



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 04:22 PM UTC

PDB ID : 5VFR / pdb_00005vfr
EMDB ID : EMD-8665
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 : 4.90 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:

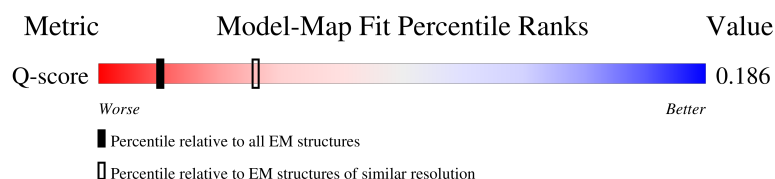
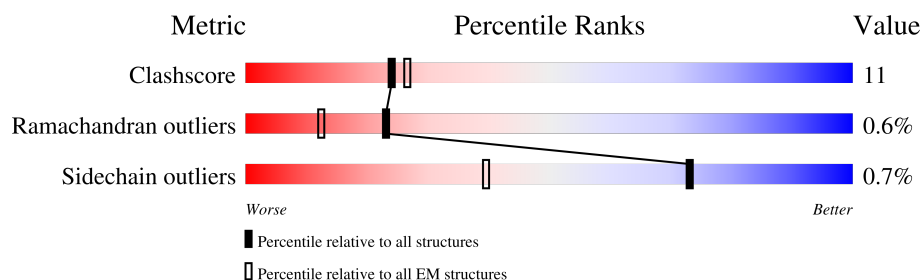
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.90 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	1274 (4.40 - 5.40)

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

Mol	Chain	Length	Quality of chain
1	U	911	
2	V	480	
3	W	456	
4	X	380	

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Mol	Chain	Length	Quality of chain
5	Y	378	
6	Z	286	
7	a	373	
8	b	191	
9	c	287	
10	d	257	
11	e	70	
12	G	240	
12	g	240	
13	H	232	
13	h	232	
14	I	250	
14	i	250	
15	J	243	
15	j	243	
16	K	234	
16	k	234	
17	L	238	
17	l	238	
18	M	245	
18	m	245	
19	N	191	
19	n	191	
20	O	220	
20	o	220	

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Mol	Chain	Length	Quality of chain
21	P	204	
21	p	204	
22	Q	199	
22	q	199	
23	R	201	
23	r	201	
24	S	213	
24	s	213	
25	T	215	
25	t	215	
26	A	399	
27	B	389	
28	C	392	
29	D	380	
30	E	375	
31	F	396	
32	f	908	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	AGS	F	501	-	-	X	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 99908 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	472	Total	C	N	O	S	0	0
			3799	2413	675	697	14		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	241	Total	C	N	O	S	0	0
			1905	1212	320	365	8		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	c	278	Total	C	N	O	S	0	0
			2187	1389	374	406	18		

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

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

- Molecule 11 is a protein called Sem1.

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

- Molecule 12 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 13 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	230	Total	C	N	O	S	0	0
			1688	1070	284	329	5		

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

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

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

- Molecule 15 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 16 is a protein called Proteasome subunit alpha type-5.

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

- Molecule 17 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 18 is a protein called Proteasome subunit alpha type-3.

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

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

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

- Molecule 20 is a protein called Proteasome subunit beta type-7.

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

- Molecule 21 is a protein called Proteasome subunit beta type-3.

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

- Molecule 22 is a protein called Proteasome subunit beta type-2.

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

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

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

- Molecule 24 is a protein called Proteasome subunit beta type-1.

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

- Molecule 25 is a protein called Proteasome subunit beta type-4.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	342	Total	C	N	O	S	0	0
			2672	1684	475	497	16		

- Molecule 27 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B	350	Total	C	N	O	S	0	0
			2706	1703	458	533	12		

- Molecule 28 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	C	363	Total	C	N	O	S	0	0
			2859	1804	513	525	17		

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

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

- Molecule 30 is a protein called 26S proteasome regulatory subunit 10B.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	F	376	Total	C	N	O	S	0	0
			2859	1802	496	546	15		

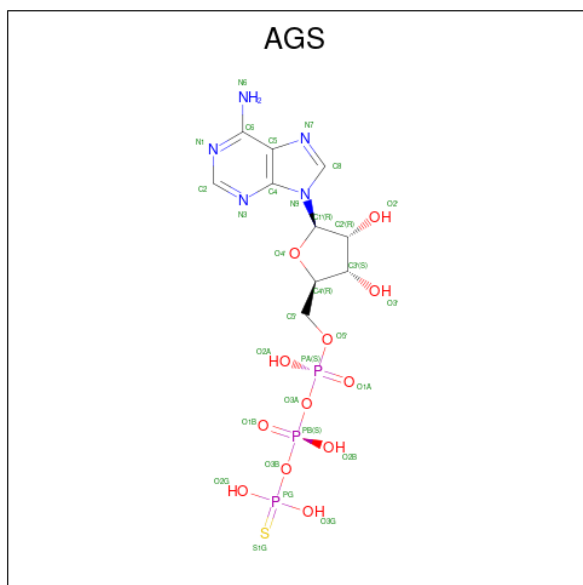
- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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).



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

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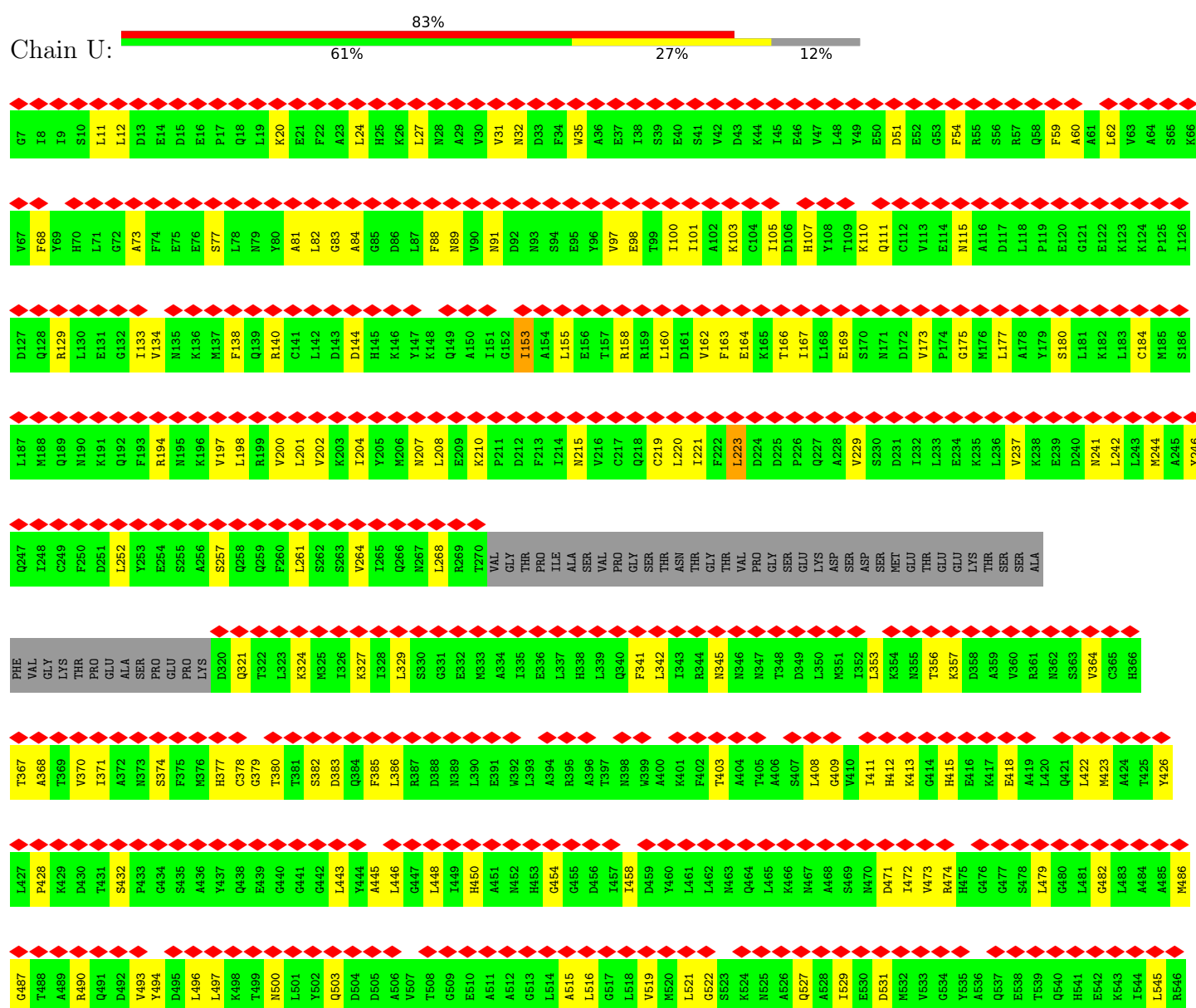
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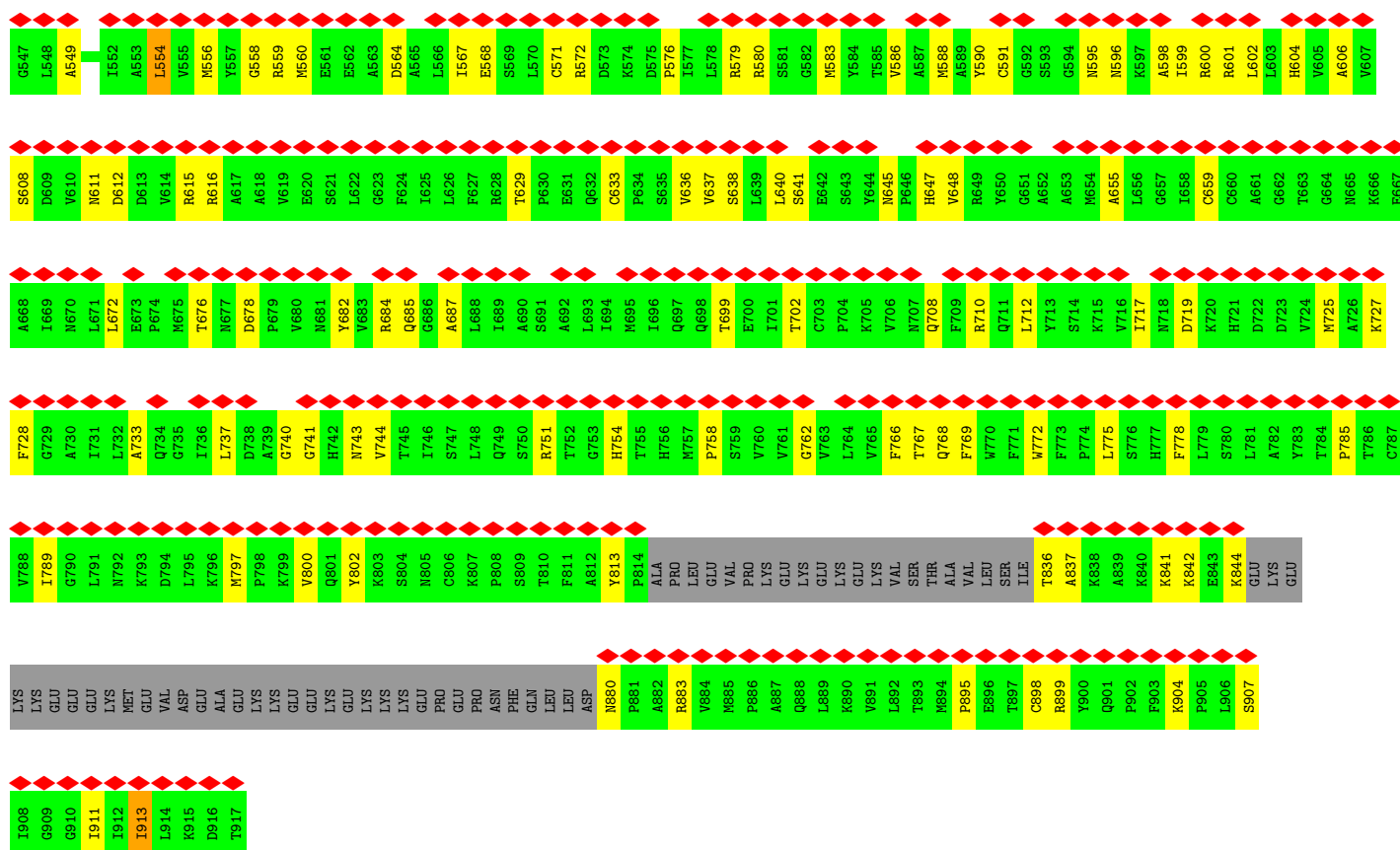
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			Total	C	N	O	P	S	
34	F	1	31	10	5	12	3	1	0

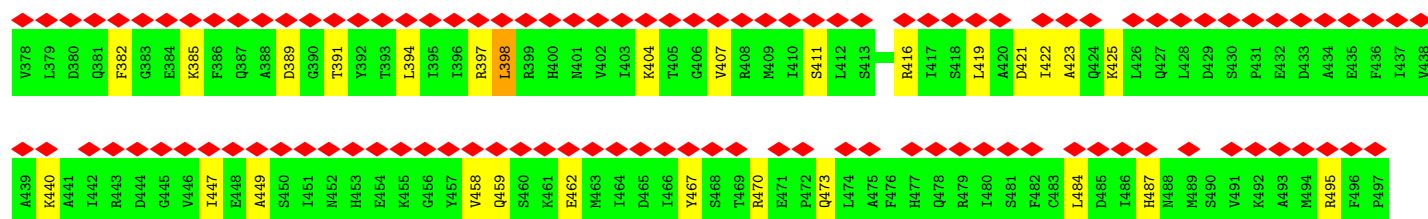
3 Residue-property plots

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.

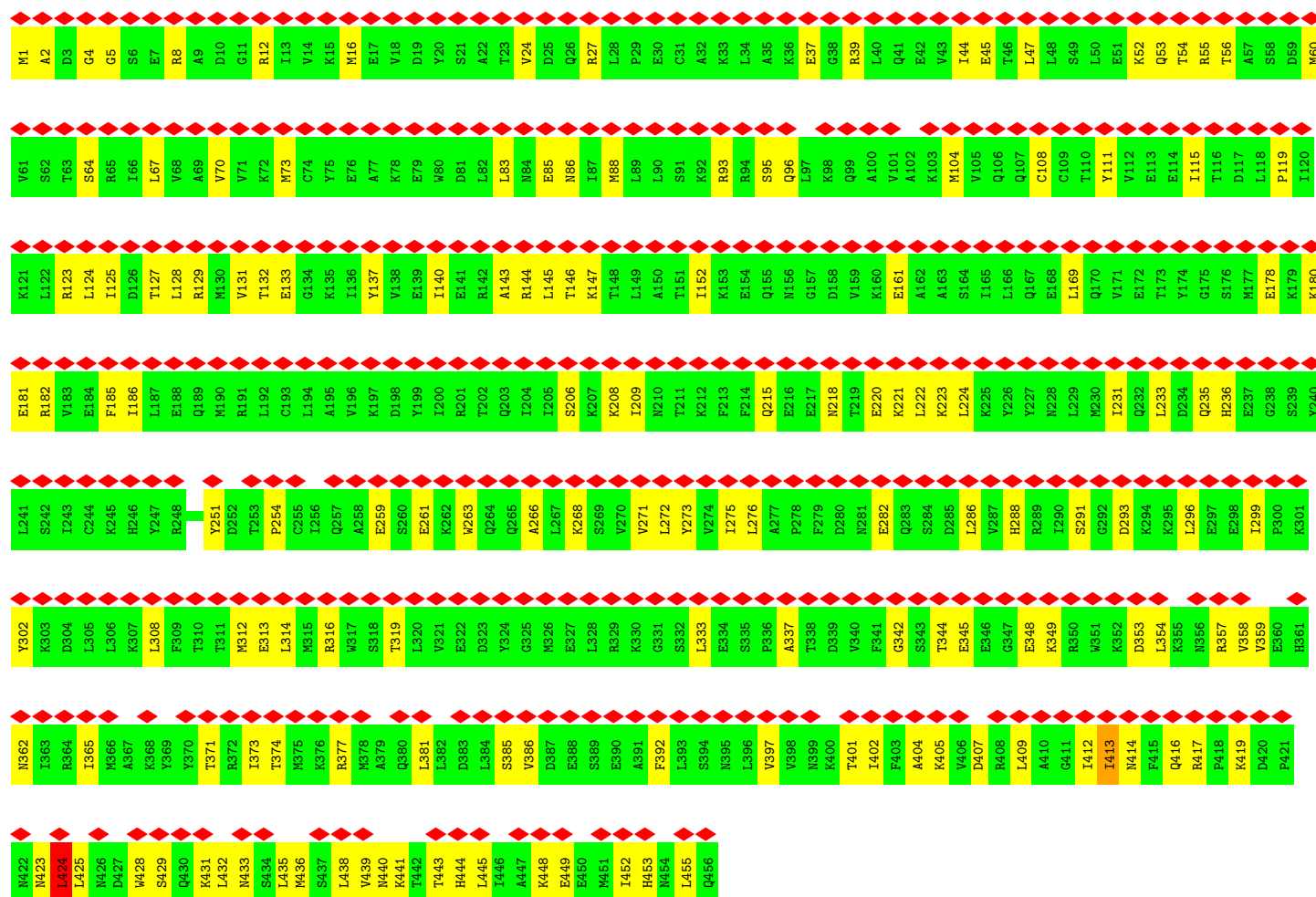
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 1



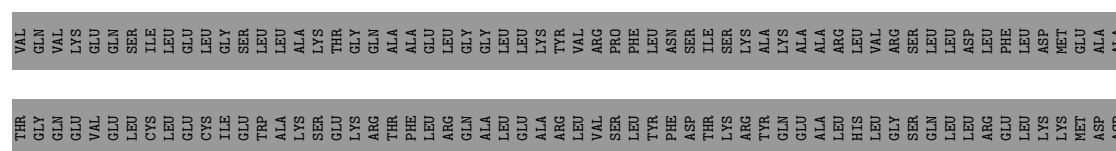


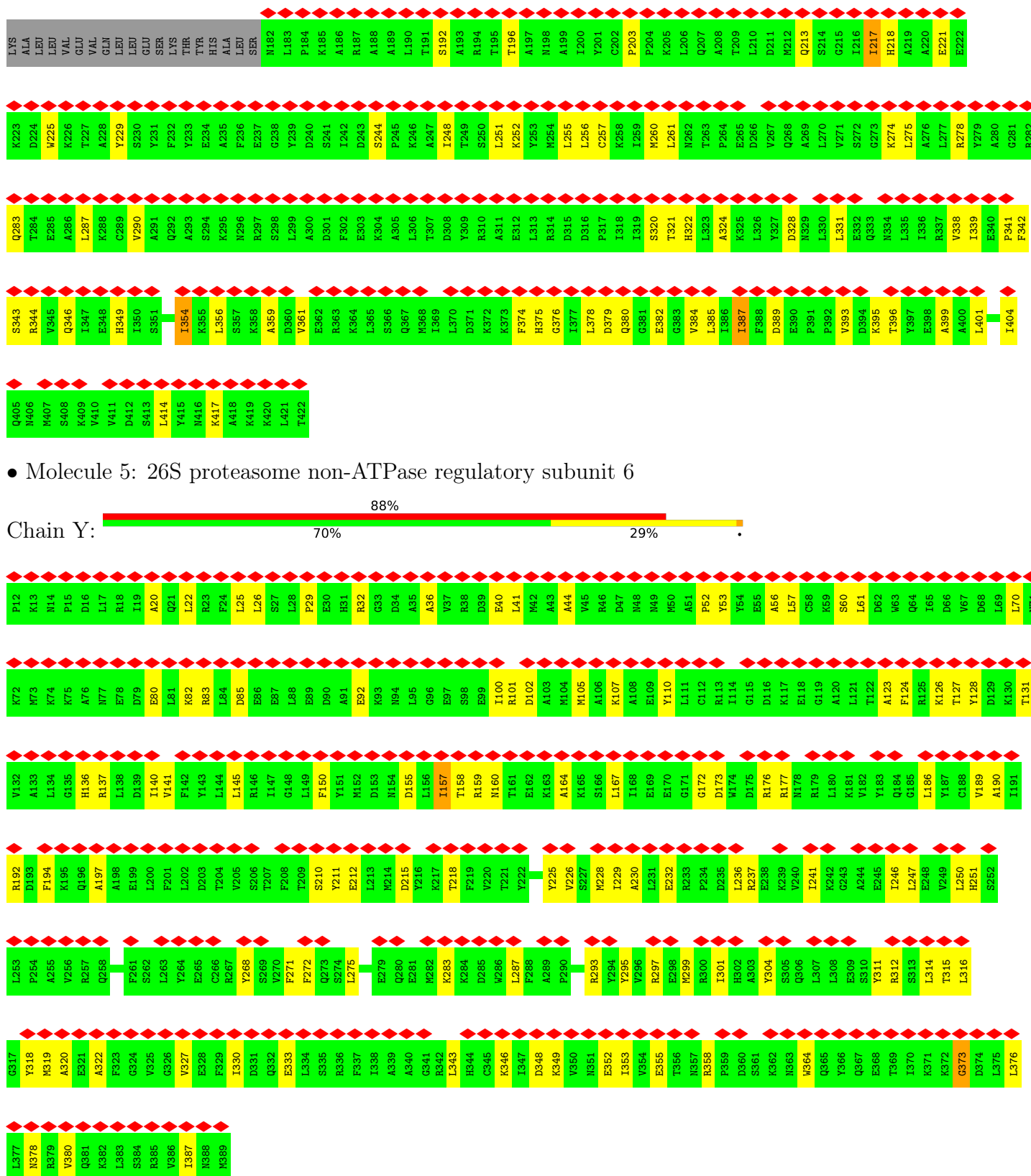


• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

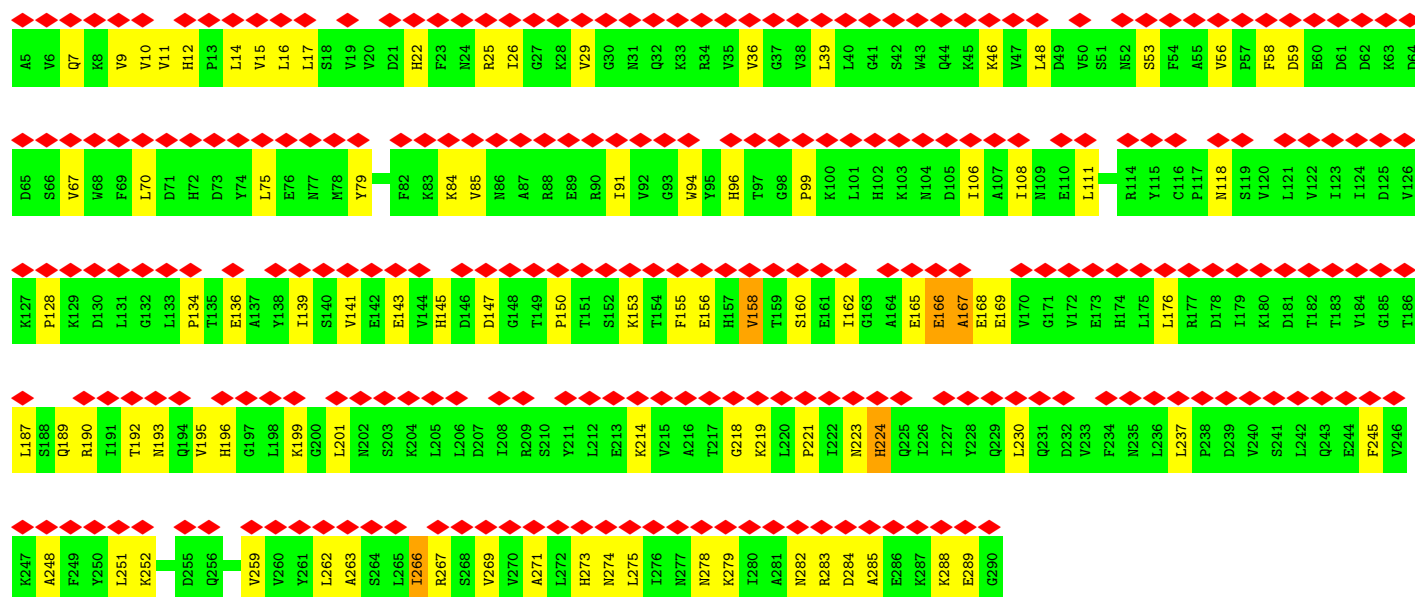


• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

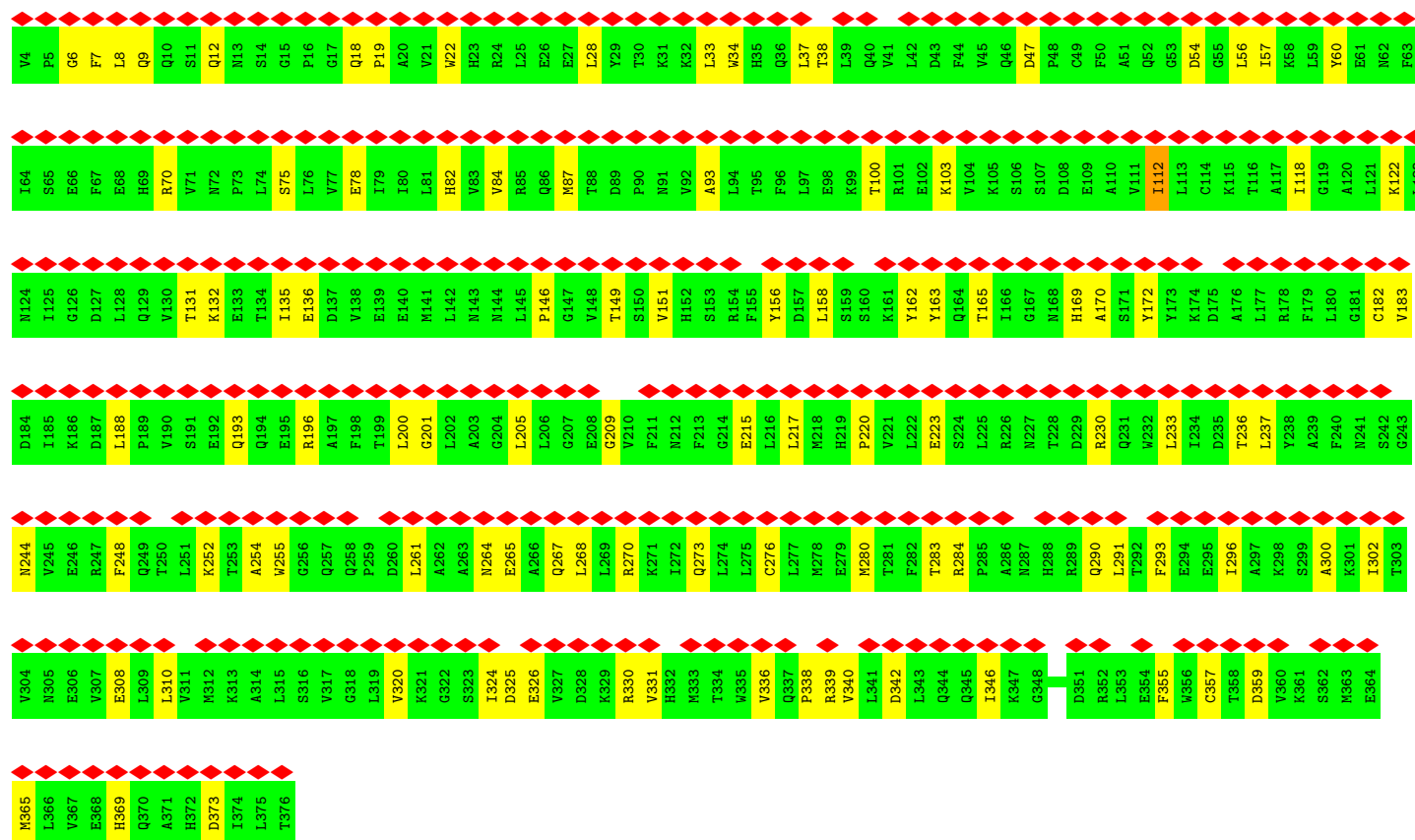
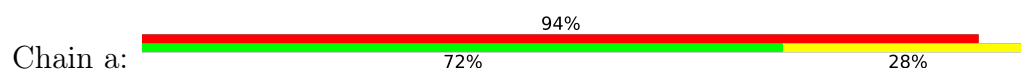




• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7



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

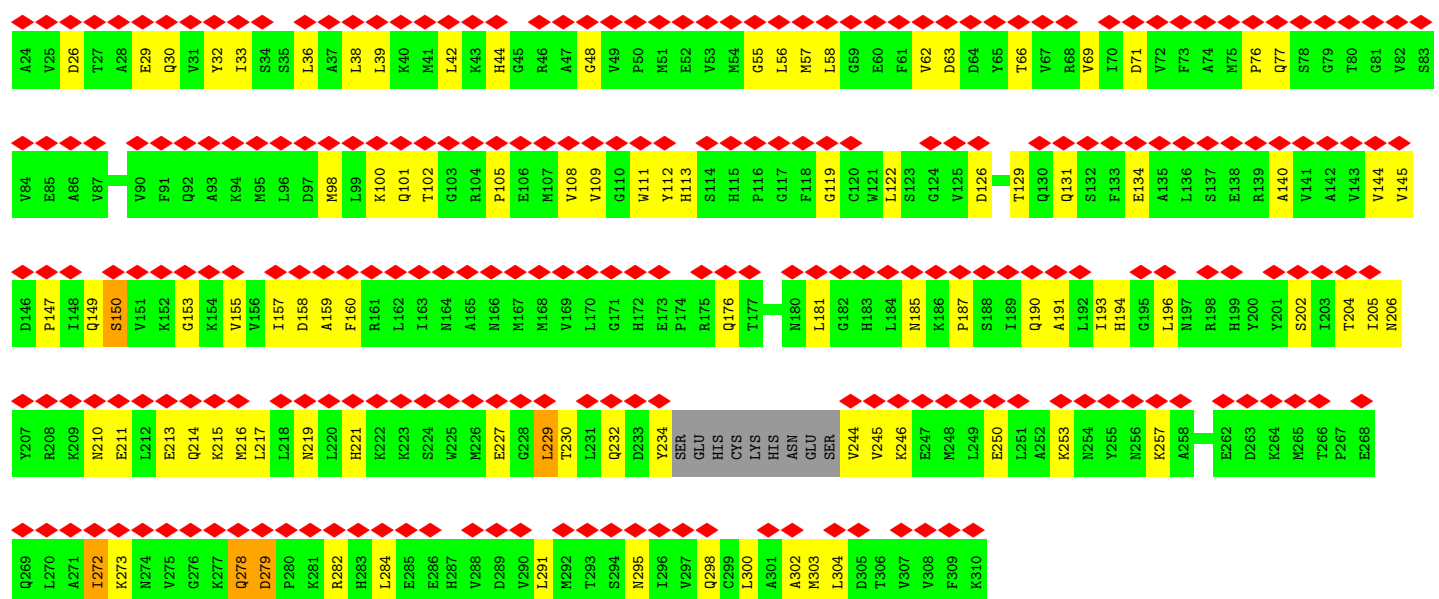
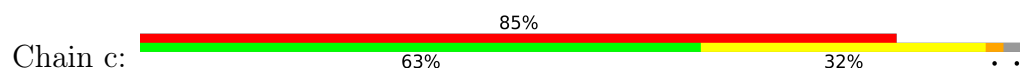


• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

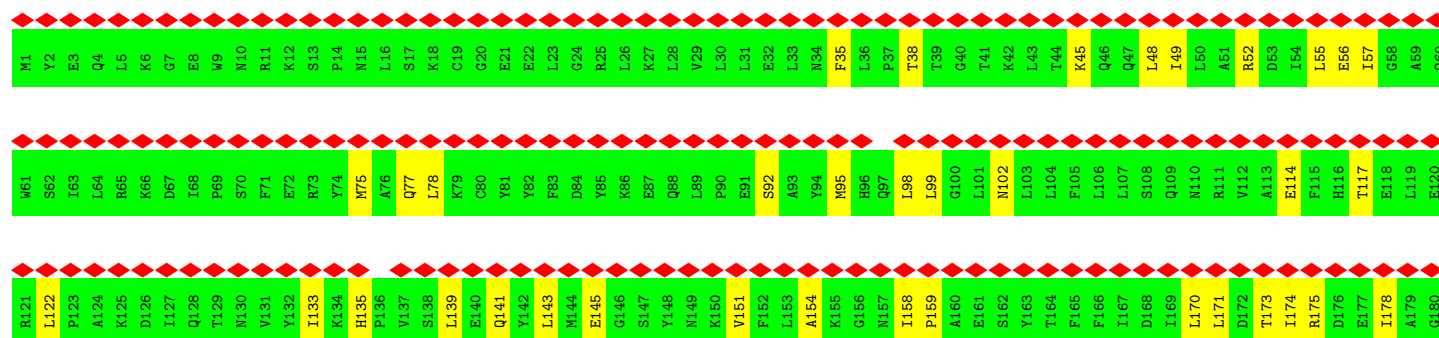
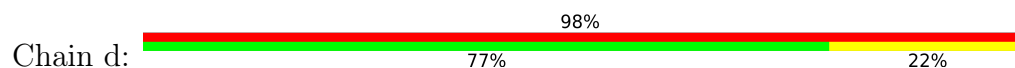


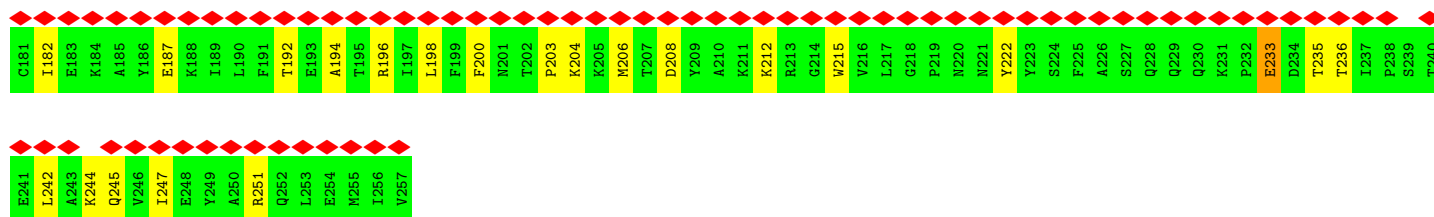


• Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

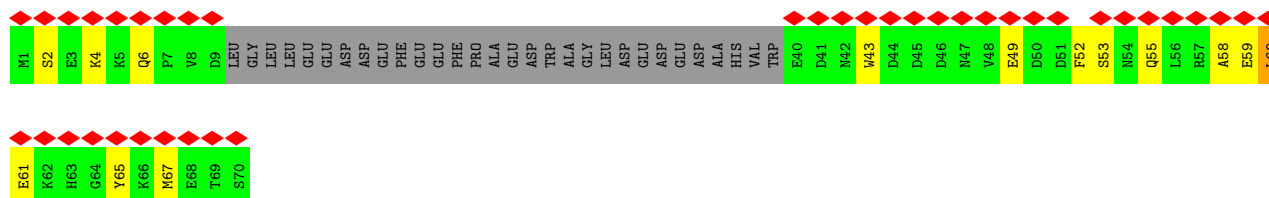


• Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

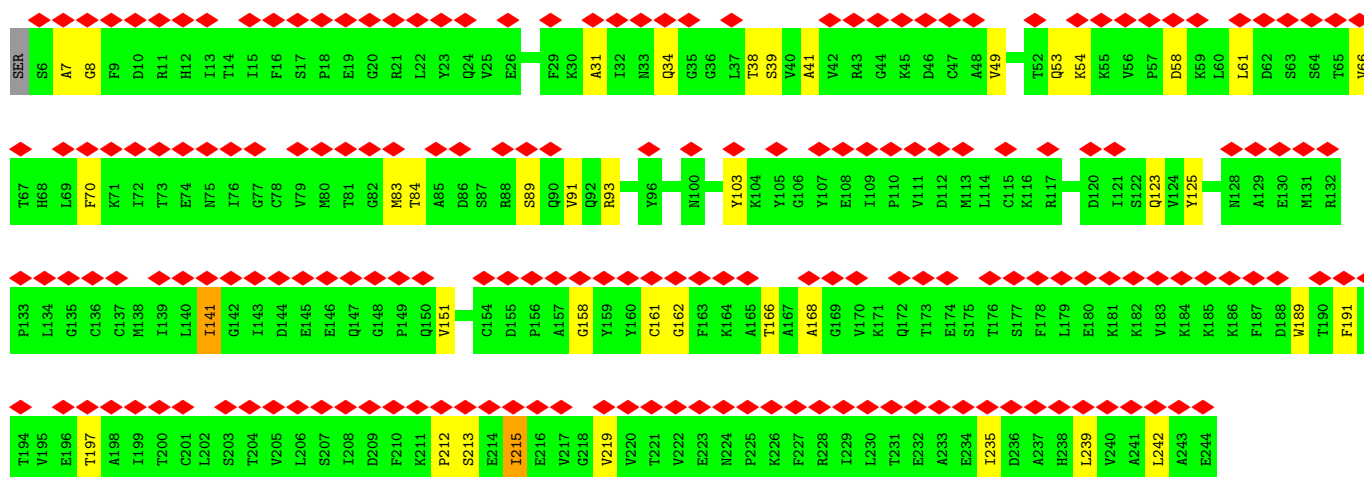
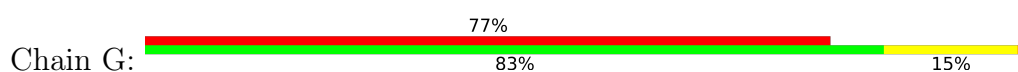




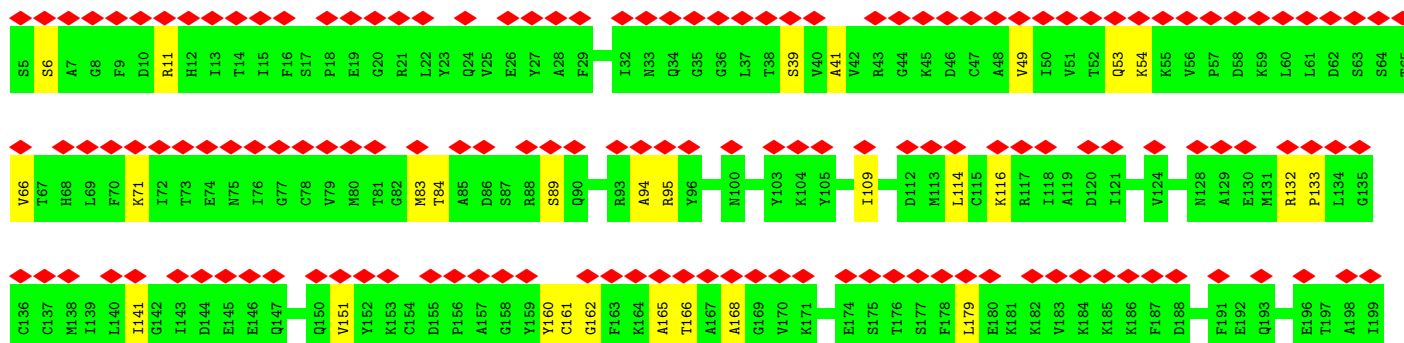
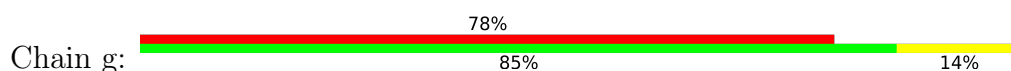
• Molecule 11: Sem1



• Molecule 12: Proteasome subunit alpha type-6

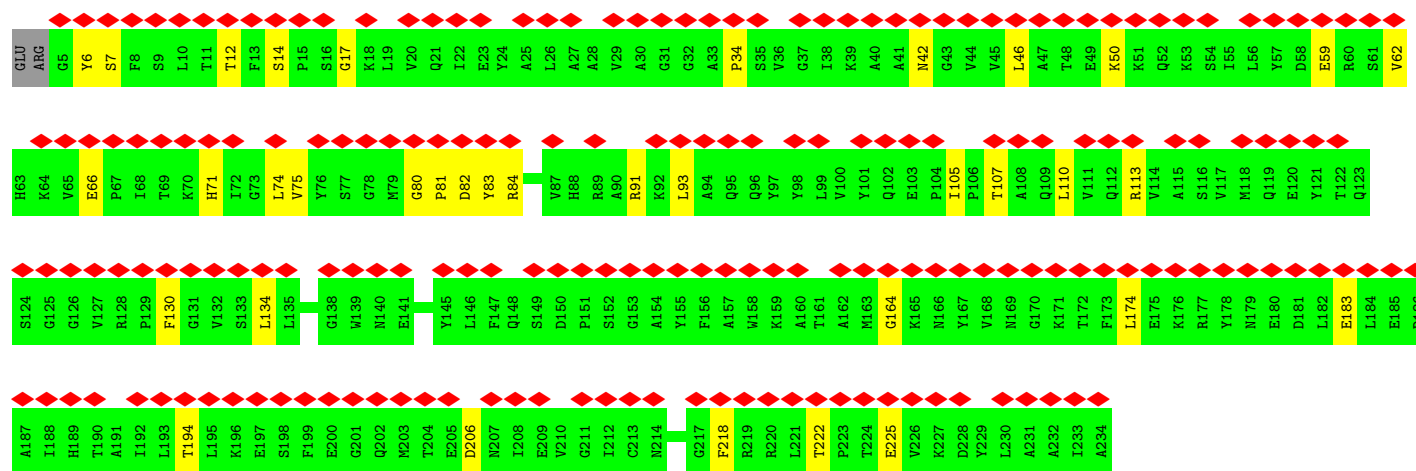
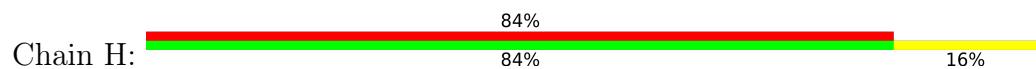


• Molecule 12: Proteasome subunit alpha type-6

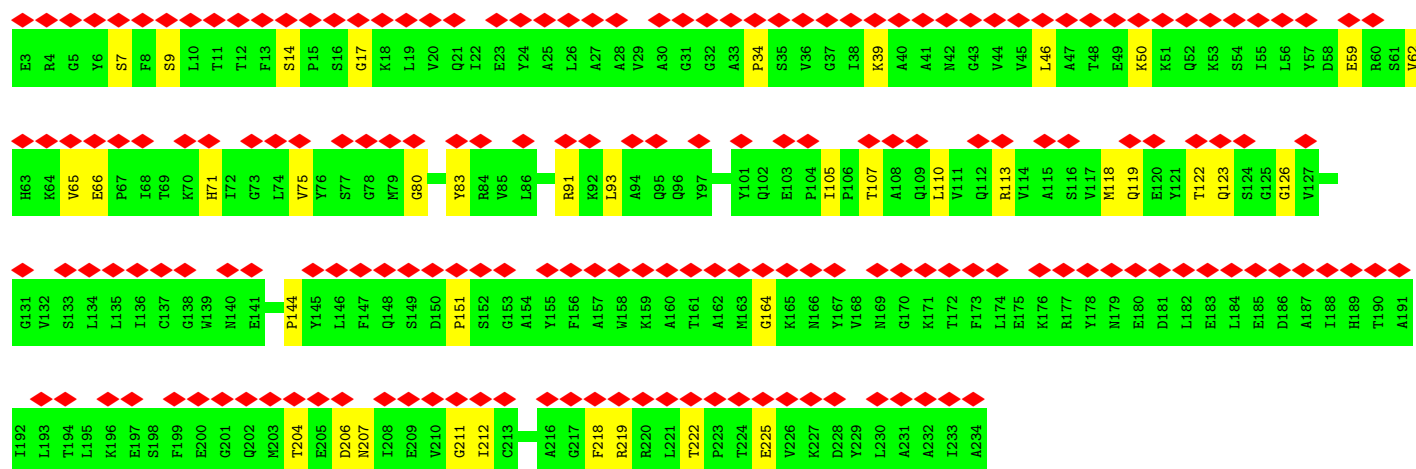
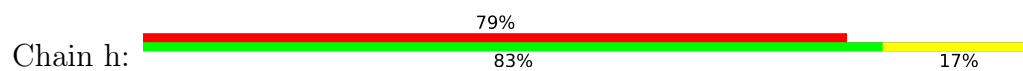




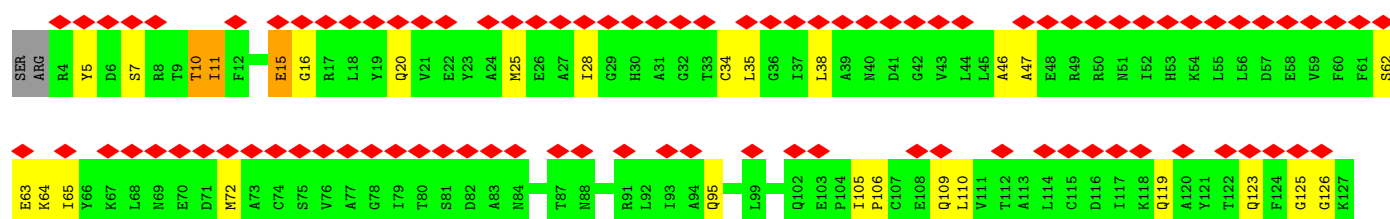
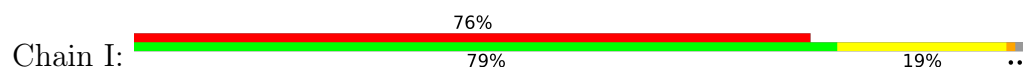
• Molecule 13: Proteasome subunit alpha type-2

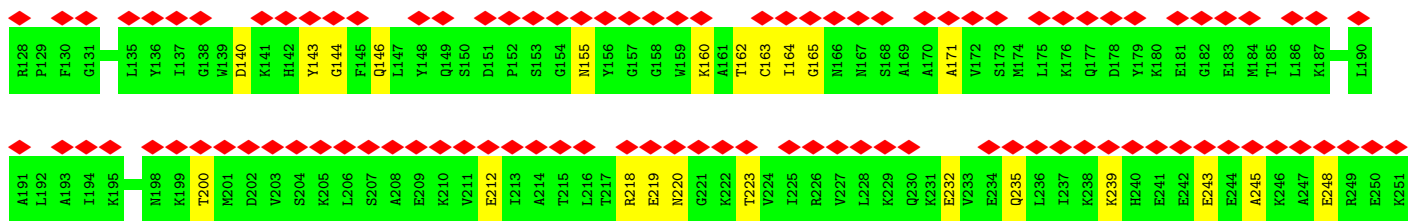


• Molecule 13: Proteasome subunit alpha type-2

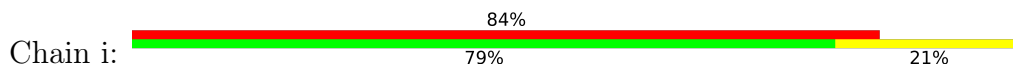


• Molecule 14: Proteasome subunit alpha type-4

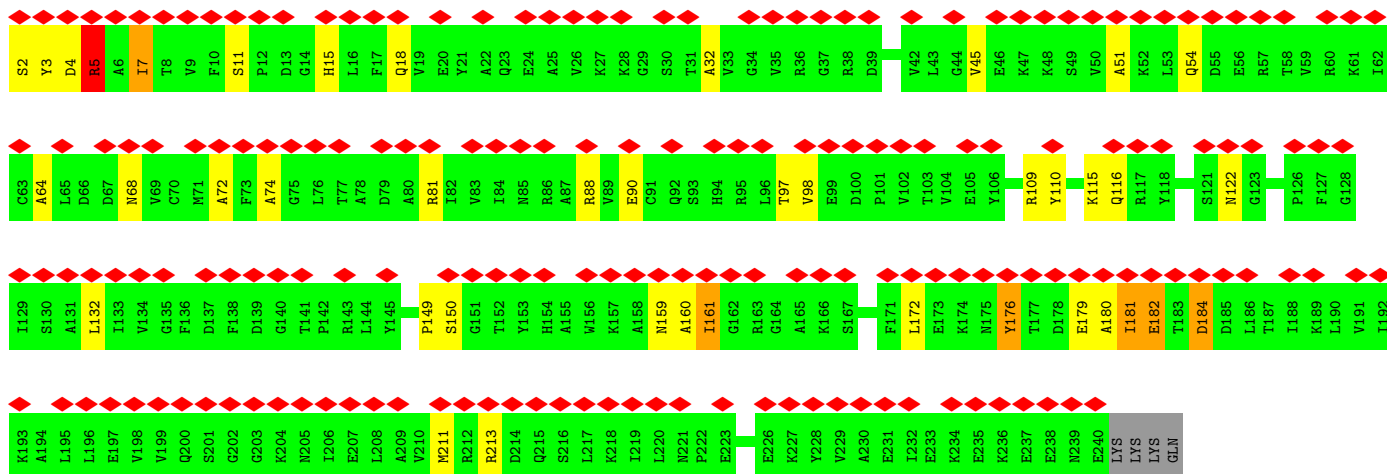
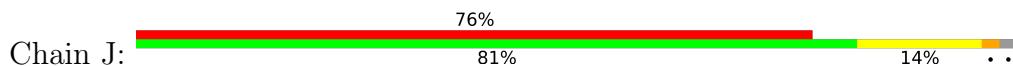




