	433	ALA	Peptide
3	I	184	MET	Peptide
4	J	199	VAL	Mainchain
5	K	121	LEU	Peptide
15	U	699	THR	Peptide
16	V	263	LEU	Peptide

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Mol	Chain	Res	Type	Group
16	V	317	PRO	Peptide
17	W	137	TYR	Peptide
17	W	313	GLU	Peptide
20	Z	183	THR	Peptide
20	Z	219	LYS	Peptide
20	Z	221	PRO	Peptide
21	a	165	THR	Peptide
22	b	21	PHE	Peptide
23	c	187	PRO	Peptide
23	c	189	ILE	Peptide
23	c	79	GLY	Peptide
24	d	255	MET	Peptide
1	g	222	VAL	Peptide
3	i	40	ASN	Mainchain
4	j	199	VAL	Mainchain

5.2 Too-close contacts

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	G	1826	0	1796	23	0
1	g	1826	0	1796	24	0
2	H	1708	0	1594	23	0
2	h	1708	0	1594	21	0
3	I	1912	0	1851	39	0
3	i	1912	0	1851	39	0
4	J	1704	0	1517	31	0
4	j	1704	0	1517	28	0
5	K	1722	0	1673	39	0
5	k	1722	0	1673	37	0
6	L	1850	0	1822	47	0
6	l	1850	0	1822	38	0
7	M	1856	0	1814	51	0
7	m	1856	0	1814	53	0
8	N	1430	0	1398	20	0
8	n	1430	0	1398	21	0
9	O	1643	0	1644	25	0
9	o	1643	0	1644	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	P	1585	0	1598	22	0
10	p	1585	0	1598	24	0
11	Q	1570	0	1547	35	0
11	q	1570	0	1547	33	0
12	R	1548	0	1499	18	0
12	r	1548	0	1499	17	0
13	S	1641	0	1618	19	0
13	s	1641	0	1618	21	0
14	T	1667	0	1628	20	0
14	t	1667	0	1628	25	0
15	U	6287	0	6338	132	0
16	V	3852	0	3893	102	0
17	W	3703	0	3822	107	0
18	X	3009	0	3113	56	0
19	Y	3115	0	3120	58	0
20	Z	2281	0	2312	65	0
21	a	2995	0	3012	61	0
22	b	1458	0	1505	34	0
23	c	2260	0	2276	50	0
24	d	2116	0	2146	62	0
25	e	334	0	294	22	0
26	B	2720	0	2686	33	0
27	A	2894	0	2847	63	0
28	E	2860	0	2828	56	0
29	F	2858	0	2853	40	0
30	C	2820	0	2927	46	0
31	D	3039	0	3076	65	0
32	f	5319	0	5329	461	0
33	c	1	0	0	0	0
34	A	31	0	12	2	0
34	B	31	0	12	3	0
34	C	31	0	12	2	0
34	D	31	0	12	7	0
34	E	31	0	12	7	0
34	F	31	0	12	5	0
All	All	101431	0	100447	2101	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 10.

