



Full wwPDB EM Validation Report ⓘ

Apr 20, 2026 – 05:09 PM JST

PDB ID : 9K57 / pdb_00009k57
EMDB ID : EMD-62083
Title : Structure of substrate-engaged single-cap human proteasome in state EA2
Authors : Wu, Z.; Chen, E.; Mao, Y.
Deposited on : 2024-10-21
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

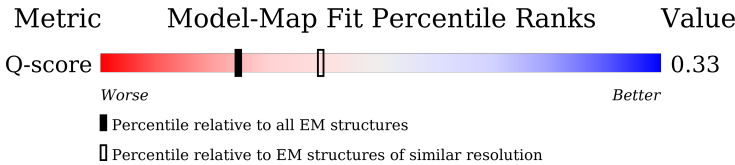
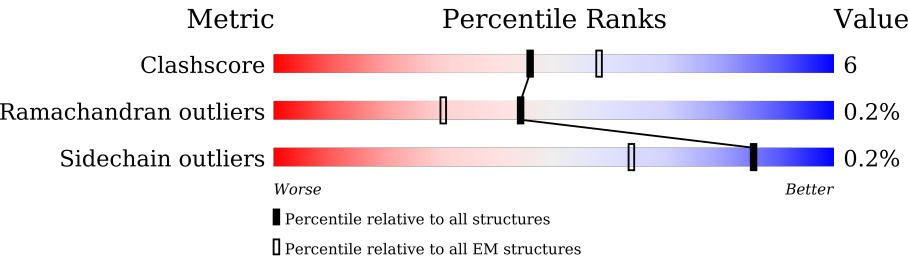
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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

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

The reported resolution of this entry is 4.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	433	<div> <div>14%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>9%</div> </div> </div>
2	B	440	<div> <div>22%</div> <div> <div></div> <div>68%</div> <div>20%</div> <div>13%</div> </div> </div>
3	C	398	<div> <div>19%</div> <div> <div></div> <div>69%</div> <div>21%</div> <div>• 9%</div> </div> </div>
4	D	418	<div> <div>14%</div> <div> <div></div> <div>71%</div> <div>19%</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	u	76	
34	v	10	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 105927 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	394	Total	C	N	O	S	0	0
			3096	1951	543	584	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	384	Total	C	N	O	S	0	0
			3018	1901	515	587	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	363	Total	C	N	O	S	0	0
			2864	1808	515	525	16		

- 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
			3039	1923	524	579	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	415	Total	C	N	O	S	0	0
			3251	2038	561	634	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	244	Total	C	N	O	S	0	0
			1889	1198	316	362	13		
7	g	244	Total	C	N	O	S	0	0
			1880	1193	318	356	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
			1805	1152	305	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	250	Total	C	N	O	S	0	0
			1955	1234	336	375	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
			1880	1179	333	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	234	Total	C	N	O	S	0	0
			1777	1117	295	354	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	238	Total	C	N	O	S	0	0
			1866	1169	336	350	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	240	Total	C	N	O	S	0	0
			1876	1191	321	353	11		
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	202	Total	C	N	O	S	0	0
			1514	949	258	295	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
			1649	1038	279	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	0	0
			1588	1017	270	292	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1588	1017	270	292	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
			1559	982	274	294	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
			1654	1047	284	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	818	Total	C	N	O	S	0	0
			6373	4047	1084	1197	45		

- 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		

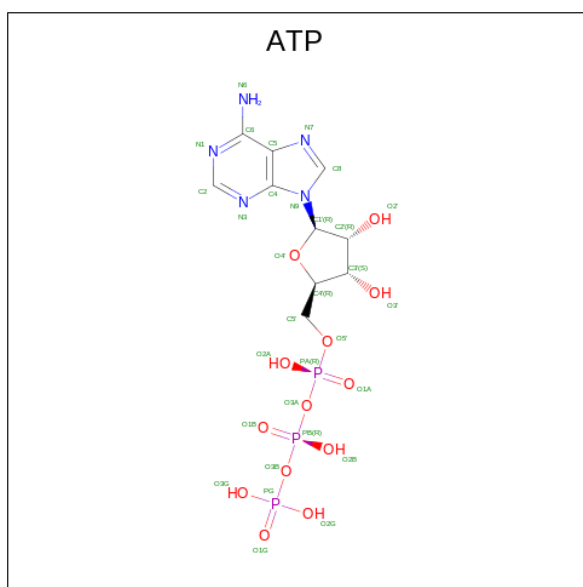
- Molecule 33 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	u	76	Total	C	N	O	S	0	0
			601	378	105	117	1		

- Molecule 34 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	v	10	Total	C	N	O	0	0
			53	32	11	10		

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

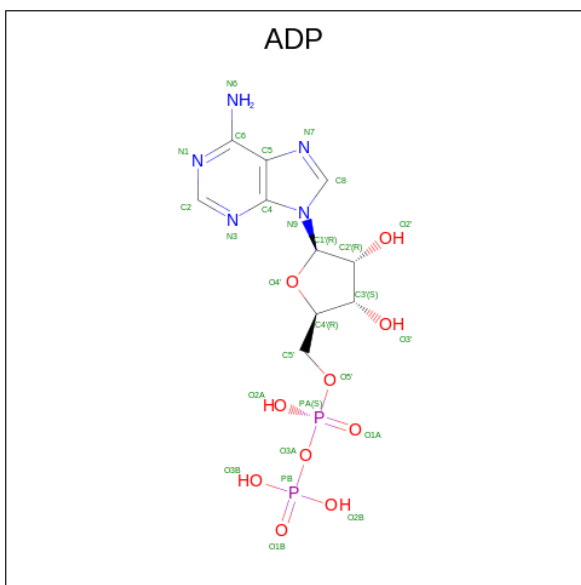


Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- 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	D	1	Total	Mg	0
			1	1	
36	E	1	Total	Mg	0
			1	1	
36	F	1	Total	Mg	0
			1	1	

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



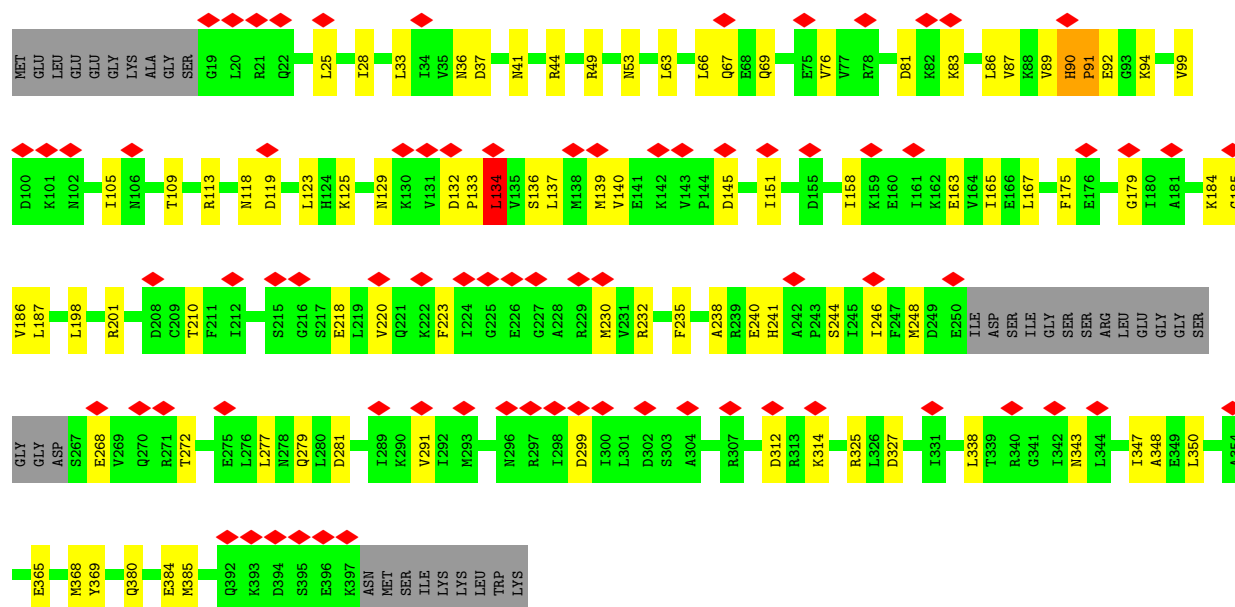
Mol	Chain	Residues	Atoms					AltConf
37	C	1	Total 27	C 10	N 5	O 10	P 2	0
37	F	1	Total 27	C 10	N 5	O 10	P 2	0

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

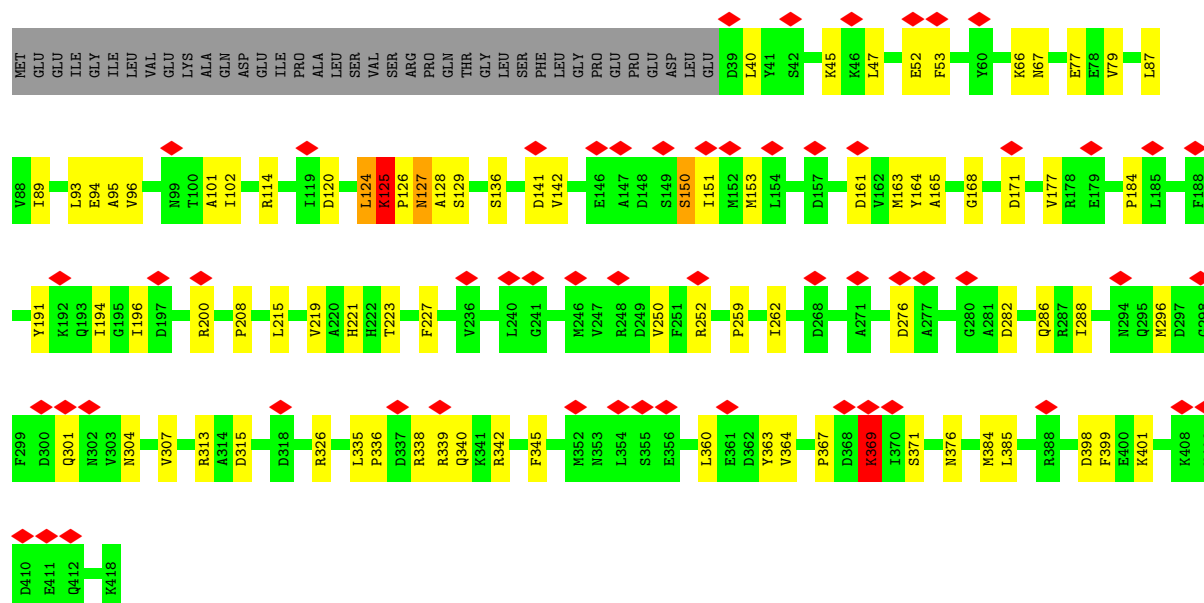
Mol	Chain	Residues	Atoms	AltConf
38	c	1	Total Zn 1 1	0




• Molecule 3: 26S proteasome regulatory subunit 8

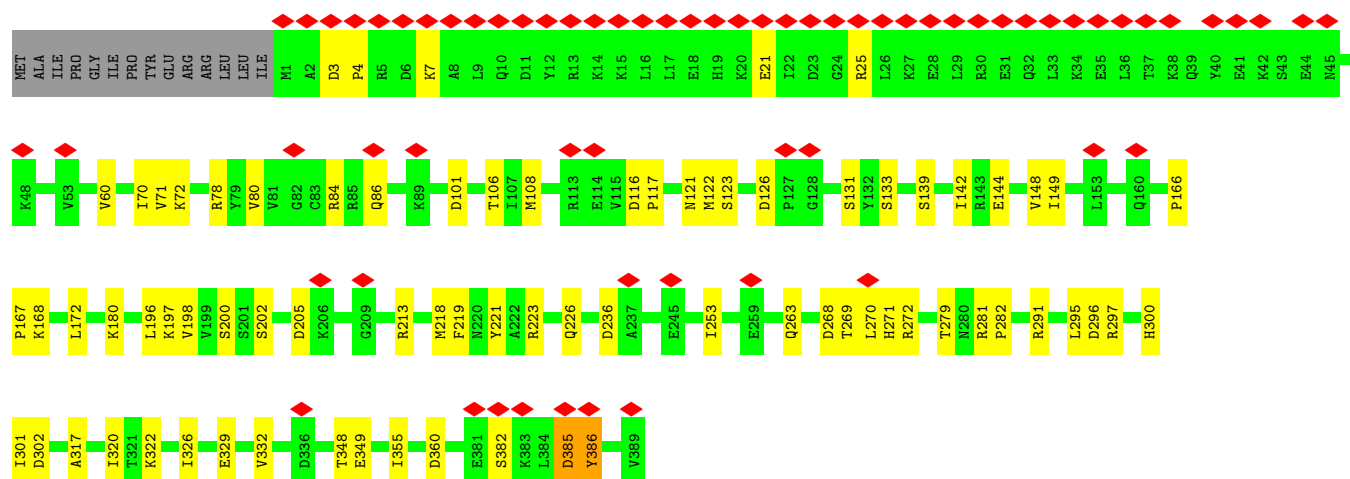


• Molecule 4: 26S proteasome regulatory subunit 6B




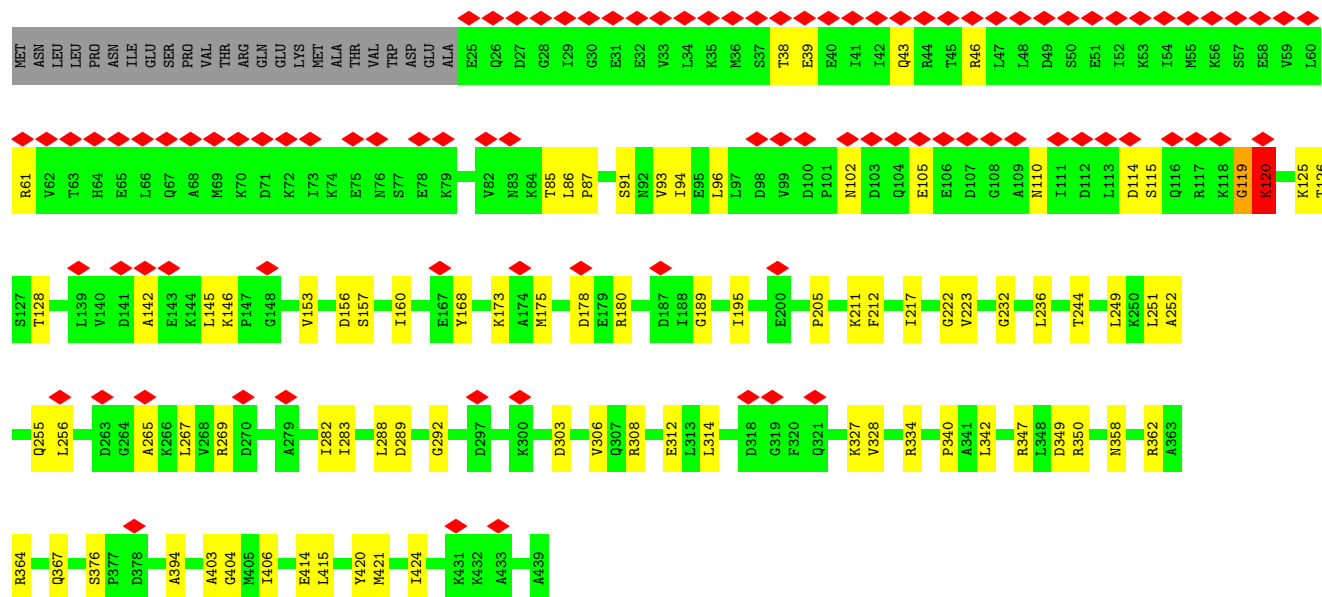
• Molecule 5: Proteasome 26S subunit, ATPase 6

Chain E: 



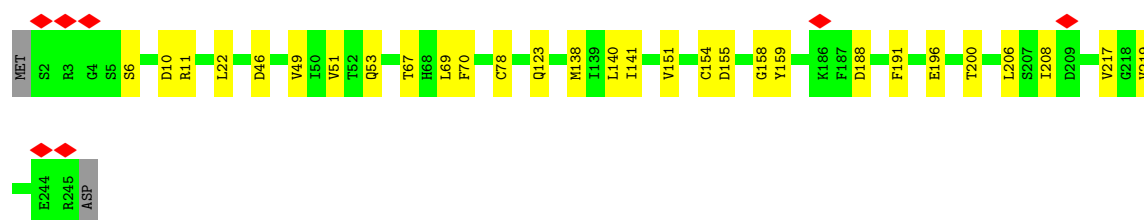
• Molecule 6: 26S proteasome regulatory subunit 6A

Chain F: 

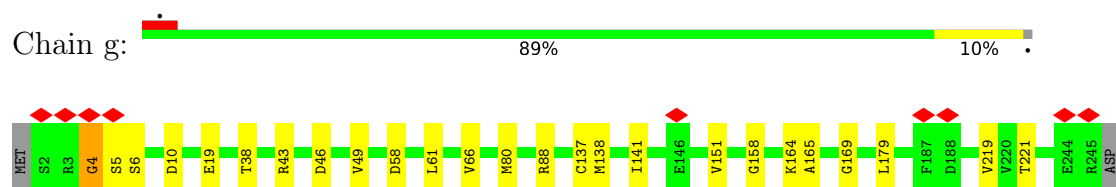


• Molecule 7: Proteasome subunit alpha type-6

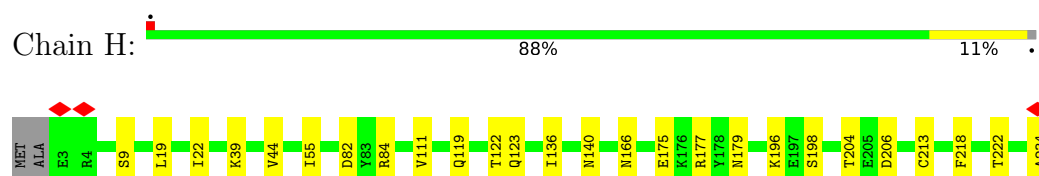
Chain G: 



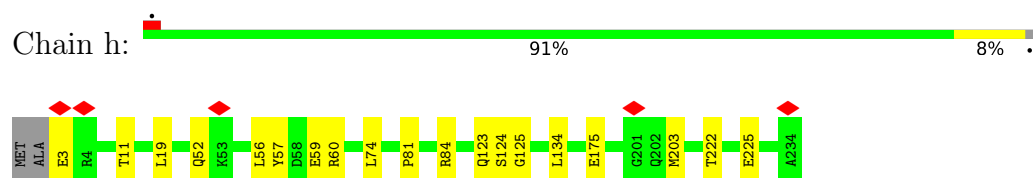
- Molecule 7: Proteasome subunit alpha type-6



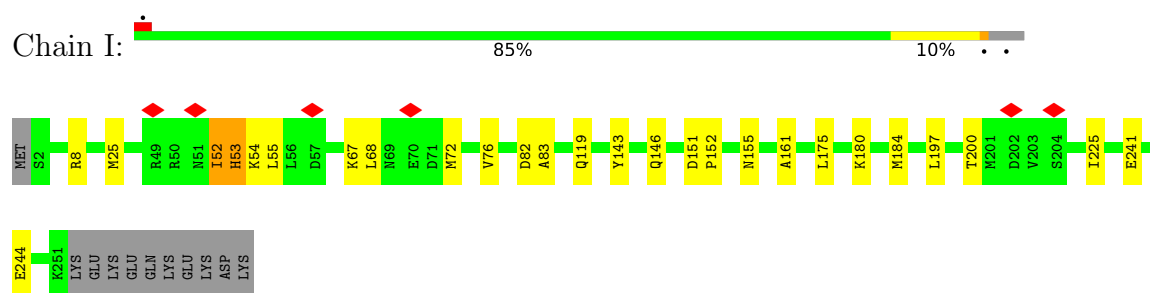
- Molecule 8: Proteasome subunit alpha type-2



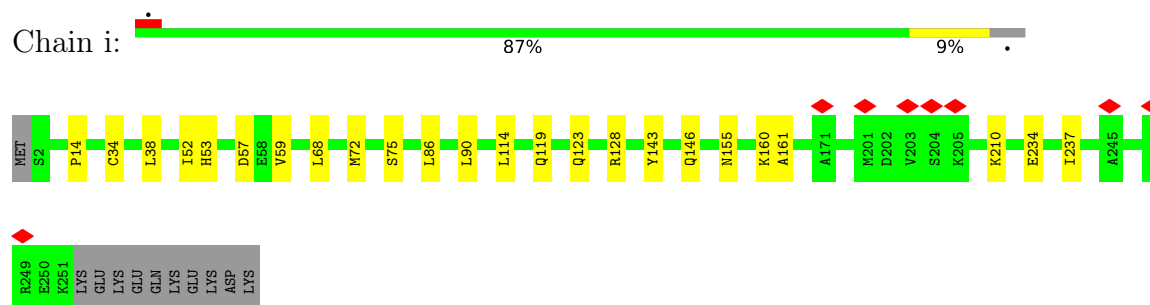
- Molecule 8: Proteasome subunit alpha type-2



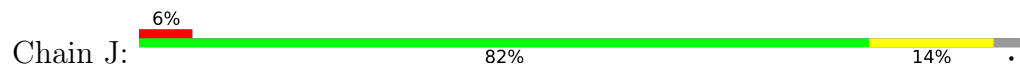
- Molecule 9: Proteasome subunit alpha type-4

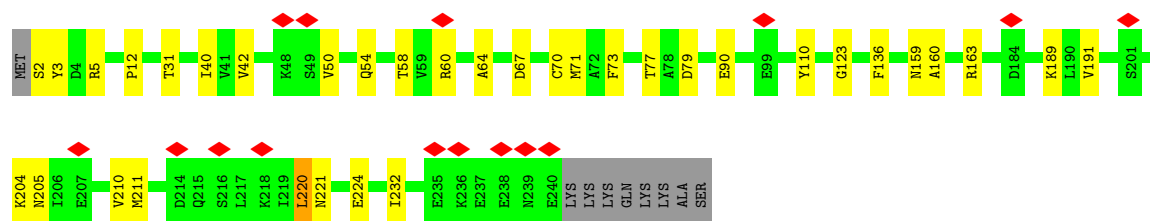


- Molecule 9: Proteasome subunit alpha type-4

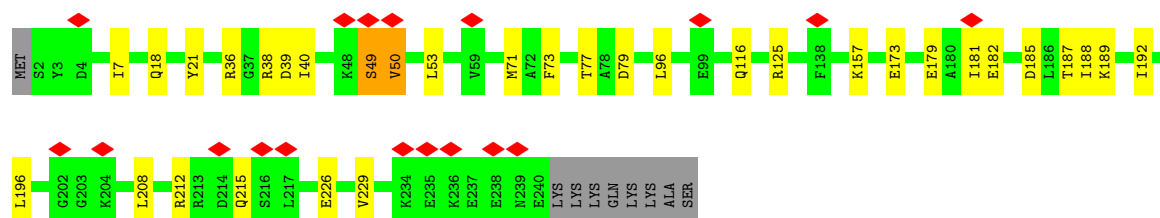
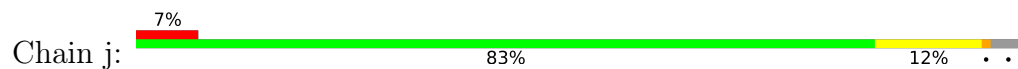


- Molecule 10: Proteasome subunit alpha type-7

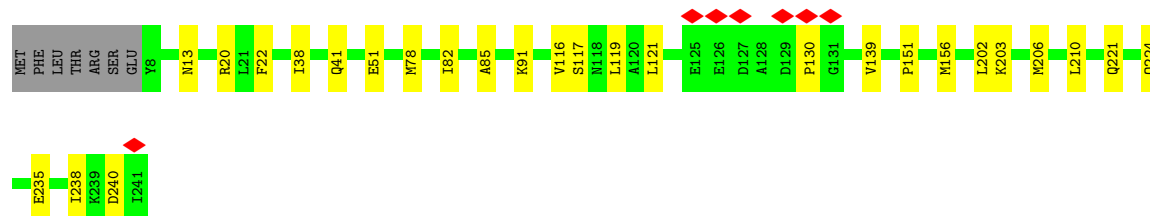
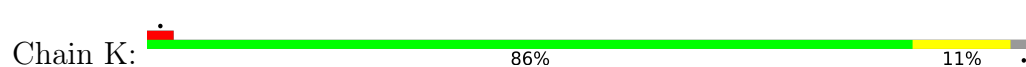




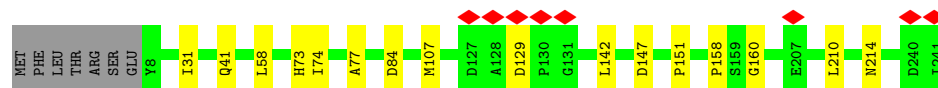
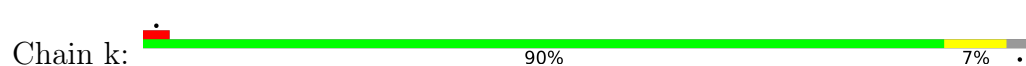
- Molecule 10: Proteasome subunit alpha type-7



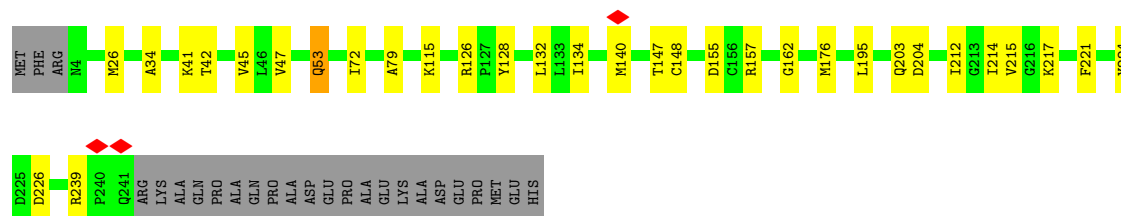
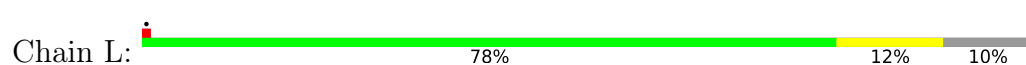
- Molecule 11: Proteasome subunit alpha type-5



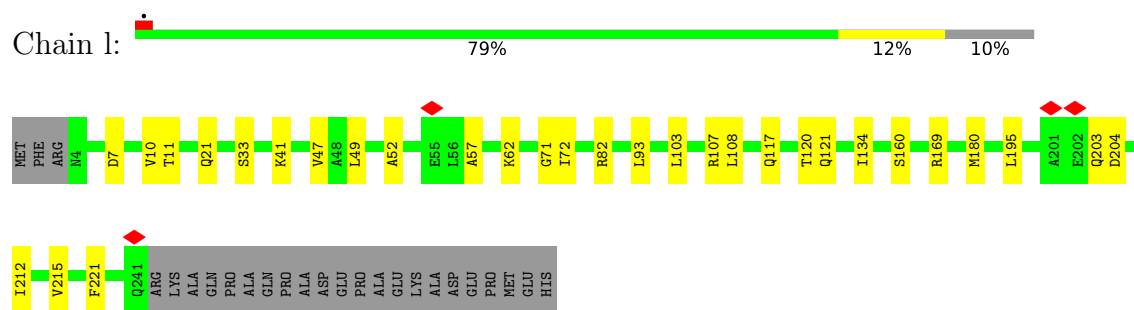
- Molecule 11: Proteasome subunit alpha type-5



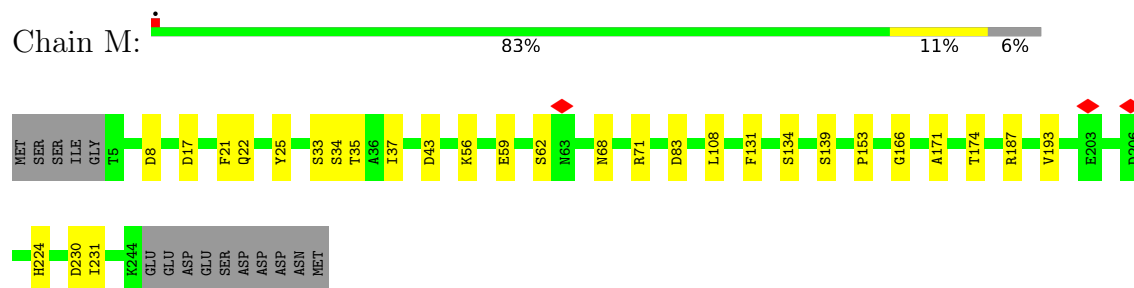
- Molecule 12: Proteasome subunit alpha type-1