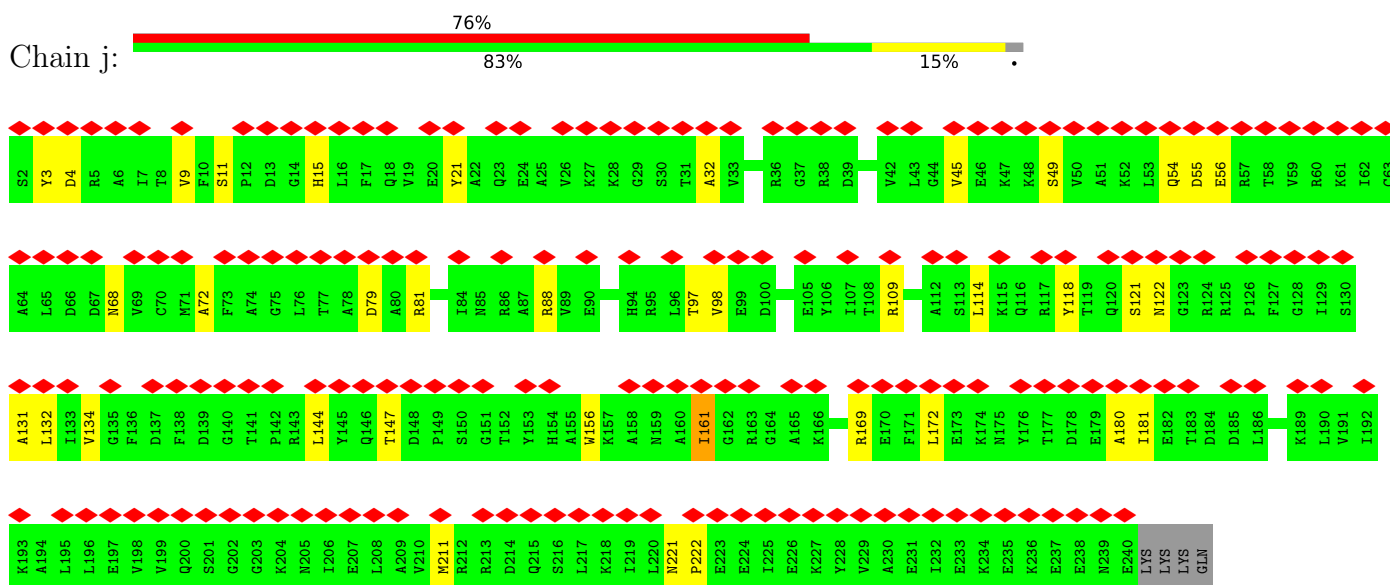
• Molecule 14: Proteasome subunit alpha type-4



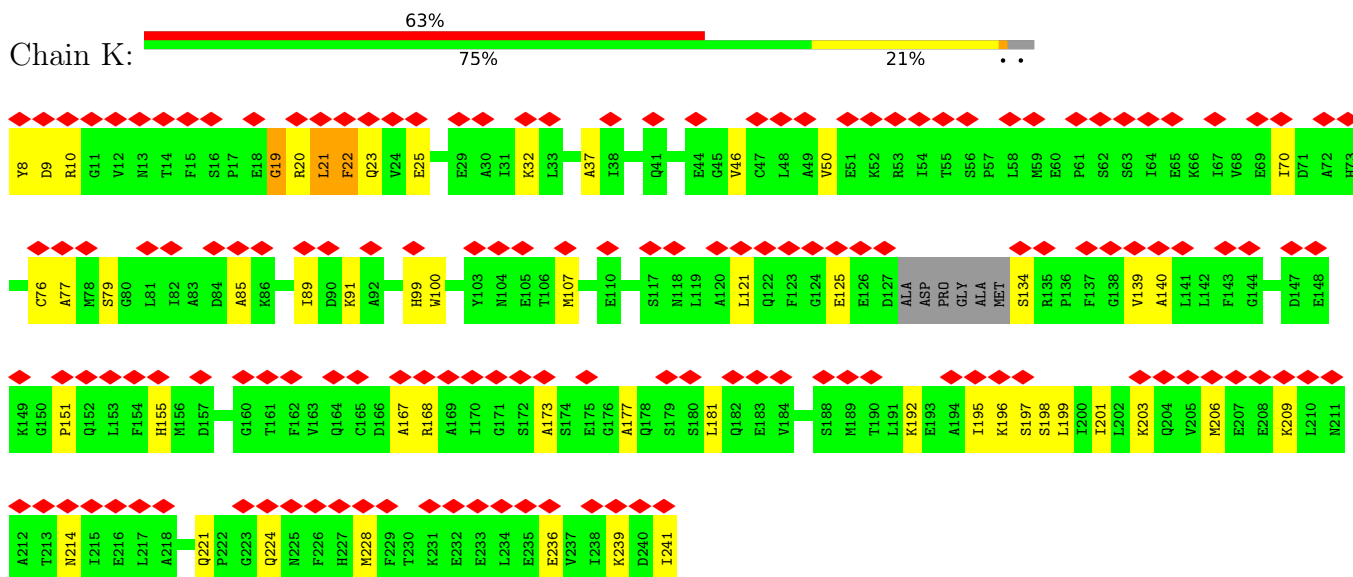
• Molecule 15: Proteasome subunit alpha type-7



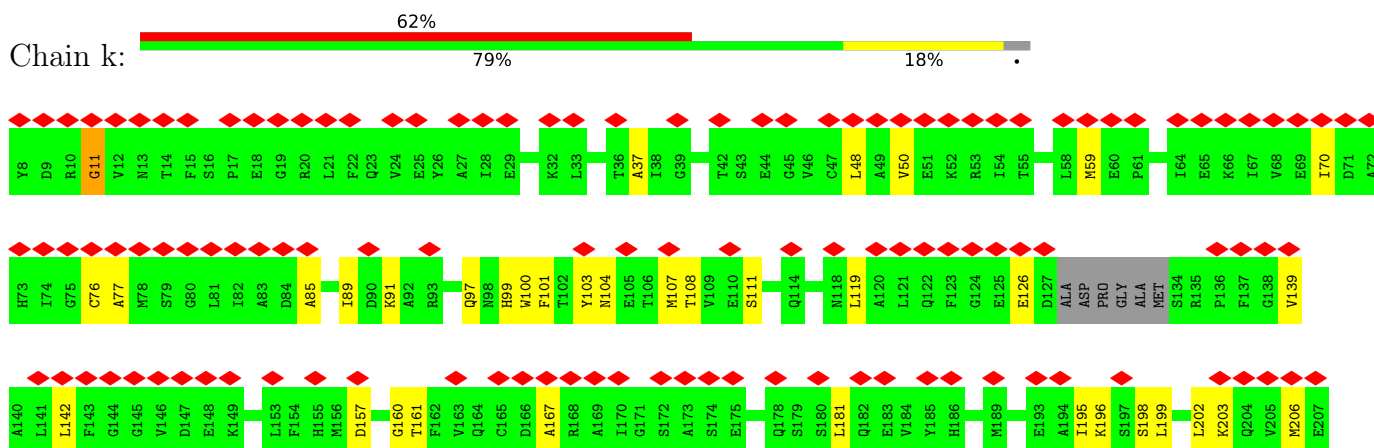
• Molecule 15: Proteasome subunit alpha type-7

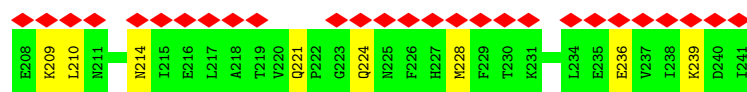


• Molecule 16: Proteasome subunit alpha type-5

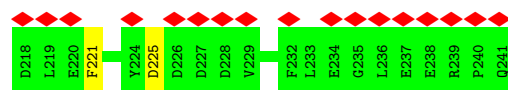
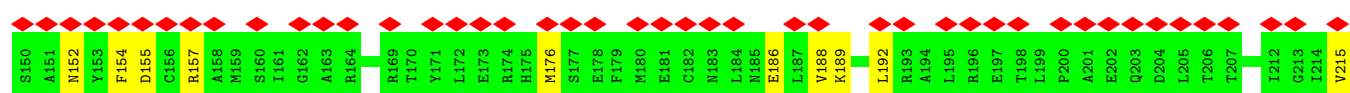
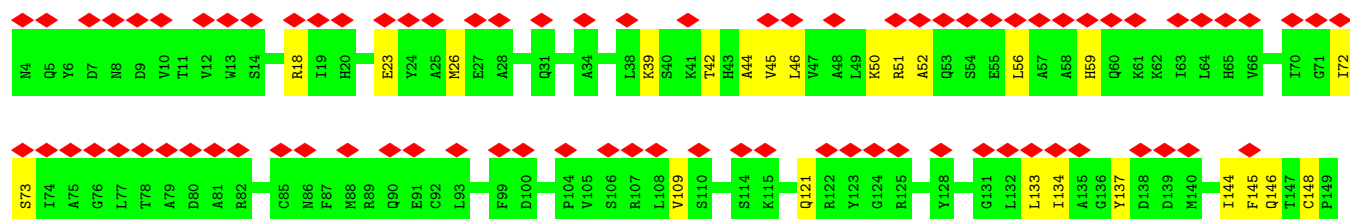
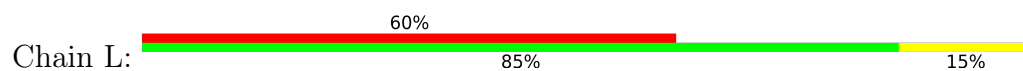


• Molecule 16: Proteasome subunit alpha type-5

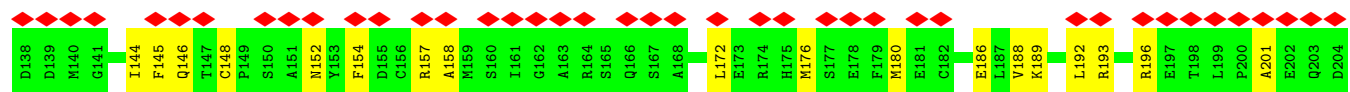
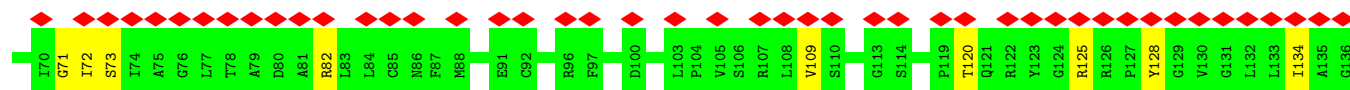
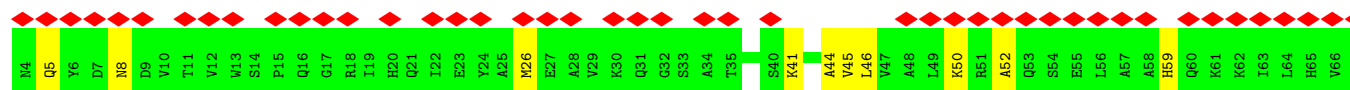
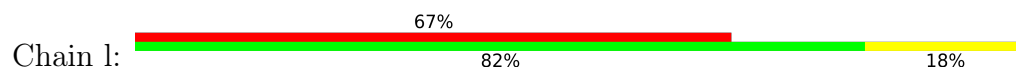




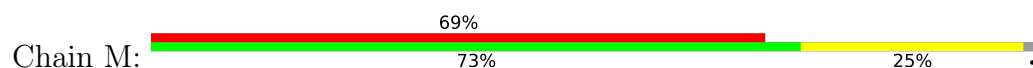
• Molecule 17: Proteasome subunit alpha type-1

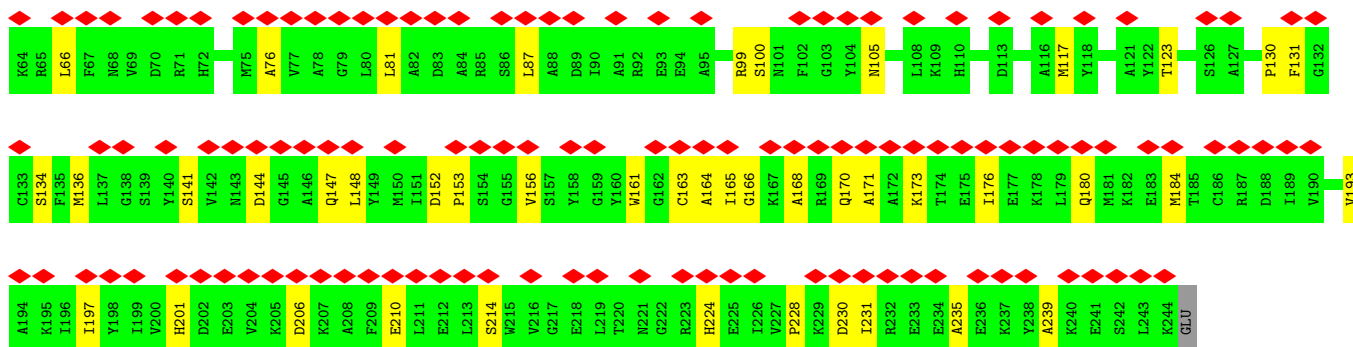


• Molecule 17: Proteasome subunit alpha type-1

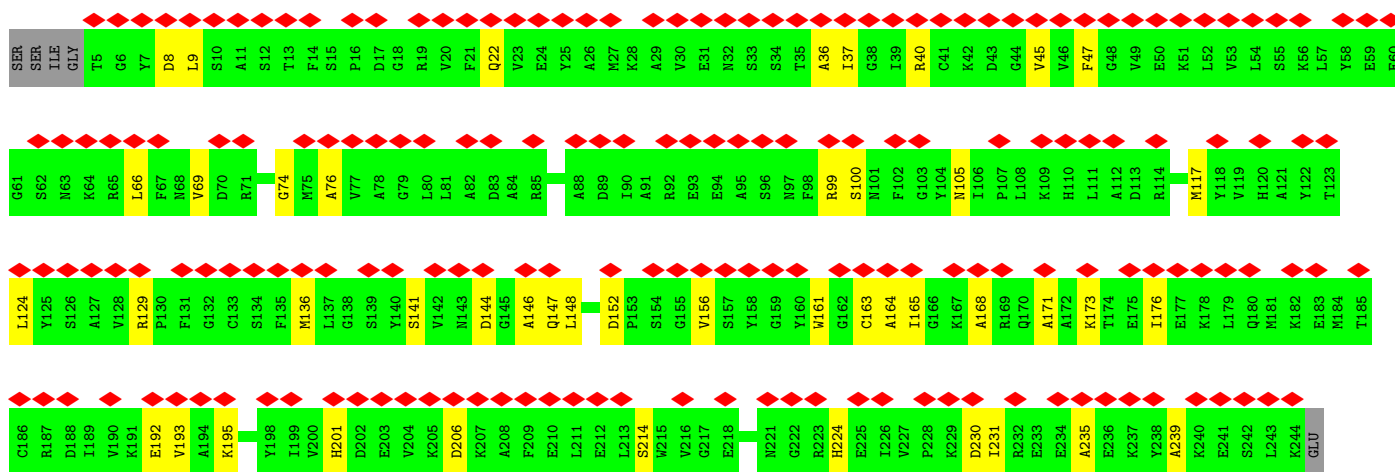
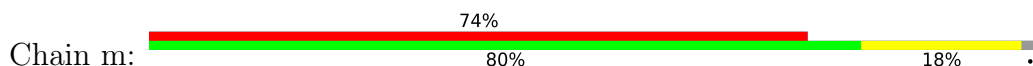


• Molecule 18: Proteasome subunit alpha type-3

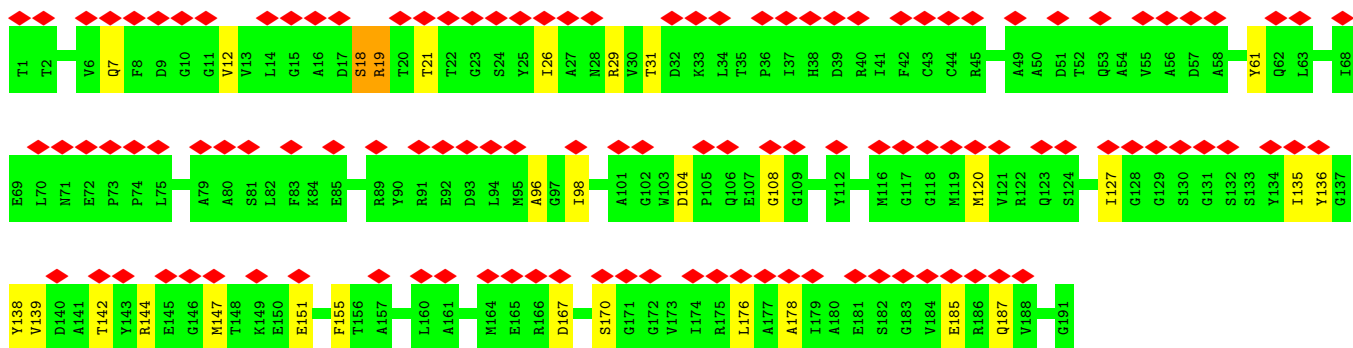
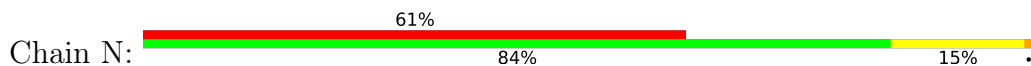




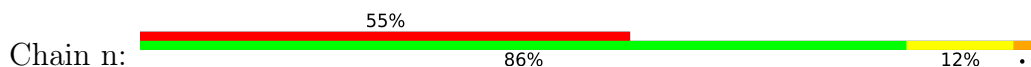
• Molecule 18: Proteasome subunit alpha type-3

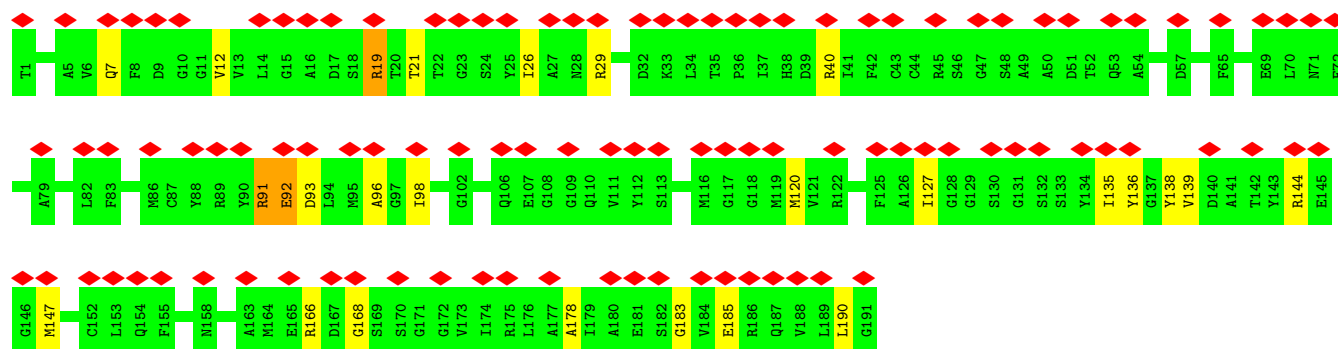


• Molecule 19: Proteasome subunit beta type-6

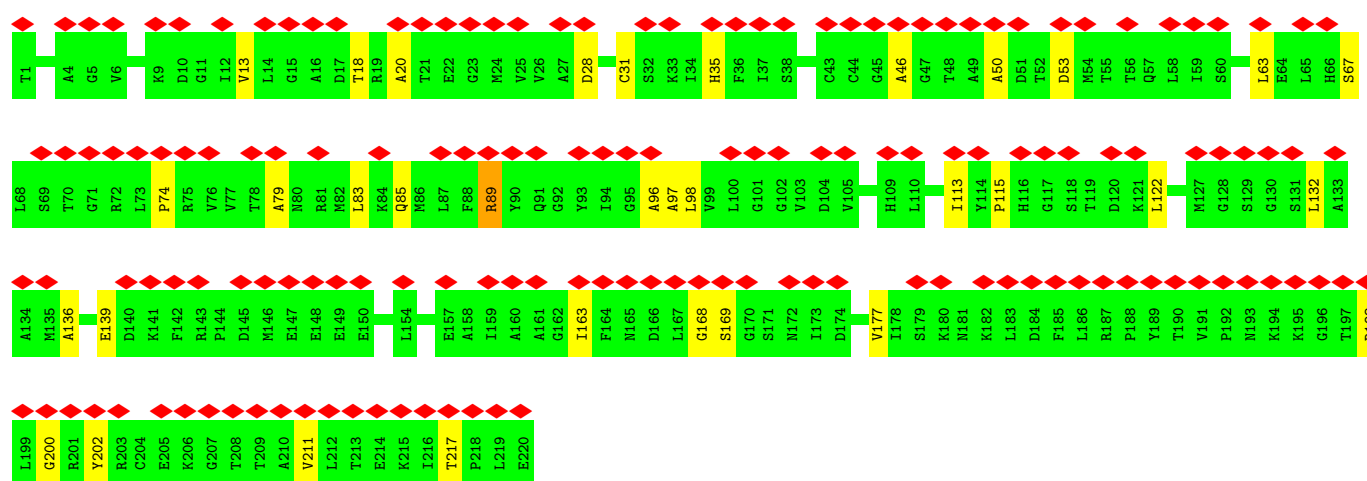
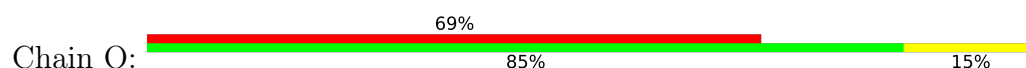


• Molecule 19: Proteasome subunit beta type-6

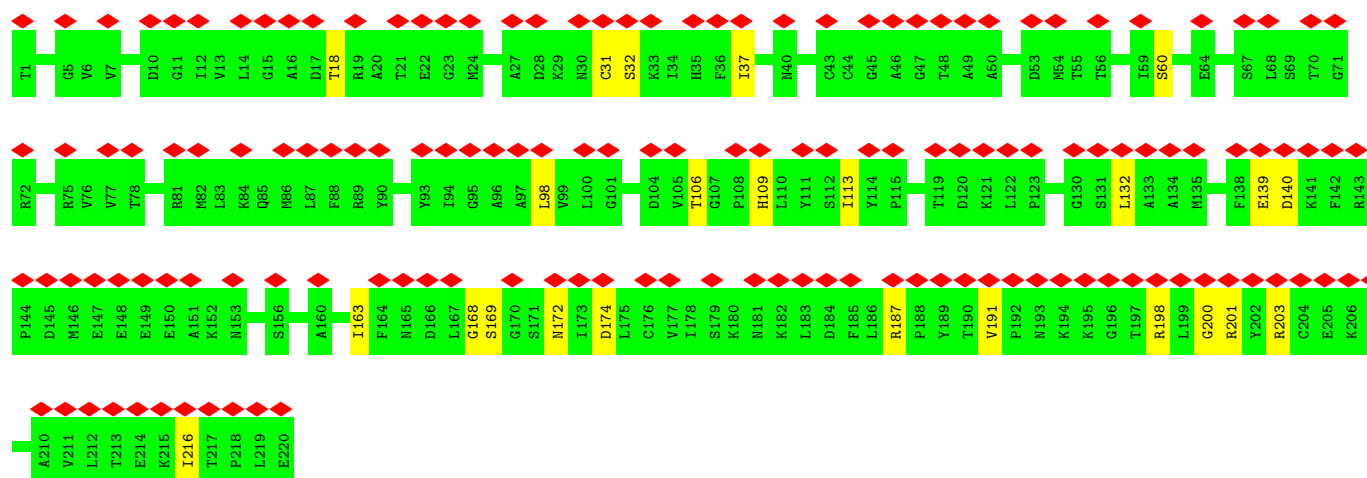
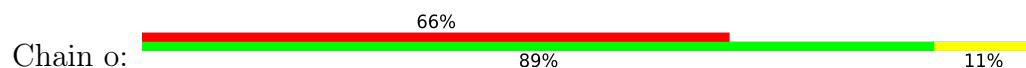




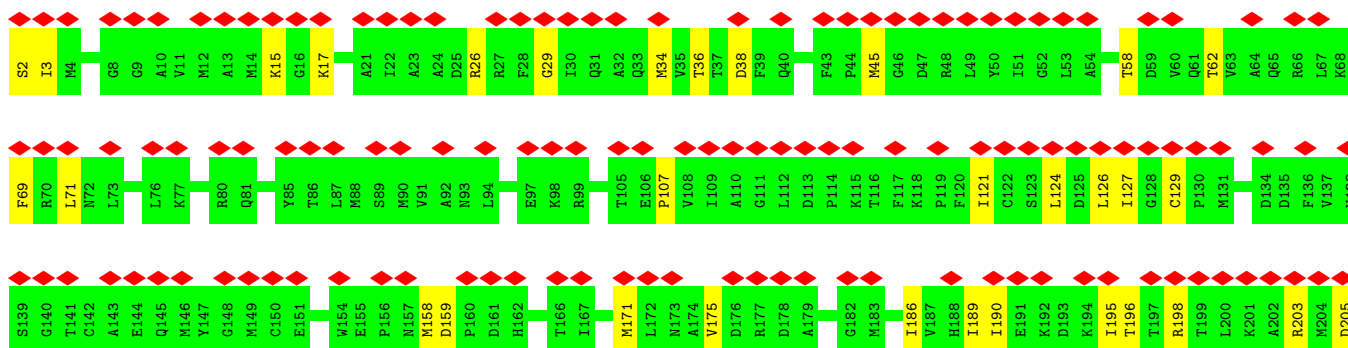
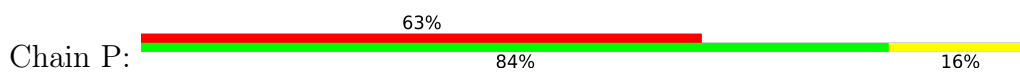
• Molecule 20: Proteasome subunit beta type-7



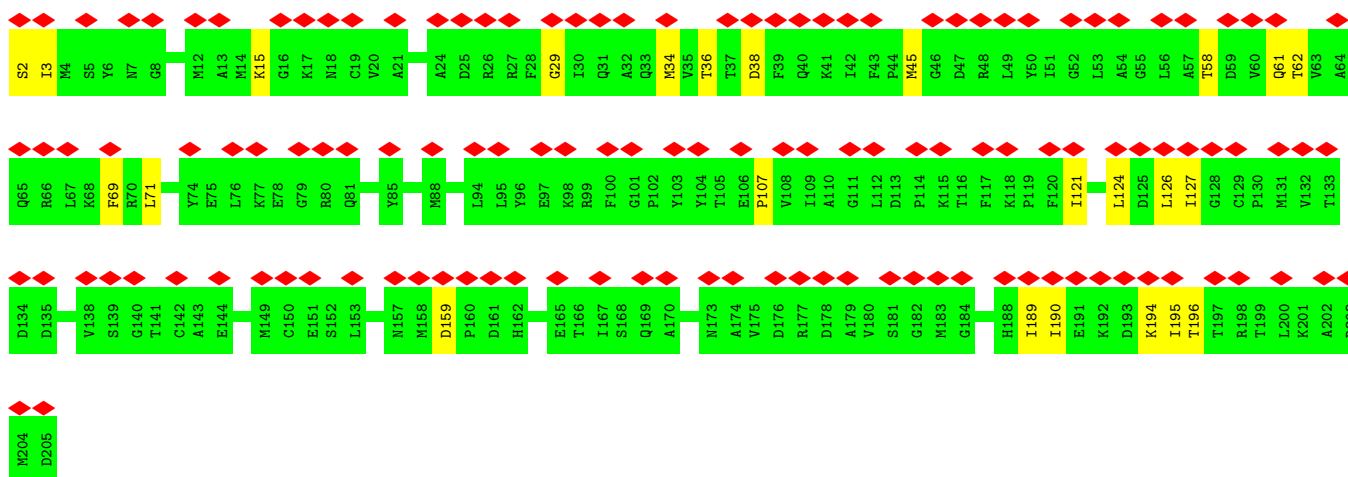
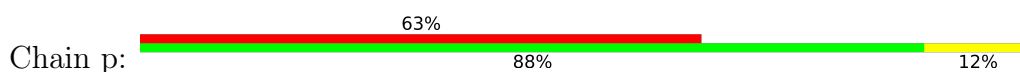
• Molecule 20: Proteasome subunit beta type-7



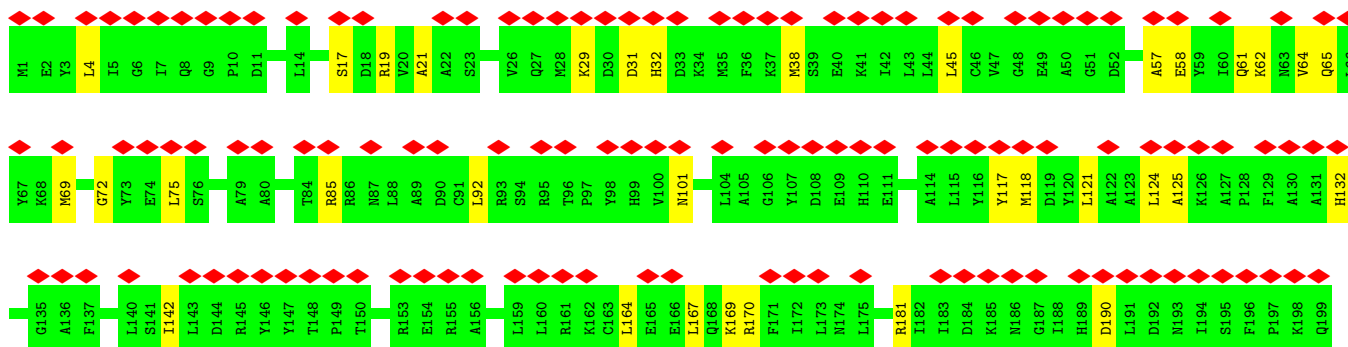
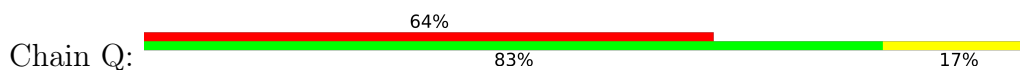
• Molecule 21: Proteasome subunit beta type-3



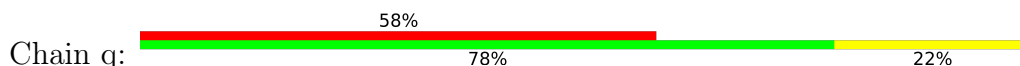
• Molecule 21: Proteasome subunit beta type-3

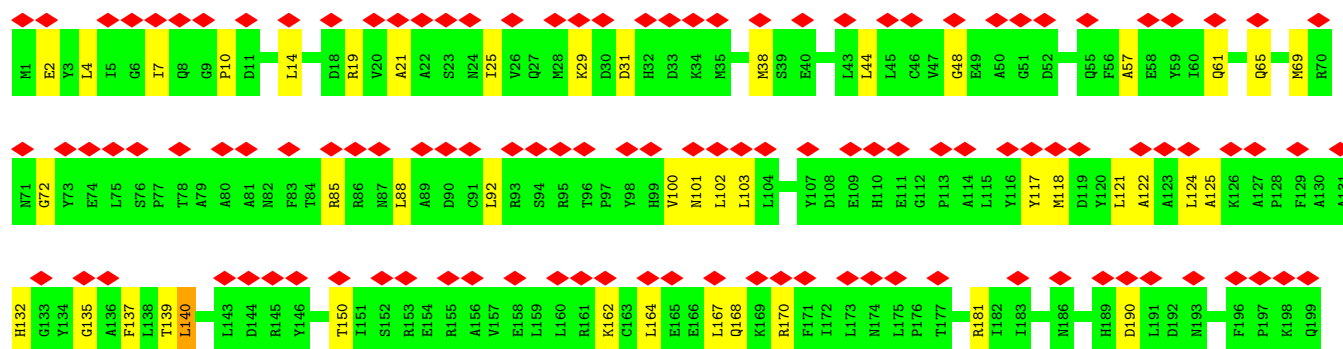


• Molecule 22: Proteasome subunit beta type-2

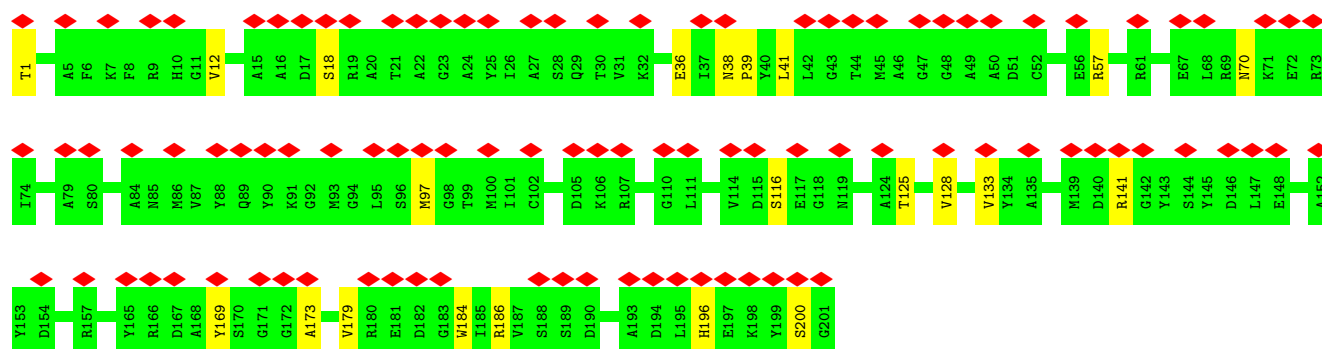


• Molecule 22: Proteasome subunit beta type-2

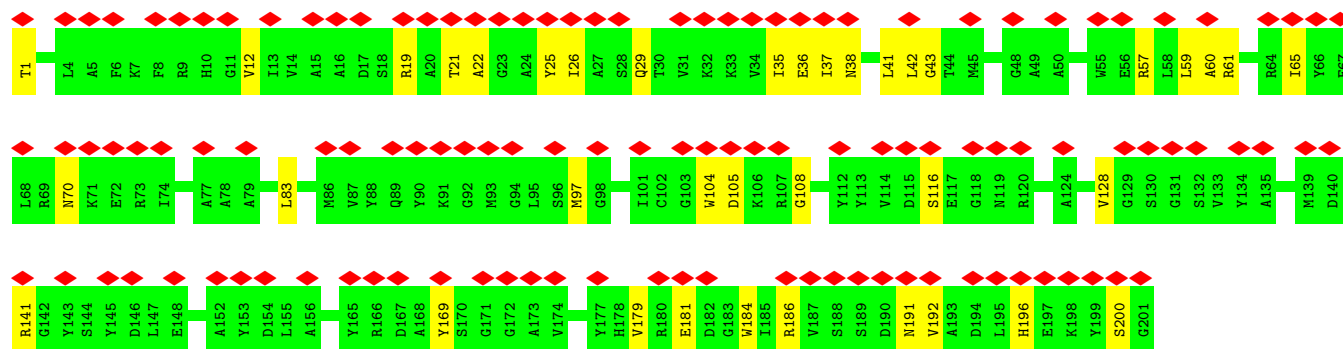
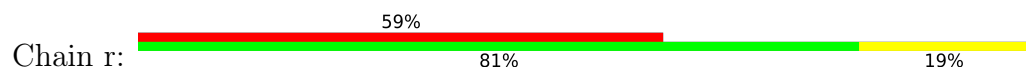




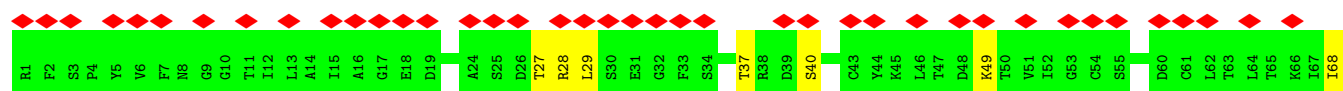
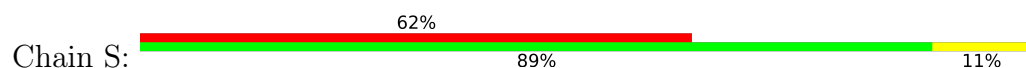
• Molecule 23: Proteasome subunit beta type-5

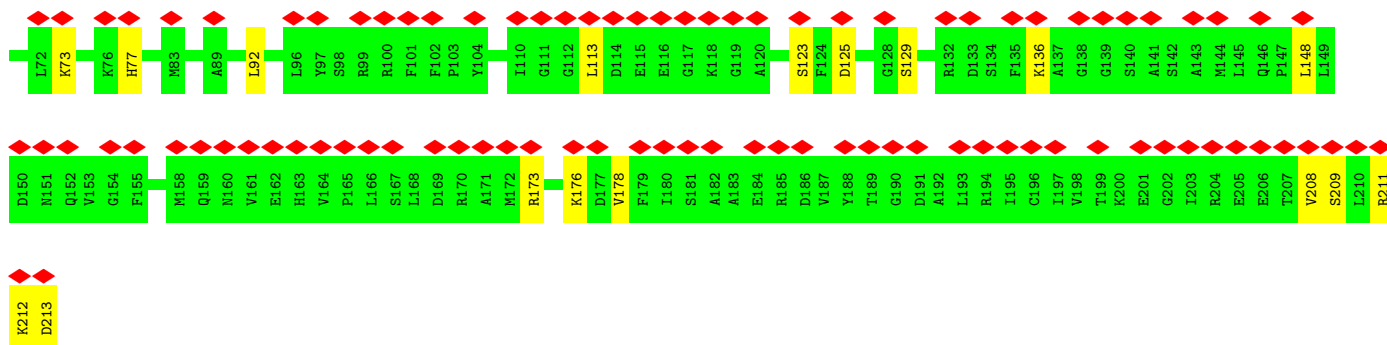


• Molecule 23: Proteasome subunit beta type-5

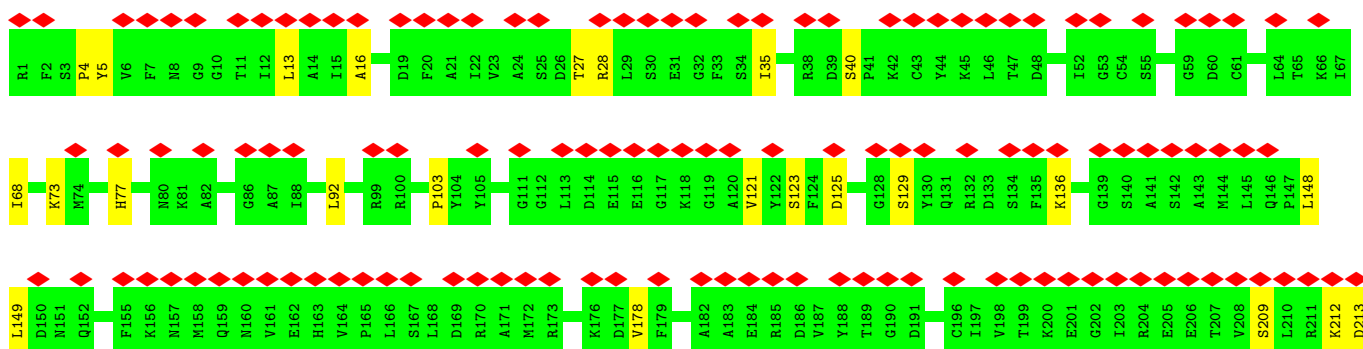
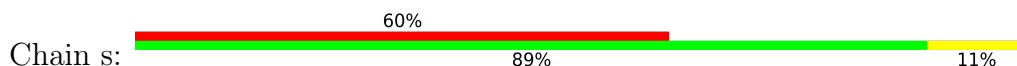


• Molecule 24: Proteasome subunit beta type-1

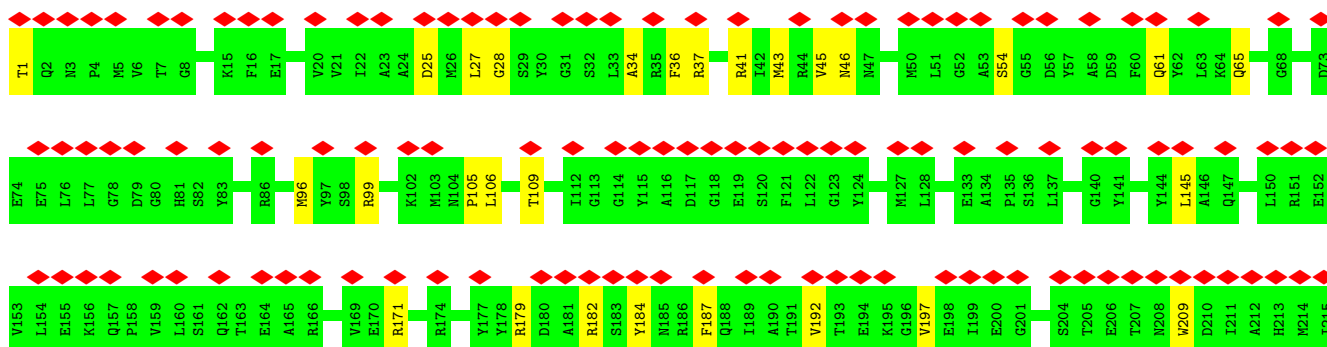
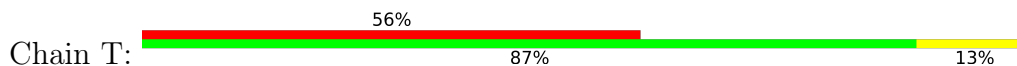




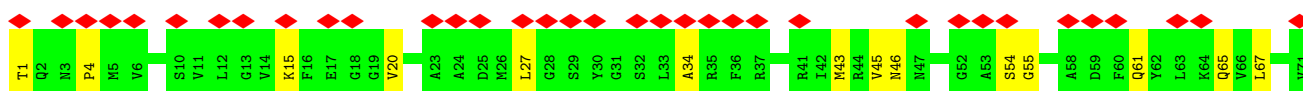
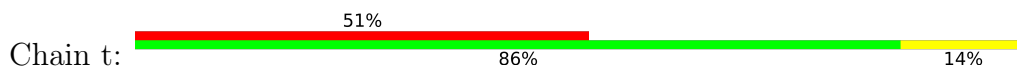
• Molecule 24: Proteasome subunit beta type-1

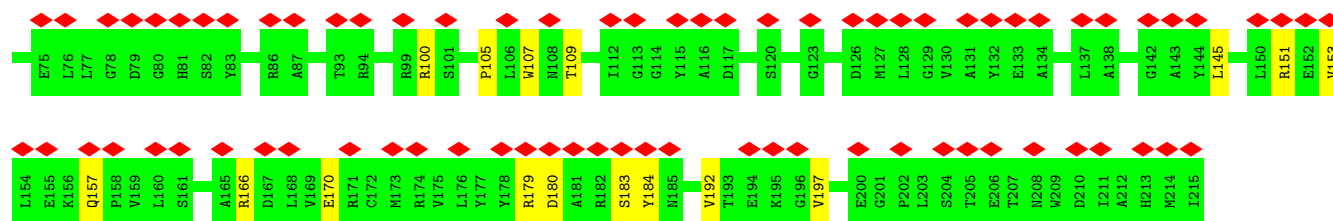


• Molecule 25: Proteasome subunit beta type-4

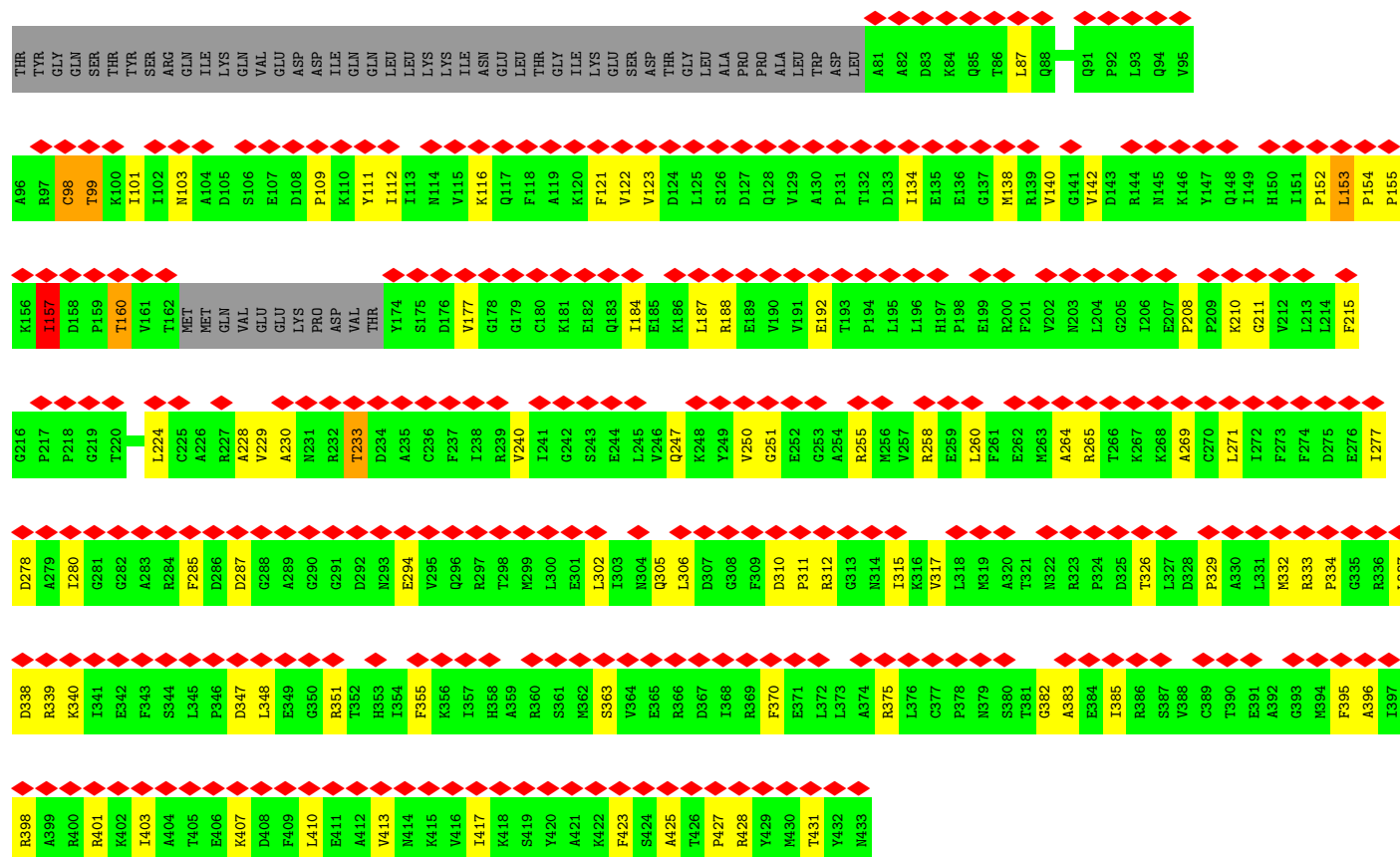
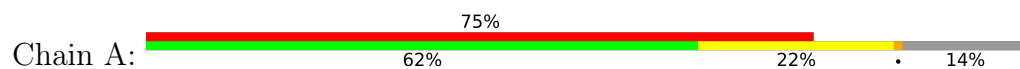