All (2101) 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)
32:f:494:ARG:HD3	32:f:496:ASP:OD1	1.26	1.33
32:f:753:ALA:O	32:f:754:LYS:HE2	1.27	1.31
32:f:796:LEU:O	32:f:799:VAL:HG22	1.30	1.30
32:f:742:ALA:HA	32:f:745:LEU:CD2	1.66	1.26
31:D:214:MET:HE3	34:D:501:AGS:N7	1.51	1.22
32:f:376:PHE:CE1	32:f:798:THR:CG2	2.23	1.21
32:f:471:LEU:CG	32:f:509:LYS:HE3	1.73	1.18
32:f:696:LEU:HD13	32:f:752:HIS:CD2	1.80	1.17
32:f:311:VAL:HB	32:f:490:ALA:HB1	1.17	1.15
32:f:494:ARG:HE	32:f:495:GLU:N	1.44	1.14
32:f:692:LEU:HD12	32:f:748:LEU:HD21	1.19	1.14
32:f:389:LYS:CG	32:f:418:LEU:HD21	1.79	1.12
32:f:479:LEU:HD21	32:f:513:GLU:CB	1.80	1.12
32:f:479:LEU:CD2	32:f:513:GLU:HB2	1.79	1.11
32:f:494:ARG:NH2	32:f:495:GLU:HG2	1.64	1.11
32:f:494:ARG:HH21	32:f:495:GLU:HG2	1.02	1.10
32:f:376:PHE:CE1	32:f:798:THR:HG21	1.85	1.10
31:D:167:ILE:HA	31:D:214:MET:HE1	1.31	1.08
27:A:63:THR:CB	32:f:613:LEU:HD11	1.82	1.08
32:f:389:LYS:HG2	32:f:418:LEU:HD21	1.29	1.08
32:f:483:PHE:CE2	32:f:799:VAL:HB	1.88	1.08
32:f:692:LEU:HD12	32:f:748:LEU:CD2	1.82	1.08
32:f:471:LEU:HG	32:f:509:LYS:CE	1.83	1.08
32:f:742:ALA:O	32:f:745:LEU:HG	1.54	1.06
32:f:780:PRO:HB3	32:f:800:LEU:HA	1.37	1.06
32:f:471:LEU:HD12	32:f:509:LYS:CG	1.87	1.05
32:f:753:ALA:O	32:f:754:LYS:CE	2.08	1.02
32:f:494:ARG:CD	32:f:496:ASP:OD1	2.06	1.02
27:A:169:LYS:HE2	32:f:714:SER:HA	1.41	1.01
32:f:696:LEU:HD13	32:f:752:HIS:HD2	1.14	1.00
27:A:333:ARG:HH21	27:A:336:ARG:NH2	1.58	0.99
32:f:494:ARG:HG3	32:f:497:VAL:HG12	1.44	0.99
32:f:692:LEU:CD1	32:f:748:LEU:HD21	1.93	0.99
31:D:167:ILE:HG12	31:D:214:MET:SD	2.02	0.99
32:f:337:LEU:HD13	32:f:420:TRP:HZ3	1.26	0.98
32:f:479:LEU:HD21	32:f:513:GLU:HB2	0.99	0.98
32:f:742:ALA:HA	32:f:745:LEU:HD23	1.46	0.97
32:f:359:GLY:O	32:f:363:SER:HB3	1.63	0.97
32:f:372:LEU:HD11	32:f:406:GLY:HA3	1.47	0.96
32:f:780:PRO:CB	32:f:800:LEU:HA	1.96	0.96
32:f:224:ASN:O	32:f:228:LYS:HB3	1.66	0.95
31:D:214:MET:CE	34:D:501:AGS:N7	2.29	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:456:ARG:HB3	32:f:489:TYR:CE2	2.00	0.95
32:f:311:VAL:HB	32:f:490:ALA:CB	1.96	0.94
23:c:219:ASN:O	23:c:223:LYS:HB3	1.66	0.94
32:f:376:PHE:CD1	32:f:416:MET:HE1	2.01	0.94
32:f:95:PRO:O	32:f:99:LEU:HB2	1.67	0.94
32:f:494:ARG:HE	32:f:495:GLU:H	1.16	0.94
27:A:333:ARG:CZ	34:F:501:AGS:O1A	2.16	0.93
32:f:376:PHE:CE1	32:f:416:MET:HE1	2.03	0.93
32:f:471:LEU:HG	32:f:509:LYS:HE3	0.96	0.93
32:f:315:GLU:HG2	32:f:491:GLY:HA2	1.51	0.93
32:f:388:ASP:OD2	32:f:390:LEU:HB2	1.67	0.93
27:A:63:THR:CB	32:f:613:LEU:CD1	2.46	0.93
32:f:358:PHE:CZ	32:f:381:VAL:HG21	2.03	0.92
32:f:691:PRO:CB	32:f:749:ALA:HB2	1.99	0.91
32:f:376:PHE:CE1	32:f:798:THR:HB	2.06	0.90
27:A:333:ARG:HH21	27:A:336:ARG:CZ	1.84	0.90
32:f:366:ASP:OD1	32:f:367:SER:N	2.04	0.90
32:f:483:PHE:CZ	32:f:799:VAL:HB	2.06	0.90
32:f:369:ARG:HB3	32:f:370:MET:SD	2.13	0.89
32:f:311:VAL:CB	32:f:490:ALA:HB1	2.03	0.89
32:f:742:ALA:HA	32:f:745:LEU:HD21	1.53	0.89
27:A:322:ASN:OD1	27:A:323:ARG:HG2	1.72	0.89
32:f:363:SER:O	32:f:365:VAL:N	2.04	0.89
32:f:389:LYS:HG2	32:f:418:LEU:CD2	2.02	0.88
32:f:318:THR:O	32:f:322:SER:HB3	1.74	0.88
32:f:376:PHE:CE1	32:f:798:THR:CB	2.55	0.88
17:W:82:LEU:O	17:W:86:ASN:HB2	1.72	0.88
32:f:378:ASN:HB3	32:f:391:LEU:HG	1.56	0.88
32:f:122:ALA:O	32:f:126:ILE:HB	1.72	0.88
32:f:223:GLU:O	32:f:227:ALA:HB3	1.73	0.88
32:f:337:LEU:HD13	32:f:420:TRP:CZ3	2.10	0.87
32:f:378:ASN:HB3	32:f:391:LEU:CG	2.05	0.87
32:f:376:PHE:HE1	32:f:798:THR:CG2	1.89	0.86
32:f:691:PRO:HB2	32:f:749:ALA:HB2	1.58	0.85
32:f:123:ALA:O	32:f:127:SER:HB2	1.76	0.85
32:f:126:ILE:O	32:f:130:ALA:HB3	1.77	0.85
32:f:696:LEU:CD1	32:f:752:HIS:HD2	1.90	0.85
32:f:129:LEU:O	32:f:133:MET:HB3	1.75	0.85
32:f:494:ARG:HH21	32:f:495:GLU:CG	1.88	0.84
32:f:471:LEU:HD12	32:f:509:LYS:HG2	1.58	0.84
32:f:88:SER:CB	32:f:92:VAL:HG23	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:301:HIS:O	32:f:305:LEU:HB2	1.77	0.83
32:f:714:SER:O	32:f:718:ASP:HB2	1.78	0.83
32:f:695:ALA:HB3	32:f:752:HIS:HB2	1.59	0.83
32:f:336:GLU:HG3	32:f:337:LEU:HD22	1.60	0.82
24:d:209:TYR:O	24:d:213:ARG:HB2	1.80	0.82
32:f:376:PHE:CZ	32:f:416:MET:SD	2.73	0.82
32:f:796:LEU:O	32:f:799:VAL:CG2	2.22	0.82
32:f:225:ALA:O	32:f:229:VAL:HB	1.79	0.82
32:f:376:PHE:HE1	32:f:798:THR:CB	1.91	0.81
32:f:378:ASN:O	32:f:381:VAL:HG12	1.80	0.81
31:D:167:ILE:HA	31:D:214:MET:CE	2.10	0.81
32:f:494:ARG:NE	32:f:495:GLU:N	2.26	0.81
32:f:376:PHE:CE1	32:f:416:MET:CE	2.64	0.81
27:A:417:ILE:O	27:A:421:ALA:HB2	1.80	0.81
3:i:49:ARG:HH12	3:i:212:GLU:HB2	1.46	0.80
32:f:88:SER:HB2	32:f:92:VAL:HG23	1.63	0.80
32:f:742:ALA:C	32:f:745:LEU:HG	2.06	0.80
17:W:98:LYS:O	17:W:102:ALA:HB3	1.81	0.80
32:f:503:PRO:O	32:f:507:ASP:HB2	1.82	0.80
31:D:167:ILE:HG12	31:D:214:MET:CE	2.12	0.79
32:f:635:LYS:HZ2	32:f:641:GLU:HG3	1.47	0.79
32:f:479:LEU:CD2	32:f:513:GLU:CB	2.50	0.79
32:f:471:LEU:HD12	32:f:509:LYS:HG3	1.62	0.79
32:f:456:ARG:HB3	32:f:489:TYR:HE2	1.47	0.78
32:f:612:LEU:O	32:f:616:CYS:HB2	1.83	0.78
32:f:745:LEU:HD12	32:f:746:ARG:N	1.99	0.78
32:f:494:ARG:HE	32:f:494:ARG:C	1.92	0.78
32:f:691:PRO:HB3	32:f:749:ALA:HB2	1.66	0.78
32:f:695:ALA:C	32:f:752:HIS:HB3	2.09	0.77
27:A:169:LYS:CE	32:f:714:SER:HA	2.15	0.77
32:f:232:TYR:O	32:f:236:CYS:HB2	1.82	0.77
32:f:392:THR:HG22	32:f:417:ILE:CD1	2.14	0.77
32:f:796:LEU:HG	32:f:799:VAL:HG21	1.66	0.77
32:f:784:ASP:HB2	32:f:800:LEU:HD21	1.66	0.77
32:f:184:LEU:HG	32:f:185:LEU:N	1.98	0.76
32:f:376:PHE:CE1	32:f:798:THR:HG22	2.20	0.76
32:f:635:LYS:HZ3	32:f:641:GLU:CD	1.94	0.76
21:a:64:ILE:O	21:a:68:GLU:HB2	1.86	0.76
32:f:494:ARG:NE	32:f:495:GLU:H	1.80	0.76
32:f:478:ARG:HD3	32:f:504:VAL:HG13	1.68	0.75
32:f:635:LYS:NZ	32:f:641:GLU:CG	2.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:376:PHE:HE1	32:f:798:THR:HG21	1.49	0.75
32:f:389:LYS:CG	32:f:418:LEU:CD2	2.63	0.75
32:f:684:PRO:O	32:f:688:ARG:HB2	1.87	0.75
6:l:101:ARG:HH12	6:l:104:PRO:HD3	1.51	0.75
32:f:358:PHE:O	32:f:362:GLY:HA3	1.87	0.75
31:D:133:HIS:HD2	31:D:136:SER:H	1.35	0.75
32:f:675:PHE:O	32:f:679:LEU:HB2	1.85	0.75
7:m:67:PHE:HB2	7:m:75:MET:HB2	1.69	0.75
15:U:140:ARG:O	15:U:144:ASP:HB2	1.87	0.74
32:f:471:LEU:CD1	32:f:509:LYS:CE	2.65	0.74
21:a:8:LEU:O	21:a:12:GLN:HB2	1.86	0.74
32:f:664:GLU:HB3	32:f:696:LEU:HG	1.69	0.74
32:f:211:ILE:O	32:f:215:ASP:HB2	1.88	0.74
32:f:392:THR:CG2	32:f:417:ILE:HG21	2.18	0.74
32:f:376:PHE:CZ	32:f:798:THR:HB	2.22	0.73
32:f:357:ARG:O	32:f:361:SER:HB2	1.87	0.73
29:F:68:ALA:O	29:F:72:LYS:HB2	1.89	0.73
32:f:494:ARG:CG	32:f:497:VAL:HG12	2.16	0.73
32:f:742:ALA:HA	32:f:745:LEU:CG	2.18	0.72
32:f:389:LYS:CD	32:f:418:LEU:HD21	2.20	0.72
32:f:691:PRO:HG2	32:f:745:LEU:HD13	1.70	0.72
8:N:166:ARG:NH2	8:n:140:ASP:OD2	2.22	0.72
5:K:91:LYS:HE2	5:K:119:LEU:HD11	1.72	0.72
21:a:247:ARG:HH22	21:a:269:LEU:HD22	1.55	0.72
32:f:370:MET:SD	32:f:370:MET:N	2.57	0.72
4:j:114:LEU:O	4:j:118:TYR:HB2	1.90	0.71
27:A:333:ARG:NH2	27:A:336:ARG:NH2	2.36	0.71
10:P:149:MET:HE3	13:s:147:PRO:HB2	1.72	0.71
11:Q:118:MET:HE1	11:Q:124:LEU:HD23	1.72	0.71
21:a:368:GLU:O	21:a:372:HIS:HB2	1.90	0.71
32:f:311:VAL:O	32:f:490:ALA:O	2.09	0.71
32:f:311:VAL:CG2	32:f:527:VAL:O	2.39	0.71
16:V:394:LEU:O	16:V:398:LEU:HB2	1.90	0.71
3:I:64:LYS:HG3	3:I:76:VAL:HG12	1.71	0.71
7:m:175:GLU:HG3	7:m:196:ILE:HG21	1.72	0.71
32:f:222:ASP:O	32:f:226:TYR:HB3	1.91	0.71
32:f:494:ARG:NH2	32:f:495:GLU:CG	2.48	0.71
4:j:72:ALA:HB3	4:j:132:LEU:HB2	1.72	0.70
32:f:88:SER:HB3	32:f:92:VAL:HG23	1.72	0.70
32:f:625:LYS:O	32:f:629:LYS:HB2	1.91	0.70
32:f:315:GLU:CG	32:f:491:GLY:HA2	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:337:LEU:CD1	32:f:420:TRP:CZ3	2.74	0.70
32:f:389:LYS:HG2	32:f:418:LEU:HD11	1.72	0.70
7:M:175:GLU:HG3	7:M:196:ILE:HG21	1.73	0.70
16:V:159:LEU:HD13	16:V:178:SER:HB2	1.74	0.70
32:f:797:LEU:O	32:f:800:LEU:HD13	1.91	0.70
16:V:415:SER:HB2	19:Y:346:LYS:HB3	1.73	0.70
24:d:203:PRO:HG2	24:d:206:MET:H	1.57	0.70
5:k:45:GLY:HA3	5:k:221:GLN:HG3	1.72	0.70
11:q:118:MET:HE1	11:q:124:LEU:HD23	1.74	0.69
32:f:130:ALA:O	32:f:134:SER:HB3	1.92	0.69
19:Y:92:GLU:HB3	19:Y:100:ILE:HD11	1.74	0.69
30:C:69:GLN:HB3	30:C:118:ASN:HD21	1.57	0.69
32:f:392:THR:HG22	32:f:417:ILE:HD12	1.74	0.69
32:f:635:LYS:HZ2	32:f:641:GLU:CG	2.04	0.69
32:f:688:ARG:HA	32:f:745:LEU:HD22	1.75	0.69
3:I:49:ARG:HH12	3:I:212:GLU:HB2	1.57	0.69
5:K:177:ALA:O	5:K:181:LEU:HB2	1.93	0.69
16:V:311:ASN:O	16:V:315:LYS:HB2	1.92	0.69
17:W:190:MET:HB2	17:W:202:THR:HG23	1.75	0.69
24:d:250:ALA:O	24:d:254:GLU:HB2	1.93	0.69
17:W:441:LYS:HD2	17:W:444:HIS:HE1	1.58	0.69
21:a:19:PRO:HA	21:a:22:TRP:HB2	1.74	0.68
20:Z:35:VAL:HB	20:Z:97:THR:HB	1.74	0.68
32:f:376:PHE:CD1	32:f:798:THR:HG21	2.26	0.68
32:f:664:GLU:O	32:f:665:GLU:O	2.10	0.68
32:f:695:ALA:HB3	32:f:752:HIS:CB	2.23	0.68
4:J:48:LYS:H	4:J:205:ASN:HB3	1.59	0.68
32:f:625:LYS:HA	32:f:657:ILE:HD11	1.75	0.68
5:K:99:HIS:HB2	5:K:107:MET:HE3	1.75	0.68
6:L:73:SER:HB3	6:L:133:LEU:HB2	1.75	0.68
32:f:494:ARG:HD3	32:f:496:ASP:CG	2.16	0.68
7:M:76:ALA:HB3	7:M:136:MET:HB2	1.76	0.68
19:Y:160:ASN:HA	19:Y:163:LYS:HB2	1.75	0.68
24:d:234:ASP:HA	24:d:236:THR:H	1.57	0.68
6:L:148:CYS:HG	6:L:150:SER:HG	1.37	0.67
7:m:37:ILE:HD11	7:m:193:VAL:HG13	1.76	0.67
32:f:311:VAL:HG21	32:f:527:VAL:O	1.94	0.67
4:J:7:ILE:HG12	4:J:123:GLY:HA2	1.75	0.67
13:S:27:THR:HB	13:S:40:SER:H	1.60	0.67
16:V:285:TRP:HD1	16:V:315:LYS:HE2	1.59	0.67
21:a:122:LYS:HD3	21:a:131:THR:HG22	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:332:ASN:ND2	34:B:501:AGS:S1G	2.67	0.67
32:f:353:LEU:HG	32:f:387:GLN:HG3	1.75	0.67
2:h:4:ARG:NH2	7:m:126:SER:OG	2.28	0.67
11:q:117:TYR:HB3	11:q:125:ALA:HB3	1.76	0.67
11:Q:57:ALA:O	11:Q:61:GLN:HB3	1.95	0.67
14:T:180:ASP:HB3	14:T:183:SER:HB3	1.76	0.67
32:f:372:LEU:HD23	32:f:372:LEU:C	2.20	0.67
5:K:219:THR:HB	5:K:221:GLN:HE22	1.58	0.67
7:M:141:SER:HB3	7:M:144:ASP:HB2	1.77	0.67
13:S:147:PRO:HB2	10:p:149:MET:HE3	1.75	0.67
20:Z:45:LYS:HB3	20:Z:47:VAL:HG12	1.76	0.67
32:f:315:GLU:HG2	32:f:491:GLY:CA	2.24	0.67
32:f:367:SER:HB3	32:f:370:MET:SD	2.34	0.67
32:f:372:LEU:HD23	32:f:372:LEU:O	1.93	0.67
32:f:376:PHE:CE1	32:f:416:MET:SD	2.88	0.67
32:f:800:LEU:HD12	32:f:800:LEU:N	2.10	0.67
18:X:406:ASN:HA	18:X:409:LYS:HD3	1.76	0.66
22:b:161:ASN:HB2	22:b:165:GLY:HA3	1.77	0.66
4:j:92:GLN:HG3	11:q:62:LYS:HD2	1.77	0.66
32:f:578:ALA:O	32:f:582:VAL:HB	1.95	0.66
15:U:519:VAL:HG23	15:U:520:MET:HG2	1.78	0.66
32:f:478:ARG:O	32:f:482:ILE:HB	1.94	0.66
11:q:57:ALA:O	11:q:61:GLN:HB3	1.95	0.66
18:X:417:LYS:HE2	19:Y:383:LEU:HB3	1.77	0.66
32:f:337:LEU:HD11	32:f:422:VAL:HG21	1.77	0.66
32:f:460:ASP:N	32:f:460:ASP:OD1	2.29	0.66
11:Q:117:TYR:HB3	11:Q:125:ALA:HB3	1.77	0.66
19:Y:276:ALA:HA	25:e:60:LEU:HD11	1.78	0.66
7:m:141:SER:HB3	7:m:144:ASP:HB2	1.77	0.66
32:f:628:ASP:HB2	32:f:657:ILE:HD13	1.77	0.66
4:j:154:HIS:NE2	5:k:59:MET:SD	2.70	0.66
5:k:76:CYS:SG	5:k:77:ALA:N	2.69	0.66
13:s:13:LEU:HD11	13:s:149:LEU:HD11	1.77	0.66
15:U:662:GLY:HA2	15:U:696:ILE:HD11	1.79	0.65
17:W:308:LEU:O	17:W:361:HIS:NE2	2.29	0.65
32:f:804:LEU:H	32:f:804:LEU:HD12	1.60	0.65
4:J:32:ALA:HB2	4:J:45:VAL:HG23	1.79	0.65
21:a:186:LYS:HB2	21:a:193:GLN:HE21	1.60	0.65
32:f:80:ARG:HB3	32:f:95:PRO:HB2	1.78	0.65
2:H:3:GLU:HG3	2:H:4:ARG:HG3	1.78	0.65
16:V:259:LEU:HD11	16:V:294:ARG:HD2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:64:LYS:HG3	3:i:76:VAL:HG12	1.78	0.65
3:i:123:GLN:NE2	4:j:118:TYR:OH	2.26	0.65
32:f:742:ALA:O	32:f:745:LEU:CG	2.38	0.65
15:U:187:LEU:HD22	31:D:45:LYS:HG2	1.78	0.65
20:Z:190:ARG:NH2	21:a:371:ALA:O	2.29	0.65
7:M:67:PHE:HB2	7:M:75:MET:HB2	1.77	0.65
13:S:13:LEU:HD11	13:S:149:LEU:HD11	1.79	0.65
5:k:91:LYS:HE2	5:k:119:LEU:HD11	1.77	0.65
5:k:99:HIS:HB2	5:k:107:MET:HE3	1.79	0.65
32:f:379:GLY:O	32:f:417:ILE:HG12	1.97	0.65
24:d:122:LEU:HB3	24:d:125:LYS:HB2	1.78	0.65
24:d:251:ARG:NH1	24:d:255:MET:SD	2.70	0.65
27:A:297:ARG:HH22	29:F:306:VAL:HG21	1.62	0.65
6:L:107:ARG:NH2	14:T:79:ASP:OD2	2.30	0.65
22:b:54:LEU:HD13	22:b:84:ILE:HG13	1.78	0.65
32:f:389:LYS:HG2	32:f:418:LEU:CG	2.27	0.65
32:f:804:LEU:HD12	32:f:804:LEU:N	2.12	0.65
1:G:158:GLY:O	2:H:84:ARG:NH2	2.30	0.64
5:K:76:CYS:SG	5:K:77:ALA:N	2.70	0.64
19:Y:32:ARG:HH12	19:Y:36:ALA:H	1.45	0.64
6:l:73:SER:HB3	6:l:133:LEU:HB2	1.78	0.64
6:L:186:GLU:HA	6:L:189:LYS:HG2	1.79	0.64
15:U:625:ILE:HG13	15:U:626:LEU:HG	1.79	0.64
1:g:158:GLY:O	2:h:84:ARG:NH2	2.31	0.64
6:l:186:GLU:HA	6:l:189:LYS:HG2	1.79	0.64
21:a:212:ASN:HD22	21:a:241:ASN:HA	1.63	0.64
28:E:97:ARG:NH1	28:E:114:GLU:OE1	2.30	0.64
32:f:93:PRO:HB2	32:f:137:ARG:HE	1.63	0.64
32:f:804:LEU:H	32:f:804:LEU:CD1	2.10	0.64
7:M:214:SER:OG	7:M:224:HIS:NE2	2.31	0.64
17:W:401:THR:HG23	17:W:402:ILE:HD12	1.78	0.64
32:f:664:GLU:HA	32:f:697:ILE:HA	1.80	0.64
18:X:141:LYS:HE3	18:X:179:ALA:HB1	1.80	0.64
15:U:11:LEU:HD21	24:d:77:GLN:HE21	1.61	0.64
13:s:27:THR:HB	13:s:40:SER:H	1.63	0.64
32:f:692:LEU:HG	32:f:752:HIS:CE1	2.32	0.64
9:O:164:PHE:O	13:s:38:ARG:NH2	2.30	0.64
15:U:155:LEU:O	15:U:158:ARG:NH1	2.31	0.64
4:j:38:ARG:HH12	4:j:182:GLU:HA	1.63	0.64
14:T:27:LEU:HD22	14:T:184:TYR:HB2	1.80	0.64
17:W:36:LYS:HG3	17:W:86:ASN:HD22	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:138:GLU:O	32:f:142:TYR:HB2	1.97	0.64
5:K:209:LYS:O	5:K:214:ASN:ND2	2.31	0.63
32:f:313:GLU:O	32:f:317:LEU:HB2	1.98	0.63
14:t:27:LEU:HD22	14:t:184:TYR:HB2	1.81	0.63
14:T:9:THR:O	14:T:41:ARG:NH2	2.31	0.63
15:U:771:PHE:HA	23:c:177:THR:HG22	1.81	0.63
32:f:483:PHE:CE2	32:f:799:VAL:CB	2.75	0.63
32:f:654:VAL:HA	32:f:657:ILE:HD12	1.81	0.63
4:J:72:ALA:HB3	4:J:132:LEU:HB2	1.81	0.63
16:V:337:LEU:O	16:V:401:ASN:ND2	2.32	0.63
9:o:161:ALA:O	9:o:165:ASN:ND2	2.31	0.63
32:f:366:ASP:O	32:f:367:SER:HB2	1.97	0.63
28:E:97:ARG:HH12	28:E:114:GLU:HB3	1.63	0.63
31:D:92:PHE:HA	31:D:103:VAL:HG12	1.80	0.63
32:f:494:ARG:HH21	32:f:495:GLU:H	1.46	0.63
15:U:188:MET:HG2	15:U:194:ARG:HB2	1.80	0.63
15:U:759:SER:HA	15:U:782:ALA:HA	1.81	0.63
28:E:317:ALA:HA	28:E:320:ILE:HD12	1.81	0.63
7:M:40:ARG:NH1	7:M:146:ALA:O	2.32	0.63
20:Z:98:GLY:HA3	20:Z:123:ILE:HG23	1.81	0.63
2:h:118:MET:HE2	2:h:151:PRO:HA	1.81	0.63
15:U:456:ASP:O	15:U:460:TYR:HB2	1.99	0.63
4:j:116:GLN:NE2	4:j:150:SER:O	2.32	0.63
32:f:339:ILE:HG23	32:f:340:MET:HG2	1.81	0.63
15:U:353:LEU:O	15:U:357:LYS:HB2	1.98	0.62
21:a:140:GLU:O	21:a:143:ASN:ND2	2.32	0.62
7:m:214:SER:OG	7:m:224:HIS:NE2	2.27	0.62
32:f:392:THR:HG23	32:f:417:ILE:HG21	1.81	0.62
5:K:85:ALA:HB2	5:K:139:VAL:HG21	1.80	0.62
6:L:196:ARG:HH21	6:L:239:ARG:HG3	1.64	0.62
19:Y:314:LEU:HD21	19:Y:319:MET:HE3	1.81	0.62
27:A:339:ARG:NH1	29:F:426:GLU:OE2	2.33	0.62
16:V:33:GLN:HE21	16:V:85:ALA:HA	1.65	0.62
31:D:83:GLN:HB3	31:D:87:LEU:HD11	1.81	0.62
6:L:50:LYS:HE2	6:L:61:LYS:HA	1.80	0.62
10:P:205:ASP:HB3	12:r:192:VAL:HG11	1.81	0.62
1:g:141:ILE:HG22	1:g:151:VAL:HG22	1.80	0.62
4:j:32:ALA:O	4:j:159:ASN:ND2	2.32	0.62
6:l:189:LYS:HZ2	6:l:193:ARG:HH12	1.46	0.62
28:E:177:GLY:HA3	29:F:344:ARG:HD3	1.81	0.62
16:V:224:LEU:O	16:V:228:ARG:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:66:GLU:OE2	2:h:91:ARG:NH2	2.33	0.62
4:j:32:ALA:HB2	4:j:45:VAL:HG23	1.82	0.62
4:J:92:GLN:HG3	11:Q:62:LYS:HD2	1.82	0.61
4:J:154:HIS:NE2	5:K:59:MET:SD	2.70	0.61
18:X:379:ASP:HB2	18:X:384:VAL:H	1.65	0.61
28:E:116:ASP:HB2	28:E:217:GLU:HG2	1.82	0.61
32:f:389:LYS:HD3	32:f:389:LYS:N	2.15	0.61
32:f:687:ARG:HH21	32:f:742:ALA:HB2	1.64	0.61
15:U:70:HIS:O	16:V:236:ARG:NH2	2.33	0.61
25:e:56:LEU:HB2	25:e:59:GLU:HB2	1.81	0.61
13:s:148:LEU:HD23	13:s:178:VAL:HG12	1.82	0.61
1:g:53:GLN:HA	1:g:215:ILE:HA	1.83	0.61
2:h:3:GLU:HG3	2:h:4:ARG:HG3	1.83	0.61
7:m:40:ARG:NH1	7:m:146:ALA:O	2.33	0.61
24:d:19:CYS:SG	24:d:65:ARG:NH1	2.73	0.61
14:t:9:THR:O	14:t:41:ARG:NH2	2.32	0.61
29:F:94:ILE:HD12	29:F:123:VAL:HG12	1.83	0.61
4:J:32:ALA:O	4:J:159:ASN:ND2	2.34	0.61
15:U:542:GLU:OE1	15:U:546:ARG:NH1	2.33	0.61
16:V:224:LEU:HB2	16:V:227:VAL:HB	1.82	0.61
16:V:280:ALA:HB1	16:V:284:GLU:HB3	1.82	0.61
17:W:155:GLN:HE21	17:W:161:GLU:HB3	1.65	0.61
4:j:7:ILE:HG12	4:j:123:GLY:HA2	1.81	0.61
32:f:234:THR:O	32:f:238:ASN:HB2	2.00	0.61
16:V:79:VAL:HG13	16:V:81:GLN:H	1.63	0.61
27:A:161:VAL:HA	27:A:164:MET:HE3	1.81	0.61
28:E:182:LEU:HD22	34:E:401:AGS:H2'	1.80	0.61
32:f:471:LEU:O	32:f:471:LEU:HD23	2.01	0.61
17:W:409:LEU:HD21	18:X:344:ARG:HG2	1.83	0.61
28:E:226:GLN:HG3	28:E:272:ARG:HD2	1.81	0.61
28:E:280:ASN:ND2	34:E:401:AGS:O3G	2.34	0.61
32:f:471:LEU:CD1	32:f:509:LYS:HE2	2.30	0.61
10:P:65:GLN:OE1	11:Q:86:ARG:NH2	2.34	0.61
23:c:41:MET:HE3	23:c:145:VAL:HB	1.82	0.61
23:c:220:LEU:O	23:c:224:SER:HB3	2.01	0.61
23:c:282:ARG:NH1	31:D:122:GLU:O	2.34	0.61
32:f:376:PHE:CG	32:f:416:MET:HE1	2.35	0.61
15:U:247:GLN:HE22	15:U:912:ILE:HG22	1.66	0.61
16:V:479:ARG:NH2	19:Y:374:ASP:OD1	2.34	0.61
30:C:328:ILE:HG23	34:C:401:AGS:H2	1.82	0.61
3:i:174:MET:HE2	3:i:199:LYS:HD3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:196:GLU:OE1	26:B:349:ARG:NH1	2.34	0.61
32:f:378:ASN:HB2	32:f:391:LEU:HD11	1.82	0.61
27:A:264:ALA:HB1	27:A:315:ILE:HG12	1.82	0.60
32:f:494:ARG:NE	32:f:496:ASP:H	1.99	0.60
6:l:107:ARG:NH2	14:t:79:ASP:OD2	2.34	0.60
15:U:424:ALA:HA	15:U:427:LEU:HD13	1.82	0.60
15:U:559:ARG:HB3	15:U:562:GLU:HB2	1.83	0.60
16:V:470:ARG:NH1	24:d:241:GLU:OE2	2.34	0.60
30:C:232:ARG:HH11	30:C:279:GLN:HE21	1.49	0.60
32:f:232:TYR:O	32:f:236:CYS:CB	2.49	0.60
32:f:337:LEU:CD1	32:f:420:TRP:HZ3	2.04	0.60
13:S:38:ARG:NH2	9:o:164:PHE:O	2.34	0.60
15:U:82:LEU:O	15:U:129:ARG:NE	2.34	0.60
22:b:116:PRO:HA	22:b:146:GLU:HG3	1.84	0.60
32:f:376:PHE:CZ	32:f:416:MET:HE1	2.36	0.60
3:I:143:TYR:HB2	3:I:146:GLN:HE21	1.67	0.60
13:s:54:CYS:SG	13:s:108:ASN:ND2	2.75	0.60
16:V:212:TYR:OH	16:V:287:ARG:NH2	2.34	0.60
9:o:1:THR:HG23	9:o:33:LYS:HE3	1.82	0.60
32:f:695:ALA:CB	32:f:752:HIS:HB2	2.31	0.60
15:U:694:ILE:HG23	15:U:695:MET:HG3	1.83	0.60
17:W:429:SER:O	17:W:433:ASN:HB2	2.02	0.60
31:D:353:ASN:ND2	31:D:392:TYR:O	2.35	0.60
6:L:152:ASN:HA	7:M:85:ARG:HH22	1.66	0.60
7:M:37:ILE:HD11	7:M:193:VAL:HG13	1.84	0.60
7:m:76:ALA:HB3	7:m:136:MET:HB2	1.83	0.60
32:f:378:ASN:O	32:f:381:VAL:CG1	2.49	0.60
32:f:801:VAL:HG13	32:f:801:VAL:O	2.01	0.60
6:L:120:THR:O	7:M:129:ARG:NH1	2.34	0.60
17:W:136:ILE:HG13	17:W:144:ARG:HB2	1.83	0.60
17:W:220:GLU:HG3	17:W:221:LYS:HG2	1.83	0.60
19:Y:12:PRO:O	19:Y:113:ARG:NH2	2.35	0.60
2:h:34:PRO:HA	2:h:164:GLY:HA3	1.84	0.60
26:B:122:ILE:HD11	26:B:130:GLU:HB3	1.83	0.60
32:f:337:LEU:HD22	32:f:337:LEU:N	2.17	0.60
32:f:389:LYS:HG2	32:f:418:LEU:CD1	2.32	0.60
17:W:435:LEU:HD13	23:c:239:LYS:HE3	1.84	0.59
3:i:106:PRO:HD2	3:i:109:GLN:HE21	1.66	0.59
7:m:144:ASP:O	7:m:147:GLN:NE2	2.34	0.59
28:E:139:SER:HA	28:E:142:ILE:HD12	1.84	0.59
31:D:167:ILE:CA	31:D:214:MET:HE1	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:101:ILE:O	15:U:105:ILE:HB	2.02	0.59
5:k:209:LYS:O	5:k:214:ASN:ND2	2.35	0.59
6:l:120:THR:O	7:m:129:ARG:NH1	2.30	0.59
28:E:207:TYR:OH	29:F:129:ARG:NH2	2.35	0.59
32:f:380:PHE:CB	32:f:751:TYR:HE2	2.14	0.59
1:G:53:GLN:HA	1:G:215:ILE:HA	1.83	0.59
16:V:497:PRO:HD2	20:Z:278:ASN:HD21	1.66	0.59
2:h:222:THR:OG1	2:h:225:GLU:OE1	2.20	0.59
3:i:149:GLN:NE2	3:i:163:CYS:O	2.36	0.59
32:f:782:HIS:HA	32:f:785:ARG:HG2	1.83	0.59
17:W:135:LYS:HE2	17:W:147:LYS:HE2	1.83	0.59
19:Y:67:VAL:O	19:Y:71:ASN:ND2	2.35	0.59
6:l:196:ARG:HH21	6:l:239:ARG:HG3	1.66	0.59
27:A:90:GLU:HA	27:A:93:LEU:HD23	1.83	0.59
32:f:315:GLU:CB	32:f:491:GLY:HA2	2.32	0.59
32:f:378:ASN:CB	32:f:391:LEU:HD11	2.33	0.59
32:f:477:MET:O	32:f:481:SER:HB2	2.02	0.59
7:m:92:ARG:NH2	14:t:73:ASP:OD1	2.35	0.59
24:d:247:ILE:O	24:d:251:ARG:HB2	2.03	0.59
27:A:413:VAL:HG13	27:A:417:ILE:HD12	1.84	0.59
31:D:292:LEU:O	31:D:296:MET:HB2	2.02	0.59
15:U:408:LEU:HG	15:U:423:MET:HE2	1.85	0.59
16:V:443:ARG:NH2	24:d:180:GLY:O	2.35	0.59
16:V:476:PHE:HB3	20:Z:260:VAL:HG21	1.85	0.59
17:W:65:ARG:HG3	17:W:67:LEU:H	1.68	0.59
7:m:47:PHE:HB2	7:m:214:SER:HB3	1.84	0.59
28:E:198:VAL:HG12	28:E:200:SER:H	1.67	0.59
32:f:494:ARG:NH2	32:f:495:GLU:H	2.00	0.59
10:P:190:ILE:HG22	10:P:195:ILE:HG23	1.85	0.59
20:Z:179:ILE:HG23	23:c:222:LYS:HE2	1.85	0.59
5:k:219:THR:HB	5:k:221:GLN:HE22	1.66	0.59
34:B:501:AGS:S1G	34:B:501:AGS:O1B	2.61	0.59
28:E:97:ARG:NH2	28:E:112:PRO:O	2.36	0.59
31:D:249:ASP:OD1	31:D:252:ARG:NH2	2.34	0.59
32:f:376:PHE:HE1	32:f:798:THR:HB	1.53	0.59
32:f:501:LEU:HD22	32:f:518:THR:HG23	1.84	0.59
32:f:541:THR:O	32:f:545:LYS:HB2	2.03	0.59
1:G:141:ILE:HG22	1:G:151:VAL:HG22	1.85	0.59
21:a:34:TRP:HZ3	21:a:64:ILE:HG23	1.67	0.59
26:B:224:LEU:HD21	26:B:235:LEU:HD12	1.85	0.59
32:f:358:PHE:HZ	32:f:381:VAL:HG21	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:94:ALA:HB1	3:I:105:ILE:HG21	1.83	0.59
10:P:107:PRO:HG2	10:P:124:LEU:HB2	1.85	0.59
10:P:189:ILE:HG23	10:P:196:THR:HB	1.85	0.59
18:X:296:ASN:O	18:X:337:ARG:NH2	2.36	0.59
32:f:438:ASP:N	32:f:438:ASP:OD1	2.35	0.59
32:f:494:ARG:CZ	32:f:496:ASP:H	2.16	0.59
15:U:128:GLN:O	15:U:132:GLY:HA3	2.03	0.58
17:W:76:GLU:OE2	17:W:123:ARG:NH1	2.36	0.58
32:f:618:GLU:HG2	32:f:623:LYS:HD2	1.85	0.58
6:L:205:LEU:HD13	6:L:233:LEU:HD22	1.84	0.58
15:U:472:ILE:HG13	15:U:473:VAL:HG23	1.85	0.58
13:S:148:LEU:HD23	13:S:178:VAL:HG12	1.84	0.58
32:f:780:PRO:O	32:f:800:LEU:HG	2.03	0.58
16:V:416:ARG:NH1	19:Y:351:ASN:OD1	2.36	0.58
20:Z:88:ARG:HE	28:E:86:GLN:HE22	1.50	0.58
11:q:3:TYR:CZ	11:q:131:ALA:HA	2.38	0.58
27:A:94:GLN:NE2	27:A:143:ASP:OD1	2.37	0.58
17:W:268:LYS:HA	17:W:271:VAL:HG12	1.84	0.58
7:m:51:LYS:O	7:m:210:GLU:N	2.34	0.58
30:C:221:GLN:HG3	30:C:227:GLY:HA2	1.85	0.58
9:O:1:THR:HG23	9:O:33:LYS:HE3	1.85	0.58
1:g:32:ILE:HA	1:g:82:GLY:HA2	1.85	0.58
34:A:501:AGS:S1G	34:A:501:AGS:O1B	2.61	0.58
28:E:70:ILE:HG12	28:E:80:VAL:HG22	1.84	0.58
32:f:22:GLY:O	32:f:26:GLU:HB2	2.04	0.58
32:f:88:SER:HB2	32:f:92:VAL:CG2	2.33	0.58
32:f:89:MET:HG2	32:f:90:THR:HG23	1.84	0.58
17:W:142:ARG:HH21	17:W:182:ARG:HB2	1.68	0.58
22:b:141:ILE:HA	22:b:171:VAL:HB	1.85	0.58
23:c:233:ASP:O	23:c:237:HIS:ND1	2.36	0.58
4:j:176:TYR:HE1	5:k:58:LEU:HD23	1.69	0.58
7:M:47:PHE:HB2	7:M:214:SER:HB3	1.86	0.58
23:c:149:GLN:HB3	31:D:81:ARG:HH21	1.67	0.58
24:d:61:TRP:HB3	24:d:65:ARG:HH11	1.69	0.58
4:j:211:MET:HG2	4:j:213:ARG:H	1.68	0.58
10:p:65:GLN:OE1	11:q:86:ARG:NH2	2.36	0.58
6:L:189:LYS:HZ3	6:L:193:ARG:HH22	1.52	0.58
21:a:188:LEU:HD11	21:a:193:GLN:HG3	1.84	0.58
30:C:63:LEU:HG	31:D:79:VAL:HG22	1.85	0.58
32:f:378:ASN:HB3	32:f:391:LEU:CD2	2.34	0.58
32:f:487:LEU:HD23	32:f:524:MET:HE1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:192:VAL:HG11	10:p:205:ASP:HB3	1.86	0.58
14:T:1:THR:N	14:T:105:PRO:O	2.37	0.58
24:d:155:LYS:HE2	24:d:167:ILE:HB	1.86	0.58
7:m:34:SER:OG	7:m:65:ARG:NH2	2.30	0.58
34:F:501:AGS:S1G	34:F:501:AGS:O1B	2.62	0.58
32:f:140:LEU:O	32:f:144:LEU:HB2	2.04	0.58
2:H:4:ARG:NH2	7:M:126:SER:OG	2.37	0.57
6:L:196:ARG:NH1	6:L:237:GLU:O	2.37	0.57
16:V:290:TYR:OH	16:V:294:ARG:NH2	2.37	0.57
13:s:4:PRO:O	14:t:100:ARG:NH2	2.33	0.57
27:A:312:ARG:HH21	27:A:315:ILE:HG22	1.69	0.57
34:F:501:AGS:O1B	34:F:501:AGS:O2A	2.20	0.57
31:D:167:ILE:CG1	31:D:214:MET:CE	2.82	0.57
32:f:695:ALA:CB	32:f:752:HIS:CB	2.82	0.57
4:J:2:SER:OG	4:J:3:TYR:N	2.37	0.57
7:M:51:LYS:O	7:M:210:GLU:N	2.36	0.57
17:W:343:SER:O	17:W:347:GLY:N	2.37	0.57
32:f:780:PRO:HB2	32:f:800:LEU:HB3	1.86	0.57
4:J:176:TYR:HE1	5:K:58:LEU:HD23	1.68	0.57
8:N:29:ARG:HH21	14:t:179:ARG:HG2	1.69	0.57
17:W:169:LEU:O	17:W:182:ARG:NH1	2.31	0.57
26:B:168:ASP:HB3	26:B:171:VAL:HB	1.86	0.57
3:I:218:ARG:NH1	3:I:223:THR:OG1	2.37	0.57
24:d:237:ILE:HA	24:d:240:THR:HG22	1.86	0.57
32:f:127:SER:O	32:f:131:MET:CB	2.52	0.57
32:f:269:ALA:HB2	32:f:277:LEU:HD22	1.87	0.57
2:H:59:GLU:HG2	2:H:206:ASP:HB3	1.86	0.57
9:O:140:ASP:OD2	14:t:171:ARG:NH2	2.38	0.57
15:U:363:SER:HB2	23:c:175:ARG:HH21	1.70	0.57
16:V:190:ASP:HA	16:V:200:ARG:HH21	1.69	0.57
3:I:106:PRO:HD2	3:I:109:GLN:HE21	1.68	0.57
11:Q:135:GLY:HA2	11:Q:171:PHE:HZ	1.69	0.57
15:U:187:LEU:HD13	31:D:45:LYS:HE2	1.87	0.57
17:W:62:SER:OG	17:W:75:TYR:OH	2.22	0.57
10:p:190:ILE:HG22	10:p:195:ILE:HG23	1.86	0.57
16:V:148:ARG:NH1	16:V:192:MET:O	2.37	0.57
16:V:494:MET:O	20:Z:278:ASN:ND2	2.38	0.57
18:X:173:GLU:HA	18:X:176:THR:HG22	1.87	0.57
24:d:203:PRO:HB2	24:d:205:LYS:H	1.69	0.57
26:B:133:VAL:HB	26:B:158:ALA:HA	1.87	0.57
32:f:635:LYS:NZ	32:f:641:GLU:HG3	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:751:ARG:HH12	15:U:907:SER:HB2	1.69	0.57
19:Y:42:MET:O	19:Y:46:ARG:NH2	2.37	0.57
20:Z:16:LEU:HD21	23:c:216:MET:HE2	1.86	0.57
14:t:180:ASP:HB3	14:t:183:SER:HB3	1.87	0.57
26:B:375:ALA:HB2	26:B:413:LYS:HB3	1.86	0.57
28:E:210:GLU:OE2	28:E:213:ARG:NH2	2.36	0.57
31:D:341:LYS:NZ	31:D:367:PRO:O	2.37	0.57
32:f:353:LEU:H	32:f:387:GLN:HG2	1.68	0.57
1:G:114:LEU:HD22	1:G:140:LEU:HD21	1.85	0.57
16:V:228:ARG:O	16:V:232:HIS:ND1	2.38	0.57
24:d:47:GLN:O	24:d:51:ALA:HB2	2.04	0.57
2:h:39:LYS:HE2	2:h:144:PRO:HG2	1.84	0.57
6:l:196:ARG:NH1	6:l:237:GLU:O	2.37	0.57
3:I:161:ALA:HB1	3:I:175:LEU:HD13	1.87	0.56
15:U:418:GLU:HA	15:U:421:GLN:HE21	1.70	0.56
19:Y:261:PHE:O	19:Y:265:GLU:HB2	2.04	0.56
6:L:101:ARG:HH12	6:L:104:PRO:HD3	1.70	0.56
9:O:17:ASP:O	9:O:33:LYS:NZ	2.36	0.56
25:e:45:ASP:O	25:e:49:GLU:HB2	2.05	0.56
27:A:212:VAL:HG22	27:A:339:ARG:HB2	1.87	0.56
30:C:99:VAL:HG12	30:C:123:LEU:HD12	1.87	0.56
32:f:226:TYR:O	32:f:230:CYS:CB	2.53	0.56
32:f:471:LEU:CD1	32:f:509:LYS:HE3	2.26	0.56
32:f:536:SER:O	32:f:540:GLN:HB2	2.05	0.56
32:f:780:PRO:CB	32:f:800:LEU:CA	2.79	0.56
22:b:142:ASN:HD22	22:b:172:THR:HA	1.69	0.56
24:d:131:VAL:O	24:d:135:HIS:HB3	2.05	0.56
1:g:201:CYS:SG	1:g:202:LEU:N	2.78	0.56
8:n:120:MET:H	14:t:61:GLN:HE22	1.52	0.56
28:E:291:ARG:NH1	34:D:501:AGS:O2A	2.38	0.56
32:f:129:LEU:O	32:f:133:MET:CB	2.50	0.56
32:f:358:PHE:CE1	32:f:381:VAL:HG21	2.40	0.56
32:f:742:ALA:CA	32:f:745:LEU:HG	2.35	0.56
11:Q:170:ARG:NH2	12:r:125:THR:OG1	2.39	0.56
15:U:885:MET:HG2	15:U:887:ALA:H	1.69	0.56
21:a:321:LYS:O	21:a:334:THR:OG1	2.23	0.56
1:g:123:GLN:O	1:g:127:GLN:N	2.38	0.56
32:f:456:ARG:HD3	32:f:489:TYR:OH	2.04	0.56
15:U:108:TYR:HH	15:U:159:ARG:HH12	1.54	0.56
7:m:8:ASP:O	7:m:22:GLN:NE2	2.37	0.56
32:f:456:ARG:HB3	32:f:489:TYR:CZ	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:742:ALA:CA	32:f:745:LEU:HD21	2.32	0.56
15:U:13:ASP:OD1	15:U:44:LYS:NZ	2.38	0.56
15:U:742:HIS:O	15:U:883:ARG:NH2	2.38	0.56
19:Y:101:ARG:HE	19:Y:127:THR:HA	1.71	0.56
19:Y:231:LEU:HD12	19:Y:234:PRO:HD2	1.87	0.56
21:a:45:VAL:HG11	21:a:79:ILE:HA	1.88	0.56
10:p:189:ILE:HG23	10:p:196:THR:HB	1.86	0.56
32:f:380:PHE:CG	32:f:751:TYR:HE2	2.24	0.56
32:f:742:ALA:HA	32:f:745:LEU:HG	1.87	0.56
16:V:365:GLN:NE2	25:e:50:ASP:OD1	2.39	0.56
31:D:214:MET:HE3	34:D:501:AGS:C8	2.30	0.56
32:f:494:ARG:CZ	32:f:495:GLU:H	2.17	0.56
32:f:688:ARG:HH12	32:f:788:MET:HA	1.71	0.56
15:U:97:VAL:HA	15:U:100:ILE:HG12	1.88	0.56
18:X:222:GLU:HA	18:X:225:TRP:HE1	1.71	0.56
32:f:353:LEU:HG	32:f:387:GLN:CG	2.36	0.56
18:X:149:LEU:O	18:X:153:LEU:HB2	2.05	0.56
18:X:338:VAL:HG23	18:X:339:ILE:HG13	1.88	0.56
21:a:12:GLN:HG3	21:a:22:TRP:HB3	1.87	0.56
26:B:201:VAL:HG21	26:B:328:ILE:HD11	1.88	0.56
32:f:780:PRO:HB2	32:f:800:LEU:CB	2.36	0.56
6:L:158:ALA:HB1	6:L:172:LEU:HD13	1.88	0.56
15:U:898:CYS:SG	15:U:899:ARG:N	2.76	0.56
21:a:33:LEU:HA	22:b:18:ASN:HD22	1.71	0.56
16:V:30:PRO:HA	16:V:33:GLN:HB2	1.86	0.55
18:X:90:ARG:HH22	18:X:128:ALA:HB3	1.72	0.55
19:Y:50:MET:HE2	19:Y:74:LYS:HB3	1.89	0.55
23:c:157:ILE:HG12	23:c:205:ILE:HG21	1.88	0.55
6:l:50:LYS:HE2	6:l:61:LYS:HA	1.88	0.55
11:q:181:ARG:NH1	11:q:190:ASP:OD1	2.39	0.55
32:f:623:LYS:O	32:f:627:GLU:CB	2.54	0.55
23:c:138:GLU:O	23:c:161:ARG:NH2	2.39	0.55
25:e:40:GLU:OE2	25:e:44:ASP:N	2.39	0.55
2:H:66:GLU:OE2	2:H:91:ARG:NH2	2.40	0.55
2:H:222:THR:OG1	2:H:225:GLU:OE1	2.21	0.55
10:P:36:THR:OG1	10:P:38:ASP:OD1	2.22	0.55
14:T:27:LEU:HD11	14:T:34:ALA:HB1	1.88	0.55
17:W:440:ASN:HB3	20:Z:230:LEU:HD21	1.89	0.55
32:f:317:LEU:O	32:f:321:MET:HB2	2.05	0.55
32:f:336:GLU:CG	32:f:337:LEU:HD22	2.36	0.55
11:Q:23:SER:OG	11:Q:24:ASN:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:43:MET:HE3	14:T:45:VAL:HG22	1.89	0.55
20:Z:172:VAL:HG13	23:c:217:LEU:HD21	1.89	0.55
30:C:164:VAL:HG13	30:C:165:ILE:HG13	1.88	0.55
7:M:144:ASP:O	7:M:147:GLN:NE2	2.35	0.55
17:W:173:THR:HG23	17:W:182:ARG:HH11	1.70	0.55
22:b:100:ARG:NH1	22:b:102:GLY:O	2.40	0.55
23:c:163:ILE:HG22	23:c:199:HIS:HA	1.89	0.55
11:q:23:SER:OG	11:q:24:ASN:N	2.40	0.55
32:f:426:LEU:O	32:f:430:ASP:HB3	2.07	0.55
3:I:38:LEU:HD23	3:I:147:LEU:HG	1.87	0.55
6:L:155:ASP:HB3	7:M:62:SER:HB2	1.89	0.55
15:U:46:GLU:OE2	15:U:80:TYR:OH	2.23	0.55
24:d:62:SER:HA	24:d:65:ARG:HG2	1.88	0.55
31:D:167:ILE:CG1	31:D:214:MET:HE2	2.37	0.55
32:f:684:PRO:O	32:f:688:ARG:CB	2.54	0.55
1:G:70:PHE:HD2	1:G:91:VAL:HG21	1.71	0.55
21:a:212:ASN:OD1	21:a:213:PHE:N	2.39	0.55
22:b:14:GLU:HB3	22:b:82:GLY:H	1.71	0.55
3:i:171:ALA:HB2	3:i:200:THR:HG21	1.87	0.55
11:q:48:GLY:HA3	11:q:100:VAL:HA	1.87	0.55
13:s:169:ASP:OD2	13:s:173:ARG:NH2	2.38	0.55
9:O:46:ALA:HB3	9:O:97:ALA:HB3	1.89	0.55
15:U:678:ASP:O	15:U:684:ARG:NH1	2.40	0.55
16:V:452:ASN:OD1	16:V:455:LYS:NZ	2.40	0.55
8:n:144:ARG:H	8:n:147:MET:HE3	1.72	0.55
32:f:403:LYS:O	32:f:407:MET:N	2.40	0.55
32:f:692:LEU:HD12	32:f:748:LEU:HD23	1.84	0.55
17:W:340:VAL:HA	17:W:350:ARG:HD2	1.88	0.55
20:Z:192:THR:HA	20:Z:195:VAL:HB	1.88	0.55
22:b:15:TYR:O	22:b:25:ARG:NH1	2.40	0.55
27:A:277:ILE:HG22	27:A:280:ILE:HD12	1.88	0.55
29:F:358:ASN:O	29:F:362:ARG:NH1	2.40	0.55
32:f:313:GLU:O	32:f:317:LEU:CB	2.55	0.55
19:Y:141:VAL:HG11	19:Y:164:ALA:HB2	1.88	0.55
20:Z:88:ARG:NH2	28:E:86:GLN:OE1	2.40	0.55
6:l:189:LYS:HA	6:l:192:LEU:HG	1.89	0.55
13:s:125:ASP:OD1	13:s:129:SER:N	2.37	0.55
17:W:73:MET:O	17:W:77:ALA:HB2	2.07	0.54
18:X:322:HIS:O	18:X:326:LEU:HB3	2.06	0.54
21:a:261:LEU:O	21:a:265:GLU:HB2	2.07	0.54
7:m:52:LEU:HA	7:m:209:PHE:HA	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:p:36:THR:OG1	10:p:38:ASP:OD1	2.22	0.54
14:t:43:MET:HE3	14:t:45:VAL:HG22	1.89	0.54
30:C:155:ASP:HA	30:C:158:ILE:HD12	1.89	0.54
32:f:138:GLU:O	32:f:142:TYR:CB	2.56	0.54
32:f:301:HIS:O	32:f:305:LEU:CB	2.53	0.54
32:f:471:LEU:HD12	32:f:509:LYS:CE	2.36	0.54
6:L:109:VAL:HG21	6:L:145:PHE:HD2	1.73	0.54
5:k:54:ILE:HA	5:k:59:MET:HE1	1.88	0.54
1:G:201:CYS:SG	1:G:202:LEU:N	2.80	0.54
6:L:151:ALA:O	7:M:85:ARG:NH2	2.39	0.54
17:W:93:ARG:NH1	17:W:137:TYR:O	2.40	0.54
21:a:120:ALA:HA	21:a:123:LEU:HD13	1.89	0.54
2:h:9:SER:HA	2:h:126:GLY:H	1.73	0.54
12:r:35:ILE:N	12:r:43:GLY:O	2.40	0.54
30:C:301:LEU:HD13	30:C:305:LEU:HD23	1.88	0.54
32:f:575:ALA:O	32:f:579:ALA:HB2	2.07	0.54
32:f:663:GLY:O	32:f:697:ILE:HB	2.07	0.54
2:H:231:ALA:HB2	18:X:87:ARG:HH11	1.72	0.54
13:S:172:MET:HE1	13:S:195:ILE:HG21	1.89	0.54
16:V:368:ARG:NH1	25:e:50:ASP:OD2	2.41	0.54
17:W:395:ASN:HA	17:W:398:VAL:HG22	1.90	0.54
19:Y:71:ASN:HA	19:Y:74:LYS:HG2	1.90	0.54
28:E:351:GLY:HA3	29:F:217:ILE:HD13	1.89	0.54
32:f:80:ARG:O	32:f:84:SER:HB3	2.07	0.54
32:f:278:VAL:HA	32:f:281:ILE:HG22	1.89	0.54
2:H:67:PRO:HG2	9:O:68:LEU:HD11	1.90	0.54
16:V:200:ARG:HD2	16:V:242:HIS:HD2	1.72	0.54
30:C:86:LEU:HD11	30:C:94:LYS:HD2	1.90	0.54
32:f:15:GLN:NE2	32:f:47:GLU:OE1	2.41	0.54
32:f:229:VAL:O	32:f:233:LEU:CB	2.56	0.54
5:K:70:ILE:HD11	5:K:89:ILE:HD12	1.90	0.54
13:S:169:ASP:OD2	13:S:173:ARG:NH2	2.40	0.54
21:a:252:LYS:HA	21:a:255:TRP:HD1	1.73	0.54
3:i:33:THR:HG23	3:i:168:SER:HB2	1.89	0.54
27:A:244:GLU:O	27:A:247:GLN:NE2	2.41	0.54
28:E:198:VAL:HB	28:E:232:MET:HG2	1.90	0.54
28:E:322:LYS:NZ	28:E:328:TYR:OH	2.39	0.54
32:f:273:ASN:ND2	32:f:310:ASP:OD2	2.41	0.54
11:Q:181:ARG:NH1	11:Q:190:ASP:OD1	2.41	0.54
17:W:155:GLN:NE2	17:W:161:GLU:OE1	2.41	0.54
21:a:54:ASP:HA	21:a:57:ILE:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:d:45:LYS:HG2	24:d:48:LEU:HD12	1.87	0.54
24:d:75:MET:HE3	24:d:79:LYS:HB2	1.88	0.54
6:l:151:ALA:O	7:m:85:ARG:NH2	2.40	0.54
31:D:391:ARG:NH2	31:D:398:ASP:OD2	2.41	0.54
32:f:8:LYS:O	32:f:12:GLN:HB2	2.08	0.54
32:f:229:VAL:O	32:f:233:LEU:HB2	2.07	0.54
32:f:281:ILE:O	32:f:285:CYS:CB	2.56	0.54
8:N:144:ARG:H	8:N:147:MET:HE3	1.72	0.54
23:c:179:SER:O	23:c:183:HIS:ND1	2.33	0.54
26:B:315:GLN:O	26:B:322:ARG:NH1	2.41	0.54
31:D:170:MET:HG2	31:D:173:GLN:HB2	1.89	0.54
10:P:58:THR:OG1	11:Q:121:LEU:O	2.18	0.54
12:R:12:VAL:HB	12:R:179:VAL:HB	1.90	0.54
15:U:45:ILE:HG21	15:U:64:ALA:HB2	1.90	0.54
17:W:431:LYS:HB3	23:c:239:LYS:HG2	1.89	0.54
24:d:188:LYS:HB2	24:d:221:ASN:HD21	1.73	0.54
3:i:218:ARG:NH1	3:i:223:THR:OG1	2.41	0.54
