



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 09:42 PM UTC

PDB ID : 9WBG / pdb_00009wbg
EMDB ID : EMD-65839
Title : Structure of human 26S proteasome complexed with midnolin, 19S proteasome with Ubl and Catch domain resolved
Authors : Zhu, C.; Qin, L.; Liang, L.
Deposited on : 2025-08-14
Resolution : 4.23 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:

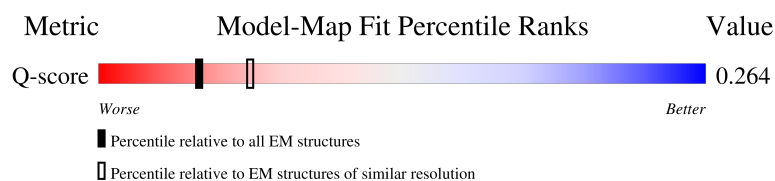
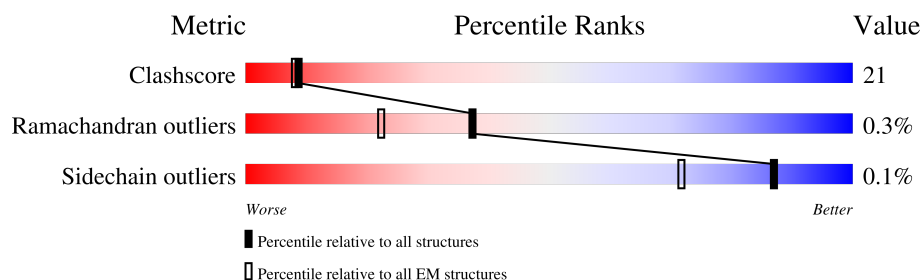
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.23 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	4685 (3.74 - 4.73)

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	f	856	<div> <div>5%</div> <div>12%</div> <div>10%</div> <div>77%</div> </div>
2	C	406	<div> <div>25%</div> <div>50%</div> <div>40%</div> <div>10%</div> </div>
3	D	418	<div> <div>12%</div> <div>52%</div> <div>39%</div> <div>9%</div> </div>
4	V	534	<div> <div>22%</div> <div>45%</div> <div>38%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
5	W	456	
6	X	422	
7	Y	389	
8	Z	324	
9	a	376	
10	b	377	
11	d	350	
12	e	70	
13	v	7	
14	U	953	
15	c	590	
16	A	433	
17	B	440	
18	E	389	
19	F	439	
20	w	337	

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
22	ATP	D	501	-	-	X	-

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 50206 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 Maltose/maltodextrin-binding periplasmic protein, Midnolin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	f	196	Total	C	N	O	S	0	0
			1488	925	274	283	6		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	-387	MET	-	initiating methionine	UNP P0AEX9
f	-386	GLY	-	expression tag	UNP P0AEX9
f	-385	HIS	-	expression tag	UNP P0AEX9
f	-384	HIS	-	expression tag	UNP P0AEX9
f	-383	HIS	-	expression tag	UNP P0AEX9
f	-382	HIS	-	expression tag	UNP P0AEX9
f	-381	HIS	-	expression tag	UNP P0AEX9
f	-380	HIS	-	expression tag	UNP P0AEX9
f	-13	ASP	-	linker	UNP P0AEX9
f	-12	TYR	-	linker	UNP P0AEX9
f	-11	ASP	-	linker	UNP P0AEX9
f	-10	ILE	-	linker	UNP P0AEX9
f	-9	PRO	-	linker	UNP P0AEX9
f	-8	THR	-	linker	UNP P0AEX9
f	-7	THR	-	linker	UNP P0AEX9
f	-6	GLU	-	linker	UNP P0AEX9
f	-5	ASN	-	linker	UNP P0AEX9
f	-4	LEU	-	linker	UNP P0AEX9
f	-3	TYR	-	linker	UNP P0AEX9
f	-2	PHE	-	linker	UNP P0AEX9
f	-1	GLN	-	linker	UNP P0AEX9
f	0	GLY	-	linker	UNP P0AEX9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	364	Total	C	N	O	S	0	0
			2870	1811	516	527	16		

- Molecule 3 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	380	Total	C	N	O	S	0	0
			3035	1921	523	578	13		

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	442	Total	C	N	O	S	0	0
			3592	2290	639	650	13		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	440	Total	C	N	O	S	0	0
			3582	2269	609	681	23		

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	384	Total	C	N	O	S	0	0
			3040	1935	513	580	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	376	Total	C	N	O	S	0	0
			3103	1979	531	576	17		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 11 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	270	Total	C	N	O	S	0	0
			2193	1417	360	407	9		

- Molecule 12 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	e	48	Total	C	N	O	0	0
			409	249	63	97		

- Molecule 13 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	v	7	Total	C	N	O	0	0
			35	21	7	7		

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	818	Total	C	N	O	S	0	0
			6371	4046	1085	1196	44		

- Molecule 15 is a protein called Ubiquitin C-terminal hydrolase PSMD14, Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	293	Total	C	N	O	S	0	0
			2304	1457	396	432	19		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	311	GLU	-	linker	UNP O00487
c	312	ASN	-	linker	UNP O00487
c	313	LEU	-	linker	UNP O00487
c	314	TYR	-	linker	UNP O00487
c	315	PHE	-	linker	UNP O00487
c	316	GLN	-	linker	UNP O00487
c	317	GLY	-	linker	UNP O00487
c	318	ALA	-	linker	UNP O00487
c	555	HIS	-	expression tag	UNP A0ACC5U4E7
c	556	HIS	-	expression tag	UNP A0ACC5U4E7
c	557	HIS	-	expression tag	UNP A0ACC5U4E7
c	558	HIS	-	expression tag	UNP A0ACC5U4E7
c	559	HIS	-	expression tag	UNP A0ACC5U4E7
c	560	HIS	-	expression tag	UNP A0ACC5U4E7
c	561	SER	-	expression tag	UNP A0ACC5U4E7
c	562	ALA	-	expression tag	UNP A0ACC5U4E7
c	563	TRP	-	expression tag	UNP A0ACC5U4E7
c	564	SER	-	expression tag	UNP A0ACC5U4E7
c	565	HIS	-	expression tag	UNP A0ACC5U4E7
c	566	PRO	-	expression tag	UNP A0ACC5U4E7
c	567	GLN	-	expression tag	UNP A0ACC5U4E7
c	568	PHE	-	expression tag	UNP A0ACC5U4E7
c	569	GLU	-	expression tag	UNP A0ACC5U4E7
c	570	LYS	-	expression tag	UNP A0ACC5U4E7
c	571	GLY	-	expression tag	UNP A0ACC5U4E7
c	572	GLY	-	expression tag	UNP A0ACC5U4E7
c	573	GLY	-	expression tag	UNP A0ACC5U4E7
c	574	SER	-	expression tag	UNP A0ACC5U4E7
c	575	GLY	-	expression tag	UNP A0ACC5U4E7
c	576	GLY	-	expression tag	UNP A0ACC5U4E7
c	577	GLY	-	expression tag	UNP A0ACC5U4E7
c	578	SER	-	expression tag	UNP A0ACC5U4E7
c	579	GLY	-	expression tag	UNP A0ACC5U4E7
c	580	GLY	-	expression tag	UNP A0ACC5U4E7
c	581	SER	-	expression tag	UNP A0ACC5U4E7
c	582	ALA	-	expression tag	UNP A0ACC5U4E7
c	583	TRP	-	expression tag	UNP A0ACC5U4E7
c	584	SER	-	expression tag	UNP A0ACC5U4E7
c	585	HIS	-	expression tag	UNP A0ACC5U4E7
c	586	PRO	-	expression tag	UNP A0ACC5U4E7
c	587	GLN	-	expression tag	UNP A0ACC5U4E7
c	588	PHE	-	expression tag	UNP A0ACC5U4E7
c	589	GLU	-	expression tag	UNP A0ACC5U4E7

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Chain	Residue	Modelled	Actual	Comment	Reference
c	590	LYS	-	expression tag	UNP A0ACC5U4E7

- Molecule 16 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A	366	Total	C	N	O	S	0	0
			2863	1805	503	537	18		

- Molecule 17 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B	340	Total	C	N	O	S	0	0
			2647	1663	451	521	12		

- Molecule 18 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E	347	Total	C	N	O	S	0	0
			2721	1713	484	508	16		

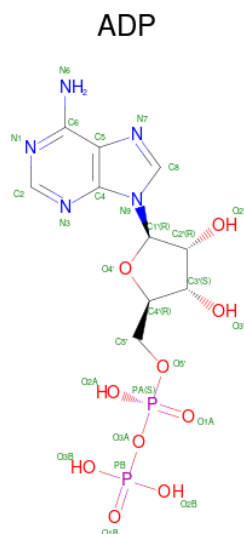
- Molecule 19 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	F	372	Total	C	N	O	S	0	0
			2902	1823	501	562	16		

- Molecule 20 is a protein called Early growth response protein 1.

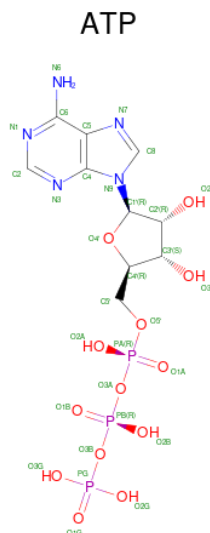
Mol	Chain	Residues	Atoms				AltConf	Trace
20	w	17	Total	C	N	O	0	0
			135	89	23	23		

- Molecule 21 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
22	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
22	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
24	B	1	Total	Mg	0
			1	1	
24	E	1	Total	Mg	0
			1	1	
24	F	1	Total	Mg	0
			1	1	

GLU	ASN	ARG	ALA	THR	ARG	CYS	LYS	GLU	GLU	LEU	GLN	LEU	LEU	LEU	GLN	GLY	GLN	LYS	ARG	LEU	ARG	VAL	VAL	ALA
LEU	GLY	LEU	ASP	PHE	GLU	ASP	ASP	TRP	GLU	TRP	LYS	PRO	GLU	VAL	VAL	ASN	PRO	ILE	LYS	SER	GLU	PHE	VAL	ALA

• Molecule 2: 26S proteasome regulatory subunit 8

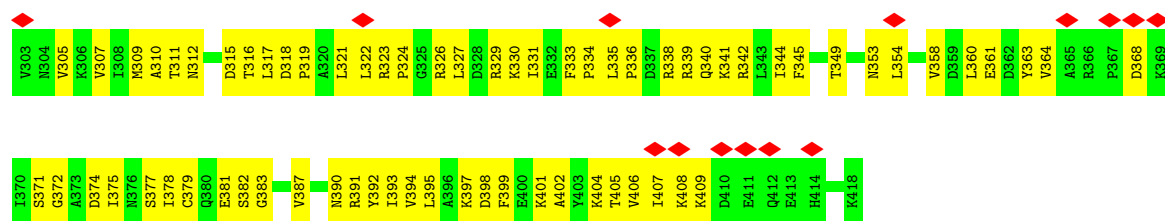


G356	A357	E358	V359	K360	T364	E365	M368	G369	A370	L371	R372	R373	R374	R375	V376	H377	V378	T379	Q380	F381	D382	F383	E384	M385	A386	V387	A388	K389	V390	M391	Q392	K393	D394	S395	E396	K397	ASN	MET	SER	ILE	LYS	LYS	LEU	TRP	LYS										
A285	T286	K287	K290	V291	A294	T295	N296	A297	L298	D299	I300	L301	R302	S303	A304	L305	R306	P307	R308	G309	R310	I311	D312	R313	K314	I315	E316	F317	P318	P319	P320	N321	A324	R325	L326	D327	I328	L329	K330	I331	H332	M336	N337	L338	T339	R340	N343	L344	R345	K346	I347	A348	E349		
F223	I224	G225	E226	G227	A228	R229	V231	R232	E233	L234	F235	H237	A238	R239	H241	A242	I246	F247	M248	D249	I250	ILE	ASP	SER	ILE	GLY	SER	SER	ARG	LEU	GLU	GLY	GLY	SER	GLY	GLY	ASP	E268	V269	Q270	R271	T272	M273	L274	E275	L276	T277	Q279	L280	D281	G282	F283	E284		
D155	K156	Q157	I158	K159	E160	I161	E163	V164	I165	E166	L167	P168	V169	F175	E176	A177	L178	G179	I180	A181	Q182	P183	K184	G185	V186	L187	L188	Y189	G190	P191	P192	G193	T194	G195	K196	T197	L198	L199	A200	R201	A202	V203	A204	S206	C209	T210	F211	T212	R213	S217	E218	L219	V220	Q221	K222
G70	S71	V77	R78	A79	M80	D81	K82	L86	H90	P91	D104	I105	M106	D107	V108	T109	F110	M111	C112	R113	R117	M118	D119	L122	L123	H124	L127	P128	N129	K130	V131	D132	P133	L134	V135	S136	L137	M138	M139	V140	E141	K142	V143	T147	V148	E149	M150	I151	G152	G153	L154				
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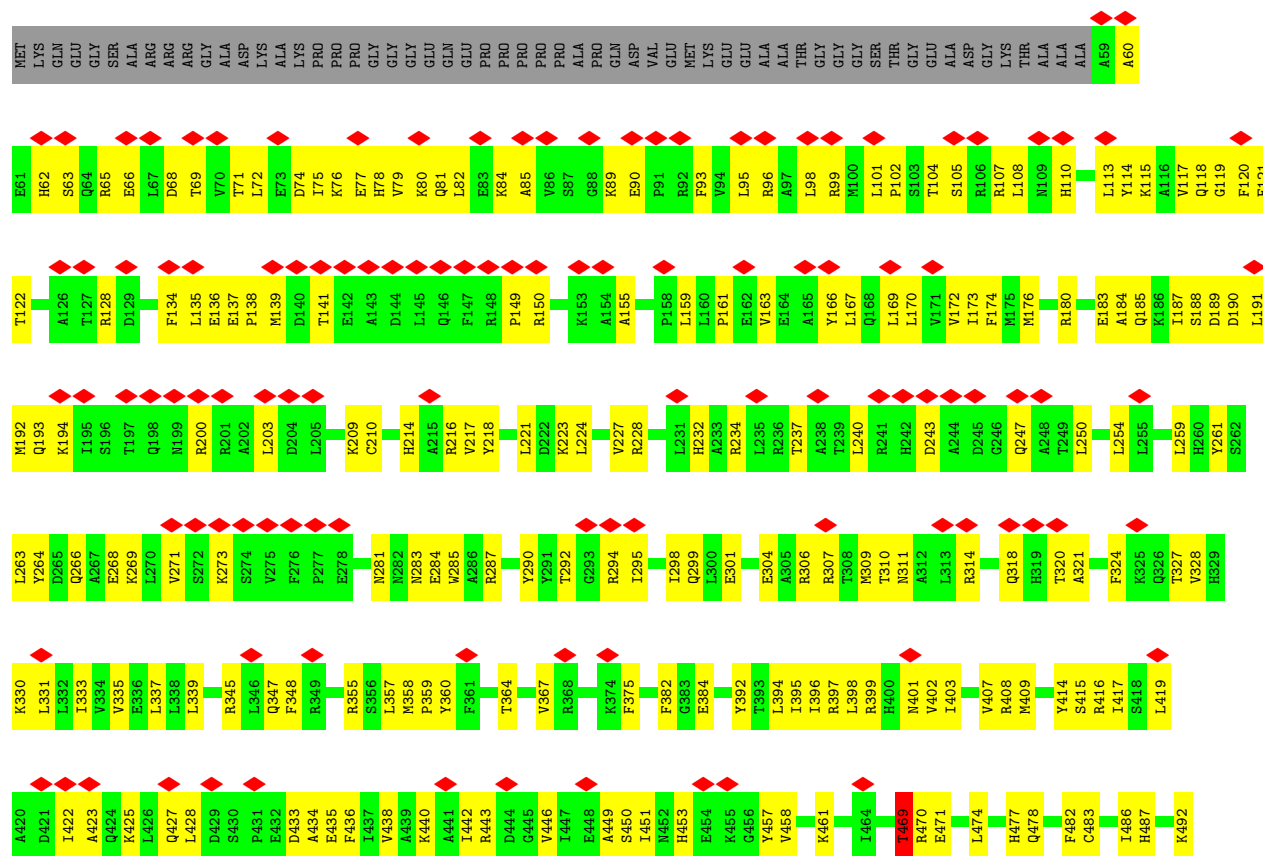
• Molecule 3: 26S proteasome regulatory subunit 6B



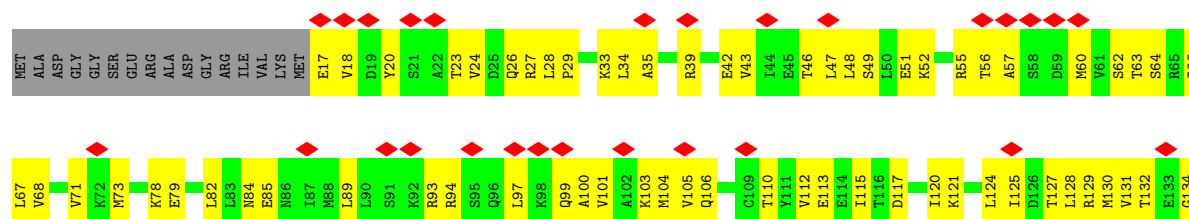
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K70	A75	Q76	E77	K80	R81	I85	Q91	E94	A95	Y96	D97	Q98	N99	I102	V103	G104	S109	M110	Y111	Y112	I115	R121	E122	L123	L124	N127	V130	A131	L132	H133	K134	H135	S136	L139	V142	E146	A147	D148	S149	S150	I151	M152	M153	L154	T155												
S156	D157	Q158	M163	Y164	A165	D166	I167	G168	G169	M170	D171	I172	Q173	K174	Q175	E176	V177	A178	E179	L183	P184	F188	E189	L190	Y191	K192	Q193	I194	G195	I196	V202	L203	M204	Y205	P208	G209	C210	G211	T212	T213	M214	L215	A216	K217	H222	A225	V231	G232	S233	E234	F235						
V236	Q237	K238	Y239	L240	G241	E242	R245	M246	V247	R248	D249	V250	F251	R252	E256	H257	A258	P259	I262	F263	L264	D265	E266	I267	I270	T272	K273	R274	F275	D276	A277	Q278	T279	D282	R283	E284	V285	L288	L289	E291	L292	L293	K294	Q295	G296	D297	G298	F299	D300	Q301	H302						

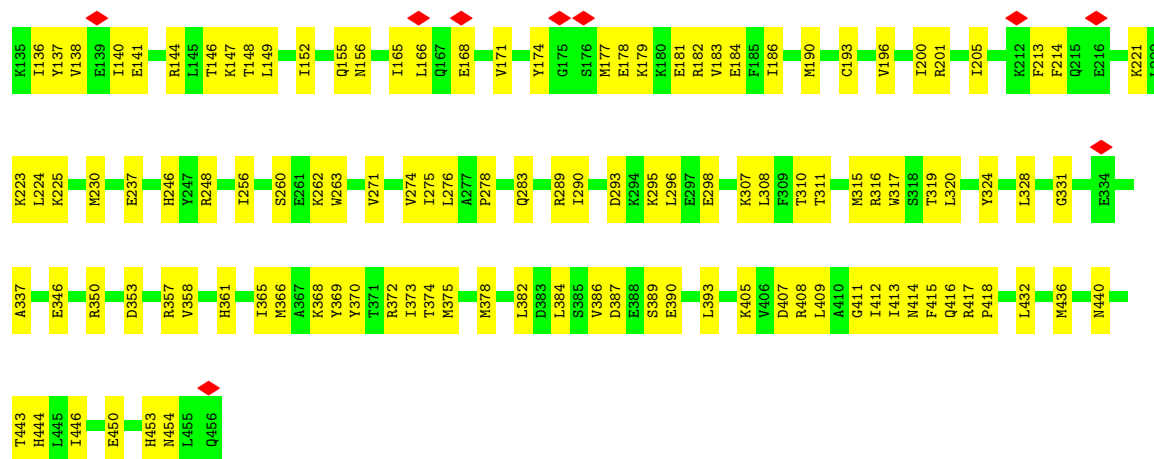


• Molecule 4: 26S proteasome non-ATPase regulatory subunit 3

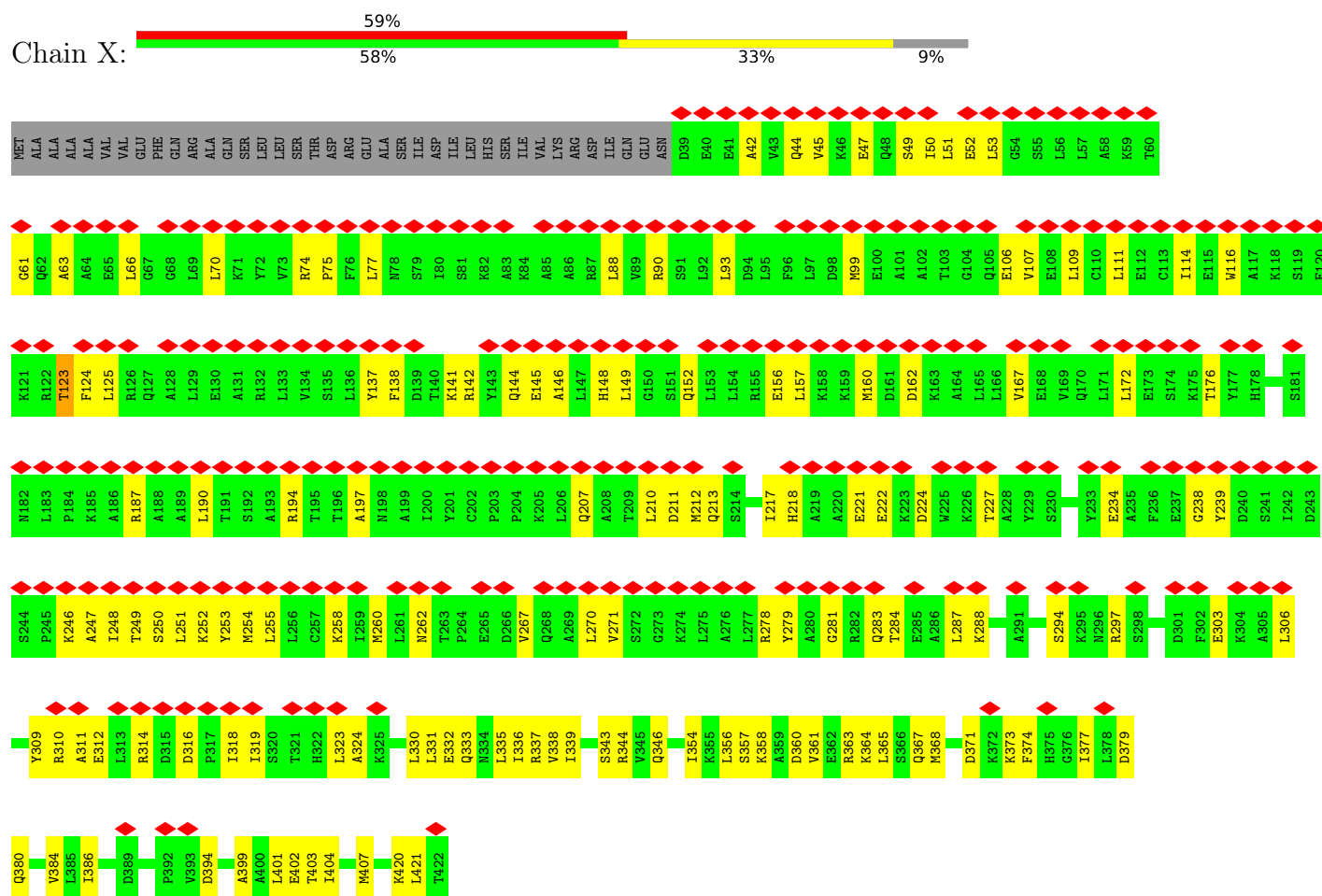


• Molecule 5: 26S proteasome non-ATPase regulatory subunit 12

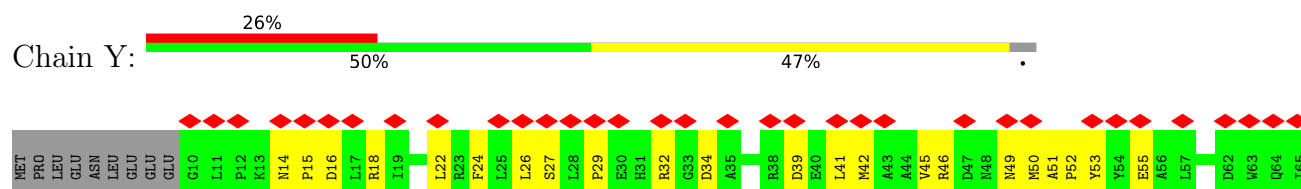


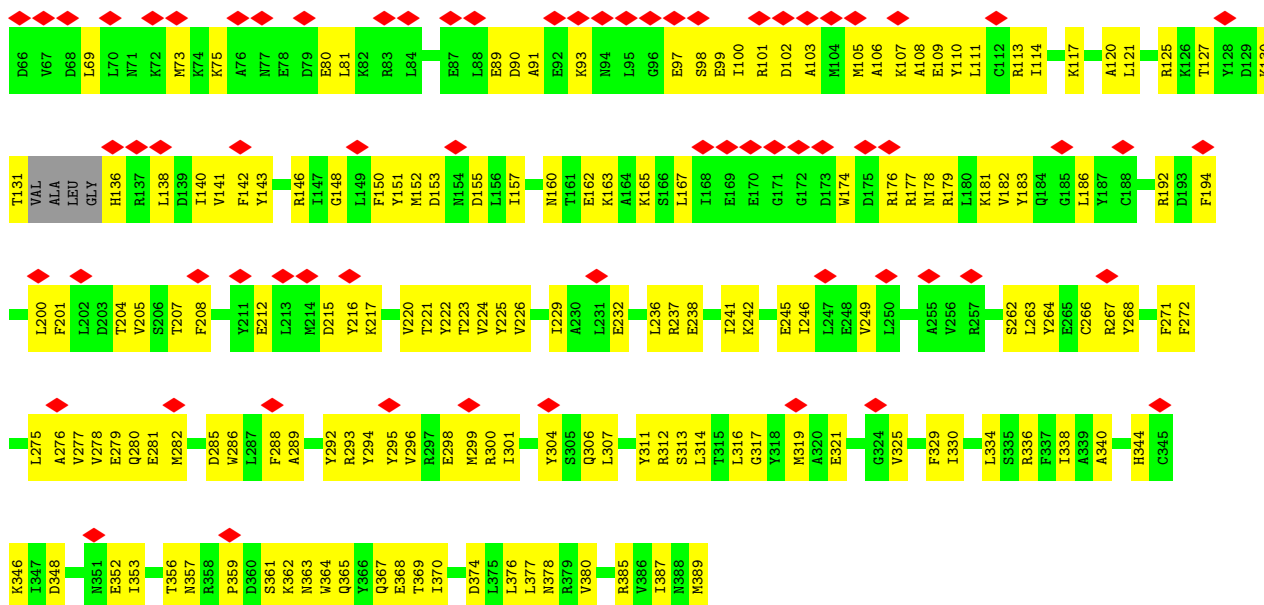


• Molecule 6: 26S proteasome non-ATPase regulatory subunit 11

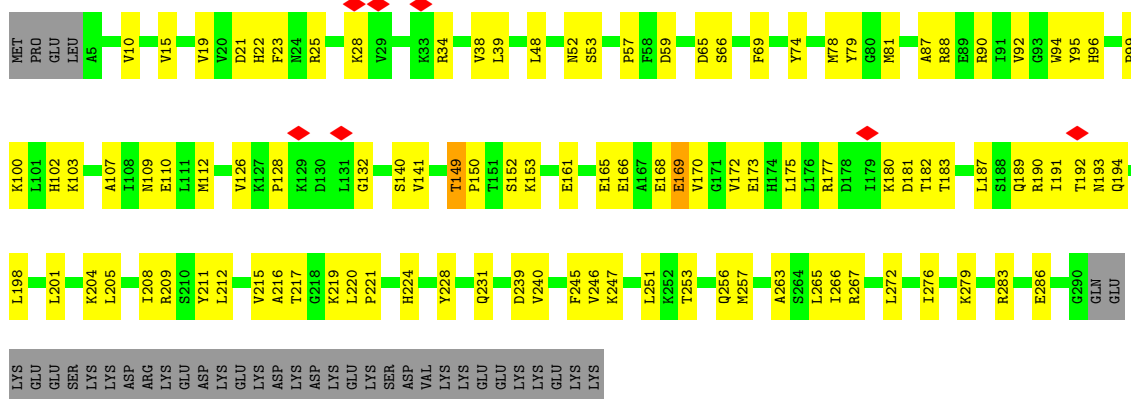


• Molecule 7: 26S proteasome non-ATPase regulatory subunit 6

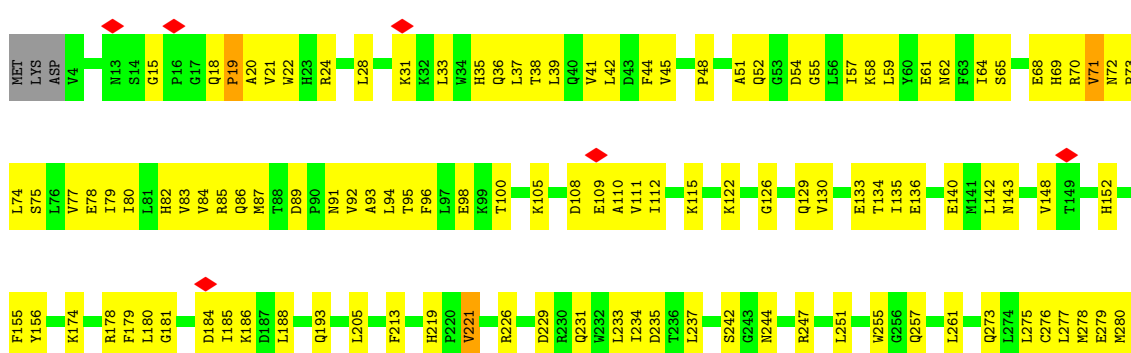


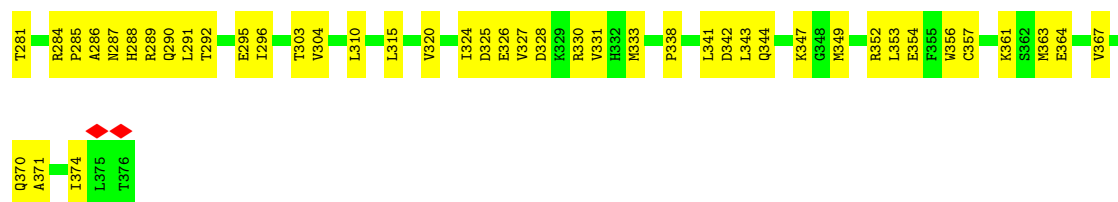


• Molecule 8: 26S proteasome non-ATPase regulatory subunit 7

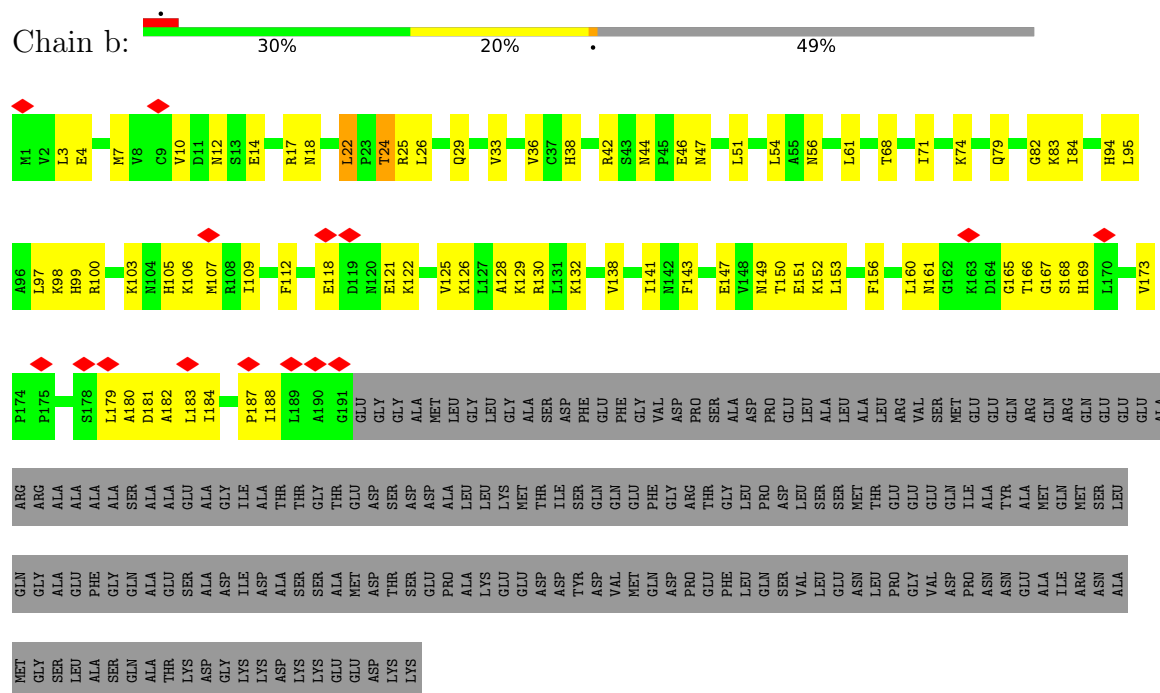


• Molecule 9: 26S proteasome non-ATPase regulatory subunit 13

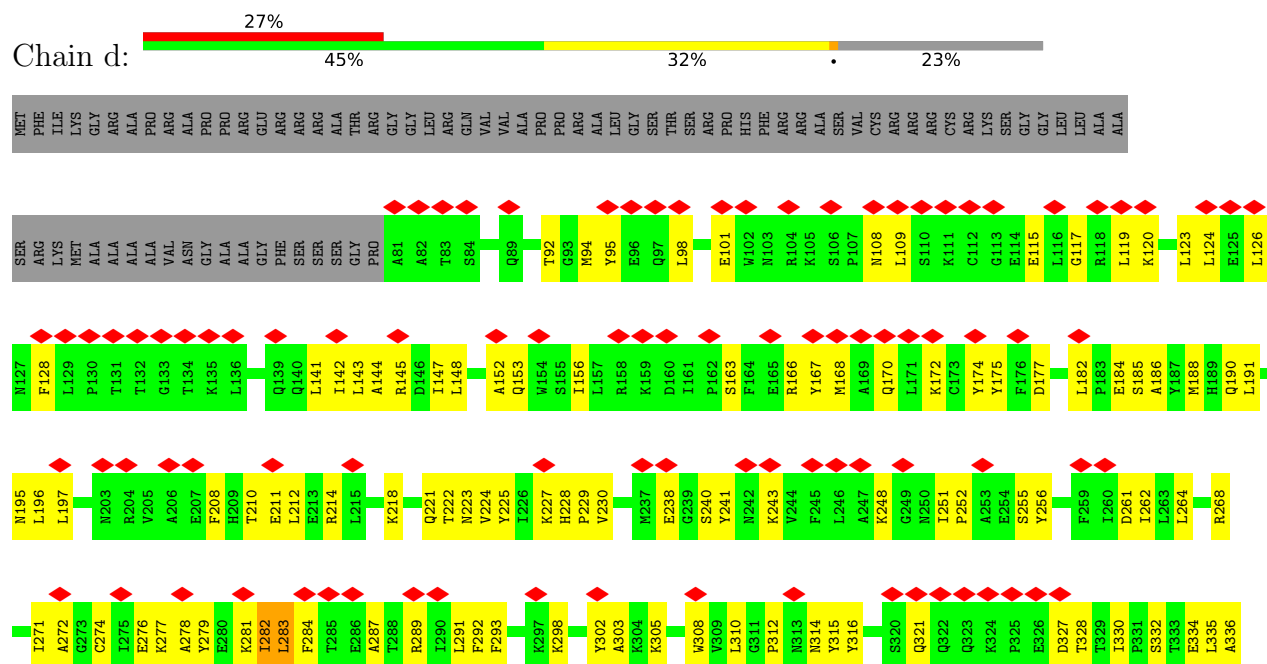




• Molecule 10: 26S proteasome non-ATPase regulatory subunit 4

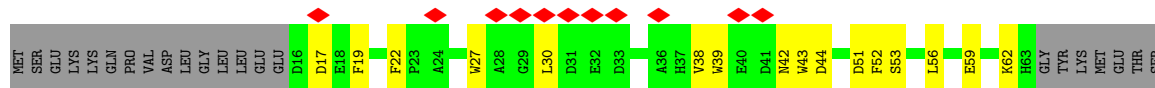


• Molecule 11: 26S proteasome non-ATPase regulatory subunit 8

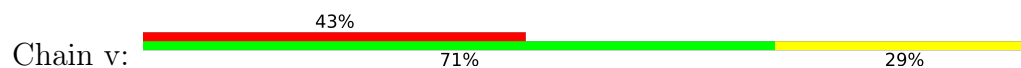




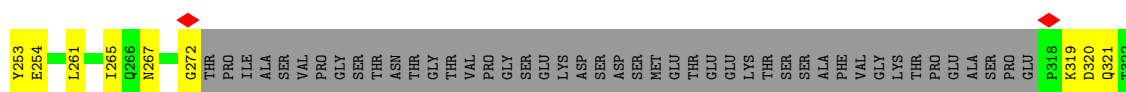
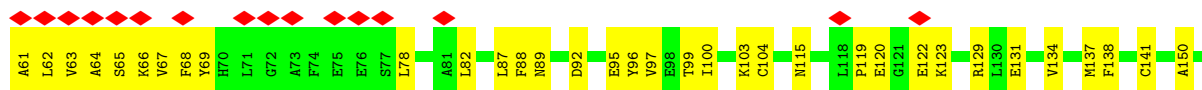
• Molecule 12: 26S proteasome complex subunit SEM1