• Molecule 25: Proteasome subunit beta type-4

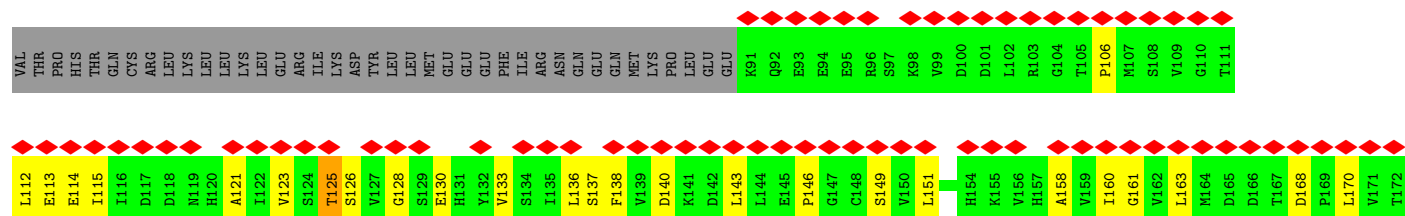
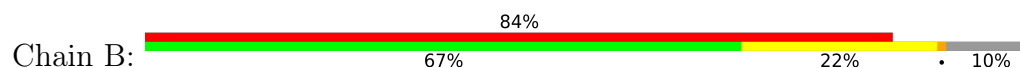


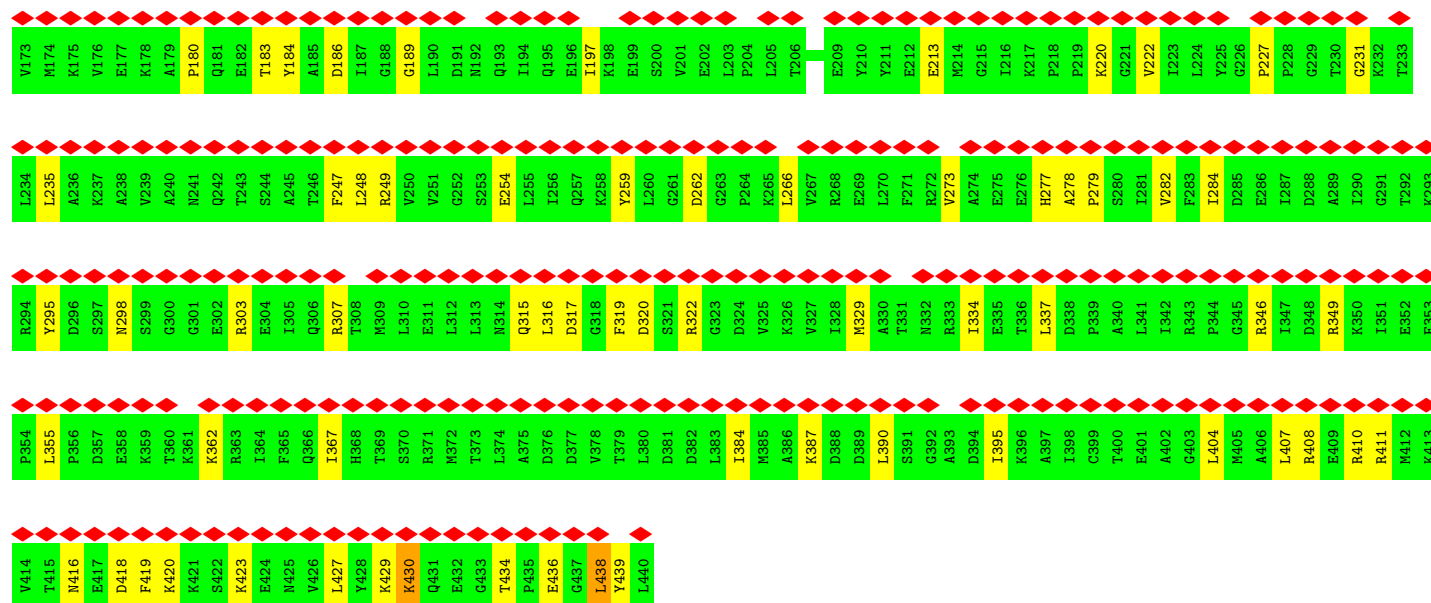


• Molecule 26: 26S proteasome regulatory subunit 7

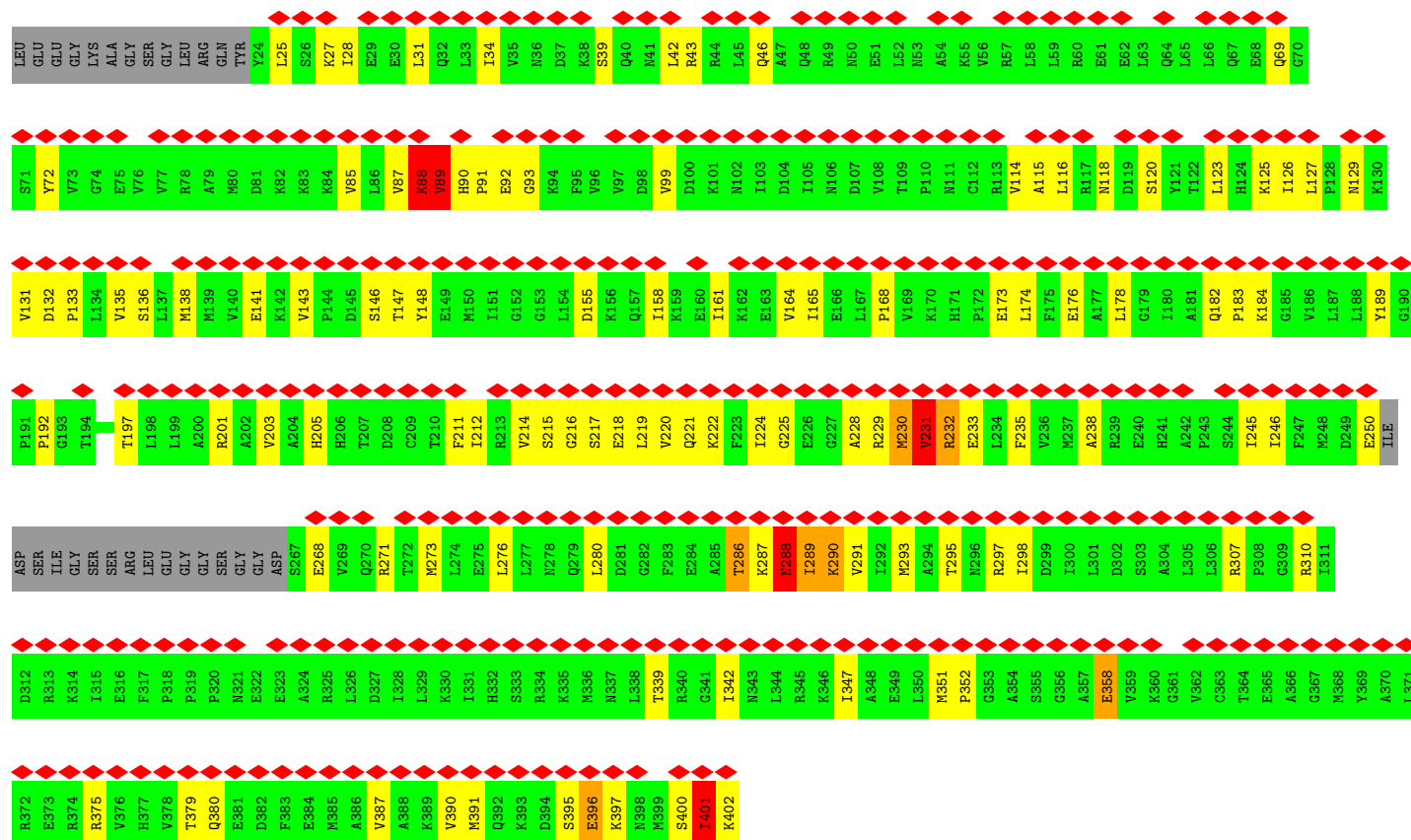
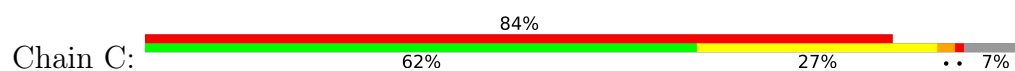


• Molecule 27: 26S proteasome regulatory subunit 4

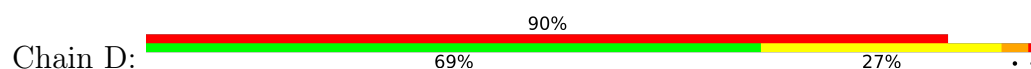


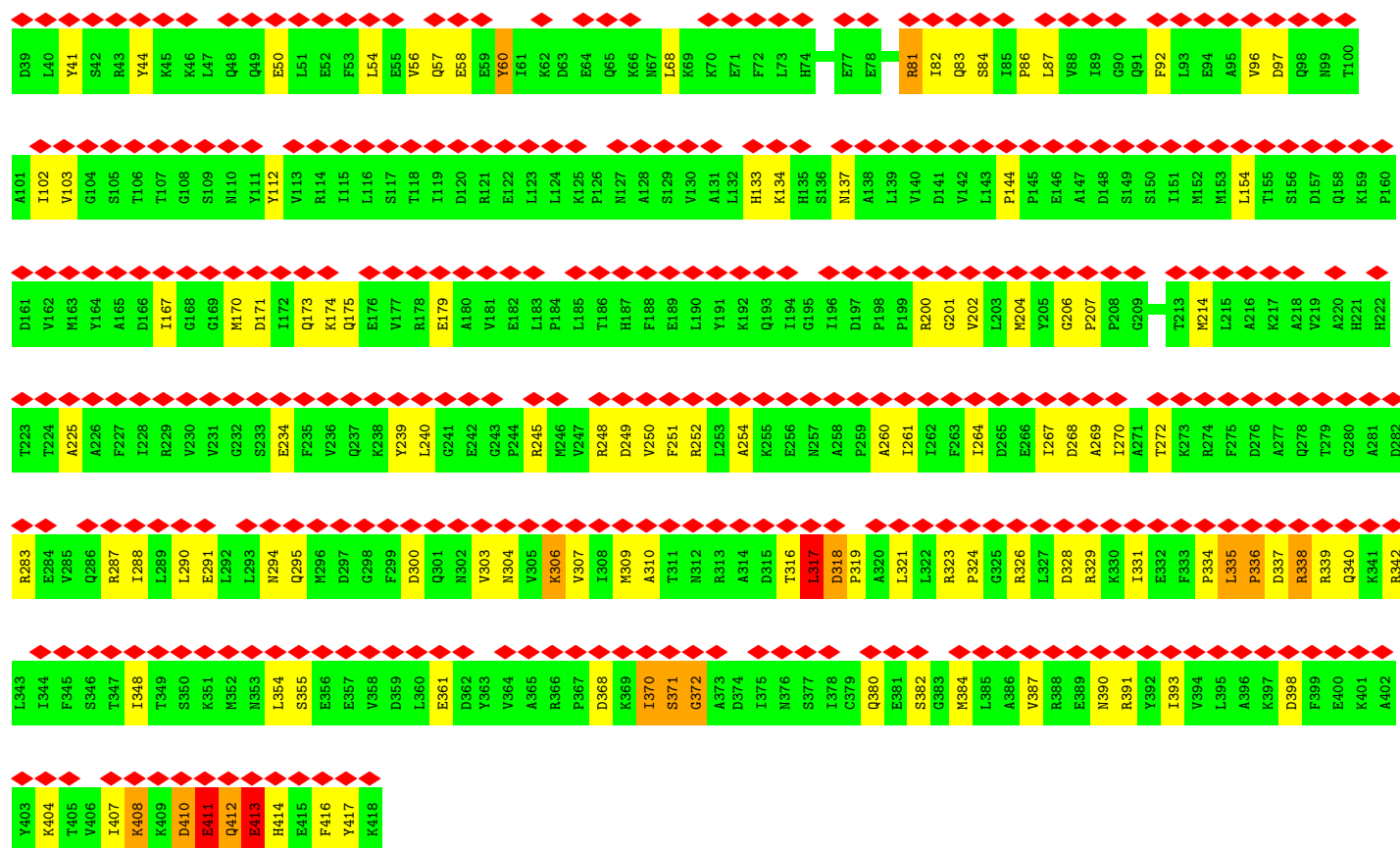


• Molecule 28: 26S proteasome regulatory subunit 8

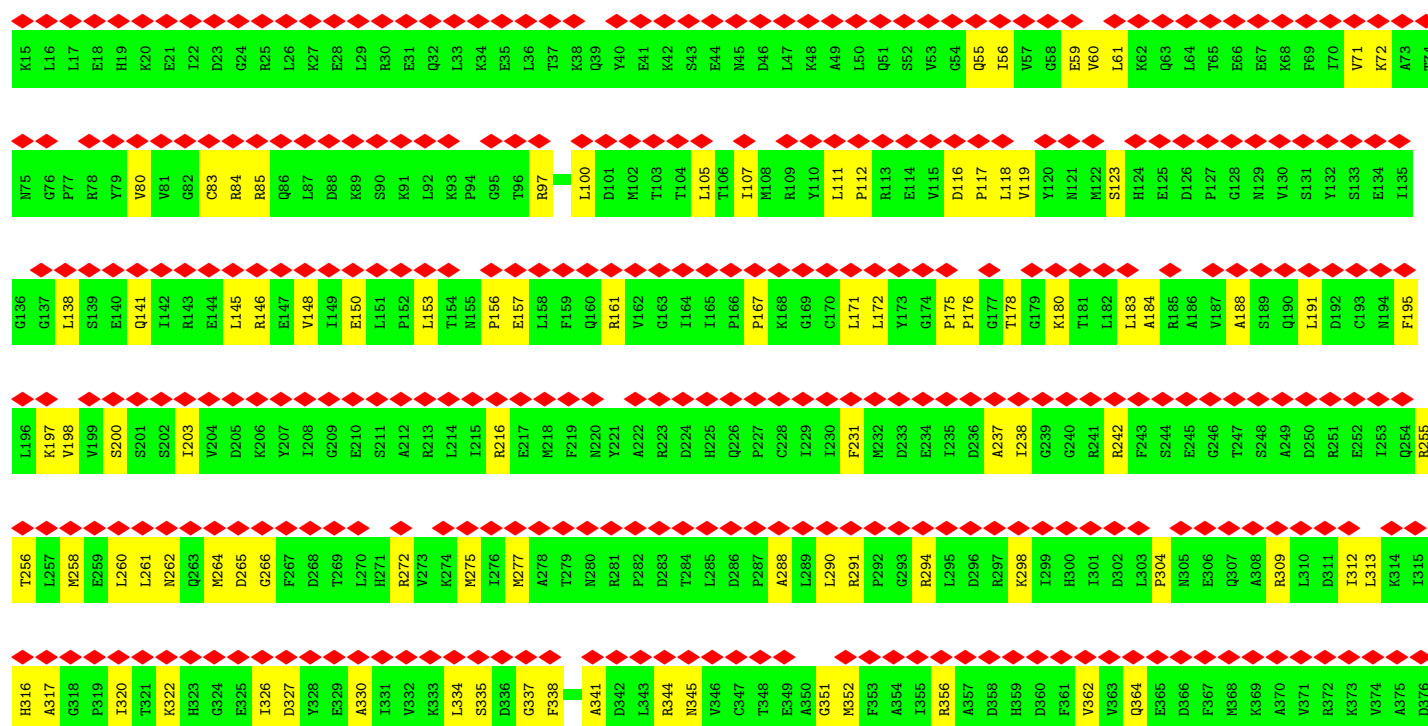
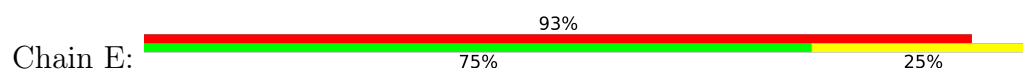


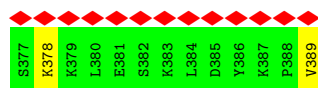
• Molecule 29: 26S proteasome regulatory subunit 6B



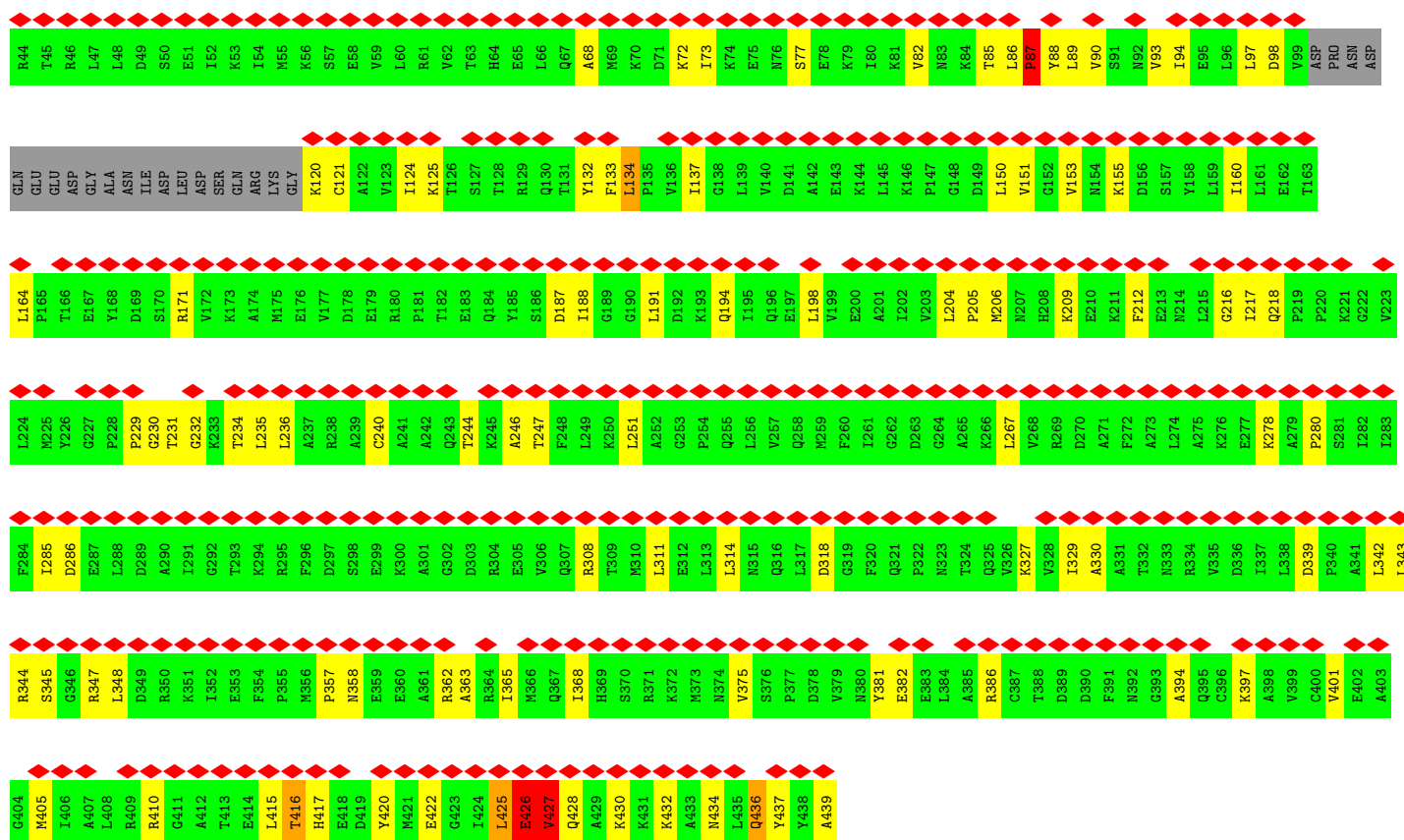
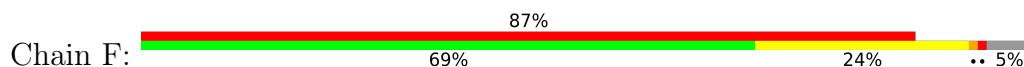


• Molecule 30: 26S proteasome regulatory subunit 10B

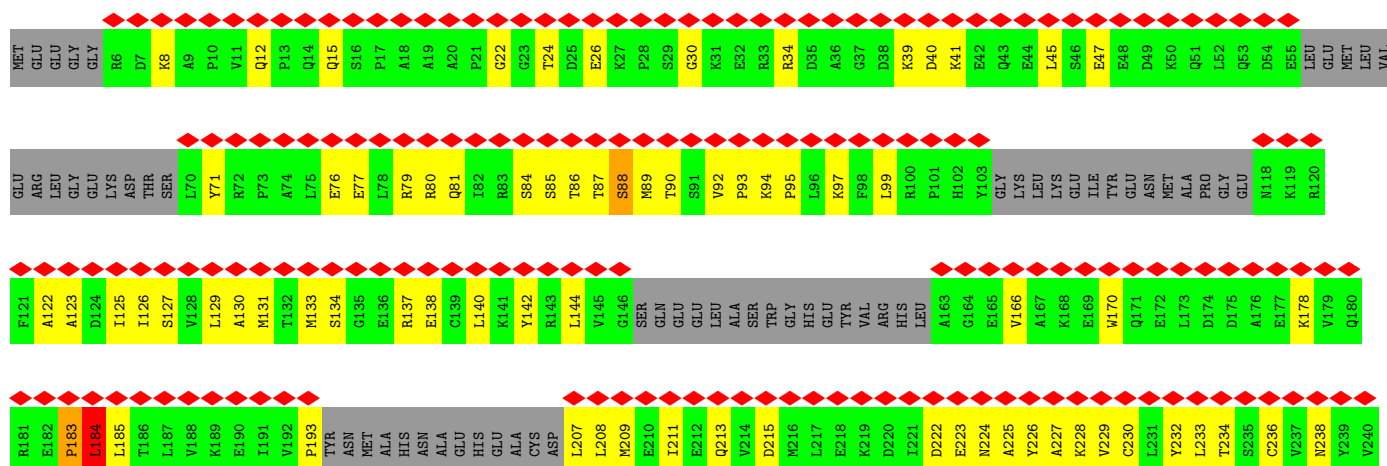
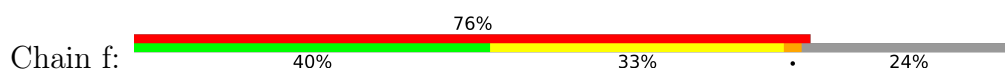




• Molecule 31: 26S proteasome regulatory subunit 6A



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



ARG	LYS	ASN	PRO	ASN	TYR	ASP	LEU	P241	H301	S361	D421	S481	T541	A601	A661	V721	V781	PRO
			VAL	VAL	VAL	GLY	ALA	E242	G302	G362	V422	I482	I542	G602	M662	S722	H782	VAL
			VAL	PRO	ASN	ASP	ASP	P243	V303	S363	D423	F483	M543	S603	G663	Y723	H783	SER
			VAL	TYR	ASN	ASP	ALA	E244	F304	S364	G424	G484	E544	G604	E664	N724	D784	ARG
			GLN	GLY	ASP	ASP	GLN	N245	L305	V365	G425	G485	K545	N605	I665	S725	R785	VAL
			ALA	GLY	ASP	ASP	ALA	S246	E306	D366	L426	L486	S546	V606	I666	T726	Q786	GLY
			VAL	L248	A247	L249	VAL	A247	L307	S367	T427	L487	E547	L607	G667	F727	L787	GLN
			ASP	L249	L248	ASP	VAL	L248	S308	A368	Q428	A488	T548	K608	A668	A728	W788	VAL
			VAL	R250	R249	VAL	VAL	R249	E309	R369	I429	Y489	E549	V609	E669	S789	S789	ASP
			GLY	C251	C251	GLY	GLY	C251	V311	M370	D430	A490	L550	Q611	M670	Q727	Q790	VAL
			GLN	A252	A252	GLN	GLN	A252	E312	N371	K431	G491	K551	Q611	A671	W791	V791	GLY
			ALA	L253	L253	ALA	ALA	L253	E313	L372	Y432	S492	T552	L612	L672	Y792	A792	GLY
			GLY	G254	G254	GLY	GLY	G254	E314	A373	L433	M493	T553	L613	R673	S793	V793	SER
			PRO	V255	V255	PRO	PRO	V255	Y314	S374	Y434	R494	Y554	H614	T674	A794	A794	GLY
			LYS	F256	F256	LYS	LYS	F256	E315	S375	S435	E495	A555	I615	P675	F795	G795	THR
			THR	R257	R257	THR	THR	R257	D316	F376	S436	D496	R556	O616	G676	L796	L796	ASN
			ILE	K258	K258	ILE	ILE	K258	L317	V377	E437	Y497	W557	S617	G676	A739	L797	ASN
			GLY	F259	F259	GLY	GLY	F259	T318	N378	D438	L498	L558	E618	H678	R740	T798	THR
			ALA	R260	R260	ALA	ALA	R260	E319	G379	Y439	T499	P559	H619	L679	L741	V799	THR
			THR	R261	R261	THR	THR	R261	I320	F380	I440	L500	L560	F620	R680	A742	L800	GLY
			PRO	F262	F262	PRO	PRO	F262	M321	V381	K441	L501	G561	D621	Y681	A743	W801	THR
			VAL	P263	P263	VAL	VAL	P263	S322	N382	S442	L502	L562	S622	G682	M744	S802	HIS
			LEU	E264	E264	LEU	LEU	E264	N323	ALA	G443	P503	G563	K623	E683	L745	F803	THR
			GLY	A265	A265	GLY	GLY	A265	Q324	PHE	A444	V504	L564	E624	P684	R746	L804	THR
			LEU	L266	L266	LEU	LEU	L266	Q325	GLY	L445	G506	N565	K625	T685	Q747	A804	PRO
			ALA	R267	R267	ALA	ALA	R267	L326	Q387	A447	D507	H567	E626	L686	L748	VAL	VAL
			THR	L268	L268	THR	THR	L268	N327	D388	C448	K508	G568	D628	R687	A749	ARG	ARG
			GLY	A269	A269	GLY	GLY	A269	S328	K389	G449	S509	K569	K629	G688	Q750	ASN	ASN
			THR	L270	L270	THR	THR	L270	N329	L390	C449	S510	G570	D630	A689	Y751	LEU	LEU
			LEU	M271	M271	LEU	LEU	M271	F330	L391	I450	S511	E571	K631	V690	H752	GLY	GLY
			ALA	L272	L272	ALA	ALA	L272	L331	T392	V451	S512	A572	K632	P691	A753	ALA	ALA
			THR	N273	N273	THR	THR	N273	A332	D393	N452	M512	I573	E633	L692	K754	HIS	HIS
			GLY	D274	D274	GLY	GLY	D274	L333	D394	G454	E513	E574	F634	A693	PRO	VAL	VAL
			LEU	M275	M275	LEU	LEU	M275	A334	G395	G455	V514	A575	K635	L694	ASN	ASN	ASN
			ILE	E276	E276	ILE	ILE	E276	R335	N396	V455	A515	I576	D636	A695	VAL	VAL	VAL
			VAL	L277	L277	VAL	VAL	L277	E336	K397	R456	G516	L577	K637	L696	THR	THR	THR
			THR	V278	V278	THR	THR	V278	L337	W398	M457	V517	A577	D638	I697	S698	VAL	VAL
			PRO	E279	E279	PRO	PRO	E279	D338	L399	C459	T518	A578	K639	V699	ARG	ALA	ALA
			LEU	D280	D280	LEU	LEU	D280	I339	Y400	G459	A519	L580	K639	SER	PRO	PRO	PRO
			GLY	I281	I281	GLY	GLY	I281	M340	K401	D460	L520	L580	K640	ASN	ASN	ASN	ASN
			THR	F282	F282	THR	THR	F282	E341	N402	P461	A521	V582	E641	PRO	PRO	PRO	PRO
			LEU	T283	T283	LEU	LEU	T283	P342	O403	L463	G523	V583	P643	ARG	ARG	ARG	ARG
			VAL	S284	S284	VAL	VAL	S284	K343	D404	A464	M524	E584	A644	LEU	LEU	LEU	LEU
			GLY	C285	C285	GLY	GLY	C285	V344	H405	A464	I525	E585	D645	ASN	ASN	ASN	ASN
			THR	K286	K286	THR	THR	K286	P345	G406	L465	T526	E586	N646	ILE	ILE	ILE	ILE
			LEU	D287	D287	LEU	LEU	D287	D346	M407	L466	A526	P586	N646	LEU	LEU	LEU	LEU
			PRO	V288	V288	PRO	PRO	V288	D347	L408	S467	V527	F587	N647	ASP	THR	THR	THR
			LEU	V289	V289	LEU	LEU	V289	I348	S409	D468	G528	F588	N648	LEU	LEU	LEU	LEU
			VAL	VAL	VAL	VAL	VAL	VAL	Y349	A410	Y469	S529	R588	A648	THR	THR	THR	THR
			GLN	GLN	GLN	GLN	GLN	GLN	K350	V470	V470	C530	S589	H649	LYS	LYS	LYS	LYS
			LYS	LYS	LYS	LYS	LYS	LYS	T351	A411	L471	G532	F590	Q650	PHE	PHE	PHE	PHE
			GLN	GLN	GLN	GLN	GLN	GLN	A412	A412	H472	D533	N591	Q651	S714	S714	S714	S714
			THR	GLN	GLN	GLN	GLN	GLN	H352	S413	M473	V534	N592	V652	H715	H715	H715	H715
			ALA	ALA	ALA	ALA	ALA	ALA	L353	L414	S474	V534	L594	V654	D716	D716	D716	D716
			PHE	ALA	ALA	PHE	PHE	ALA	E354	G415	M475	T535	L594	L655	A717	A717	A717	A717
			LEU	PHE	PHE	LEU	LEU	PHE	N355	M416	T476	S536	V595	L655	D718	D718	D718	D718
			LEU	PHE	PHE	LEU	LEU	PHE	N356	I417	T477	S536	V596	L656	P719	P719	P719	P719
			LEU	PHE	PHE	LEU	LEU	PHE	N357	L418	M477	T537	D596	L657	E720	E720	E720	E720
			LEU	PHE	PHE	LEU	LEU	PHE	R357	L419	R478	T538	C598	L659				
			LEU	PHE	PHE	LEU	LEU	PHE	G359	W420	C480	Q540	Y600	I660				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	33278	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	0.017	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	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: ZN, AGS

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	U	0.29	0/6396	0.74	5/8646 (0.1%)
2	V	0.34	0/3874	0.81	2/5234 (0.0%)
3	W	0.31	0/3751	0.82	1/5042 (0.0%)
4	X	0.30	0/1936	0.73	1/2614 (0.0%)
5	Y	0.31	0/3173	0.75	0/4273
6	Z	0.31	0/2324	0.84	1/3150 (0.0%)
7	a	0.30	0/3053	0.78	0/4133
8	b	0.32	0/1478	0.79	4/2001 (0.2%)
9	c	0.36	1/2226 (0.0%)	0.87	4/3007 (0.1%)
10	d	0.31	0/2162	0.79	2/2919 (0.1%)
11	e	0.39	0/338	1.03	2/450 (0.4%)
12	G	0.28	0/1853	0.69	0/2515
12	g	0.26	0/1859	0.61	0/2523
13	H	0.27	0/1723	0.65	2/2346 (0.1%)
13	h	0.25	0/1743	0.57	0/2372
14	I	0.29	0/1925	0.77	3/2606 (0.1%)
14	i	0.28	0/1942	0.70	0/2628
15	J	0.36	0/1728	0.87	7/2358 (0.3%)
15	j	0.34	0/1728	0.80	2/2358 (0.1%)
16	K	0.29	0/1755	0.79	9/2375 (0.4%)
16	k	0.26	0/1747	0.61	0/2364
17	L	0.30	0/1885	0.65	0/2552
17	l	0.27	0/1885	0.64	0/2552
18	M	0.27	0/1891	0.67	2/2552 (0.1%)
18	m	0.26	0/1891	0.62	2/2552 (0.1%)
19	N	0.26	0/1454	0.66	2/1967 (0.1%)
19	n	0.28	0/1454	0.68	0/1967
20	O	0.26	0/1670	0.59	0/2265
20	o	0.29	0/1670	0.67	0/2265
21	P	0.25	0/1614	0.54	0/2177
21	p	0.28	0/1614	0.56	0/2177
22	Q	0.34	0/1603	0.73	0/2174

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	q	0.34	0/1603	0.71	1/2174 (0.0%)
23	R	0.27	0/1579	0.51	0/2134
23	r	0.25	0/1579	0.51	0/2134
24	S	0.27	0/1671	0.57	0/2253
24	s	0.27	0/1671	0.55	0/2253
25	T	0.27	0/1700	0.57	0/2305
25	t	0.26	0/1700	0.57	0/2305
26	A	0.29	0/2717	0.81	6/3665 (0.2%)
27	B	0.28	0/2745	0.78	3/3709 (0.1%)
28	C	0.35	0/2896	0.94	14/3895 (0.4%)
29	D	0.39	1/3090 (0.0%)	1.00	17/4168 (0.4%)
30	E	0.27	0/2904	0.67	0/3924
31	F	0.28	0/2897	0.76	12/3912 (0.3%)
32	f	0.33	1/5393 (0.0%)	0.87	20/7271 (0.3%)
All	All	0.30	3/101490 (0.0%)	0.74	124/137216 (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	U	0	2
2	V	0	1
3	W	0	1
5	Y	0	1
6	Z	0	5
8	b	0	1
9	c	0	5
15	J	0	2
15	j	0	1
16	K	0	3
16	k	0	1
20	O	0	1
26	A	0	3
27	B	0	1
28	C	0	10
29	D	0	8
31	F	0	5
All	All	0	51

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	c	279	ASP	C-N	6.82	1.42	1.33
29	D	144	PRO	C-N	5.23	1.39	1.33
32	f	494	ARG	CA-C	5.21	1.59	1.52

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	414	HIS	N-CA-C	10.74	126.71	113.50
32	f	488	ALA	N-CA-C	10.52	122.82	111.36
16	K	21	LEU	CA-C-N	9.92	139.56	121.70
16	K	21	LEU	C-N-CA	9.92	139.56	121.70
29	D	335	LEU	CA-C-N	9.72	129.67	119.85
29	D	335	LEU	C-N-CA	9.72	129.67	119.85
18	M	6	GLY	CA-C-N	9.40	138.63	121.70
18	M	6	GLY	C-N-CA	9.40	138.63	121.70
15	J	2	SER	CA-C-N	8.82	138.40	121.54
15	J	2	SER	C-N-CA	8.82	138.40	121.54
9	c	278	GLN	CA-C-N	8.68	142.97	121.80
9	c	278	GLN	C-N-CA	8.68	142.97	121.80
16	K	8	TYR	CA-C-N	7.88	136.60	121.54
16	K	8	TYR	C-N-CA	7.88	136.60	121.54
13	H	7	SER	CA-C-N	7.71	135.59	121.70
13	H	7	SER	C-N-CA	7.71	135.59	121.70
31	F	436	GLN	CA-C-N	7.71	136.28	121.54
31	F	436	GLN	C-N-CA	7.71	136.28	121.54
28	C	401	ILE	N-CA-C	7.40	124.74	109.34
16	K	19	GLY	CA-C-N	7.29	134.82	121.70
16	K	19	GLY	C-N-CA	7.29	134.82	121.70
28	C	286	THR	CA-C-N	7.01	134.93	121.54
28	C	286	THR	C-N-CA	7.01	134.93	121.54
32	f	493	ASN	N-CA-C	-6.98	95.94	110.80
32	f	472	HIS	CA-C-N	6.93	130.43	120.79
32	f	472	HIS	C-N-CA	6.93	130.43	120.79
32	f	493	ASN	CA-C-N	-6.93	111.05	120.82
32	f	493	ASN	C-N-CA	-6.93	111.05	120.82
28	C	401	ILE	CA-C-N	6.83	133.99	121.70
28	C	401	ILE	C-N-CA	6.83	133.99	121.70
4	X	354	ILE	N-CA-C	-6.70	107.35	113.71
29	D	412	GLN	CA-C-N	6.54	133.48	121.70
29	D	412	GLN	C-N-CA	6.54	133.48	121.70
26	A	157	ILE	CA-C-N	6.49	137.64	121.80
26	A	157	ILE	C-N-CA	6.49	137.64	121.80
29	D	410	ASP	CA-C-N	6.45	133.31	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	410	ASP	C-N-CA	6.45	133.31	121.70
15	J	182	GLU	CA-C-N	6.42	133.25	121.70
15	J	182	GLU	C-N-CA	6.42	133.25	121.70
32	f	492	SER	N-CA-C	-6.33	104.38	111.28
27	B	439	TYR	CA-C-N	6.22	132.90	121.70
27	B	439	TYR	C-N-CA	6.22	132.90	121.70
28	C	297	ARG	CA-C-N	6.21	133.15	121.97
28	C	297	ARG	C-N-CA	6.21	133.15	121.97
32	f	370	MET	N-CA-C	-6.14	104.67	111.36
32	f	324	VAL	CA-C-N	6.10	133.19	121.54
32	f	324	VAL	C-N-CA	6.10	133.19	121.54
32	f	663	GLY	N-CA-C	6.10	121.32	110.95
26	A	98	CYS	N-CA-C	6.05	117.57	110.97
26	A	153	LEU	N-CA-C	-6.05	96.44	109.81
2	V	96	ARG	N-CA-C	6.03	119.67	111.17
15	J	7	ILE	CB-CG1-CD1	5.96	126.31	113.80
32	f	489	TYR	N-CA-C	5.96	118.47	109.23
28	C	89	VAL	CA-C-N	5.84	128.08	120.26
28	C	89	VAL	C-N-CA	5.84	128.08	120.26
28	C	396	GLU	CA-CB-CG	5.83	125.75	114.10
15	j	49	SER	CA-C-N	5.82	128.90	120.98
15	j	49	SER	C-N-CA	5.82	128.90	120.98
1	U	223	LEU	CA-C-N	5.82	131.08	122.82
1	U	223	LEU	C-N-CA	5.82	131.08	122.82
32	f	365	VAL	N-CA-C	5.80	121.41	109.34
29	D	300	ASP	CA-C-N	5.73	132.48	121.54
29	D	300	ASP	C-N-CA	5.73	132.48	121.54
32	f	374	SER	CA-C-N	-5.67	112.69	120.28
32	f	374	SER	C-N-CA	-5.67	112.69	120.28
26	A	99	THR	N-CA-C	5.64	118.07	111.02
32	f	379	GLY	CA-C-N	-5.64	113.47	122.66
32	f	379	GLY	C-N-CA	-5.64	113.47	122.66
28	C	88	LYS	CA-C-N	5.63	132.10	121.97
28	C	88	LYS	C-N-CA	5.63	132.10	121.97
10	d	233	GLU	CA-C-N	5.60	132.24	121.54
10	d	233	GLU	C-N-CA	5.60	132.24	121.54
31	F	434	ASN	CA-C-N	5.60	131.77	121.70
31	F	434	ASN	C-N-CA	5.60	131.77	121.70
14	I	15	GLU	CA-C-N	5.59	131.76	121.70
14	I	15	GLU	C-N-CA	5.59	131.76	121.70
29	D	60	TYR	N-CA-C	5.58	117.16	111.14
31	F	426	GLU	CA-C-N	5.53	131.92	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	F	426	GLU	C-N-CA	5.53	131.92	121.97
32	f	337	LEU	N-CA-C	5.51	122.53	110.80
28	C	287	LYS	N-CA-C	5.50	122.53	110.80
14	I	10	THR	N-CA-C	-5.48	100.46	109.40
19	N	18	SER	CA-C-N	5.42	131.89	121.54
19	N	18	SER	C-N-CA	5.42	131.89	121.54
8	b	100	ARG	CA-C-N	5.42	130.71	121.29
8	b	100	ARG	C-N-CA	5.42	130.71	121.29
31	F	427	VAL	CA-C-N	5.41	130.24	122.40
31	F	427	VAL	C-N-CA	5.41	130.24	122.40
16	K	20	ARG	N-CA-CB	5.39	119.66	110.50
9	c	229	LEU	CA-C-N	5.36	131.78	121.54
9	c	229	LEU	C-N-CA	5.36	131.78	121.54
22	q	140	LEU	CA-CB-CG	5.31	134.90	116.30
31	F	427	VAL	N-CA-C	5.31	120.39	109.34
16	K	9	ASP	CA-C-N	5.29	131.65	121.54
16	K	9	ASP	C-N-CA	5.29	131.65	121.54
3	W	424	LEU	N-CA-C	5.28	122.05	110.80
27	B	138	PHE	N-CA-C	-5.25	108.14	114.75
29	D	317	LEU	CA-C-N	5.25	134.60	121.80
29	D	317	LEU	C-N-CA	5.25	134.60	121.80
1	U	595	ASN	CA-C-N	5.23	131.53	121.54
1	U	595	ASN	C-N-CA	5.23	131.53	121.54
8	b	165	GLY	CA-C-N	5.22	129.53	122.07
8	b	165	GLY	C-N-CA	5.22	129.53	122.07
15	J	181	ILE	CA-C-N	5.22	131.09	121.70
15	J	181	ILE	C-N-CA	5.22	131.09	121.70
29	D	338	ARG	CA-C-N	-5.21	111.60	121.54
29	D	338	ARG	C-N-CA	-5.21	111.60	121.54
31	F	437	TYR	CB-CA-C	-5.20	100.07	110.42
29	D	154	LEU	CA-C-N	5.17	131.42	121.54
29	D	154	LEU	C-N-CA	5.17	131.42	121.54
11	e	58	ALA	CA-C-N	5.15	131.38	121.54
11	e	58	ALA	C-N-CA	5.15	131.38	121.54
2	V	279	GLN	CA-CB-CG	5.14	124.37	114.10
6	Z	176	LEU	CA-CB-CG	5.12	134.23	116.30
29	D	336	PRO	N-CA-C	5.08	119.45	111.38
18	m	231	ILE	CA-C-N	5.07	131.23	121.54
18	m	231	ILE	C-N-CA	5.07	131.23	121.54
26	A	160	THR	N-CA-C	-5.06	108.85	114.62
31	F	432	LYS	CA-C-N	5.05	130.80	121.70
31	F	432	LYS	C-N-CA	5.05	130.80	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	767	THR	N-CA-C	5.05	119.66	111.37
28	C	231	VAL	N-CA-C	5.03	119.79	109.34
32	f	404	ASP	N-CA-C	5.02	117.15	111.02
32	f	493	ASN	CA-C-O	-5.00	113.36	120.51

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	A	157	ILE	Peptide
26	A	233	THR	Peptide
26	A	311	PRO	Peptide
27	B	278	ALA	Peptide
28	C	129	ASN	Peptide
28	C	132	ASP	Peptide
28	C	230	MET	Peptide
28	C	288	ASN	Peptide
28	C	358	GLU	Peptide
28	C	397	LYS	Peptide
28	C	400	SER	Peptide
28	C	88	LYS	Peptide
28	C	89	VAL	Peptide
28	C	90	HIS	Peptide
29	D	318	ASP	Peptide
29	D	354	LEU	Peptide
29	D	355	SER	Peptide
29	D	370	ILE	Peptide
29	D	371	SER	Peptide
29	D	413	GLU	Peptide
29	D	417	TYR	Peptide
29	D	84	SER	Peptide
31	F	343	LEU	Peptide
31	F	425	LEU	Peptide
31	F	426	GLU	Peptide
31	F	86	LEU	Peptide
31	F	87	PRO	Peptide
15	J	184	ASP	Mainchain
15	J	5	ARG	Peptide
16	K	121	LEU	Peptide
16	K	19	GLY	Peptide
16	K	22	PHE	Peptide
20	O	200	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	U	432	SER	Peptide
1	U	598	ALA	Peptide
2	V	194	LYS	Peptide
3	W	313	GLU	Peptide
5	Y	373	GLY	Peptide
6	Z	143	GLU	Peptide
6	Z	158	VAL	Peptide
6	Z	166	GLU	Peptide
6	Z	219	LYS	Peptide
6	Z	224	HIS	Peptide
8	b	101	GLN	Peptide
9	c	150	SER	Peptide
9	c	155	VAL	Peptide
9	c	272	ILE	Peptide
9	c	278	GLN	Peptide
9	c	33	ILE	Peptide
15	j	180	ALA	Peptide
16	k	11	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	6287	0	6338	154	0
2	V	3799	0	3850	100	0
3	W	3703	0	3822	106	0
4	X	1905	0	1951	45	0
5	Y	3115	0	3120	80	0
6	Z	2281	0	2312	73	0
7	a	2995	0	3012	71	0
8	b	1458	0	1505	42	0
9	c	2187	0	2215	66	0
10	d	2116	0	2146	38	0
11	e	334	0	294	11	0
12	G	1820	0	1791	23	0
12	g	1826	0	1796	20	0
13	H	1688	0	1575	21	0
13	h	1708	0	1594	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	I	1895	0	1833	30	0
14	i	1912	0	1851	30	0
15	J	1704	0	1517	24	0
15	j	1704	0	1517	27	0
16	K	1729	0	1680	30	0
16	k	1722	0	1673	30	0
17	L	1850	0	1822	25	0
17	l	1850	0	1822	27	0
18	M	1856	0	1814	38	0
18	m	1856	0	1814	30	0
19	N	1430	0	1398	19	0
19	n	1430	0	1398	19	0
20	O	1643	0	1644	21	0
20	o	1643	0	1644	16	0
21	P	1585	0	1598	22	0
21	p	1585	0	1598	17	0
22	Q	1570	0	1547	21	0
22	q	1570	0	1547	27	0
23	R	1548	0	1499	14	0
23	r	1548	0	1499	28	0
24	S	1641	0	1618	13	0
24	s	1641	0	1618	14	0
25	T	1667	0	1628	20	0
25	t	1667	0	1628	22	0
26	A	2672	0	2700	57	0
27	B	2706	0	2731	64	0
28	C	2859	0	2971	79	0
29	D	3040	0	3076	94	0
30	E	2860	0	2828	60	0
31	F	2859	0	2853	85	0
32	f	5319	0	5329	461	0
33	c	1	0	0	0	0
34	A	31	0	12	3	0
34	B	31	0	12	4	0
34	D	31	0	12	7	0
34	F	31	0	12	9	0
All	All	99908	0	99064	2151	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 11.