32:f:477:MET:O	32:f:481:SER:CB	2.56	0.54
15:U:842:LYS:H	15:U:882:ALA:HB2	1.73	0.54
16:V:78:HIS:HB3	16:V:164:GLU:HB3	1.88	0.54
16:V:252:ASN:ND2	16:V:284:GLU:OE2	2.41	0.54
28:E:81:VAL:HG12	28:E:105:LEU:HD13	1.90	0.54
29:F:413:THR:OG1	29:F:414:GLU:OE1	2.25	0.54
34:C:401:AGS:O2A	34:C:401:AGS:O1B	2.25	0.54
32:f:8:LYS:O	32:f:12:GLN:CB	2.56	0.54
32:f:253:LEU:O	32:f:257:ARG:HB2	2.07	0.54
32:f:586:PRO:HA	32:f:589:SER:HB2	1.89	0.54
3:I:171:ALA:HB2	3:I:200:THR:HG21	1.90	0.53
18:X:323:LEU:O	18:X:327:TYR:HB2	2.07	0.53
21:a:163:TYR:CG	21:a:172:TYR:HB2	2.43	0.53
21:a:254:ALA:O	21:a:258:GLN:NE2	2.40	0.53
3:i:135:LEU:HG	3:i:164:ILE:HD11	1.89	0.53
29:F:295:ARG:HH22	29:F:311:LEU:HD21	1.73	0.53
4:J:114:LEU:O	4:J:118:TYR:HB2	2.07	0.53
18:X:338:VAL:HB	18:X:350:ILE:HD11	1.89	0.53
6:l:72:ILE:HG22	6:l:134:ILE:HG12	1.90	0.53
31:D:119:ILE:O	31:D:121:ARG:NH1	2.42	0.53
32:f:211:ILE:O	32:f:215:ASP:CB	2.56	0.53
3:I:216:LEU:HD12	3:I:225:ILE:HG12	1.89	0.53
8:N:96:ALA:HB1	8:N:98:ILE:HG12	1.89	0.53
15:U:31:VAL:HG22	15:U:35:TRP:HD1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:107:HIS:HA	15:U:110:LYS:HE3	1.90	0.53
15:U:353:LEU:O	15:U:357:LYS:CB	2.56	0.53
17:W:99:GLN:O	17:W:103:LYS:HB2	2.08	0.53
18:X:122:ARG:HG2	18:X:125:LEU:H	1.73	0.53
11:q:135:GLY:HA2	11:q:171:PHE:HZ	1.73	0.53
32:f:376:PHE:CD1	32:f:416:MET:CE	2.83	0.53
6:L:42:THR:O	6:L:137:TYR:OH	2.26	0.53
13:S:123:SER:HB3	13:S:136:LYS:HG3	1.90	0.53
31:D:368:ASP:OD2	31:D:403:TYR:OH	2.24	0.53
15:U:38:ILE:HB	15:U:67:VAL:HG21	1.90	0.53
22:b:12:ASN:HB2	22:b:80:PRO:HA	1.90	0.53
13:s:123:SER:HB3	13:s:136:LYS:HG3	1.90	0.53
28:E:75:ASN:HD22	29:F:130:GLN:HG2	1.72	0.53
32:f:314:TYR:CE1	32:f:490:ALA:HB3	2.43	0.53
2:H:185:GLU:HB3	18:X:122:ARG:HH21	1.74	0.53
6:L:72:ILE:HG22	6:L:134:ILE:HG12	1.90	0.53
11:Q:48:GLY:HA3	11:Q:100:VAL:HA	1.91	0.53
13:S:4:PRO:O	14:T:100:ARG:NH2	2.34	0.53
23:c:59:GLY:HA2	23:c:70:ILE:HG22	1.91	0.53
32:f:377:VAL:HG22	32:f:751:TYR:HB2	1.88	0.53
32:f:600:TYR:HB3	32:f:608:LYS:HE2	1.91	0.53
17:W:426:ASN:ND2	20:Z:244:GLU:O	2.38	0.53
21:a:163:TYR:HE1	21:a:169:HIS:HA	1.74	0.53
32:f:76:GLU:OE1	32:f:79:ARG:NH2	2.41	0.53
32:f:80:ARG:O	32:f:84:SER:CB	2.57	0.53
32:f:306:GLU:HB3	32:f:339:ILE:HD12	1.91	0.53
11:Q:3:TYR:CZ	11:Q:131:ALA:HA	2.44	0.53
13:S:125:ASP:OD1	13:S:129:SER:N	2.37	0.53
16:V:227:VAL:HA	16:V:230:PHE:HB3	1.91	0.53
16:V:319:HIS:HD2	25:e:4:LYS:HG3	1.72	0.53
16:V:440:LYS:HA	16:V:443:ARG:HB3	1.91	0.53
18:X:96:PHE:HZ	18:X:105:GLN:HB3	1.74	0.53
20:Z:190:ARG:HH22	21:a:374:ILE:HG13	1.74	0.53
7:m:230:ASP:OD1	7:m:230:ASP:N	2.42	0.53
32:f:714:SER:C	32:f:718:ASP:HB2	2.33	0.53
17:W:93:ARG:H	17:W:96:GLN:HE21	1.56	0.53
18:X:420:LYS:HZ2	20:Z:279:LYS:HD2	1.74	0.53
22:b:16:MET:HA	22:b:25:ARG:HD2	1.91	0.53
14:t:1:THR:N	14:t:105:PRO:O	2.39	0.53
32:f:612:LEU:O	32:f:616:CYS:CB	2.56	0.53
17:W:144:ARG:HA	17:W:147:LYS:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:372:ARG:HG2	17:W:414:ASN:HB3	1.91	0.53
18:X:255:LEU:HB2	18:X:287:LEU:HD13	1.91	0.53
18:X:395:LYS:HD2	20:Z:257:MET:HG2	1.90	0.53
6:l:152:ASN:HA	7:m:85:ARG:HH22	1.74	0.53
12:R:21:THR:HG22	12:R:26:ILE:HG12	1.92	0.52
15:U:458:ILE:HA	15:U:481:LEU:HD11	1.91	0.52
17:W:346:GLU:OE2	17:W:350:ARG:NE	2.42	0.52
18:X:320:SER:O	18:X:324:ALA:HB3	2.08	0.52
23:c:183:HIS:O	23:c:187:PRO:HD2	2.09	0.52
27:A:333:ARG:NH2	34:F:501:AGS:O1A	2.41	0.52
34:E:401:AGS:O1B	29:F:344:ARG:NH1	2.41	0.52
23:c:236:GLU:O	23:c:240:HIS:ND1	2.40	0.52
32:f:468:ASP:OD2	32:f:475:ASN:N	2.42	0.52
15:U:510:GLU:HG3	15:U:543:LYS:HB3	1.91	0.52
17:W:274:VAL:O	17:W:283:GLN:NE2	2.42	0.52
27:A:394:MET:HA	27:A:397:ILE:HD12	1.91	0.52
15:U:26:LYS:HG2	24:d:36:LEU:HD22	1.91	0.52
16:V:218:TYR:HA	16:V:221:LEU:HG	1.90	0.52
21:a:73:PRO:HG3	21:a:104:VAL:HG11	1.91	0.52
22:b:30:GLN:HG3	22:b:75:LEU:HD13	1.91	0.52
5:k:20:ARG:HG3	5:k:21:LEU:H	1.75	0.52
6:l:193:ARG:HA	6:l:196:ARG:HG2	1.91	0.52
10:p:107:PRO:HG2	10:p:124:LEU:HB2	1.91	0.52
11:q:19:ARG:HH21	11:q:31:ASP:HB2	1.74	0.52
27:A:307:ASP:HB2	27:A:336:ARG:HG2	1.92	0.52
31:D:167:ILE:HG12	31:D:214:MET:HE2	1.90	0.52
31:D:173:GLN:HE22	31:D:334:PRO:HD2	1.74	0.52
32:f:378:ASN:HB3	32:f:391:LEU:CD1	2.39	0.52
16:V:346:LEU:HB2	16:V:349:ARG:HB3	1.91	0.52
27:A:309:PHE:HA	29:F:238:ARG:HD3	1.91	0.52
29:F:212:PHE:O	29:F:216:GLY:N	2.39	0.52
32:f:262:PHE:HB3	32:f:281:ILE:HD11	1.91	0.52
32:f:376:PHE:CZ	32:f:798:THR:CG2	2.91	0.52
32:f:515:ALA:HB1	32:f:558:LEU:HD21	1.91	0.52
32:f:800:LEU:N	32:f:800:LEU:CD1	2.73	0.52
15:U:255:SER:HB2	15:U:752:THR:HG21	1.92	0.52
15:U:458:ILE:O	15:U:462:LEU:HB2	2.09	0.52
15:U:889:LEU:HD13	15:U:908:ILE:HG13	1.92	0.52
17:W:142:ARG:NH2	17:W:176:SER:O	2.41	0.52
24:d:111:ARG:HB3	24:d:114:GLU:HB2	1.92	0.52
11:q:57:ALA:O	11:q:61:GLN:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:95:LEU:O	16:V:96:ARG:NH1	2.40	0.52
16:V:171:VAL:O	16:V:175:MET:N	2.32	0.52
16:V:203:LEU:O	16:V:207:ALA:HB2	2.09	0.52
16:V:464:ILE:HD12	16:V:465:ASP:HB2	1.91	0.52
21:a:70:ARG:HH21	22:b:80:PRO:HD2	1.75	0.52
24:d:234:ASP:OD1	24:d:236:THR:OG1	2.27	0.52
26:B:310:LEU:HD21	27:A:276:GLU:HB3	1.92	0.52
29:F:233:LYS:N	34:F:501:AGS:O2B	2.42	0.52
32:f:537:THR:OG1	32:f:538:ILE:N	2.42	0.52
32:f:641:GLU:HG3	32:f:641:GLU:O	2.09	0.52
1:G:5:SER:HB2	1:G:19:GLU:HG3	1.90	0.52
19:Y:148:GLY:O	19:Y:153:ASP:N	2.43	0.52
20:Z:142:GLU:OE2	20:Z:153:LYS:NZ	2.38	0.52
1:g:58:ASP:HB3	1:g:61:LEU:HB2	1.91	0.52
7:m:215:TRP:HH2	7:m:219:LEU:HD22	1.75	0.52
8:n:96:ALA:HB1	8:n:98:ILE:HG12	1.90	0.52
9:o:46:ALA:HB3	9:o:97:ALA:HB3	1.91	0.52
32:f:268:LEU:O	32:f:272:LEU:HB2	2.10	0.52
32:f:366:ASP:O	32:f:367:SER:CB	2.57	0.52
32:f:440:ILE:O	32:f:444:ALA:HB2	2.10	0.52
4:J:158:ALA:HB3	5:K:58:LEU:HD22	1.91	0.52
7:M:34:SER:OG	7:M:65:ARG:NH2	2.37	0.52
16:V:316:ALA:O	25:e:4:LYS:NZ	2.40	0.52
23:c:29:GLU:OE1	23:c:180:ASN:ND2	2.43	0.52
29:F:224:LEU:HB2	29:F:348:LEU:HD23	1.92	0.52
29:F:341:ALA:O	29:F:347:ARG:NH1	2.42	0.52
30:C:287:LYS:HG3	30:C:288:ASN:H	1.75	0.52
4:j:2:SER:OG	4:j:3:TYR:N	2.42	0.52
26:B:259:TYR:OH	31:D:275:PHE:O	2.28	0.52
28:E:291:ARG:HD2	28:E:294:ARG:HG3	1.92	0.52
30:C:168:PRO:HG3	30:C:175:PHE:HE2	1.75	0.52
31:D:167:ILE:CA	31:D:214:MET:CE	2.86	0.52
31:D:341:LYS:HE2	31:D:370:ILE:HB	1.92	0.52
32:f:463:LEU:HD22	32:f:466:LEU:CD1	2.40	0.52
5:K:15:PHE:HA	5:K:21:LEU:HA	1.92	0.51
6:L:189:LYS:HA	6:L:192:LEU:HG	1.92	0.51
7:M:8:ASP:O	7:M:22:GLN:NE2	2.42	0.51
15:U:216:VAL:O	15:U:220:LEU:HB2	2.09	0.51
16:V:480:ILE:HG13	20:Z:260:VAL:HG22	1.92	0.51
17:W:259:GLU:HG2	17:W:262:LYS:HB3	1.92	0.51
20:Z:12:HIS:ND1	20:Z:50:VAL:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:m:53:VAL:HB	7:m:208:ALA:HB3	1.92	0.51
27:A:241:ILE:HG22	27:A:243:SER:H	1.75	0.51
32:f:688:ARG:HA	32:f:745:LEU:CD2	2.38	0.51
3:I:108:GLU:OE2	3:I:148:TYR:OH	2.23	0.51
11:Q:57:ALA:O	11:Q:61:GLN:CB	2.57	0.51
28:E:291:ARG:NH1	34:D:501:AGS:O2B	2.43	0.51
31:D:352:MET:HG3	31:D:354:LEU:HB2	1.92	0.51
32:f:24:THR:HG22	32:f:71:TYR:HB2	1.91	0.51
3:I:180:LYS:HD2	3:I:183:GLU:HB2	1.92	0.51
6:l:37:GLY:HA2	6:l:46:LEU:HA	1.92	0.51
7:m:10:SER:HB3	7:m:13:THR:HG23	1.91	0.51
32:f:392:THR:HG22	32:f:417:ILE:HD13	1.92	0.51
3:I:63:GLU:CD	3:I:64:LYS:H	2.18	0.51
7:M:228:PRO:HB2	7:M:231:ILE:HB	1.91	0.51
8:N:7:GLN:HA	8:N:12:VAL:HA	1.91	0.51
17:W:312:MET:HE1	17:W:362:ASN:HD22	1.75	0.51
20:Z:137:ALA:O	20:Z:157:HIS:ND1	2.44	0.51
23:c:241:ASN:HD21	23:c:300:LEU:HB3	1.75	0.51
5:k:85:ALA:HB2	5:k:139:VAL:HG21	1.93	0.51
32:f:127:SER:O	32:f:131:MET:HB3	2.10	0.51
32:f:523:GLY:O	32:f:527:VAL:N	2.43	0.51
32:f:556:ARG:NH1	32:f:786:GLN:OE1	2.44	0.51
5:K:20:ARG:HG3	5:K:21:LEU:H	1.75	0.51
8:N:27:ALA:O	14:t:179:ARG:NH1	2.43	0.51
9:O:16:ALA:HB3	9:O:174:ASP:HB2	1.93	0.51
15:U:213:PHE:HE2	15:U:244:MET:HB2	1.76	0.51
15:U:357:LYS:HE3	15:U:392:TRP:CD2	2.46	0.51
19:Y:82:LYS:HA	19:Y:85:ASP:HB2	1.92	0.51
3:i:216:LEU:HD12	3:i:225:ILE:HG12	1.93	0.51
32:f:632:LYS:HD2	32:f:661:ALA:HA	1.92	0.51
32:f:714:SER:O	32:f:718:ASP:CB	2.55	0.51
17:W:32:ALA:HB1	17:W:86:ASN:HD21	1.76	0.51
19:Y:268:TYR:HB3	19:Y:323:PHE:HD1	1.74	0.51
21:a:33:LEU:HD13	21:a:36:GLN:HB2	1.91	0.51
22:b:2:VAL:O	22:b:47:ASN:ND2	2.39	0.51
1:g:39:SER:OG	1:g:168:ALA:O	2.27	0.51
14:t:27:LEU:HD11	14:t:34:ALA:HB1	1.93	0.51
32:f:485:LEU:HD12	32:f:488:ALA:HB3	1.92	0.51
32:f:502:LEU:HG	32:f:540:GLN:HE22	1.75	0.51
7:M:192:GLU:HA	7:M:195:LYS:HE3	1.93	0.51
11:Q:162:LYS:HB3	12:r:141:ARG:NH2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:126:ILE:HG23	15:U:130:LEU:HD23	1.93	0.51
21:a:216:LEU:HA	21:a:219:HIS:HB2	1.92	0.51
22:b:90:ILE:HD13	22:b:127:LEU:HD13	1.93	0.51
24:d:49:ILE:HD12	24:d:52:ARG:HH11	1.75	0.51
1:g:163:PHE:HD1	2:h:58:ASP:H	1.57	0.51
8:n:142:THR:HB	8:n:155:PHE:HE1	1.75	0.51
32:f:337:LEU:HD22	32:f:337:LEU:H	1.75	0.51
32:f:455:VAL:HG12	32:f:457:ASN:H	1.76	0.51
3:I:3:ARG:HB2	4:J:5:ARG:HH12	1.75	0.51
3:I:135:LEU:HG	3:I:164:ILE:HD11	1.93	0.51
16:V:319:HIS:CD2	25:e:4:LYS:HG3	2.45	0.51
19:Y:101:ARG:NH2	19:Y:126:LYS:O	2.35	0.51
5:k:93:ARG:NH1	12:r:68:LEU:O	2.44	0.51
28:E:80:VAL:HB	31:D:87:LEU:HB2	1.93	0.51
32:f:389:LYS:HD2	32:f:418:LEU:HD21	1.92	0.51
32:f:463:LEU:HD22	32:f:466:LEU:HD11	1.93	0.51
32:f:623:LYS:O	32:f:627:GLU:HB2	2.11	0.51
7:M:230:ASP:OD1	7:M:230:ASP:N	2.42	0.51
17:W:320:LEU:O	17:W:324:TYR:HB2	2.11	0.51
17:W:427:ASP:OD2	23:c:243:SER:OG	2.27	0.51
23:c:71:ASP:HB2	23:c:104:ARG:HH11	1.76	0.51
4:j:159:ASN:OD1	4:j:160:ALA:N	2.44	0.51
32:f:337:LEU:N	32:f:337:LEU:CD2	2.73	0.51
32:f:380:PHE:CG	32:f:751:TYR:CE2	2.99	0.51
19:Y:311:TYR:HD2	19:Y:314:LEU:HD12	1.75	0.51
24:d:200:PHE:HB3	24:d:203:PRO:HB3	1.93	0.51
5:k:99:HIS:O	5:k:103:TYR:HB2	2.10	0.51
7:m:36:ALA:N	7:m:165:ILE:O	2.42	0.51
12:r:21:THR:HG22	12:r:26:ILE:HG12	1.93	0.51
13:s:5:TYR:OH	13:s:103:PRO:O	2.27	0.51
26:B:214:MET:HG2	27:A:363:SER:HB2	1.92	0.51
31:D:248:ARG:HG2	31:D:295:GLN:HE22	1.76	0.51
32:f:647:GLY:HA2	32:f:655:LEU:HG	1.93	0.51
1:G:190:THR:H	1:G:193:GLN:HB3	1.76	0.50
6:L:44:ALA:HB1	6:L:144:ILE:HD11	1.94	0.50
15:U:167:ILE:HD12	15:U:204:ILE:HG21	1.92	0.50
16:V:306:ARG:HD3	16:V:339:LEU:HD11	1.93	0.50
18:X:420:LYS:HZ1	20:Z:276:ILE:HD13	1.75	0.50
7:m:34:SER:OG	7:m:35:THR:N	2.44	0.50
32:f:336:GLU:HG3	32:f:337:LEU:H	1.76	0.50
32:f:631:LYS:HA	32:f:634:LYS:HZ2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:d:182:ILE:HD12	24:d:186:TYR:HD2	1.76	0.50
34:E:401:AGS:O1A	34:E:401:AGS:O2B	2.28	0.50
32:f:536:SER:HA	32:f:539:LEU:HB3	1.93	0.50
7:M:10:SER:HB3	7:M:13:THR:HG23	1.93	0.50
16:V:353:LEU:HG	16:V:357:LEU:HD23	1.93	0.50
17:W:377:ARG:HA	17:W:380:GLN:HG2	1.93	0.50
20:Z:249:PHE:HE2	24:d:235:THR:HA	1.76	0.50
22:b:109:ILE:HB	22:b:138:VAL:HG22	1.94	0.50
9:o:96:ALA:H	9:o:115:PRO:HB3	1.76	0.50
28:E:197:LYS:HG2	28:E:231:PHE:HB3	1.93	0.50
32:f:657:ILE:HA	32:f:660:ILE:HD12	1.94	0.50
32:f:745:LEU:HD12	32:f:745:LEU:C	2.36	0.50
10:P:2:SER:OG	10:P:3:ILE:N	2.44	0.50
15:U:469:SER:OG	15:U:470:ASN:N	2.44	0.50
5:k:203:LYS:HA	5:k:206:MET:HG2	1.93	0.50
28:E:101:ASP:OD2	28:E:104:THR:N	2.44	0.50
32:f:790:GLN:HG3	32:f:792:ALA:H	1.76	0.50
3:I:57:ASP:HB3	3:I:59:VAL:HG13	1.93	0.50
4:J:180:ALA:HB1	4:J:190:LEU:HD22	1.93	0.50
5:K:117:SER:HB3	6:L:82:ARG:HH22	1.75	0.50
8:N:18:SER:HB2	8:N:31:THR:H	1.77	0.50
13:S:150:ASP:OD2	10:p:177:ARG:NH2	2.41	0.50
15:U:235:LYS:O	15:U:239:GLU:HB2	2.11	0.50
15:U:630:PRO:HG2	15:U:663:THR:HG21	1.94	0.50
16:V:210:CYS:O	16:V:214:HIS:HB2	2.11	0.50
17:W:178:GLU:OE1	17:W:181:GLU:N	2.36	0.50
22:b:157:VAL:HG21	22:b:170:LEU:HB2	1.93	0.50
28:E:57:VAL:HG13	28:E:97:ARG:HD3	1.94	0.50
32:f:343:LYS:NZ	32:f:804:LEU:HD23	2.26	0.50
2:H:118:MET:HE2	2:H:151:PRO:HA	1.93	0.50
12:R:141:ARG:NH2	11:q:162:LYS:HB3	2.26	0.50
15:U:410:VAL:HG13	15:U:780:SER:HB3	1.93	0.50
15:U:719:ASP:O	15:U:727:LYS:NZ	2.41	0.50
16:V:368:ARG:NH2	25:e:47:ASN:OD1	2.44	0.50
18:X:331:LEU:HD23	18:X:364:LYS:HG2	1.94	0.50
14:t:46:ASN:OD1	14:t:46:ASN:N	2.43	0.50
32:f:226:TYR:O	32:f:230:CYS:HB2	2.11	0.50
2:H:39:LYS:HE2	2:H:144:PRO:HG2	1.93	0.50
4:J:159:ASN:OD1	4:J:160:ALA:N	2.44	0.50
16:V:39:GLU:O	16:V:43:THR:HB	2.12	0.50
16:V:264:TYR:O	16:V:266:GLN:N	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:102:ALA:HA	17:W:105:VAL:HG22	1.94	0.50
18:X:90:ARG:NH2	18:X:125:LEU:O	2.45	0.50
18:X:122:ARG:HD2	18:X:125:LEU:HB2	1.93	0.50
23:c:111:TRP:NE1	23:c:130:GLN:OE1	2.38	0.50
4:j:156:TRP:CD1	5:k:59:MET:HA	2.46	0.50
10:p:7:ASN:ND2	10:p:29:GLY:O	2.38	0.50
30:C:72:TYR:HB2	30:C:116:LEU:HB3	1.92	0.50
30:C:91:PRO:HG2	30:C:92:GLU:HG3	1.94	0.50
30:C:161:ILE:HA	30:C:164:VAL:HG12	1.92	0.50
30:C:307:ARG:HH21	30:C:310:ARG:HH21	1.59	0.50
31:D:407:ILE:HG22	31:D:409:LYS:H	1.77	0.50
7:M:236:GLU:HA	7:M:239:ALA:HB3	1.92	0.50
21:a:135:ILE:HG12	21:a:158:LEU:HD13	1.94	0.50
1:g:144:ASP:OD2	9:o:72:ARG:NH2	2.32	0.50
5:k:37:ALA:HB2	5:k:50:VAL:HG23	1.94	0.50
32:f:311:VAL:CB	32:f:490:ALA:CB	2.77	0.50
32:f:347:ASP:O	32:f:351:THR:OG1	2.25	0.50
9:O:18:THR:HB	9:O:31:CYS:H	1.77	0.50
14:T:46:ASN:OD1	14:T:46:ASN:N	2.42	0.50
15:U:607:VAL:O	15:U:615:ARG:NH1	2.38	0.50
16:V:185:GLN:O	16:V:189:ASP:HB2	2.12	0.50
24:d:148:TYR:HH	24:d:181:CYS:HG	1.60	0.50
5:k:117:SER:HB3	6:l:82:ARG:HH22	1.77	0.50
6:l:65:HIS:O	6:l:89:ARG:NH2	2.36	0.50
7:m:163:CYS:SG	7:m:164:ALA:N	2.85	0.50
9:o:18:THR:HB	9:o:31:CYS:H	1.77	0.50
26:B:387:LYS:HB3	26:B:390:LEU:HD23	1.93	0.50
34:E:401:AGS:S1G	29:F:347:ARG:NH2	2.83	0.50
31:D:95:ALA:HA	31:D:101:ALA:HA	1.94	0.50
32:f:234:THR:HG23	32:f:637:LYS:HE2	1.94	0.50
32:f:392:THR:CG2	32:f:417:ILE:HD13	2.42	0.50
32:f:479:LEU:CD2	32:f:513:GLU:HB3	2.39	0.50
32:f:675:PHE:O	32:f:679:LEU:CB	2.59	0.50
3:I:149:GLN:NE2	3:I:163:CYS:O	2.45	0.49
6:L:65:HIS:O	6:L:89:ARG:NH2	2.38	0.49
16:V:32:PRO:O	16:V:36:GLU:HB3	2.12	0.49
16:V:349:ARG:HA	16:V:353:LEU:HD23	1.93	0.49
19:Y:173:ASP:OD2	19:Y:176:ARG:NH2	2.44	0.49
3:i:99:LEU:O	11:q:86:ARG:NH2	2.45	0.49
26:B:223:ILE:HG13	26:B:347:ILE:HG21	1.94	0.49
30:C:217:SER:HB3	30:C:220:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:479:LEU:HA	32:f:517:VAL:HG21	1.93	0.49
32:f:691:PRO:HB3	32:f:749:ALA:CB	2.39	0.49
32:f:691:PRO:HA	32:f:694:LEU:HB3	1.93	0.49
4:J:156:TRP:CD1	5:K:59:MET:HA	2.47	0.49
6:L:146:GLN:HE21	6:L:154:PHE:HD2	1.58	0.49
16:V:108:LEU:HA	16:V:111:TYR:HD2	1.76	0.49
2:h:40:ALA:HB1	2:h:182:LEU:HB2	1.95	0.49
14:t:192:VAL:HG12	14:t:197:VAL:HG22	1.95	0.49
26:B:136:LEU:HD12	26:B:160:ILE:HA	1.94	0.49
26:B:303:ARG:O	26:B:307:ARG:NH2	2.45	0.49
15:U:220:LEU:HD13	15:U:248:ILE:HD11	1.94	0.49
17:W:131:VAL:O	17:W:144:ARG:NH2	2.46	0.49
17:W:152:ILE:HD11	17:W:165:ILE:HB	1.95	0.49
20:Z:202:ASN:OD1	20:Z:203:SER:N	2.45	0.49
32:f:531:ASN:HA	32:f:569:LYS:HA	1.93	0.49
7:M:198:TYR:CG	7:M:239:ALA:HB1	2.46	0.49
15:U:347:ASN:ND2	15:U:813:TYR:O	2.45	0.49
15:U:460:TYR:HD2	15:U:461:LEU:HD12	1.77	0.49
20:Z:184:VAL:HA	20:Z:188:SER:HB2	1.94	0.49
24:d:175:ARG:HH11	24:d:199:PHE:HD2	1.58	0.49
27:A:122:VAL:HB	29:F:88:TYR:HB2	1.94	0.49
34:A:501:AGS:O2A	34:A:501:AGS:O2B	2.30	0.49
31:D:321:LEU:HB3	31:D:327:LEU:HD12	1.94	0.49
16:V:211:TYR:HA	16:V:214:HIS:HB3	1.94	0.49
17:W:441:LYS:NZ	20:Z:203:SER:OG	2.44	0.49
27:A:177:VAL:HG13	27:A:224:LEU:HD12	1.94	0.49
28:E:180:LYS:HG2	28:E:301:ILE:HD12	1.94	0.49
32:f:94:LYS:HA	32:f:97:LYS:HG2	1.94	0.49
15:U:36:ALA:HB2	15:U:70:HIS:HE1	1.77	0.49
17:W:183:VAL:HA	17:W:186:ILE:HG22	1.94	0.49
19:Y:210:SER:HB3	19:Y:213:LEU:HB2	1.94	0.49
24:d:164:THR:HA	24:d:167:ILE:HG12	1.95	0.49
24:d:236:THR:O	24:d:240:THR:N	2.36	0.49
6:l:166:GLN:OE1	6:l:169:ARG:NH1	2.46	0.49
28:E:177:GLY:N	34:E:401:AGS:O2G	2.45	0.49
30:C:191:PRO:HG2	30:C:319:PRO:HG3	1.94	0.49
13:S:177:ASP:OD2	9:o:200:GLY:N	2.45	0.49
16:V:203:LEU:HA	16:V:206:VAL:HB	1.94	0.49
19:Y:215:ASP:HB3	19:Y:218:THR:HG23	1.95	0.49
19:Y:238:GLU:HA	19:Y:242:LYS:HB2	1.95	0.49
24:d:207:THR:O	24:d:211:LYS:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:190:THR:H	1:g:193:GLN:HB3	1.78	0.49
5:k:70:ILE:HD11	5:k:89:ILE:HD12	1.94	0.49
7:m:152:ASP:OD1	7:m:156:VAL:N	2.45	0.49
10:p:58:THR:OG1	11:q:121:LEU:O	2.22	0.49
28:E:97:ARG:HE	28:E:111:LEU:HB2	1.78	0.49
31:D:88:VAL:HG23	31:D:132:LEU:HB2	1.95	0.49
32:f:333:LEU:HA	32:f:338:ASP:HB2	1.95	0.49
32:f:372:LEU:C	32:f:372:LEU:CD2	2.85	0.49
32:f:387:GLN:N	32:f:387:GLN:NE2	2.60	0.49
32:f:478:ARG:NE	32:f:504:VAL:HG22	2.27	0.49
4:J:32:ALA:HB3	4:J:161:ILE:HD11	1.94	0.49
5:K:182:GLN:NE2	6:L:55:GLU:OE1	2.44	0.49
17:W:248:ARG:HD2	17:W:286:LEU:HD11	1.94	0.49
17:W:272:LEU:HD12	17:W:336:PRO:HB2	1.95	0.49
18:X:255:LEU:HD22	18:X:267:VAL:HG13	1.95	0.49
32:f:471:LEU:CG	32:f:509:LYS:CE	2.56	0.49
6:L:156:CYS:HA	7:M:58:TYR:HA	1.95	0.49
16:V:440:LYS:O	16:V:444:ASP:HB2	2.13	0.49
21:a:84:VAL:HG21	21:a:121:LEU:HD11	1.95	0.49
24:d:114:GLU:HA	24:d:117:THR:HG22	1.95	0.49
24:d:176:ASP:HA	24:d:179:ALA:HB3	1.94	0.49
4:j:11:SER:OG	4:j:15:HIS:N	2.38	0.49
6:l:117:GLN:O	6:l:120:THR:OG1	2.27	0.49
7:m:198:TYR:CG	7:m:239:ALA:HB1	2.48	0.49
10:p:113:ASP:OD2	10:p:116:THR:OG1	2.28	0.49
11:q:81:ALA:O	11:q:84:THR:OG1	2.27	0.49
28:E:294:ARG:NH2	34:D:501:AGS:S1G	2.74	0.49
30:C:147:THR:HG22	30:C:150:MET:HE3	1.94	0.49
32:f:517:VAL:O	32:f:521:ALA:CB	2.60	0.49
32:f:517:VAL:O	32:f:521:ALA:HB3	2.12	0.49
6:L:46:LEU:HD13	6:L:73:SER:HB2	1.94	0.49
10:P:177:ARG:NH2	13:s:150:ASP:OD2	2.40	0.49
15:U:418:GLU:O	15:U:422:LEU:HB2	2.13	0.49
19:Y:204:THR:HA	19:Y:219:PHE:HE2	1.78	0.49
6:l:84:LEU:HD12	6:l:130:VAL:HG21	1.94	0.49
27:A:103:ASN:HA	27:A:136:GLU:HG2	1.95	0.49
32:f:514:VAL:O	32:f:518:THR:OG1	2.25	0.49
3:I:174:MET:HE3	3:I:174:MET:HB2	1.63	0.48
5:K:167:ALA:H	6:L:56:LEU:HD13	1.77	0.48
7:M:152:ASP:OD1	7:M:156:VAL:N	2.44	0.48
18:X:394:ASP:O	18:X:398:GLU:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:d:250:ALA:O	24:d:254:GLU:CB	2.59	0.48
2:h:118:MET:HE3	2:h:130:PHE:HB2	1.95	0.48
26:B:106:PRO:HB3	30:C:121:TYR:HB2	1.95	0.48
28:E:167:PRO:O	28:E:274:LYS:NZ	2.39	0.48
28:E:322:LYS:HD3	28:E:326:ILE:HG13	1.94	0.48
32:f:253:LEU:O	32:f:257:ARG:CB	2.61	0.48
9:o:110:LEU:HD21	9:o:125:VAL:HG22	1.95	0.48
27:A:333:ARG:NH2	27:A:336:ARG:CZ	2.66	0.48
29:F:281:SER:OG	29:F:325:GLN:O	2.30	0.48
30:C:182:GLN:HG3	30:C:287:LYS:HE3	1.95	0.48
32:f:487:LEU:HD22	32:f:801:VAL:HG11	1.95	0.48
3:I:47:ALA:HB3	3:I:212:GLU:HB3	1.94	0.48
4:J:11:SER:OG	4:J:15:HIS:N	2.36	0.48
10:P:61:GLN:HE22	11:Q:124:LEU:HB2	1.77	0.48
12:R:59:LEU:HD22	12:R:83:LEU:HB2	1.96	0.48
15:U:17:PRO:O	15:U:20:LYS:N	2.45	0.48
15:U:36:ALA:O	16:V:264:TYR:OH	2.31	0.48
16:V:46:GLY:O	16:V:50:GLU:HB2	2.12	0.48
17:W:55:ARG:NH1	17:W:75:TYR:O	2.47	0.48
19:Y:347:ILE:HG13	19:Y:354:VAL:HG22	1.94	0.48
22:b:122:LYS:HA	22:b:125:VAL:HG12	1.94	0.48
27:A:415:LYS:NZ	27:A:420:TYR:OH	2.46	0.48
28:E:235:ILE:HD11	28:E:277:MET:HB3	1.94	0.48
30:C:46:GLN:HB3	31:D:61:ILE:HG21	1.93	0.48
31:D:300:ASP:HB2	31:D:303:VAL:HG23	1.96	0.48
5:K:54:ILE:HA	5:K:59:MET:HE1	1.96	0.48
9:O:31:CYS:SG	9:O:32:SER:N	2.85	0.48
11:Q:88:LEU:HB3	11:Q:122:ALA:HB2	1.95	0.48
15:U:568:GLU:OE2	15:U:572:ARG:NH2	2.46	0.48
17:W:111:TYR:O	17:W:115:ILE:N	2.45	0.48
17:W:447:ALA:HB1	20:Z:226:ILE:HG21	1.94	0.48
18:X:262:ASN:ND2	18:X:329:ASN:OD1	2.47	0.48
24:d:183:GLU:HA	24:d:215:TRP:HZ2	1.78	0.48
30:C:248:MET:HE1	30:C:273:MET:HG2	1.96	0.48
9:O:96:ALA:H	9:O:115:PRO:HB3	1.79	0.48
14:T:178:TYR:OH	14:T:208:ASN:N	2.40	0.48
16:V:110:HIS:HA	16:V:113:LEU:HB2	1.95	0.48
19:Y:192:ARG:NH2	19:Y:290:PRO:O	2.46	0.48
19:Y:261:PHE:O	19:Y:265:GLU:CB	2.61	0.48
26:B:232:LYS:HD2	26:B:330:ALA:HB1	1.96	0.48
27:A:300:LEU:HD23	27:A:303:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:C:57:ARG:NH1	31:D:71:GLU:OE1	2.39	0.48
30:C:333:SER:HB2	30:C:338:LEU:HD11	1.95	0.48
32:f:445:LEU:HG	32:f:462:ALA:HB2	1.95	0.48
32:f:456:ARG:HD3	32:f:489:TYR:CZ	2.49	0.48
32:f:597:VAL:HG22	32:f:630:ASP:HB2	1.95	0.48
10:P:62:THR:OG1	11:Q:85:ARG:NH2	2.43	0.48
23:c:118:PHE:HE2	28:E:103:THR:HB	1.78	0.48
1:g:71:LYS:O	1:g:95:ARG:NH2	2.45	0.48
3:i:108:GLU:OE2	3:i:148:TYR:OH	2.30	0.48
6:l:109:VAL:HG21	6:l:145:PHE:HD2	1.78	0.48
14:T:192:VAL:HG12	14:T:197:VAL:HG22	1.96	0.48
15:U:92:ASP:OD2	15:U:140:ARG:NH1	2.47	0.48
18:X:194:ARG:HD2	18:X:210:LEU:HD21	1.94	0.48
23:c:241:ASN:ND2	23:c:300:LEU:O	2.46	0.48
8:n:40:ARG:NH1	8:n:180:ALA:O	2.46	0.48
3:I:105:ILE:HA	3:I:106:PRO:HD3	1.78	0.48
5:K:91:LYS:NZ	5:K:95:GLU:OE2	2.41	0.48
15:U:428:PRO:HB3	15:U:439:GLU:HB2	1.95	0.48
17:W:361:HIS:HA	17:W:364:ARG:HH11	1.79	0.48
19:Y:132:VAL:HA	19:Y:137:ARG:HH12	1.79	0.48
22:b:50:GLY:H	22:b:64:LEU:HD12	1.78	0.48
26:B:264:PRO:HA	26:B:311:GLU:HG2	1.96	0.48
31:D:129:SER:HG	31:D:252:ARG:HH12	1.55	0.48
32:f:166:VAL:O	32:f:170:TRP:HB2	2.14	0.48
32:f:392:THR:HA	32:f:414:LEU:CD2	2.44	0.48
4:J:119:THR:HG22	4:J:126:PRO:HB3	1.96	0.48
14:T:45:VAL:HB	14:T:49:THR:HG23	1.96	0.48
15:U:173:VAL:HG13	15:U:176:MET:HB2	1.96	0.48
18:X:90:ARG:HH21	18:X:129:LEU:HG	1.77	0.48
19:Y:224:VAL:HG11	19:Y:256:VAL:HG13	1.96	0.48
4:j:158:ALA:HB3	5:k:58:LEU:HD22	1.94	0.48
26:B:310:LEU:HD11	27:A:276:GLU:HG2	1.96	0.48
30:C:33:LEU:HD22	31:D:47:LEU:HD13	1.95	0.48
32:f:336:GLU:HB3	32:f:337:LEU:HD23	1.95	0.48
12:R:133:VAL:HG21	11:q:137:PHE:HB3	1.95	0.48
16:V:130:PHE:O	16:V:134:PHE:N	2.47	0.48
17:W:237:GLU:HG2	17:W:238:GLY:H	1.77	0.48
11:q:138:LEU:HD13	11:q:171:PHE:HE1	1.79	0.48
14:t:136:SER:HB2	14:t:150:LEU:HD13	1.95	0.48
26:B:347:ILE:O	26:B:350:LYS:NZ	2.42	0.48
32:f:252:ALA:O	32:f:256:PHE:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:331:LEU:O	32:f:335:ARG:NH1	2.47	0.48
32:f:336:GLU:HG3	32:f:337:LEU:CD2	2.38	0.48
32:f:336:GLU:CG	32:f:337:LEU:CD2	2.92	0.48
32:f:343:LYS:O	32:f:347:ASP:N	2.40	0.48
2:H:107:THR:HA	2:H:110:LEU:HD13	1.95	0.47
5:K:45:GLY:HA3	5:K:221:GLN:HG3	1.94	0.47
15:U:208:LEU:HD23	15:U:210:LYS:H	1.79	0.47
17:W:190:MET:HB3	17:W:205:ILE:HD11	1.96	0.47
27:A:282:GLY:O	27:A:328:ASP:N	2.47	0.47
29:F:94:ILE:HD11	29:F:125:LYS:HB2	1.96	0.47
30:C:113:ARG:NH2	30:C:129:ASN:O	2.47	0.47
32:f:30:GLY:O	32:f:34:ARG:HB2	2.14	0.47
32:f:140:LEU:O	32:f:144:LEU:CB	2.61	0.47
32:f:695:ALA:CB	32:f:752:HIS:HB3	2.44	0.47
1:G:89:SER:OG	7:M:117:MET:SD	2.70	0.47
10:P:58:THR:O	11:Q:85:ARG:NH2	2.47	0.47
12:R:97:MET:O	12:R:116:SER:N	2.47	0.47
16:V:342:ILE:HD12	16:V:343:PRO:HD2	1.96	0.47
9:o:106:THR:OG1	9:o:109:HIS:NE2	2.39	0.47
34:E:401:AGS:O1B	34:E:401:AGS:O2G	2.31	0.47
30:C:137:LEU:HD11	30:C:220:VAL:HG22	1.96	0.47
32:f:127:SER:O	32:f:131:MET:HB2	2.13	0.47
32:f:376:PHE:CZ	32:f:416:MET:CE	2.95	0.47
32:f:692:LEU:HG	32:f:752:HIS:HE1	1.77	0.47
24:d:67:ASP:O	24:d:71:PHE:N	2.46	0.47
5:k:41:GLN:HE21	5:k:151:PRO:HG2	1.78	0.47
7:m:15:SER:OG	7:m:18:GLY:N	2.42	0.47
7:m:99:ARG:NH2	7:m:105:ASN:OD1	2.47	0.47
32:f:389:LYS:HB3	32:f:392:THR:HG21	1.95	0.47
32:f:453:SER:O	32:f:488:ALA:O	2.31	0.47
10:P:126:LEU:HD12	10:P:127:ILE:HG23	1.95	0.47
15:U:167:ILE:HB	15:U:177:LEU:HD21	1.96	0.47
16:V:440:LYS:NZ	24:d:177:GLU:OE2	2.40	0.47
21:a:76:LEU:O	21:a:80:ILE:HB	2.14	0.47
23:c:94:LYS:HG2	23:c:98:MET:HE3	1.96	0.47
24:d:78:LEU:HD23	24:d:81:TYR:HD2	1.78	0.47
24:d:129:THR:OG1	24:d:130:ASN:N	2.47	0.47
3:i:162:THR:OG1	3:i:163:CYS:N	2.47	0.47
27:A:169:LYS:HZ3	32:f:714:SER:CB	2.28	0.47
30:C:196:LYS:HB3	30:C:294:ALA:HB1	1.96	0.47
32:f:424:GLY:HA2	32:f:427:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:538:ILE:HA	32:f:541:THR:HG22	1.97	0.47
11:Q:102:LEU:HD22	11:Q:102:LEU:HA	1.76	0.47
15:U:173:VAL:HG11	15:U:177:LEU:HD13	1.95	0.47
17:W:124:LEU:HD13	17:W:151:THR:HG22	1.97	0.47
24:d:195:THR:HG23	24:d:201:ASN:HA	1.96	0.47
24:d:208:ASP:O	24:d:212:LYS:HB3	2.15	0.47
3:i:174:MET:HE3	3:i:174:MET:HB2	1.79	0.47
29:F:314:LEU:HD21	29:F:342:LEU:HD23	1.97	0.47
6:L:117:GLN:O	6:L:120:THR:OG1	2.29	0.47
10:P:159:ASP:N	10:P:159:ASP:OD1	2.45	0.47
18:X:339:ILE:HG21	18:X:374:PHE:HE1	1.79	0.47
1:g:114:LEU:HD22	1:g:140:LEU:HD21	1.95	0.47
4:j:38:ARG:NH1	4:j:181:ILE:O	2.47	0.47
4:j:195:LEU:O	4:j:201:SER:OG	2.29	0.47
6:l:42:THR:O	6:l:137:TYR:OH	2.31	0.47
10:p:26:ARG:HH21	10:p:38:ASP:HA	1.80	0.47
13:s:36:HIS:O	14:t:151:ARG:NH2	2.36	0.47
32:f:209:MET:SD	32:f:213:GLN:NE2	2.87	0.47
32:f:315:GLU:HA	32:f:318:THR:HG22	1.95	0.47
32:f:688:ARG:CA	32:f:745:LEU:HD22	2.44	0.47
9:O:106:THR:OG1	9:O:109:HIS:NE2	2.39	0.47
15:U:84:ALA:HB3	15:U:88:PHE:HB2	1.97	0.47
15:U:383:ASP:HB3	15:U:386:LEU:HB2	1.95	0.47
16:V:365:GLN:HE22	25:e:50:ASP:HA	1.79	0.47
16:V:416:ARG:HA	16:V:459:GLN:HA	1.96	0.47
19:Y:192:ARG:NH1	25:e:40:GLU:OE1	2.48	0.47
21:a:373:ASP:O	21:a:376:THR:OG1	2.33	0.47
22:b:53:THR:OG1	22:b:54:LEU:N	2.47	0.47
22:b:131:LEU:HA	22:b:134:GLU:HB2	1.96	0.47
11:q:88:LEU:HB3	11:q:122:ALA:HB2	1.95	0.47
28:E:248:SER:HA	28:E:251:ARG:HD3	1.95	0.47
29:F:97:LEU:N	29:F:121:CYS:O	2.48	0.47
29:F:311:LEU:HD23	29:F:314:LEU:HD12	1.97	0.47
29:F:430:LYS:HD3	29:F:432:LYS:HG3	1.97	0.47
31:D:280:GLY:HA2	31:D:283:ARG:HE	1.80	0.47
32:f:559:PRO:HA	32:f:562:LEU:HB2	1.96	0.47
32:f:645:ASP:HB3	32:f:648:ALA:HB3	1.95	0.47
7:M:54:LEU:HB2	7:M:57:LEU:HG	1.96	0.47
7:M:55:SER:H	7:M:57:LEU:HD23	1.79	0.47
15:U:219:CYS:SG	15:U:220:LEU:N	2.87	0.47
16:V:79:VAL:HG22	16:V:80:LYS:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:323:GLY:O	16:V:326:GLN:N	2.47	0.47
21:a:324:ILE:HG13	21:a:331:VAL:HG13	1.97	0.47
22:b:25:ARG:NH2	22:b:145:GLU:OE1	2.32	0.47
22:b:156:PHE:O	22:b:160:LEU:HB2	2.15	0.47
26:B:286:GLU:OE2	34:B:501:AGS:O2G	2.33	0.47
27:A:140:VAL:HG12	27:A:152:PRO:HA	1.96	0.47
2:H:6:TYR:HE2	2:H:126:GLY:HA3	1.80	0.47
7:M:175:GLU:N	7:M:175:GLU:OE1	2.47	0.47
13:S:36:HIS:O	14:T:151:ARG:NH2	2.48	0.47
15:U:229:VAL:HG13	15:U:264:VAL:HG21	1.97	0.47
15:U:408:LEU:O	15:U:412:HIS:ND1	2.33	0.47
16:V:131:LEU:HD23	16:V:134:PHE:HD2	1.79	0.47
17:W:38:GLY:H	17:W:44:ILE:HD12	1.79	0.47
18:X:172:LEU:HD12	18:X:175:LYS:HD3	1.97	0.47
18:X:321:THR:O	18:X:325:LYS:HB2	2.15	0.47
19:Y:174:TRP:CD1	30:C:338:LEU:H	2.32	0.47
20:Z:34:ARG:HH11	20:Z:58:PHE:HE2	1.61	0.47
20:Z:228:TYR:HD2	21:a:338:PRO:HB2	1.80	0.47
20:Z:244:GLU:HA	20:Z:247:LYS:HD3	1.97	0.47
30:C:141:GLU:O	31:D:323:ARG:NH1	2.47	0.47
7:M:163:CYS:SG	7:M:164:ALA:N	2.88	0.47
15:U:789:ILE:HB	15:U:911:ILE:HA	1.97	0.47
16:V:106:ARG:O	16:V:110:HIS:ND1	2.40	0.47
21:a:42:LEU:O	21:a:46:GLN:CB	2.63	0.47
24:d:51:ALA:HA	24:d:54:ILE:HG12	1.97	0.47
6:l:146:GLN:HE21	6:l:154:PHE:HD2	1.62	0.47
27:A:88:GLN:HA	27:A:91:GLN:HG2	1.97	0.47
29:F:375:VAL:HG22	29:F:415:LEU:HD12	1.96	0.47
32:f:376:PHE:CZ	32:f:798:THR:HG22	2.50	0.47
32:f:475:ASN:O	32:f:478:ARG:HB3	2.15	0.47
32:f:479:LEU:HD23	32:f:513:GLU:CB	2.42	0.47
32:f:541:THR:O	32:f:545:LYS:CB	2.63	0.47
32:f:626:GLU:OE1	32:f:782:HIS:NE2	2.47	0.47
2:H:93:LEU:HD11	2:H:113:ARG:HB3	1.95	0.46
3:I:136:TYR:HB2	3:I:148:TYR:HB2	1.97	0.46
4:J:73:PHE:HA	4:J:131:ALA:HA	1.97	0.46
5:K:196:LYS:HA	5:K:199:LEU:HG	1.98	0.46
14:T:136:SER:HB2	14:T:150:LEU:HD13	1.96	0.46
16:V:303:SER:HA	16:V:306:ARG:HG2	1.97	0.46
3:i:63:GLU:CD	3:i:64:LYS:H	2.23	0.46
32:f:664:GLU:O	32:f:665:GLU:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:37:ALA:HB3	5:K:170:ILE:HD11	1.97	0.46
15:U:202:VAL:HG11	15:U:219:CYS:SG	2.55	0.46
16:V:179:LYS:HD2	16:V:214:HIS:ND1	2.30	0.46
17:W:162:ALA:HB1	17:W:192:LEU:HB3	1.97	0.46
18:X:111:LEU:HD23	18:X:114:ILE:HD12	1.97	0.46
18:X:191:THR:HG23	30:C:381:GLU:HG3	1.97	0.46
2:h:80:GLY:HA2	2:h:83:TYR:HB3	1.97	0.46
32:f:248:LEU:O	32:f:252:ALA:CB	2.62	0.46
32:f:392:THR:HB	32:f:414:LEU:HD22	1.98	0.46
6:L:146:GLN:HE22	6:L:159:MET:HE2	1.79	0.46
7:M:99:ARG:NH2	7:M:105:ASN:OD1	2.48	0.46
7:M:170:GLN:HA	7:M:173:LYS:HG2	1.98	0.46
12:R:38:ASN:HD22	12:R:41:LEU:HD12	1.80	0.46
13:S:145:LEU:HD22	13:S:178:VAL:HB	1.97	0.46
16:V:81:GLN:HB2	16:V:86:VAL:HB	1.97	0.46
17:W:312:MET:HE2	17:W:314:LEU:HA	1.98	0.46
20:Z:222:ILE:H	20:Z:222:ILE:HG13	1.39	0.46
20:Z:258:VAL:HG11	23:c:249:LEU:HD22	1.95	0.46
13:s:176:LYS:HE2	13:s:208:VAL:HG21	1.97	0.46
30:C:337:ASN:ND2	30:C:376:VAL:O	2.49	0.46
32:f:226:TYR:O	32:f:230:CYS:HB3	2.16	0.46
32:f:281:ILE:O	32:f:285:CYS:HB3	2.15	0.46
6:L:18:ARG:NH1	6:L:23:GLU:OE2	2.47	0.46
13:S:176:LYS:HE2	13:S:208:VAL:HG21	1.96	0.46
15:U:506:ALA:HB1	15:U:543:LYS:HB2	1.97	0.46
15:U:770:TRP:HD1	23:c:178:THR:HB	1.79	0.46
16:V:201:ARG:HE	16:V:242:HIS:HB3	1.79	0.46
18:X:335:LEU:HA	18:X:338:VAL:HG22	1.98	0.46
24:d:234:ASP:HA	24:d:236:THR:N	2.29	0.46
4:j:7:ILE:HD13	4:j:7:ILE:HA	1.84	0.46
6:l:158:ALA:HB1	6:l:172:LEU:HD13	1.97	0.46
7:m:228:PRO:HB2	7:m:231:ILE:HB	1.97	0.46
11:q:11:ASP:N	11:q:11:ASP:OD1	2.48	0.46
32:f:691:PRO:HG2	32:f:745:LEU:CD1	2.41	0.46
32:f:695:ALA:O	32:f:752:HIS:HB3	2.15	0.46
3:I:50:ARG:HD3	3:I:50:ARG:HA	1.64	0.46
4:J:7:ILE:HD13	4:J:7:ILE:HA	1.83	0.46
5:K:117:SER:O	6:L:82:ARG:NH2	2.48	0.46
11:Q:19:ARG:HH21	11:Q:31:ASP:HB2	1.79	0.46
15:U:94:SER:OG	15:U:95:GLU:N	2.48	0.46
17:W:187:LEU:HB2	17:W:226:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:424:LEU:HA	17:W:427:ASP:HB3	1.98	0.46
21:a:272:ILE:HA	21:a:275:LEU:HB3	1.97	0.46
5:k:206:MET:HE1	5:k:210:LEU:HD13	1.97	0.46
28:E:60:VAL:HG22	28:E:71:VAL:HG12	1.97	0.46
32:f:178:LYS:NZ	32:f:215:ASP:O	2.42	0.46
16:V:268:GLU:O	16:V:272:SER:OG	2.24	0.46
17:W:93:ARG:N	17:W:96:GLN:HE21	2.13	0.46
20:Z:109:ASN:HD22	20:Z:155:PHE:HE1	1.63	0.46
24:d:33:LEU:HD11	24:d:38:THR:HG21	1.96	0.46
8:n:29:ARG:HH22	9:o:139:GLU:CD	2.22	0.46
12:r:38:ASN:HD22	12:r:41:LEU:HD12	1.80	0.46
32:f:193:PRO:C	32:f:208:LEU:HD12	2.40	0.46
5:K:236:GLU:HA	5:K:239:LYS:HE3	1.96	0.46
7:M:52:LEU:HA	7:M:209:PHE:HA	1.97	0.46
7:M:110:HIS:NE2	8:N:70:LEU:HD23	2.30	0.46
15:U:374:SER:HB3	15:U:407:SER:HB3	1.97	0.46
17:W:444:HIS:HB3	20:Z:230:LEU:HD22	1.97	0.46
20:Z:39:LEU:H	20:Z:94:TRP:HA	1.81	0.46
24:d:111:ARG:O	24:d:115:PHE:N	2.46	0.46
7:m:40:ARG:HA	7:m:45:VAL:HA	1.97	0.46
32:f:79:ARG:HE	32:f:95:PRO:HG3	1.80	0.46
32:f:376:PHE:CZ	32:f:798:THR:CB	2.91	0.46
6:L:225:ASP:OD1	6:L:225:ASP:N	2.47	0.46
15:U:545:LEU:HB3	15:U:577:ILE:HG21	1.96	0.46
17:W:73:MET:O	17:W:77:ALA:CB	2.64	0.46
21:a:172:TYR:HE2	21:a:200:LEU:HA	1.80	0.46
23:c:34:SER:HB3	23:c:70:ILE:HA	1.97	0.46
4:j:116:GLN:OE1	4:j:119:THR:OG1	2.34	0.46
7:m:110:HIS:NE2	8:n:70:LEU:HD23	2.31	0.46
32:f:797:LEU:HD22	32:f:797:LEU:HA	1.76	0.46
17:W:23:THR:HA	17:W:26:GLN:HB2	1.98	0.46
24:d:16:LEU:O	24:d:20:GLY:N	2.47	0.46
6:l:205:LEU:HD13	6:l:233:LEU:HD22	1.98	0.46
7:m:192:GLU:HA	7:m:195:LYS:HE3	1.97	0.46
27:A:322:ASN:OD1	27:A:323:ARG:N	2.49	0.46
32:f:378:ASN:HB3	32:f:391:LEU:HD21	1.97	0.46
32:f:742:ALA:CA	32:f:745:LEU:CD2	2.62	0.46
11:Q:26:VAL:HG12	11:q:138:LEU:HD11	1.98	0.46
15:U:697:GLN:NE2	15:U:742:HIS:O	2.49	0.46
7:m:30:VAL:HG11	7:m:134:SER:HB3	1.98	0.46
27:A:369:ARG:HH21	27:A:372:LEU:HG	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:353:LEU:H	32:f:387:GLN:CG	2.29	0.46
7:M:100:SER:O	14:T:65:GLN:NE2	2.49	0.45
20:Z:70:LEU:HD12	20:Z:111:LEU:HD13	1.98	0.45
20:Z:210:SER:O	20:Z:214:LYS:HG2	2.17	0.45
24:d:118:GLU:HG2	24:d:121:ARG:HH12	1.81	0.45
11:q:62:LYS:HD3	11:q:62:LYS:HA	1.77	0.45
26:B:266:LEU:HD21	30:C:229:ARG:HB3	1.98	0.45
27:A:284:ARG:NH2	27:A:328:ASP:OD2	2.49	0.45
32:f:378:ASN:CB	32:f:391:LEU:CD1	2.94	0.45
32:f:389:LYS:HD3	32:f:389:LYS:H	1.81	0.45
6:L:37:GLY:HA2	6:L:46:LEU:HA	1.98	0.45
15:U:512:ALA:O	15:U:516:LEU:HB2	2.15	0.45
15:U:596:ASN:HD22	15:U:599:ILE:HG21	1.81	0.45
19:Y:60:SER:OG	19:Y:61:LEU:N	2.48	0.45
21:a:80:ILE:HA	21:a:83:VAL:HB	1.98	0.45
5:k:117:SER:O	6:l:82:ARG:NH2	2.49	0.45
27:A:346:PRO:O	27:A:351:ARG:NH1	2.49	0.45
12:R:125:THR:OG1	11:q:170:ARG:NH2	2.50	0.45
16:V:210:CYS:O	16:V:214:HIS:CB	2.65	0.45
17:W:130:MET:HB3	17:W:135:LYS:HG3	1.98	0.45
18:X:318:ILE:O	18:X:322:HIS:ND1	2.48	0.45
8:n:18:SER:HB2	8:n:31:THR:H	1.81	0.45
10:p:159:ASP:N	10:p:159:ASP:OD1	2.49	0.45
32:f:316:ASP:HA	32:f:319:GLU:HG2	1.99	0.45
32:f:796:LEU:HD12	32:f:799:VAL:HG11	1.98	0.45
4:J:201:SER:HA	4:J:206:ILE:HD11	1.98	0.45
15:U:146:LYS:HE2	15:U:148:LYS:HB2	1.99	0.45
17:W:268:LYS:HE3	17:W:272:LEU:HD11	1.98	0.45
22:b:5:SER:HB3	22:b:64:LEU:HD21	1.99	0.45
23:c:228:GLY:C	23:c:230:THR:H	2.25	0.45
25:e:62:LYS:HA	25:e:65:TYR:HB2	1.98	0.45
28:E:237:ALA:HB1	29:F:308:ARG:HG3	1.99	0.45
29:F:314:LEU:HD21	29:F:342:LEU:HA	1.99	0.45
32:f:509:LYS:HB3	32:f:514:VAL:HG21	1.99	0.45
32:f:675:PHE:CG	32:f:694:LEU:HD23	2.51	0.45
3:I:174:MET:HE2	3:I:199:LYS:HD3	1.98	0.45
9:O:19:ARG:NH1	9:O:169:SER:O	2.50	0.45
11:Q:81:ALA:O	11:Q:84:THR:OG1	2.31	0.45
17:W:28:LEU:O	17:W:32:ALA:HB2	2.16	0.45
17:W:141:GLU:HB3	17:W:172:GLU:HG2	1.99	0.45