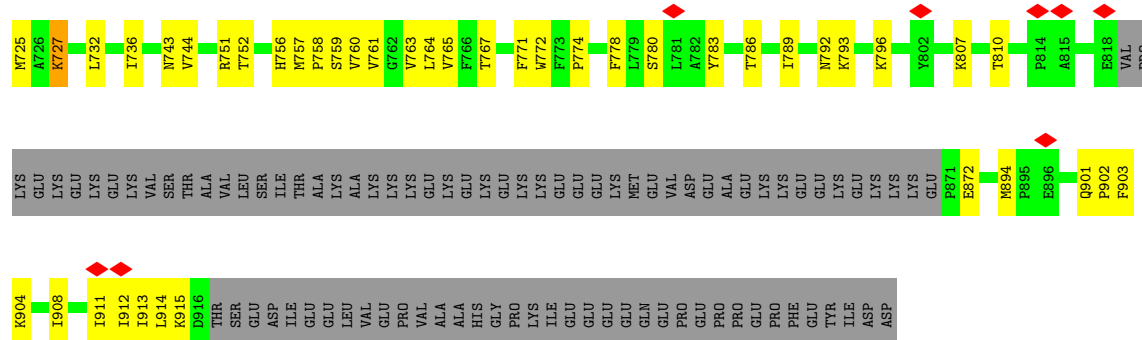


• Molecule 13: Substrate

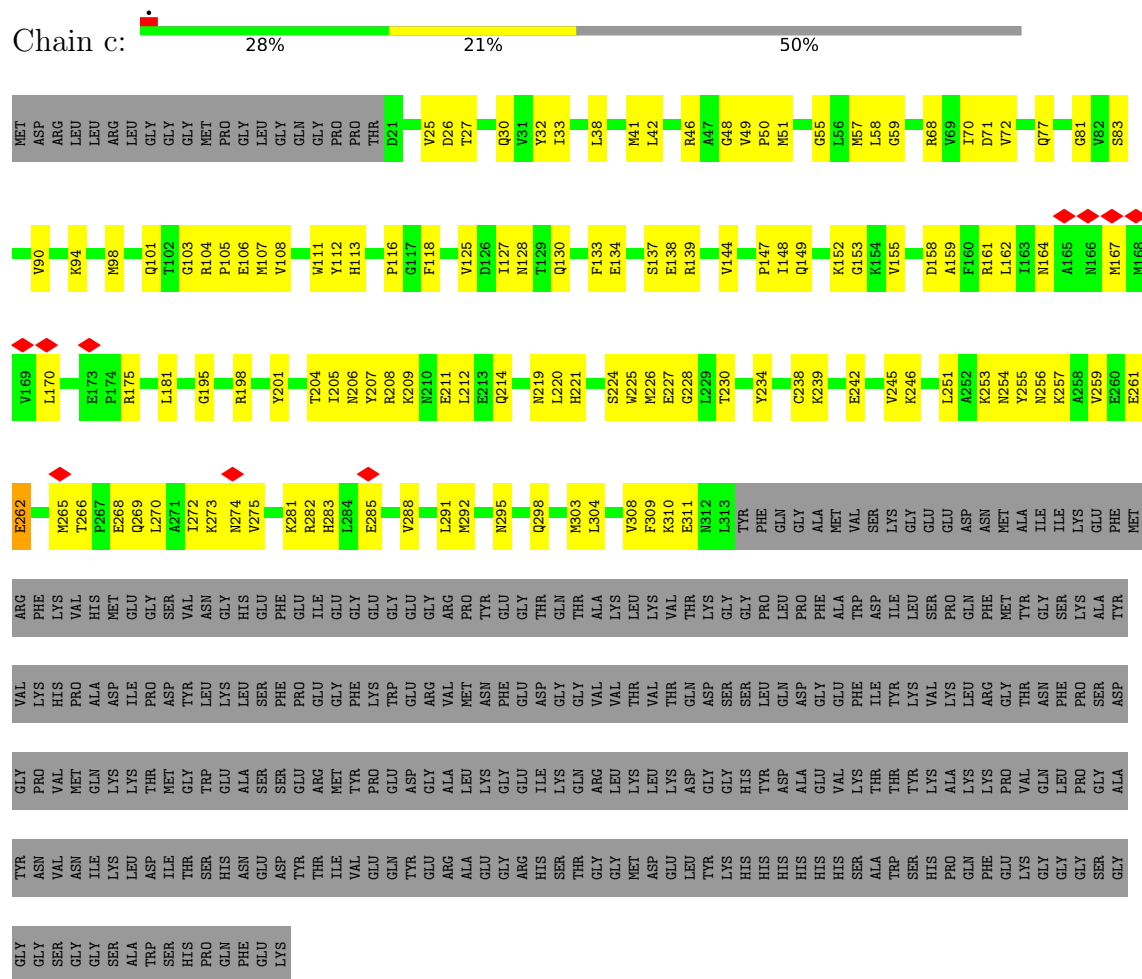


• Molecule 14: 26S proteasome non-ATPase regulatory subunit 1

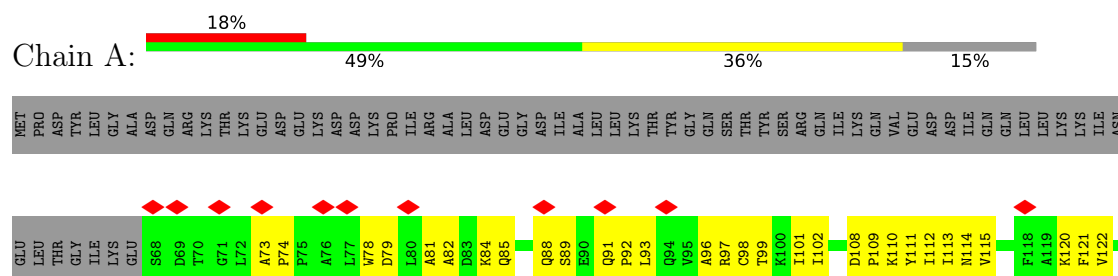


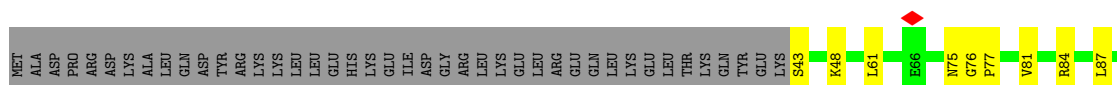
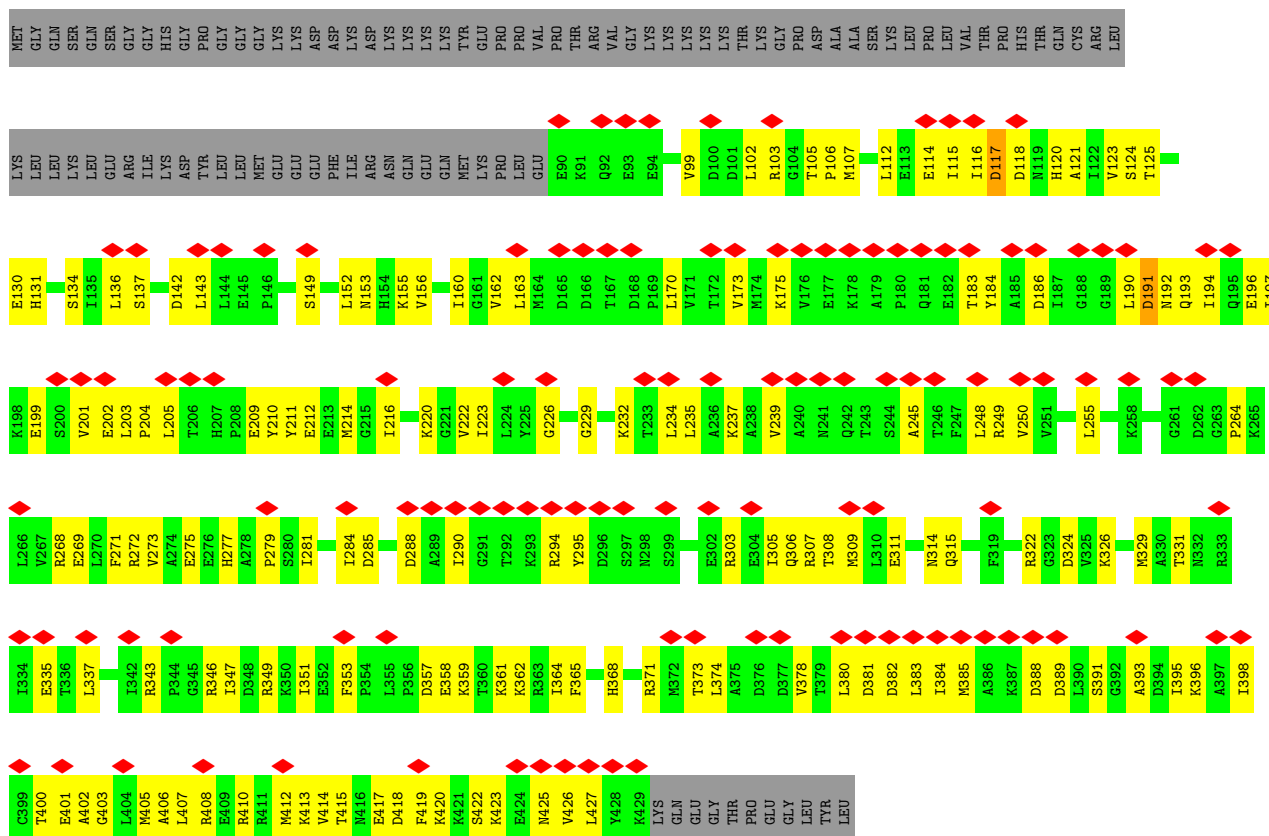


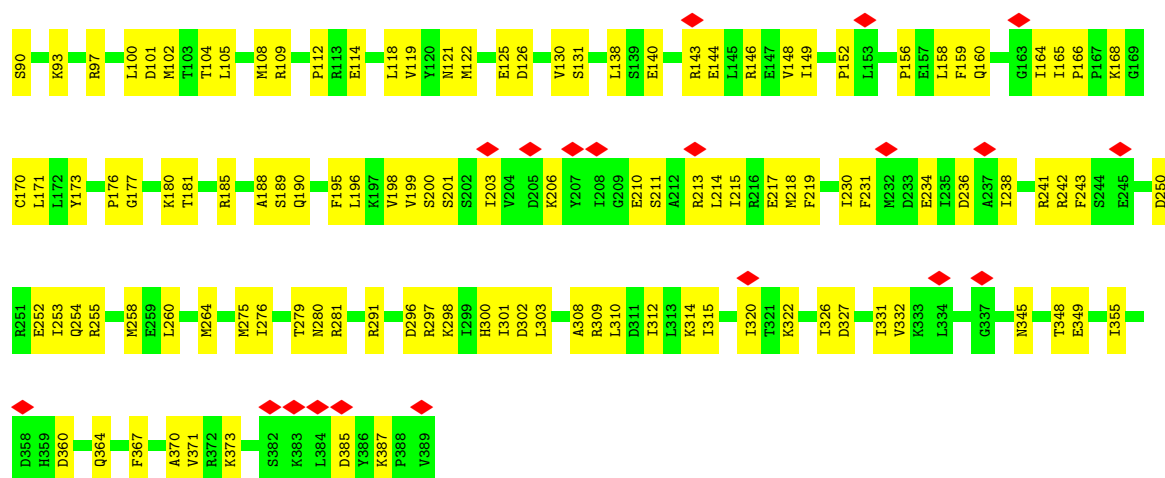
• Molecule 15: Ubiquitin C-terminal hydrolase PSMD14, Uncharacterized protein



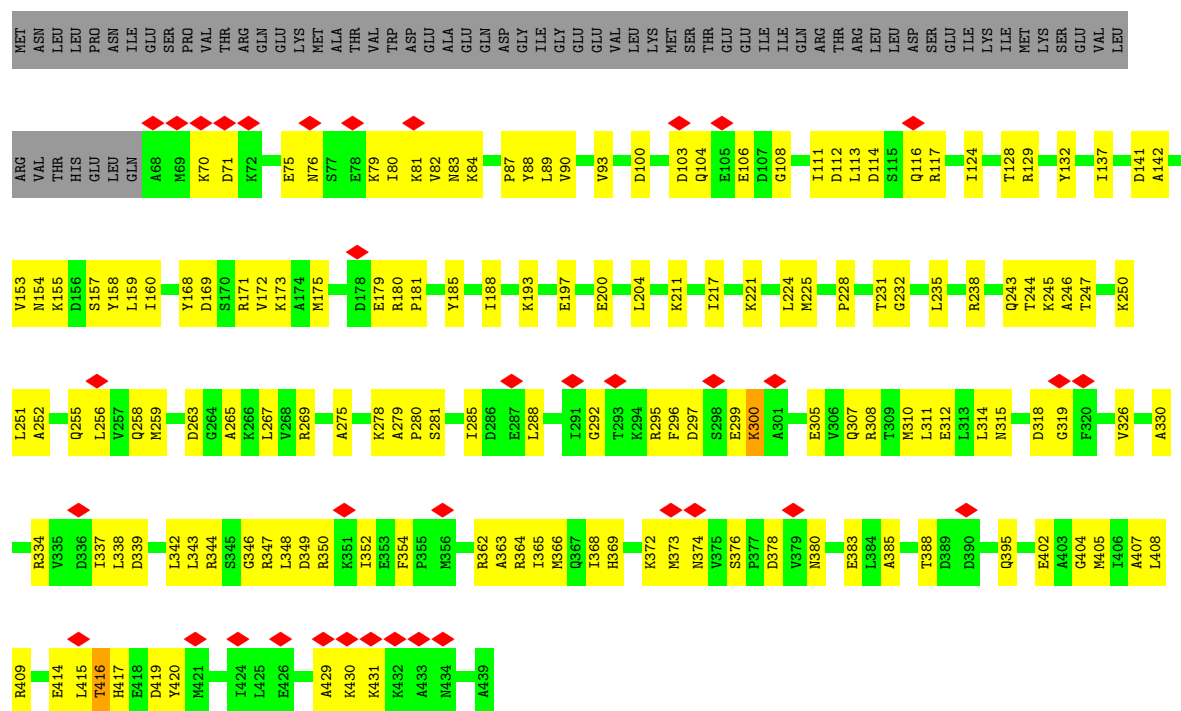
• Molecule 16: 26S proteasome regulatory subunit 7



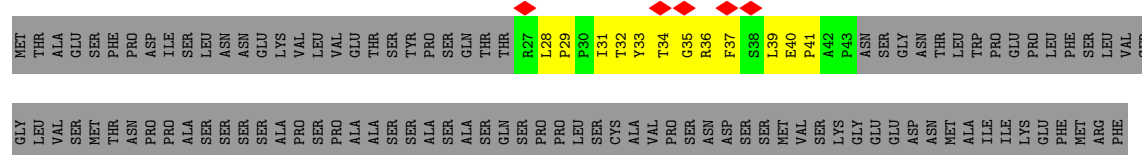




• Molecule 19: 26S proteasome regulatory subunit 6A



• Molecule 20: Early growth response protein 1



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7251	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.243	Depositor
Minimum map value	-0.140	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	340.0, 340.0, 340.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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, MG, ATP, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	f	0.22	0/1513	0.47	0/2046
2	C	0.20	0/2908	0.47	0/3912
3	D	0.21	0/3085	0.48	0/4163
4	V	0.20	0/3662	0.46	0/4946
5	W	0.20	0/3630	0.45	0/4884
6	X	0.16	0/3084	0.41	0/4157
7	Y	0.22	0/3160	0.52	0/4254
8	Z	0.21	0/2324	0.48	0/3150
9	a	0.18	0/3053	0.47	0/4133
10	b	0.18	0/1478	0.46	0/2001
11	d	0.22	0/2239	0.52	0/3025
12	e	0.19	0/420	0.42	0/572
14	U	0.18	0/6486	0.41	2/8777 (0.0%)
15	c	0.23	0/2347	0.48	0/3174
16	A	0.19	0/2914	0.44	0/3937
17	B	0.18	0/2684	0.47	0/3623
18	E	0.20	0/2765	0.46	0/3730
19	F	0.19	0/2942	0.45	0/3967
20	w	0.23	0/140	0.55	0/192
All	All	0.20	0/50834	0.46	2/68643 (0.0%)

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
9	a	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	U	685	GLN	CA-CB-CG	5.12	124.34	114.10
14	U	727	LYS	CA-CB-CG	5.06	124.21	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	a	221	VAL	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	f	1488	0	1509	100	0
2	C	2870	0	2976	162	0
3	D	3035	0	3070	147	0
4	V	3592	0	3647	191	0
5	W	3582	0	3693	159	0
6	X	3040	0	3134	116	0
7	Y	3103	0	3104	163	0
8	Z	2281	0	2312	109	0
9	a	2995	0	3012	148	0
10	b	1458	0	1505	68	0
11	d	2193	0	2221	111	0
12	e	409	0	316	18	0
13	v	35	0	9	2	0
14	U	6371	0	6409	248	0
15	c	2304	0	2315	115	0
16	A	2863	0	2895	136	0
17	B	2647	0	2684	137	0
18	E	2721	0	2770	106	0
19	F	2902	0	2957	146	0
20	w	135	0	137	24	0
21	C	27	0	12	7	0
21	F	27	0	12	3	0
22	A	31	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	B	31	0	12	6	0
22	D	31	0	12	9	0
22	E	31	0	12	1	0
23	c	1	0	0	0	0
24	B	1	0	0	0	0
24	E	1	0	0	0	0
24	F	1	0	0	0	0
All	All	50206	0	50747	2131	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 21.