All (2151) 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	1.35
32:f:753:ALA:O	32:f:754:LYS:HE2	1.27	1.31
31:F:230:GLY:O	34:F:501:AGS:H8	1.14	1.29
32:f:796:LEU:O	32:f:799:VAL:HG22	1.30	1.26
32:f:742:ALA:HA	32:f:745:LEU:CD2	1.66	1.25
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	1.19
31:F:229:PRO:O	34:F:501:AGS:H5'1	1.45	1.16
32:f:696:LEU:HD13	32:f:752:HIS:CD2	1.80	1.16
32:f:494:ARG:HE	32:f:495:GLU:N	1.44	1.15
32:f:494:ARG:HH21	32:f:495:GLU:HG2	1.01	1.14
32:f:311:VAL:HB	32:f:490:ALA:HB1	1.17	1.13
32:f:479:LEU:HD21	32:f:513:GLU:CB	1.80	1.11
32:f:479:LEU:CD2	32:f:513:GLU:HB2	1.79	1.11
32:f:389:LYS:HG2	32:f:418:LEU:HD21	1.29	1.11
32:f:494:ARG:NH2	32:f:495:GLU:HG2	1.64	1.11
32:f:389:LYS:CG	32:f:418:LEU:HD21	1.79	1.10
32:f:376:PHE:CE1	32:f:798:THR:HG21	1.85	1.10
32:f:696:LEU:HD13	32:f:752:HIS:HD2	1.14	1.10
32:f:692:LEU:HD12	32:f:748:LEU:CD2	1.82	1.10
32:f:692:LEU:HD12	32:f:748:LEU:HD21	1.19	1.09
32:f:483:PHE:CE2	32:f:799:VAL:HB	1.88	1.08
27:B:279:PRO:HD3	32:f:718:ASP:OD2	1.51	1.07
32:f:471:LEU:HG	32:f:509:LYS:CE	1.83	1.07
32:f:742:ALA:O	32:f:745:LEU:HG	1.54	1.07
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	1.03
32:f:494:ARG:CD	32:f:496:ASP:OD1	2.06	1.03
29:D:338:ARG:O	29:D:339:ARG:HB2	1.57	1.01
32:f:337:LEU:HD13	32:f:420:TRP:HZ3	1.26	1.00
32:f:753:ALA:O	32:f:754:LYS:CE	2.08	1.00
31:F:230:GLY:O	34:F:501:AGS:C8	2.11	0.98
32:f:692:LEU:CD1	32:f:748:LEU:HD21	1.93	0.97
32:f:359:GLY:O	32:f:363:SER:HB3	1.63	0.97
32:f:479:LEU:HD21	32:f:513:GLU:HB2	0.99	0.97
32:f:494:ARG:HG3	32:f:497:VAL:HG12	1.43	0.96
32:f:471:LEU:HG	32:f:509:LYS:HE3	0.96	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	0.96
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	0.95
32:f:376:PHE:CD1	32:f:416:MET:HE1	2.01	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:742:ALA:HA	32:f:745:LEU:HD23	1.46	0.95
32:f:388:ASP:OD2	32:f:390:LEU:HB2	1.67	0.95
32:f:95:PRO:O	32:f:99:LEU:HB2	1.67	0.94
32:f:372:LEU:HD11	32:f:406:GLY:HA3	1.47	0.93
32:f:358:PHE:CZ	32:f:381:VAL:HG21	2.03	0.93
32:f:691:PRO:CB	32:f:749:ALA:HB2	1.99	0.93
32:f:376:PHE:CE1	32:f:416:MET:HE1	2.03	0.92
29:D:338:ARG:O	29:D:339:ARG:CB	2.12	0.91
32:f:494:ARG:HE	32:f:495:GLU:H	1.16	0.91
32:f:363:SER:O	32:f:365:VAL:N	2.04	0.91
31:F:188:ILE:CD1	31:F:235:LEU:HD13	2.01	0.91
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:315:GLU:HG2	32:f:491:GLY:HA2	1.51	0.90
32:f:376:PHE:CE1	32:f:798:THR:HB	2.06	0.89
32:f:369:ARG:HB3	32:f:370:MET:SD	2.13	0.89
32:f:376:PHE:CE1	32:f:798:THR:CB	2.55	0.89
29:D:336:PRO:HB2	29:D:340:GLN:HG3	1.51	0.88
32:f:742:ALA:HA	32:f:745:LEU:HD21	1.53	0.88
1:U:134:VAL:O	1:U:138:PHE:HB2	1.73	0.88
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: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:378:ASN:HB3	32:f:391:LEU:HG	1.56	0.88
32:f:311:VAL:CB	32:f:490:ALA:HB1	2.03	0.87
32:f:129:LEU:O	32:f:133:MET:HB3	1.75	0.87
3:W:60:MET:O	3:W:64:SER:HB3	1.75	0.87
28:C:387:VAL:O	28:C:391:MET:HB3	1.75	0.87
32:f:378:ASN:HB3	32:f:391:LEU:CG	2.05	0.86
5:Y:124:PHE:O	5:Y:128:TYR:HB2	1.75	0.86
32:f:123:ALA:O	32:f:127:SER:HB2	1.76	0.86
29:D:372:GLY:O	34:D:501:AGS:N6	2.09	0.86
32:f:337:LEU:HD13	32:f:420:TRP:CZ3	2.10	0.86
32:f:635:LYS:HZ2	32:f:641:GLU:HG3	1.41	0.86
32:f:691:PRO:HB2	32:f:749:ALA:HB2	1.58	0.86
32:f:494:ARG:HH21	32:f:495:GLU:CG	1.88	0.85
32:f:471:LEU:HD12	32:f:509:LYS:HG2	1.58	0.85
32:f:796:LEU:O	32:f:799:VAL:CG2	2.22	0.85
6:Z:262:LEU:O	6:Z:266:ILE:HB	1.77	0.85
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:376:PHE:HE1	32:f:798:THR:CG2	1.89	0.84
29:D:372:GLY:O	34:D:501:AGS:C6	2.25	0.84
32:f:695:ALA:HB3	32:f:752:HIS:HB2	1.59	0.84
32:f:696:LEU:CD1	32:f:752:HIS:HD2	1.90	0.84
32:f:301:HIS:O	32:f:305:LEU:HB2	1.77	0.84
32:f:376:PHE:HE1	32:f:798:THR:CB	1.91	0.83
32:f:336:GLU:HG3	32:f:337:LEU:HD22	1.60	0.83
9:c:44:HIS:O	9:c:48:GLY:HA3	1.79	0.83
6:Z:263:ALA:O	6:Z:267:ARG:HB2	1.77	0.83
32:f:126:ILE:O	32:f:130:ALA:HB3	1.77	0.83
32:f:714:SER:O	32:f:718:ASP:HB2	1.78	0.82
10:d:194:ALA:O	10:d:198:LEU:HB2	1.77	0.82
32:f:376:PHE:CZ	32:f:416:MET:SD	2.73	0.82
32:f:494:ARG:NE	32:f:495:GLU:N	2.26	0.82
32:f:479:LEU:CD2	32:f:513:GLU:CB	2.50	0.82
32:f:471:LEU:HD12	32:f:509:LYS:HG3	1.62	0.82
32:f:378:ASN:O	32:f:381:VAL:HG12	1.80	0.81
32:f:225:ALA:O	32:f:229:VAL:HB	1.79	0.81
32:f:742:ALA:C	32:f:745:LEU:HG	2.06	0.81
32:f:376:PHE:CE1	32:f:416:MET:CE	2.64	0.80
32:f:456:ARG:HB3	32:f:489:TYR:HE2	1.47	0.80
31:F:232:GLY:HA3	31:F:235:LEU:HD23	1.62	0.79
31:F:394:ALA:HA	34:F:501:AGS:HI1'	1.63	0.79
32:f:635:LYS:HZ2	32:f:641:GLU:CG	1.95	0.79
32:f:88:SER:HB2	32:f:92:VAL:HG23	1.63	0.79
32:f:503:PRO:O	32:f:507:ASP:HB2	1.82	0.79
7:a:131:THR:O	7:a:135:ILE:HB	1.82	0.79
32:f:232:TYR:O	32:f:236:CYS:HB2	1.82	0.79
32:f:612:LEU:O	32:f:616:CYS:HB2	1.83	0.79
32:f:494:ARG:HE	32:f:494:ARG:C	1.92	0.78
32:f:695:ALA:C	32:f:752:HIS:HB3	2.09	0.78
27:B:279:PRO:CD	32:f:718:ASP:OD2	2.30	0.78
32:f:184:LEU:HG	32:f:185:LEU:N	1.98	0.78
32:f:392:THR:HG22	32:f:417:ILE:CD1	2.14	0.77
32:f:494:ARG:NE	32:f:495:GLU:H	1.80	0.77
32:f:370:MET:SD	32:f:370:MET:N	2.57	0.77
32:f:376:PHE:CE1	32:f:798:THR:HG22	2.20	0.77
6:Z:285:ALA:O	6:Z:289:GLU:HB2	1.85	0.77
32:f:691:PRO:HB3	32:f:749:ALA:HB2	1.66	0.77
32:f:675:PHE:O	32:f:679:LEU:HB2	1.85	0.76
32:f:745:LEU:HD12	32:f:746:ARG:N	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:494:ARG:NH2	32:f:495:GLU:CG	2.48	0.76
31:F:188:ILE:HD13	31:F:235:LEU:HD13	1.65	0.76
32:f:796:LEU:HG	32:f:799:VAL:HG21	1.66	0.76
32:f:478:ARG:HD3	32:f:504:VAL:HG13	1.68	0.76
32:f:494:ARG:CG	32:f:497:VAL:HG12	2.16	0.75
27:B:279:PRO:CG	32:f:714:SER:N	2.50	0.75
1:U:527:GLN:O	1:U:531:ASP:HB2	1.86	0.75
27:B:279:PRO:HG3	32:f:714:SER:N	2.02	0.75
32:f:358:PHE:O	32:f:362:GLY:HA3	1.87	0.75
32:f:784:ASP:HB2	32:f:800:LEU:HD21	1.66	0.75
32:f:376:PHE:CZ	32:f:798:THR:HB	2.22	0.75
32:f:635:LYS:NZ	32:f:641:GLU:CG	2.50	0.75
3:W:222:LEU:HD22	3:W:223:LYS:HZ2	1.51	0.75
9:c:217:LEU:O	9:c:221:HIS:HB2	1.86	0.74
15:J:51:ALA:H	15:J:54:GLN:HE22	1.32	0.74
32:f:357:ARG:O	32:f:361:SER:HB2	1.87	0.74
32:f:471:LEU:CD1	32:f:509:LYS:CE	2.65	0.74
32:f:392:THR:CG2	32:f:417:ILE:HG21	2.18	0.74
3:W:131:VAL:HB	3:W:144:ARG:HH21	1.52	0.74
32:f:211:ILE:O	32:f:215:ASP:HB2	1.88	0.73
32:f:684:PRO:O	32:f:688:ARG:HB2	1.87	0.73
18:m:47:PHE:HB2	18:m:214:SER:HB3	1.71	0.72
32:f:691:PRO:HG2	32:f:745:LEU:HD13	1.70	0.72
28:C:238:ALA:HB1	28:C:289:ILE:HG13	1.72	0.72
32:f:389:LYS:CD	32:f:418:LEU:HD21	2.20	0.72
32:f:742:ALA:HA	32:f:745:LEU:CG	2.18	0.72
6:Z:245:PHE:HB3	6:Z:248:ALA:HB3	1.71	0.72
28:C:131:VAL:HG22	28:C:133:PRO:HD2	1.72	0.72
29:D:335:LEU:HB3	29:D:336:PRO:HD2	1.72	0.72
32:f:664:GLU:HB3	32:f:696:LEU:HG	1.69	0.71
32:f:389:LYS:HG2	32:f:418:LEU:HD11	1.72	0.71
32:f:797:LEU:O	32:f:800:LEU:HD13	1.91	0.71
24:S:27:THR:HB	24:S:40:SER:H	1.53	0.71
4:X:274:LYS:O	4:X:278:ARG:HB2	1.90	0.71
28:C:164:VAL:HG13	28:C:165:ILE:HG13	1.73	0.71
32:f:311:VAL:O	32:f:490:ALA:O	2.09	0.71
7:a:248:PHE:O	7:a:252:LYS:HB2	1.91	0.70
32:f:311:VAL:CG2	32:f:527:VAL:O	2.39	0.70
1:U:596:ASN:HA	1:U:599:ILE:HG22	1.72	0.70
1:U:202:VAL:HG12	1:U:215:ASN:HB2	1.72	0.70
32:f:625:LYS:O	32:f:629:LYS:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:88:SER:HB3	32:f:92:VAL:HG23	1.72	0.70
32:f:130:ALA:O	32:f:134:SER:HB3	1.92	0.70
32:f:392:THR:HG22	32:f:417:ILE:HD12	1.74	0.70
8:b:156:PHE:O	8:b:160:LEU:HB2	1.92	0.69
32:f:337:LEU:CD1	32:f:420:TRP:CZ3	2.74	0.69
6:Z:195:VAL:O	6:Z:199:LYS:HB2	1.91	0.69
29:D:234:GLU:HB2	30:E:216:ARG:HH22	1.56	0.69
32:f:315:GLU:CG	32:f:491:GLY:HA2	2.20	0.69
32:f:471:LEU:CG	32:f:509:LYS:CE	2.56	0.69
28:C:201:ARG:O	28:C:205:HIS:HB2	1.93	0.69
32:f:695:ALA:HB3	32:f:752:HIS:CB	2.23	0.69
7:a:230:ARG:HE	7:a:233:LEU:HB2	1.55	0.69
32:f:688:ARG:HA	32:f:745:LEU:HD22	1.75	0.69
32:f:635:LYS:HZ3	32:f:641:GLU:CD	2.01	0.69
5:Y:268:TYR:HB2	5:Y:322:ALA:HB1	1.75	0.69
32:f:625:LYS:HA	32:f:657:ILE:HD11	1.75	0.69
22:Q:118:MET:HE1	22:Q:124:LEU:HD23	1.75	0.69
32:f:222:ASP:O	32:f:226:TYR:HB3	1.91	0.69
22:Q:117:TYR:HB3	22:Q:125:ALA:HB3	1.75	0.68
32:f:376:PHE:CD1	32:f:798:THR:HG21	2.26	0.68
6:Z:274:ASN:O	6:Z:278:ASN:HB2	1.93	0.68
14:I:119:GLN:HE21	14:I:123:GLN:HE22	1.40	0.68
32:f:372:LEU:O	32:f:372:LEU:HD23	1.93	0.68
16:K:177:ALA:O	16:K:181:LEU:HB2	1.93	0.68
32:f:353:LEU:HG	32:f:387:GLN:HG3	1.75	0.68
32:f:664:GLU:O	32:f:665:GLU:O	2.10	0.68
32:f:742:ALA:O	32:f:745:LEU:CG	2.38	0.68
5:Y:316:LEU:O	5:Y:320:ALA:HB2	1.93	0.68
1:U:242:LEU:HD21	1:U:321:GLN:HB3	1.75	0.68
7:a:296:ILE:O	7:a:300:ALA:HB3	1.93	0.68
9:c:131:GLN:HA	9:c:134:GLU:HG2	1.74	0.68
32:f:478:ARG:O	32:f:482:ILE:HB	1.94	0.68
14:I:143:TYR:HB2	14:I:146:GLN:HE21	1.57	0.67
32:f:367:SER:HB3	32:f:370:MET:SD	2.34	0.67
1:U:545:LEU:O	1:U:549:ALA:HB2	1.94	0.67
14:i:143:TYR:HB2	14:i:146:GLN:HE21	1.59	0.67
8:b:140:ILE:HG22	8:b:170:LEU:HD13	1.76	0.67
25:T:27:LEU:HD22	25:T:184:TYR:HB2	1.75	0.67
32:f:389:LYS:CG	32:f:418:LEU:CD2	2.63	0.67
13:h:39:LYS:HE2	13:h:144:PRO:HG2	1.77	0.67
17:L:186:GLU:HA	17:L:189:LYS:HG2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:800:LEU:HD12	32:f:800:LEU:N	2.10	0.67
3:W:67:LEU:HD13	3:W:115:ILE:HG13	1.77	0.67
29:D:82:ILE:HG23	29:D:83:GLN:HG2	1.77	0.67
2:V:55:THR:HA	2:V:59:ALA:H	1.59	0.67
3:W:128:LEU:HA	3:W:144:ARG:HH22	1.57	0.67
22:Q:169:LYS:HD3	22:Q:170:ARG:HG3	1.77	0.67
32:f:372:LEU:HD23	32:f:372:LEU:C	2.20	0.67
1:U:356:THR:HG22	1:U:717:ILE:HD13	1.77	0.66
29:D:323:ARG:HE	29:D:324:PRO:HD2	1.59	0.66
32:f:494:ARG:HD3	32:f:496:ASP:CG	2.16	0.66
5:Y:127:THR:HG23	5:Y:140:ILE:HD11	1.75	0.66
32:f:376:PHE:CE1	32:f:416:MET:SD	2.88	0.66
1:U:708:GLN:O	1:U:712:LEU:HB2	1.95	0.66
6:Z:214:LYS:HA	6:Z:218:GLY:HA3	1.77	0.66
6:Z:284:ASP:O	6:Z:288:LYS:HB2	1.95	0.66
14:i:106:PRO:HD2	14:i:109:GLN:HE21	1.61	0.66
15:j:72:ALA:HB3	15:j:132:LEU:HB2	1.77	0.66
10:d:141:GLN:O	10:d:145:GLU:HB2	1.95	0.66
31:F:150:LEU:HB3	31:F:164:LEU:HD12	1.77	0.66
32:f:578:ALA:O	32:f:582:VAL:HB	1.95	0.66
23:r:19:ARG:HH21	23:r:29:GLN:HE22	1.43	0.66
32:f:804:LEU:H	32:f:804:LEU:HD12	1.60	0.66
1:U:717:ILE:HG13	1:U:727:LYS:HD3	1.76	0.66
28:C:201:ARG:HE	28:C:211:PHE:HE2	1.42	0.66
30:E:56:ILE:HB	30:E:100:LEU:HB2	1.76	0.66
27:B:186:ASP:OD1	34:B:501:AGS:N6	2.29	0.66
31:F:191:LEU:CD1	31:F:235:LEU:HD21	2.26	0.66
32:f:311:VAL:HG21	32:f:527:VAL:O	1.94	0.66
7:a:8:LEU:O	7:a:12:GLN:HB2	1.95	0.66
14:I:106:PRO:HD2	14:I:109:GLN:HE21	1.61	0.66
32:f:315:GLU:HG2	32:f:491:GLY:CA	2.24	0.66
18:m:99:ARG:NH2	18:m:105:ASN:OD1	2.29	0.65
6:Z:17:LEU:HD22	9:c:36:LEU:HB3	1.78	0.65
32:f:483:PHE:CE2	32:f:799:VAL:CB	2.75	0.65
24:s:27:THR:HB	24:s:40:SER:H	1.62	0.65
26:A:339:ARG:NH1	31:F:405:MET:SD	2.69	0.65
32:f:471:LEU:CD1	32:f:509:LYS:HE3	2.26	0.65
26:A:329:PRO:HA	26:A:332:MET:HB2	1.78	0.65
29:D:207:PRO:HD2	29:D:335:LEU:CD1	2.26	0.65
32:f:804:LEU:HD12	32:f:804:LEU:N	2.12	0.65
32:f:337:LEU:HD11	32:f:422:VAL:HG21	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:36:ALA:O	5:Y:40:GLU:HB3	1.95	0.65
9:c:144:VAL:HB	9:c:158:ASP:HB3	1.79	0.65
22:q:117:TYR:HB3	22:q:125:ALA:HB3	1.77	0.65
22:q:118:MET:HE1	22:q:124:LEU:HD23	1.78	0.65
32:f:379:GLY:O	32:f:417:ILE:HG12	1.97	0.65
4:X:248:ILE:HG13	4:X:283:GLN:HB2	1.77	0.65
31:F:235:LEU:HD12	31:F:236:LEU:N	2.12	0.65
32:f:366:ASP:O	32:f:367:SER:HB2	1.97	0.65
32:f:628:ASP:HB2	32:f:657:ILE:HD13	1.77	0.65
32:f:692:LEU:HG	32:f:752:HIS:CE1	2.32	0.65
1:U:368:ALA:HA	1:U:371:ILE:HB	1.79	0.65
4:X:354:ILE:HG21	4:X:361:VAL:HG21	1.79	0.65
5:Y:40:GLU:HG3	5:Y:52:PRO:HB3	1.78	0.65
16:k:160:GLY:O	17:l:82:ARG:NH2	2.29	0.64
28:C:141:GLU:HG3	28:C:214:VAL:HA	1.79	0.64
28:C:182:GLN:O	28:C:288:ASN:ND2	2.31	0.64
2:V:470:ARG:HD3	2:V:473:GLN:HE21	1.61	0.64
29:D:239:TYR:O	29:D:287:ARG:NH2	2.31	0.64
32:f:460:ASP:N	32:f:460:ASP:OD1	2.29	0.64
9:c:227:GLU:HB3	9:c:232:GLN:HB2	1.80	0.64
29:D:92:PHE:HA	29:D:103:VAL:HG12	1.78	0.64
13:H:59:GLU:HG2	13:H:206:ASP:HB3	1.79	0.64
17:l:186:GLU:HA	17:l:189:LYS:HG2	1.78	0.64
19:n:19:ARG:NH2	19:n:168:GLY:O	2.29	0.64
32:f:138:GLU:O	32:f:142:TYR:HB2	1.97	0.64
5:Y:172:GLY:HA3	5:Y:177:ARG:HD2	1.78	0.64
9:c:30:GLN:HB3	9:c:66:THR:HG22	1.77	0.64
1:U:789:ILE:HB	1:U:911:ILE:HA	1.78	0.64
7:a:365:MET:O	7:a:369:HIS:HB2	1.98	0.64
22:q:21:ALA:HB3	22:q:29:LYS:HB3	1.80	0.64
32:f:313:GLU:O	32:f:317:LEU:HB2	1.98	0.64
14:I:15:GLU:H	14:I:16:GLY:HA2	1.63	0.64
32:f:389:LYS:HG2	32:f:418:LEU:CG	2.27	0.64
7:a:54:ASP:HA	7:a:57:ILE:HG22	1.80	0.64
9:c:119:GLY:O	9:c:190:GLN:NE2	2.30	0.64
32:f:494:ARG:HH21	32:f:495:GLU:H	1.46	0.64
32:f:664:GLU:HA	32:f:697:ILE:HA	1.80	0.64
5:Y:247:LEU:O	5:Y:251:HIS:HB2	1.98	0.64
13:H:12:THR:OG1	14:I:20:GLN:NE2	2.32	0.63
14:i:161:ALA:HB3	15:j:54:GLN:HE22	1.63	0.63
16:k:99:HIS:HB2	16:k:107:MET:HE3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:E:83:CYS:HA	30:E:107:ILE:HB	1.79	0.63
32:f:804:LEU:H	32:f:804:LEU:CD1	2.10	0.63
3:W:88:MET:SD	3:W:96:GLN:NE2	2.71	0.63
5:Y:228:MET:SD	5:Y:295:TYR:OH	2.56	0.63
10:d:203:PRO:HD2	10:d:206:MET:HG2	1.79	0.63
22:Q:57:ALA:O	22:Q:61:GLN:HB3	1.98	0.63
32:f:80:ARG:HB3	32:f:95:PRO:HB2	1.78	0.63
1:U:345:ASN:HD21	1:U:883:ARG:HD2	1.64	0.63
7:a:34:TRP:HD1	8:b:19:GLY:H	1.45	0.63
13:h:118:MET:HE2	13:h:151:PRO:HA	1.79	0.63
29:D:206:GLY:HA3	29:D:335:LEU:HD11	1.80	0.63
29:D:323:ARG:HB2	29:D:326:ARG:HB2	1.80	0.63
32:f:654:VAL:HA	32:f:657:ILE:HD12	1.81	0.63
2:V:394:LEU:O	2:V:398:LEU:HB2	1.97	0.63
3:W:431:LYS:O	3:W:435:LEU:HB2	1.99	0.63
12:g:41:ALA:HB3	12:g:166:THR:HB	1.81	0.63
12:g:53:GLN:HA	12:g:215:ILE:HA	1.79	0.63
1:U:77:SER:O	1:U:81:ALA:HB2	1.99	0.63
1:U:408:LEU:O	1:U:412:HIS:ND1	2.31	0.63
12:G:53:GLN:HA	12:G:215:ILE:HA	1.81	0.63
28:C:161:ILE:HG23	28:C:165:ILE:HD12	1.80	0.63
1:U:725:MET:HA	1:U:728:PHE:HB2	1.81	0.63
12:G:34:GLN:NE2	18:M:17:ASP:O	2.32	0.63
26:A:240:VAL:HG21	26:A:260:LEU:HD21	1.81	0.63
25:t:27:LEU:HD22	25:t:184:TYR:HB2	1.79	0.62
32:f:93:PRO:HB2	32:f:137:ARG:HE	1.63	0.62
32:f:687:ARG:HH21	32:f:742:ALA:HB2	1.64	0.62
1:U:529:ILE:HG12	1:U:556:MET:HE3	1.82	0.62
16:k:70:ILE:HD11	16:k:89:ILE:HD12	1.82	0.62
7:a:273:GLN:HG2	7:a:300:ALA:HB1	1.81	0.62
16:K:21:LEU:HB3	16:K:23:GLN:H	1.65	0.62
17:L:73:SER:HB3	17:L:133:LEU:HB2	1.82	0.62
25:T:1:THR:N	25:T:105:PRO:O	2.30	0.62
25:t:1:THR:N	25:t:105:PRO:O	2.32	0.62
32:f:339:ILE:HG23	32:f:340:MET:HG2	1.81	0.62
1:U:719:ASP:O	1:U:727:LYS:NZ	2.32	0.62
28:C:143:VAL:O	28:C:201:ARG:NH1	2.33	0.62
8:b:142:ASN:ND2	8:b:146:GLU:OE1	2.32	0.62
16:K:76:CYS:SG	16:K:77:ALA:N	2.73	0.62
18:M:47:PHE:HB2	18:M:214:SER:HB3	1.79	0.62
27:B:133:VAL:HB	27:B:158:ALA:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:89:ASN:HB3	1:U:133:ILE:HG23	1.82	0.62
30:E:97:ARG:NH2	30:E:112:PRO:O	2.33	0.62
30:E:175:PRO:O	30:E:180:LYS:NZ	2.32	0.62
22:Q:21:ALA:HB3	22:Q:29:LYS:HB3	1.82	0.62
15:j:88:ARG:NH1	22:q:69:MET:O	2.33	0.62
18:m:8:ASP:O	18:m:22:GLN:NE2	2.33	0.62
28:C:141:GLU:HG2	28:C:212:ILE:HG22	1.81	0.62
3:W:358:VAL:O	3:W:362:ASN:HB2	1.99	0.61
3:W:293:ASP:HB3	3:W:296:LEU:HB2	1.82	0.61
6:Z:192:THR:O	6:Z:196:HIS:ND1	2.34	0.61
30:E:97:ARG:HE	30:E:111:LEU:HB2	1.65	0.61
19:n:91:ARG:HG3	19:n:92:GLU:HG2	1.81	0.61
31:F:286:ASP:OD1	34:F:501:AGS:S1G	2.59	0.61
32:f:389:LYS:HD3	32:f:389:LYS:N	2.15	0.61
32:f:392:THR:HG23	32:f:417:ILE:HG21	1.81	0.61
15:J:109:ARG:NH2	23:R:70:ASN:OD1	2.33	0.61
18:m:173:LYS:HA	18:m:176:ILE:HB	1.81	0.61
1:U:252:LEU:HD11	1:U:264:VAL:HG11	1.83	0.61
16:K:32:LYS:HZ3	16:K:173:ALA:H	1.48	0.61
16:K:203:LYS:HA	16:K:206:MET:HG2	1.83	0.61
28:C:184:LYS:HE2	28:C:280:LEU:HD13	1.83	0.61
34:D:501:AGS:O3G	30:E:294:ARG:NH2	2.33	0.61
31:F:422:GLU:HA	31:F:425:LEU:HB2	1.83	0.61
32:f:494:ARG:NE	32:f:496:ASP:H	1.99	0.61
16:K:99:HIS:HB2	16:K:107:MET:HE3	1.83	0.61
25:t:54:SER:HB3	25:t:109:THR:HB	1.82	0.61
28:C:218:GLU:O	29:D:248:ARG:NH2	2.34	0.61
32:f:378:ASN:HB2	32:f:391:LEU:HD11	1.82	0.61
32:f:471:LEU:CD1	32:f:509:LYS:HE2	2.30	0.61
7:a:156:TYR:OH	7:a:196:ARG:NH1	2.34	0.61
21:p:61:GLN:HE22	22:q:124:LEU:HB2	1.66	0.61
27:B:407:LEU:HD13	28:C:178:LEU:HD11	1.83	0.61
32:f:234:THR:O	32:f:238:ASN:HB2	2.00	0.61
32:f:315:GLU:CB	32:f:491:GLY:HA2	2.31	0.60
32:f:695:ALA:CB	32:f:752:HIS:HB2	2.31	0.60
16:k:100:TRP:O	23:r:57:ARG:NH2	2.33	0.60
22:q:19:ARG:HH21	22:q:31:ASP:HB2	1.65	0.60
29:D:57:GLN:HA	29:D:60:TYR:HB3	1.83	0.60
25:T:27:LEU:HD11	25:T:34:ALA:HB1	1.83	0.60
28:C:127:LEU:HD22	29:D:96:VAL:HG21	1.83	0.60
3:W:137:TYR:HD2	3:W:140:ILE:H	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:k:48:LEU:HD21	16:k:77:ALA:HB2	1.82	0.60
30:E:288:ALA:O	30:E:294:ARG:NH1	2.34	0.60
32:f:376:PHE:CG	32:f:416:MET:HE1	2.35	0.60
1:U:321:GLN:HA	1:U:324:LYS:HB3	1.84	0.60
7:a:230:ARG:HH21	7:a:233:LEU:HD13	1.66	0.60
23:r:1:THR:N	23:r:169:TYR:O	2.35	0.60
24:s:28:ARG:NH2	24:s:213:ASP:O	2.35	0.60
30:E:265:ASP:OD2	30:E:291:ARG:NH1	2.34	0.60
32:f:471:LEU:O	32:f:471:LEU:HD23	2.01	0.60
2:V:179:LYS:HG2	2:V:182:LYS:HD2	1.82	0.60
16:K:209:LYS:O	16:K:214:ASN:ND2	2.34	0.60
12:g:83:MET:SD	12:g:132:ARG:NH1	2.70	0.60
28:C:133:PRO:HG2	28:C:233:GLU:HG2	1.83	0.60
32:f:376:PHE:CZ	32:f:416:MET:HE1	2.36	0.60
1:U:740:GLY:O	1:U:743:ASN:ND2	2.35	0.60
10:d:135:HIS:O	10:d:139:LEU:HB2	2.02	0.60
13:H:42:ASN:ND2	13:H:183:GLU:OE1	2.34	0.60
15:J:115:LYS:HE2	15:J:149:PRO:HA	1.84	0.60
32:f:389:LYS:HG2	32:f:418:LEU:CD1	2.32	0.60
1:U:12:LEU:HD22	1:U:20:LYS:HD3	1.82	0.60
3:W:381:LEU:HD21	7:a:308:GLU:HG2	1.84	0.60
18:M:173:LYS:HA	18:M:176:ILE:HB	1.82	0.60
24:S:173:ARG:HH11	20:o:200:GLY:HA2	1.67	0.60
14:i:16:GLY:N	15:j:21:TYR:OH	2.35	0.60
28:C:115:ALA:HB3	28:C:125:LYS:HB3	1.83	0.60
32:f:337:LEU:HD22	32:f:337:LEU:N	2.17	0.60
32:f:801:VAL:HG13	32:f:801:VAL:O	2.01	0.60
7:a:182:CYS:SG	7:a:183:VAL:N	2.75	0.60
19:n:29:ARG:NH1	20:o:139:GLU:OE1	2.30	0.60
3:W:140:ILE:HA	3:W:143:ALA:HB3	1.84	0.59
5:Y:44:ALA:HB2	5:Y:52:PRO:HB2	1.82	0.59
11:e:2:SER:HA	11:e:6:GLN:HE21	1.67	0.59
18:M:99:ARG:NH2	18:M:105:ASN:OD1	2.35	0.59
29:D:410:ASP:H	29:D:411:GLU:HG2	1.67	0.59
1:U:246:TYR:OH	1:U:911:ILE:O	2.20	0.59
2:V:329:HIS:HD2	2:V:345:ARG:HH21	1.49	0.59
3:W:231:ILE:O	3:W:235:GLN:HB2	2.01	0.59
3:W:417:ARG:HG3	3:W:419:LYS:H	1.67	0.59
7:a:283:THR:OG1	7:a:339:ARG:NH2	2.35	0.59
32:f:89:MET:HG2	32:f:90:THR:HG23	1.84	0.59
5:Y:192:ARG:HH12	5:Y:295:TYR:HB2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:382:SER:HB2	29:D:398:ASP:HB3	1.84	0.59
30:E:330:ALA:O	30:E:334:LEU:HB2	2.02	0.59
32:f:380:PHE:CB	32:f:751:TYR:HE2	2.14	0.59
32:f:494:ARG:NH2	32:f:495:GLU:H	1.99	0.59
2:V:349:ARG:HG3	2:V:357:LEU:HD21	1.84	0.59
5:Y:348:ASP:HB3	5:Y:353:ILE:H	1.68	0.59
1:U:166:THR:HA	1:U:169:GLU:HB3	1.84	0.59
12:G:93:ARG:NH1	12:G:125:TYR:OH	2.33	0.59
18:m:141:SER:HB3	18:m:144:ASP:HB2	1.84	0.59
30:E:341:ALA:HB3	31:F:344:ARG:HH12	1.67	0.59
31:F:98:ASP:OD1	31:F:120:LYS:N	2.35	0.59
32:f:378:ASN:O	32:f:381:VAL:CG1	2.49	0.59
2:V:326:GLN:HB3	2:V:353:LEU:HD22	1.84	0.59
4:X:417:LYS:HG2	6:Z:283:ARG:HH22	1.65	0.59
15:J:179:GLU:HG2	15:J:180:ALA:HB2	1.85	0.59
25:t:43:MET:HE3	25:t:45:VAL:HG22	1.84	0.59
26:A:348:LEU:HD23	26:A:351:ARG:HH21	1.68	0.59
32:f:232:TYR:O	32:f:236:CYS:CB	2.49	0.59
2:V:148:ARG:NH2	2:V:197:THR:O	2.36	0.59
3:W:4:GLY:O	3:W:8:ARG:NH2	2.35	0.59
21:P:107:PRO:HG2	21:P:124:LEU:HB2	1.84	0.59
15:j:131:ALA:H	15:j:147:THR:HG1	1.50	0.59
30:E:184:ALA:O	30:E:197:LYS:NZ	2.36	0.59
32:f:618:GLU:HG2	32:f:623:LYS:HD2	1.85	0.59
32:f:782:HIS:HA	32:f:785:ARG:HG2	1.83	0.59
5:Y:155:ASP:O	5:Y:159:ARG:HB2	2.03	0.59
24:s:148:LEU:HD23	24:s:178:VAL:HG12	1.85	0.59
32:f:477:MET:O	32:f:481:SER:HB2	2.02	0.59
5:Y:272:PHE:HB3	11:e:67:MET:HE2	1.84	0.59
6:Z:128:PRO:O	9:c:219:ASN:ND2	2.36	0.59
10:d:208:ASP:O	10:d:212:LYS:HB2	2.02	0.59
14:I:25:MET:HA	14:I:28:ILE:HD12	1.83	0.59
32:f:541:THR:O	32:f:545:LYS:HB2	2.02	0.59
26:A:285:PHE:O	31:F:171:ARG:NH1	2.36	0.58
28:C:218:GLU:HG3	29:D:248:ARG:HH21	1.68	0.58
30:E:275:MET:HB3	30:E:277:MET:HE2	1.84	0.58
1:U:576:PRO:O	1:U:580:ARG:HB2	2.03	0.58
7:a:201:GLY:O	7:a:205:LEU:HB2	2.02	0.58
32:f:376:PHE:CD1	32:f:416:MET:CE	2.83	0.58
32:f:378:ASN:CB	32:f:391:LEU:HD11	2.33	0.58
32:f:780:PRO:O	32:f:800:LEU:HG	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:173:VAL:HG22	1:U:175:GLY:H	1.68	0.58
18:M:141:SER:HB3	18:M:144:ASP:HB2	1.85	0.58
12:g:234:GLU:O	12:g:238:HIS:ND1	2.35	0.58
26:A:258:ARG:HD3	26:A:305:GLN:HE22	1.69	0.58
27:B:189:GLY:HA3	34:B:501:AGS:H2	1.84	0.58
27:B:427:LEU:HD23	27:B:430:LYS:HA	1.84	0.58
32:f:127:SER:O	32:f:131:MET:CB	2.52	0.58
32:f:487:LEU:HD23	32:f:524:MET:HE1	1.85	0.58
1:U:219:CYS:O	1:U:223:LEU:HB3	2.04	0.58
2:V:237:THR:OG1	2:V:241:ARG:NH2	2.36	0.58
5:Y:387:ILE:HD13	6:Z:283:ARG:HG2	1.85	0.58
32:f:22:GLY:O	32:f:26:GLU:HB2	2.04	0.58
32:f:353:LEU:H	32:f:387:GLN:HG2	1.68	0.58
32:f:501:LEU:HD22	32:f:518:THR:HG23	1.84	0.58
2:V:338:LEU:HD13	2:V:397:ARG:HD2	1.86	0.58
7:a:19:PRO:HA	7:a:22:TRP:HB2	1.86	0.58
13:H:81:PRO:HG2	29:D:416:PHE:HE1	1.69	0.58
8:b:50:GLY:H	8:b:64:LEU:HD12	1.69	0.58
9:c:190:GLN:O	9:c:194:HIS:ND1	2.37	0.58
30:E:171:LEU:HB3	30:E:298:LYS:HG3	1.86	0.58
32:f:456:ARG:HD3	32:f:489:TYR:OH	2.03	0.58
1:U:134:VAL:O	1:U:138:PHE:CB	2.49	0.58
1:U:522:GLY:O	1:U:559:ARG:NH2	2.37	0.58
1:U:554:LEU:HG	1:U:588:MET:HE1	1.86	0.58
24:S:123:SER:HB3	24:S:136:LYS:HG3	1.84	0.58
14:i:218:ARG:NH1	14:i:223:THR:OG1	2.37	0.58
14:i:219:GLU:OE2	14:i:220:ASN:ND2	2.37	0.58
18:m:76:ALA:HB3	18:m:136:MET:HB2	1.84	0.58
34:D:501:AGS:O2B	30:E:291:ARG:NH1	2.37	0.58
31:F:314:LEU:HD21	31:F:342:LEU:HD23	1.86	0.58
26:A:333:ARG:HH11	26:A:334:PRO:HD2	1.70	0.57
28:C:358:GLU:HG3	29:D:324:PRO:HG3	1.86	0.57
32:f:494:ARG:CZ	32:f:496:ASP:H	2.16	0.57
3:W:362:ASN:HA	3:W:365:ILE:HG12	1.86	0.57
4:X:346:GLN:HE21	4:X:349:HIS:HB2	1.67	0.57
5:Y:346:LYS:H	5:Y:355:GLU:HB3	1.69	0.57
9:c:160:PHE:HA	9:c:202:SER:HA	1.84	0.57
18:m:163:CYS:SG	18:m:164:ALA:N	2.77	0.57
28:C:225:GLY:H	28:C:228:ALA:HB3	1.69	0.57
32:f:456:ARG:HB3	32:f:489:TYR:CZ	2.39	0.57
2:V:79:VAL:HG22	2:V:80:LYS:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:J:116:GLN:NE2	15:J:150:SER:O	2.37	0.57
29:D:175:GLN:NE2	29:D:179:GLU:OE2	2.36	0.57
32:f:378:ASN:HB3	32:f:391:LEU:CD2	2.34	0.57
3:W:186:ILE:HD11	3:W:208:LYS:HG3	1.85	0.57
4:X:225:TRP:O	4:X:229:TYR:HB2	2.05	0.57
29:D:240:LEU:O	29:D:245:ARG:NH1	2.37	0.57
1:U:184:CYS:SG	29:D:41:TYR:OH	2.61	0.57
7:a:118:ILE:O	7:a:122:LYS:HB2	2.04	0.57
19:N:96:ALA:HB1	19:N:98:ILE:HG12	1.87	0.57
25:T:43:MET:HE3	25:T:45:VAL:HG22	1.86	0.57
28:C:173:GLU:HA	28:C:176:GLU:HB2	1.87	0.57
32:f:140:LEU:O	32:f:144:LEU:HB2	2.04	0.57
32:f:695:ALA:CB	32:f:752:HIS:CB	2.82	0.57
32:f:780:PRO:HB2	32:f:800:LEU:HB3	1.86	0.57
1:U:367:THR:HG22	1:U:403:THR:HG21	1.87	0.57
1:U:612:ASP:HB3	1:U:647:HIS:HB2	1.87	0.57
20:o:174:ASP:OD2	20:o:187:ARG:NH1	2.38	0.57
22:q:181:ARG:NH1	22:q:190:ASP:OD1	2.38	0.57
27:B:112:LEU:HD21	27:B:123:VAL:HG12	1.85	0.57
32:f:129:LEU:O	32:f:133:MET:CB	2.50	0.57
21:p:15:LYS:HE3	21:p:121:ILE:HG12	1.86	0.57
27:B:316:LEU:O	27:B:322:ARG:NH1	2.37	0.57
27:B:436:GLU:HB2	27:B:438:LEU:H	1.68	0.57
29:D:87:LEU:HB2	30:E:80:VAL:HB	1.87	0.57
31:F:401:VAL:HG12	31:F:405:MET:HE2	1.87	0.57
9:c:153:GLY:H	29:D:81:ARG:HE	1.52	0.57
18:M:8:ASP:O	18:M:22:GLN:NE2	2.36	0.57
23:R:1:THR:N	23:R:169:TYR:O	2.38	0.57
15:j:32:ALA:HB2	15:j:45:VAL:HG23	1.86	0.57
31:F:188:ILE:CG1	31:F:235:LEU:HD13	2.35	0.57
32:f:376:PHE:HE1	32:f:798:THR:HG21	1.49	0.57
32:f:742:ALA:CA	32:f:745:LEU:HG	2.35	0.57
3:W:52:LYS:HD2	3:W:55:ARG:HH21	1.70	0.57
6:Z:248:ALA:HA	6:Z:251:LEU:HB3	1.86	0.57
9:c:181:LEU:O	9:c:185:ASN:HB2	2.04	0.57
10:d:208:ASP:O	10:d:212:LYS:CB	2.53	0.57
17:L:18:ARG:NH1	17:L:23:GLU:OE2	2.37	0.57
16:k:76:CYS:SG	16:k:77:ALA:N	2.78	0.57
19:n:7:GLN:HA	19:n:12:VAL:HA	1.87	0.57
22:q:164:LEU:O	22:q:168:GLN:NE2	2.38	0.57
29:D:317:LEU:HD22	29:D:321:LEU:HG	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:357:PRO:O	31:F:362:ARG:NH1	2.37	0.57
32:f:358:PHE:CE1	32:f:381:VAL:HG21	2.40	0.57
2:V:55:THR:H	2:V:59:ALA:HB3	1.70	0.56
3:W:436:MET:HA	3:W:439:VAL:HG22	1.87	0.56
23:R:97:MET:O	23:R:116:SER:N	2.37	0.56
13:h:34:PRO:HA	13:h:164:GLY:HA3	1.87	0.56
23:r:21:THR:HG22	23:r:26:ILE:HG12	1.87	0.56
27:B:362:LYS:HG2	27:B:384:ILE:HD13	1.87	0.56
30:E:156:PRO:HG3	30:E:272:ARG:HH21	1.70	0.56
32:f:317:LEU:O	32:f:321:MET:HB2	2.05	0.56
3:W:129:ARG:O	3:W:133:GLU:HB3	2.06	0.56
26:A:134:ILE:HG23	26:A:140:VAL:HG11	1.87	0.56
1:U:500:ASN:HA	1:U:503:GLN:HG2	1.87	0.56
1:U:612:ASP:HA	1:U:615:ARG:HD3	1.86	0.56
2:V:228:ARG:O	2:V:232:HIS:ND1	2.35	0.56
8:b:157:VAL:HA	8:b:168:SER:HB2	1.87	0.56
13:h:222:THR:OG1	13:h:225:GLU:OE1	2.21	0.56
27:B:197:ILE:HG21	27:B:235:LEU:HD11	1.87	0.56
28:C:85:VAL:HG21	28:C:123:LEU:HG	1.86	0.56
28:C:135:VAL:HA	28:C:138:MET:HB3	1.87	0.56
30:E:290:LEU:HD13	30:E:389:VAL:HG22	1.87	0.56
32:f:353:LEU:HG	32:f:387:GLN:CG	2.36	0.56
1:U:568:GLU:O	1:U:572:ARG:HB2	2.06	0.56
1:U:733:ALA:O	1:U:737:LEU:HB2	2.05	0.56
17:L:44:ALA:HB1	17:L:144:ILE:HD11	1.87	0.56
27:B:248:LEU:HD12	27:B:282:VAL:HG22	1.86	0.56
31:F:68:ALA:O	31:F:72:LYS:HB2	2.06	0.56
31:F:251:LEU:HD23	31:F:285:ILE:HG12	1.86	0.56
32:f:380:PHE:CG	32:f:751:TYR:HE2	2.24	0.56
32:f:494:ARG:CZ	32:f:495:GLU:H	2.17	0.56
1:U:600:ARG:HE	29:D:56:VAL:HG22	1.71	0.56
5:Y:297:ARG:NH2	11:e:55:GLN:OE1	2.38	0.56
23:R:12:VAL:HB	23:R:179:VAL:HB	1.86	0.56
28:C:99:VAL:HA	28:C:123:LEU:HB3	1.87	0.56
29:D:170:MET:HG2	29:D:173:GLN:HB2	1.87	0.56
31:F:94:ILE:HD11	31:F:125:LYS:HB2	1.88	0.56
3:W:125:ILE:HD12	3:W:128:LEU:HD12	1.88	0.56
7:a:244:ASN:ND2	7:a:276:CYS:SG	2.79	0.56
10:d:204:LYS:O	10:d:208:ASP:HB2	2.06	0.56
16:K:22:PHE:H	16:K:25:GLU:HB3	1.70	0.56
19:n:91:ARG:O	19:n:93:ASP:N	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:279:PRO:HG2	32:f:714:SER:N	2.19	0.56
32:f:269:ALA:HB2	32:f:277:LEU:HD22	1.86	0.56
32:f:471:LEU:HD12	32:f:509:LYS:CE	2.36	0.56
2:V:100:MET:H	2:V:104:THR:HG21	1.71	0.56
3:W:124:LEU:HA	3:W:127:THR:HG22	1.88	0.56
9:c:211:GLU:O	9:c:215:LYS:HB3	2.06	0.56
25:t:145:LEU:HB3	25:t:179:ARG:HH21	1.71	0.56
30:E:178:THR:H	30:E:180:LYS:HZ3	1.54	0.56
1:U:380:THR:HG23	1:U:382:SER:H	1.70	0.56
2:V:67:LEU:HD11	2:V:205:LEU:HB3	1.86	0.56
5:Y:330:ILE:HA	5:Y:333:GLU:HB3	1.86	0.56
20:O:163:ILE:HG12	20:O:169:SER:H	1.70	0.56
25:T:145:LEU:HB3	25:T:179:ARG:HH21	1.71	0.56
32:f:684:PRO:O	32:f:688:ARG:CB	2.54	0.56
3:W:359:VAL:HG21	3:W:392:PHE:HB3	1.87	0.56
15:J:4:ASP:O	15:J:18:GLN:NE2	2.39	0.56
29:D:201:GLY:HA2	29:D:306:LYS:HA	1.87	0.56
7:a:252:LYS:HD2	7:a:255:TRP:HB2	1.88	0.56
28:C:221:GLN:HB3	29:D:240:LEU:HB3	1.87	0.56
32:f:226:TYR:O	32:f:230:CYS:CB	2.53	0.56
32:f:536:SER:O	32:f:540:GLN:HB2	2.05	0.56
32:f:623:LYS:O	32:f:627:GLU:CB	2.54	0.56
8:b:34:ASN:O	8:b:38:HIS:ND1	2.32	0.55
16:K:100:TRP:O	23:R:57:ARG:NH2	2.39	0.55
19:N:19:ARG:NH1	19:N:170:SER:O	2.40	0.55
20:O:96:ALA:H	20:O:115:PRO:HB3	1.71	0.55
20:o:163:ILE:HG12	20:o:169:SER:H	1.69	0.55
26:A:116:LYS:HE3	27:B:128:GLY:HA3	1.88	0.55
28:C:339:THR:HG21	28:C:379:THR:HG22	1.88	0.55
30:E:304:PRO:O	30:E:309:ARG:NH1	2.39	0.55
32:f:742:ALA:CA	32:f:745:LEU:HD21	2.32	0.55
2:V:255:LEU:HD22	2:V:291:TYR:HB3	1.87	0.55
5:Y:26:LEU:HD11	5:Y:60:SER:HB2	1.87	0.55
16:k:206:MET:HE1	16:k:210:LEU:HD13	1.87	0.55
17:l:26:MET:HE1	17:l:148:CYS:HB2	1.88	0.55
5:Y:157:ILE:HD12	5:Y:158:THR:HG23	1.87	0.55
8:b:39:SER:O	8:b:43:SER:HB2	2.05	0.55
16:K:37:ALA:HB2	16:K:50:VAL:HG23	1.87	0.55
21:P:15:LYS:HE3	21:P:121:ILE:HG12	1.88	0.55
21:p:107:PRO:HG2	21:p:124:LEU:HB2	1.87	0.55
32:f:780:PRO:HB2	32:f:800:LEU:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:220:LEU:HD11	1:U:252:LEU:HD13	1.88	0.55
1:U:655:ALA:O	1:U:659:CYS:HB3	2.06	0.55
2:V:88:GLY:HA3	2:V:118:GLN:HE21	1.70	0.55
2:V:440:LYS:NZ	10:d:143:LEU:O	2.39	0.55
2:V:462:GLU:HG3	5:Y:346:LYS:HD2	1.88	0.55
6:Z:56:VAL:HG13	6:Z:58:PHE:HB2	1.88	0.55
1:U:571:CYS:HA	1:U:579:ARG:HG2	1.88	0.55
6:Z:16:LEU:HD21	9:c:216:MET:HE2	1.89	0.55
27:B:125:THR:OG1	27:B:126:SER:N	2.37	0.55
29:D:248:ARG:NH2	29:D:291:GLU:OE1	2.40	0.55
30:E:60:VAL:HA	30:E:71:VAL:HG12	1.87	0.55
32:f:301:HIS:O	32:f:305:LEU:CB	2.53	0.55
16:K:221:GLN:HB2	16:K:224:GLN:HB3	1.88	0.55
29:D:200:ARG:NH2	29:D:303:VAL:O	2.36	0.55
32:f:347:ASP:O	32:f:351:THR:OG1	2.25	0.55
32:f:438:ASP:N	32:f:438:ASP:OD1	2.35	0.55
32:f:586:PRO:HA	32:f:589:SER:HB2	1.89	0.55
2:V:495:ARG:HD2	28:C:42:LEU:HB3	1.87	0.55
13:H:34:PRO:HA	13:H:164:GLY:HA3	1.88	0.55
12:G:70:PHE:HD2	12:G:91:VAL:HG21	1.70	0.55
14:I:38:LEU:HG	14:I:160:LYS:HB3	1.87	0.55
14:I:239:LYS:NZ	14:I:243:GLU:OE2	2.40	0.55
17:L:72:ILE:HG22	17:L:134:ILE:HG12	1.89	0.55
32:f:80:ARG:O	32:f:84:SER:HB3	2.07	0.55
6:Z:70:LEU:HD12	6:Z:111:LEU:HD13	1.88	0.55
18:M:51:LYS:O	18:M:210:GLU:N	2.37	0.55
24:S:73:LYS:O	24:S:77:HIS:ND1	2.36	0.55
15:j:131:ALA:N	15:j:147:THR:OG1	2.35	0.55
16:k:97:GLN:HG3	23:r:61:ARG:HG3	1.87	0.55
32:f:742:ALA:HA	32:f:745:LEU:HG	1.88	0.55
1:U:710:ARG:HG2	1:U:737:LEU:HD21	1.89	0.55
3:W:423:ASN:O	3:W:425:LEU:N	2.40	0.55
3:W:445:LEU:HD11	6:Z:230:LEU:HD21	1.87	0.55
21:P:29:GLY:HA3	21:P:34:MET:HA	1.89	0.55
18:m:235:ALA:O	18:m:239:ALA:N	2.38	0.55
31:F:194:GLN:O	31:F:198:LEU:HB2	2.07	0.55
32:f:688:ARG:HH12	32:f:788:MET:HA	1.71	0.55
13:H:222:THR:OG1	13:H:225:GLU:OE1	2.22	0.54
13:h:66:GLU:OE2	13:h:91:ARG:NH2	2.40	0.54
29:D:249:ASP:OD1	29:D:252:ARG:NH2	2.39	0.54
29:D:251:PHE:HE2	29:D:295:GLN:HB3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:338:ARG:O	29:D:339:ARG:CG	2.54	0.54
32:f:278:VAL:HA	32:f:281:ILE:HG22	1.89	0.54
1:U:68:PHE:HB3	1:U:73:ALA:HB3	1.88	0.54
19:n:21:THR:HG22	19:n:26:ILE:HG13	1.89	0.54
23:r:38:ASN:HD22	23:r:41:LEU:HD12	1.71	0.54
27:B:186:ASP:OD1	27:B:186:ASP:N	2.39	0.54
32:f:229:VAL:O	32:f:233:LEU:HB2	2.07	0.54
6:Z:106:ILE:HA	6:Z:155:PHE:HE2	1.73	0.54
8:b:138:VAL:HB	8:b:160:LEU:HD11	1.89	0.54
32:f:8:LYS:O	32:f:12:GLN:HB2	2.08	0.54
32:f:15:GLN:NE2	32:f:47:GLU:OE1	2.41	0.54
32:f:253:LEU:O	32:f:257:ARG:HB2	2.07	0.54
32:f:313:GLU:O	32:f:317:LEU:CB	2.55	0.54
1:U:241:ASN:HD22	1:U:244:MET:HE3	1.72	0.54
2:V:89:LYS:HD2	2:V:118:GLN:HE22	1.72	0.54
2:V:95:LEU:O	2:V:111:TYR:OH	2.23	0.54
4:X:395:LYS:HA	9:c:257:LYS:HE2	1.89	0.54
9:c:282:ARG:HG3	9:c:284:LEU:HD13	1.89	0.54
19:N:29:ARG:NH1	20:O:139:GLU:OE1	2.33	0.54
26:A:188:ARG:O	26:A:192:GLU:HB3	2.08	0.54
32:f:426:LEU:O	32:f:430:ASP:HB3	2.07	0.54
32:f:575:ALA:O	32:f:579:ALA:HB2	2.07	0.54
1:U:741:GLY:O	1:U:883:ARG:NH2	2.40	0.54
1:U:898:CYS:SG	1:U:899:ARG:N	2.81	0.54
12:g:161:CYS:SG	12:g:162:GLY:N	2.80	0.54
17:l:50:LYS:HB3	17:l:59:HIS:HB3	1.90	0.54
21:p:194:LYS:NZ	21:p:196:THR:OG1	2.41	0.54
29:D:269:ALA:HB3	30:E:258:MET:HE1	1.90	0.54
32:f:138:GLU:O	32:f:142:TYR:CB	2.55	0.54
32:f:780:PRO:CB	32:f:800:LEU:CA	2.79	0.54
3:W:273:TYR:HA	3:W:276:LEU:HD13	1.89	0.54
8:b:150:THR:HG1	8:b:154:THR:HG1	1.55	0.54
10:d:49:ILE:HD12	10:d:52:ARG:HH11	1.72	0.54
13:H:66:GLU:OE2	13:H:91:ARG:NH2	2.41	0.54
24:S:148:LEU:HD23	24:S:178:VAL:HG12	1.88	0.54
17:l:109:VAL:HG21	17:l:145:PHE:HD2	1.73	0.54
24:s:123:SER:HB3	24:s:136:LYS:HG3	1.89	0.54
28:C:114:VAL:HA	28:C:126:ILE:HA	1.89	0.54
32:f:377:VAL:HG22	32:f:751:TYR:HB2	1.88	0.54
2:V:30:PRO:HA	2:V:33:GLN:HB2	1.90	0.54
3:W:83:LEU:HG	3:W:88:MET:HE1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:H:93:LEU:HD11	13:H:113:ARG:HB3	1.88	0.54
14:I:10:THR:HG22	14:I:11:ILE:HG13	1.90	0.54
18:M:235:ALA:O	18:M:239:ALA:N	2.38	0.54
21:p:190:ILE:HG22	21:p:195:ILE:HG23	1.88	0.54
27:B:259:TYR:HB2	27:B:262:ASP:HB2	1.90	0.54
27:B:404:LEU:O	27:B:408:ARG:HB2	2.07	0.54
32:f:88:SER:HB2	32:f:92:VAL:CG2	2.33	0.54
32:f:273:ASN:ND2	32:f:310:ASP:OD2	2.41	0.54
9:c:159:ALA:HB3	9:c:205:ILE:HD11	1.88	0.54
18:M:180:GLN:HB3	18:M:184:MET:HE3	1.89	0.54
22:Q:4:LEU:HD22	22:Q:17:SER:HB2	1.90	0.54
14:i:239:LYS:NZ	14:i:243:GLU:OE2	2.41	0.54
26:A:265:ARG:NH2	26:A:310:ASP:O	2.41	0.54
32:f:635:LYS:NZ	32:f:641:GLU:HG3	2.16	0.54
1:U:140:ARG:O	1:U:144:ASP:HB2	2.08	0.54
1:U:490:ARG:HB2	1:U:493:VAL:HG12	1.90	0.54
2:V:250:LEU:HA	2:V:253:LEU:HD12	1.89	0.54
6:Z:106:ILE:HD11	6:Z:153:LYS:HB3	1.90	0.54
8:b:26:LEU:O	8:b:30:GLN:HB2	2.06	0.54
17:L:46:LEU:HD13	17:L:73:SER:HB2	1.88	0.54
31:F:240:CYS:O	31:F:244:THR:OG1	2.26	0.54
32:f:8:LYS:O	32:f:12:GLN:CB	2.56	0.54
32:f:477:MET:O	32:f:481:SER:CB	2.56	0.54
1:U:446:LEU:O	1:U:450:HIS:ND1	2.33	0.54
3:W:282:GLU:O	3:W:286:LEU:CB	2.56	0.54
9:c:126:ASP:HA	9:c:129:THR:HG22	1.90	0.54
14:I:171:ALA:HB2	14:I:200:THR:HG21	1.90	0.54
14:I:219:GLU:OE2	14:I:220:ASN:ND2	2.41	0.54
15:J:172:LEU:O	15:J:176:TYR:HB2	2.08	0.54
18:M:163:CYS:SG	18:M:164:ALA:N	2.81	0.54
22:Q:181:ARG:NH1	22:Q:190:ASP:OD1	2.40	0.54
17:l:45:VAL:HG11	17:l:188:VAL:HG22	1.89	0.54
29:D:268:ASP:OD2	30:E:242:ARG:NH1	2.41	0.54
29:D:391:ARG:HG2	29:D:393:ILE:H	1.73	0.54
31:F:417:HIS:HA	31:F:420:TYR:HD2	1.73	0.54
2:V:224:LEU:HB2	2:V:227:VAL:HB	1.90	0.53
5:Y:145:LEU:HD23	5:Y:157:ILE:HG22	1.90	0.53
6:Z:201:LEU:HD22	7:a:357:CYS:HA	1.89	0.53
16:K:125:GLU:HG3	16:K:134:SER:HB2	1.89	0.53
12:g:141:ILE:HG22	12:g:151:VAL:HG22	1.90	0.53
30:E:345:ASN:HB2	31:F:345:SER:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:191:LEU:HD12	31:F:235:LEU:HD21	1.90	0.53
31:F:339:ASP:H	31:F:342:LEU:HD12	1.73	0.53
32:f:229:VAL:O	32:f:233:LEU:CB	2.56	0.53
1:U:645:ASN:OD1	1:U:645:ASN:N	2.41	0.53
8:b:97:LEU:HA	8:b:100:ARG:HG3	1.90	0.53
10:d:35:PHE:HD1	10:d:48:LEU:HD13	1.73	0.53
11:e:61:GLU:O	11:e:65:TYR:N	2.37	0.53
22:Q:19:ARG:HH21	22:Q:31:ASP:HB2	1.73	0.53
21:p:189:ILE:HG23	21:p:196:THR:HB	1.89	0.53
26:A:123:VAL:HA	31:F:87:PRO:HB3	1.91	0.53
26:A:347:ASP:O	26:A:351:ARG:NH2	2.41	0.53
27:B:410:ARG:HH22	28:C:174:LEU:HD22	1.72	0.53
32:f:262:PHE:HB3	32:f:281:ILE:HD11	1.91	0.53
32:f:600:TYR:HB3	32:f:608:LYS:HE2	1.91	0.53
5:Y:373:GLY:HA2	5:Y:376:LEU:HB3	1.90	0.53
8:b:24:THR:HG22	8:b:26:LEU:H	1.73	0.53
29:D:380:GLN:HB3	30:E:167:PRO:HG3	1.89	0.53
31:F:73:ILE:O	31:F:77:SER:CB	2.57	0.53
2:V:404:LYS:HA	2:V:407:VAL:HG12	1.90	0.53
3:W:397:VAL:HG22	4:X:341:PRO:HB2	1.88	0.53
7:a:78:GLU:O	7:a:82:HIS:ND1	2.33	0.53
15:J:74:ALA:HB2	15:J:161:ILE:HD13	1.90	0.53
26:A:140:VAL:HG12	26:A:152:PRO:HB3	1.89	0.53
27:B:170:LEU:HD22	27:B:254:GLU:HB3	1.90	0.53
3:W:409:LEU:HB3	4:X:384:VAL:HG21	1.90	0.53
9:c:58:LEU:HA	9:c:108:VAL:HA	1.89	0.53
25:T:99:ARG:HG2	25:T:106:LEU:HG	1.90	0.53
17:l:120:THR:O	18:m:129:ARG:NH1	2.37	0.53
25:t:15:LYS:HG2	25:t:20:VAL:HG22	1.91	0.53
28:C:133:PRO:O	28:C:136:SER:OG	2.25	0.53
29:D:170:MET:HB3	29:D:174:LYS:HG3	1.89	0.53
32:f:688:ARG:HA	32:f:745:LEU:CD2	2.38	0.53
9:c:36:LEU:HD11	9:c:71:ASP:HA	1.89	0.53
14:I:62:SER:OG	14:I:65:ILE:O	2.26	0.53
17:L:189:LYS:HA	17:L:192:LEU:HG	1.91	0.53
30:E:146:ARG:NH1	30:E:150:GLU:OE1	2.41	0.53
32:f:76:GLU:OE1	32:f:79:ARG:NH2	2.41	0.53
32:f:281:ILE:O	32:f:285:CYS:CB	2.56	0.53
32:f:515:ALA:HB1	32:f:558:LEU:HD21	1.91	0.53
9:c:98:MET:HA	9:c:101:GLN:HG2	1.90	0.53
9:c:190:GLN:HB2	9:c:193:ILE:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:231:GLY:HA2	34:B:501:AGS:H5'2	1.91	0.53
27:B:420:LYS:HD2	27:B:423:LYS:HE3	1.90	0.53
31:F:235:LEU:CD1	31:F:236:LEU:HG	2.39	0.53
32:f:378:ASN:HB3	32:f:391:LEU:CD1	2.39	0.53
2:V:252:ASN:ND2	2:V:284:GLU:OE2	2.42	0.53
5:Y:107:LYS:HA	5:Y:110:TYR:HB3	1.91	0.53
5:Y:237:ARG:O	5:Y:241:ILE:HB	2.09	0.53
6:Z:12:HIS:HB3	6:Z:14:LEU:HD13	1.91	0.53
15:J:11:SER:OG	15:J:15:HIS:N	2.36	0.53
15:J:181:ILE:H	15:J:182:GLU:HA	1.73	0.53
20:O:50:ALA:HB2	21:P:129:CYS:HB2	1.91	0.53
21:P:45:MET:HE3	21:P:71:LEU:HD22	1.91	0.53
21:P:189:ILE:HG23	21:P:196:THR:HB	1.91	0.53
23:R:125:THR:OG1	22:q:170:ARG:NH2	2.42	0.53
29:D:264:ILE:HB	29:D:307:VAL:HG13	1.90	0.53
31:F:394:ALA:HB2	34:F:501:AGS:H4'	1.90	0.53
32:f:714:SER:C	32:f:718:ASP:HB2	2.33	0.53
1:U:904:LYS:HB3	1:U:913:ILE:HG12	1.91	0.53
2:V:195:ILE:HG21	28:C:28:ILE:HG12	1.90	0.53
7:a:84:VAL:HA	7:a:87:MET:HB2	1.91	0.53
14:i:154:GLY:O	15:j:81:ARG:NH1	2.42	0.53
28:C:192:PRO:O	29:D:323:ARG:NH2	2.41	0.53
32:f:663:GLY:O	32:f:697:ILE:HB	2.07	0.53
2:V:117:VAL:HA	2:V:121:PHE:HB2	1.91	0.53
6:Z:266:ILE:HG23	9:c:291:LEU:HD13	1.91	0.53
9:c:150:SER:OG	29:D:81:ARG:NH1	2.42	0.53
12:G:123:GLN:NE2	13:H:82:ASP:OD1	2.42	0.53
12:g:54:LYS:NZ	12:g:213:SER:O	2.37	0.53
27:B:390:LEU:HD13	27:B:395:ILE:HD11	1.90	0.53
28:C:88:LYS:HE2	28:C:93:GLY:HA2	1.90	0.53
30:E:320:ILE:HG23	30:E:362:VAL:HG21	1.91	0.53
32:f:314:TYR:CE1	32:f:490:ALA:HB3	2.43	0.53
2:V:37:MET:HE1	2:V:108:LEU:HD22	1.90	0.52
3:W:143:ALA:HA	3:W:146:THR:HG22	1.90	0.52
3:W:428:TRP:O	3:W:432:LEU:HB2	2.09	0.52
11:e:59:GLU:O	11:e:61:GLU:N	2.33	0.52
18:M:214:SER:OG	18:M:224:HIS:NE2	2.40	0.52
17:l:201:ALA:O	17:l:239:ARG:NH1	2.42	0.52
28:C:229:ARG:HG3	28:C:230:MET:HG2	1.90	0.52
31:F:90:VAL:HB	31:F:164:LEU:HD11	1.90	0.52
3:W:16:MET:HE1	3:W:24:VAL:HG22	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:193:ILE:HA	9:c:196:LEU:HB2	1.91	0.52
9:c:210:ASN:O	9:c:214:GLN:N	2.31	0.52
10:d:114:GLU:HA	10:d:117:THR:HG22	1.90	0.52
10:d:192:THR:OG1	10:d:196:ARG:NH1	2.43	0.52
15:J:72:ALA:HB3	15:J:132:LEU:HB2	1.92	0.52
24:s:35:ILE:HB	25:t:151:ARG:HH12	1.74	0.52
32:f:80:ARG:O	32:f:84:SER:CB	2.57	0.52
32:f:403:LYS:O	32:f:407:MET:N	2.40	0.52
1:U:83:GLY:HA2	1:U:129:ARG:HH21	1.72	0.52
13:H:50:LYS:NZ	13:H:62:VAL:O	2.42	0.52
23:r:97:MET:HB3	23:r:116:SER:HB3	1.91	0.52
30:E:157:GLU:O	30:E:161:ARG:N	2.43	0.52
32:f:306:GLU:HB3	32:f:339:ILE:HD12	1.91	0.52
1:U:155:LEU:O	1:U:158:ARG:NH1	2.40	0.52
7:a:172:TYR:HE2	7:a:200:LEU:HA	1.74	0.52
7:a:270:ARG:NH1	7:a:310:LEU:O	2.43	0.52
9:c:56:LEU:HA	9:c:111:TRP:HA	1.90	0.52
16:k:77:ALA:HB3	16:k:142:LEU:HB2	1.91	0.52
20:o:37:ILE:HD13	20:o:60:SER:HB2	1.91	0.52
29:D:206:GLY:CA	29:D:335:LEU:HD11	2.38	0.52
29:D:319:PRO:O	29:D:323:ARG:NH2	2.37	0.52
32:f:24:THR:HG22	32:f:71:TYR:HB2	1.91	0.52
2:V:349:ARG:HB3	11:e:43:TRP:HZ2	1.73	0.52
4:X:218:HIS:HA	4:X:221:GLU:HB2	1.91	0.52
5:Y:141:VAL:HG21	5:Y:164:ALA:HB2	1.90	0.52
21:P:159:ASP:N	21:P:159:ASP:OD1	2.41	0.52
32:f:343:LYS:HZ2	32:f:804:LEU:HD23	1.74	0.52
32:f:366:ASP:O	32:f:367:SER:CB	2.57	0.52
32:f:537:THR:OG1	32:f:538:ILE:N	2.42	0.52
2:V:131:LEU:HD23	2:V:134:PHE:HD2	1.75	0.52
6:Z:84:LYS:HG2	9:c:76:PRO:HB3	1.90	0.52
15:J:68:ASN:HA	15:J:211:MET:HE1	1.91	0.52
23:R:196:HIS:O	23:R:200:SER:HB3	2.10	0.52
26:A:287:ASP:HA	31:F:267:LEU:HB2	1.90	0.52
27:B:151:LEU:HB2	27:B:161:GLY:H	1.74	0.52
1:U:428:PRO:HB3	1:U:443:LEU:HD11	1.90	0.52
1:U:629:THR:OG1	29:D:50:GLU:OE2	2.28	0.52
1:U:762:GLY:O	1:U:766:PHE:HB2	2.10	0.52
2:V:407:VAL:O	2:V:411:SER:OG	2.27	0.52
3:W:152:ILE:HG12	3:W:161:GLU:HB3	1.90	0.52
3:W:282:GLU:O	3:W:286:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:414:LEU:HD23	4:X:417:LYS:HD2	1.91	0.52
5:Y:102:ASP:HA	5:Y:105:MET:HG2	1.91	0.52
6:Z:145:HIS:HB3	6:Z:147:ASP:H	1.75	0.52
18:M:170:GLN:HA	18:M:173:LYS:HE2	1.90	0.52
20:O:18:THR:HB	20:O:31:CYS:H	1.75	0.52
25:T:54:SER:HB3	25:T:109:THR:HB	1.92	0.52
21:p:29:GLY:HA3	21:p:34:MET:HA	1.92	0.52
26:A:347:ASP:OD1	26:A:347:ASP:N	2.43	0.52
29:D:328:ASP:O	29:D:329:ARG:NE	2.43	0.52
31:F:234:THR:OG1	34:F:501:AGS:O2A	2.24	0.52
14:i:126:GLY:HA3	15:j:3:TYR:HE2	1.74	0.52
23:r:12:VAL:HB	23:r:179:VAL:HB	1.92	0.52
25:t:27:LEU:HD11	25:t:34:ALA:HB1	1.90	0.52
32:f:468:ASP:OD2	32:f:475:ASN:N	2.42	0.52
1:U:377:HIS:HB3	1:U:380:THR:HB	1.92	0.52
2:V:47:SER:HA	2:V:50:GLU:HB2	1.90	0.52
3:W:440:ASN:O	3:W:444:HIS:ND1	2.42	0.52
7:a:325:ASP:HB3	7:a:330:ARG:HB2	1.92	0.52
9:c:100:LYS:HG2	9:c:105:PRO:HB3	1.92	0.52
14:I:47:ALA:HB3	14:I:212:GLU:HB3	1.92	0.52
16:k:203:LYS:HA	16:k:206:MET:HG2	1.91	0.52
27:B:284:ILE:HB	27:B:329:MET:HG2	1.91	0.52
32:f:502:LEU:HG	32:f:540:GLN:HE22	1.75	0.52
2:V:148:ARG:NH1	2:V:192:MET:O	2.43	0.52
3:W:407:ASP:HB2	4:X:344:ARG:HG3	1.92	0.52
8:b:26:LEU:O	8:b:30:GLN:CB	2.58	0.52
8:b:181:ASP:O	8:b:185:SER:HB2	2.09	0.52
16:K:228:MET:N	16:K:228:MET:SD	2.83	0.52
15:j:131:ALA:N	15:j:147:THR:HG1	2.07	0.52
26:A:177:VAL:HG22	26:A:228:ALA:HB1	1.92	0.52
27:B:279:PRO:HD3	32:f:718:ASP:CG	2.31	0.52
31:F:188:ILE:HG12	31:F:235:LEU:HD13	1.92	0.52
32:f:127:SER:O	32:f:131:MET:HB3	2.10	0.52
32:f:440:ILE:O	32:f:444:ALA:HB2	2.10	0.52
19:N:144:ARG:H	19:N:147:MET:HE3	1.74	0.51
13:h:71:HIS:HA	13:h:218:PHE:H	1.75	0.51
23:r:97:MET:O	23:r:116:SER:N	2.41	0.51
26:A:278:ASP:OD1	26:A:326:THR:OG1	2.27	0.51
32:f:268:LEU:O	32:f:272:LEU:HB2	2.10	0.51
32:f:463:LEU:HD22	32:f:466:LEU:CD1	2.40	0.51
32:f:790:GLN:HG3	32:f:792:ALA:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:5:GLY:HA3	3:W:47:LEU:HD13	1.91	0.51
9:c:211:GLU:O	9:c:215:LYS:CB	2.58	0.51
19:N:21:THR:HG22	19:N:26:ILE:HG13	1.91	0.51
14:i:140:ASP:OD1	14:i:144:GLY:N	2.40	0.51
17:l:5:GLN:O	17:l:8:ASN:ND2	2.43	0.51
24:s:209:SER:OG	24:s:212:LYS:NZ	2.44	0.51
31:F:363:ALA:HB1	31:F:381:TYR:HB3	1.91	0.51
32:f:389:LYS:HD2	32:f:418:LEU:HD21	1.92	0.51
4:X:192:SER:O	4:X:196:THR:HB	2.09	0.51
6:Z:12:HIS:NE2	6:Z:165:GLU:OE1	2.38	0.51
9:c:234:TYR:HA	9:c:304:LEU:HD13	1.93	0.51
24:s:5:TYR:OH	24:s:103:PRO:O	2.22	0.51
27:B:416:ASN:HA	27:B:419:PHE:HD2	1.75	0.51
29:D:267:ILE:HB	29:D:309:MET:HB3	1.93	0.51
32:f:485:LEU:HD12	32:f:488:ALA:HB3	1.92	0.51
32:f:556:ARG:NH1	32:f:786:GLN:OE1	2.44	0.51
32:f:800:LEU:N	32:f:800:LEU:CD1	2.73	0.51
3:W:27:ARG:NH1	3:W:54:THR:OG1	2.44	0.51
3:W:344:THR:O	3:W:348:GLU:HB3	2.10	0.51
3:W:452:ILE:HD12	6:Z:214:LYS:HG3	1.92	0.51
6:Z:141:VAL:HG21	6:Z:156:GLU:HG2	1.92	0.51
8:b:132:LYS:NZ	8:b:161:ASN:O	2.43	0.51
13:h:107:THR:HA	13:h:110:LEU:HD13	1.93	0.51
30:E:61:LEU:HD11	30:E:72:LYS:HB2	1.93	0.51
31:F:82:VAL:HA	31:F:85:THR:HG23	1.92	0.51
32:f:336:GLU:CG	32:f:337:LEU:HD22	2.36	0.51
32:f:612:LEU:O	32:f:616:CYS:CB	2.56	0.51
1:U:105:ILE:HB	28:C:25:LEU:HD11	1.93	0.51
3:W:373:ILE:HG22	3:W:414:ASN:HB3	1.92	0.51
7:a:373:ASP:HB2	10:d:251:ARG:HH22	1.75	0.51
12:G:84:THR:HB	18:M:156:VAL:HG22	1.91	0.51
17:L:215:VAL:HB	17:L:221:PHE:HD1	1.76	0.51
18:M:76:ALA:HB3	18:M:136:MET:HB2	1.92	0.51
25:T:209:TRP:HB2	19:n:190:LEU:HD22	1.93	0.51
32:f:632:LYS:HD2	32:f:661:ALA:HA	1.92	0.51
2:V:354:LYS:HA	2:V:357:LEU:HG	1.93	0.51
7:a:146:PRO:O	7:a:149:THR:OG1	2.26	0.51
9:c:282:ARG:HE	9:c:284:LEU:HD22	1.75	0.51
10:d:175:ARG:HH12	10:d:200:PHE:HD2	1.59	0.51
16:K:70:ILE:HD11	16:K:89:ILE:HD12	1.93	0.51
18:M:37:ILE:HD11	18:M:193:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:k:37:ALA:HB2	16:k:50:VAL:HG23	1.92	0.51
19:n:178:ALA:HB3	19:n:185:GLU:HB2	1.92	0.51
26:A:160:THR:HG23	26:A:247:GLN:HG3	1.92	0.51
29:D:173:GLN:NE2	29:D:334:PRO:O	2.43	0.51
32:f:647:GLY:HA2	32:f:655:LEU:HG	1.93	0.51
2:V:167:LEU:HG	2:V:171:VAL:HG11	1.92	0.51
2:V:171:VAL:HG13	2:V:172:VAL:HG23	1.93	0.51
4:X:401:LEU:HD23	4:X:404:ILE:HD12	1.92	0.51
5:Y:215:ASP:O	5:Y:218:THR:OG1	2.28	0.51
18:M:27:MET:HA	18:M:153:PRO:HG2	1.92	0.51
12:g:89:SER:OG	18:m:117:MET:SD	2.67	0.51
17:l:189:LYS:HZ3	17:l:193:ARG:HH22	1.59	0.51
31:F:397:LYS:HE3	31:F:401:VAL:HG21	1.92	0.51
3:W:405:LYS:HA	4:X:342:PHE:HB2	1.93	0.51
18:m:214:SER:OG	18:m:224:HIS:NE2	2.36	0.51
29:D:270:ILE:HG22	29:D:288:ILE:HG21	1.92	0.51
32:f:692:LEU:HD12	32:f:748:LEU:HD23	1.84	0.51
5:Y:36:ALA:O	5:Y:40:GLU:CB	2.59	0.51
5:Y:293:ARG:NH1	11:e:49:GLU:OE2	2.44	0.51
6:Z:9:VAL:HG12	6:Z:48:LEU:HB3	1.92	0.51
29:D:412:GLN:N	29:D:413:GLU:O	2.43	0.51
32:f:336:GLU:HG3	32:f:337:LEU:H	1.76	0.51
32:f:337:LEU:N	32:f:337:LEU:CD2	2.73	0.51
32:f:343:LYS:NZ	32:f:804:LEU:HD23	2.26	0.51
32:f:531:ASN:HA	32:f:569:LYS:HA	1.93	0.51
1:U:54:PHE:HE2	1:U:60:ALA:HB2	1.76	0.51
2:V:80:LYS:HE2	2:V:88:GLY:H	1.75	0.51
6:Z:39:LEU:H	6:Z:94:TRP:HA	1.75	0.51
20:O:35:HIS:NE2	20:O:53:ASP:OD1	2.44	0.51
23:R:18:SER:OG	23:R:173:ALA:N	2.44	0.51
12:g:84:THR:HB	18:m:156:VAL:HG22	1.92	0.51
19:n:144:ARG:H	19:n:147:MET:HE3	1.76	0.51
30:E:84:ARG:O	30:E:85:ARG:NE	2.39	0.51
30:E:262:ASN:O	30:E:266:GLY:N	2.44	0.51
32:f:479:LEU:HA	32:f:517:VAL:HG21	1.93	0.51
32:f:635:LYS:NZ	32:f:641:GLU:CD	2.66	0.51
1:U:638:SER:O	1:U:641:SER:OG	2.25	0.50
3:W:254:PRO:HB2	3:W:263:TRP:HD1	1.75	0.50
5:Y:271:PHE:O	5:Y:275:LEU:CB	2.59	0.50
8:b:124:LEU:HD22	8:b:152:LYS:HA	1.94	0.50
9:c:250:GLU:HA	9:c:253:LYS:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:P:2:SER:OG	21:P:3:ILE:N	2.44	0.50
24:S:28:ARG:NH2	24:S:213:ASP:O	2.44	0.50
14:i:90:LEU:HD12	14:i:114:LEU:HD22	1.92	0.50
23:r:196:HIS:O	23:r:200:SER:HB3	2.10	0.50
26:A:87:LEU:HD11	27:B:137:SER:H	1.77	0.50
26:A:395:PHE:HA	26:A:398:ARG:HD2	1.94	0.50
27:B:106:PRO:HD3	28:C:120:SER:HB3	1.93	0.50
29:D:207:PRO:HD2	29:D:335:LEU:HD11	1.92	0.50
32:f:337:LEU:HD22	32:f:337:LEU:H	1.75	0.50
32:f:380:PHE:CG	32:f:751:TYR:CE2	2.99	0.50
32:f:523:GLY:O	32:f:527:VAL:N	2.43	0.50
2:V:32:PRO:HA	2:V:35:VAL:HG22	1.92	0.50
3:W:108:CYS:HA	3:W:111:TYR:HB2	1.92	0.50
3:W:152:ILE:HA	3:W:161:GLU:HG3	1.93	0.50
5:Y:194:PHE:HB3	5:Y:230:ALA:HB2	1.93	0.50
8:b:137:ASN:OD1	8:b:161:ASN:ND2	2.38	0.50
12:G:41:ALA:HB3	12:G:166:THR:HB	1.94	0.50
21:P:205:ASP:O	23:r:19:ARG:NH1	2.39	0.50
1:U:379:GLY:HA2	1:U:412:HIS:HA	1.93	0.50
3:W:371:THR:OG1	3:W:416:GLN:NE2	2.44	0.50
3:W:443:THR:HG22	9:c:229:LEU:HD13	1.94	0.50
8:b:26:LEU:HD11	8:b:80:PRO:HG3	1.92	0.50
14:i:123:GLN:NE2	15:j:79:ASP:OD1	2.44	0.50
17:l:41:LYS:NZ	17:l:180:MET:O	2.44	0.50
24:s:4:PRO:O	25:t:100:ARG:NH2	2.44	0.50
28:C:307:ARG:HB3	28:C:310:ARG:HG3	1.92	0.50
30:E:327:ASP:H	30:E:364:GLN:HG3	1.75	0.50
32:f:455:VAL:HG12	32:f:457:ASN:H	1.76	0.50
1:U:194:ARG:O	1:U:198:LEU:HB2	2.11	0.50
1:U:486:MET:HE1	1:U:758:PRO:HB3	1.94	0.50
5:Y:210:SER:HB3	5:Y:212:GLU:HG2	1.94	0.50
7:a:254:ALA:HA	7:a:261:LEU:HD21	1.92	0.50
17:L:109:VAL:HG21	17:L:145:PHE:HD2	1.75	0.50
17:l:189:LYS:HA	17:l:192:LEU:HG	1.94	0.50
23:r:35:ILE:N	23:r:43:GLY:O	2.45	0.50
27:B:315:GLN:NE2	27:B:320:ASP:OD2	2.44	0.50
28:C:69:GLN:NE2	28:C:118:ASN:OD1	2.39	0.50
28:C:224:ILE:HG22	28:C:268:GLU:HG3	1.93	0.50
32:f:226:TYR:O	32:f:230:CYS:HB2	2.11	0.50
32:f:392:THR:HG22	32:f:417:ILE:HD13	1.92	0.50
32:f:671:ALA:O	32:f:674:THR:OG1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:714:SER:O	32:f:718:ASP:CB	2.55	0.50
32:f:745:LEU:HD12	32:f:745:LEU:C	2.36	0.50
1:U:423:MET:HB3	1:U:426:TYR:HB2	1.94	0.50
2:V:416:ARG:HG3	2:V:459:GLN:HA	1.92	0.50
3:W:268:LYS:HA	3:W:271:VAL:HG12	1.94	0.50
5:Y:316:LEU:HD13	5:Y:327:VAL:HG22	1.94	0.50
12:g:212:PRO:HB3	12:g:235:ILE:HG22	1.94	0.50
27:B:168:ASP:N	27:B:168:ASP:OD1	2.44	0.50
32:f:392:THR:CG2	32:f:417:ILE:HD13	2.42	0.50
32:f:517:VAL:O	32:f:521:ALA:CB	2.60	0.50
5:Y:315:THR:OG1	5:Y:316:LEU:N	2.43	0.50
7:a:18:GLN:NE2	7:a:47:ASP:OD2	2.41	0.50
29:D:202:VAL:HG23	29:D:331:ILE:H	1.75	0.50
32:f:211:ILE:O	32:f:215:ASP:CB	2.56	0.50
32:f:358:PHE:HZ	32:f:381:VAL:HG21	1.66	0.50
32:f:691:PRO:HA	32:f:694:LEU:HB3	1.93	0.50
1:U:208:LEU:HD23	1:U:210:LYS:H	1.77	0.50
2:V:459:GLN:HE21	10:d:187:GLU:HG3	1.76	0.50
9:c:32:TYR:HE1	9:c:206:ASN:HD21	1.59	0.50
9:c:227:GLU:HB2	9:c:230:THR:HA	1.93	0.50
14:i:119:GLN:HE21	14:i:123:GLN:HE22	1.59	0.50
22:q:88:LEU:HB3	22:q:122:ALA:HB2	1.94	0.50
31:F:209:LYS:HA	31:F:212:PHE:HD2	1.77	0.50
2:V:147:PHE:HB3	2:V:149:PRO:HD2	1.94	0.50
4:X:356:LEU:HD13	4:X:359:ALA:HB3	1.92	0.50
7:a:342:ASP:O	7:a:346:ILE:N	2.44	0.50
8:b:31:ASP:HA	8:b:34:ASN:HD22	1.76	0.50
17:L:50:LYS:HB3	17:L:59:HIS:HB3	1.94	0.50
14:i:25:MET:HA	14:i:28:ILE:HD12	1.93	0.50
28:C:148:TYR:HE1	28:C:203:VAL:HA	1.77	0.50
32:f:336:GLU:HG3	32:f:337:LEU:CD2	2.38	0.50
5:Y:232:GLU:O	5:Y:236:LEU:N	2.45	0.50
8:b:97:LEU:O	8:b:100:ARG:NE	2.41	0.50
13:h:46:LEU:HD13	13:h:75:VAL:HG13	1.94	0.50
32:f:623:LYS:O	32:f:627:GLU:HB2	2.11	0.50
1:U:364:VAL:O	1:U:368:ALA:N	2.33	0.49
24:s:68:ILE:HD11	24:s:92:LEU:HD13	1.93	0.49
32:f:372:LEU:C	32:f:372:LEU:CD2	2.85	0.49
32:f:463:LEU:HD22	32:f:466:LEU:HD11	1.93	0.49
32:f:536:SER:HA	32:f:539:LEU:HB3	1.93	0.49
1:U:27:LEU:O	1:U:31:VAL:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:51:ASP:OD2	1:U:54:PHE:N	2.46	0.49
1:U:494:TYR:HD1	1:U:516:LEU:HD11	1.76	0.49
2:V:259:LEU:HD11	2:V:294:ARG:HD2	1.93	0.49
4:X:339:ILE:HG21	4:X:374:PHE:HE1	1.76	0.49
7:a:135:ILE:HG12	7:a:158:LEU:HD13	1.93	0.49
14:i:171:ALA:HB2	14:i:200:THR:HG21	1.94	0.49
26:A:111:TYR:O	26:A:123:VAL:N	2.40	0.49
27:B:115:ILE:HG12	27:B:146:PRO:HG3	1.94	0.49
27:B:222:VAL:HG22	27:B:349:ARG:HB2	1.94	0.49
30:E:55:GLN:O	31:F:133:PHE:N	2.43	0.49
30:E:337:GLY:O	30:E:378:LYS:NZ	2.42	0.49
32:f:517:VAL:O	32:f:521:ALA:HB3	2.12	0.49
1:U:324:LYS:HA	1:U:327:LYS:HB2	1.94	0.49
1:U:493:VAL:O	1:U:497:LEU:HB2	2.12	0.49
3:W:70:VAL:HA	3:W:73:MET:HG2	1.94	0.49
5:Y:271:PHE:O	5:Y:275:LEU:HB3	2.12	0.49
7:a:188:LEU:HD11	7:a:193:GLN:HG3	1.94	0.49
9:c:44:HIS:O	9:c:48:GLY:CA	2.56	0.49
13:H:107:THR:HA	13:H:110:LEU:HD13	1.93	0.49
21:P:126:LEU:HD12	21:P:127:ILE:HG23	1.94	0.49
13:h:50:LYS:NZ	13:h:62:VAL:O	2.46	0.49
20:o:163:ILE:HA	20:o:168:GLY:HA3	1.94	0.49
27:B:186:ASP:HB2	27:B:367:ILE:HD13	1.94	0.49
28:C:146:SER:OG	28:C:147:THR:N	2.44	0.49
32:f:657:ILE:HA	32:f:660:ILE:HD12	1.94	0.49
3:W:52:LYS:HA	3:W:55:ARG:HB3	1.93	0.49
4:X:255:LEU:HD12	4:X:287:LEU:HD13	1.94	0.49
4:X:324:ALA:O	4:X:328:ASP:HB2	2.12	0.49
25:T:171:ARG:NH2	20:o:140:ASP:OD1	2.44	0.49
15:j:169:ARG:HA	15:j:172:LEU:HB2	1.95	0.49
31:F:73:ILE:O	31:F:77:SER:HB3	2.13	0.49
32:f:343:LYS:O	32:f:347:ASP:N	2.40	0.49
32:f:376:PHE:CZ	32:f:416:MET:CE	2.95	0.49
5:Y:82:LYS:HA	5:Y:85:ASP:HB2	1.95	0.49
6:Z:278:ASN:O	6:Z:282:ASN:HB2	2.12	0.49
20:o:18:THR:HB	20:o:31:CYS:H	1.76	0.49
32:f:691:PRO:HG2	32:f:745:LEU:CD1	2.41	0.49
3:W:344:THR:OG1	3:W:345:GLU:OE1	2.30	0.49
7:a:193:GLN:HG2	7:a:196:ARG:HD3	1.93	0.49