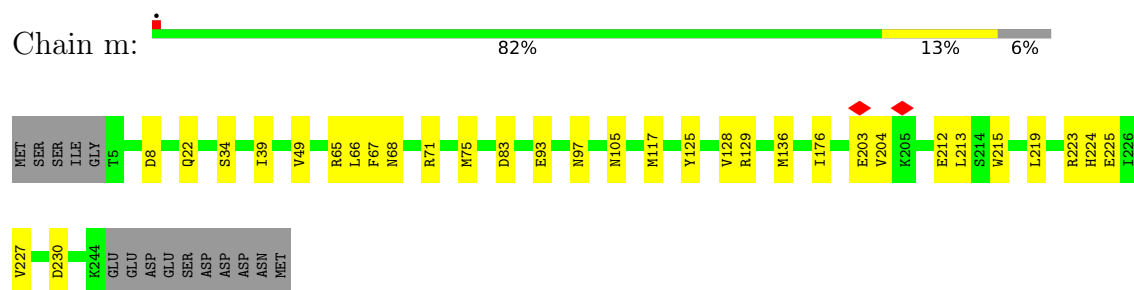
- Molecule 12: Proteasome subunit alpha type-1



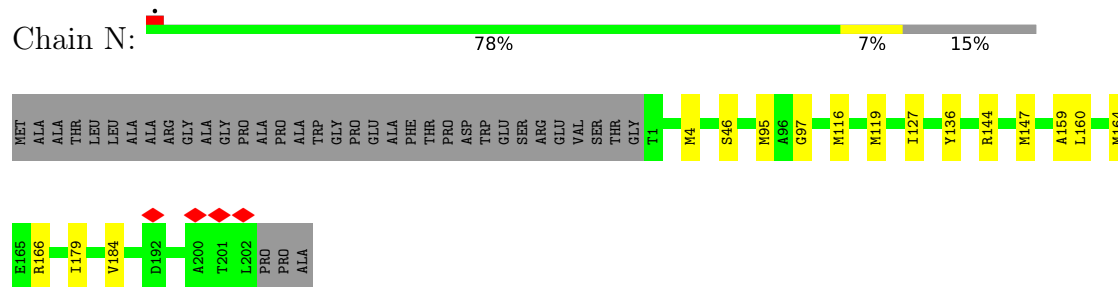
- Molecule 13: Proteasome subunit alpha type-3



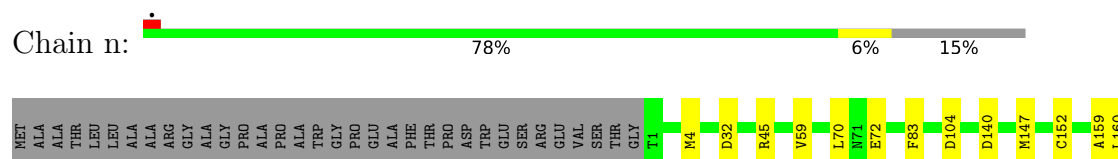
- Molecule 13: Proteasome subunit alpha type-3

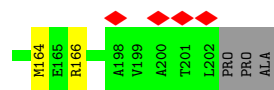


- Molecule 14: Proteasome subunit beta type-6



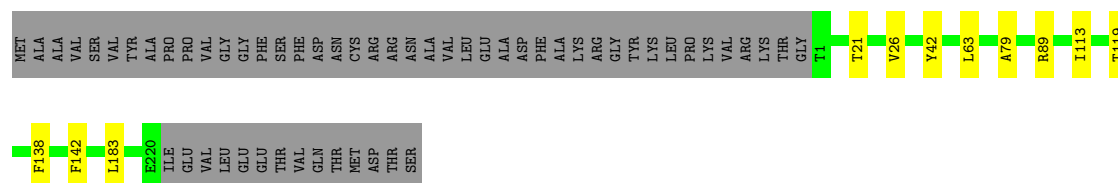
- Molecule 14: Proteasome subunit beta type-6





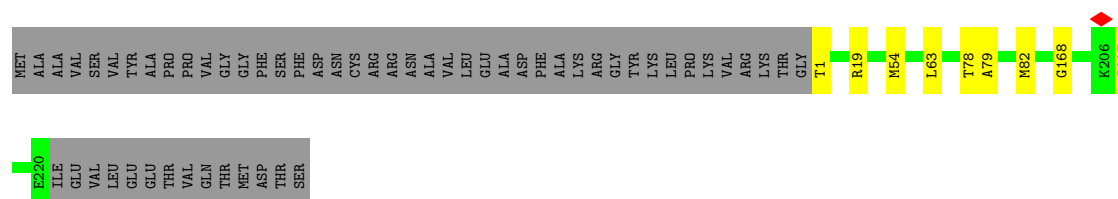
• Molecule 15: Proteasome subunit beta type-7

Chain O: 75% 21%



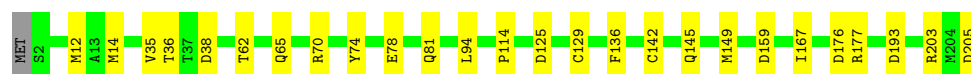
• Molecule 15: Proteasome subunit beta type-7

Chain o: 76% 21%



• Molecule 16: Proteasome subunit beta type-3

Chain P: 87% 13%



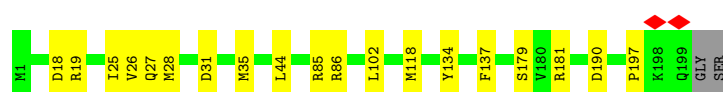
• Molecule 16: Proteasome subunit beta type-3

Chain p: 84% 16%



• Molecule 17: Proteasome subunit beta type-2

Chain Q: 90% 9%



• Molecule 17: Proteasome subunit beta type-2

Chain q: 87% 12%



- Molecule 18: Proteasome subunit beta type-5

Chain R:



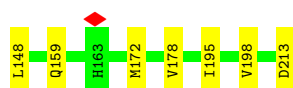
- Molecule 18: Proteasome subunit beta type-5

Chain r:



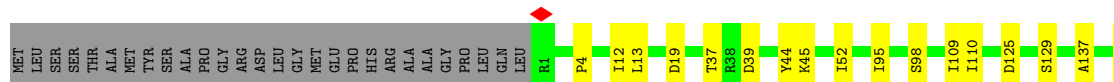
- Molecule 19: Proteasome subunit beta type-1

Chain S:



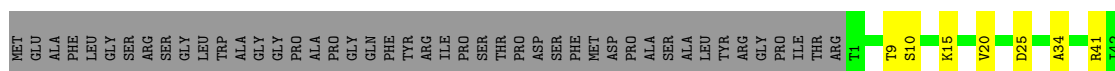
- Molecule 19: Proteasome subunit beta type-1

Chain s:

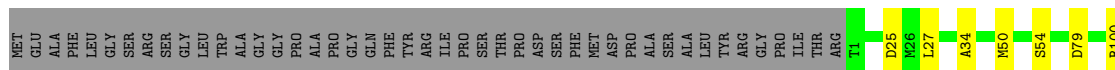


- Molecule 20: Proteasome subunit beta type-4

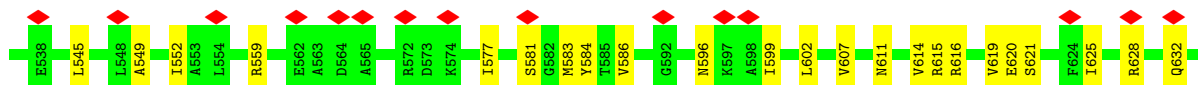
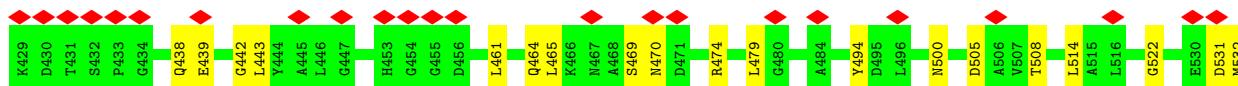
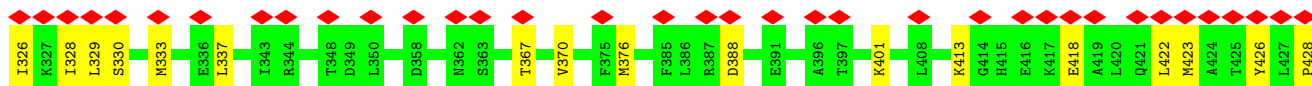
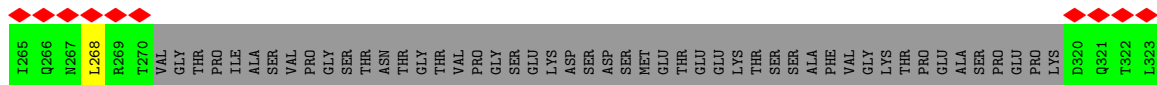
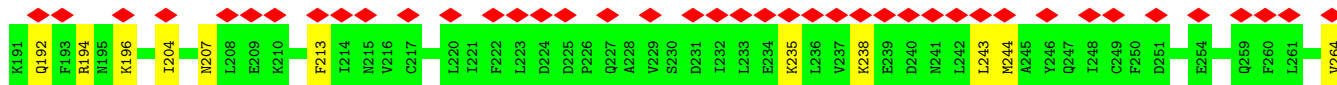
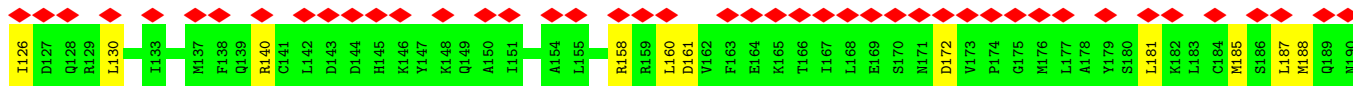
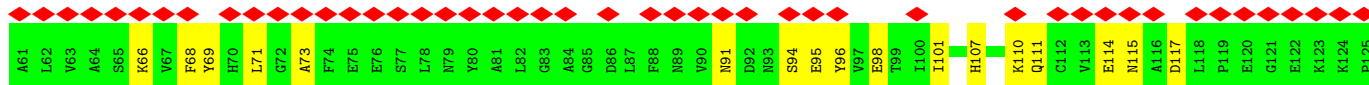
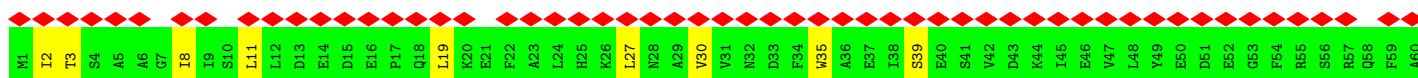
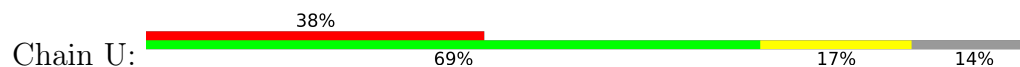
Chain T:



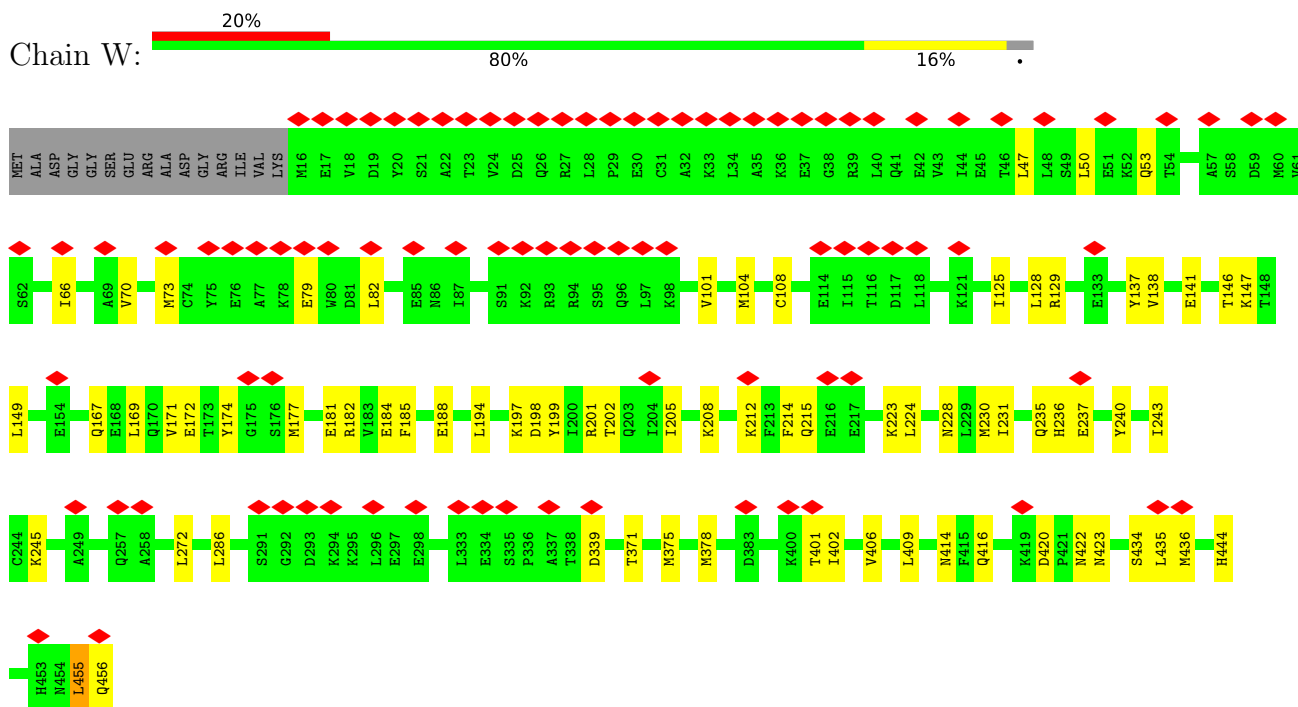
• Molecule 20: Proteasome subunit beta type-4



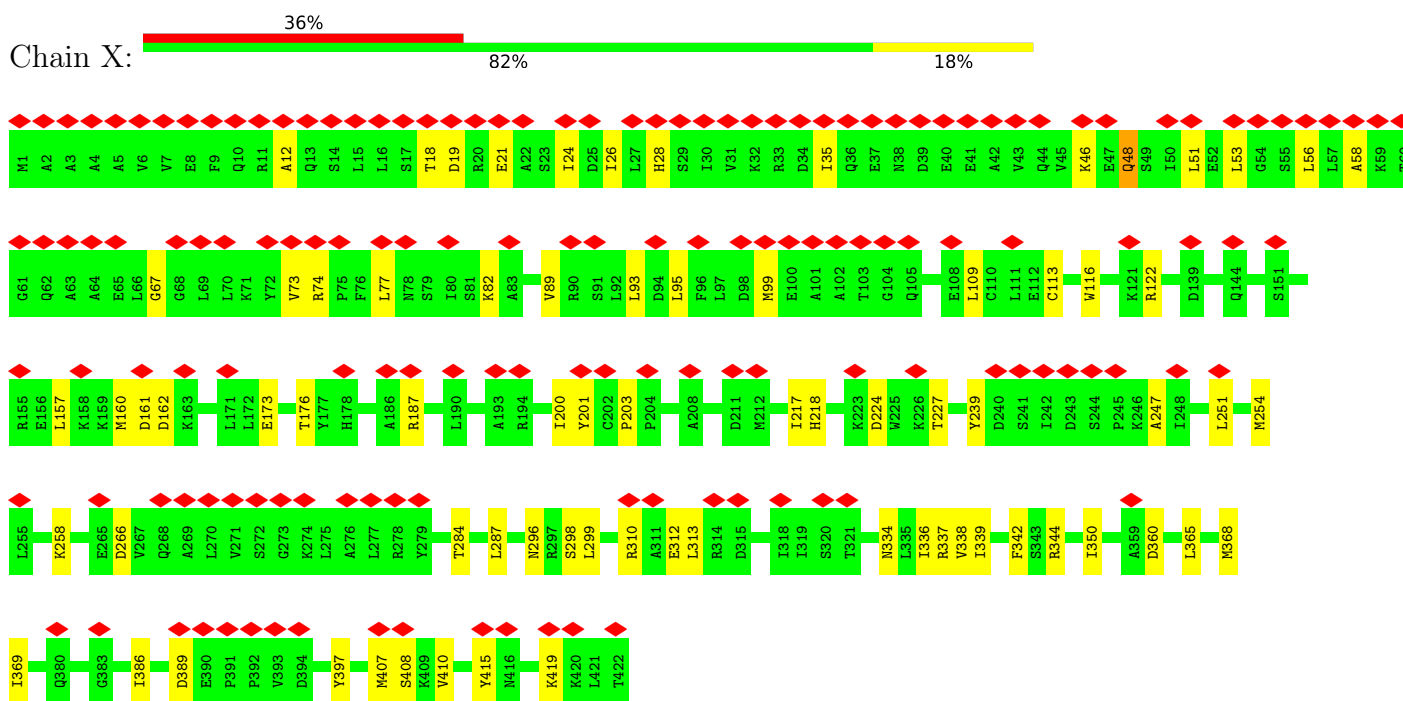
• Molecule 21: 26S proteasome non-ATPase regulatory subunit 1



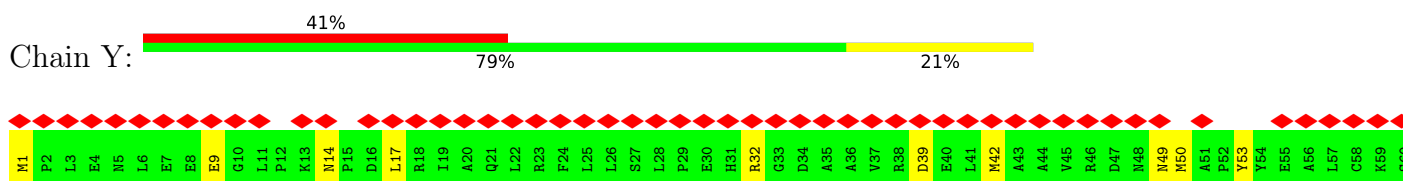
- Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

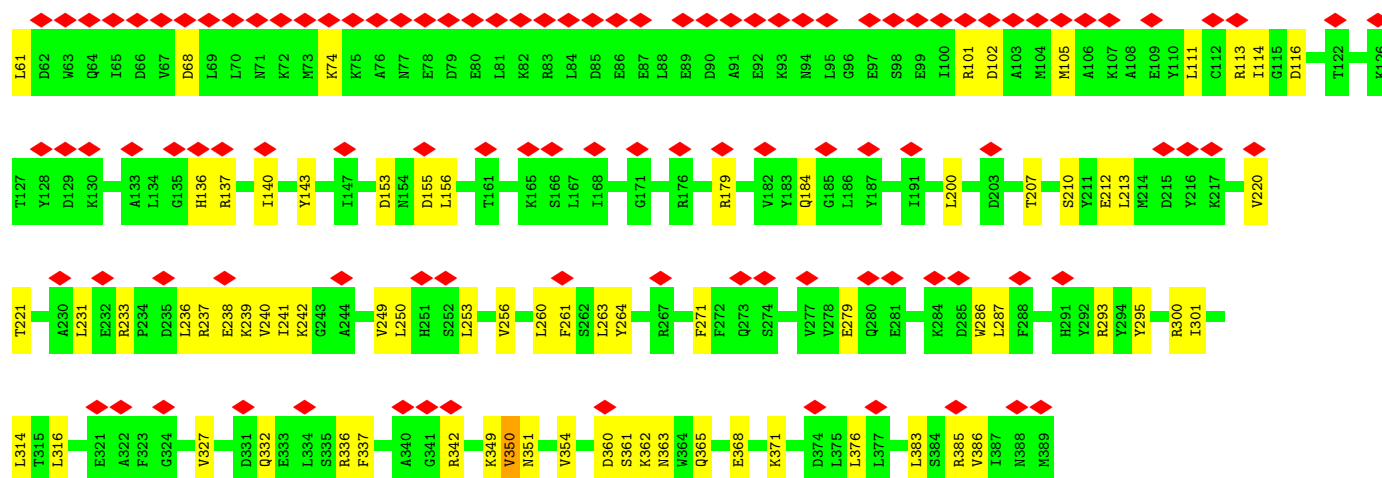


- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

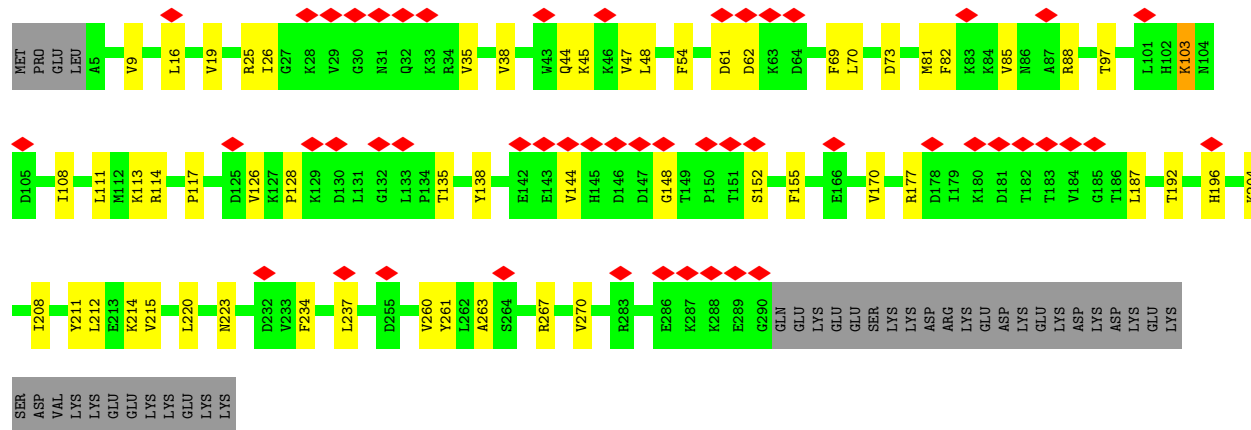


- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

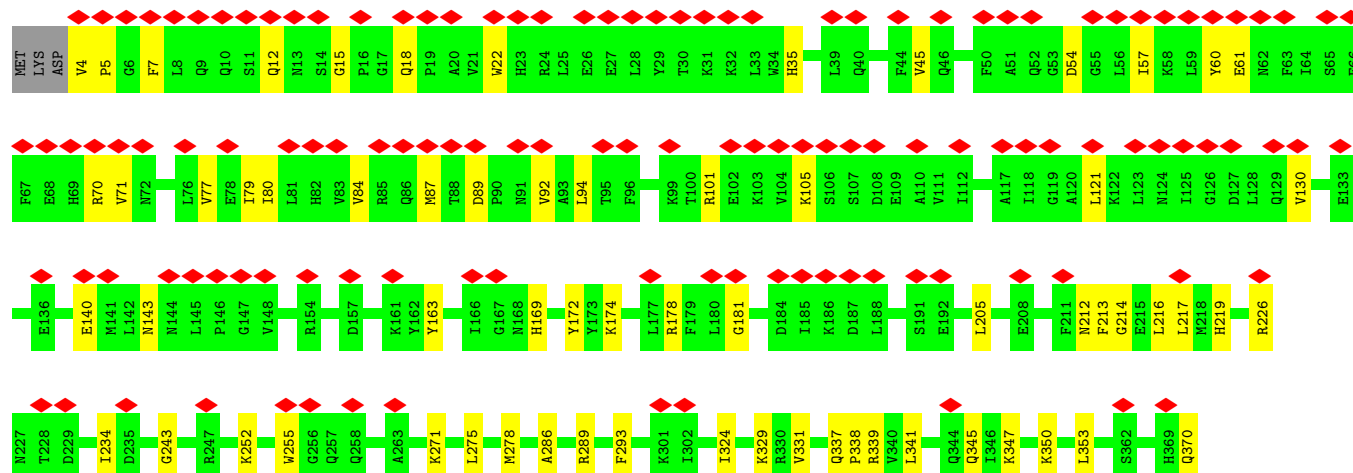
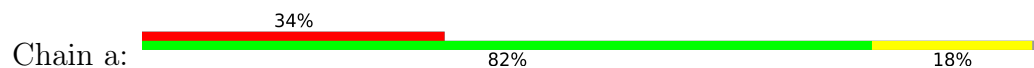