All (2131) 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)
14:U:685:GLN:HE21	14:U:725:MET:HB3	1.29	0.97
8:Z:263:ALA:HB1	15:c:288:VAL:HG23	1.46	0.93
17:B:223:ILE:HG12	17:B:329:MET:HB3	1.52	0.91
9:a:70:ARG:HD3	10:b:17:ARG:HH12	1.31	0.91
6:X:283:GLN:HG3	6:X:312:GLU:HG3	1.53	0.90
7:Y:15:PRO:HD2	7:Y:146:ARG:HB3	1.52	0.89
3:D:168:GLY:H	22:D:501:ATP:HN62	1.19	0.89
14:U:540:GLN:HB2	15:c:68:ARG:HH22	1.38	0.89
3:D:60:TYR:HD1	14:U:603:LEU:HD13	1.38	0.87
3:D:60:TYR:CD1	14:U:603:LEU:HD13	2.10	0.87
19:F:224:LEU:HD23	19:F:348:LEU:HD13	1.53	0.87
14:U:203:LYS:HA	14:U:206:MET:HE3	1.57	0.85
18:E:198:VAL:HG12	18:E:200:SER:H	1.40	0.85
6:X:278:ARG:NH1	6:X:278:ARG:O	2.09	0.84
11:d:302:TYR:HD2	11:d:305:LYS:HZ3	1.20	0.84
4:V:85:ALA:HA	4:V:90:GLU:HB2	1.57	0.84
2:C:46:GLN:HE21	14:U:639:LEU:HD21	1.44	0.83
8:Z:59:ASP:HB2	10:b:95:LEU:HD21	1.59	0.83
14:U:603:LEU:HD12	14:U:604:HIS:N	1.93	0.83
6:X:61:GLY:HA2	6:X:99:MET:HE1	1.61	0.82
3:D:214:MET:HE1	22:D:501:ATP:C8	2.15	0.82
5:W:64:SER:HA	5:W:103:LYS:HE2	1.63	0.81
1:f:107:MET:HE2	15:c:125:VAL:HG21	1.62	0.80
1:f:297:GLY:HA2	20:w:28:LEU:HG	1.63	0.80
6:X:194:ARG:HE	6:X:210:LEU:HD21	1.46	0.80
6:X:70:LEU:HD23	6:X:109:LEU:HD22	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:d:168:MET:HE3	11:d:195:ASN:HB2	1.61	0.80
1:f:145:VAL:HG23	1:f:150:MET:HE2	1.65	0.79
2:C:356:GLY:HA3	21:C:501:ADP:C8	2.17	0.79
9:a:54:ASP:HA	9:a:57:ILE:HB	1.63	0.79
5:W:417:ARG:HE	5:W:418:PRO:HD2	1.45	0.79
11:d:335:LEU:HD11	15:c:303:MET:HG3	1.62	0.79
8:Z:228:TYR:HD1	9:a:338:PRO:HB2	1.48	0.78
7:Y:91:ALA:HB1	7:Y:100:ILE:HG22	1.65	0.78
5:W:66:ILE:HG13	5:W:67:LEU:HD12	1.66	0.78
14:U:894:MET:HE3	14:U:902:PRO:HD3	1.66	0.77
4:V:443:ARG:HA	11:d:277:LYS:HD2	1.67	0.77
2:C:90:HIS:HB3	2:C:91:PRO:HD2	1.66	0.77
7:Y:266:CYS:SG	7:Y:306:GLN:NE2	2.57	0.77
3:D:103:VAL:HG21	3:D:132:LEU:HD21	1.66	0.77
16:A:220:THR:HG21	16:A:343:PHE:HB3	1.65	0.77
17:B:197:ILE:HG21	17:B:235:LEU:HD11	1.64	0.77
7:Y:237:ARG:HA	7:Y:241:ILE:HD12	1.66	0.77
8:Z:69:PHE:HB3	10:b:95:LEU:HD22	1.65	0.77
15:c:261:GLU:HB3	15:c:265:MET:HE1	1.67	0.77
5:W:224:LEU:HD11	5:W:256:ILE:HD11	1.66	0.77
16:A:396:ALA:HB3	17:B:214:MET:HE1	1.67	0.76
5:W:331:GLY:HA3	5:W:337:ALA:HB2	1.66	0.76
9:a:61:GLU:HA	9:a:64:ILE:HG12	1.67	0.76
4:V:309:MET:HE1	4:V:331:LEU:HD23	1.68	0.76
15:c:269:GLN:HG3	15:c:273:LYS:HE2	1.67	0.76
11:d:282:ILE:HG23	11:d:283:LEU:H	1.51	0.76
4:V:71:THR:HG22	4:V:107:ARG:HD2	1.67	0.75
17:B:368:HIS:HA	17:B:371:ARG:HH12	1.50	0.75
5:W:179:LYS:HA	5:W:182:ARG:HD3	1.66	0.75
3:D:121:ARG:HB2	15:c:274:ASN:HD22	1.52	0.75
9:a:291:LEU:HD13	9:a:296:ILE:HD11	1.69	0.74
8:Z:193:ASN:HB2	15:c:228:GLY:HA2	1.68	0.74
9:a:284:ARG:HD3	9:a:285:PRO:HD2	1.69	0.74
14:U:208:LEU:HD23	14:U:210:LYS:H	1.51	0.74
2:C:90:HIS:CE1	3:D:110:ASN:H	2.06	0.74
3:D:378:ILE:HG12	3:D:406:VAL:HG11	1.70	0.74
17:B:281:ILE:HG23	17:B:326:LYS:HB2	1.70	0.74
3:D:213:THR:HG22	3:D:217:LYS:HE3	1.69	0.74
14:U:218:GLN:HG2	14:U:752:THR:HG21	1.68	0.74
19:F:255:GLN:O	19:F:258:GLN:NE2	2.21	0.74
10:b:151:GLU:HB2	10:b:153:LEU:HD23	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:744:VAL:HG21	14:U:783:TYR:HB3	1.68	0.73
17:B:343:ARG:HG2	17:B:346:ARG:HB2	1.69	0.73
7:Y:176:ARG:HD2	7:Y:179:ARG:HH21	1.52	0.73
16:A:122:VAL:HG12	19:F:88:TYR:HB2	1.71	0.73
18:E:310:LEU:HD11	18:E:314:LYS:HE2	1.68	0.73
9:a:226:ARG:HB3	9:a:234:ILE:HD11	1.71	0.73
1:f:288:LEU:HG	20:w:33:TYR:HD2	1.52	0.73
4:V:90:GLU:HB3	4:V:93:PHE:CE1	2.24	0.72
6:X:74:ARG:HH12	6:X:77:LEU:HD22	1.52	0.72
18:E:231:PHE:HD1	18:E:276:ILE:HG13	1.54	0.72
1:f:34:ALA:HB1	1:f:95:LYS:HZ3	1.54	0.72
8:Z:34:ARG:HH12	8:Z:102:HIS:HB2	1.54	0.72
5:W:55:ARG:NH1	5:W:94:ARG:O	2.23	0.72
6:X:157:LEU:HD11	6:X:162:ASP:HB2	1.69	0.72
17:B:255:LEU:HD21	17:B:308:THR:HG21	1.71	0.72
8:Z:246:VAL:HG12	11:d:330:ILE:HD11	1.72	0.72
18:E:345:ASN:ND2	19:F:349:ASP:OD1	2.22	0.72
18:E:143:ARG:HH21	18:E:146:ARG:HE	1.37	0.72
14:U:115:ASN:HD21	14:U:123:LYS:HD2	1.55	0.72
4:V:192:MET:HE3	4:V:214:HIS:CD2	2.25	0.72
2:C:161:ILE:HG21	2:C:199:LEU:HD21	1.72	0.71
3:D:204:MET:HE1	3:D:331:ILE:HD13	1.70	0.71
4:V:192:MET:HE3	4:V:214:HIS:CG	2.25	0.71
5:W:24:VAL:HB	5:W:27:ARG:HH21	1.54	0.71
6:X:248:ILE:HG22	6:X:279:TYR:HB3	1.70	0.71
18:E:109:ARG:NH2	19:F:114:ASP:O	2.23	0.71
7:Y:298:GLU:HA	7:Y:301:ILE:HD12	1.72	0.71
6:X:222:GLU:HG2	6:X:224:ASP:H	1.55	0.71
9:a:87:MET:HE3	9:a:93:ALA:HA	1.72	0.71
16:A:162:THR:O	16:A:165:GLN:NE2	2.24	0.71
11:d:153:GLN:HE22	11:d:255:SER:HB3	1.54	0.71
16:A:84:LYS:O	16:A:88:GLN:HB2	1.90	0.71
7:Y:52:PRO:HD2	7:Y:114:ILE:HB	1.70	0.71
17:B:368:HIS:NE2	17:B:396:LYS:HE2	2.05	0.71
5:W:67:LEU:HD23	5:W:104:MET:SD	2.31	0.71
14:U:462:LEU:HA	14:U:481:LEU:HD11	1.73	0.71
16:A:366:ARG:NH1	16:A:367:ASP:O	2.23	0.71
17:B:149:SER:HB2	17:B:163:LEU:HB3	1.73	0.71
3:D:335:LEU:HD11	3:D:371:SER:HA	1.73	0.70
14:U:82:LEU:HD22	14:U:129:ARG:HB3	1.73	0.70
7:Y:344:HIS:HB3	7:Y:357:ASN:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:89:GLU:HG3	7:Y:93:LYS:HE3	1.74	0.70
8:Z:149:THR:HB	8:Z:150:PRO:HD3	1.73	0.70
16:A:85:GLN:HA	16:A:89:SER:HB3	1.74	0.70
1:f:133:LEU:HA	1:f:156:LEU:HD13	1.73	0.70
2:C:60:ARG:HH12	14:U:644:TYR:HB2	1.56	0.70
2:C:163:GLU:HB2	2:C:313:ARG:HH12	1.55	0.70
3:D:55:GLU:OE1	14:U:600:ARG:NH2	2.25	0.70
8:Z:21:ASP:OD2	15:c:104:ARG:NH2	2.20	0.70
9:a:87:MET:HE1	9:a:96:PHE:HB3	1.73	0.70
7:Y:24:PHE:HD2	7:Y:286:TRP:HB2	1.57	0.69
16:A:97:ARG:HG3	17:B:131:HIS:HA	1.72	0.69
6:X:51:LEU:HD21	6:X:88:LEU:HG	1.74	0.69
15:c:70:ILE:HD12	15:c:104:ARG:HH11	1.57	0.69
3:D:211:GLY:N	22:D:501:ATP:O2B	2.20	0.69
9:a:349:MET:SD	9:a:352:ARG:NH2	2.64	0.69
17:B:349:ARG:HG3	17:B:351:ILE:HD11	1.72	0.69
14:U:757:MET:SD	14:U:758:PRO:HD3	2.33	0.69
19:F:299:GLU:HG3	19:F:300:LYS:H	1.57	0.69
3:D:173:GLN:HE22	3:D:334:PRO:HD2	1.58	0.69
9:a:126:GLY:HA3	9:a:129:GLN:HE22	1.57	0.69
15:c:51:MET:HE1	15:c:81:GLY:HA2	1.74	0.69
16:A:312:ARG:NH1	16:A:315:ILE:H	1.90	0.69
5:W:24:VAL:HA	5:W:27:ARG:HE	1.56	0.68
17:B:249:ARG:NH2	17:B:285:ASP:OD2	2.27	0.68
3:D:279:THR:HA	13:v:1:UNK:HA	1.74	0.68
6:X:363:ARG:NH1	6:X:363:ARG:O	2.26	0.68
9:a:52:GLN:O	9:a:86:GLN:NE2	2.26	0.68
14:U:120:GLU:HA	14:U:123:LYS:HE2	1.75	0.68
4:V:117:VAL:O	4:V:128:ARG:NH2	2.26	0.68
3:D:372:GLY:HA3	22:D:501:ATP:C8	2.27	0.68
4:V:191:LEU:HD13	4:V:210:CYS:SG	2.34	0.68
18:E:203:ILE:HD11	18:E:238:ILE:HG13	1.76	0.68
15:c:26:ASP:OD1	15:c:27:THR:N	2.27	0.68
18:E:327:ASP:OD1	18:E:364:GLN:NE2	2.26	0.68
6:X:187:ARG:NH2	6:X:217:ILE:O	2.27	0.68
11:d:251:ILE:HD11	11:d:256:TYR:HB2	1.76	0.68
2:C:165:ILE:O	2:C:290:LYS:NZ	2.27	0.68
8:Z:190:ARG:NH2	9:a:367:VAL:O	2.26	0.68
4:V:122:THR:HG21	4:V:155:ALA:HA	1.76	0.67
14:U:599:ILE:HG22	14:U:603:LEU:HD23	1.76	0.67
9:a:371:ALA:HB2	11:d:340:ILE:HD11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F:295:ARG:NH2	19:F:310:MET:SD	2.66	0.67
4:V:189:ASP:O	4:V:193:GLN:NE2	2.26	0.67
7:Y:26:LEU:HD13	7:Y:32:ARG:HA	1.76	0.67
1:f:131:ASP:HB3	1:f:136:ARG:HB2	1.75	0.67
2:C:235:PHE:HE2	2:C:276:LEU:HD22	1.60	0.67
9:a:108:ASP:O	9:a:110:ALA:N	2.27	0.67
1:f:124:LEU:HD13	1:f:139:LEU:HD11	1.77	0.67
4:V:453:HIS:H	11:d:283:LEU:HD11	1.59	0.67
7:Y:293:ARG:HH22	12:e:51:ASP:HA	1.59	0.67
3:D:341:LYS:HG2	3:D:345:PHE:HE2	1.60	0.67
17:B:294:ARG:NH1	17:B:295:TYR:O	2.27	0.67
10:b:51:LEU:HB2	10:b:71:ILE:HD11	1.77	0.66
6:X:74:ARG:NH1	6:X:74:ARG:O	2.27	0.66
19:F:112:ASP:O	19:F:117:ARG:NH2	2.26	0.66
19:F:311:LEU:HD13	19:F:314:LEU:HD12	1.77	0.66
7:Y:313:SER:HB3	7:Y:353:ILE:HD11	1.77	0.66
17:B:250:VAL:HG23	17:B:284:ILE:HD12	1.77	0.66
18:E:242:ARG:HH22	18:E:258:MET:HB3	1.59	0.66
5:W:373:ILE:HD12	9:a:326:GLU:HG2	1.78	0.66
9:a:188:LEU:O	9:a:193:GLN:NE2	2.28	0.66
1:f:321:GLN:OE1	1:f:321:GLN:N	2.28	0.66
3:D:167:ILE:HG23	3:D:170:MET:HE3	1.77	0.66
4:V:95:LEU:HA	4:V:98:LEU:HB2	1.77	0.66
7:Y:336:ARG:NH2	12:e:44:ASP:OD1	2.28	0.66
14:U:751:ARG:NH1	14:U:908:ILE:O	2.28	0.66
4:V:188:SER:HA	4:V:191:LEU:HG	1.77	0.66
6:X:252:LYS:HZ3	6:X:284:THR:HA	1.61	0.66
9:a:35:HIS:CE1	10:b:17:ARG:HB2	2.31	0.66
4:V:78:HIS:HD1	4:V:166:TYR:HH	1.44	0.66
4:V:264:TYR:HE1	11:d:214:ARG:HE	1.43	0.66
19:F:80:ILE:HG22	19:F:84:LYS:NZ	2.11	0.66
4:V:423:ALA:HA	4:V:428:LEU:HD12	1.77	0.66
9:a:286:ALA:HA	9:a:289:ARG:HE	1.61	0.66
4:V:285:TRP:CD1	7:Y:385:ARG:HH22	2.14	0.65
11:d:123:LEU:HB3	11:d:128:PHE:HB2	1.77	0.65
2:C:221:GLN:HA	2:C:224:ILE:HG22	1.79	0.65
6:X:377:ILE:HG23	7:Y:312:ARG:NH2	2.10	0.65
6:X:420:LYS:O	8:Z:283:ARG:NH2	2.30	0.65
8:Z:59:ASP:OD2	10:b:99:HIS:NE2	2.28	0.65
5:W:131:VAL:HG13	5:W:132:THR:HG23	1.78	0.65
14:U:461:LEU:HB3	14:U:481:LEU:HG	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:269:ILE:HG21	1:f:272:PHE:HB2	1.77	0.65
2:C:47:ALA:HA	2:C:50:ASN:HD22	1.59	0.65
3:D:204:MET:HB2	3:D:310:ALA:HA	1.78	0.65
14:U:771:PHE:HD1	15:c:181:LEU:HD21	1.60	0.65
17:B:220:LYS:HG3	17:B:326:LYS:HD3	1.78	0.65
1:f:299:PRO:HD3	20:w:31:ILE:HG21	1.78	0.65
7:Y:29:PRO:HA	7:Y:32:ARG:HE	1.62	0.65
4:V:469:THR:HB	4:V:471:GLU:OE1	1.97	0.65
5:W:274:VAL:O	5:W:283:GLN:NE2	2.29	0.65
2:C:47:ALA:HB3	4:V:496:PHE:CE2	2.32	0.64
4:V:185:GLN:HG3	4:V:221:LEU:HD22	1.79	0.64
5:W:125:ILE:O	5:W:129:ARG:HG2	1.97	0.64
14:U:685:GLN:NE2	14:U:725:MET:HB3	2.07	0.64
15:c:138:GLU:HG2	15:c:139:ARG:HG2	1.79	0.64
16:A:216:GLY:H	16:A:222:LYS:HD3	1.62	0.64
9:a:140:GLU:HA	9:a:143:ASN:HD21	1.63	0.64
7:Y:14:ASN:HB2	7:Y:143:TYR:HE1	1.61	0.64
14:U:763:VAL:O	14:U:767:THR:HG23	1.98	0.64
19:F:363:ALA:HB2	19:F:385:ALA:HB2	1.80	0.64
4:V:65:ARG:NH2	4:V:139:MET:O	2.24	0.64
2:C:27:LYS:HG2	3:D:44:TYR:CE1	2.33	0.64
1:f:287:THR:HG22	20:w:32:THR:HG22	1.80	0.64
5:W:454:ASN:ND2	8:Z:220:LEU:HD22	2.13	0.64
18:E:281:ARG:NH2	19:F:295:ARG:HG2	2.13	0.64
4:V:324:PHE:HA	4:V:327:THR:HG22	1.78	0.64
15:c:147:PRO:HG2	15:c:148:ILE:HD12	1.78	0.64
2:C:117:ARG:HD3	2:C:122:THR:HG23	1.80	0.64
18:E:84:ARG:HB2	18:E:87:LEU:HD13	1.80	0.64
9:a:77:VAL:HG21	9:a:110:ALA:HB1	1.80	0.63
2:C:235:PHE:HA	2:C:238:ALA:HB3	1.79	0.63
6:X:379:ASP:HB2	7:Y:312:ARG:HH11	1.62	0.63
8:Z:216:ALA:HA	9:a:343:LEU:HD11	1.80	0.63
9:a:51:ALA:HB3	9:a:85:ARG:HH22	1.63	0.63
9:a:91:ASN:OD1	9:a:92:VAL:N	2.31	0.63
11:d:248:LYS:HG3	11:d:264:LEU:HD11	1.79	0.63
14:U:780:SER:HA	14:U:783:TYR:HD2	1.63	0.63
15:c:77:GLN:NE2	19:F:108:GLY:O	2.22	0.63
18:E:122:MET:HE1	18:E:196:LEU:HD13	1.80	0.63
19:F:344:ARG:HH21	19:F:346:GLY:HA3	1.61	0.63
2:C:310:ARG:HG3	2:C:311:ILE:HD12	1.78	0.63
7:Y:90:ASP:HA	7:Y:93:LYS:HD2	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:19:PRO:HA	9:a:22:TRP:HE3	1.63	0.63
2:C:201:ARG:HD2	2:C:211:PHE:HD1	1.62	0.63
11:d:98:LEU:HD13	11:d:115:GLU:HB3	1.80	0.63
11:d:224:VAL:O	11:d:228:HIS:ND1	2.30	0.63
16:A:97:ARG:HH22	16:A:144:ARG:HA	1.63	0.63
7:Y:217:LYS:NZ	7:Y:249:VAL:O	2.31	0.63
16:A:78:TRP:CE3	16:A:79:ASP:HB3	2.34	0.63
18:E:90:SER:O	18:E:93:LYS:NZ	2.32	0.63
1:f:112:ARG:HD3	19:F:82:VAL:HG21	1.80	0.63
1:f:148:HIS:HA	20:w:41:PRO:HA	1.80	0.63
9:a:15:GLY:HA3	9:a:22:TRP:CH2	2.34	0.63
9:a:374:ILE:HD11	11:d:344:ARG:HA	1.80	0.63
4:V:120:PHE:HB3	4:V:167:LEU:HD13	1.81	0.63
15:c:270:LEU:HA	15:c:273:LYS:HG2	1.81	0.63
16:A:78:TRP:HZ2	17:B:99:VAL:HG23	1.62	0.63
18:E:302:ASP:OD1	18:E:303:LEU:N	2.31	0.63
16:A:394:MET:HE2	17:B:349:ARG:HH22	1.64	0.63
1:f:131:ASP:O	1:f:136:ARG:N	2.32	0.62
2:C:41:ASN:OD1	2:C:44:ARG:NH2	2.31	0.62
8:Z:209:ARG:NH1	9:a:354:GLU:OE2	2.32	0.62
9:a:44:PHE:O	9:a:48:PRO:HD3	1.99	0.62
10:b:33:VAL:HA	10:b:36:VAL:HG12	1.80	0.62
18:E:144:GLU:HB3	18:E:297:ARG:HH22	1.63	0.62
18:E:348:THR:HA	19:F:217:ILE:HD11	1.79	0.62
9:a:363:MET:SD	15:c:304:LEU:HD11	2.38	0.62
11:d:282:ILE:H	11:d:316:TYR:H	1.47	0.62
16:A:212:VAL:HG12	16:A:339:ARG:HB2	1.81	0.62
9:a:315:LEU:HD23	9:a:320:VAL:HG23	1.81	0.62
14:U:535:TYR:HE2	14:U:544:ILE:HG21	1.65	0.62
19:F:339:ASP:HB3	19:F:342:LEU:HD13	1.81	0.62
1:f:293:GLN:HG2	20:w:31:ILE:HD11	1.81	0.62
3:D:62:LYS:NZ	11:d:349:ILE:O	2.27	0.62
5:W:221:LYS:HG3	5:W:225:LYS:HE2	1.80	0.62
7:Y:348:ASP:O	7:Y:352:GLU:N	2.31	0.62
14:U:524:LYS:HA	14:U:556:MET:HE1	1.82	0.62
16:A:272:ILE:HG12	16:A:315:ILE:HD11	1.82	0.62
18:E:253:ILE:HG21	19:F:308:ARG:HH12	1.63	0.62
2:C:31:LEU:HD23	2:C:34:ILE:HD12	1.79	0.62
16:A:213:LEU:HB2	16:A:337:LEU:HD12	1.81	0.62
17:B:102:LEU:HD21	17:B:136:LEU:HD21	1.82	0.62
19:F:93:VAL:HA	19:F:124:ILE:HG22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:129:ARG:NH2	5:W:146:THR:HA	2.15	0.62
2:C:273:MET:HE3	2:C:277:LEU:HD11	1.82	0.62
5:W:24:VAL:HG11	5:W:62:SER:HB3	1.82	0.62
1:f:288:LEU:HB2	20:w:31:ILE:HG13	1.82	0.62
7:Y:18:ARG:HH12	7:Y:22:LEU:HD21	1.65	0.61
10:b:36:VAL:HG23	10:b:188:ILE:HG23	1.82	0.61
14:U:362:ASN:HD21	14:U:724:VAL:HG11	1.63	0.61
4:V:188:SER:HB3	4:V:214:HIS:ND1	2.14	0.61
9:a:257:GLN:OE1	9:a:257:GLN:N	2.33	0.61
10:b:54:LEU:HB3	10:b:84:ILE:HG23	1.81	0.61
11:d:101:GLU:OE2	11:d:108:ASN:ND2	2.32	0.61
15:c:206:ASN:OD1	15:c:207:TYR:N	2.33	0.61
2:C:195:GLY:H	21:C:501:ADP:H5'2	1.65	0.61
14:U:78:LEU:HD22	14:U:103:LYS:HG3	1.81	0.61
15:c:158:ASP:OD1	15:c:159:ALA:N	2.33	0.61
16:A:135:GLU:H	16:A:138:MET:HE3	1.65	0.61
3:D:179:GLU:HG2	3:D:183:LEU:HD23	1.82	0.61
7:Y:101:ARG:HH22	7:Y:130:LYS:HG3	1.64	0.61
7:Y:105:MET:O	7:Y:109:GLU:N	2.26	0.61
11:d:268:ARG:O	11:d:271:ILE:HG12	2.00	0.61
7:Y:205:VAL:HG21	7:Y:246:ILE:HD11	1.82	0.61
9:a:52:GLN:OE1	9:a:86:GLN:NE2	2.34	0.61
17:B:279:PRO:HA	17:B:324:ASP:HB3	1.82	0.61
18:E:43:SER:OG	19:F:76:ASN:ND2	2.32	0.61
4:V:477:HIS:ND1	11:d:342:TYR:OH	2.31	0.61
9:a:38:THR:O	9:a:42:LEU:HG	2.00	0.61
14:U:374:SER:HB2	14:U:407:SER:HB2	1.81	0.61
15:c:111:TRP:HB3	15:c:133:PHE:HE2	1.66	0.61
17:B:232:LYS:HG2	17:B:353:PHE:CD2	2.35	0.61
8:Z:190:ARG:HH21	9:a:371:ALA:HB3	1.66	0.61
19:F:75:GLU:OE2	19:F:79:LYS:NZ	2.28	0.61
4:V:209:LYS:HA	4:V:209:LYS:HE3	1.83	0.61
4:V:355:ARG:HH12	12:e:30:LEU:H	1.48	0.61
17:B:120:HIS:HB2	17:B:134:SER:HA	1.83	0.61
1:f:36:HIS:CD2	1:f:95:LYS:HE3	2.35	0.61
15:c:253:LYS:NZ	15:c:253:LYS:O	2.33	0.61
2:C:235:PHE:CE2	2:C:276:LEU:HD22	2.35	0.61
2:C:272:THR:O	2:C:276:LEU:HG	2.01	0.61
2:C:324:ALA:O	2:C:328:ILE:HG13	2.01	0.60
2:C:369:TYR:HA	2:C:372:ARG:HD2	1.82	0.60
3:D:383:GLY:HA3	18:E:164:ILE:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:114:TYR:CD1	4:V:138:PRO:HG3	2.36	0.60
7:Y:279:GLU:HA	7:Y:282:MET:HE2	1.83	0.60
14:U:185:MET:HE3	14:U:198:LEU:HD21	1.83	0.60
17:B:106:PRO:O	17:B:107:MET:HE2	2.01	0.60
2:C:277:LEU:HD13	2:C:310:ARG:HD2	1.83	0.60
17:B:273:VAL:HG22	17:B:277:HIS:CE1	2.37	0.60
9:a:89:ASP:HB3	9:a:92:VAL:HG12	1.81	0.60
11:d:152:ALA:O	11:d:156:ILE:HG12	2.00	0.60
3:D:77:GLU:OE1	15:c:152:LYS:HB2	2.00	0.60
1:f:154:LEU:HD23	1:f:284:PHE:HZ	1.65	0.60
8:Z:78:MET:SD	15:c:98:MET:HE3	2.41	0.60
11:d:123:LEU:HA	11:d:126:LEU:HG	1.84	0.60
15:c:113:HIS:CE1	15:c:144:VAL:HG22	2.37	0.60
19:F:81:LYS:HA	19:F:84:LYS:HG2	1.82	0.60
6:X:360:ASP:OD1	6:X:361:VAL:N	2.35	0.60
11:d:334:GLU:OE1	11:d:334:GLU:N	2.27	0.60
15:c:98:MET:HA	15:c:101:GLN:HG2	1.83	0.60
16:A:178:GLY:O	22:A:501:ATP:N6	2.33	0.60
17:B:402:ALA:HA	17:B:405:MET:HE3	1.84	0.60
19:F:171:ARG:HH22	19:F:258:GLN:HE22	1.49	0.60
1:f:112:ARG:HH22	19:F:79:LYS:HE2	1.67	0.60
9:a:72:ASN:O	9:a:74:LEU:N	2.35	0.60
9:a:364:GLU:HA	9:a:367:VAL:HG12	1.84	0.60
11:d:327:ASP:OD1	11:d:328:THR:N	2.35	0.60
1:f:280:PHE:N	20:w:39:LEU:O	2.28	0.60
2:C:218:GLU:HG3	3:D:275:PHE:HB2	1.82	0.60
14:U:489:ALA:HA	14:U:520:MET:HE1	1.82	0.60
17:B:124:SER:HA	17:B:130:GLU:HA	1.84	0.60
17:B:380:LEU:HD13	17:B:383:LEU:HD12	1.82	0.60
2:C:227:GLY:HA3	2:C:229:ARG:HE	1.66	0.60
3:D:211:GLY:HA2	3:D:214:MET:HE3	1.82	0.60
4:V:101:LEU:O	4:V:104:THR:OG1	2.20	0.60
6:X:137:TYR:OH	6:X:145:GLU:OE1	2.20	0.60
7:Y:316:LEU:HA	7:Y:319:MET:SD	2.41	0.60
7:Y:361:SER:O	7:Y:365:GLN:NE2	2.34	0.60
11:d:123:LEU:HD13	11:d:126:LEU:HD11	1.84	0.60
14:U:352:ILE:HG13	14:U:353:LEU:HD12	1.84	0.60
14:U:568:GLU:HA	14:U:601:ARG:HH22	1.66	0.60
17:B:190:LEU:HB3	17:B:193:GLN:HB2	1.84	0.60
10:b:121:GLU:HG2	10:b:152:LYS:HD2	1.84	0.60
11:d:124:LEU:HD11	14:U:19:LEU:HD23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:9:ILE:HG21	14:U:41:SER:HB2	1.84	0.60
19:F:247:THR:HG21	19:F:278:LYS:HB3	1.83	0.60
3:D:391:ARG:NH2	3:D:398:ASP:OD2	2.34	0.59
5:W:256:ILE:HG23	5:W:262:LYS:HB3	1.83	0.59
2:C:57:ARG:HE	14:U:644:TYR:HA	1.67	0.59
4:V:90:GLU:HB3	4:V:93:PHE:CD1	2.37	0.59
10:b:122:LYS:O	10:b:126:LYS:HG2	2.02	0.59
14:U:654:MET:HE2	14:U:654:MET:HA	1.83	0.59
3:D:183:LEU:HG	3:D:191:TYR:HE1	1.68	0.59
3:D:284:GLU:O	3:D:288:ILE:HG12	2.02	0.59
4:V:93:PHE:HB3	4:V:96:ARG:HD3	1.84	0.59
4:V:95:LEU:HD21	7:Y:389:MET:HE1	1.85	0.59
6:X:255:LEU:HD22	6:X:267:VAL:HG23	1.85	0.59
4:V:337:LEU:HD22	4:V:367:VAL:HG11	1.84	0.59
2:C:49:ARG:NE	3:D:64:GLU:OE1	2.35	0.59
2:C:90:HIS:HE1	3:D:110:ASN:ND2	2.01	0.59
2:C:160:GLU:OE1	17:B:408:ARG:NH2	2.35	0.59
5:W:374:THR:HG23	9:a:327:VAL:HG22	1.84	0.59
7:Y:138:LEU:HD22	7:Y:167:LEU:HD23	1.83	0.59
14:U:244:MET:HG2	14:U:903:PHE:CZ	2.38	0.59
16:A:293:ASN:OD1	16:A:294:GLU:N	2.35	0.59
16:A:312:ARG:HH11	16:A:315:ILE:H	1.50	0.59
17:B:234:LEU:HD11	22:B:501:ATP:C4	2.37	0.59
18:E:242:ARG:NH2	18:E:258:MET:HB3	2.17	0.59
19:F:157:SER:OG	19:F:159:LEU:HD23	2.03	0.59
19:F:405:MET:O	19:F:409:ARG:HG2	2.02	0.59
5:W:373:ILE:HG12	5:W:378:MET:HE3	1.83	0.59
10:b:4:GLU:N	10:b:47:ASN:OD1	2.35	0.59
15:c:25:VAL:HG23	15:c:175:ARG:HG2	1.84	0.59
2:C:219:LEU:HD11	3:D:289:LEU:HD23	1.83	0.59
3:D:130:VAL:HG12	3:D:142:VAL:HG22	1.84	0.59
3:D:363:TYR:HE2	3:D:399:PHE:HB3	1.68	0.59
5:W:409:LEU:HD22	6:X:344:ARG:HH12	1.66	0.59
10:b:24:THR:HG22	10:b:26:LEU:H	1.68	0.59
17:B:284:ILE:HG23	17:B:329:MET:HG3	1.85	0.59
4:V:321:ALA:HA	12:e:19:PHE:HB2	1.83	0.59
7:Y:81:LEU:HD12	7:Y:110:TYR:HE2	1.66	0.59
8:Z:189:GLN:N	8:Z:189:GLN:OE1	2.34	0.59
4:V:118:GLN:HA	4:V:128:ARG:HH22	1.66	0.59
14:U:542:GLU:HA	14:U:545:LEU:HD12	1.84	0.59
17:B:364:ILE:HG23	17:B:368:HIS:CE1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:292:CYS:HB3	1:f:305:THR:HG23	1.85	0.58
4:V:259:LEU:HD21	4:V:295:ILE:HG22	1.84	0.58
5:W:260:SER:HA	5:W:263:TRP:NE1	2.17	0.58
19:F:256:LEU:HD23	19:F:267:LEU:HD23	1.85	0.58
3:D:177:VAL:HG11	3:D:215:LEU:HD21	1.85	0.58
6:X:310:ARG:HB2	6:X:314:ARG:HE	1.67	0.58
16:A:163:MET:O	16:A:164:MET:HE2	2.03	0.58
2:C:213:ARG:HH21	2:C:247:PHE:HE2	1.51	0.58
15:c:48:GLY:O	15:c:51:MET:N	2.37	0.58
16:A:183:GLN:N	16:A:183:GLN:OE1	2.36	0.58
18:E:281:ARG:HH21	19:F:295:ARG:HG2	1.69	0.58
9:a:226:ARG:NH1	9:a:229:ASP:OD2	2.28	0.58
14:U:722:ASP:OD1	14:U:727:LYS:NZ	2.36	0.58
15:c:161:ARG:NH1	15:c:201:TYR:OH	2.33	0.58
3:D:248:ARG:HB3	3:D:295:GLN:NE2	2.19	0.58
3:D:275:PHE:HD1	3:D:282:ASP:HB3	1.68	0.58
3:D:353:ASN:HB3	3:D:393:ILE:HD12	1.84	0.58
5:W:29:PRO:O	5:W:33:LYS:HG2	2.03	0.58
2:C:231:VAL:HG13	2:C:232:ARG:HG3	1.85	0.58
4:V:311:ASN:OD1	4:V:314:ARG:NH2	2.37	0.58
4:V:324:PHE:CE2	12:e:19:PHE:HB3	2.38	0.58
4:V:414:TYR:CD2	4:V:417:ILE:HD13	2.38	0.58
8:Z:52:ASN:OD1	8:Z:53:SER:N	2.36	0.58
10:b:165:GLY:O	10:b:167:GLY:N	2.36	0.58
15:c:269:GLN:HE22	15:c:272:ILE:HB	1.69	0.58
16:A:334:PRO:HG3	19:F:395:GLN:HG3	1.84	0.58
10:b:181:ASP:OD1	10:b:182:ALA:N	2.36	0.58
19:F:221:LYS:N	19:F:349:ASP:OD2	2.23	0.58
3:D:311:THR:HG21	3:D:317:LEU:HD11	1.83	0.58
12:e:52:PHE:CE2	12:e:56:LEU:HD23	2.39	0.58
9:a:15:GLY:HA3	9:a:22:TRP:HH2	1.69	0.58
15:c:130:GLN:HE21	15:c:134:GLU:HG2	1.68	0.58
17:B:398:ILE:HD11	17:B:427:LEU:HG	1.86	0.58
14:U:719:ASP:OD1	14:U:720:LYS:N	2.37	0.57
16:A:357:ILE:HG13	16:A:360:ARG:NH2	2.19	0.57
17:B:103:ARG:HG2	17:B:160:ILE:HG21	1.86	0.57
1:f:42:ARG:NH1	1:f:44:ASP:OD1	2.35	0.57
3:D:115:ILE:HG22	3:D:139:LEU:HD12	1.85	0.57
3:D:349:THR:HB	3:D:354:LEU:HD11	1.85	0.57
7:Y:46:ARG:HD2	7:Y:69:LEU:HD22	1.86	0.57
14:U:2:ILE:HG23	14:U:3:THR:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:724:VAL:HA	14:U:727:LYS:HG2	1.87	0.57
19:F:305:GLU:HA	19:F:308:ARG:HE	1.68	0.57
3:D:392:TYR:CZ	5:W:134:GLY:HA2	2.40	0.57
7:Y:194:PHE:HD1	7:Y:226:VAL:HG23	1.68	0.57
9:a:273:GLN:HB3	9:a:310:LEU:HD11	1.86	0.57
14:U:134:VAL:HA	14:U:137:MET:HG3	1.84	0.57
18:E:76:GLY:H	18:E:77:PRO:HD2	1.68	0.57
19:F:305:GLU:OE1	19:F:308:ARG:NH2	2.37	0.57
19:F:318:ASP:HB3	19:F:347:ARG:HG2	1.87	0.57
1:f:144:ARG:HA	1:f:149:MET:HA	1.87	0.57
2:C:279:GLN:NE2	2:C:280:LEU:HG	2.20	0.57
7:Y:237:ARG:HB2	7:Y:264:TYR:CZ	2.39	0.57
11:d:224:VAL:HB	11:d:228:HIS:HE1	1.69	0.57
11:d:312:PRO:HB2	11:d:315:TYR:CD1	2.38	0.57
14:U:506:ALA:HA	14:U:544:ILE:HD11	1.86	0.57
15:c:46:ARG:HH11	15:c:49:VAL:HG21	1.68	0.57
17:B:331:THR:HG21	17:B:337:LEU:HD21	1.84	0.57
1:f:287:THR:HA	20:w:32:THR:HA	1.85	0.57
4:V:139:MET:HA	4:V:139:MET:HE3	1.87	0.57
4:V:375:PHE:HB3	4:V:399:ARG:HH11	1.69	0.57
2:C:52:LEU:HB3	3:D:68:LEU:CD2	2.35	0.57
5:W:375:MET:HB3	5:W:413:ILE:HD11	1.86	0.57
15:c:254:ASN:HA	15:c:257:LYS:HG2	1.86	0.57
2:C:42:LEU:HD11	3:D:57:GLN:HG3	1.87	0.57
3:D:60:TYR:HE2	14:U:640:LEU:HD21	1.70	0.57
3:D:133:HIS:ND1	3:D:135:HIS:O	2.37	0.57
5:W:346:GLU:HG3	5:W:350:ARG:HH12	1.67	0.57
7:Y:52:PRO:HG2	7:Y:114:ILE:HD12	1.87	0.57
11:d:252:PRO:HG2	11:d:256:TYR:HE2	1.69	0.57
15:c:127:ILE:HG23	15:c:162:LEU:HD21	1.87	0.57
22:A:501:ATP:O1G	17:B:343:ARG:NH2	2.37	0.57
2:C:60:ARG:NH1	14:U:644:TYR:HB2	2.20	0.57
2:C:336:MET:HA	2:C:336:MET:HE3	1.86	0.57
7:Y:237:ARG:HB2	7:Y:264:TYR:CE1	2.40	0.57
10:b:166:THR:O	10:b:169:HIS:NE2	2.38	0.57
17:B:112:LEU:HD21	17:B:115:ILE:HD11	1.86	0.57
1:f:70:ARG:HH12	15:c:128:ASN:C	2.13	0.57
2:C:369:TYR:HE2	2:C:385:MET:HB3	1.70	0.57
8:Z:190:ARG:HH22	9:a:367:VAL:HG22	1.69	0.57
8:Z:194:GLN:O	8:Z:198:LEU:HG	2.04	0.57
10:b:147:GLU:HB2	10:b:151:GLU:OE2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:E:281:ARG:HH22	19:F:296:PHE:C	2.13	0.57
18:E:327:ASP:H	18:E:364:GLN:NE2	2.03	0.57
1:f:34:ALA:HB1	1:f:95:LYS:NZ	2.18	0.56
7:Y:102:ASP:HA	7:Y:105:MET:HE3	1.86	0.56
7:Y:103:ALA:O	7:Y:106:ALA:HB3	2.05	0.56
9:a:42:LEU:HA	9:a:79:ILE:HD11	1.87	0.56
14:U:624:PHE:CE2	14:U:760:VAL:HG23	2.40	0.56
14:U:633:CYS:O	14:U:637:VAL:HG22	2.05	0.56
17:B:422:SER:O	17:B:426:VAL:HG22	2.05	0.56
4:V:114:TYR:O	4:V:117:VAL:HG12	2.04	0.56
8:Z:81:MET:HE1	15:c:94:LYS:HG3	1.86	0.56
9:a:38:THR:HG21	9:a:71:VAL:HG21	1.87	0.56
11:d:95:TYR:CD1	11:d:143:LEU:HG	2.40	0.56
16:A:96:ALA:HA	16:A:142:VAL:O	2.06	0.56
18:E:97:ARG:NH2	18:E:112:PRO:O	2.37	0.56
3:D:77:GLU:O	3:D:80:LYS:HG2	2.05	0.56
4:V:375:PHE:HB3	4:V:399:ARG:NH1	2.20	0.56
4:V:408:ARG:HA	4:V:408:ARG:HH11	1.70	0.56
5:W:440:ASN:O	5:W:443:THR:OG1	2.22	0.56
9:a:35:HIS:HE1	10:b:14:GLU:O	1.89	0.56
9:a:142:LEU:HD12	9:a:152:HIS:CD2	2.40	0.56
9:a:277:LEU:HA	9:a:280:MET:HE2	1.86	0.56
16:A:154:PRO:HG3	17:B:116:ILE:HD13	1.86	0.56
16:A:241:ILE:HB	16:A:244:GLU:CD	2.31	0.56
16:A:357:ILE:HG13	16:A:360:ARG:HH21	1.71	0.56
18:E:81:VAL:HG21	18:E:100:LEU:HD11	1.88	0.56
1:f:139:LEU:HG	1:f:141:LEU:HD21	1.87	0.56
5:W:307:LYS:HA	5:W:310:THR:HG22	1.86	0.56
7:Y:298:GLU:O	7:Y:301:ILE:HB	2.06	0.56
8:Z:152:SER:OG	8:Z:153:LYS:N	2.34	0.56
14:U:254:GLU:OE2	14:U:751:ARG:NE	2.38	0.56
16:A:200:ARG:HA	16:A:203:ASN:ND2	2.21	0.56
8:Z:25:ARG:HD3	15:c:104:ARG:CZ	2.36	0.56
14:U:24:LEU:HG	14:U:59:PHE:HD2	1.70	0.56
18:E:176:PRO:HG3	18:E:280:ASN:HD21	1.69	0.56
2:C:190:GLY:HA3	2:C:317:PHE:HB2	1.86	0.56
2:C:236:VAL:O	2:C:240:GLU:HG3	2.05	0.56
4:V:264:TYR:CE2	11:d:210:THR:HB	2.41	0.56
2:C:150:MET:HE1	2:C:198:LEU:HD11	1.87	0.56
3:D:344:ILE:HG23	3:D:375:ILE:HD13	1.86	0.56
8:Z:25:ARG:HA	8:Z:28:LYS:HE3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:d:128:PHE:HE2	11:d:170:GLN:HG2	1.71	0.56
2:C:296:ASN:OD1	2:C:297:ARG:NE	2.39	0.56
4:V:93:PHE:HB3	4:V:96:ARG:CD	2.36	0.56
5:W:35:ALA:HB1	5:W:73:MET:HG2	1.87	0.56
7:Y:312:ARG:HA	7:Y:356:THR:HG23	1.87	0.56
10:b:97:LEU:HD12	10:b:107:MET:SD	2.46	0.56
14:U:31:VAL:HG23	14:U:38:ILE:HG21	1.87	0.56
14:U:192:GLN:HG3	14:U:196:LYS:HE2	1.88	0.56
19:F:318:ASP:OD1	19:F:319:GLY:N	2.34	0.56
1:f:139:LEU:HB3	1:f:154:LEU:HB2	1.87	0.56
10:b:161:ASN:HB3	10:b:168:SER:HB2	1.88	0.56
16:A:158:ASP:O	16:A:161:VAL:N	2.37	0.56
16:A:333:ARG:HE	16:A:336:ARG:NH1	2.04	0.56
19:F:129:ARG:O	19:F:129:ARG:HD3	2.06	0.56
19:F:224:LEU:HD23	19:F:348:LEU:CD1	2.33	0.56
5:W:129:ARG:NH1	5:W:146:THR:OG1	2.39	0.55
5:W:174:TYR:O	5:W:182:ARG:NH1	2.39	0.55
7:Y:275:LEU:HA	7:Y:278:VAL:HG12	1.87	0.55
11:d:282:ILE:HB	11:d:315:TYR:HA	1.86	0.55
4:V:451:ILE:HG13	4:V:458:VAL:HG22	1.87	0.55
9:a:374:ILE:HD13	11:d:344:ARG:HH11	1.72	0.55
14:U:13:ASP:HB3	14:U:44:LYS:HZ3	1.70	0.55
16:A:85:GLN:HE22	17:B:136:LEU:HA	1.70	0.55
18:E:180:LYS:HG2	18:E:301:ILE:HD13	1.88	0.55
2:C:372:ARG:NH2	3:D:175:GLN:OE1	2.39	0.55
5:W:35:ALA:HB2	5:W:43:VAL:HG21	1.89	0.55
8:Z:109:ASN:ND2	8:Z:140:SER:HB3	2.22	0.55
10:b:173:VAL:HG23	10:b:183:LEU:HD22	1.87	0.55
14:U:69:TYR:CE1	14:U:99:THR:HG21	2.42	0.55
17:B:190:LEU:O	17:B:192:ASN:N	2.39	0.55
6:X:212:MET:HE1	6:X:250:SER:HA	1.87	0.55
15:c:220:LEU:HD23	15:c:221:HIS:HD2	1.70	0.55
18:E:370:ALA:O	18:E:373:LYS:HG3	2.07	0.55
19:F:225:MET:HE1	19:F:352:ILE:HB	1.88	0.55
1:f:117:VAL:HA	1:f:143:LEU:HD22	1.87	0.55
4:V:425:LYS:O	4:V:427:GLN:NE2	2.40	0.55
14:U:13:ASP:HB3	14:U:44:LYS:NZ	2.21	0.55
1:f:283:THR:HG22	20:w:36:ARG:HG3	1.87	0.55
5:W:178:GLU:OE2	5:W:181:GLU:N	2.40	0.55
9:a:324:ILE:HG22	9:a:331:VAL:HG23	1.88	0.55
15:c:285:GLU:HA	15:c:288:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:351:ARG:O	16:A:354:ILE:HG22	2.07	0.55
19:F:251:LEU:HD11	19:F:256:LEU:HD11	1.87	0.55
7:Y:50:MET:HB3	7:Y:53:TYR:HB3	1.89	0.55
14:U:230:SER:OG	14:U:267:ASN:ND2	2.40	0.55
15:c:33:ILE:HD13	15:c:205:ILE:HG23	1.87	0.55
2:C:201:ARG:HD2	2:C:211:PHE:CD1	2.41	0.55
4:V:450:SER:HB3	4:V:461:LYS:HE3	1.89	0.55
5:W:51:GLU:CD	5:W:55:ARG:HE	2.15	0.55
10:b:51:LEU:HD23	10:b:61:LEU:HD23	1.89	0.55
14:U:46:GLU:O	14:U:50:GLU:HG2	2.07	0.55
15:c:224:SER:N	15:c:227:GLU:OE2	2.39	0.55
16:A:151:ILE:HD12	16:A:152:PRO:HD2	1.89	0.55
17:B:142:ASP:OD1	17:B:143:LEU:N	2.37	0.55
2:C:182:GLN:HE21	2:C:287:LYS:HG2	1.71	0.55
3:D:55:GLU:O	3:D:58:GLU:HG2	2.06	0.55
3:D:374:ASP:O	3:D:378:ILE:HG13	2.06	0.55
9:a:344:GLN:HA	9:a:347:LYS:HE2	1.88	0.55
11:d:120:LYS:HE3	14:U:19:LEU:HD11	1.88	0.55
14:U:115:ASN:ND2	14:U:123:LYS:HD2	2.22	0.55
16:A:74:PRO:O	16:A:78:TRP:N	2.40	0.55
16:A:351:ARG:HG3	16:A:374:ALA:HB1	1.88	0.55
16:A:351:ARG:NH2	16:A:378:PRO:O	2.39	0.55
19:F:235:LEU:HD22	21:F:501:ADP:H2'	1.89	0.55
1:f:117:VAL:HG22	1:f:143:LEU:HB3	1.89	0.54
2:C:59:LEU:HD22	3:D:75:ALA:HB1	1.89	0.54
3:D:124:LEU:HD12	15:c:275:VAL:HG13	1.89	0.54
11:d:142:ILE:HA	11:d:145:ARG:HD2	1.87	0.54
19:F:285:ILE:HB	19:F:330:ALA:HB2	1.90	0.54
6:X:371:ASP:OD1	7:Y:237:ARG:NH2	2.41	0.54
7:Y:39:ASP:O	7:Y:42:MET:HG2	2.06	0.54
8:Z:263:ALA:HB3	15:c:292:MET:HE2	1.88	0.54
14:U:568:GLU:HG3	14:U:601:ARG:HH22	1.72	0.54
16:A:212:VAL:HA	16:A:339:ARG:O	2.07	0.54
18:E:165:ILE:HD12	18:E:166:PRO:HD2	1.88	0.54
19:F:79:LYS:HA	19:F:82:VAL:HG12	1.89	0.54
2:C:222:LYS:HE2	2:C:223:PHE:CE1	2.42	0.54
22:D:501:ATP:H5'2	18:E:291:ARG:NH2	2.23	0.54
7:Y:52:PRO:O	7:Y:55:GLU:HG2	2.08	0.54
9:a:142:LEU:HG	9:a:155:PHE:HD1	1.72	0.54
14:U:69:TYR:CZ	14:U:99:THR:HG21	2.41	0.54
19:F:224:LEU:O	19:F:225:MET:HE2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:294:ASP:OD1	1:f:298:ARG:N	2.41	0.54
2:C:20:LEU:HD21	14:U:137:MET:HE1	1.90	0.54
2:C:27:LYS:O	2:C:30:GLU:HG2	2.07	0.54
4:V:284:GLU:HA	4:V:287:ARG:HD2	1.89	0.54
8:Z:34:ARG:HD2	8:Z:96:HIS:HB2	1.88	0.54
9:a:290:GLN:NE2	9:a:330:ARG:HE	2.06	0.54
16:A:397:ILE:HD12	17:B:210:TYR:HB3	1.90	0.54
18:E:199:VAL:HG13	19:F:315:ASN:HD22	1.72	0.54
18:E:250:ASP:HA	18:E:253:ILE:HG12	1.88	0.54
4:V:150:ARG:CZ	4:V:159:LEU:HB3	2.37	0.54
14:U:399:TRP:O	14:U:402:PHE:HB3	2.07	0.54
16:A:358:HIS:CE1	16:A:386:ARG:HB2	2.42	0.54
18:E:97:ARG:HH12	18:E:114:GLU:HB3	1.72	0.54
6:X:401:LEU:O	6:X:404:ILE:HG22	2.07	0.54
14:U:2:ILE:HG12	14:U:3:THR:H	1.72	0.54
15:c:255:TYR:HE1	15:c:281:LYS:HG2	1.72	0.54
18:E:108:MET:HA	18:E:108:MET:HE3	1.89	0.54
6:X:357:SER:OG	6:X:358:LYS:N	2.40	0.54
7:Y:160:ASN:HA	7:Y:163:LYS:HG2	1.90	0.54
7:Y:272:PHE:HZ	7:Y:304:TYR:HE1	1.53	0.54
9:a:287:ASN:OD1	9:a:288:HIS:N	2.40	0.54
19:F:80:ILE:HG22	19:F:84:LYS:HZ2	1.70	0.54
1:f:145:VAL:N	1:f:148:HIS:O	2.33	0.54
2:C:311:ILE:HD12	2:C:311:ILE:H	1.73	0.54
5:W:432:LEU:HG	5:W:436:MET:HE3	1.90	0.54
11:d:197:LEU:HD22	11:d:229:PRO:HB3	1.90	0.54
19:F:405:MET:HE2	19:F:405:MET:N	2.23	0.54
1:f:272:PHE:HB3	1:f:320:TYR:CD2	2.43	0.54
2:C:127:LEU:HB3	2:C:128:PRO:HD2	1.90	0.54
3:D:345:PHE:CG	3:D:375:ILE:HD11	2.43	0.54
5:W:390:GLU:HA	5:W:393:LEU:HG	1.90	0.54
6:X:248:ILE:HG13	6:X:249:THR:H	1.72	0.54
11:d:166:ARG:O	11:d:170:GLN:NE2	2.40	0.54
11:d:289:ARG:HH12	11:d:292:PHE:HE1	1.56	0.54
16:A:139:ARG:HG2	16:A:153:LEU:HB2	1.89	0.54
1:f:129:VAL:O	1:f:133:LEU:HG	2.07	0.54
4:V:82:LEU:HD11	4:V:163:VAL:CG1	2.38	0.54
5:W:60:MET:HE1	5:W:97:LEU:HB3	1.90	0.54
5:W:324:TYR:HB3	5:W:328:LEU:HD23	1.90	0.54
10:b:83:LYS:NZ	10:b:118:GLU:OE2	2.34	0.54
19:F:385:ALA:HA	19:F:388:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:117:VAL:HG13	1:f:143:LEU:HD13	1.89	0.53
3:D:168:GLY:N	22:D:501:ATP:HN62	1.97	0.53
3:D:390:ASN:O	5:W:136:ILE:HG12	2.08	0.53
4:V:224:LEU:HA	4:V:227:VAL:HG12	1.89	0.53
10:b:79:GLN:CD	10:b:79:GLN:H	2.15	0.53
15:c:226:MET:O	15:c:230:THR:HG23	2.08	0.53
15:c:227:GLU:OE1	15:c:227:GLU:N	2.38	0.53
2:C:276:LEU:O	2:C:279:GLN:HG3	2.08	0.53
4:V:119:GLY:HA3	4:V:149:PRO:HD2	1.90	0.53
9:a:288:HIS:CD2	9:a:290:GLN:HB3	2.43	0.53
14:U:757:MET:HA	14:U:760:VAL:HG12	1.89	0.53
15:c:55:GLY:HA3	15:c:112:TYR:CE2	2.44	0.53
18:E:364:GLN:HA	18:E:367:PHE:HD2	1.73	0.53
2:C:58:LEU:O	2:C:62:GLU:HG3	2.08	0.53
1:f:90:VAL:HG23	1:f:94:SER:HB2	1.90	0.53
5:W:446:ILE:HG23	8:Z:211:TYR:CD1	2.43	0.53
8:Z:239:ASP:OD1	8:Z:240:VAL:N	2.41	0.53
10:b:150:THR:OG1	10:b:153:LEU:N	2.41	0.53
11:d:310:LEU:HD12	11:d:316:TYR:HE1	1.74	0.53
14:U:45:ILE:HD11	14:U:63:VAL:HB	1.91	0.53
14:U:445:ALA:O	14:U:449:ILE:HG12	2.08	0.53
17:B:373:THR:HG23	17:B:414:VAL:HG12	1.89	0.53
19:F:373:MET:HA	19:F:373:MET:HE3	1.89	0.53
2:C:152:GLY:CA	21:C:501:ADP:HN62	2.22	0.53
6:X:354:ILE:HG23	6:X:356:LEU:HD13	1.89	0.53
8:Z:79:TYR:OH	8:Z:90:ARG:HG3	2.08	0.53
9:a:281:THR:OG1	9:a:333:MET:HG2	2.08	0.53
17:B:193:GLN:HG2	17:B:353:PHE:CE1	2.44	0.53
18:E:131:SER:HA	18:E:190:GLN:HE21	1.73	0.53
2:C:152:GLY:HA3	21:C:501:ADP:HN62	1.72	0.53
3:D:102:ILE:HD13	3:D:112:TYR:HA	1.90	0.53
5:W:186:ILE:HG13	5:W:190:MET:HE3	1.90	0.53
9:a:35:HIS:O	9:a:39:LEU:HG	2.08	0.53
10:b:125:VAL:O	10:b:129:LYS:HG2	2.09	0.53
11:d:282:ILE:HG23	11:d:283:LEU:N	2.20	0.53
15:c:164:ASN:OD1	15:c:167:MET:HG2	2.08	0.53
17:B:303:ARG:O	17:B:307:ARG:HD3	2.08	0.53
18:E:122:MET:SD	18:E:196:LEU:HB3	2.48	0.53
2:C:360:LYS:O	2:C:364:THR:HG23	2.09	0.53
7:Y:24:PHE:HE2	7:Y:286:TRP:HE3	1.57	0.53
8:Z:177:ARG:NH2	15:c:153:GLY:HA2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F:281:SER:HB2	19:F:326:VAL:HG12	1.90	0.53
2:C:189:TYR:CZ	2:C:316:GLU:HB2	2.44	0.53
2:C:328:ILE:HG12	21:C:501:ADP:N6	2.23	0.53
3:D:205:TYR:CE2	3:D:330:LYS:HB3	2.44	0.53
14:U:21:GLU:OE1	14:U:21:GLU:N	2.40	0.53
14:U:351:MET:O	14:U:354:LYS:HG2	2.09	0.53
17:B:170:LEU:HA	17:B:173:VAL:HG12	1.90	0.53
17:B:268:ARG:HG3	17:B:311:GLU:OE2	2.09	0.53
2:C:232:ARG:HH12	17:B:173:VAL:HG22	1.73	0.53
3:D:60:TYR:CE2	14:U:640:LEU:HD21	2.44	0.53
3:D:94:GLU:N	3:D:94:GLU:OE2	2.41	0.53
3:D:202:VAL:HG12	3:D:329:ARG:HB3	1.91	0.53
4:V:234:ARG:HA	4:V:237:THR:HG22	1.89	0.53
6:X:252:LYS:HE3	6:X:283:GLN:HB3	1.90	0.53
7:Y:279:GLU:OE2	12:e:53:SER:OG	2.27	0.53
9:a:303:THR:HG22	9:a:304:VAL:H	1.74	0.53
10:b:109:ILE:HG22	10:b:138:VAL:HA	1.89	0.53
14:U:697:GLN:NE2	14:U:744:VAL:O	2.42	0.53
2:C:57:ARG:NE	14:U:644:TYR:HA	2.23	0.53
2:C:307:ARG:NH2	17:B:229:GLY:HA3	2.24	0.53
4:V:304:GLU:HA	4:V:307:ARG:HG2	1.91	0.53
10:b:3:LEU:HB3	10:b:105:HIS:CG	2.44	0.53
11:d:119:LEU:HD21	11:d:147:ILE:HG21	1.90	0.53
14:U:599:ILE:O	14:U:603:LEU:HG	2.08	0.53
18:E:255:ARG:HA	18:E:258:MET:HE2	1.90	0.53
4:V:324:PHE:CE2	12:e:22:PHE:HB2	2.44	0.52
7:Y:282:MET:HB2	7:Y:288:PHE:HB3	1.90	0.52
7:Y:296:VAL:O	7:Y:300:ARG:HG3	2.09	0.52
7:Y:336:ARG:NH1	7:Y:340:ALA:HB2	2.24	0.52
7:Y:377:LEU:HA	7:Y:380:VAL:HG12	1.90	0.52
9:a:108:ASP:OD1	9:a:109:GLU:N	2.38	0.52
16:A:274:PHE:N	16:A:318:LEU:O	2.31	0.52
16:A:277:ILE:HG21	16:A:319:MET:HB2	1.91	0.52
19:F:111:ILE:HG12	19:F:113:LEU:H	1.74	0.52
19:F:407:ALA:HB2	19:F:415:LEU:HD13	1.90	0.52
3:D:43:ARG:HA	3:D:46:LYS:HE3	1.91	0.52
3:D:122:GLU:CD	15:c:282:ARG:HH22	2.15	0.52
4:V:104:THR:HG22	4:V:107:ARG:NH2	2.23	0.52
14:U:16:GLU:HG3	14:U:18:GLN:H	1.74	0.52
14:U:596:ASN:OD1	14:U:597:LYS:N	2.42	0.52
19:F:275:ALA:O	19:F:281:SER:OG	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:264:LYS:HD2	1:f:289:HIS:CD2	2.44	0.52
4:V:283:ASN:HD22	12:e:19:PHE:HZ	1.56	0.52
4:V:345:ARG:HD3	12:e:43:TRP:CD2	2.44	0.52
4:V:417:ILE:HG23	4:V:422:ILE:HD11	1.91	0.52
11:d:163:SER:HA	11:d:166:ARG:HD3	1.91	0.52
14:U:617:ALA:O	14:U:620:GLU:HB2	2.09	0.52
14:U:682:TYR:O	14:U:685:GLN:HB2	2.09	0.52
15:c:57:MET:HG2	15:c:72:VAL:HG12	1.92	0.52
16:A:142:VAL:HA	16:A:148:GLN:O	2.09	0.52
3:D:64:GLU:HB2	14:U:607:VAL:HG11	1.90	0.52
5:W:136:ILE:HG13	5:W:137:TYR:N	2.25	0.52
8:Z:149:THR:HG23	9:a:178:ARG:HA	1.92	0.52
10:b:132:LYS:HB2	10:b:160:LEU:HD12	1.91	0.52
14:U:241:ASN:HD22	14:U:244:MET:HE2	1.75	0.52
16:A:98:CYS:N	17:B:130:GLU:OE1	2.38	0.52
16:A:274:PHE:O	16:A:319:MET:HA	2.08	0.52
1:f:303:ILE:HG23	1:f:306:ILE:HD11	1.91	0.52
5:W:115:ILE:HG23	5:W:121:LYS:HD3	1.92	0.52
6:X:190:LEU:HD13	6:X:213:GLN:HG3	1.91	0.52
14:U:695:MET:SD	14:U:698:GLN:HB2	2.49	0.52
15:c:125:VAL:HA	15:c:128:ASN:HD22	1.74	0.52
18:E:130:VAL:O	18:E:189:SER:OG	2.27	0.52
18:E:148:VAL:HG13	18:E:149:ILE:HG12	1.91	0.52
5:W:141:GLU:OE1	5:W:141:GLU:N	2.42	0.52
6:X:309:TYR:HB3	6:X:312:GLU:HB2	1.89	0.52
19:F:251:LEU:HD22	19:F:285:ILE:HD12	1.90	0.52
2:C:175:PHE:O	2:C:179:GLY:N	2.43	0.52
2:C:184:LYS:HG2	2:C:290:LYS:HG2	1.92	0.52
5:W:230:MET:HB3	5:W:246:HIS:CE1	2.45	0.52
9:a:278:MET:HA	9:a:278:MET:HE3	1.90	0.52
16:A:73:ALA:HB3	16:A:78:TRP:HA	1.91	0.52
19:F:279:ALA:HB3	19:F:280:PRO:HD3	1.92	0.52
6:X:284:THR:O	6:X:288:LYS:HD3	2.10	0.52
11:d:184:GLU:HG3	11:d:188:MET:HE3	1.92	0.52
14:U:213:PHE:HA	14:U:216:VAL:HG12	1.91	0.52
16:A:415:LYS:O	16:A:419:SER:HB3	2.10	0.52
17:B:306:GLN:HA	17:B:309:MET:HG2	1.90	0.52
6:X:47:GLU:HA	6:X:50:ILE:HG12	1.91	0.52
6:X:248:ILE:HG13	6:X:249:THR:N	2.25	0.52
6:X:368:MET:HB2	6:X:373:LYS:HB2	1.92	0.52
11:d:108:ASN:O	11:d:109:LEU:HG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:d:252:PRO:HG2	11:d:256:TYR:CE2	2.45	0.52
16:A:206:ILE:HA	19:F:372:LYS:NZ	2.25	0.52
19:F:258:GLN:HB2	19:F:263:ASP:HB3	1.92	0.52
19:F:376:SER:OG	19:F:378:ASP:OD1	2.26	0.52
2:C:339:THR:N	2:C:378:VAL:H	2.07	0.52
3:D:291:GLU:OE2	3:D:295:GLN:NE2	2.33	0.52
7:Y:110:TYR:HA	7:Y:113:ARG:HB3	1.91	0.52
7:Y:186:LEU:HA	7:Y:222:TYR:OH	2.10	0.52
8:Z:57:PRO:HD3	8:Z:74:TYR:CZ	2.45	0.52
11:d:321:GLN:H	11:d:321:GLN:CD	2.18	0.52
17:B:162:VAL:HG22	17:B:163:LEU:H	1.74	0.52
18:E:196:LEU:HB2	18:E:230:ILE:HG22	1.91	0.52
18:E:250:ASP:OD1	18:E:250:ASP:N	2.42	0.52
1:f:47:VAL:HG12	1:f:59:ARG:NH1	2.25	0.51
2:C:178:LEU:HD21	17:B:403:GLY:CA	2.39	0.51
2:C:376:VAL:HB	3:D:193:GLN:NE2	2.25	0.51
4:V:104:THR:HG22	4:V:107:ARG:HH21	1.74	0.51
4:V:108:LEU:HD11	4:V:170:LEU:HD12	1.90	0.51
6:X:149:LEU:O	6:X:152:GLN:HG3	2.10	0.51
10:b:22:LEU:HD11	10:b:179:LEU:HA	1.91	0.51
16:A:270:CYS:SG	16:A:271:LEU:N	2.84	0.51
17:B:196:GLU:HG3	17:B:349:ARG:HH11	1.75	0.51
7:Y:46:ARG:HD3	7:Y:69:LEU:HD13	1.92	0.51
7:Y:117:LYS:HD3	7:Y:151:TYR:CE1	2.46	0.51
4:V:68:ASP:O	4:V:72:LEU:HG	2.10	0.51
4:V:183:GLU:HG3	4:V:184:ALA:H	1.75	0.51
4:V:436:PHE:HB3	4:V:440:LYS:NZ	2.25	0.51
5:W:140:ILE:HG22	5:W:144:ARG:HH21	1.74	0.51
5:W:260:SER:HA	5:W:263:TRP:CD1	2.46	0.51
6:X:207:GLN:HE22	6:X:238:GLY:HA3	1.75	0.51
9:a:133:GLU:HA	9:a:136:GLU:HG2	1.92	0.51
11:d:293:PHE:HA	11:d:298:LYS:HE3	1.91	0.51
16:A:120:LYS:HB2	19:F:90:VAL:HG21	1.90	0.51
16:A:295:VAL:HG21	17:B:307:ARG:NH2	2.25	0.51
17:B:419:PHE:O	17:B:422:SER:OG	2.26	0.51
18:E:252:GLU:OE1	18:E:255:ARG:NH2	2.36	0.51
1:f:132:PHE:CE1	1:f:154:LEU:HB3	2.45	0.51
2:C:232:ARG:NH1	17:B:173:VAL:HG22	2.25	0.51
5:W:84:ASN:HD21	5:W:124:LEU:HD23	1.74	0.51
7:Y:177:ARG:O	7:Y:181:LYS:HG2	2.09	0.51
8:Z:173:GLU:OE1	15:c:153:GLY:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:308:VAL:HG12	15:c:309:PHE:CD2	2.46	0.51
17:B:155:LYS:HE2	17:B:156:VAL:HG13	1.92	0.51
17:B:275:GLU:OE2	17:B:322:ARG:HG2	2.11	0.51
3:D:273:LYS:HG2	3:D:319:PRO:HD3	1.93	0.51
5:W:100:ALA:O	5:W:103:LYS:HG3	2.11	0.51
5:W:141:GLU:HG3	5:W:144:ARG:HH22	1.76	0.51
6:X:335:LEU:HD13	6:X:368:MET:HE1	1.92	0.51
14:U:261:LEU:HD11	14:U:329:LEU:HB3	1.91	0.51
14:U:656:LEU:O	14:U:694:ILE:HD11	2.10	0.51
1:f:31:MET:HB3	1:f:47:VAL:O	2.10	0.51
2:C:332:HIS:HD2	2:C:359:VAL:HG12	1.75	0.51
7:Y:148:GLY:O	7:Y:152:MET:N	2.44	0.51
9:a:140:GLU:HA	9:a:143:ASN:ND2	2.26	0.51
14:U:54:PHE:HD1	14:U:56:SER:H	1.57	0.51
18:E:176:PRO:HG3	18:E:280:ASN:ND2	2.26	0.51
2:C:218:GLU:HA	2:C:221:GLN:HG2	1.92	0.51
2:C:267:SER:HA	2:C:270:GLN:HE22	1.75	0.51
22:D:501:ATP:H5'2	18:E:291:ARG:HH21	1.76	0.51
4:V:74:ASP:OD2	4:V:107:ARG:NH1	2.43	0.51
4:V:398:LEU:HA	4:V:401:ASN:OD1	2.11	0.51
5:W:128:LEU:HA	5:W:131:VAL:HG12	1.92	0.51
6:X:335:LEU:O	6:X:339:ILE:HG12	2.11	0.51
8:Z:170:VAL:HA	15:c:152:LYS:NZ	2.25	0.51
10:b:14:GLU:HB2	10:b:82:GLY:H	1.76	0.51
14:U:62:LEU:O	14:U:66:LYS:HG3	2.11	0.51
16:A:405:THR:HG23	16:A:407:LYS:HG2	1.91	0.51
17:B:269:GLU:OE2	17:B:272:ARG:NH2	2.44	0.51
18:E:234:GLU:OE1	18:E:236:ASP:HB2	2.10	0.51
2:C:105:ILE:HD12	2:C:108:VAL:HG11	1.93	0.51
4:V:355:ARG:NH1	12:e:30:LEU:H	2.08	0.51
6:X:252:LYS:NZ	6:X:284:THR:HA	2.25	0.51
4:V:161:PRO:HB2	4:V:203:LEU:HD21	1.92	0.51
4:V:367:VAL:HG23	4:V:402:VAL:HG23	1.92	0.51
5:W:453:HIS:CE1	8:Z:221:PRO:HD3	2.46	0.51
7:Y:174:TRP:O	7:Y:177:ARG:HG2	2.10	0.51
9:a:70:ARG:HD3	10:b:17:ARG:NH1	2.13	0.51
10:b:18:ASN:O	10:b:25:ARG:HG3	2.10	0.51
11:d:94:MET:HE1	11:d:119:LEU:HD13	1.92	0.51
11:d:332:SER:HB2	15:c:303:MET:SD	2.51	0.51
14:U:324:LYS:HA	14:U:327:LYS:NZ	2.26	0.51
5:W:34:LEU:HB3	5:W:39:ARG:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:145:GLU:O	6:X:148:HIS:ND1	2.43	0.51
12:e:59:GLU:HA	12:e:62:LYS:HE3	1.93	0.51
14:U:624:PHE:HZ	14:U:763:VAL:HG13	1.76	0.51
18:E:210:GLU:O	18:E:213:ARG:HG2	2.11	0.51
3:D:315:ASP:OD1	3:D:316:THR:N	2.43	0.50
3:D:318:ASP:HB3	3:D:321:LEU:HG	1.92	0.50
4:V:102:PRO:O	4:V:105:SER:OG	2.29	0.50
11:d:337:LYS:HA	11:d:340:ILE:HG22	1.92	0.50
14:U:551:GLY:O	14:U:555:VAL:HG23	2.11	0.50
16:A:89:SER:O	16:A:93:LEU:HB2	2.10	0.50
19:F:430:LYS:HD2	19:F:431:LYS:O	2.11	0.50
1:f:132:PHE:CZ	1:f:154:LEU:HB3	2.46	0.50
4:V:159:LEU:HD12	4:V:163:VAL:HG23	1.92	0.50
5:W:48:LEU:HD11	5:W:93:ARG:HD2	1.92	0.50
6:X:167:VAL:HG21	6:X:197:ALA:HB2	1.93	0.50
6:X:258:LYS:HE3	6:X:270:LEU:HD11	1.93	0.50
6:X:377:ILE:HG23	7:Y:312:ARG:HH22	1.74	0.50
7:Y:90:ASP:HA	7:Y:93:LYS:HB2	1.92	0.50
14:U:662:GLY:HA2	14:U:696:ILE:HG22	1.93	0.50
15:c:310:LYS:HD3	15:c:311:GLU:H	1.76	0.50
16:A:108:ASP:OD2	16:A:110:LYS:NZ	2.29	0.50
17:B:184:TYR:HE1	17:B:194:ILE:HG23	1.76	0.50
17:B:201:VAL:HB	17:B:326:LYS:HG3	1.93	0.50
1:f:132:PHE:CD1	1:f:139:LEU:HB2	2.46	0.50
2:C:165:ILE:HD11	2:C:186:VAL:HG11	1.91	0.50
3:D:179:GLU:O	3:D:184:PRO:HD3	2.11	0.50
4:V:269:LYS:HG2	4:V:273:LYS:NZ	2.27	0.50
4:V:408:ARG:HD3	4:V:446:VAL:HG12	1.94	0.50
15:c:58:LEU:HB2	15:c:71:ASP:OD1	2.11	0.50
16:A:223:THR:O	16:A:227:ARG:HG3	2.11	0.50
17:B:374:LEU:HD22	17:B:378:VAL:HG11	1.93	0.50
17:B:401:GLU:HG3	17:B:426:VAL:HG11	1.93	0.50
19:F:172:VAL:HG23	19:F:267:LEU:HD12	1.93	0.50
19:F:265:ALA:O	19:F:269:ARG:HG2	2.11	0.50
2:C:338:LEU:HD22	2:C:383:PHE:CZ	2.46	0.50
4:V:138:PRO:HB2	4:V:141:THR:HB	1.93	0.50
4:V:409:MET:N	4:V:409:MET:HE2	2.26	0.50
4:V:487:HIS:HB2	8:Z:267:ARG:HH12	1.75	0.50
14:U:761:VAL:O	14:U:765:VAL:HG12	2.11	0.50
16:A:205:GLY:O	19:F:372:LYS:NZ	2.42	0.50
4:V:134:PHE:CD2	4:V:187:ILE:HD11	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:324:PHE:O	4:V:328:VAL:HG22	2.10	0.50
4:V:469:THR:HG22	4:V:470:ARG:H	1.76	0.50
5:W:315:MET:HB3	5:W:320:LEU:HD21	1.93	0.50
7:Y:201:PHE:HD2	7:Y:226:VAL:HG11	1.77	0.50
8:Z:99:PRO:C	8:Z:100:LYS:HD3	2.36	0.50
8:Z:132:GLY:O	15:c:219:ASN:ND2	2.34	0.50
11:d:272:ALA:O	11:d:276:GLU:N	2.43	0.50
14:U:568:GLU:HA	14:U:601:ARG:NH2	2.26	0.50
17:B:396:LYS:HE3	22:B:501:ATP:N3	2.26	0.50
18:E:300:HIS:NE2	18:E:302:ASP:HB2	2.26	0.50
19:F:154:ASN:OD1	19:F:155:LYS:N	2.45	0.50
4:V:82:LEU:HD11	4:V:163:VAL:HG13	1.94	0.50
4:V:474:LEU:O	4:V:478:GLN:HG3	2.12	0.50
6:X:367:GLN:NE2	6:X:371:ASP:OD2	2.45	0.50
7:Y:100:ILE:HG13	7:Y:101:ARG:N	2.27	0.50
7:Y:364:TRP:HE3	7:Y:365:GLN:HG3	1.76	0.50
8:Z:109:ASN:HD21	8:Z:140:SER:HB3	1.75	0.50
9:a:188:LEU:HD11	9:a:193:GLN:HB3	1.94	0.50
10:b:56:ASN:OD1	10:b:82:GLY:HA3	2.12	0.50
11:d:261:ASP:OD1	11:d:262:ILE:N	2.44	0.50
14:U:261:LEU:HD21	14:U:329:LEU:O	2.12	0.50
18:E:171:LEU:HD11	18:E:279:THR:HG22	1.94	0.50
19:F:185:TYR:H	19:F:243:GLN:HE21	1.59	0.50
5:W:386:VAL:O	5:W:389:SER:HB3	2.12	0.50
14:U:772:TRP:CD1	14:U:774:PRO:HD2	2.47	0.50
5:W:183:VAL:HA	5:W:186:ILE:HG22	1.93	0.50
7:Y:208:PHE:HB3	7:Y:216:TYR:CE1	2.47	0.50
15:c:152:LYS:HA	15:c:152:LYS:HE3	1.94	0.50
16:A:286:ASP:OD1	19:F:337:ILE:HG13	2.12	0.50
17:B:425:ASN:OD1	17:B:426:VAL:HG13	2.12	0.50
1:f:143:LEU:HB2	1:f:150:MET:CG	2.41	0.50
1:f:288:LEU:HD12	20:w:31:ILE:HD12	1.94	0.50
2:C:376:VAL:HB	3:D:193:GLN:HE22	1.77	0.50
7:Y:49:ASN:HA	7:Y:73:MET:HE1	1.92	0.50
15:c:220:LEU:HD23	15:c:221:HIS:CD2	2.47	0.50
17:B:357:ASP:OD2	17:B:359:LYS:NZ	2.44	0.50
1:f:264:LYS:HD2	1:f:289:HIS:NE2	2.27	0.49
3:D:339:ARG:NH1	3:D:342:ARG:HE	2.09	0.49
4:V:419:LEU:HA	4:V:422:ILE:HD12	1.94	0.49
5:W:454:ASN:HD22	8:Z:220:LEU:HD22	1.76	0.49
7:Y:51:ALA:HB3	7:Y:52:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:353:LEU:HB3	14:U:385:PHE:CE2	2.47	0.49
14:U:583:MET:HG2	14:U:602:LEU:HD22	1.94	0.49
14:U:622:LEU:HA	14:U:625:ILE:HG22	1.93	0.49
16:A:81:ALA:O	16:A:84:LYS:HG2	2.12	0.49
18:E:76:GLY:H	18:E:77:PRO:CD	2.25	0.49
18:E:138:LEU:HD21	18:E:301:ILE:HG23	1.94	0.49
1:f:267:ALA:N	20:w:33:TYR:OH	2.45	0.49
7:Y:215:ASP:OD1	7:Y:216:TYR:N	2.42	0.49
7:Y:348:ASP:HB3	7:Y:353:ILE:HG22	1.94	0.49
10:b:180:ALA:O	10:b:184:ILE:HG12	2.12	0.49
14:U:323:LEU:O	14:U:327:LYS:HG3	2.12	0.49
14:U:723:ASP:OD1	14:U:724:VAL:N	2.45	0.49
14:U:807:LYS:HB3	14:U:872:GLU:OE2	2.12	0.49
19:F:154:ASN:HB3	19:F:158:TYR:H	1.77	0.49
19:F:193:LYS:O	19:F:197:GLU:HG3	2.12	0.49
3:D:342:ARG:NH1	3:D:361:GLU:OE1	2.45	0.49
7:Y:365:GLN:O	7:Y:369:THR:HG23	2.11	0.49
8:Z:175:LEU:HD21	15:c:38:LEU:HD23	1.95	0.49
9:a:186:LYS:HD2	9:a:221:VAL:HG21	1.94	0.49
14:U:119:PRO:HD2	14:U:122:GLU:OE2	2.13	0.49
19:F:365:ILE:HG23	19:F:369:HIS:CE1	2.47	0.49
2:C:44:ARG:HA	4:V:496:PHE:CZ	2.47	0.49
2:C:249:ASP:OD1	2:C:250:GLU:N	2.44	0.49
3:D:194:ILE:HG23	3:D:196:ILE:HG13	1.94	0.49
8:Z:22:HIS:HA	8:Z:25:ARG:HE	1.77	0.49
8:Z:87:ALA:N	19:F:106:GLU:OE1	2.32	0.49
10:b:61:LEU:HD11	10:b:74:LYS:HE2	1.94	0.49
14:U:807:LYS:HB2	14:U:810:THR:HG22	1.94	0.49
16:A:172:VAL:HG12	16:A:228:ALA:HB2	1.93	0.49
16:A:310:ASP:HB3	19:F:250:LYS:HZ2	1.76	0.49
16:A:362:MET:HE1	17:B:214:MET:HG3	1.95	0.49
2:C:338:LEU:HD22	2:C:383:PHE:HZ	1.76	0.49
4:V:74:ASP:HA	4:V:77:GLU:CD	2.38	0.49
4:V:185:GLN:HG2	4:V:218:TYR:HE1	1.77	0.49
7:Y:162:GLU:O	7:Y:165:LYS:HG2	2.12	0.49
9:a:54:ASP:O	9:a:58:LYS:N	2.45	0.49
14:U:427:LEU:HD21	14:U:439:GLU:HA	1.95	0.49
16:A:102:ILE:HD11	16:A:114:ASN:HB2	1.94	0.49
18:E:349:GLU:OE1	18:E:373:LYS:HE2	2.12	0.49
5:W:46:THR:O	5:W:49:SER:OG	2.20	0.49
7:Y:97:GLU:O	7:Y:99:GLU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:439:GLU:O	14:U:443:LEU:HG	2.12	0.49
14:U:620:GLU:OE2	14:U:651:GLY:HA2	2.13	0.49
16:A:96:ALA:C	16:A:97:ARG:HD3	2.38	0.49
1:f:56:LEU:O	1:f:60:LEU:HG	2.13	0.49
6:X:399:ALA:O	6:X:403:THR:HG23	2.13	0.49
9:a:242:SER:O	9:a:279:GLU:HG3	2.13	0.49
9:a:288:HIS:HD2	9:a:290:GLN:HB3	1.77	0.49
15:c:42:LEU:HD11	15:c:155:VAL:HG11	1.93	0.49
16:A:210:LYS:HE2	16:A:312:ARG:NH2	2.28	0.49
16:A:348:LEU:HA	16:A:351:ARG:HG2	1.95	0.49
2:C:51:GLU:O	2:C:55:LYS:HG2	2.13	0.49
3:D:326:ARG:O	3:D:327:LEU:HD22	2.12	0.49
5:W:27:ARG:CZ	5:W:66:ILE:HG22	2.43	0.49
8:Z:180:LYS:NZ	8:Z:181:ASP:O	2.44	0.49
9:a:18:GLN:O	9:a:20:ALA:N	2.45	0.49
11:d:141:LEU:HD13	11:d:182:LEU:HD13	1.93	0.49
11:d:281:LYS:O	11:d:282:ILE:HG22	2.13	0.49
17:B:273:VAL:O	17:B:277:HIS:ND1	2.45	0.49
2:C:71:SER:OG	3:D:112:TYR:HB3	2.12	0.49
3:D:323:ARG:CZ	3:D:324:PRO:HD2	2.42	0.49
14:U:381:THR:HA	14:U:412:HIS:HD2	1.78	0.49
15:c:251:LEU:HD21	15:c:283:HIS:HB3	1.94	0.49
16:A:81:ALA:HB2	17:B:137:SER:HB2	1.95	0.49
19:F:179:GLU:HG2	19:F:181:PRO:HD3	1.94	0.49
19:F:231:THR:HG21	19:F:354:PHE:HB3	1.95	0.49
1:f:69:GLU:OE1	1:f:69:GLU:N	2.36	0.49
3:D:96:VAL:HG13	3:D:97:ASP:OD1	2.12	0.49
3:D:342:ARG:HB2	3:D:364:VAL:HG11	1.95	0.49
3:D:401:LYS:O	3:D:404:LYS:HG3	2.13	0.49
5:W:308:LEU:HD23	5:W:320:LEU:HD11	1.95	0.49
8:Z:165:GLU:HB3	8:Z:168:GLU:OE1	2.13	0.49
11:d:144:ALA:HA	11:d:147:ILE:HG12	1.95	0.49
14:U:12:LEU:HD11	14:U:48:LEU:HD12	1.95	0.49
14:U:199:ARG:HH11	14:U:223:LEU:HD13	1.77	0.49
16:A:345:LEU:HD11	16:A:381:THR:HG22	1.94	0.49
2:C:117:ARG:NH1	2:C:124:HIS:HA	2.28	0.48
4:V:299:GLN:HB2	4:V:301:GLU:OE2	2.13	0.48
7:Y:113:ARG:HG2	7:Y:113:ARG:HH11	1.78	0.48
8:Z:88:ARG:NH1	19:F:104:GLN:HE22	2.11	0.48
9:a:234:ILE:H	9:a:234:ILE:HD12	1.77	0.48
14:U:421:GLN:OE1	14:U:421:GLN:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:98:CYS:HB2	16:A:139:ARG:HG3	1.94	0.48
18:E:168:LYS:N	18:E:296:ASP:OD2	2.30	0.48
18:E:312:ILE:HA	18:E:315:ILE:HG22	1.95	0.48
1:f:74:LEU:O	1:f:96:LEU:HG	2.13	0.48
4:V:216:ARG:O	4:V:216:ARG:HD3	2.13	0.48
6:X:141:LYS:O	6:X:141:LYS:HD3	2.12	0.48
8:Z:191:ILE:HG23	8:Z:192:THR:N	2.29	0.48
14:U:327:LYS:HB2	14:U:333:MET:HE1	1.95	0.48
14:U:678:ASP:OD1	14:U:679:PRO:HD2	2.13	0.48
16:A:198:PRO:O	16:A:202:VAL:HG23	2.14	0.48
18:E:156:PRO:HB2	18:E:160:GLN:HE22	1.78	0.48
18:E:215:ILE:HA	18:E:218:MET:HE3	1.95	0.48
2:C:160:GLU:HA	17:B:408:ARG:HH22	1.78	0.48
2:C:196:LYS:HD2	2:C:294:ALA:HB1	1.96	0.48
3:D:275:PHE:HE1	3:D:285:VAL:HB	1.78	0.48
4:V:337:LEU:HD21	4:V:364:THR:HG23	1.95	0.48
8:Z:263:ALA:CB	15:c:291:LEU:HD11	2.43	0.48
9:a:28:LEU:HB3	9:a:37:LEU:HB2	1.95	0.48
10:b:25:ARG:HB3	10:b:143:PHE:CE2	2.48	0.48
14:U:348:THR:HG22	14:U:376:MET:HE3	1.94	0.48
14:U:675:MET:HE2	14:U:675:MET:HB3	1.70	0.48
1:f:132:PHE:CD2	1:f:139:LEU:HD22	2.49	0.48
4:V:63:SER:O	4:V:66:GLU:HG3	2.12	0.48
4:V:134:PHE:HD2	4:V:187:ILE:HD11	1.77	0.48
8:Z:94:TRP:CD1	8:Z:112:MET:HG2	2.48	0.48
8:Z:217:THR:HG23	8:Z:219:LYS:HG3	1.95	0.48
9:a:184:ASP:OD1	9:a:185:ILE:N	2.46	0.48
14:U:201:LEU:HA	14:U:204:ILE:HG22	1.94	0.48
14:U:568:GLU:HB3	14:U:572:ARG:HE	1.78	0.48
14:U:603:LEU:HD12	14:U:604:HIS:H	1.71	0.48
14:U:642:GLU:O	14:U:642:GLU:HG2	2.11	0.48
16:A:255:ARG:HG3	16:A:256:MET:HE2	1.95	0.48
16:A:353:HIS:HA	16:A:356:LYS:HE3	1.96	0.48
17:B:365:PHE:CZ	17:B:395:ILE:HD12	2.47	0.48
1:f:128:GLN:NE2	1:f:137:SER:OG	2.46	0.48
2:C:235:PHE:HB3	2:C:239:ARG:HH21	1.78	0.48
3:D:381:GLU:HG3	3:D:402:ALA:HB1	1.96	0.48
5:W:17:GLU:HG2	5:W:18:VAL:HG13	1.96	0.48
6:X:125:LEU:H	6:X:125:LEU:HD12	1.78	0.48
7:Y:102:ASP:O	7:Y:105:MET:HG2	2.13	0.48
8:Z:126:VAL:O	8:Z:128:PRO:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:54:ASP:OD1	9:a:55:GLY:N	2.47	0.48
15:c:41:MET:HE2	15:c:112:TYR:CG	2.48	0.48
16:A:197:HIS:HB2	16:A:200:ARG:HE	1.79	0.48
16:A:224:LEU:HD11	22:A:501:ATP:H2'	1.95	0.48
1:f:278:GLY:C	20:w:41:PRO:HD3	2.39	0.48
2:C:36:ASN:HB3	4:V:89:LYS:CD	2.44	0.48
4:V:435:GLU:HG3	4:V:453:HIS:CE1	2.47	0.48
5:W:140:ILE:HG23	5:W:177:MET:HE1	1.96	0.48
5:W:373:ILE:HG23	5:W:413:ILE:HB	1.95	0.48
6:X:252:LYS:HD2	6:X:287:LEU:HD12	1.94	0.48
7:Y:263:LEU:HD12	7:Y:271:PHE:CZ	2.48	0.48
10:b:25:ARG:HB3	10:b:143:PHE:CZ	2.49	0.48
11:d:177:ASP:HB2	14:U:2:ILE:HG22	1.94	0.48
14:U:42:VAL:HG21	14:U:68:PHE:CE1	2.47	0.48
14:U:427:LEU:HD22	14:U:442:GLY:HA3	1.95	0.48
15:c:130:GLN:O	15:c:134:GLU:HG2	2.12	0.48
16:A:109:PRO:C	16:A:110:LYS:HZ2	2.20	0.48
17:B:117:ASP:OD2	17:B:118:ASP:N	2.47	0.48
19:F:224:LEU:HD11	19:F:288:LEU:HD22	1.96	0.48
19:F:376:SER:HB2	19:F:415:LEU:O	2.13	0.48
1:f:265:PRO:HB3	1:f:315:SER:OG	2.13	0.48