13:H:74:LEU:HD21	13:H:134:LEU:HD22	1.95	0.49
16:K:236:GLU:HA	16:K:239:LYS:HE3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:n:178:ALA:N	19:n:185:GLU:O	2.40	0.49
12:g:49:VAL:HG22	12:g:219:VAL:HG23	1.95	0.49
19:n:120:MET:H	25:t:61:GLN:HE22	1.60	0.49
22:q:44:LEU:HD11	22:q:102:LEU:HD22	1.95	0.49
29:D:272:THR:HG22	29:D:316:THR:HG22	1.94	0.49
32:f:487:LEU:HD22	32:f:801:VAL:HG11	1.95	0.49
1:U:82:LEU:O	1:U:129:ARG:NE	2.33	0.49
1:U:353:LEU:HD13	1:U:385:PHE:HZ	1.77	0.49
2:V:467:TYR:HE2	2:V:470:ARG:HB3	1.77	0.49
5:Y:225:TYR:HA	5:Y:228:MET:HE3	1.94	0.49
21:P:190:ILE:HG22	21:P:195:ILE:HG23	1.94	0.49
34:F:501:AGS:O1B	34:F:501:AGS:O2G	2.30	0.49
32:f:478:ARG:NE	32:f:504:VAL:HG22	2.27	0.49
1:U:751:ARG:HH21	1:U:907:SER:HB3	1.77	0.49
4:X:374:PHE:HZ	4:X:385:LEU:HD21	1.78	0.49
5:Y:197:ALA:HB3	5:Y:226:VAL:HG21	1.95	0.49
6:Z:262:LEU:HB2	9:c:298:GLN:HE22	1.78	0.49
16:K:167:ALA:H	17:L:56:LEU:HD13	1.77	0.49
21:P:203:ARG:HH12	23:r:191:ASN:HD21	1.60	0.49
24:S:209:SER:OG	24:S:212:LYS:NZ	2.46	0.49
12:g:109:ILE:HD13	12:g:114:LEU:HD12	1.94	0.49
26:A:230:ALA:HB2	26:A:271:LEU:HD12	1.95	0.49
27:B:411:ARG:NH2	27:B:418:ASP:OD2	2.46	0.49
30:E:326:ILE:HA	30:E:364:GLN:HG3	1.95	0.49
31:F:427:VAL:HG23	31:F:430:LYS:H	1.77	0.49
2:V:29:PRO:HG3	2:V:83:GLU:HG3	1.93	0.49
2:V:43:THR:O	2:V:47:SER:OG	2.22	0.49
2:V:290:TYR:OH	2:V:294:ARG:NH2	2.46	0.49
3:W:1:MET:N	3:W:37:GLU:OE1	2.46	0.49
6:Z:274:ASN:O	6:Z:278:ASN:CB	2.60	0.49
30:E:322:LYS:HD3	30:E:326:ILE:HG13	1.95	0.49
1:U:353:LEU:O	1:U:357:LYS:HB2	2.12	0.48
1:U:772:TRP:HB3	1:U:775:LEU:HG	1.94	0.48
4:X:399:ALA:HB2	9:c:257:LYS:HE3	1.95	0.48
6:Z:10:VAL:N	6:Z:48:LEU:O	2.45	0.48
10:d:92:SER:HB3	10:d:95:MET:HB2	1.94	0.48
10:d:178:ILE:O	10:d:182:ILE:HB	2.13	0.48
14:I:162:THR:OG1	14:I:163:CYS:N	2.46	0.48
14:I:245:ALA:HA	14:I:248:GLU:HG2	1.94	0.48
17:L:52:ALA:HB2	17:L:59:HIS:CD2	2.48	0.48
22:Q:92:LEU:HD11	22:Q:121:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:R:38:ASN:HD22	23:R:41:LEU:HD12	1.77	0.48
28:C:245:ILE:HG12	28:C:290:LYS:HB2	1.96	0.48
29:D:290:LEU:O	29:D:294:ASN:HB2	2.12	0.48
29:D:337:ASP:OD2	29:D:339:ARG:NH2	2.46	0.48
32:f:336:GLU:HB3	32:f:337:LEU:HD23	1.95	0.48
32:f:641:GLU:HG3	32:f:641:GLU:O	2.09	0.48
1:U:370:VAL:O	1:U:374:SER:OG	2.29	0.48
1:U:655:ALA:O	1:U:659:CYS:CB	2.61	0.48
2:V:311:ASN:O	2:V:315:LYS:HB2	2.14	0.48
2:V:314:ARG:NH2	5:Y:378:ASN:HD22	2.11	0.48
4:X:343:SER:HB2	4:X:387:ILE:HB	1.95	0.48
8:b:51:LEU:HD21	8:b:61:LEU:HB2	1.96	0.48
10:d:56:GLU:OE2	10:d:92:SER:OG	2.30	0.48
16:K:192:LYS:HA	16:K:195:ILE:HD12	1.96	0.48
19:N:18:SER:OG	19:N:19:ARG:N	2.45	0.48
22:Q:38:MET:O	22:Q:65:GLN:NE2	2.46	0.48
18:m:40:ARG:NH1	18:m:146:ALA:O	2.46	0.48
21:p:2:SER:OG	21:p:3:ILE:N	2.46	0.48
21:p:45:MET:HE3	21:p:71:LEU:HD22	1.94	0.48
26:A:121:PHE:HB3	31:F:87:PRO:HB2	1.95	0.48
28:C:43:ARG:HA	28:C:46:GLN:HB2	1.95	0.48
30:E:197:LYS:HG2	30:E:231:PHE:HB3	1.94	0.48
32:f:127:SER:O	32:f:131:MET:HB2	2.13	0.48
32:f:387:GLN:N	32:f:387:GLN:NE2	2.60	0.48
1:U:77:SER:O	1:U:81:ALA:CB	2.62	0.48
1:U:672:LEU:HD22	1:U:687:ALA:HA	1.95	0.48
7:a:290:GLN:NE2	7:a:325:ASP:OD2	2.46	0.48
13:H:46:LEU:HD13	13:H:75:VAL:HG13	1.94	0.48
12:g:165:ALA:HB1	12:g:179:LEU:HD13	1.95	0.48
26:A:264:ALA:HB1	26:A:315:ILE:HG12	1.94	0.48
29:D:96:VAL:HG23	29:D:102:ILE:HD11	1.94	0.48
32:f:695:ALA:CB	32:f:752:HIS:HB3	2.44	0.48
3:W:128:LEU:O	3:W:132:THR:OG1	2.28	0.48
3:W:206:SER:HB2	3:W:233:LEU:HD11	1.93	0.48
3:W:337:ALA:O	3:W:342:GLY:N	2.46	0.48
5:Y:348:ASP:OD1	5:Y:349:LYS:N	2.46	0.48
18:M:66:LEU:HD13	18:M:214:SER:HB2	1.95	0.48
22:Q:4:LEU:HD12	22:Q:45:LEU:HB3	1.96	0.48
23:R:133:VAL:HG21	22:q:137:PHE:HB3	1.95	0.48
25:T:41:ARG:HH21	25:T:54:SER:HA	1.79	0.48
14:i:178:ASP:OD2	14:i:195:LYS:NZ	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:303:ARG:O	27:B:307:ARG:NH2	2.46	0.48
32:f:453:SER:O	32:f:488:ALA:O	2.32	0.48
32:f:597:VAL:HG22	32:f:630:ASP:HB2	1.95	0.48
3:W:169:LEU:HD13	3:W:208:LYS:HG2	1.95	0.48
5:Y:53:TYR:O	5:Y:57:LEU:HB2	2.13	0.48
27:B:429:LYS:NZ	28:C:189:TYR:OH	2.45	0.48
31:F:235:LEU:HD12	31:F:236:LEU:HG	1.95	0.48
32:f:30:GLY:O	32:f:34:ARG:HB2	2.14	0.48
32:f:376:PHE:HE1	32:f:798:THR:HB	1.53	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
1:U:107:HIS:HA	1:U:110:LYS:HG2	1.96	0.48
1:U:415:HIS:NE2	1:U:418:GLU:OE1	2.36	0.48
3:W:405:LYS:HG2	4:X:344:ARG:HG2	1.95	0.48
5:Y:105:MET:HB2	5:Y:127:THR:HG21	1.94	0.48
5:Y:186:LEU:HA	5:Y:189:VAL:HG12	1.96	0.48
12:G:161:CYS:SG	12:G:162:GLY:N	2.86	0.48
18:M:201:HIS:HE1	18:M:206:ASP:HB2	1.78	0.48
32:f:559:PRO:HA	32:f:562:LEU:HB2	1.96	0.48
6:Z:59:ASP:HB3	8:b:95:LEU:HD21	1.94	0.48
18:M:35:THR:HA	18:M:166:GLY:HA3	1.96	0.48
28:C:89:VAL:O	28:C:92:GLU:N	2.47	0.48
28:C:201:ARG:O	28:C:205:HIS:CB	2.61	0.48
29:D:102:ILE:HG13	29:D:112:TYR:HD1	1.78	0.48
31:F:330:ALA:HB3	31:F:348:LEU:HD21	1.95	0.48
32:f:94:LYS:HA	32:f:97:LYS:HG2	1.94	0.48
32:f:140:LEU:O	32:f:144:LEU:CB	2.61	0.48
32:f:209:MET:SD	32:f:213:GLN:NE2	2.87	0.48
32:f:252:ALA:O	32:f:256:PHE:HB2	2.14	0.48
32:f:333:LEU:HA	32:f:338:ASP:HB2	1.95	0.48
1:U:24:LEU:HB2	1:U:59:PHE:CE2	2.49	0.48
1:U:153:ILE:HG22	1:U:162:VAL:HG11	1.95	0.48
3:W:86:ASN:HB3	3:W:93:ARG:HH22	1.77	0.48
6:Z:223:ASN:ND2	7:a:340:VAL:O	2.47	0.48
7:a:163:TYR:HE1	7:a:169:HIS:HA	1.79	0.48
15:J:211:MET:HG2	15:J:213:ARG:H	1.77	0.48
16:k:104:ASN:OD1	23:r:57:ARG:NH1	2.47	0.48
18:m:168:ALA:HB1	18:m:171:ALA:HB3	1.95	0.48
31:F:98:ASP:HA	31:F:120:LYS:HB2	1.96	0.48
32:f:389:LYS:HB3	32:f:392:THR:HG21	1.95	0.48
32:f:645:ASP:HB3	32:f:648:ALA:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:50:GLU:HA	2:V:54:LYS:HG3	1.96	0.48
3:W:221:LYS:HG3	3:W:224:LEU:HD12	1.94	0.48
5:Y:283:LYS:HZ2	11:e:60:LEU:HD22	1.78	0.48
7:a:291:LEU:O	7:a:331:VAL:N	2.47	0.48
9:c:63:ASP:OD1	9:c:66:THR:OG1	2.23	0.48
18:m:100:SER:O	25:t:65:GLN:NE2	2.47	0.48
26:A:224:LEU:HD11	34:A:501:AGS:H2'	1.95	0.48
26:A:277:ILE:HG22	26:A:280:ILE:HD12	1.95	0.48
32:f:234:THR:HG23	32:f:637:LYS:HE2	1.94	0.48
32:f:253:LEU:O	32:f:257:ARG:CB	2.61	0.48
32:f:311:VAL:CB	32:f:490:ALA:CB	2.77	0.48
32:f:392:THR:HA	32:f:414:LEU:CD2	2.44	0.48
2:V:57:ALA:O	2:V:201:ARG:NH1	2.38	0.48
7:a:215:GLU:HA	7:a:340:VAL:HG21	1.95	0.48
12:G:54:LYS:NZ	12:G:213:SER:O	2.43	0.48
18:M:40:ARG:HE	18:M:161:TRP:CD1	2.31	0.48
25:T:96:MET:HE1	25:T:106:LEU:HB2	1.96	0.48
17:l:196:ARG:HH21	17:l:239:ARG:HG3	1.77	0.48
20:o:98:LEU:HB2	20:o:113:ILE:HB	1.96	0.48
22:q:57:ALA:O	22:q:61:GLN:HB3	2.13	0.48
28:C:220:VAL:HA	28:C:224:ILE:HD12	1.96	0.48
7:a:18:GLN:HG3	7:a:22:TRP:CD1	2.49	0.47
8:b:84:ILE:HG21	8:b:115:SER:HB2	1.95	0.47
19:N:135:ILE:O	19:N:139:VAL:HB	2.13	0.47
13:h:9:SER:OG	13:h:123:GLN:O	2.29	0.47
20:o:216:ILE:HG23	21:p:194:LYS:HE2	1.95	0.47
32:f:248:LEU:O	32:f:252:ALA:CB	2.62	0.47
32:f:424:GLY:HA2	32:f:427:THR:HG22	1.96	0.47
32:f:479:LEU:CD2	32:f:513:GLU:HB3	2.39	0.47
32:f:632:LYS:NZ	32:f:660:ILE:O	2.46	0.47
3:W:169:LEU:O	3:W:182:ARG:NH1	2.47	0.47
4:X:260:MET:HE2	4:X:321:THR:HB	1.96	0.47
28:C:87:VAL:HG11	28:C:116:LEU:HD22	1.96	0.47
30:E:59:GLU:HG2	30:E:97:ARG:HA	1.96	0.47
32:f:331:LEU:O	32:f:335:ARG:NH1	2.47	0.47
1:U:160:LEU:HA	1:U:163:PHE:HB3	1.96	0.47
2:V:116:ALA:O	2:V:120:PHE:HB2	2.13	0.47
2:V:263:LEU:O	10:d:117:THR:OG1	2.32	0.47
3:W:429:SER:O	3:W:433:ASN:CB	2.62	0.47
3:W:449:GLU:O	3:W:453:HIS:ND1	2.39	0.47
5:Y:102:ASP:HB2	5:Y:136:HIS:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:h:9:SER:HA	13:h:126:GLY:H	1.80	0.47
18:m:9:LEU:O	18:m:22:GLN:NE2	2.47	0.47
18:m:69:VAL:H	18:m:74:GLY:HA2	1.79	0.47
26:A:413:VAL:HG13	26:A:417:ILE:HD12	1.97	0.47
27:B:125:THR:H	27:B:128:GLY:HA2	1.79	0.47
32:f:166:VAL:O	32:f:170:TRP:HB2	2.14	0.47
2:V:419:LEU:O	2:V:423:ALA:HB2	2.13	0.47
18:M:168:ALA:HB1	18:M:171:ALA:HB3	1.97	0.47
18:m:66:LEU:HD13	18:m:214:SER:HB2	1.97	0.47
2:V:349:ARG:HH11	2:V:354:LYS:HB2	1.80	0.47
9:c:57:MET:HE3	9:c:109:VAL:HG23	1.96	0.47
12:G:49:VAL:HG22	12:G:219:VAL:HG23	1.96	0.47
19:N:176:LEU:HD12	19:N:187:GLN:HE21	1.78	0.47
25:T:37:ARG:HD3	19:n:166:ARG:HH12	1.79	0.47
14:i:161:ALA:HB1	14:i:175:LEU:HD13	1.95	0.47
15:j:134:VAL:HG22	15:j:144:LEU:HB2	1.96	0.47
28:C:342:ILE:HG13	28:C:380:GLN:HB2	1.96	0.47
29:D:214:MET:HE1	34:D:501:AGS:C5	2.44	0.47
32:f:675:PHE:O	32:f:679:LEU:CB	2.59	0.47
1:U:177:LEU:HA	1:U:180:SER:HB3	1.95	0.47
6:Z:14:LEU:HA	9:c:39:LEU:HD13	1.95	0.47
13:H:6:TYR:HE2	13:H:14:SER:HA	1.80	0.47
16:k:195:ILE:O	16:k:198:SER:OG	2.32	0.47
27:B:248:LEU:HB2	27:B:282:VAL:HA	1.96	0.47
28:C:168:PRO:HG3	28:C:182:GLN:HG2	1.96	0.47
1:U:378:CYS:HB3	1:U:413:LYS:HB3	1.95	0.47
1:U:604:HIS:O	1:U:608:SER:OG	2.24	0.47
3:W:44:ILE:HA	3:W:47:LEU:HB2	1.95	0.47
3:W:385:SER:OG	3:W:386:VAL:N	2.48	0.47
3:W:407:ASP:H	3:W:413:ILE:HG12	1.80	0.47
5:Y:20:ALA:HB2	5:Y:150:PHE:CD1	2.50	0.47
5:Y:229:ILE:HD11	5:Y:295:TYR:HE1	1.80	0.47
5:Y:316:LEU:O	5:Y:320:ALA:CB	2.61	0.47
17:L:26:MET:HE1	17:L:148:CYS:HB2	1.97	0.47
18:M:30:VAL:HG11	18:M:134:SER:HB3	1.97	0.47
22:Q:101:ASN:HB3	22:Q:132:HIS:CD2	2.49	0.47
16:k:228:MET:N	16:k:228:MET:SD	2.88	0.47
21:p:58:THR:OG1	22:q:121:LEU:O	2.20	0.47
25:t:46:ASN:OD1	25:t:46:ASN:N	2.48	0.47
26:A:98:CYS:SG	26:A:99:THR:N	2.86	0.47
27:B:434:THR:HA	27:B:436:GLU:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:311:LEU:HD23	31:F:314:LEU:HD12	1.96	0.47
32:f:336:GLU:CG	32:f:337:LEU:CD2	2.92	0.47
32:f:626:GLU:OE1	32:f:782:HIS:NE2	2.47	0.47
2:V:90:GLU:HB2	2:V:127:THR:HG22	1.97	0.47
2:V:484:LEU:HA	2:V:487:HIS:HD2	1.79	0.47
5:Y:131:THR:O	5:Y:137:ARG:NH1	2.48	0.47
9:c:26:ASP:O	9:c:176:GLN:NE2	2.48	0.47
16:K:173:ALA:HB2	26:A:375:ARG:HG3	1.97	0.47
18:M:152:ASP:OD1	18:M:156:VAL:N	2.46	0.47
27:B:220:LYS:HB3	27:B:322:ARG:HH21	1.79	0.47
29:D:207:PRO:CD	29:D:335:LEU:HD11	2.45	0.47
30:E:188:ALA:HB2	30:E:197:LYS:HZ1	1.80	0.47
31:F:382:GLU:O	31:F:386:ARG:HB2	2.15	0.47
32:f:315:GLU:HA	32:f:318:THR:HG22	1.95	0.47
1:U:471:ASP:HA	1:U:474:ARG:HB2	1.95	0.47
2:V:389:ASP:HB3	2:V:391:THR:HG22	1.97	0.47
13:H:71:HIS:HA	13:H:218:PHE:H	1.79	0.47
17:l:158:ALA:HB1	17:l:172:LEU:HD22	1.96	0.47
28:C:31:LEU:HD23	28:C:34:ILE:HD12	1.96	0.47
28:C:114:VAL:HG12	28:C:126:ILE:HG12	1.97	0.47
32:f:692:LEU:HG	32:f:752:HIS:HE1	1.77	0.47
3:W:180:LYS:HG2	3:W:218:ASN:HB3	1.97	0.47
4:X:379:ASP:OD2	4:X:382:GLU:N	2.47	0.47
21:P:205:ASP:HB3	23:r:192:VAL:HG11	1.97	0.47
13:h:93:LEU:HD11	13:h:113:ARG:HB3	1.97	0.47
16:k:85:ALA:HB2	16:k:139:VAL:HG21	1.97	0.47
18:m:136:MET:HE3	18:m:148:LEU:HD11	1.96	0.47
21:p:159:ASP:N	21:p:159:ASP:OD1	2.46	0.47
30:E:352:MET:O	30:E:356:ARG:N	2.44	0.47
32:f:691:PRO:HB3	32:f:749:ALA:CB	2.39	0.47
3:W:272:LEU:HD23	3:W:275:ILE:HD13	1.95	0.46
7:a:112:ILE:HB	7:a:151:VAL:HG21	1.97	0.46
10:d:242:LEU:HD23	10:d:245:GLN:HG3	1.96	0.46
12:g:132:ARG:HD3	18:m:124:LEU:HD23	1.97	0.46
28:C:201:ARG:HH21	28:C:211:PHE:HD2	1.62	0.46
29:D:207:PRO:CD	29:D:335:LEU:CD1	2.92	0.46
29:D:251:PHE:CE2	29:D:295:GLN:HB3	2.50	0.46
31:F:365:ILE:HA	31:F:368:ILE:HD12	1.97	0.46
32:f:79:ARG:HE	32:f:95:PRO:HG3	1.80	0.46
32:f:281:ILE:O	32:f:285:CYS:HB3	2.15	0.46
2:V:148:ARG:HH12	2:V:193:GLN:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:320:VAL:HB	7:a:336:VAL:HG23	1.98	0.46
18:M:63:ASN:HB2	18:M:81:LEU:HD21	1.97	0.46
13:h:59:GLU:HG2	13:h:206:ASP:HB3	1.98	0.46
13:h:119:GLN:O	13:h:122:THR:OG1	2.25	0.46
14:i:180:LYS:HD3	14:i:192:LEU:HD13	1.98	0.46
16:k:196:LYS:HA	16:k:199:LEU:HG	1.97	0.46
1:U:558:GLY:HA2	1:U:560:MET:HE2	1.96	0.46
1:U:800:VAL:HB	1:U:842:LYS:HE2	1.95	0.46
3:W:236:HIS:HE1	3:W:345:GLU:HG2	1.80	0.46
5:Y:101:ARG:NH2	5:Y:126:LYS:O	2.49	0.46
5:Y:173:ASP:HB3	5:Y:176:ARG:HG2	1.96	0.46
10:d:215:TRP:HZ2	10:d:222:TYR:HB3	1.80	0.46
18:M:136:MET:HE3	18:M:148:LEU:HD11	1.97	0.46
16:k:101:PHE:HB2	23:r:61:ARG:HD2	1.97	0.46
17:l:44:ALA:HB1	17:l:144:ILE:HD11	1.98	0.46
27:B:279:PRO:HG2	32:f:714:SER:CA	2.45	0.46
2:V:362:LEU:HD23	2:V:382:PHE:HE2	1.79	0.46
2:V:421:ASP:O	2:V:425:LYS:HB2	2.16	0.46
3:W:12:ARG:O	3:W:27:ARG:NH2	2.48	0.46
9:c:122:LEU:H	9:c:193:ILE:HD11	1.79	0.46
20:O:98:LEU:HB2	20:O:113:ILE:HB	1.96	0.46
24:S:176:LYS:HE2	24:S:208:VAL:HG21	1.97	0.46
28:C:197:THR:O	28:C:201:ARG:HB3	2.15	0.46
31:F:339:ASP:HB2	31:F:342:LEU:HG	1.96	0.46
1:U:408:LEU:HD23	1:U:423:MET:HG2	1.98	0.46
4:X:378:LEU:HB2	5:Y:311:TYR:HB3	1.97	0.46
6:Z:70:LEU:HD11	6:Z:108:ILE:HG23	1.97	0.46
19:N:178:ALA:HB3	19:N:185:GLU:HB2	1.98	0.46
34:A:501:AGS:O2A	34:A:501:AGS:O2B	2.31	0.46
27:B:140:ASP:HB3	27:B:143:LEU:HG	1.97	0.46
1:U:560:MET:HE1	1:U:591:CYS:H	1.80	0.46
3:W:220:GLU:HG3	3:W:221:LYS:HD3	1.98	0.46
17:L:39:LYS:HD3	17:L:144:ILE:HG12	1.98	0.46
13:h:65:VAL:HG11	13:h:211:GLY:HA3	1.96	0.46
27:B:273:VAL:HG13	27:B:277:HIS:HE1	1.79	0.46
30:E:153:LEU:HD11	30:E:191:LEU:HD22	1.97	0.46
32:f:378:ASN:HB3	32:f:391:LEU:HD21	1.98	0.46
32:f:541:THR:O	32:f:545:LYS:CB	2.63	0.46
5:Y:312:ARG:NE	5:Y:355:GLU:OE1	2.48	0.46
6:Z:150:PRO:HA	7:a:146:PRO:HG2	1.97	0.46
7:a:34:TRP:HA	7:a:37:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:l:46:LEU:HD13	17:l:73:SER:HB2	1.97	0.46
17:l:52:ALA:HB2	17:l:59:HIS:CD2	2.51	0.46
31:F:375:VAL:HG22	31:F:415:LEU:HD12	1.97	0.46
32:f:193:PRO:C	32:f:208:LEU:HD12	2.40	0.46
32:f:675:PHE:CG	32:f:694:LEU:HD23	2.51	0.46
3:W:145:LEU:HD22	3:W:185:PHE:CG	2.50	0.46
4:X:287:LEU:HA	4:X:290:VAL:HB	1.98	0.46
5:Y:145:LEU:HG	5:Y:160:ASN:HD21	1.80	0.46
11:e:49:GLU:HA	11:e:52:PHE:HB2	1.98	0.46
17:L:225:ASP:OD1	17:L:225:ASP:N	2.49	0.46
21:P:62:THR:OG1	22:Q:85:ARG:NH2	2.49	0.46
25:t:180:ASP:HB3	25:t:183:SER:HB3	1.97	0.46
26:A:187:LEU:HD21	26:A:229:VAL:HG22	1.98	0.46
28:C:165:ILE:HG12	28:C:290:LYS:HD2	1.98	0.46
32:f:226:TYR:O	32:f:230:CYS:HB3	2.16	0.46
1:U:221:ILE:HD12	1:U:754:HIS:HB2	1.97	0.46
7:a:7:PHE:HZ	7:a:56:LEU:HB3	1.81	0.46
17:L:157:ARG:HD2	17:L:176:MET:HE3	1.98	0.46
29:D:204:MET:HB2	29:D:310:ALA:HB2	1.98	0.46
32:f:392:THR:HB	32:f:414:LEU:HD22	1.97	0.46
32:f:664:GLU:C	32:f:665:GLU:O	2.59	0.46
1:U:479:LEU:HD23	1:U:778:PHE:HZ	1.81	0.46
2:V:87:SER:HB2	2:V:125:ASN:HA	1.98	0.46
9:c:55:GLY:HA3	9:c:112:TYR:CZ	2.50	0.46
16:K:85:ALA:HB2	16:K:139:VAL:HG21	1.98	0.46
18:M:15:SER:OG	18:M:18:GLY:N	2.45	0.46
30:E:145:LEU:HA	30:E:148:VAL:HG12	1.97	0.46
31:F:137:ILE:HG23	31:F:160:ILE:HD12	1.98	0.46
32:f:378:ASN:CB	32:f:391:LEU:CD1	2.94	0.46
32:f:475:ASN:O	32:f:478:ARG:HB3	2.15	0.46
2:V:210:CYS:O	2:V:214:HIS:ND1	2.36	0.45
6:Z:22:HIS:HA	6:Z:25:ARG:HG2	1.97	0.45
10:d:78:LEU:HD13	10:d:98:LEU:HD22	1.98	0.45
12:G:58:ASP:HB3	12:G:61:LEU:HB2	1.98	0.45
19:N:127:ILE:HD13	19:N:136:TYR:HB2	1.99	0.45
14:i:62:SER:OG	14:i:65:ILE:O	2.33	0.45
15:j:68:ASN:HA	15:j:211:MET:HE1	1.98	0.45
16:k:167:ALA:HB3	16:k:181:LEU:HD21	1.96	0.45
25:t:153:VAL:O	25:t:157:GLN:N	2.46	0.45
25:t:192:VAL:HG12	25:t:197:VAL:HG22	1.97	0.45
32:f:125:ILE:HA	32:f:129:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:802:TYR:HB3	1:U:895:PRO:HD3	1.98	0.45
2:V:357:LEU:HB2	2:V:360:TYR:HB3	1.97	0.45
3:W:2:ALA:HA	3:W:47:LEU:HD11	1.98	0.45
3:W:144:ARG:HA	3:W:147:LYS:HG2	1.98	0.45
4:X:393:VAL:HG12	4:X:396:THR:H	1.81	0.45
10:d:151:VAL:HG21	10:d:174:ILE:HD11	1.98	0.45
10:d:244:LYS:HA	10:d:247:ILE:HD12	1.97	0.45
18:M:37:ILE:HG12	18:M:197:ILE:HD11	1.98	0.45
13:h:80:GLY:HA2	13:h:83:TYR:HB3	1.97	0.45
18:m:37:ILE:HD11	18:m:193:VAL:HG13	1.98	0.45
22:q:7:ILE:HB	22:q:14:LEU:HB3	1.98	0.45
29:D:225:ALA:HB1	29:D:260:ALA:HB1	1.99	0.45
31:F:93:VAL:HG23	31:F:151:VAL:HG21	1.98	0.45
32:f:538:ILE:HA	32:f:541:THR:HG22	1.97	0.45
32:f:796:LEU:HG	32:f:799:VAL:CG2	2.42	0.45
1:U:583:MET:HA	1:U:586:VAL:HG12	1.98	0.45
13:h:7:SER:O	15:j:3:TYR:OH	2.35	0.45
19:n:96:ALA:HB1	19:n:98:ILE:HG12	1.97	0.45
22:q:135:GLY:O	22:q:139:THR:OG1	2.31	0.45
23:r:104:TRP:NE1	23:r:181:GLU:HG3	2.31	0.45
29:D:317:LEU:HB3	29:D:318:ASP:H	1.40	0.45
29:D:338:ARG:O	29:D:339:ARG:HG3	2.16	0.45
31:F:73:ILE:O	31:F:77:SER:OG	2.30	0.45
32:f:796:LEU:HD12	32:f:799:VAL:HG11	1.98	0.45
3:W:39:ARG:H	3:W:44:ILE:HD12	1.82	0.45
7:a:170:ALA:HB3	7:a:209:GLY:H	1.80	0.45
7:a:355:PHE:O	7:a:359:ASP:HB2	2.16	0.45
9:c:217:LEU:O	9:c:221:HIS:CB	2.62	0.45
19:N:167:ASP:OD2	19:N:170:SER:N	2.44	0.45
20:O:63:LEU:HD11	20:O:79:ALA:HB2	1.98	0.45
20:o:106:THR:OG1	20:o:109:HIS:NE2	2.38	0.45
23:r:36:GLU:OE2	23:r:186:ARG:NH2	2.49	0.45
23:r:105:ASP:N	23:r:108:GLY:O	2.46	0.45
28:C:39:SER:O	28:C:43:ARG:HB2	2.15	0.45
3:W:215:GLN:O	3:W:218:ASN:ND2	2.50	0.45
6:Z:85:VAL:O	9:c:77:GLN:NE2	2.49	0.45
10:d:170:LEU:HA	10:d:173:THR:HG22	1.99	0.45
14:I:105:ILE:HD11	14:I:109:GLN:HG3	1.97	0.45
17:L:146:GLN:HE21	17:L:154:PHE:HD2	1.63	0.45
23:R:36:GLU:OE2	23:R:186:ARG:NH2	2.50	0.45
24:s:35:ILE:O	25:t:151:ARG:NH2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:170:LEU:HD11	27:B:266:LEU:HD13	1.98	0.45
32:f:353:LEU:H	32:f:387:GLN:CG	2.29	0.45
32:f:533:ASP:OD1	32:f:565:ASN:ND2	2.50	0.45
32:f:608:LYS:HA	32:f:611:GLN:HB3	1.99	0.45
4:X:380:GLN:HE22	5:Y:318:TYR:HB2	1.82	0.45
9:c:38:LEU:HD12	9:c:157:ILE:HD12	1.98	0.45
10:d:45:LYS:HA	10:d:48:LEU:HD12	1.98	0.45
15:j:121:SER:OG	15:j:122:ASN:N	2.48	0.45
29:D:404:LYS:HA	29:D:408:LYS:HD3	1.97	0.45
32:f:316:ASP:HA	32:f:319:GLU:HG2	1.98	0.45
2:V:159:LEU:HD13	2:V:178:SER:HB2	1.99	0.45
3:W:251:TYR:HA	3:W:266:ALA:HB1	1.97	0.45
3:W:308:LEU:HG	3:W:312:MET:HG3	1.99	0.45
4:X:252:LYS:HD3	4:X:287:LEU:HD21	1.99	0.45
4:X:376:GLY:HA3	4:X:387:ILE:HA	1.98	0.45
5:Y:53:TYR:HA	5:Y:56:ALA:HB3	1.99	0.45
5:Y:358:ARG:HH12	5:Y:364:TRP:HB3	1.80	0.45
6:Z:259:VAL:HG13	9:c:298:GLN:HG3	1.97	0.45
14:I:125:GLY:HA2	14:I:126:GLY:HA2	1.59	0.45
14:I:164:ILE:HG22	14:I:165:GLY:H	1.80	0.45
13:h:212:ILE:HD11	13:h:219:ARG:HD3	1.99	0.45
14:i:216:LEU:HD12	14:i:225:ILE:HG12	1.99	0.45
15:j:109:ARG:NH2	23:r:70:ASN:OD1	2.50	0.45
34:B:501:AGS:S1G	34:B:501:AGS:O1B	2.75	0.45
30:E:172:LEU:HD11	30:E:183:LEU:HD22	1.99	0.45
31:F:217:ILE:HG13	31:F:218:GLN:H	1.82	0.45
32:f:376:PHE:CZ	32:f:798:THR:HG22	2.50	0.45
1:U:383:ASP:HB3	1:U:386:LEU:HB2	1.99	0.45
1:U:678:ASP:O	1:U:684:ARG:NH1	2.49	0.45
2:V:487:HIS:CE1	6:Z:271:ALA:HA	2.52	0.45
3:W:397:VAL:HG23	3:W:404:ALA:HB3	1.99	0.45
6:Z:36:VAL:HG22	6:Z:96:HIS:HB2	1.99	0.45
6:Z:75:LEU:O	6:Z:79:TYR:HB2	2.17	0.45
8:b:97:LEU:HD23	8:b:107:MET:HG2	1.98	0.45
12:G:39:SER:OG	12:G:168:ALA:O	2.34	0.45
13:h:105:ILE:HG12	13:h:110:LEU:HD12	1.99	0.45
15:j:156:TRP:CD1	16:k:59:MET:HA	2.51	0.45
17:l:59:HIS:ND1	17:l:208:LYS:O	2.50	0.45
17:l:125:ARG:NH2	17:l:128:TYR:OH	2.50	0.45
23:r:59:LEU:HD22	23:r:83:LEU:HB2	1.98	0.45
31:F:124:ILE:O	31:F:132:TYR:N	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:410:ARG:NH2	31:F:416:THR:OG1	2.41	0.45
32:f:178:LYS:NZ	32:f:215:ASP:O	2.42	0.45
1:U:98:GLU:HA	1:U:101:ILE:HG12	1.99	0.45
3:W:438:LEU:HD23	3:W:441:LYS:HG3	1.99	0.45
6:Z:67:VAL:HG13	8:b:92:VAL:HG23	1.99	0.45
14:I:140:ASP:OD1	14:I:144:GLY:N	2.47	0.45
23:r:21:THR:HA	23:r:26:ILE:HA	1.99	0.45
25:t:4:PRO:HG3	25:t:107:TRP:CE2	2.51	0.45
27:B:149:SER:HB3	27:B:163:LEU:HD13	1.98	0.45
27:B:183:THR:OG1	27:B:184:TYR:N	2.49	0.45
29:D:171:ASP:O	29:D:175:GLN:HB2	2.16	0.45
1:U:91:ASN:HB2	1:U:97:VAL:HG21	1.99	0.45
1:U:111:GLN:NE2	1:U:115:ASN:OD1	2.40	0.45
1:U:257:SER:O	1:U:261:LEU:N	2.47	0.45
1:U:474:ARG:HH22	1:U:496:LEU:HD12	1.81	0.45
1:U:733:ALA:O	1:U:737:LEU:CB	2.65	0.45
1:U:762:GLY:O	1:U:766:PHE:CB	2.65	0.45
2:V:175:MET:HB3	2:V:179:LYS:HZ3	1.82	0.45
4:X:244:SER:O	4:X:248:ILE:HB	2.17	0.45
5:Y:246:ILE:HG13	5:Y:250:LEU:HD23	1.99	0.45
7:a:162:TYR:O	7:a:165:THR:OG1	2.27	0.45
7:a:264:ASN:HB3	7:a:267:GLN:HB2	1.98	0.45
7:a:280:MET:O	7:a:284:ARG:NH1	2.50	0.45
15:J:122:ASN:HD21	16:K:125:GLU:HB3	1.82	0.45
12:g:71:LYS:O	12:g:95:ARG:NH2	2.50	0.45
26:A:251:GLY:O	26:A:255:ARG:N	2.45	0.45
26:A:363:SER:OG	27:B:213:GLU:O	2.29	0.45
29:D:251:PHE:HE1	29:D:304:ASN:HD22	1.64	0.45
30:E:119:VAL:O	30:E:123:SER:OG	2.31	0.45
32:f:45:LEU:HD22	32:f:86:THR:HG21	1.99	0.45
32:f:380:PHE:CD2	32:f:380:PHE:O	2.70	0.45
5:Y:387:ILE:HG21	6:Z:283:ARG:HG2	1.99	0.44
9:c:153:GLY:H	29:D:81:ARG:NE	2.12	0.44
10:d:75:MET:HE2	10:d:102:ASN:HB2	1.99	0.44
18:M:9:LEU:O	18:M:22:GLN:NE2	2.49	0.44
18:M:36:ALA:O	18:M:165:ILE:N	2.47	0.44
18:m:192:GLU:HA	18:m:195:LYS:HE3	1.99	0.44
32:f:420:TRP:CG	32:f:421:ASP:H	2.34	0.44
1:U:177:LEU:HD23	1:U:201:LEU:HD22	1.99	0.44
1:U:342:LEU:HD13	1:U:378:CYS:HB2	1.99	0.44
1:U:682:TYR:O	1:U:685:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:41:LEU:HD11	5:Y:70:LEU:HD11	1.99	0.44
7:a:131:THR:HB	7:a:135:ILE:HD12	1.99	0.44
12:G:38:THR:HB	12:G:53:GLN:HE22	1.83	0.44
15:J:32:ALA:HB2	15:J:45:VAL:HG23	2.00	0.44
20:O:217:THR:HB	21:P:195:ILE:HB	1.99	0.44
24:S:125:ASP:OD1	24:S:129:SER:N	2.43	0.44
14:i:38:LEU:HG	14:i:160:LYS:HB3	1.99	0.44
18:m:152:ASP:OD1	18:m:156:VAL:N	2.47	0.44
31:F:212:PHE:O	31:F:216:GLY:N	2.50	0.44
32:f:354:GLU:HG3	32:f:355:ASN:H	1.82	0.44
1:U:341:PHE:HD1	1:U:880:ASN:HB2	1.82	0.44
1:U:769:PHE:HA	1:U:775:LEU:HB2	1.99	0.44
3:W:349:LYS:O	3:W:353:ASP:HB2	2.17	0.44
5:Y:314:LEU:HD11	5:Y:319:MET:HE3	1.99	0.44
7:a:112:ILE:HD13	7:a:151:VAL:HG11	1.98	0.44
9:c:38:LEU:HD23	9:c:42:LEU:HD23	1.99	0.44
10:d:200:PHE:O	10:d:203:PRO:HD3	2.17	0.44
20:O:20:ALA:HB3	20:O:28:ASP:HB3	1.99	0.44
20:O:46:ALA:HB3	20:O:97:ALA:HB3	1.99	0.44
16:k:157:ASP:OD1	16:k:161:THR:N	2.50	0.44
26:A:101:ILE:HD12	26:A:138:MET:HB3	1.99	0.44
32:f:379:GLY:O	32:f:417:ILE:CG1	2.65	0.44
32:f:446:LEU:HD13	32:f:480:GLY:HA2	2.00	0.44
3:W:316:ARG:O	3:W:319:THR:OG1	2.29	0.44
8:b:100:ARG:NH1	8:b:105:HIS:O	2.51	0.44
17:L:45:VAL:HG11	17:L:188:VAL:HG22	1.99	0.44
21:P:26:ARG:HD3	21:P:186:ILE:HB	1.99	0.44
17:l:189:LYS:HZ3	17:l:193:ARG:HH12	1.65	0.44
28:C:228:ALA:HB1	28:C:231:VAL:HA	1.98	0.44
28:C:347:ILE:HG22	28:C:351:MET:HE3	1.99	0.44
31:F:394:ALA:CA	34:F:501:AGS:H1'	2.40	0.44
31:F:426:GLU:O	31:F:428:GLN:N	2.44	0.44
32:f:355:ASN:HA	32:f:358:PHE:HD2	1.83	0.44
32:f:797:LEU:HD22	32:f:797:LEU:HA	1.76	0.44
1:U:813:TYR:OH	1:U:841:LYS:NZ	2.50	0.44
2:V:62:HIS:HA	2:V:65:ARG:HB3	2.00	0.44
2:V:227:VAL:HA	2:V:230:PHE:HB3	2.00	0.44
7:a:280:MET:HE1	7:a:296:ILE:HG13	1.99	0.44
13:H:14:SER:OG	13:H:17:GLY:N	2.51	0.44
18:M:230:ASP:OD1	18:M:230:ASP:N	2.50	0.44
29:D:214:MET:HE3	34:D:501:AGS:C8	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:E:198:VAL:HG12	30:E:200:SER:H	1.81	0.44
30:E:237:ALA:HB1	31:F:308:ARG:HE	1.82	0.44
30:E:344:ARG:HD3	31:F:218:GLN:HE22	1.83	0.44
32:f:283:THR:O	32:f:287:ASP:HB2	2.18	0.44
32:f:357:ARG:NH2	32:f:754:LYS:HG3	2.33	0.44
32:f:646:MET:HA	32:f:649:HIS:HD1	1.82	0.44
32:f:695:ALA:O	32:f:752:HIS:HB3	2.15	0.44
2:V:294:ARG:HH21	2:V:331:LEU:HD23	1.82	0.44
4:X:213:GLN:O	4:X:217:ILE:HB	2.18	0.44
13:H:80:GLY:HA2	13:H:83:TYR:HB3	2.00	0.44
18:M:228:PRO:HB2	18:M:231:ILE:HB	1.99	0.44
15:j:97:THR:OG1	15:j:98:VAL:N	2.51	0.44
28:C:184:LYS:HB3	28:C:288:ASN:ND2	2.33	0.44
1:U:229:VAL:HG13	1:U:268:LEU:HD11	2.00	0.44
4:X:328:ASP:HA	4:X:331:LEU:HD13	2.00	0.44
5:Y:60:SER:OG	5:Y:61:LEU:N	2.49	0.44
5:Y:315:THR:HG1	5:Y:352:GLU:CD	2.23	0.44
6:Z:189:GLN:HG3	9:c:300:LEU:HD13	2.00	0.44
7:a:122:LYS:HD3	7:a:131:THR:HG22	2.00	0.44
9:c:211:GLU:HA	9:c:214:GLN:HB3	1.98	0.44
12:G:31:ALA:HB1	12:G:83:MET:HE3	2.00	0.44
26:A:211:GLY:HA3	26:A:337:LEU:HD23	1.99	0.44
30:E:261:LEU:HD22	30:E:294:ARG:NH1	2.33	0.44
32:f:282:PHE:HE2	32:f:317:LEU:HD21	1.83	0.44
32:f:376:PHE:CZ	32:f:798:THR:CB	2.91	0.44
32:f:412:ALA:HA	32:f:447:ALA:HB2	2.00	0.44
32:f:698:SER:OG	32:f:716:ASP:OD1	2.36	0.44
32:f:742:ALA:CA	32:f:745:LEU:CD2	2.62	0.44
1:U:633:CYS:HA	1:U:636:VAL:HG22	1.99	0.44
2:V:29:PRO:HA	2:V:32:PRO:HD2	2.00	0.44
2:V:171:VAL:HG22	2:V:175:MET:HE3	2.00	0.44
4:X:225:TRP:O	4:X:229:TYR:CB	2.64	0.44
22:Q:64:VAL:HG13	22:Q:75:LEU:HD12	2.00	0.44
17:l:215:VAL:HB	17:l:221:PHE:HD1	1.82	0.44
18:m:40:ARG:HE	18:m:161:TRP:CD1	2.35	0.44
26:A:98:CYS:HB3	27:B:130:GLU:HB2	2.00	0.44
28:C:293:MET:HE2	28:C:295:THR:HB	2.00	0.44
28:C:395:SER:OG	28:C:396:GLU:N	2.50	0.44
29:D:342:ARG:NH2	29:D:361:GLU:OE2	2.50	0.44
31:F:285:ILE:N	31:F:329:ILE:O	2.51	0.44
32:f:664:GLU:HA	32:f:697:ILE:CA	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:690:VAL:O	32:f:694:LEU:HB2	2.18	0.44
2:V:189:ASP:HB3	2:V:234:ARG:HH12	1.82	0.44
5:Y:190:ALA:HA	5:Y:287:LEU:HB2	1.98	0.44
8:b:145:GLU:HA	8:b:173:VAL:HG13	2.00	0.44
12:G:89:SER:OG	18:M:117:MET:SD	2.71	0.44
18:m:230:ASP:OD1	18:m:230:ASP:N	2.51	0.44
27:B:438:LEU:HD22	27:B:438:LEU:HA	1.88	0.44
30:E:138:LEU:HB3	30:E:141:GLN:HB2	1.99	0.44
32:f:22:GLY:O	32:f:26:GLU:CB	2.66	0.44
32:f:281:ILE:O	32:f:285:CYS:HB2	2.18	0.44
1:U:564:ASP:OD1	1:U:590:TYR:OH	2.30	0.43
2:V:96:ARG:NH1	2:V:114:TYR:OH	2.51	0.43
4:X:379:ASP:HB3	4:X:384:VAL:H	1.82	0.43
5:Y:229:ILE:HG13	5:Y:299:MET:SD	2.58	0.43
7:a:34:TRP:H	8:b:18:ASN:HB2	1.83	0.43
15:J:88:ARG:NH1	22:Q:69:MET:O	2.50	0.43
19:N:120:MET:H	25:T:61:GLN:HE22	1.66	0.43
22:Q:164:LEU:HA	22:Q:167:LEU:HD12	1.99	0.43
14:i:162:THR:OG1	14:i:163:CYS:N	2.51	0.43
31:F:89:LEU:HD22	31:F:155:LYS:HG2	2.00	0.43
32:f:311:VAL:CA	32:f:490:ALA:HB1	2.48	0.43
32:f:509:LYS:HB3	32:f:514:VAL:HG21	1.99	0.43
4:X:256:LEU:HD23	4:X:322:HIS:CD2	2.53	0.43
12:G:103:TYR:HB2	19:N:61:TYR:CD1	2.53	0.43
14:I:63:GLU:OE1	14:I:64:LYS:NZ	2.40	0.43
15:J:159:ASN:OD1	15:J:160:ALA:N	2.51	0.43
16:K:46:VAL:HG23	16:K:151:PRO:HB2	2.00	0.43
29:D:86:PRO:HB2	29:D:134:LYS:HE3	1.99	0.43
29:D:97:ASP:OD1	29:D:97:ASP:N	2.51	0.43
31:F:246:ALA:HB1	31:F:280:PRO:HB2	2.00	0.43
32:f:664:GLU:O	32:f:665:GLU:C	2.57	0.43
32:f:688:ARG:HG3	32:f:745:LEU:HB3	1.99	0.43
1:U:197:VAL:HA	1:U:200:VAL:HG12	2.01	0.43
2:V:470:ARG:HD2	10:d:242:LEU:HD12	2.00	0.43
3:W:254:PRO:HB2	3:W:263:TRP:CD1	2.52	0.43
3:W:312:MET:HB3	3:W:362:ASN:HD21	1.83	0.43
8:b:20:ASP:OD1	8:b:20:ASP:N	2.51	0.43
8:b:54:LEU:HD13	8:b:84:ILE:HA	2.00	0.43
9:c:134:GLU:HB3	9:c:140:ALA:HB3	2.00	0.43
14:i:44:LEU:HA	14:i:215:THR:HA	1.99	0.43
17:l:146:GLN:HE21	17:l:154:PHE:HD2	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:478:ARG:HD3	32:f:504:VAL:CG1	2.45	0.43
1:U:24:LEU:HA	1:U:27:LEU:HD12	2.00	0.43
2:V:447:ILE:HG23	2:V:449:ALA:H	1.83	0.43
3:W:45:GLU:HG2	3:W:95:SER:HB2	1.99	0.43
5:Y:20:ALA:HB2	5:Y:150:PHE:HD1	1.82	0.43
8:b:52:ILE:HD11	8:b:58:CYS:HB3	1.99	0.43
8:b:90:ILE:HG13	8:b:109:ILE:HG21	1.99	0.43
21:P:17:LYS:HB2	21:P:158:MET:H	1.83	0.43
16:k:97:GLN:HG2	23:r:65:ILE:HG13	1.99	0.43
17:l:72:ILE:HG22	17:l:134:ILE:HG12	2.01	0.43
28:C:27:LYS:HA	29:D:44:TYR:CZ	2.54	0.43
29:D:387:VAL:HA	29:D:390:ASN:HA	2.00	0.43
32:f:494:ARG:HE	32:f:494:ARG:CA	2.32	0.43
1:U:676:THR:HA	1:U:684:ARG:HG2	2.01	0.43
2:V:184:ALA:HA	2:V:187:ILE:HD12	1.99	0.43
2:V:422:ILE:HA	2:V:425:LYS:HE2	1.99	0.43
3:W:145:LEU:HD13	3:W:185:PHE:HB2	2.00	0.43
8:b:110:ILE:HG22	8:b:139:ASP:HB2	2.01	0.43
10:d:38:THR:O	10:d:45:LYS:NZ	2.51	0.43
20:O:163:ILE:HA	20:O:168:GLY:HA3	1.99	0.43
25:T:145:LEU:HD23	20:o:132:LEU:HB3	1.99	0.43
24:s:13:LEU:HD11	24:s:149:LEU:HD11	2.00	0.43
26:A:396:ALA:HA	26:A:401:ARG:HB2	1.99	0.43
28:C:147:THR:OG1	28:C:148:TYR:N	2.52	0.43
29:D:133:HIS:HB3	29:D:137:ASN:N	2.34	0.43
31:F:187:ASP:HA	31:F:368:ILE:HD13	2.00	0.43
32:f:286:LYS:HD3	32:f:326:LEU:HD23	2.00	0.43
1:U:567:ILE:HG22	1:U:601:ARG:HH12	1.83	0.43
2:V:484:LEU:HA	2:V:487:HIS:CD2	2.52	0.43
6:Z:26:ILE:HA	6:Z:29:VAL:HG22	2.00	0.43
7:a:87:MET:HE1	7:a:93:ALA:HB2	2.00	0.43
7:a:100:THR:HA	7:a:103:LYS:HG2	2.00	0.43
7:a:220:PRO:HA	7:a:223:GLU:HG2	2.00	0.43
7:a:252:LYS:HA	7:a:255:TRP:HB2	2.00	0.43
12:G:212:PRO:HB3	12:G:235:ILE:HG22	2.00	0.43
25:T:25:ASP:HA	25:T:187:PHE:HA	2.01	0.43
15:j:32:ALA:HB3	15:j:161:ILE:HD11	2.00	0.43
18:m:40:ARG:HA	18:m:45:VAL:HA	2.01	0.43
21:p:62:THR:OG1	22:q:85:ARG:NH2	2.51	0.43
27:B:121:ALA:O	27:B:133:VAL:N	2.52	0.43
28:C:250:GLU:HG3	29:D:290:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:77:GLU:O	32:f:81:GLN:HB2	2.19	0.43
32:f:303:VAL:HG22	32:f:339:ILE:HA	2.00	0.43
32:f:494:ARG:NE	32:f:494:ARG:CA	2.82	0.43
32:f:513:GLU:HG3	32:f:557:TRP:HZ3	1.84	0.43
1:U:482:GLY:HA3	1:U:515:ALA:HB1	2.00	0.43
3:W:178:GLU:OE2	3:W:181:GLU:N	2.41	0.43
3:W:445:LEU:HD12	3:W:448:LYS:HZ1	1.83	0.43
5:Y:123:ALA:O	5:Y:127:THR:HG22	2.19	0.43
7:a:38:THR:HG23	7:a:75:SER:HB3	2.00	0.43
8:b:30:GLN:HG3	8:b:75:LEU:HB3	1.99	0.43
10:d:55:LEU:HD23	10:d:55:LEU:HA	1.81	0.43
19:N:142:THR:HB	19:N:155:PHE:HE1	1.84	0.43
17:l:157:ARG:HD2	17:l:176:MET:HE3	2.01	0.43
22:q:101:ASN:HB3	22:q:132:HIS:CD2	2.53	0.43
26:A:154:PRO:HB2	26:A:157:ILE:HG23	2.00	0.43
27:B:227:PRO:HG2	27:B:355:LEU:HG	2.01	0.43
28:C:224:ILE:HG23	28:C:231:VAL:HG21	2.01	0.43
29:D:283:ARG:HB3	29:D:287:ARG:HH11	1.84	0.43
1:U:62:LEU:HD12	1:U:84:ALA:HB1	2.01	0.43
2:V:419:LEU:O	2:V:423:ALA:CB	2.67	0.43
5:Y:92:GLU:HA	5:Y:100:ILE:HD13	1.99	0.43
6:Z:15:VAL:HG21	6:Z:53:SER:N	2.34	0.43
6:Z:136:GLU:HA	6:Z:160:SER:HB3	2.01	0.43
6:Z:139:ILE:HG22	6:Z:158:VAL:HG21	2.00	0.43
9:c:245:VAL:HG12	9:c:246:LYS:HG3	2.00	0.43
14:I:232:GLU:HA	14:I:235:GLN:HG2	2.00	0.43
16:K:197:SER:O	16:K:201:ILE:HG12	2.19	0.43
12:g:94:ALA:HB1	12:g:114:LEU:HD21	2.00	0.43
26:A:250:VAL:HA	26:A:294:GLU:HG2	2.01	0.43
28:C:352:PRO:HD3	28:C:391:MET:SD	2.58	0.43
30:E:238:ILE:HD11	30:E:256:THR:HG21	2.00	0.43
32:f:130:ALA:O	32:f:134:SER:CB	2.64	0.43
32:f:228:LYS:O	32:f:232:TYR:HB3	2.19	0.43
32:f:248:LEU:O	32:f:252:ALA:HB3	2.19	0.43
1:U:602:LEU:O	1:U:606:ALA:HB2	2.18	0.43
1:U:699:THR:O	1:U:702:THR:OG1	2.30	0.43
2:V:419:LEU:HD23	2:V:458:VAL:HG23	2.00	0.43
4:X:257:CYS:O	4:X:261:LEU:N	2.48	0.43
9:c:29:GLU:O	9:c:204:THR:OG1	2.36	0.43
9:c:113:HIS:CE1	9:c:144:VAL:HG22	2.54	0.43
10:d:99:LEU:HD21	10:d:122:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:g:116:LYS:HG2	12:g:160:TYR:CZ	2.53	0.43
14:i:105:ILE:HD11	14:i:109:GLN:HG3	2.00	0.43
30:E:116:ASP:O	30:E:118:LEU:N	2.52	0.43
32:f:402:ASN:OD1	32:f:403:LYS:N	2.52	0.43
32:f:536:SER:O	32:f:540:GLN:CB	2.66	0.43
1:U:472:ILE:HD12	1:U:473:VAL:HG23	2.01	0.43
10:d:215:TRP:HE1	10:d:222:TYR:HD1	1.67	0.43
14:I:5:TYR:HA	15:J:5:ARG:NH2	2.33	0.43
16:K:89:ILE:HD13	16:K:89:ILE:HA	1.86	0.43
16:k:91:LYS:HE2	16:k:119:LEU:HD11	2.00	0.43
24:s:125:ASP:OD1	24:s:129:SER:N	2.45	0.43
27:B:334:ILE:HA	27:B:337:LEU:HD23	2.00	0.43
27:B:387:LYS:HB2	27:B:430:LYS:HE3	2.01	0.43
28:C:250:GLU:HB3	28:C:293:MET:HE1	1.99	0.43
28:C:273:MET:HA	28:C:276:LEU:HD12	2.01	0.43
28:C:375:ARG:HH22	28:C:379:THR:HG23	1.84	0.43
30:E:312:ILE:O	30:E:316:HIS:ND1	2.42	0.43
32:f:368:ALA:O	32:f:372:LEU:HB2	2.18	0.43
2:V:391:THR:HG23	2:V:394:LEU:HD23	2.00	0.42
3:W:308:LEU:HA	3:W:312:MET:HA	2.01	0.42
3:W:374:THR:HA	3:W:412:ILE:HA	2.01	0.42
6:Z:7:GLN:OE1	6:Z:46:LYS:NZ	2.52	0.42
14:I:34:CYS:H	14:I:164:ILE:HG13	1.84	0.42
18:M:100:SER:HA	25:T:65:GLN:HE21	1.84	0.42
24:S:68:ILE:HD11	24:S:92:LEU:HD13	2.01	0.42
23:r:42:LEU:HD21	23:r:184:TRP:CD2	2.54	0.42
29:D:272:THR:HA	29:D:316:THR:HA	2.01	0.42
31:F:231:THR:HG22	31:F:357:PRO:HD3	2.00	0.42
32:f:688:ARG:CA	32:f:745:LEU:HD22	2.44	0.42
32:f:794:ALA:HA	32:f:797:LEU:HB2	2.01	0.42
2:V:289:LEU:HA	2:V:292:THR:HG22	2.02	0.42
2:V:339:LEU:HB3	2:V:341:GLU:HG2	2.00	0.42
2:V:487:HIS:CE1	6:Z:274:ASN:HB2	2.54	0.42
3:W:288:HIS:HA	3:W:291:SER:HB3	2.00	0.42
3:W:401:THR:HG23	3:W:402:ILE:HD12	2.01	0.42
6:Z:17:LEU:HG	9:c:213:GLU:HG3	2.00	0.42
7:a:6:GLY:HA2	7:a:9:GLN:HB2	2.00	0.42
8:b:31:ASP:HA	8:b:34:ASN:HB2	2.00	0.42
15:J:180:ALA:HA	15:J:181:ILE:HA	1.83	0.42
17:L:42:THR:O	17:L:137:TYR:OH	2.35	0.42
17:L:51:ARG:NH1	31:F:439:ALA:OXT	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:104:ASP:N	19:N:108:GLY:O	2.50	0.42
15:j:55:ASP:OD1	15:j:56:GLU:N	2.52	0.42
15:j:114:LEU:O	15:j:118:TYR:HB2	2.19	0.42
16:k:99:HIS:O	16:k:103:TYR:HB2	2.19	0.42
21:p:126:LEU:HD12	21:p:127:ILE:HG23	2.00	0.42
22:q:103:LEU:HD23	22:q:132:HIS:CE1	2.53	0.42
27:B:113:GLU:HG2	27:B:114:GLU:HB2	2.00	0.42
28:C:401:ILE:HG22	28:C:402:LYS:HG2	2.01	0.42
30:E:351:GLY:HA3	31:F:217:ILE:HD13	2.01	0.42
32:f:376:PHE:CZ	32:f:798:THR:CG2	2.91	0.42
32:f:389:LYS:HD3	32:f:389:LYS:H	1.81	0.42
6:Z:14:LEU:HG	9:c:39:LEU:HD22	2.00	0.42
8:b:58:CYS:SG	8:b:88:THR:OG1	2.72	0.42
9:c:145:VAL:HG22	9:c:147:PRO:HD3	2.01	0.42
16:K:167:ALA:HB3	16:K:181:LEU:HD21	2.01	0.42
17:L:50:LYS:HD3	17:L:59:HIS:HB2	2.00	0.42
16:k:236:GLU:HA	16:k:239:LYS:HG2	2.01	0.42
17:l:148:CYS:SG	17:l:152:ASN:N	2.84	0.42
22:q:19:ARG:HE	22:q:31:ASP:HA	1.85	0.42
30:E:191:LEU:HB2	30:E:195:PHE:CZ	2.54	0.42
30:E:313:LEU:O	30:E:317:ALA:N	2.52	0.42
32:f:631:LYS:HA	32:f:634:LYS:HZ2	1.84	0.42
32:f:635:LYS:HD3	32:f:641:GLU:HG2	2.01	0.42
1:U:204:ILE:HD12	1:U:207:ASN:HD22	1.85	0.42
1:U:454:GLY:HA3	1:U:458:ILE:HG13	2.01	0.42
2:V:326:GLN:NE2	2:V:348:PHE:O	2.40	0.42
3:W:374:THR:HG22	3:W:412:ILE:HG13	2.00	0.42
4:X:320:SER:O	4:X:324:ALA:HB2	2.20	0.42
7:a:217:LEU:HD21	7:a:237:LEU:HB3	2.00	0.42
9:c:191:ALA:HA	9:c:194:HIS:CE1	2.55	0.42
12:G:141:ILE:HG22	12:G:151:VAL:HG22	2.01	0.42
14:I:155:ASN:HA	15:J:81:ARG:HH22	1.84	0.42
15:J:90:GLU:HG2	15:J:110:TYR:CG	2.55	0.42
20:O:85:GLN:O	20:O:89:ARG:HB2	2.19	0.42
18:m:144:ASP:O	18:m:147:GLN:NE2	2.51	0.42
23:r:37:ILE:HG23	23:r:60:ALA:HB2	2.02	0.42
26:A:123:VAL:HG12	31:F:87:PRO:HG3	2.00	0.42
26:A:355:PHE:CD2	26:A:370:PHE:HB3	2.54	0.42
31:F:97:LEU:N	31:F:121:CYS:O	2.45	0.42
32:f:80:ARG:HE	32:f:99:LEU:HD13	1.85	0.42
32:f:479:LEU:HD23	32:f:513:GLU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:623:LYS:O	32:f:627:GLU:HB3	2.17	0.42
3:W:344:THR:O	3:W:348:GLU:CB	2.67	0.42
6:Z:11:VAL:HB	6:Z:162:ILE:HG23	2.02	0.42
12:G:158:GLY:O	13:H:84:ARG:NH2	2.52	0.42
14:I:35:LEU:HG	14:I:46:ALA:HB3	2.00	0.42
14:i:164:ILE:HG22	14:i:165:GLY:H	1.84	0.42
20:o:172:ASN:HB3	20:o:191:VAL:HG22	2.01	0.42
23:r:22:ALA:N	23:r:25:TYR:O	2.43	0.42
24:s:73:LYS:O	24:s:77:HIS:ND1	2.41	0.42
28:C:155:ASP:HA	28:C:158:ILE:HD12	2.01	0.42
30:E:255:ARG:HA	30:E:258:MET:HE3	2.02	0.42
31:F:318:ASP:HB3	31:F:347:ARG:HE	1.83	0.42
32:f:380:PHE:CB	32:f:751:TYR:CE2	2.99	0.42
1:U:11:LEU:HD21	10:d:77:GLN:HE21	1.85	0.42
7:a:265:GLU:HG3	7:a:268:LEU:HD12	2.01	0.42
9:c:244:VAL:HG12	9:c:245:VAL:HG23	2.01	0.42
19:N:18:SER:HB2	19:N:31:THR:H	1.85	0.42
23:R:141:ARG:NH2	22:q:162:LYS:HB3	2.34	0.42
13:h:14:SER:OG	13:h:17:GLY:N	2.53	0.42
17:l:225:ASP:OD1	17:l:225:ASP:N	2.52	0.42
18:m:201:HIS:CE1	18:m:206:ASP:H	2.37	0.42
26:A:233:THR:HB	26:A:269:ALA:HB1	2.01	0.42
29:D:170:MET:HE3	29:D:170:MET:HB2	1.93	0.42
4:X:251:LEU:HD11	4:X:275:LEU:HG	2.00	0.42
5:Y:80:GLU:HA	5:Y:83:ARG:HG2	2.02	0.42
6:Z:167:ALA:O	6:Z:169:GLU:N	2.53	0.42
6:Z:193:ASN:HA	6:Z:196:HIS:CE1	2.54	0.42
9:c:303:MET:HE3	9:c:303:MET:HB3	1.88	0.42
16:K:21:LEU:HA	16:K:22:PHE:HB2	2.02	0.42
20:O:13:VAL:HG22	20:O:177:VAL:HG22	2.02	0.42
24:S:211:ARG:NH2	24:S:213:ASP:OD2	2.47	0.42
21:p:36:THR:OG1	21:p:38:ASP:OD1	2.27	0.42
31:F:206:MET:HE3	31:F:246:ALA:HB2	2.01	0.42
32:f:389:LYS:O	32:f:392:THR:OG1	2.37	0.42
32:f:573:ILE:HG22	32:f:576:ILE:HB	2.01	0.42
32:f:645:ASP:O	32:f:649:HIS:ND1	2.51	0.42
2:V:487:HIS:CE1	6:Z:274:ASN:HD22	2.37	0.42
3:W:206:SER:HA	3:W:209:ILE:HG12	2.02	0.42
6:Z:166:GLU:HB3	6:Z:167:ALA:H	1.75	0.42
15:J:64:ALA:O	15:J:88:ARG:NH1	2.53	0.42
19:N:144:ARG:NH2	19:N:151:GLU:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:P:58:THR:OG1	22:Q:121:LEU:O	2.22	0.42
26:A:208:PRO:HG2	26:A:210:LYS:HE2	2.01	0.42
26:A:407:LYS:HA	26:A:410:LEU:HD12	2.01	0.42
29:D:133:HIS:HB3	29:D:137:ASN:H	1.84	0.42
32:f:122:ALA:HB1	32:f:126:ILE:HD12	2.01	0.42
32:f:471:LEU:HD11	32:f:509:LYS:HE2	2.00	0.42
32:f:664:GLU:HB3	32:f:696:LEU:CG	2.43	0.42
1:U:374:SER:HB3	1:U:411:ILE:HG12	2.02	0.42
2:V:94:VAL:HG11	2:V:134:PHE:HB3	2.02	0.42
2:V:338:LEU:HD22	2:V:397:ARG:HG3	2.02	0.42
2:V:350:GLN:HG3	2:V:352:SER:H	1.85	0.42
2:V:359:PRO:HG2	2:V:385:LYS:HG2	2.02	0.42
12:G:191:PHE:HE1	12:G:219:VAL:HG21	1.85	0.42
13:H:105:ILE:HG12	13:H:110:LEU:HD12	2.00	0.42
20:O:132:LEU:HB3	25:t:145:LEU:HD23	2.02	0.42
26:A:383:ALA:HB2	34:A:501:AGS:H5'2	2.02	0.42
28:C:89:VAL:H	28:C:89:VAL:HG23	1.55	0.42
32:f:359:GLY:O	32:f:363:SER:CB	2.50	0.42
32:f:374:SER:O	32:f:375:SER:C	2.59	0.42
1:U:59:PHE:HA	1:U:62:LEU:HB2	2.01	0.42
1:U:237:VAL:HA	1:U:321:GLN:HE21	1.85	0.42
5:Y:380:VAL:HG23	6:Z:279:LYS:HE2	2.02	0.42
7:a:33:LEU:HA	8:b:20:ASP:HB3	2.00	0.42
7:a:57:ILE:HG13	7:a:60:TYR:HB3	2.01	0.42
10:d:99:LEU:HB3	10:d:133:ILE:HD11	2.01	0.42
12:G:7:ALA:HA	12:G:8:GLY:HA3	1.78	0.42
13:H:174:LEU:HD21	13:H:194:THR:HG21	2.01	0.42
15:J:32:ALA:HB3	15:J:161:ILE:HD11	2.02	0.42
18:M:123:THR:HG22	18:M:130:PRO:HB3	2.02	0.42
20:O:83:LEU:HD23	20:O:83:LEU:HA	1.93	0.42
21:P:36:THR:OG1	21:P:38:ASP:OD1	2.27	0.42
19:n:135:ILE:O	19:n:139:VAL:HB	2.18	0.42
21:p:58:THR:O	22:q:85:ARG:NH2	2.53	0.42
24:s:16:ALA:HB2	24:s:121:VAL:HG23	2.02	0.42
27:B:136:LEU:HD12	27:B:160:ILE:HG23	2.02	0.42
29:D:171:ASP:O	29:D:175:GLN:CB	2.68	0.42
31:F:247:THR:HG21	31:F:278:LYS:HE3	2.01	0.42
32:f:86:THR:HG23	32:f:87:THR:H	1.85	0.42
32:f:282:PHE:HD1	32:f:282:PHE:HA	1.74	0.42
32:f:688:ARG:HA	32:f:745:LEU:CB	2.49	0.42
3:W:259:GLU:HG2	3:W:261:GLU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:247:LEU:HA	5:Y:250:LEU:HG	2.02	0.41
14:i:229:LYS:N	14:i:232:GLU:OE2	2.53	0.41
16:k:209:LYS:O	16:k:214:ASN:ND2	2.53	0.41
18:m:99:ARG:HH21	18:m:105:ASN:HA	1.85	0.41
23:r:196:HIS:O	23:r:200:SER:CB	2.67	0.41
26:A:184:ILE:HA	26:A:187:LEU:HB3	2.02	0.41
26:A:302:LEU:O	26:A:306:LEU:HB2	2.20	0.41
27:B:247:PHE:HE2	27:B:249:ARG:HB2	1.85	0.41
32:f:629:LYS:HE2	32:f:660:ILE:HG21	2.02	0.41
1:U:545:LEU:O	1:U:549:ALA:CB	2.65	0.41
2:V:337:LEU:HD23	2:V:342:ILE:HG21	2.02	0.41
14:I:105:ILE:HG12	14:I:110:LEU:HB2	2.02	0.41
16:K:196:LYS:HA	16:K:199:LEU:HG	2.02	0.41
20:O:198:ARG:NH2	20:O:202:TYR:H	2.19	0.41
22:Q:142:ILE:HG21	23:r:141:ARG:HH21	1.84	0.41
23:R:196:HIS:O	23:R:200:SER:CB	2.68	0.41
26:A:333:ARG:HA	26:A:334:PRO:HD3	1.85	0.41
27:B:295:TYR:HB2	27:B:298:ASN:HB2	2.02	0.41
29:D:348:ILE:HG13	34:D:501:AGS:H2	2.02	0.41
31:F:191:LEU:HD12	31:F:235:LEU:CD2	2.50	0.41
31:F:382:GLU:O	31:F:386:ARG:CB	2.68	0.41
32:f:81:GLN:O	32:f:85:SER:HB2	2.21	0.41
3:W:115:ILE:HG12	3:W:119:PRO:HG2	2.02	0.41
3:W:299:ILE:HG22	3:W:302:TYR:H	1.85	0.41
3:W:405:LYS:HD2	3:W:419:LYS:HE3	2.01	0.41
6:Z:269:VAL:HG12	6:Z:273:HIS:CE1	2.55	0.41
7:a:233:LEU:HA	7:a:236:THR:HG22	2.02	0.41
16:K:241:ILE:HD12	16:K:241:ILE:HA	1.94	0.41
22:Q:29:LYS:HE3	22:Q:32:HIS:HA	2.03	0.41
25:T:46:ASN:OD1	25:T:46:ASN:N	2.53	0.41
12:g:6:SER:HB2	12:g:11:ARG:HE	1.84	0.41
15:j:11:SER:OG	15:j:15:HIS:N	2.44	0.41
15:j:221:ASN:HA	15:j:222:PRO:HD3	1.90	0.41
20:o:32:SER:HA	20:o:187:ARG:HH12	1.85	0.41
26:A:103:ASN:O	26:A:112:ILE:N	2.53	0.41
26:A:153:LEU:O	26:A:155:PRO:HD3	2.20	0.41
30:E:260:LEU:HD22	30:E:264:MET:HE3	2.02	0.41
32:f:170:TRP:CZ3	32:f:208:LEU:HB3	2.56	0.41
1:U:637:VAL:HG22	1:U:640:LEU:HD12	2.03	0.41
1:U:836:THR:OG1	1:U:837:ALA:N	2.54	0.41
2:V:44:GLY:O	2:V:48:THR:OG1	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:320:SER:O	4:X:324:ALA:CB	2.68	0.41
17:L:155:ASP:HB3	18:M:62:SER:HB2	2.02	0.41
12:g:39:SER:OG	12:g:168:ALA:O	2.29	0.41
18:m:36:ALA:O	18:m:165:ILE:N	2.48	0.41
19:n:127:ILE:HD13	19:n:136:TYR:HB2	2.02	0.41
20:o:203:ARG:HD2	20:o:203:ARG:HA	1.80	0.41
29:D:54:LEU:O	29:D:58:GLU:HB2	2.20	0.41
32:f:389:LYS:CD	32:f:389:LYS:N	2.83	0.41
1:U:409:GLY:HA3	1:U:445:ALA:HB1	2.01	0.41
5:Y:22:LEU:HA	5:Y:25:LEU:HB3	2.02	0.41
6:Z:190:ARG:HA	6:Z:193:ASN:HB2	2.03	0.41
22:Q:57:ALA:O	22:Q:61:GLN:CB	2.68	0.41
16:k:108:THR:O	16:k:111:SER:OG	2.31	0.41
19:n:127:ILE:HG21	19:n:136:TYR:HB2	2.02	0.41
26:A:338:ASP:OD1	26:A:338:ASP:N	2.54	0.41
26:A:423:PHE:HE2	26:A:425:ALA:HB3	1.86	0.41
2:V:99:ARG:HB3	2:V:144:ASP:O	2.20	0.41
3:W:53:GLN:O	3:W:56:THR:OG1	2.30	0.41
4:X:375:HIS:HB3	4:X:389:ASP:HB3	2.02	0.41
5:Y:25:LEU:HD12	5:Y:29:PRO:HG2	2.02	0.41
7:a:28:LEU:HG	7:a:33:LEU:HD11	2.02	0.41
16:K:155:HIS:CG	16:K:168:ARG:HG2	2.56	0.41
17:L:121:GLN:HE22	18:M:131:PHE:HE1	1.68	0.41
17:L:148:CYS:SG	17:L:152:ASN:N	2.85	0.41
20:O:211:VAL:HG11	21:P:198:ARG:HD3	2.03	0.41
22:q:92:LEU:HD11	22:q:121:LEU:HD23	2.02	0.41
25:t:166:ARG:NH1	25:t:170:GLU:OE2	2.54	0.41
26:A:153:LEU:HG	26:A:154:PRO:HD2	2.02	0.41
26:A:312:ARG:HH22	26:A:317:VAL:N	2.17	0.41
28:C:246:ILE:HB	28:C:291:VAL:HG12	2.03	0.41
31:F:124:ILE:HG21	31:F:153:VAL:HG21	2.03	0.41
32:f:8:LYS:HA	32:f:8:LYS:HD2	1.94	0.41
1:U:100:ILE:HA	1:U:103:LYS:HZ1	1.85	0.41
1:U:370:VAL:O	1:U:374:SER:CB	2.69	0.41
1:U:611:ASN:HD22	1:U:612:ASP:H	1.66	0.41
2:V:32:PRO:O	2:V:36:GLU:HB2	2.19	0.41
5:Y:140:ILE:HD13	5:Y:140:ILE:HA	1.92	0.41
5:Y:301:ILE:HD11	5:Y:343:LEU:HB2	2.01	0.41
10:d:233:GLU:HG3	10:d:236:THR:HG23	2.01	0.41
14:I:95:GLN:HG3	21:P:69:PHE:CD1	2.55	0.41
15:J:97:THR:OG1	15:J:98:VAL:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:i:20:GLN:HB3	14:i:129:PRO:HG3	2.03	0.41
19:n:40:ARG:HH12	19:n:183:GLY:HA2	1.85	0.41
29:D:167:ILE:HG12	29:D:214:MET:HG2	2.03	0.41
29:D:384:MET:HA	29:D:387:VAL:HB	2.03	0.41
32:f:338:ASP:HA	32:f:341:GLU:HG3	2.02	0.41
32:f:479:LEU:HD11	32:f:514:VAL:HG23	2.03	0.41
1:U:81:ALA:HB1	1:U:88:PHE:CZ	2.56	0.41
1:U:516:LEU:HD12	1:U:516:LEU:HA	1.87	0.41
1:U:797:MET:HA	1:U:844:LYS:HD3	2.02	0.41
3:W:448:LYS:HE3	6:Z:230:LEU:HD22	2.02	0.41
10:d:171:LEU:HD23	10:d:174:ILE:HD12	2.03	0.41
14:I:34:CYS:HB2	14:I:164:ILE:HG13	2.02	0.41
12:g:132:ARG:HA	12:g:133:PRO:HD3	1.81	0.41
19:n:166:ARG:HA	19:n:166:ARG:HD3	1.93	0.41
1:U:204:ILE:HA	1:U:207:ASN:HB2	2.02	0.41
1:U:487:GLY:HA2	1:U:521:LEU:HB3	2.03	0.41
2:V:251:LEU:HD21	2:V:275:VAL:HG12	2.03	0.41
2:V:287:ARG:HD3	11:e:4:LYS:HE3	2.02	0.41
3:W:354:LEU:HD12	3:W:357:ARG:HB2	2.02	0.41
3:W:452:ILE:HB	6:Z:214:LYS:HE2	2.02	0.41
5:Y:137:ARG:HD3	5:Y:167:LEU:HB3	2.03	0.41
7:a:70:ARG:HE	8:b:26:LEU:HD13	1.85	0.41
8:b:22:LEU:HD23	8:b:180:ALA:H	1.86	0.41
8:b:84:ILE:HG12	8:b:117:VAL:HG23	2.02	0.41
13:H:82:ASP:HB3	13:H:130:PHE:HD1	1.85	0.41
16:K:195:ILE:O	16:K:198:SER:OG	2.32	0.41
17:L:52:ALA:HB2	17:L:59:HIS:HD2	1.85	0.41
18:M:144:ASP:O	18:M:147:GLN:NE2	2.49	0.41
19:N:7:GLN:HA	19:N:12:VAL:HA	2.02	0.41
25:T:28:GLY:HA3	25:T:36:PHE:HB2	2.03	0.41
15:j:4:ASP:HB3	16:k:126:GLU:HB3	2.03	0.41
15:j:132:LEU:HD11	15:j:161:ILE:HG12	2.03	0.41
25:t:54:SER:OG	25:t:55:GLY:N	2.54	0.41
28:C:219:LEU:HB3	28:C:222:LYS:HB3	2.03	0.41
28:C:232:ARG:HG2	28:C:235:PHE:CD2	2.55	0.41
31:F:205:PRO:HB2	31:F:327:LYS:HE3	2.03	0.41
31:F:314:LEU:HD21	31:F:342:LEU:HA	2.03	0.41
32:f:8:LYS:HD3	32:f:39:LYS:HD2	2.02	0.41
32:f:40:ASP:HB3	32:f:41:LYS:H	1.70	0.41
32:f:303:VAL:HG13	32:f:339:ILE:HG13	2.02	0.41
32:f:333:LEU:HD23	32:f:338:ASP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:478:ARG:HD3	32:f:504:VAL:HG22	2.03	0.41
32:f:483:PHE:HE2	32:f:799:VAL:HB	1.69	0.41
32:f:512:MET:HE1	32:f:554:TYR:HA	2.02	0.41
32:f:533:ASP:OD1	32:f:533:ASP:N	2.53	0.41
1:U:264:VAL:HG22	1:U:268:LEU:HD13	2.02	0.41
1:U:474:ARG:HH21	1:U:500:ASN:ND2	2.18	0.41
2:V:204:ASP:HA	2:V:207:ALA:HB3	2.03	0.41
3:W:377:ARG:HE	7:a:326:GLU:HG2	1.86	0.41
5:Y:301:ILE:HA	5:Y:304:TYR:HB2	2.03	0.41
6:Z:118:ASN:OD1	6:Z:118:ASN:N	2.54	0.41
8:b:26:LEU:HA	8:b:29:GLN:HE21	1.86	0.41
11:e:49:GLU:O	11:e:53:SER:N	2.54	0.41
21:P:171:MET:O	21:P:175:VAL:HB	2.21	0.41
17:l:71:GLY:HA3	17:l:221:PHE:CZ	2.56	0.41
26:A:112:ILE:HG12	26:A:122:VAL:HG22	2.02	0.41
28:C:215:SER:O	28:C:217:SER:N	2.53	0.41
28:C:268:GLU:OE2	28:C:271:ARG:NH2	2.54	0.41
29:D:368:ASP:HB3	29:D:370:ILE:HG23	2.03	0.41
32:f:86:THR:O	32:f:87:THR:HB	2.21	0.41
32:f:479:LEU:HD23	32:f:513:GLU:CB	2.42	0.41
32:f:620:PHE:HD2	32:f:623:LYS:HG2	1.85	0.41
1:U:164:GLU:HA	1:U:167:ILE:HG12	2.02	0.40
1:U:445:ALA:HA	1:U:448:LEU:HD12	2.03	0.40
1:U:615:ARG:HE	1:U:648:VAL:HG21	1.87	0.40
1:U:616:ARG:HD3	1:U:768:GLN:NE2	2.36	0.40
4:X:378:LEU:HG	4:X:385:LEU:HD13	2.02	0.40
7:a:132:LYS:O	7:a:136:GLU:HB2	2.21	0.40
24:S:49:LYS:HD2	24:S:113:LEU:HB2	2.03	0.40
22:q:10:PRO:HG3	22:q:150:THR:HA	2.03	0.40
22:q:38:MET:O	22:q:65:GLN:NE2	2.53	0.40
26:A:382:GLY:HA2	26:A:385:ILE:HD12	2.03	0.40
28:C:72:TYR:HA	29:D:112:TYR:H	1.86	0.40
29:D:68:LEU:HD23	29:D:68:LEU:HA	1.86	0.40
30:E:175:PRO:HA	30:E:176:PRO:HD3	1.98	0.40
31:F:134:LEU:HD13	31:F:137:ILE:HA	2.02	0.40
32:f:298:LEU:HA	32:f:301:HIS:CD2	2.55	0.40
32:f:509:LYS:O	32:f:554:TYR:OH	2.36	0.40
1:U:516:LEU:HA	1:U:519:VAL:HG22	2.04	0.40
2:V:338:LEU:HD11	2:V:394:LEU:HA	2.02	0.40
5:Y:210:SER:OG	5:Y:211:TYR:N	2.54	0.40
6:Z:252:LYS:NZ	9:c:302:ALA:O	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:189:TRP:HZ3	12:G:197:THR:HG21	1.85	0.40
19:N:138:TYR:HB3	19:n:138:TYR:HB3	2.03	0.40
25:T:192:VAL:HG12	25:T:197:VAL:HG22	2.04	0.40
22:q:48:GLY:HA3	22:q:100:VAL:HA	2.03	0.40
25:t:67:LEU:HD23	25:t:67:LEU:HA	1.91	0.40
29:D:250:VAL:O	29:D:254:ALA:HB2	2.21	0.40
30:E:335:SER:HB3	30:E:338:PHE:CD2	2.55	0.40
32:f:183:PRO:HB2	32:f:184:LEU:H	1.63	0.40
32:f:380:PHE:CD2	32:f:751:TYR:CE2	3.09	0.40
32:f:545:LYS:HE2	32:f:555:ALA:HA	2.03	0.40
32:f:780:PRO:HB2	32:f:800:LEU:CA	2.50	0.40
1:U:329:LEU:HD23	1:U:329:LEU:HA	1.94	0.40
1:U:418:GLU:O	1:U:422:LEU:HB2	2.22	0.40
1:U:744:VAL:HG12	1:U:785:PRO:HA	2.04	0.40
3:W:104:MET:HB3	3:W:123:ARG:HE	1.87	0.40
6:Z:269:VAL:O	6:Z:273:HIS:ND1	2.51	0.40
7:a:273:GLN:HE22	7:a:302:ILE:HD13	1.87	0.40
12:G:239:LEU:HD12	12:G:242:LEU:HD11	2.04	0.40
18:M:6:GLY:HA3	18:M:7:TYR:HB2	2.02	0.40
20:O:122:LEU:HD23	20:O:122:LEU:HA	1.94	0.40
14:i:125:GLY:O	15:j:3:TYR:OH	2.37	0.40
14:i:232:GLU:HA	14:i:235:GLN:HG2	2.03	0.40
20:o:198:ARG:HB2	20:o:201:ARG:HH11	1.87	0.40
27:B:319:PHE:HB3	27:B:320:ASP:H	1.74	0.40
30:E:203:ILE:HD12	30:E:238:ILE:HG12	2.03	0.40
1:U:32:ASN:HA	1:U:35:TRP:CE2	2.57	0.40
3:W:452:ILE:HG22	6:Z:221:PRO:HB2	2.02	0.40
6:Z:267:ARG:HH12	9:c:295:ASN:HB2	1.86	0.40
6:Z:271:ALA:O	6:Z:275:LEU:HB2	2.21	0.40
7:a:293:PHE:HA	7:a:296:ILE:HD13	2.03	0.40
14:I:218:ARG:NH1	14:I:223:THR:OG1	2.53	0.40
20:O:136:ALA:HB2	25:t:179:ARG:HH22	1.87	0.40
24:S:29:LEU:HB3	24:S:37:THR:HG22	2.03	0.40
16:k:199:LEU:HA	16:k:202:LEU:HD12	2.04	0.40
16:k:221:GLN:HB2	16:k:224:GLN:HB3	2.02	0.40
22:q:102:LEU:HB2	22:q:118:MET:HB2	2.03	0.40
27:B:112:LEU:HD23	27:B:112:LEU:HA	1.90	0.40
27:B:317:ASP:HB3	27:B:346:ARG:HG2	2.03	0.40
32:f:89:MET:SD	32:f:89:MET:N	2.94	0.40
4:X:192:SER:O	4:X:196:THR:CB	2.70	0.40
4:X:338:VAL:HG23	4:X:339:ILE:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:189:GLN:O	6:Z:192:THR:OG1	2.30	0.40
10:d:154:ALA:HB1	10:d:158:ILE:HD11	2.02	0.40
14:I:72:MET:HE3	14:I:72:MET:HB2	2.00	0.40
16:K:79:SER:HB2	16:K:140:ALA:H	1.86	0.40
20:O:67:SER:HB3	20:O:74:PRO:HG3	2.04	0.40
22:Q:58:GLU:O	22:Q:62:LYS:HB2	2.20	0.40
23:R:39:PRO:HA	23:R:184:TRP:HE1	1.87	0.40
25:T:182:ARG:HA	25:T:182:ARG:HD3	1.87	0.40
13:h:204:THR:N	13:h:207:ASN:OD1	2.54	0.40
14:i:95:GLN:HG3	21:p:69:PHE:CD1	2.56	0.40
16:k:99:HIS:CG	16:k:107:MET:HB2	2.57	0.40
26:A:215:PHE:HE1	26:A:340:LYS:HB3	1.85	0.40
28:C:183:PRO:O	28:C:290:LYS:NZ	2.53	0.40
29:D:260:ALA:O	29:D:261:ILE:HG13	2.22	0.40
31:F:188:ILE:HD13	31:F:235:LEU:CD1	2.43	0.40
31:F:204:LEU:HD23	31:F:204:LEU:HA	1.93	0.40
31:F:422:GLU:O	31:F:426:GLU:N	2.53	0.40
32:f:687:ARG:O	32:f:745:LEU:HD22	2.21	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	U	798/911 (88%)	735 (92%)	63 (8%)	0	100	100
2	V	470/480 (98%)	400 (85%)	68 (14%)	2 (0%)	30	67
3	W	454/456 (100%)	394 (87%)	58 (13%)	2 (0%)	30	67
4	X	239/380 (63%)	222 (93%)	16 (7%)	1 (0%)	30	67
5	Y	376/378 (100%)	336 (89%)	40 (11%)	0	100	100
6	Z	284/286 (99%)	240 (84%)	39 (14%)	5 (2%)	6	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	a	371/373 (100%)	339 (91%)	31 (8%)	1 (0%)	36	71
8	b	189/191 (99%)	160 (85%)	29 (15%)	0	100	100
9	c	274/287 (96%)	237 (86%)	33 (12%)	4 (2%)	8	38
10	d	255/257 (99%)	219 (86%)	34 (13%)	2 (1%)	16	52
11	e	36/70 (51%)	26 (72%)	9 (25%)	1 (3%)	4	24
12	G	237/240 (99%)	215 (91%)	22 (9%)	0	100	100
12	g	238/240 (99%)	220 (92%)	18 (8%)	0	100	100
13	H	228/232 (98%)	210 (92%)	18 (8%)	0	100	100
13	h	230/232 (99%)	219 (95%)	11 (5%)	0	100	100
14	I	246/250 (98%)	222 (90%)	23 (9%)	1 (0%)	30	67
14	i	248/250 (99%)	218 (88%)	29 (12%)	1 (0%)	30	67
15	J	237/243 (98%)	222 (94%)	12 (5%)	3 (1%)	9	41
15	j	237/243 (98%)	220 (93%)	15 (6%)	2 (1%)	16	52
16	K	224/234 (96%)	205 (92%)	18 (8%)	1 (0%)	30	67
16	k	224/234 (96%)	203 (91%)	20 (9%)	1 (0%)	30	67
17	L	236/238 (99%)	221 (94%)	15 (6%)	0	100	100
17	l	236/238 (99%)	221 (94%)	15 (6%)	0	100	100
18	M	238/245 (97%)	216 (91%)	22 (9%)	0	100	100
18	m	238/245 (97%)	219 (92%)	19 (8%)	0	100	100
19	N	189/191 (99%)	179 (95%)	9 (5%)	1 (0%)	24	63
19	n	189/191 (99%)	179 (95%)	7 (4%)	3 (2%)	7	37
20	O	218/220 (99%)	204 (94%)	14 (6%)	0	100	100
20	o	218/220 (99%)	209 (96%)	9 (4%)	0	100	100
21	P	202/204 (99%)	190 (94%)	12 (6%)	0	100	100
21	p	202/204 (99%)	190 (94%)	12 (6%)	0	100	100
22	Q	197/199 (99%)	181 (92%)	15 (8%)	1 (0%)	24	63
22	q	197/199 (99%)	179 (91%)	16 (8%)	2 (1%)	12	47
23	R	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
23	r	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
24	S	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
24	s	211/213 (99%)	198 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	T	213/215 (99%)	203 (95%)	10 (5%)	0	100	100
25	t	213/215 (99%)	203 (95%)	10 (5%)	0	100	100
26	A	338/399 (85%)	269 (80%)	64 (19%)	5 (2%)	8	38
27	B	348/389 (90%)	300 (86%)	46 (13%)	2 (1%)	21	58
28	C	359/392 (92%)	290 (81%)	59 (16%)	10 (3%)	4	24
29	D	378/380 (100%)	298 (79%)	74 (20%)	6 (2%)	7	37
30	E	373/375 (100%)	343 (92%)	29 (8%)	1 (0%)	36	71
31	F	372/396 (94%)	334 (90%)	33 (9%)	5 (1%)	9	41
32	f	669/908 (74%)	579 (86%)	82 (12%)	8 (1%)	10	42
All	All	12738/13558 (94%)	11445 (90%)	1222 (10%)	71 (1%)	23	58

