



## Full wwPDB EM Validation Report ⓘ

Apr 20, 2026 – 08:35 PM JST

PDB ID : 9K53 / pdb\_00009k53  
EMDB ID : EMD-62079  
Title : Structure of substrate-engaged human 26S proteasome RP-CP subcomplex in state ED2.1  
Authors : Wu, Z.; Chen, E.; Mao, Y.  
Deposited on : 2024-10-21  
Resolution : 2.50 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](mailto: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>.

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

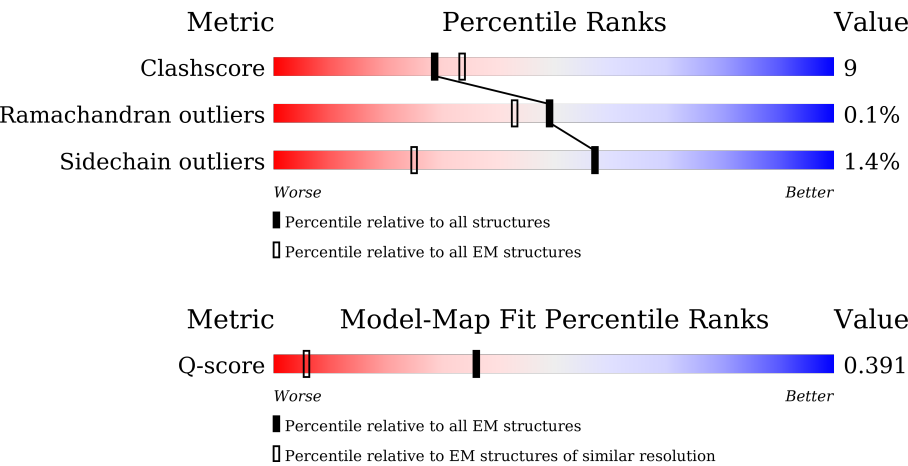
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.50 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.




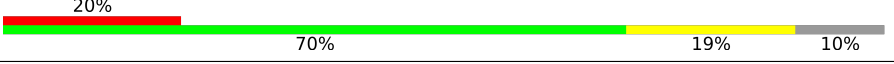
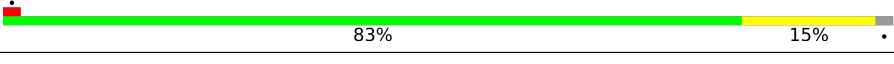


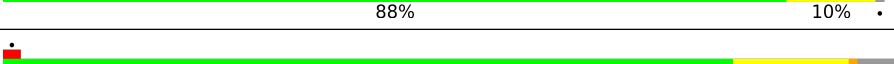
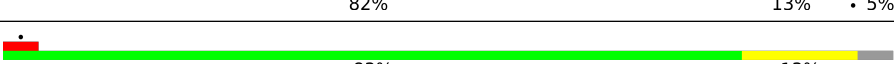
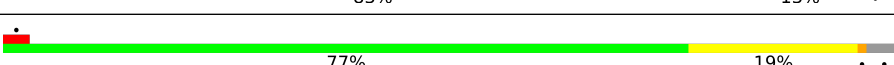
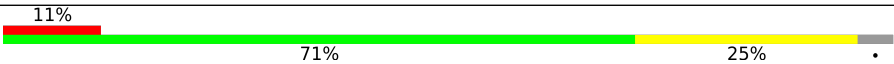
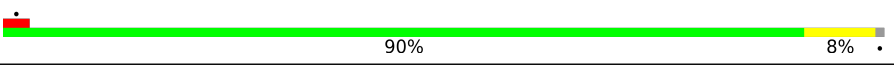

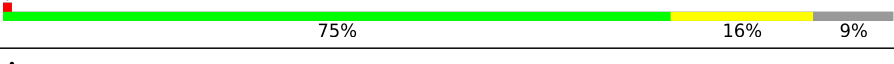
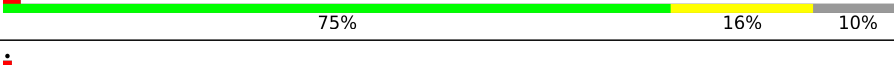

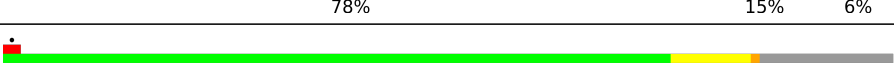










Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 ( 2.00 - 3.00 )

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  $\geq 3$ , 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	A	433	<div><div>14%</div><div><div></div><div>73%</div><div>22%</div><div>5%</div></div></div>
2	B	440	<div><div>13%</div><div><div></div><div>67%</div><div>25%</div><div>• 7%</div></div></div>
3	C	398	<div><div>8%</div><div><div></div><div>78%</div><div>20%</div><div>••</div></div></div>
4	D	418	<div><div>10%</div><div><div></div><div>64%</div><div>26%</div><div>• 9%</div></div></div>

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Mol	Chain	Length	Quality of chain
5	E	403	
6	F	439	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	263	
12	l	263	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	Q	201	
17	q	201	
18	R	263	

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Mol	Chain	Length	Quality of chain
18	r	263	
19	S	241	
19	s	241	
20	T	264	
20	t	264	
21	U	953	
22	V	534	
23	W	456	
24	X	422	
25	Y	389	
26	Z	324	
27	a	376	
28	b	377	
29	c	310	
30	d	350	
31	e	70	
32	f	908	
33	v	36	
34	y	5	
34	z	5	

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 106358 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 26S proteasome regulatory subunit 7.

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

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4.

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

- Molecule 3 is a protein called 26S proteasome regulatory subunit 8.

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

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

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

- Molecule 5 is a protein called Proteasome 26S subunit, ATPase 6.

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

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

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

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	240	Total	C	N	O	S	0	0
			1867	1187	312	355	13		
7	g	244	Total	C	N	O	S	0	0
			1879	1193	318	355	13		

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	232	Total	C	N	O	S	0	0
			1801	1149	304	342	6		
8	h	232	Total	C	N	O	S	0	0
			1805	1154	307	338	6		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	248	Total	C	N	O	S	0	0
			1933	1222	330	371	10		
9	i	250	Total	C	N	O	S	0	0
			1955	1234	336	375	10		

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1861	1166	327	363	5		
10	j	239	Total	C	N	O	S	0	0
			1861	1168	332	356	5		

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	238	Total	C	N	O	S	0	0
			1813	1139	302	361	11		
11	k	234	Total	C	N	O	S	0	0
			1782	1119	295	357	11		

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	240	Total	C	N	O	S	0	0
			1876	1175	338	352	11		
12	l	238	Total	C	N	O	S	0	0
			1861	1165	335	350	11		

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	242	Total	C	N	O	S	1	0
			1893	1202	323	356	12		
13	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	203	Total	C	N	O	S	0	0
			1521	954	259	296	12		
14	n	202	Total	C	N	O	S	0	0
			1510	947	258	293	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1645	1035	278	320	12		
15	o	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

- Molecule 16 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1587	1010	264	294	19		
16	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 17 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	1	0
			1591	1019	270	292	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1578	1012	267	290	9		

- Molecule 18 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		
18	r	201	Total	C	N	O	S	0	0
			1549	977	270	293	9		

- Molecule 19 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1641	1041	281	309	10		
19	s	213	Total	C	N	O	S	0	0
			1650	1044	283	313	10		

- Molecule 20 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	216	Total	C	N	O	S	0	0
			1683	1062	291	318	12		
20	t	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	878	Total	C	N	O	S	0	0
			6867	4352	1163	1306	46		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	444	Total	C	N	O	S	0	0
			3612	2301	645	653	13		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.



Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	441	Total	C	N	O	S	0	0
			3596	2277	613	682	24		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	422	Total	C	N	O	S	0	0
			3335	2116	567	639	13		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	389	Total	C	N	O	S	0	0
			3202	2041	545	598	18		

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

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

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

- Molecule 31 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	e	50	Total	C	N	O	0	0
			425	260	65	100		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	844	Total	C	N	O	S	0	0
			6529	4126	1108	1250	45		

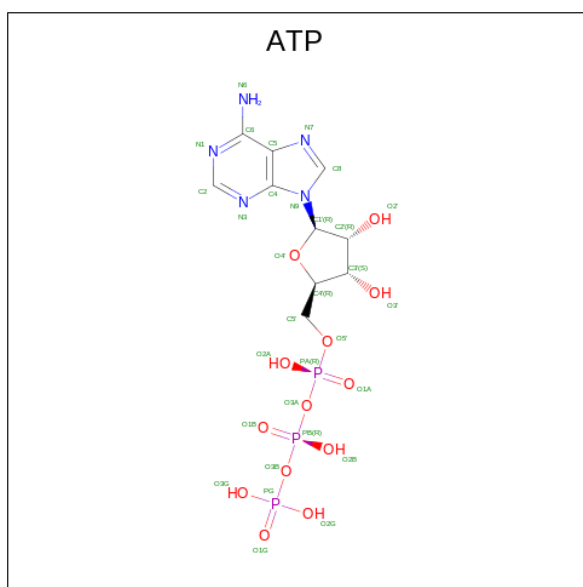
- Molecule 33 is a protein called Substrate binding RP.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	v	36	Total	C	N	O	0	0
			180	108	36	36		

- Molecule 34 is a protein called Substrates binding CP.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	y	5	Total	C	N	O	0	0
			25	15	5	5		
34	z	5	Total	C	N	O	0	0
			25	15	5	5		

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).

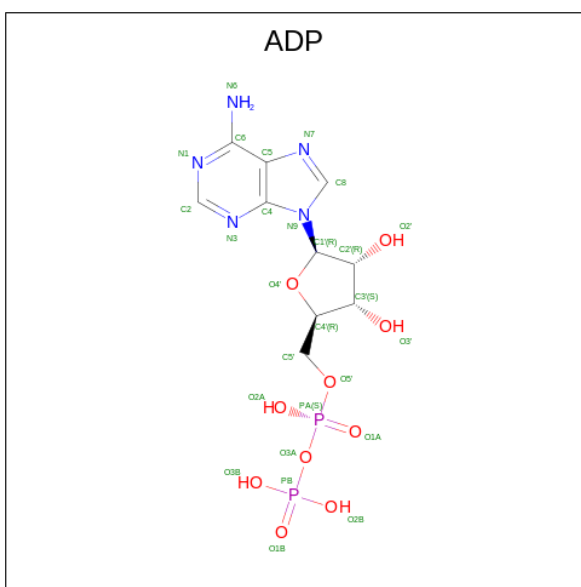


Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

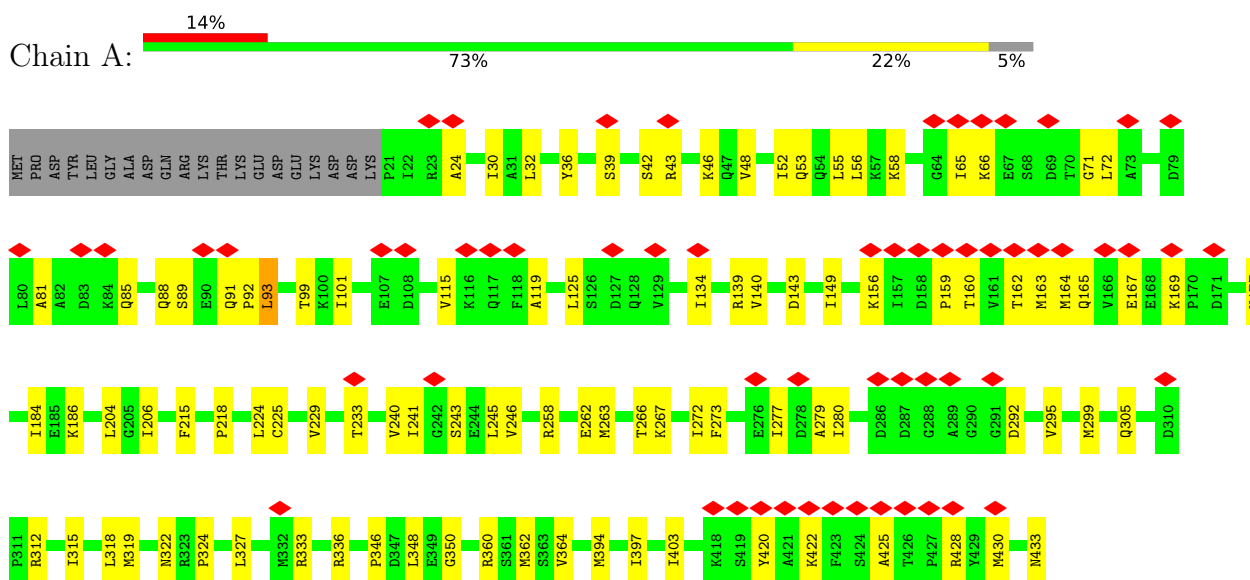
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

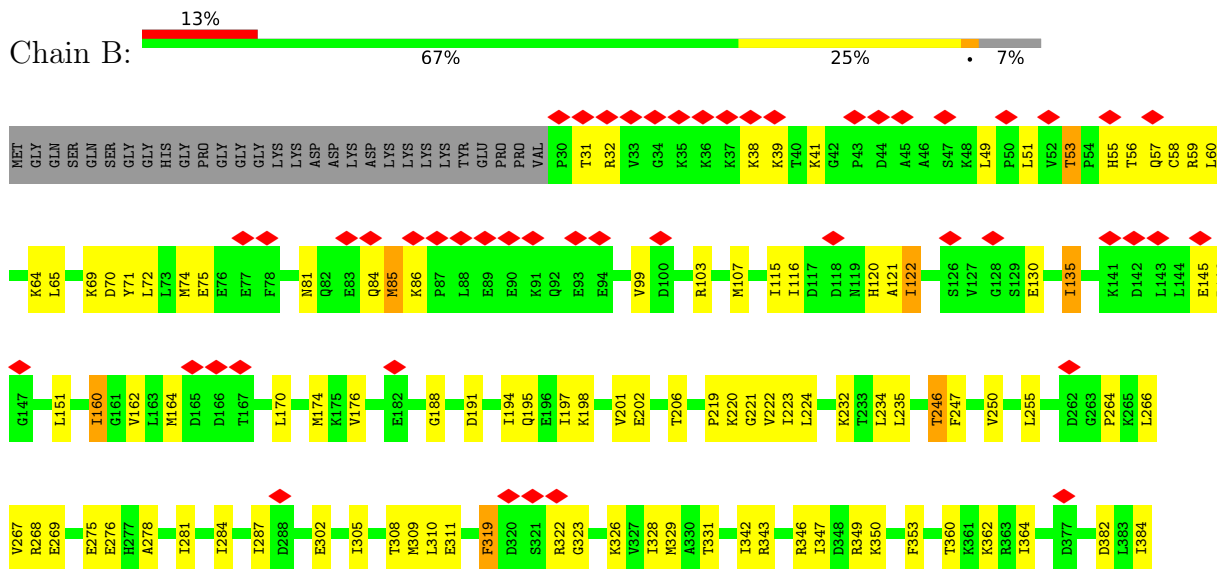
### 3 Residue-property plots [i](#)

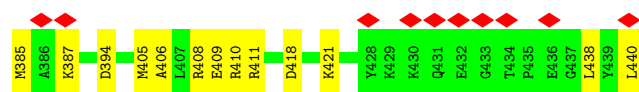
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 26S proteasome regulatory subunit 7

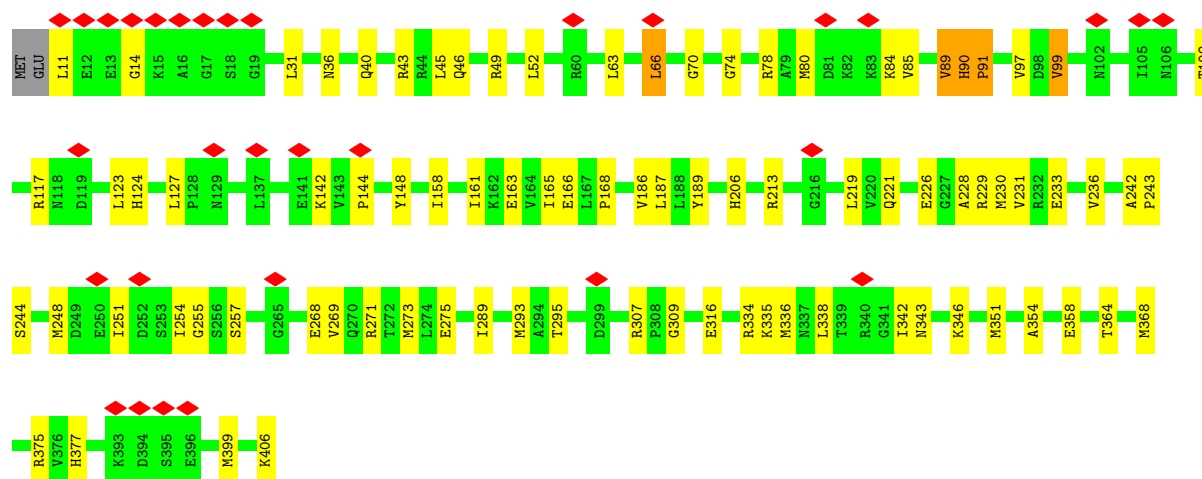
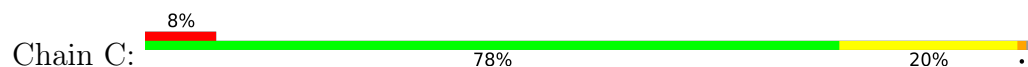


- Molecule 2: 26S proteasome regulatory subunit 4

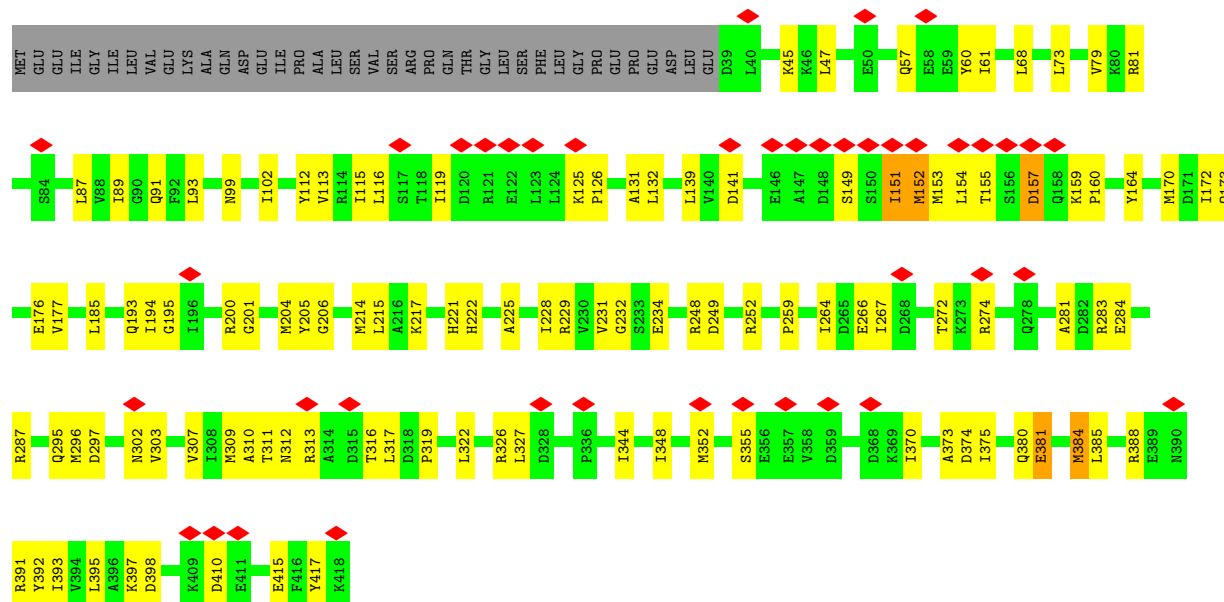




• Molecule 3: 26S proteasome regulatory subunit 8

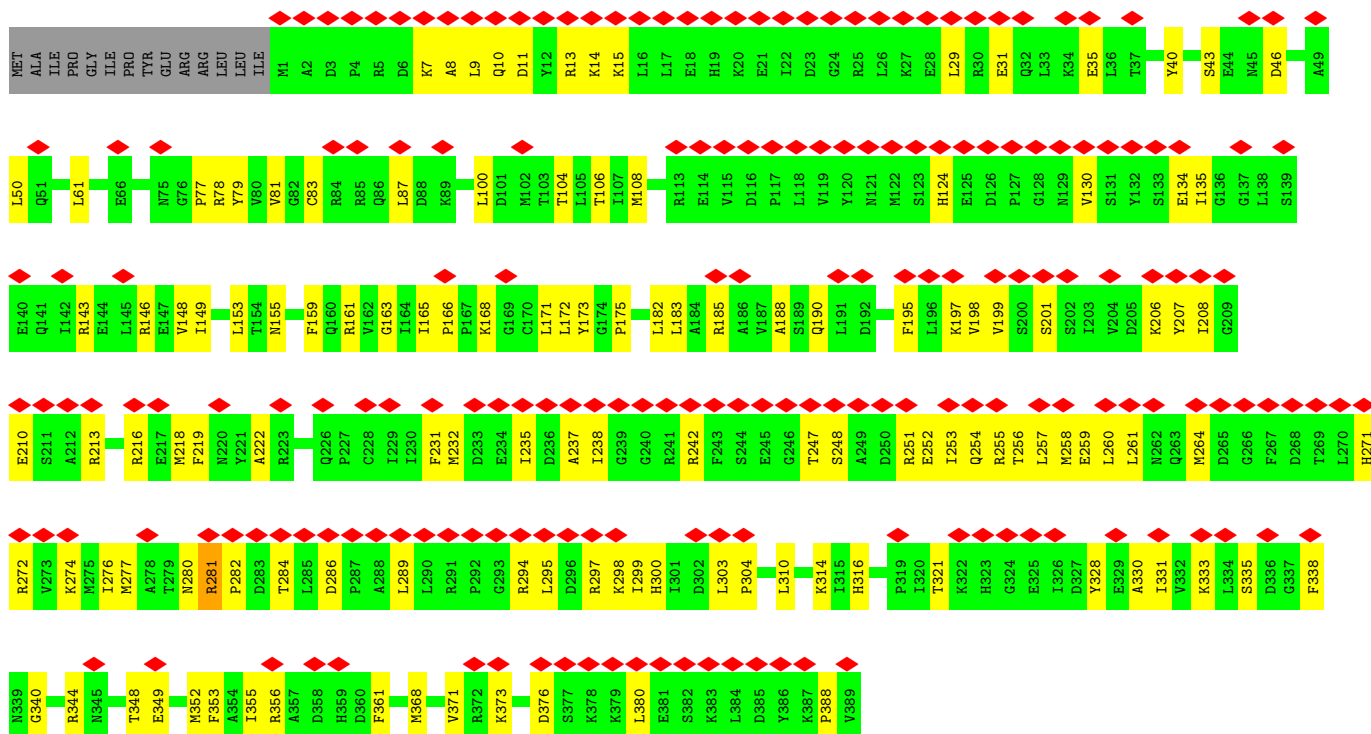


• Molecule 4: 26S proteasome regulatory subunit 6B

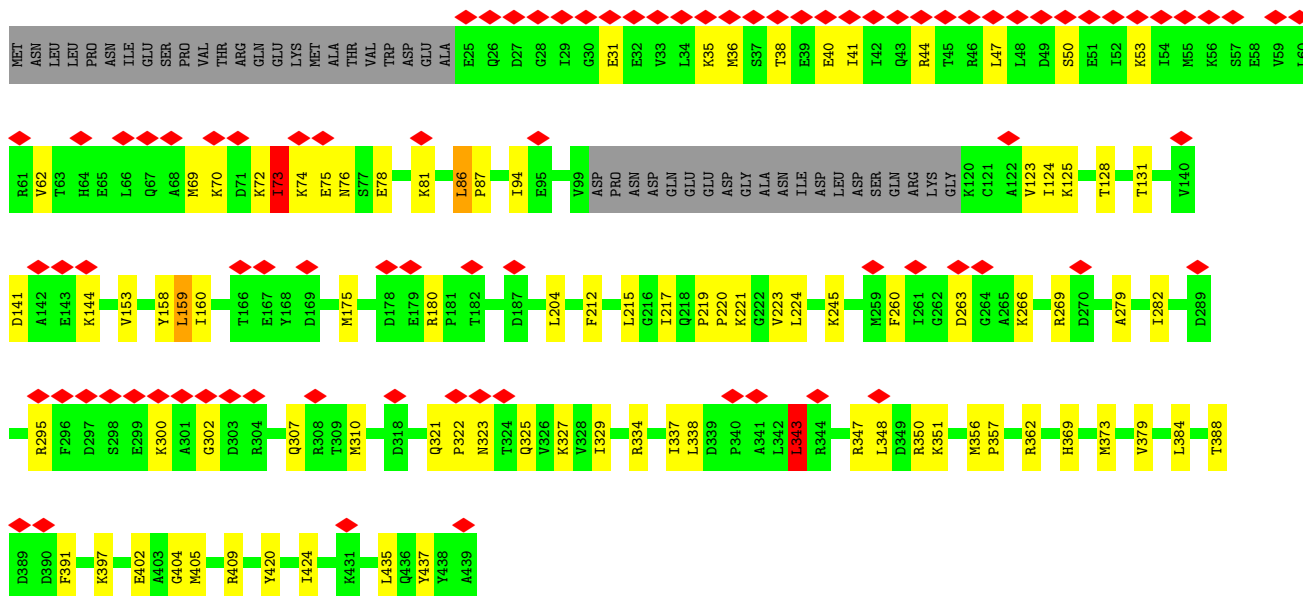


• Molecule 5: Proteasome 26S subunit, ATPase 6

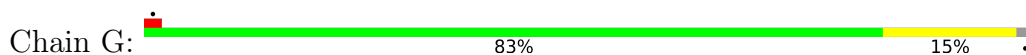




• Molecule 6: 26S proteasome regulatory subunit 6A

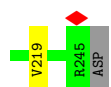
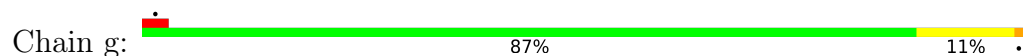


• Molecule 7: Proteasome subunit alpha type-6

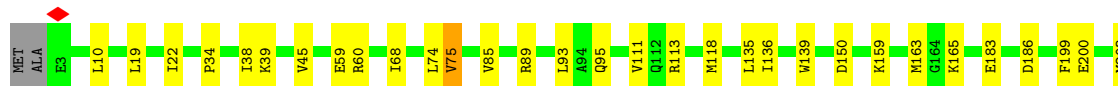
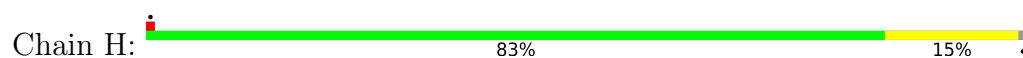




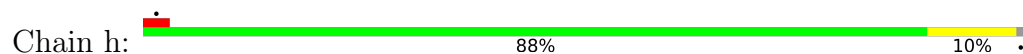
• Molecule 7: Proteasome subunit alpha type-6



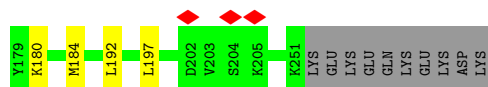
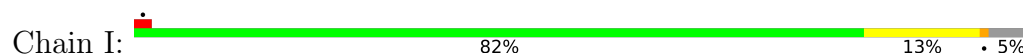
• Molecule 8: Proteasome subunit alpha type-2



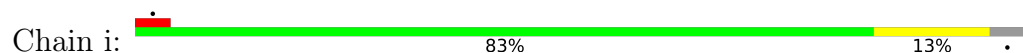
• Molecule 8: Proteasome subunit alpha type-2



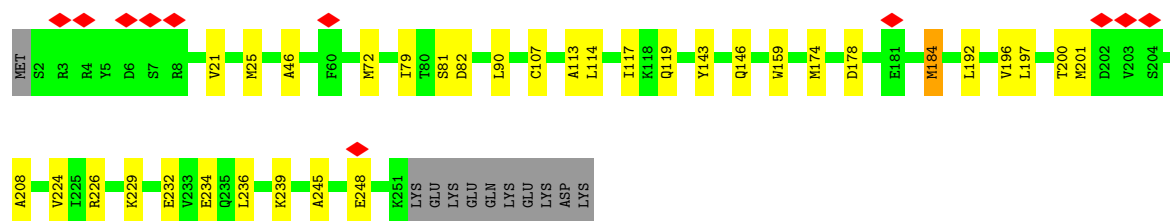
• Molecule 9: Proteasome subunit alpha type-4



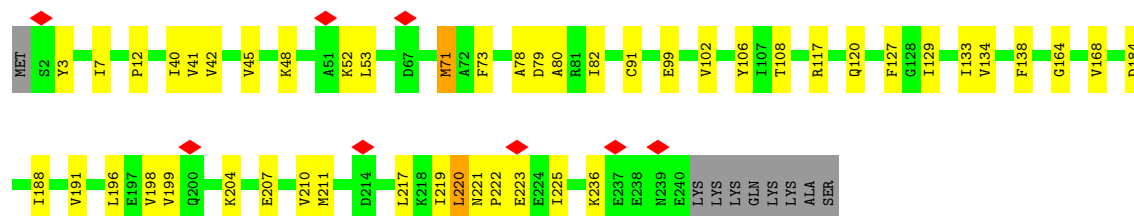
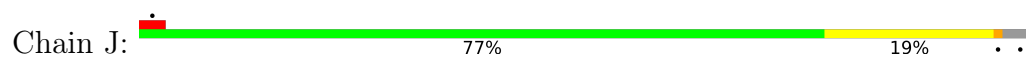
• Molecule 9: Proteasome subunit alpha type-4



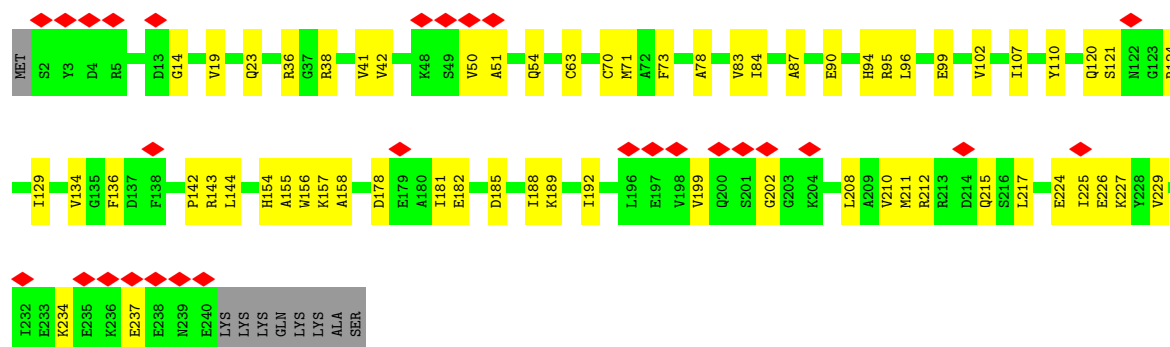




- Molecule 10: Proteasome subunit alpha type-7



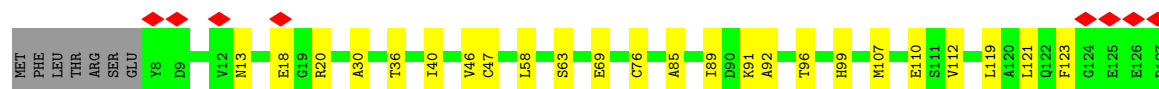
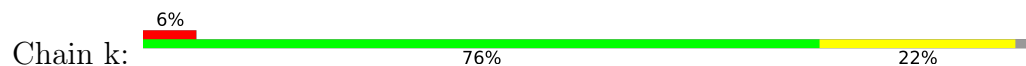
- Molecule 10: Proteasome subunit alpha type-7

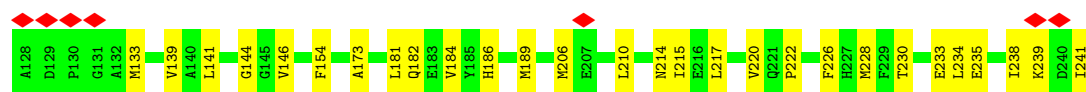


- Molecule 11: Proteasome subunit alpha type-5

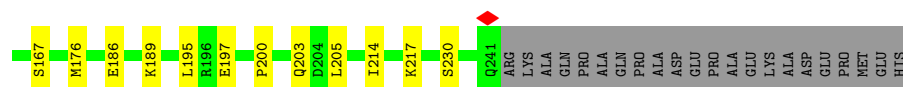
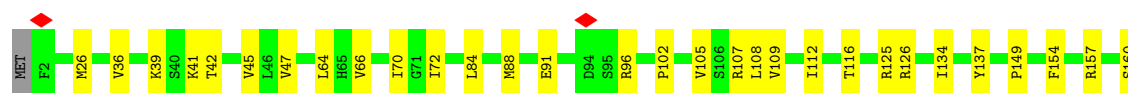
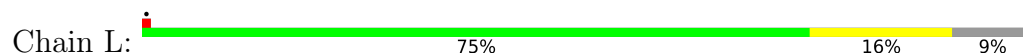


- Molecule 11: Proteasome subunit alpha type-5

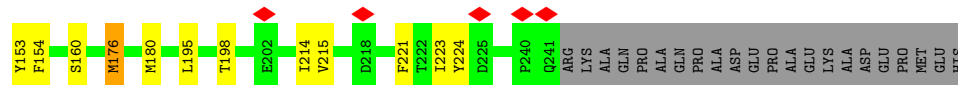




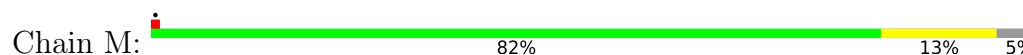
- Molecule 12: Proteasome subunit alpha type-1



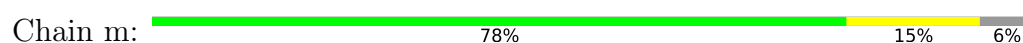
- Molecule 12: Proteasome subunit alpha type-1




- Molecule 13: Proteasome subunit alpha type-3

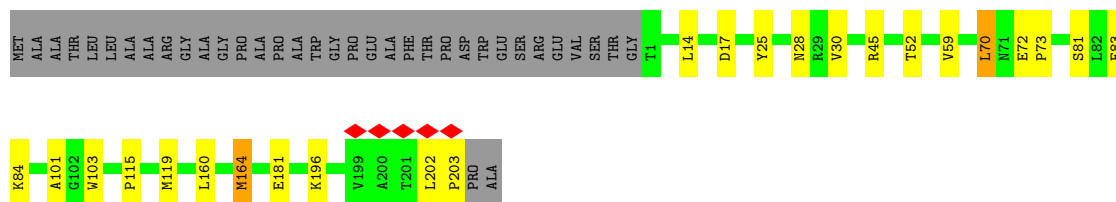


- Molecule 13: Proteasome subunit alpha type-3




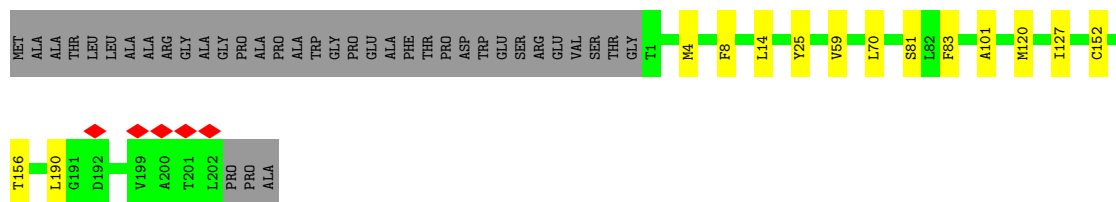
- Molecule 14: Proteasome subunit beta type-6

Chain N: 



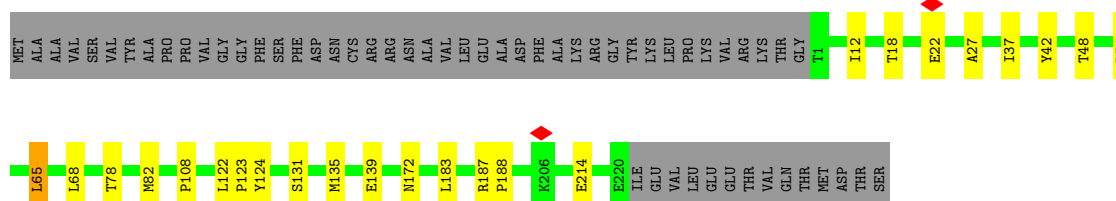
- Molecule 14: Proteasome subunit beta type-6

Chain n: 



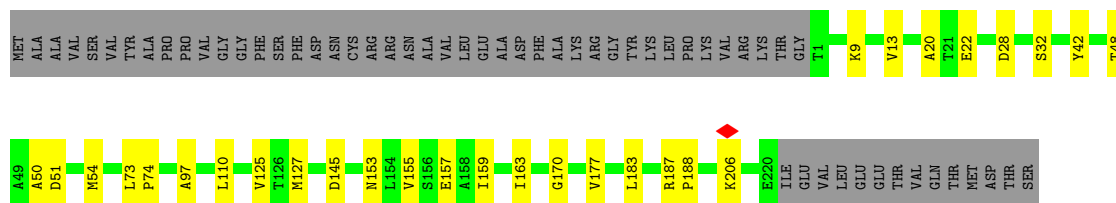
- Molecule 15: Proteasome subunit beta type-7

Chain O: 




- Molecule 15: Proteasome subunit beta type-7

Chain o: 

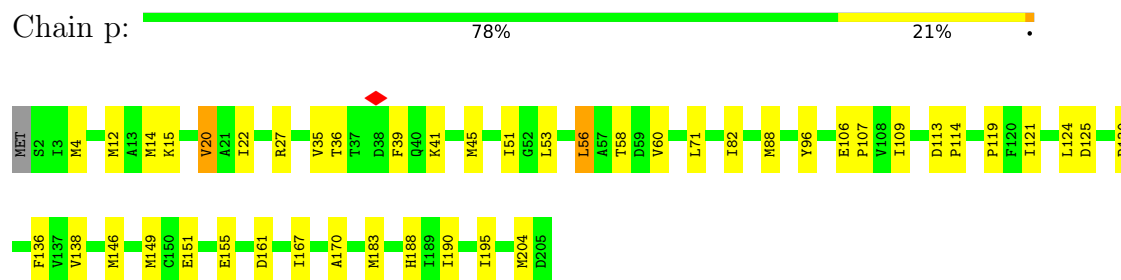


- Molecule 16: Proteasome subunit beta type-3

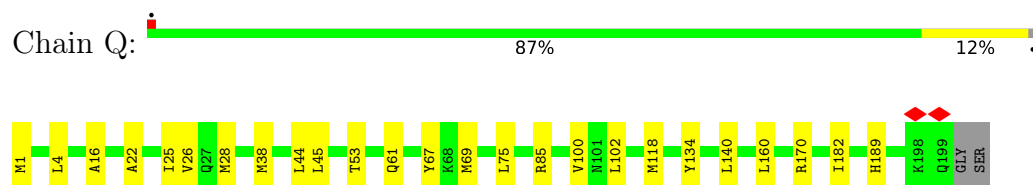
Chain P: 