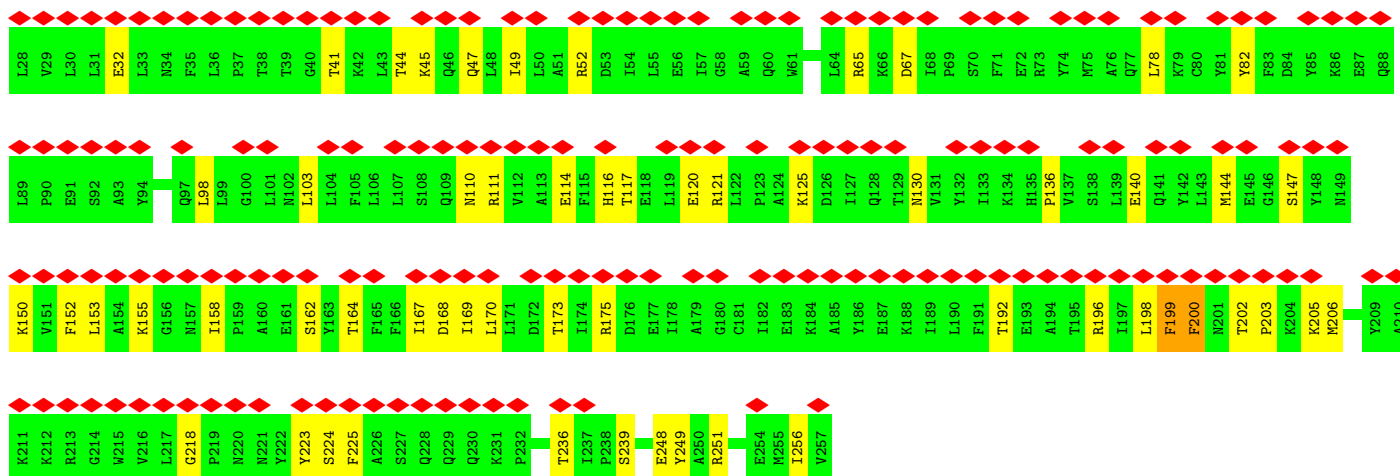


• Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

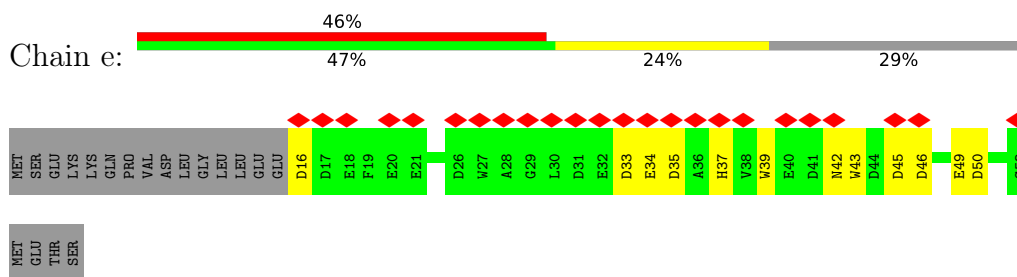


• Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

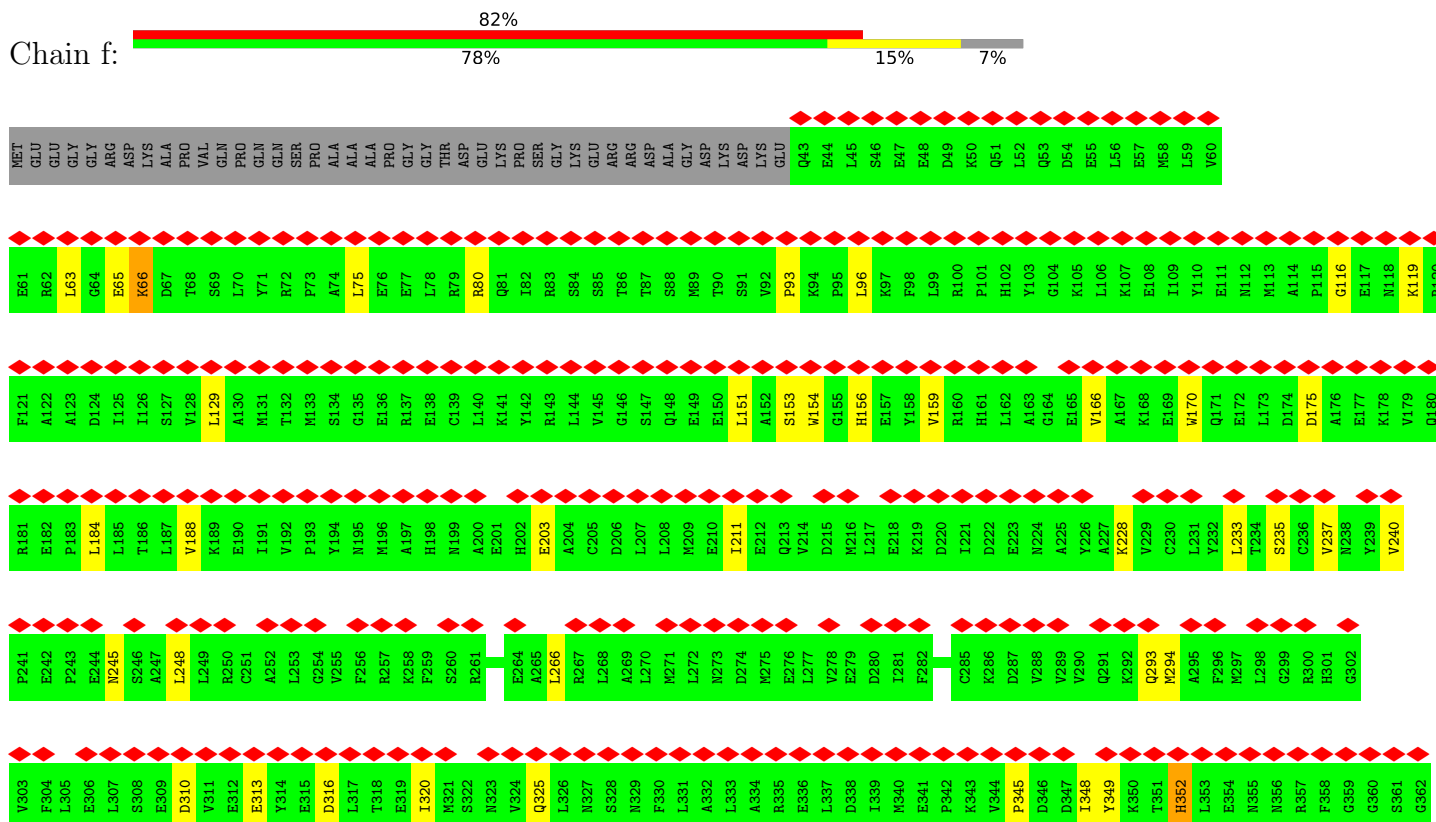


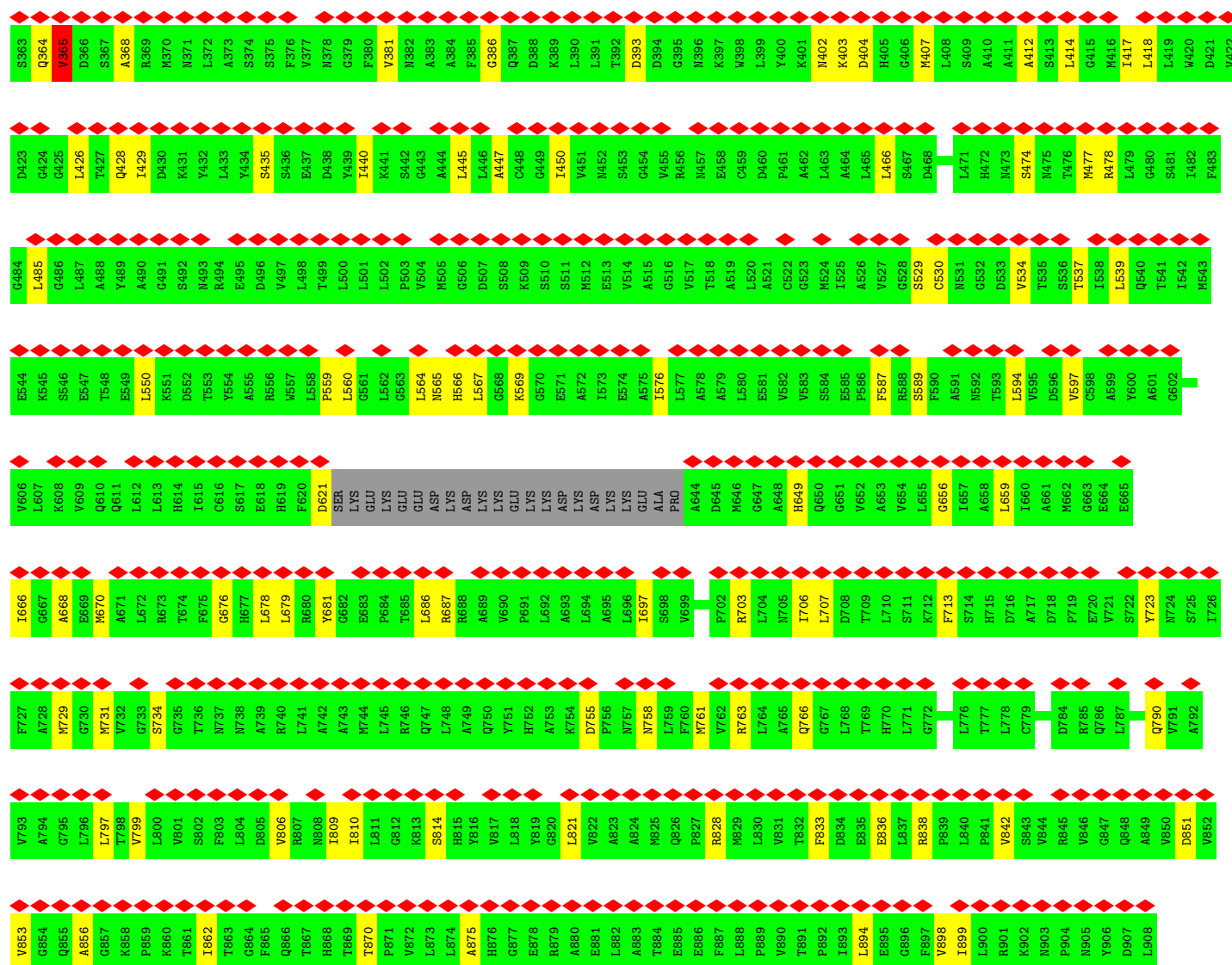


• Molecule 31: 26S proteasome complex subunit SEM1

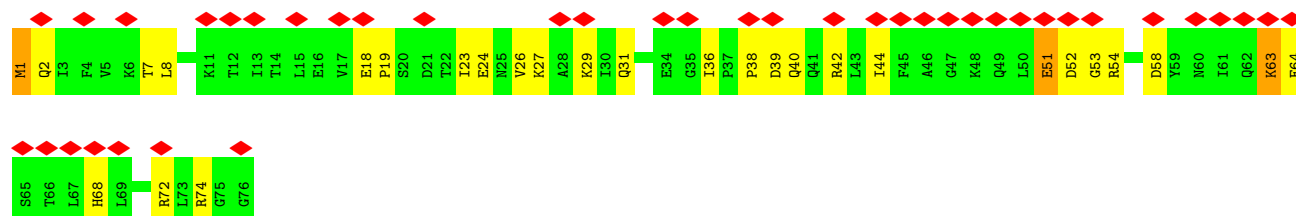


• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2

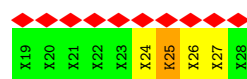




• Molecule 33: Ubiquitin



• Molecule 34: Substrate



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14171	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.022	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00589	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: ZN, ATP, ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/3148	0.58	0/4250
2	B	0.23	0/3061	0.57	0/4129
3	C	0.26	0/2902	0.58	0/3904
4	D	0.28	0/3089	0.59	0/4168
5	E	0.24	0/3145	0.54	0/4233
6	F	0.25	0/3292	0.53	0/4435
7	G	0.25	0/1923	0.48	0/2601
7	g	0.27	0/1914	0.50	0/2590
8	H	0.27	0/1844	0.50	0/2499
8	h	0.25	0/1844	0.43	0/2497
9	I	0.27	0/1985	0.52	0/2677
9	i	0.23	0/1985	0.47	0/2677
10	J	0.25	0/1906	0.52	0/2573
10	j	0.24	0/1887	0.48	0/2549
11	K	0.26	0/1804	0.48	0/2436
11	k	0.23	0/1809	0.43	0/2444
12	L	0.25	0/1901	0.43	0/2570
12	l	0.24	0/1896	0.49	0/2565
13	M	0.23	0/1911	0.42	0/2573
13	m	0.23	0/1916	0.42	0/2580
14	N	0.27	0/1540	0.44	0/2085
14	n	0.27	0/1536	0.45	0/2080
15	O	0.26	0/1676	0.44	0/2271
15	o	0.24	0/1686	0.44	0/2282
16	P	0.26	0/1616	0.50	0/2180
16	p	0.26	0/1620	0.51	0/2184
17	Q	0.27	0/1621	0.47	0/2194
17	q	0.25	0/1621	0.43	0/2194
18	R	0.24	0/1590	0.42	0/2147
18	r	0.26	0/1590	0.42	0/2147
19	S	0.26	0/1671	0.50	0/2252
19	s	0.26	0/1684	0.50	0/2268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.28	0/1716	0.48	0/2323
20	t	0.26	0/1720	0.46	0/2328
21	U	0.22	0/6488	0.53	0/8782
22	V	0.20	0/3681	0.45	0/4969
23	W	0.21	0/3644	0.48	0/4901
24	X	0.21	0/3381	0.51	2/4558 (0.0%)
25	Y	0.22	0/3261	0.53	2/4393 (0.0%)
26	Z	0.23	0/2324	0.61	1/3150 (0.0%)
27	a	0.22	0/3053	0.58	1/4133 (0.0%)
28	b	0.22	0/1478	0.59	0/2001
29	c	0.26	0/2302	0.61	2/3110 (0.1%)
30	d	0.26	0/2162	0.61	2/2919 (0.1%)
31	e	0.25	0/437	0.70	3/595 (0.5%)
32	f	0.20	0/6640	0.49	0/8988
33	u	0.20	0/607	0.40	0/816
34	v	0.17	0/8	0.07	0/8
All	All	0.24	0/107515	0.51	13/145208 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	19	VAL	N-CA-C	-7.43	105.53	112.96
25	Y	239	LYS	CA-C-N	-6.14	114.55	121.85
25	Y	239	LYS	C-N-CA	-6.14	114.55	121.85
29	c	185	ASN	CA-C-N	5.79	136.87	122.74
29	c	185	ASN	C-N-CA	5.79	136.87	122.74
30	d	198	LEU	CA-C-N	5.63	132.30	121.54
30	d	198	LEU	C-N-CA	5.63	132.30	121.54
31	e	61	GLU	N-CA-CB	5.49	119.34	110.40
24	X	48	GLN	N-CA-CB	5.38	119.17	110.40
24	X	310	ARG	CA-CB-CG	5.34	124.78	114.10
31	e	60	LEU	CA-C-N	-5.15	112.12	121.14
31	e	60	LEU	C-N-CA	-5.15	112.12	121.14
27	a	130	VAL	N-CA-C	-5.12	107.85	113.43

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3096	0	3139	51	0
2	B	3018	0	3082	64	0
3	C	2864	0	2971	61	0
4	D	3039	0	3076	69	0
5	E	3097	0	3173	56	0
6	F	3251	0	3319	63	0
7	G	1889	0	1885	18	0
7	g	1880	0	1875	15	0
8	H	1805	0	1784	17	0
8	h	1805	0	1798	15	0
9	I	1955	0	1955	19	0
9	i	1955	0	1955	16	0
10	J	1880	0	1892	21	0
10	j	1861	0	1865	24	0
11	K	1777	0	1762	15	0
11	k	1782	0	1766	11	0
12	L	1866	0	1852	23	0
12	l	1861	0	1839	21	0
13	M	1876	0	1861	19	0
13	m	1881	0	1868	23	0
14	N	1514	0	1487	11	0
14	n	1510	0	1483	9	0
15	O	1649	0	1659	7	0
15	o	1659	0	1681	8	0
16	P	1587	0	1598	17	0
16	p	1591	0	1609	22	0
17	Q	1588	0	1584	16	0
17	q	1588	0	1584	17	0
18	R	1559	0	1523	15	0
18	r	1559	0	1523	9	0
19	S	1641	0	1639	13	0
19	s	1654	0	1656	18	0
20	T	1683	0	1662	20	0
20	t	1687	0	1666	12	0
21	U	6373	0	6411	114	0
22	V	3612	0	3682	65	0
23	W	3596	0	3713	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	X	3335	0	3435	50	0
25	Y	3202	0	3204	58	0
26	Z	2281	0	2312	43	0
27	a	2995	0	3012	41	0
28	b	1458	0	1505	34	0
29	c	2260	0	2276	55	0
30	d	2116	0	2146	47	0
31	e	425	0	328	14	0
32	f	6529	0	6541	81	0
33	u	601	0	629	29	0
34	v	53	0	22	3	0
35	A	31	0	12	1	0
35	B	31	0	12	2	0
35	D	31	0	12	3	0
35	E	31	0	12	1	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	D	1	0	0	0	0
36	E	1	0	0	0	0
36	F	1	0	0	0	0
37	C	27	0	12	1	0
37	F	27	0	12	1	0
38	c	1	0	0	0	0
All	All	105927	0	106359	1313	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 6.