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	W	424	LEU
9	c	279	ASP
11	e	60	LEU
15	J	184	ASP
16	K	10	ARG
19	n	91	ARG
19	n	92	GLU
28	C	89	VAL
28	C	231	VAL
28	C	232	ARG
28	C	289	ILE
28	C	298	ILE
31	F	427	VAL
32	f	337	LEU
32	f	364	GLN
32	f	367	SER
32	f	665	GLU
3	W	314	LEU
6	Z	167	ALA
6	Z	168	GLU
9	c	273	LYS
10	d	235	THR
15	J	176	TYR
16	k	11	GLY
26	A	431	THR

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Mol	Chain	Res	Type
27	B	430	LYS
28	C	216	GLY
29	D	408	LYS
29	D	411	GLU
32	f	183	PRO
32	f	365	VAL
9	c	149	GLN
15	J	3	TYR
22	q	2	GLU
26	A	428	ARG
27	B	180	PRO
28	C	288	ASN
32	f	184	LEU
32	f	326	LEU
4	X	203	PRO
6	Z	224	HIS
7	a	338	PRO
19	N	19	ARG
22	Q	72	GLY
19	n	19	ARG
22	q	72	GLY
28	C	401	ILE
29	D	371	SER
29	D	413	GLU
31	F	358	ASN
31	F	436	GLN
2	V	299	GLN
28	C	91	PRO
28	C	290	LYS
6	Z	99	PRO
6	Z	134	PRO
9	c	187	PRO
14	I	7	SER
15	j	9	VAL
15	j	181	ILE
29	D	407	ILE
31	F	88	TYR
26	A	157	ILE
26	A	427	PRO
10	d	159	PRO
14	i	221	GLY
29	D	372	GLY