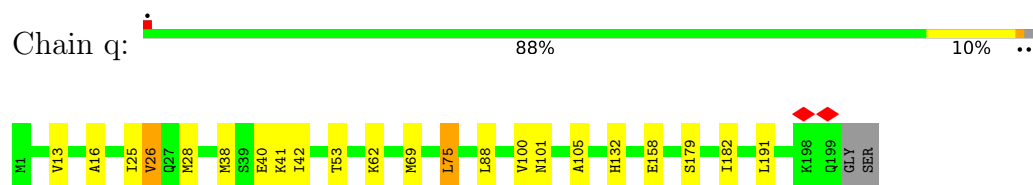
- Molecule 16: Proteasome subunit beta type-3



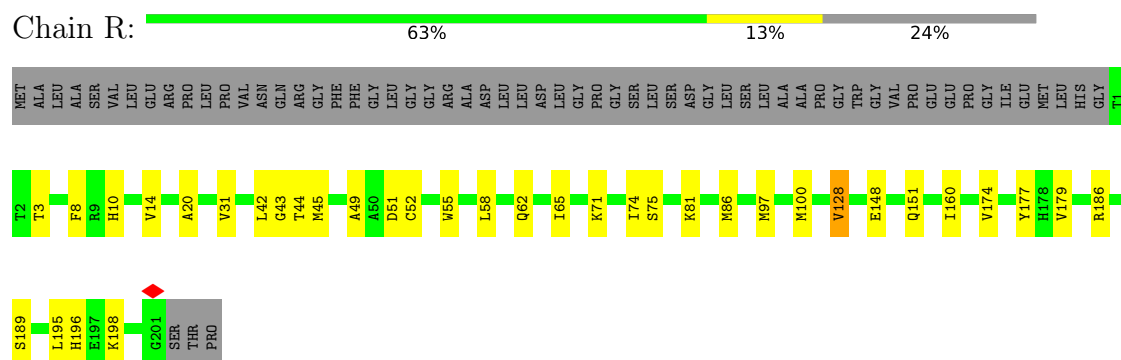
- Molecule 17: Proteasome subunit beta type-2



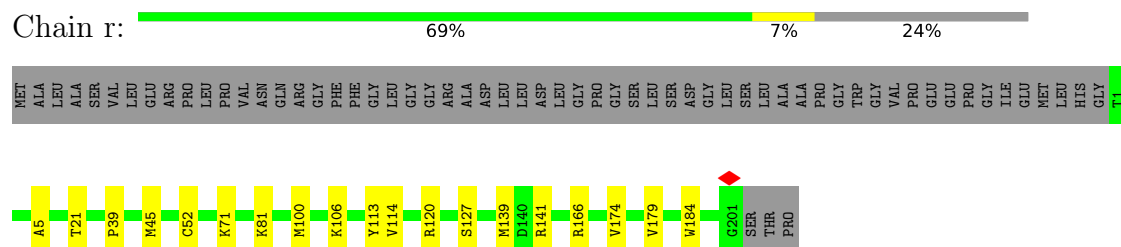
- Molecule 17: Proteasome subunit beta type-2



- Molecule 18: Proteasome subunit beta type-5

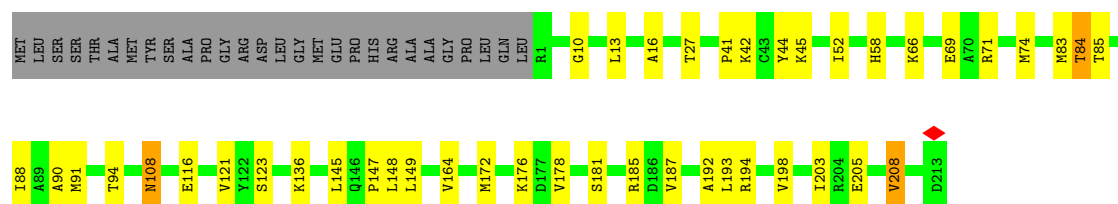


- Molecule 18: Proteasome subunit beta type-5



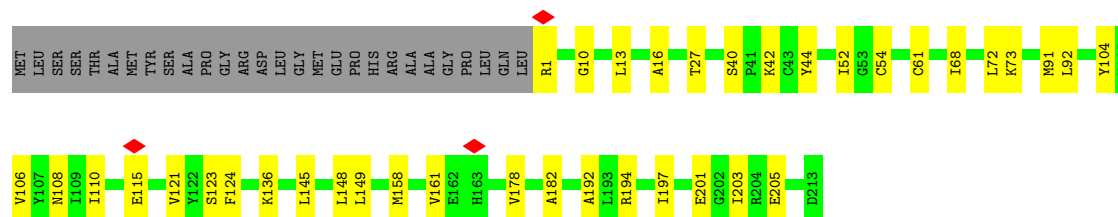
- Molecule 19: Proteasome subunit beta type-1

Chain S: 



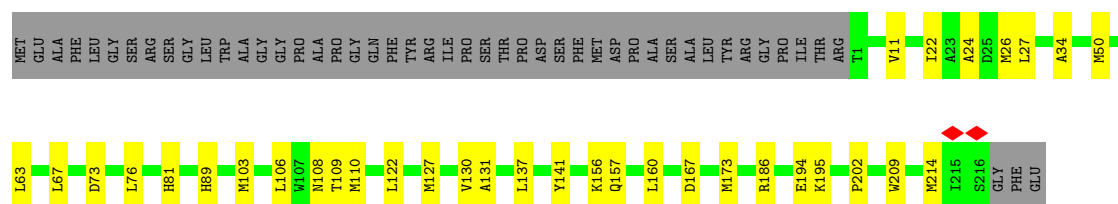
- Molecule 19: Proteasome subunit beta type-1

Chain s: 



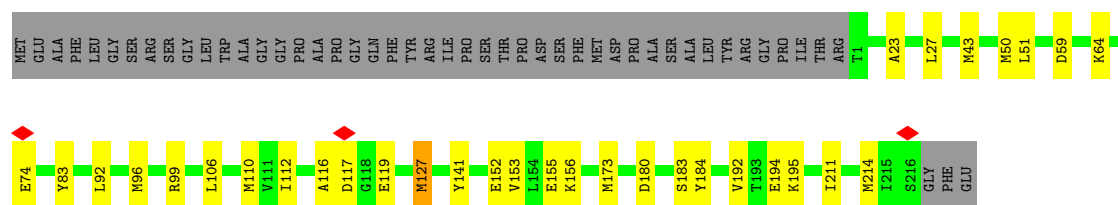
- Molecule 20: Proteasome subunit beta type-4

Chain T: 



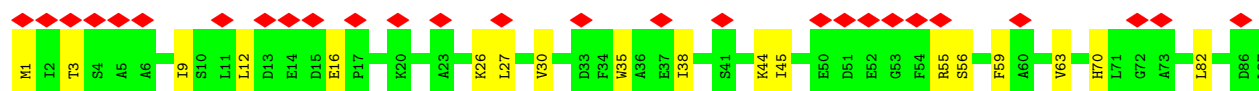
- Molecule 20: Proteasome subunit beta type-4

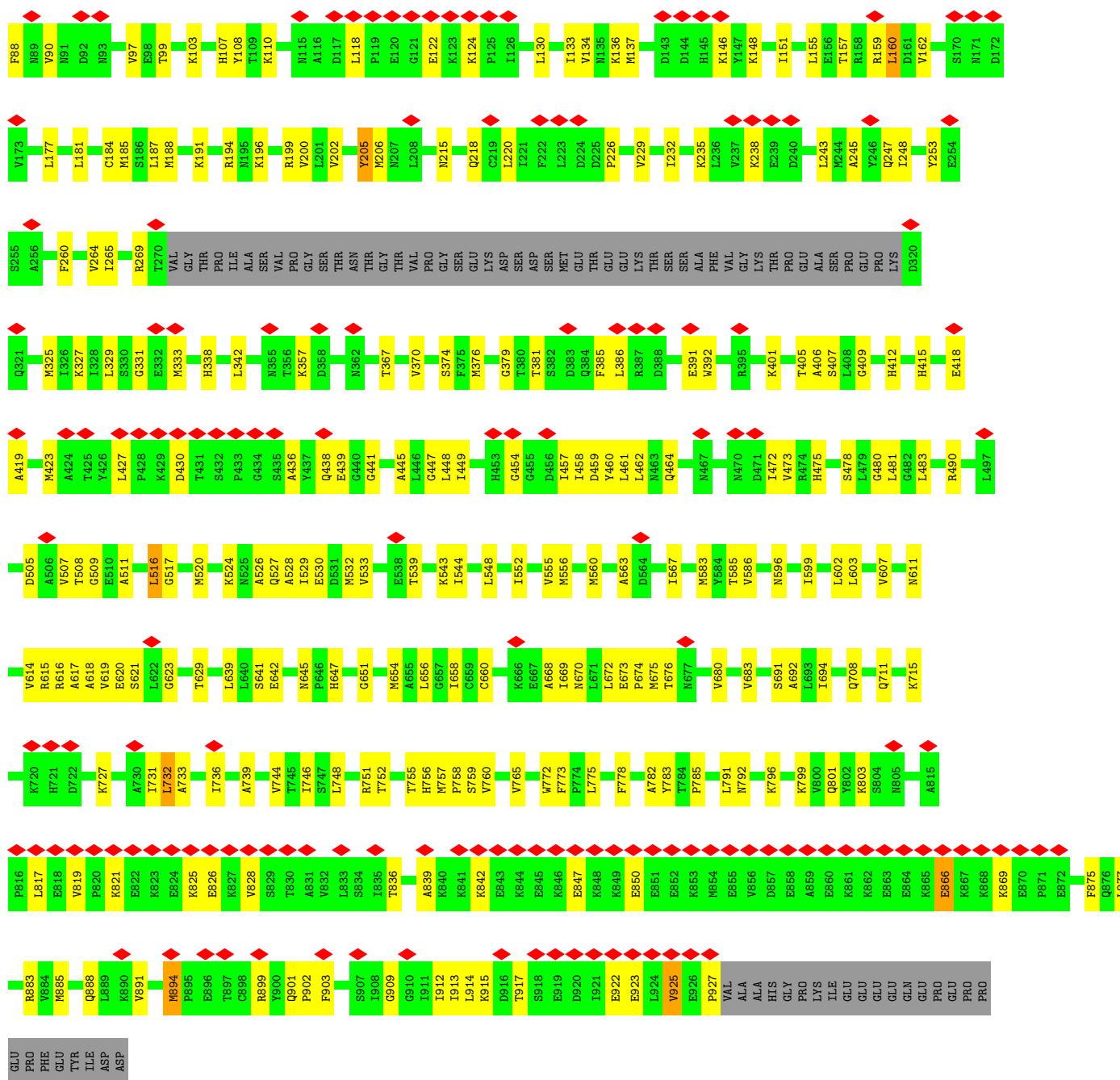
Chain t: 



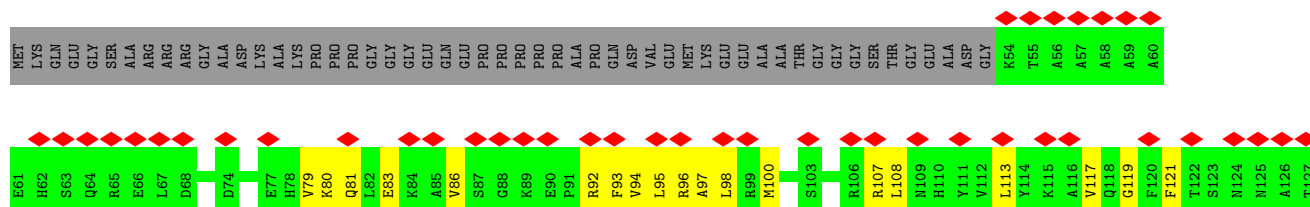
- Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

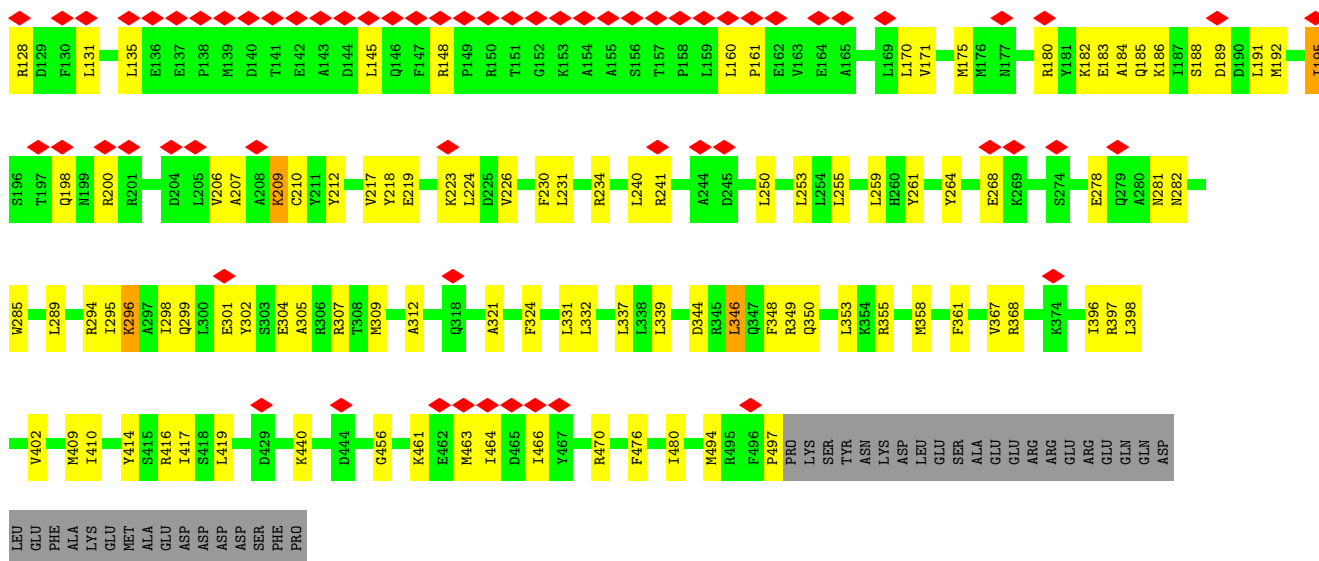
Chain U: 



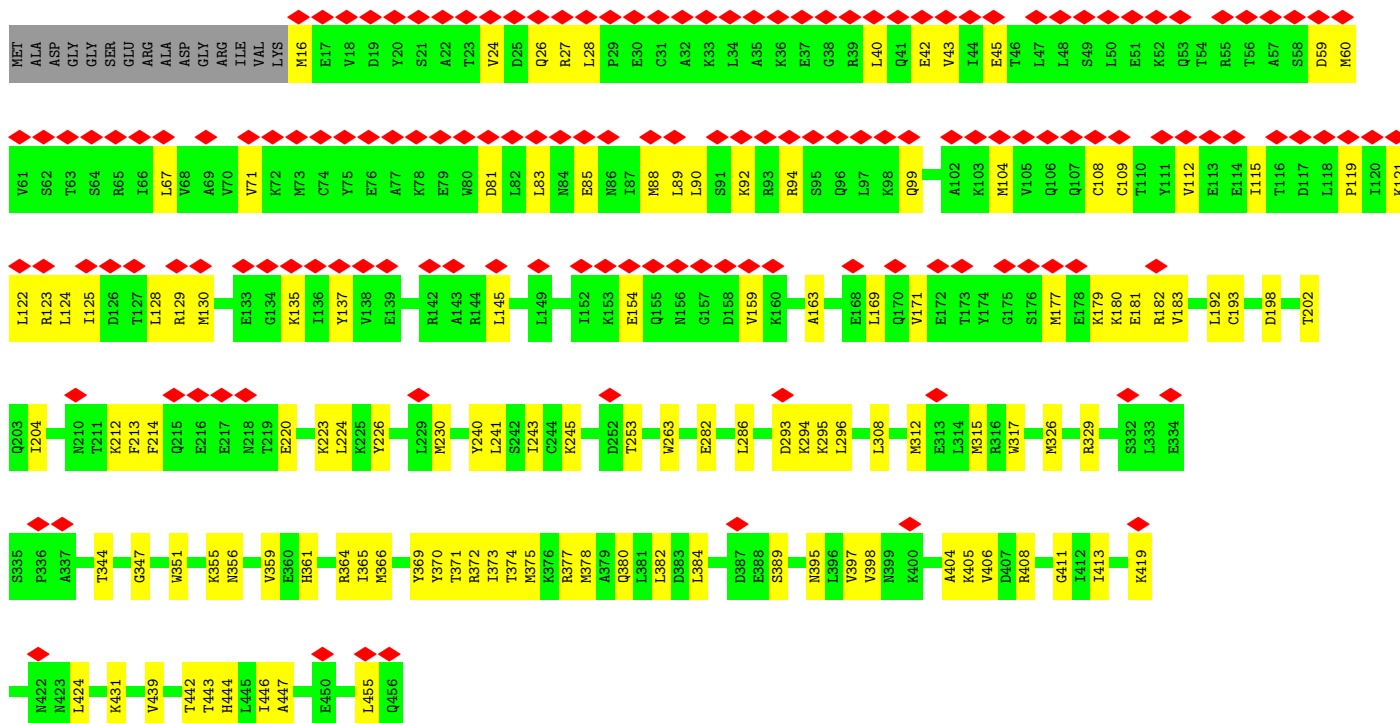
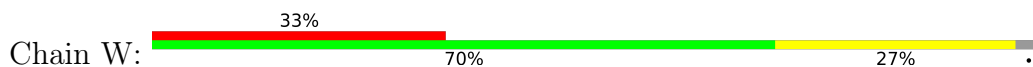


- Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

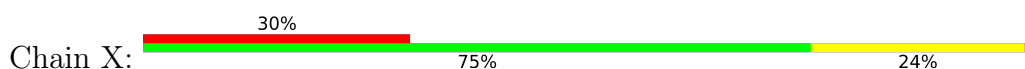


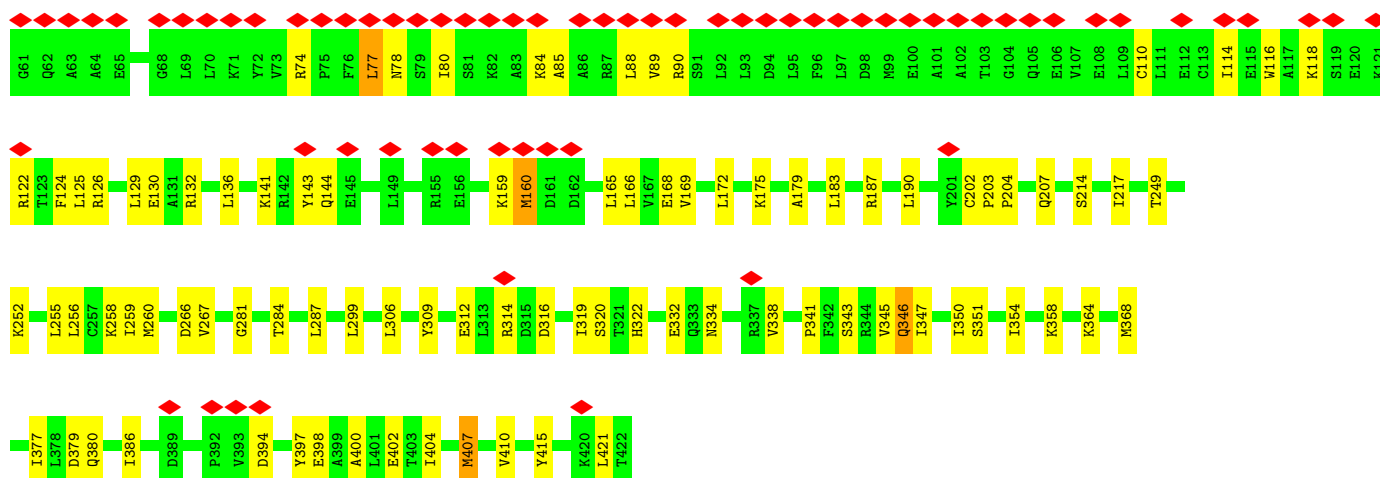


• Molecule 23: 26S proteasome non-ATPase regulatory subunit 12



• Molecule 24: 26S proteasome non-ATPase regulatory subunit 11





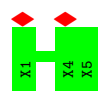
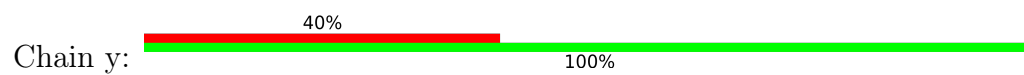




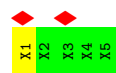
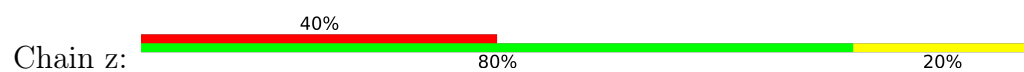




- Molecule 34: Substrates binding CP



- Molecule 34: Substrates binding CP



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	856683	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 ( $e^-/\text{\AA}^2$ )	44	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00594	Depositor
Map size (Å)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.17	0/3283	0.41	0/4433
2	B	0.19	0/3254	0.48	0/4388
3	C	0.20	0/3146	0.49	1/4226 (0.0%)
4	D	0.21	0/3090	0.54	2/4168 (0.0%)
5	E	0.19	0/3145	0.46	0/4233
6	F	0.19	0/3137	0.47	0/4223
7	G	0.13	0/1901	0.36	0/2572
7	g	0.17	0/1913	0.40	0/2589
8	H	0.14	0/1840	0.39	0/2495
8	h	0.13	0/1844	0.35	0/2497
9	I	0.20	0/1963	0.43	0/2650
9	i	0.14	0/1985	0.35	0/2677
10	J	0.17	0/1887	0.38	0/2553
10	j	0.14	0/1887	0.39	0/2549
11	K	0.14	0/1841	0.38	0/2486
11	k	0.15	0/1809	0.39	0/2444
12	L	0.14	0/1911	0.34	0/2584
12	l	0.14	0/1896	0.35	0/2565
13	M	0.13	0/1931	0.37	0/2600
13	m	0.13	0/1916	0.32	0/2580
14	N	0.20	0/1548	0.37	0/2097
14	n	0.13	0/1536	0.36	0/2080
15	O	0.13	0/1672	0.38	1/2267 (0.0%)
15	o	0.12	0/1686	0.36	0/2282
16	P	0.21	0/1616	0.42	0/2180
16	p	0.16	0/1620	0.42	0/2184
17	Q	0.13	0/1627	0.38	0/2202
17	q	0.18	0/1611	0.44	0/2182
18	R	0.15	0/1590	0.39	0/2147
18	r	0.14	0/1580	0.40	0/2135
19	S	0.16	0/1671	0.43	0/2252
19	s	0.13	0/1680	0.36	0/2264

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
20	T	0.16	0/1716	0.44	0/2323
20	t	0.17	0/1720	0.42	0/2328
21	U	0.16	0/6984	0.41	0/9435
22	V	0.18	0/3681	0.42	0/4969
23	W	0.14	0/3644	0.37	0/4901
24	X	0.17	0/3381	0.37	0/4558
25	Y	0.16	0/3261	0.39	1/4393 (0.0%)
26	Z	0.22	0/2324	0.49	0/3150
27	a	0.18	0/3053	0.46	0/4133
28	b	0.14	0/1478	0.42	0/2001
29	c	0.19	0/2302	0.51	0/3110
30	d	0.16	0/2162	0.44	0/2919
31	e	0.34	0/437	0.55	0/595
32	f	0.16	0/6640	0.48	2/8988 (0.0%)
All	All	0.17	0/107799	0.42	7/145587 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	f	113	MET	CA-C-N	14.78	140.94	120.39
32	f	113	MET	C-N-CA	14.78	140.94	120.39
25	Y	236	LEU	N-CA-C	-5.83	105.06	111.82
3	C	221	GLN	CB-CA-C	-5.56	110.15	116.54
4	D	384	MET	CB-CG-SD	5.37	128.82	112.70
4	D	384	MET	CA-CB-CG	5.31	124.71	114.10
15	O	37	ILE	N-CA-C	-5.29	107.68	112.12