All (1313) 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)
33:u:1:MET:SD	33:u:1:MET:N	2.35	0.99
29:c:96:LEU:HD12	33:u:8:LEU:HD22	1.46	0.94
3:C:89:VAL:HB	3:C:92:GLU:HB2	1.53	0.91
29:c:96:LEU:CD1	33:u:8:LEU:HD22	2.07	0.85
5:E:282:PRO:HD2	5:E:386:TYR:HB3	1.66	0.77
33:u:63:LYS:O	33:u:63:LYS:HG2	1.85	0.77
22:V:486:ILE:HA	22:V:489:MET:HE2	1.67	0.76
33:u:1:MET:HG3	33:u:63:LYS:CB	2.16	0.75
29:c:96:LEU:HD12	33:u:8:LEU:CD2	2.17	0.75
4:D:125:LYS:HG2	29:c:276:GLY:HA2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:457:TYR:HE1	25:Y:350:VAL:HG11	1.51	0.74
9:I:143:TYR:HB2	9:I:146:GLN:HE21	1.52	0.74
29:c:192:LEU:HA	29:c:196:LEU:HB2	1.70	0.74
17:Q:25:ILE:HG23	17:Q:26:VAL:HG13	1.69	0.73
27:a:70:ARG:HH21	28:b:80:PRO:HG2	1.54	0.72
6:F:93:VAL:HG11	6:F:145:LEU:HD21	1.70	0.72
33:u:51:GLU:OE1	33:u:51:GLU:HA	1.91	0.71
24:X:82:LYS:HB3	24:X:122:ARG:HH22	1.56	0.71
7:g:80:MET:HE1	7:g:138:MET:HG3	1.71	0.71
3:C:44:ARG:HG3	22:V:496:PHE:HE2	1.54	0.71
10:J:50:VAL:HB	10:J:54:GLN:HB2	1.73	0.71
33:u:23:ILE:HB	33:u:52:ASP:HA	1.73	0.70
3:C:53:ASN:HD21	21:U:643:SER:HA	1.56	0.70
27:a:35:HIS:NE2	28:b:14:GLU:O	2.24	0.70
3:C:90:HIS:CD2	3:C:91:PRO:HD3	2.27	0.69
21:U:328:ILE:HG13	21:U:329:LEU:HG	1.74	0.69
2:B:82:GLN:HG2	32:f:681:TYR:HB3	1.74	0.69
28:b:25:ARG:NH2	28:b:145:GLU:OE1	2.27	0.68
32:f:828:ARG:HH21	32:f:875:ALA:HA	1.59	0.68
28:b:14:GLU:HG2	28:b:82:GLY:H	1.56	0.68
4:D:163:MET:HG3	4:D:165:ALA:H	1.58	0.68
19:S:27:THR:HB	19:S:40:SER:H	1.59	0.67
5:E:148:VAL:HG13	5:E:149:ILE:HG23	1.77	0.67
1:A:161:VAL:HA	1:A:164:MET:HE3	1.75	0.67
30:d:32:GLU:OE1	30:d:47:GLN:NE2	2.28	0.67
26:Z:111:LEU:HG	26:Z:114:ARG:HH12	1.59	0.67
10:j:212:ARG:HH11	10:j:215:GLN:HE22	1.40	0.67
3:C:86:LEU:HD21	3:C:94:LYS:HD3	1.75	0.66
30:d:202:THR:HG23	30:d:206:MET:HG3	1.78	0.66
32:f:151:LEU:HB3	32:f:159:VAL:HG22	1.78	0.66
4:D:124:LEU:O	4:D:125:LYS:HB2	1.95	0.66
2:B:387:LYS:HB3	2:B:390:LEU:HB3	1.78	0.65
21:U:479:LEU:HG	21:U:514:LEU:HD11	1.79	0.65
27:a:243:GLY:HA2	27:a:275:LEU:HG	1.76	0.65
9:I:8:ARG:HH21	10:J:5:ARG:HH22	1.44	0.65
21:U:243:LEU:HG	21:U:913:ILE:HG23	1.79	0.65
5:E:84:ARG:NH2	5:E:108:MET:SD	2.69	0.65
7:g:88:ARG:HB3	13:m:117:MET:HE1	1.79	0.65
30:d:192:THR:OG1	30:d:196:ARG:NH1	2.30	0.64
1:A:295:VAL:HG11	2:B:307:ARG:HH21	1.62	0.64
28:b:157:VAL:HG21	28:b:170:LEU:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:3:GLU:O	30:d:25:ARG:NH2	2.29	0.64
23:W:245:LYS:HZ2	23:W:286:LEU:HD11	1.61	0.64
1:A:101:ILE:HD11	1:A:111:TYR:HB3	1.78	0.64
5:E:202:SER:HA	6:F:269:ARG:HH22	1.61	0.64
32:f:402:ASN:HB2	32:f:407:MET:HB3	1.79	0.64
11:K:78:MET:HE1	11:K:82:ILE:HA	1.79	0.64
32:f:842:VAL:H	32:f:870:THR:HG22	1.63	0.64
23:W:47:LEU:HD22	23:W:66:ILE:HD11	1.80	0.64
1:A:390:THR:HA	2:B:216:ILE:HD11	1.80	0.63
21:U:11:LEU:HD22	21:U:19:LEU:HD21	1.80	0.63
29:c:57:MET:HE3	29:c:112:TYR:HB3	1.78	0.63
4:D:336:PRO:HB3	4:D:340:GLN:HB2	1.80	0.63
21:U:898:CYS:SG	21:U:899:ARG:N	2.70	0.63
26:Z:16:LEU:HD22	26:Z:135:THR:HG21	1.80	0.63
29:c:187:PRO:HB3	29:c:196:LEU:HG	1.79	0.63
30:d:49:ILE:HD12	30:d:52:ARG:HH21	1.63	0.63
24:X:298:SER:HA	24:X:334:ASN:HD21	1.64	0.63
30:d:120:GLU:HG3	30:d:121:ARG:HG3	1.80	0.63
19:S:148:LEU:HD23	19:S:178:VAL:HG12	1.80	0.63
27:a:370:GLN:O	30:d:251:ARG:NH2	2.31	0.63
4:D:126:PRO:HD3	29:c:277:LYS:HZ2	1.64	0.63
32:f:666:ILE:HG22	32:f:670:MET:HE1	1.80	0.63
4:D:66:LYS:HG3	30:d:256:ILE:HD11	1.81	0.63
4:D:384:MET:HE1	5:E:167:PRO:HD3	1.80	0.62
29:c:195:GLY:O	29:c:198:ARG:HB2	1.99	0.62
15:O:113:ILE:HG12	15:O:119:THR:HG22	1.80	0.62
21:U:461:LEU:HA	21:U:464:GLN:HG2	1.81	0.62
25:Y:361:SER:O	25:Y:365:GLN:NE2	2.32	0.62
21:U:798:PRO:O	21:U:880:ASN:ND2	2.33	0.62
6:F:364:ARG:NH2	6:F:367:GLN:OE1	2.33	0.62
22:V:457:TYR:CE1	25:Y:350:VAL:HG11	2.33	0.62
3:C:137:LEU:HD11	3:C:220:VAL:HG13	1.81	0.62
21:U:264:VAL:O	21:U:268:LEU:HB2	2.00	0.62
4:D:96:VAL:HG23	4:D:102:ILE:HD11	1.81	0.62
21:U:522:GLY:O	21:U:559:ARG:NH2	2.32	0.62
33:u:1:MET:HG3	33:u:63:LYS:HB3	1.82	0.62
32:f:676:GLY:HA2	32:f:679:LEU:HD12	1.81	0.62
1:A:236:CYS:H	32:f:352:HIS:HE1	1.47	0.61
23:W:231:ILE:HG22	23:W:235:GLN:HE22	1.63	0.61
25:Y:49:ASN:HB3	25:Y:114:ILE:HG22	1.80	0.61
1:A:297:ARG:HH12	6:F:306:VAL:HG21	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:HD22	1:A:337:LEU:HD12	1.82	0.61
2:B:290:ILE:HG12	2:B:305:ILE:HG23	1.82	0.61
4:D:129:SER:OG	4:D:252:ARG:NH1	2.33	0.61
22:V:349:ARG:NH2	31:e:39:TRP:O	2.34	0.61
23:W:147:LYS:NZ	23:W:184:GLU:OE1	2.33	0.61
21:U:160:LEU:HD11	21:U:196:LYS:HB3	1.81	0.61
25:Y:105:MET:SD	25:Y:136:HIS:NE2	2.71	0.61
29:c:187:PRO:CB	29:c:196:LEU:HG	2.30	0.61
15:o:78:THR:HG22	15:o:82:MET:HE2	1.81	0.61
5:E:86:GLN:OE1	26:Z:88:ARG:NH2	2.33	0.61
4:D:345:PHE:HB3	4:D:360:LEU:HD23	1.82	0.61
24:X:218:HIS:NE2	24:X:227:THR:OG1	2.34	0.61
2:B:249:ARG:NH2	3:C:279:GLN:OE1	2.34	0.60
4:D:126:PRO:HD3	29:c:277:LYS:NZ	2.15	0.60
11:K:13:ASN:HB3	12:L:126:ARG:HB3	1.82	0.60
29:c:135:ALA:HB3	33:u:36:ILE:HD11	1.82	0.60
31:e:50:ASP:OD1	31:e:55:GLN:NE2	2.34	0.60
21:U:235:LYS:HA	21:U:238:LYS:HD2	1.83	0.60
22:V:397:ARG:HH21	30:d:116:HIS:HB3	1.67	0.60
21:U:801:GLN:HB3	21:U:877:LEU:HD22	1.83	0.60
10:j:38:ARG:HH22	10:j:182:GLU:HG3	1.66	0.60
28:b:35:ILE:HD12	28:b:184:ILE:HD13	1.82	0.60
1:A:75:PRO:HB2	2:B:91:LYS:HE3	1.82	0.60
21:U:66:LYS:NZ	21:U:95:GLU:OE2	2.35	0.60
26:Z:208:ILE:HG23	27:a:353:LEU:HD21	1.83	0.60
4:D:168:GLY:H	35:D:501:ATP:HN62	1.49	0.60
2:B:222:VAL:HG22	2:B:349:ARG:HB2	1.84	0.60
4:D:77:GLU:OE2	26:Z:177:ARG:NH2	2.34	0.60
6:F:85:THR:HG22	6:F:87:PRO:HD2	1.82	0.60
5:E:269:THR:O	5:E:271:HIS:ND1	2.33	0.60
25:Y:349:LYS:O	25:Y:351:ASN:N	2.35	0.60
6:F:153:VAL:HG22	6:F:160:ILE:HG22	1.83	0.59
30:d:110:ASN:ND2	30:d:173:THR:OG1	2.34	0.59
2:B:204:PRO:HG3	2:B:211:TYR:HE2	1.67	0.59
3:C:83:LYS:HA	3:C:105:ILE:HD11	1.82	0.59
27:a:347:LYS:HD3	27:a:350:LYS:HZ1	1.67	0.59
3:C:132:ASP:CG	3:C:133:PRO:HD2	2.27	0.59
19:s:4:PRO:O	20:t:100:ARG:NH2	2.36	0.59
30:d:125:LYS:HE3	30:d:130:ASN:HB2	1.85	0.59
1:A:284:ARG:HD3	1:A:300:LEU:HD21	1.84	0.59
21:U:599:ILE:HD13	21:U:625:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:160:SER:O	12:l:169:ARG:NH1	2.36	0.59
22:V:345:ARG:NH1	31:e:46:ASP:OD2	2.35	0.59
29:c:51:MET:HE1	29:c:79:GLY:HA3	1.85	0.59
10:j:116:GLN:NE2	11:k:84:ASP:OD1	2.35	0.59
7:G:123:GLN:NE2	8:H:82:ASP:OD1	2.36	0.58
29:c:27:THR:OG1	29:c:176:GLN:NE2	2.34	0.58
16:P:12:MET:HE3	16:P:167:ILE:HG13	1.85	0.58
32:f:474:SER:HB3	32:f:477:MET:HE3	1.84	0.58
20:T:25:ASP:OD1	20:T:41:ARG:NH2	2.37	0.58
22:V:321:ALA:HB1	22:V:324:PHE:HB3	1.85	0.58
23:W:129:ARG:NH1	23:W:146:THR:OG1	2.35	0.58
33:u:40:GLN:HA	33:u:72:ARG:HB2	1.85	0.58
21:U:619:VAL:HG11	21:U:648:VAL:HG13	1.84	0.58
23:W:409:LEU:HD21	24:X:344:ARG:HG2	1.85	0.58
23:W:422:ASN:HD21	29:c:235:SER:HA	1.67	0.58
3:C:140:VAL:O	4:D:326:ARG:NH2	2.36	0.58
4:D:208:PRO:HB2	5:E:291:ARG:HD3	1.85	0.58
30:d:44:THR:OG1	30:d:47:GLN:NE2	2.36	0.58
5:E:355:ILE:HD11	6:F:211:LYS:HG2	1.85	0.58
17:Q:102:LEU:HB2	17:Q:118:MET:HB2	1.85	0.58
18:R:64:ARG:NH1	18:R:67:GLU:OE2	2.37	0.58
25:Y:231:LEU:HG	25:Y:236:LEU:HD12	1.85	0.58
12:L:203:GLN:O	12:L:239:ARG:NH2	2.37	0.58
10:j:49:SER:O	10:j:50:VAL:C	2.47	0.58
12:L:115:LYS:NZ	12:L:128:TYR:OH	2.36	0.58
17:q:168:GLN:NE2	17:q:175:LEU:O	2.37	0.58
3:C:90:HIS:CG	3:C:91:PRO:HD3	2.39	0.58
4:D:163:MET:HE3	4:D:164:TYR:H	1.69	0.58
23:W:436:MET:HE1	26:Z:237:LEU:HD22	1.86	0.58
27:a:278:MET:O	27:a:339:ARG:NH2	2.37	0.58
3:C:36:ASN:O	22:V:89:LYS:NZ	2.35	0.58
3:C:49:ARG:NH1	21:U:639:LEU:O	2.37	0.58
23:W:108:CYS:HB3	23:W:128:LEU:HD11	1.86	0.58
12:l:41:LYS:HG2	12:l:180:MET:HE3	1.85	0.58
19:s:148:LEU:HD23	19:s:178:VAL:HG12	1.85	0.58
5:E:281:ARG:HB3	5:E:386:TYR:CZ	2.39	0.57
24:X:284:THR:HA	24:X:287:LEU:HD12	1.86	0.57
27:a:163:TYR:HE1	27:a:169:HIS:HA	1.68	0.57
22:V:74:ASP:OD2	22:V:107:ARG:NH2	2.36	0.57
30:d:155:LYS:HZ3	30:d:167:ILE:HD12	1.69	0.57
22:V:338:LEU:HG	22:V:398:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:184:ILE:HA	28:b:187:PRO:HD2	1.85	0.57
32:f:435:SER:HB3	32:f:440:ILE:HG21	1.85	0.57
10:j:36:ARG:HH21	10:j:157:LYS:HG2	1.69	0.57
12:l:33:SER:OG	12:l:62:LYS:NZ	2.34	0.57
3:C:41:ASN:OD1	3:C:44:ARG:NH2	2.37	0.57
9:I:25:MET:HE1	9:I:151:ASP:HB2	1.86	0.57
16:p:65:GLN:OE1	17:q:86:ARG:NH2	2.37	0.57
2:B:181:GLN:O	2:B:241:ASN:ND2	2.37	0.57
2:B:287:ILE:HB	2:B:329:MET:HE2	1.85	0.57
7:g:61:LEU:HD21	7:g:66:VAL:HG11	1.85	0.57
1:A:347:ASP:OD1	1:A:348:LEU:N	2.34	0.57
21:U:628:ARG:NH1	21:U:749:GLN:OE1	2.38	0.57
26:Z:215:VAL:HA	26:Z:220:LEU:HB2	1.86	0.57
3:C:28:ILE:HD11	4:D:47:LEU:HD12	1.86	0.57
3:C:198:LEU:HD23	37:C:501:ADP:H5'2	1.86	0.57
24:X:48:GLN:HA	24:X:51:LEU:HG	1.87	0.57
26:Z:113:LYS:NZ	26:Z:117:PRO:O	2.38	0.57
32:f:417:ILE:HG22	32:f:418:LEU:HD12	1.86	0.57
8:h:3:GLU:N	13:m:125:TYR:HB3	2.19	0.57
8:h:59:GLU:HG2	8:h:60:ARG:HD3	1.85	0.57
9:I:180:LYS:HB2	9:I:184:MET:HE3	1.87	0.57
13:M:37:ILE:HD11	13:M:193:VAL:HG13	1.86	0.57
27:a:94:LEU:HD21	27:a:121:LEU:HD11	1.87	0.57
5:E:21:GLU:OE2	5:E:25:ARG:NH2	2.38	0.57
21:U:423:MET:HB2	21:U:426:TYR:HB2	1.86	0.57
3:C:185:GLY:N	3:C:312:ASP:OD2	2.37	0.56
5:E:168:LYS:N	5:E:296:ASP:OD2	2.35	0.56
13:m:8:ASP:O	13:m:22:GLN:NE2	2.35	0.56
12:l:117:GLN:NE2	13:m:83:ASP:OD1	2.37	0.56
1:A:307:ASP:OD2	1:A:333:ARG:NH2	2.39	0.56
3:C:235:PHE:HA	3:C:238:ALA:HB3	1.87	0.56
5:E:281:ARG:HB3	5:E:386:TYR:CE2	2.40	0.56
5:E:322:LYS:HD3	5:E:326:ILE:HG13	1.86	0.56
6:F:283:ILE:HD11	6:F:328:VAL:HG22	1.87	0.56
12:L:157:ARG:NH1	12:L:176:MET:SD	2.77	0.56
21:U:791:LEU:O	21:U:914:LEU:N	2.36	0.56
25:Y:9:GLU:O	25:Y:179:ARG:NH2	2.34	0.56
10:j:71:MET:HE1	10:j:73:PHE:HB3	1.88	0.56
23:W:401:THR:HG23	23:W:402:ILE:HD12	1.87	0.56
25:Y:137:ARG:HA	25:Y:140:ILE:HD12	1.88	0.56
1:A:113:ILE:HG22	1:A:121:PHE:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:152:PHE:HB2	30:d:199:PHE:HE2	1.69	0.56
32:f:235:SER:HB3	32:f:853:VAL:HG21	1.88	0.56
1:A:284:ARG:O	6:F:334:ARG:NH1	2.34	0.56
16:P:159:ASP:N	16:P:159:ASP:OD1	2.37	0.56
21:U:619:VAL:HG23	21:U:651:GLY:HA3	1.87	0.56
21:U:461:LEU:HG	21:U:464:GLN:NE2	2.19	0.56
25:Y:220:VAL:HG21	25:Y:249:VAL:HG11	1.88	0.56
9:i:86:LEU:HD22	9:i:114:LEU:HD11	1.88	0.56
5:E:223:ARG:NH1	5:E:268:ASP:OD2	2.39	0.56
6:F:180:ARG:NH1	6:F:244:THR:O	2.39	0.56
7:G:138:MET:HB3	7:G:154:CYS:HB3	1.88	0.56
4:D:150:SER:HB2	4:D:250:VAL:HG22	1.87	0.56
6:F:96:LEU:HD21	6:F:120:LYS:CB	2.36	0.56
6:F:195:ILE:HG12	6:F:236:LEU:HD21	1.87	0.56
21:U:91:ASN:O	21:U:140:ARG:NH2	2.38	0.56
30:d:147:SER:HA	30:d:150:LYS:HE2	1.88	0.56
6:F:404:GLY:HA2	6:F:415:LEU:HD21	1.88	0.55
15:O:21:THR:HG22	15:O:26:VAL:HA	1.87	0.55
17:Q:26:VAL:HG21	18:R:136:TYR:HE2	1.70	0.55
14:n:32:ASP:O	14:n:45:ARG:NH2	2.39	0.55
17:q:151:ILE:HG13	17:q:155:ARG:HG3	1.87	0.55
13:M:8:ASP:O	13:M:22:GLN:NE2	2.36	0.55
22:V:121:PHE:O	22:V:128:ARG:NH1	2.36	0.55
25:Y:368:GLU:OE1	25:Y:371:LYS:NZ	2.40	0.55
14:n:4:MET:HE1	14:n:159:ALA:HB3	1.88	0.55
19:s:52:ILE:HG13	19:s:110:ILE:HG12	1.88	0.55
27:a:84:VAL:HA	27:a:87:MET:HG2	1.87	0.55
28:b:124:LEU:HD21	28:b:152:LYS:HB3	1.88	0.55
7:g:141:ILE:HG22	7:g:151:VAL:HG22	1.89	0.55
2:B:197:ILE:HG13	2:B:235:LEU:HD21	1.88	0.55
29:c:125:VAL:HG12	33:u:74:ARG:O	2.07	0.55
12:l:52:ALA:HB1	12:l:57:ALA:HB3	1.87	0.55
33:u:1:MET:HG3	33:u:63:LYS:HB2	1.88	0.55
6:F:314:LEU:HD21	6:F:342:LEU:HB3	1.89	0.55
12:L:41:LYS:HG3	12:L:42:THR:HG23	1.89	0.55
24:X:35:ILE:HD12	24:X:46:LYS:HD3	1.87	0.55
1:A:239:ARG:HG3	2:B:319:PHE:HZ	1.72	0.55
3:C:69:GLN:HB2	3:C:118:ASN:HD21	1.72	0.55
5:E:123:SER:O	5:E:197:LYS:NZ	2.38	0.55
32:f:567:LEU:O	32:f:790:GLN:NE2	2.40	0.55
1:A:274:PHE:HB2	1:A:319:MET:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:72:ILE:HG22	12:L:134:ILE:HG12	1.87	0.55
12:l:121:GLN:HG3	13:m:129:ARG:HG2	1.89	0.55
33:u:39:ASP:O	33:u:42:ARG:NH1	2.40	0.55
16:P:149:MET:HE3	19:s:147:PRO:HB2	1.87	0.55
21:U:584:TYR:OH	21:U:768:GLN:NE2	2.40	0.55
9:i:68:LEU:HB2	9:i:72:MET:HB2	1.89	0.55
22:V:417:ILE:HD12	22:V:422:ILE:HB	1.88	0.54
26:Z:9:VAL:HG12	26:Z:48:LEU:HB3	1.88	0.54
25:Y:210:SER:HB3	25:Y:213:LEU:HD23	1.89	0.54
26:Z:44:GLN:HE21	26:Z:47:VAL:HG13	1.71	0.54
9:i:155:ASN:OD1	10:j:77:THR:OG1	2.25	0.54
5:E:348:THR:HA	6:F:217:ILE:HD11	1.88	0.54
6:F:61:ARG:NH1	33:u:53:GLY:O	2.40	0.54
21:U:333:MET:O	21:U:337:LEU:HB2	2.07	0.54
22:V:343:PRO:O	31:e:43:TRP:NE1	2.40	0.54
30:d:152:PHE:HA	30:d:155:LYS:HB2	1.89	0.54
18:R:166:ARG:NH1	16:p:34:MET:O	2.41	0.54
21:U:461:LEU:HG	21:U:464:GLN:HE21	1.72	0.54
23:W:197:LYS:NZ	23:W:199:TYR:OH	2.37	0.54
26:Z:82:PHE:HA	26:Z:85:VAL:HG12	1.88	0.54
26:Z:126:VAL:HB	29:c:212:LEU:HD21	1.89	0.54
7:g:43:ARG:HH21	7:g:164:LYS:HG2	1.71	0.54
11:k:41:GLN:NE2	11:k:151:PRO:O	2.41	0.54
20:t:25:ASP:HA	20:t:187:PHE:HA	1.87	0.54
4:D:114:ARG:NH2	4:D:136:SER:OG	2.41	0.54
5:E:385:ASP:O	5:E:386:TYR:HB2	2.08	0.54
6:F:96:LEU:HD21	6:F:120:LYS:HB2	1.90	0.54
21:U:770:TRP:O	29:c:177:THR:OG1	2.26	0.54
22:V:199:ASN:OD1	22:V:241:ARG:NH2	2.40	0.54
25:Y:332:GLN:OE1	25:Y:336:ARG:NE	2.39	0.54
22:V:95:LEU:HD12	22:V:96:ARG:HE	1.73	0.54
22:V:132:LEU:HD23	22:V:135:LEU:HD21	1.89	0.54
23:W:224:LEU:O	23:W:228:ASN:ND2	2.41	0.54
26:Z:25:ARG:HH11	29:c:104:ARG:H	1.55	0.54
30:d:78:LEU:HD13	30:d:98:LEU:HD21	1.89	0.54
2:B:171:VAL:O	2:B:175:LYS:HB2	2.08	0.54
21:U:643:SER:O	21:U:649:ARG:NH1	2.40	0.54
22:V:85:ALA:HB2	22:V:93:PHE:HB2	1.89	0.54
23:W:172:GLU:HA	23:W:182:ARG:HD3	1.88	0.54
18:r:106:LYS:HG3	18:r:107:ARG:HD2	1.90	0.54
22:V:121:PHE:HB3	22:V:128:ARG:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ASP:HB2	2:B:322:ARG:HH12	1.73	0.54
2:B:378:VAL:HG12	2:B:416:ASN:HA	1.90	0.54
23:W:420:ASP:HB3	23:W:423:ASN:H	1.73	0.54
26:Z:263:ALA:HB1	29:c:288:VAL:HG13	1.90	0.54
31:e:59:GLU:O	31:e:63:HIS:ND1	2.38	0.54
4:D:313:ARG:NH2	4:D:315:ASP:OD2	2.42	0.53
5:E:198:VAL:HG12	5:E:200:SER:H	1.73	0.53
21:U:532:MET:HE2	21:U:552:ILE:HG21	1.90	0.53
11:k:160:GLY:O	12:l:82:ARG:NH2	2.40	0.53
4:D:153:MET:HG2	4:D:227:PHE:HB3	1.89	0.53
9:I:53:HIS:CG	9:I:54:LYS:H	2.26	0.53
17:Q:35:MET:HE3	17:Q:181:ARG:HH11	1.73	0.53
19:S:147:PRO:HB2	16:p:149:MET:HE3	1.89	0.53
21:U:654:MET:HE2	21:U:767:THR:HG22	1.90	0.53
21:U:666:LYS:HA	21:U:669:ILE:HD12	1.90	0.53
2:B:272:ARG:O	2:B:276:GLU:HB3	2.08	0.53
11:K:91:LYS:HG2	11:K:119:LEU:HD11	1.90	0.53
22:V:465:ASP:HB3	22:V:468:SER:HB3	1.91	0.53
27:a:12:GLN:HG3	27:a:22:TRP:HB3	1.90	0.53
17:q:52:ASP:OD1	18:r:88:TYR:OH	2.23	0.53
35:E:401:ATP:O3G	6:F:347:ARG:NH2	2.40	0.53
6:F:232:GLY:HA2	37:F:501:ADP:H5'1	1.89	0.53
32:f:723:TYR:HB3	32:f:761:MET:HE3	1.90	0.53
10:j:40:ILE:HG22	10:j:212:ARG:HG2	1.90	0.53
1:A:236:CYS:H	32:f:352:HIS:CE1	2.24	0.53
3:C:347:ILE:HD12	3:C:350:LEU:HD12	1.90	0.53
17:Q:134:TYR:HB3	17:q:25:ILE:HD11	1.91	0.53
21:U:694:ILE:HG23	21:U:695:MET:HG2	1.89	0.53
16:p:126:LEU:HG	16:p:127:ILE:HG23	1.90	0.53
1:A:258:ARG:HH12	6:F:255:GLN:HA	1.74	0.53
2:B:196:GLU:OE2	2:B:349:ARG:NH1	2.33	0.53
4:D:342:ARG:HB3	4:D:364:VAL:HG11	1.89	0.53
23:W:171:VAL:HG12	23:W:182:ARG:HG3	1.91	0.53
32:f:151:LEU:HD23	32:f:159:VAL:HA	1.89	0.53
32:f:529:SER:OG	32:f:565:ASN:OD1	2.26	0.53
16:P:177:ARG:NH2	19:s:150:ASP:OD2	2.34	0.53
21:U:607:VAL:O	21:U:615:ARG:NH1	2.42	0.53
9:I:67:LYS:HE3	9:I:225:ILE:HD12	1.90	0.53
19:S:21:ALA:HB3	19:S:198:VAL:HB	1.91	0.53
22:V:416:ARG:HH11	22:V:459:GLN:HE21	1.57	0.53
32:f:530:CYS:SG	32:f:569:LYS:NZ	2.82	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:215:TRP:CD1	13:m:227:VAL:HG22	2.43	0.53
6:F:43:GLN:HA	6:F:46:ARG:HG2	1.91	0.53
9:I:52:ILE:O	9:I:53:HIS:C	2.51	0.53
22:V:337:LEU:HD21	22:V:364:THR:HG23	1.91	0.53
24:X:365:LEU:HA	24:X:368:MET:HG3	1.91	0.53
10:j:181:ILE:HA	10:j:187:THR:HG22	1.90	0.53
20:t:27:LEU:HD22	20:t:184:TYR:HB2	1.91	0.53
2:B:234:LEU:HD12	35:B:501:ATP:H2'	1.91	0.53
4:D:95:ALA:HA	4:D:101:ALA:HA	1.91	0.53
16:P:14:MET:HG2	16:P:136:PHE:HB3	1.89	0.53
21:U:749:GLN:NE2	21:U:750:SER:O	2.38	0.53
31:e:16:ASP:OD1	31:e:16:ASP:N	2.41	0.53
9:i:57:ASP:HB3	9:i:59:VAL:HG23	1.91	0.53
16:p:124:LEU:HD23	16:p:128:GLY:HA2	1.91	0.53
1:A:94:GLN:HE22	1:A:96:ALA:HB2	1.74	0.52
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.91	0.52
27:a:140:GLU:O	27:a:143:ASN:ND2	2.42	0.52
28:b:62:THR:HA	28:b:70:ARG:HH12	1.74	0.52
11:k:210:LEU:HA	11:k:214:ASN:HD21	1.74	0.52
12:l:103:LEU:HD23	12:l:108:LEU:HB2	1.91	0.52
4:D:151:ILE:HD12	4:D:153:MET:H	1.72	0.52
21:U:111:GLN:HE21	21:U:115:ASN:ND2	2.07	0.52
21:U:401:LYS:HB3	21:U:438:GLN:HB2	1.91	0.52
28:b:51:LEU:N	28:b:62:THR:OG1	2.42	0.52
10:j:7:ILE:O	10:j:18:GLN:NE2	2.42	0.52
27:a:341:LEU:HD13	27:a:345:GLN:HB2	1.90	0.52
20:t:27:LEU:HD11	20:t:34:ALA:HB1	1.91	0.52
3:C:163:GLU:HA	3:C:167:LEU:HD13	1.91	0.52
23:W:125:ILE:HG21	23:W:149:LEU:HD13	1.92	0.52
24:X:95:LEU:O	24:X:99:MET:HB2	2.09	0.52
27:a:205:LEU:O	27:a:271:LYS:NZ	2.42	0.52
21:U:71:LEU:HD13	22:V:273:LYS:HE3	1.91	0.52
22:V:289:LEU:HB3	22:V:312:ALA:HB2	1.91	0.52
8:h:81:PRO:HA	8:h:84:ARG:HE	1.73	0.52
13:m:68:ASN:OD1	13:m:224:HIS:ND1	2.42	0.52
4:D:384:MET:HE1	5:E:166:PRO:HA	1.92	0.52
5:E:172:LEU:HD22	5:E:301:ILE:HD11	1.90	0.52
14:N:4:MET:HE1	14:N:159:ALA:HB3	1.91	0.52
24:X:160:MET:HE2	24:X:162:ASP:HB2	1.92	0.52
26:Z:192:THR:O	26:Z:196:HIS:ND1	2.32	0.52
12:l:120:THR:O	13:m:129:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:46:ALA:HB3	18:R:98:GLY:HA3	1.91	0.52
3:C:365:GLU:HA	3:C:368:MET:HE2	1.91	0.52
14:N:127:ILE:HD11	14:N:136:TYR:HD1	1.75	0.52
21:U:532:MET:HE2	21:U:552:ILE:HD13	1.92	0.52
27:a:45:VAL:HG21	27:a:79:ILE:HG22	1.91	0.52
9:I:155:ASN:OD1	10:J:77:THR:OG1	2.27	0.52
21:U:772:TRP:HD1	21:U:775:LEU:HB2	1.75	0.52
22:V:124:ASN:HA	22:V:128:ARG:HD3	1.91	0.52
9:i:52:ILE:HD11	9:i:210:LYS:HE2	1.91	0.52
2:B:252:GLY:HA2	2:B:255:LEU:HD23	1.91	0.52
3:C:89:VAL:O	3:C:90:HIS:C	2.53	0.52
5:E:148:VAL:HB	5:E:297:ARG:HH21	1.74	0.52
8:H:111:VAL:HG22	8:H:136:ILE:HD12	1.92	0.52
9:I:119:GLN:NE2	10:J:79:ASP:OD1	2.43	0.52
22:V:102:PRO:O	22:V:106:ARG:NH1	2.43	0.52
23:W:406:VAL:HG23	24:X:342:PHE:HB3	1.92	0.52
3:C:248:MET:SD	3:C:248:MET:N	2.83	0.51
22:V:284:GLU:OE2	22:V:287:ARG:NH1	2.42	0.51
2:B:76:GLU:HA	2:B:79:ILE:HG22	1.91	0.51
24:X:218:HIS:HE2	24:X:224:ASP:HB3	1.76	0.51
25:Y:300:ARG:HD3	25:Y:337:PHE:HZ	1.75	0.51
27:a:278:MET:HG2	27:a:339:ARG:HH22	1.75	0.51
32:f:237:VAL:HB	32:f:248:LEU:HD11	1.93	0.51
2:B:118:ASP:OD1	2:B:118:ASP:N	2.42	0.51
2:B:387:LYS:HG3	2:B:389:ASP:H	1.75	0.51
5:E:144:GLU:OE2	5:E:297:ARG:NH1	2.43	0.51
22:V:228:ARG:HH22	22:V:261:TYR:HB2	1.73	0.51
1:A:101:ILE:HG22	1:A:138:MET:H	1.75	0.51
1:A:119:ALA:HB2	6:F:128:THR:HG23	1.93	0.51
1:A:128:GLN:HG2	1:A:129:VAL:HG13	1.92	0.51
4:D:335:LEU:HD11	4:D:371:SER:HA	1.91	0.51
5:E:349:GLU:OE1	6:F:350:ARG:NH1	2.43	0.51
6:F:96:LEU:CD2	6:F:120:LYS:HB2	2.41	0.51
8:H:177:ARG:NH1	24:X:161:ASP:OD1	2.43	0.51
8:H:204:THR:OG1	8:H:206:ASP:OD1	2.28	0.51
12:L:26:MET:HE1	12:L:148:CYS:HB3	1.92	0.51
21:U:66:LYS:HD2	21:U:69:TYR:HE1	1.75	0.51
21:U:158:ARG:NH2	21:U:192:GLN:OE1	2.42	0.51
32:f:96:LEU:HD13	32:f:129:LEU:HD13	1.92	0.51
3:C:113:ARG:NH2	3:C:129:ASN:O	2.43	0.51
17:Q:19:ARG:NH1	17:Q:179:SER:OG	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:461:LYS:NZ	22:V:462:GLU:O	2.44	0.51
23:W:444:HIS:CE1	26:Z:204:LYS:HB3	2.45	0.51
24:X:239:TYR:HB3	24:X:247:ALA:HB2	1.92	0.51
24:X:407:MET:HA	24:X:410:VAL:HG22	1.91	0.51
27:a:212:ASN:OD1	27:a:213:PHE:N	2.43	0.51
1:A:181:LYS:HA	1:A:184:ILE:HD12	1.93	0.51
21:U:505:ASP:HB3	21:U:508:THR:HG22	1.93	0.51
22:V:467:TYR:OH	24:X:397:TYR:OH	2.29	0.51
5:E:226:GLN:HG2	5:E:272:ARG:HH21	1.76	0.51
5:E:282:PRO:CD	5:E:386:TYR:HB3	2.39	0.51
15:O:63:LEU:HD11	15:O:79:ALA:HB2	1.93	0.51
23:W:147:LYS:HE3	23:W:188:GLU:HG3	1.93	0.51
24:X:21:GLU:HA	24:X:24:ILE:HD12	1.93	0.51
25:Y:237:ARG:NH1	25:Y:264:TYR:OH	2.44	0.51
32:f:851:ASP:N	32:f:851:ASP:OD1	2.44	0.51
1:A:103:ASN:HA	1:A:136:GLU:HG2	1.93	0.51
1:A:108:ASP:OD2	1:A:110:LYS:NZ	2.35	0.51
12:L:226:ASP:OD1	12:L:226:ASP:N	2.44	0.51
21:U:895:PRO:HD2	21:U:902:PRO:HG3	1.93	0.51
28:b:6:THR:HB	28:b:49:VAL:HG22	1.93	0.51
32:f:566:HIS:HB3	32:f:569:LYS:HE2	1.92	0.51
3:C:44:ARG:HG3	22:V:496:PHE:CE2	2.41	0.51
6:F:282:ILE:HG22	6:F:327:LYS:HB2	1.93	0.51
21:U:660:CYS:HB2	21:U:694:ILE:HD11	1.93	0.51
24:X:74:ARG:HH22	24:X:116:TRP:HB2	1.76	0.51
13:m:49:VAL:HB	13:m:212:GLU:HB3	1.92	0.51
9:I:68:LEU:HB2	9:I:72:MET:HB2	1.93	0.50
26:Z:73:ASP:OD2	28:b:70:ARG:NH2	2.44	0.50
30:d:111:ARG:HB3	30:d:114:GLU:HB2	1.93	0.50
3:C:165:ILE:HD11	3:C:186:VAL:HG21	1.92	0.50
6:F:421:MET:HA	6:F:424:ILE:HD12	1.93	0.50
9:I:53:HIS:CG	9:I:54:LYS:N	2.79	0.50
16:P:38:ASP:OD1	16:P:38:ASP:N	2.44	0.50
16:P:125:ASP:OD1	16:P:129:CYS:N	2.33	0.50