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Mol	Chain	Res	Type
30	E	117	PRO
2	V	277	PRO
26	A	109	PRO
31	F	87	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	685/779 (88%)	682 (100%)	3 (0%)	84	83
2	V	409/414 (99%)	406 (99%)	3 (1%)	76	79
3	W	416/416 (100%)	411 (99%)	5 (1%)	63	74
4	X	208/327 (64%)	206 (99%)	2 (1%)	68	76
5	Y	334/334 (100%)	332 (99%)	2 (1%)	78	81
6	Z	257/257 (100%)	253 (98%)	4 (2%)	55	69
7	a	333/333 (100%)	331 (99%)	2 (1%)	78	81
8	b	167/167 (100%)	165 (99%)	2 (1%)	63	74
9	c	243/252 (96%)	239 (98%)	4 (2%)	55	69
10	d	231/231 (100%)	230 (100%)	1 (0%)	84	83
11	e	38/63 (60%)	38 (100%)	0	100	100
12	G	192/205 (94%)	189 (98%)	3 (2%)	55	69
12	g	193/205 (94%)	191 (99%)	2 (1%)	68	76
13	H	162/190 (85%)	162 (100%)	0	100	100
13	h	164/190 (86%)	164 (100%)	0	100	100
14	I	191/210 (91%)	190 (100%)	1 (0%)	81	82
14	i	193/210 (92%)	191 (99%)	2 (1%)	68	76
15	J	152/207 (73%)	149 (98%)	3 (2%)	48	66
15	j	152/207 (73%)	151 (99%)	1 (1%)	76	79
16	K	187/196 (95%)	186 (100%)	1 (0%)	81	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	k	186/196 (95%)	186 (100%)	0	100	100
17	L	198/204 (97%)	198 (100%)	0	100	100
17	l	198/204 (97%)	198 (100%)	0	100	100
18	M	192/202 (95%)	191 (100%)	1 (0%)	81	82
18	m	192/202 (95%)	192 (100%)	0	100	100
19	N	148/148 (100%)	148 (100%)	0	100	100
19	n	148/148 (100%)	148 (100%)	0	100	100
20	O	177/181 (98%)	176 (99%)	1 (1%)	78	81
20	o	177/181 (98%)	177 (100%)	0	100	100
21	P	172/173 (99%)	172 (100%)	0	100	100
21	p	172/173 (99%)	172 (100%)	0	100	100
22	Q	164/170 (96%)	164 (100%)	0	100	100
22	q	164/170 (96%)	160 (98%)	4 (2%)	43	63
23	R	153/156 (98%)	152 (99%)	1 (1%)	76	79
23	r	153/156 (98%)	152 (99%)	1 (1%)	76	79
24	S	174/178 (98%)	174 (100%)	0	100	100
24	s	174/178 (98%)	174 (100%)	0	100	100
25	T	175/178 (98%)	175 (100%)	0	100	100
25	t	175/178 (98%)	175 (100%)	0	100	100
26	A	286/343 (83%)	284 (99%)	2 (1%)	76	79
27	B	300/345 (87%)	298 (99%)	2 (1%)	76	79
28	C	315/340 (93%)	312 (99%)	3 (1%)	68	76
29	D	333/333 (100%)	329 (99%)	4 (1%)	63	74
30	E	298/329 (91%)	297 (100%)	1 (0%)	86	84
31	F	296/340 (87%)	294 (99%)	2 (1%)	76	79
32	f	580/763 (76%)	564 (97%)	16 (3%)	38	59
All	All	10607/11562 (92%)	10528 (99%)	79 (1%)	73	79

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	153	ILE
1	U	554	LEU

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Mol	Chain	Res	Type
1	U	913	ILE
2	V	195	ILE
2	V	328	VAL
2	V	398	LEU
3	W	85	GLU
3	W	333	LEU
3	W	413	ILE
3	W	424	LEU
3	W	455	LEU
4	X	217	ILE
4	X	387	ILE
5	Y	32	ARG
5	Y	157	ILE
6	Z	91	ILE
6	Z	187	LEU
6	Z	237	LEU
6	Z	266	ILE
7	a	112	ILE
7	a	324	ILE
8	b	54	LEU
8	b	90	ILE
9	c	62	VAL
9	c	69	VAL
9	c	102	THR
9	c	272	ILE
10	d	57	ILE
12	G	66	VAL
12	G	141	ILE
12	G	215	ILE
14	I	11	ILE
15	J	5	ARG
15	J	7	ILE
15	J	161	ILE
16	K	91	LYS
18	M	87	LEU
20	O	89	ARG
23	R	128	VAL
12	g	66	VAL
12	g	215	ILE
14	i	206	LEU
14	i	228	LEU
15	j	161	ILE

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Mol	Chain	Res	Type
22	q	4	LEU
22	q	25	ILE
22	q	140	LEU
22	q	167	LEU
23	r	128	VAL
26	A	142	VAL
26	A	403	ILE
27	B	125	THR
27	B	438	LEU
28	C	88	LYS
28	C	286	THR
28	C	390	VAL
29	D	81	ARG
29	D	306	LYS
29	D	317	LEU
29	D	411	GLU
30	E	105	LEU
31	F	134	LEU
31	F	416	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 (141) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	189	GLN
1	U	207	ASN
1	U	355	ASN

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Mol	Chain	Res	Type
1	U	389	ASN
1	U	491	GLN
1	U	500	ASN
1	U	503	GLN
1	U	611	ASN
1	U	698	GLN
1	U	743	ASN
1	U	756	HIS
2	V	33	GLN
2	V	242	HIS
2	V	281	ASN
2	V	311	ASN
2	V	459	GLN
2	V	473	GLN
2	V	487	HIS
3	W	106	GLN
3	W	218	ASN
3	W	235	GLN
3	W	361	HIS
3	W	380	GLN
3	W	454	ASN
4	X	292	GLN
4	X	296	ASN
5	Y	154	ASN
5	Y	351	ASN
5	Y	365	GLN
5	Y	378	ASN
6	Z	96	HIS
6	Z	102	HIS
6	Z	174	HIS
6	Z	231	GLN
6	Z	256	GLN
7	a	40	GLN
7	a	152	HIS
7	a	244	ASN
7	a	273	GLN
7	a	370	GLN
8	b	34	ASN
8	b	47	ASN
9	c	183	HIS
9	c	190	GLN
9	c	199	HIS

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Mol	Chain	Res	Type
9	c	214	GLN
10	d	77	GLN
10	d	228	GLN
11	e	63	HIS
12	G	68	HIS
12	G	75	ASN
12	G	100	ASN
12	G	123	GLN
13	H	71	HIS
13	H	102	GLN
13	H	119	GLN
13	H	123	GLN
14	I	20	GLN
14	I	102	GLN
14	I	109	GLN
14	I	119	GLN
14	I	146	GLN
15	J	54	GLN
15	J	122	ASN
15	J	175	ASN
16	K	99	HIS
16	K	114	GLN
16	K	178	GLN
16	K	214	ASN
17	L	53	GLN
17	L	90	GLN
17	L	117	GLN
17	L	146	GLN
17	L	152	ASN
19	N	158	ASN
21	P	93	ASN
22	Q	71	ASN
22	Q	87	ASN
22	Q	132	HIS
23	R	38	ASN
24	S	58	HIS
25	T	61	GLN
25	T	65	GLN
12	g	12	HIS
12	g	224	ASN
13	h	95	GLN
13	h	166	ASN

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Mol	Chain	Res	Type
13	h	169	ASN
14	i	30	HIS
14	i	40	ASN
14	i	109	GLN
14	i	119	GLN
14	i	146	GLN
16	k	99	HIS
16	k	152	GLN
16	k	214	ASN
16	k	225	ASN
17	l	53	GLN
17	l	90	GLN
18	m	68	ASN
18	m	110	HIS
18	m	180	GLN
19	n	154	GLN
19	n	158	ASN
20	o	66	HIS
20	o	116	HIS
21	p	61	GLN
22	q	71	ASN
22	q	99	HIS
22	q	132	HIS
23	r	38	ASN
23	r	85	ASN
24	s	159	GLN
25	t	61	GLN
25	t	65	GLN
25	t	81	HIS
25	t	213	HIS
26	A	247	GLN
26	A	305	GLN
27	B	195	GLN
27	B	315	GLN
27	B	332	ASN
28	C	241	HIS
28	C	270	GLN
28	C	332	HIS
28	C	377	HIS
29	D	49	GLN
29	D	187	HIS
29	D	257	ASN

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Mol	Chain	Res	Type
29	D	304	ASN
30	E	86	GLN
31	F	243	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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	B	501	-	32,33,33	0.84	2 (6%)	45,52,52	1.06	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	AGS	D	501	-	32,33,33	0.60	1 (3%)	45,52,52	0.83	1 (2%)
34	AGS	A	501	-	32,33,33	0.72	1 (3%)	45,52,52	0.78	1 (2%)
34	AGS	F	501	-	32,33,33	0.54	0	45,52,52	0.76	1 (2%)

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	B	501	-	-	4/21/38/38	0/3/3/3
34	AGS	D	501	-	-	2/21/38/38	0/3/3/3
34	AGS	A	501	-	-	8/21/38/38	0/3/3/3
34	AGS	F	501	-	-	5/21/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	501	AGS	PA-O3A	-2.26	1.57	1.59
34	B	501	AGS	PB-O3A	-2.15	1.57	1.59
34	A	501	AGS	PA-O3A	-2.09	1.57	1.59
34	D	501	AGS	PG-S1G	2.06	1.95	1.90

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	501	AGS	PB-O3B-PG	-5.16	114.27	133.17
34	A	501	AGS	PB-O3B-PG	-4.41	117.01	133.17
34	D	501	AGS	PB-O3B-PG	-4.22	117.73	133.17
34	F	501	AGS	PB-O3B-PG	-2.87	122.65	133.17

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	501	AGS	C5'-O5'-PA-O1A
34	A	501	AGS	C5'-O5'-PA-O2A
34	A	501	AGS	C5'-O5'-PA-O3A
34	B	501	AGS	C5'-O5'-PA-O1A
34	F	501	AGS	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
34	D	501	AGS	O4'-C4'-C5'-O5'
34	D	501	AGS	C3'-C4'-C5'-O5'
34	A	501	AGS	O4'-C4'-C5'-O5'
34	A	501	AGS	C3'-C4'-C5'-O5'
34	F	501	AGS	PA-O3A-PB-O1B
34	A	501	AGS	C4'-C5'-O5'-PA
34	B	501	AGS	C2'-C1'-N9-C8
34	A	501	AGS	PA-O3A-PB-O2B
34	F	501	AGS	O4'-C4'-C5'-O5'
34	F	501	AGS	PB-O3B-PG-O3G
34	B	501	AGS	O4'-C1'-N9-C8
34	A	501	AGS	PA-O3A-PB-O1B
34	B	501	AGS	O4'-C4'-C5'-O5'
34	F	501	AGS	C3'-C4'-C5'-O5'

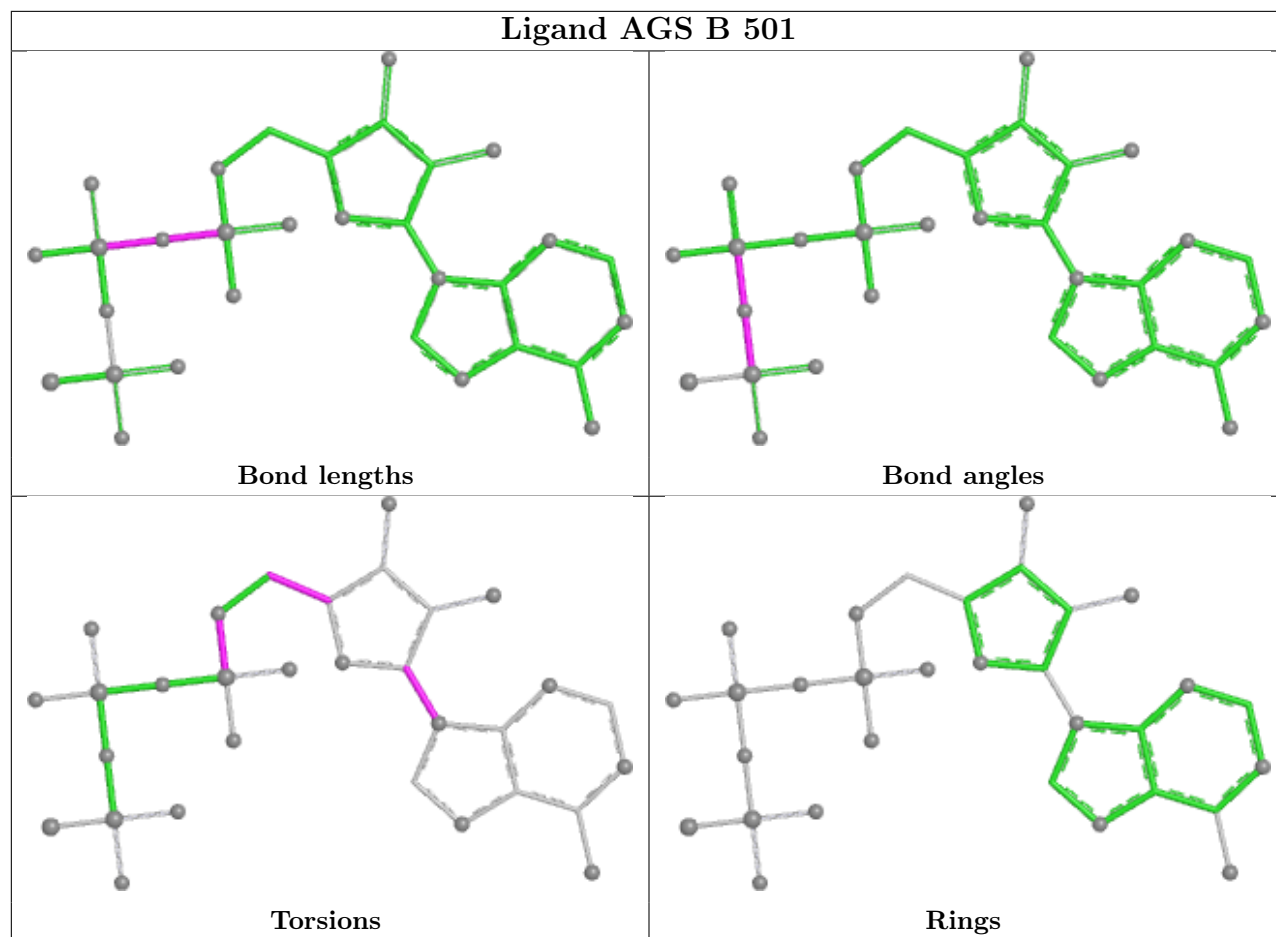
There are no ring outliers.