21:a:281:THR:HG23	21:a:336:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:29:GLU:H	23:c:180:ASN:ND2	2.14	0.45
23:c:115:HIS:HE1	23:c:122:LEU:HD23	1.81	0.45
2:h:10:LEU:H	2:h:10:LEU:HG	1.58	0.45
29:F:68:ALA:O	29:F:72:LYS:CB	2.62	0.45
29:F:197:GLU:HB3	29:F:350:ARG:HH21	1.81	0.45
32:f:125:ILE:HA	32:f:129:LEU:HD12	1.98	0.45
32:f:664:GLU:HA	32:f:697:ILE:CA	2.46	0.45
5:K:203:LYS:HA	5:K:206:MET:HG2	1.98	0.45
7:M:59:GLU:O	7:M:61:GLY:N	2.49	0.45
10:P:113:ASP:OD2	10:P:116:THR:OG1	2.27	0.45
15:U:362:ASN:HA	15:U:366:HIS:HE1	1.82	0.45
16:V:200:ARG:HD2	16:V:242:HIS:CD2	2.49	0.45
17:W:377:ARG:O	17:W:381:LEU:HB2	2.17	0.45
19:Y:349:LYS:O	19:Y:351:ASN:N	2.50	0.45
20:Z:213:GLU:OE2	20:Z:217:THR:OG1	2.33	0.45
20:Z:227:ILE:O	20:Z:231:GLN:CB	2.64	0.45
21:a:374:ILE:HG21	24:d:251:ARG:HG2	1.98	0.45
7:m:17:ASP:OD2	7:m:19:ARG:NH2	2.49	0.45
8:n:7:GLN:HA	8:n:12:VAL:HA	1.98	0.45
27:A:189:GLU:O	27:A:193:THR:OG1	2.34	0.45
30:C:190:GLY:O	30:C:196:LYS:NZ	2.49	0.45
32:f:45:LEU:HD22	32:f:86:THR:HG21	1.99	0.45
32:f:688:ARG:HG3	32:f:745:LEU:HB3	1.99	0.45
5:K:10:ARG:H	5:K:10:ARG:HD3	1.82	0.45
17:W:359:VAL:HG23	17:W:382:LEU:HD22	1.98	0.45
24:d:170:LEU:HA	24:d:173:THR:HG22	1.97	0.45
1:g:191:PHE:HE1	1:g:219:VAL:HG21	1.82	0.45
6:l:225:ASP:OD1	6:l:225:ASP:N	2.50	0.45
30:C:186:VAL:HB	30:C:292:ILE:HG12	1.99	0.45
32:f:533:ASP:OD1	32:f:565:ASN:ND2	2.50	0.45
2:H:80:GLY:HA2	2:H:83:TYR:HB3	1.99	0.45
8:N:141:ALA:HB2	8:n:162:LEU:HD11	1.98	0.45
15:U:402:PHE:HD2	15:U:437:TYR:HB3	1.82	0.45
17:W:308:LEU:HD12	17:W:315:MET:HE1	1.99	0.45
6:l:160:SER:O	6:l:169:ARG:NH2	2.50	0.45
11:q:164:LEU:HB3	11:q:196:PHE:HZ	1.81	0.45
26:B:107:MET:HB2	30:C:96:VAL:HB	1.98	0.45
30:C:221:GLN:HE21	30:C:227:GLY:HA2	1.81	0.45
2:H:9:SER:HA	2:H:125:GLY:HA2	1.98	0.45
6:L:84:LEU:HD12	6:L:130:VAL:HG21	1.99	0.45
15:U:804:SER:HB3	15:U:839:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:808:PRO:HA	15:U:811:PHE:HD2	1.82	0.45
19:Y:215:ASP:O	19:Y:218:THR:OG1	2.33	0.45
22:b:91:ARG:HH12	22:b:130:ARG:HE	1.63	0.45
1:g:54:LYS:N	1:g:214:GLU:O	2.46	0.45
9:o:31:CYS:SG	9:o:32:SER:N	2.89	0.45
9:o:41:ILE:HG12	9:o:102:GLY:HA3	1.98	0.45
10:p:103:TYR:HA	11:q:93:ARG:HH22	1.82	0.45
13:s:171:ALA:HA	13:s:174:LEU:HD12	1.97	0.45
32:f:664:GLU:C	32:f:665:GLU:O	2.59	0.45
1:G:191:PHE:HE1	1:G:219:VAL:HG21	1.82	0.45
4:J:38:ARG:HH12	4:J:182:GLU:HA	1.81	0.45
5:K:123:PHE:HB2	5:K:134:SER:O	2.16	0.45
6:L:193:ARG:HA	6:L:196:ARG:HG2	1.97	0.45
15:U:461:LEU:HB2	15:U:481:LEU:HD13	1.99	0.45
18:X:201:TYR:OH	31:D:337:ASP:OD2	2.35	0.45
21:a:115:LYS:HD3	21:a:118:ILE:HD12	1.99	0.45
3:i:90:LEU:HD12	3:i:114:LEU:HD22	1.99	0.45
5:k:182:GLN:NE2	6:l:55:GLU:OE1	2.50	0.45
11:q:4:LEU:HD22	11:q:17:SER:HB2	1.98	0.45
27:A:355:PHE:O	27:A:359:ALA:HB3	2.17	0.45
30:C:369:TYR:HD1	30:C:372:ARG:HE	1.64	0.45
32:f:608:LYS:HA	32:f:611:GLN:HB3	1.99	0.45
3:I:140:ASP:OD1	3:I:144:GLY:N	2.48	0.44
7:M:40:ARG:HE	7:M:161:TRP:CD1	2.35	0.44
15:U:194:ARG:HH22	15:U:222:PHE:HB3	1.81	0.44
15:U:257:SER:OG	15:U:258:GLN:N	2.50	0.44
18:X:322:HIS:O	18:X:326:LEU:CB	2.65	0.44
19:Y:203:ASP:OD1	19:Y:203:ASP:N	2.50	0.44
20:Z:140:SER:HA	20:Z:155:PHE:HA	1.99	0.44
7:m:34:SER:HG	7:m:65:ARG:HH22	1.62	0.44
12:r:12:VAL:HB	12:r:179:VAL:HB	1.99	0.44
26:B:103:ARG:HG2	26:B:160:ILE:HG23	1.98	0.44
26:B:268:ARG:HH12	27:A:244:GLU:HA	1.81	0.44
27:A:335:GLY:N	27:A:338:ASP:OD1	2.47	0.44
32:f:130:ALA:O	32:f:134:SER:CB	2.64	0.44
32:f:379:GLY:O	32:f:417:ILE:CG1	2.65	0.44
8:N:136:TYR:HA	8:N:139:VAL:HG12	1.99	0.44
15:U:27:LEU:O	15:U:31:VAL:HB	2.16	0.44
15:U:714:SER:HA	15:U:717:ILE:HG22	1.99	0.44
19:Y:122:THR:O	19:Y:126:LYS:HB2	2.17	0.44
19:Y:348:ASP:OD1	19:Y:349:LYS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:68:THR:HA	22:b:71:ILE:HD13	1.98	0.44
4:j:32:ALA:HB3	4:j:161:ILE:HD11	1.98	0.44
7:m:170:GLN:HA	7:m:173:LYS:HE2	1.97	0.44
8:n:40:ARG:NH2	8:n:181:GLU:O	2.50	0.44
10:p:126:LEU:HD12	10:p:127:ILE:HG23	2.00	0.44
30:C:336:MET:HE2	30:C:378:VAL:HG21	2.00	0.44
32:f:354:GLU:HG3	32:f:355:ASN:H	1.82	0.44
3:I:154:GLY:O	4:J:81:ARG:NH1	2.51	0.44
5:K:177:ALA:O	5:K:181:LEU:CB	2.65	0.44
9:O:41:ILE:HG12	9:O:102:GLY:HA3	1.99	0.44
10:P:17:LYS:HB2	10:P:158:MET:H	1.83	0.44
13:S:68:ILE:HD11	13:S:92:LEU:HD13	1.98	0.44
17:W:63:THR:OG1	17:W:111:TYR:OH	2.26	0.44
21:a:100:THR:HG22	21:a:103:LYS:HE2	2.00	0.44
23:c:190:GLN:HB3	23:c:193:ILE:H	1.83	0.44
28:E:56:ILE:HB	28:E:100:LEU:HB2	1.98	0.44
28:E:216:ARG:HH22	31:D:234:GLU:HA	1.83	0.44
32:f:420:TRP:CG	32:f:421:ASP:H	2.34	0.44
32:f:446:LEU:HD13	32:f:480:GLY:HA2	2.00	0.44
15:U:583:MET:HE1	15:U:602:LEU:HA	1.98	0.44
15:U:611:ASN:HB3	15:U:614:VAL:HG12	1.98	0.44
16:V:68:ASP:O	16:V:71:THR:OG1	2.27	0.44
22:b:95:LEU:O	22:b:99:HIS:ND1	2.43	0.44
2:h:93:LEU:HD11	2:h:113:ARG:HB3	2.00	0.44
9:o:50:ALA:HB2	10:p:129:CYS:HB2	1.99	0.44
12:r:77:ALA:O	12:r:120:ARG:NH2	2.46	0.44
32:f:357:ARG:NH2	32:f:754:LYS:HG3	2.33	0.44
3:I:10:THR:HG22	4:J:125:ARG:HB3	1.99	0.44
3:I:119:GLN:NE2	4:J:79:ASP:OD1	2.51	0.44
19:Y:336:ARG:HH22	25:e:56:LEU:HD21	1.81	0.44
31:D:82:ILE:HG21	31:D:116:LEU:HD11	1.99	0.44
31:D:173:GLN:NE2	31:D:332:GLU:O	2.50	0.44
32:f:286:LYS:HD3	32:f:326:LEU:HD23	2.00	0.44
32:f:804:LEU:N	32:f:804:LEU:CD1	2.74	0.44
9:O:67:SER:HB3	9:O:74:PRO:HG3	1.99	0.44
17:W:99:GLN:O	17:W:103:LYS:CB	2.65	0.44
22:b:12:ASN:OD1	22:b:53:THR:OG1	2.35	0.44
24:d:47:GLN:O	24:d:51:ALA:CB	2.65	0.44
27:A:59:ILE:O	27:A:63:THR:CB	2.65	0.44
29:F:401:VAL:HG12	29:F:405:MET:HE2	1.98	0.44
1:G:172:GLN:HA	1:G:175:SER:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:113:ILE:HG12	9:O:119:THR:HG22	2.00	0.44
15:U:141:CYS:HB3	15:U:150:ALA:HB2	2.00	0.44
17:W:55:ARG:NH1	17:W:79:GLU:HG3	2.33	0.44
17:W:320:LEU:HD21	17:W:354:LEU:HD21	1.99	0.44
2:h:38:ILE:HG12	2:h:160:ALA:HB1	2.00	0.44
11:q:102:LEU:HD22	11:q:102:LEU:HA	1.72	0.44
27:A:125:LEU:HB2	27:A:129:VAL:HG21	1.99	0.44
28:E:364:GLN:HA	28:E:367:PHE:HD2	1.83	0.44
31:D:338:ARG:HH12	31:D:365:ALA:HA	1.83	0.44
32:f:638:ASP:OD1	32:f:638:ASP:N	2.50	0.44
6:L:92:CYS:HA	6:L:103:LEU:HD12	2.00	0.44
13:S:145:LEU:HD21	13:S:182:ALA:HB2	1.99	0.44
15:U:248:ILE:O	15:U:252:LEU:HB2	2.18	0.44
17:W:98:LYS:O	17:W:102:ALA:CB	2.58	0.44
23:c:29:GLU:HB3	23:c:203:ILE:HG13	1.99	0.44
23:c:282:ARG:HB2	31:D:125:LYS:HZ1	1.83	0.44
9:o:13:VAL:HG22	9:o:177:VAL:HG22	2.00	0.44
30:C:235:PHE:HE1	30:C:280:LEU:HD23	1.83	0.44
32:f:374:SER:O	32:f:375:SER:C	2.59	0.44
4:J:121:SER:OG	4:J:122:ASN:N	2.48	0.44
6:L:7:ASP:OD1	6:L:20:HIS:ND1	2.51	0.44
8:N:127:ILE:HD12	8:N:136:TYR:CD1	2.53	0.44
15:U:475:HIS:HA	15:U:511:ALA:HB2	1.98	0.44
17:W:282:GLU:O	17:W:286:LEU:HB2	2.18	0.44
24:d:54:ILE:HA	24:d:57:ILE:HG22	2.00	0.44
5:k:146:VAL:HG11	5:k:222:PRO:HG3	2.00	0.44
5:k:221:GLN:HB2	5:k:224:GLN:HB3	1.99	0.44
9:o:17:ASP:OD1	9:o:17:ASP:N	2.49	0.44
29:F:432:LYS:HA	29:F:433:ALA:HB3	2.00	0.44
30:C:85:VAL:HG21	30:C:123:LEU:HD11	2.00	0.44
32:f:380:PHE:CD2	32:f:380:PHE:O	2.70	0.44
1:G:27:TYR:HA	1:G:30:LYS:HZ3	1.82	0.43
5:K:93:ARG:NH1	12:R:68:LEU:O	2.51	0.43
7:M:120:HIS:O	7:M:123:THR:OG1	2.34	0.43
8:N:133:SER:O	8:n:134:TYR:HA	2.17	0.43
9:O:175:LEU:HD12	9:O:186:LEU:HD21	1.99	0.43
15:U:64:ALA:HA	15:U:67:VAL:HG12	1.98	0.43
17:W:150:ALA:HA	17:W:153:LYS:HB2	2.00	0.43
19:Y:377:LEU:HA	19:Y:380:VAL:HG22	1.98	0.43
24:d:248:GLU:OE2	24:d:252:GLN:NE2	2.51	0.43
1:g:102:LYS:HD3	1:g:108:GLU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:149:GLN:NE2	3:i:162:THR:OG1	2.50	0.43
3:i:229:LYS:N	3:i:232:GLU:OE2	2.49	0.43
7:m:27:MET:HA	7:m:153:PRO:HG2	2.00	0.43
9:o:187:ARG:HB2	9:o:188:PRO:HD3	2.00	0.43
26:B:181:GLN:HB3	26:B:182:GLU:H	1.64	0.43
32:f:698:SER:OG	32:f:716:ASP:OD1	2.36	0.43
1:G:32:ILE:HA	1:G:82:GLY:HA2	2.01	0.43
3:I:155:ASN:HA	4:J:81:ARG:HH22	1.83	0.43
7:M:139:SER:OG	7:M:140:TYR:N	2.52	0.43
12:R:164:THR:HG22	12:R:170:SER:HB3	1.99	0.43
17:W:363:ILE:HA	17:W:366:MET:HB2	1.99	0.43
18:X:341:PRO:HB2	18:X:342:PHE:HD1	1.83	0.43
21:a:323:SER:O	21:a:332:HIS:N	2.49	0.43
3:i:57:ASP:HB3	3:i:59:VAL:HG13	1.99	0.43
4:j:48:LYS:H	4:j:205:ASN:HB3	1.83	0.43
7:m:100:SER:O	14:t:65:GLN:NE2	2.51	0.43
28:E:144:GLU:HG2	28:E:297:ARG:HH22	1.83	0.43
32:f:380:PHE:CB	32:f:751:TYR:CE2	2.99	0.43
32:f:646:MET:HA	32:f:649:HIS:HD1	1.82	0.43
32:f:690:VAL:O	32:f:694:LEU:HB2	2.18	0.43
4:J:61:LYS:HD2	4:J:73:PHE:CZ	2.53	0.43
4:J:176:TYR:CE2	5:K:57:PRO:HB2	2.53	0.43
8:N:19:ARG:NH2	14:t:180:ASP:O	2.52	0.43
9:O:51:ASP:HB3	9:O:94:ILE:HG23	2.00	0.43
16:V:89:LYS:HA	16:V:92:ARG:HH11	1.84	0.43
16:V:161:PRO:HA	16:V:164:GLU:HB2	2.01	0.43
17:W:37:GLU:HB3	17:W:39:ARG:HG2	1.99	0.43
19:Y:44:ALA:HA	19:Y:49:ASN:HD22	1.83	0.43
7:m:92:ARG:HH21	14:t:73:ASP:HA	1.84	0.43
32:f:311:VAL:CA	32:f:490:ALA:HB1	2.48	0.43
32:f:536:SER:O	32:f:540:GLN:CB	2.66	0.43
32:f:664:GLU:HB3	32:f:696:LEU:CG	2.43	0.43
1:G:185:LYS:O	1:G:187:PHE:N	2.51	0.43
15:U:402:PHE:CD2	15:U:437:TYR:HB3	2.52	0.43
19:Y:23:ARG:HH22	19:Y:52:PRO:HB2	1.82	0.43
1:g:215:ILE:H	1:g:215:ILE:HG13	1.64	0.43
10:p:27:ARG:HB2	10:p:183:MET:HB2	2.00	0.43
12:r:97:MET:O	12:r:116:SER:N	2.48	0.43
32:f:494:ARG:HE	32:f:494:ARG:CA	2.32	0.43
32:f:645:ASP:O	32:f:649:HIS:ND1	2.51	0.43
3:I:229:LYS:N	3:I:232:GLU:OE2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:154:PHE:HB3	5:K:162:PHE:HE1	1.84	0.43
15:U:536:ALA:HB1	15:U:545:LEU:HD23	2.00	0.43
15:U:554:LEU:HG	15:U:588:MET:HE1	2.00	0.43
16:V:184:ALA:HA	16:V:187:ILE:HD12	2.01	0.43
17:W:444:HIS:HB3	20:Z:230:LEU:HD13	2.00	0.43
19:Y:143:TYR:HD1	19:Y:146:ARG:HH12	1.66	0.43
3:i:3:ARG:NH1	5:k:11:GLY:HA2	2.33	0.43
6:l:89:ARG:NH1	13:s:77:HIS:HB3	2.34	0.43
10:p:27:ARG:NH1	10:p:180:VAL:O	2.51	0.43
27:A:217:PRO:O	27:A:220:THR:OG1	2.31	0.43
29:F:217:ILE:HG13	29:F:218:GLN:H	1.84	0.43
32:f:281:ILE:O	32:f:285:CYS:HB2	2.18	0.43
32:f:282:PHE:HE2	32:f:317:LEU:HD21	1.83	0.43
32:f:283:THR:O	32:f:287:ASP:HB2	2.18	0.43
32:f:355:ASN:HA	32:f:358:PHE:HD2	1.83	0.43
32:f:513:GLU:HG3	32:f:557:TRP:HZ3	1.84	0.43
32:f:794:ALA:HA	32:f:797:LEU:HB2	2.01	0.43
2:H:171:LYS:HE3	3:I:55:LEU:HD12	2.01	0.43
11:Q:137:PHE:HB3	12:r:133:VAL:HG21	1.99	0.43
15:U:62:LEU:HD12	15:U:84:ALA:HB1	2.01	0.43
15:U:74:PHE:O	15:U:78:LEU:HB2	2.18	0.43
15:U:135:ASN:HA	15:U:138:PHE:HB3	2.01	0.43
15:U:191:LYS:HD2	15:U:194:ARG:HH11	1.83	0.43
18:X:80:ILE:HB	18:X:84:LYS:HE3	2.00	0.43
18:X:309:TYR:HB3	18:X:312:GLU:HB2	2.00	0.43
20:Z:259:VAL:HG11	23:c:298:GLN:HB3	1.99	0.43
23:c:31:VAL:HG23	23:c:203:ILE:HG12	2.01	0.43
5:k:210:LEU:HA	5:k:214:ASN:HD22	1.83	0.43
12:r:105:ASP:N	12:r:108:GLY:O	2.50	0.43
14:t:4:PRO:HG3	14:t:107:TRP:CE2	2.54	0.43
28:E:171:LEU:HD23	28:E:298:LYS:HG3	2.01	0.43
32:f:22:GLY:O	32:f:26:GLU:CB	2.66	0.43
32:f:368:ALA:O	32:f:372:LEU:HB2	2.18	0.43
32:f:494:ARG:NE	32:f:494:ARG:CA	2.82	0.43
1:G:58:ASP:HB3	1:G:61:LEU:HB2	1.99	0.43
1:G:144:ASP:OD2	9:O:72:ARG:NH2	2.48	0.43
10:P:49:LEU:HD21	10:P:87:LEU:HD22	2.00	0.43
10:P:113:ASP:HB2	10:P:118:LYS:HB3	2.00	0.43
17:W:155:GLN:HG3	17:W:161:GLU:HG3	2.01	0.43
17:W:231:ILE:O	17:W:235:GLN:HB2	2.18	0.43
19:Y:210:SER:OG	19:Y:211:TYR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:315:THR:OG1	19:Y:316:LEU:N	2.51	0.43
21:a:270:ARG:HH12	21:a:310:LEU:HA	1.84	0.43
32:f:248:LEU:O	32:f:252:ALA:HB3	2.19	0.43
32:f:402:ASN:OD1	32:f:403:LYS:N	2.52	0.43
1:G:208:ILE:HG22	1:G:210:PHE:HB3	2.00	0.43
3:I:162:THR:OG1	3:I:163:CYS:N	2.51	0.43
5:K:192:LYS:HA	5:K:195:ILE:HD12	2.00	0.43
6:L:89:ARG:NH1	13:S:77:HIS:HB3	2.34	0.43
6:L:204:ASP:OD1	6:L:204:ASP:N	2.52	0.43
7:M:192:GLU:O	7:M:196:ILE:HD12	2.19	0.43
9:O:17:ASP:N	9:O:17:ASP:OD1	2.51	0.43
16:V:95:LEU:HA	16:V:137:GLU:HB3	1.99	0.43
16:V:218:TYR:HB3	16:V:224:LEU:HD22	2.01	0.43
16:V:340:GLY:N	16:V:401:ASN:HD21	2.17	0.43
3:i:40:ASN:O	3:i:42:GLY:N	2.52	0.43
5:k:203:LYS:HE2	5:k:241:ILE:HG12	2.01	0.43
7:m:40:ARG:HE	7:m:161:TRP:CD1	2.36	0.43
9:o:16:ALA:HB3	9:o:174:ASP:HB2	2.01	0.43
28:E:310:LEU:HD11	28:E:314:LYS:HE3	2.01	0.43
31:D:83:GLN:HB2	31:D:84:SER:H	1.49	0.43
32:f:358:PHE:O	32:f:362:GLY:CA	2.63	0.43
32:f:688:ARG:HA	32:f:745:LEU:CB	2.49	0.43
12:R:104:TRP:NE1	12:R:181:GLU:HG3	2.34	0.43
17:W:78:LYS:HA	17:W:81:ASP:HB3	2.01	0.43
17:W:135:LYS:HB3	17:W:136:ILE:H	1.33	0.43
7:m:175:GLU:N	7:m:175:GLU:OE1	2.48	0.43
28:E:64:LEU:HG	28:E:65:THR:HG23	2.00	0.43
31:D:115:ILE:HG22	31:D:139:LEU:HB2	2.00	0.43
32:f:207:LEU:HD13	32:f:207:LEU:HA	1.86	0.43
32:f:478:ARG:HD3	32:f:504:VAL:CG1	2.45	0.43
5:K:203:LYS:HB3	5:K:210:LEU:HD22	2.01	0.43
11:Q:85:ARG:HG3	11:Q:124:LEU:HG	2.00	0.43
15:U:268:LEU:HD22	15:U:329:LEU:HD11	2.00	0.43
17:W:109:CYS:HA	17:W:112:VAL:HG12	2.00	0.43
18:X:297:ARG:HB3	18:X:333:GLN:HB3	1.99	0.43
20:Z:138:TYR:HB3	20:Z:155:PHE:HB3	2.01	0.43
24:d:94:TYR:O	24:d:98:LEU:HB2	2.19	0.43
4:j:82:ILE:HD13	4:j:82:ILE:HA	1.92	0.43
5:k:195:ILE:O	5:k:198:SER:OG	2.33	0.43
6:l:204:ASP:OD1	6:l:204:ASP:N	2.52	0.43
7:m:59:GLU:O	7:m:61:GLY:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:m:179:LEU:HD23	7:m:179:LEU:HA	1.80	0.43
28:E:282:PRO:HB2	28:E:388:PRO:HB3	2.01	0.43
32:f:228:LYS:O	32:f:232:TYR:HB3	2.19	0.43
8:N:134:TYR:HA	8:n:133:SER:O	2.18	0.42
20:Z:239:ASP:OD1	20:Z:239:ASP:N	2.51	0.42
21:a:35:HIS:NE2	22:b:17:ARG:HB2	2.35	0.42
23:c:157:ILE:HG23	23:c:205:ILE:HD13	1.99	0.42
3:i:174:MET:SD	3:i:196:VAL:HG13	2.59	0.42
9:o:167:LEU:HD23	9:o:167:LEU:HA	1.81	0.42
27:A:169:LYS:NZ	32:f:714:SER:CB	2.82	0.42
32:f:303:VAL:HG22	32:f:339:ILE:HA	2.00	0.42
32:f:635:LYS:NZ	32:f:641:GLU:CD	2.66	0.42
1:G:49:VAL:HG22	1:G:219:VAL:HG23	2.01	0.42
12:R:144:SER:H	12:R:147:LEU:HD11	1.84	0.42
16:V:94:VAL:HG22	16:V:138:PRO:HD3	2.00	0.42
17:W:15:LYS:HA	17:W:18:VAL:HB	2.00	0.42
20:Z:138:TYR:HA	20:Z:157:HIS:HA	2.01	0.42
25:e:6:GLN:OE1	25:e:9:ASP:N	2.37	0.42
1:g:5:SER:HB2	1:g:19:GLU:HG3	2.00	0.42
11:q:23:SER:HB2	11:q:28:MET:HG3	2.01	0.42
13:s:145:LEU:HD22	13:s:178:VAL:HB	2.01	0.42
30:C:274:LEU:O	30:C:278:ASN:ND2	2.52	0.42
31:D:234:GLU:HG2	31:D:246:MET:HE1	2.01	0.42
32:f:122:ALA:HB1	32:f:126:ILE:HD12	2.01	0.42
32:f:378:ASN:HB3	32:f:391:LEU:HD11	2.01	0.42
6:L:101:ARG:HH22	6:L:107:ARG:NH1	2.18	0.42
6:L:170:THR:HG21	29:F:383:GLU:HG2	2.01	0.42
11:Q:11:ASP:N	11:Q:11:ASP:OD1	2.51	0.42
18:X:134:VAL:HG21	18:X:149:LEU:HD22	2.01	0.42
18:X:394:ASP:O	18:X:398:GLU:HB3	2.18	0.42
19:Y:69:LEU:HA	19:Y:72:LYS:HE3	2.02	0.42
20:Z:7:GLN:N	20:Z:46:LYS:HG2	2.34	0.42
21:a:245:VAL:HA	21:a:272:ILE:HD12	2.01	0.42
4:j:38:ARG:NH2	4:j:182:GLU:O	2.52	0.42
7:m:139:SER:OG	7:m:140:TYR:N	2.53	0.42
12:r:59:LEU:HD22	12:r:83:LEU:HB2	2.01	0.42
32:f:412:ALA:HA	32:f:447:ALA:HB2	2.00	0.42
32:f:573:ILE:HG22	32:f:576:ILE:HB	2.01	0.42
32:f:664:GLU:CB	32:f:696:LEU:HG	2.45	0.42
3:I:135:LEU:HA	3:I:135:LEU:HD23	1.82	0.42
11:Q:10:PRO:HG3	11:Q:150:THR:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:423:ALA:HB2	16:V:434:ALA:HB2	2.01	0.42
18:X:236:PHE:HB2	18:X:254:MET:HE1	2.00	0.42
19:Y:186:LEU:HA	19:Y:189:VAL:HG12	2.01	0.42
22:b:100:ARG:HH12	22:b:103:LYS:HA	1.84	0.42
23:c:250:GLU:O	23:c:253:LYS:HG2	2.19	0.42
8:n:136:TYR:HA	8:n:139:VAL:HG12	2.00	0.42
26:B:273:VAL:HG13	26:B:277:HIS:CE1	2.54	0.42
32:f:471:LEU:HD11	32:f:509:LYS:HE2	2.00	0.42
6:L:45:VAL:HG11	6:L:188:VAL:HG22	2.02	0.42
11:Q:32:HIS:CD2	11:Q:33:ASP:H	2.36	0.42
17:W:247:TYR:HA	17:W:250:ILE:HG13	2.01	0.42
18:X:323:LEU:O	18:X:327:TYR:CB	2.67	0.42
25:e:49:GLU:HA	25:e:52:PHE:HB2	2.02	0.42
25:e:61:GLU:O	25:e:65:TYR:N	2.51	0.42
27:A:143:ASP:OD2	27:A:146:LYS:N	2.37	0.42
27:A:355:PHE:O	27:A:359:ALA:CB	2.67	0.42
30:C:293:MET:HE2	30:C:295:THR:HB	2.00	0.42
31:D:372:GLY:HA3	34:D:501:AGS:H2	2.01	0.42
1:G:84:THR:HB	7:M:156:VAL:HG22	2.00	0.42
2:H:8:PHE:O	2:H:126:GLY:N	2.52	0.42
5:K:108:THR:O	5:K:111:SER:OG	2.32	0.42
6:L:148:CYS:SG	6:L:150:SER:OG	2.61	0.42
11:Q:4:LEU:HD22	11:Q:17:SER:HB2	2.00	0.42
18:X:318:ILE:HG22	18:X:321:THR:H	1.83	0.42
21:a:292:THR:HG23	21:a:294:GLU:H	1.84	0.42
21:a:325:ASP:OD1	21:a:326:GLU:N	2.52	0.42
22:b:91:ARG:HH12	22:b:130:ARG:HH21	1.66	0.42
23:c:39:LEU:HD23	23:c:42:LEU:HD21	2.02	0.42
24:d:192:THR:HA	24:d:195:THR:HB	2.00	0.42
3:i:77:ALA:HB3	3:i:164:ILE:HG21	2.01	0.42
3:i:105:ILE:HA	3:i:106:PRO:HD3	1.81	0.42
3:i:118:LYS:HZ3	3:i:150:SER:HB2	1.85	0.42
27:A:66:LYS:O	27:A:70:THR:CB	2.68	0.42
31:D:152:MET:O	31:D:154:LEU:N	2.52	0.42
32:f:80:ARG:HE	32:f:99:LEU:HD13	1.85	0.42
32:f:623:LYS:O	32:f:627:GLU:HB3	2.17	0.42
5:K:221:GLN:HB2	5:K:224:GLN:HB3	2.00	0.42
6:L:82:ARG:HA	6:L:85:CYS:HB3	2.01	0.42
7:M:53:VAL:HB	7:M:208:ALA:HB3	2.02	0.42
9:O:122:LEU:HD23	9:O:122:LEU:HA	1.90	0.42
21:a:148:VAL:HB	21:a:151:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:163:ILE:HD12	23:c:163:ILE:HA	1.86	0.42
24:d:72:GLU:HA	24:d:75:MET:HB3	2.02	0.42
3:i:50:ARG:HD3	3:i:50:ARG:HA	1.66	0.42
5:k:108:THR:O	5:k:111:SER:OG	2.35	0.42
8:n:19:ARG:HD2	8:n:171:GLY:HA3	2.00	0.42
12:r:196:HIS:O	12:r:200:SER:HB3	2.19	0.42
13:s:73:LYS:O	13:s:77:HIS:ND1	2.37	0.42
26:B:361:LYS:HD2	26:B:384:ILE:HG23	2.00	0.42
28:E:83:CYS:HB2	28:E:89:LYS:HE2	2.02	0.42
32:f:77:GLU:O	32:f:81:GLN:HB2	2.19	0.42
3:I:95:GLN:HG2	10:P:73:LEU:HG	2.02	0.42
7:M:66:LEU:HD13	7:M:214:SER:HB2	2.02	0.42
9:O:112:SER:HB3	9:O:125:VAL:HG11	2.01	0.42
15:U:636:VAL:HG23	15:U:637:VAL:HG23	2.02	0.42
16:V:82:LEU:HD23	16:V:125:ASN:ND2	2.35	0.42
16:V:190:ASP:HA	16:V:200:ARG:NH2	2.33	0.42
19:Y:293:ARG:HH21	25:e:52:PHE:HB3	1.83	0.42
3:i:118:LYS:NZ	3:i:150:SER:HB2	2.35	0.42
3:i:185:THR:O	3:i:187:LYS:N	2.48	0.42
3:i:185:THR:C	3:i:187:LYS:H	2.28	0.42
5:k:48:LEU:HD21	5:k:77:ALA:HB2	2.02	0.42
11:q:32:HIS:CD2	11:q:33:ASP:H	2.38	0.42
14:t:166:ARG:NH1	14:t:170:GLU:OE2	2.53	0.42
27:A:99:THR:HG22	27:A:115:VAL:HG13	2.01	0.42
28:E:101:ASP:HB3	28:E:105:LEU:H	1.85	0.42
28:E:243:PHE:HZ	29:F:304:ARG:HE	1.68	0.42
28:E:262:ASN:HD22	31:D:231:VAL:HG13	1.84	0.42
32:f:298:LEU:HA	32:f:301:HIS:CD2	2.55	0.42
32:f:512:MET:HE1	32:f:554:TYR:HA	2.02	0.42
15:U:70:HIS:CD2	16:V:236:ARG:HH21	2.38	0.42
15:U:342:LEU:HD21	15:U:744:VAL:HG13	2.02	0.42
19:Y:138:LEU:HD22	19:Y:176:ARG:HE	1.85	0.42
20:Z:263:ALA:O	20:Z:267:ARG:HB3	2.20	0.42
24:d:158:ILE:HG22	24:d:160:ALA:H	1.85	0.42
3:i:47:ALA:HB1	3:i:64:LYS:HD2	2.00	0.42
5:k:200:ILE:HA	5:k:203:LYS:HE3	2.00	0.42
29:F:235:LEU:HD23	29:F:238:ARG:HH11	1.84	0.42
2:H:14:SER:OG	2:H:18:LYS:N	2.48	0.42
2:H:181:ASP:OD1	2:H:181:ASP:N	2.51	0.42
3:I:95:GLN:HG3	10:P:69:PHE:CD1	2.55	0.42
15:U:24:LEU:HA	15:U:27:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:82:LEU:O	17:W:86:ASN:CB	2.57	0.42
20:Z:14:LEU:HG	23:c:39:LEU:HB3	2.02	0.42
1:g:172:GLN:HA	1:g:175:SER:HB3	2.01	0.42
5:k:99:HIS:CG	5:k:107:MET:HB2	2.55	0.42
6:l:26:MET:HE1	6:l:148:CYS:HB2	2.02	0.42
9:o:19:ARG:NH1	9:o:169:SER:O	2.53	0.42
10:p:62:THR:OG1	11:q:85:ARG:NH2	2.53	0.42
13:s:28:ARG:HB2	13:s:190:GLY:HA2	2.02	0.42
27:A:215:PHE:CD2	27:A:324:PRO:HG3	2.55	0.42
28:E:144:GLU:HG2	28:E:297:ARG:NH2	2.35	0.42
28:E:268:ASP:OD2	31:D:229:ARG:NH2	2.53	0.42
32:f:333:LEU:HD23	32:f:338:ASP:HB3	2.02	0.42
32:f:388:ASP:O	32:f:390:LEU:N	2.49	0.42
32:f:479:LEU:HD23	32:f:513:GLU:HB3	2.02	0.42
7:M:170:GLN:HA	7:M:173:LYS:HE2	2.01	0.41
7:M:198:TYR:CD2	7:M:239:ALA:HB1	2.55	0.41
12:R:37:ILE:HG23	12:R:60:ALA:HB2	2.03	0.41
14:T:178:TYR:HB3	8:n:29:ARG:NH2	2.34	0.41
15:U:633:CYS:HA	15:U:636:VAL:HG22	2.01	0.41
17:W:203:GLN:HA	17:W:206:SER:HB3	2.02	0.41
18:X:228:ALA:HA	18:X:231:TYR:HD2	1.85	0.41
18:X:364:LYS:HE3	18:X:368:MET:HE3	2.02	0.41
27:A:362:MET:HG3	27:A:364:VAL:HG13	2.02	0.41
28:E:156:PRO:HA	28:E:159:PHE:HD2	1.85	0.41
28:E:349:GLU:OE1	29:F:350:ARG:NH1	2.53	0.41
32:f:338:ASP:HA	32:f:341:GLU:HG3	2.02	0.41
2:H:14:SER:OG	2:H:17:GLY:N	2.53	0.41
11:Q:23:SER:HB2	11:Q:28:MET:HG3	2.00	0.41
11:Q:164:LEU:HB3	11:Q:196:PHE:HZ	1.85	0.41
1:g:131:MET:HE3	1:g:131:MET:HB2	1.91	0.41
7:M:52:LEU:HD13	7:M:206:ASP:OD2	2.20	0.41
13:S:5:TYR:OH	13:S:103:PRO:O	2.21	0.41
15:U:326:ILE:O	15:U:330:SER:OG	2.35	0.41
15:U:433:PRO:HD2	15:U:439:GLU:HB3	2.02	0.41
17:W:408:ARG:HD2	18:X:346:GLN:HE22	1.85	0.41
17:W:446:ILE:HD13	20:Z:157:HIS:HB3	2.01	0.41
18:X:70:LEU:O	18:X:74:ARG:HG3	2.20	0.41
20:Z:72:HIS:CD2	20:Z:114:ARG:HH21	2.39	0.41
21:a:58:LYS:NZ	21:a:87:MET:SD	2.93	0.41
22:b:126:LYS:O	22:b:130:ARG:HB2	2.21	0.41
2:h:119:GLN:O	2:h:122:THR:OG1	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:j:116:GLN:HE21	5:k:83:ALA:HB3	1.86	0.41
7:m:120:HIS:O	7:m:123:THR:OG1	2.34	0.41
32:f:170:TRP:CZ3	32:f:208:LEU:HB3	2.55	0.41
32:f:620:PHE:HD2	32:f:623:LYS:HG2	1.85	0.41
16:V:163:VAL:HA	16:V:175:MET:HE2	2.02	0.41
17:W:188:GLU:O	17:W:191:ARG:HG2	2.20	0.41
19:Y:336:ARG:HH12	25:e:56:LEU:HD21	1.84	0.41
20:Z:273:HIS:CE1	20:Z:277:ASN:HD21	2.38	0.41
1:g:159:TYR:HB3	2:h:81:PRO:HG3	2.03	0.41
2:h:14:SER:OG	2:h:17:GLY:N	2.54	0.41
8:n:127:ILE:HD12	8:n:136:TYR:CD1	2.56	0.41
10:p:4:MET:HE2	10:p:104:TYR:HD1	1.86	0.41
12:r:115:ASP:HB2	12:r:119:ASN:H	1.84	0.41
13:s:28:ARG:O	13:s:42:LYS:NZ	2.53	0.41
27:A:426:THR:O	27:A:426:THR:OG1	2.31	0.41
32:f:81:GLN:O	32:f:85:SER:HB2	2.21	0.41
32:f:86:THR:HG23	32:f:87:THR:H	1.85	0.41
32:f:275:MET:SD	32:f:275:MET:N	2.90	0.41
32:f:796:LEU:HG	32:f:799:VAL:CG2	2.42	0.41
1:G:163:PHE:HB3	2:H:57:TYR:HA	2.01	0.41
5:K:157:ASP:OD2	5:K:159:SER:OG	2.37	0.41
5:K:207:GLU:HB3	27:A:372:LEU:HD21	2.02	0.41
17:W:186:ILE:HG13	17:W:189:GLN:HE22	1.85	0.41
20:Z:136:GLU:OE2	20:Z:157:HIS:ND1	2.52	0.41
21:a:100:THR:HA	21:a:103:LYS:HG2	2.02	0.41
22:b:51:LEU:N	22:b:62:THR:OG1	2.40	0.41
5:k:196:LYS:HA	5:k:199:LEU:HG	2.02	0.41
7:m:42:LYS:HD3	7:m:182:LYS:O	2.21	0.41
7:m:56:LYS:H	7:m:57:LEU:HD23	1.85	0.41
10:p:49:LEU:HD21	10:p:87:LEU:HD22	2.01	0.41
11:q:7:ILE:N	11:q:14:LEU:O	2.54	0.41
31:D:202:VAL:HG23	31:D:329:ARG:HB2	2.01	0.41
32:f:8:LYS:HD3	32:f:39:LYS:HD2	2.02	0.41
32:f:635:LYS:HD3	32:f:641:GLU:HG2	2.01	0.41
32:f:671:ALA:O	32:f:674:THR:OG1	2.26	0.41
8:N:104:ASP:N	8:N:108:GLY:O	2.53	0.41
8:N:120:MET:H	14:T:61:GLN:HE22	1.69	0.41
16:V:203:LEU:O	16:V:207:ALA:CB	2.68	0.41
16:V:482:PHE:CZ	19:Y:381:GLN:HG2	2.56	0.41
18:X:214:SER:O	18:X:218:HIS:ND1	2.38	0.41
20:Z:16:LEU:HD13	23:c:220:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:a:142:LEU:HD12	21:a:151:VAL:HG22	2.01	0.41
3:i:94:ALA:HB1	3:i:105:ILE:HG21	2.01	0.41
6:l:46:LEU:HD13	6:l:73:SER:HB2	2.02	0.41
26:B:338:ASP:OD1	27:A:429:TYR:OH	2.38	0.41
32:f:629:LYS:HE2	32:f:660:ILE:HG21	2.02	0.41
4:J:108:THR:HG22	4:J:133:ILE:HD13	2.03	0.41
15:U:36:ALA:C	16:V:264:TYR:HH	2.29	0.41
15:U:341:PHE:HZ	15:U:883:ARG:HB3	1.85	0.41
16:V:257:ASN:O	16:V:261:TYR:N	2.44	0.41
16:V:310:THR:HA	16:V:332:LEU:HD11	2.03	0.41
17:W:56:THR:HG21	17:W:103:LYS:HE2	2.01	0.41
17:W:170:GLN:O	17:W:173:THR:OG1	2.30	0.41
22:b:4:GLU:HA	22:b:106:LYS:N	2.35	0.41
10:p:113:ASP:HB2	10:p:118:LYS:HB3	2.03	0.41
31:D:187:HIS:HB3	31:D:190:LEU:HD12	2.02	0.41
31:D:225:ALA:HB1	31:D:260:ALA:HA	2.03	0.41
32:f:545:LYS:HE2	32:f:555:ALA:HA	2.03	0.41
6:L:152:ASN:HA	7:M:85:ARG:NH2	2.34	0.41
8:N:29:ARG:NH2	14:t:178:TYR:HB3	2.36	0.41
9:O:49:ALA:O	9:O:52:THR:OG1	2.38	0.41
14:T:96:MET:HE1	14:T:106:LEU:HD12	2.03	0.41
17:W:155:GLN:HG2	17:W:157:GLY:H	1.86	0.41
1:g:103:TYR:HB2	8:n:61:TYR:CD1	2.56	0.41
3:i:136:TYR:HB2	3:i:148:TYR:HB2	2.03	0.41
6:l:152:ASN:ND2	7:m:81:LEU:HB3	2.36	0.41
26:B:144:LEU:HD21	26:B:162:VAL:HG23	2.03	0.41
32:f:687:ARG:O	32:f:745:LEU:HD22	2.21	0.41
1:G:215:ILE:H	1:G:215:ILE:HG13	1.61	0.41
1:G:217:VAL:HG12	1:G:230:LEU:HD13	2.02	0.41
2:H:15:PRO:HA	3:I:23:TYR:CE2	2.56	0.41
3:I:178:ASP:OD2	3:I:195:LYS:NZ	2.38	0.41
3:I:232:GLU:HA	3:I:235:GLN:HG2	2.02	0.41
4:J:20:GLU:N	4:J:20:GLU:OE1	2.54	0.41
6:L:199:LEU:HA	6:L:199:LEU:HD23	1.84	0.41
8:N:14:LEU:HD11	8:N:101:ALA:HB3	2.02	0.41
9:O:110:LEU:HD21	9:O:125:VAL:HG22	2.03	0.41
11:Q:21:ALA:HB3	11:Q:29:LYS:HB3	2.03	0.41
11:Q:47:VAL:HB	11:Q:102:LEU:HD23	2.03	0.41
12:R:22:ALA:N	12:R:25:TYR:O	2.45	0.41
12:R:35:ILE:N	12:R:43:GLY:O	2.53	0.41
12:R:38:ASN:O	12:R:184:TRP:NE1	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:115:ASP:HB2	12:R:119:ASN:H	1.86	0.41
15:U:35:TRP:HB3	15:U:70:HIS:CE1	2.56	0.41
15:U:248:ILE:O	15:U:252:LEU:CB	2.69	0.41
15:U:398:ASN:H	15:U:401:LYS:HE2	1.86	0.41
15:U:500:ASN:OD1	15:U:508:THR:OG1	2.39	0.41
15:U:612:ASP:HB3	15:U:647:HIS:CG	2.55	0.41
15:U:669:ILE:HG21	15:U:705:LYS:HG3	2.03	0.41
15:U:803:LYS:HB2	15:U:838:LYS:HB2	2.01	0.41
16:V:263:LEU:HD13	24:d:121:ARG:HH21	1.85	0.41
16:V:379:LEU:HD22	16:V:395:ILE:HG12	2.03	0.41
17:W:35:ALA:HB2	17:W:48:LEU:HD21	2.03	0.41
17:W:448:LYS:NZ	20:Z:207:ASP:OD1	2.53	0.41
20:Z:201:LEU:HA	20:Z:201:LEU:HD23	1.91	0.41
20:Z:223:ASN:O	20:Z:225:GLN:N	2.49	0.41
20:Z:272:LEU:O	20:Z:276:ILE:HG12	2.21	0.41
21:a:8:LEU:O	21:a:12:GLN:CB	2.65	0.41
21:a:212:ASN:ND2	21:a:241:ASN:OD1	2.53	0.41
21:a:214:GLY:HA2	21:a:217:LEU:HD13	2.03	0.41
21:a:349:MET:O	21:a:353:LEU:HB2	2.21	0.41
23:c:29:GLU:O	23:c:204:THR:OG1	2.35	0.41
23:c:33:ILE:HG12	23:c:207:TYR:HA	2.02	0.41
3:i:118:LYS:HE3	3:i:118:LYS:HB2	1.90	0.41
27:A:312:ARG:HH22	27:A:317:VAL:HG23	1.86	0.41
29:F:185:TYR:CE2	29:F:243:GLN:HG3	2.56	0.41
31:D:231:VAL:HB	31:D:234:GLU:HB2	2.02	0.41
32:f:86:THR:O	32:f:87:THR:HB	2.21	0.41
32:f:89:MET:SD	32:f:89:MET:N	2.94	0.41
32:f:303:VAL:HG13	32:f:339:ILE:HG13	2.02	0.41
32:f:479:LEU:HG	32:f:513:GLU:O	2.21	0.41
32:f:533:ASP:OD1	32:f:533:ASP:N	2.53	0.41
9:O:189:TYR:HD2	9:O:190:THR:HG22	1.86	0.41
14:T:9:THR:OG1	14:T:10:SER:N	2.53	0.41
15:U:194:ARG:NH2	15:U:222:PHE:HB3	2.36	0.41
15:U:487:GLY:HA2	15:U:521:LEU:HB3	2.02	0.41
16:V:285:TRP:CD1	16:V:315:LYS:HE2	2.48	0.41
16:V:393:THR:HB	16:V:397:ARG:HH12	1.86	0.41
17:W:317:TRP:CD1	17:W:320:LEU:HD22	2.56	0.41
18:X:254:MET:HE2	18:X:254:MET:HB3	1.73	0.41
20:Z:169:GLU:O	20:Z:173:GLU:HB2	2.21	0.41
20:Z:228:TYR:CD2	21:a:338:PRO:HB2	2.56	0.41
20:Z:259:VAL:HG21	23:c:298:GLN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:a:27:GLU:OE1	21:a:31:LYS:NZ	2.52	0.41
2:h:100:VAL:HG13	10:p:93:ASN:HD22	1.86	0.41
7:m:54:LEU:HD23	7:m:54:LEU:HA	1.96	0.41
14:t:67:LEU:HD23	14:t:67:LEU:HA	1.93	0.41
31:D:99:ASN:HA	31:D:115:ILE:HD11	2.03	0.41
5:K:170:ILE:C	5:K:174:SER:HB2	2.46	0.40
7:M:175:GLU:HG3	7:M:196:ILE:HG12	2.02	0.40
10:P:7:ASN:ND2	10:P:29:GLY:O	2.41	0.40
17:W:9:ALA:HA	17:W:12:ARG:HB2	2.03	0.40
21:a:245:VAL:HG21	21:a:300:ALA:HA	2.03	0.40
25:e:45:ASP:HA	25:e:48:VAL:HB	2.03	0.40
25:e:49:GLU:O	25:e:53:SER:N	2.54	0.40
25:e:60:LEU:HD12	25:e:60:LEU:HA	1.87	0.40
2:h:59:GLU:HG2	2:h:206:ASP:HB3	2.04	0.40
3:i:100:GLN:HE21	11:q:83:PHE:HE1	1.69	0.40
3:i:118:LYS:NZ	3:i:151:ASP:O	2.35	0.40
5:k:170:ILE:C	5:k:174:SER:HB2	2.46	0.40
5:k:177:ALA:O	5:k:181:LEU:HB2	2.21	0.40
6:l:82:ARG:HA	6:l:85:CYS:HB3	2.01	0.40
13:s:16:ALA:HB2	13:s:121:VAL:HG23	2.03	0.40
14:t:7:THR:OG1	14:t:182:ARG:NH2	2.53	0.40
26:B:197:ILE:HG21	26:B:235:LEU:HD11	2.02	0.40
27:A:254:ALA:O	27:A:258:ARG:HD3	2.21	0.40
29:F:304:ARG:HB3	29:F:308:ARG:CZ	2.50	0.40
29:F:405:MET:HB2	29:F:405:MET:HE3	1.88	0.40
31:D:87:LEU:HD23	31:D:87:LEU:HA	1.91	0.40
32:f:780:PRO:HB2	32:f:800:LEU:CA	2.50	0.40
5:K:15:PHE:HE2	6:L:127:PRO:HD2	1.86	0.40
7:M:161:TRP:HE1	7:M:181:MET:HE2	1.86	0.40
8:N:142:THR:HB	8:N:155:PHE:HE1	1.85	0.40
9:O:167:LEU:HD23	9:O:167:LEU:HA	1.83	0.40
11:Q:102:LEU:HD13	11:Q:103:LEU:HG	2.03	0.40
11:Q:135:GLY:O	11:Q:139:THR:OG1	2.23	0.40
11:Q:138:LEU:HD13	11:Q:171:PHE:HE1	1.86	0.40
14:T:25:ASP:HA	14:T:187:PHE:HA	2.04	0.40
16:V:379:LEU:HD13	16:V:395:ILE:HG12	2.03	0.40
17:W:426:ASN:O	17:W:430:GLN:HB3	2.21	0.40
18:X:89:VAL:O	18:X:93:LEU:HB2	2.20	0.40
23:c:202:SER:OG	23:c:203:ILE:N	2.53	0.40
23:c:238:CYS:HA	23:c:241:ASN:HD22	1.85	0.40
24:d:192:THR:HG23	24:d:196:ARG:HH12	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:d:203:PRO:HG2	24:d:206:MET:N	2.29	0.40
3:i:64:LYS:HE2	3:i:64:LYS:HB2	1.89	0.40
3:i:75:SER:HB2	3:i:135:LEU:HD12	2.02	0.40
3:i:140:ASP:CG	3:i:143:TYR:H	2.29	0.40
4:j:221:ASN:HA	4:j:222:PRO:HD3	1.81	0.40
7:m:110:HIS:NE2	8:n:70:LEU:HA	2.36	0.40
10:p:34:MET:HE3	10:p:34:MET:HB2	1.99	0.40
12:r:144:SER:HB3	12:r:147:LEU:HD21	2.03	0.40
27:A:421:ALA:HA	27:A:424:SER:HB3	2.03	0.40
28:E:164:ILE:HG21	31:D:380:GLN:HA	2.02	0.40
32:f:380:PHE:CD2	32:f:751:TYR:CE2	3.09	0.40
3:I:17:ARG:HD2	3:I:22:GLU:HG3	2.03	0.40
7:M:54:LEU:HD23	7:M:54:LEU:HA	1.87	0.40
16:V:195:ILE:HD13	30:C:31:LEU:HD11	2.03	0.40
16:V:346:LEU:HD13	16:V:349:ARG:HD3	2.03	0.40
19:Y:101:ARG:HB3	19:Y:130:LYS:HD3	2.02	0.40
19:Y:197:ALA:HB3	19:Y:226:VAL:HG21	2.03	0.40
1:g:188:ASP:O	1:g:193:GLN:HG2	2.20	0.40
4:j:92:GLN:HG2	11:q:66:LEU:HD22	2.02	0.40
7:m:40:ARG:HH21	7:m:161:TRP:NE1	2.19	0.40
26:B:317:ASP:HB2	26:B:346:ARG:HG2	2.02	0.40
32:f:392:THR:CG2	32:f:417:ILE:CG2	2.94	0.40
32:f:479:LEU:HD11	32:f:514:VAL:HG23	2.03	0.40
1:G:102:LYS:HA	1:G:102:LYS:HD2	1.92	0.40
15:U:373:ASN:HA	15:U:376:MET:HG2	2.03	0.40
15:U:900:TYR:HB3	15:U:914:LEU:HG	2.04	0.40
19:Y:266:CYS:HA	19:Y:271:PHE:HZ	1.85	0.40
20:Z:118:ASN:OD1	20:Z:118:ASN:N	2.55	0.40
20:Z:123:ILE:O	20:Z:136:GLU:N	2.54	0.40
24:d:69:PRO:HA	24:d:72:GLU:HG2	2.02	0.40
1:g:6:SER:OG	1:g:10:ASP:OD1	2.33	0.40
6:l:33:SER:HB3	6:l:51:ARG:HE	1.87	0.40
6:l:146:GLN:HE22	6:l:159:MET:HE2	1.87	0.40
7:m:66:LEU:HD13	7:m:214:SER:HB2	2.03	0.40
8:n:19:ARG:NH1	8:n:168:GLY:O	2.54	0.40
12:r:144:SER:H	12:r:147:LEU:HD11	1.86	0.40
30:C:161:ILE:HG22	30:C:203:VAL:HG11	2.03	0.40
3:I:118:LYS:HE3	3:I:118:LYS:HB2	1.96	0.40
7:M:179:LEU:HD23	7:M:179:LEU:HA	1.94	0.40
8:N:18:SER:HB2	8:N:30:VAL:HA	2.03	0.40
15:U:742:HIS:HB3	15:U:883:ARG:HH22	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:131:LEU:HA	16:V:134:PHE:HB2	2.04	0.40
17:W:60:MET:O	17:W:64:SER:HB3	2.22	0.40
17:W:333:LEU:HD12	17:W:334:GLU:H	1.87	0.40
19:Y:315:THR:HG23	19:Y:317:GLY:H	1.86	0.40
20:Z:195:VAL:HG13	20:Z:199:LYS:HD3	2.04	0.40
20:Z:221:PRO:C	20:Z:223:ASN:H	2.28	0.40
21:a:328:ASP:HB2	21:a:330:ARG:HG3	2.03	0.40
6:l:170:THR:HA	6:l:173:GLU:OE1	2.22	0.40
32:f:183:PRO:HB2	32:f:184:LEU:H	1.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	238/240 (99%)	225 (94%)	11 (5%)	2 (1%)	16	49
1	g	238/240 (99%)	225 (94%)	12 (5%)	1 (0%)	30	61
2	H	230/232 (99%)	218 (95%)	11 (5%)	1 (0%)	30	61
2	h	230/232 (99%)	221 (96%)	8 (4%)	1 (0%)	30	61
3	I	248/250 (99%)	223 (90%)	22 (9%)	3 (1%)	10	41
3	i	248/250 (99%)	218 (88%)	26 (10%)	4 (2%)	7	36
4	J	237/243 (98%)	225 (95%)	8 (3%)	4 (2%)	7	35
4	j	237/243 (98%)	223 (94%)	10 (4%)	4 (2%)	7	35
5	K	224/234 (96%)	206 (92%)	17 (8%)	1 (0%)	30	61
5	k	224/234 (96%)	207 (92%)	16 (7%)	1 (0%)	30	61
6	L	236/238 (99%)	221 (94%)	14 (6%)	1 (0%)	30	61
6	l	236/238 (99%)	219 (93%)	17 (7%)	0	100	100
7	M	238/245 (97%)	215 (90%)	20 (8%)	3 (1%)	9	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	m	238/245 (97%)	213 (90%)	23 (10%)	2 (1%)	16	49
8	N	189/191 (99%)	183 (97%)	5 (3%)	1 (0%)	24	57
8	n	189/191 (99%)	183 (97%)	5 (3%)	1 (0%)	24	57
9	O	218/220 (99%)	204 (94%)	13 (6%)	1 (0%)	24	57
9	o	218/220 (99%)	208 (95%)	9 (4%)	1 (0%)	24	57
10	P	202/204 (99%)	190 (94%)	11 (5%)	1 (0%)	24	57
10	p	202/204 (99%)	190 (94%)	12 (6%)	0	100	100
11	Q	197/199 (99%)	184 (93%)	13 (7%)	0	100	100
11	q	197/199 (99%)	184 (93%)	13 (7%)	0	100	100
12	R	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
12	r	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
13	S	211/213 (99%)	199 (94%)	12 (6%)	0	100	100
13	s	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
14	T	213/215 (99%)	203 (95%)	10 (5%)	0	100	100
14	t	213/215 (99%)	204 (96%)	9 (4%)	0	100	100
15	U	798/911 (88%)	741 (93%)	57 (7%)	0	100	100
16	V	478/480 (100%)	420 (88%)	56 (12%)	2 (0%)	30	61
17	W	454/456 (100%)	401 (88%)	51 (11%)	2 (0%)	30	61
18	X	378/380 (100%)	360 (95%)	18 (5%)	0	100	100
19	Y	376/378 (100%)	331 (88%)	44 (12%)	1 (0%)	36	65
20	Z	284/286 (99%)	249 (88%)	32 (11%)	3 (1%)	11	43
21	a	371/373 (100%)	336 (91%)	34 (9%)	1 (0%)	36	65
22	b	189/191 (99%)	166 (88%)	22 (12%)	1 (0%)	24	57
23	c	285/309 (92%)	251 (88%)	31 (11%)	3 (1%)	11	43
24	d	255/257 (99%)	208 (82%)	43 (17%)	4 (2%)	7	36
25	e	36/70 (51%)	23 (64%)	13 (36%)	0	100	100
26	B	355/369 (96%)	326 (92%)	27 (8%)	2 (1%)	21	54
27	A	376/433 (87%)	326 (87%)	48 (13%)	2 (0%)	24	57
28	E	373/403 (93%)	333 (89%)	40 (11%)	0	100	100
29	F	372/439 (85%)	345 (93%)	25 (7%)	2 (0%)	24	57
30	C	354/389 (91%)	313 (88%)	39 (11%)	2 (1%)	21	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	D	378/418 (90%)	327 (86%)	43 (11%)	8 (2%)	5	31
32	f	669/848 (79%)	579 (86%)	82 (12%)	8 (1%)	10	41
All	All	12941/13640 (95%)	11811 (91%)	1056 (8%)	74 (1%)	23	54