29:c:30:GLN:HB3	29:c:66:THR:HG22	1.93	0.50
2:B:249:ARG:HG3	2:B:283:PHE:HD2	1.77	0.50
6:F:223:VAL:HG12	6:F:350:ARG:HB2	1.93	0.50
22:V:235:LEU:HA	22:V:250:LEU:HD13	1.92	0.50
25:Y:293:ARG:HH12	31:e:49:GLU:HG2	1.76	0.50
15:o:1:THR:N	15:o:168:GLY:O	2.44	0.50
33:u:1:MET:CG	33:u:63:LYS:HB2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:u:44:ILE:HB	33:u:68:HIS:HB2	1.94	0.50
2:B:107:MET:HB3	2:B:151:LEU:HD12	1.92	0.50
2:B:288:ASP:N	2:B:288:ASP:OD1	2.41	0.50
21:U:649:ARG:HE	21:U:675:MET:HE1	1.77	0.50
25:Y:316:LEU:HD13	25:Y:327:VAL:HG13	1.93	0.50
32:f:703:ARG:HB2	32:f:706:ILE:HG12	1.93	0.50
15:o:63:LEU:HD11	15:o:79:ALA:HB2	1.93	0.50
2:B:223:ILE:HG22	2:B:350:LYS:HA	1.93	0.50
2:B:251:VAL:HG23	2:B:285:ASP:HB3	1.94	0.50
4:D:171:ASP:OD1	4:D:171:ASP:N	2.44	0.50
6:F:102:ASN:H	6:F:115:SER:HB2	1.77	0.50
6:F:252:ALA:HB3	6:F:255:GLN:HB2	1.93	0.50
26:Z:45:LYS:HD2	26:Z:47:VAL:H	1.75	0.50
27:a:347:LYS:HA	27:a:350:LYS:HZ3	1.77	0.50
32:f:156:HIS:NE2	32:f:203:GLU:OE1	2.44	0.50
9:i:161:ALA:HB3	10:j:53:LEU:HD23	1.94	0.50
13:m:34:SER:OG	13:m:65:ARG:NH1	2.39	0.50
18:r:7:LYS:HD2	18:r:109:PRO:HB2	1.93	0.50
2:B:269:GLU:HA	2:B:272:ARG:HG2	1.92	0.50
7:G:49:VAL:HG22	7:G:219:VAL:HG22	1.94	0.50
21:U:701:ILE:HD12	21:U:809:SER:HB2	1.94	0.50
22:V:452:ASN:HB3	22:V:457:TYR:HB2	1.94	0.50
28:b:117:VAL:HG22	28:b:119:ASP:H	1.77	0.50
29:c:54:MET:O	29:c:77:GLN:NE2	2.45	0.50
29:c:136:LEU:HD11	33:u:7:THR:HG21	1.94	0.50
32:f:404:ASP:OD1	32:f:404:ASP:N	2.44	0.50
9:i:234:GLU:HA	9:i:237:ILE:HG12	1.94	0.50
13:M:71:ARG:HH21	20:T:72:ILE:HG12	1.77	0.50
17:Q:18:ASP:N	17:Q:18:ASP:OD1	2.42	0.50
20:T:63:LEU:HD21	20:T:106:LEU:HD13	1.93	0.50
30:d:200:PHE:CD1	30:d:205:LYS:HD3	2.46	0.50
32:f:799:VAL:HG21	32:f:821:LEU:HG	1.92	0.50
2:B:401:GLU:OE2	2:B:422:SER:OG	2.30	0.50
6:F:303:ASP:OD1	6:F:303:ASP:N	2.44	0.50
21:U:94:SER:HA	21:U:98:GLU:HG3	1.93	0.50
21:U:111:GLN:HE21	21:U:115:ASN:HD21	1.60	0.50
22:V:263:LEU:HD23	30:d:121:ARG:HH22	1.77	0.50
9:I:197:LEU:HA	9:I:200:THR:HG22	1.94	0.49
21:U:95:GLU:CD	21:U:96:TYR:H	2.20	0.49
10:j:185:ASP:OD1	10:j:185:ASP:N	2.44	0.49
2:B:183:THR:OG1	2:B:184:TYR:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:230:MET:HG3	3:C:232:ARG:H	1.77	0.49
4:D:126:PRO:C	4:D:128:ALA:N	2.70	0.49
13:M:230:ASP:N	13:M:230:ASP:OD1	2.45	0.49
21:U:698:GLN:HG2	21:U:702:THR:HG21	1.94	0.49
26:Z:35:VAL:H	26:Z:97:THR:HG22	1.76	0.49
35:D:501:ATP:O3G	5:E:291:ARG:NE	2.45	0.49
5:E:3:ASP:OD1	5:E:3:ASP:N	2.45	0.49
5:E:131:SER:OG	5:E:133:SER:OG	2.30	0.49
5:E:253:ILE:HG13	6:F:308:ARG:HH22	1.76	0.49
18:R:7:LYS:HG2	18:R:12:VAL:HG22	1.94	0.49
22:V:140:ASP:OD1	22:V:140:ASP:N	2.44	0.49
25:Y:286:TRP:HD1	25:Y:287:LEU:HD12	1.76	0.49
30:d:236:THR:O	30:d:239:SER:OG	2.25	0.49
10:j:96:LEU:HA	17:q:62:LYS:HE2	1.93	0.49
12:l:215:VAL:HB	12:l:221:PHE:HD1	1.77	0.49
2:B:373:THR:OG1	2:B:412:MET:O	2.29	0.49
3:C:76:VAL:HG22	3:C:87:VAL:HG22	1.94	0.49
20:T:34:ALA:O	14:n:166:ARG:NH1	2.42	0.49
25:Y:240:VAL:HG23	25:Y:241:ILE:HG13	1.94	0.49
32:f:386:GLY:HA2	32:f:418:LEU:HG	1.94	0.49
12:l:203:GLN:NE2	12:l:204:ASP:O	2.45	0.49
1:A:55:LEU:HD11	2:B:76:GLU:HG2	1.94	0.49
3:C:380:GLN:NE2	3:C:384:GLU:OE1	2.45	0.49
21:U:117:ASP:OD1	21:U:117:ASP:N	2.45	0.49
22:V:346:LEU:O	22:V:350:GLN:NE2	2.38	0.49
27:a:226:ARG:HB3	27:a:234:ILE:HD11	1.93	0.49
12:l:33:SER:HG	12:l:62:LYS:NZ	2.10	0.49
16:p:7:ASN:ND2	16:p:29:GLY:O	2.38	0.49
3:C:343:ASN:HD21	25:Y:1:MET:HE2	1.78	0.49
18:R:52:CYS:HA	18:R:97:MET:HE2	1.95	0.49
23:W:240:TYR:HA	23:W:243:ILE:HD12	1.94	0.49
1:A:214:LEU:HD12	1:A:343:PHE:HE2	1.77	0.49
3:C:134:LEU:O	3:C:137:LEU:HB3	2.13	0.49
3:C:369:TYR:CE2	3:C:385:MET:HB3	2.47	0.49
4:D:67:ASN:ND2	21:U:607:VAL:O	2.46	0.49
15:O:42:TYR:HE2	15:O:183:LEU:HD11	1.78	0.49
19:S:131:GLN:OE1	19:S:132:ARG:N	2.36	0.49
20:T:9:THR:O	20:T:41:ARG:NH1	2.45	0.49
20:T:25:ASP:HA	20:T:187:PHE:HA	1.95	0.49
23:W:70:VAL:HA	23:W:73:MET:HE2	1.95	0.49
23:W:174:TYR:O	23:W:182:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:191:ASN:HD21	16:p:203:ARG:HH12	1.60	0.49
24:X:360:ASP:OD1	24:X:360:ASP:N	2.46	0.49
32:f:687:ARG:HG2	32:f:713:PHE:HZ	1.77	0.49
12:l:7:ASP:O	12:l:21:GLN:NE2	2.42	0.49
12:l:47:VAL:HG12	12:l:195:LEU:HD22	1.95	0.49
4:D:52:GLU:HG2	21:U:596:ASN:HD21	1.76	0.49
4:D:338:ARG:HH21	24:X:201:TYR:HA	1.78	0.49
3:C:184:LYS:N	3:C:312:ASP:OD2	2.44	0.49
4:D:126:PRO:O	4:D:127:ASN:C	2.56	0.49
27:a:89:ASP:HB3	27:a:92:VAL:HG22	1.95	0.49
8:h:175:GLU:OE2	9:i:53:HIS:NE2	2.40	0.49
13:m:93:GLU:OE2	13:m:97:ASN:ND2	2.41	0.49
1:A:75:PRO:HA	1:A:78:TRP:NE1	2.28	0.48
17:Q:197:PRO:HD2	17:q:199:GLN:H	1.78	0.48
18:R:179:VAL:HG22	18:R:184:TRP:HB3	1.95	0.48
24:X:73:VAL:O	24:X:77:LEU:N	2.46	0.48
28:b:84:ILE:HD12	28:b:115:SER:HB2	1.94	0.48
28:b:180:ALA:HA	28:b:183:LEU:HB2	1.95	0.48
30:d:164:THR:HA	30:d:167:ILE:HG12	1.95	0.48
7:g:158:GLY:O	8:h:84:ARG:NH2	2.46	0.48
19:s:95:ILE:O	19:s:98:SER:OG	2.29	0.48
16:P:142:CYS:HB2	16:P:145:GLN:HE21	1.77	0.48
21:U:161:ASP:OD1	21:U:161:ASP:N	2.44	0.48
22:V:150:ARG:NH1	22:V:157:THR:O	2.47	0.48
28:b:22:LEU:HB2	28:b:23:PRO:HD3	1.93	0.48
28:b:124:LEU:HD13	28:b:156:PHE:HB2	1.94	0.48
30:d:200:PHE:HB3	30:d:203:PRO:HD3	1.96	0.48
20:T:54:SER:OG	20:T:55:GLY:N	2.46	0.48
21:U:423:MET:HE1	21:U:442:GLY:HA3	1.95	0.48
22:V:177:ASN:O	22:V:179:LYS:NZ	2.46	0.48
32:f:755:ASP:OD2	32:f:758:ASN:ND2	2.36	0.48
16:p:12:MET:HE1	16:p:14:MET:HE3	1.95	0.48
11:K:203:LYS:HB2	11:K:210:LEU:HD22	1.95	0.48
12:L:212:ILE:HB	12:L:224:TYR:HB2	1.95	0.48
13:M:8:ASP:HB2	13:M:25:TYR:HE2	1.78	0.48
14:N:127:ILE:HD11	14:N:136:TYR:CD1	2.48	0.48
26:Z:267:ARG:HA	26:Z:270:VAL:HG12	1.94	0.48
28:b:139:ASP:OD1	28:b:169:HIS:N	2.44	0.48
30:d:140:GLU:HG3	30:d:144:MET:HE2	1.95	0.48
30:d:158:ILE:HG21	30:d:162:SER:HA	1.95	0.48
32:f:560:LEU:O	32:f:564:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:ASP:OD1	2:B:388:ASP:N	2.47	0.48
4:D:296:MET:HE1	4:D:326:ARG:HB3	1.94	0.48
6:F:96:LEU:HD12	6:F:145:LEU:HD22	1.94	0.48
21:U:725:MET:HE3	29:c:181:LEU:HG	1.94	0.48
32:f:393:ASP:OD1	32:f:393:ASP:N	2.46	0.48
4:D:124:LEU:C	4:D:126:PRO:HD2	2.38	0.48
21:U:8:ILE:HD12	21:U:27:LEU:HB3	1.94	0.48
21:U:35:TRP:HB2	22:V:273:LYS:HZ3	1.77	0.48
22:V:282:ASN:OD1	25:Y:385:ARG:NH2	2.46	0.48
24:X:365:LEU:O	24:X:369:ILE:HG22	2.13	0.48
12:l:47:VAL:HG22	12:l:212:ILE:HG12	1.96	0.48
1:A:252:GLU:OE2	1:A:255:ARG:NH2	2.46	0.48
4:D:276:ASP:N	4:D:282:ASP:OD2	2.44	0.48
11:K:235:GLU:HA	11:K:238:ILE:HG12	1.96	0.48
12:L:176:MET:HE1	13:M:56:LYS:HB3	1.96	0.48
19:S:52:ILE:HD11	19:S:108:ASN:HD21	1.77	0.48
21:U:678:ASP:O	21:U:684:ARG:NH1	2.40	0.48
27:a:54:ASP:HA	27:a:57:ILE:HG22	1.96	0.48
1:A:189:GLU:O	1:A:193:THR:OG1	2.32	0.48
29:c:146:ASP:OD2	29:c:149:GLN:N	2.40	0.48
29:c:267:PRO:O	29:c:268:GLU:C	2.57	0.48
11:k:77:ALA:HB3	11:k:142:LEU:HB2	1.95	0.48
2:B:376:ASP:OD1	2:B:376:ASP:N	2.47	0.48
3:C:338:LEU:O	25:Y:207:THR:OG1	2.24	0.48
6:F:249:LEU:HD23	6:F:283:ILE:HG22	1.95	0.48
10:J:40:ILE:HD11	10:J:210:VAL:HB	1.96	0.48
11:K:240:ASP:N	11:K:240:ASP:OD1	2.46	0.48
17:Q:181:ARG:HG2	17:Q:190:ASP:HA	1.96	0.48
24:X:389:ASP:OD1	24:X:389:ASP:N	2.46	0.48
30:d:175:ARG:HH22	30:d:200:PHE:HE1	1.61	0.48
32:f:414:LEU:HD21	32:f:428:GLN:HE22	1.79	0.48
9:i:90:LEU:HD21	9:i:114:LEU:HD22	1.95	0.48
4:D:53:PHE:CZ	21:U:632:GLN:HB3	2.49	0.48
4:D:89:ILE:HD11	5:E:70:ILE:HD12	1.96	0.48
6:F:175:MET:SD	6:F:249:LEU:HD11	2.53	0.48
7:G:46:ASP:OD1	7:G:46:ASP:N	2.47	0.48
21:U:611:ASN:HB3	21:U:614:VAL:HG12	1.96	0.48
23:W:236:HIS:ND1	23:W:237:GLU:OE2	2.40	0.48
32:f:63:LEU:HD21	32:f:75:LEU:HG	1.96	0.48
2:B:117:ASP:OD1	2:B:117:ASP:N	2.46	0.47
6:F:288:LEU:O	6:F:292:GLY:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:55:ILE:HD12	8:H:55:ILE:H	1.79	0.47
10:J:90:GLU:HG3	10:J:110:TYR:CZ	2.49	0.47
16:P:35:VAL:HG12	16:P:36:THR:HG23	1.95	0.47
33:u:1:MET:CB	33:u:63:LYS:HB2	2.44	0.47
1:A:394:MET:HE3	2:B:349:ARG:HH21	1.77	0.47
3:C:145:ASP:HA	3:C:201:ARG:HG2	1.97	0.47
6:F:376:SER:HB3	6:F:414:GLU:HG3	1.95	0.47
10:J:220:LEU:HD13	10:J:224:GLU:HB2	1.95	0.47
12:L:155:ASP:HB3	13:M:62:SER:HB2	1.96	0.47
22:V:430:SER:HB3	22:V:433:ASP:HB3	1.95	0.47
22:V:479:ARG:HB3	26:Z:261:TYR:CE1	2.49	0.47
24:X:67:GLY:HA2	24:X:109:LEU:HD21	1.95	0.47
25:Y:286:TRP:CD1	25:Y:287:LEU:HD12	2.49	0.47
26:Z:62:ASP:OD1	26:Z:62:ASP:N	2.46	0.47
26:Z:144:VAL:HG22	26:Z:152:SER:H	1.78	0.47
30:d:114:GLU:HA	30:d:117:THR:HG22	1.95	0.47
2:B:252:GLY:N	2:B:285:ASP:O	2.44	0.47
9:I:241:GLU:HA	9:I:244:GLU:HG3	1.95	0.47
18:R:122:SER:OG	18:R:123:GLY:N	2.48	0.47
20:T:20:VAL:HG11	20:T:122:LEU:HD13	1.96	0.47
26:Z:170:VAL:HG22	29:c:152:LYS:HA	1.94	0.47
27:a:293:PHE:HB3	27:a:329:LYS:HB3	1.96	0.47
29:c:88:ASP:N	29:c:88:ASP:OD1	2.46	0.47
31:e:33:ASP:OD1	31:e:34:GLU:N	2.45	0.47
32:f:175:ASP:N	32:f:175:ASP:OD1	2.45	0.47
32:f:266:LEU:HD22	32:f:294:MET:HG3	1.95	0.47
7:g:165:ALA:HB3	8:h:56:LEU:HD22	1.96	0.47
3:C:99:VAL:HG12	3:C:123:LEU:HD22	1.96	0.47
3:C:299:ASP:OD1	3:C:299:ASP:N	2.47	0.47
4:D:161:ASP:HA	4:D:221:HIS:CD2	2.49	0.47
18:R:27:ALA:O	16:p:177:ARG:NH1	2.47	0.47
19:S:125:ASP:OD1	19:S:129:SER:N	2.47	0.47
21:U:464:GLN:HG3	21:U:465:LEU:HD12	1.97	0.47
26:Z:26:ILE:HD11	26:Z:35:VAL:HG22	1.95	0.47
30:d:52:ARG:HH11	30:d:82:TYR:HE1	1.62	0.47
30:d:150:LYS:HG3	30:d:153:LEU:HD12	1.96	0.47
32:f:166:VAL:HG13	32:f:184:LEU:HD22	1.97	0.47
32:f:313:GLU:HG2	32:f:316:ASP:HB2	1.96	0.47
4:D:120:ASP:N	4:D:120:ASP:OD1	2.47	0.47
8:h:3:GLU:OE2	13:m:128:VAL:HG13	2.15	0.47
29:c:189:ILE:O	29:c:193:ILE:HB	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:52:GLN:HB3	8:h:57:TYR:HD2	1.80	0.47
1:A:143:ASP:OD1	1:A:143:ASP:N	2.47	0.47
3:C:25:LEU:HD12	4:D:40:LEU:HD21	1.97	0.47
3:C:175:PHE:O	3:C:179:GLY:N	2.38	0.47
3:C:241:HIS:O	3:C:244:SER:OG	2.29	0.47
4:D:141:ASP:N	4:D:141:ASP:OD1	2.47	0.47
7:G:6:SER:OG	7:G:11:ARG:NH1	2.47	0.47
8:H:9:SER:OG	8:H:123:GLN:O	2.31	0.47
18:R:144:SER:OG	18:R:145:TYR:N	2.48	0.47
21:U:428:PRO:HA	21:U:439:GLU:HB2	1.97	0.47
23:W:177:MET:SD	23:W:181:GLU:HB3	2.55	0.47
24:X:415:TYR:HA	25:Y:383:LEU:HD11	1.96	0.47
27:a:252:LYS:HA	27:a:255:TRP:HE3	1.80	0.47
30:d:248:GLU:HA	30:d:251:ARG:HG2	1.96	0.47
8:h:11:THR:HG22	8:h:19:LEU:HD22	1.97	0.47
13:m:67:PHE:HB2	13:m:75:MET:HB3	1.96	0.47
16:p:30:ILE:HG22	16:p:31:GLN:H	1.80	0.47
1:A:430:MET:HE3	10:J:12:PRO:HB3	1.97	0.47
2:B:145:GLU:HG2	2:B:148:CYS:HB2	1.97	0.47
5:E:126:ASP:HB2	5:E:197:LYS:HE3	1.96	0.47
8:H:166:ASN:HD22	8:H:198:SER:HB3	1.79	0.47
12:L:41:LYS:O	12:L:217:LYS:NZ	2.47	0.47
23:W:177:MET:O	23:W:182:ARG:NH2	2.47	0.47
24:X:419:LYS:HZ1	25:Y:386:VAL:HG11	1.80	0.47
32:f:474:SER:O	32:f:478:ARG:HB2	2.15	0.47
13:m:71:ARG:HH21	13:m:105:ASN:HD21	1.63	0.47
6:F:358:ASN:O	6:F:362:ARG:NH1	2.48	0.47
8:H:213:CYS:HB2	8:H:218:PHE:HD1	1.79	0.47
11:K:221:GLN:HB2	11:K:224:GLN:HG3	1.96	0.47
15:O:26:VAL:O	19:s:185:ARG:NH1	2.43	0.47
24:X:58:ALA:HA	24:X:99:MET:HG3	1.97	0.47
33:u:1:MET:CG	33:u:63:LYS:CB	2.91	0.47
8:H:119:GLN:NE2	9:I:82:ASP:OD1	2.48	0.47
16:P:203:ARG:NH2	16:P:205:ASP:OD2	2.42	0.47
32:f:153:SER:HG	32:f:154:TRP:CD1	2.32	0.47
8:h:123:GLN:OE1	9:i:128:ARG:NE	2.48	0.47
18:R:192:VAL:HG11	16:p:205:ASP:HB3	1.95	0.46
21:U:3:THR:O	22:V:266:GLN:NE2	2.48	0.46
21:U:772:TRP:CD1	21:U:775:LEU:HB2	2.51	0.46
22:V:477:HIS:ND1	30:d:249:TYR:OH	2.48	0.46
23:W:147:LYS:HB2	23:W:185:PHE:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:332:GLN:HE22	25:Y:336:ARG:HH21	1.63	0.46
28:b:7:MET:HG3	28:b:97:LEU:HD11	1.97	0.46
28:b:26:LEU:HD11	28:b:80:PRO:HG3	1.97	0.46
9:i:123:GLN:HA	10:j:125:ARG:HE	1.79	0.46
5:E:4:PRO:HG2	5:E:7:LYS:HB3	1.98	0.46
23:W:194:LEU:HG	23:W:202:THR:HG21	1.97	0.46
24:X:187:ARG:HH21	24:X:217:ILE:HG22	1.81	0.46
27:a:214:GLY:HA2	27:a:217:LEU:HD13	1.98	0.46
28:b:1:MET:N	28:b:43:SER:O	2.35	0.46
29:c:279:ASP:HB2	29:c:283:HIS:HB2	1.96	0.46
30:d:4:GLN:OE1	30:d:18:LYS:NZ	2.49	0.46
4:D:200:ARG:HH22	4:D:301:GLN:HA	1.80	0.46
5:E:72:LYS:HB2	5:E:78:ARG:HG2	1.97	0.46
6:F:168:TYR:HB3	6:F:173:LYS:HE3	1.96	0.46
17:Q:27:GLN:O	17:q:170:ARG:NH1	2.44	0.46
22:V:215:ALA:O	22:V:219:GLU:HG3	2.15	0.46
26:Z:70:LEU:HD11	26:Z:108:ILE:HG23	1.98	0.46
29:c:98:MET:HA	29:c:101:GLN:HG2	1.97	0.46
30:d:170:LEU:HA	30:d:173:THR:HG22	1.97	0.46
32:f:188:VAL:HG21	32:f:211:ILE:HD12	1.96	0.46
9:i:143:TYR:HB2	9:i:146:GLN:HE21	1.81	0.46
4:D:363:TYR:HE2	4:D:399:PHE:HB3	1.79	0.46
7:G:191:PHE:HE1	7:G:219:VAL:HG11	1.80	0.46
23:W:212:LYS:HD3	23:W:215:GLN:HE22	1.79	0.46
32:f:228:LYS:HZ3	32:f:856:ALA:HA	1.80	0.46
33:u:54:ARG:NH2	33:u:58:ASP:HB3	2.30	0.46
5:E:236:ASP:OD2	5:E:279:THR:OG1	2.31	0.46
21:U:636:VAL:HG23	21:U:637:VAL:HG23	1.98	0.46
22:V:95:LEU:O	22:V:99:ARG:HB2	2.14	0.46
25:Y:238:GLU:HA	25:Y:242:LYS:HB2	1.97	0.46
27:a:286:ALA:HA	27:a:289:ARG:HB3	1.98	0.46
7:g:10:ASP:OD1	7:g:10:ASP:N	2.47	0.46
16:p:27:ARG:HB2	16:p:183:MET:HB2	1.96	0.46
2:B:223:ILE:HG13	2:B:329:MET:HB3	1.98	0.46
4:D:45:LYS:HB3	21:U:187:LEU:HD13	1.97	0.46
7:G:51:VAL:HG23	7:G:217:VAL:HG22	1.97	0.46
26:Z:187:LEU:HB3	29:c:293:THR:HG22	1.97	0.46
26:Z:234:PHE:HA	26:Z:237:LEU:HD23	1.97	0.46
29:c:131:GLN:HA	29:c:134:GLU:HB2	1.98	0.46
29:c:150:SER:HB3	29:c:156:VAL:HG22	1.98	0.46
30:d:23:LEU:HG	30:d:27:LYS:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:222:THR:HG23	8:h:225:GLU:H	1.81	0.46
2:B:68:ILE:HA	32:f:670:MET:HE3	1.97	0.46
21:U:172:ASP:OD1	21:U:172:ASP:N	2.48	0.46
24:X:173:GLU:HA	24:X:176:THR:HG22	1.97	0.46
26:Z:69:PHE:HE1	28:b:60:VAL:HG11	1.81	0.46
32:f:348:ILE:HD13	32:f:381:VAL:HG21	1.96	0.46
19:s:145:LEU:HD22	19:s:178:VAL:HB	1.97	0.46
1:A:124:ASP:HB2	6:F:86:LEU:HD22	1.97	0.46
23:W:198:ASP:O	23:W:202:THR:OG1	2.31	0.46
24:X:12:ALA:HB2	24:X:26:ILE:HG21	1.97	0.46
25:Y:233:ARG:HH21	25:Y:264:TYR:HA	1.81	0.46
26:Z:223:ASN:OD1	26:Z:223:ASN:N	2.49	0.46
27:a:324:ILE:HG13	27:a:331:VAL:HG13	1.98	0.46
28:b:161:ASN:HB2	28:b:166:THR:H	1.78	0.46
29:c:149:GLN:HB2	29:c:156:VAL:HG21	1.98	0.46
5:E:196:LEU:HD21	5:E:221:TYR:HE2	1.81	0.46
6:F:153:VAL:HA	6:F:160:ILE:HA	1.98	0.46
26:Z:138:TYR:HB3	26:Z:155:PHE:HB3	1.98	0.46
12:l:72:ILE:HG22	12:l:134:ILE:HG12	1.98	0.46
16:p:178:ASP:HB3	16:p:181:SER:HB2	1.98	0.46
4:D:177:VAL:HG11	4:D:215:LEU:HD21	1.97	0.46
6:F:289:ASP:OD1	6:F:289:ASP:N	2.47	0.46
21:U:469:SER:OG	21:U:470:ASN:N	2.48	0.46
23:W:50:LEU:HD23	23:W:53:GLN:HE22	1.80	0.46
23:W:205:ILE:HA	23:W:208:LYS:HE3	1.98	0.46
28:b:91:ARG:HG2	28:b:130:ARG:HH12	1.80	0.46
16:p:193:ASP:OD1	16:p:193:ASP:N	2.48	0.46
2:B:168:ASP:OD2	2:B:171:VAL:HG23	2.16	0.45
12:L:215:VAL:HB	12:L:221:PHE:HD1	1.81	0.45
19:s:12:ILE:HG13	19:s:109:ILE:HD12	1.97	0.45
3:C:218:GLU:O	4:D:286:GLN:NE2	2.49	0.45
11:K:41:GLN:NE2	11:K:151:PRO:O	2.50	0.45
21:U:337:LEU:HD23	21:U:911:ILE:HD12	1.97	0.45
22:V:345:ARG:NE	31:e:42:ASN:O	2.49	0.45
24:X:200:ILE:HD13	24:X:203:PRO:HB3	1.99	0.45
17:q:38:MET:O	17:q:65:GLN:NE2	2.45	0.45
5:E:121:ASN:OD1	6:F:146:LYS:NZ	2.36	0.45
19:S:16:ALA:HB2	19:S:121:VAL:HG23	1.97	0.45
21:U:388:ASP:OD1	21:U:388:ASP:N	2.46	0.45
25:Y:102:ASP:HA	25:Y:105:MET:HG2	1.99	0.45
25:Y:241:ILE:HG12	25:Y:261:PHE:HE1	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:292:MET:O	29:c:296:ILE:HG12	2.16	0.45
32:f:116:GLY:H	32:f:119:LYS:HB3	1.81	0.45
9:i:38:LEU:HD23	9:i:160:LYS:HG2	1.98	0.45
16:p:159:ASP:OD1	16:p:159:ASP:N	2.40	0.45
3:C:37:ASP:OD1	3:C:37:ASP:N	2.50	0.45
8:H:119:GLN:O	8:H:122:THR:OG1	2.31	0.45
21:U:701:ILE:HG21	21:U:810:THR:HG22	1.98	0.45
32:f:345:PRO:HA	32:f:348:ILE:HD12	1.97	0.45
2:B:140:ASP:O	2:B:142:ASP:N	2.48	0.45
3:C:66:LEU:O	4:D:114:ARG:NH2	2.48	0.45
5:E:60:VAL:HA	5:E:71:VAL:HG12	1.97	0.45
8:H:175:GLU:HG2	9:I:54:LYS:HE2	1.99	0.45
10:J:64:ALA:HA	10:J:70:CYS:HA	1.98	0.45
11:K:117:SER:HB3	11:K:156:MET:HE2	1.99	0.45
11:K:121:LEU:HD12	12:L:79:ALA:HB3	1.99	0.45
13:M:35:THR:HA	13:M:166:GLY:HA3	1.99	0.45
13:M:108:LEU:HD22	13:M:139:SER:HB3	1.99	0.45
14:N:144:ARG:H	14:N:147:MET:HE3	1.81	0.45
19:S:71:ARG:HA	19:S:74:MET:SD	2.57	0.45
22:V:461:LYS:HD2	22:V:461:LYS:HA	1.78	0.45
23:W:79:GLU:HB3	23:W:82:LEU:HB2	1.98	0.45
23:W:375:MET:HA	23:W:378:MET:HE2	1.98	0.45
25:Y:250:LEU:HD21	25:Y:260:LEU:HD12	1.97	0.45
2:B:339:PRO:HA	2:B:342:ILE:HG12	1.98	0.45
22:V:294:ARG:HH12	22:V:391:THR:HG22	1.82	0.45
22:V:366:ALA:HA	22:V:374:LYS:HE3	1.99	0.45
30:d:224:SER:OG	30:d:225:PHE:N	2.50	0.45
1:A:73:ALA:HA	2:B:140:ASP:HB3	1.99	0.45
2:B:120:HIS:HA	2:B:134:SER:HA	1.98	0.45
3:C:151:ILE:HG21	3:C:158:ILE:HD11	1.97	0.45
10:J:159:ASN:OD1	10:J:160:ALA:N	2.49	0.45
19:S:213:ASP:OD2	15:o:19:ARG:NH2	2.50	0.45
21:U:27:LEU:HA	21:U:30:VAL:HG22	1.98	0.45
21:U:68:PHE:HB3	21:U:73:ALA:HB3	1.99	0.45
8:h:124:SER:OG	8:h:125:GLY:N	2.49	0.45
16:p:123:SER:HB3	16:p:137:VAL:HB	1.98	0.45
2:B:231:GLY:N	35:B:501:ATP:O2B	2.50	0.45
21:U:744:VAL:HA	21:U:785:PRO:HA	1.98	0.45
23:W:137:TYR:HD1	23:W:138:VAL:HG13	1.82	0.45
24:X:342:PHE:HZ	24:X:350:ILE:HD13	1.80	0.45
32:f:539:LEU:HB2	32:f:576:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:597:VAL:HG11	32:f:656:GLY:HA3	1.99	0.45
32:f:809:ILE:HG23	32:f:814:SER:HB2	1.98	0.45
16:p:67:LEU:HD11	16:p:91:VAL:HG22	1.99	0.45
1:A:220:THR:N	35:A:501:ATP:O1B	2.44	0.45
2:B:170:LEU:HD13	2:B:174:MET:HE1	1.99	0.45
4:D:124:LEU:HD11	4:D:142:VAL:HG12	1.99	0.45
5:E:360:ASP:N	5:E:360:ASP:OD1	2.49	0.45
7:G:67:THR:HG22	7:G:69:LEU:H	1.82	0.45
12:L:34:ALA:HA	12:L:162:GLY:HA3	1.99	0.45
17:Q:28:MET:HB3	18:R:126:PHE:HE1	1.82	0.45
20:T:53:ALA:HB2	20:T:110:MET:HG3	1.99	0.45
25:Y:350:VAL:HG23	25:Y:351:ASN:H	1.82	0.45
28:b:67:ASP:OD1	28:b:67:ASP:N	2.49	0.45
32:f:668:ALA:HA	32:f:697:ILE:HD11	1.98	0.45
7:g:46:ASP:O	7:g:221:THR:OG1	2.33	0.45
10:j:188:ILE:HD12	10:j:208:LEU:HD21	1.99	0.45
11:k:73:HIS:CD2	11:k:74:ILE:HG13	2.51	0.45
1:A:100:LYS:O	1:A:114:ASN:N	2.50	0.45
2:B:387:LYS:HE2	2:B:427:LEU:HD13	1.99	0.45
3:C:119:ASP:OD1	3:C:119:ASP:N	2.49	0.45
17:Q:137:PHE:HB3	18:r:133:VAL:HG21	1.98	0.45
21:U:413:LYS:HD2	21:U:780:SER:HB2	1.98	0.45
26:Z:61:ASP:OD2	28:b:91:ARG:NH2	2.50	0.45
27:a:77:VAL:HA	27:a:80:ILE:HG22	1.98	0.45
27:a:370:GLN:HG3	30:d:251:ARG:HH22	1.82	0.45
14:n:160:LEU:O	14:n:164:MET:HG2	2.17	0.45
20:t:50:MET:HE3	20:t:192:VAL:HB	1.99	0.45
4:D:45:LYS:HD2	21:U:187:LEU:HD22	1.99	0.44
5:E:219:PHE:HD2	5:E:263:GLN:HB3	1.82	0.44
6:F:403:ALA:HA	6:F:406:ILE:HD12	1.98	0.44
10:J:204:LYS:HD2	10:J:205:ASN:HB3	1.99	0.44
13:M:134:SER:HB2	13:M:153:PRO:HD3	1.99	0.44
20:T:146:ALA:HB1	20:T:172:CYS:HB3	1.99	0.44
24:X:161:ASP:OD1	24:X:161:ASP:N	2.43	0.44
13:m:203:GLU:HG2	13:m:204:VAL:HG13	1.99	0.44
16:p:67:LEU:HD21	16:p:87:LEU:HD11	1.99	0.44
19:s:125:ASP:OD1	19:s:129:SER:N	2.49	0.44
3:C:63:LEU:HD21	4:D:79:VAL:HA	1.99	0.44
3:C:325:ARG:NH2	3:C:348:ALA:O	2.49	0.44
6:F:189:GLY:HA3	6:F:364:ARG:HG2	1.98	0.44
10:J:189:LYS:HA	10:J:232:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:444:HIS:CD2	26:Z:208:ILE:HD12	2.53	0.44
29:c:266:THR:O	29:c:267:PRO:C	2.60	0.44
9:i:34:CYS:HG	9:i:75:SER:HG	1.58	0.44
6:F:91:SER:HA	6:F:126:THR:HA	1.98	0.44
20:T:92:LEU:HD23	20:T:92:LEU:HA	1.84	0.44
27:a:163:TYR:CD1	27:a:172:TYR:HB2	2.52	0.44
10:j:179:GLU:HA	10:j:182:GLU:HB2	1.98	0.44
34:v:24:UNK:O	34:v:26:UNK:N	2.50	0.44
1:A:210:LYS:NZ	1:A:313:GLY:O	2.46	0.44
6:F:119:GLY:O	6:F:120:LYS:C	2.59	0.44
11:K:116:VAL:HB	11:K:156:MET:HE1	1.99	0.44
12:L:47:VAL:HG12	12:L:195:LEU:HD22	2.00	0.44
14:N:95:MET:HE3	14:N:116:MET:HE1	1.99	0.44
16:P:74:TYR:CZ	16:P:78:GLU:HG3	2.52	0.44
19:S:68:ILE:HD11	19:S:92:LEU:HD13	1.99	0.44
25:Y:39:ASP:HA	25:Y:42:MET:HE2	2.00	0.44
25:Y:279:GLU:HB2	25:Y:295:TYR:HE2	1.82	0.44
19:s:13:LEU:HD13	19:s:137:ALA:HB2	1.98	0.44
33:u:26:VAL:HA	33:u:29:LYS:HE2	1.98	0.44
1:A:142:VAL:HG22	1:A:149:ILE:HA	1.99	0.44
3:C:240:GLU:OE1	3:C:241:HIS:NE2	2.50	0.44
17:Q:31:ASP:OD1	17:Q:31:ASP:N	2.49	0.44
25:Y:50:MET:HE3	25:Y:53:TYR:HD2	1.83	0.44
25:Y:301:ILE:HG21	25:Y:342:ARG:HD3	1.99	0.44
30:d:168:ASP:OD1	30:d:169:ILE:N	2.50	0.44
30:d:200:PHE:HB3	30:d:203:PRO:HG3	1.99	0.44
31:e:45:ASP:OD1	31:e:45:ASP:N	2.49	0.44
32:f:447:ALA:HA	32:f:450:ILE:HD12	1.99	0.44
32:f:589:SER:HB3	32:f:649:HIS:CE1	2.53	0.44
1:A:146:LYS:HD3	1:A:148:GLN:HG2	2.00	0.44
1:A:234:ASP:OD1	1:A:234:ASP:N	2.50	0.44
18:R:182:ASP:OD1	18:R:182:ASP:N	2.50	0.44
23:W:167:GLN:O	23:W:201:ARG:NH2	2.51	0.44
23:W:339:ASP:OD1	23:W:339:ASP:N	2.50	0.44
30:d:218:GLY:HA3	30:d:223:TYR:HE2	1.81	0.44
13:m:39:ILE:HD11	13:m:176:ILE:HG12	2.00	0.44
13:m:66:LEU:HD12	13:m:212:GLU:HG2	2.00	0.44
13:m:230:ASP:OD1	13:m:230:ASP:N	2.50	0.44
6:F:94:ILE:HD11	6:F:125:LYS:HB2	1.99	0.44
10:J:2:SER:OG	10:J:3:TYR:N	2.50	0.44