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3229	0	3261	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3207	0	3277	93	0
3	C	3105	0	3219	64	0
4	D	3040	0	3076	89	0
5	E	3097	0	3174	95	0
6	F	3098	0	3187	69	0
7	G	1867	0	1867	23	0
7	g	1879	0	1872	22	0
8	H	1801	0	1773	20	0
8	h	1805	0	1798	15	0
9	I	1933	0	1923	28	0
9	i	1955	0	1955	24	0
10	J	1861	0	1846	31	0
10	j	1861	0	1865	50	0
11	K	1813	0	1796	11	0
11	k	1782	0	1766	37	0
12	L	1876	0	1856	30	0
12	l	1861	0	1839	28	0
13	M	1893	0	1885	21	0
13	m	1881	0	1868	27	0
14	N	1521	0	1494	16	0
14	n	1510	0	1483	10	0
15	O	1645	0	1648	20	0
15	o	1659	0	1681	18	0
16	P	1587	0	1598	19	0
16	p	1591	0	1609	32	0
17	Q	1591	0	1589	18	0
17	q	1578	0	1569	18	0
18	R	1559	0	1523	23	0
18	r	1549	0	1506	14	0
19	S	1641	0	1639	27	0
19	s	1650	0	1645	22	0
20	T	1683	0	1662	28	0
20	t	1687	0	1666	23	0
21	U	6867	0	6929	187	0
22	V	3612	0	3682	92	0
23	W	3596	0	3713	84	0
24	X	3335	0	3435	81	0
25	Y	3202	0	3204	81	0
26	Z	2281	0	2312	89	0
27	a	2995	0	3012	81	0
28	b	1458	0	1505	66	0
29	c	2260	0	2276	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	d	2116	0	2146	51	0
31	e	425	0	328	12	0
32	f	6529	0	6541	173	0
33	v	180	0	50	1	0
34	y	25	0	7	0	0
34	z	25	0	7	1	0
35	A	31	0	12	0	0
35	B	31	0	12	1	0
35	C	31	0	12	0	0
35	F	31	0	12	1	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
36	F	1	0	0	0	0
37	D	27	0	12	3	0
38	c	1	0	0	0	0
All	All	106358	0	106622	2008	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (2008) 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)
20:T:108:ASN:HB3	20:T:110:MET:HE1	1.36	1.08
16:p:88:MET:HE3	16:p:130:PRO:HB2	1.44	1.00
12:l:61:LYS:HE2	12:l:61:LYS:H	1.36	0.91
19:S:147:PRO:HB2	16:p:149:MET:HE1	1.55	0.89
29:c:113:HIS:NE2	29:c:115:HIS:CE1	2.41	0.88
10:j:36:ARG:HH21	10:j:157:LYS:HG2	1.39	0.87
30:d:203:PRO:HD2	30:d:206:MET:HE1	1.56	0.86
28:b:110:ILE:HG22	28:b:139:ASP:HB2	1.58	0.85
32:f:407:MET:HE3	32:f:407:MET:H	1.41	0.85
32:f:415:GLY:HA3	32:f:447:ALA:HB1	1.57	0.84
16:p:71:LEU:HD11	16:p:82:ILE:HG21	1.58	0.84
24:X:258:LYS:HD3	24:X:266:ASP:HB3	1.60	0.84
32:f:216:MET:HE3	32:f:216:MET:H	1.43	0.83
28:b:157:VAL:HG21	28:b:170:LEU:HB2	1.59	0.82
21:U:333:MET:HE3	21:U:333:MET:H	1.44	0.82
22:V:309:MET:HE1	22:V:331:LEU:HB3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:143:TYR:HB2	9:i:146:GLN:HE21	1.44	0.81
31:e:25:GLU:HG3	31:e:27:TRP:H	1.47	0.80
4:D:157:ASP:H	4:D:159:LYS:HZ2	1.30	0.80
18:R:45:MET:HE1	18:R:49:ALA:HA	1.65	0.79
26:Z:209:ARG:HH22	27:a:354:GLU:HA	1.48	0.79
7:g:128:ASN:HB2	7:g:131:MET:HE1	1.63	0.79
4:D:200:ARG:HH12	4:D:302:ASN:HA	1.48	0.78
5:E:148:VAL:HB	5:E:297:ARG:HH21	1.47	0.78
30:d:164:THR:HA	30:d:167:ILE:HG12	1.63	0.78
9:I:22:GLU:HA	9:I:25:MET:HB2	1.66	0.78
10:j:158:ALA:H	11:k:58:LEU:HD11	1.49	0.78
21:U:894:MET:HE1	21:U:901:GLN:HB3	1.65	0.78
25:Y:69:LEU:O	25:Y:73:MET:HB2	1.84	0.77
11:k:210:LEU:HA	11:k:214:ASN:HD21	1.50	0.76
23:W:405:LYS:HG2	24:X:343:SER:HB3	1.66	0.76
4:D:152:MET:HE3	4:D:152:MET:H	1.50	0.76
6:F:53:LYS:HD2	28:b:27:GLN:HB3	1.68	0.75
3:C:165:ILE:HG22	3:C:166:GLU:HG3	1.66	0.75
13:m:37:ILE:HD11	13:m:193:VAL:HG13	1.69	0.75
16:p:149:MET:HG2	16:p:170:ALA:HA	1.68	0.75
25:Y:231:LEU:HD11	25:Y:239:LYS:HZ2	1.51	0.75
13:M:27:MET:HE3	13:M:27:MET:HA	1.69	0.74
21:U:505:ASP:HB3	21:U:508:THR:HG22	1.67	0.74
20:t:92:LEU:HD12	20:t:112:ILE:HD11	1.69	0.74
5:E:168:LYS:HZ3	5:E:274:LYS:HD3	1.52	0.74
22:V:175:MET:HE1	22:V:180:ARG:H	1.52	0.74
11:k:13:ASN:HB2	12:l:126:ARG:HB3	1.69	0.74
21:U:656:LEU:HD11	21:U:668:ALA:HB1	1.69	0.73
22:V:289:LEU:HB3	22:V:312:ALA:HB2	1.69	0.73
26:Z:102:HIS:HD2	26:Z:104:ASN:HB3	1.53	0.73
27:a:222:LEU:HB2	27:a:226:ARG:HH21	1.54	0.73
2:B:385:MET:O	2:B:385:MET:HE3	1.87	0.73
7:G:80:MET:HE3	7:G:80:MET:HA	1.70	0.73
23:W:112:VAL:HG21	23:W:125:ILE:HD11	1.70	0.73
32:f:398:TRP:HA	32:f:401:LYS:HD3	1.71	0.72
26:Z:176:LEU:HD23	26:Z:177:ARG:H	1.52	0.72
29:c:167:MET:HB3	29:c:170:LEU:HB3	1.71	0.72
1:A:164:MET:HE1	1:A:241:ILE:HG12	1.72	0.72
5:E:124:HIS:HE1	5:E:197:LYS:HB2	1.55	0.72
9:I:143:TYR:HB2	9:I:146:GLN:HE21	1.55	0.72
22:V:231:LEU:HD13	22:V:250:LEU:HD23	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:6:THR:HB	28:b:49:VAL:HG22	1.72	0.72
4:D:352:MET:HE3	4:D:352:MET:HA	1.72	0.71
5:E:352:MET:HE2	5:E:352:MET:HA	1.71	0.71
21:U:457:ILE:O	21:U:461:LEU:HD12	1.90	0.71
7:g:191:PHE:HE1	7:g:219:VAL:HG21	1.55	0.71
31:e:59:GLU:HA	31:e:62:LYS:HD3	1.73	0.71
3:C:406:LYS:HE2	9:I:80:THR:HG22	1.73	0.71
21:U:235:LYS:HA	21:U:238:LYS:HD2	1.72	0.71
1:A:394:MET:HE1	2:B:219:PRO:HD3	1.72	0.71
11:K:235:GLU:HA	11:K:238:ILE:HG12	1.72	0.71
2:B:41:LYS:HB2	2:B:278:ALA:HB2	1.73	0.71
21:U:133:ILE:HG12	21:U:137:MET:HE1	1.73	0.71
1:A:422:LYS:HD3	1:A:425:ALA:HB3	1.73	0.70
29:c:226:MET:HA	29:c:226:MET:HE3	1.73	0.70
6:F:224:LEU:HB2	6:F:348:LEU:HD13	1.72	0.70
4:D:93:LEU:HD12	4:D:102:ILE:HG22	1.73	0.70
15:O:135:MET:HE2	15:O:139:GLU:HG2	1.73	0.70
21:U:243:LEU:HD21	21:U:913:ILE:HD13	1.73	0.70
21:U:619:VAL:HG23	21:U:651:GLY:HA3	1.73	0.70
21:U:902:PRO:HA	21:U:915:LYS:H	1.55	0.70
23:W:154:GLU:HG2	23:W:159:VAL:HG12	1.72	0.70
21:U:338:HIS:HE1	21:U:785:PRO:HB3	1.56	0.70
21:U:611:ASN:HB3	21:U:614:VAL:HG12	1.74	0.70
21:U:641:SER:HB2	21:U:675:MET:HE2	1.72	0.70
32:f:487:LEU:HD21	32:f:822:VAL:HG21	1.73	0.70
13:M:67:PHE:HB2	13:M:75:MET:HB3	1.74	0.70
29:c:303:MET:HE1	30:d:242:LEU:HB2	1.73	0.70
32:f:268:LEU:HA	32:f:271:MET:SD	2.31	0.70
20:t:23:ALA:HB1	20:t:173:MET:HE2	1.72	0.70
24:X:255:LEU:HD22	24:X:267:VAL:HG13	1.74	0.70
28:b:65:THR:HG22	28:b:70:ARG:HH21	1.56	0.70
22:V:355:ARG:HH12	22:V:358:MET:HG2	1.56	0.70
24:X:397:TYR:HE1	26:Z:257:MET:HG2	1.56	0.70
32:f:478:ARG:HH12	32:f:509:LYS:HD2	1.57	0.69
1:A:32:LEU:O	1:A:36:TYR:HB2	1.92	0.69
6:F:50:SER:HA	6:F:53:LYS:HE2	1.74	0.69
3:C:248:MET:HE3	3:C:248:MET:HA	1.73	0.69
3:C:351:MET:HA	3:C:351:MET:HE3	1.73	0.69
21:U:185:MET:HG3	21:U:218:GLN:HE22	1.56	0.69
9:i:174:MET:HE3	9:i:196:VAL:HG23	1.74	0.69
10:j:120:GLN:HE21	11:k:133:MET:HE1	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:LEU:HB2	2:B:266:LEU:HD11	1.75	0.69
21:U:338:HIS:CE1	21:U:785:PRO:HB3	2.28	0.69
2:B:220:LYS:HB3	2:B:322:ARG:HH21	1.57	0.69
21:U:799:LYS:H	21:U:923:GLU:HB3	1.57	0.69
22:V:470:ARG:HH22	26:Z:249:PHE:HB3	1.58	0.69
24:X:309:TYR:HB3	24:X:312:GLU:HB2	1.74	0.69
26:Z:39:LEU:HD13	26:Z:95:TYR:HB3	1.75	0.69
23:W:366:MET:O	23:W:370:TYR:HB2	1.92	0.69
29:c:32:TYR:HB3	29:c:208:ARG:HH11	1.58	0.69
29:c:145:VAL:HG22	29:c:157:ILE:HG13	1.73	0.68
30:d:145:GLU:HG2	30:d:146:GLY:H	1.59	0.68
5:E:8:ALA:HB1	6:F:40:GLU:HG3	1.74	0.68
24:X:203:PRO:HB2	24:X:207:GLN:HB2	1.74	0.68
27:a:245:VAL:HG21	27:a:301:LYS:HG2	1.75	0.68
5:E:251:ARG:HH22	5:E:284:THR:HB	1.59	0.68
7:G:202:LEU:HA	7:G:205:VAL:HG12	1.75	0.68
9:i:178:ASP:OD2	9:i:192:LEU:HD11	1.93	0.68
15:o:187:ARG:HB3	15:o:188:PRO:HD3	1.74	0.68
29:c:57:MET:HE1	29:c:112:TYR:HB3	1.76	0.68
6:F:36:MET:HA	6:F:36:MET:HE3	1.75	0.68
18:R:148:GLU:HB2	18:R:151:GLN:HG3	1.76	0.68
20:t:92:LEU:O	20:t:96:MET:HG2	1.95	0.67
16:P:12:MET:HG3	16:P:138:VAL:HG12	1.75	0.67
22:V:494:MET:HE2	22:V:494:MET:HA	1.77	0.67
4:D:319:PRO:HA	4:D:322:LEU:HG	1.75	0.67
5:E:149:ILE:HD11	5:E:274:LYS:HB3	1.77	0.67
7:G:80:MET:HG3	7:G:87:SER:HB3	1.75	0.67
7:G:206:LEU:HB3	7:G:208:ILE:HG12	1.76	0.67
12:L:84:LEU:O	12:L:88:MET:HG3	1.95	0.67
21:U:866:GLU:HG2	21:U:869:LYS:HZ3	1.58	0.67
23:W:112:VAL:HA	23:W:115:ILE:HD12	1.76	0.67
2:B:188:GLY:HA3	2:B:364:ILE:HD13	1.76	0.67
3:C:248:MET:HB3	3:C:251:ILE:HD11	1.76	0.67
10:J:120:GLN:HE21	11:K:133:MET:HE3	1.59	0.67
19:s:148:LEU:HD23	19:s:178:VAL:HG12	1.77	0.67
28:b:100:ARG:HD2	28:b:107:MET:HE1	1.76	0.66
10:j:157:LYS:HB2	11:k:58:LEU:HD21	1.76	0.66
1:A:206:ILE:HG12	6:F:404:GLY:HA3	1.76	0.66
9:I:119:GLN:HG3	10:J:78:ALA:HB1	1.76	0.66
23:W:293:ASP:HB2	23:W:296:LEU:HD23	1.75	0.66
8:H:111:VAL:HG22	8:H:136:ILE:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:53:LEU:HB3	16:P:60:VAL:HG22	1.77	0.66
10:j:192:ILE:HG21	10:j:229:VAL:HG12	1.77	0.66
28:b:63:THR:HG22	28:b:64:LEU:H	1.60	0.66
17:Q:4:LEU:HD22	17:Q:45:LEU:HD23	1.78	0.66
27:a:78:GLU:HA	27:a:81:LEU:HD23	1.78	0.66
28:b:26:LEU:HD21	28:b:78:VAL:HG21	1.77	0.66
15:O:22:GLU:HG2	15:O:27:ALA:HB2	1.77	0.66
15:O:124:TYR:HE1	15:O:135:MET:HE1	1.59	0.66
19:S:181:SER:HB3	16:p:151:GLU:HG3	1.78	0.66
3:C:99:VAL:HA	3:C:123:LEU:HB2	1.78	0.66
4:D:281:ALA:HB2	33:v:13:UNK:HA	1.78	0.66
22:V:107:ARG:H	22:V:108:LEU:HD12	1.60	0.66
5:E:199:VAL:HG23	5:E:201:SER:H	1.61	0.66
25:Y:66:ASP:HB3	25:Y:69:LEU:HB3	1.78	0.66
26:Z:9:VAL:HG12	26:Z:48:LEU:HB3	1.78	0.66
8:H:75:VAL:HG12	8:H:135:LEU:HB2	1.78	0.65
20:T:156:LYS:HE2	20:T:156:LYS:H	1.61	0.65
27:a:374:ILE:HG22	30:d:255:MET:HE1	1.78	0.65
29:c:29:GLU:HB2	29:c:203:ILE:HD11	1.77	0.65
22:V:414:TYR:HD2	22:V:417:ILE:HD11	1.61	0.65
11:k:133:MET:HE2	11:k:133:MET:HA	1.78	0.65
6:F:94:ILE:HD11	6:F:125:LYS:HB2	1.78	0.65
5:E:175:PRO:HG3	5:E:303:LEU:HG	1.78	0.65
13:M:27:MET:HE1	13:M:153:PRO:HD2	1.78	0.65
25:Y:299:MET:HE2	25:Y:299:MET:HA	1.77	0.65
24:X:24:ILE:HG12	24:X:56:LEU:HD13	1.78	0.65
5:E:353:PHE:HA	5:E:356:ARG:HD2	1.77	0.65
21:U:819:VAL:HG22	21:U:821:LYS:H	1.60	0.65
4:D:384:MET:HB2	4:D:388:ARG:HH21	1.61	0.65
21:U:922:GLU:HG3	21:U:923:GLU:HG2	1.78	0.65
24:X:143:TYR:HD2	24:X:144:GLN:HG2	1.62	0.65
32:f:413:SER:HA	32:f:416:MET:HE3	1.79	0.65
4:D:309:MET:HE1	4:D:311:THR:HG23	1.79	0.64
6:F:356:MET:SD	6:F:357:PRO:HD2	2.37	0.64
2:B:405:MET:HA	2:B:405:MET:HE3	1.80	0.64
7:g:141:ILE:HG22	7:g:151:VAL:HG22	1.79	0.64
6:F:373:MET:HA	6:F:373:MET:HE3	1.79	0.64
16:P:123:SER:HB3	16:P:137:VAL:HG11	1.77	0.64
12:l:61:LYS:HE2	12:l:61:LYS:N	2.10	0.64
16:p:4:MET:HA	16:p:4:MET:HE3	1.80	0.64
21:U:16:GLU:HG3	30:d:27:LYS:HZ2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:49:VAL:HG22	7:G:219:VAL:HG12	1.79	0.64
11:k:228:MET:HE2	11:k:228:MET:HA	1.79	0.64
23:W:370:TYR:HB3	23:W:373:ILE:HD11	1.80	0.64
5:E:29:LEU:HB3	6:F:62:VAL:HG11	1.80	0.63
3:C:90:HIS:HB3	3:C:91:PRO:HD3	1.78	0.63
4:D:151:ILE:C	4:D:153:MET:H	2.07	0.63
19:S:193:LEU:HB3	19:S:208:VAL:HG12	1.81	0.63
25:Y:312:ARG:HA	25:Y:356:THR:HG22	1.80	0.63
16:p:53:LEU:HB3	16:p:60:VAL:HG22	1.80	0.63
15:O:78:THR:O	15:O:82:MET:HG3	1.98	0.63
28:b:100:ARG:HH12	28:b:105:HIS:HB2	1.63	0.63
10:j:96:LEU:HB2	17:q:62:LYS:HG3	1.79	0.63
2:B:266:LEU:HA	2:B:269:GLU:HG3	1.78	0.63
21:U:509:GLY:HA3	21:U:544:ILE:HG12	1.81	0.63
27:a:372:HIS:HA	27:a:375:LEU:HD12	1.81	0.63
29:c:52:GLU:HG2	29:c:82:VAL:HG21	1.79	0.63
30:d:96:HIS:HB3	30:d:130:ASN:HD21	1.63	0.63
32:f:807:ARG:HA	32:f:811:LEU:HD12	1.79	0.63
10:j:41:VAL:HG11	10:j:134:VAL:HB	1.81	0.63
9:I:53:HIS:CG	9:I:54:LYS:H	2.15	0.63
24:X:110:CYS:O	24:X:114:ILE:HG12	1.98	0.63
10:j:121:SER:HB2	10:j:124:ARG:HD2	1.79	0.63
4:D:45:LYS:HG2	21:U:187:LEU:HB2	1.81	0.63
10:J:99:GLU:OE1	18:R:81:LYS:HG2	1.99	0.62
23:W:89:LEU:HA	23:W:92:LYS:HE3	1.80	0.62
24:X:256:LEU:HD22	24:X:319:ILE:HG22	1.80	0.62
32:f:412:ALA:HA	32:f:447:ALA:HB2	1.81	0.62
10:J:42:VAL:HG22	10:J:210:VAL:HG12	1.81	0.62
2:B:191:ASP:O	2:B:195:GLN:HG3	1.99	0.62
4:D:177:VAL:HG21	4:D:215:LEU:HD21	1.82	0.62
27:a:289:ARG:HB3	27:a:333:MET:HE3	1.80	0.62
12:L:167:SER:HB3	12:L:197:GLU:HG3	1.81	0.62
21:U:457:ILE:H	21:U:457:ILE:HD12	1.65	0.62
26:Z:187:LEU:HG	29:c:293:THR:HG22	1.81	0.62
26:Z:67:VAL:HG12	28:b:95:LEU:HD22	1.81	0.62
32:f:205:CYS:O	32:f:209:MET:HG2	2.00	0.62
23:W:329:ARG:HE	23:W:351:TRP:HE1	1.48	0.62
21:U:751:ARG:HD2	21:U:909:GLY:H	1.64	0.61
22:V:349:ARG:HH12	31:e:37:HIS:HE1	1.48	0.61
17:q:25:ILE:HG23	17:q:26:VAL:HG12	1.82	0.61
4:D:154:LEU:HD11	4:D:229:ARG:HE	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:385:LEU:HD23	4:D:398:ASP:HB2	1.82	0.61
6:F:343:LEU:HD12	6:F:347:ARG:HB3	1.82	0.61
7:g:60:LEU:HD12	13:m:173:LYS:HG2	1.82	0.61
10:J:52:LYS:HG3	10:J:53:LEU:HG	1.82	0.61
6:F:35:LYS:HD2	6:F:38:THR:HB	1.82	0.61
22:V:81:GLN:HB3	22:V:93:PHE:HB3	1.82	0.61
29:c:94:LYS:O	29:c:98:MET:HG2	2.01	0.61
32:f:470:VAL:HG13	32:f:471:LEU:HG	1.80	0.61
11:k:107:MET:HE3	11:k:112:VAL:HG22	1.81	0.61
6:F:94:ILE:HD12	6:F:123:VAL:HG12	1.82	0.61
25:Y:233:ARG:N	25:Y:234:PRO:HD3	2.15	0.61
28:b:86:PHE:CE1	28:b:90:ILE:HD11	2.36	0.61
21:U:620:GLU:HG3	21:U:651:GLY:HA2	1.83	0.61
30:d:237:ILE:H	30:d:237:ILE:HD12	1.66	0.61
2:B:418:ASP:HA	2:B:421:LYS:HD3	1.83	0.61
17:Q:38:MET:HA	17:Q:38:MET:HE3	1.82	0.61
21:U:792:ASN:HB3	21:U:914:LEU:HB3	1.82	0.61
24:X:407:MET:HE1	29:c:252:ALA:HB1	1.83	0.61
25:Y:279:GLU:HG3	25:Y:296:VAL:HG21	1.82	0.61
29:c:155:VAL:HB	29:c:157:ILE:HD13	1.82	0.61
21:U:381:THR:HG22	21:U:412:HIS:HA	1.83	0.61
32:f:460:ASP:HB3	32:f:463:LEU:HB2	1.82	0.61
2:B:115:ILE:HD11	2:B:146:PRO:HD3	1.83	0.61
3:C:49:ARG:HD2	21:U:639:LEU:HD21	1.82	0.61
23:W:382:LEU:HB2	23:W:384:LEU:HD22	1.81	0.61
26:Z:224:HIS:HA	26:Z:228:TYR:CE2	2.36	0.61
6:F:86:LEU:HB3	6:F:87:PRO:HD3	1.83	0.60
25:Y:72:LYS:HA	25:Y:75:LYS:HE3	1.83	0.60
27:a:163:TYR:HB2	27:a:172:TYR:CD1	2.36	0.60
32:f:566:HIS:HB3	32:f:569:LYS:HD2	1.82	0.60
7:g:59:LYS:HD2	7:g:60:LEU:HD23	1.83	0.60
3:C:226:GLU:HA	3:C:229:ARG:HG2	1.82	0.60
6:F:141:ASP:H	6:F:144:LYS:HE2	1.65	0.60
27:a:254:ALA:HA	27:a:261:LEU:HD23	1.83	0.60
2:B:70:ASP:O	2:B:74:MET:HG2	2.02	0.60
10:J:222:PRO:HA	10:J:225:ILE:HB	1.83	0.60
2:B:232:LYS:HG2	2:B:353:PHE:HD2	1.66	0.60
21:U:903:PHE:HB2	21:U:915:LYS:HB2	1.84	0.60
22:V:414:TYR:CD2	22:V:417:ILE:HD11	2.36	0.60
23:W:67:LEU:HD12	23:W:90:LEU:HD13	1.83	0.60
5:E:282:PRO:HD2	5:E:388:PRO:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:100:MET:HE2	18:R:128:VAL:HG23	1.84	0.60
17:Q:38:MET:HE1	17:Q:61:GLN:HA	1.84	0.60
26:Z:63:LYS:HB3	28:b:91:ARG:NH1	2.16	0.60
28:b:109:ILE:HB	28:b:138:VAL:HG22	1.83	0.60
5:E:231:PHE:HA	5:E:276:ILE:HD11	1.84	0.60
4:D:60:TYR:HB2	21:U:603:LEU:HD11	1.84	0.60
9:I:180:LYS:HB2	9:I:184:MET:HE3	1.83	0.60
24:X:316:ASP:HB2	24:X:320:SER:HB3	1.83	0.60
24:X:404:ILE:HG21	25:Y:372:LYS:HB3	1.82	0.60
10:J:71:MET:HE3	10:J:73:PHE:HB3	1.84	0.60
27:a:226:ARG:HH12	27:a:233:LEU:HB3	1.67	0.60
27:a:212:ASN:HD22	27:a:240:PHE:HB3	1.66	0.59
5:E:135:ILE:HG12	5:E:182:LEU:HB3	1.83	0.59
19:S:13:LEU:HD11	19:S:149:LEU:HD11	1.83	0.59
21:U:386:LEU:HD23	21:U:386:LEU:H	1.67	0.59
24:X:319:ILE:HD12	24:X:320:SER:N	2.16	0.59
27:a:321:LYS:HZ1	27:a:336:VAL:HG22	1.66	0.59
1:A:139:ARG:HH22	1:A:156:LYS:H	1.50	0.59
20:T:156:LYS:HE2	20:T:156:LYS:N	2.16	0.59
27:a:335:TRP:HE1	27:a:337:GLN:HB3	1.67	0.59
32:f:521:ALA:HA	32:f:524:MET:HE3	1.82	0.59
12:l:88:MET:HB3	12:l:108:LEU:HD11	1.85	0.59
29:c:168:MET:HE2	29:c:168:MET:N	2.17	0.59
32:f:379:GLY:HA2	32:f:417:ILE:HD11	1.84	0.59
16:P:29:GLY:HA2	16:P:35:VAL:HG23	1.85	0.59
30:d:18:LYS:HB3	30:d:61:TRP:HH2	1.67	0.59
4:D:267:ILE:HG13	4:D:309:MET:SD	2.42	0.59
4:D:313:ARG:HH12	4:D:316:THR:HG22	1.68	0.59
26:Z:106:ILE:HA	26:Z:153:LYS:HE2	1.85	0.59
2:B:281:ILE:HG22	2:B:326:LYS:HB3	1.84	0.59
7:G:79:VAL:HG12	7:G:139:ILE:HB	1.83	0.59
22:V:108:LEU:HD21	22:V:170:LEU:HD21	1.84	0.59
13:m:42:LYS:HE2	13:m:183:GLU:HA	1.83	0.59
21:U:711:GLN:O	21:U:715:LYS:HE3	2.03	0.59
23:W:94:ARG:HE	23:W:94:ARG:H	1.49	0.59
4:D:164:TYR:HB2	4:D:222:HIS:CD2	2.38	0.59
32:f:216:MET:H	32:f:216:MET:CE	2.14	0.59
5:E:143:ARG:HA	5:E:146:ARG:HB3	1.84	0.59
6:F:41:ILE:HD13	6:F:44:ARG:HE	1.66	0.59
22:V:212:TYR:HA	22:V:253:LEU:HD11	1.85	0.59
32:f:407:MET:H	32:f:407:MET:CE	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:184:MET:HE2	9:I:184:MET:HA	1.85	0.58
23:W:419:LYS:HE3	23:W:424:LEU:HD22	1.85	0.58
25:Y:231:LEU:HD12	25:Y:234:PRO:HD2	1.83	0.58
32:f:94:LYS:HA	32:f:97:LYS:HD3	1.84	0.58
32:f:379:GLY:HA3	32:f:416:MET:HE1	1.85	0.58
1:A:177:VAL:HG22	1:A:224:LEU:HD13	1.85	0.58
2:B:360:THR:O	2:B:364:ILE:HG12	2.03	0.58
10:J:45:VAL:HG12	10:J:207:GLU:HB3	1.85	0.58
10:J:79:ASP:HB3	10:J:127:PHE:HD2	1.68	0.58
21:U:528:ALA:O	21:U:532:MET:HG2	2.03	0.58
27:a:34:TRP:HZ3	27:a:68:GLU:HA	1.69	0.58
1:A:277:ILE:HD13	1:A:327:LEU:HD11	1.84	0.58
4:D:116:LEU:HB3	4:D:119:ILE:HD12	1.84	0.58
4:D:266:GLU:HB2	4:D:311:THR:HG22	1.85	0.58
7:G:61:LEU:HD12	7:G:62:ASP:H	1.68	0.58
24:X:249:THR:HA	24:X:252:LYS:HD3	1.85	0.58
28:b:100:ARG:HH22	28:b:105:HIS:N	2.01	0.58
32:f:131:MET:HE1	32:f:161:HIS:HB3	1.83	0.58
17:q:38:MET:HB3	17:q:42:ILE:HB	1.84	0.58
20:t:74:GLU:HG3	20:t:83:TYR:CE2	2.38	0.58
2:B:201:VAL:HG21	2:B:328:ILE:HD11	1.86	0.58
2:B:342:ILE:HA	2:B:347:ILE:HD11	1.86	0.58
3:C:364:THR:O	3:C:368:MET:HG2	2.04	0.58
22:V:175:MET:O	22:V:175:MET:HE3	2.03	0.58
28:b:70:ARG:HH11	28:b:70:ARG:HG3	1.69	0.58
21:U:517:GLY:HA2	21:U:520:MET:HE2	1.85	0.58
24:X:347:ILE:HD12	24:X:358:LYS:HD3	1.84	0.58
23:W:372:ARG:HH11	27:a:327:VAL:HG21	1.69	0.58
24:X:314:ARG:O	24:X:314:ARG:HD3	2.04	0.58
28:b:8:VAL:HG12	28:b:110:ILE:HD11	1.85	0.58
28:b:25:ARG:CZ	28:b:145:GLU:H	2.17	0.58
32:f:350:LYS:HB3	32:f:353:LEU:HD21	1.86	0.58
7:g:180:GLU:HB3	8:h:56:LEU:HD21	1.85	0.58
3:C:63:LEU:HD23	4:D:79:VAL:HG22	1.85	0.58
17:Q:25:ILE:HG22	17:Q:26:VAL:HG13	1.86	0.58
19:S:198:VAL:HG22	19:S:203:ILE:HG12	1.85	0.58
25:Y:319:MET:HB2	25:Y:330:ILE:HD13	1.86	0.58
29:c:299:CYS:O	29:c:303:MET:HG3	2.03	0.58
1:A:258:ARG:HA	1:A:305:GLN:HE22	1.69	0.58
32:f:520:LEU:HD21	32:f:557:TRP:HB3	1.86	0.58
11:k:181:LEU:HA	11:k:184:VAL:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:214:MET:HE1	37:D:502:ADP:H2'	1.85	0.57
11:K:116:VAL:HG12	11:K:156:MET:HE1	1.85	0.57
20:T:109:THR:C	20:T:110:MET:HE3	2.28	0.57
27:a:252:LYS:HD2	27:a:255:TRP:HE1	1.69	0.57
32:f:822:VAL:HA	32:f:825:MET:HG3	1.86	0.57
10:j:95:ARG:HD2	17:q:62:LYS:HE3	1.86	0.57
17:q:13:VAL:HG11	17:q:105:ALA:HB1	1.85	0.57
19:s:123:SER:HB3	19:s:136:LYS:HG2	1.86	0.57
27:a:13:ASN:HA	27:a:18:GLN:HG2	1.86	0.57
30:d:238:PRO:HA	30:d:241:GLU:HG2	1.86	0.57
12:l:47:VAL:HG22	12:l:195:LEU:HD22	1.85	0.57
12:l:72:ILE:HG21	12:l:88:MET:HE1	1.85	0.57
20:t:99:ARG:HD3	20:t:106:LEU:HG	1.85	0.57
2:B:31:THR:HG23	2:B:32:ARG:HG2	1.85	0.57
9:I:53:HIS:CG	9:I:54:LYS:N	2.71	0.57
21:U:56:SER:HB3	21:U:59:PHE:HB2	1.86	0.57
22:V:368:ARG:HH12	31:e:43:TRP:HB3	1.69	0.57
23:W:16:MET:HE1	23:W:59:ASP:HA	1.87	0.57
29:c:41:MET:HA	29:c:41:MET:HE3	1.86	0.57
19:s:158:MET:HE3	19:s:161:VAL:HG11	1.85	0.57
23:W:369:TYR:HB2	27:a:312:MET:HE1	1.87	0.57
32:f:133:MET:H	32:f:133:MET:HE3	1.69	0.57
1:A:55:LEU:HA	1:A:58:LYS:HE2	1.86	0.57
21:U:543:LYS:HD3	29:c:65:TYR:HE1	1.69	0.57
18:r:113:TYR:O	18:r:120:ARG:HA	2.05	0.57
3:C:254:ILE:HG22	3:C:269:VAL:HG13	1.84	0.57
6:F:125:LYS:HG3	6:F:131:THR:HG22	1.86	0.57
26:Z:106:ILE:HG23	26:Z:153:LYS:HG3	1.86	0.57
27:a:269:LEU:HD23	27:a:272:ILE:HD11	1.87	0.57
30:d:98:LEU:HA	30:d:101:LEU:HD12	1.86	0.57
15:o:153:ASN:O	15:o:157:GLU:HG2	2.05	0.57
3:C:268:GLU:HA	3:C:271:ARG:HG3	1.86	0.57
11:K:50:VAL:HG22	11:K:216:GLU:HB2	1.86	0.57
15:O:123:PRO:HB3	20:t:214:MET:HE3	1.86	0.57
26:Z:102:HIS:CD2	26:Z:104:ASN:HB3	2.36	0.57
26:Z:146:ASP:HB2	26:Z:149:THR:HB	1.86	0.57
23:W:308:LEU:HB3	23:W:315:MET:HE1	1.85	0.57
2:B:103:ARG:HB3	2:B:160:ILE:HG21	1.86	0.57
32:f:478:ARG:HH11	32:f:510:SER:HB3	1.69	0.57
3:C:307:ARG:HH11	3:C:309:GLY:HA3	1.68	0.57
5:E:7:LYS:HA	5:E:10:GLN:NE2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:24:VAL:O	23:W:28:LEU:HG	2.05	0.56
15:o:32:SER:HB2	15:o:187:ARG:HH21	1.70	0.56
17:q:182:ILE:HD11	17:q:191:LEU:HD11	1.86	0.56
2:B:438:LEU:HD13	9:I:25:MET:HE1	1.87	0.56
3:C:142:LYS:HG2	3:C:144:PRO:HD3	1.87	0.56
3:C:254:ILE:O	3:C:254:ILE:HD12	2.04	0.56
21:U:90:VAL:HG13	21:U:136:LYS:HD3	1.86	0.56
27:a:35:HIS:CE1	28:b:17:ARG:HB2	2.40	0.56
5:E:348:THR:HA	6:F:217:ILE:HD12	1.87	0.56
6:F:78:GLU:HA	6:F:81:LYS:HG2	1.86	0.56
12:L:47:VAL:HG12	12:L:195:LEU:HD22	1.87	0.56
18:R:62:GLN:HA	18:R:65:ILE:HD12	1.85	0.56
21:U:376:MET:HA	21:U:739:ALA:HA	1.86	0.56
21:U:520:MET:HG3	21:U:555:VAL:HG23	1.88	0.56
26:Z:25:ARG:HH21	29:c:104:ARG:H	1.53	0.56
28:b:24:THR:HG22	28:b:26:LEU:H	1.70	0.56
32:f:82:ILE:O	32:f:86:THR:HG22	2.05	0.56
32:f:845:ARG:HG2	32:f:865:PHE:HB2	1.88	0.56
7:g:206:LEU:HB3	7:g:208:ILE:HD13	1.87	0.56
13:m:179:LEU:HD21	13:m:192:GLU:HB3	1.87	0.56
6:F:295:ARG:HG2	6:F:307:GLN:HE21	1.71	0.56
22:V:304:GLU:HA	22:V:307:ARG:HG2	1.88	0.56
10:j:185:ASP:O	10:j:189:LYS:HG2	2.06	0.56
2:B:284:ILE:HD13	2:B:287:ILE:HD13	1.87	0.56
21:U:448:LEU:HA	21:U:483:LEU:HD23	1.86	0.56
28:b:25:ARG:HH22	28:b:145:GLU:HB2	1.71	0.56
30:d:61:TRP:HB3	30:d:65:ARG:HH22	1.70	0.56
13:M:108:LEU:HD22	13:M:139:SER:HB3	1.87	0.56
21:U:801:GLN:HB3	21:U:877:LEU:HB3	1.88	0.56
21:U:902:PRO:HB3	21:U:914:LEU:HG	1.87	0.56
21:U:925:VAL:HG22	21:U:927:PRO:HD3	1.86	0.56
20:t:153:VAL:HA	20:t:156:LYS:NZ	2.20	0.56
2:B:71:TYR:CE1	32:f:667:GLY:HA2	2.40	0.56
12:L:88:MET:HE3	12:L:112:ILE:HD11	1.87	0.56
21:U:333:MET:H	21:U:333:MET:CE	2.16	0.56
21:U:616:ARG:HG3	21:U:647:HIS:HB3	1.87	0.56
5:E:188:ALA:HB2	5:E:195:PHE:HE2	1.70	0.56
23:W:344:THR:HG23	23:W:347:GLY:H	1.71	0.56
26:Z:190:ARG:O	26:Z:194:GLN:HG2	2.06	0.56
30:d:6:LYS:HD2	30:d:10:ASN:HD21	1.71	0.56
32:f:447:ALA:O	32:f:451:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:665:GLU:O	32:f:669:GLU:HG2	2.06	0.56
20:t:110:MET:HA	20:t:110:MET:HE3	1.86	0.56
5:E:247:THR:HG22	5:E:248:SER:H	1.70	0.56
13:M:197:ILE:HG21	13:M:211:LEU:HD13	1.88	0.56
20:T:195:LYS:HE2	20:T:195:LYS:N	2.20	0.56
24:X:397:TYR:CE1	26:Z:257:MET:HG2	2.40	0.56
27:a:87:MET:HG3	27:a:88:THR:N	2.21	0.56
2:B:247:PHE:CD2	2:B:281:ILE:HD11	2.41	0.56
25:Y:50:MET:N	25:Y:73:MET:HE1	2.20	0.56
4:D:57:GLN:O	4:D:61:ILE:HG12	2.06	0.55
32:f:789:SER:O	32:f:793:VAL:HG12	2.06	0.55
6:F:402:GLU:HA	6:F:405:MET:HE3	1.88	0.55
19:S:58:HIS:HB3	20:T:130:VAL:HG22	1.88	0.55
11:k:91:LYS:HG2	11:k:119:LEU:HD11	1.87	0.55
1:A:36:TYR:HE1	32:f:157:GLU:HG3	1.71	0.55
7:G:187:PHE:HB2	7:G:189:TRP:CD1	2.42	0.55
2:B:198:LYS:HG2	2:B:202:GLU:OE2	2.05	0.55
20:T:209:TRP:HB2	14:n:190:LEU:HD13	1.89	0.55
21:U:458:ILE:HD13	21:U:490:ARG:HH22	1.72	0.55
23:W:119:PRO:O	23:W:123:ARG:HG2	2.06	0.55
26:Z:212:LEU:HD21	27:a:350:LYS:HG3	1.89	0.55
32:f:407:MET:HB2	32:f:440:ILE:HD11	1.89	0.55
22:V:121:PHE:HB3	22:V:128:ARG:HD2	1.89	0.55
25:Y:81:LEU:HD22	25:Y:107:LYS:HZ1	1.72	0.55
16:p:138:VAL:HB	16:p:146:MET:HE2	1.89	0.55
3:C:43:ARG:HD2	22:V:497:PRO:HA	1.88	0.55
25:Y:191:ILE:HA	31:e:39:TRP:NE1	2.22	0.55
32:f:477:MET:C	32:f:477:MET:HE2	2.32	0.55
9:i:46:ALA:HB1	9:i:197:LEU:HD11	1.88	0.55
8:H:203:MET:HA	8:H:207:ASN:HD21	1.71	0.55
19:S:13:LEU:HD12	19:S:145:LEU:HD13	1.89	0.55
22:V:96:ARG:O	22:V:100:MET:HE3	2.07	0.55
22:V:97:ALA:HA	22:V:100:MET:HE1	1.88	0.55
22:V:145:LEU:HD23	22:V:145:LEU:H	1.72	0.55
24:X:126:ARG:O	24:X:130:GLU:HG2	2.06	0.55
26:Z:21:ASP:O	26:Z:25:ARG:HG3	2.06	0.55
32:f:408:LEU:HB3	32:f:439:TYR:HB3	1.86	0.55
6:F:73:ILE:HG23	6:F:74:LYS:N	2.22	0.55
14:N:72:GLU:HG2	14:N:73:PRO:HD2	1.87	0.55
20:T:173:MET:HE2	20:T:173:MET:HA	1.89	0.55
21:U:439:GLU:HG3	21:U:473:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:252:LYS:HA	27:a:255:TRP:CE2	2.42	0.55
32:f:137:ARG:HD3	32:f:168:LYS:NZ	2.22	0.55
2:B:221:GLY:HA3	2:B:347:ILE:HA	1.89	0.55
5:E:15:LYS:HB3	6:F:47:LEU:HG	1.88	0.55
5:E:258:MET:HA	5:E:258:MET:HE3	1.87	0.55
10:J:42:VAL:HG11	10:J:191:VAL:HG21	1.88	0.55
21:U:883:ARG:HH22	21:U:885:MET:HE1	1.72	0.55
25:Y:151:TYR:C	25:Y:152:MET:HE2	2.32	0.55
25:Y:283:LYS:HA	25:Y:288:PHE:CZ	2.41	0.55
30:d:190:LEU:HD22	30:d:191:PHE:H	1.72	0.55
32:f:502:LEU:HG	32:f:503:PRO:HD3	1.88	0.55
32:f:585:GLU:HG3	32:f:586:PRO:HD3	1.88	0.55
7:g:138:MET:HA	7:g:138:MET:HE3	1.88	0.55
11:k:46:VAL:HG11	11:k:144:GLY:HA3	1.89	0.55
13:m:108:LEU:HD13	13:m:147:GLN:HB2	1.89	0.55
3:C:307:ARG:HD2	3:C:309:GLY:H	1.73	0.54
5:E:314:LYS:HZ2	5:E:328:TYR:HD2	1.55	0.54
7:G:165:ALA:HB1	7:G:179:LEU:HD13	1.89	0.54
25:Y:75:LYS:HD2	25:Y:76:ALA:N	2.22	0.54
23:W:171:VAL:HG12	23:W:182:ARG:HG3	1.89	0.54
29:c:221:HIS:CD2	29:c:222:LYS:HG2	2.42	0.54
32:f:470:VAL:HG23	32:f:482:ILE:HG22	1.89	0.54
2:B:49:LEU:HD21	32:f:669:GLU:HG3	1.88	0.54
21:U:744:VAL:HG21	21:U:783:TYR:HB3	1.89	0.54
23:W:455:LEU:HD11	26:Z:103:LYS:HA	1.89	0.54
26:Z:25:ARG:HH12	29:c:99:LEU:HD21	1.72	0.54
26:Z:191:ILE:HG21	27:a:374:ILE:HD11	1.88	0.54
30:d:145:GLU:HG2	30:d:146:GLY:N	2.22	0.54
8:h:79:MET:H	8:h:132:VAL:HG12	1.71	0.54
9:i:113:ALA:O	9:i:117:ILE:HG23	2.08	0.54
16:P:34:MET:C	16:P:34:MET:HE3	2.33	0.54
21:U:12:LEU:HB2	21:U:44:LYS:HZ2	1.73	0.54
21:U:27:LEU:HD11	21:U:38:ILE:HD13	1.89	0.54
24:X:377:ILE:HG22	24:X:386:ILE:HB	1.90	0.54
19:s:16:ALA:HB2	19:s:121:VAL:HG23	1.90	0.54
1:A:319:MET:HE3	1:A:319:MET:N	2.23	0.54
10:J:40:ILE:HD11	10:J:210:VAL:HB	1.89	0.54
12:L:107:ARG:NH2	20:T:81:HIS:HB2	2.22	0.54
20:T:11:VAL:HG13	20:T:24:ALA:HB2	1.90	0.54
22:V:98:LEU:HB3	22:V:209:LYS:HE2	1.89	0.54
25:Y:92:GLU:HG3	25:Y:100:ILE:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:152:MET:HE2	25:Y:152:MET:N	2.22	0.54
32:f:96:LEU:HD13	32:f:129:LEU:HD13	1.90	0.54
16:p:35:VAL:HG12	16:p:36:THR:HG23	1.90	0.54
3:C:251:ILE:H	3:C:295:THR:HB	1.71	0.54
7:G:212:PRO:HB2	7:G:232:GLU:HG3	1.89	0.54
22:V:117:VAL:HG11	22:V:131:LEU:HD11	1.88	0.54
23:W:377:ARG:HA	23:W:380:GLN:HG2	1.89	0.54
24:X:364:LYS:O	24:X:368:MET:HG2	2.06	0.54
15:o:97:ALA:HB1	15:o:127:MET:HE3	1.90	0.54
5:E:210:GLU:HG3	5:E:213:ARG:HH21	1.73	0.54
6:F:69:MET:O	6:F:73:ILE:HG22	2.08	0.54
6:F:343:LEU:H	6:F:343:LEU:HD22	1.73	0.54
21:U:151:ILE:O	21:U:155:LEU:HG	2.07	0.54
26:Z:223:ASN:ND2	26:Z:227:ILE:HG12	2.23	0.54
7:g:120:ASP:O	7:g:124:VAL:HG23	2.08	0.54
9:i:201:MET:HE2	9:i:201:MET:HA	1.88	0.54
18:r:45:MET:HE3	18:r:52:CYS:HB2	1.89	0.54
2:B:309:MET:HE3	2:B:310:LEU:N	2.23	0.54
12:L:200:PRO:HD2	12:L:203:GLN:HG3	1.90	0.54
19:S:41:PRO:HB3	19:S:194:ARG:HD3	1.89	0.54
26:Z:77:ASN:HB3	29:c:98:MET:HE1	1.90	0.54
26:Z:192:THR:HG22	27:a:375:LEU:HD23	1.88	0.54
10:j:211:MET:HG3	10:j:217:LEU:HB3	1.90	0.54
2:B:60:LEU:O	2:B:64:LYS:HG2	2.08	0.54
2:B:250:VAL:HB	2:B:284:ILE:HG22	1.90	0.54
5:E:260:LEU:O	5:E:264:MET:HG3	2.08	0.54
12:L:45:VAL:HG12	12:L:214:ILE:HG12	1.89	0.54
12:L:64:LEU:HD12	12:L:72:ILE:HD11	1.89	0.54
21:U:9:ILE:HA	21:U:12:LEU:HD12	1.88	0.54
25:Y:201:PHE:HB3	25:Y:223:THR:OG1	2.08	0.54
11:k:217:LEU:HB2	11:k:234:LEU:HD21	1.90	0.54
5:E:172:LEU:HA	5:E:299:ILE:HG23	1.90	0.54
20:T:122:LEU:HG	20:T:137:LEU:HD12	1.89	0.54
24:X:334:ASN:HB3	24:X:354:ILE:HD11	1.90	0.54
26:Z:19:VAL:HG21	26:Z:124:ILE:HD13	1.90	0.54
27:a:317:VAL:HG23	27:a:319:LEU:HG	1.90	0.54
30:d:204:LYS:HD2	30:d:204:LYS:C	2.32	0.54
2:B:197:ILE:HG22	2:B:222:VAL:HG11	1.91	0.53
5:E:208:ILE:HG21	5:E:259:GLU:HG3	1.89	0.53
6:F:72:LYS:O	6:F:74:LYS:N	2.42	0.53
18:R:51:ASP:O	18:R:55:TRP:HD1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:196:HIS:CE1	16:p:204:MET:HG3	2.44	0.53
21:U:55:ARG:H	21:U:55:ARG:HE	1.54	0.53
22:V:397:ARG:HH21	30:d:116:HIS:HB3	1.72	0.53
26:Z:169:GLU:HA	26:Z:172:VAL:HG12	1.89	0.53
32:f:788:MET:C	32:f:788:MET:HE3	2.33	0.53
3:C:148:TYR:HB2	3:C:206:HIS:CE1	2.43	0.53
4:D:73:LEU:HD22	26:Z:184:VAL:HG21	1.91	0.53
27:a:308:GLU:O	27:a:312:MET:HG2	2.08	0.53
29:c:52:GLU:HG3	29:c:114:SER:O	2.08	0.53
22:V:350:GLN:HB2	22:V:353:LEU:HB2	1.91	0.53
25:Y:105:MET:SD	25:Y:127:THR:HG21	2.48	0.53
28:b:62:THR:HB	28:b:70:ARG:NH1	2.24	0.53
12:l:55:GLU:HG2	12:l:56:LEU:HG	1.90	0.53
2:B:176:VAL:HB	2:B:247:PHE:HB3	1.91	0.53
3:C:49:ARG:HH12	21:U:642:GLU:HB2	1.73	0.53
8:H:34:PRO:HD3	8:H:165:LYS:HE3	1.91	0.53
10:J:196:LEU:HA	10:J:199:VAL:HG12	1.90	0.53
14:N:81:SER:HA	14:N:84:LYS:HE3	1.91	0.53
21:U:107:HIS:HA	21:U:110:LYS:HE3	1.90	0.53
22:V:301:GLU:OE2	22:V:304:GLU:HB3	2.09	0.53
32:f:416:MET:HB3	32:f:450:ILE:HG21	1.90	0.53
13:m:175:GLU:HB3	13:m:196:ILE:HG12	1.91	0.53
22:V:160:LEU:HD22	22:V:200:ARG:HH12	1.73	0.53
25:Y:288:PHE:CE1	25:Y:292:TYR:HB2	2.44	0.53
32:f:93:PRO:HG2	32:f:96:LEU:HB2	1.91	0.53
8:h:119:GLN:HG3	9:i:81:SER:HB2	1.90	0.53
7:G:193:GLN:O	7:G:197:THR:HG23	2.08	0.53
12:L:72:ILE:HG22	12:L:134:ILE:HG12	1.90	0.53
23:W:115:ILE:HD13	23:W:124:LEU:HD21	1.91	0.53
28:b:100:ARG:HH22	28:b:105:HIS:H	1.56	0.53
8:h:9:SER:HA	8:h:125:GLY:HA2	1.89	0.53
16:p:14:MET:HG3	16:p:136:PHE:HB3	1.90	0.53
21:U:419:ALA:HB2	21:U:449:ILE:HG21	1.90	0.53
21:U:615:ARG:O	21:U:619:VAL:HG22	2.08	0.53
22:V:175:MET:SD	22:V:183:GLU:HB2	2.49	0.53
23:W:329:ARG:HH21	23:W:351:TRP:CD1	2.27	0.53
23:W:404:ALA:HB1	23:W:413:ILE:HD11	1.91	0.53
28:b:55:ALA:HB1	28:b:82:GLY:HA3	1.90	0.53
28:b:121:GLU:O	28:b:125:VAL:HG13	2.08	0.53
32:f:182:GLU:HA	32:f:185:LEU:HD12	1.91	0.53
5:E:198:VAL:HG11	5:E:232:MET:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:14:LEU:HD21	14:N:101:ALA:HB3	1.91	0.53
21:U:108:TYR:HB2	21:U:130:LEU:HD22	1.90	0.53
21:U:245:ALA:HA	21:U:248:ILE:HG12	1.91	0.53
12:l:44:ALA:HB3	12:l:215:VAL:HG12	1.90	0.53
17:q:53:THR:HG22	17:q:100:VAL:HG12	1.91	0.53
19:s:44:TYR:HB2	19:s:52:ILE:HG22	1.91	0.53
3:C:99:VAL:HG12	3:C:123:LEU:HD12	1.91	0.53
5:E:81:VAL:HG11	5:E:100:LEU:HD11	1.91	0.53
5:E:261:LEU:HB3	5:E:294:ARG:HE	1.74	0.53
19:S:148:LEU:HD12	19:S:178:VAL:HG12	1.90	0.53
22:V:92:ARG:HA	22:V:95:LEU:HD12	1.91	0.53
24:X:172:LEU:HD12	24:X:175:LYS:HD3	1.91	0.53
9:i:119:GLN:HG3	10:j:78:ALA:HB1	1.91	0.53
10:J:211:MET:HE2	10:J:217:LEU:HD12	1.91	0.53
22:V:344:ASP:OD2	22:V:346:LEU:HB2	2.09	0.53
23:W:245:LYS:HE3	23:W:286:LEU:HD11	1.91	0.53
23:W:443:THR:HA	23:W:446:ILE:HG12	1.90	0.53
25:Y:50:MET:HE3	25:Y:53:TYR:HD2	1.73	0.53
19:s:145:LEU:HD21	19:s:182:ALA:HB2	1.91	0.53
4:D:125:LYS:HB2	4:D:126:PRO:HD3	1.91	0.52
21:U:423:MET:HE2	21:U:423:MET:N	2.25	0.52
21:U:759:SER:HA	21:U:782:ALA:HA	1.91	0.52
23:W:94:ARG:H	23:W:94:ARG:NE	2.07	0.52
32:f:196:MET:HE2	32:f:196:MET:C	2.34	0.52
11:k:36:THR:HG22	11:k:173:ALA:H	1.74	0.52
20:T:186:ARG:HD2	20:T:202:PRO:HB2	1.90	0.52
24:X:380:GLN:HB3	25:Y:315:THR:HG22	1.91	0.52
25:Y:382:LYS:O	25:Y:386:VAL:HG23	2.09	0.52
1:A:204:LEU:HB3	1:A:206:ILE:HD12	1.91	0.52
6:F:310:MET:C	6:F:310:MET:HE3	2.35	0.52
21:U:756:HIS:HB3	21:U:758:PRO:HD2	1.92	0.52
22:V:296:LYS:HG2	22:V:301:GLU:HB3	1.90	0.52
22:V:461:LYS:HB2	22:V:463:MET:H	1.75	0.52
11:k:85:ALA:HB2	11:k:139:VAL:HG11	1.89	0.52
15:o:73:LEU:HD23	15:o:74:PRO:HD2	1.92	0.52
2:B:49:LEU:HD22	2:B:51:LEU:HD23	1.90	0.52
6:F:282:ILE:HD13	6:F:329:ILE:HD13	1.90	0.52
19:S:71:ARG:HA	19:S:74:MET:SD	2.48	0.52
24:X:43:VAL:O	24:X:47:GLU:HG2	2.09	0.52
27:a:65:SER:HA	27:a:68:GLU:HB2	1.90	0.52
29:c:216:MET:O	29:c:220:LEU:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:71:MET:HE1	10:j:73:PHE:HB3	1.90	0.52
2:B:224:LEU:HD23	2:B:353:PHE:HE2	1.75	0.52
4:D:152:MET:SD	4:D:228:ILE:HG23	2.50	0.52
23:W:198:ASP:O	23:W:202:THR:HG23	2.10	0.52
32:f:522:CYS:HB3	32:f:534:VAL:HG21	1.92	0.52
2:B:56:THR:HG23	2:B:58:CYS:HB2	1.90	0.52
3:C:148:TYR:OH	3:C:158:ILE:HG23	2.09	0.52
11:K:121:LEU:HD23	11:K:160:GLY:HA3	1.90	0.52
14:N:45:ARG:HD2	14:N:52:THR:HB	1.92	0.52
14:N:202:LEU:HD23	14:N:203:PRO:HD2	1.92	0.52
16:P:20:VAL:HG23	16:P:190:ILE:HB	1.92	0.52
26:Z:195:VAL:HA	26:Z:198:LEU:HD12	1.91	0.52
2:B:223:ILE:HD13	2:B:329:MET:HG3	1.90	0.52
21:U:888:GLN:HA	21:U:891:VAL:HG22	1.91	0.52
25:Y:84:LEU:O	25:Y:87:GLU:HG3	2.10	0.52
26:Z:15:VAL:HG11	26:Z:50:VAL:HG12	1.92	0.52
26:Z:124:ILE:HA	26:Z:135:THR:HG22	1.92	0.52
26:Z:182:THR:HG23	26:Z:184:VAL:HG12	1.91	0.52
32:f:679:LEU:HG	32:f:690:VAL:HG11	1.90	0.52
3:C:161:ILE:HD11	3:C:186:VAL:HG11	1.91	0.52
27:a:278:MET:HA	27:a:281:THR:HG22	1.92	0.52
30:d:206:MET:N	30:d:206:MET:HE3	2.24	0.52
32:f:56:LEU:HD22	32:f:99:LEU:HD21	1.90	0.52
32:f:268:LEU:O	32:f:272:LEU:HB2	2.10	0.52
32:f:836:GLU:HB2	32:f:838:ARG:HE	1.74	0.52
10:j:199:VAL:HG12	10:j:202:GLY:H	1.75	0.52
4:D:119:ILE:HD13	4:D:139:LEU:HD12	1.92	0.52
4:D:160:PRO:HB3	4:D:221:HIS:CG	2.45	0.52
21:U:405:THR:HG23	21:U:441:GLY:HA3	1.91	0.52
23:W:108:CYS:HB3	23:W:128:LEU:HD11	1.91	0.52