1:f:269:ILE:HB	1:f:320:TYR:CE1	2.47	0.48
2:C:248:MET:HE2	2:C:269:VAL:HG22	1.96	0.48
3:D:99:ASN:HA	3:D:115:ILE:HG12	1.95	0.48
3:D:170:MET:O	3:D:174:LYS:HG3	2.13	0.48
4:V:71:THR:O	4:V:75:ILE:HG13	2.13	0.48
4:V:189:ASP:OD1	4:V:218:TYR:OH	2.20	0.48
4:V:487:HIS:HB2	8:Z:267:ARG:NH1	2.28	0.48
5:W:155:GLN:NE2	5:W:156:ASN:OD1	2.46	0.48
8:Z:231:GLN:HE21	9:a:341:LEU:HD11	1.77	0.48
9:a:18:GLN:O	9:a:21:VAL:HG22	2.14	0.48
9:a:58:LYS:HA	9:a:61:GLU:CD	2.39	0.48
9:a:235:ASP:HB3	9:a:251:LEU:HD21	1.96	0.48
9:a:370:GLN:HB2	11:d:340:ILE:HD13	1.96	0.48
14:U:626:LEU:HD21	14:U:632:GLN:HB2	1.96	0.48
16:A:113:ILE:HG22	16:A:121:PHE:H	1.77	0.48
16:A:259:GLU:O	16:A:262:GLU:HG3	2.14	0.48
18:E:201:SER:OG	19:F:312:GLU:OE1	2.30	0.48
20:w:31:ILE:HG13	20:w:31:ILE:O	2.14	0.48
3:D:208:PRO:HD3	3:D:312:ASN:HD21	1.79	0.48
5:W:103:LYS:O	5:W:106:GLN:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:220:VAL:HG21	7:Y:249:VAL:HG21	1.95	0.48
10:b:180:ALA:HA	10:b:183:LEU:HD13	1.95	0.48
11:d:224:VAL:HB	11:d:228:HIS:CE1	2.49	0.48
14:U:272:GLY:O	14:U:319:LYS:NZ	2.45	0.48
14:U:463:ASN:HA	14:U:466:LYS:HE3	1.96	0.48
14:U:602:LEU:HD13	14:U:621:SER:HB3	1.95	0.48
19:F:362:ARG:HE	19:F:388:THR:HG23	1.79	0.48
1:f:314:LEU:O	1:f:317:THR:OG1	2.26	0.48
2:C:130:LYS:HG3	2:C:131:VAL:H	1.79	0.48
3:D:121:ARG:HB2	15:c:274:ASN:ND2	2.23	0.48
4:V:183:GLU:HG3	4:V:184:ALA:N	2.28	0.48
4:V:415:SER:HB2	7:Y:346:LYS:HE3	1.95	0.48
5:W:85:GLU:O	5:W:89:LEU:HG	2.13	0.48
9:a:205:LEU:HA	9:a:213:PHE:HZ	1.78	0.48
17:B:234:LEU:HA	17:B:237:LYS:HG2	1.95	0.48
19:F:180:ARG:HH12	19:F:246:ALA:H	1.61	0.48
6:X:368:MET:HG3	6:X:374:PHE:HE1	1.79	0.48
8:Z:204:LYS:O	8:Z:208:ILE:HG12	2.14	0.48
11:d:303:ALA:HA	11:d:308:TRP:HE3	1.78	0.48
14:U:78:LEU:HD11	14:U:104:CYS:HB2	1.96	0.48
2:C:184:LYS:HD3	2:C:280:LEU:HD22	1.96	0.47
5:W:407:ASP:HB3	5:W:412:ILE:HB	1.95	0.47
6:X:222:GLU:OE1	6:X:222:GLU:N	2.43	0.47
6:X:379:ASP:HB2	7:Y:312:ARG:NH1	2.27	0.47
7:Y:143:TYR:HD1	7:Y:146:ARG:HH21	1.61	0.47
9:a:72:ASN:O	9:a:74:LEU:HG	2.14	0.47
10:b:126:LYS:O	10:b:130:ARG:HG2	2.14	0.47
14:U:253:TYR:CZ	14:U:331:GLY:HA3	2.49	0.47
14:U:765:VAL:HG11	14:U:778:PHE:CD1	2.49	0.47
14:U:771:PHE:CD1	15:c:181:LEU:HD21	2.46	0.47
18:E:213:ARG:O	18:E:217:GLU:OE1	2.32	0.47
19:F:251:LEU:HB3	19:F:285:ILE:HD13	1.95	0.47
8:Z:23:PHE:HD2	8:Z:126:VAL:HG11	1.78	0.47
11:d:287:ALA:HB3	11:d:314:ASN:ND2	2.28	0.47
14:U:792:ASN:OD1	14:U:796:LYS:N	2.45	0.47
1:f:143:LEU:HB2	1:f:150:MET:SD	2.55	0.47
2:C:52:LEU:HB3	3:D:68:LEU:HD21	1.96	0.47
3:D:372:GLY:HA2	3:D:375:ILE:HG22	1.95	0.47
4:V:228:ARG:HH21	4:V:232:HIS:CE1	2.32	0.47
5:W:29:PRO:O	5:W:33:LYS:NZ	2.45	0.47
16:A:365:GLU:HG2	16:A:368:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F:374:ASN:HB3	19:F:414:GLU:HA	1.96	0.47
3:D:264:ILE:O	3:D:309:MET:HA	2.14	0.47
5:W:120:ILE:O	5:W:124:LEU:HG	2.14	0.47
7:Y:268:TYR:HE2	7:Y:307:LEU:HD13	1.78	0.47
17:B:184:TYR:CE1	17:B:194:ILE:HG23	2.49	0.47
17:B:349:ARG:HG3	17:B:351:ILE:CD1	2.43	0.47
17:B:381:ASP:OD1	17:B:382:ASP:N	2.47	0.47
18:E:144:GLU:HB3	18:E:297:ARG:NH2	2.29	0.47
1:f:143:LEU:O	1:f:150:MET:N	2.48	0.47
4:V:269:LYS:HG2	4:V:273:LYS:HZ1	1.79	0.47
7:Y:387:ILE:O	8:Z:279:LYS:NZ	2.44	0.47
9:a:42:LEU:HD22	9:a:78:GLU:OE2	2.13	0.47
9:a:80:ILE:O	9:a:84:VAL:HG23	2.14	0.47
10:b:169:HIS:HB2	10:b:187:PRO:HB3	1.96	0.47
11:d:268:ARG:HH21	11:d:292:PHE:HB3	1.79	0.47
14:U:265:ILE:HD11	14:U:329:LEU:HB2	1.95	0.47
14:U:540:GLN:O	15:c:68:ARG:NH2	2.47	0.47
18:E:119:VAL:HA	18:E:122:MET:HB3	1.95	0.47
2:C:52:LEU:HB3	3:D:68:LEU:HD22	1.95	0.47
5:W:101:VAL:HA	5:W:104:MET:CE	2.45	0.47
6:X:271:VAL:HG21	6:X:288:LYS:HE3	1.96	0.47
7:Y:279:GLU:HA	7:Y:282:MET:HG2	1.96	0.47
9:a:31:LYS:HB3	9:a:33:LEU:HD23	1.97	0.47
14:U:448:LEU:HA	14:U:483:LEU:HD22	1.97	0.47
16:A:146:LYS:NZ	19:F:87:PRO:HG3	2.30	0.47
1:f:141:LEU:O	1:f:151:PHE:HA	2.14	0.47
2:C:30:GLU:O	2:C:34:ILE:HG13	2.15	0.47
2:C:113:ARG:HB2	2:C:128:PRO:O	2.15	0.47
4:V:451:ILE:HG23	11:d:279:TYR:CE1	2.49	0.47
7:Y:106:ALA:O	7:Y:109:GLU:HG3	2.14	0.47
8:Z:57:PRO:HD3	8:Z:74:TYR:CE1	2.50	0.47
10:b:14:GLU:HB2	10:b:82:GLY:N	2.30	0.47
10:b:100:ARG:HE	10:b:103:LYS:HA	1.79	0.47
10:b:128:ALA:HB2	10:b:156:PHE:CD1	2.49	0.47
14:U:62:LEU:HD22	14:U:87:LEU:HB3	1.95	0.47
14:U:497:LEU:HB3	14:U:516:LEU:HG	1.97	0.47
14:U:789:ILE:HB	14:U:911:ILE:HD12	1.96	0.47
14:U:901:GLN:O	14:U:915:LYS:N	2.45	0.47
15:c:130:GLN:O	15:c:130:GLN:NE2	2.43	0.47
15:c:209:LYS:HG3	15:c:214:GLN:HE21	1.80	0.47
16:A:120:LYS:O	19:F:90:VAL:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:415:LYS:O	16:A:415:LYS:NZ	2.33	0.47
19:F:292:GLY:O	19:F:338:LEU:HA	2.14	0.47
5:W:129:ARG:HH21	5:W:149:LEU:HB3	1.80	0.47
5:W:361:HIS:O	5:W:365:ILE:HG12	2.14	0.47
6:X:106:GLU:HG2	6:X:107:VAL:N	2.30	0.47
6:X:137:TYR:CD2	6:X:146:ALA:HB2	2.50	0.47
14:U:131:GLU:HA	14:U:134:VAL:HG22	1.97	0.47
14:U:345:ASN:O	14:U:743:ASN:ND2	2.48	0.47
18:E:215:ILE:HD13	18:E:260:LEU:HB2	1.97	0.47
19:F:172:VAL:O	19:F:175:MET:HB2	2.15	0.47
3:D:163:MET:HA	3:D:222:HIS:HE1	1.80	0.47
5:W:79:GLU:CG	5:W:82:LEU:HB2	2.45	0.47
5:W:200:ILE:HG13	5:W:201:ARG:H	1.80	0.47
6:X:137:TYR:HD2	6:X:146:ALA:HB2	1.79	0.47
6:X:316:ASP:OD2	6:X:319:ILE:HG12	2.15	0.47
6:X:331:LEU:HD21	6:X:364:LYS:HG3	1.97	0.47
7:Y:138:LEU:O	7:Y:142:PHE:HD1	1.98	0.47
10:b:147:GLU:O	10:b:149:ASN:N	2.47	0.47
11:d:94:MET:HE1	11:d:119:LEU:HB2	1.97	0.47
15:c:266:THR:HG22	15:c:268:GLU:HG3	1.97	0.47
3:D:407:ILE:HG22	3:D:409:LYS:HG2	1.95	0.47
4:V:449:ALA:HA	4:V:461:LYS:H	1.80	0.47
5:W:263:TRP:HH2	5:W:298:GLU:HB3	1.80	0.47
5:W:278:PRO:HG3	5:W:357:ARG:NH2	2.30	0.47
7:Y:27:SER:O	7:Y:32:ARG:NH2	2.47	0.47
8:Z:107:ALA:O	8:Z:110:GLU:HG3	2.15	0.47
10:b:38:HIS:HB3	10:b:42:ARG:CZ	2.45	0.47
14:U:583:MET:SD	14:U:621:SER:HB2	2.54	0.47
16:A:120:LYS:HE2	19:F:90:VAL:HG21	1.98	0.47
18:E:126:ASP:OD1	18:E:185:ARG:NH2	2.40	0.47
19:F:232:GLY:N	21:F:501:ADP:O1A	2.47	0.47
19:F:299:GLU:HG3	19:F:300:LYS:N	2.26	0.47
19:F:307:GLN:O	19:F:311:LEU:HD23	2.15	0.47
2:C:224:ILE:HD11	2:C:233:GLU:C	2.40	0.46
4:V:62:HIS:HA	4:V:65:ARG:HB2	1.97	0.46
14:U:756:HIS:CD2	14:U:758:PRO:HD2	2.49	0.46
16:A:381:THR:O	16:A:385:ILE:HG12	2.15	0.46
18:E:355:ILE:HG23	19:F:211:LYS:HZ2	1.79	0.46
1:f:264:LYS:HD2	1:f:289:HIS:HE2	1.80	0.46
2:C:299:ASP:OD1	2:C:299:ASP:N	2.49	0.46
3:D:124:LEU:HD12	3:D:124:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:248:ARG:HB3	3:D:295:GLN:HE22	1.80	0.46
6:X:190:LEU:HD22	6:X:217:ILE:HG21	1.97	0.46
6:X:333:GLN:O	6:X:336:ILE:HG12	2.15	0.46
8:Z:215:VAL:HA	8:Z:220:LEU:HB2	1.97	0.46
14:U:9:ILE:HG22	14:U:44:LYS:HD3	1.97	0.46
14:U:49:TYR:CE1	14:U:61:ALA:HB2	2.50	0.46
14:U:682:TYR:HA	14:U:685:GLN:HG3	1.98	0.46
1:f:31:MET:HE1	1:f:91:GLY:CA	2.46	0.46
1:f:129:VAL:HG21	1:f:303:ILE:HG12	1.96	0.46
1:f:262:SER:O	1:f:263:ARG:HD3	2.15	0.46
2:C:178:LEU:HD21	17:B:403:GLY:HA3	1.97	0.46
4:V:80:LYS:O	4:V:84:LYS:HD3	2.14	0.46
4:V:188:SER:HA	4:V:191:LEU:CG	2.44	0.46
7:Y:127:THR:O	7:Y:131:THR:OG1	2.23	0.46
8:Z:240:VAL:HB	8:Z:245:PHE:HE2	1.80	0.46
14:U:446:LEU:HD21	14:U:457:ILE:HD12	1.95	0.46
14:U:528:ALA:O	14:U:532:MET:HG2	2.15	0.46
14:U:624:PHE:CZ	14:U:763:VAL:HG13	2.50	0.46
16:A:381:THR:O	16:A:384:GLU:HG2	2.16	0.46
18:E:170:CYS:SG	18:E:171:LEU:N	2.88	0.46
1:f:141:LEU:HB3	1:f:143:LEU:HG	1.96	0.46
3:D:60:TYR:HH	14:U:640:LEU:HD11	1.79	0.46
4:V:200:ARG:HB2	4:V:203:LEU:HD23	1.97	0.46
4:V:375:PHE:CE1	4:V:399:ARG:HB2	2.51	0.46
4:V:483:CYS:SG	8:Z:265:LEU:HA	2.56	0.46
7:Y:39:ASP:HA	7:Y:42:MET:HE3	1.97	0.46
8:Z:253:THR:HG23	8:Z:257:MET:HE1	1.97	0.46
10:b:106:LYS:O	10:b:107:MET:HE2	2.14	0.46
14:U:544:ILE:HD12	14:U:544:ILE:H	1.80	0.46
15:c:195:GLY:HA2	15:c:198:ARG:HH11	1.79	0.46
16:A:180:CYS:SG	16:A:181:LYS:N	2.89	0.46
16:A:261:PHE:CD2	16:A:305:GLN:HB3	2.51	0.46
17:B:412:MET:SD	17:B:413:LYS:N	2.88	0.46
18:E:101:ASP:HB2	18:E:108:MET:SD	2.55	0.46
18:E:177:GLY:N	19:F:344:ARG:HD2	2.31	0.46
18:E:211:SER:HA	18:E:214:LEU:HD12	1.96	0.46
4:V:173:ILE:HD12	4:V:176:MET:HE3	1.97	0.46
5:W:372:ARG:NH1	9:a:327:VAL:HB	2.30	0.46
6:X:271:VAL:HG21	6:X:288:LYS:NZ	2.31	0.46
7:Y:336:ARG:HH12	7:Y:340:ALA:HB2	1.79	0.46
19:F:307:GLN:HA	19:F:310:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F:337:ILE:O	19:F:337:ILE:HG22	2.14	0.46
1:f:116:SER:HB3	1:f:119:GLN:HG3	1.97	0.46
2:C:167:LEU:HD21	17:B:407:LEU:HD21	1.98	0.46
3:D:387:VAL:HG22	18:E:158:LEU:HD22	1.97	0.46
3:D:395:LEU:HD12	3:D:397:LYS:H	1.80	0.46
4:V:121:PHE:HE1	4:V:159:LEU:HD11	1.81	0.46
4:V:237:THR:HA	4:V:240:LEU:HG	1.98	0.46
4:V:273:LYS:NZ	14:U:36:ALA:HB1	2.31	0.46
4:V:348:PHE:HE1	4:V:357:LEU:HB3	1.81	0.46
7:Y:52:PRO:CD	7:Y:114:ILE:HB	2.44	0.46
7:Y:181:LYS:HD2	7:Y:200:LEU:HD22	1.97	0.46
7:Y:285:ASP:OD1	7:Y:286:TRP:N	2.48	0.46
8:Z:256:GLN:HB3	15:c:295:ASN:HD21	1.79	0.46
14:U:336:GLU:OE1	14:U:337:LEU:HD22	2.14	0.46
16:A:224:LEU:HD11	22:A:501:ATP:H5'2	1.97	0.46
16:A:241:ILE:HG23	16:A:276:GLU:OE1	2.16	0.46
17:B:362:LYS:HB2	17:B:384:ILE:HG21	1.97	0.46
17:B:393:ALA:HB2	22:B:501:ATP:H5'1	1.96	0.46
2:C:151:ILE:HG12	2:C:198:LEU:HD21	1.96	0.46
4:V:306:ARG:O	4:V:310:THR:HG23	2.15	0.46
5:W:372:ARG:CZ	9:a:325:ASP:HB3	2.46	0.46
8:Z:78:MET:HA	8:Z:78:MET:HE3	1.97	0.46
9:a:244:ASN:ND2	9:a:247:ARG:HG2	2.30	0.46
15:c:269:GLN:NE2	15:c:272:ILE:HB	2.30	0.46
17:B:103:ARG:HE	17:B:160:ILE:CG2	2.29	0.46
17:B:264:PRO:HB2	17:B:268:ARG:HH21	1.81	0.46
4:V:104:THR:HA	4:V:107:ARG:HG2	1.97	0.46
5:W:89:LEU:O	5:W:93:ARG:HG2	2.16	0.46
8:Z:25:ARG:O	8:Z:28:LYS:HG2	2.16	0.46
9:a:42:LEU:HD21	9:a:75:SER:HB2	1.98	0.46
10:b:3:LEU:HB3	10:b:105:HIS:CD2	2.51	0.46
14:U:183:LEU:HD12	14:U:184:CYS:N	2.31	0.46
14:U:446:LEU:HD22	14:U:461:LEU:HD11	1.98	0.46
18:E:181:THR:O	18:E:185:ARG:HG2	2.15	0.46
3:D:405:THR:HA	3:D:408:LYS:HE2	1.96	0.46
5:W:129:ARG:HH22	5:W:146:THR:HA	1.77	0.46
5:W:387:ASP:HA	5:W:390:GLU:OE2	2.16	0.46
7:Y:178:ASN:O	7:Y:182:VAL:HG23	2.15	0.46
15:c:234:TYR:HE1	15:c:298:GLN:HE21	1.63	0.46
16:A:354:ILE:HG13	16:A:358:HIS:CD2	2.51	0.46
17:B:245:ALA:HB1	17:B:279:PRO:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:156:LEU:HA	20:w:33:TYR:HA	1.99	0.46
3:D:205:TYR:HE2	3:D:330:LYS:HB3	1.79	0.46
4:V:170:LEU:HA	4:V:173:ILE:HG22	1.97	0.46
4:V:214:HIS:HA	4:V:217:VAL:HG12	1.98	0.46
5:W:375:MET:SD	5:W:375:MET:N	2.75	0.46
5:W:408:ARG:NH2	6:X:346:GLN:OE1	2.48	0.46
6:X:310:ARG:O	6:X:314:ARG:HG2	2.16	0.46
7:Y:136:HIS:O	7:Y:140:ILE:HG12	2.16	0.46
8:Z:15:VAL:O	8:Z:19:VAL:HG23	2.15	0.46
9:a:24:ARG:O	9:a:28:LEU:HG	2.16	0.46
10:b:112:PHE:CE1	10:b:141:ILE:HG13	2.51	0.46
11:d:224:VAL:HA	11:d:227:LYS:HB3	1.97	0.46
11:d:303:ALA:HB1	11:d:310:LEU:HD11	1.98	0.46
14:U:166:THR:O	14:U:170:SER:OG	2.33	0.46
14:U:697:GLN:HE22	14:U:786:THR:HG21	1.81	0.46
16:A:187:LEU:O	16:A:191:VAL:HG22	2.16	0.46
17:B:417:GLU:HG2	17:B:418:ASP:N	2.31	0.46
19:F:200:GLU:HA	19:F:204:LEU:HD23	1.97	0.46
11:d:208:PHE:HE1	11:d:229:PRO:HB2	1.80	0.45
14:U:24:LEU:HD11	14:U:60:ALA:HA	1.97	0.45
14:U:64:ALA:O	14:U:67:VAL:HG22	2.16	0.45
14:U:517:GLY:O	14:U:554:LEU:HD22	2.15	0.45
17:B:264:PRO:HB2	17:B:268:ARG:NH2	2.31	0.45
3:D:273:LYS:O	3:D:274:ARG:HD3	2.17	0.45
4:V:451:ILE:C	11:d:279:TYR:HE1	2.24	0.45
5:W:20:TYR:HE1	5:W:57:ALA:HB3	1.81	0.45
5:W:23:THR:O	5:W:26:GLN:HG3	2.16	0.45
5:W:369:TYR:CD1	9:a:315:LEU:HD13	2.52	0.45
5:W:373:ILE:O	5:W:413:ILE:N	2.48	0.45
9:a:58:LYS:HA	9:a:61:GLU:OE2	2.15	0.45
9:a:91:ASN:O	9:a:94:LEU:HG	2.16	0.45
9:a:303:THR:HG22	9:a:304:VAL:N	2.31	0.45
11:d:166:ARG:HH21	14:U:13:ASP:CG	2.24	0.45
14:U:34:PHE:HB3	14:U:37:GLU:OE1	2.15	0.45
14:U:793:LYS:NZ	14:U:914:LEU:O	2.42	0.45
15:c:256:ASN:HA	15:c:259:VAL:HG12	1.97	0.45
16:A:111:TYR:HE2	16:A:125:LEU:HB3	1.81	0.45
16:A:280:ILE:HG23	16:A:295:VAL:HG13	1.98	0.45
18:E:188:ALA:HA	18:E:195:PHE:CE2	2.51	0.45
4:V:185:GLN:HG2	4:V:218:TYR:CE1	2.51	0.45
6:X:251:LEU:O	6:X:254:MET:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:399:ALA:HA	6:X:402:GLU:HG3	1.97	0.45
7:Y:138:LEU:HD12	7:Y:142:PHE:HE1	1.80	0.45
7:Y:317:GLY:O	7:Y:321:GLU:HG2	2.16	0.45
7:Y:367:GLN:O	7:Y:370:ILE:HG22	2.16	0.45
8:Z:140:SER:HB2	8:Z:153:LYS:NZ	2.31	0.45
16:A:340:LYS:HE2	19:F:429:ALA:HB1	1.98	0.45
17:B:190:LEU:HB2	17:B:194:ILE:HG13	1.97	0.45
2:C:270:GLN:HB2	2:C:305:LEU:HD11	1.98	0.45
4:V:243:ASP:O	4:V:247:GLN:HG3	2.17	0.45
4:V:290:TYR:CD2	4:V:328:VAL:HG12	2.52	0.45
8:Z:165:GLU:OE2	8:Z:166:GLU:HG3	2.17	0.45
9:a:18:GLN:HB2	9:a:22:TRP:CZ3	2.52	0.45
11:d:168:MET:HE2	11:d:191:LEU:HG	1.98	0.45
15:c:282:ARG:HE	15:c:283:HIS:CD2	2.35	0.45
16:A:99:THR:HG21	16:A:115:VAL:HG22	1.97	0.45
16:A:300:LEU:HD23	16:A:303:ILE:HD12	1.99	0.45
17:B:420:LYS:HA	17:B:423:LYS:HD3	1.99	0.45
18:E:331:ILE:HG23	18:E:371:VAL:HG11	1.98	0.45
18:E:385:ASP:OD2	18:E:387:LYS:HG2	2.15	0.45
1:f:138:PRO:HB3	15:c:170:LEU:HD21	1.98	0.45
2:C:20:LEU:HD13	14:U:141:CYS:SG	2.57	0.45
2:C:296:ASN:O	2:C:297:ARG:HG2	2.17	0.45
4:V:218:TYR:CD2	4:V:227:VAL:HB	2.52	0.45
5:W:79:GLU:HG3	5:W:82:LEU:HB2	1.98	0.45
5:W:124:LEU:O	5:W:128:LEU:HG	2.17	0.45
5:W:148:THR:O	5:W:152:ILE:HG12	2.17	0.45
5:W:200:ILE:HG13	5:W:201:ARG:N	2.31	0.45
5:W:375:MET:HE1	5:W:411:GLY:C	2.41	0.45
6:X:297:ARG:HG3	6:X:337:ARG:HD3	1.98	0.45
6:X:399:ALA:HB1	15:c:245:VAL:HG12	1.98	0.45
8:Z:212:LEU:HD21	9:a:353:LEU:HD12	1.99	0.45
10:b:44:ASN:ND2	10:b:46:GLU:OE1	2.49	0.45
10:b:94:HIS:CE1	10:b:98:LYS:HD2	2.51	0.45
14:U:141:CYS:HB3	14:U:150:ALA:HB2	1.99	0.45
14:U:501:LEU:HB2	14:U:512:ALA:HB1	1.97	0.45
14:U:901:GLN:NE2	14:U:902:PRO:HD2	2.32	0.45
18:E:364:GLN:HA	18:E:367:PHE:CD2	2.50	0.45
19:F:228:PRO:HG2	19:F:231:THR:OG1	2.17	0.45
1:f:51:GLU:O	1:f:85:LEU:N	2.50	0.45
2:C:375:ARG:NH2	2:C:382:ASP:OD2	2.50	0.45
3:D:210:CYS:N	22:D:501:ATP:O2B	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:345:PHE:HB2	3:D:360:LEU:HD12	1.99	0.45
6:X:332:GLU:O	6:X:336:ILE:HG23	2.17	0.45
8:Z:193:ASN:OD1	8:Z:194:GLN:N	2.48	0.45
10:b:138:VAL:HG12	10:b:160:LEU:HD23	1.98	0.45
17:B:209:GLU:HA	17:B:212:GLU:HG2	1.99	0.45
17:B:214:MET:HG2	17:B:216:ILE:HG23	1.97	0.45
19:F:100:ASP:OD1	19:F:100:ASP:N	2.50	0.45
3:D:225:ALA:HB1	3:D:259:PRO:O	2.16	0.45
4:V:110:HIS:CE1	4:V:174:PHE:HE2	2.35	0.45
4:V:384:GLU:OE1	4:V:384:GLU:N	2.29	0.45
5:W:317:TRP:CD1	5:W:358:VAL:HG11	2.52	0.45
6:X:335:LEU:HA	6:X:338:VAL:HG12	1.99	0.45
7:Y:42:MET:HA	7:Y:45:VAL:HG22	1.99	0.45
9:a:122:LYS:HB3	9:a:130:VAL:HG11	1.97	0.45
14:U:542:GLU:O	14:U:545:LEU:HB2	2.17	0.45
17:B:284:ILE:CG2	17:B:329:MET:HG3	2.46	0.45
18:E:196:LEU:HD12	18:E:230:ILE:HG22	1.99	0.45
19:F:307:GLN:HA	19:F:310:MET:HG2	1.98	0.45
19:F:408:LEU:HD22	19:F:409:ARG:NH1	2.31	0.45
1:f:132:PHE:CZ	1:f:156:LEU:HB2	2.52	0.45
3:D:66:LYS:NZ	3:D:70:LYS:HG3	2.32	0.45
5:W:17:GLU:N	5:W:57:ALA:O	2.50	0.45
5:W:147:LYS:NZ	5:W:184:GLU:OE1	2.46	0.45
5:W:308:LEU:O	5:W:311:THR:HG22	2.17	0.45
6:X:247:ALA:O	6:X:250:SER:OG	2.31	0.45
6:X:365:LEU:HA	6:X:368:MET:HG2	1.98	0.45
7:Y:15:PRO:HB2	7:Y:150:PHE:CD2	2.52	0.45
7:Y:16:ASP:OD2	7:Y:18:ARG:HB3	2.17	0.45
8:Z:69:PHE:HB3	10:b:95:LEU:CD2	2.43	0.45
9:a:255:TRP:HB2	9:a:261:LEU:HD13	1.99	0.45
14:U:247:GLN:OE1	14:U:912:ILE:HD12	2.16	0.45
14:U:416:GLU:OE1	14:U:453:HIS:ND1	2.47	0.45
17:B:358:GLU:HA	17:B:361:LYS:HD2	1.99	0.45
19:F:366:MET:HE1	19:F:388:THR:HG21	1.98	0.45
2:C:20:LEU:HD21	14:U:137:MET:CE	2.45	0.45
4:V:419:LEU:HD13	4:V:422:ILE:HD12	1.99	0.45
6:X:248:ILE:O	6:X:252:LYS:HG2	2.17	0.45
6:X:281:GLY:H	6:X:284:THR:HB	1.81	0.45
7:Y:300:ARG:HH11	7:Y:300:ARG:HG2	1.82	0.45
8:Z:140:SER:CA	8:Z:153:LYS:HZ1	2.30	0.45
8:Z:182:THR:O	8:Z:183:THR:OG1	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:246:LYS:HD3	15:c:246:LYS:HA	1.62	0.45
17:B:388:ASP:OD1	17:B:389:ASP:N	2.50	0.45
18:E:241:ARG:HH12	19:F:297:ASP:CG	2.24	0.45
1:f:58:LYS:O	1:f:62:GLN:HG3	2.17	0.45
4:V:261:TYR:HB2	4:V:263:LEU:HG	1.99	0.45
6:X:44:GLN:O	6:X:47:GLU:HG3	2.17	0.45
7:Y:14:ASN:HD21	7:Y:113:ARG:HD3	1.81	0.45
7:Y:325:VAL:HB	7:Y:329:PHE:HD2	1.82	0.45
11:d:172:LYS:NZ	11:d:211:GLU:OE1	2.50	0.45
14:U:357:LYS:O	14:U:360:VAL:HG12	2.17	0.45
14:U:583:MET:SD	14:U:583:MET:C	3.00	0.45
16:A:331:LEU:O	16:A:337:LEU:HD23	2.17	0.45
1:f:313:LEU:O	1:f:317:THR:HG23	2.17	0.44
2:C:82:LYS:HA	2:C:82:LYS:HE3	1.99	0.44
2:C:211:PHE:HE2	2:C:247:PHE:HB2	1.81	0.44
2:C:364:THR:O	2:C:368:MET:HG2	2.17	0.44
4:V:169:LEU:HA	4:V:172:VAL:HG12	2.00	0.44
4:V:436:PHE:HB3	4:V:440:LYS:HZ3	1.82	0.44
5:W:382:LEU:HD23	5:W:384:LEU:HB2	1.99	0.44
13:v:2:UNK:O	18:E:206:LYS:NZ	2.33	0.44
14:U:654:MET:HE2	14:U:690:ALA:HB2	2.00	0.44
16:A:261:PHE:CE2	16:A:305:GLN:HB3	2.53	0.44
19:F:75:GLU:O	19:F:79:LYS:HG2	2.17	0.44
1:f:156:LEU:HD11	1:f:288:LEU:HD11	1.98	0.44
2:C:118:ASN:ND2	2:C:119:ASP:OD2	2.50	0.44
2:C:296:ASN:HD21	2:C:297:ARG:HH21	1.65	0.44
5:W:66:ILE:HG13	5:W:67:LEU:N	2.32	0.44
5:W:366:MET:O	5:W:370:TYR:HB2	2.17	0.44
6:X:211:ASP:HB3	6:X:234:GLU:HG3	1.99	0.44
7:Y:138:LEU:O	7:Y:141:VAL:HG12	2.17	0.44
11:d:172:LYS:HB3	11:d:172:LYS:HE2	1.76	0.44
16:A:241:ILE:HG23	17:B:314:ASN:HD22	1.82	0.44
18:E:101:ASP:O	18:E:105:LEU:HD23	2.17	0.44
19:F:169:ASP:O	19:F:173:LYS:HG2	2.16	0.44
1:f:107:MET:SD	15:c:83:SER:OG	2.74	0.44
3:D:245:ARG:HA	3:D:248:ARG:HG3	1.99	0.44
5:W:28:LEU:HB2	5:W:29:PRO:HD3	1.99	0.44
5:W:248:ARG:HD2	5:W:290:ILE:HD11	1.98	0.44
5:W:373:ILE:HD12	9:a:326:GLU:CG	2.45	0.44
5:W:436:MET:SD	15:c:226:MET:HG3	2.58	0.44
6:X:111:LEU:O	6:X:114:ILE:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:121:LEU:HD21	7:Y:125:ARG:HH22	1.81	0.44
9:a:80:ILE:HA	9:a:83:VAL:HG22	2.00	0.44
10:b:10:VAL:HG13	10:b:29:GLN:CD	2.43	0.44
11:d:119:LEU:O	11:d:123:LEU:HD23	2.17	0.44
14:U:320:ASP:OD1	14:U:321:GLN:N	2.50	0.44
14:U:417:LYS:HD2	14:U:418:GLU:HB2	2.00	0.44
14:U:673:GLU:HG3	14:U:674:PRO:HD3	1.98	0.44
16:A:180:CYS:O	16:A:181:LYS:HD2	2.18	0.44
17:B:199:GLU:HG2	17:B:203:LEU:HD22	1.99	0.44
19:F:251:LEU:HD23	19:F:252:ALA:N	2.32	0.44
2:C:104:ASP:OD2	2:C:105:ILE:N	2.50	0.44
3:D:231:VAL:HA	3:D:265:ASP:OD1	2.17	0.44
4:V:268:GLU:O	4:V:271:VAL:HG12	2.18	0.44
5:W:117:ASP:HB3	5:W:120:ILE:HD11	2.00	0.44
5:W:276:LEU:O	5:W:357:ARG:NE	2.49	0.44
6:X:123:THR:OG1	6:X:124:PHE:N	2.50	0.44
7:Y:111:LEU:C	7:Y:120:ALA:HB2	2.43	0.44
7:Y:334:LEU:O	7:Y:338:ILE:HG12	2.17	0.44
11:d:117:GLY:O	11:d:120:LYS:HG2	2.17	0.44
11:d:238:GLU:OE2	11:d:243:LYS:NZ	2.42	0.44
15:c:175:ARG:HD3	15:c:201:TYR:CE1	2.53	0.44
16:A:122:VAL:HG13	16:A:122:VAL:O	2.17	0.44
16:A:249:TYR:CD1	19:F:259:MET:HE1	2.52	0.44
17:B:222:VAL:HG22	17:B:349:ARG:HB3	1.98	0.44
2:C:310:ARG:HD3	2:C:310:ARG:HA	1.86	0.44
2:C:365:GLU:HB3	2:C:386:ALA:HB1	2.00	0.44
2:C:380:GLN:HA	2:C:383:PHE:HD2	1.82	0.44
4:V:477:HIS:CE1	11:d:338:GLN:NE2	2.85	0.44
5:W:409:LEU:HD12	6:X:384:VAL:HG11	1.99	0.44
6:X:252:LYS:HD2	6:X:287:LEU:CD1	2.48	0.44
6:X:310:ARG:HG3	6:X:311:ALA:N	2.32	0.44
9:a:33:LEU:HB3	9:a:36:GLN:OE1	2.18	0.44
9:a:41:VAL:O	9:a:45:VAL:HG23	2.18	0.44
14:U:178:ALA:O	14:U:181:LEU:HG	2.18	0.44
14:U:601:ARG:O	14:U:605:VAL:HG23	2.17	0.44
2:C:53:ASN:ND2	14:U:642:GLU:O	2.49	0.44
2:C:218:GLU:OE1	2:C:218:GLU:N	2.38	0.44
6:X:421:LEU:HD11	8:Z:279:LYS:HG2	1.99	0.44
8:Z:193:ASN:OD1	8:Z:194:GLN:HG2	2.17	0.44
16:A:146:LYS:HG3	16:A:148:GLN:HG2	2.00	0.44
17:B:398:ILE:HD12	17:B:423:LYS:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F:103:ASP:OD1	19:F:103:ASP:N	2.49	0.44
3:D:377:SER:O	3:D:381:GLU:HG2	2.17	0.44
4:V:223:LYS:HD2	4:V:223:LYS:HA	1.78	0.44
5:W:110:THR:O	5:W:113:GLU:HG3	2.17	0.44
6:X:379:ASP:OD1	6:X:380:GLN:N	2.51	0.44
8:Z:65:ASP:OD1	8:Z:66:SER:N	2.51	0.44
8:Z:180:LYS:HD2	8:Z:180:LYS:HA	1.82	0.44
14:U:96:TYR:O	14:U:100:ILE:HG12	2.17	0.44
14:U:541:HIS:HB2	14:U:544:ILE:HD13	2.00	0.44
19:F:84:LYS:HG3	19:F:84:LYS:O	2.17	0.44
1:f:155:GLN:HG2	20:w:35:GLY:HA2	1.99	0.44
4:V:69:THR:HA	4:V:72:LEU:HD12	2.00	0.44
4:V:93:PHE:HD2	4:V:96:ARG:HD2	1.82	0.44
4:V:453:HIS:CE1	11:d:279:TYR:OH	2.70	0.44
5:W:115:ILE:HG23	5:W:121:LYS:CD	2.48	0.44
5:W:225:LYS:HB2	5:W:225:LYS:HE3	1.79	0.44
5:W:372:ARG:HH12	9:a:328:ASP:H	1.64	0.44
9:a:290:GLN:HE21	9:a:330:ARG:HE	1.66	0.44
15:c:90:VAL:C	15:c:94:LYS:HZ2	2.25	0.44
15:c:239:LYS:O	15:c:242:GLU:HB2	2.18	0.44
18:E:211:SER:O	18:E:214:LEU:HB2	2.18	0.44
18:E:243:PHE:N	18:E:254:GLN:OE1	2.39	0.44
1:f:159:GLN:HG2	20:w:29:PRO:HB2	1.99	0.44
2:C:142:LYS:NZ	3:D:297:ASP:OD1	2.49	0.44
3:D:341:LYS:HG2	3:D:345:PHE:CE2	2.47	0.44
4:V:60:ALA:O	4:V:63:SER:OG	2.28	0.44
5:W:271:VAL:HA	5:W:274:VAL:HG12	2.00	0.44
7:Y:75:LYS:HE2	7:Y:75:LYS:HB3	1.81	0.44
7:Y:238:GLU:HA	7:Y:242:LYS:HZ3	1.83	0.44
8:Z:267:ARG:HG2	8:Z:267:ARG:HH11	1.82	0.44
11:d:142:ILE:O	11:d:145:ARG:HG2	2.18	0.44
14:U:218:GLN:O	14:U:222:PHE:HD1	2.01	0.44
17:B:153:ASN:HB2	17:B:160:ILE:HD11	1.99	0.44
17:B:271:PHE:HD2	17:B:315:GLN:HB3	1.82	0.44
2:C:391:MET:O	2:C:395:SER:OG	2.24	0.43
3:D:214:MET:HE1	22:D:501:ATP:N9	2.31	0.43
4:V:451:ILE:HA	4:V:458:VAL:HA	1.99	0.43
5:W:214:PHE:HB3	5:W:223:LYS:HG3	1.99	0.43
6:X:74:ARG:HB3	6:X:75:PRO:HD3	2.00	0.43
6:X:187:ARG:NH2	6:X:221:GLU:OE1	2.52	0.43
6:X:207:GLN:NE2	6:X:238:GLY:HA3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:212:GLU:H	7:Y:212:GLU:CD	2.18	0.43
7:Y:238:GLU:HA	7:Y:242:LYS:NZ	2.32	0.43
7:Y:359:PRO:C	7:Y:361:SER:H	2.25	0.43
7:Y:363:ASN:O	7:Y:367:GLN:HG2	2.18	0.43
12:e:42:ASN:OD1	12:e:43:TRP:N	2.51	0.43
14:U:15:ASP:OD1	14:U:15:ASP:N	2.51	0.43
16:A:113:ILE:HG13	16:A:114:ASN:H	1.83	0.43
19:F:128:THR:HG22	19:F:128:THR:O	2.17	0.43
19:F:338:LEU:HB3	19:F:343:LEU:HD21	2.00	0.43
19:F:343:LEU:HD13	19:F:348:LEU:HD23	2.00	0.43
20:w:40:GLU:N	20:w:40:GLU:OE1	2.51	0.43
1:f:276:ALA:HB1	1:f:277:PRO:HD2	2.00	0.43
5:W:171:VAL:HA	5:W:174:TYR:CD2	2.54	0.43
6:X:42:ALA:HA	6:X:45:VAL:HG12	1.99	0.43
7:Y:282:MET:HE1	7:Y:295:TYR:HB3	1.99	0.43
10:b:150:THR:HG1	10:b:153:LEU:N	2.15	0.43
14:U:695:MET:O	14:U:695:MET:HE3	2.18	0.43
16:A:309:PHE:HB3	19:F:250:LYS:HZ1	1.82	0.43
17:B:175:LYS:NZ	17:B:248:LEU:HD21	2.32	0.43
17:B:365:PHE:CE1	17:B:395:ILE:HG23	2.53	0.43
18:E:355:ILE:HG23	19:F:211:LYS:NZ	2.33	0.43
19:F:168:TYR:HB2	19:F:173:LYS:HE2	2.00	0.43
2:C:248:MET:HG3	2:C:249:ASP:N	2.33	0.43
2:C:339:THR:H	2:C:378:VAL:H	1.65	0.43
2:C:346:LYS:HA	2:C:349:GLU:HG2	2.00	0.43
3:D:205:TYR:O	3:D:333:PHE:N	2.50	0.43
4:V:136:GLU:OE2	4:V:137:GLU:HG3	2.18	0.43
4:V:309:MET:HE1	4:V:331:LEU:CD2	2.43	0.43
4:V:415:SER:HB2	7:Y:346:LYS:HB3	2.00	0.43
7:Y:277:VAL:O	7:Y:281:GLU:HG2	2.18	0.43
14:U:247:GLN:OE1	14:U:913:ILE:HG22	2.18	0.43
16:A:91:GLN:HB3	16:A:92:PRO:HD3	1.99	0.43
16:A:339:ARG:HE	19:F:402:GLU:CD	2.25	0.43
17:B:288:ASP:HB3	17:B:331:THR:HG23	2.00	0.43
2:C:25:LEU:O	2:C:29:GLU:HG2	2.18	0.43
5:W:52:LYS:O	5:W:56:THR:OG1	2.34	0.43
5:W:60:MET:CE	5:W:99:GLN:HB3	2.48	0.43
7:Y:212:GLU:OE1	7:Y:212:GLU:N	2.34	0.43
9:a:231:GLN:HA	9:a:234:ILE:HD13	2.01	0.43
14:U:89:ASN:HB3	14:U:92:ASP:OD2	2.19	0.43
14:U:557:TYR:HA	14:U:588:MET:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:563:ALA:O	14:U:567:ILE:HG12	2.18	0.43
14:U:902:PRO:HB2	14:U:904:LYS:O	2.18	0.43
16:A:157:ILE:O	16:A:157:ILE:HG22	2.19	0.43
16:A:216:GLY:O	16:A:222:LYS:NZ	2.51	0.43
3:D:103:VAL:O	3:D:110:ASN:HB2	2.18	0.43
3:D:322:LEU:HD12	3:D:330:LYS:NZ	2.33	0.43
4:V:355:ARG:HA	4:V:358:MET:HE2	2.00	0.43
4:V:408:ARG:HA	4:V:408:ARG:HD2	1.80	0.43
5:W:414:ASN:HD21	5:W:416:GLN:HE21	1.66	0.43
6:X:142:ARG:NH1	6:X:144:GLN:H	2.16	0.43
6:X:252:LYS:HZ3	6:X:284:THR:CA	2.29	0.43
7:Y:69:LEU:O	7:Y:73:MET:HG2	2.18	0.43
7:Y:223:THR:HA	7:Y:226:VAL:HG12	2.01	0.43
7:Y:389:MET:HE3	7:Y:389:MET:HB3	1.62	0.43
9:a:135:ILE:HG13	9:a:136:GLU:N	2.32	0.43
14:U:34:PHE:HB3	14:U:37:GLU:CD	2.43	0.43
14:U:59:PHE:O	14:U:63:VAL:HG23	2.18	0.43
14:U:88:PHE:HE1	14:U:97:VAL:HG22	1.83	0.43
14:U:327:LYS:CB	14:U:333:MET:HE1	2.48	0.43
14:U:352:ILE:O	14:U:356:THR:HG23	2.19	0.43
14:U:357:LYS:HD3	14:U:385:PHE:CZ	2.53	0.43
14:U:711:GLN:O	14:U:715:LYS:HG2	2.17	0.43
14:U:732:LEU:O	14:U:736:ILE:HG12	2.17	0.43
15:c:59:GLY:HA3	15:c:68:ARG:O	2.18	0.43
17:B:364:ILE:HG23	17:B:368:HIS:HE1	1.79	0.43
19:F:378:ASP:OD1	19:F:378:ASP:N	2.52	0.43
1:f:42:ARG:NH1	1:f:43:TYR:O	2.51	0.43
1:f:288:LEU:HD23	1:f:288:LEU:HA	1.72	0.43
2:C:211:PHE:HE2	2:C:247:PHE:CB	2.31	0.43
2:C:389:LYS:HG2	2:C:393:LYS:NZ	2.33	0.43
4:V:234:ARG:HE	4:V:237:THR:HG21	1.84	0.43
4:V:399:ARG:O	4:V:399:ARG:HD2	2.18	0.43
4:V:403:ILE:O	4:V:407:VAL:HG13	2.18	0.43
5:W:190:MET:HE1	5:W:205:ILE:O	2.18	0.43
5:W:237:GLU:OE1	5:W:237:GLU:N	2.52	0.43
5:W:373:ILE:CD1	9:a:326:GLU:HG2	2.45	0.43
5:W:450:GLU:HA	5:W:454:ASN:OD1	2.18	0.43
6:X:253:TYR:HE1	6:X:318:ILE:HB	1.83	0.43
7:Y:177:ARG:HE	7:Y:181:LYS:HZ1	1.65	0.43
11:d:144:ALA:HB1	11:d:174:TYR:CE2	2.54	0.43
14:U:549:ALA:HB1	14:U:581:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:708:GLN:O	14:U:712:LEU:HD23	2.19	0.43
15:c:226:MET:C	15:c:230:THR:HG23	2.44	0.43
15:c:282:ARG:HH21	15:c:283:HIS:CD2	2.36	0.43
17:B:103:ARG:HE	17:B:160:ILE:HG22	1.84	0.43
17:B:364:ILE:HG22	17:B:395:ILE:HG21	2.00	0.43
17:B:415:THR:HG1	17:B:417:GLU:CD	2.26	0.43
19:F:244:THR:C	19:F:245:LYS:HD2	2.44	0.43
2:C:68:GLU:O	3:D:136:SER:HB2	2.19	0.43
2:C:191:PRO:O	2:C:194:THR:OG1	2.22	0.43
2:C:343:ASN:O	2:C:346:LYS:HG2	2.19	0.43
4:V:120:PHE:HB3	4:V:167:LEU:CD1	2.48	0.43
4:V:434:ALA:O	4:V:438:VAL:HG22	2.18	0.43
5:W:20:TYR:O	5:W:24:VAL:HG22	2.19	0.43
5:W:171:VAL:O	5:W:182:ARG:NH1	2.52	0.43
7:Y:42:MET:HE2	7:Y:42:MET:HB3	1.92	0.43
9:a:80:ILE:HG21	9:a:100:THR:HG21	2.00	0.43
14:U:173:VAL:O	14:U:177:LEU:HD23	2.18	0.43
14:U:712:LEU:HA	14:U:715:LYS:HG2	2.01	0.43
15:c:116:PRO:HD2	15:c:118:PHE:HE1	1.83	0.43
15:c:282:ARG:HE	15:c:283:HIS:HD2	1.67	0.43
16:A:192:GLU:OE2	16:A:232:ARG:HG2	2.19	0.43
17:B:203:LEU:N	17:B:204:PRO:HD2	2.34	0.43
1:f:298:ARG:HG3	1:f:299:PRO:HD2	2.01	0.43
2:C:347:ILE:CD1	2:C:383:PHE:HB3	2.48	0.43
3:D:273:LYS:HE2	3:D:316:THR:HA	2.00	0.43
7:Y:80:GLU:OE2	7:Y:110:TYR:OH	2.31	0.43
9:a:18:GLN:HB3	9:a:21:VAL:HG22	2.01	0.43
10:b:68:THR:O	10:b:71:ILE:HG22	2.19	0.43
10:b:121:GLU:OE2	10:b:152:LYS:HG3	2.18	0.43
14:U:490:ARG:HB2	14:U:493:VAL:HG22	2.00	0.43
14:U:556:MET:HE2	14:U:556:MET:HA	2.01	0.43
14:U:620:GLU:OE2	14:U:654:MET:HB2	2.18	0.43
14:U:780:SER:HA	14:U:783:TYR:CD2	2.50	0.43
19:F:137:ILE:O	19:F:160:ILE:HG12	2.19	0.43
19:F:299:GLU:CG	19:F:300:LYS:H	2.27	0.43
19:F:417:HIS:HA	19:F:420:TYR:CD2	2.54	0.43
2:C:194:THR:HB	2:C:317:PHE:HB3	2.01	0.43
4:V:318:GLN:O	4:V:320:THR:N	2.52	0.43
5:W:43:VAL:O	5:W:47:LEU:HG	2.19	0.43
5:W:105:VAL:HG11	5:W:138:VAL:HG11	2.00	0.43
5:W:140:ILE:HA	5:W:177:MET:HE1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:295:LYS:HD2	5:W:295:LYS:HA	1.89	0.43
6:X:77:LEU:HD13	6:X:116:TRP:HE1	1.83	0.43
6:X:172:LEU:O	6:X:176:THR:HG23	2.18	0.43
7:Y:106:ALA:HA	7:Y:109:GLU:HG3	2.01	0.43
9:a:226:ARG:HA	9:a:226:ARG:NE	2.34	0.43
10:b:10:VAL:HG13	10:b:29:GLN:OE1	2.18	0.43
11:d:94:MET:SD	11:d:115:GLU:HG3	2.59	0.43
11:d:223:ASN:OD1	11:d:225:TYR:HB2	2.19	0.43
11:d:336:ALA:HB2	15:c:303:MET:HE1	1.99	0.43
14:U:214:ILE:O	14:U:217:CYS:HB3	2.19	0.43
15:c:211:GLU:HG2	15:c:212:LEU:N	2.33	0.43
17:B:183:THR:OG1	17:B:186:ASP:HB2	2.19	0.43
17:B:204:PRO:HB3	17:B:211:TYR:HD2	1.84	0.43
19:F:185:TYR:CZ	19:F:243:GLN:HG3	2.54	0.43
19:F:188:ILE:HG23	21:F:501:ADP:N6	2.34	0.43
1:f:36:HIS:CG	1:f:95:LYS:HE3	2.54	0.43
1:f:145:VAL:HG21	20:w:39:LEU:HD23	2.00	0.43
1:f:152:VAL:HG23	20:w:37:PHE:HB3	2.00	0.43
2:C:189:TYR:O	2:C:316:GLU:HA	2.19	0.43
2:C:192:PRO:HA	21:C:501:ADP:O2B	2.18	0.43
2:C:369:TYR:CD1	2:C:372:ARG:HD2	2.54	0.43
3:D:66:LYS:HZ1	3:D:70:LYS:HG3	1.83	0.43
4:V:333:ILE:HG12	4:V:347:GLN:HE22	1.84	0.43
5:W:42:GLU:CD	5:W:42:GLU:H	2.27	0.43
7:Y:353:ILE:HD12	7:Y:353:ILE:HA	1.93	0.43
8:Z:201:LEU:HD22	8:Z:204:LYS:HZ1	1.84	0.43
9:a:174:LYS:O	9:a:178:ARG:HG2	2.18	0.43
9:a:180:LEU:HD22	9:a:219:HIS:CE1	2.54	0.43
10:b:138:VAL:CG1	10:b:160:LEU:HD23	2.49	0.43
11:d:330:ILE:O	11:d:332:SER:N	2.52	0.43
12:e:53:SER:O	12:e:56:LEU:HG	2.19	0.43
16:A:178:GLY:HA2	16:A:353:HIS:HD2	1.83	0.43
16:A:354:ILE:O	16:A:357:ILE:HG22	2.19	0.43
18:E:168:LYS:HG3	18:E:275:MET:SD	2.59	0.43
1:f:279:VAL:HG13	20:w:40:GLU:HB3	2.01	0.42
3:D:383:GLY:O	3:D:387:VAL:HG23	2.19	0.42
5:W:103:LYS:HA	5:W:106:GLN:HG2	2.01	0.42
5:W:117:ASP:O	5:W:120:ILE:HG13	2.19	0.42
6:X:218:HIS:NE2	6:X:227:THR:OG1	2.51	0.42
6:X:294:SER:HA	6:X:330:LEU:HD11	2.01	0.42
6:X:403:THR:O	6:X:407:MET:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:220:VAL:O	7:Y:224:VAL:HG23	2.18	0.42
7:Y:289:ALA:O	7:Y:292:TYR:HD2	2.01	0.42
8:Z:228:TYR:CD1	9:a:338:PRO:HB2	2.39	0.42
8:Z:247:LYS:O	8:Z:251:LEU:HG	2.18	0.42
8:Z:283:ARG:HA	8:Z:286:GLU:HG2	2.00	0.42
11:d:148:LEU:HD22	11:d:167:TYR:HD1	1.84	0.42
14:U:7:GLY:O	14:U:10:SER:OG	2.30	0.42
14:U:203:LYS:O	14:U:206:MET:HG2	2.19	0.42
14:U:667:GLU:O	14:U:671:LEU:HD23	2.19	0.42
15:c:41:MET:HE2	15:c:112:TYR:CD2	2.54	0.42
16:A:98:CYS:HB2	16:A:139:ARG:CG	2.49	0.42
16:A:143:ASP:OD1	16:A:148:GLN:N	2.50	0.42
18:E:327:ASP:H	18:E:364:GLN:HE22	1.66	0.42
19:F:80:ILE:HG22	19:F:84:LYS:HZ1	1.81	0.42
4:V:228:ARG:NH2	14:U:33:ASP:OD1	2.51	0.42
5:W:117:ASP:O	5:W:121:LYS:HG2	2.19	0.42
5:W:387:ASP:HA	5:W:390:GLU:CD	2.44	0.42
6:X:271:VAL:HG21	6:X:288:LYS:CE	2.48	0.42
8:Z:103:LYS:HB2	8:Z:103:LYS:HE3	1.69	0.42
9:a:70:ARG:HG3	9:a:73:PRO:HG3	2.01	0.42
9:a:148:VAL:O	9:a:152:HIS:ND1	2.52	0.42
11:d:92:THR:O	11:d:95:TYR:HB3	2.18	0.42
11:d:218:LYS:HA	11:d:221:GLN:HE21	1.83	0.42
14:U:705:LYS:HA	14:U:708:GLN:HG2	2.00	0.42
16:A:309:PHE:HB3	19:F:250:LYS:NZ	2.34	0.42
16:A:417:ILE:O	16:A:421:ALA:HB2	2.18	0.42
19:F:70:LYS:HG2	19:F:71:ASP:N	2.34	0.42
19:F:364:ARG:O	19:F:368:ILE:HG12	2.20	0.42
19:F:416:THR:O	19:F:419:ASP:HB2	2.19	0.42
3:D:189:GLU:OE1	3:D:189:GLU:N	2.45	0.42
3:D:391:ARG:HH21	3:D:394:VAL:HA	1.83	0.42
4:V:114:TYR:HD1	4:V:115:LYS:HE2	1.84	0.42
4:V:283:ASN:HB2	4:V:284:GLU:OE1	2.20	0.42
4:V:330:LYS:HD3	4:V:360:TYR:OH	2.20	0.42
5:W:271:VAL:O	5:W:275:ILE:HG13	2.19	0.42
6:X:49:SER:O	6:X:52:GLU:HG2	2.19	0.42
7:Y:155:ASP:OD1	7:Y:155:ASP:N	2.51	0.42
8:Z:263:ALA:O	8:Z:266:ILE:HG22	2.18	0.42
9:a:65:SER:C	9:a:69:HIS:HB3	2.44	0.42
9:a:95:THR:O	9:a:98:GLU:HG3	2.19	0.42
14:U:596:ASN:O	14:U:600:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:695:MET:SD	14:U:706:VAL:HG22	2.59	0.42
16:A:284:ARG:HH11	16:A:300:LEU:HD21	1.84	0.42
16:A:299:MET:HE3	16:A:328:ASP:OD2	2.20	0.42
17:B:191:ASP:H	17:B:194:ILE:HD12	1.85	0.42
18:E:143:ARG:HH21	18:E:146:ARG:NE	2.10	0.42
1:f:29:ALA:HA	1:f:30:PRO:HD3	1.83	0.42
2:C:160:GLU:O	2:C:164:VAL:HG23	2.20	0.42
2:C:326:LEU:O	2:C:329:LEU:HG	2.20	0.42
3:D:335:LEU:HD12	3:D:336:PRO:HD3	2.02	0.42
4:V:121:PHE:CE1	4:V:159:LEU:HD11	2.54	0.42
4:V:269:LYS:C	4:V:273:LYS:HZ2	2.27	0.42
4:V:273:LYS:HZ1	14:U:36:ALA:HB1	1.84	0.42
4:V:433:ASP:OD2	11:d:240:SER:HB3	2.19	0.42
5:W:121:LYS:O	5:W:125:ILE:HG13	2.19	0.42
5:W:165:ILE:O	5:W:168:GLU:HG2	2.19	0.42
5:W:368:LYS:HE3	5:W:369:TYR:CE2	2.53	0.42
7:Y:232:GLU:O	7:Y:236:LEU:N	2.37	0.42
7:Y:387:ILE:HG21	8:Z:276:ILE:CD1	2.49	0.42
14:U:510:GLU:HB2	14:U:543:LYS:HG2	2.01	0.42
15:c:125:VAL:HA	15:c:128:ASN:ND2	2.34	0.42
17:B:123:VAL:HG21	17:B:152:LEU:HD21	2.01	0.42
18:E:140:GLU:O	18:E:144:GLU:HG3	2.20	0.42
18:E:349:GLU:HG2	19:F:350:ARG:HH21	1.84	0.42
19:F:79:LYS:O	19:F:83:ASN:ND2	2.52	0.42
2:C:187:LEU:HD23	2:C:314:LYS:HG2	2.00	0.42
3:D:122:GLU:OE1	15:c:282:ARG:NH2	2.39	0.42
3:D:341:LYS:O	3:D:344:ILE:HG22	2.20	0.42
4:V:79:VAL:HA	4:V:82:LEU:HG	2.00	0.42
4:V:359:PRO:HB3	4:V:382:PHE:HD2	1.85	0.42
4:V:419:LEU:HD11	4:V:451:ILE:HD11	2.02	0.42
4:V:451:ILE:CG1	4:V:458:VAL:HG22	2.49	0.42
14:U:690:ALA:O	14:U:694:ILE:HG12	2.20	0.42
17:B:405:MET:CG	17:B:418:ASP:HB2	2.50	0.42
3:D:146:GLU:OE2	18:E:61:LEU:HB3	2.20	0.42
3:D:276:ASP:O	3:D:279:THR:HG22	2.20	0.42
4:V:492:LYS:HB2	4:V:492:LYS:HE2	1.84	0.42
5:W:440:ASN:O	5:W:444:HIS:ND1	2.52	0.42
6:X:323:LEU:HD12	6:X:324:ALA:N	2.35	0.42
7:Y:24:PHE:CE2	7:Y:286:TRP:HE3	2.37	0.42
7:Y:107:LYS:HG3	7:Y:111:LEU:HD23	2.01	0.42
7:Y:245:GLU:O	7:Y:249:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:387:ILE:HG21	8:Z:276:ILE:HD13	2.01	0.42
8:Z:187:LEU:O	8:Z:191:ILE:HG22	2.19	0.42
11:d:211:GLU:OE1	11:d:214:ARG:NH2	2.53	0.42
15:c:134:GLU:HA	15:c:137:SER:O	2.19	0.42
16:A:377:CYS:HB3	16:A:380:SER:OG	2.19	0.42
17:B:226:GLY:HA3	17:B:353:PHE:HB2	2.01	0.42
17:B:412:MET:SD	17:B:413:LYS:HB2	2.60	0.42
17:B:420:LYS:HE3	17:B:420:LYS:HB2	1.84	0.42
18:E:320:ILE:HB	18:E:322:LYS:NZ	2.34	0.42
19:F:380:ASN:ND2	19:F:383:GLU:OE1	2.52	0.42
1:f:297:GLY:HA3	20:w:29:PRO:HD2	2.01	0.42
3:D:379:CYS:O	3:D:382:SER:OG	2.28	0.42
4:V:114:TYR:CE2	4:V:138:PRO:HD3	2.54	0.42
4:V:250:LEU:O	4:V:254:LEU:HG	2.18	0.42
5:W:375:MET:HE1	5:W:412:ILE:N	2.35	0.42
7:Y:22:LEU:HD12	7:Y:41:LEU:HD13	2.01	0.42
7:Y:192:ARG:HD2	12:e:39:TRP:HB3	2.02	0.42
7:Y:314:LEU:HB3	7:Y:319:MET:HE3	2.01	0.42
8:Z:140:SER:HB2	8:Z:153:LYS:HZ1	1.85	0.42
8:Z:182:THR:C	8:Z:183:THR:HG1	2.23	0.42
9:a:233:LEU:O	9:a:237:LEU:HD23	2.20	0.42
10:b:3:LEU:HD13	10:b:105:HIS:CE1	2.55	0.42
11:d:175:TYR:HA	11:d:188:MET:HE1	2.01	0.42
11:d:310:LEU:HD12	11:d:316:TYR:CE1	2.54	0.42
17:B:202:GLU:O	17:B:205:LEU:HG	2.20	0.42
18:E:180:LYS:N	22:E:401:ATP:O1B	2.53	0.42
3:D:336:PRO:HB3	3:D:340:GLN:OE1	2.19	0.42
4:V:76:LYS:O	4:V:80:LYS:HG2	2.19	0.42
5:W:60:MET:HE2	5:W:99:GLN:HB3	2.01	0.42
5:W:248:ARG:HH21	5:W:289:ARG:HE	1.68	0.42
6:X:404:ILE:CD1	7:Y:376:LEU:HD13	2.50	0.42
7:Y:22:LEU:HD23	7:Y:22:LEU:HA	1.78	0.42
7:Y:142:PHE:HD2	7:Y:183:TYR:CE2	2.37	0.42
9:a:94:LEU:HD22	9:a:122:LYS:NZ	2.34	0.42
9:a:361:LYS:O	9:a:364:GLU:HG3	2.20	0.42
19:F:116:GLN:O	19:F:116:GLN:CD	2.63	0.42
1:f:121:LEU:HD22	1:f:306:ILE:HD12	2.01	0.42
2:C:321:ASN:O	2:C:325:ARG:HG3	2.20	0.42
3:D:299:PHE:HE2	3:D:305:VAL:HB	1.84	0.42
4:V:482:PHE:O	4:V:486:ILE:HG12	2.20	0.42
5:W:316:ARG:O	5:W:319:THR:OG1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:239:TYR:CZ	6:X:246:LYS:HD2	2.54	0.42
10:b:7:MET:HA	10:b:7:MET:HE2	2.01	0.42
11:d:94:MET:HE3	11:d:94:MET:HB3	1.79	0.42
14:U:138:PHE:CE2	14:U:162:VAL:HG11	2.54	0.42
14:U:373:ASN:ND2	14:U:385:PHE:HB3	2.34	0.42
16:A:235:ALA:HB1	16:A:269:ALA:O	2.20	0.42
18:E:118:LEU:HD23	18:E:118:LEU:HA	1.86	0.42
19:F:314:LEU:HD21	19:F:342:LEU:HG	2.01	0.42
3:D:189:GLU:O	3:D:192:LYS:HG3	2.19	0.42
5:W:112:VAL:HA	5:W:115:ILE:HG22	2.02	0.42
6:X:50:ILE:HA	6:X:53:LEU:HG	2.01	0.42
6:X:394:ASP:OD2	7:Y:362:LYS:NZ	2.53	0.42
9:a:65:SER:HA	9:a:69:HIS:HB3	2.02	0.42
9:a:68:GLU:OE1	9:a:71:VAL:HG23	2.19	0.42
9:a:156:TYR:HB3	9:a:179:PHE:HB2	2.02	0.42
9:a:292:THR:HG23	9:a:295:GLU:H	1.83	0.42
10:b:38:HIS:HB3	10:b:42:ARG:NH2	2.35	0.42
14:U:325:MET:HE1	14:U:328:ILE:HD12	2.01	0.42
15:c:70:ILE:HD11	15:c:106:GLU:HB2	2.02	0.42
17:B:410:ARG:HG3	17:B:410:ARG:O	2.20	0.42
18:E:121:ASN:O	18:E:125:GLU:HB2	2.19	0.42
18:E:219:PHE:HZ	18:E:264:MET:CE	2.33	0.42
2:C:90:HIS:CG	3:D:109:SER:HB2	2.55	0.41
2:C:190:GLY:O	2:C:296:ASN:HB3	2.20	0.41
2:C:340:ARG:HB3	7:Y:207:THR:OG1	2.19	0.41
2:C:370:ALA:HB2	2:C:378:VAL:HG13	2.01	0.41
3:D:81:ARG:NH1	15:c:149:GLN:HG2	2.35	0.41
4:V:110:HIS:HA	4:V:113:LEU:HG	2.01	0.41
4:V:314:ARG:NH1	7:Y:378:ASN:ND2	2.68	0.41
5:W:63:THR:O	5:W:67:LEU:HD13	2.20	0.41
5:W:193:CYS:O	5:W:196:VAL:HG22	2.20	0.41
15:c:50:PRO:HB3	18:E:104:THR:HG21	2.01	0.41
16:A:244:GLU:HG2	17:B:268:ARG:NH1	2.34	0.41
17:B:232:LYS:HZ3	22:B:501:ATP:PB	2.39	0.41
2:C:196:LYS:HG2	2:C:317:PHE:CD2	2.56	0.41
2:C:307:ARG:HG3	2:C:310:ARG:HH21	1.85	0.41
3:D:262:ILE:HB	3:D:307:VAL:HG12	2.02	0.41
4:V:173:ILE:HA	4:V:176:MET:HE3	2.02	0.41
4:V:416:ARG:HG3	4:V:457:TYR:CD2	2.54	0.41
5:W:68:VAL:HA	5:W:71:VAL:HG12	2.01	0.41
6:X:90:ARG:HD2	6:X:93:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:272:LEU:O	8:Z:276:ILE:HG12	2.19	0.41
9:a:105:LYS:HD3	9:a:105:LYS:HA	1.81	0.41
11:d:196:LEU:HB3	11:d:208:PHE:HE1	1.85	0.41
11:d:221:GLN:NE2	11:d:222:THR:HG23	2.35	0.41
11:d:240:SER:OG	11:d:243:LYS:HD2	2.19	0.41
11:d:241:TYR:CD2	11:d:271:ILE:HG22	2.56	0.41
14:U:122:GLU:O	14:U:122:GLU:HG2	2.20	0.41
16:A:355:PHE:CE2	16:A:374:ALA:HA	2.55	0.41
19:F:153:VAL:HG12	19:F:160:ILE:HA	2.00	0.41
1:f:139:LEU:HD12	1:f:139:LEU:HA	1.94	0.41
2:C:232:ARG:HD3	2:C:279:GLN:HG2	2.03	0.41
2:C:236:VAL:O	2:C:239:ARG:HG2	2.19	0.41
2:C:340:ARG:CZ	7:Y:204:THR:HG23	2.50	0.41
3:D:293:LEU:HG	3:D:326:ARG:NE	2.35	0.41
3:D:338:ARG:HH21	3:D:341:LYS:HE3	1.83	0.41
5:W:89:LEU:O	5:W:93:ARG:NH1	2.53	0.41
6:X:148:HIS:CE1	6:X:149:LEU:HG	2.55	0.41
14:U:227:GLN:OE1	14:U:267:ASN:ND2	2.50	0.41
17:B:223:ILE:HD12	17:B:347:ILE:HG21	2.02	0.41
18:E:360:ASP:OD1	18:E:360:ASP:N	2.52	0.41
19:F:137:ILE:HD13	19:F:142:ALA:HB2	2.01	0.41
19:F:180:ARG:HH12	19:F:246:ALA:N	2.18	0.41
19:F:225:MET:HE1	19:F:352:ILE:HD13	2.02	0.41
2:C:90:HIS:HB3	2:C:91:PRO:CD	2.43	0.41
3:D:157:ASP:OD1	3:D:158:GLN:N	2.53	0.41
3:D:278:GLN:OE1	3:D:278:GLN:N	2.52	0.41
4:V:78:HIS:O	4:V:81:GLN:HG2	2.21	0.41
4:V:443:ARG:HD3	11:d:274:CYS:SG	2.60	0.41
6:X:222:GLU:HG2	6:X:224:ASP:N	2.29	0.41
8:Z:256:GLN:HB3	15:c:295:ASN:ND2	2.36	0.41
9:a:21:VAL:HG21	9:a:44:PHE:CE1	2.55	0.41
9:a:356:TRP:CD1	9:a:356:TRP:C	2.98	0.41
11:d:228:HIS:CD2	11:d:252:PRO:HD3	2.54	0.41
15:c:261:GLU:O	15:c:262:GLU:HB2	2.20	0.41
15:c:303:MET:HE3	15:c:303:MET:HB3	1.92	0.41
16:A:206:ILE:CD1	19:F:404:GLY:HA3	2.50	0.41
17:B:114:GLU:O	17:B:121:ALA:HB1	2.20	0.41
17:B:155:LYS:HG3	17:B:156:VAL:HG22	2.01	0.41
18:E:309:ARG:HE	18:E:332:VAL:HG13	1.85	0.41
18:E:387:LYS:HE2	18:E:387:LYS:HA	2.01	0.41
19:F:87:PRO:HB2	19:F:155:LYS:HZ2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:31:LEU:HD12	3:D:44:TYR:CE1	2.55	0.41
2:C:169:VAL:HG23	2:C:290:LYS:NZ	2.36	0.41
5:W:374:THR:HG22	5:W:411:GLY:O	2.20	0.41
7:Y:162:GLU:HA	7:Y:165:LYS:HG2	2.03	0.41
10:b:12:ASN:OD1	10:b:12:ASN:O	2.38	0.41
11:d:119:LEU:HD21	11:d:147:ILE:CG2	2.50	0.41
11:d:337:LYS:O	11:d:340:ILE:HG22	2.21	0.41
14:U:167:ILE:HG21	14:U:204:ILE:HG12	2.02	0.41
14:U:579:ARG:NH1	14:U:609:ASP:OD1	2.53	0.41
15:c:32:TYR:HD2	15:c:208:ARG:HB2	1.85	0.41
16:A:208:PRO:O	16:A:210:LYS:NZ	2.51	0.41
18:E:75:ASN:HA	19:F:129:ARG:CZ	2.50	0.41
18:E:130:VAL:H	18:E:189:SER:CB	2.33	0.41
18:E:297:ARG:C	18:E:298:LYS:HD3	2.45	0.41
2:C:196:LYS:H	21:C:501:ADP:PA	2.44	0.41
2:C:380:GLN:HA	2:C:383:PHE:CD2	2.55	0.41
3:D:279:THR:HG23	3:D:282:ASP:H	1.85	0.41
4:V:180:ARG:NH2	4:V:183:GLU:OE1	2.54	0.41
7:Y:221:THR:HG22	7:Y:225:TYR:CE2	2.56	0.41
7:Y:319:MET:HG2	7:Y:330:ILE:HD13	2.03	0.41
8:Z:10:VAL:HG12	8:Z:161:GLU:HG2	2.02	0.41
8:Z:205:LEU:HB3	9:a:357:CYS:SG	2.61	0.41
8:Z:263:ALA:HA	8:Z:266:ILE:HG22	2.03	0.41
10:b:106:LYS:C	10:b:107:MET:HE2	2.45	0.41
11:d:342:TYR:O	11:d:346:LEU:HD23	2.21	0.41
14:U:587:ALA:HB2	14:U:621:SER:OG	2.21	0.41
16:A:200:ARG:HA	16:A:203:ASN:HD22	1.85	0.41
16:A:273:PHE:CZ	16:A:275:ASP:HB3	2.55	0.41
17:B:335:GLU:OE1	17:B:335:GLU:N	2.45	0.41
1:f:139:LEU:HG	1:f:141:LEU:CD2	2.49	0.41
1:f:139:LEU:HD23	1:f:154:LEU:HD12	2.02	0.41
1:f:156:LEU:HD23	1:f:157:ALA:N	2.35	0.41
2:C:113:ARG:HB3	2:C:127:LEU:HB2	2.02	0.41
4:V:163:VAL:O	4:V:167:LEU:HG	2.21	0.41
4:V:190:ASP:O	4:V:194:LYS:HG2	2.20	0.41
4:V:266:GLN:NE2	14:U:36:ALA:HB3	2.35	0.41
4:V:392:TYR:O	4:V:395:ILE:HG22	2.21	0.41
5:W:366:MET:HE1	5:W:415:PHE:CZ	2.56	0.41
5:W:373:ILE:HG13	5:W:374:THR:O	2.20	0.41
6:X:63:ALA:HA	6:X:66:LEU:HD12	2.02	0.41
6:X:156:GLU:O	6:X:160:MET:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:105:MET:HA	7:Y:108:ALA:HB3	2.02	0.41
8:Z:38:VAL:O	8:Z:53:SER:OG	2.27	0.41
9:a:71:VAL:HG13	10:b:14:GLU:OE2	2.21	0.41
9:a:344:GLN:HA	9:a:347:LYS:HG2	2.02	0.41
11:d:170:GLN:NE2	14:U:11:LEU:HG	2.35	0.41
14:U:35:TRP:HE3	14:U:35:TRP:H	1.67	0.41
17:B:162:VAL:HG22	17:B:163:LEU:N	2.36	0.41
17:B:396:LYS:O	17:B:400:THR:HG22	2.20	0.41
19:F:153:VAL:HG12	19:F:160:ILE:HG22	2.03	0.41
1:f:107:MET:SD	1:f:107:MET:N	2.94	0.41
3:D:172:ILE:HG13	3:D:173:GLN:N	2.35	0.41
4:V:99:ARG:HH22	12:e:17:ASP:HB2	1.85	0.41
5:W:78:LYS:HE3	5:W:78:LYS:HB3	1.97	0.41
5:W:293:ASP:HB3	5:W:296:LEU:HB2	2.02	0.41
6:X:260:MET:C	6:X:262:ASN:H	2.29	0.41
6:X:344:ARG:HG2	6:X:386:ILE:HG13	2.02	0.41
7:Y:201:PHE:CD2	7:Y:226:VAL:HG11	2.55	0.41
7:Y:229:ILE:HD12	7:Y:295:TYR:HD1	1.86	0.41
7:Y:293:ARG:O	7:Y:294:TYR:C	2.64	0.41
8:Z:256:GLN:HB3	15:c:295:ASN:OD1	2.21	0.41
9:a:59:LEU:O	9:a:62:ASN:HB2	2.21	0.41
11:d:190:GLN:HB2	11:d:225:TYR:CD2	2.56	0.41
14:U:248:ILE:O	14:U:252:LEU:HG	2.20	0.41
14:U:527:GLN:OE1	14:U:527:GLN:N	2.43	0.41
14:U:535:TYR:CE2	14:U:544:ILE:HG21	2.51	0.41
14:U:712:LEU:HD13	14:U:715:LYS:HD2	2.01	0.41
14:U:764:LEU:O	14:U:767:THR:OG1	2.37	0.41
15:c:49:VAL:HA	15:c:50:PRO:HA	1.94	0.41
16:A:97:ARG:HH12	16:A:144:ARG:CB	2.34	0.41
17:B:406:ALA:HB2	17:B:414:VAL:HG23	2.03	0.41
19:F:141:ASP:N	19:F:141:ASP:OD1	2.54	0.41
20:w:35:GLY:C	20:w:36:ARG:HD2	2.45	0.41
1:f:140:THR:HA	1:f:152:VAL:O	2.21	0.41
1:f:155:GLN:O	20:w:34:THR:OG1	2.25	0.41
1:f:264:LYS:O	1:f:266:GLY:N	2.50	0.41
1:f:298:ARG:HE	1:f:301:ARG:HE	1.69	0.41
2:C:188:LEU:HD23	2:C:317:PHE:CZ	2.55	0.41
2:C:218:GLU:HA	2:C:221:GLN:CG	2.51	0.41
3:D:91:GLN:N	3:D:104:GLY:O	2.40	0.41
3:D:177:VAL:HG11	3:D:215:LEU:CD2	2.50	0.41
4:V:281:ASN:ND2	4:V:284:GLU:OE2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:368:MET:HG3	6:X:374:PHE:CE1	2.56	0.41
7:Y:311:TYR:CD2	7:Y:314:LEU:HD21	2.56	0.41
8:Z:39:LEU:HD11	8:Z:95:TYR:HB3	2.03	0.41
8:Z:141:VAL:O	8:Z:153:LYS:HD2	2.21	0.41
8:Z:149:THR:HG21	9:a:181:GLY:HA3	2.03	0.41
8:Z:190:ARG:NH2	9:a:367:VAL:HG22	2.35	0.41
9:a:35:HIS:CE1	10:b:14:GLU:O	2.70	0.41
9:a:112:ILE:HD12	9:a:112:ILE:H	1.86	0.41
11:d:185:SER:OG	11:d:186:ALA:N	2.54	0.41
12:e:38:VAL:O	12:e:38:VAL:HG12	2.21	0.41
14:U:24:LEU:HD21	14:U:60:ALA:N	2.36	0.41
14:U:64:ALA:HA	14:U:67:VAL:HG22	2.02	0.41
14:U:95:GLU:OE2	14:U:95:GLU:N	2.54	0.41
14:U:208:LEU:O	14:U:211:PRO:HD3	2.20	0.41
14:U:416:GLU:CD	14:U:453:HIS:HD1	2.28	0.41
14:U:712:LEU:O	14:U:716:VAL:HG22	2.20	0.41
15:c:30:GLN:HE22	15:c:204:THR:HB	1.84	0.41
16:A:101:ILE:HG13	16:A:112:ILE:O	2.21	0.41
16:A:101:ILE:HG23	16:A:137:GLY:H	1.86	0.41
16:A:251:GLY:N	16:A:294:GLU:OE2	2.46	0.41
17:B:105:THR:OG1	17:B:106:PRO:HD3	2.21	0.41
17:B:120:HIS:CB	17:B:134:SER:HA	2.49	0.41
17:B:235:LEU:O	17:B:239:VAL:HG23	2.21	0.41
17:B:382:ASP:HA	17:B:385:MET:SD	2.61	0.41
19:F:180:ARG:NH2	19:F:244:THR:O	2.54	0.41
1:f:121:LEU:O	1:f:124:LEU:HB2	2.21	0.41
1:f:141:LEU:HD12	1:f:143:LEU:HD21	2.03	0.41
2:C:148:TYR:OH	2:C:203:VAL:HG22	2.21	0.41
2:C:340:ARG:NH2	7:Y:207:THR:O	2.51	0.41
3:D:163:MET:HA	3:D:222:HIS:CE1	2.54	0.41
4:V:117:VAL:HB	4:V:135:LEU:HD11	2.03	0.41
4:V:292:THR:O	4:V:295:ILE:HG12	2.20	0.41
4:V:335:VAL:O	4:V:339:LEU:HD12	2.21	0.41
5:W:166:LEU:HD23	5:W:166:LEU:HA	1.85	0.41
7:Y:101:ARG:NH2	7:Y:130:LYS:HG3	2.34	0.41
7:Y:262:SER:HA	7:Y:267:ARG:HG2	2.02	0.41
7:Y:293:ARG:HA	7:Y:293:ARG:HD3	1.72	0.41
7:Y:364:TRP:O	7:Y:368:GLU:OE1	2.39	0.41
8:Z:224:HIS:HB3	8:Z:228:TYR:HE2	1.86	0.41
9:a:35:HIS:NE2	10:b:17:ARG:HB2	2.36	0.41
9:a:111:VAL:O	9:a:115:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:d:212:LEU:HD21	11:d:230:VAL:HG12	2.02	0.41
11:d:291:LEU:O	11:d:292:PHE:HB2	2.21	0.41
14:U:62:LEU:O	14:U:65:SER:OG	2.32	0.41
14:U:682:TYR:HA	14:U:685:GLN:CG	2.51	0.41
17:B:232:LYS:HB2	22:B:501:ATP:O1B	2.21	0.41
17:B:234:LEU:HD11	22:B:501:ATP:H2'	2.02	0.41
18:E:308:ALA:O	18:E:312:ILE:HG13	2.21	0.41
2:C:338:LEU:HA	2:C:378:VAL:HG23	2.02	0.40
3:D:66:LYS:NZ	3:D:66:LYS:O	2.51	0.40
4:V:294:ARG:NH1	4:V:298:ILE:HD11	2.36	0.40
5:W:353:ASP:O	5:W:357:ARG:HG2	2.21	0.40
5:W:405:LYS:HG3	6:X:343:SER:HB3	2.03	0.40
6:X:138:PHE:CE1	6:X:176:THR:HA	2.56	0.40
7:Y:153:ASP:O	7:Y:157:ILE:HG12	2.21	0.40
8:Z:74:TYR:CE2	15:c:98:MET:SD	3.14	0.40
9:a:291:LEU:HB2	9:a:331:VAL:CG1	2.51	0.40
9:a:356:TRP:O	9:a:356:TRP:HD1	2.04	0.40
14:U:583:MET:HE2	14:U:617:ALA:C	2.45	0.40
14:U:759:SER:O	14:U:763:VAL:HG12	2.21	0.40
15:c:107:MET:HG2	15:c:108:VAL:H	1.85	0.40
15:c:225:TRP:NE1	15:c:226:MET:SD	2.94	0.40
16:A:101:ILE:HD11	16:A:111:TYR:HB3	2.03	0.40
17:B:290:ILE:HG22	17:B:305:ILE:HG23	2.03	0.40
18:E:152:PRO:HB3	18:E:166:PRO:HG3	2.03	0.40
18:E:322:LYS:HE3	18:E:326:ILE:HD11	2.03	0.40
19:F:185:TYR:H	19:F:243:GLN:NE2	2.19	0.40
1:f:143:LEU:C	1:f:150:MET:HG2	2.47	0.40
2:C:201:ARG:NH1	2:C:201:ARG:O	2.55	0.40
3:D:276:ASP:O	3:D:282:ASP:HB2	2.21	0.40
4:V:89:LYS:O	4:V:89:LYS:HG2	2.20	0.40
6:X:303:GLU:HA	6:X:306:LEU:HG	2.03	0.40
7:Y:34:ASP:OD1	7:Y:34:ASP:N	2.51	0.40
8:Z:48:LEU:HD11	8:Z:92:VAL:HG11	2.02	0.40
8:Z:219:LYS:O	8:Z:220:LEU:HD23	2.21	0.40
9:a:82:HIS:HE1	9:a:85:ARG:HH21	1.68	0.40
9:a:130:VAL:O	9:a:134:THR:OG1	2.33	0.40
9:a:275:LEU:O	9:a:278:MET:HB2	2.20	0.40
11:d:227:LYS:HD3	11:d:227:LYS:C	2.46	0.40
12:e:27:TRP:CD1	12:e:27:TRP:H	2.40	0.40
14:U:583:MET:HE1	14:U:584:TYR:CE1	2.56	0.40
16:A:274:PHE:HB3	16:A:277:ILE:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:305:ILE:HG22	17:B:309:MET:CE	2.50	0.40
2:C:271:ARG:O	2:C:275:GLU:HG3	2.20	0.40
3:D:81:ARG:NH1	15:c:149:GLN:HA	2.36	0.40
3:D:358:VAL:HG11	3:D:399:PHE:HE2	1.86	0.40
3:D:387:VAL:HG11	18:E:159:PHE:HE1	1.86	0.40
4:V:167:LEU:HD23	4:V:167:LEU:HA	1.90	0.40
4:V:392:TYR:O	4:V:396:ILE:HG12	2.20	0.40
4:V:442:ILE:HD11	11:d:278:ALA:HB2	2.03	0.40
6:X:363:ARG:NH1	6:X:367:GLN:HB2	2.36	0.40
7:Y:374:ASP:O	7:Y:377:LEU:HG	2.21	0.40
8:Z:38:VAL:HA	8:Z:94:TRP:HA	2.03	0.40
9:a:39:LEU:HA	9:a:42:LEU:HD12	2.03	0.40
9:a:342:ASP:OD1	9:a:343:LEU:N	2.55	0.40
14:U:204:ILE:HA	14:U:207:ASN:OD1	2.21	0.40
14:U:405:THR:HA	14:U:408:LEU:HD13	2.03	0.40
15:c:238:CYS:O	15:c:242:GLU:HG2	2.20	0.40
16:A:272:ILE:H	16:A:315:ILE:HD11	1.86	0.40
2:C:78:ARG:HB3	2:C:80:MET:HE3	2.04	0.40
2:C:212:ILE:O	2:C:246:ILE:HD12	2.21	0.40
2:C:307:ARG:HH21	17:B:229:GLY:HA3	1.86	0.40
3:D:96:VAL:HG11	3:D:112:TYR:HE1	1.87	0.40
4:V:117:VAL:O	4:V:121:PHE:HB2	2.22	0.40
4:V:453:HIS:ND1	11:d:284:PHE:HA	2.36	0.40
5:W:127:THR:O	5:W:130:MET:HG3	2.22	0.40
5:W:179:LYS:HB3	5:W:213:PHE:CE1	2.57	0.40
5:W:372:ARG:NH2	9:a:325:ASP:HB3	2.37	0.40
5:W:408:ARG:HH11	5:W:408:ARG:C	2.29	0.40
6:X:368:MET:HA	6:X:373:LYS:HG3	2.03	0.40
7:Y:276:ALA:O	7:Y:280:GLN:HG2	2.22	0.40
8:Z:25:ARG:HD3	15:c:104:ARG:NH2	2.36	0.40
9:a:126:GLY:HA3	9:a:129:GLN:NE2	2.31	0.40
9:a:276:CYS:SG	9:a:280:MET:HE1	2.62	0.40
11:d:184:GLU:OE2	11:d:184:GLU:N	2.54	0.40
14:U:31:VAL:HG11	14:U:66:LYS:HE2	2.04	0.40
14:U:707:ASN:HA	14:U:710:ARG:HE	1.86	0.40
16:A:284:ARG:O	19:F:334:ARG:NH1	2.55	0.40
16:A:309:PHE:O	19:F:238:ARG:HD3	2.21	0.40
17:B:391:SER:O	17:B:395:ILE:HG12	2.20	0.40
18:E:102:MET:HE2	19:F:132:TYR:HE2	1.86	0.40
2:C:63:LEU:O	2:C:67:GLN:NE2	2.53	0.40
2:C:169:VAL:HG23	2:C:290:LYS:HZ3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:394:LEU:HG	4:V:397:ARG:NH2	2.37	0.40
6:X:111:LEU:HA	6:X:114:ILE:HG22	2.03	0.40
6:X:252:LYS:HZ1	6:X:283:GLN:C	2.30	0.40
7:Y:271:PHE:HZ	7:Y:299:MET:HE3	1.86	0.40
8:Z:169:GLU:O	8:Z:172:VAL:HG12	2.21	0.40
9:a:70:ARG:O	9:a:71:VAL:C	2.65	0.40
9:a:193:GLN:H	9:a:193:GLN:HG2	1.74	0.40
11:d:279:TYR:CD2	11:d:284:PHE:HB3	2.57	0.40
14:U:519:VAL:HG12	14:U:520:MET:CE	2.51	0.40
14:U:568:GLU:HG3	14:U:601:ARG:HH12	1.87	0.40
15:c:103:GLY:O	15:c:105:PRO:HD3	2.21	0.40
16:A:121:PHE:HE2	19:F:89:LEU:HD13	1.86	0.40
18:E:48:LYS:HD2	18:E:48:LYS:HA	1.89	0.40
18:E:173:TYR:CZ	18:E:300:HIS:HB2	2.56	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	f	192/856 (22%)	173 (90%)	19 (10%)	0	100	100
2	C	360/406 (89%)	334 (93%)	25 (7%)	1 (0%)	36	71
3	D	378/418 (90%)	351 (93%)	26 (7%)	1 (0%)	36	71
4	V	440/534 (82%)	414 (94%)	25 (6%)	1 (0%)	43	77
5	W	438/456 (96%)	416 (95%)	22 (5%)	0	100	100
6	X	382/422 (90%)	364 (95%)	17 (4%)	1 (0%)	36	71
7	Y	372/389 (96%)	348 (94%)	23 (6%)	1 (0%)	36	71
8	Z	284/324 (88%)	273 (96%)	10 (4%)	1 (0%)	30	66
9	a	371/376 (99%)	338 (91%)	31 (8%)	2 (0%)	24	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	b	189/377 (50%)	168 (89%)	19 (10%)	2 (1%)	11	45
11	d	268/350 (77%)	248 (92%)	18 (7%)	2 (1%)	18	55
12	e	46/70 (66%)	35 (76%)	11 (24%)	0	100	100
14	U	812/953 (85%)	771 (95%)	41 (5%)	0	100	100
15	c	291/590 (49%)	279 (96%)	11 (4%)	1 (0%)	36	71
16	A	364/433 (84%)	330 (91%)	33 (9%)	1 (0%)	36	71
17	B	338/440 (77%)	310 (92%)	26 (8%)	2 (1%)	21	58
18	E	345/389 (89%)	318 (92%)	27 (8%)	0	100	100
19	F	370/439 (84%)	344 (93%)	25 (7%)	1 (0%)	36	71
20	w	15/337 (4%)	13 (87%)	2 (13%)	0	100	100
All	All	6255/8559 (73%)	5827 (93%)	411 (7%)	17 (0%)	37	71