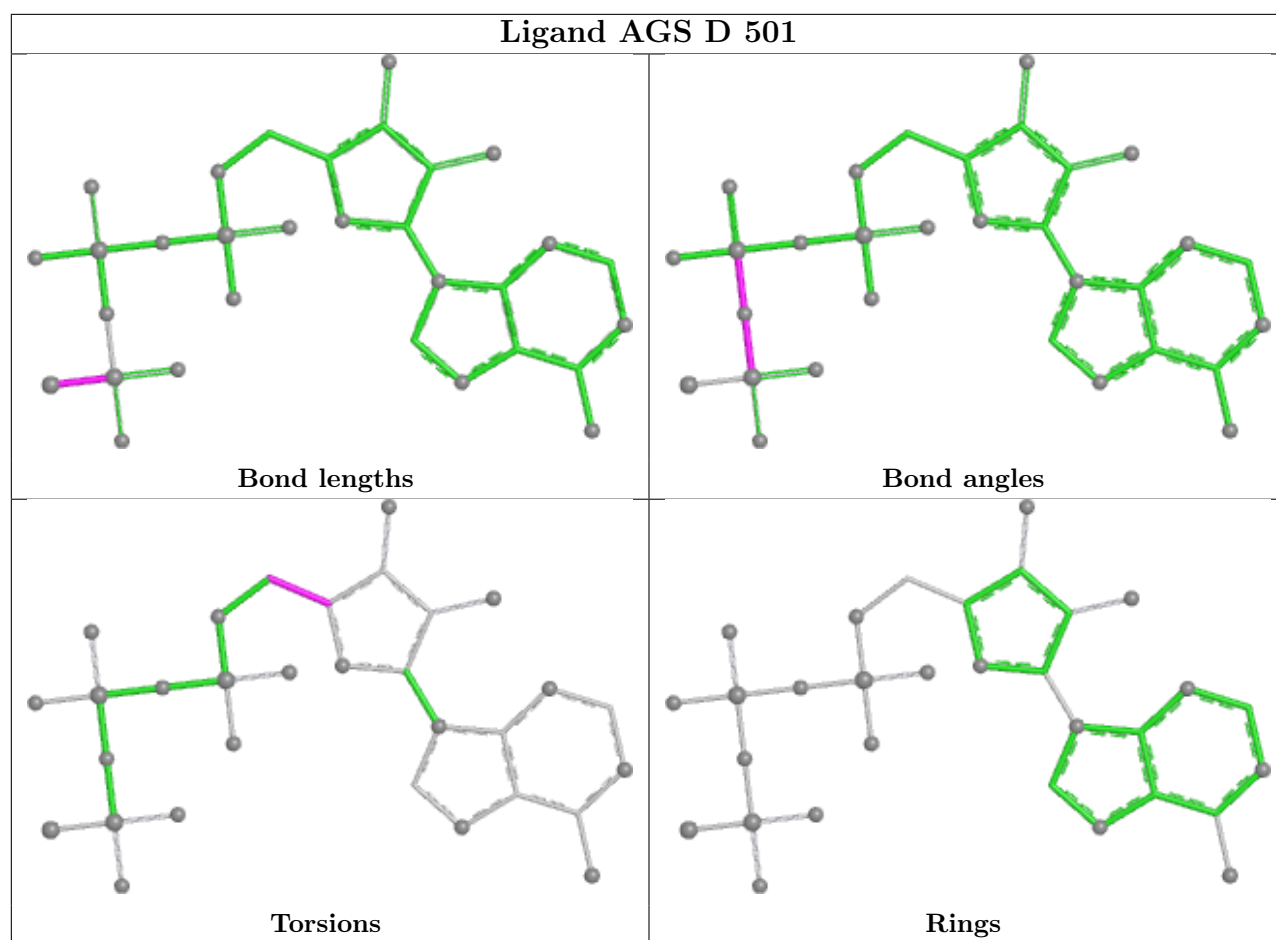
4 monomers are involved in 23 short contacts:

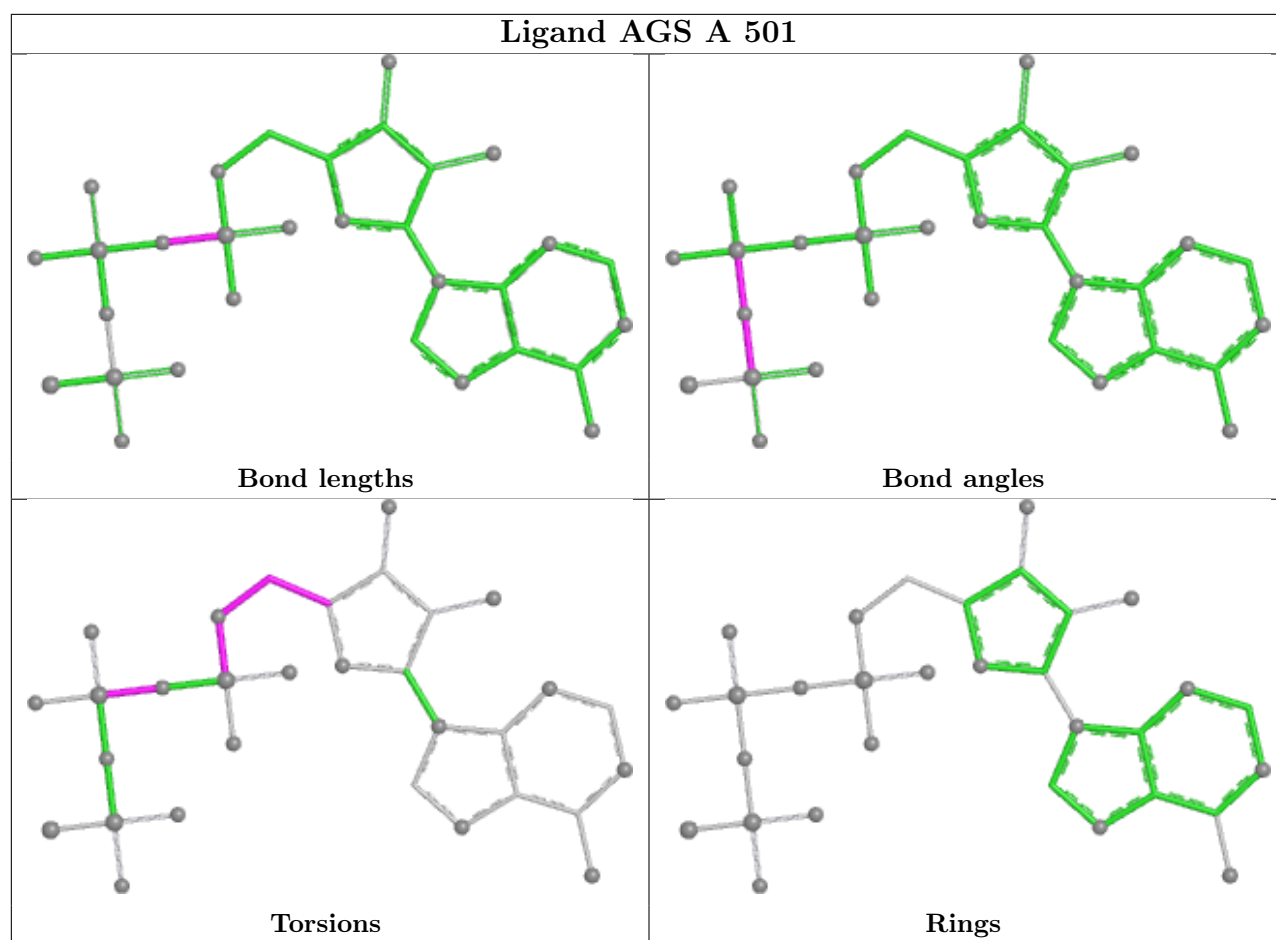
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	B	501	AGS	4	0
34	D	501	AGS	7	0
34	A	501	AGS	3	0
34	F	501	AGS	9	0

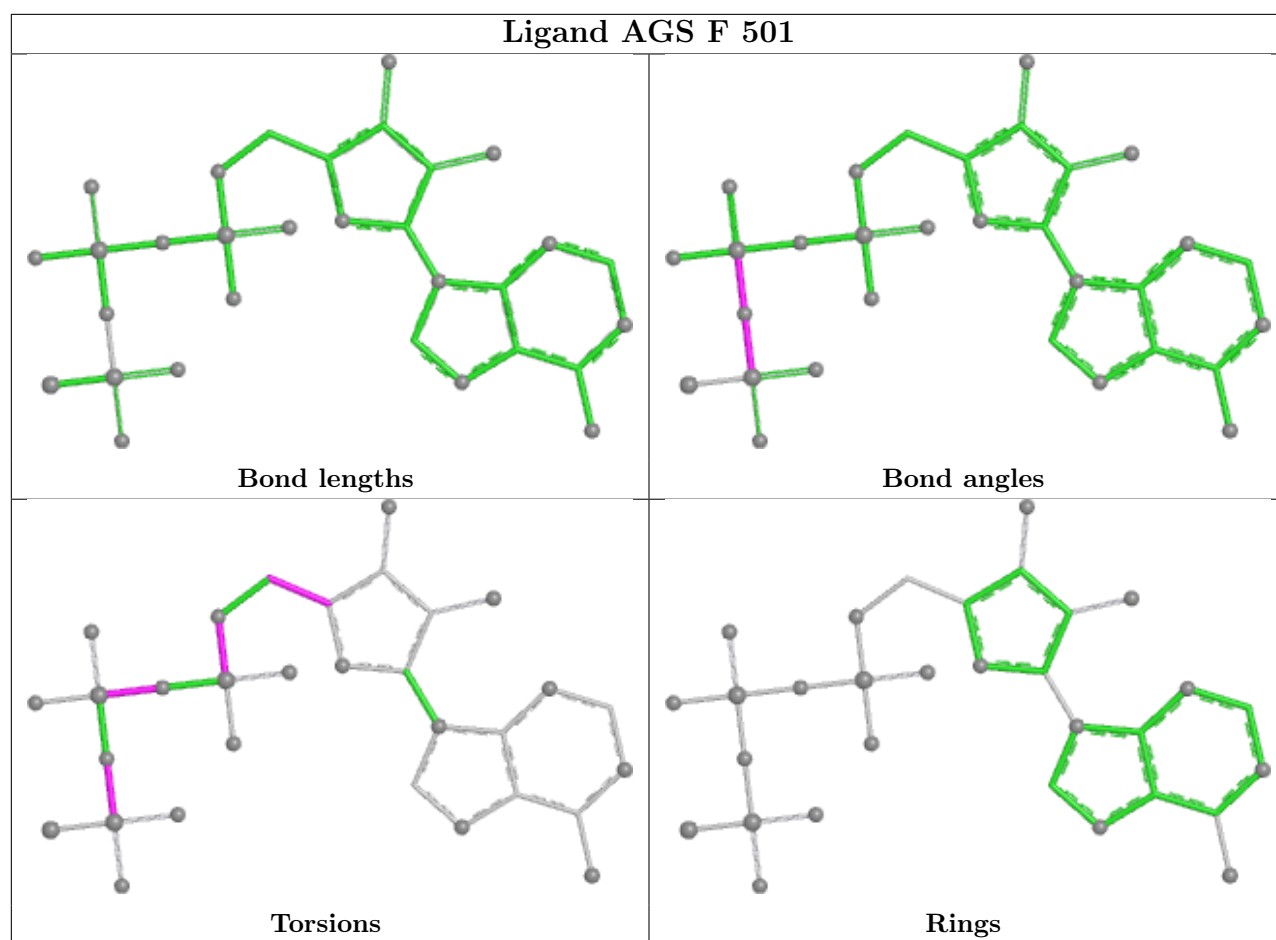
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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.

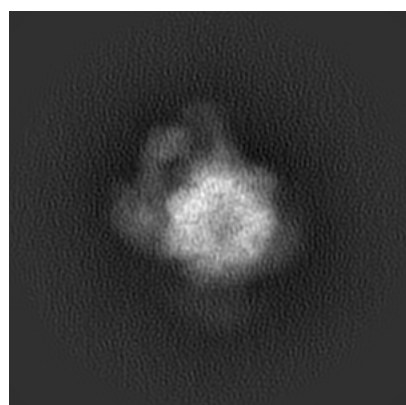
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8665. These allow visual inspection of the internal detail of the map and identification of artifacts.

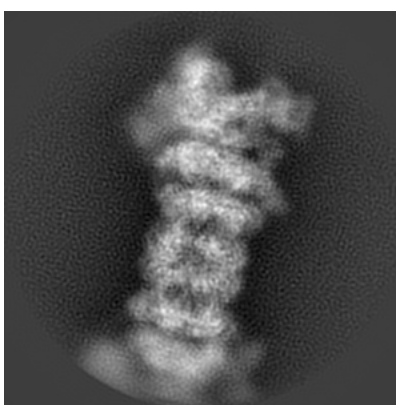
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

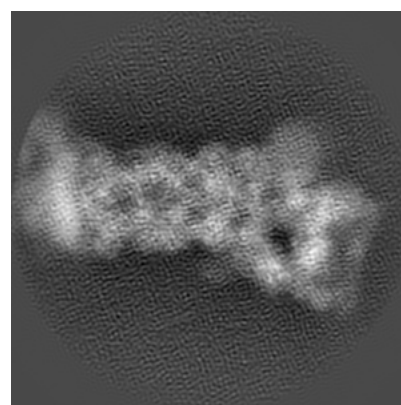
6.1.1 Primary map



X



Y

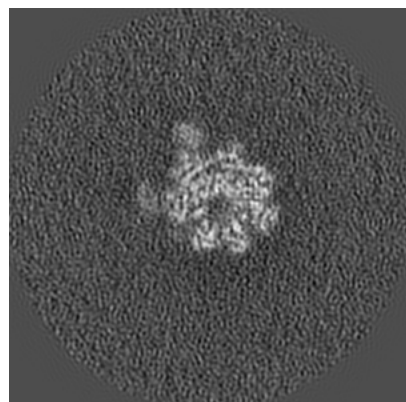


Z

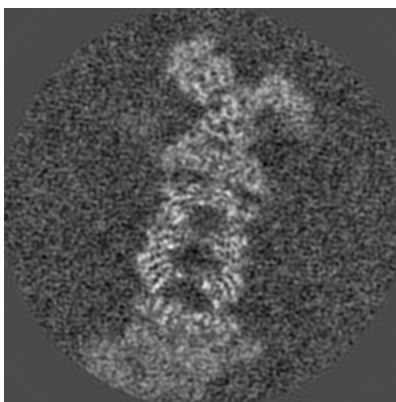
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

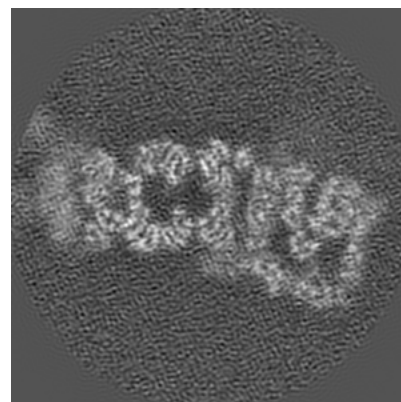
6.2.1 Primary map



X Index: 280



Y Index: 280

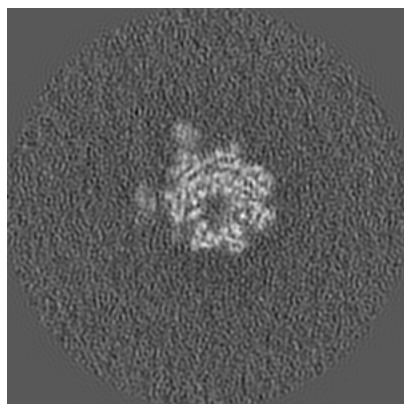


Z Index: 280

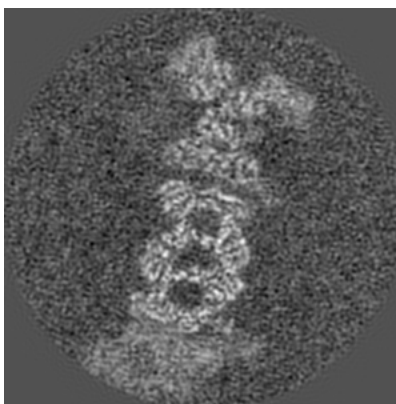
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

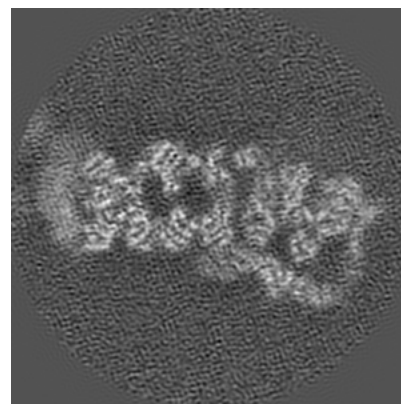
6.3.1 Primary map



X Index: 278



Y Index: 273

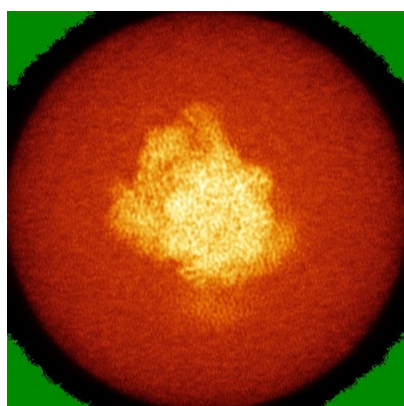


Z Index: 286

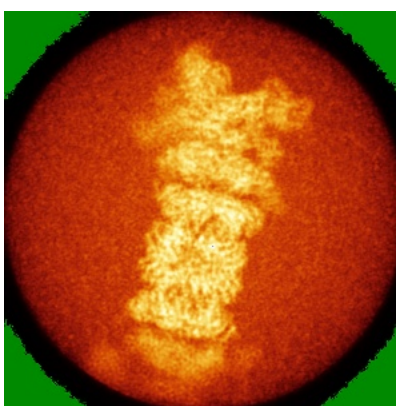
The images above show the largest variance slices of the map in three orthogonal directions.

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

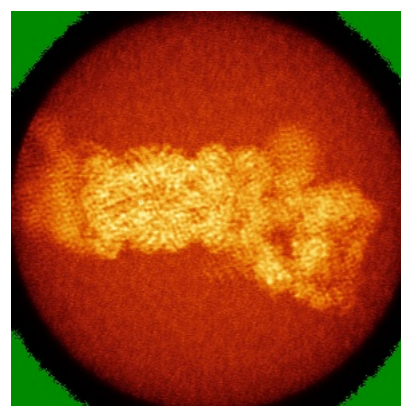
6.4.1 Primary map



X



Y

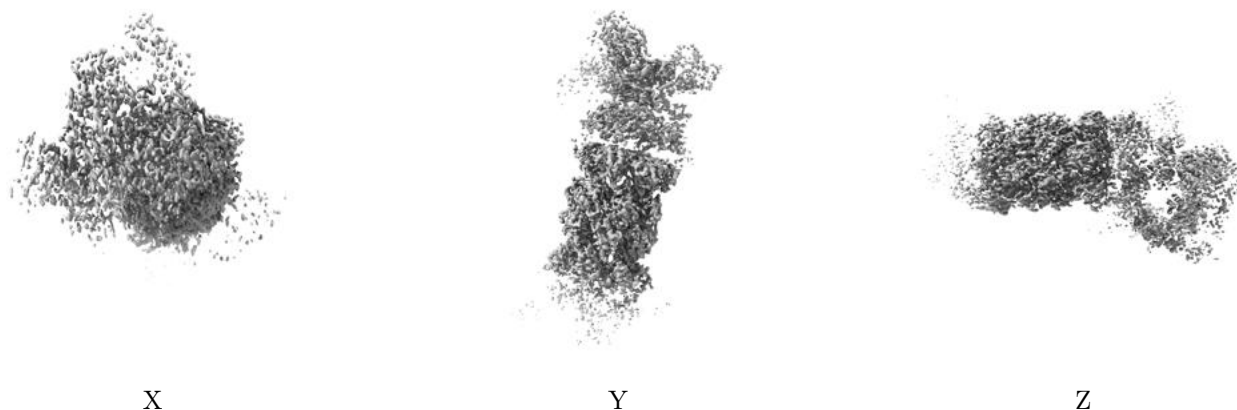


Z

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.

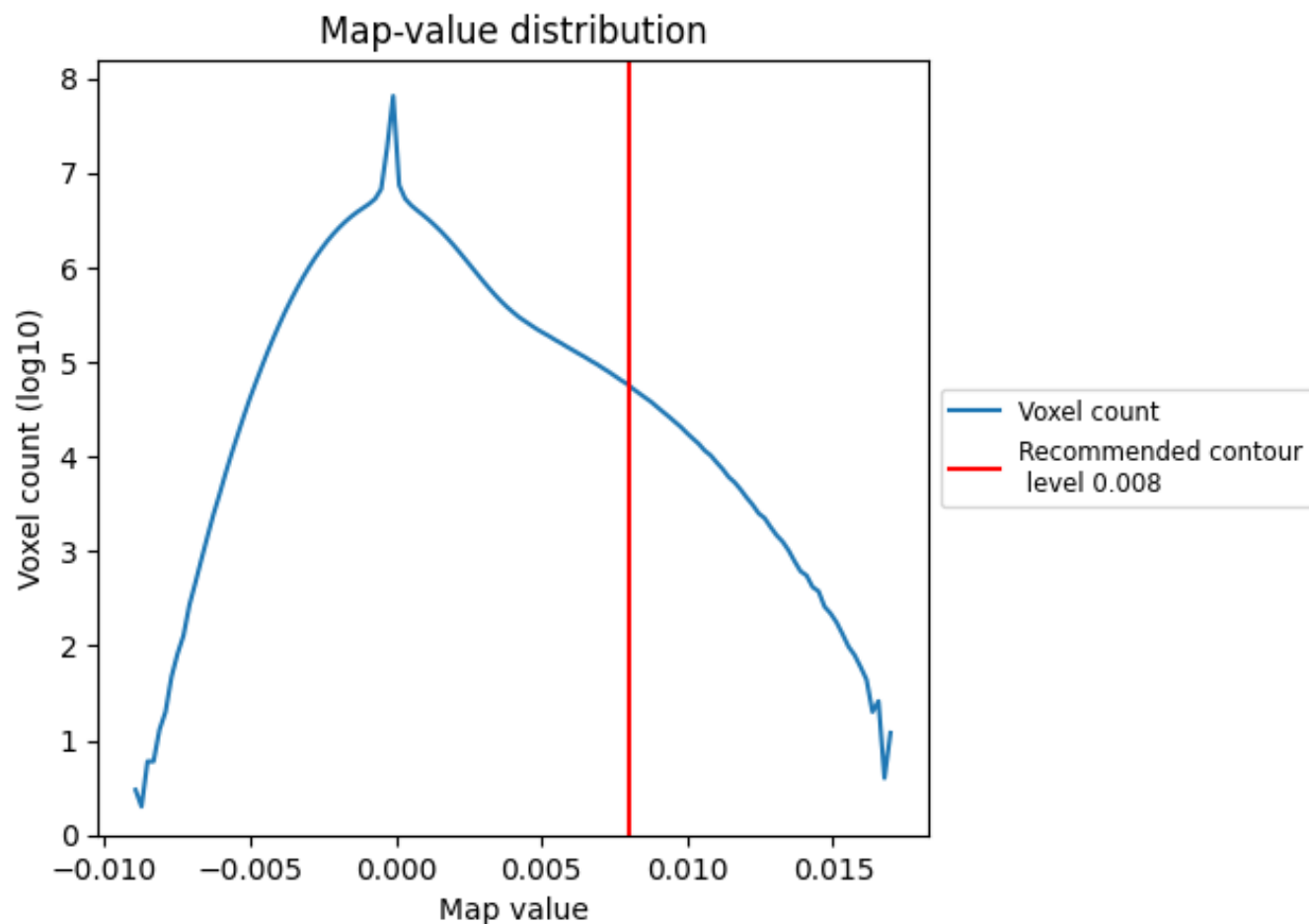
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

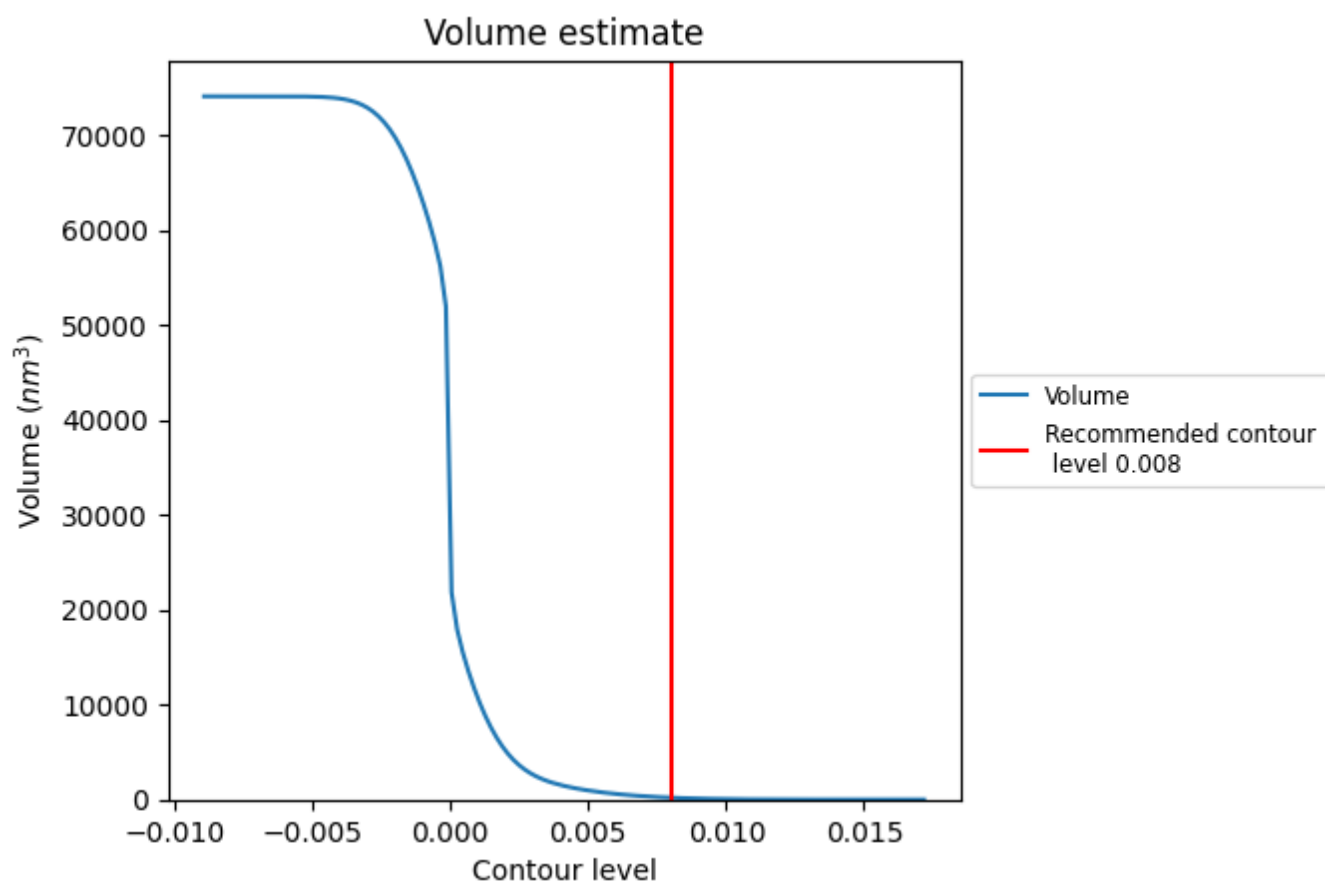
This section contains the results of statistical analysis of the map.

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.

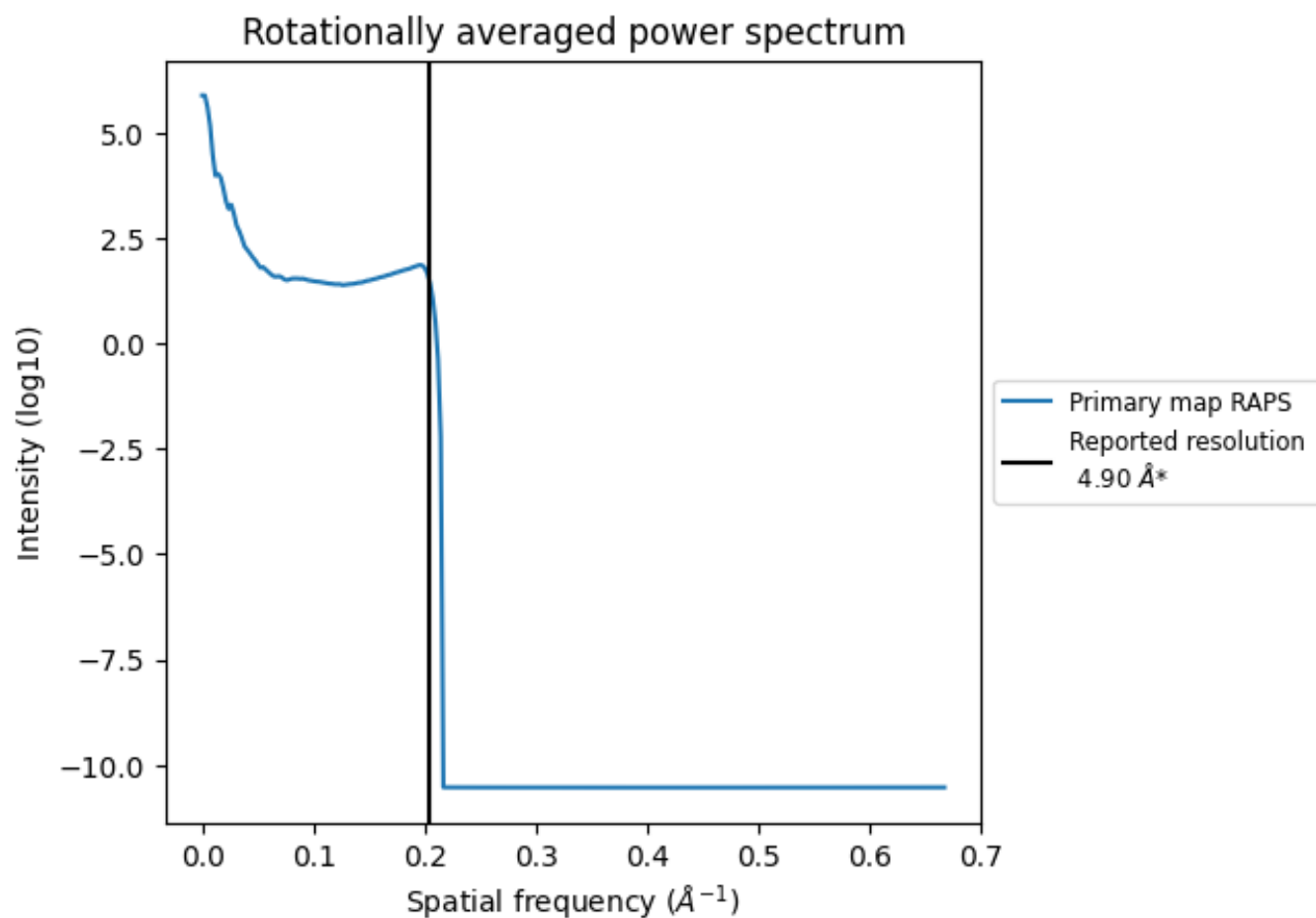
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 199 nm³; this corresponds to an approximate mass of 180 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 0.204 $\text{\AA}^{-1}$

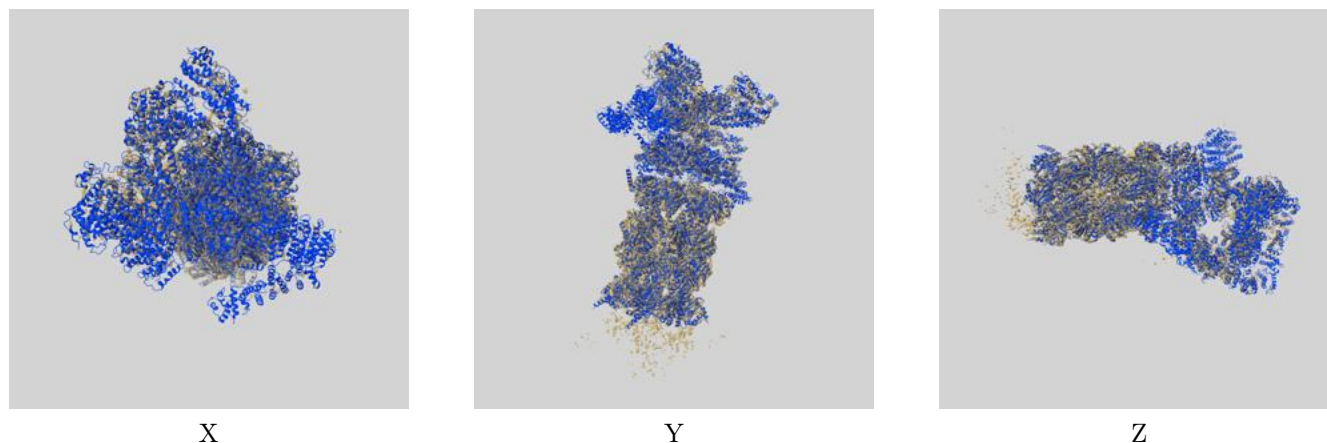
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

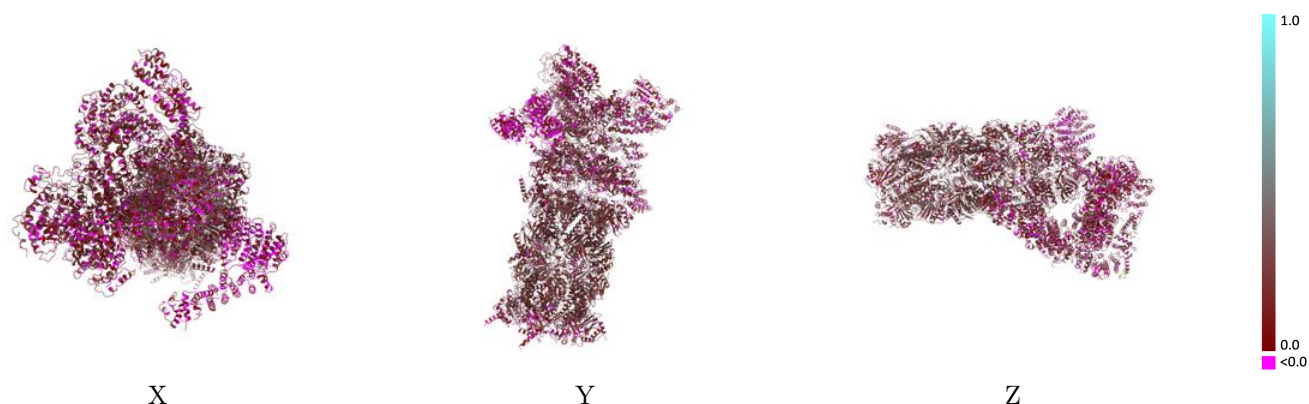
This section contains information regarding the fit between EMDB map EMD-8665 and PDB model 5VFR. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



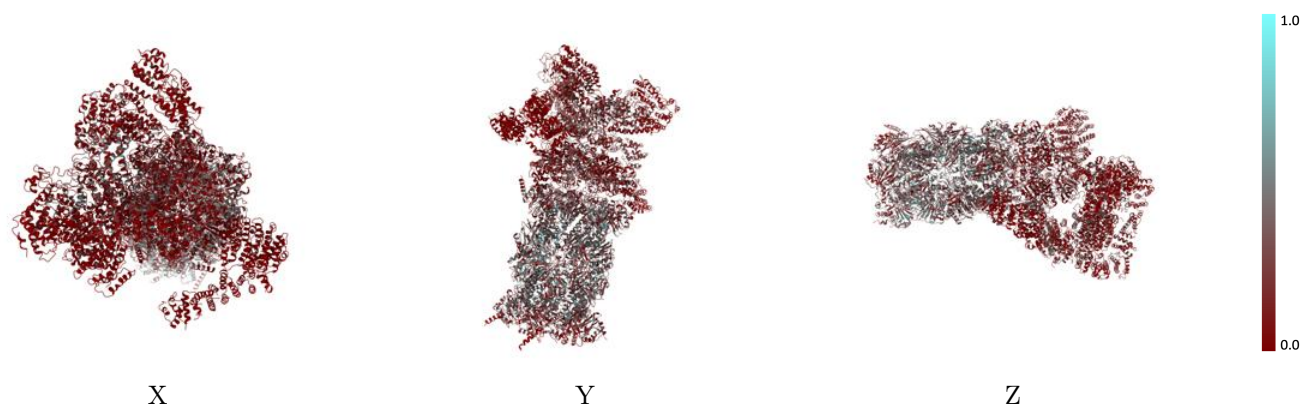
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



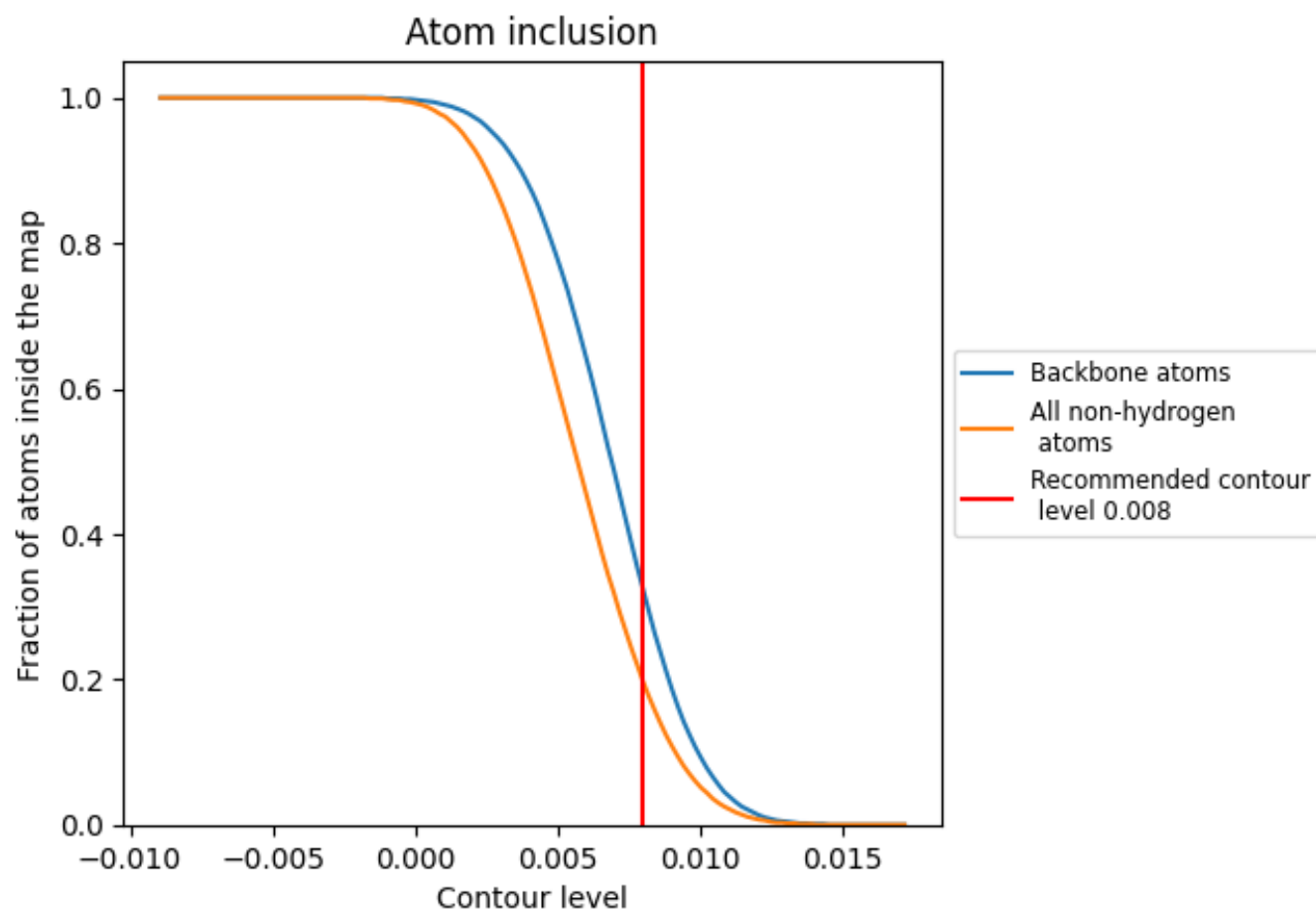
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 32% of all backbone atoms, 20% 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	 0.1970	 0.1860
A	 0.1520	 0.1910
B	 0.1050	 0.1900
C	 0.1190	 0.1960
D	 0.1460	 0.1980
E	 0.1200	 0.2070
F	 0.1280	 0.2010
G	 0.2490	 0.2070
H	 0.2100	 0.2030
I	 0.2340	 0.2090
J	 0.2470	 0.2200
K	 0.3090	 0.2120
L	 0.3360	 0.2280
M	 0.2830	 0.2150
N	 0.3350	 0.2540
O	 0.2910	 0.2390
P	 0.3380	 0.2470
Q	 0.3400	 0.2390
R	 0.4270	 0.2710
S	 0.3460	 0.2450
T	 0.3900	 0.2640
U	 0.1060	 0.1580
V	 0.0700	 0.1380
W	 0.0870	 0.1360
X	 0.0740	 0.1310
Y	 0.1580	 0.1480
Z	 0.1580	 0.1450
a	 0.0980	 0.1480
b	 0.0490	 0.0980
c	 0.1770	 0.1640
d	 0.0480	 0.1520
e	 0.0700	 0.1860
f	 0.0040	 0.0220
g	 0.2400	 0.2120
h	 0.2190	 0.2030



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Chain	Atom inclusion	Q-score
i	 0.1970	 0.1760
j	 0.2430	 0.1990
k	 0.2920	 0.2100
l	 0.3080	 0.2060
m	 0.2660	 0.2030
n	 0.3570	 0.2410
o	 0.3190	 0.2460
p	 0.3480	 0.2360
q	 0.3720	 0.2570
r	 0.3810	 0.2470
s	 0.3510	 0.2470
t	 0.3820	 0.2450