27:a:289:ARG:CB	27:a:333:MET:HE3	2.39	0.52
32:f:686:LEU:O	32:f:690:VAL:HG23	2.09	0.52
8:h:160:ALA:HB1	8:h:174:LEU:HD23	1.92	0.52
3:C:338:LEU:HD12	3:C:342:ILE:HG13	1.92	0.52
19:S:16:ALA:HB2	19:S:121:VAL:HG23	1.90	0.52
21:U:196:LYS:HA	21:U:199:ARG:HG2	1.91	0.52
21:U:530:GLU:HA	21:U:533:VAL:HG22	1.92	0.52
22:V:113:LEU:HB3	22:V:135:LEU:HD13	1.92	0.52
25:Y:128:TYR:HB2	25:Y:140:ILE:HG21	1.91	0.52
27:a:156:TYR:CE2	27:a:178:ARG:HB3	2.44	0.52
12:l:40:SER:O	12:l:142:PRO:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:176:MET:HE2	13:m:57:LEU:HD23	1.92	0.52
12:L:157:ARG:HG2	13:M:59:GLU:HG2	1.90	0.51
21:U:459:ASP:HA	21:U:462:LEU:HD12	1.92	0.51
22:V:79:VAL:O	22:V:83:GLU:HG2	2.10	0.51
23:W:42:GLU:O	23:W:45:GLU:HG3	2.10	0.51
27:a:156:TYR:HB3	27:a:179:PHE:HB2	1.91	0.51
27:a:278:MET:HG2	27:a:335:TRP:CZ2	2.45	0.51
32:f:128:VAL:HG21	32:f:154:TRP:CZ3	2.45	0.51
32:f:399:LEU:HD22	32:f:432:TYR:HE1	1.75	0.51
32:f:524:MET:HA	32:f:527:VAL:HG22	1.93	0.51
32:f:806:VAL:HG23	32:f:810:ILE:HB	1.92	0.51
15:O:131:SER:O	15:O:135:MET:HB2	2.10	0.51
23:W:193:CYS:HB3	23:W:202:THR:HG22	1.91	0.51
25:Y:50:MET:HE2	25:Y:50:MET:O	2.11	0.51
28:b:51:LEU:HD11	28:b:61:LEU:HD23	1.93	0.51
5:E:11:ASP:HA	5:E:14:LYS:HG2	1.92	0.51
17:q:38:MET:HA	17:q:38:MET:HE3	1.92	0.51
1:A:163:MET:HE2	1:A:163:MET:C	2.36	0.51
2:B:170:LEU:O	2:B:174:MET:HE1	2.10	0.51
17:Q:85:ARG:HA	17:Q:118:MET:HE1	1.93	0.51
28:b:127:LEU:HD23	28:b:130:ARG:HH21	1.75	0.51
32:f:791:VAL:HG12	32:f:823:ALA:HB1	1.93	0.51
11:k:96:THR:HA	11:k:107:MET:HE2	1.93	0.51
3:C:354:ALA:HB1	3:C:358:GLU:OE1	2.10	0.51
5:E:331:ILE:HA	5:E:368:MET:HE1	1.92	0.51
8:H:199:PHE:O	8:H:200:GLU:HG2	2.11	0.51
23:W:112:VAL:HG23	23:W:124:LEU:HD11	1.93	0.51
25:Y:282:MET:HE2	25:Y:291:HIS:CG	2.46	0.51
20:T:63:LEU:HD21	20:T:106:LEU:HD13	1.93	0.51
24:X:415:TYR:CE2	25:Y:383:LEU:HB2	2.45	0.51
28:b:100:ARG:HE	28:b:103:LYS:HD2	1.76	0.51
10:j:70:CYS:HB2	10:j:217:LEU:HD22	1.93	0.51
16:p:45:MET:HE3	16:p:71:LEU:HD22	1.92	0.51
1:A:177:VAL:HG12	1:A:184:ILE:HD11	1.93	0.51
8:H:95:GLN:HG3	15:O:65:LEU:HG	1.93	0.51
21:U:556:MET:HE3	21:U:563:ALA:HA	1.93	0.51
26:Z:227:ILE:HG22	26:Z:228:TYR:N	2.26	0.51
27:a:122:LYS:NZ	27:a:130:VAL:HG22	2.26	0.51
28:b:4:GLU:HG2	28:b:106:LYS:HB2	1.92	0.51
12:L:154:PHE:HD1	13:M:63:ASN:HD21	1.59	0.51
7:g:130:GLU:HG2	7:g:131:MET:SD	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:4:MET:HE2	14:n:156:THR:HA	1.93	0.51
4:D:248:ARG:HA	4:D:295:GLN:OE1	2.11	0.51
9:I:178:ASP:OD1	9:I:192:LEU:HD11	2.10	0.51
24:X:80:ILE:HB	24:X:84:LYS:HE3	1.93	0.51
10:j:225:ILE:O	10:j:229:VAL:HG13	2.10	0.51
4:D:131:ALA:HB3	4:D:141:ASP:HB2	1.92	0.51
10:J:184:ASP:O	10:J:188:ILE:HG12	2.11	0.51
21:U:118:LEU:HD22	21:U:122:GLU:HG3	1.93	0.51
21:U:159:ARG:HB3	21:U:162:VAL:HG12	1.93	0.51
21:U:436:ALA:HB3	21:U:472:ILE:HD11	1.93	0.51
23:W:81:ASP:O	23:W:85:GLU:HG2	2.11	0.51
28:b:161:ASN:HD21	28:b:168:SER:H	1.58	0.51
29:c:270:LEU:HA	29:c:273:LYS:HG2	1.93	0.51
32:f:113:MET:HE1	32:f:119:LYS:HA	1.92	0.51
32:f:370:MET:HE2	32:f:370:MET:N	2.25	0.51
10:j:38:ARG:HH12	10:j:182:GLU:HA	1.74	0.51
13:m:90:ILE:O	13:m:93:GLU:HG3	2.11	0.51
2:B:174:MET:N	2:B:174:MET:HE3	2.26	0.50
8:H:19:LEU:H	8:H:19:LEU:HD12	1.75	0.50
20:T:27:LEU:HD11	20:T:34:ALA:HB1	1.93	0.50
22:V:321:ALA:HB1	22:V:324:PHE:HB3	1.92	0.50
25:Y:213:LEU:HB3	25:Y:214:MET:HG3	1.92	0.50
27:a:68:GLU:HG3	27:a:71:VAL:HG23	1.93	0.50
29:c:33:ILE:HD11	29:c:207:TYR:HD2	1.74	0.50
19:s:10:GLY:HA3	19:s:42:LYS:HE2	1.93	0.50
20:t:27:LEU:HD22	20:t:184:TYR:HB2	1.93	0.50
6:F:220:PRO:HG2	6:F:350:ARG:HD2	1.93	0.50
6:F:388:THR:HB	6:F:391:PHE:HD2	1.75	0.50
21:U:406:ALA:HA	21:U:445:ALA:HB2	1.93	0.50
15:o:50:ALA:O	15:o:54:MET:HG2	2.12	0.50
16:P:149:MET:HG2	16:P:170:ALA:HA	1.94	0.50
21:U:374:SER:HB3	21:U:407:SER:HB3	1.94	0.50
21:U:458:ILE:HG21	21:U:490:ARG:NH2	2.27	0.50
24:X:35:ILE:HD12	24:X:46:LYS:HD2	1.93	0.50
25:Y:191:ILE:HA	31:e:39:TRP:HE1	1.76	0.50
28:b:70:ARG:HG3	28:b:70:ARG:NH1	2.26	0.50
1:A:333:ARG:HH21	1:A:336:ARG:CZ	2.25	0.50
4:D:153:MET:HA	4:D:153:MET:HE3	1.94	0.50
5:E:185:ARG:HH12	5:E:231:PHE:HE2	1.60	0.50
5:E:286:ASP:HB3	5:E:289:LEU:HG	1.92	0.50
8:H:93:LEU:HD13	8:H:113:ARG:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:326:MET:HE2	23:W:326:MET:N	2.27	0.50
27:a:148:VAL:HG12	27:a:150:SER:H	1.76	0.50
27:a:246:GLU:O	27:a:250:THR:HG22	2.12	0.50
18:r:5:ALA:HB3	18:r:100:MET:HE1	1.93	0.50
3:C:78:ARG:HE	3:C:80:MET:HE1	1.77	0.50
4:D:91:GLN:HE22	4:D:93:LEU:HD21	1.76	0.50
4:D:264:ILE:HB	4:D:309:MET:HG2	1.94	0.50
19:S:66:LYS:HA	19:S:69:GLU:OE1	2.11	0.50
22:V:296:LYS:HB3	22:V:305:ALA:HB2	1.93	0.50
30:d:190:LEU:HD13	30:d:191:PHE:N	2.26	0.50
16:p:106:GLU:OE2	16:p:125:ASP:HA	2.11	0.50
1:A:24:ALA:HB1	2:B:410:ARG:HG2	1.93	0.50
8:H:139:TRP:CD1	8:H:215:GLU:HA	2.47	0.50
9:I:53:HIS:CE1	9:I:55:LEU:HB2	2.46	0.50
13:M:90:ILE:O	13:M:93:GLU:HG3	2.12	0.50
20:T:103:MET:HA	20:T:103:MET:HE3	1.94	0.50
21:U:691:SER:O	21:U:694:ILE:HG22	2.12	0.50
23:W:179:LYS:HB3	23:W:180:LYS:HE2	1.93	0.50
30:d:131:VAL:HA	30:d:134:LYS:HB3	1.94	0.50
32:f:539:LEU:O	32:f:543:MET:HG2	2.11	0.50
15:o:163:ILE:HG12	15:o:170:GLY:HA2	1.93	0.50
21:U:757:MET:HG3	21:U:758:PRO:HD3	1.94	0.50
30:d:45:LYS:HA	30:d:48:LEU:HB2	1.94	0.50
10:j:134:VAL:HG12	10:j:144:LEU:HD13	1.92	0.50
4:D:99:ASN:HA	4:D:115:ILE:HG12	1.94	0.50
21:U:146:LYS:HE2	21:U:148:LYS:HD3	1.93	0.50
27:a:248:PHE:HD2	27:a:249:GLN:HG2	1.76	0.50
30:d:23:LEU:O	30:d:27:LYS:HG2	2.12	0.50
30:d:45:LYS:HG2	30:d:48:LEU:HD12	1.93	0.50
30:d:53:ASP:O	30:d:57:ILE:HG12	2.12	0.50
10:j:212:ARG:HB3	10:j:215:GLN:HG3	1.94	0.50
13:m:45:VAL:HG23	13:m:146:ALA:HB1	1.92	0.50
1:A:88:GLN:O	1:A:92:PRO:HD2	2.12	0.50
5:E:148:VAL:HB	5:E:297:ARG:NH2	2.22	0.50
6:F:141:ASP:HB3	6:F:144:LYS:HG3	1.93	0.50
25:Y:188:CYS:HB3	25:Y:193:ASP:HB3	1.94	0.50
27:a:122:LYS:HZ1	27:a:130:VAL:HG22	1.77	0.50
27:a:268:LEU:O	27:a:272:ILE:HG12	2.12	0.50
32:f:355:ASN:HD22	32:f:357:ARG:HE	1.60	0.50
32:f:490:ALA:HA	32:f:525:ILE:HA	1.94	0.50
1:A:71:GLY:HA2	2:B:162:VAL:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:61:LEU:HD12	5:E:78:ARG:HD3	1.94	0.49
20:T:194:GLU:HB2	20:T:195:LYS:NZ	2.26	0.49
22:V:337:LEU:HB3	22:V:398:LEU:HD21	1.94	0.49
24:X:39:ASP:HB3	24:X:42:ALA:HB3	1.94	0.49
19:s:68:ILE:HD11	19:s:92:LEU:HD13	1.94	0.49
1:A:243:SER:HB3	2:B:268:ARG:HH22	1.77	0.49
2:B:135:ILE:H	2:B:135:ILE:HD12	1.77	0.49
2:B:281:ILE:C	2:B:281:ILE:HD12	2.37	0.49
3:C:228:ALA:O	3:C:231:VAL:HG12	2.11	0.49
7:G:51:VAL:HG12	7:G:217:VAL:HG22	1.94	0.49
12:L:66:VAL:HB	12:L:70:ILE:HG22	1.94	0.49
24:X:1:MET:HE1	24:X:36:GLN:HB2	1.94	0.49
12:l:69:HIS:CE1	12:l:102:PRO:HB3	2.46	0.49
3:C:399:MET:O	3:C:399:MET:HE3	2.13	0.49
5:E:146:ARG:HH12	5:E:190:GLN:CD	2.20	0.49
17:Q:102:LEU:HB2	17:Q:118:MET:HB2	1.93	0.49
21:U:660:CYS:HB2	21:U:694:ILE:HD11	1.94	0.49
28:b:147:GLU:HG3	28:b:150:THR:HG22	1.94	0.49
32:f:548:THR:HA	32:f:551:LYS:HD3	1.92	0.49
32:f:847:GLY:N	32:f:862:ILE:HD11	2.27	0.49
8:h:93:LEU:HD13	8:h:113:ARG:HB3	1.94	0.49
2:B:220:LYS:HA	2:B:326:LYS:HD3	1.95	0.49
2:B:223:ILE:HG23	2:B:350:LYS:HA	1.93	0.49
4:D:160:PRO:HB3	4:D:221:HIS:CD2	2.47	0.49
5:E:237:ALA:N	5:E:242:ARG:HH22	2.10	0.49
19:S:45:LYS:HG3	19:S:203:ILE:HD12	1.95	0.49
24:X:143:TYR:CZ	25:Y:252:SER:HB2	2.46	0.49
27:a:180:LEU:HD21	27:a:221:VAL:HG11	1.95	0.49
28:b:18:ASN:HD21	28:b:25:ARG:NH2	2.11	0.49
10:j:188:ILE:H	10:j:188:ILE:HD12	1.77	0.49
1:A:240:VAL:HG23	1:A:272:ILE:HD11	1.94	0.49
1:A:333:ARG:NH1	35:F:501:ATP:H5'1	2.28	0.49
3:C:257:SER:HB3	4:D:283:ARG:HH22	1.77	0.49
5:E:146:ARG:HH12	5:E:190:GLN:NE2	2.10	0.49
10:J:41:VAL:HG23	10:J:211:MET:HB3	1.94	0.49
21:U:817:LEU:HD11	21:U:819:VAL:HG12	1.94	0.49
24:X:77:LEU:HD11	24:X:85:ALA:HB1	1.94	0.49
12:l:71:GLY:HA3	12:l:221:PHE:CZ	2.47	0.49
12:l:84:LEU:O	12:l:88:MET:HG3	2.12	0.49
16:p:190:ILE:HG23	16:p:195:ILE:HG12	1.94	0.49
1:A:177:VAL:HG12	1:A:177:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:232:MET:SD	5:E:235:ILE:HB	2.53	0.49
6:F:124:ILE:HD11	6:F:160:ILE:HD11	1.94	0.49
20:T:73:ASP:HA	20:T:76:LEU:HD12	1.94	0.49
24:X:400:ALA:HB1	26:Z:262:LEU:HD21	1.95	0.49
1:A:72:LEU:HD21	2:B:99:VAL:HG11	1.95	0.49
7:G:43:ARG:HH21	7:G:164:LYS:HG2	1.78	0.49
10:J:164:GLY:O	10:J:168:VAL:HG23	2.13	0.49
22:V:185:GLN:HB2	22:V:218:TYR:HE1	1.78	0.49
23:W:130:MET:C	23:W:130:MET:HE2	2.37	0.49
28:b:7:MET:HB3	28:b:109:ILE:HG12	1.94	0.49
28:b:26:LEU:O	28:b:29:GLN:HG2	2.12	0.49
10:j:136:PHE:HD1	10:j:142:PRO:HA	1.77	0.49
2:B:302:GLU:O	2:B:305:ILE:HG13	2.13	0.49
4:D:177:VAL:HG11	4:D:215:LEU:HD21	1.95	0.49
5:E:173:TYR:HE1	5:E:300:HIS:CD2	2.31	0.49
6:F:31:GLU:O	6:F:35:LYS:HB2	2.12	0.49
23:W:395:ASN:HA	23:W:398:VAL:HG22	1.93	0.49
30:d:68:ILE:HD12	30:d:69:PRO:N	2.28	0.49
32:f:368:ALA:HA	32:f:371:ASN:HD21	1.78	0.49
32:f:486:GLY:C	32:f:524:MET:HE1	2.37	0.49
10:j:120:GLN:OE1	10:j:120:GLN:HA	2.13	0.49
4:D:155:THR:HA	4:D:159:LYS:HD3	1.94	0.49
9:I:69:ASN:OD1	9:I:72:MET:HG2	2.13	0.49
28:b:90:ILE:HG21	28:b:131:LEU:HD11	1.95	0.49
30:d:51:ALA:HA	30:d:54:ILE:HG12	1.94	0.49
13:m:197:ILE:HG21	13:m:211:LEU:HD11	1.93	0.49
18:r:127:SER:HB2	18:r:139:MET:HE1	1.95	0.49
1:A:48:VAL:HG11	2:B:65:LEU:HB3	1.95	0.49
5:E:281:ARG:N	5:E:282:PRO:HD3	2.28	0.49
5:E:289:LEU:HD23	5:E:294:ARG:HD3	1.94	0.49
10:J:71:MET:HG3	10:J:133:ILE:HG12	1.94	0.49
21:U:475:HIS:NE2	21:U:507:VAL:HG13	2.28	0.49
23:W:406:VAL:HG23	23:W:413:ILE:HB	1.94	0.49
26:Z:177:ARG:HA	26:Z:180:LYS:HD3	1.95	0.49
12:l:9:ASP:HB3	12:l:12:VAL:HG23	1.94	0.49
1:A:164:MET:SD	1:A:240:VAL:HA	2.53	0.48
1:A:262:GLU:O	1:A:266:THR:HG23	2.12	0.48
4:D:297:ASP:HB3	4:D:326:ARG:NH2	2.28	0.48
5:E:171:LEU:HG	5:E:173:TYR:HD2	1.77	0.48
11:K:91:LYS:HG2	11:K:119:LEU:HD13	1.94	0.48
21:U:415:HIS:HB3	21:U:418:GLU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:50:PHE:HD2	27:a:52:GLN:HB3	1.78	0.48
9:i:90:LEU:HG	9:i:114:LEU:HD13	1.94	0.48
15:o:9:LYS:HD3	15:o:145:ASP:OD2	2.12	0.48
1:A:346:PRO:HB3	1:A:350:GLY:HA3	1.94	0.48
2:B:408:ARG:HD2	3:C:163:GLU:OE2	2.12	0.48
5:E:40:TYR:CE1	6:F:72:LYS:HD3	2.48	0.48
21:U:124:LYS:HD3	21:U:124:LYS:HA	1.65	0.48
23:W:224:LEU:HD21	23:W:253:THR:HG21	1.95	0.48
26:Z:208:ILE:HD11	27:a:353:LEU:HD11	1.94	0.48
30:d:23:LEU:HG	30:d:27:LYS:HE2	1.95	0.48
32:f:120:ARG:HD3	32:f:147:SER:HB3	1.94	0.48
32:f:235:SER:HB3	32:f:853:VAL:HG21	1.95	0.48
4:D:214:MET:HA	4:D:217:LYS:HD2	1.95	0.48
5:E:232:MET:HE2	5:E:277:MET:HA	1.95	0.48
11:K:46:VAL:HG12	11:K:220:VAL:HB	1.95	0.48
15:O:124:TYR:CE1	15:O:135:MET:HE1	2.45	0.48
19:S:71:ARG:HD2	19:S:74:MET:SD	2.52	0.48
23:W:312:MET:HG2	23:W:365:ILE:HG22	1.96	0.48
27:a:289:ARG:HG3	27:a:332:HIS:CD2	2.49	0.48
28:b:100:ARG:HH21	28:b:103:LYS:HA	1.78	0.48
20:t:194:GLU:HG2	20:t:195:LYS:HD2	1.95	0.48
6:F:73:ILE:HG23	6:F:74:LYS:H	1.77	0.48
18:R:195:LEU:HA	18:R:198:LYS:HB3	1.93	0.48
32:f:718:ASP:HB3	32:f:721:VAL:HB	1.96	0.48
7:g:59:LYS:H	7:g:59:LYS:HZ1	1.62	0.48
4:D:81:ARG:HG3	29:c:152:LYS:HE3	1.95	0.48
13:M:229:LYS:HA	13:M:232:ARG:HG2	1.95	0.48
15:O:18:THR:OG1	15:O:172:ASN:HB2	2.14	0.48
21:U:516:LEU:HG	21:U:532:MET:HE1	1.95	0.48
23:W:71:VAL:HB	23:W:104:MET:HE1	1.95	0.48
32:f:89:MET:O	32:f:89:MET:HE2	2.12	0.48
2:B:121:ALA:HB2	2:B:135:ILE:HD11	1.95	0.48
11:K:103:TYR:HE1	19:S:91:MET:HE2	1.79	0.48
23:W:378:MET:HE1	23:W:389:SER:HB3	1.95	0.48
32:f:237:VAL:HG23	32:f:248:LEU:HD11	1.96	0.48
10:j:51:ALA:O	10:j:54:GLN:HG3	2.13	0.48
6:F:175:MET:N	6:F:175:MET:HE3	2.28	0.48
15:O:135:MET:O	15:O:135:MET:HE3	2.12	0.48
22:V:476:PHE:HB3	26:Z:260:VAL:HG21	1.96	0.48
27:a:290:GLN:HG2	27:a:330:ARG:HD3	1.95	0.48
32:f:445:LEU:HG	32:f:466:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:181:MET:C	13:m:181:MET:HE2	2.38	0.48
13:m:228:PRO:HD2	13:m:231:ILE:HD12	1.94	0.48
22:V:419:LEU:HD12	22:V:456:GLY:HA2	1.96	0.48
25:Y:159:ARG:O	25:Y:162:GLU:HG3	2.13	0.48
32:f:115:PRO:HA	32:f:119:LYS:HD3	1.96	0.48
15:o:42:TYR:HE1	15:o:183:LEU:HD11	1.77	0.48
2:B:75:GLU:OE2	32:f:673:ARG:HG2	2.14	0.48
5:E:108:MET:H	5:E:108:MET:HE2	1.79	0.48
5:E:171:LEU:HB3	5:E:298:LYS:HG2	1.96	0.48
12:L:125:ARG:HH12	12:L:126:ARG:NH1	2.12	0.48
19:S:10:GLY:HA3	19:S:42:LYS:HE2	1.96	0.48
30:d:29:VAL:HG21	30:d:54:ILE:HD11	1.95	0.48
32:f:223:GLU:HG2	32:f:259:PHE:CE1	2.49	0.48
32:f:234:THR:O	32:f:237:VAL:HG12	2.13	0.48
1:A:52:ILE:HD13	2:B:69:LYS:HA	1.95	0.48
2:B:264:PRO:HB3	2:B:311:GLU:HG2	1.95	0.48
10:J:102:VAL:HG13	10:J:106:TYR:HD2	1.79	0.48
27:a:112:ILE:O	27:a:116:THR:HG23	2.14	0.48
29:c:120:CYS:HA	29:c:144:VAL:HG11	1.95	0.48
32:f:298:LEU:HD13	32:f:305:LEU:HG	1.96	0.48
32:f:647:GLY:HA3	32:f:685:THR:HG21	1.95	0.48
9:i:90:LEU:HD21	9:i:114:LEU:HD22	1.96	0.48
13:m:150:MET:HG2	13:m:163:CYS:SG	2.54	0.48
19:s:72:LEU:HD12	19:s:91:MET:HE1	1.95	0.48
2:B:194:ILE:O	2:B:197:ILE:HD12	2.14	0.47
3:C:45:LEU:HB3	4:D:61:ILE:HG21	1.96	0.47
3:C:117:ARG:HD3	3:C:124:HIS:CG	2.49	0.47
5:E:9:LEU:O	5:E:13:ARG:HG2	2.15	0.47
17:Q:170:ARG:HD2	17:q:26:VAL:HG23	1.95	0.47
18:R:42:LEU:HD12	18:R:179:VAL:HG22	1.96	0.47
22:V:470:ARG:NH2	26:Z:249:PHE:HB3	2.25	0.47
25:Y:100:ILE:HG13	25:Y:101:ARG:N	2.29	0.47
25:Y:224:VAL:HG22	25:Y:260:LEU:HD11	1.96	0.47
29:c:279:ASP:HB3	29:c:283:HIS:HB3	1.95	0.47
7:g:59:LYS:HE3	7:g:59:LYS:HB3	1.52	0.47
10:j:154:HIS:HB2	10:j:156:TRP:HE1	1.79	0.47
1:A:362:MET:HE3	1:A:364:VAL:HG12	1.94	0.47
6:F:153:VAL:HG13	6:F:158:TYR:HA	1.96	0.47
6:F:223:VAL:HG22	6:F:350:ARG:HB2	1.96	0.47
6:F:420:TYR:O	6:F:424:ILE:HD13	2.14	0.47
7:G:113:MET:HE2	7:G:113:MET:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:229:VAL:HA	21:U:232:ILE:HG12	1.96	0.47
22:V:480:ILE:HB	26:Z:260:VAL:HG13	1.97	0.47
24:X:190:LEU:HD21	24:X:214:SER:HA	1.95	0.47
24:X:351:SER:HA	24:X:354:ILE:HG22	1.96	0.47
25:Y:21:GLN:HA	25:Y:286:TRP:HB3	1.96	0.47
29:c:192:LEU:HA	29:c:196:LEU:HB3	1.95	0.47
32:f:289:VAL:O	32:f:292:LYS:HG2	2.15	0.47
32:f:472:HIS:HB3	32:f:477:MET:HE1	1.96	0.47
1:A:52:ILE:HD11	2:B:72:LEU:HG	1.96	0.47
9:I:95:GLN:HG3	16:P:73:LEU:HG	1.95	0.47
21:U:527:GLN:O	21:U:530:GLU:HG3	2.13	0.47
21:U:583:MET:O	21:U:586:VAL:HG12	2.13	0.47
21:U:654:MET:HE2	21:U:654:MET:HA	1.95	0.47
24:X:346:GLN:HE21	24:X:346:GLN:N	2.12	0.47
25:Y:220:VAL:HA	25:Y:223:THR:HG22	1.97	0.47
26:Z:257:MET:HA	26:Z:257:MET:HE2	1.95	0.47
32:f:155:GLY:O	32:f:159:VAL:HG23	2.13	0.47
32:f:547:GLU:HA	32:f:550:LEU:HB2	1.95	0.47
32:f:760:PHE:O	32:f:764:LEU:HG	2.14	0.47
10:j:99:GLU:OE1	18:r:81:LYS:HG2	2.13	0.47
10:j:156:TRP:HE3	11:k:58:LEU:HD12	1.79	0.47
6:F:221:LYS:HD3	6:F:322:PRO:HA	1.95	0.47
7:G:48:ALA:HB3	7:G:220:VAL:HG12	1.96	0.47
21:U:260:PHE:O	21:U:264:VAL:HG13	2.13	0.47
25:Y:231:LEU:HB2	25:Y:234:PRO:HG2	1.96	0.47
27:a:6:GLY:HA2	27:a:9:GLN:HB2	1.96	0.47
27:a:346:ILE:HA	27:a:349:MET:HE2	1.96	0.47
28:b:38:HIS:O	28:b:42:ARG:HD3	2.14	0.47
16:p:12:MET:HE2	16:p:167:ILE:HG13	1.96	0.47
2:B:266:LEU:HD12	2:B:267:VAL:N	2.30	0.47
3:C:36:ASN:O	3:C:40:GLN:HG2	2.15	0.47
3:C:233:GLU:HA	3:C:236:VAL:HG12	1.96	0.47
21:U:202:VAL:HA	21:U:205:TYR:HB2	1.97	0.47
21:U:602:LEU:HD11	21:U:621:SER:HB2	1.97	0.47
21:U:847:GLU:HA	21:U:850:GLU:HG2	1.97	0.47
22:V:355:ARG:NH1	22:V:355:ARG:HA	2.30	0.47
23:W:361:HIS:HA	23:W:364:ARG:HE	1.79	0.47
23:W:371:THR:HG22	23:W:372:ARG:HG3	1.97	0.47
24:X:394:ASP:HB2	24:X:398:GLU:OE1	2.14	0.47
32:f:268:LEU:HD12	32:f:268:LEU:H	1.79	0.47
13:m:50:GLU:HG2	13:m:197:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:t:50:MET:HE2	20:t:192:VAL:HG12	1.96	0.47
1:A:299:MET:HE2	1:A:299:MET:HB3	1.82	0.47
4:D:417:TYR:CE1	7:G:21:ARG:HB2	2.49	0.47
17:Q:4:LEU:HD13	17:Q:45:LEU:HB3	1.95	0.47
18:R:45:MET:HE3	18:R:52:CYS:HB2	1.96	0.47
21:U:367:THR:HA	21:U:370:VAL:HG22	1.96	0.47
24:X:187:ARG:HH21	24:X:217:ILE:HG22	1.79	0.47
25:Y:77:ASN:O	25:Y:81:LEU:HG	2.14	0.47
5:E:321:THR:OG1	5:E:361:PHE:HA	2.15	0.47
18:R:186:ARG:HH21	18:R:189:SER:HB2	1.80	0.47
21:U:327:LYS:O	21:U:333:MET:HE1	2.14	0.47
21:U:773:PHE:HB2	29:c:177:THR:HB	1.96	0.47
23:W:240:TYR:HA	23:W:243:ILE:HD12	1.97	0.47
25:Y:81:LEU:HD22	25:Y:107:LYS:NZ	2.29	0.47
25:Y:236:LEU:HA	25:Y:239:LYS:NZ	2.30	0.47
29:c:39:LEU:HD23	29:c:42:LEU:HD21	1.97	0.47
29:c:278:GLN:C	29:c:280:PRO:HD3	2.40	0.47
10:j:87:ALA:HB1	10:j:107:ILE:HD11	1.96	0.47
11:k:76:CYS:SG	11:k:141:LEU:HD23	2.55	0.47
14:n:4:MET:HB2	14:n:127:ILE:HG22	1.95	0.47
15:o:42:TYR:CE1	15:o:183:LEU:HD11	2.50	0.47
16:p:39:PHE:HD2	16:p:41:LYS:HE3	1.79	0.47
17:q:16:ALA:HA	17:q:179:SER:O	2.14	0.47
13:M:169:ARG:O	13:M:173:LYS:HG3	2.15	0.47
28:b:110:ILE:HD12	28:b:110:ILE:O	2.15	0.47
11:k:210:LEU:HD12	11:k:215:ILE:HG21	1.96	0.47
5:E:218:MET:C	5:E:218:MET:HE2	2.40	0.47
24:X:77:LEU:HD23	24:X:78:ASN:ND2	2.29	0.47
24:X:332:GLU:HB3	24:X:368:MET:HE1	1.96	0.47
26:Z:14:LEU:HD12	29:c:39:LEU:HB3	1.95	0.47
27:a:245:VAL:HG11	27:a:301:LYS:HD3	1.96	0.47
32:f:398:TRP:HD1	32:f:401:LYS:HZ3	1.62	0.47
11:k:146:VAL:HG11	11:k:222:PRO:HA	1.96	0.47
16:p:204:MET:HA	16:p:204:MET:HE3	1.97	0.47
5:E:155:ASN:HD21	23:W:204:ILE:HG23	1.80	0.47
5:E:206:LYS:HA	5:E:255:ARG:NH2	2.30	0.47
20:T:22:ILE:HG23	20:T:50:MET:HE3	1.97	0.47
21:U:134:VAL:HG11	21:U:162:VAL:HG21	1.96	0.47
25:Y:121:LEU:HB3	25:Y:125:ARG:HH12	1.79	0.47
26:Z:22:HIS:HA	26:Z:25:ARG:HD3	1.97	0.47
28:b:32:ALA:O	28:b:35:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:284:LEU:HD12	29:c:284:LEU:HA	1.76	0.47
7:g:191:PHE:CE1	7:g:219:VAL:HG21	2.43	0.47
9:i:200:THR:HG23	9:i:201:MET:HE3	1.96	0.47
2:B:59:ARG:HE	32:f:209:MET:HE2	1.79	0.46
20:T:127:MET:HB2	20:T:127:MET:HE3	1.81	0.46
22:V:302:TYR:HB3	22:V:339:LEU:HG	1.97	0.46
30:d:205:LYS:HA	30:d:208:ASP:HB3	1.97	0.46
32:f:659:LEU:HD11	32:f:797:LEU:HD11	1.97	0.46
1:A:394:MET:HG2	2:B:349:ARG:HH22	1.80	0.46
3:C:187:LEU:HD13	3:C:293:MET:HG3	1.97	0.46
3:C:406:LYS:HB3	9:I:80:THR:HG22	1.97	0.46
4:D:391:ARG:HH12	4:D:397:LYS:HZ3	1.62	0.46
10:J:91:CYS:HA	10:J:102:VAL:HG21	1.98	0.46
12:L:176:MET:HE1	13:M:57:LEU:HA	1.98	0.46
16:P:27:ARG:HB2	16:P:183:MET:HB2	1.97	0.46
19:S:90:ALA:O	19:S:94:THR:HG23	2.15	0.46
19:S:194:ARG:HG2	19:S:205:GLU:OE2	2.15	0.46
21:U:184:CYS:HA	21:U:188:MET:SD	2.55	0.46
23:W:241:LEU:HD21	23:W:282:GLU:OE1	2.15	0.46
26:Z:134:PRO:HB3	29:c:220:LEU:HG	1.97	0.46
28:b:22:LEU:HD22	28:b:22:LEU:H	1.79	0.46
32:f:560:LEU:HA	32:f:594:LEU:HD11	1.97	0.46
4:D:206:GLY:O	4:D:312:ASN:HA	2.15	0.46
4:D:303:VAL:HG23	4:D:303:VAL:O	2.14	0.46
6:F:357:PRO:O	6:F:362:ARG:HG3	2.16	0.46
15:O:123:PRO:HG3	20:t:211:ILE:HG23	1.97	0.46
20:T:195:LYS:HE2	20:T:195:LYS:H	1.80	0.46
23:W:121:LYS:O	23:W:125:ILE:HG12	2.15	0.46
23:W:163:ALA:HA	23:W:192:LEU:HD13	1.98	0.46
25:Y:285:ASP:O	25:Y:288:PHE:HB2	2.15	0.46
26:Z:165:GLU:O	26:Z:168:GLU:HG2	2.16	0.46
27:a:248:PHE:CD2	27:a:249:GLN:HG2	2.50	0.46
29:c:231:LEU:C	29:c:233:ASP:H	2.22	0.46
20:t:43:MET:SD	20:t:64:LYS:HG3	2.55	0.46
1:A:99:THR:HG22	1:A:115:VAL:HG22	1.97	0.46
12:L:41:LYS:HG2	12:L:42:THR:HG23	1.98	0.46
12:L:186:GLU:HA	12:L:189:LYS:HE2	1.96	0.46
21:U:583:MET:HE1	21:U:617:ALA:HB3	1.96	0.46
27:a:96:PHE:O	27:a:99:LYS:HG2	2.15	0.46
28:b:138:VAL:HB	28:b:160:LEU:HD21	1.98	0.46
29:c:42:LEU:HD12	29:c:43:LYS:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:66:LYS:HB2	32:f:66:LYS:HE2	1.59	0.46
32:f:137:ARG:HD3	32:f:168:LYS:HZ1	1.80	0.46
32:f:351:THR:HA	32:f:354:GLU:CD	2.41	0.46
32:f:809:ILE:HG23	32:f:814:SER:HB2	1.97	0.46
1:A:160:THR:HA	1:A:163:MET:SD	2.54	0.46
4:D:232:GLY:HA3	4:D:266:GLU:O	2.16	0.46
9:I:46:ALA:HB1	9:I:197:LEU:HD11	1.98	0.46
10:J:220:LEU:HD12	10:J:225:ILE:HG13	1.97	0.46
14:N:70:LEU:HD13	14:N:70:LEU:HA	1.80	0.46
15:O:48:THR:HB	15:O:51:ASP:HB2	1.97	0.46
18:R:43:GLY:HA2	18:R:100:MET:O	2.15	0.46
19:S:27:THR:OG1	19:S:192:ALA:HB3	2.16	0.46
27:a:41:VAL:HG12	27:a:79:ILE:HD11	1.96	0.46
28:b:7:MET:HE2	28:b:52:ILE:HG12	1.97	0.46
28:b:184:ILE:HA	28:b:188:ILE:HG12	1.98	0.46
12:l:36:VAL:HG22	12:l:160:SER:HB2	1.96	0.46
12:l:88:MET:HG2	12:l:112:ILE:HD11	1.97	0.46
17:q:28:MET:HE1	18:r:113:TYR:CD2	2.50	0.46
1:A:428:ARG:HA	1:A:430:MET:HE2	1.98	0.46
3:C:244:SER:OG	3:C:289:ILE:HG12	2.16	0.46
4:D:297:ASP:HB3	4:D:326:ARG:HH21	1.79	0.46
6:F:300:LYS:C	6:F:302:GLY:H	2.23	0.46
8:H:118:MET:HE2	8:H:150:ASP:C	2.40	0.46
9:I:45:LEU:HG	9:I:137:ILE:HD13	1.97	0.46
18:R:14:VAL:HG22	18:R:177:TYR:HB2	1.98	0.46
21:U:529:ILE:HG22	21:U:555:VAL:HG11	1.97	0.46
24:X:143:TYR:CD2	24:X:144:GLN:HG2	2.46	0.46
24:X:306:LEU:HD21	24:X:314:ARG:NH2	2.31	0.46
26:Z:68:TRP:CG	26:Z:104:ASN:HD21	2.34	0.46
28:b:8:VAL:HA	28:b:110:ILE:HD12	1.98	0.46
29:c:32:TYR:HB3	29:c:208:ARG:NH1	2.25	0.46
7:g:177:SER:O	7:g:180:GLU:HG3	2.15	0.46
16:p:15:LYS:HE3	16:p:121:ILE:HG12	1.98	0.46
20:t:59:ASP:HB3	20:t:106:LEU:HD22	1.96	0.46
2:B:81:ASN:HB3	32:f:617:SER:HB2	1.97	0.46
21:U:191:LYS:HA	21:U:194:ARG:HB3	1.98	0.46
23:W:442:THR:O	23:W:446:ILE:HG23	2.16	0.46
25:Y:153:ASP:HB3	25:Y:156:LEU:HB3	1.98	0.46
25:Y:343:LEU:HD23	25:Y:343:LEU:HA	1.85	0.46
32:f:62:ARG:HD2	32:f:70:LEU:HD21	1.97	0.46
32:f:338:ASP:HA	32:f:340:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:79:ILE:HB	9:i:82:ASP:HB2	1.96	0.46
10:j:42:VAL:HG12	10:j:210:VAL:HG22	1.98	0.46
15:o:110:LEU:HD21	15:o:125:VAL:HG22	1.97	0.46
1:A:263:MET:HE1	1:A:267:LYS:HE3	1.97	0.46
21:U:55:ARG:H	21:U:55:ARG:NE	2.11	0.46
22:V:135:LEU:HD21	22:V:171:VAL:HG13	1.97	0.46
23:W:26:GLN:HE22	23:W:27:ARG:HD3	1.81	0.46
23:W:455:LEU:HG	26:Z:101:LEU:HD12	1.98	0.46
25:Y:49:ASN:HA	25:Y:73:MET:SD	2.55	0.46
32:f:505:MET:HG3	32:f:506:GLY:N	2.31	0.46
32:f:539:LEU:HG	32:f:543:MET:HE3	1.98	0.46
17:q:75:LEU:HD23	17:q:75:LEU:HA	1.78	0.46
2:B:235:LEU:HD12	2:B:353:PHE:HZ	1.81	0.46
2:B:275:GLU:OE2	2:B:323:GLY:HA3	2.16	0.46
9:I:119:GLN:OE1	10:J:82:ILE:HG13	2.15	0.46
14:N:28:ASN:HD21	15:O:122:LEU:HD21	1.80	0.46
21:U:26:LYS:O	21:U:30:VAL:HG22	2.15	0.46
29:c:279:ASP:HB2	29:c:284:LEU:HD13	1.97	0.46
7:g:54:LYS:HB2	7:g:216:GLU:OE2	2.16	0.46
9:i:236:LEU:HA	9:i:239:LYS:HE2	1.96	0.46
16:p:107:PRO:HG2	16:p:124:LEU:HB2	1.97	0.46
5:E:159:PHE:O	5:E:163:GLY:HA2	2.16	0.46
17:Q:44:LEU:HD11	17:Q:102:LEU:HD22	1.96	0.46
20:T:26:MET:HE2	20:T:26:MET:HB3	1.74	0.46
21:U:177:LEU:HD23	21:U:177:LEU:H	1.80	0.46
21:U:401:LYS:O	21:U:405:THR:HG22	2.15	0.46
21:U:746:ILE:HD12	21:U:746:ILE:O	2.16	0.46
22:V:282:ASN:OD1	25:Y:385:ARG:HG2	2.16	0.46
22:V:414:TYR:HB3	22:V:417:ILE:CD1	2.45	0.46
23:W:119:PRO:O	23:W:122:LEU:HG	2.16	0.46
25:Y:50:MET:HE2	25:Y:53:TYR:HB3	1.98	0.46
25:Y:217:LYS:O	25:Y:221:THR:HG23	2.15	0.46
27:a:278:MET:HE3	27:a:278:MET:HB2	1.76	0.46
7:g:59:LYS:HE2	13:m:177:GLU:HG2	1.98	0.46
10:J:221:ASN:ND2	10:J:223:GLU:HB2	2.30	0.45
24:X:141:LYS:HE2	24:X:179:ALA:HB1	1.98	0.45
24:X:260:MET:SD	24:X:322:HIS:HB3	2.57	0.45
26:Z:211:TYR:OH	26:Z:227:ILE:HG13	2.16	0.45
30:d:42:LYS:HD2	30:d:45:LYS:HB2	1.98	0.45
32:f:386:GLY:HA2	32:f:418:LEU:HG	1.98	0.45
19:s:13:LEU:HD11	19:s:149:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:27:THR:HB	19:s:40:SER:H	1.81	0.45
1:A:91:GLN:HB2	1:A:92:PRO:HD3	1.98	0.45
5:E:251:ARG:HH21	5:E:254:GLN:HG3	1.81	0.45
12:L:137:TYR:CZ	12:L:217:LYS:HA	2.51	0.45
17:Q:67:TYR:CD1	17:Q:75:LEU:HG	2.51	0.45
21:U:136:LYS:HZ2	21:U:137:MET:N	2.14	0.45
21:U:765:VAL:HG11	21:U:778:PHE:CD2	2.51	0.45
26:Z:101:LEU:HB2	26:Z:105:ASP:OD2	2.16	0.45
26:Z:202:ASN:O	26:Z:206:LEU:HG	2.15	0.45
28:b:25:ARG:NH1	28:b:145:GLU:H	2.13	0.45
32:f:271:MET:HE2	32:f:271:MET:C	2.40	0.45
14:n:14:LEU:HD21	14:n:101:ALA:HB3	1.97	0.45
4:D:89:ILE:HB	5:E:78:ARG:HB3	1.99	0.45
21:U:692:ALA:HB2	21:U:733:ALA:HB1	1.98	0.45
22:V:295:ILE:O	22:V:299:GLN:HG2	2.17	0.45
26:Z:213:GLU:HA	27:a:350:LYS:NZ	2.31	0.45
28:b:124:LEU:HD13	28:b:156:PHE:HB2	1.98	0.45
31:e:62:LYS:C	31:e:64:GLY:H	2.24	0.45
32:f:275:MET:HA	32:f:275:MET:HE3	1.97	0.45
7:g:123:GLN:HG3	8:h:81:PRO:HB3	1.98	0.45
20:t:116:ALA:O	20:t:119:GLU:HG3	2.16	0.45
2:B:174:MET:HE3	2:B:174:MET:H	1.80	0.45
21:U:391:GLU:H	21:U:391:GLU:HG3	1.62	0.45
21:U:596:ASN:HA	21:U:599:ILE:HG22	1.98	0.45
21:U:839:ALA:HA	21:U:842:LYS:HE3	1.98	0.45
22:V:183:GLU:HA	22:V:186:LYS:NZ	2.31	0.45
22:V:206:VAL:HA	22:V:209:LYS:HE3	1.98	0.45
22:V:409:MET:C	22:V:409:MET:HE2	2.41	0.45
23:W:375:MET:HE2	23:W:411:GLY:HA2	1.98	0.45
30:d:237:ILE:N	30:d:238:PRO:HD2	2.31	0.45
5:E:198:VAL:HB	5:E:232:MET:HA	1.98	0.45
6:F:81:LYS:HE2	6:F:81:LYS:HB2	1.79	0.45
18:R:58:LEU:HB3	18:R:86:MET:HE1	1.98	0.45
21:U:247:GLN:HE21	21:U:912:ILE:HA	1.82	0.45
21:U:342:LEU:HD13	21:U:379:GLY:HA3	1.98	0.45
22:V:161:PRO:HB3	22:V:198:GLN:NE2	2.30	0.45
22:V:476:PHE:O	22:V:480:ILE:HG22	2.16	0.45
23:W:446:ILE:HG13	23:W:447:ALA:N	2.31	0.45
25:Y:83:ARG:O	25:Y:86:GLU:HG3	2.17	0.45
32:f:99:LEU:HB2	32:f:129:LEU:HD11	1.97	0.45
32:f:373:ALA:HB2	32:f:760:PHE:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:417:ILE:HG22	32:f:418:LEU:HD12	1.98	0.45
9:i:21:VAL:O	9:i:25:MET:HG3	2.17	0.45
2:B:409:GLU:HG3	2:B:411:ARG:HE	1.81	0.45
5:E:352:MET:HE1	6:F:212:PHE:HE1	1.81	0.45
6:F:351:LYS:HA	6:F:351:LYS:HE2	1.99	0.45
8:H:85:VAL:O	8:H:89:ARG:HG2	2.17	0.45
21:U:639:LEU:HD12	21:U:639:LEU:HA	1.81	0.45
27:a:8:LEU:HA	27:a:11:SER:OG	2.17	0.45
1:A:81:ALA:O	1:A:85:GLN:HG3	2.17	0.45
1:A:89:SER:HA	1:A:93:LEU:HD23	1.97	0.45
3:C:127:LEU:HD21	4:D:112:TYR:CE1	2.52	0.45
19:S:116:GLU:OE1	19:S:116:GLU:N	2.50	0.45
21:U:669:ILE:HA	21:U:672:LEU:HD12	1.98	0.45
22:V:255:LEU:HD23	22:V:255:LEU:HA	1.87	0.45
26:Z:16:LEU:HD23	26:Z:17:LEU:H	1.81	0.45
26:Z:37:GLY:HA3	26:Z:95:TYR:CE1	2.52	0.45
30:d:208:ASP:O	30:d:211:LYS:HG3	2.16	0.45
32:f:323:ASN:HB3	32:f:326:LEU:HB2	1.98	0.45
1:A:43:ARG:HA	1:A:46:LYS:HB2	1.99	0.45
1:A:279:ALA:HB2	2:B:310:LEU:HD23	1.97	0.45
3:C:11:LEU:HB3	3:C:14:GLY:HA3	1.98	0.45
10:J:3:TYR:CD2	10:J:12:PRO:HD3	2.52	0.45
13:M:191:LYS:HB3	13:M:238:TYR:CD2	2.52	0.45
21:U:88:PHE:HE1	21:U:97:VAL:HG12	1.82	0.45
22:V:224:LEU:HD12	22:V:261:TYR:HE1	1.82	0.45
27:a:245:VAL:C	27:a:246:GLU:HG3	2.42	0.45
29:c:246:LYS:HA	29:c:246:LYS:HD2	1.78	0.45
32:f:592:ASN:O	32:f:596:ASP:HB2	2.16	0.45
10:j:71:MET:SD	10:j:84:ILE:HD11	2.57	0.45
4:D:200:ARG:HH22	4:D:302:ASN:HA	1.82	0.45
5:E:207:TYR:HD1	5:E:208:ILE:N	2.15	0.45
6:F:369:HIS:CE1	6:F:397:LYS:HG3	2.52	0.45
21:U:191:LYS:HE3	21:U:560:MET:HG3	1.98	0.45
21:U:673:GLU:O	21:U:676:THR:HG22	2.17	0.45
23:W:356:ASN:O	23:W:359:VAL:HG12	2.17	0.45
29:c:231:LEU:O	29:c:232:GLN:HB3	2.17	0.45
30:d:51:ALA:O	30:d:55:LEU:HG	2.17	0.45
30:d:201:ASN:C	30:d:203:PRO:HD3	2.42	0.45
32:f:193:PRO:HA	32:f:196:MET:SD	2.57	0.45
32:f:445:LEU:HD22	32:f:469:TYR:HD2	1.82	0.45
8:h:89:ARG:O	8:h:93:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:146:VAL:HG23	11:k:220:VAL:HG12	1.99	0.45
11:k:186:HIS:O	11:k:189:MET:HG3	2.16	0.45
12:l:180:MET:HA	12:l:180:MET:HE3	1.98	0.45
16:p:15:LYS:HB2	16:p:121:ILE:HD13	1.99	0.45
1:A:119:ALA:HB2	6:F:128:THR:HG22	1.98	0.45
2:B:53:THR:HA	2:B:55:HIS:CE1	2.52	0.45
2:B:64:LYS:HE2	32:f:239:TYR:CE1	2.51	0.45
3:C:226:GLU:O	3:C:230:MET:HG3	2.17	0.45
4:D:200:ARG:NH1	4:D:302:ASN:HA	2.23	0.45
5:E:216:ARG:HA	5:E:219:PHE:HB2	1.98	0.45
6:F:384:LEU:HD21	6:F:420:TYR:HB3	1.99	0.45
8:H:68:ILE:HD11	8:H:74:LEU:HD12	1.99	0.45
10:J:117:ARG:HA	10:J:120:GLN:OE1	2.17	0.45
14:N:17:ASP:HB3	14:N:164:MET:HE2	1.99	0.45
21:U:454:GLY:HA2	21:U:458:ILE:HD11	1.99	0.45
27:a:60:TYR:CZ	27:a:64:ILE:HD11	2.52	0.45
29:c:141:VAL:HG22	29:c:161:ARG:HE	1.82	0.45
29:c:214:GLN:O	29:c:217:LEU:HG	2.17	0.45
10:j:142:PRO:O	10:j:143:ARG:HD2	2.17	0.45
19:s:108:ASN:HB2	19:s:124:PHE:HB2	1.99	0.45
20:t:51:LEU:HD21	20:t:110:MET:HE2	1.99	0.45
6:F:73:ILE:O	6:F:76:ASN:N	2.50	0.44
15:O:42:TYR:HE2	15:O:183:LEU:HD11	1.81	0.44
17:Q:16:ALA:HB2	17:Q:160:LEU:HD11	1.99	0.44
21:U:45:ILE:HG21	21:U:63:VAL:HG23	1.98	0.44
21:U:103:LYS:HB2	21:U:103:LYS:HE3	1.71	0.44
21:U:405:THR:CG2	21:U:441:GLY:HA3	2.47	0.44
22:V:414:TYR:HB3	22:V:417:ILE:HD11	1.98	0.44
22:V:480:ILE:HB	26:Z:260:VAL:HG22	1.99	0.44
25:Y:91:ALA:HB1	25:Y:100:ILE:HG22	1.99	0.44
28:b:124:LEU:HD21	28:b:152:LYS:HB3	1.97	0.44
28:b:189:LEU:H	28:b:189:LEU:HD12	1.82	0.44
32:f:785:ARG:HH21	32:f:876:HIS:HA	1.82	0.44
12:l:64:LEU:HD12	12:l:72:ILE:HD11	1.98	0.44
16:p:20:VAL:HG13	16:p:119:PRO:HB3	1.99	0.44
1:A:433:ASN:HA	11:K:53:ARG:HH21	1.82	0.44
2:B:281:ILE:HG22	2:B:326:LYS:CB	2.47	0.44
16:P:131:MET:HE2	16:P:131:MET:HB2	1.87	0.44
24:X:6:VAL:HG13	24:X:10:GLN:HE22	1.82	0.44
25:Y:288:PHE:CZ	25:Y:292:TYR:HB2	2.52	0.44
27:a:96:PHE:HA	27:a:99:LYS:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:94:LYS:H	32:f:94:LYS:HD3	1.82	0.44
32:f:576:ILE:O	32:f:580:LEU:HG	2.17	0.44
7:g:180:GLU:HA	7:g:183:VAL:HG12	1.99	0.44
8:h:59:GLU:HG2	8:h:60:ARG:HE	1.83	0.44
3:C:46:GLN:HE22	21:U:639:LEU:HB2	1.82	0.44
4:D:225:ALA:HB1	4:D:259:PRO:O	2.17	0.44
12:L:217:LYS:HD2	12:L:217:LYS:C	2.42	0.44
19:S:44:TYR:HB2	19:S:52:ILE:HG23	2.00	0.44
21:U:82:LEU:HD23	21:U:82:LEU:HA	1.89	0.44
25:Y:283:LYS:HD2	25:Y:288:PHE:CZ	2.52	0.44
27:a:249:GLN:HA	27:a:252:LYS:HB2	1.99	0.44
27:a:335:TRP:CD1	27:a:337:GLN:H	2.35	0.44
28:b:28:ALA:HB3	28:b:143:PHE:HZ	1.82	0.44
17:q:40:GLU:OE2	17:q:41:LYS:HG3	2.17	0.44
18:r:39:PRO:HA	18:r:184:TRP:HE1	1.82	0.44
20:t:152:GLU:O	20:t:155:GLU:HG3	2.17	0.44
2:B:308:THR:O	2:B:311:GLU:HG3	2.17	0.44
6:F:72:LYS:O	6:F:73:ILE:C	2.60	0.44
6:F:180:ARG:HH22	6:F:245:LYS:HA	1.82	0.44
7:G:217:VAL:HG12	7:G:230:LEU:HD23	2.00	0.44
18:R:160:ILE:HG21	18:R:174:VAL:HG13	1.99	0.44
21:U:801:GLN:HB3	21:U:877:LEU:HD22	2.00	0.44
22:V:416:ARG:C	22:V:417:ILE:HD12	2.42	0.44
26:Z:174:HIS:CD2	29:c:155:VAL:HG22	2.53	0.44
27:a:267:GLN:O	27:a:271:LYS:HG3	2.17	0.44
17:q:158:GLU:N	17:q:158:GLU:OE2	2.49	0.44
18:r:141:ARG:HD2	18:r:141:ARG:HA	1.69	0.44
20:t:127:MET:HE2	20:t:127:MET:HB2	1.81	0.44
1:A:215:PHE:CD2	1:A:324:PRO:HG3	2.52	0.44
1:A:292:ASP:HB2	1:A:295:VAL:HB	1.99	0.44
3:C:142:LYS:HE2	3:C:142:LYS:HB3	1.81	0.44
4:D:172:ILE:O	4:D:176:GLU:HG2	2.18	0.44
4:D:380:GLN:O	4:D:384:MET:HE3	2.18	0.44
5:E:165:ILE:N	5:E:166:PRO:HD2	2.32	0.44
6:F:159:LEU:HA	6:F:159:LEU:HD13	1.72	0.44
7:G:101:TRP:CD1	7:G:109:ILE:HB	2.52	0.44
18:R:20:ALA:HB2	18:R:31:VAL:HG21	2.00	0.44
25:Y:375:LEU:HD23	25:Y:375:LEU:HA	1.80	0.44
26:Z:186:THR:HA	26:Z:190:ARG:HG3	1.98	0.44
26:Z:262:LEU:O	26:Z:266:ILE:HG12	2.18	0.44
27:a:268:LEU:HD23	27:a:268:LEU:HA	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:234:TYR:HA	29:c:237:HIS:HB3	1.98	0.44
32:f:282:PHE:HA	32:f:294:MET:HE1	1.99	0.44
9:i:192:LEU:O	9:i:196:VAL:HG12	2.18	0.44
10:j:19:VAL:O	10:j:23:GLN:HG2	2.17	0.44
15:o:54:MET:HG3	16:p:96:TYR:CE2	2.52	0.44
2:B:343:ARG:HE	2:B:346:ARG:HE	1.65	0.44
3:C:52:LEU:HD22	4:D:68:LEU:HB3	2.00	0.44
5:E:219:PHE:HA	5:E:222:ALA:HB3	2.00	0.44
5:E:231:PHE:HD1	5:E:232:MET:N	2.15	0.44
6:F:220:PRO:HG2	6:F:350:ARG:HH11	1.82	0.44
14:N:103:TRP:CH2	14:N:181:GLU:HG2	2.53	0.44
16:P:12:MET:HE3	16:P:12:MET:HB3	1.71	0.44
17:Q:140:LEU:HD13	18:r:166:ARG:NH1	2.33	0.44
18:R:74:ILE:HG13	18:R:75:SER:N	2.33	0.44
22:V:304:GLU:HA	22:V:307:ARG:CG	2.48	0.44
22:V:466:ILE:HD11	26:Z:247:LYS:HE3	1.99	0.44
31:e:58:ALA:O	31:e:62:LYS:HB3	2.17	0.44
1:A:159:PRO:O	1:A:162:THR:HG22	2.18	0.44
4:D:327:LEU:HD23	4:D:327:LEU:HA	1.79	0.44
6:F:435:LEU:HB3	6:F:437:TYR:CE1	2.53	0.44
10:J:108:THR:HG22	10:J:133:ILE:HD12	1.98	0.44
14:N:59:VAL:HG11	14:N:83:PHE:CE2	2.53	0.44
15:O:214:GLU:HG3	16:P:198:ARG:HG2	1.99	0.44
18:R:55:TRP:HE3	18:R:86:MET:HE3	1.82	0.44
21:U:727:LYS:O	21:U:731:ILE:HG22	2.18	0.44
25:Y:237:ARG:HA	25:Y:241:ILE:HD12	2.00	0.44
26:Z:78:MET:HE2	29:c:98:MET:HE2	2.00	0.44
15:o:20:ALA:HB3	15:o:28:ASP:HB3	1.99	0.44
1:A:225:CYS:O	1:A:229:VAL:HG22	2.18	0.44
10:J:219:ILE:HD12	10:J:219:ILE:HA	1.83	0.44
12:L:39:LYS:HE2	12:L:157:ARG:HA	1.99	0.44
14:N:25:TYR:OH	15:O:135:MET:HG2	2.18	0.44
14:N:115:PRO:HG2	14:N:119:MET:HB3	1.99	0.44
21:U:526:ALA:O	21:U:529:ILE:HG13	2.17	0.44