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	Y	98	SER
8	Z	149	THR
15	c	262	GLU
16	A	82	ALA
17	B	117	ASP
2	C	90	HIS
11	d	283	LEU
17	B	191	ASP
3	D	368	ASP
11	d	282	ILE
4	V	469	THR
6	X	123	THR
10	b	22	LEU
19	F	300	LYS
10	b	24	THR
9	a	71	VAL
9	a	19	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	f	165/690 (24%)	165 (100%)	0	100	100
2	C	315/352 (90%)	314 (100%)	1 (0%)	86	84
3	D	332/366 (91%)	332 (100%)	0	100	100
4	V	388/460 (84%)	387 (100%)	1 (0%)	86	84
5	W	404/416 (97%)	404 (100%)	0	100	100
6	X	330/362 (91%)	330 (100%)	0	100	100
7	Y	333/344 (97%)	333 (100%)	0	100	100
8	Z	257/295 (87%)	256 (100%)	1 (0%)	84	82
9	a	333/336 (99%)	333 (100%)	0	100	100
10	b	167/312 (54%)	167 (100%)	0	100	100
11	d	237/294 (81%)	237 (100%)	0	100	100
12	e	43/63 (68%)	43 (100%)	0	100	100
14	U	695/816 (85%)	695 (100%)	0	100	100
15	c	257/500 (51%)	257 (100%)	0	100	100
16	A	310/372 (83%)	309 (100%)	1 (0%)	86	84
17	B	296/385 (77%)	295 (100%)	1 (0%)	86	84
18	E	298/341 (87%)	298 (100%)	0	100	100
19	F	316/379 (83%)	315 (100%)	1 (0%)	86	84
20	w	15/289 (5%)	15 (100%)	0	100	100
All	All	5491/7372 (74%)	5485 (100%)	6 (0%)	87	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	109	THR
4	V	469	THR
8	Z	169	GLU
16	A	403	ILE
17	B	125	THR
19	F	416	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	f	36	HIS
1	f	291	ASN
2	C	32	GLN
2	C	50	ASN
2	C	53	ASN
2	C	90	HIS
2	C	106	ASN
2	C	171	HIS
2	C	241	HIS
2	C	392	GLN
3	D	48	GLN
3	D	65	GLN
3	D	173	GLN
3	D	221	HIS
3	D	222	HIS
3	D	301	GLN
3	D	312	ASN
3	D	376	ASN
4	V	193	GLN
4	V	198	GLN
4	V	247	GLN
4	V	260	HIS
4	V	283	ASN
4	V	299	GLN
4	V	318	GLN
4	V	347	GLN
4	V	377	GLN
4	V	459	GLN
4	V	488	ASN
5	W	84	ASN
5	W	107	GLN
5	W	236	HIS
5	W	246	HIS
5	W	416	GLN
6	X	178	HIS
6	X	207	GLN
6	X	322	HIS
6	X	367	GLN
7	Y	14	ASN
7	Y	31	HIS
7	Y	154	ASN
7	Y	160	ASN
7	Y	184	GLN