10:J:71:MET:HE1	10:J:73:PHE:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:20:ARG:NH2	11:K:22:PHE:HA	2.33	0.44
12:L:53:GLN:HE21	12:L:53:GLN:HB2	1.61	0.44
12:L:157:ARG:NE	13:M:59:GLU:OE2	2.49	0.44
14:N:179:ILE:HG12	14:N:184:VAL:HG22	2.00	0.44
16:P:176:ASP:OD2	19:s:157:ASN:ND2	2.42	0.44
16:P:193:ASP:OD1	16:P:193:ASP:N	2.51	0.44
24:X:28:HIS:CE1	24:X:53:LEU:HD11	2.53	0.44
26:Z:260:VAL:HA	29:c:292:MET:HE1	2.00	0.44
28:b:152:LYS:HA	28:b:155:ALA:HB3	1.99	0.44
29:c:198:ARG:O	29:c:199:HIS:HB2	2.18	0.44
32:f:233:LEU:HD22	32:f:248:LEU:HB2	1.99	0.44
10:J:31:THR:OG1	10:J:163:ARG:O	2.29	0.44
20:T:15:LYS:HE2	20:T:135:PRO:HA	2.00	0.44
23:W:371:THR:HG23	23:W:416:GLN:HG2	1.99	0.44
24:X:74:ARG:HH12	24:X:113:CYS:HA	1.82	0.44
24:X:122:ARG:HE	24:X:122:ARG:HB2	1.53	0.44
27:a:15:GLY:O	27:a:18:GLN:NE2	2.48	0.44
10:j:39:ASP:OD1	10:j:39:ASP:N	2.50	0.44
3:C:268:GLU:O	3:C:272:THR:OG1	2.27	0.44
5:E:139:SER:HA	5:E:142:ILE:HD12	2.00	0.44
6:F:38:THR:HG22	6:F:39:GLU:HG2	2.00	0.44
14:N:166:ARG:NH2	14:n:140:ASP:OD2	2.40	0.44
21:U:751:ARG:HH21	21:U:908:ILE:HD13	1.83	0.44
23:W:455:LEU:HB2	23:W:456:GLN:NE2	2.33	0.44
25:Y:350:VAL:HG23	25:Y:351:ASN:N	2.33	0.44
12:l:49:LEU:HG	12:l:195:LEU:HD21	2.00	0.44
6:F:96:LEU:HD11	6:F:142:ALA:HB1	1.99	0.43
8:H:19:LEU:HB2	8:H:22:ILE:HG12	1.99	0.43
10:J:5:ARG:O	10:J:123:GLY:N	2.51	0.43
21:U:474:ARG:NH2	21:U:500:ASN:OD1	2.51	0.43
22:V:397:ARG:HE	30:d:116:HIS:CD2	2.36	0.43
22:V:467:TYR:HD2	25:Y:362:LYS:HZ3	1.65	0.43
24:X:258:LYS:HD3	24:X:266:ASP:HB2	1.99	0.43
31:e:37:HIS:HD2	31:e:39:TRP:H	1.65	0.43
32:f:836:GLU:OE1	32:f:838:ARG:NH2	2.51	0.43
2:B:90:GLU:H	2:B:94:GLU:HB3	1.83	0.43
3:C:125:LYS:HZ2	4:D:96:VAL:HG11	1.83	0.43
3:C:134:LEU:O	3:C:137:LEU:N	2.51	0.43
5:E:385:ASP:O	5:E:386:TYR:CB	2.66	0.43
14:N:166:ARG:NH1	20:t:34:ALA:O	2.47	0.43
22:V:81:GLN:HB3	22:V:93:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:89:VAL:HG12	24:X:93:LEU:HD23	2.00	0.43
7:g:58:ASP:OD1	7:g:58:ASP:N	2.50	0.43
12:l:10:VAL:HG13	12:l:11:THR:HG23	1.99	0.43
7:G:10:ASP:OD1	7:G:10:ASP:N	2.50	0.43
10:J:136:PHE:HD2	10:J:211:MET:HE2	1.83	0.43
25:Y:68:ASP:OD1	25:Y:68:ASP:N	2.50	0.43
29:c:269:GLN:HA	29:c:272:ILE:HG22	2.00	0.43
33:u:24:GLU:HB3	33:u:52:ASP:HB3	2.00	0.43
7:G:206:LEU:HB3	7:G:208:ILE:HG23	2.01	0.43
16:P:65:GLN:OE1	17:Q:86:ARG:NH2	2.50	0.43
22:V:365:GLN:HE22	22:V:374:LYS:HD2	1.84	0.43
23:W:230:MET:HE3	23:W:230:MET:HB3	1.88	0.43
25:Y:184:GLN:HB3	25:Y:200:LEU:HD13	1.99	0.43
32:f:65:GLU:O	32:f:66:LYS:C	2.61	0.43
16:p:134:ASP:OD1	16:p:134:ASP:N	2.50	0.43
17:q:19:ARG:HD2	17:q:179:SER:HB3	1.99	0.43
17:q:25:ILE:HG23	17:q:26:VAL:HG22	1.99	0.43
2:B:288:ASP:OD2	2:B:333:ARG:NE	2.44	0.43
4:D:184:PRO:HG3	4:D:191:TYR:CZ	2.53	0.43
5:E:101:ASP:HB3	5:E:106:THR:H	1.82	0.43
16:P:70:ARG:HD2	16:P:94:LEU:HD12	2.00	0.43
20:T:92:LEU:HD12	20:T:112:ILE:HD11	2.00	0.43
21:U:8:ILE:HA	21:U:11:LEU:HD12	2.00	0.43
24:X:296:ASN:O	24:X:337:ARG:NH1	2.52	0.43
32:f:894:LEU:HA	32:f:898:VAL:HG21	1.99	0.43
15:o:54:MET:HG3	16:p:96:TYR:CZ	2.53	0.43
7:G:196:GLU:O	7:G:200:THR:OG1	2.21	0.43
11:K:51:GLU:HB2	11:K:206:MET:HE3	2.01	0.43
32:f:426:LEU:HA	32:f:429:ILE:HG22	1.99	0.43
32:f:559:PRO:HG2	32:f:594:LEU:HD23	2.01	0.43
8:H:179:ASN:OD1	8:H:179:ASN:N	2.52	0.43
13:M:68:ASN:OD1	13:M:224:HIS:ND1	2.51	0.43
20:T:43:MET:HB3	20:T:51:LEU:HB3	2.00	0.43
21:U:326:ILE:O	21:U:330:SER:OG	2.32	0.43
21:U:443:LEU:HD22	21:U:464:GLN:HE22	1.84	0.43
21:U:586:VAL:HG13	21:U:602:LEU:HD12	2.00	0.43
25:Y:74:LYS:HD2	25:Y:74:LYS:HA	1.85	0.43
25:Y:113:ARG:HD2	25:Y:113:ARG:HA	1.83	0.43
25:Y:155:ASP:N	25:Y:155:ASP:OD1	2.52	0.43
27:a:7:PHE:HE2	27:a:60:TYR:HB2	1.84	0.43
32:f:659:LEU:HD13	32:f:797:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:147:MET:HB3	14:n:152:CYS:SG	2.59	0.43
1:A:115:VAL:HG21	1:A:118:PHE:HB2	2.00	0.43
4:D:194:ILE:HG22	4:D:196:ILE:HG23	2.01	0.43
6:F:114:ASP:OD1	6:F:114:ASP:N	2.43	0.43
18:R:141:ARG:HH21	17:q:162:LYS:HE2	1.83	0.43
19:S:159:GLN:NE2	15:o:207:GLY:O	2.52	0.43
22:V:228:ARG:NH2	22:V:257:ASN:O	2.47	0.43
32:f:763:ARG:NH1	32:f:766:GLN:OE1	2.49	0.43
9:i:119:GLN:NE2	10:j:79:ASP:OD1	2.52	0.43
10:j:185:ASP:O	10:j:189:LYS:HG2	2.18	0.43
19:s:37:THR:OG1	19:s:39:ASP:OD1	2.36	0.43
33:u:31:GLN:OE1	33:u:38:PRO:HD3	2.19	0.43
5:E:180:LYS:HG2	5:E:301:ILE:HD12	2.00	0.43
11:K:38:ILE:HD12	11:K:202:LEU:HG	2.00	0.43
21:U:111:GLN:NE2	21:U:114:GLU:OE1	2.52	0.43
21:U:710:ARG:HE	21:U:737:LEU:HD23	1.83	0.43
29:c:150:SER:HB2	29:c:155:VAL:HA	2.00	0.43
13:m:136:MET:HE2	13:m:136:MET:HB3	1.85	0.43
13:m:213:LEU:HB2	13:m:227:VAL:HG21	2.00	0.43
18:r:35:ILE:N	18:r:43:GLY:O	2.52	0.43
20:t:107:TRP:CE2	20:t:127:MET:HE1	2.54	0.43
33:u:54:ARG:HG2	33:u:54:ARG:HH11	1.83	0.43
1:A:171:ASP:OD1	1:A:171:ASP:N	2.50	0.43
1:A:333:ARG:HH21	1:A:336:ARG:CZ	2.32	0.43
6:F:265:ALA:HB1	6:F:312:GLU:OE1	2.18	0.43
10:J:42:VAL:HG22	10:J:210:VAL:HG12	2.00	0.43
14:N:46:SER:OG	14:N:97:GLY:O	2.35	0.43
32:f:93:PRO:HB2	32:f:96:LEU:HD23	2.00	0.43
32:f:293:GLN:HE22	32:f:899:ILE:HB	1.83	0.43
32:f:320:ILE:HA	32:f:325:GLN:HE22	1.83	0.43
7:g:165:ALA:HB1	7:g:179:LEU:HD13	2.00	0.43
19:s:44:TYR:HB2	19:s:52:ILE:HG22	2.00	0.43
1:A:214:LEU:HD12	1:A:343:PHE:CE2	2.53	0.42
2:B:221:GLY:HA3	2:B:347:ILE:HA	2.00	0.42
4:D:376:ASN:ND2	35:D:501:ATP:O2'	2.40	0.42
5:E:117:PRO:HD3	6:F:94:ILE:HG23	2.01	0.42
13:M:33:SER:OG	13:M:34:SER:N	2.52	0.42
21:U:545:LEU:HB3	21:U:577:ILE:HG21	2.01	0.42
21:U:879:ASP:OD1	21:U:879:ASP:N	2.50	0.42
29:c:187:PRO:HB3	29:c:196:LEU:CG	2.48	0.42
29:c:233:ASP:O	29:c:237:HIS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:103:LEU:HD12	30:d:103:LEU:HA	1.87	0.42
32:f:240:VAL:O	32:f:245:ASN:ND2	2.48	0.42
8:h:203:MET:HE2	8:h:203:MET:HB3	1.90	0.42
11:k:31:ILE:HD11	11:k:158:PRO:HD2	2.01	0.42
2:B:318:GLY:H	2:B:322:ARG:HH21	1.67	0.42
6:F:120:LYS:NZ	6:F:120:LYS:H	2.17	0.42
7:G:188:ASP:OD1	7:G:188:ASP:N	2.53	0.42
9:I:76:VAL:HG11	9:I:83:ALA:HB1	2.00	0.42
22:V:218:TYR:HD2	22:V:227:VAL:HG22	1.84	0.42
23:W:214:PHE:CZ	23:W:223:LYS:HA	2.54	0.42
24:X:344:ARG:HG3	24:X:386:ILE:HG12	1.99	0.42
20:t:124:TYR:HB2	20:t:137:LEU:HD13	2.01	0.42
3:C:137:LEU:HD12	3:C:223:PHE:HB2	2.01	0.42
4:D:94:GLU:HG2	4:D:102:ILE:HD13	2.02	0.42
19:S:172:MET:HE1	19:S:195:ILE:HG21	2.01	0.42
21:U:126:ILE:HD12	21:U:130:LEU:HD11	2.01	0.42
25:Y:249:VAL:O	25:Y:253:LEU:N	2.52	0.42
25:Y:360:ASP:HB2	25:Y:363:ASN:HB2	2.01	0.42
26:Z:128:PRO:HD2	29:c:215:LYS:NZ	2.33	0.42
26:Z:192:THR:HG22	27:a:375:LEU:HD12	2.01	0.42
27:a:216:LEU:HA	27:a:219:HIS:HB2	2.02	0.42
30:d:103:LEU:HD23	30:d:136:PRO:HB2	2.00	0.42
32:f:833:PHE:HB2	32:f:899:ILE:HG12	2.00	0.42
9:i:14:PRO:HA	10:j:21:TYR:CZ	2.54	0.42
11:k:107:MET:HE3	11:k:107:MET:HB3	1.86	0.42
19:s:145:LEU:HD21	19:s:182:ALA:HB2	2.00	0.42
15:O:89:ARG:HD2	15:O:89:ARG:HA	1.75	0.42
21:U:549:ALA:HB1	21:U:581:SER:HB2	2.01	0.42
24:X:56:LEU:HD23	24:X:56:LEU:HA	1.87	0.42
24:X:299:LEU:N	24:X:334:ASN:OD1	2.52	0.42
29:c:202:SER:OG	29:c:203:ILE:N	2.52	0.42
32:f:364:GLN:O	32:f:365:VAL:C	2.63	0.42
32:f:862:ILE:H	32:f:862:ILE:HG13	1.67	0.42
12:l:107:ARG:NE	20:t:79:ASP:OD2	2.41	0.42
34:v:25:LYS:O	34:v:26:UNK:C	2.67	0.42
6:F:222:GLY:O	6:F:349:ASP:N	2.42	0.42
6:F:256:LEU:HD23	6:F:267:LEU:HD23	2.01	0.42
8:H:39:LYS:HG3	8:H:44:VAL:HG22	2.00	0.42
11:K:85:ALA:HB2	11:K:139:VAL:HG11	2.01	0.42
12:L:45:VAL:HG12	12:L:214:ILE:HG23	2.02	0.42
12:L:140:MET:HE1	20:T:81:HIS:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:19:LEU:HB2	30:d:27:LYS:NZ	2.34	0.42
21:U:39:SER:OG	22:V:273:LYS:NZ	2.40	0.42
21:U:98:GLU:HA	21:U:101:ILE:HG12	2.02	0.42
23:W:272:LEU:HD23	23:W:272:LEU:HA	1.83	0.42
29:c:37:ALA:O	29:c:41:MET:HG2	2.19	0.42
32:f:349:TYR:CE1	32:f:763:ARG:HD2	2.55	0.42
2:B:355:LEU:HD12	2:B:356:PRO:HD2	2.01	0.42
7:G:78:CYS:HB3	7:G:140:LEU:HD23	2.01	0.42
8:H:196:LYS:HE3	8:H:234:ALA:HB2	2.01	0.42
20:T:50:MET:HE2	20:T:197:VAL:HG13	2.02	0.42
21:U:204:ILE:HA	21:U:207:ASN:HB2	2.01	0.42
24:X:251:LEU:HA	24:X:254:MET:HG2	2.01	0.42
31:e:35:ASP:HB3	31:e:37:HIS:ND1	2.35	0.42
32:f:412:ALA:HA	32:f:447:ALA:HB2	2.00	0.42
19:s:4:PRO:HB3	20:t:103:MET:HE1	2.01	0.42
20:t:180:ASP:HB3	20:t:183:SER:HB3	2.01	0.42
2:B:176:VAL:HG21	2:B:247:PHE:HD2	1.85	0.42
4:D:125:LYS:HD3	29:c:275:VAL:HG13	2.01	0.42
5:E:317:ALA:O	5:E:322:LYS:NZ	2.39	0.42
12:L:42:THR:HA	12:L:217:LYS:NZ	2.35	0.42
21:U:188:MET:HG2	21:U:194:ARG:HG3	2.01	0.42
21:U:443:LEU:HD22	21:U:464:GLN:NE2	2.33	0.42
21:U:616:ARG:HH11	21:U:650:TYR:HE2	1.66	0.42
21:U:714:SER:HA	21:U:717:ILE:HG22	2.01	0.42
26:Z:144:VAL:HA	26:Z:152:SER:HB3	2.02	0.42
29:c:106:GLU:O	29:c:107:MET:HE2	2.20	0.42
29:c:187:PRO:HB2	29:c:196:LEU:HG	1.99	0.42
32:f:621:ASP:N	32:f:621:ASP:OD1	2.52	0.42
8:h:52:GLN:HB3	8:h:57:TYR:CD2	2.54	0.42
15:o:79:ALA:HA	15:o:82:MET:HE3	2.02	0.42
3:C:33:LEU:HA	3:C:36:ASN:HD22	1.84	0.42
4:D:338:ARG:NH1	4:D:339:ARG:HB2	2.34	0.42
7:G:158:GLY:O	8:H:84:ARG:NH2	2.53	0.42
12:L:204:ASP:OD1	12:L:204:ASP:N	2.51	0.42
25:Y:101:ARG:HG2	25:Y:105:MET:HE3	2.00	0.42
25:Y:153:ASP:HB3	25:Y:156:LEU:HB3	2.02	0.42
27:a:174:LYS:HG3	27:a:178:ARG:HH12	1.85	0.42
29:c:96:LEU:HD11	33:u:8:LEU:HD22	1.95	0.42
29:c:175:ARG:HD3	29:c:181:LEU:HD11	2.01	0.42
13:m:215:TRP:HE1	13:m:227:VAL:HA	1.85	0.42
1:A:276:GLU:HG2	2:B:310:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:335:LEU:HD23	4:D:369:LYS:HG2	2.02	0.42
5:E:317:ALA:HA	5:E:320:ILE:HD12	2.02	0.42
6:F:105:GLU:OE2	6:F:110:ASN:HA	2.19	0.42
6:F:205:PRO:HG3	6:F:212:PHE:HE2	1.84	0.42
21:U:2:ILE:H	21:U:2:ILE:HG13	1.74	0.42
21:U:620:GLU:HG3	21:U:651:GLY:HA2	2.02	0.42
32:f:466:LEU:HB3	32:f:485:LEU:HB3	2.02	0.42
1:A:306:LEU:O	1:A:312:ARG:NH1	2.50	0.42
2:B:171:VAL:O	2:B:175:LYS:CB	2.68	0.42
9:I:53:HIS:HE1	9:I:55:LEU:HD12	1.85	0.42
21:U:900:TYR:HB3	21:U:914:LEU:HG	2.02	0.42
24:X:18:THR:OG1	24:X:19:ASP:N	2.53	0.42
26:Z:212:LEU:HA	26:Z:215:VAL:HG12	2.01	0.42
27:a:163:TYR:CG	27:a:172:TYR:HB2	2.55	0.42
32:f:534:VAL:HA	32:f:537:THR:HG22	2.01	0.42
32:f:707:LEU:HD22	32:f:729:MET:HG3	2.01	0.42
7:g:137:CYS:SG	7:g:138:MET:N	2.92	0.42
8:h:74:LEU:HD12	8:h:134:LEU:HD22	2.02	0.42
33:u:27:LYS:HB3	33:u:38:PRO:HB3	2.02	0.42
13:M:187:ARG:HH12	13:M:231:ILE:HG12	1.85	0.41
22:V:345:ARG:HH21	31:e:43:TRP:HA	1.84	0.41
25:Y:212:GLU:HG2	25:Y:213:LEU:HD22	2.02	0.41
26:Z:103:LYS:HZ2	26:Z:103:LYS:HG3	1.74	0.41
32:f:170:TRP:CD1	32:f:211:ILE:HA	2.55	0.41
10:j:192:ILE:HG22	10:j:196:LEU:HD23	2.01	0.41
11:k:147:ASP:N	11:k:147:ASP:OD1	2.53	0.41
13:m:215:TRP:CH2	13:m:219:LEU:HD11	2.55	0.41
18:r:97:MET:O	18:r:116:SER:N	2.53	0.41
1:A:300:LEU:HA	1:A:303:ILE:HG22	2.01	0.41
5:E:205:ASP:OD1	5:E:205:ASP:N	2.52	0.41
22:V:90:GLU:HG2	22:V:92:ARG:H	1.84	0.41
27:a:61:GLU:HG3	27:a:79:ILE:HD12	2.02	0.41
27:a:101:ARG:O	27:a:105:LYS:NZ	2.53	0.41
29:c:96:LEU:HD23	29:c:96:LEU:HA	1.87	0.41
30:d:65:ARG:HG3	30:d:67:ASP:HB2	2.02	0.41
32:f:678:LEU:HD22	32:f:686:LEU:HD21	2.02	0.41
10:j:173:GLU:HG2	11:k:58:LEU:HD23	2.03	0.41
1:A:391:GLU:HA	1:A:394:MET:HE2	2.02	0.41
3:C:136:SER:HA	3:C:139:MET:HE3	2.02	0.41
5:E:300:HIS:NE2	5:E:302:ASP:OD1	2.53	0.41
6:F:178:ASP:N	6:F:178:ASP:OD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:25:MET:HE2	9:I:152:PRO:HD2	2.01	0.41
10:J:58:THR:HA	10:J:60:ARG:HH11	1.85	0.41
17:Q:44:LEU:HD11	17:Q:102:LEU:HD22	2.01	0.41
21:U:107:HIS:ND1	21:U:110:LYS:HE3	2.35	0.41
21:U:367:THR:HA	21:U:370:VAL:HG22	2.02	0.41
28:b:26:LEU:HD21	28:b:80:PRO:HG3	2.02	0.41
13:m:223:ARG:NE	13:m:225:GLU:OE2	2.41	0.41
14:n:59:VAL:HG11	14:n:83:PHE:CZ	2.55	0.41
16:p:22:ILE:HG23	16:p:188:HIS:HB2	2.01	0.41
17:q:13:VAL:HG21	17:q:105:ALA:HB1	2.03	0.41
20:T:173:MET:HE1	20:T:187:PHE:CZ	2.56	0.41
21:U:418:GLU:HG2	21:U:422:LEU:HB2	2.03	0.41
23:W:70:VAL:HG22	23:W:73:MET:HE2	2.03	0.41
23:W:146:THR:HG21	23:W:169:LEU:HD21	2.03	0.41
23:W:414:ASN:OD1	23:W:414:ASN:N	2.53	0.41
28:b:30:GLN:HG3	28:b:75:LEU:HD13	2.02	0.41
32:f:806:VAL:HG23	32:f:810:ILE:HB	2.02	0.41
34:v:25:LYS:C	34:v:27:UNK:N	2.77	0.41
1:A:140:VAL:HA	1:A:152:PRO:HA	2.02	0.41
2:B:150:VAL:HG12	2:B:162:VAL:HG23	2.01	0.41
4:D:126:PRO:O	4:D:128:ALA:N	2.54	0.41
4:D:259:PRO:HB3	4:D:304:ASN:HB2	2.01	0.41
25:Y:263:LEU:HB2	25:Y:271:PHE:CE1	2.56	0.41
30:d:41:THR:O	30:d:44:THR:HG22	2.21	0.41
32:f:550:LEU:HD13	32:f:587:PHE:HB2	2.02	0.41
32:f:731:MET:O	32:f:734:SER:OG	2.33	0.41
14:n:70:LEU:HB3	14:n:72:GLU:OE1	2.21	0.41
16:p:47:ASP:OD1	16:p:47:ASP:N	2.51	0.41
18:r:52:CYS:SG	18:r:97:MET:HG2	2.61	0.41
18:r:100:MET:HE2	18:r:111:LEU:HD11	2.02	0.41
5:E:329:GLU:HA	5:E:332:VAL:HG12	2.00	0.41
15:O:138:PHE:O	15:O:142:PHE:HB2	2.20	0.41
21:U:376:MET:HE2	21:U:376:MET:HB3	1.92	0.41
22:V:131:LEU:HD22	22:V:171:VAL:HG11	2.02	0.41
25:Y:14:ASN:HB3	25:Y:143:TYR:HE1	1.85	0.41
29:c:213:GLU:HA	29:c:216:MET:HG3	2.03	0.41
10:j:226:GLU:HA	10:j:229:VAL:HG12	2.02	0.41
14:n:104:ASP:OD1	14:n:104:ASP:N	2.53	0.41
3:C:81:ASP:OD1	3:C:81:ASP:N	2.53	0.41
3:C:327:ASP:N	3:C:327:ASP:OD1	2.51	0.41
5:E:122:MET:HE2	5:E:218:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:161:ALA:HB1	9:I:175:LEU:HD13	2.01	0.41
13:M:43:ASP:OD1	13:M:43:ASP:N	2.54	0.41
13:M:83:ASP:HB3	13:M:131:PHE:HD1	1.85	0.41
20:T:9:THR:OG1	20:T:10:SER:N	2.51	0.41
25:Y:32:ARG:NH2	25:Y:61:LEU:O	2.52	0.41
28:b:93:ALA:O	28:b:97:LEU:HD13	2.20	0.41
19:s:45:LYS:HE3	19:s:203:ILE:HD12	2.03	0.41
2:B:224:LEU:HD21	2:B:235:LEU:HD23	2.03	0.41
2:B:303:ARG:O	2:B:307:ARG:HD3	2.21	0.41
4:D:87:LEU:O	5:E:80:VAL:N	2.49	0.41
21:U:213:PHE:HZ	21:U:244:MET:HG3	1.86	0.41
25:Y:314:LEU:O	25:Y:354:VAL:N	2.51	0.41
26:Z:148:GLY:HA3	27:a:181:GLY:HA3	2.03	0.41
27:a:71:VAL:HG22	28:b:17:ARG:NH1	2.35	0.41
28:b:4:GLU:OE1	28:b:6:THR:OG1	2.29	0.41
32:f:310:ASP:OD1	32:f:310:ASP:N	2.53	0.41
32:f:368:ALA:HB1	32:f:403:LYS:HG3	2.03	0.41
15:o:63:LEU:HA	15:o:63:LEU:HD23	1.90	0.41
17:q:118:MET:HE2	17:q:124:LEU:HD13	2.02	0.41
3:C:246:ILE:HB	3:C:291:VAL:HA	2.03	0.41
5:E:168:LYS:HG2	5:E:270:LEU:HD22	2.02	0.41
5:E:382:SER:HB3	6:F:340:PRO:HG3	2.03	0.41
6:F:175:MET:HE3	6:F:251:LEU:HD13	2.03	0.41
7:G:155:ASP:OD1	7:G:159:TYR:N	2.48	0.41
13:M:171:ALA:HA	13:M:174:THR:HG22	2.03	0.41
14:N:160:LEU:O	14:N:164:MET:HG2	2.20	0.41
16:P:62:THR:OG1	17:Q:85:ARG:NH2	2.54	0.41
16:P:81:GLN:OE1	16:P:114:PRO:HG3	2.21	0.41
21:U:181:LEU:O	21:U:185:MET:HG2	2.20	0.41
22:V:134:PHE:HZ	22:V:186:LYS:HD3	1.86	0.41
22:V:193:GLN:O	22:V:197:THR:OG1	2.35	0.41
22:V:414:TYR:CE2	25:Y:349:LYS:HE3	2.56	0.41
23:W:141:GLU:H	23:W:141:GLU:HG2	1.74	0.41
24:X:408:SER:HA	25:Y:376:LEU:HD11	2.03	0.41
25:Y:17:LEU:HD21	25:Y:213:LEU:HA	2.01	0.41
26:Z:211:TYR:HA	26:Z:214:LYS:HE2	2.01	0.41
27:a:4:VAL:HG23	27:a:5:PRO:HD3	2.02	0.41
28:b:8:VAL:HA	28:b:110:ILE:HG13	2.03	0.41
29:c:54:MET:H	29:c:77:GLN:HE22	1.68	0.41
7:g:49:VAL:HG22	7:g:219:VAL:HG12	2.03	0.41
2:B:71:TYR:HA	2:B:74:MET:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:389:ASP:N	2:B:389:ASP:OD1	2.53	0.41
4:D:150:SER:O	4:D:151:ILE:C	2.63	0.41
5:E:295:LEU:HA	5:E:295:LEU:HD23	1.77	0.41
6:F:415:LEU:HD13	6:F:420:TYR:HE1	1.86	0.41
20:T:65:GLN:HE21	20:T:65:GLN:HB3	1.71	0.41
21:U:494:TYR:OH	21:U:531:ASP:OD2	2.38	0.41
21:U:583:MET:HA	21:U:586:VAL:HG12	2.03	0.41
23:W:101:VAL:HA	23:W:104:MET:HE2	2.02	0.41
23:W:434:SER:OG	23:W:435:LEU:N	2.54	0.41
25:Y:221:THR:HG22	25:Y:256:VAL:HG21	2.03	0.41
27:a:337:GLN:HA	27:a:338:PRO:HD3	1.91	0.41
11:k:129:ASP:OD1	11:k:129:ASP:N	2.53	0.41
12:l:93:LEU:HD23	12:l:93:LEU:HA	1.85	0.41
2:B:284:ILE:HB	2:B:329:MET:SD	2.60	0.40
4:D:219:VAL:O	4:D:223:THR:HB	2.20	0.40
4:D:385:LEU:HD21	4:D:401:LYS:HD2	2.04	0.40
5:E:116:ASP:OD1	5:E:213:ARG:NH1	2.54	0.40
6:F:156:ASP:OD2	6:F:157:SER:N	2.55	0.40
8:H:140:ASN:OD1	8:H:140:ASN:N	2.54	0.40
12:L:132:LEU:HB2	12:L:147:THR:HB	2.02	0.40
13:M:8:ASP:HB3	13:M:21:PHE:HD2	1.86	0.40
21:U:639:LEU:HD12	21:U:639:LEU:HA	1.88	0.40
21:U:749:GLN:HE22	21:U:754:HIS:N	2.20	0.40
22:V:173:ILE:HD13	22:V:173:ILE:HA	1.83	0.40
25:Y:111:LEU:HB3	25:Y:116:ASP:HB3	2.02	0.40
25:Y:300:ARG:HD3	25:Y:337:PHE:CZ	2.56	0.40
28:b:11:ASP:HB3	28:b:16:MET:HE3	2.04	0.40
30:d:45:LYS:O	30:d:49:ILE:HG12	2.20	0.40
32:f:80:ARG:HA	32:f:80:ARG:HD2	1.87	0.40
12:l:71:GLY:HA3	12:l:221:PHE:CZ	2.56	0.40
17:q:11:ASP:OD1	17:q:11:ASP:N	2.53	0.40
17:q:108:ASP:HB3	17:q:111:GLU:HG3	2.03	0.40
2:B:287:ILE:O	2:B:290:ILE:HG22	2.21	0.40
4:D:93:LEU:HD12	4:D:102:ILE:HG22	2.03	0.40
21:U:696:ILE:HD13	21:U:746:ILE:HG12	2.03	0.40
24:X:312:GLU:HG2	24:X:313:LEU:HD22	2.02	0.40
24:X:338:VAL:HG23	24:X:339:ILE:HG13	2.03	0.40
26:Z:81:MET:HB3	29:c:91:PHE:HE1	1.85	0.40
30:d:203:PRO:HG2	30:d:205:LYS:HB2	2.03	0.40
7:g:38:THR:HA	7:g:169:GLY:HA3	2.03	0.40
19:s:19:ASP:N	19:s:19:ASP:OD1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ARG:O	1:A:192:GLU:HG3	2.21	0.40
3:C:187:LEU:HD23	3:C:314:LYS:HD2	2.03	0.40
3:C:277:LEU:O	3:C:281:ASP:HB2	2.22	0.40
4:D:315:ASP:OD1	4:D:315:ASP:N	2.53	0.40
4:D:385:LEU:HD23	4:D:398:ASP:HA	2.03	0.40
7:G:22:LEU:HD23	7:G:22:LEU:HA	1.90	0.40
14:N:119:MET:N	14:N:119:MET:SD	2.84	0.40
20:T:126:ASP:OD1	20:T:130:VAL:N	2.54	0.40
21:U:906:LEU:HD12	21:U:906:LEU:HA	1.92	0.40
26:Z:38:VAL:HB	26:Z:54:PHE:CZ	2.57	0.40
1:A:333:ARG:HH11	6:F:394:ALA:HB2	1.86	0.40
10:J:42:VAL:HG11	10:J:191:VAL:HG21	2.03	0.40
10:J:67:ASP:OD1	10:J:67:ASP:N	2.51	0.40
22:V:349:ARG:NH1	31:e:37:HIS:HE2	2.20	0.40
24:X:157:LEU:HA	24:X:157:LEU:HD23	1.86	0.40
24:X:336:ILE:HD13	24:X:336:ILE:HA	1.96	0.40
32:f:445:LEU:HD11	32:f:466:LEU:HA	2.02	0.40
10:j:18:GLN:OE1	10:j:18:GLN:N	2.53	0.40
3:C:63:LEU:O	3:C:67:GLN:NE2	2.32	0.40
4:D:262:ILE:HB	4:D:307:VAL:HG22	2.04	0.40
4:D:288:ILE:HD13	4:D:288:ILE:HA	1.87	0.40
7:G:70:PHE:HB2	7:G:78:CYS:SG	2.62	0.40
13:M:17:ASP:N	13:M:17:ASP:OD1	2.44	0.40
21:U:126:ILE:HB	21:U:130:LEU:HD21	2.04	0.40
21:U:602:LEU:HD21	21:U:621:SER:HB2	2.03	0.40
24:X:74:ARG:NH2	24:X:116:TRP:HB2	2.37	0.40
7:g:4:GLY:HA3	7:g:19:GLU:OE1	2.21	0.40
17:q:18:ASP:OD1	17:q:18:ASP:N	2.55	0.40
18:r:9:ARG:NH2	18:r:146:ASP:OD1	2.37	0.40
20:t:54:SER:O	20:t:108:ASN:ND2	2.43	0.40
33:u:2:GLN:O	33:u:64:GLU:N	2.54	0.40
33:u:18:GLU:HG3	33:u:19:PRO:HD2	2.02	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	392/433 (90%)	349 (89%)	43 (11%)	0	100	100
2	B	382/440 (87%)	346 (91%)	35 (9%)	1 (0%)	36	70
3	C	359/398 (90%)	328 (91%)	29 (8%)	2 (1%)	21	58
4	D	378/418 (90%)	336 (89%)	38 (10%)	4 (1%)	11	44
5	E	387/403 (96%)	350 (90%)	35 (9%)	2 (0%)	24	61
6	F	413/439 (94%)	377 (91%)	34 (8%)	2 (0%)	24	61
7	G	242/246 (98%)	229 (95%)	13 (5%)	0	100	100
7	g	242/246 (98%)	221 (91%)	19 (8%)	2 (1%)	16	52
8	H	230/234 (98%)	218 (95%)	12 (5%)	0	100	100
8	h	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
9	I	248/261 (95%)	240 (97%)	7 (3%)	1 (0%)	30	65
9	i	248/261 (95%)	242 (98%)	6 (2%)	0	100	100
10	J	237/248 (96%)	225 (95%)	12 (5%)	0	100	100
10	j	237/248 (96%)	224 (94%)	12 (5%)	1 (0%)	30	65
11	K	232/241 (96%)	221 (95%)	10 (4%)	1 (0%)	30	65
11	k	232/241 (96%)	223 (96%)	9 (4%)	0	100	100
12	L	236/263 (90%)	230 (98%)	6 (2%)	0	100	100
12	l	236/263 (90%)	226 (96%)	10 (4%)	0	100	100
13	M	238/255 (93%)	233 (98%)	5 (2%)	0	100	100
13	m	238/255 (93%)	231 (97%)	7 (3%)	0	100	100
14	N	200/239 (84%)	196 (98%)	4 (2%)	0	100	100
14	n	200/239 (84%)	194 (97%)	6 (3%)	0	100	100
15	O	218/277 (79%)	208 (95%)	10 (5%)	0	100	100
15	o	218/277 (79%)	211 (97%)	7 (3%)	0	100	100
16	P	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
16	p	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
17	Q	197/201 (98%)	189 (96%)	8 (4%)	0	100	100
17	q	197/201 (98%)	192 (98%)	5 (2%)	0	100	100
18	R	199/263 (76%)	194 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	r	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
19	S	211/241 (88%)	203 (96%)	8 (4%)	0	100	100
19	s	211/241 (88%)	201 (95%)	10 (5%)	0	100	100
20	T	214/264 (81%)	206 (96%)	8 (4%)	0	100	100
20	t	214/264 (81%)	203 (95%)	11 (5%)	0	100	100
21	U	812/953 (85%)	754 (93%)	58 (7%)	0	100	100
22	V	442/534 (83%)	426 (96%)	15 (3%)	1 (0%)	43	76
23	W	439/456 (96%)	429 (98%)	10 (2%)	0	100	100
24	X	420/422 (100%)	398 (95%)	22 (5%)	0	100	100
25	Y	387/389 (100%)	357 (92%)	29 (8%)	1 (0%)	36	70
26	Z	284/324 (88%)	250 (88%)	34 (12%)	0	100	100
27	a	371/376 (99%)	339 (91%)	32 (9%)	0	100	100
28	b	189/377 (50%)	168 (89%)	20 (11%)	1 (0%)	24	61
29	c	285/310 (92%)	254 (89%)	29 (10%)	2 (1%)	18	55
30	d	255/350 (73%)	218 (86%)	35 (14%)	2 (1%)	16	52
31	e	48/70 (69%)	40 (83%)	8 (17%)	0	100	100
32	f	840/908 (92%)	803 (96%)	35 (4%)	2 (0%)	43	76
33	u	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
34	v	1/10 (10%)	0	0	1 (100%)	0	0
All	All	13366/14962 (89%)	12548 (94%)	792 (6%)	26 (0%)	44	76