21:U:825:LYS:HG3	21:U:826:GLU:H	1.83	0.44
27:a:50:PHE:CD2	27:a:52:GLN:HB3	2.53	0.44
29:c:158:ASP:HB3	29:c:160:PHE:CE1	2.52	0.44
30:d:240:THR:O	30:d:244:LYS:HG2	2.18	0.44
32:f:517:VAL:HG22	32:f:557:TRP:HZ3	1.83	0.44
32:f:849:ALA:HB2	32:f:879:ARG:HG3	2.00	0.44
10:j:136:PHE:HE1	10:j:142:PRO:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ILE:HD12	2:B:268:ARG:HH21	1.82	0.44
5:E:43:SER:HA	5:E:46:ASP:OD2	2.18	0.44
5:E:304:PRO:HB3	5:E:338:PHE:HD1	1.82	0.44
12:L:112:ILE:O	12:L:116:THR:HG23	2.17	0.44
24:X:88:LEU:HD12	24:X:89:VAL:N	2.33	0.44
24:X:122:ARG:HD2	24:X:125:LEU:HB2	1.99	0.44
24:X:124:PHE:CE1	24:X:160:MET:HE1	2.53	0.44
28:b:188:ILE:HG13	28:b:189:LEU:N	2.33	0.44
10:j:157:LYS:H	11:k:58:LEU:HD11	1.82	0.44
16:p:138:VAL:HG11	16:p:146:MET:HB3	1.99	0.44
3:C:293:MET:HB3	3:C:293:MET:HE2	1.69	0.43
5:E:83:CYS:HB3	5:E:87:LEU:HD23	2.00	0.43
6:F:245:LYS:H	6:F:245:LYS:HD2	1.83	0.43
8:H:205:GLU:HB3	8:H:227:LYS:HE3	2.00	0.43
17:Q:1:MET:HE1	17:Q:134:TYR:CE2	2.52	0.43
22:V:189:ASP:HA	22:V:192:MET:SD	2.58	0.43
22:V:223:LYS:HB3	22:V:226:VAL:HG22	1.99	0.43
22:V:461:LYS:HD3	22:V:461:LYS:N	2.32	0.43
23:W:212:LYS:HD2	23:W:212:LYS:HA	1.81	0.43
30:d:194:ALA:O	30:d:198:LEU:HB2	2.18	0.43
32:f:256:PHE:HB3	32:f:265:ALA:HB2	2.00	0.43
32:f:513:GLU:OE2	32:f:514:VAL:HG13	2.18	0.43
10:j:136:PHE:CD1	10:j:142:PRO:HA	2.53	0.43
19:s:73:LYS:HB2	19:s:73:LYS:HE3	1.86	0.43
1:A:165:GLN:HG2	1:A:167:GLU:HG3	2.00	0.43
1:A:362:MET:O	1:A:364:VAL:HG13	2.18	0.43
4:D:309:MET:HE3	4:D:309:MET:C	2.43	0.43
6:F:219:PRO:HA	6:F:220:PRO:HD3	1.92	0.43
11:K:20:ARG:HE	11:K:22:PHE:HE1	1.65	0.43
21:U:205:TYR:CE1	21:U:215:ASN:HB3	2.53	0.43
21:U:325:MET:HE2	21:U:325:MET:HB2	1.81	0.43
21:U:427:LEU:HD13	21:U:430:ASP:HB2	2.00	0.43
22:V:86:VAL:HG21	22:V:160:LEU:HD13	2.00	0.43
24:X:299:LEU:HD12	24:X:299:LEU:HA	1.79	0.43
29:c:303:MET:HB3	29:c:303:MET:HE2	1.76	0.43
30:d:163:TYR:O	30:d:167:ILE:HG23	2.18	0.43
32:f:257:ARG:HD3	32:f:281:ILE:HD12	2.00	0.43
16:p:12:MET:HG2	16:p:146:MET:HE3	1.99	0.43
19:s:52:ILE:HG13	19:s:110:ILE:HG12	1.99	0.43
1:A:65:ILE:HG21	32:f:680:ARG:HD2	1.99	0.43
3:C:189:TYR:CZ	3:C:316:GLU:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:219:LEU:HG	3:C:230:MET:HE1	2.00	0.43
21:U:26:LYS:HZ2	30:d:36:LEU:HB2	1.82	0.43
21:U:623:GLY:HA3	21:U:658:ILE:HG13	2.00	0.43
25:Y:214:MET:HE1	25:Y:219:PHE:CA	2.49	0.43
26:Z:48:LEU:HD12	26:Z:49:ASP:H	1.83	0.43
27:a:81:LEU:HA	27:a:84:VAL:HG22	2.01	0.43
27:a:309:LEU:H	27:a:309:LEU:HD22	1.83	0.43
32:f:55:GLU:O	32:f:58:MET:HE3	2.18	0.43
32:f:75:LEU:HD22	32:f:121:PHE:HB3	1.98	0.43
13:m:185:THR:HG23	13:m:187:ARG:H	1.84	0.43
16:p:20:VAL:HG23	16:p:190:ILE:HB	1.99	0.43
19:s:197:ILE:O	19:s:203:ILE:HA	2.19	0.43
1:A:315:ILE:HD13	1:A:315:ILE:HA	1.83	0.43
1:A:360:ARG:HB3	1:A:360:ARG:CZ	2.47	0.43
23:W:226:TYR:CE1	23:W:230:MET:HE3	2.54	0.43
23:W:263:TRP:CZ3	23:W:295:LYS:HB3	2.54	0.43
27:a:131:THR:HA	27:a:134:THR:HG22	2.01	0.43
27:a:306:GLU:HA	27:a:309:LEU:HD23	2.00	0.43
28:b:30:GLN:OE1	28:b:75:LEU:HB3	2.17	0.43
10:j:83:VAL:HG21	10:j:129:ILE:HD11	2.00	0.43
12:l:65:HIS:HB2	12:l:223:ILE:HD11	2.01	0.43
16:p:27:ARG:HB2	16:p:183:MET:HB3	1.99	0.43
20:t:180:ASP:HB3	20:t:183:SER:HB3	2.01	0.43
1:A:66:LYS:H	1:A:66:LYS:HD2	1.83	0.43
2:B:49:LEU:HG	32:f:670:MET:HE1	2.01	0.43
2:B:164:MET:HA	2:B:164:MET:HE3	2.00	0.43
4:D:201:GLY:HA2	4:D:307:VAL:O	2.18	0.43
5:E:130:VAL:HG13	5:E:185:ARG:HG2	1.99	0.43
13:M:173:LYS:O	13:M:177:GLU:HG3	2.19	0.43
21:U:1:MET:HG3	21:U:3:THR:HG22	2.01	0.43
21:U:59:PHE:O	21:U:63:VAL:HG22	2.18	0.43
21:U:253:TYR:CZ	21:U:331:GLY:HA3	2.53	0.43
21:U:401:LYS:HE3	21:U:438:GLN:HB2	2.01	0.43
21:U:567:ILE:HD11	21:U:585:THR:HB	2.00	0.43
24:X:183:LEU:HD23	24:X:183:LEU:HA	1.84	0.43
24:X:334:ASN:O	24:X:338:VAL:HG22	2.18	0.43
28:b:126:LYS:HA	28:b:129:LYS:HE3	2.01	0.43
11:k:238:ILE:HD12	11:k:241:ILE:HG13	2.00	0.43
12:l:146:GLN:O	12:l:153:TYR:HA	2.19	0.43
4:D:344:ILE:HG22	4:D:375:ILE:HG21	2.00	0.43
4:D:392:TYR:HB2	5:E:161:ARG:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:415:GLU:CD	4:D:415:GLU:H	2.26	0.43
5:E:31:GLU:O	5:E:35:GLU:HG2	2.18	0.43
5:E:276:ILE:HD12	5:E:276:ILE:O	2.18	0.43
16:P:20:VAL:HG13	16:P:119:PRO:HB3	2.01	0.43
16:P:155:GLU:HG2	16:P:158:MET:SD	2.58	0.43
21:U:206:MET:C	21:U:206:MET:HE2	2.43	0.43
26:Z:96:HIS:O	26:Z:123:ILE:HA	2.19	0.43
32:f:130:ALA:HA	32:f:133:MET:SD	2.58	0.43
7:g:132:ARG:HA	7:g:133:PRO:HD3	1.85	0.43
9:i:245:ALA:O	9:i:248:GLU:HG3	2.19	0.43
1:A:81:ALA:HB1	1:A:85:GLN:HE21	1.82	0.43
1:A:273:PHE:CD1	1:A:318:LEU:HD12	2.53	0.43
2:B:194:ILE:O	2:B:198:LYS:HB2	2.19	0.43
2:B:440:LEU:HA	10:J:48:LYS:HZ1	1.84	0.43
3:C:336:MET:HE3	4:D:195:GLY:O	2.18	0.43
5:E:333:LYS:HB3	5:E:333:LYS:HE2	1.73	0.43
7:G:43:ARG:HB2	7:G:151:VAL:HG23	2.00	0.43
21:U:732:LEU:O	21:U:736:ILE:HG12	2.18	0.43
21:U:803:LYS:HD2	21:U:875:PHE:HB3	2.00	0.43
22:V:264:TYR:O	22:V:268:GLU:HG3	2.18	0.43
23:W:177:MET:SD	23:W:181:GLU:HB3	2.58	0.43
24:X:141:LYS:HA	24:X:141:LYS:HD2	1.86	0.43
24:X:281:GLY:H	24:X:284:THR:HG22	1.83	0.43
25:Y:141:VAL:HG11	25:Y:164:ALA:HB2	2.01	0.43
26:Z:150:PRO:HB3	27:a:184:ASP:CG	2.44	0.43
29:c:38:LEU:HA	29:c:41:MET:HG2	1.99	0.43
32:f:131:MET:HE1	32:f:161:HIS:CB	2.48	0.43
32:f:291:GLN:HA	32:f:294:MET:SD	2.59	0.43
8:h:116:SER:O	8:h:120:GLU:HG2	2.18	0.43
8:h:189:HIS:NE2	8:h:233:ILE:HG13	2.33	0.43
15:o:48:THR:HB	15:o:51:ASP:HB2	2.01	0.43
16:p:51:ILE:HG13	16:p:109:ILE:HG12	2.01	0.43
18:r:179:VAL:HG22	18:r:184:TRP:HB3	2.00	0.43
1:A:139:ARG:HH12	1:A:156:LYS:N	2.16	0.43
5:E:376:ASP:O	5:E:380:LEU:HG	2.18	0.43
6:F:73:ILE:O	6:F:74:LYS:C	2.61	0.43
16:P:88:MET:HG3	16:P:122:CYS:SG	2.59	0.43
16:P:177:ARG:HA	16:P:177:ARG:HD3	1.83	0.43
20:T:157:GLN:HG3	20:T:160:LEU:HD23	2.01	0.43
21:U:427:LEU:HD22	21:U:430:ASP:OD2	2.19	0.43
21:U:602:LEU:HD21	21:U:618:ALA:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:27:LEU:HD12	24:X:56:LEU:HD21	2.00	0.43
24:X:143:TYR:CE2	25:Y:252:SER:HB2	2.54	0.43
27:a:160:SER:O	27:a:163:TYR:HB3	2.19	0.43
28:b:22:LEU:HD21	28:b:177:PRO:HB3	2.00	0.43
29:c:100:LYS:HE2	29:c:100:LYS:HB3	1.88	0.43
29:c:154:LYS:H	29:c:154:LYS:HD3	1.83	0.43
29:c:189:ILE:HA	29:c:192:LEU:HG	2.01	0.43
32:f:104:GLY:O	32:f:108:GLU:HG2	2.18	0.43
32:f:340:MET:N	32:f:340:MET:SD	2.92	0.43
32:f:467:SER:HB2	32:f:500:LEU:HD11	2.01	0.43
32:f:482:ILE:HD13	32:f:518:THR:OG1	2.19	0.43
9:i:72:MET:HE1	9:i:107:CYS:HA	2.01	0.43
13:m:191:LYS:HB3	13:m:238:TYR:CD2	2.53	0.43
18:r:71:LYS:HB2	18:r:71:LYS:NZ	2.34	0.43
1:A:125:LEU:HD12	1:A:149:ILE:HB	2.01	0.43
2:B:232:LYS:HG2	2:B:353:PHE:CD2	2.52	0.43
2:B:234:LEU:HD22	35:B:501:ATP:H2'	2.01	0.43
3:C:74:GLY:HA3	3:C:89:VAL:HG12	2.00	0.43
5:E:153:LEU:HD21	5:E:274:LYS:HG2	2.01	0.43
5:E:171:LEU:HB2	5:E:295:LEU:HD22	2.01	0.43
19:S:172:MET:HE2	19:S:176:LYS:HE3	2.00	0.43
21:U:680:VAL:HB	21:U:683:VAL:HG12	2.00	0.43
21:U:772:TRP:HB3	21:U:775:LEU:HG	2.01	0.43
22:V:175:MET:HE1	22:V:180:ARG:N	2.28	0.43
23:W:192:LEU:HD23	23:W:192:LEU:HA	1.86	0.43
26:Z:45:LYS:HD3	26:Z:45:LYS:HA	1.79	0.43
26:Z:146:ASP:CB	26:Z:149:THR:HB	2.47	0.43
27:a:335:TRP:NE1	27:a:337:GLN:HB3	2.34	0.43
8:h:19:LEU:HD23	8:h:19:LEU:HA	1.87	0.43
9:i:174:MET:O	9:i:178:ASP:OD1	2.37	0.43
1:A:348:LEU:HA	1:A:348:LEU:HD23	1.81	0.43
2:B:49:LEU:HD23	2:B:49:LEU:HA	1.80	0.43
2:B:362:LYS:HG2	2:B:384:ILE:HD13	2.01	0.43
4:D:204:MET:O	4:D:310:ALA:HA	2.18	0.43
7:G:197:THR:HA	7:G:200:THR:HG22	2.01	0.43
8:H:159:LYS:HE3	9:I:57:ASP:HA	2.01	0.43
21:U:583:MET:SD	21:U:583:MET:C	3.02	0.43
21:U:670:ASN:HA	21:U:673:GLU:HG3	2.01	0.43
22:V:463:MET:HB2	22:V:464:ILE:H	1.65	0.43
23:W:71:VAL:HG23	23:W:83:LEU:HD11	2.00	0.43
23:W:214:PHE:HB3	23:W:223:LYS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:316:ASP:CB	24:X:320:SER:HB3	2.48	0.43
24:X:379:ASP:OD1	25:Y:312:ARG:HG2	2.19	0.43
26:Z:111:LEU:HG	26:Z:114:ARG:HH21	1.84	0.43
26:Z:263:ALA:HB3	29:c:292:MET:HE1	2.01	0.43
32:f:524:MET:HA	32:f:527:VAL:CG2	2.48	0.43
9:i:229:LYS:HB2	9:i:232:GLU:OE1	2.19	0.43
10:j:94:HIS:ND1	10:j:102:VAL:HG12	2.34	0.43
12:l:105:VAL:O	12:l:109:VAL:HG23	2.19	0.43
14:n:8:PHE:HB3	14:n:152:CYS:SG	2.59	0.43
2:B:39:LYS:HG2	2:B:276:GLU:HG2	2.00	0.42
2:B:107:MET:SD	2:B:151:LEU:HB3	2.59	0.42
3:C:228:ALA:HB1	3:C:275:GLU:HG2	2.00	0.42
3:C:334:ARG:HE	3:C:335:LYS:HG2	1.84	0.42
4:D:395:LEU:HD12	4:D:397:LYS:NZ	2.34	0.42
5:E:316:HIS:CD2	5:E:344:ARG:HG2	2.54	0.42
6:F:321:GLN:HE21	6:F:323:ASN:ND2	2.17	0.42
19:S:185:ARG:HG3	16:p:151:GLU:OE1	2.18	0.42
21:U:220:LEU:HD13	21:U:220:LEU:HA	1.88	0.42
23:W:431:LYS:HB3	23:W:431:LYS:HE2	1.63	0.42
24:X:202:CYS:O	24:X:204:PRO:HD3	2.18	0.42
24:X:407:MET:HA	24:X:410:VAL:HG12	2.01	0.42
26:Z:112:MET:C	26:Z:112:MET:HE3	2.44	0.42
28:b:103:LYS:HD2	28:b:103:LYS:HA	1.82	0.42
29:c:211:GLU:OE2	29:c:215:LYS:HG3	2.19	0.42
30:d:135:HIS:HB3	30:d:136:PRO:HD3	2.01	0.42
32:f:213:GLN:HB3	32:f:216:MET:HE1	2.01	0.42
13:m:81:LEU:HD12	13:m:81:LEU:HA	1.93	0.42
17:q:88:LEU:HD12	17:q:88:LEU:HA	1.86	0.42
18:r:106:LYS:HB2	18:r:106:LYS:HE2	1.88	0.42
6:F:266:LYS:HD2	6:F:269:ARG:HH21	1.84	0.42
7:G:187:PHE:HD1	7:G:189:TRP:HE1	1.66	0.42
18:R:3:THR:HG21	18:R:44:THR:HB	2.01	0.42
27:a:362:SER:HA	27:a:365:MET:HE2	2.00	0.42
32:f:72:ARG:HB2	32:f:73:PRO:HD3	2.02	0.42
32:f:474:SER:HB3	32:f:477:MET:SD	2.59	0.42
10:j:90:GLU:HG3	10:j:110:TYR:CD1	2.54	0.42
11:k:210:LEU:HD12	11:k:215:ILE:HD13	1.99	0.42
16:p:22:ILE:HG23	16:p:188:HIS:HB2	2.01	0.42
19:s:115:GLU:H	19:s:115:GLU:CD	2.27	0.42
3:C:375:ARG:NE	3:C:377:HIS:HB2	2.34	0.42
4:D:284:GLU:O	4:D:287:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:355:ILE:HG13	6:F:215:LEU:HG	2.01	0.42
9:I:107:CYS:O	9:I:111:VAL:HG23	2.19	0.42
16:P:12:MET:HB2	16:P:146:MET:HE2	2.02	0.42
21:U:462:LEU:HG	21:U:481:LEU:HD11	2.01	0.42
21:U:475:HIS:HE1	21:U:507:VAL:HG22	1.84	0.42
24:X:8:GLU:HB3	24:X:30:ILE:HD11	2.01	0.42
26:Z:236:LEU:HD23	27:a:335:TRP:HB3	2.01	0.42
27:a:70:ARG:HH21	28:b:17:ARG:HA	1.84	0.42
29:c:37:ALA:O	29:c:41:MET:HG2	2.20	0.42
32:f:659:LEU:O	32:f:662:MET:HG3	2.20	0.42
32:f:740:ARG:O	32:f:744:MET:SD	2.77	0.42
20:t:106:LEU:HD23	20:t:106:LEU:HA	1.92	0.42
3:C:242:ALA:HB3	3:C:243:PRO:HD3	2.01	0.42
5:E:340:GLY:O	5:E:344:ARG:HG3	2.19	0.42
12:L:36:VAL:HG13	12:L:160:SER:HB2	2.02	0.42
21:U:99:THR:HG22	21:U:103:LYS:HE2	2.00	0.42
21:U:524:LYS:HG3	21:U:556:MET:SD	2.59	0.42
22:V:80:LYS:HE3	22:V:80:LYS:HB3	1.89	0.42
22:V:240:LEU:HD12	22:V:241:ARG:HG3	2.02	0.42
23:W:317:TRP:CE2	23:W:355:LYS:HD3	2.54	0.42
24:X:114:ILE:HD12	24:X:130:GLU:OE2	2.19	0.42
28:b:33:VAL:HA	28:b:36:VAL:HG12	2.00	0.42
29:c:265:MET:O	29:c:269:GLN:NE2	2.51	0.42
32:f:230:CYS:HA	32:f:233:LEU:HD12	2.01	0.42
10:j:38:ARG:NH1	10:j:182:GLU:HA	2.34	0.42
11:k:18:GLU:HG3	11:k:20:ARG:HG3	2.02	0.42
2:B:122:ILE:HD11	2:B:130:GLU:HB3	2.02	0.42
9:I:52:ILE:HA	9:I:56:LEU:HD23	2.01	0.42
9:I:86:LEU:HD22	9:I:114:LEU:HD11	2.01	0.42
10:J:236:LYS:HE3	10:J:236:LYS:HB2	1.86	0.42
21:U:748:LEU:HD12	21:U:760:VAL:HG22	2.01	0.42
23:W:220:GLU:O	23:W:224:LEU:HG	2.19	0.42
24:X:114:ILE:O	24:X:118:LYS:HG3	2.19	0.42
29:c:180:ASN:O	29:c:183:HIS:HB2	2.20	0.42
10:j:36:ARG:HG2	10:j:142:PRO:HB2	2.00	0.42
10:j:70:CYS:HB3	10:j:134:VAL:HG22	2.02	0.42
15:o:155:VAL:O	15:o:159:ILE:HG12	2.20	0.42
1:A:218:PRO:HB3	1:A:322:ASN:HD21	1.84	0.42
2:B:38:LYS:HE2	2:B:38:LYS:HB2	1.83	0.42
3:C:375:ARG:HE	3:C:377:HIS:HB2	1.84	0.42
10:J:80:ALA:HA	10:J:129:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:176:MET:CE	13:M:57:LEU:HA	2.49	0.42
21:U:548:LEU:O	21:U:552:ILE:HG23	2.19	0.42
22:V:209:LYS:H	22:V:209:LYS:HG3	1.57	0.42
22:V:230:PHE:HE1	22:V:234:ARG:HE	1.68	0.42
22:V:348:PHE:CD1	22:V:361:PHE:HB2	2.55	0.42
24:X:90:ARG:HH12	24:X:125:LEU:HD12	1.85	0.42
24:X:125:LEU:O	24:X:129:LEU:HG	2.19	0.42
24:X:421:LEU:HD11	26:Z:280:ILE:HG12	2.01	0.42
26:Z:40:LEU:HD23	26:Z:91:ILE:HA	2.01	0.42
32:f:345:PRO:HG3	32:f:378:ASN:HB2	2.02	0.42
32:f:760:PHE:CE2	32:f:764:LEU:HD11	2.55	0.42
7:g:85:ALA:HB1	13:m:120:HIS:HD2	1.84	0.42
9:i:184:MET:HB3	9:i:184:MET:HE3	1.70	0.42
15:o:22:GLU:HB3	34:z:1:UNK:HA	2.00	0.42
1:A:125:LEU:HD21	1:A:134:ILE:HG13	2.01	0.42
2:B:191:ASP:HA	2:B:194:ILE:HB	2.02	0.42
3:C:31:LEU:HD12	3:C:31:LEU:HA	1.81	0.42
4:D:87:LEU:HB3	4:D:132:LEU:O	2.18	0.42
5:E:130:VAL:HB	5:E:134:GLU:OE1	2.20	0.42
5:E:251:ARG:HE	5:E:254:GLN:HB2	1.83	0.42
5:E:310:LEU:O	5:E:314:LYS:HG2	2.20	0.42
18:R:52:CYS:SG	18:R:97:MET:HG3	2.60	0.42
20:T:141:TYR:HE2	14:n:25:TYR:HB2	1.84	0.42
21:U:672:LEU:HA	21:U:675:MET:HG2	2.01	0.42
22:V:206:VAL:HA	22:V:209:LYS:CE	2.49	0.42
23:W:135:LYS:HB3	23:W:137:TYR:CZ	2.54	0.42
24:X:415:TYR:CZ	25:Y:383:LEU:HB2	2.54	0.42
28:b:16:MET:N	28:b:16:MET:SD	2.93	0.42
30:d:15:ASN:ND2	30:d:18:LYS:HD2	2.35	0.42
31:e:62:LYS:HG2	31:e:63:HIS:N	2.34	0.42
8:h:195:LEU:HB3	8:h:203:MET:HE1	2.02	0.42
14:n:70:LEU:HD12	14:n:70:LEU:HA	1.82	0.42
19:s:54:CYS:HB3	19:s:61:CYS:SG	2.59	0.42
1:A:169:LYS:HE3	1:A:169:LYS:HB2	1.87	0.42
4:D:205:TYR:HA	4:D:311:THR:O	2.20	0.42
5:E:238:ILE:HD12	5:E:238:ILE:HA	1.87	0.42
5:E:349:GLU:HG3	5:E:373:LYS:HZ3	1.84	0.42
15:O:68:LEU:HD23	15:O:68:LEU:HA	1.90	0.42
22:V:259:LEU:HD11	22:V:294:ARG:HD3	2.02	0.42
23:W:183:VAL:HG11	23:W:213:PHE:HE2	1.85	0.42
24:X:166:LEU:HA	24:X:169:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:240:VAL:HG11	29:c:310:LYS:HB2	2.02	0.42
28:b:121:GLU:HB3	28:b:152:LYS:HG2	2.02	0.42
29:c:122:LEU:HB2	29:c:200:TYR:CE2	2.55	0.42
32:f:45:LEU:HD13	32:f:45:LEU:HA	1.92	0.42
32:f:453:SER:HB2	32:f:487:LEU:HD23	2.02	0.42
8:h:3:GLU:N	13:m:125:TYR:HB3	2.35	0.42
1:A:394:MET:HA	1:A:397:ILE:HD12	2.02	0.42
2:B:223:ILE:HD11	2:B:331:THR:HG22	2.02	0.42
2:B:246:THR:HG23	2:B:278:ALA:HB3	2.02	0.42
5:E:256:THR:HG22	5:E:260:LEU:HD23	2.00	0.42
6:F:260:PHE:HB2	6:F:263:ASP:OD2	2.20	0.42
7:G:92:GLN:HG3	13:M:117:MET:HE3	2.02	0.42
9:I:90:LEU:HD21	9:I:114:LEU:HD22	2.02	0.42
19:S:84:THR:HG22	19:S:85:THR:H	1.85	0.42
21:U:181:LEU:O	21:U:184:CYS:HB2	2.20	0.42
21:U:409:GLY:HA3	21:U:445:ALA:HB1	2.02	0.42
23:W:130:MET:HE2	23:W:130:MET:O	2.20	0.42
25:Y:236:LEU:HG	25:Y:240:VAL:HG22	2.02	0.42
25:Y:319:MET:HE3	25:Y:319:MET:H	1.84	0.42
26:Z:57:PRO:HD3	29:c:102:THR:OG1	2.20	0.42
26:Z:197:GLY:HA3	29:c:229:LEU:HD22	2.01	0.42
26:Z:224:HIS:ND1	27:a:215:GLU:HB3	2.33	0.42
28:b:91:ARG:HH21	28:b:130:ARG:CZ	2.32	0.42
32:f:168:LYS:HE3	32:f:168:LYS:HB3	1.70	0.42
32:f:296:PHE:HE2	32:f:899:ILE:HD11	1.84	0.42
32:f:714:SER:OG	32:f:729:MET:HE3	2.20	0.42
10:j:14:GLY:HA3	11:k:30:ALA:HB2	2.01	0.42
18:r:114:VAL:HG22	18:r:120:ARG:HB3	2.01	0.42
20:t:74:GLU:HG3	20:t:83:TYR:CZ	2.55	0.42
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.85	0.42
3:C:255:GLY:HA2	3:C:273:MET:HG2	2.02	0.42
4:D:170:MET:HG3	4:D:173:GLN:OE1	2.19	0.42
5:E:280:ASN:H	5:E:281:ARG:NH1	2.18	0.42
10:J:138:PHE:CD1	10:J:138:PHE:C	2.97	0.42
13:M:185:THR:O	13:M:189:ILE:HG12	2.20	0.42
17:Q:22:ALA:C	17:Q:28:MET:HE1	2.45	0.42
19:S:123:SER:HB3	19:S:136:LYS:HG2	2.00	0.42
22:V:188:SER:HA	22:V:191:LEU:HG	2.02	0.42
24:X:78:ASN:HD21	24:X:116:TRP:HZ2	1.67	0.42
24:X:132:ARG:O	24:X:136:LEU:HD22	2.20	0.42
28:b:4:GLU:HA	28:b:106:LYS:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:61:TRP:HB3	30:d:65:ARG:NH2	2.33	0.42
32:f:204:ALA:O	32:f:207:LEU:HG	2.20	0.42
32:f:685:THR:HA	32:f:688:ARG:HD2	2.02	0.42
13:m:35:THR:HG21	13:m:168:ALA:HB3	2.01	0.42
13:m:52:LEU:HD12	13:m:52:LEU:HA	1.79	0.42
1:A:36:TYR:CE1	32:f:157:GLU:HG3	2.53	0.41
4:D:272:THR:OG1	4:D:274:ARG:HG2	2.20	0.41
4:D:381:GLU:OE1	4:D:385:LEU:HD22	2.20	0.41
8:H:213:CYS:HB2	8:H:218:PHE:HD1	1.85	0.41
13:M:181:MET:H	13:M:181:MET:HE2	1.84	0.41
18:R:71:LYS:HD3	18:R:71:LYS:HA	1.78	0.41
19:S:83:MET:HG2	19:S:88:ILE:HG13	2.02	0.41
24:X:314:ARG:HD3	24:X:314:ARG:C	2.45	0.41
25:Y:277:VAL:O	25:Y:281:GLU:HG2	2.20	0.41
26:Z:63:LYS:C	26:Z:65:ASP:H	2.27	0.41
26:Z:212:LEU:O	26:Z:215:VAL:HG12	2.20	0.41
32:f:100:ARG:HA	32:f:100:ARG:HD2	1.78	0.41
32:f:211:ILE:HG23	32:f:213:GLN:HB2	2.01	0.41
32:f:513:GLU:O	32:f:517:VAL:HG23	2.20	0.41
32:f:753:ALA:HA	32:f:759:LEU:HD11	2.02	0.41
10:j:178:ASP:HA	10:j:181:ILE:HG12	2.02	0.41
11:k:110:GLU:HB3	11:k:154:PHE:CZ	2.55	0.41
17:q:101:ASN:HB3	17:q:132:HIS:CE1	2.55	0.41
12:L:205:LEU:HD23	12:L:205:LEU:HA	1.90	0.41
17:Q:69:MET:HE2	17:Q:69:MET:HB2	1.80	0.41
21:U:160:LEU:HG	21:U:200:VAL:HG11	2.01	0.41
22:V:440:LYS:HG2	30:d:145:GLU:O	2.19	0.41
24:X:90:ARG:HH22	24:X:125:LEU:HD12	1.85	0.41
25:Y:325:VAL:HG21	31:e:60:LEU:HA	2.02	0.41
32:f:507:ASP:CG	32:f:509:LYS:HE3	2.45	0.41
10:j:234:LYS:HE2	10:j:234:LYS:HB3	1.89	0.41
13:m:110:HIS:HB2	14:n:70:LEU:HD11	2.02	0.41
15:o:13:VAL:HG22	15:o:177:VAL:HG22	2.02	0.41
19:s:104:TYR:HB3	19:s:106:VAL:HG23	2.01	0.41
1:A:42:SER:HA	2:B:57:GLN:HE22	1.85	0.41
2:B:85:MET:O	2:B:86:LYS:HG2	2.20	0.41
2:B:202:GLU:OE1	2:B:206:THR:HG21	2.21	0.41
4:D:297:ASP:OD2	4:D:326:ARG:HB2	2.21	0.41
6:F:70:LYS:HD3	6:F:70:LYS:HA	1.88	0.41
16:P:35:VAL:HG12	16:P:36:THR:HG23	2.03	0.41
18:R:8:PHE:CZ	18:R:10:HIS:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:89:HIS:CE1	20:T:131:ALA:HB1	2.56	0.41
21:U:26:LYS:HD3	30:d:36:LEU:HD13	2.03	0.41
21:U:160:LEU:HD12	21:U:160:LEU:HA	1.78	0.41
21:U:460:TYR:O	21:U:464:GLN:HG2	2.21	0.41
22:V:119:GLY:HA2	22:V:148:ARG:HD3	2.01	0.41
22:V:182:LYS:O	22:V:186:LYS:HG3	2.20	0.41
24:X:165:LEU:HA	24:X:168:GLU:OE1	2.21	0.41
30:d:79:LYS:HD3	30:d:79:LYS:HA	1.92	0.41
32:f:538:ILE:HD11	32:f:558:LEU:HD12	2.03	0.41
32:f:796:LEU:HD12	32:f:796:LEU:HA	1.89	0.41
9:i:208:ALA:HB2	9:i:234:GLU:HB3	2.01	0.41
9:i:224:VAL:HG12	9:i:226:ARG:HG3	2.01	0.41
10:j:234:LYS:O	10:j:237:GLU:HG3	2.19	0.41
11:k:92:ALA:O	11:k:96:THR:HG23	2.21	0.41
12:l:154:PHE:HE1	13:m:63:ASN:HD21	1.68	0.41
19:s:1:ARG:HA	19:s:1:ARG:HD2	1.80	0.41
19:s:201:GLU:OE1	19:s:201:GLU:N	2.53	0.41
1:A:186:LYS:HG2	6:F:409:ARG:HH22	1.86	0.41
4:D:60:TYR:HE1	21:U:607:VAL:HG21	1.85	0.41
5:E:77:PRO:HG2	5:E:79:TYR:CE2	2.55	0.41
5:E:330:ALA:O	5:E:333:LYS:HG2	2.20	0.41
12:L:157:ARG:HB2	12:L:176:MET:CE	2.50	0.41
14:N:30:VAL:O	14:N:30:VAL:HG12	2.20	0.41
17:Q:53:THR:HG22	17:Q:100:VAL:HG12	2.02	0.41
20:T:194:GLU:HB2	20:T:195:LYS:HZ1	1.85	0.41
25:Y:72:LYS:CA	25:Y:75:LYS:HE3	2.50	0.41
26:Z:188:SER:O	26:Z:192:THR:HG23	2.21	0.41
27:a:193:GLN:HB3	27:a:225:LEU:HD13	2.01	0.41
28:b:68:THR:HA	28:b:71:ILE:HD12	2.01	0.41
29:c:49:VAL:CG2	29:c:50:PRO:HD3	2.50	0.41
30:d:143:LEU:HD21	30:d:174:ILE:HD11	2.02	0.41
30:d:217:LEU:HD23	30:d:222:TYR:CE1	2.55	0.41
32:f:249:LEU:HD13	32:f:272:LEU:HG	2.02	0.41
32:f:337:LEU:HD23	32:f:337:LEU:HA	1.85	0.41
9:i:159:TRP:CZ3	10:j:54:GLN:HG2	2.56	0.41
9:i:178:ASP:OD1	9:i:178:ASP:N	2.52	0.41
12:l:133:LEU:HD23	12:l:133:LEU:HA	1.88	0.41
1:A:32:LEU:HD22	1:A:36:TYR:CD2	2.55	0.41
3:C:163:GLU:O	3:C:168:PRO:HD3	2.19	0.41
5:E:171:LEU:HD23	5:E:298:LYS:HG2	2.01	0.41
10:J:204:LYS:HD3	10:J:204:LYS:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:96:ARG:HH12	12:L:102:PRO:HG3	1.85	0.41
21:U:205:TYR:CZ	21:U:215:ASN:HB3	2.55	0.41
21:U:674:PRO:HG2	21:U:675:MET:SD	2.60	0.41
26:Z:7:GLN:OE1	26:Z:46:LYS:HB3	2.21	0.41
26:Z:15:VAL:O	26:Z:19:VAL:HG23	2.21	0.41
26:Z:91:ILE:H	26:Z:91:ILE:HG13	1.60	0.41
28:b:24:THR:HB	28:b:27:GLN:HB2	2.03	0.41
30:d:190:LEU:HB3	30:d:193:GLU:OE1	2.21	0.41
32:f:70:LEU:C	32:f:73:PRO:HD2	2.45	0.41
12:l:214:ILE:HD12	12:l:224:TYR:HE2	1.84	0.41
13:m:181:MET:HA	13:m:184:MET:HG3	2.03	0.41
2:B:84:GLN:OE1	21:U:828:VAL:HG22	2.21	0.41
3:C:343:ASN:HD22	3:C:346:LYS:HD2	1.85	0.41
4:D:296:MET:HE3	4:D:326:ARG:HG3	2.02	0.41
5:E:195:PHE:HA	5:E:231:PHE:HB2	2.02	0.41
9:I:19:TYR:HA	9:I:22:GLU:OE2	2.21	0.41
12:L:105:VAL:O	12:L:109:VAL:HG23	2.21	0.41
12:L:157:ARG:HE	13:M:59:GLU:HA	1.86	0.41
14:N:196:LYS:HE3	14:N:196:LYS:HB3	1.85	0.41
17:Q:182:ILE:HG23	17:Q:189:HIS:HB2	2.03	0.41
21:U:16:GLU:HG3	30:d:27:LYS:NZ	2.32	0.41
21:U:265:ILE:HD11	21:U:329:LEU:HB3	2.02	0.41
21:U:475:HIS:CE1	21:U:507:VAL:HG22	2.56	0.41
22:V:281:ASN:HA	25:Y:385:ARG:HH12	1.85	0.41
24:X:402:GLU:OE1	29:c:249:LEU:HD11	2.20	0.41
25:Y:113:ARG:HD2	25:Y:113:ARG:HA	1.85	0.41
30:d:241:GLU:O	30:d:245:GLN:HG3	2.21	0.41
32:f:559:PRO:HD3	32:f:587:PHE:CZ	2.55	0.41
1:A:101:ILE:HD11	1:A:140:VAL:HG11	2.02	0.41
3:C:31:LEU:HD23	4:D:47:LEU:HB2	2.03	0.41
4:D:193:GLN:HB3	4:D:194:ILE:HD12	2.02	0.41
4:D:355:SER:HB3	4:D:393:ILE:HG12	2.01	0.41
4:D:393:ILE:HD12	4:D:393:ILE:HA	1.92	0.41
5:E:335:SER:HA	5:E:371:VAL:HG11	2.03	0.41
6:F:384:LEU:HD23	6:F:384:LEU:HA	1.84	0.41
8:H:59:GLU:HB2	8:H:60:ARG:NH2	2.36	0.41
9:I:136:TYR:HE1	9:I:150:SER:HB3	1.85	0.41
20:T:167:ASP:OD2	20:T:167:ASP:C	2.63	0.41
21:U:35:TRP:CD1	21:U:70:HIS:HD1	2.39	0.41
22:V:207:ALA:HA	22:V:210:CYS:SG	2.61	0.41
26:Z:189:GLN:OE1	26:Z:190:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:26:GLU:OE1	27:a:26:GLU:HA	2.21	0.41
28:b:48:ASN:HD22	28:b:101:GLN:NE2	2.19	0.41
29:c:149:GLN:HB3	29:c:156:VAL:HG21	2.03	0.41
32:f:96:LEU:O	32:f:100:ARG:HG2	2.20	0.41
32:f:339:ILE:HG13	32:f:343:LYS:HZ3	1.85	0.41
11:k:85:ALA:O	11:k:89:ILE:HG12	2.21	0.41
11:k:121:LEU:HA	11:k:123:PHE:CE1	2.55	0.41
20:t:117:ASP:OD2	20:t:117:ASP:C	2.63	0.41
2:B:116:ILE:HB	2:B:120:HIS:O	2.21	0.41
4:D:151:ILE:C	4:D:153:MET:N	2.71	0.41
4:D:272:THR:HB	4:D:317:LEU:HA	2.02	0.41
5:E:100:LEU:HA	5:E:106:THR:O	2.21	0.41
8:H:10:LEU:HD11	8:H:22:ILE:HD11	2.03	0.41
21:U:148:LYS:HA	21:U:151:ILE:HG22	2.02	0.41
23:W:378:MET:HB3	23:W:378:MET:HE3	1.80	0.41
23:W:439:VAL:HB	26:Z:234:PHE:CE1	2.56	0.41
24:X:350:ILE:HD12	24:X:350:ILE:HA	1.99	0.41
25:Y:25:LEU:HD11	25:Y:284:LYS:NZ	2.36	0.41
27:a:239:ALA:HB1	27:a:246:GLU:HG2	2.02	0.41
30:d:182:ILE:HD12	30:d:186:TYR:HD2	1.85	0.41
32:f:94:LYS:H	32:f:94:LYS:CD	2.34	0.41
32:f:335:ARG:HA	32:f:340:MET:HE1	2.03	0.41
12:l:46:LEU:HD21	12:l:135:ALA:HB2	2.02	0.41
14:n:59:VAL:HG11	14:n:83:PHE:CE2	2.56	0.41
17:q:62:LYS:HD3	17:q:62:LYS:HA	1.77	0.41
18:r:81:LYS:HD2	18:r:81:LYS:HA	1.76	0.41
1:A:312:ARG:HG3	1:A:315:ILE:HB	2.01	0.41
3:C:70:GLY:HA3	4:D:113:VAL:HG12	2.03	0.41
4:D:60:TYR:CG	21:U:603:LEU:HD21	2.56	0.41
4:D:249:ASP:O	4:D:252:ARG:HG3	2.21	0.41
5:E:253:ILE:O	5:E:257:LEU:HG	2.21	0.41
6:F:327:LYS:HA	6:F:327:LYS:HD3	1.79	0.41
8:H:38:ILE:HB	8:H:45:VAL:HG22	2.03	0.41
17:Q:28:MET:H	17:Q:28:MET:HE2	1.86	0.41
18:R:45:MET:HE3	18:R:45:MET:HB2	1.74	0.41
21:U:708:GLN:O	21:U:711:GLN:HG2	2.21	0.41
22:V:264:TYR:CE2	22:V:298:ILE:HG21	2.56	0.41
22:V:416:ARG:HB3	25:Y:348:ASP:OD1	2.21	0.41
23:W:294:LYS:HB3	23:W:294:LYS:HE3	1.78	0.41
23:W:397:VAL:HG11	24:X:341:PRO:HA	2.03	0.41
24:X:259:ILE:HD13	24:X:259:ILE:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:229:ILE:HD11	25:Y:295:TYR:CE1	2.56	0.41
25:Y:268:TYR:HA	25:Y:271:PHE:HB3	2.02	0.41
26:Z:82:PHE:HA	26:Z:85:VAL:HG12	2.02	0.41
26:Z:190:ARG:NH1	29:c:297:VAL:HG11	2.35	0.41
26:Z:224:HIS:HA	26:Z:228:TYR:HE2	1.82	0.41
28:b:106:LYS:HA	28:b:106:LYS:HD3	1.89	0.41
32:f:133:MET:H	32:f:133:MET:CE	2.32	0.41
32:f:264:GLU:O	32:f:268:LEU:HD12	2.21	0.41
32:f:368:ALA:HA	32:f:371:ASN:ND2	2.35	0.41
32:f:545:LYS:HA	32:f:545:LYS:HD2	1.90	0.41
32:f:857:GLY:O	32:f:859:PRO:HD3	2.21	0.41
11:k:69:GLU:HB2	11:k:226:PHE:CE2	2.56	0.41
11:k:186:HIS:CE1	11:k:189:MET:HG2	2.56	0.41
3:C:336:MET:N	3:C:336:MET:SD	2.94	0.41
6:F:279:ALA:HB1	6:F:325:GLN:HE21	1.86	0.41
8:H:39:LYS:HE2	9:I:57:ASP:OD1	2.20	0.41
9:I:137:ILE:HG22	9:I:147:LEU:HD13	2.03	0.41
13:M:83:ASP:HB3	13:M:131:PHE:HD1	1.86	0.41
13:M:186:CYS:O	13:M:190:VAL:HG13	2.21	0.41
14:N:28:ASN:ND2	15:O:122:LEU:HD21	2.36	0.41
14:N:160:LEU:HD23	14:N:160:LEU:HA	1.95	0.41
21:U:357:LYS:HE3	21:U:392:TRP:CD1	2.56	0.41
21:U:791:LEU:HD12	21:U:796:LYS:O	2.21	0.41
22:V:175:MET:HG3	22:V:184:ALA:HB2	2.03	0.41
23:W:85:GLU:HA	23:W:88:MET:HG3	2.02	0.41
23:W:373:ILE:HG22	23:W:374:THR:O	2.21	0.41
24:X:255:LEU:HB2	24:X:287:LEU:HD13	2.03	0.41
24:X:407:MET:HA	24:X:410:VAL:CG1	2.51	0.41
25:Y:186:LEU:HD12	25:Y:186:LEU:HA	1.82	0.41
26:Z:72:HIS:CD2	28:b:60:VAL:HG13	2.55	0.41
26:Z:186:THR:OG1	29:c:293:THR:HG21	2.20	0.41
26:Z:273:HIS:CE1	26:Z:277:ASN:HD21	2.39	0.41
29:c:163:ILE:HG12	29:c:172:HIS:ND1	2.36	0.41
32:f:472:HIS:HB3	32:f:477:MET:CE	2.51	0.41
10:j:189:LYS:HB3	10:j:189:LYS:HE2	1.75	0.41
1:A:245:LEU:H	1:A:245:LEU:HD22	1.85	0.40
5:E:252:GLU:HA	5:E:255:ARG:NE	2.36	0.40
6:F:204:LEU:HD23	6:F:204:LEU:HA	1.93	0.40
7:G:211:LYS:HE2	7:G:211:LYS:HB2	1.90	0.40
12:L:107:ARG:HH22	20:T:81:HIS:HB2	1.84	0.40
15:O:12:ILE:HD11	15:O:108:PRO:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:67:LEU:HD12	20:T:67:LEU:HA	1.92	0.40
21:U:427:LEU:H	21:U:427:LEU:HD12	1.86	0.40
22:V:396:ILE:HD13	22:V:396:ILE:HA	1.91	0.40
23:W:129:ARG:HH22	23:W:145:LEU:HB3	1.86	0.40
23:W:370:TYR:HD1	23:W:370:TYR:HA	1.74	0.40
23:W:408:ARG:HD3	24:X:345:VAL:HG23	2.03	0.40
25:Y:110:TYR:O	25:Y:114:ILE:HG12	2.21	0.40
25:Y:371:LYS:HE3	25:Y:371:LYS:HB3	1.72	0.40
25:Y:376:LEU:O	25:Y:380:VAL:HG12	2.21	0.40
10:j:224:GLU:O	10:j:227:LYS:HG2	2.21	0.40
10:j:226:GLU:O	10:j:229:VAL:HG22	2.20	0.40
11:k:40:ILE:HB	11:k:47:CYS:SG	2.61	0.40
12:l:13:TRP:HE1	13:m:129:ARG:HB2	1.85	0.40
19:s:194:ARG:HD2	19:s:205:GLU:OE1	2.21	0.40
2:B:287:ILE:HD12	2:B:287:ILE:HA	1.91	0.40
4:D:231:VAL:HB	4:D:234:GLU:OE1	2.21	0.40
4:D:370:ILE:CG2	4:D:374:ASP:HB2	2.51	0.40
4:D:373:ALA:HA	37:D:502:ADP:H1'	2.04	0.40
9:I:72:MET:HE3	9:I:72:MET:HB3	1.93	0.40
9:I:119:GLN:O	9:I:122:THR:HG22	2.22	0.40
12:L:70:ILE:HD13	12:L:108:LEU:HD22	2.03	0.40
13:M:52:LEU:HA	13:M:209:PHE:HA	2.02	0.40
16:P:97:GLU:OE1	16:P:98:LYS:HG2	2.21	0.40
19:S:52:ILE:HD11	19:S:108:ASN:HB2	2.03	0.40
21:U:478:SER:OG	21:U:511:ALA:HB1	2.21	0.40
21:U:803:LYS:HB2	21:U:875:PHE:HA	2.04	0.40
22:V:192:MET:O	22:V:195:ILE:HG22	2.22	0.40
22:V:349:ARG:HH12	31:e:37:HIS:CE1	2.33	0.40
23:W:169:LEU:HD13	23:W:169:LEU:HA	1.97	0.40
25:Y:50:MET:HA	25:Y:114:ILE:O	2.21	0.40
25:Y:100:ILE:HG13	25:Y:101:ARG:H	1.85	0.40
25:Y:233:ARG:N	25:Y:234:PRO:CD	2.84	0.40
25:Y:283:LYS:HD2	25:Y:288:PHE:HZ	1.87	0.40
27:a:42:LEU:O	27:a:46:GLN:HG2	2.20	0.40
31:e:33:ASP:HB3	31:e:36:ALA:HB2	2.03	0.40
32:f:559:PRO:HD3	32:f:587:PHE:HZ	1.87	0.40
7:g:111:VAL:HG21	7:g:142:GLY:HA3	2.02	0.40
11:k:99:HIS:CG	11:k:107:MET:HG2	2.56	0.40
11:k:230:THR:HG22	11:k:233:GLU:HG3	2.03	0.40
16:p:113:ASP:OD1	16:p:114:PRO:HD2	2.21	0.40
1:A:39:SER:HA	1:A:42:SER:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:GLU:HG2	2:B:146:PRO:HD2	2.02	0.40
2:B:406:ALA:HA	2:B:411:ARG:NH2	2.36	0.40
3:C:84:LYS:HA	3:C:97:VAL:O	2.22	0.40
6:F:74:LYS:HE3	6:F:74:LYS:HB3	1.72	0.40
12:L:26:MET:SD	12:L:149:PRO:HD2	2.62	0.40
15:O:187:ARG:HA	15:O:188:PRO:HA	1.97	0.40
21:U:401:LYS:HZ2	21:U:438:GLN:HA	1.86	0.40
21:U:615:ARG:HH21	21:U:645:ASN:HD21	1.69	0.40
22:V:217:VAL:HG12	22:V:218:TYR:HD1	1.86	0.40
22:V:337:LEU:HD22	22:V:367:VAL:HG11	2.03	0.40
27:a:252:LYS:HD2	27:a:255:TRP:NE1	2.35	0.40
27:a:276:CYS:HA	27:a:279:GLU:HB2	2.02	0.40
12:l:121:GLN:HB3	12:l:122:ARG:NH2	2.37	0.40
13:m:180:GLN:N	13:m:180:GLN:CD	2.80	0.40
14:n:81:SER:HA	14:n:120:MET:HE1	2.03	0.40
15:o:206:LYS:HD2	16:p:161:ASP:HB3	2.03	0.40
2:B:387:LYS:HD3	2:B:387:LYS:HA	1.77	0.40
3:C:46:GLN:NE2	21:U:639:LEU:HD22	2.36	0.40
3:C:66:LEU:HA	3:C:66:LEU:HD22	1.70	0.40
4:D:173:GLN:O	4:D:177:VAL:HG22	2.22	0.40
5:E:271:HIS:C	5:E:272:ARG:HG2	2.46	0.40
5:E:373:LYS:HE3	5:E:373:LYS:HB3	1.77	0.40
6:F:334:ARG:HH11	6:F:337:ILE:HD11	1.86	0.40
21:U:913:ILE:H	21:U:913:ILE:HG13	1.65	0.40
22:V:278:GLU:HA	22:V:285:TRP:HZ2	1.86	0.40
22:V:464:ILE:HD13	22:V:464:ILE:HA	1.85	0.40
23:W:40:LEU:O	23:W:43:VAL:HG22	2.22	0.40
23:W:60:MET:HE1	23:W:99:GLN:OE1	2.21	0.40
23:W:109:CYS:O	23:W:112:VAL:HG12	2.20	0.40
24:X:74:ARG:NH2	24:X:116:TRP:HD1	2.19	0.40
27:a:210:VAL:HG23	27:a:213:PHE:HB2	2.02	0.40
28:b:107:MET:HE3	28:b:107:MET:HA	2.04	0.40
32:f:463:LEU:HG	32:f:489:TYR:OH	2.22	0.40
32:f:723:TYR:HA	32:f:761:MET:SD	2.61	0.40
32:f:814:SER:HA	32:f:816:TYR:CE2	2.57	0.40
8:h:50:LYS:HE2	8:h:50:LYS:HB3	1.89	0.40
10:j:188:ILE:HG23	10:j:208:LEU:HD13	2.02	0.40
16:p:56:LEU:HD12	16:p:56:LEU:HA	1.80	0.40
19:s:27:THR:OG1	19:s:192:ALA:HB3	2.21	0.40
1:A:30:ILE:HD13	1:A:30:ILE:HA	1.98	0.40
1:A:56:LEU:HD12	1:A:56:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:348:ILE:HD11	37:D:502:ADP:H2	1.87	0.40
4:D:385:LEU:HD12	4:D:385:LEU:HA	1.95	0.40
5:E:232:MET:CE	5:E:277:MET:HA	2.51	0.40
5:E:316:HIS:NE2	5:E:344:ARG:HG2	2.37	0.40
8:H:183:GLU:HB3	8:H:186:ASP:OD1	2.22	0.40
11:K:12:VAL:HG11	11:K:136:PRO:HD3	2.02	0.40
21:U:157:THR:HG23	21:U:159:ARG:HB2	2.01	0.40
21:U:226:PRO:HA	21:U:264:VAL:HG12	2.02	0.40
21:U:232:ILE:O	21:U:235:LYS:HG2	2.22	0.40
21:U:269:ARG:NH1	21:U:269:ARG:HB3	2.37	0.40
21:U:447:GLY:HA3	21:U:480:GLY:HA2	2.03	0.40
21:U:899:ARG:O	21:U:917:THR:HG21	2.21	0.40
22:V:219:GLU:HA	22:V:224:LEU:HD21	2.03	0.40
24:X:159:LYS:HB3	24:X:159:LYS:HE3	1.66	0.40
26:Z:185:GLY:O	26:Z:189:GLN:HG3	2.21	0.40
30:d:119:LEU:HD11	30:d:137:VAL:HG12	2.02	0.40
32:f:339:ILE:HD12	32:f:339:ILE:HA	1.90	0.40
32:f:658:ALA:HB2	32:f:693:ALA:HB1	2.03	0.40
7:g:10:ASP:HA	7:g:15:ILE:HG13	2.03	0.40
10:j:155:ALA:HB3	11:k:63:SER:HB2	2.04	0.40
11:k:235:GLU:HG3	11:k:239:LYS:HZ2	1.87	0.40
12:l:55:GLU:CD	12:l:55:GLU:H	2.29	0.40
17:q:69:MET:HE2	17:q:69:MET:HA	2.02	0.40
20:t:23:ALA:CB	20:t:173:MET:HE2	2.46	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	A	411/433 (95%)	381 (93%)	30 (7%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	409/440 (93%)	362 (88%)	46 (11%)	1 (0%)	43	63
3	C	394/398 (99%)	357 (91%)	35 (9%)	2 (0%)	24	43
4	D	378/418 (90%)	318 (84%)	57 (15%)	3 (1%)	16	31
5	E	387/403 (96%)	334 (86%)	53 (14%)	0	100	100
6	F	391/439 (89%)	354 (90%)	34 (9%)	3 (1%)	16	31
7	G	238/246 (97%)	224 (94%)	14 (6%)	0	100	100
7	g	242/246 (98%)	235 (97%)	7 (3%)	0	100	100
8	H	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
8	h	230/234 (98%)	222 (96%)	8 (4%)	0	100	100
9	I	246/261 (94%)	235 (96%)	10 (4%)	1 (0%)	30	49
9	i	248/261 (95%)	243 (98%)	5 (2%)	0	100	100
10	J	237/248 (96%)	227 (96%)	10 (4%)	0	100	100
10	j	237/248 (96%)	226 (95%)	10 (4%)	1 (0%)	30	49
11	K	236/241 (98%)	225 (95%)	11 (5%)	0	100	100
11	k	232/241 (96%)	224 (97%)	8 (3%)	0	100	100
12	L	238/263 (90%)	230 (97%)	8 (3%)	0	100	100
12	l	236/263 (90%)	227 (96%)	9 (4%)	0	100	100
13	M	241/255 (94%)	234 (97%)	7 (3%)	0	100	100
13	m	238/255 (93%)	236 (99%)	2 (1%)	0	100	100
14	N	201/239 (84%)	195 (97%)	6 (3%)	0	100	100
14	n	200/239 (84%)	194 (97%)	6 (3%)	0	100	100
15	O	218/277 (79%)	212 (97%)	6 (3%)	0	100	100
15	o	218/277 (79%)	210 (96%)	8 (4%)	0	100	100
16	P	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
16	p	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
17	Q	198/201 (98%)	189 (96%)	9 (4%)	0	100	100
17	q	197/201 (98%)	191 (97%)	6 (3%)	0	100	100
18	R	199/263 (76%)	192 (96%)	7 (4%)	0	100	100
18	r	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
19	S	211/241 (88%)	202 (96%)	9 (4%)	0	100	100
19	s	211/241 (88%)	204 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	214/264 (81%)	208 (97%)	6 (3%)	0	100	100
20	t	214/264 (81%)	206 (96%)	8 (4%)	0	100	100
21	U	874/953 (92%)	814 (93%)	60 (7%)	0	100	100
22	V	442/534 (83%)	420 (95%)	22 (5%)	0	100	100
23	W	439/456 (96%)	432 (98%)	7 (2%)	0	100	100
24	X	420/422 (100%)	405 (96%)	15 (4%)	0	100	100
25	Y	387/389 (100%)	363 (94%)	24 (6%)	0	100	100
26	Z	284/324 (88%)	257 (90%)	27 (10%)	0	100	100
27	a	371/376 (99%)	344 (93%)	27 (7%)	0	100	100
28	b	189/377 (50%)	171 (90%)	18 (10%)	0	100	100
29	c	285/310 (92%)	243 (85%)	42 (15%)	0	100	100
30	d	255/350 (73%)	219 (86%)	36 (14%)	0	100	100
31	e	48/70 (69%)	39 (81%)	9 (19%)	0	100	100
32	f	840/908 (92%)	808 (96%)	32 (4%)	0	100	100
All	All	13417/14876 (90%)	12616 (94%)	790 (6%)	11 (0%)	49	68