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Mol	Chain	Res	Type
7	Y	306	GLN
7	Y	367	GLN
7	Y	378	ASN
8	Z	22	HIS
8	Z	32	GLN
8	Z	109	ASN
8	Z	157	HIS
8	Z	273	HIS
9	a	40	GLN
9	a	62	ASN
9	a	69	HIS
9	a	86	GLN
9	a	124	ASN
9	a	143	ASN
9	a	164	GLN
9	a	219	HIS
9	a	244	ASN
9	a	288	HIS
9	a	290	GLN
10	b	30	GLN
10	b	137	ASN
11	d	89	GLN
11	d	97	GLN
11	d	153	GLN
11	d	170	GLN
11	d	181	GLN
11	d	221	GLN
11	d	338	GLN
12	e	63	HIS
14	U	58	GLN
14	U	107	HIS
14	U	189	GLN
14	U	192	GLN
14	U	195	ASN
14	U	267	ASN
14	U	340	GLN
14	U	362	ASN
14	U	389	ASN
14	U	438	GLN
14	U	595	ASN
14	U	685	GLN
14	U	756	HIS

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Mol	Chain	Res	Type
14	U	901	GLN
15	c	30	GLN
15	c	92	GLN
15	c	113	HIS
15	c	128	ASN
15	c	149	GLN
15	c	185	ASN
15	c	199	HIS
15	c	214	GLN
15	c	221	HIS
15	c	256	ASN
15	c	269	GLN
15	c	274	ASN
15	c	283	HIS
15	c	298	GLN
16	A	85	GLN
16	A	91	GLN
16	A	203	ASN
16	A	358	HIS
16	A	433	ASN
17	B	120	HIS
18	E	190	GLN
18	E	220	ASN
18	E	280	ASN
19	F	76	ASN
19	F	83	ASN
19	F	116	GLN
19	F	196	GLN
19	F	208	HIS
19	F	243	GLN
19	F	307	GLN
19	F	315	ASN
19	F	417	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	ATP	A	501	-	32,33,33	0.27	0	48,52,52	0.34	0
22	ATP	B	501	24	32,33,33	0.35	0	48,52,52	0.35	0
22	ATP	E	401	24	32,33,33	0.34	0	48,52,52	0.28	0
22	ATP	D	501	-	32,33,33	0.34	0	48,52,52	0.40	0
21	ADP	F	501	24	28,29,29	1.39	4 (14%)	43,45,45	1.94	8 (18%)
21	ADP	C	501	-	28,29,29	0.47	0	43,45,45	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	ATP	A	501	-	-	4/22/38/38	0/3/3/3
22	ATP	B	501	24	-	6/22/38/38	0/3/3/3
22	ATP	E	401	24	-	6/22/38/38	0/3/3/3
22	ATP	D	501	-	-	7/22/38/38	0/3/3/3
21	ADP	F	501	24	-	3/16/32/32	0/3/3/3
21	ADP	C	501	-	-	3/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	F	501	ADP	C5-C4	4.64	1.47	1.39
21	F	501	ADP	C5-C6	2.67	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	F	501	ADP	C5-N7	-2.34	1.34	1.39
21	F	501	ADP	C8-N7	2.17	1.35	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	F	501	ADP	C5-C4-N3	-6.33	118.00	126.72
21	F	501	ADP	N3-C4-N9	5.21	136.03	127.17
21	F	501	ADP	C2-N3-C4	3.95	121.47	111.83
21	F	501	ADP	C4-C5-N7	-3.34	106.76	110.58
21	F	501	ADP	N3-C2-N1	-3.34	123.53	128.58
21	F	501	ADP	C4-N9-C8	2.71	108.58	105.74
21	F	501	ADP	C5-N7-C8	2.62	107.57	103.45
21	F	501	ADP	C3'-C2'-C1'	2.56	106.30	101.46