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	125	LYS
5	E	385	ASP
5	E	386	TYR
11	K	130	PRO
29	c	196	LEU
10	j	50	VAL
4	D	369	LYS
25	Y	350	VAL
30	d	200	PHE
32	f	66	LYS
34	v	25	LYS

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Mol	Chain	Res	Type
3	C	91	PRO
4	D	127	ASN
22	V	496	PHE
28	b	23	PRO
7	g	5	SER
3	C	134	LEU
6	F	120	LYS
9	I	53	HIS
29	c	266	THR
6	F	119	GLY
30	d	199	PHE
32	f	365	VAL
2	B	87	PRO
4	D	367	PRO
7	g	4	GLY

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	337/372 (91%)	336 (100%)	1 (0%)	86	85
2	B	339/385 (88%)	339 (100%)	0	100	100
3	C	314/346 (91%)	310 (99%)	4 (1%)	61	72
4	D	333/366 (91%)	329 (99%)	4 (1%)	63	73
5	E	341/353 (97%)	341 (100%)	0	100	100
6	F	357/379 (94%)	356 (100%)	1 (0%)	86	85
7	G	205/210 (98%)	204 (100%)	1 (0%)	81	82
7	g	202/210 (96%)	201 (100%)	1 (0%)	81	82
8	H	188/191 (98%)	187 (100%)	1 (0%)	81	82
8	h	188/191 (98%)	188 (100%)	0	100	100
9	I	206/221 (93%)	205 (100%)	1 (0%)	81	82
9	i	206/221 (93%)	206 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	201/211 (95%)	199 (99%)	2 (1%)	68	76
10	j	196/211 (93%)	195 (100%)	1 (0%)	81	82
11	K	193/203 (95%)	193 (100%)	0	100	100
11	k	195/203 (96%)	195 (100%)	0	100	100
12	L	202/224 (90%)	201 (100%)	1 (0%)	81	82
12	l	201/224 (90%)	201 (100%)	0	100	100
13	M	196/212 (92%)	196 (100%)	0	100	100
13	m	198/212 (93%)	198 (100%)	0	100	100
14	N	157/181 (87%)	157 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	179/228 (78%)	179 (100%)	0	100	100
15	o	181/228 (79%)	181 (100%)	0	100	100
16	P	172/174 (99%)	172 (100%)	0	100	100
16	p	173/174 (99%)	173 (100%)	0	100	100
17	Q	168/171 (98%)	168 (100%)	0	100	100
17	q	168/171 (98%)	168 (100%)	0	100	100
18	R	156/202 (77%)	156 (100%)	0	100	100
18	r	156/202 (77%)	156 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	178/199 (89%)	178 (100%)	0	100	100
20	T	178/215 (83%)	178 (100%)	0	100	100
20	t	179/215 (83%)	179 (100%)	0	100	100
21	U	696/816 (85%)	696 (100%)	0	100	100
22	V	390/460 (85%)	390 (100%)	0	100	100
23	W	406/416 (98%)	405 (100%)	1 (0%)	87	87
24	X	362/362 (100%)	362 (100%)	0	100	100
25	Y	344/344 (100%)	344 (100%)	0	100	100
26	Z	257/295 (87%)	256 (100%)	1 (0%)	84	83
27	a	333/336 (99%)	333 (100%)	0	100	100
28	b	167/312 (54%)	167 (100%)	0	100	100
29	c	252/268 (94%)	250 (99%)	2 (1%)	73	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	d	231/294 (79%)	231 (100%)	0	100	100
31	e	44/63 (70%)	44 (100%)	0	100	100
32	f	711/763 (93%)	709 (100%)	2 (0%)	86	85
33	u	68/68 (100%)	65 (96%)	3 (4%)	25	48
34	v	1/1 (100%)	1 (100%)	0	100	100
All	All	11436/12683 (90%)	11409 (100%)	27 (0%)	85	87

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	403	ILE
3	C	90	HIS
3	C	109	THR
3	C	134	LEU
3	C	210	THR
4	D	124	LEU
4	D	125	LYS
4	D	150	SER
4	D	369	LYS
6	F	120	LYS
7	G	53	GLN
8	H	222	THR
9	I	52	ILE
10	J	220	LEU
10	J	221	ASN
12	L	53	GLN
23	W	455	LEU
26	Z	103	LYS
29	c	196	LEU
29	c	197	ASN
32	f	352	HIS
32	f	365	VAL
7	g	6	SER
10	j	49	SER
33	u	1	MET
33	u	51	GLU
33	u	63	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	148	GLN
1	A	150	HIS
1	A	197	HIS
1	A	203	ASN
1	A	247	GLN
1	A	433	ASN
2	B	242	GLN
2	B	332	ASN
3	C	53	ASN
3	C	64	GLN
3	C	102	ASN
3	C	171	HIS
3	C	337	ASN
3	C	343	ASN
4	D	49	GLN
4	D	110	ASN
4	D	221	HIS
4	D	222	HIS
5	E	10	GLN
5	E	155	ASN
5	E	323	HIS
5	E	359	HIS
7	G	12	HIS
7	G	147	GLN
8	H	88	HIS
9	I	142	HIS
10	J	92	GLN
10	J	175	ASN
10	J	215	GLN
11	K	13	ASN
11	K	23	GLN
11	K	73	HIS
11	K	204	GLN
12	L	16	GLN
12	L	69	HIS
12	L	86	ASN
16	P	145	GLN
17	Q	61	GLN
17	Q	99	HIS
17	Q	101	ASN
18	R	151	GLN
19	S	8	ASN

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Mol	Chain	Res	Type
20	T	157	GLN
21	U	111	GLN
21	U	145	HIS
21	U	258	GLN
21	U	267	ASN
21	U	362	ASN
21	U	366	HIS
21	U	421	GLN
21	U	464	GLN
21	U	467	ASN
21	U	604	HIS
21	U	768	GLN
22	V	124	ASN
22	V	260	HIS
22	V	377	GLN
23	W	96	GLN
23	W	203	GLN
23	W	235	GLN
23	W	453	HIS
24	X	44	GLN
24	X	78	ASN
24	X	178	HIS
24	X	198	ASN
24	X	292	GLN
24	X	296	ASN
24	X	405	GLN
25	Y	160	ASN
25	Y	184	GLN
25	Y	365	GLN
25	Y	388	ASN
26	Z	32	GLN
26	Z	193	ASN
27	a	12	GLN
27	a	23	HIS
27	a	193	GLN
27	a	258	GLN
27	a	264	ASN
28	b	76	HIS
28	b	169	HIS
29	c	77	GLN
29	c	92	GLN
29	c	115	HIS

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Mol	Chain	Res	Type
29	c	164	ASN
29	c	197	ASN
29	c	241	ASN
29	c	295	ASN
30	d	46	GLN
30	d	47	GLN
30	d	60	GLN
30	d	109	GLN
30	d	110	ASN
30	d	135	HIS
30	d	149	ASN
32	f	53	GLN
32	f	81	GLN
32	f	171	GLN
32	f	352	HIS
32	f	475	ASN
32	f	808	ASN
32	f	866	GLN
32	f	868	HIS
7	g	127	GLN
7	g	128	ASN
7	g	150	GLN
9	i	40	ASN
9	i	95	GLN
9	i	177	GLN
10	j	85	ASN
10	j	205	ASN
10	j	215	GLN
11	k	73	HIS
11	k	118	ASN
11	k	204	GLN
12	l	175	HIS
15	o	116	HIS
15	o	193	ASN
16	p	61	GLN
17	q	99	HIS
18	r	85	ASN
18	r	175	ASN
18	r	196	HIS
19	s	108	ASN
20	t	61	GLN
20	t	65	GLN

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Mol	Chain	Res	Type
20	t	81	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
35	ATP	E	401	36	29,33,33	0.32	0	44,52,52	0.45	1 (2%)
35	ATP	B	501	36	29,33,33	0.31	0	44,52,52	0.51	1 (2%)
37	ADP	F	501	36	27,29,29	1.33	4 (14%)	42,45,45	2.06	11 (26%)
37	ADP	C	501	-	27,29,29	1.35	4 (14%)	42,45,45	2.09	8 (19%)
35	ATP	D	501	36	29,33,33	0.32	0	44,52,52	0.50	0
35	ATP	A	501	36	29,33,33	0.31	0	44,52,52	0.52	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	E	401	36	-	4/22/38/38	0/3/3/3
35	ATP	B	501	36	-	6/22/38/38	0/3/3/3
37	ADP	F	501	36	-	5/16/32/32	0/3/3/3
37	ADP	C	501	-	-	5/16/32/32	0/3/3/3
35	ATP	D	501	36	-	4/22/38/38	0/3/3/3
35	ATP	A	501	36	-	3/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C	501	ADP	C5-C4	4.65	1.47	1.39
37	F	501	ADP	C5-C4	4.37	1.47	1.39
37	F	501	ADP	C5-C6	2.60	1.48	1.41
37	C	501	ADP	C5-C6	2.50	1.48	1.41
37	C	501	ADP	C5-N7	-2.47	1.34	1.39
37	F	501	ADP	C5-N7	-2.28	1.34	1.39
37	F	501	ADP	C8-N7	2.27	1.35	1.31
37	C	501	ADP	C8-N7	2.18	1.35	1.31

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	501	ADP	C5-C4-N3	-6.96	117.67	126.75
37	F	501	ADP	C5-C4-N3	-6.73	117.97	126.75
37	C	501	ADP	N3-C4-N9	5.67	136.43	127.08
37	F	501	ADP	N3-C4-N9	5.20	135.65	127.08
37	C	501	ADP	C2-N3-C4	4.12	121.49	111.75
37	F	501	ADP	C2-N3-C4	3.97	121.13	111.75
37	F	501	ADP	PA-O3A-PB	-3.91	119.42	132.83
37	F	501	ADP	C4-C5-N7	-3.42	106.45	110.62
37	C	501	ADP	PA-O3A-PB	-3.32	121.43	132.83
37	C	501	ADP	C3'-C2'-C1'	3.22	107.54	101.43
37	C	501	ADP	N3-C2-N1	-3.16	123.66	128.60
37	F	501	ADP	C5-N7-C8	2.91	107.64	103.51
37	F	501	ADP	N3-C2-N1	-2.87	124.11	128.60
37	C	501	ADP	C4-C5-N7	-2.73	107.29	110.62
37	C	501	ADP	C5-N7-C8	2.46	107.01	103.51
37	F	501	ADP	C4-N9-C8	2.46	108.39	105.73
37	F	501	ADP	C3'-C2'-C1'	2.35	105.89	101.43
37	F	501	ADP	C2'-C1'-N9	-2.15	107.86	113.30
35	A	501	ATP	PB-O3B-PG	2.07	139.94	132.83
35	B	501	ATP	PB-O3B-PG	2.03	139.79	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	F	501	ADP	N9-C8-N7	-2.03	111.14	113.91
35	E	401	ATP	PB-O3B-PG	2.00	139.70	132.83

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	501	ATP	C5'-O5'-PA-O2A
35	B	501	ATP	PB-O3B-PG-O3G
35	B	501	ATP	C5'-O5'-PA-O1A
35	B	501	ATP	C5'-O5'-PA-O2A
35	E	401	ATP	C5'-O5'-PA-O1A
35	E	401	ATP	C5'-O5'-PA-O2A
37	C	501	ADP	PA-O3A-PB-O3B
37	C	501	ADP	C5'-O5'-PA-O1A
37	F	501	ADP	O4'-C1'-N9-C8
37	F	501	ADP	O4'-C1'-N9-C4
37	F	501	ADP	O4'-C4'-C5'-O5'
35	D	501	ATP	O4'-C4'-C5'-O5'
35	D	501	ATP	C3'-C4'-C5'-O5'
35	A	501	ATP	C5'-O5'-PA-O3A
35	B	501	ATP	C5'-O5'-PA-O3A
35	E	401	ATP	C5'-O5'-PA-O3A
37	F	501	ADP	C5'-O5'-PA-O3A
35	D	501	ATP	PA-O3A-PB-O2B
35	A	501	ATP	C5'-O5'-PA-O1A
35	B	501	ATP	PB-O3B-PG-O2G
35	E	401	ATP	PB-O3B-PG-O2G
37	C	501	ADP	PA-O3A-PB-O2B
37	C	501	ADP	C5'-O5'-PA-O3A
35	D	501	ATP	PA-O3A-PB-O1B
37	C	501	ADP	C2'-C1'-N9-C8
37	F	501	ADP	C5'-O5'-PA-O1A
35	B	501	ATP	PB-O3B-PG-O1G

There are no ring outliers.