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	157	ASP
6	F	73	ILE
6	F	86	LEU
9	I	53	HIS
2	B	319	PHE
4	D	149	SER
4	D	152	MET
3	C	90	HIS
3	C	91	PRO
6	F	343	LEU
10	j	50	VAL

### 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	A	348/372 (94%)	340 (98%)	8 (2%)	44	72
2	B	357/385 (93%)	348 (98%)	9 (2%)	42	69
3	C	340/346 (98%)	334 (98%)	6 (2%)	51	77
4	D	333/366 (91%)	329 (99%)	4 (1%)	63	83
5	E	341/353 (97%)	337 (99%)	4 (1%)	63	83
6	F	340/379 (90%)	334 (98%)	6 (2%)	51	77
7	G	202/210 (96%)	201 (100%)	1 (0%)	81	92
7	g	201/210 (96%)	196 (98%)	5 (2%)	42	69
8	H	187/191 (98%)	185 (99%)	2 (1%)	65	84
8	h	188/191 (98%)	185 (98%)	3 (2%)	55	79
9	I	202/221 (91%)	199 (98%)	3 (2%)	57	80
9	i	206/221 (93%)	205 (100%)	1 (0%)	81	92
10	J	197/211 (93%)	192 (98%)	5 (2%)	42	69
10	j	196/211 (93%)	195 (100%)	1 (0%)	81	92
11	K	197/203 (97%)	196 (100%)	1 (0%)	81	92
11	k	195/203 (96%)	193 (99%)	2 (1%)	68	86
12	L	202/224 (90%)	200 (99%)	2 (1%)	68	86
12	l	201/224 (90%)	199 (99%)	2 (1%)	68	86
13	M	199/212 (94%)	197 (99%)	2 (1%)	68	86
13	m	198/212 (93%)	197 (100%)	1 (0%)	81	92
14	N	158/181 (87%)	156 (99%)	2 (1%)	61	82
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	178/228 (78%)	177 (99%)	1 (1%)	78	91
15	o	181/228 (79%)	181 (100%)	0	100	100
16	P	172/174 (99%)	169 (98%)	3 (2%)	53	78
16	p	173/174 (99%)	169 (98%)	4 (2%)	44	72
17	Q	169/171 (99%)	169 (100%)	0	100	100
17	q	166/171 (97%)	164 (99%)	2 (1%)	63	83
18	R	156/202 (77%)	155 (99%)	1 (1%)	78	91
18	r	154/202 (76%)	152 (99%)	2 (1%)	61	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	S	175/199 (88%)	170 (97%)	5 (3%)	37	65
19	s	177/199 (89%)	177 (100%)	0	100	100
20	T	178/215 (83%)	177 (99%)	1 (1%)	78	91
20	t	179/215 (83%)	177 (99%)	2 (1%)	65	84
21	U	752/816 (92%)	739 (98%)	13 (2%)	53	78
22	V	390/460 (85%)	382 (98%)	8 (2%)	47	74
23	W	406/416 (98%)	405 (100%)	1 (0%)	87	95
24	X	362/362 (100%)	357 (99%)	5 (1%)	59	81
25	Y	344/344 (100%)	339 (98%)	5 (2%)	57	80
26	Z	257/295 (87%)	247 (96%)	10 (4%)	28	55
27	a	333/336 (99%)	325 (98%)	8 (2%)	43	70
28	b	167/312 (54%)	165 (99%)	2 (1%)	63	83
29	c	252/268 (94%)	249 (99%)	3 (1%)	63	83
30	d	231/294 (79%)	227 (98%)	4 (2%)	53	78
31	e	44/63 (70%)	40 (91%)	4 (9%)	9	19
32	f	711/763 (93%)	701 (99%)	10 (1%)	59	81
All	All	11451/12614 (91%)	11287 (99%)	164 (1%)	57	81