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	10	ASP
2	H	41	ALA
3	I	40	ASN
4	J	199	VAL
7	M	60	GLU
8	N	19	ARG
10	P	31	GLN
16	V	265	ASP
20	Z	222	ILE
3	i	40	ASN
3	i	41	ASP
4	j	199	VAL
7	m	60	GLU
8	n	19	ARG
31	D	85	ILE
32	f	337	LEU
32	f	364	GLN
32	f	367	SER
32	f	665	GLU
1	G	186	LYS
3	I	186	LEU
17	W	136	ILE
23	c	190	GLN
2	h	41	ALA
30	C	89	VAL
31	D	126	PRO
32	f	183	PRO
32	f	365	VAL
4	J	137	ASP
6	L	206	THR
7	M	58	TYR
9	O	201	ARG
16	V	264	TYR
22	b	23	PRO

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Mol	Chain	Res	Type
24	d	199	PHE
24	d	232	PRO
1	g	186	LYS
3	i	64	LYS
3	i	186	LEU
7	m	58	TYR
26	B	181	GLN
26	B	356	PRO
31	D	86	PRO
31	D	148	ASP
31	D	355	SER
32	f	184	LEU
32	f	326	LEU
3	I	64	LYS
4	J	97	THR
7	M	203	GLU
19	Y	350	VAL
4	j	97	THR
4	j	98	VAL
4	j	137	ASP
30	C	90	HIS
21	a	166	ILE
23	c	188	SER
24	d	201	ASN
9	o	201	ARG
27	A	109	PRO
29	F	344	ARG
31	D	299	PHE
5	K	20	ARG
17	W	418	PRO
20	Z	223	ASN
24	d	256	ILE
5	k	21	LEU
27	A	115	VAL
31	D	125	LYS
29	F	165	PRO
4	J	98	VAL
20	Z	238	PRO
31	D	367	PRO
23	c	189	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	193/205 (94%)	189 (98%)	4 (2%)	47	65
1	g	193/205 (94%)	191 (99%)	2 (1%)	68	75
2	H	164/190 (86%)	164 (100%)	0	100	100
2	h	164/190 (86%)	163 (99%)	1 (1%)	78	79
3	I	193/210 (92%)	193 (100%)	0	100	100
3	i	193/210 (92%)	190 (98%)	3 (2%)	55	69
4	J	152/207 (73%)	150 (99%)	2 (1%)	61	72
4	j	152/207 (73%)	151 (99%)	1 (1%)	76	78
5	K	186/196 (95%)	185 (100%)	1 (0%)	81	80
5	k	186/196 (95%)	184 (99%)	2 (1%)	65	74
6	L	198/204 (97%)	197 (100%)	1 (0%)	81	80
6	l	198/204 (97%)	197 (100%)	1 (0%)	81	80
7	M	192/202 (95%)	191 (100%)	1 (0%)	81	80
7	m	192/202 (95%)	190 (99%)	2 (1%)	68	75
8	N	148/148 (100%)	147 (99%)	1 (1%)	76	78
8	n	148/148 (100%)	147 (99%)	1 (1%)	76	78
9	O	177/181 (98%)	174 (98%)	3 (2%)	53	69
9	o	177/181 (98%)	176 (99%)	1 (1%)	78	79
10	P	172/173 (99%)	172 (100%)	0	100	100
10	p	172/173 (99%)	172 (100%)	0	100	100
11	Q	164/170 (96%)	160 (98%)	4 (2%)	43	63
11	q	164/170 (96%)	162 (99%)	2 (1%)	63	73
12	R	153/156 (98%)	152 (99%)	1 (1%)	76	78
12	r	153/156 (98%)	152 (99%)	1 (1%)	76	78
13	S	174/178 (98%)	174 (100%)	0	100	100
13	s	174/178 (98%)	174 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	175/178 (98%)	174 (99%)	1 (1%)	78	79
14	t	175/178 (98%)	175 (100%)	0	100	100
15	U	685/779 (88%)	681 (99%)	4 (1%)	78	79
16	V	414/414 (100%)	410 (99%)	4 (1%)	68	75
17	W	416/416 (100%)	412 (99%)	4 (1%)	68	75
18	X	327/327 (100%)	322 (98%)	5 (2%)	57	70
19	Y	334/334 (100%)	333 (100%)	1 (0%)	86	83
20	Z	257/257 (100%)	255 (99%)	2 (1%)	73	77
21	a	333/333 (100%)	330 (99%)	3 (1%)	70	76
22	b	167/167 (100%)	167 (100%)	0	100	100
23	c	252/267 (94%)	247 (98%)	5 (2%)	48	66
24	d	231/231 (100%)	230 (100%)	1 (0%)	84	81
25	e	38/63 (60%)	38 (100%)	0	100	100
26	B	291/326 (89%)	291 (100%)	0	100	100
27	A	298/372 (80%)	295 (99%)	3 (1%)	68	75
28	E	298/353 (84%)	293 (98%)	5 (2%)	53	69
29	F	296/379 (78%)	295 (100%)	1 (0%)	86	83
30	C	310/337 (92%)	308 (99%)	2 (1%)	78	79
31	D	333/366 (91%)	333 (100%)	0	100	100
32	f	580/714 (81%)	564 (97%)	16 (3%)	38	60
All	All	10742/11631 (92%)	10650 (99%)	92 (1%)	68	76