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	F	501	ADP	C5'-O5'-PA-O1A
21	F	501	ADP	C5'-O5'-PA-O2A
21	F	501	ADP	C5'-O5'-PA-O3A
22	D	501	ATP	PB-O3B-PG-O2G
22	D	501	ATP	C5'-O5'-PA-O1A
22	D	501	ATP	C5'-O5'-PA-O3A
22	D	501	ATP	O4'-C4'-C5'-O5'
22	B	501	ATP	C5'-O5'-PA-O3A
22	E	401	ATP	PB-O3B-PG-O2G
22	E	401	ATP	C5'-O5'-PA-O1A
22	D	501	ATP	C3'-C4'-C5'-O5'
21	C	501	ADP	C3'-C4'-C5'-O5'
22	E	401	ATP	C3'-C4'-C5'-O5'
21	C	501	ADP	O4'-C4'-C5'-O5'
22	E	401	ATP	O4'-C4'-C5'-O5'
22	D	501	ATP	PB-O3B-PG-O1G
21	C	501	ADP	C5'-O5'-PA-O1A
22	D	501	ATP	C5'-O5'-PA-O2A
22	B	501	ATP	C5'-O5'-PA-O1A
22	E	401	ATP	C5'-O5'-PA-O3A
22	B	501	ATP	PB-O3A-PA-O2A
22	B	501	ATP	C4'-C5'-O5'-PA
22	E	401	ATP	PB-O3B-PG-O1G

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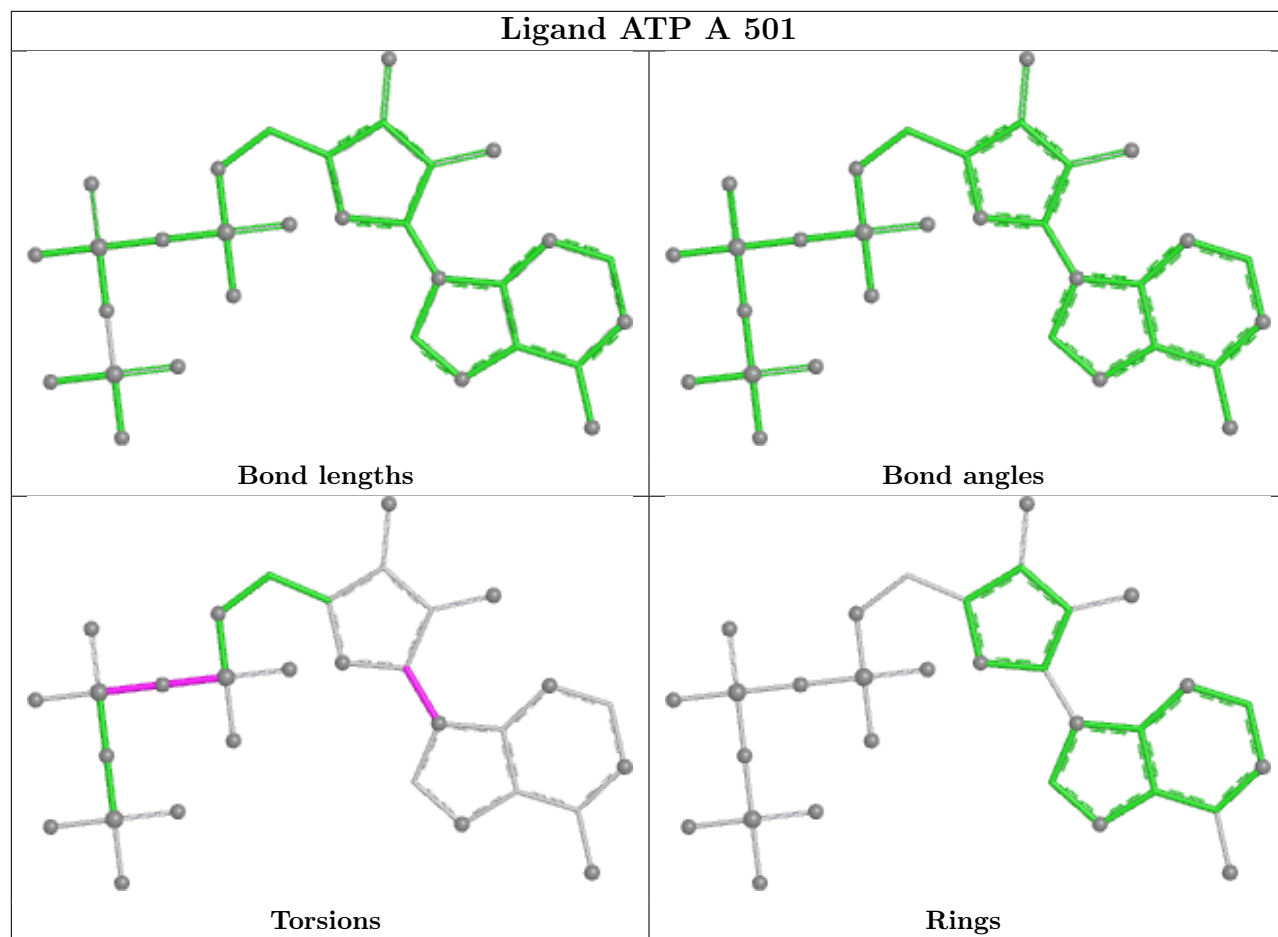
Mol	Chain	Res	Type	Atoms
22	A	501	ATP	PA-O3A-PB-O1B
22	A	501	ATP	PA-O3A-PB-O2B
22	B	501	ATP	PB-O3A-PA-O1A
22	A	501	ATP	C2'-C1'-N9-C8
22	A	501	ATP	PB-O3A-PA-O2A
22	B	501	ATP	PG-O3B-PB-O2B

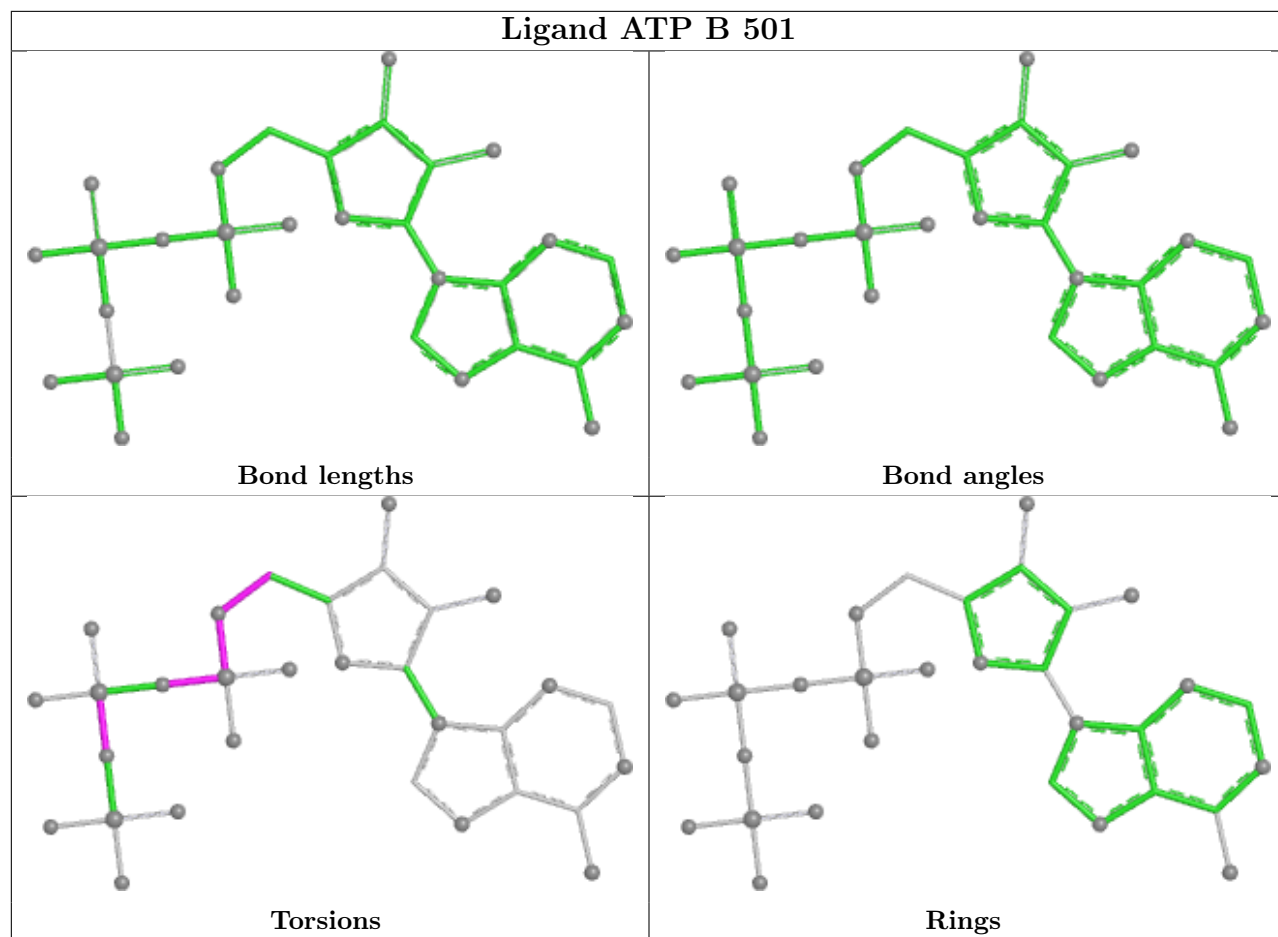
There are no ring outliers.

6 monomers are involved in 30 short contacts:

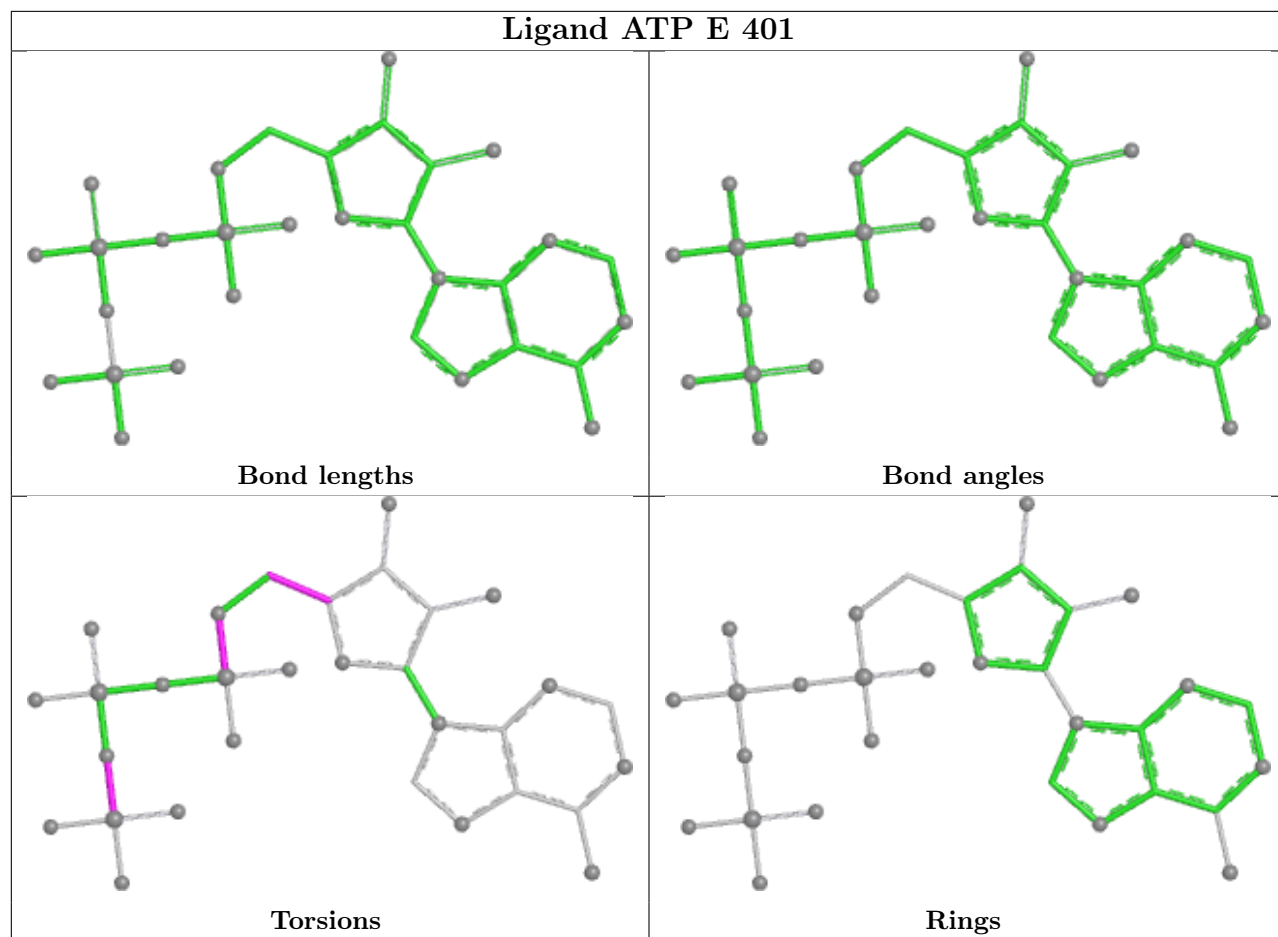
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	501	ATP	4	0
22	B	501	ATP	6	0
22	E	401	ATP	1	0
22	D	501	ATP	9	0
21	F	501	ADP	3	0
21	C	501	ADP	7	0

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

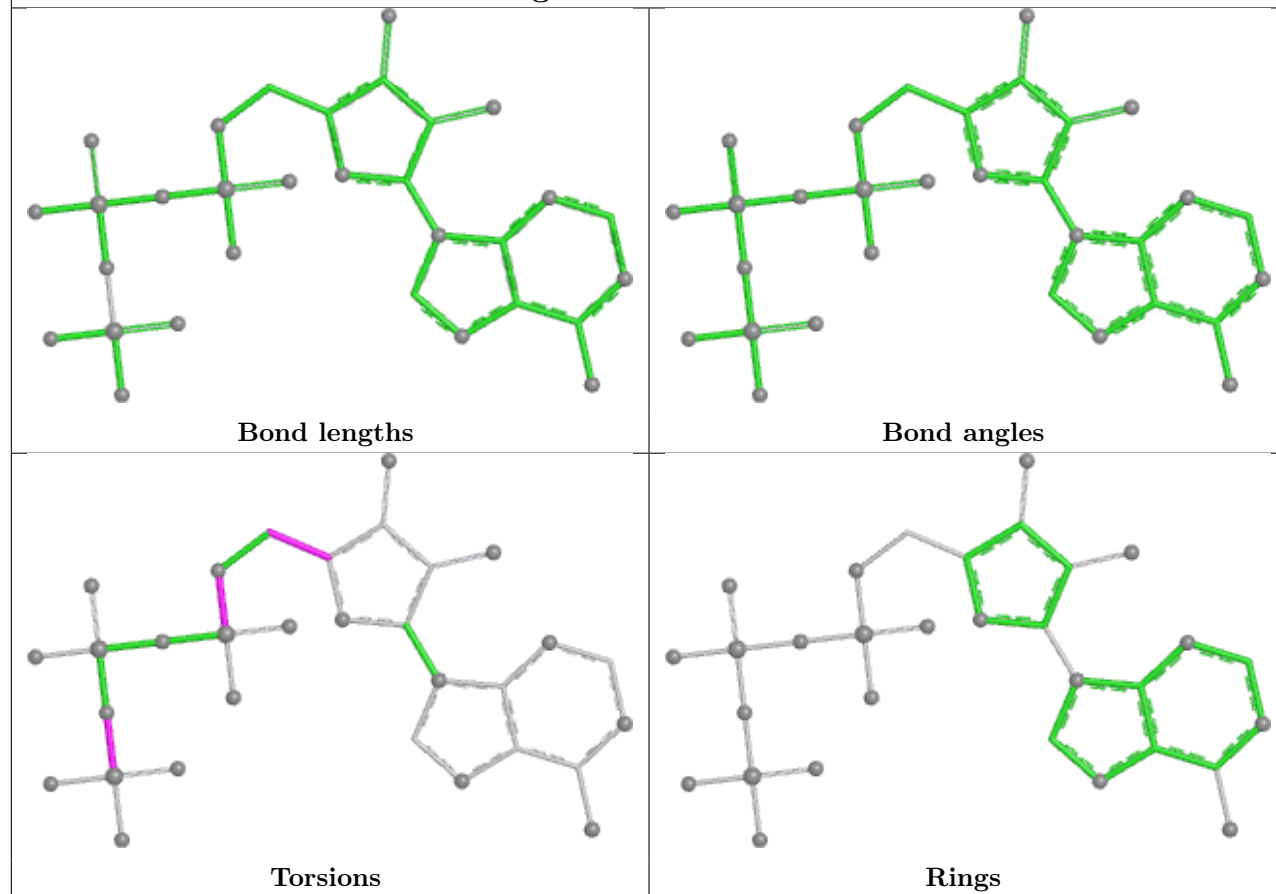




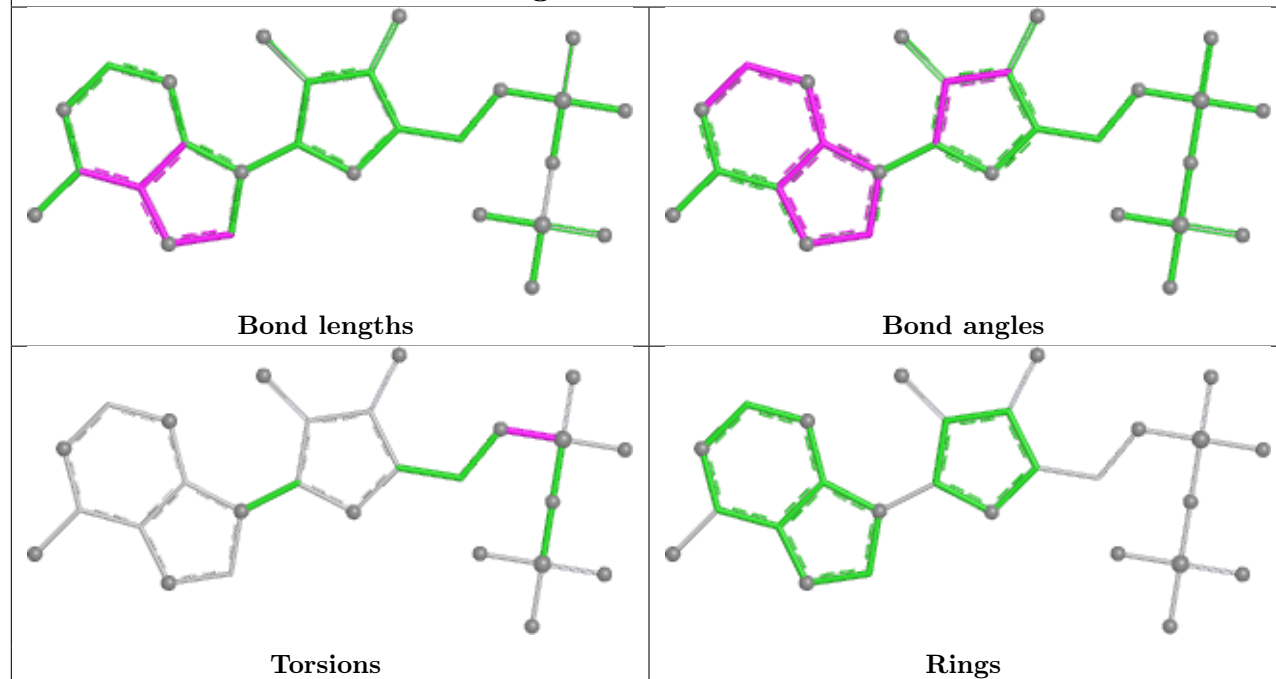
Ligand ATP E 401

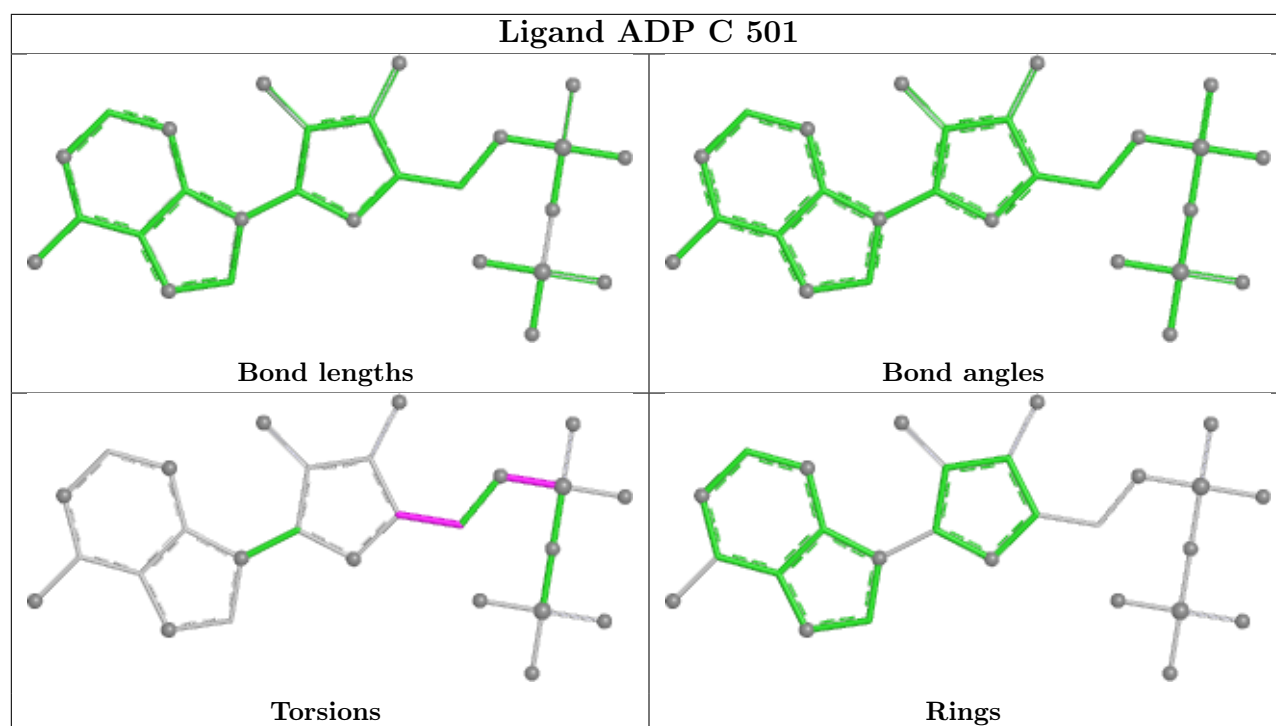


Ligand ATP D 501



Ligand ADP F 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

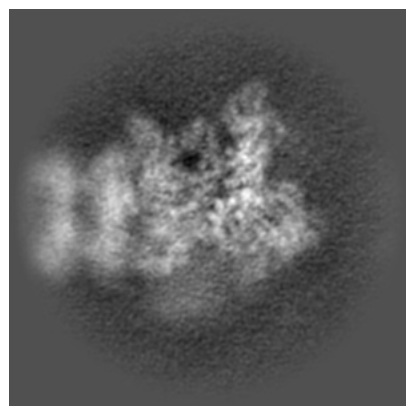
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65839. These allow visual inspection of the internal detail of the map and identification of artifacts.