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	93	LEU
1	A	143	ASP
1	A	233	THR
1	A	246	VAL
1	A	280	ILE
1	A	403	ILE
1	A	420	TYR
2	B	53	THR
2	B	85	MET
2	B	122	ILE
2	B	135	ILE
2	B	160	ILE
2	B	246	THR
2	B	319	PHE

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Mol	Chain	Res	Type
2	B	382	ASP
2	B	394	ASP
3	C	66	LEU
3	C	85	VAL
3	C	89	VAL
3	C	99	VAL
3	C	109	THR
3	C	213	ARG
4	D	151	ILE
4	D	185	LEU
4	D	381	GLU
4	D	410	ASP
5	E	50	LEU
5	E	104	THR
5	E	183	LEU
5	E	281	ARG
6	F	73	ILE
6	F	75	GLU
6	F	159	LEU
6	F	338	LEU
6	F	343	LEU
6	F	379	VAL
7	G	40	VAL
8	H	75	VAL
8	H	163	MET
9	I	6	ASP
9	I	52	ILE
9	I	92	LEU
10	J	7	ILE
10	J	71	MET
10	J	134	VAL
10	J	198	VAL
10	J	220	LEU
11	K	146	VAL
12	L	91	GLU
12	L	230	SER
13	M	142	VAL
13	M	216	VAL
14	N	70	LEU
14	N	164	MET
15	O	65	LEU
16	P	4	MET

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Mol	Chain	Res	Type
16	P	12	MET
16	P	158	MET
18	R	128	VAL
19	S	84	THR
19	S	108	ASN
19	S	164	VAL
19	S	187	VAL
19	S	208	VAL
20	T	214	MET
21	U	160	LEU
21	U	205	TYR
21	U	385	PHE
21	U	516	LEU
21	U	539	THR
21	U	629	THR
21	U	732	LEU
21	U	752	THR
21	U	755	THR
21	U	836	THR
21	U	866	GLU
21	U	894	MET
21	U	925	VAL
22	V	94	VAL
22	V	195	ILE
22	V	209	LYS
22	V	296	LYS
22	V	332	LEU
22	V	346	LEU
22	V	402	VAL
22	V	410	ILE
23	W	444	HIS
24	X	28	HIS
24	X	77	LEU
24	X	160	MET
24	X	346	GLN
24	X	407	MET
25	Y	95	LEU
25	Y	104	MET
25	Y	236	LEU
25	Y	315	THR
25	Y	377	LEU
26	Z	20	VAL

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Mol	Chain	Res	Type
26	Z	63	LYS
26	Z	91	ILE
26	Z	96	HIS
26	Z	133	LEU
26	Z	144	VAL
26	Z	149	THR
26	Z	212	LEU
26	Z	227	ILE
26	Z	249	PHE
27	a	130	VAL
27	a	163	TYR
27	a	165	THR
27	a	166	ILE
27	a	171	SER
27	a	211	PHE
27	a	277	LEU
27	a	365	MET
28	b	2	VAL
28	b	37	CYS
29	c	176	GLN
29	c	269	GLN
29	c	284	LEU
30	d	81	TYR
30	d	195	THR
30	d	217	LEU
30	d	257	VAL
31	e	60	LEU
31	e	61	GLU
31	e	62	LYS
31	e	63	HIS
32	f	179	VAL
32	f	340	MET
32	f	404	ASP
32	f	463	LEU
32	f	514	VAL
32	f	527	VAL
32	f	606	VAL
32	f	736	THR
32	f	796	LEU
32	f	891	THR
7	g	5	SER
7	g	59	LYS

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Mol	Chain	Res	Type
7	g	60	LEU
7	g	61	LEU
7	g	66	VAL
8	h	45	VAL
8	h	116	SER
8	h	222	THR
9	i	184	MET
10	j	63	CYS
11	k	182	GLN
11	k	206	MET
12	l	176	MET
12	l	198	THR
13	m	52	LEU
16	p	20	VAL
16	p	56	LEU
16	p	58	THR
16	p	155	GLU
17	q	26	VAL
17	q	75	LEU
18	r	21	THR
18	r	174	VAL
20	t	127	MET
20	t	141	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	305	GLN
1	A	322	ASN
2	B	57	GLN
2	B	277	HIS
2	B	425	ASN
3	C	32	GLN
3	C	46	GLN
3	C	171	HIS
3	C	279	GLN
4	D	57	GLN
4	D	175	GLN
5	E	39	GLN
5	E	129	ASN
5	E	155	ASN

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Mol	Chain	Res	Type
6	F	83	ASN
6	F	218	GLN
6	F	323	ASN
7	G	224	ASN
9	I	95	GLN
9	I	146	GLN
10	J	120	GLN
10	J	239	ASN
11	K	41	GLN
11	K	98	ASN
16	P	72	ASN
17	Q	101	ASN
19	S	160	ASN
20	T	3	ASN
20	T	108	ASN
21	U	171	ASN
21	U	190	ASN
21	U	338	HIS
21	U	355	ASN
21	U	711	GLN
21	U	718	ASN
21	U	754	HIS
21	U	874	ASN
22	V	185	GLN
23	W	26	GLN
23	W	86	ASN
24	X	198	ASN
24	X	207	GLN
24	X	296	ASN
25	Y	351	ASN
25	Y	363	ASN
26	Z	102	HIS
27	a	9	GLN
27	a	18	GLN
27	a	46	GLN
27	a	129	GLN
27	a	193	GLN
27	a	288	HIS
27	a	337	GLN
27	a	369	HIS
28	b	101	GLN
29	c	77	GLN

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Mol	Chain	Res	Type
29	c	274	ASN
29	c	295	ASN
30	d	46	GLN
30	d	47	GLN
30	d	130	ASN
32	f	148	GLN
32	f	493	ASN
32	f	611	GLN
32	f	737	ASN
32	f	848	GLN
8	h	102	GLN
8	h	179	ASN
9	i	95	GLN
9	i	166	ASN
9	i	235	GLN
10	j	68	ASN
11	k	178	GLN
11	k	204	GLN
12	l	59	HIS
12	l	203	GLN
13	m	63	ASN
13	m	110	HIS
13	m	201	HIS
14	n	110	GLN
14	n	193	GLN
15	o	35	HIS
16	p	93	ASN
16	p	162	HIS
16	p	169	GLN
17	q	8	GLN
17	q	101	ASN
18	r	70	ASN
19	s	151	ASN
19	s	163	HIS
20	t	2	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
35	ATP	B	501	36	29,33,33	0.29	0	44,52,52	0.52	1 (2%)
37	ADP	D	502	36	27,29,29	1.37	4 (14%)	42,45,45	2.01	9 (21%)
35	ATP	A	501	36	29,33,33	0.29	0	44,52,52	0.51	1 (2%)
35	ATP	C	501	36	29,33,33	0.31	0	44,52,52	0.54	1 (2%)
35	ATP	F	501	36	29,33,33	0.29	0	44,52,52	0.50	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ATP	B	501	36	-	2/22/38/38	0/3/3/3
37	ADP	D	502	36	-	3/16/32/32	0/3/3/3
35	ATP	A	501	36	-	3/22/38/38	0/3/3/3
35	ATP	C	501	36	-	5/22/38/38	0/3/3/3
35	ATP	F	501	36	-	6/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D	502	ADP	C5-C4	4.66	1.47	1.39
37	D	502	ADP	C5-C6	2.67	1.48	1.41
37	D	502	ADP	C8-N7	2.34	1.36	1.31
37	D	502	ADP	C5-N7	-2.28	1.34	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D	502	ADP	C5-C4-N3	-6.59	118.15	126.75
37	D	502	ADP	N3-C4-N9	5.22	135.68	127.08
37	D	502	ADP	C2-N3-C4	3.97	121.12	111.75
37	D	502	ADP	PA-O3A-PB	-3.60	120.47	132.83
37	D	502	ADP	C4-C5-N7	-3.13	106.80	110.62
37	D	502	ADP	N3-C2-N1	-3.07	123.80	128.60
37	D	502	ADP	C3'-C2'-C1'	2.71	106.58	101.43
37	D	502	ADP	C5-N7-C8	2.67	107.30	103.51
37	D	502	ADP	C4-N9-C8	2.26	108.18	105.73
35	A	501	ATP	PB-O3B-PG	2.06	139.88	132.83
35	C	501	ATP	PB-O3B-PG	2.05	139.85	132.83
35	B	501	ATP	PB-O3B-PG	2.04	139.82	132.83
35	F	501	ATP	PB-O3B-PG	2.00	139.70	132.83

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	C	501	ATP	C5'-O5'-PA-O3A
35	C	501	ATP	C3'-C4'-C5'-O5'
35	F	501	ATP	C5'-O5'-PA-O1A
35	F	501	ATP	C5'-O5'-PA-O2A
35	C	501	ATP	O4'-C4'-C5'-O5'
37	D	502	ADP	C3'-C4'-C5'-O5'
35	A	501	ATP	PB-O3B-PG-O1G
37	D	502	ADP	O4'-C4'-C5'-O5'
35	B	501	ATP	C4'-C5'-O5'-PA
35	C	501	ATP	C4'-C5'-O5'-PA
35	A	501	ATP	PB-O3B-PG-O2G
35	F	501	ATP	C5'-O5'-PA-O3A
35	C	501	ATP	C5'-O5'-PA-O2A
35	A	501	ATP	PB-O3A-PA-O2A
35	F	501	ATP	O4'-C4'-C5'-O5'
35	F	501	ATP	PG-O3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
35	F	501	ATP	PG-O3B-PB-O2B
35	B	501	ATP	C2'-C1'-N9-C8
37	D	502	ADP	C5'-O5'-PA-O1A

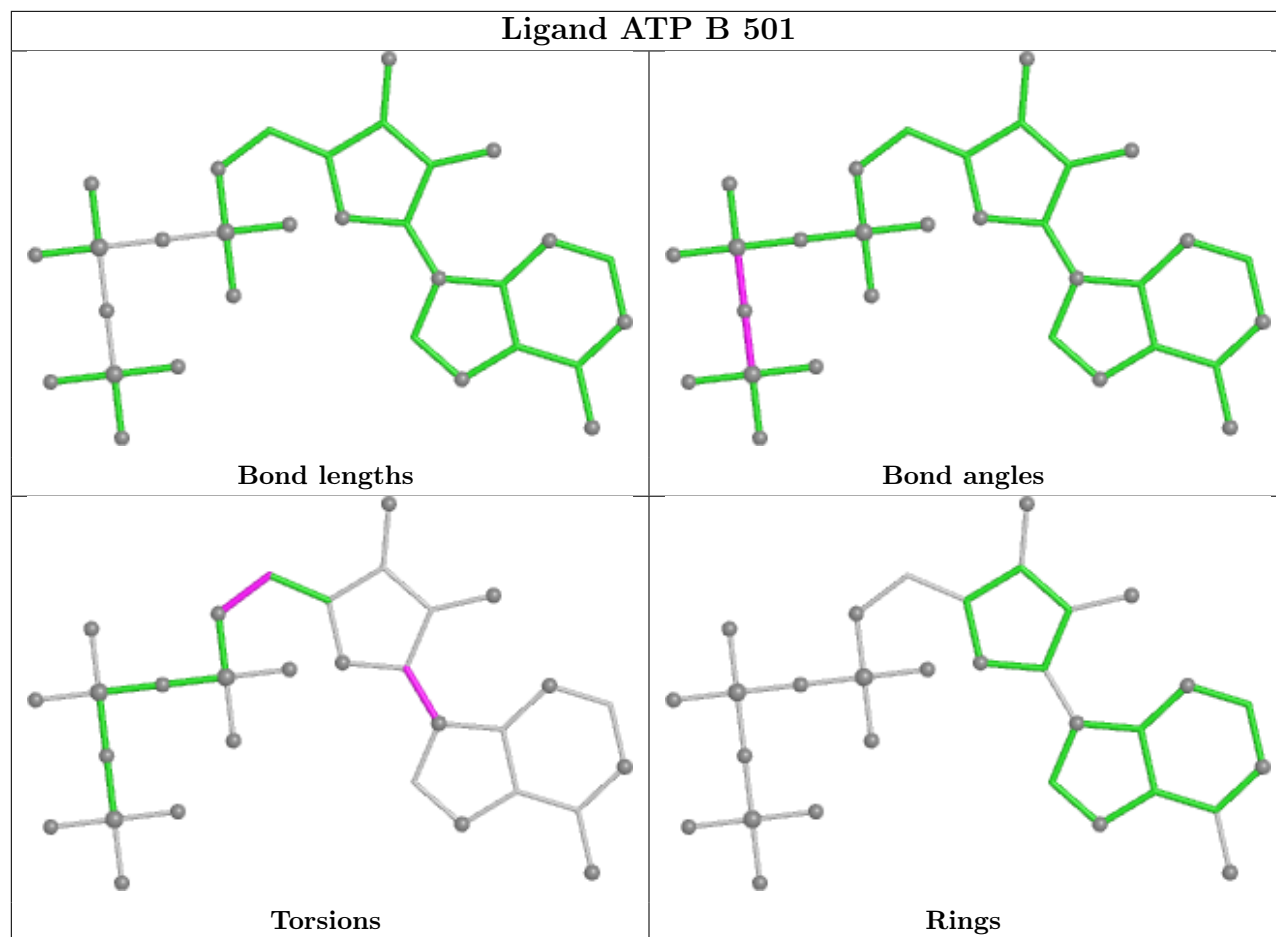
There are no ring outliers.

3 monomers are involved in 5 short contacts:

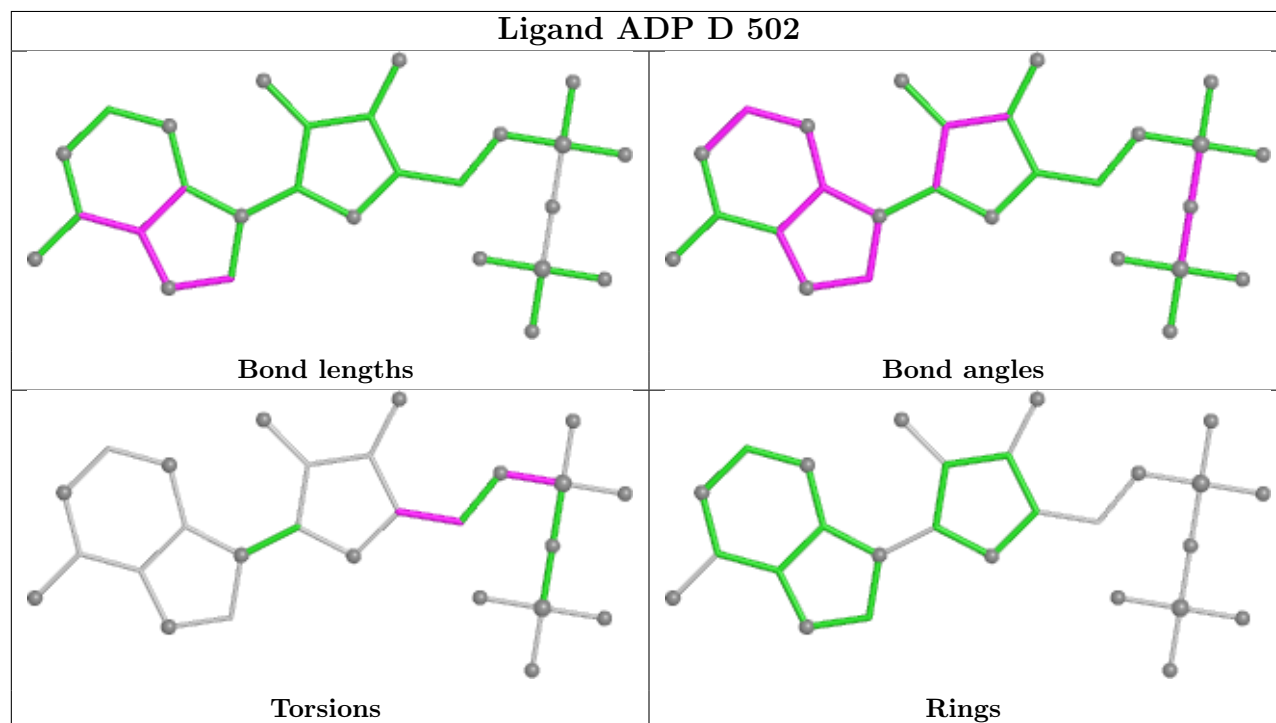
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	B	501	ATP	1	0
37	D	502	ADP	3	0
35	F	501	ATP	1	0

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

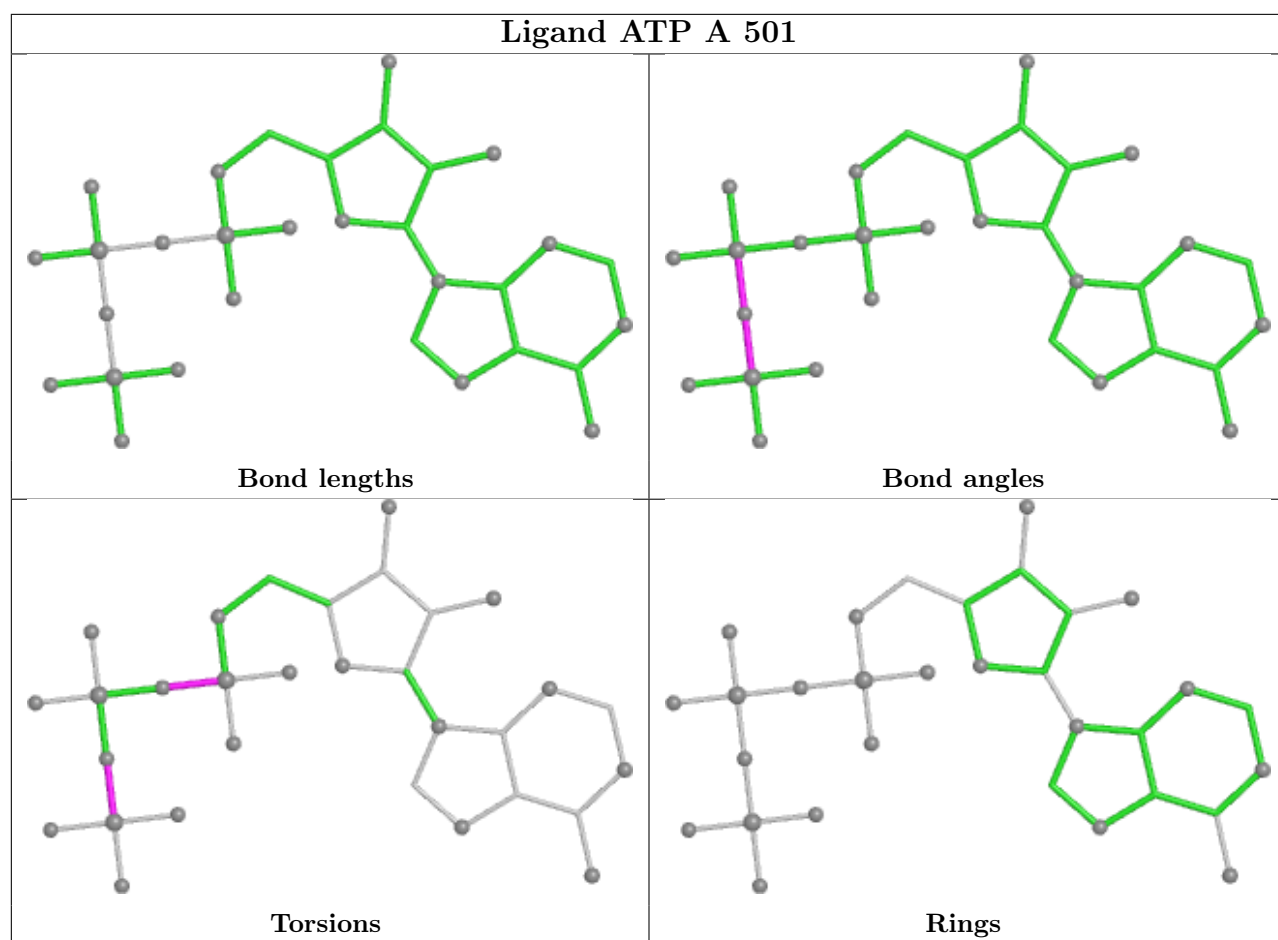
## Ligand ATP B 501

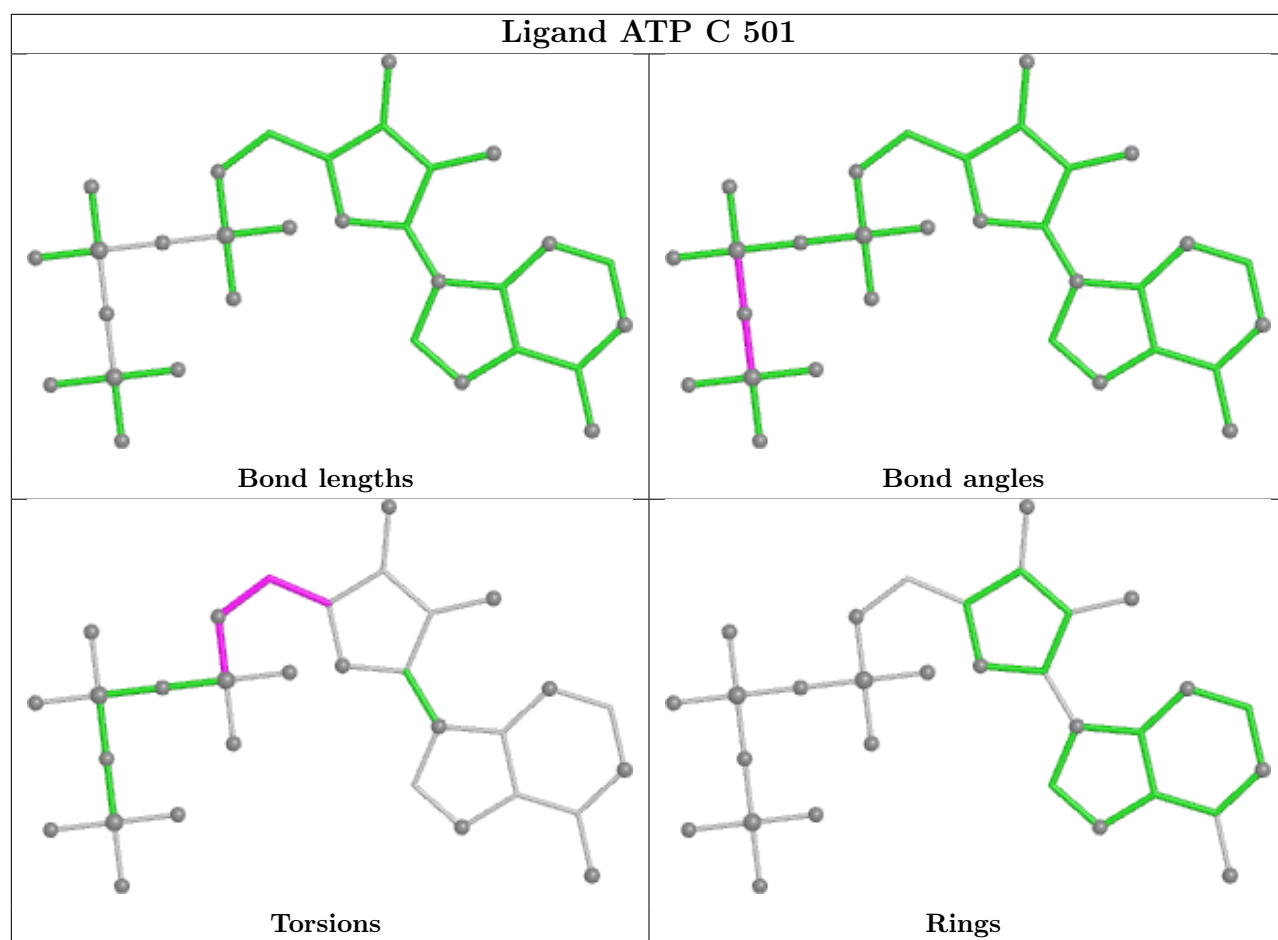


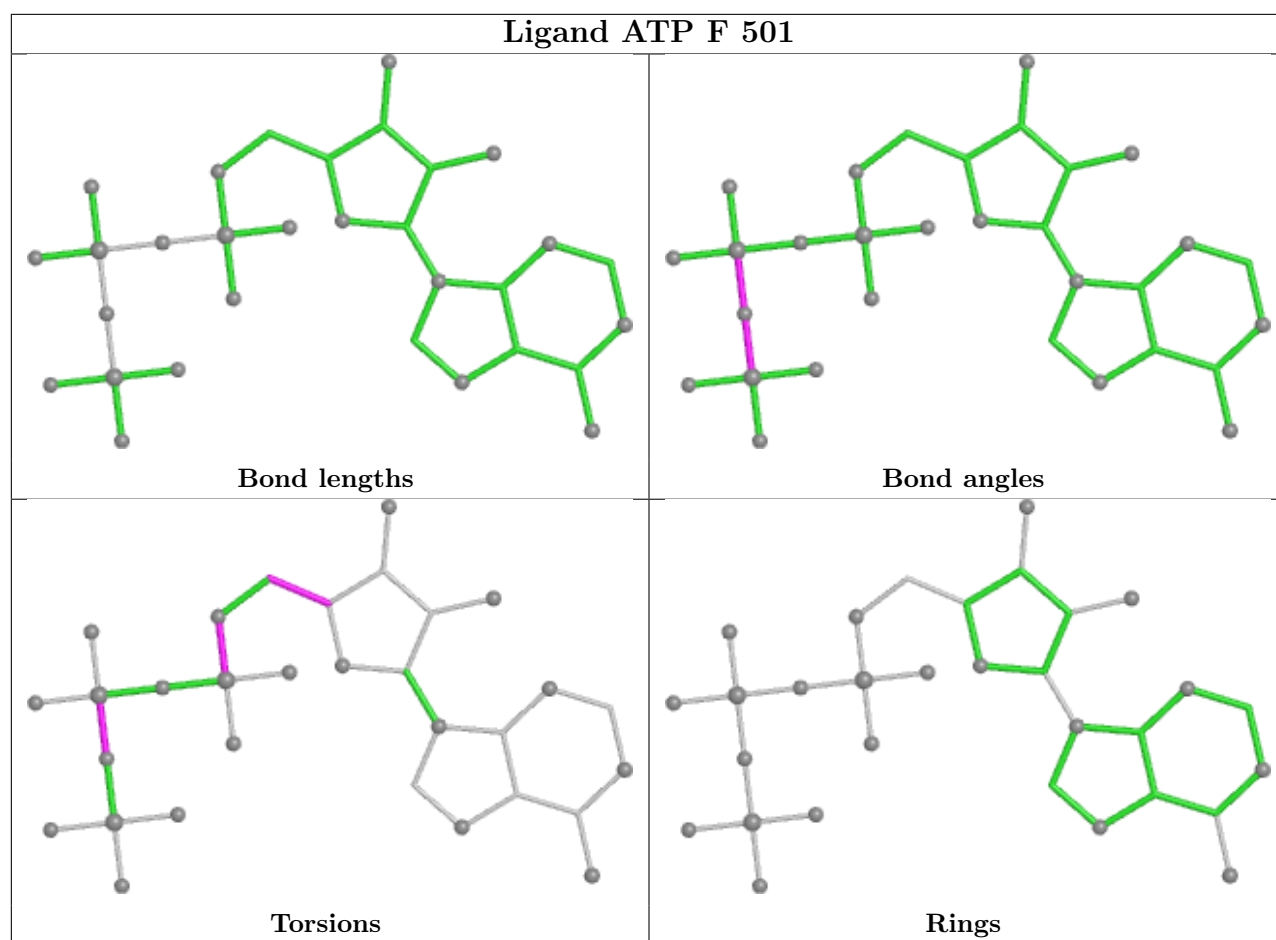
## Ligand ADP D 502











## 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.

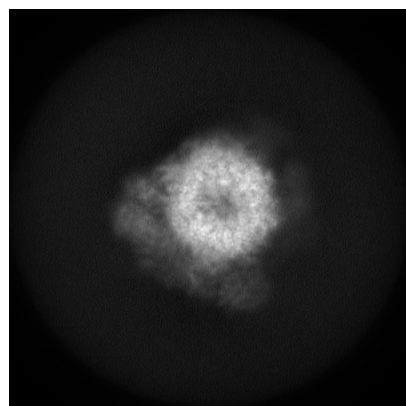
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62079. 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](#)

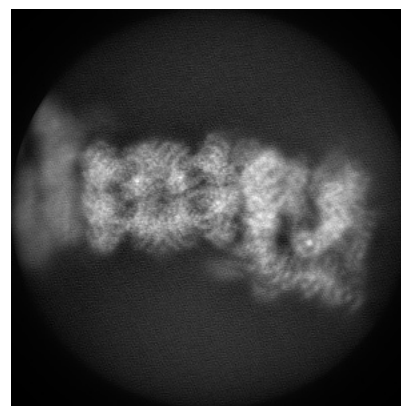
#### 6.1.1 Primary map



X

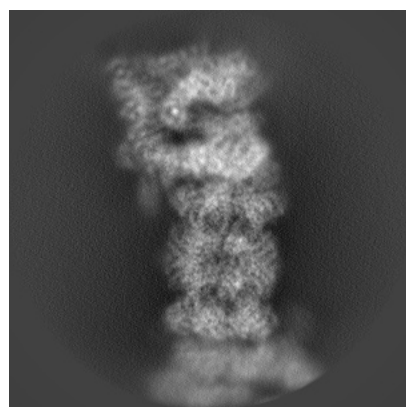


Y

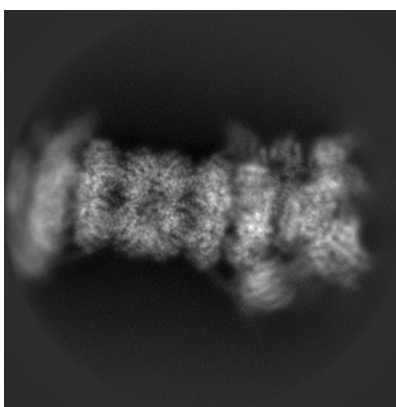


Z

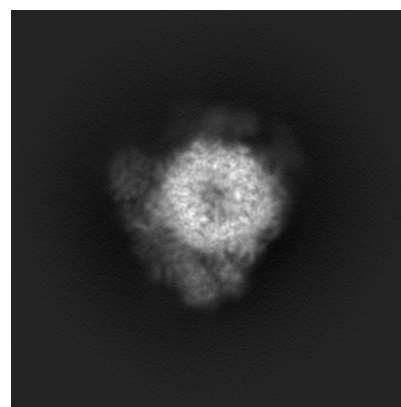
#### 6.1.2 Raw map



X



Y

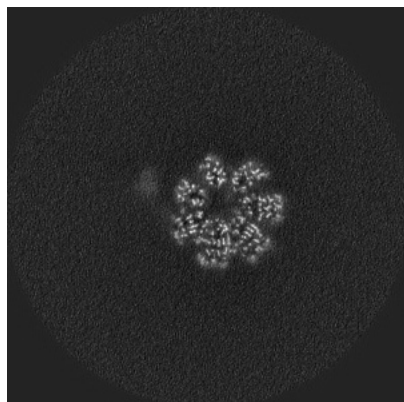


Z

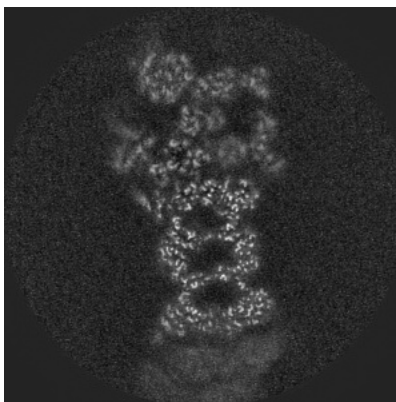
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