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	66	VAL
1	G	141	ILE
1	G	163	PHE
1	G	215	ILE
4	J	7	ILE
4	J	161	ILE
5	K	68	VAL
6	L	205	LEU
7	M	57	LEU
8	N	127	ILE

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Mol	Chain	Res	Type
9	O	89	ARG
9	O	175	LEU
9	O	186	LEU
11	Q	56	PHE
11	Q	66	LEU
11	Q	102	LEU
11	Q	171	PHE
12	R	128	VAL
14	T	100	ARG
15	U	153	ILE
15	U	529	ILE
15	U	689	ILE
15	U	913	ILE
16	V	167	LEU
16	V	194	LYS
16	V	437	ILE
16	V	464	ILE
17	W	71	VAL
17	W	90	LEU
17	W	128	LEU
17	W	333	LEU
18	X	80	ILE
18	X	217	ILE
18	X	256	LEU
18	X	369	ILE
18	X	393	VAL
19	Y	330	ILE
20	Z	187	LEU
20	Z	230	LEU
21	a	125	ILE
21	a	296	ILE
21	a	353	LEU
23	c	49	VAL
23	c	62	VAL
23	c	131	GLN
23	c	156	VAL
23	c	175	ARG
24	d	197	ILE
1	g	66	VAL
1	g	215	ILE
2	h	10	LEU
3	i	10	THR