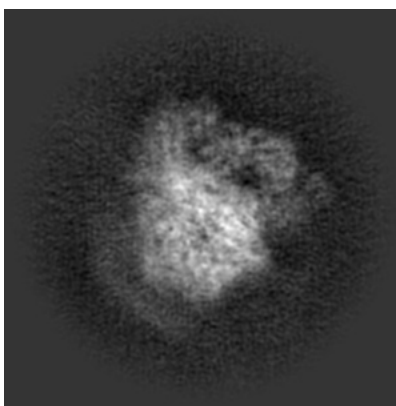
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

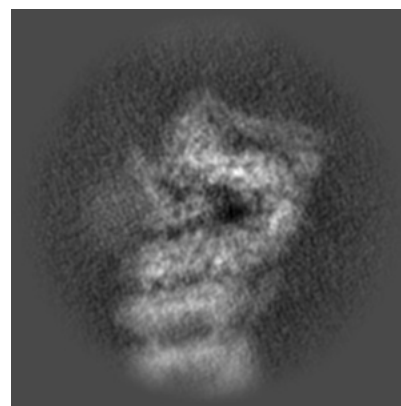
6.1.1 Primary map



X

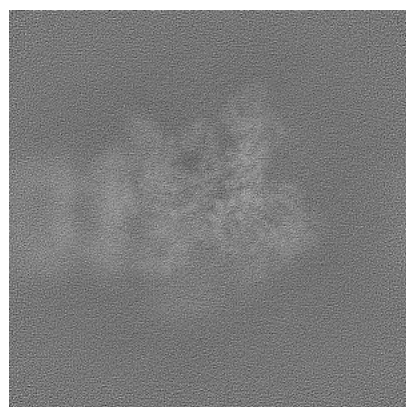


Y

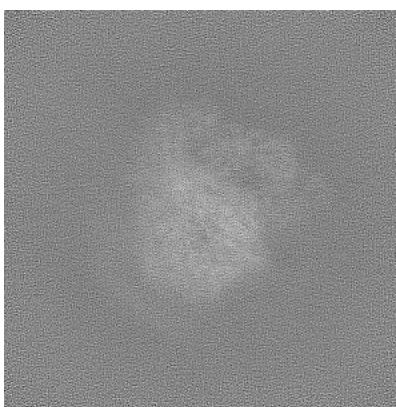


Z

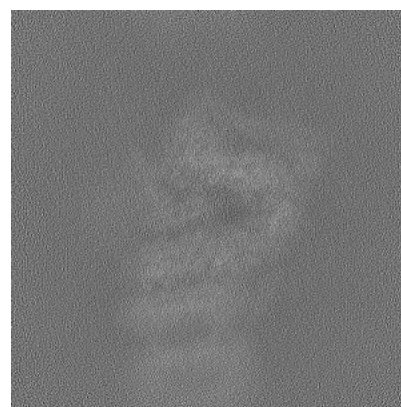
6.1.2 Raw map



X



Y

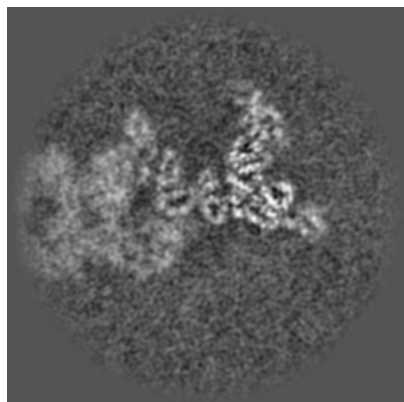


Z

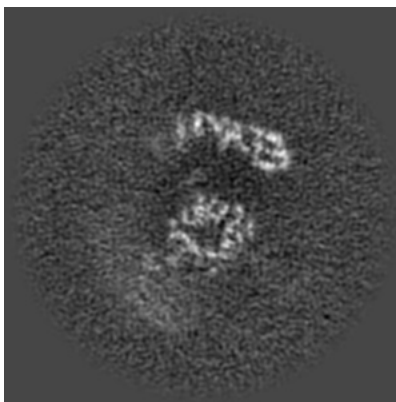
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

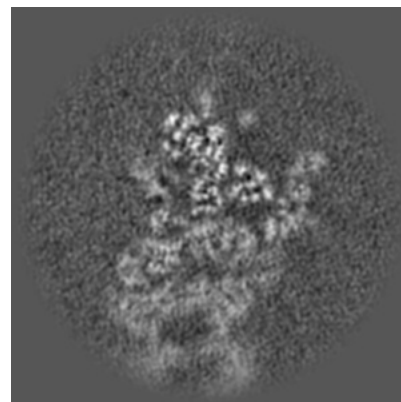
6.2.1 Primary map



X Index: 200

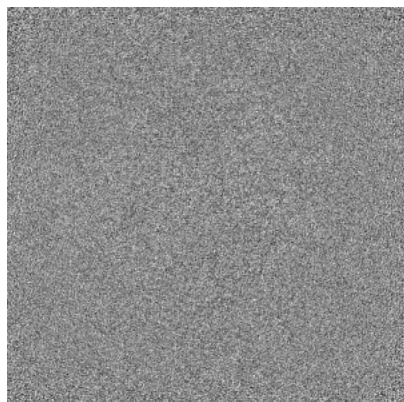


Y Index: 200

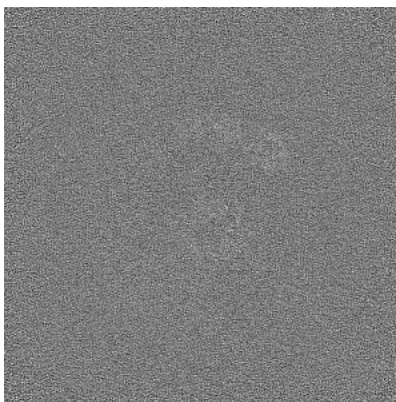


Z Index: 200

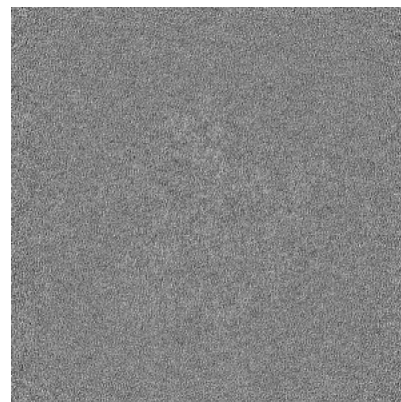
6.2.2 Raw map



X Index: 200



Y Index: 200

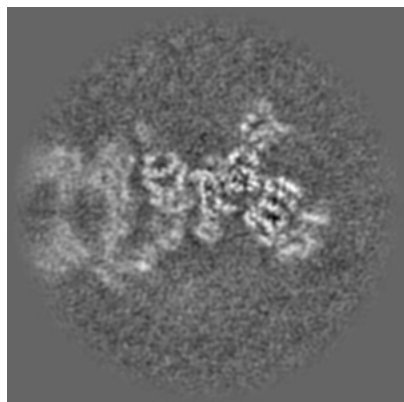


Z Index: 200

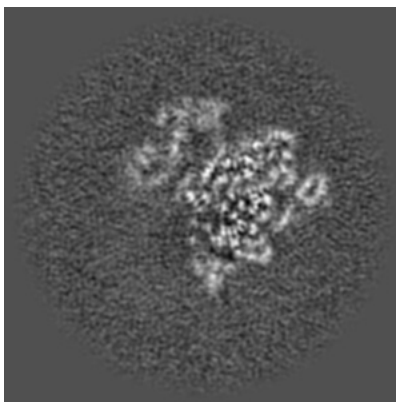
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

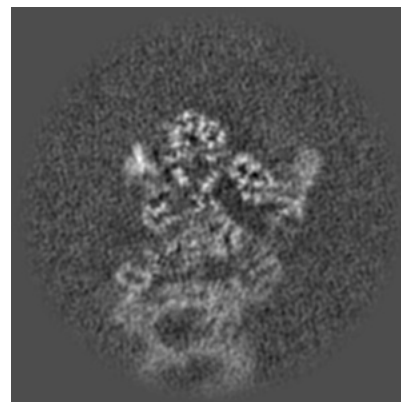
6.3.1 Primary map



X Index: 185

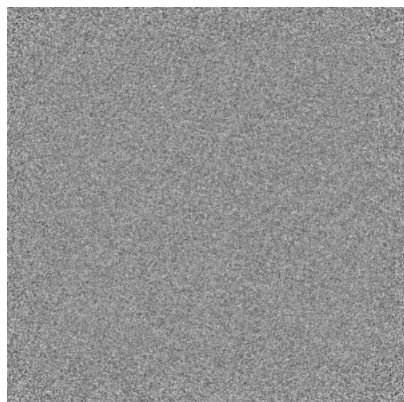


Y Index: 237

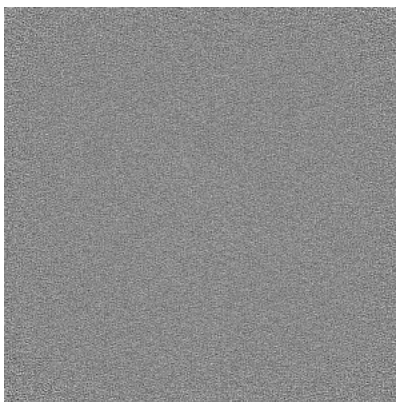


Z Index: 209

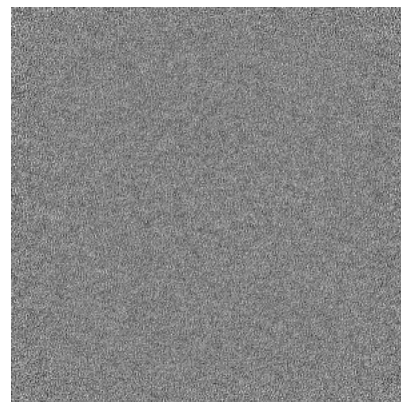
6.3.2 Raw map



X Index: 0



Y Index: 0

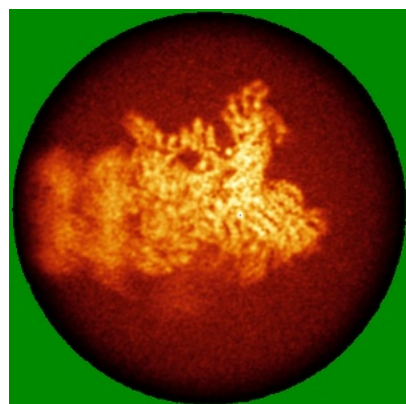


Z Index: 0

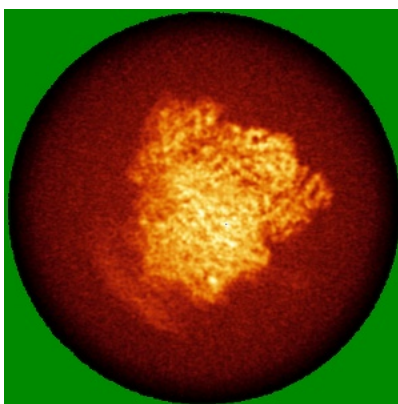
The images above show the largest variance slices of the map in three orthogonal directions.

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

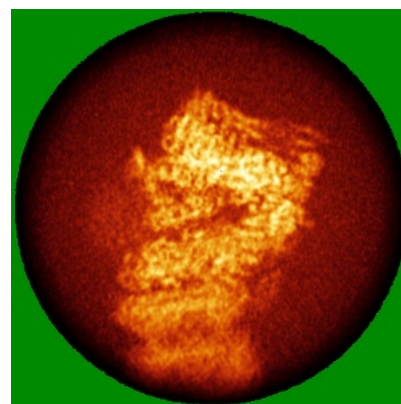
6.4.1 Primary map



X

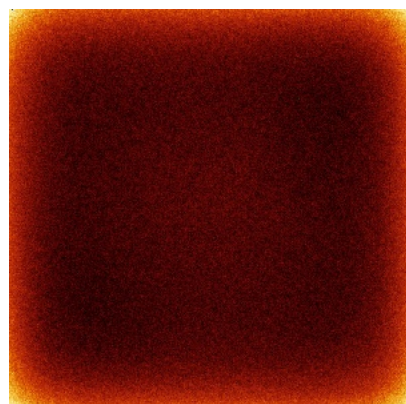


Y

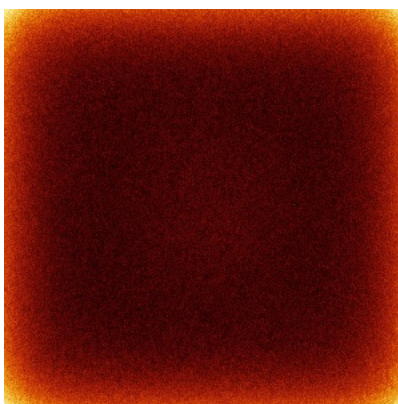


Z

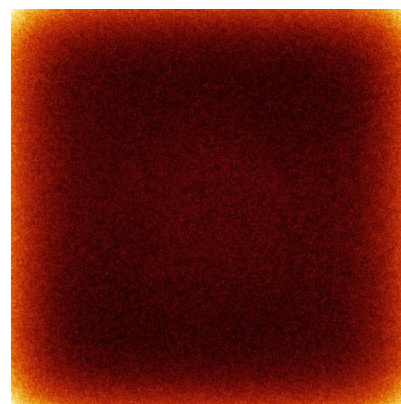
6.4.2 Raw map



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.

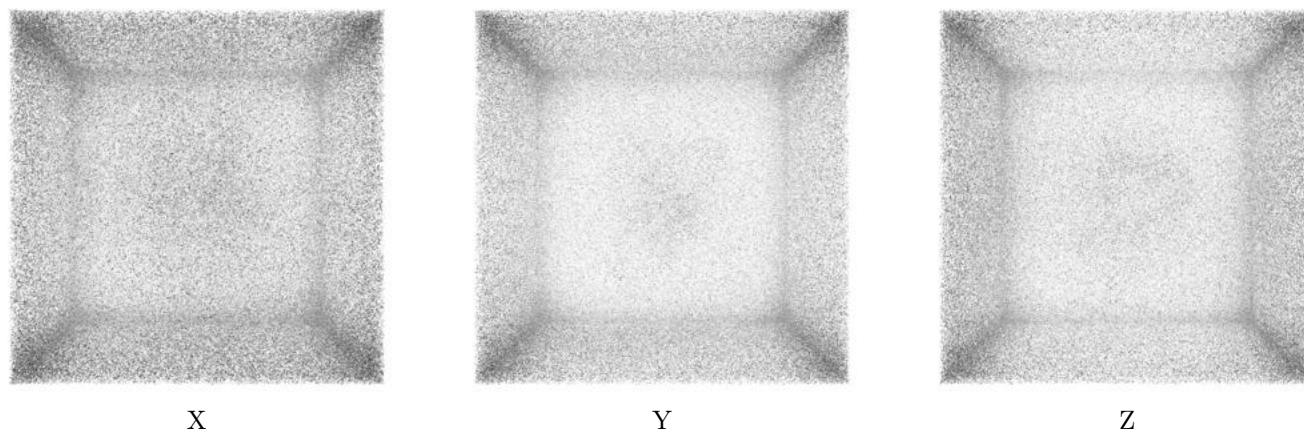
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

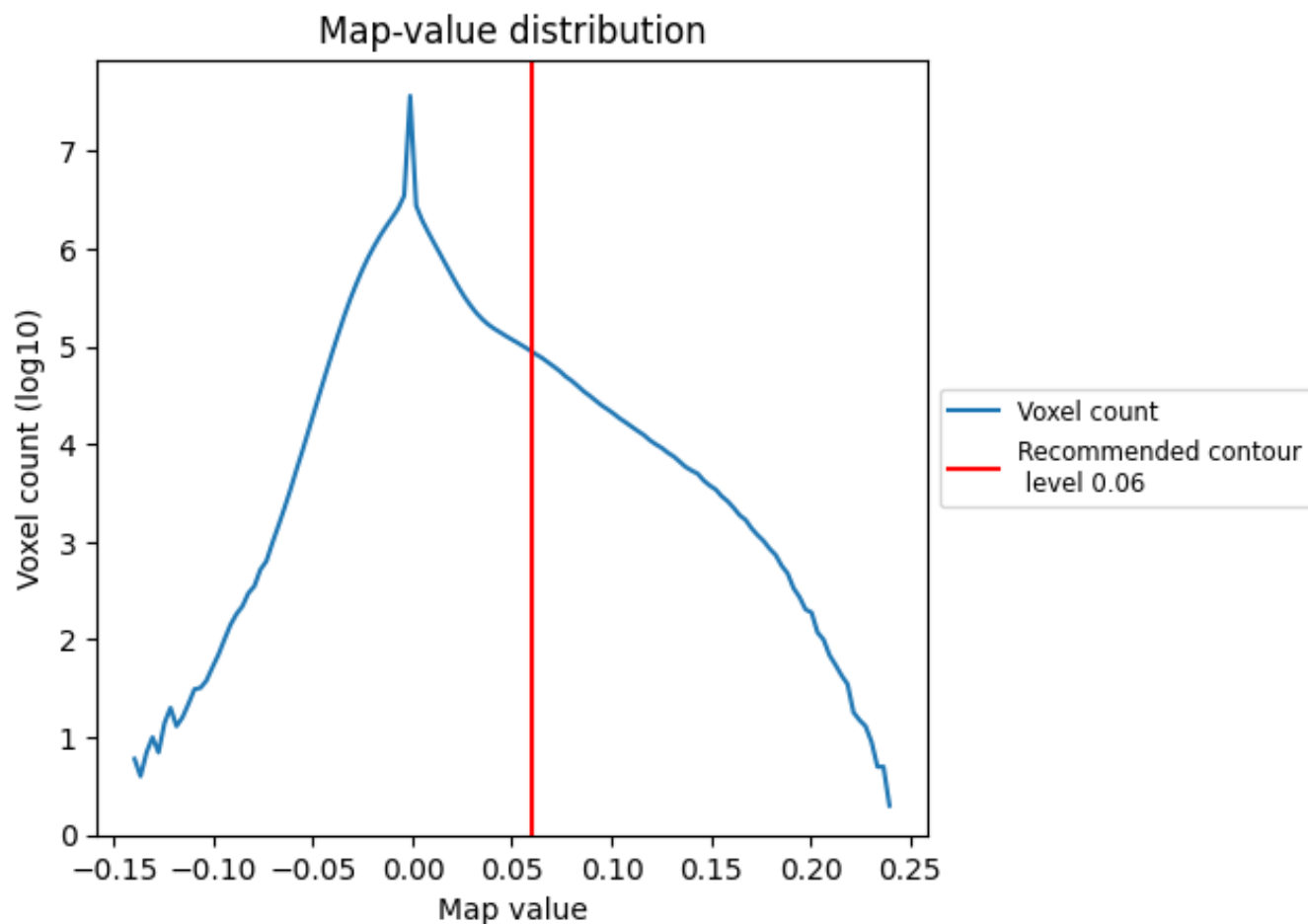
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

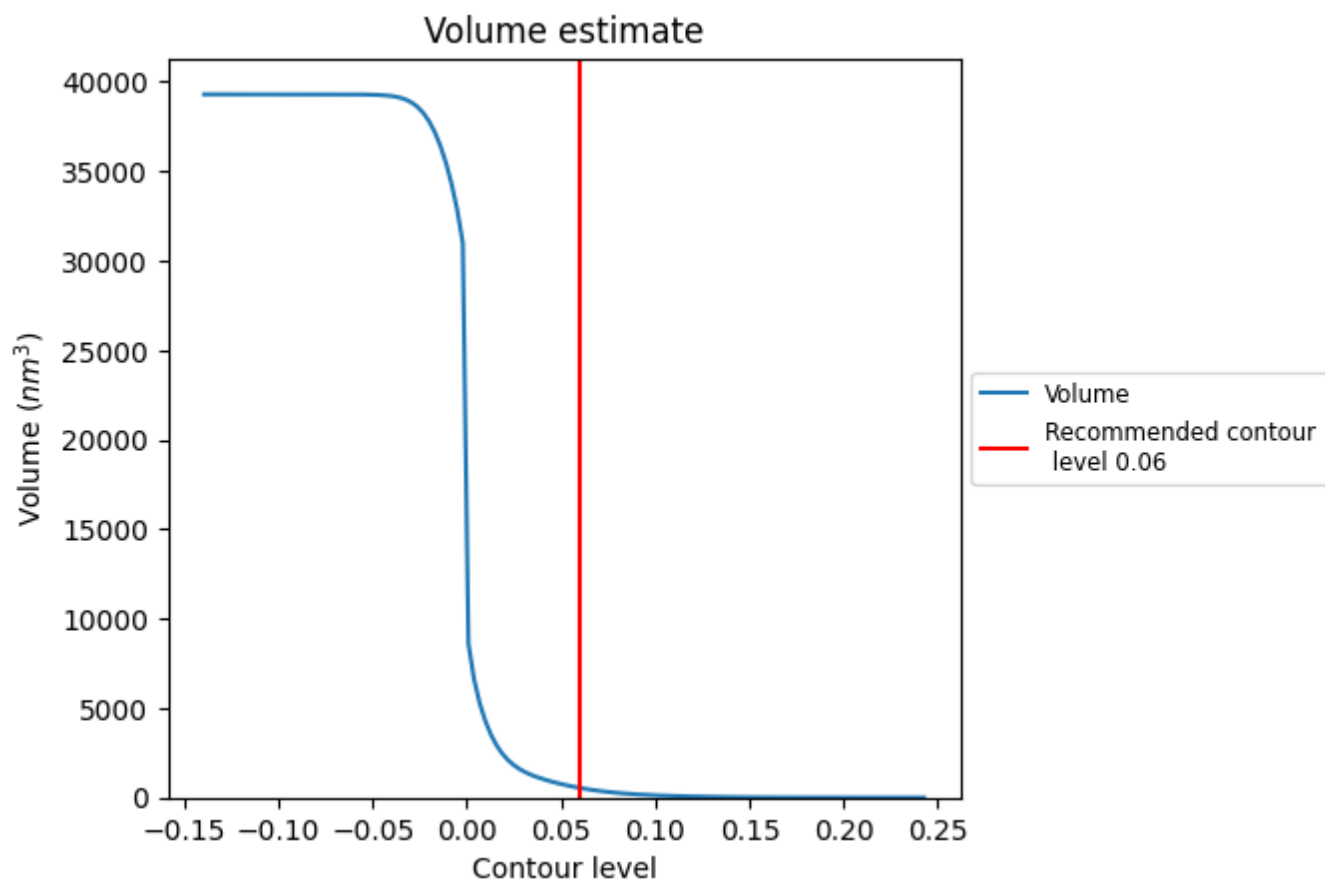
This section contains the results of statistical analysis of the map.

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.

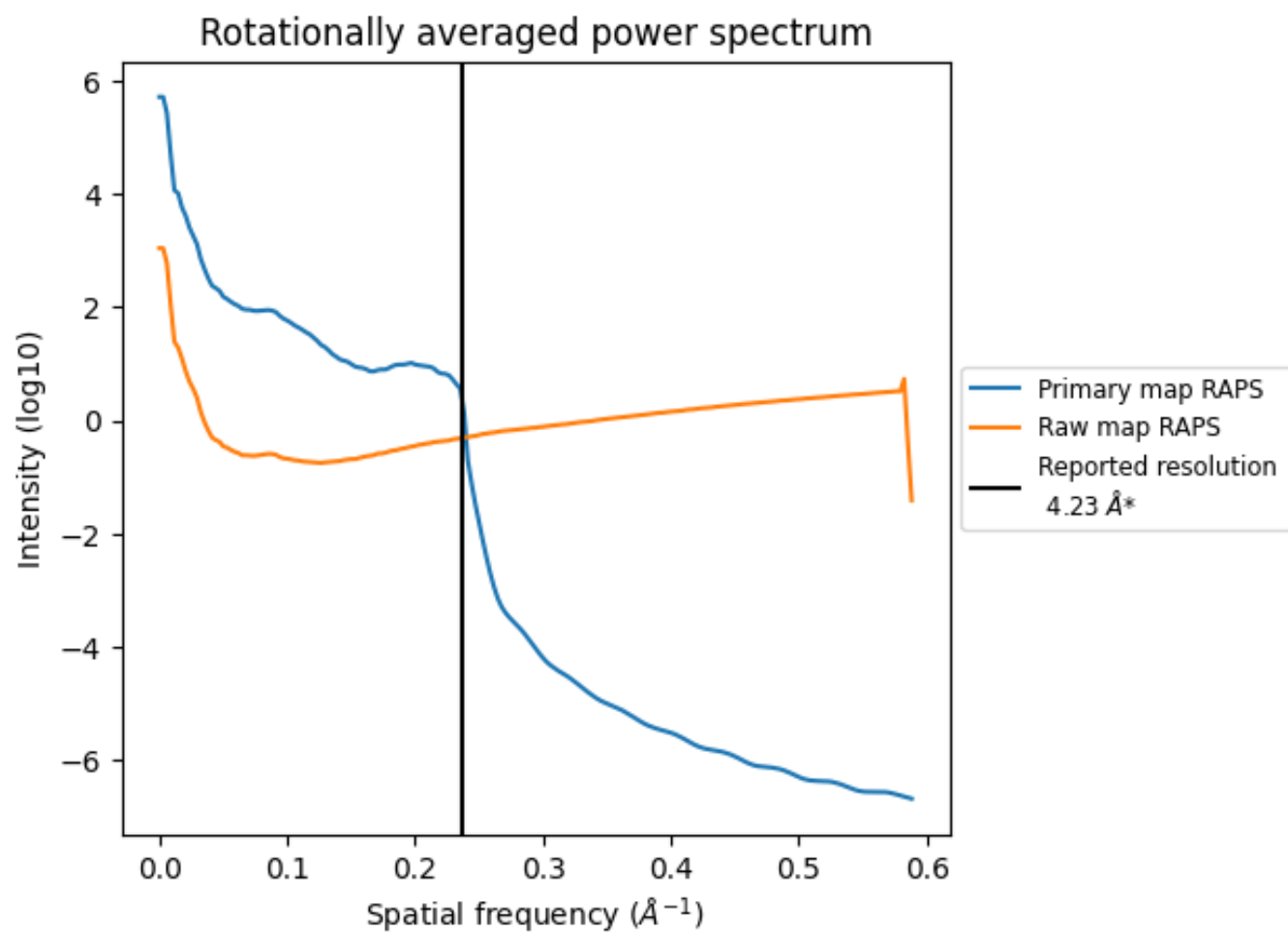
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 538 nm³; this corresponds to an approximate mass of 486 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 ⓘ

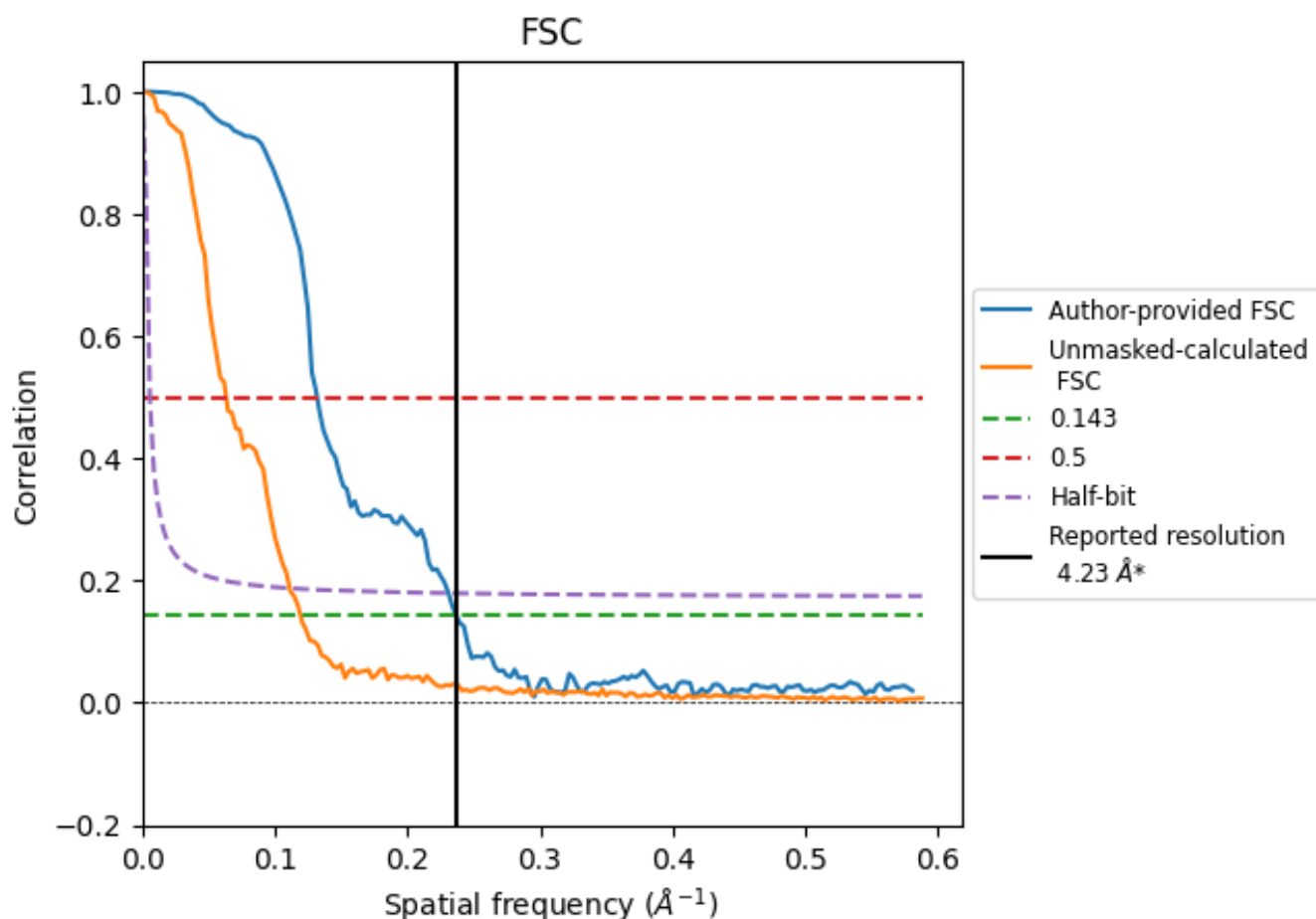


*Reported resolution corresponds to spatial frequency of 0.236 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.236 \AA^{-1}

8.2 Resolution estimates [i](#)

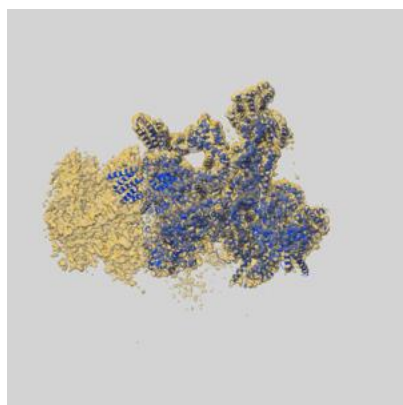
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.23	-	-
Author-provided FSC curve	4.23	7.58	4.33
Unmasked-calculated*	8.38	15.80	8.98

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.38 differs from the reported value 4.23 by more than 10 %

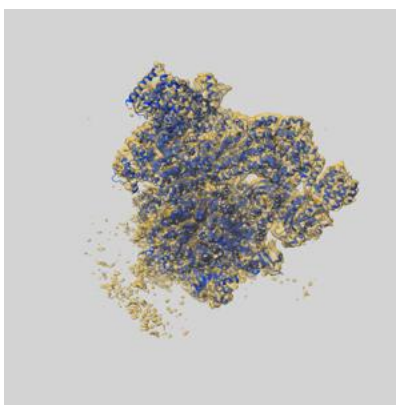
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65839 and PDB model 9WBG. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

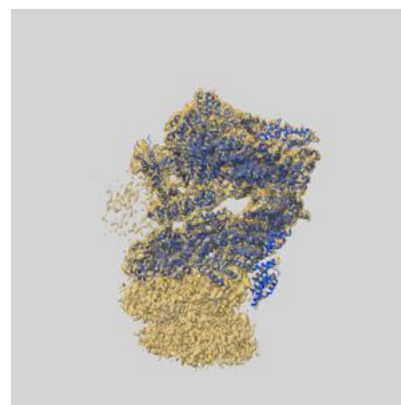
9.1 Map-model overlay [i](#)



X



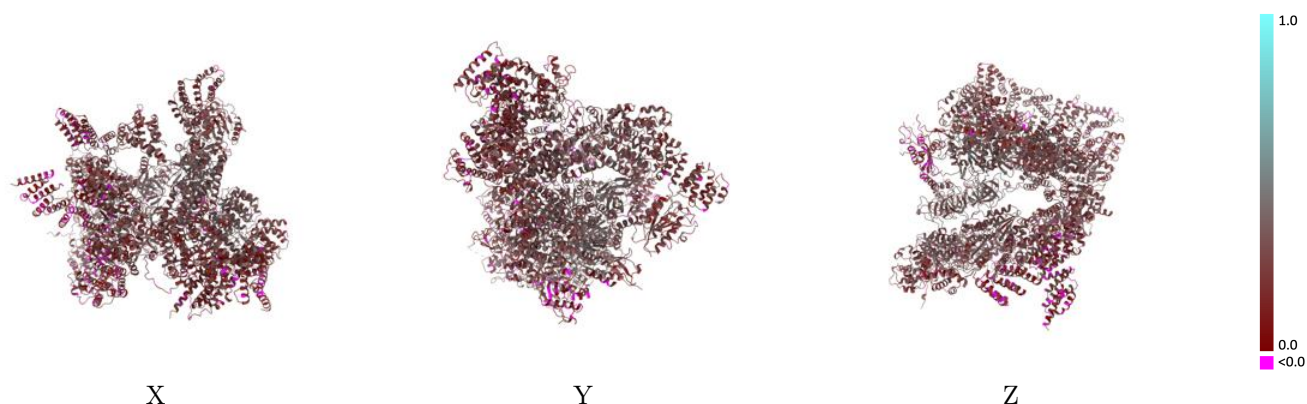
Y



Z

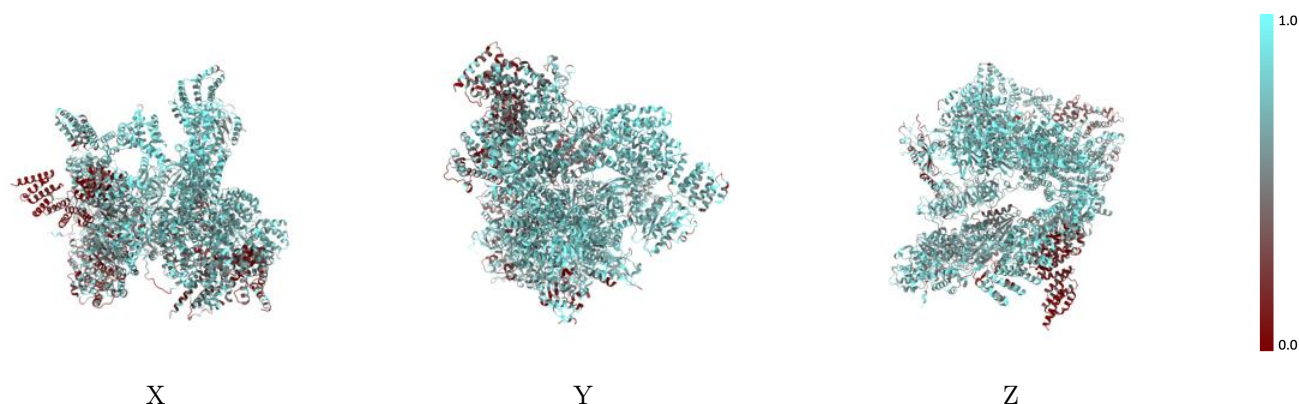
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



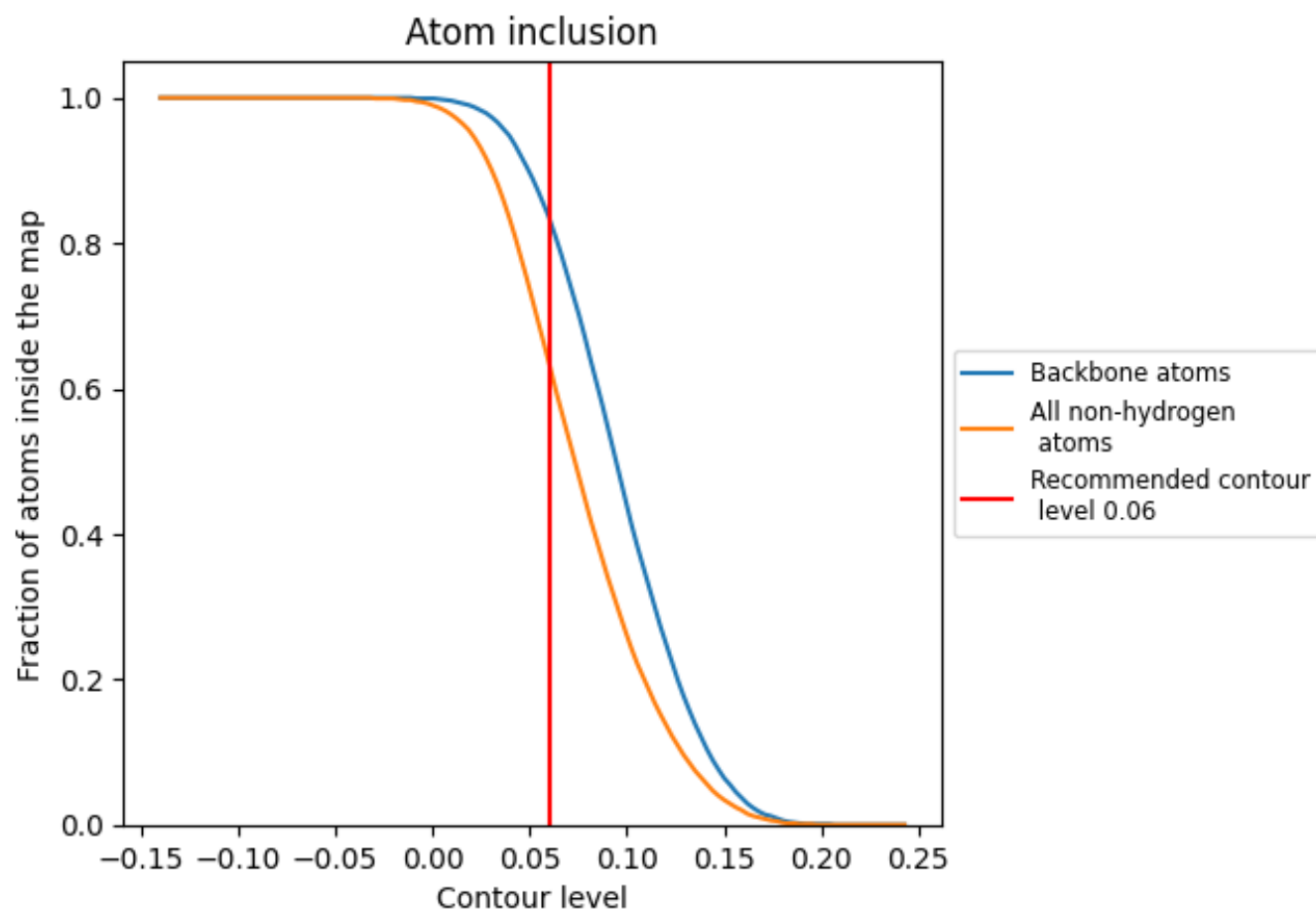
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 64% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6360	 0.2640
A	 0.6030	 0.2740
B	 0.4960	 0.2290
C	 0.5620	 0.2490
D	 0.6650	 0.2980
E	 0.7090	 0.3010
F	 0.6790	 0.2810
U	 0.7130	 0.2900
V	 0.5720	 0.2370
W	 0.7340	 0.2460
X	 0.3140	 0.1850
Y	 0.5940	 0.2320
Z	 0.7600	 0.3450
a	 0.7730	 0.2820
b	 0.7090	 0.2610
c	 0.7500	 0.3540
d	 0.5030	 0.2090
e	 0.5790	 0.2180
f	 0.6460	 0.1890
v	 0.4000	 0.3180
w	 0.6460	 0.1450