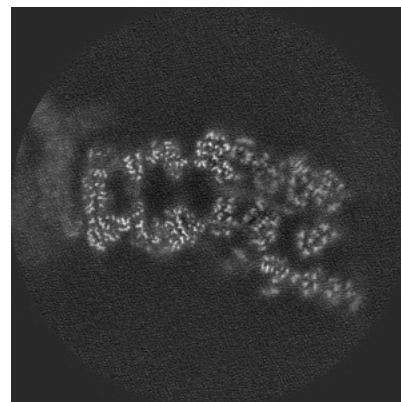
### 6.2.1 Primary map



X Index: 300

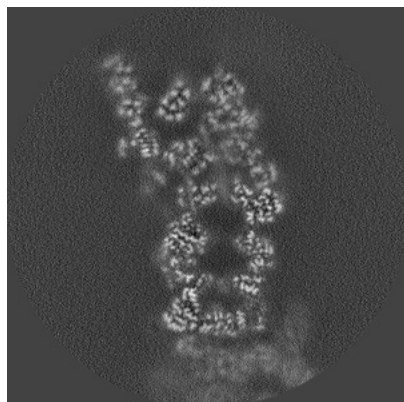


Y Index: 300

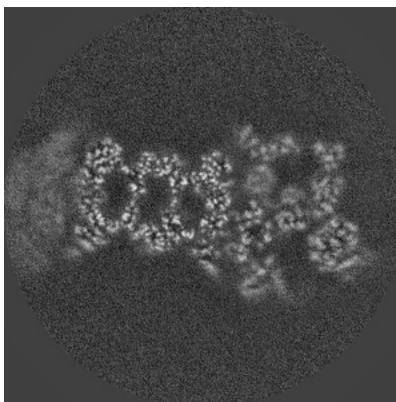


Z Index: 300

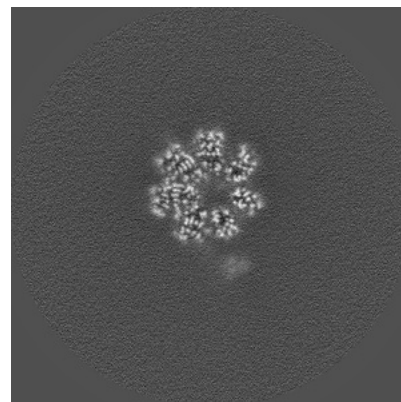
### 6.2.2 Raw map



X Index: 300



Y Index: 300

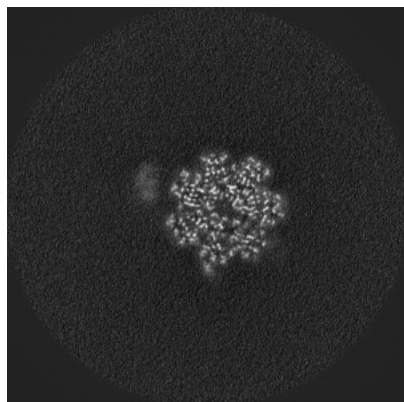


Z Index: 300

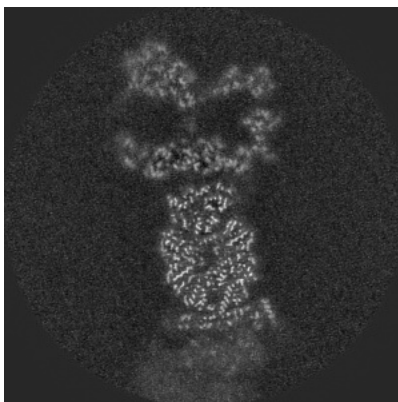
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

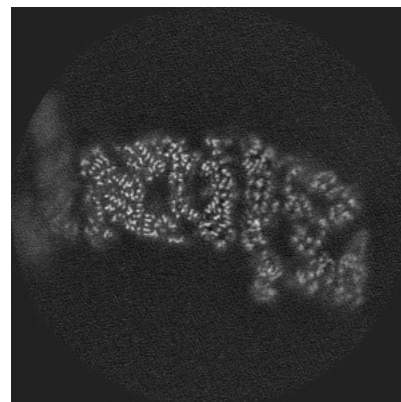
### 6.3.1 Primary map



X Index: 310

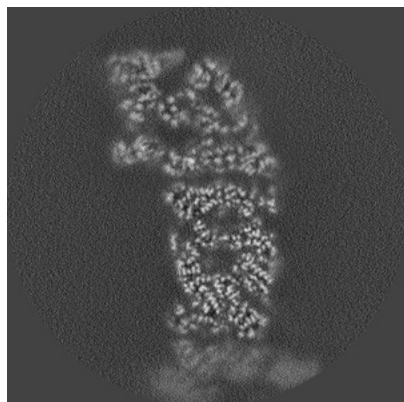


Y Index: 280

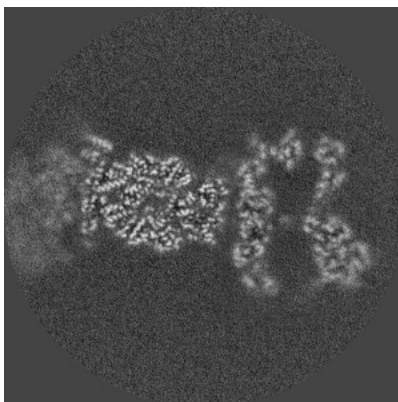


Z Index: 275

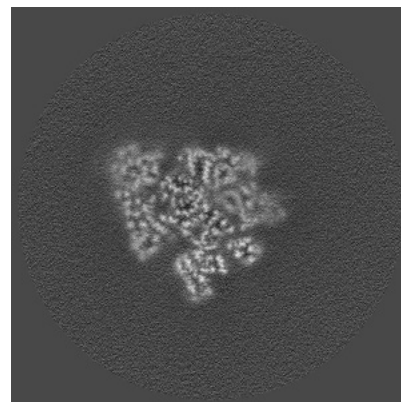
### 6.3.2 Raw map



X Index: 275



Y Index: 280



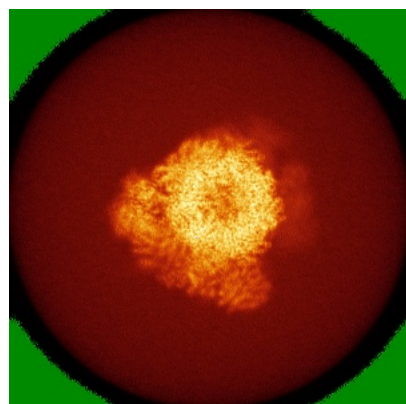
Z Index: 381

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

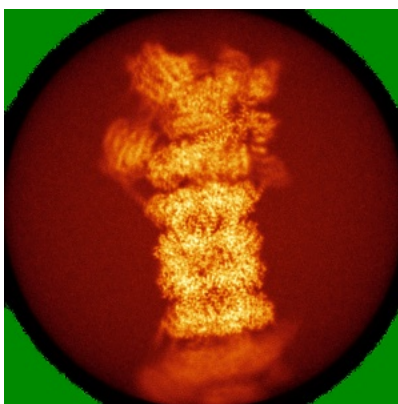


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

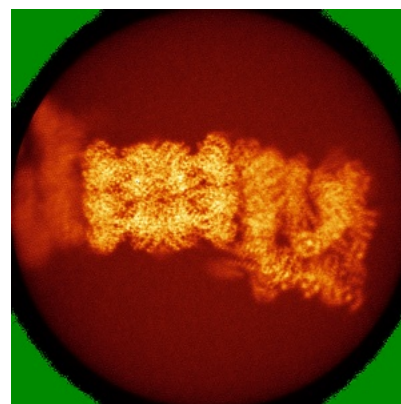
### 6.4.1 Primary map



X

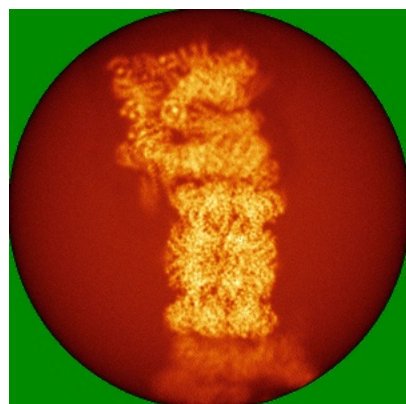


Y

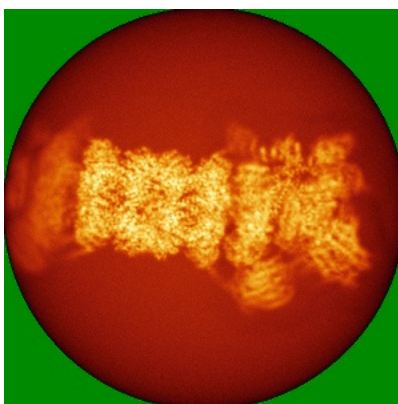


Z

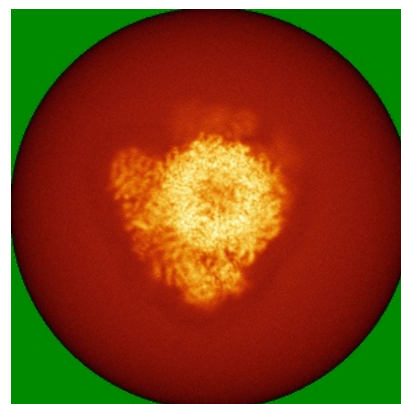
### 6.4.2 Raw map



X



Y

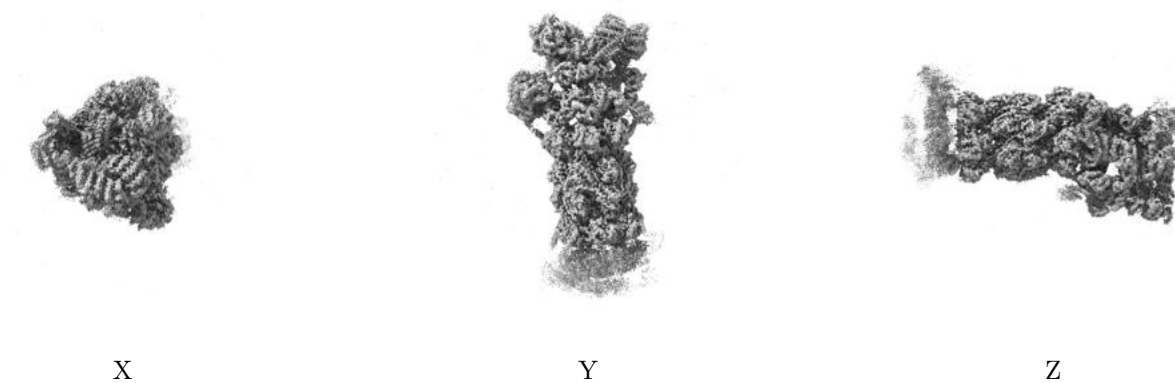


Z

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.

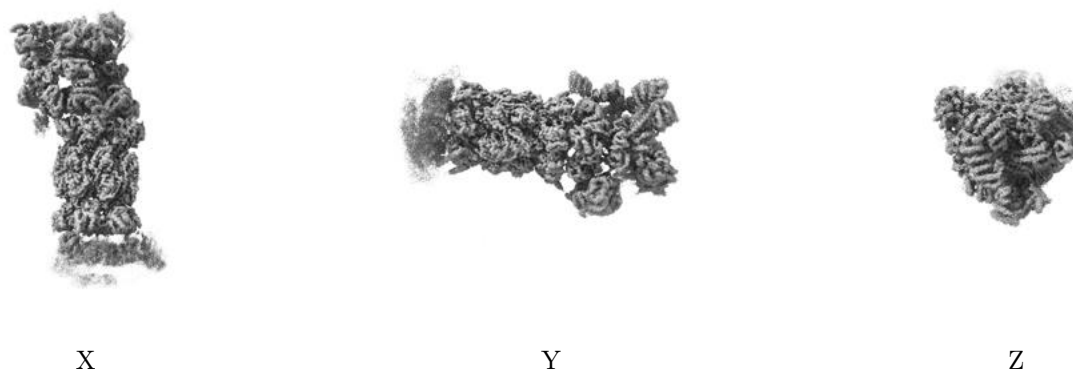
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00594. 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](#)

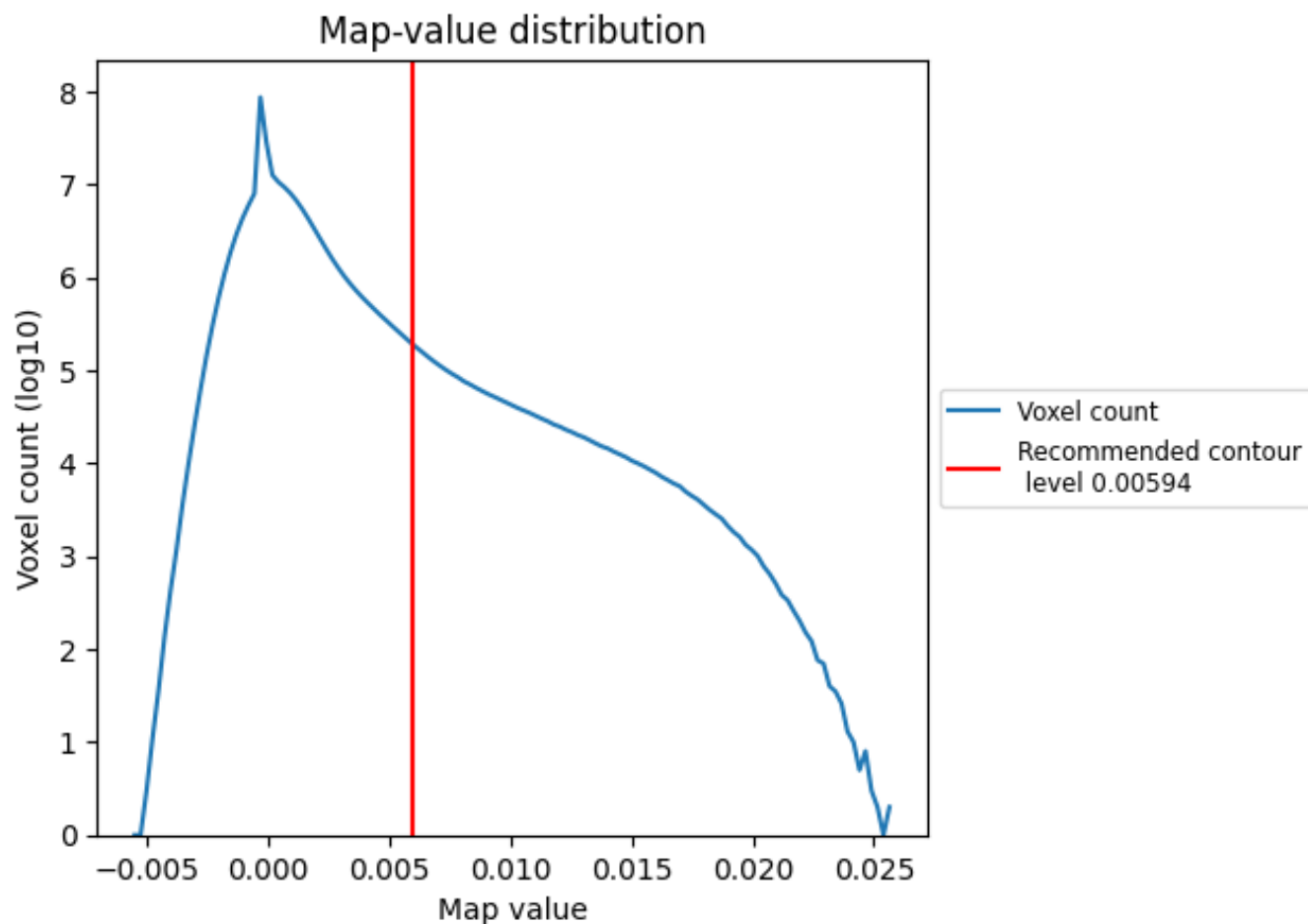
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

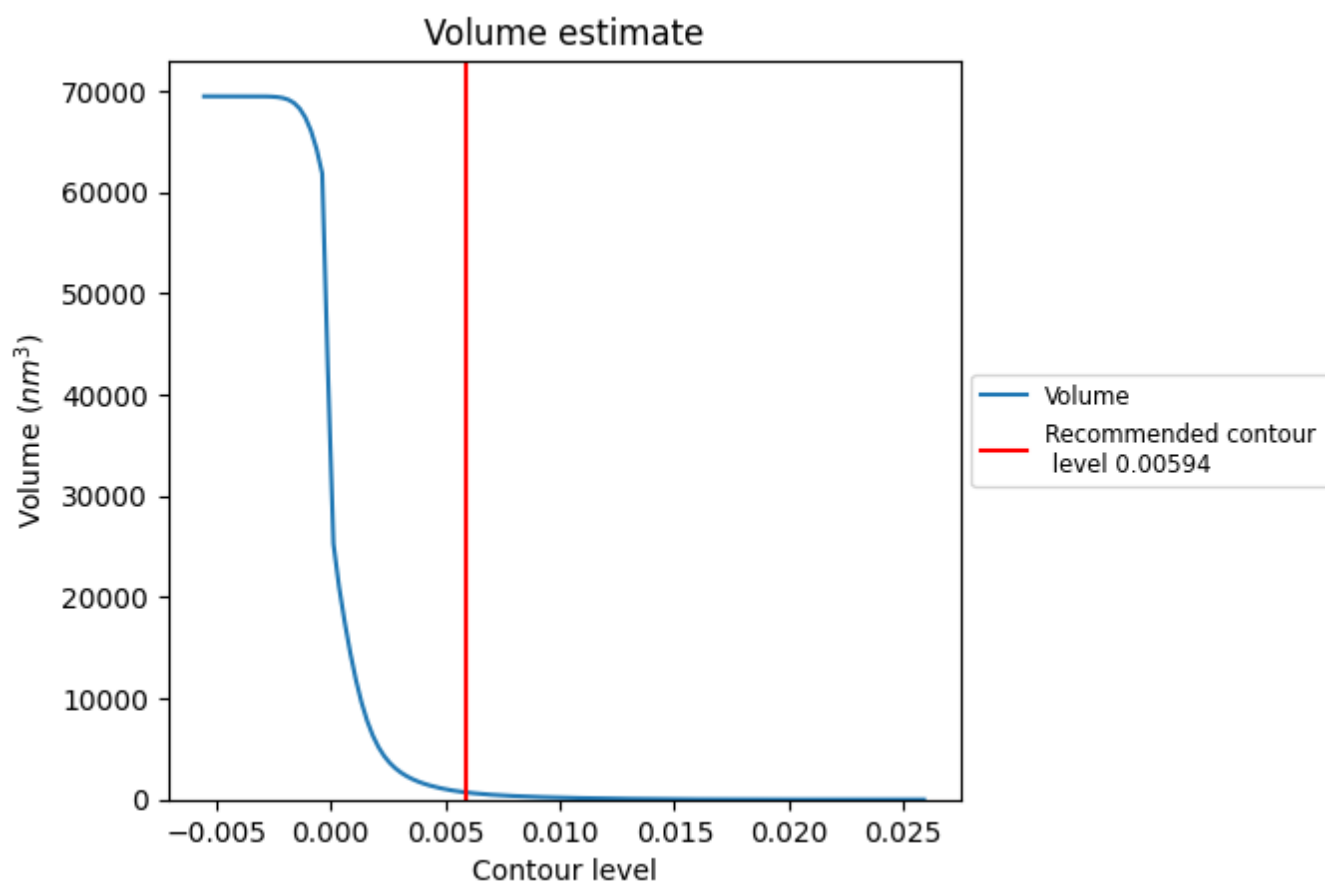
This section contains the results of statistical analysis of the map.

### 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.

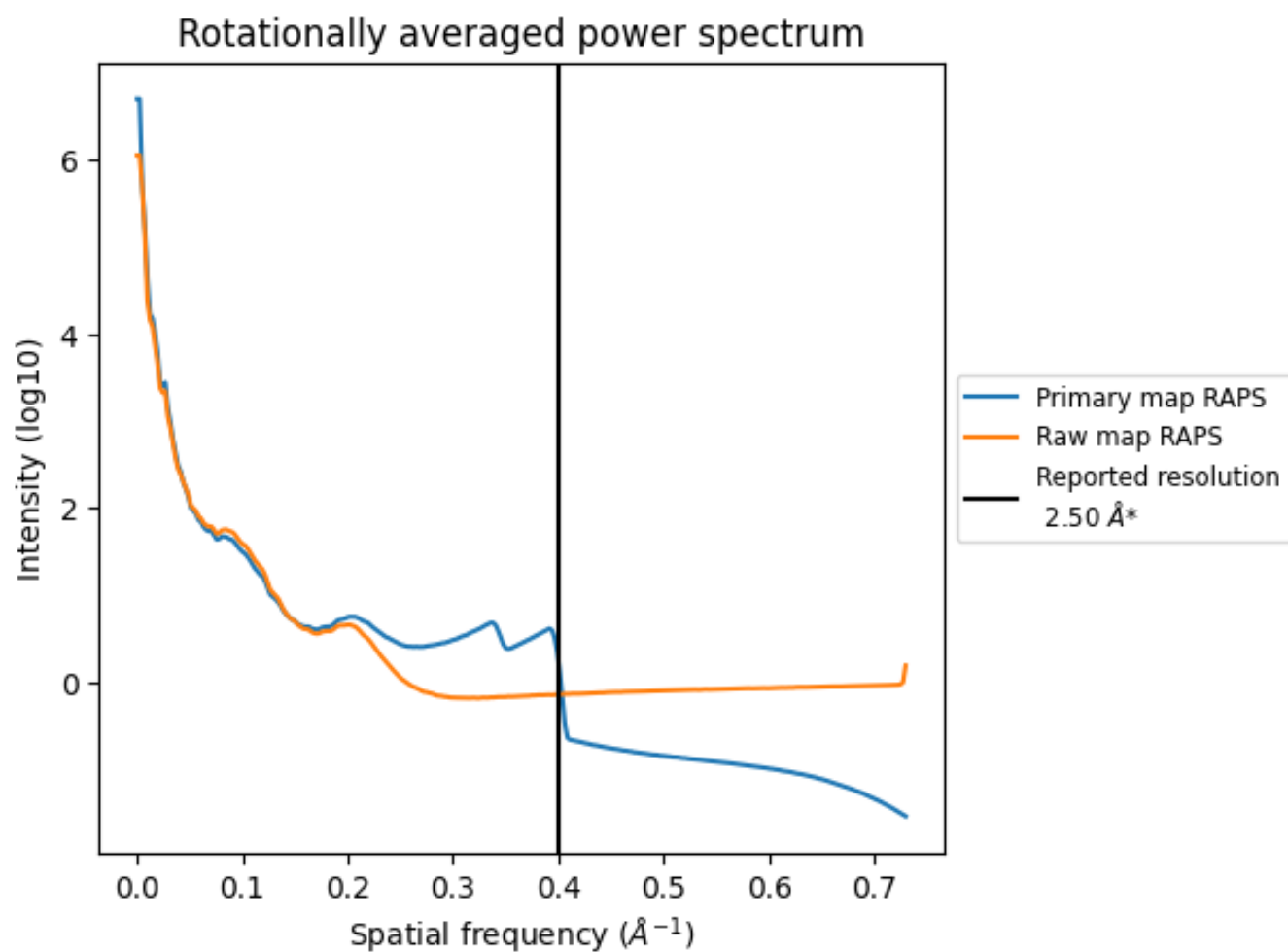
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 700 nm<sup>3</sup>; this corresponds to an approximate mass of 633 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 ⓘ

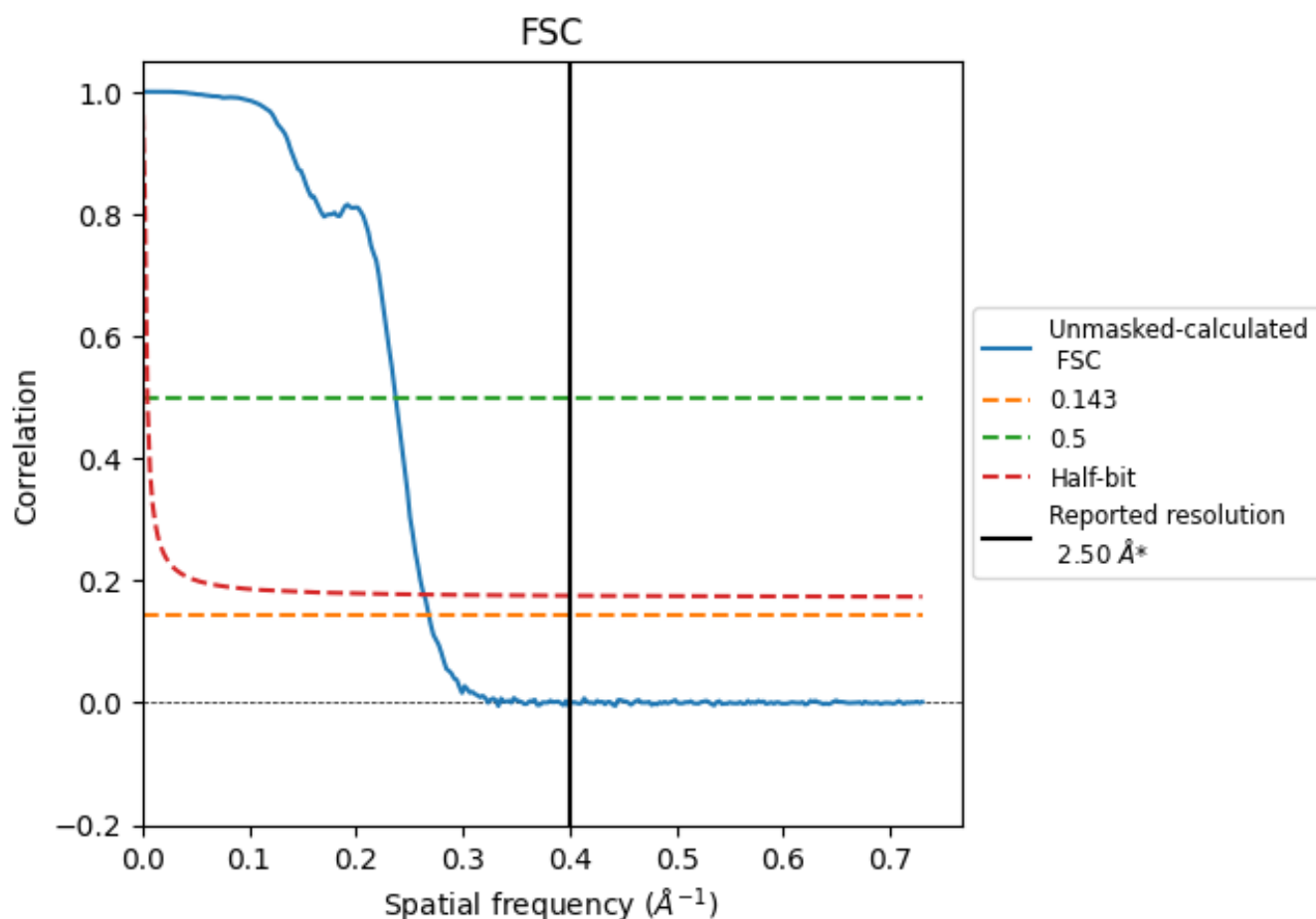


\*Reported resolution corresponds to spatial frequency of  $0.400 \text{ \AA}^{-1}$

## 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 0.400  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

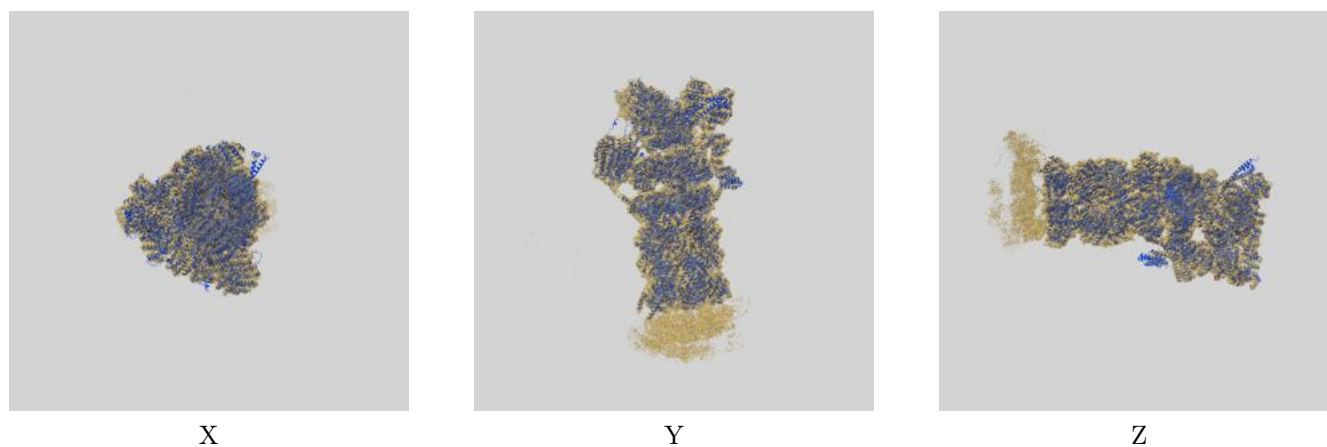
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.73	4.22	3.79

\*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 3.73 differs from the reported value 2.5 by more than 10 %

## 9 Map-model fit [i](#)

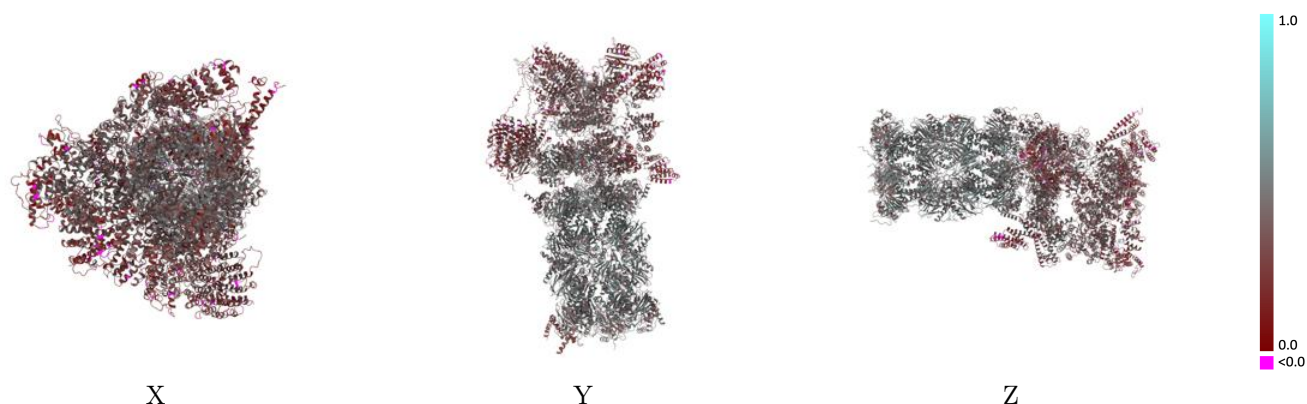
This section contains information regarding the fit between EMDB map EMD-62079 and PDB model 9K53. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

### 9.1 Map-model overlay [i](#)



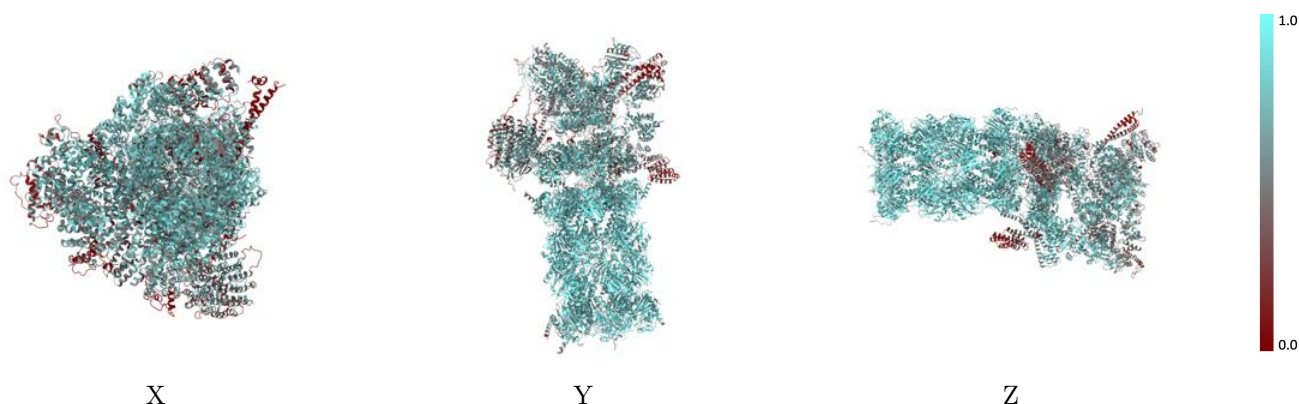
The images above show the 3D surface view of the map at the recommended contour level 0.00594 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



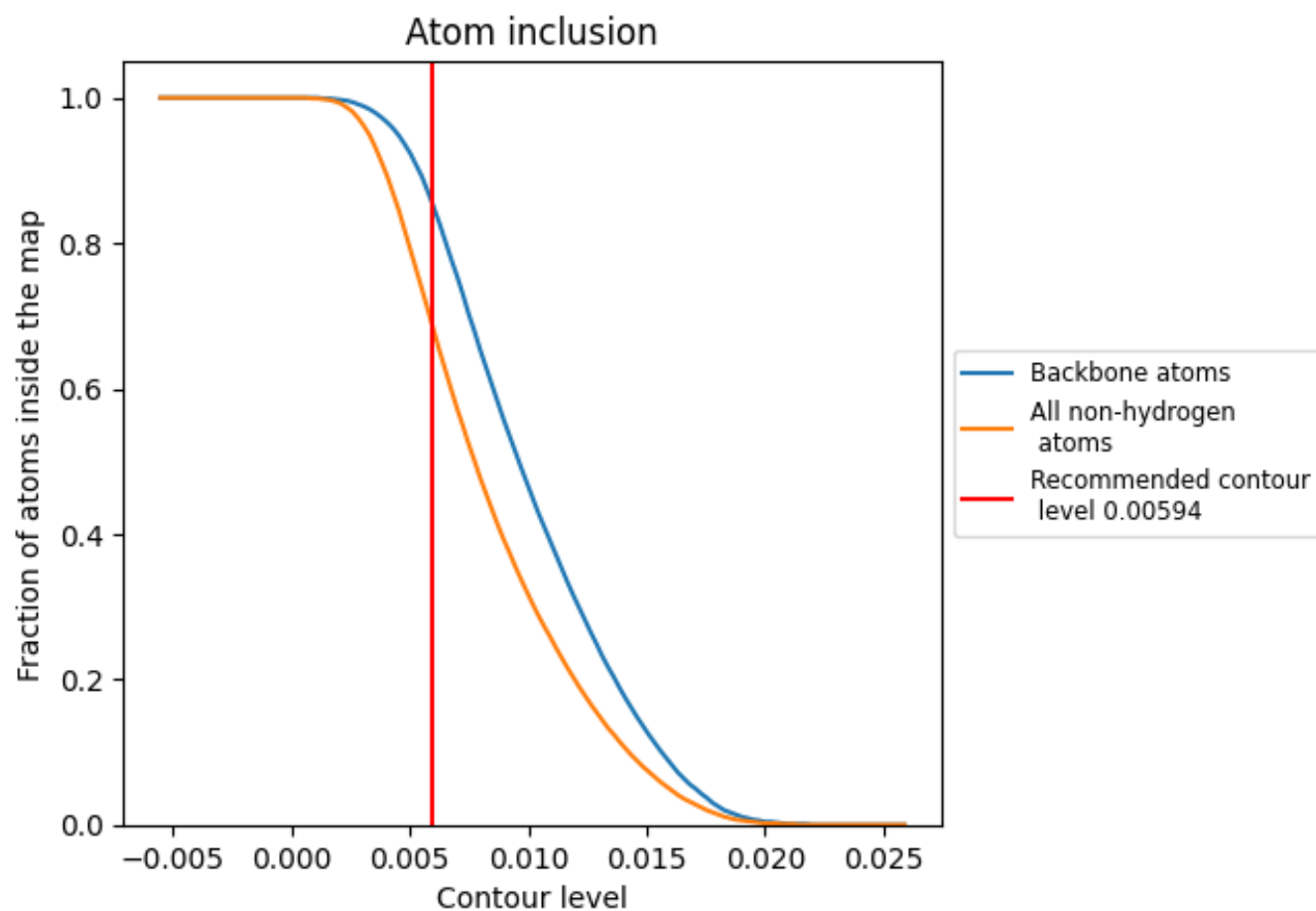
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00594).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 86% of all backbone atoms, 69% 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 (0.00594) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6880	 0.3910
A	 0.6520	 0.3820
B	 0.6450	 0.3880
C	 0.6960	 0.4050
D	 0.6680	 0.3760
E	 0.4010	 0.2570
F	 0.5800	 0.3500
G	 0.8170	 0.4710
H	 0.8410	 0.4730
I	 0.8010	 0.4670
J	 0.7830	 0.4450
K	 0.7840	 0.4560
L	 0.8340	 0.4700
M	 0.8120	 0.4690
N	 0.8550	 0.4870
O	 0.8570	 0.4880
P	 0.8680	 0.4780
Q	 0.8590	 0.4790
R	 0.8690	 0.4660
S	 0.8380	 0.4730
T	 0.8570	 0.4860
U	 0.5850	 0.3100
V	 0.5890	 0.3260
W	 0.5100	 0.3120
X	 0.5400	 0.3260
Y	 0.7380	 0.3670
Z	 0.6320	 0.3530
a	 0.5750	 0.2940
b	 0.5240	 0.3030
c	 0.6180	 0.3510
d	 0.4630	 0.2650
e	 0.5300	 0.3460
f	 0.5020	 0.2830
g	 0.7910	 0.4560
h	 0.7850	 0.4530



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Chain	Atom inclusion	Q-score
i	 0.7440	 0.4260
j	 0.7030	 0.3970
k	 0.7380	 0.4300
l	 0.8130	 0.4590
m	 0.8050	 0.4600
n	 0.8410	 0.4790
o	 0.8360	 0.4760
p	 0.8410	 0.4660
q	 0.8460	 0.4720
r	 0.8790	 0.4870
s	 0.8350	 0.4790
t	 0.8530	 0.4710
v	 0.2610	 0.3670
y	 0.5600	 0.3570
z	 0.5600	 0.3820