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Mol	Chain	Res	Type
3	i	206	LEU
3	i	228	LEU
4	j	161	ILE
5	k	10	ARG
5	k	68	VAL
6	l	205	LEU
7	m	56	LYS
7	m	57	LEU
8	n	127	ILE
9	o	89	ARG
11	q	66	LEU
11	q	102	LEU
12	r	128	VAL
27	A	153	LEU
27	A	224	LEU
27	A	403	ILE
28	E	105	LEU
28	E	138	LEU
28	E	194	ASN
28	E	257	LEU
28	E	291	ARG
29	F	134	LEU
30	C	63	LEU
30	C	109	THR
32	f	88	SER
32	f	184	LEU
32	f	207	LEU
32	f	337	LEU
32	f	370	MET
32	f	381	VAL
32	f	387	GLN
32	f	389	LYS
32	f	391	LEU
32	f	403	LYS
32	f	460	ASP
32	f	463	LEU
32	f	479	LEU
32	f	641	GLU
32	f	797	LEU
32	f	800	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (148) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	68	HIS
1	G	224	ASN
2	H	119	GLN
3	I	20	GLN
3	I	53	HIS
3	I	102	GLN
3	I	119	GLN
3	I	149	GLN
4	J	92	GLN
4	J	120	GLN
4	J	205	ASN
5	K	98	ASN
5	K	214	ASN
6	L	90	GLN
6	L	146	GLN
6	L	190	HIS
7	M	72	HIS
8	N	28	ASN
9	O	193	ASN
10	P	61	GLN
10	P	162	HIS
12	R	29	GLN
12	R	38	ASN
12	R	70	ASN
12	R	119	ASN
13	S	157	ASN
14	T	61	GLN
14	T	65	GLN
14	T	213	HIS
15	U	70	HIS
15	U	79	ASN
15	U	111	GLN
15	U	115	ASN
15	U	241	ASN
15	U	345	ASN
15	U	355	ASN
15	U	421	GLN
15	U	450	HIS
15	U	491	GLN
15	U	596	ASN
15	U	698	GLN
15	U	711	GLN
15	U	718	ASN

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Mol	Chain	Res	Type
15	U	734	GLN
15	U	749	GLN
15	U	768	GLN
16	V	242	HIS
16	V	247	GLN
16	V	252	ASN
16	V	319	HIS
16	V	326	GLN
16	V	365	GLN
16	V	477	HIS
17	W	84	ASN
17	W	86	ASN
17	W	106	GLN
17	W	203	GLN
17	W	235	GLN
17	W	399	ASN
17	W	444	HIS
17	W	453	HIS
18	X	213	GLN
18	X	262	ASN
18	X	334	ASN
18	X	380	GLN
18	X	405	GLN
19	Y	31	HIS
19	Y	49	ASN
20	Z	174	HIS
20	Z	193	ASN
20	Z	273	HIS
20	Z	277	ASN
20	Z	278	ASN
21	a	9	GLN
21	a	18	GLN
21	a	82	HIS
21	a	168	ASN
21	a	227	ASN
21	a	332	HIS
21	a	370	GLN
23	c	241	ASN
23	c	254	ASN
24	d	77	GLN
24	d	88	GLN
24	d	128	GLN

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Mol	Chain	Res	Type
24	d	220	ASN
24	d	252	GLN
1	g	12	HIS
1	g	68	HIS
1	g	127	GLN
2	h	166	ASN
3	i	40	ASN
3	i	53	HIS
3	i	100	GLN
3	i	109	GLN
3	i	123	GLN
3	i	149	GLN
5	k	41	GLN
5	k	98	ASN
5	k	155	HIS
5	k	214	ASN
6	l	90	GLN
6	l	146	GLN
6	l	152	ASN
7	m	22	GLN
7	m	72	HIS
7	m	180	GLN
8	n	28	ASN
9	o	62	ASN
9	o	66	HIS
10	p	93	ASN
10	p	169	GLN
11	q	71	ASN
12	r	29	GLN
12	r	38	ASN
13	s	108	ASN
14	t	61	GLN
14	t	65	GLN
14	t	213	HIS
27	A	148	GLN
27	A	150	HIS
27	A	293	ASN
28	E	194	ASN
28	E	220	ASN
28	E	226	GLN
28	E	271	HIS
28	E	323	HIS

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Mol	Chain	Res	Type
29	F	208	HIS
29	F	243	GLN
29	F	333	ASN
30	C	69	GLN
30	C	221	GLN
30	C	241	HIS
30	C	279	GLN
31	D	74	HIS
31	D	133	HIS
31	D	173	GLN
31	D	301	GLN
32	f	12	GLN
32	f	102	HIS
32	f	213	GLN
32	f	352	HIS
32	f	387	GLN
32	f	473	ASN
32	f	493	ASN
32	f	540	GLN
32	f	565	ASN
32	f	650	GLN

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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	AGS	A	501	-	32,33,33	1.15	3 (9%)	45,52,52	0.88	2 (4%)
34	AGS	B	501	-	32,33,33	1.18	3 (9%)	45,52,52	1.31	4 (8%)
34	AGS	C	401	-	32,33,33	0.71	2 (6%)	45,52,52	0.81	1 (2%)
34	AGS	E	401	-	32,33,33	1.17	3 (9%)	45,52,52	1.00	2 (4%)
34	AGS	F	501	-	32,33,33	1.01	4 (12%)	45,52,52	0.96	2 (4%)
34	AGS	D	501	-	32,33,33	0.61	0	45,52,52	0.87	2 (4%)

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	AGS	A	501	-	-	3/21/38/38	0/3/3/3
34	AGS	B	501	-	-	2/21/38/38	0/3/3/3
34	AGS	C	401	-	-	3/21/38/38	0/3/3/3
34	AGS	E	401	-	-	3/21/38/38	0/3/3/3
34	AGS	F	501	-	-	7/21/38/38	0/3/3/3
34	AGS	D	501	-	-	10/21/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	501	AGS	PB-O3A	-3.84	1.55	1.59
34	E	401	AGS	PB-O3B	-3.83	1.55	1.59
34	A	501	AGS	PA-O3A	-3.78	1.55	1.59
34	A	501	AGS	PB-O3A	-3.68	1.55	1.59
34	B	501	AGS	PB-O3B	-3.44	1.55	1.59
34	E	401	AGS	PA-O3A	-3.27	1.56	1.59
34	F	501	AGS	PB-O3A	-2.79	1.56	1.59
34	F	501	AGS	PB-O3B	-2.76	1.56	1.59
34	E	401	AGS	PB-O3A	-2.72	1.56	1.59
34	B	501	AGS	PA-O3A	-2.55	1.56	1.59
34	F	501	AGS	PA-O3A	-2.53	1.56	1.59
34	A	501	AGS	PB-O3B	-2.33	1.57	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	F	501	AGS	PG-S1G	2.06	1.95	1.90
34	C	401	AGS	PG-S1G	2.01	1.95	1.90
34	C	401	AGS	PB-O3B	-2.01	1.57	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	501	AGS	PB-O3B-PG	-5.97	111.31	133.17
34	F	501	AGS	PB-O3B-PG	-4.79	115.65	133.17
34	C	401	AGS	PB-O3B-PG	-4.54	116.56	133.17
34	E	401	AGS	PB-O3B-PG	-4.48	116.76	133.17
34	D	501	AGS	PB-O3B-PG	-4.40	117.06	133.17
34	A	501	AGS	PB-O3B-PG	-3.85	119.06	133.17
34	B	501	AGS	O2A-PA-O3A	2.89	115.07	107.27
34	B	501	AGS	O2B-PB-O3A	2.40	113.75	107.27
34	A	501	AGS	O3A-PB-O1B	-2.35	103.63	110.70
34	F	501	AGS	O3B-PB-O1B	-2.28	103.83	110.70
34	D	501	AGS	O3G-PG-O3B	2.20	111.99	104.64
34	B	501	AGS	C3'-C2'-C1'	2.17	105.57	101.46
34	E	401	AGS	O2B-PB-O3A	2.09	112.91	107.27

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	B	501	AGS	C5'-O5'-PA-O1A
34	F	501	AGS	C5'-O5'-PA-O3A
34	D	501	AGS	C5'-O5'-PA-O1A
34	D	501	AGS	C5'-O5'-PA-O2A
34	D	501	AGS	C5'-O5'-PA-O3A
34	D	501	AGS	O4'-C4'-C5'-O5'
34	D	501	AGS	O4'-C1'-N9-C4
34	F	501	AGS	C2'-C1'-N9-C8
34	D	501	AGS	C3'-C4'-C5'-O5'
34	A	501	AGS	O4'-C4'-C5'-O5'
34	D	501	AGS	O4'-C1'-N9-C8
34	A	501	AGS	C3'-C4'-C5'-O5'
34	F	501	AGS	C2'-C1'-N9-C4
34	C	401	AGS	PB-O3A-PA-O1A
34	F	501	AGS	PG-O3B-PB-O1B
34	B	501	AGS	C5'-O5'-PA-O3A
34	E	401	AGS	C5'-O5'-PA-O1A

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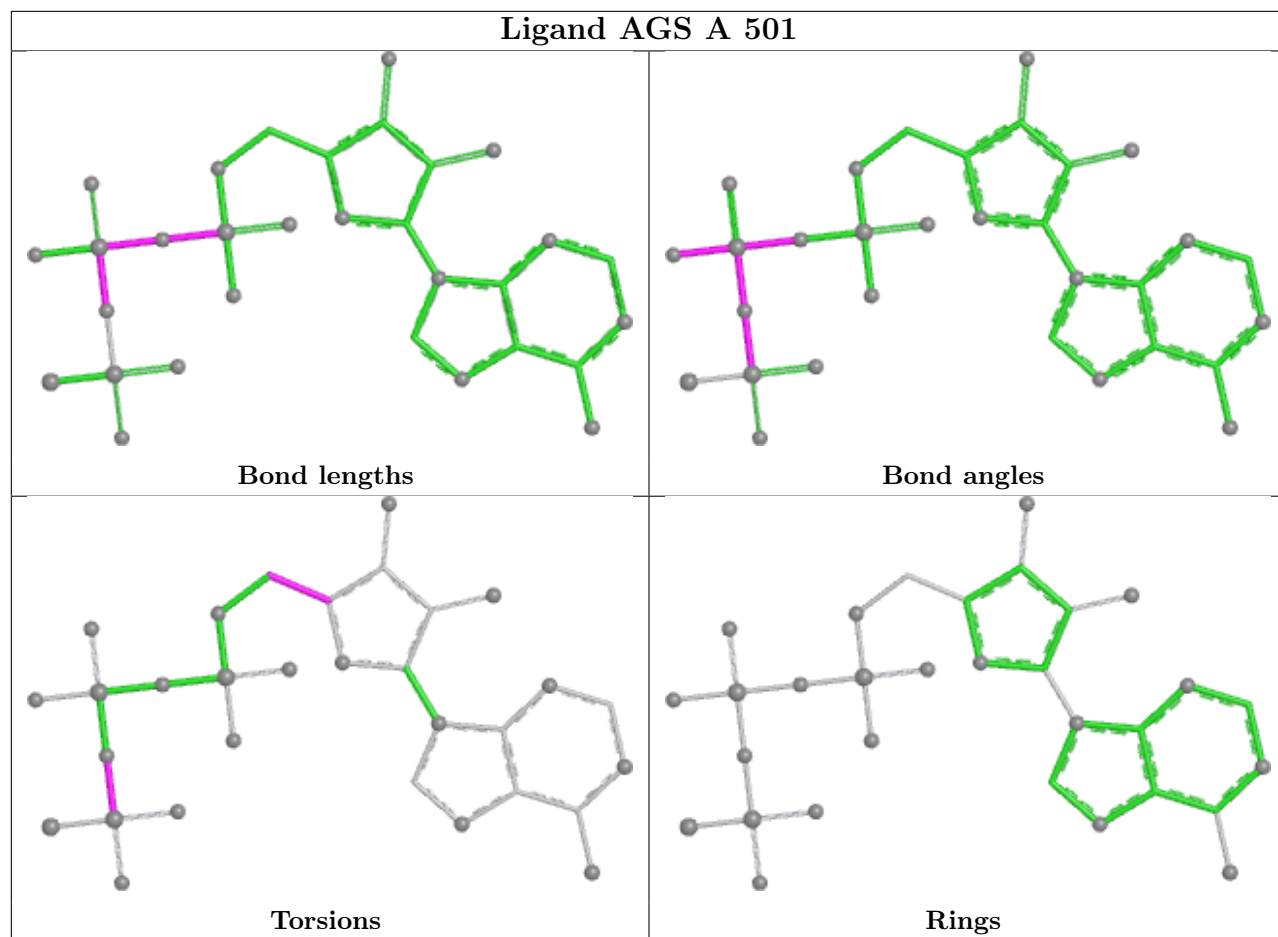
Mol	Chain	Res	Type	Atoms
34	F	501	AGS	C5'-O5'-PA-O1A
34	C	401	AGS	C5'-O5'-PA-O1A
34	D	501	AGS	C4'-C5'-O5'-PA
34	D	501	AGS	PB-O3A-PA-O2A
34	E	401	AGS	PB-O3A-PA-O1A
34	A	501	AGS	PB-O3B-PG-O3G
34	F	501	AGS	C3'-C4'-C5'-O5'
34	F	501	AGS	PG-O3B-PB-O2B
34	C	401	AGS	PB-O3A-PA-O2A
34	E	401	AGS	PB-O3A-PA-O2A
34	D	501	AGS	PB-O3A-PA-O1A

There are no ring outliers.

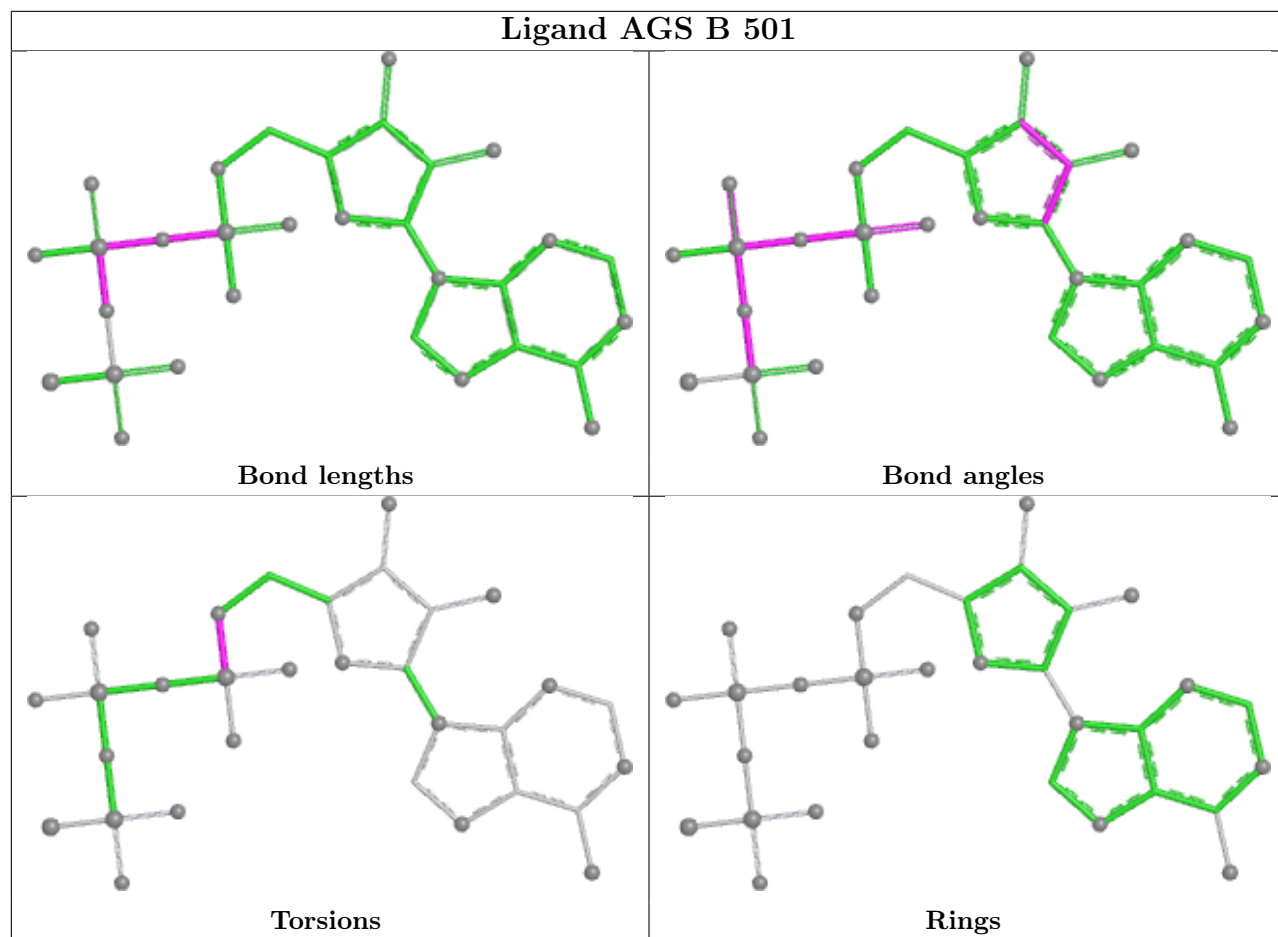
6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	A	501	AGS	2	0
34	B	501	AGS	3	0
34	C	401	AGS	2	0
34	E	401	AGS	7	0
34	F	501	AGS	5	0
34	D	501	AGS	7	0

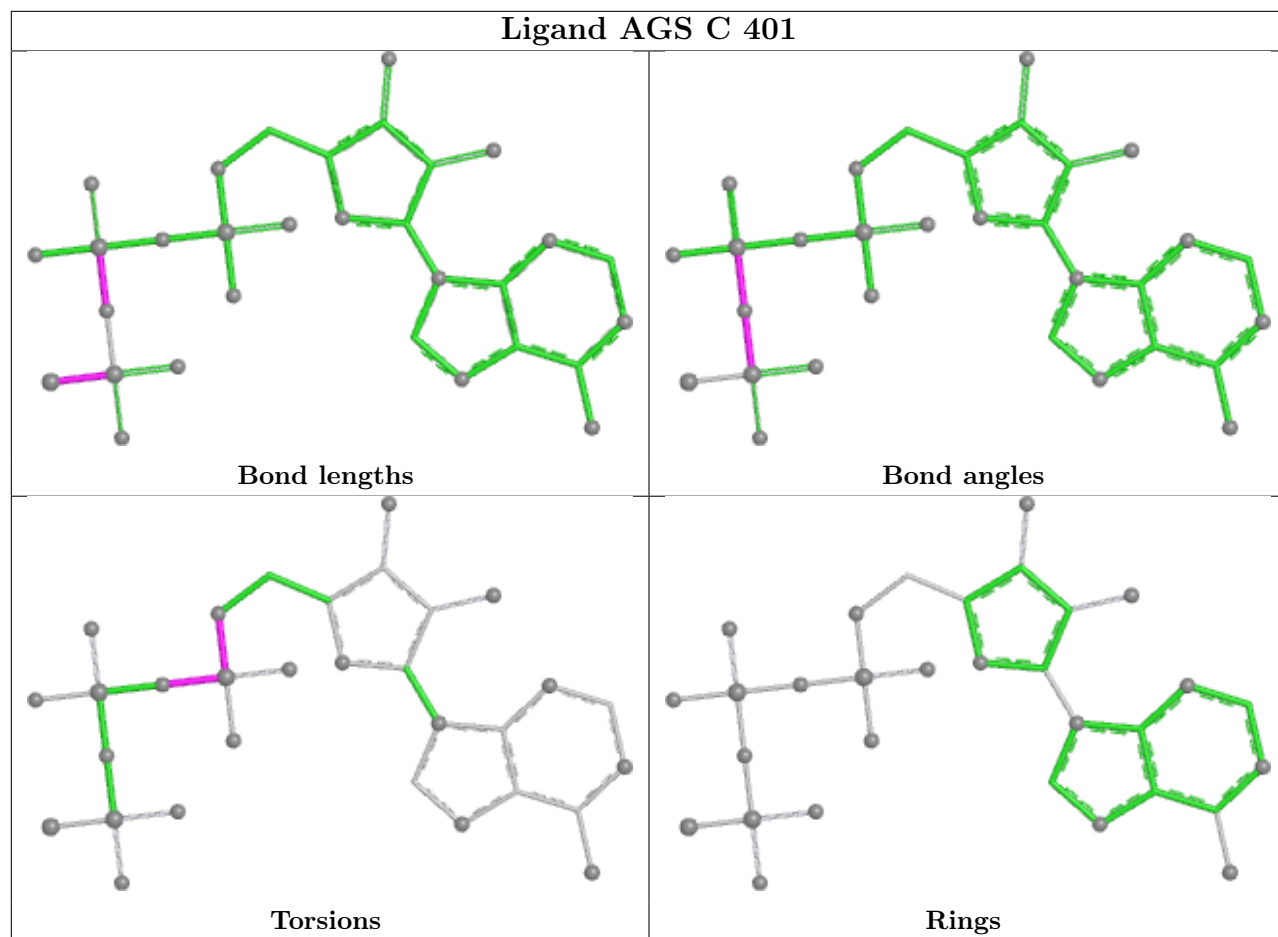
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



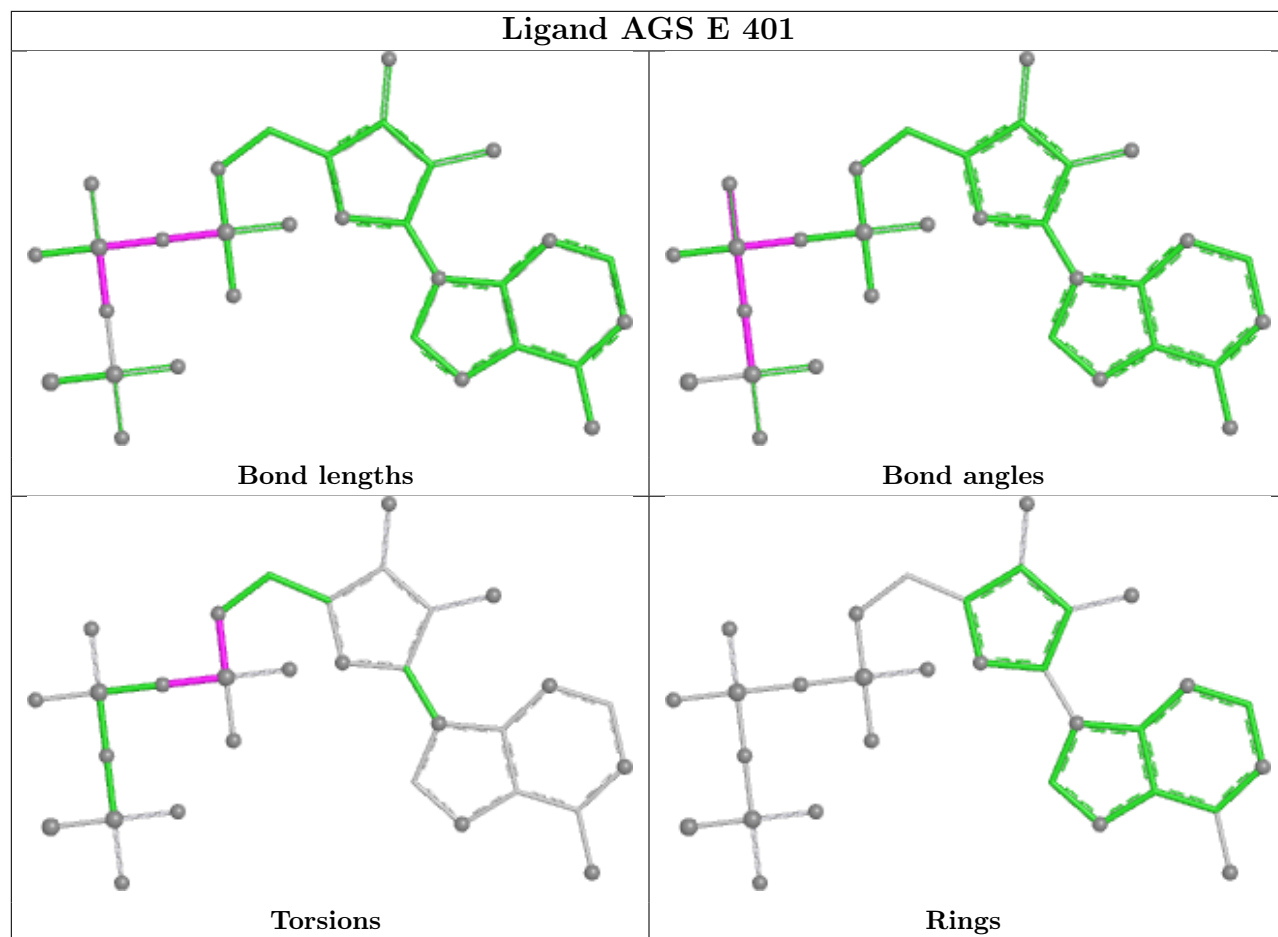
Ligand AGS B 501



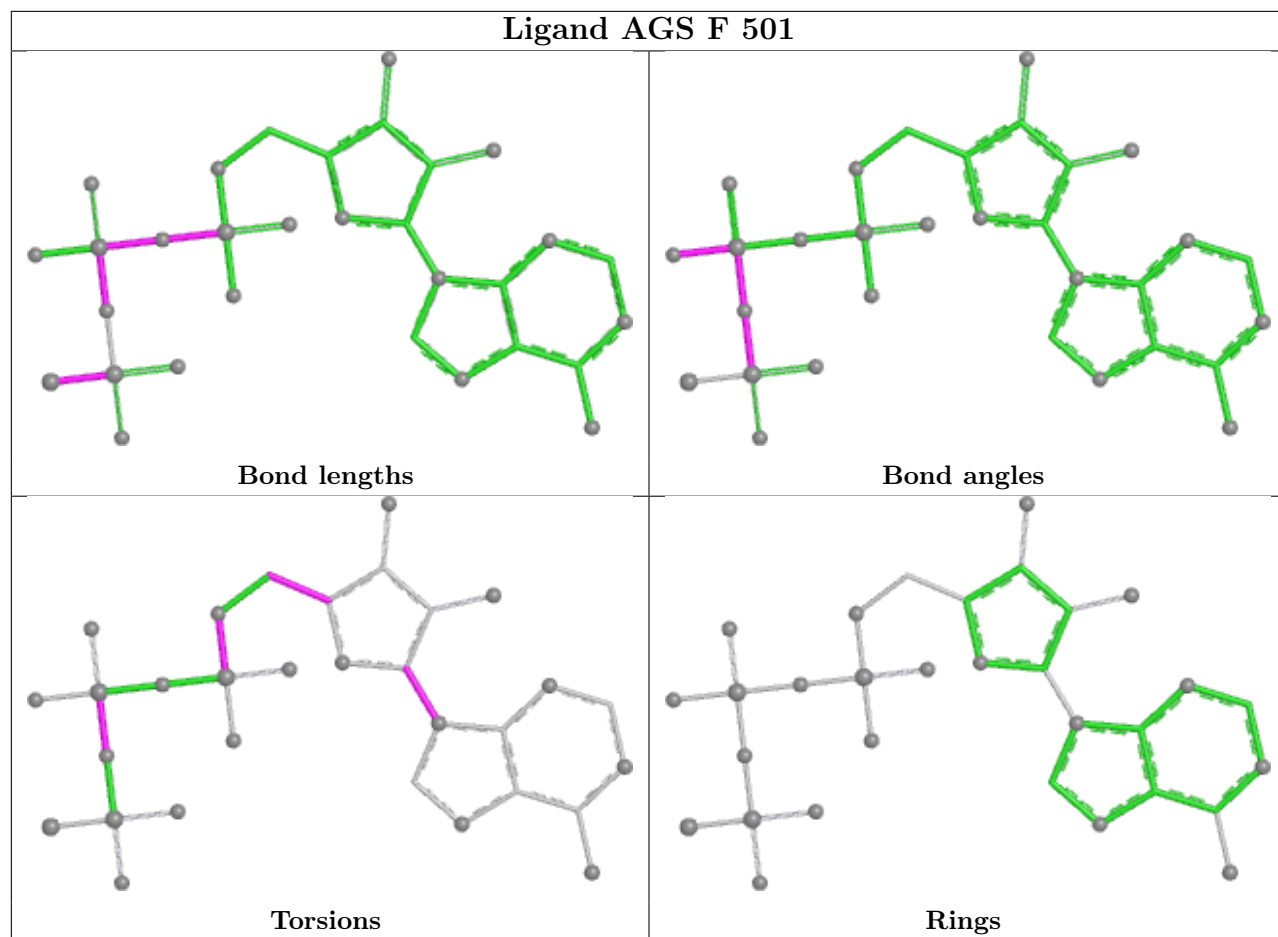
Ligand AGS C 401

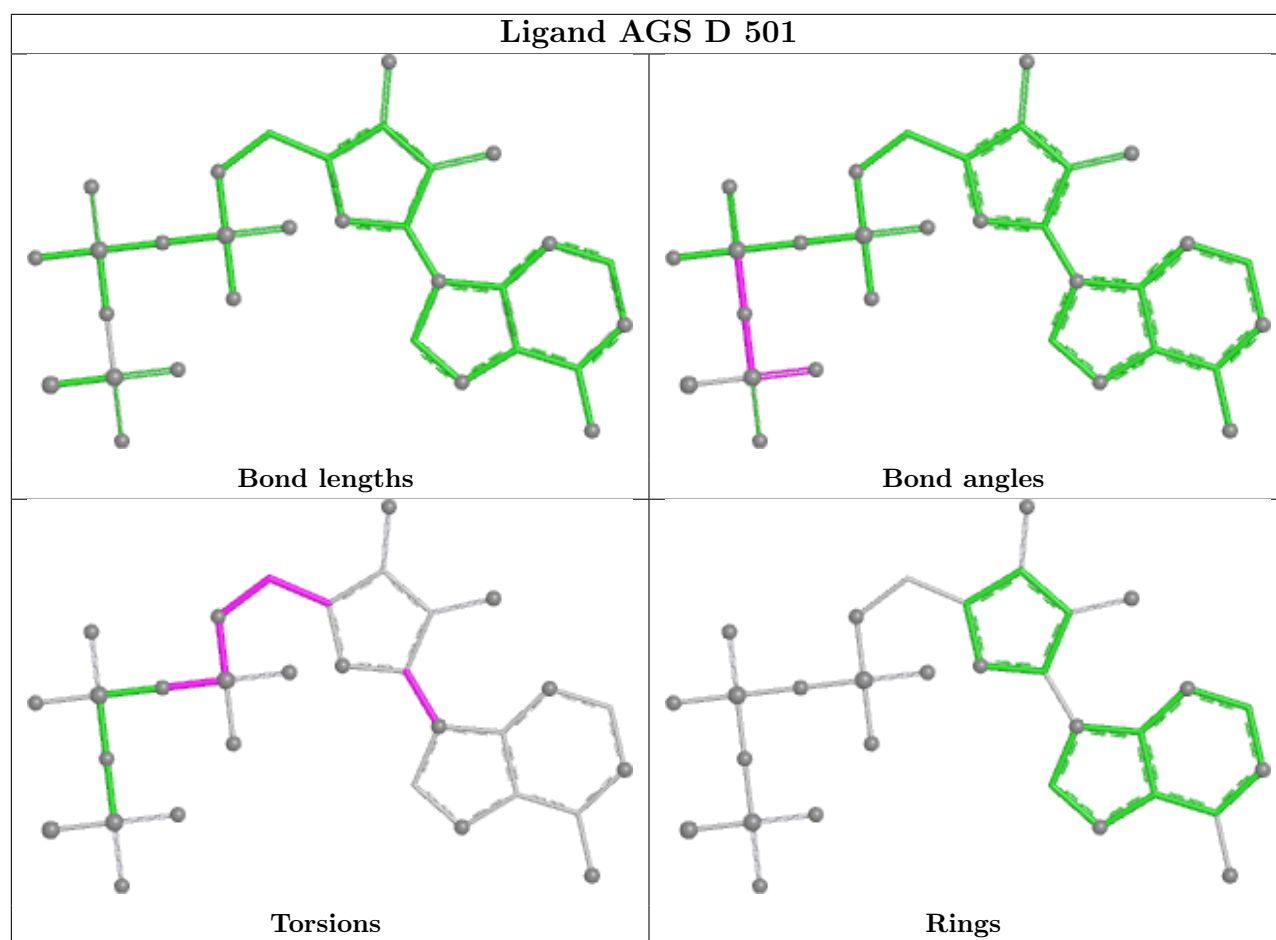


Ligand AGS E 401



Ligand AGS F 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.

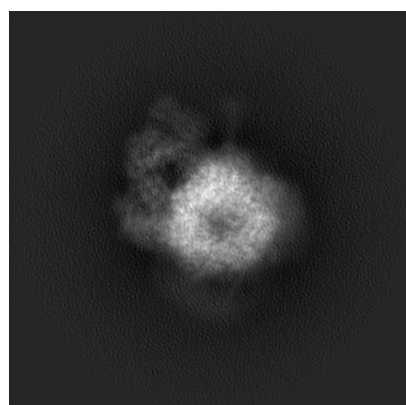
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8666. These allow visual inspection of the internal detail of the map and identification of artifacts.

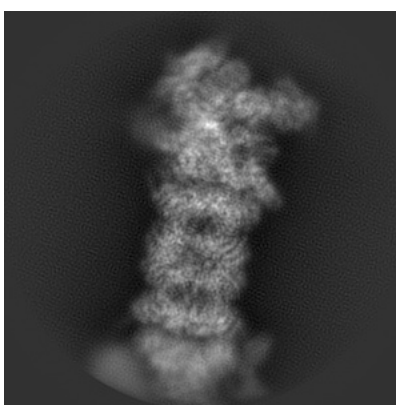
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

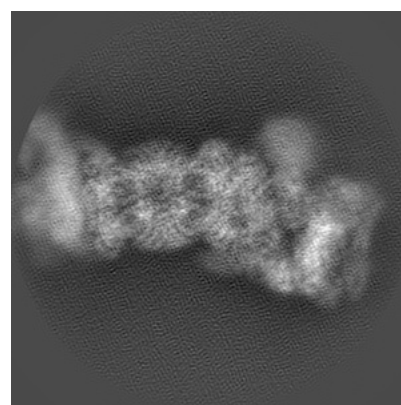
6.1.1 Primary map



X



Y

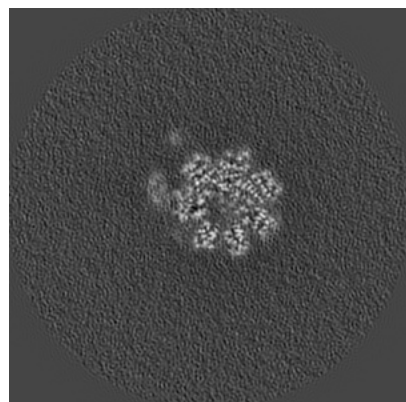


Z

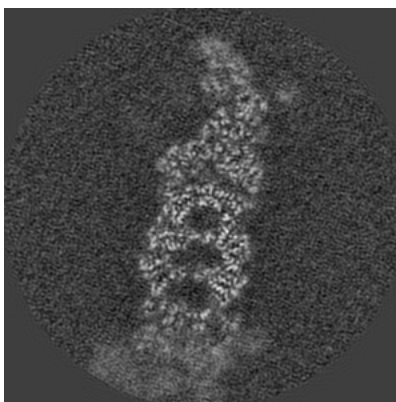
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

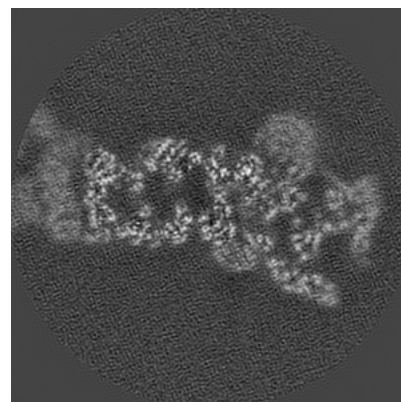
6.2.1 Primary map



X Index: 280



Y Index: 280

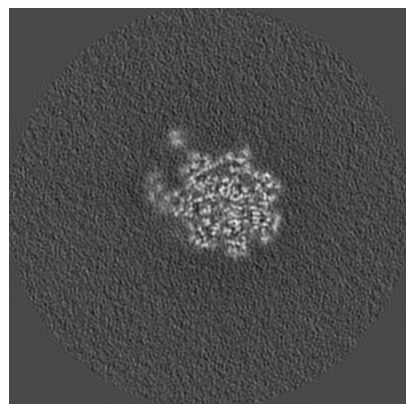


Z Index: 280

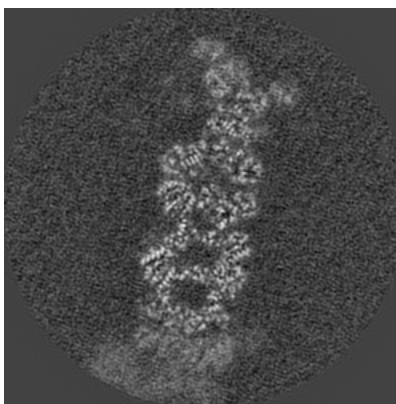
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

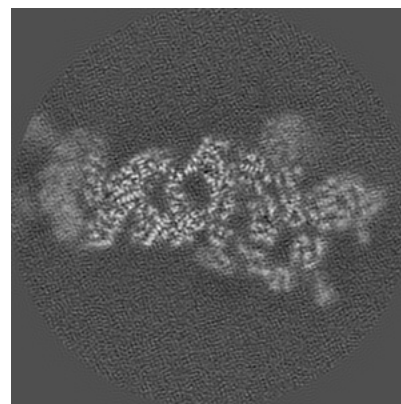
6.3.1 Primary map



X Index: 285



Y Index: 274

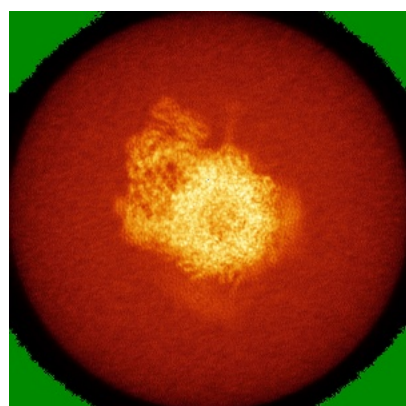


Z Index: 299

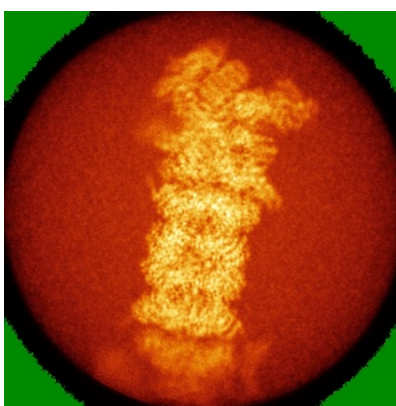
The images above show the largest variance slices of the map in three orthogonal directions.

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

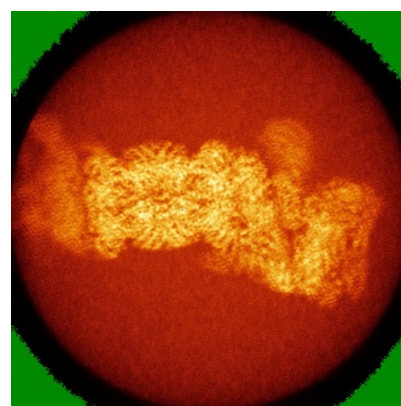
6.4.1 Primary map



X



Y

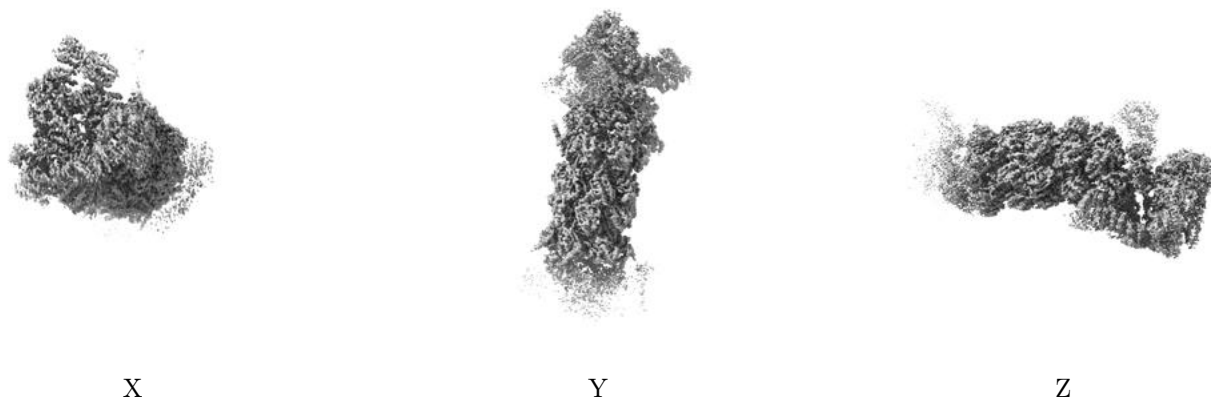


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

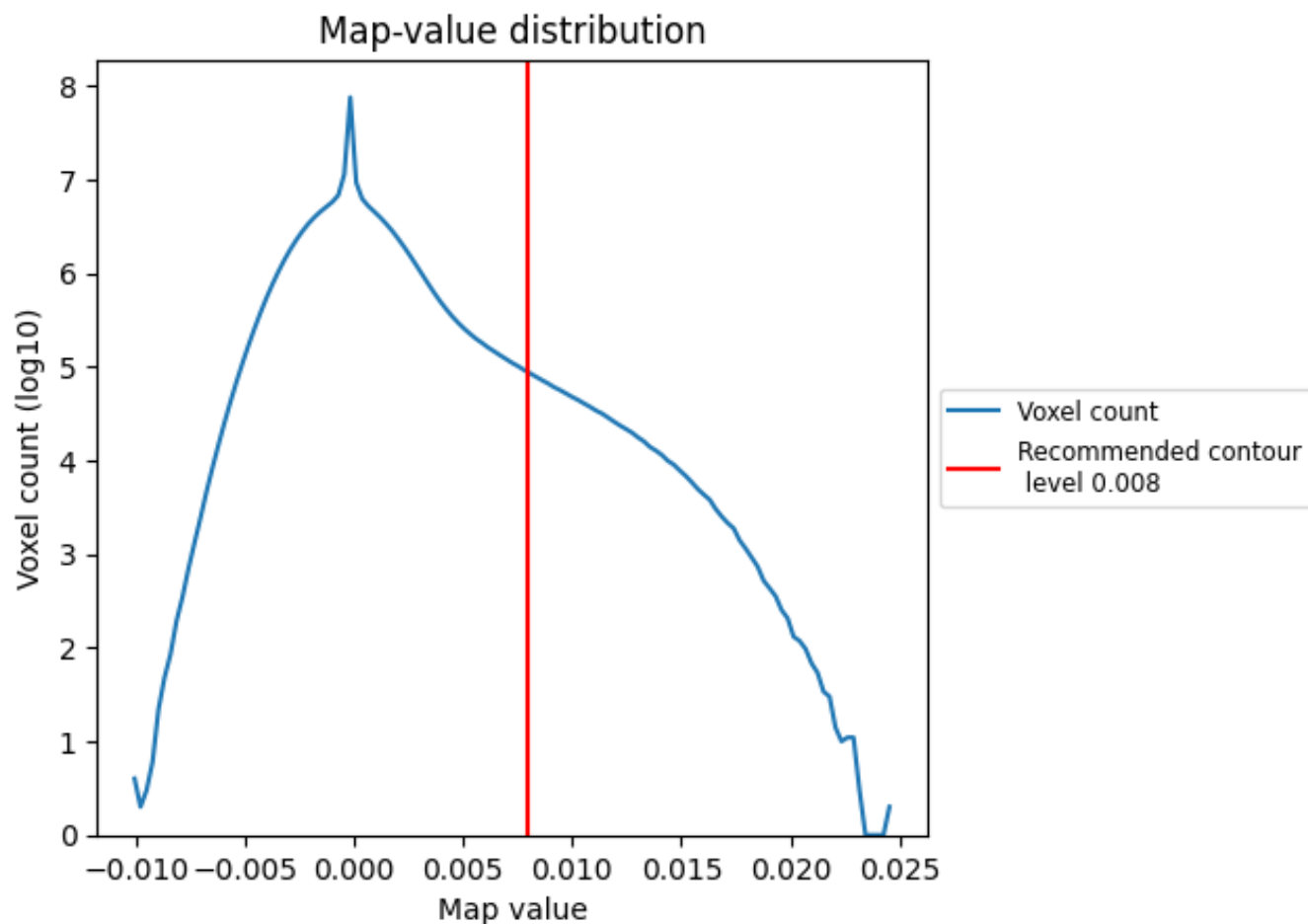
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

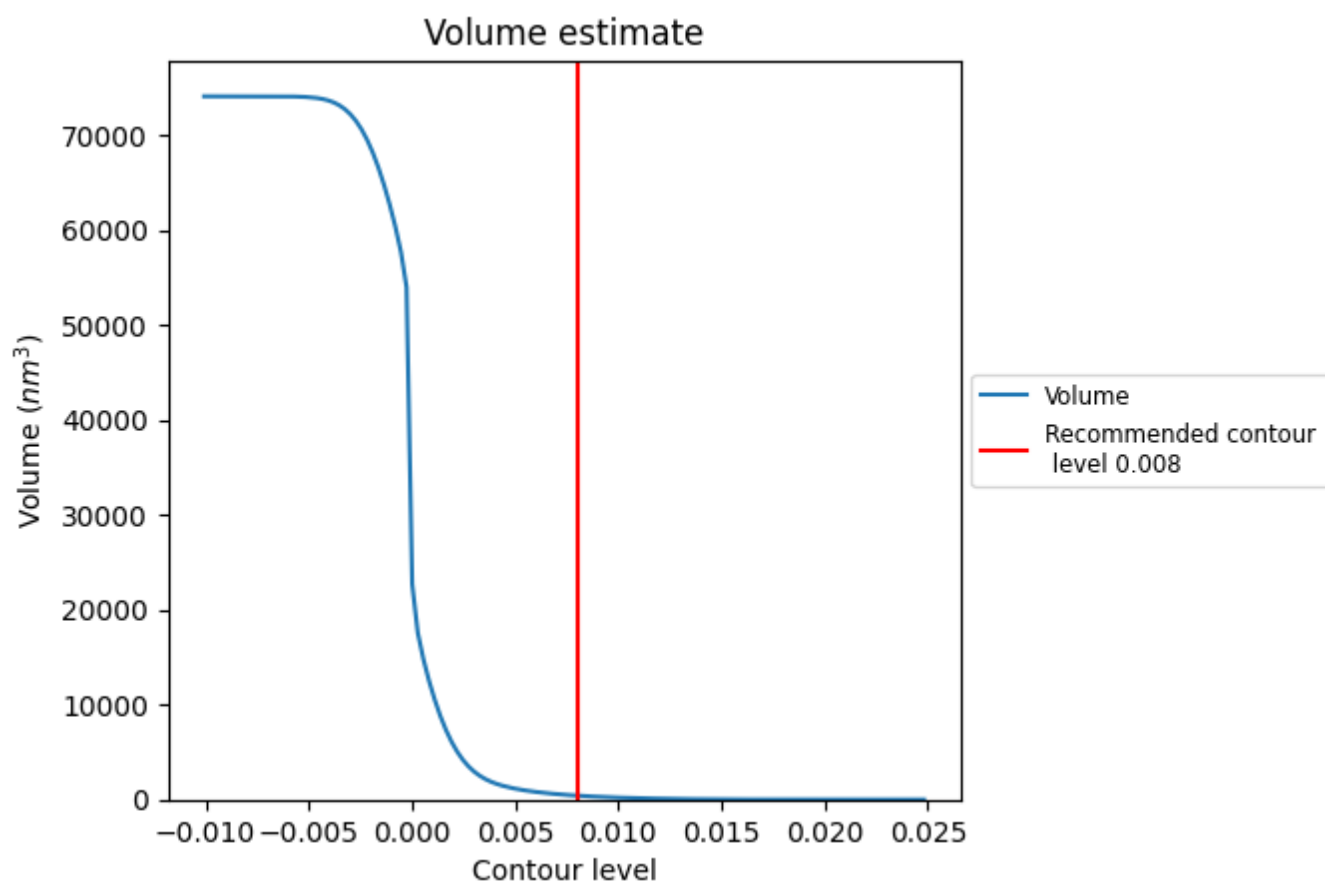
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

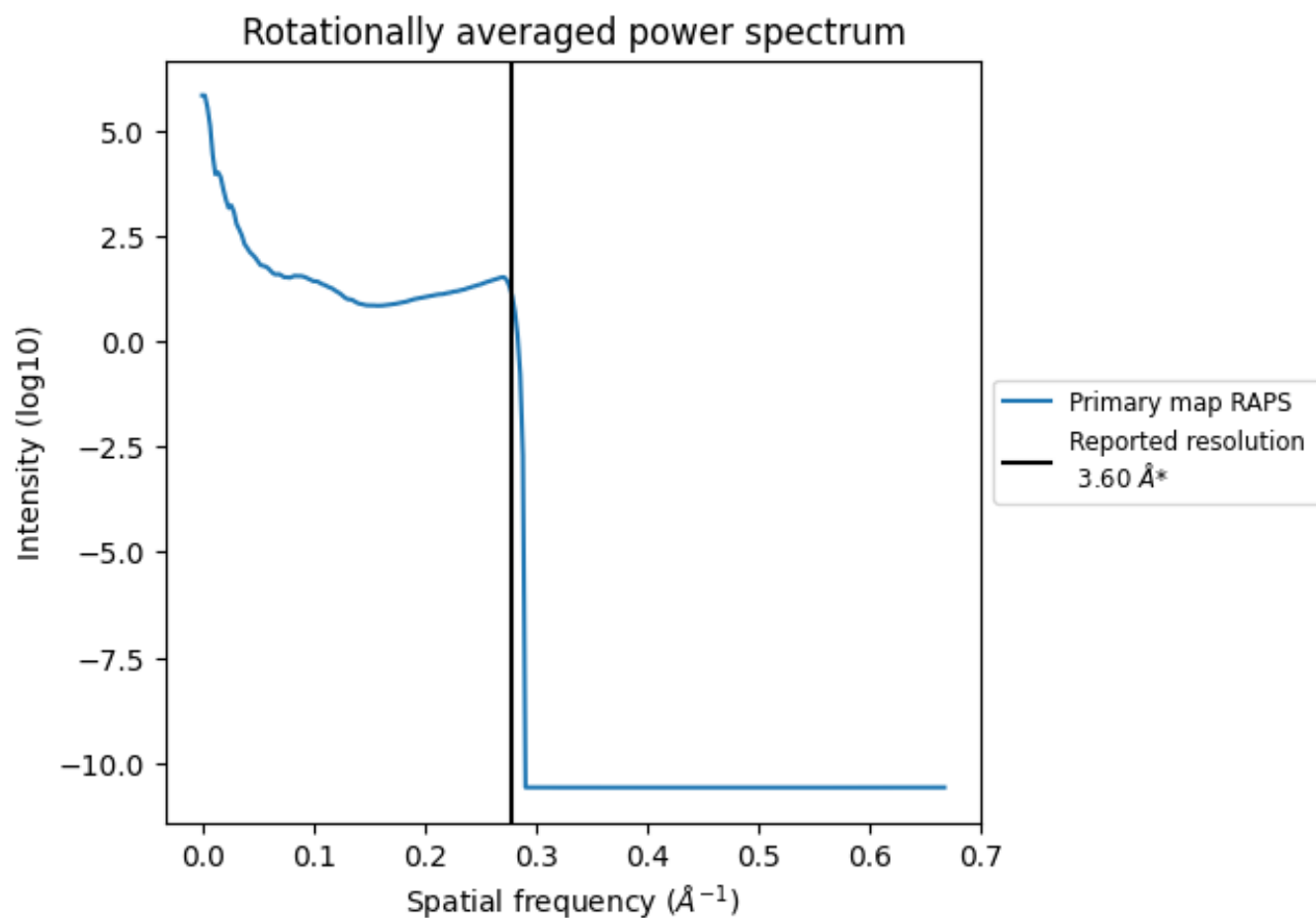
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 415 nm³; this corresponds to an approximate mass of 375 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 0.278 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

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

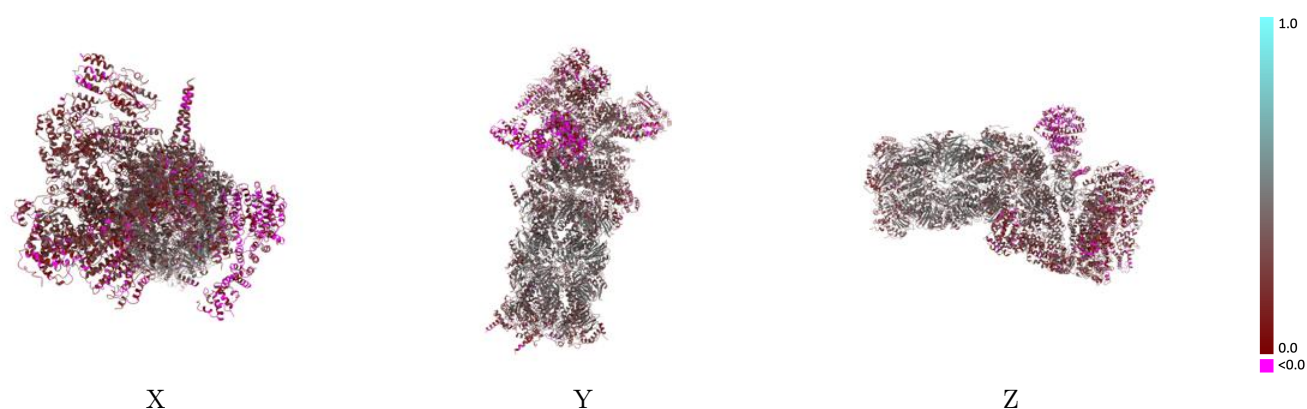
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8666 and PDB model 5VFS. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)

This section was not generated.

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

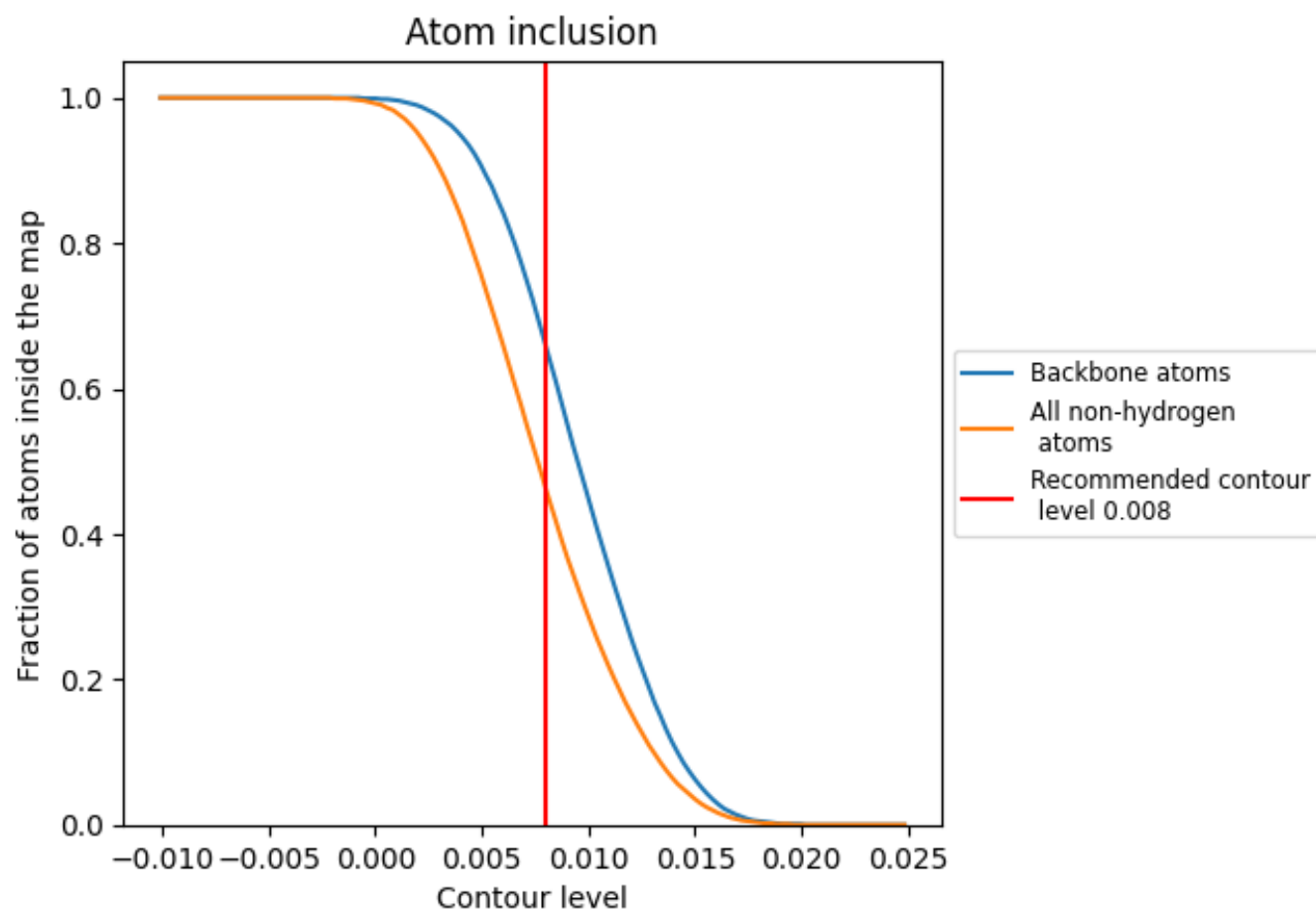


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 66% of all backbone atoms, 46% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4620	 0.3020
A	 0.5130	 0.3550
B	 0.4640	 0.3370
C	 0.4840	 0.3290
D	 0.4660	 0.3420
E	 0.4930	 0.3330
F	 0.5180	 0.3600
G	 0.5960	 0.3720
H	 0.6010	 0.3760
I	 0.5720	 0.3530
J	 0.6210	 0.3660
K	 0.5830	 0.3660
L	 0.6290	 0.3830
M	 0.5770	 0.3610
N	 0.6750	 0.4170
O	 0.6120	 0.3840
P	 0.6330	 0.4080
Q	 0.6280	 0.3870
R	 0.6880	 0.4220
S	 0.6350	 0.4210
T	 0.6740	 0.4250
U	 0.2740	 0.2080
V	 0.3050	 0.1960
W	 0.3760	 0.2090
X	 0.2510	 0.2560
Y	 0.4070	 0.2440
Z	 0.4400	 0.2730
a	 0.3200	 0.2040
b	 0.2480	 0.2000
c	 0.4280	 0.2620
d	 0.2310	 0.1720
e	 0.2520	 0.2000
f	 0.0190	 0.0470
g	 0.5170	 0.3210
h	 0.5260	 0.3250



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Chain	Atom inclusion	Q-score
i	 0.4790	 0.3020
j	 0.4750	 0.2980
k	 0.5200	 0.3240
l	 0.5460	 0.3280
m	 0.5060	 0.3060
n	 0.6510	 0.3980
o	 0.5970	 0.3950
p	 0.6330	 0.4150
q	 0.6180	 0.3730
r	 0.6670	 0.4040
s	 0.6170	 0.3910
t	 0.6550	 0.3890