6 monomers are involved in 9 short contacts:

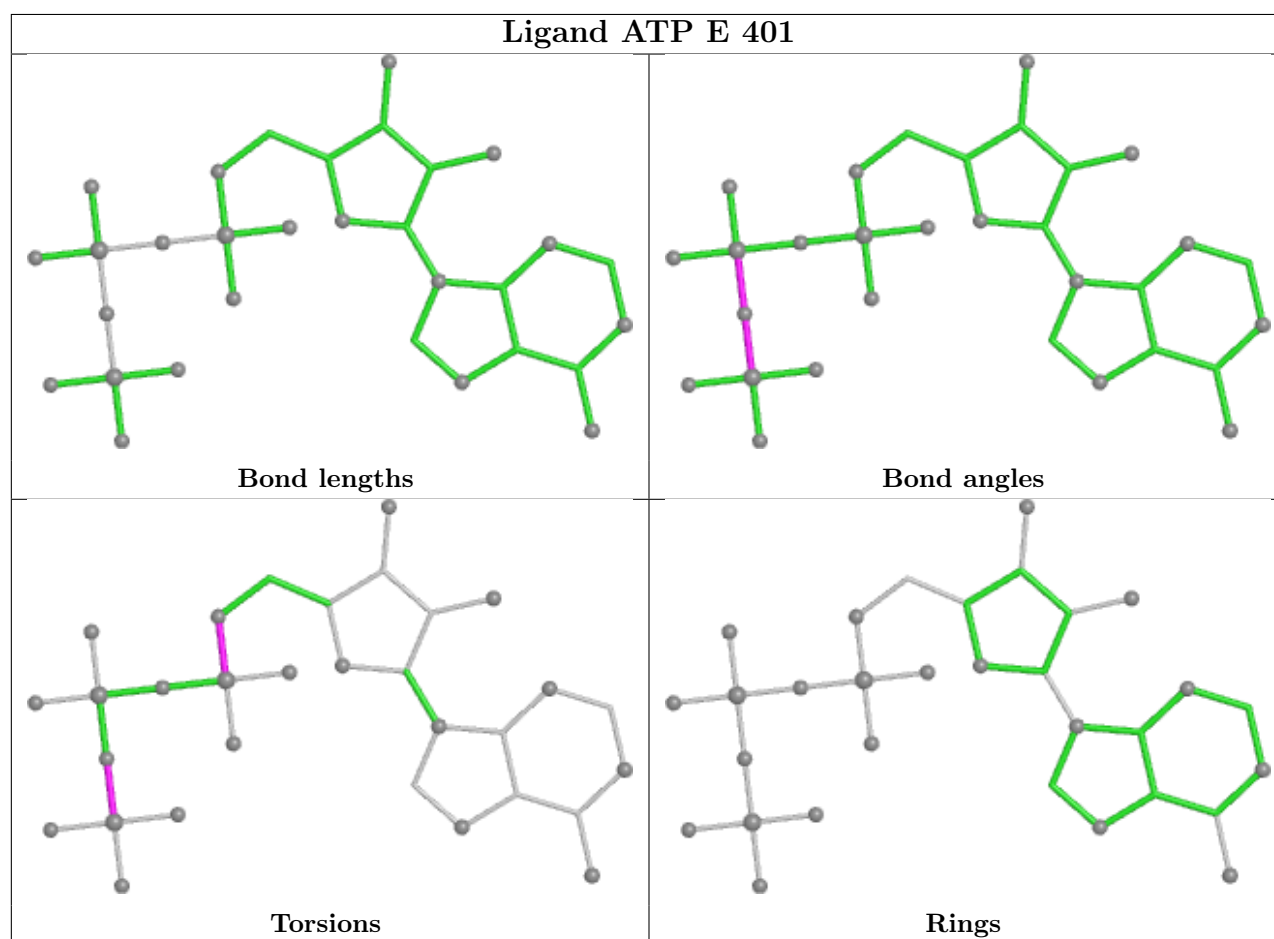
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	E	401	ATP	1	0
35	B	501	ATP	2	0

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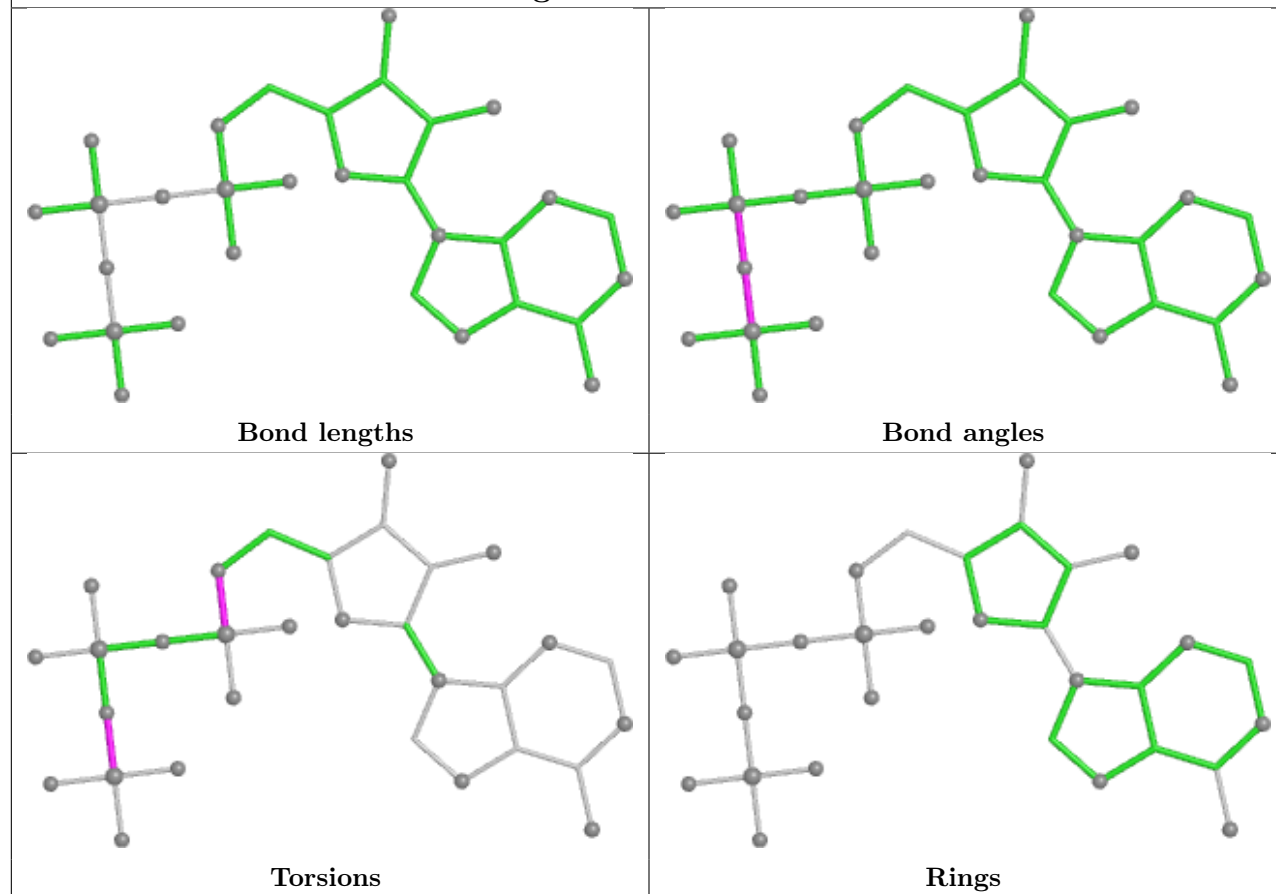
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	F	501	ADP	1	0
37	C	501	ADP	1	0
35	D	501	ATP	3	0
35	A	501	ATP	1	0

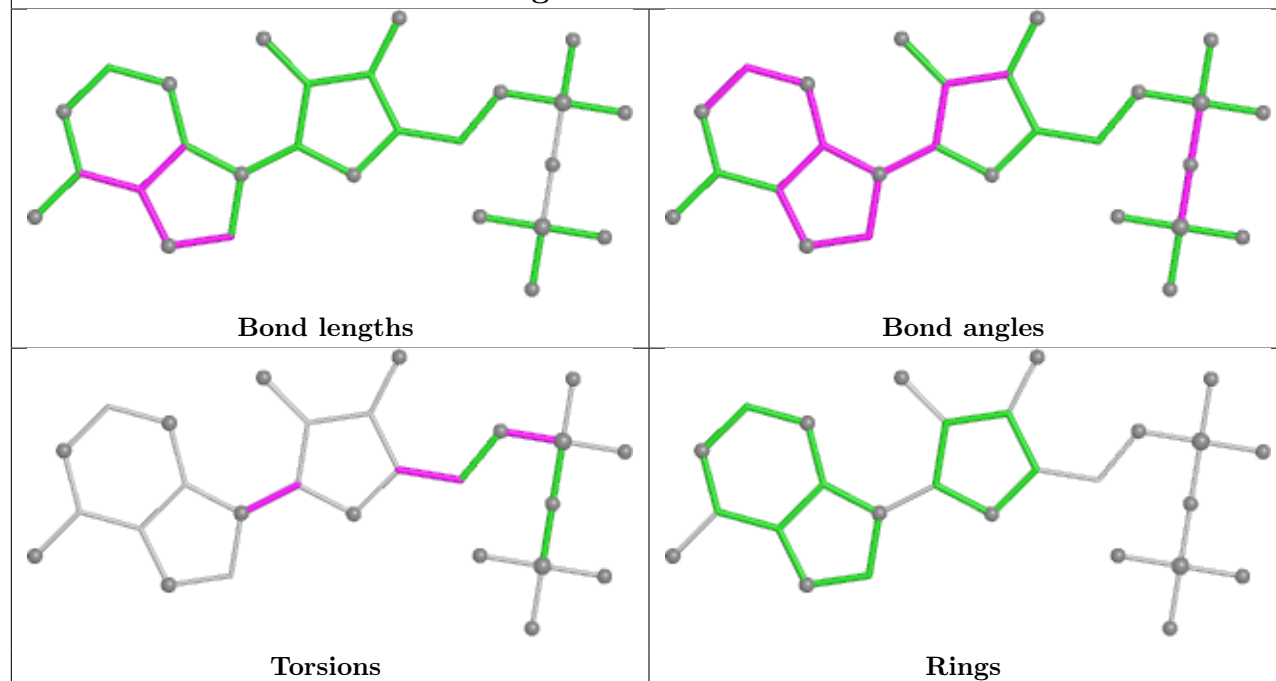
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

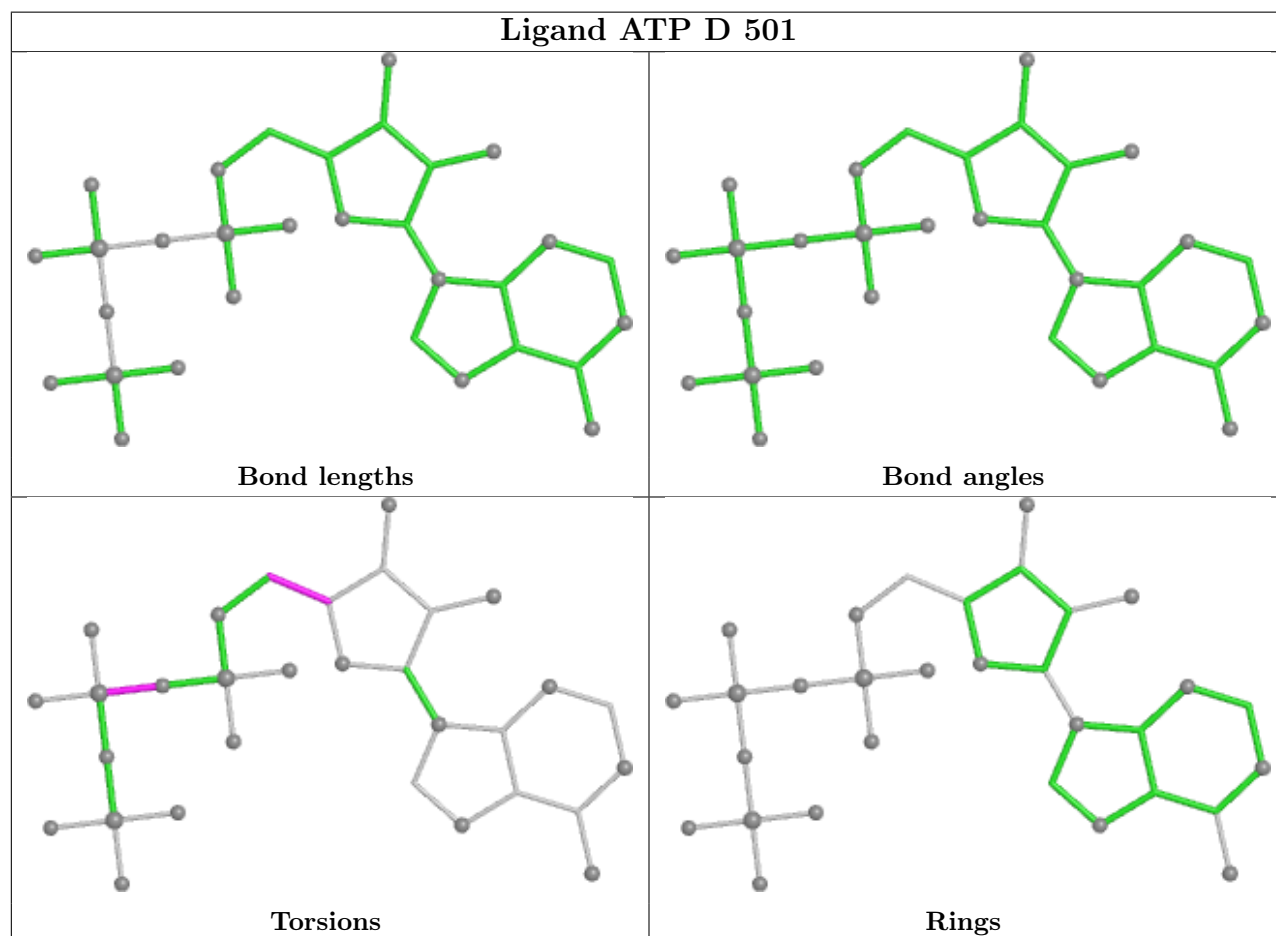
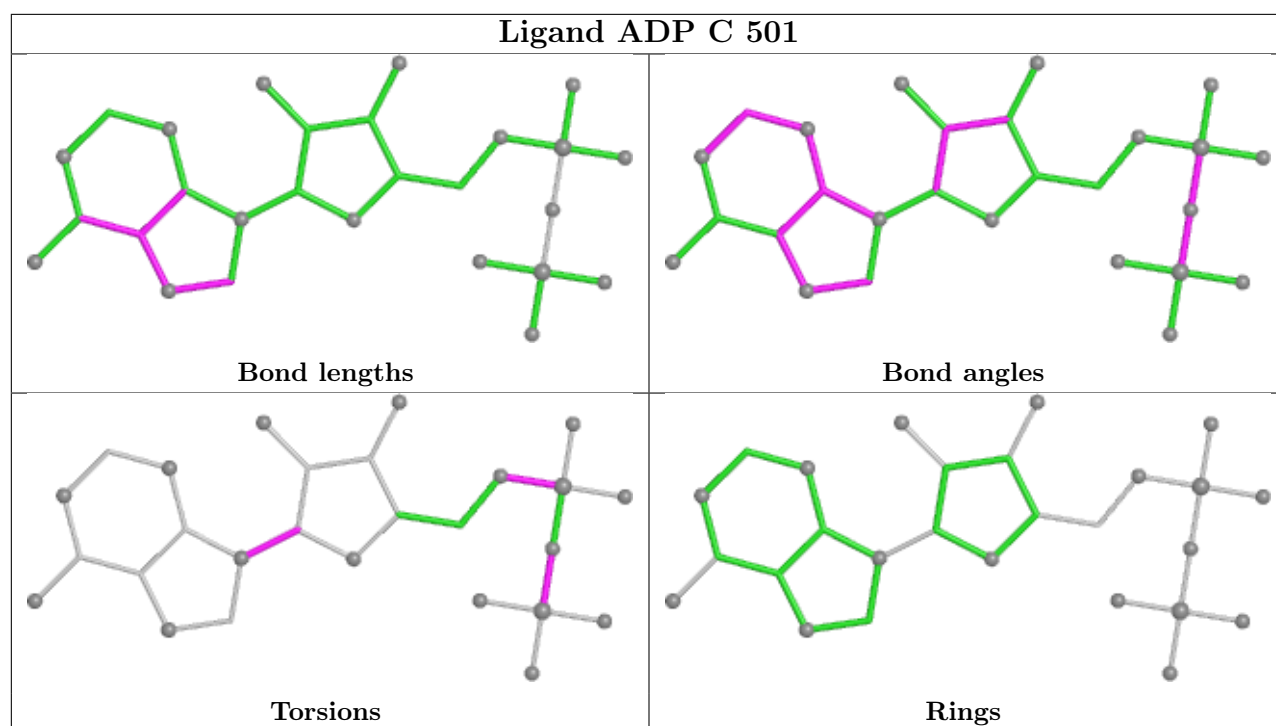


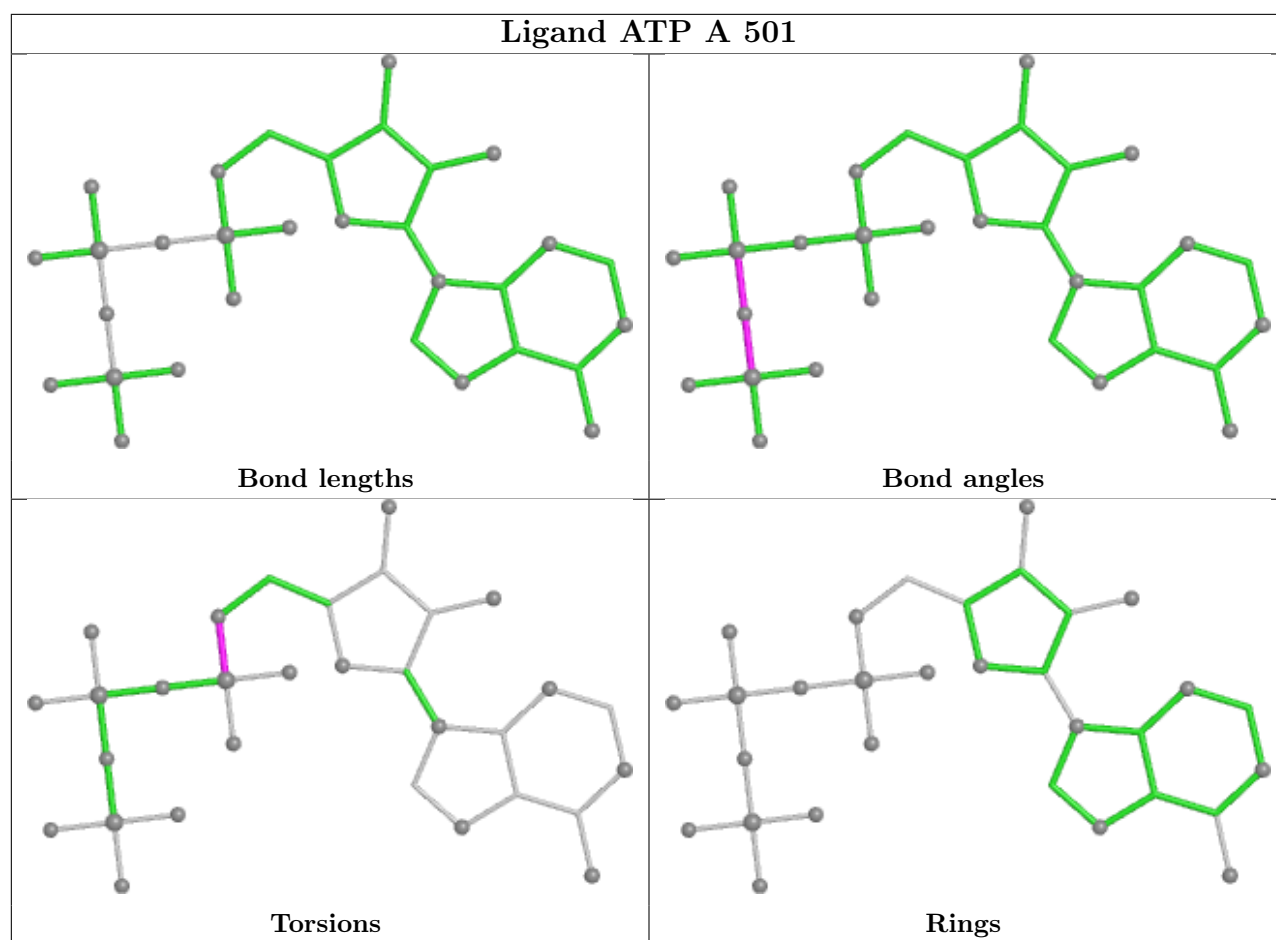
Ligand ATP B 501



Ligand ADP F 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

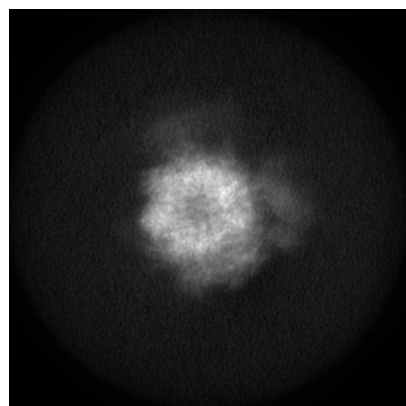
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62083. These allow visual inspection of the internal detail of the map and identification of artifacts.

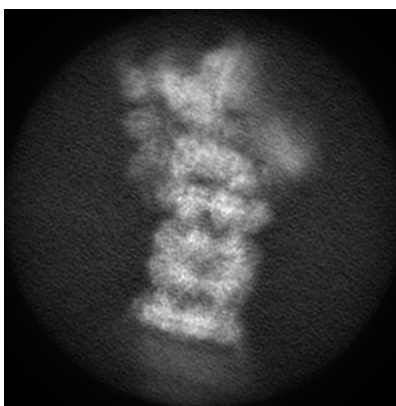
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

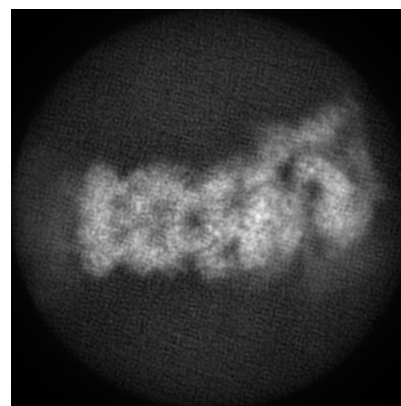
6.1.1 Primary map



X

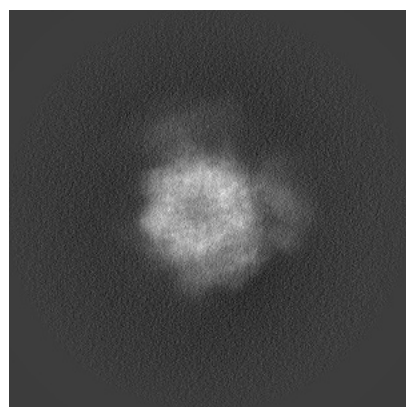


Y

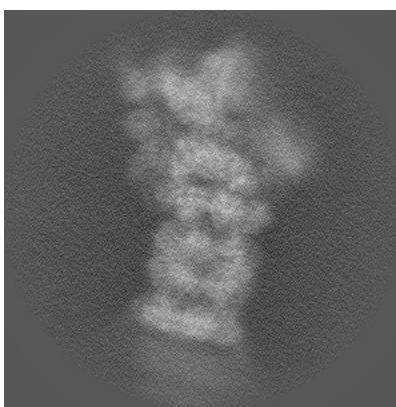


Z

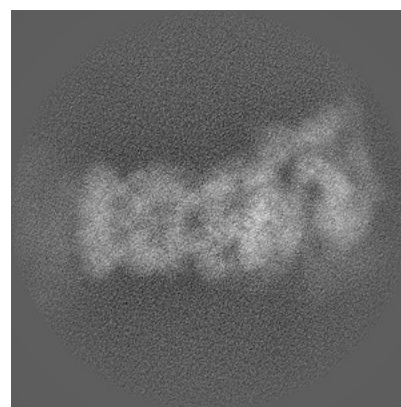
6.1.2 Raw map



X



Y

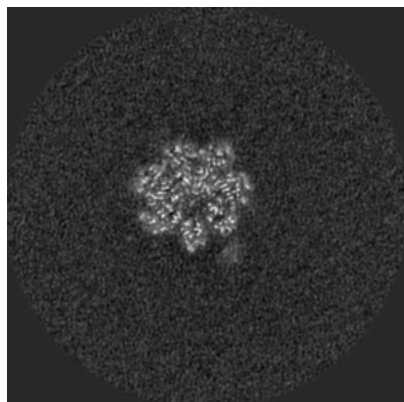


Z

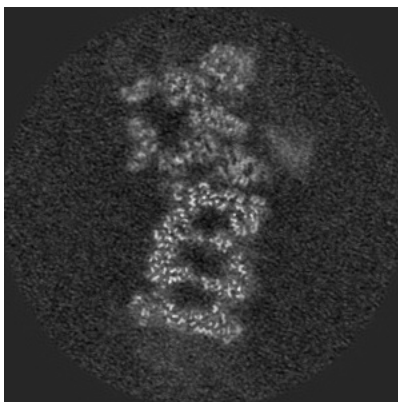
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

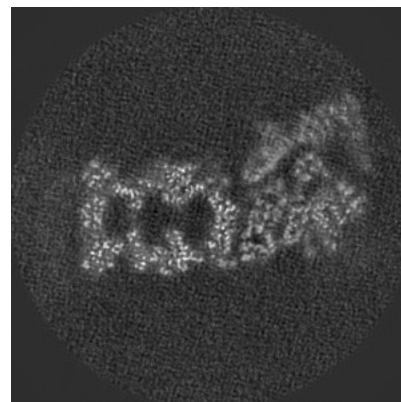
6.2.1 Primary map



X Index: 300

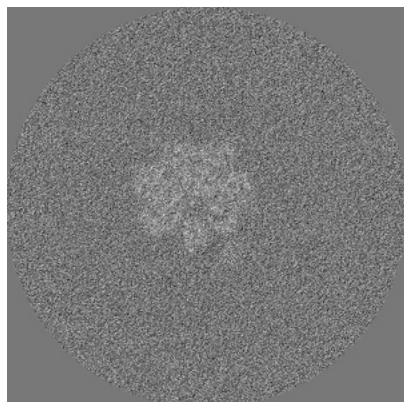


Y Index: 300

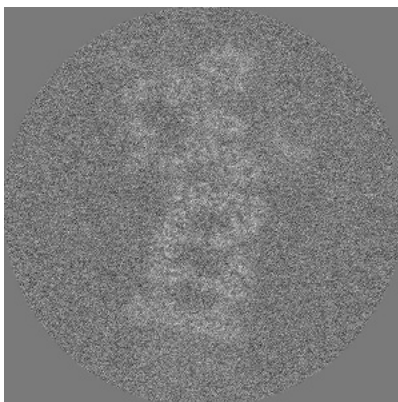


Z Index: 300

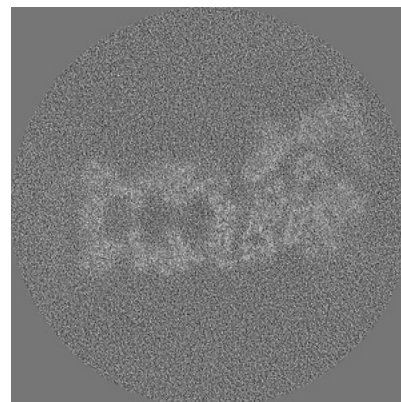
6.2.2 Raw map



X Index: 300



Y Index: 300

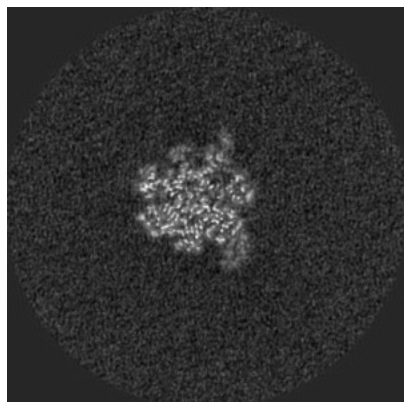


Z Index: 300

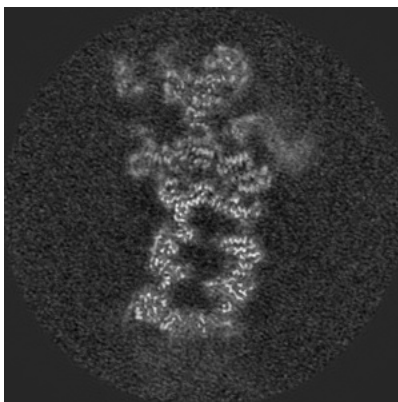
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

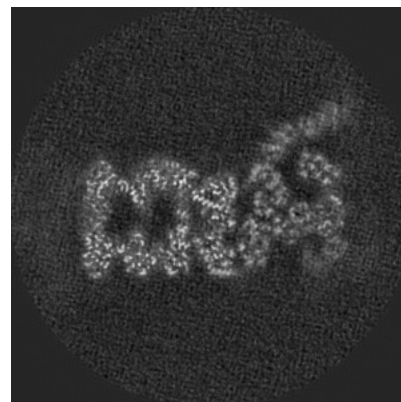
6.3.1 Primary map



X Index: 313

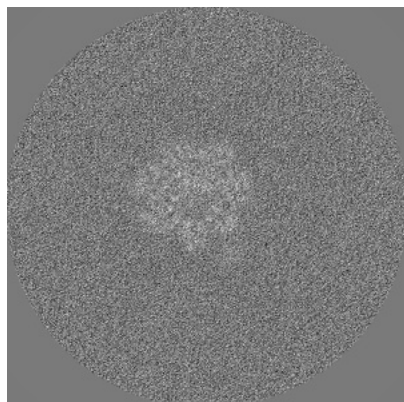


Y Index: 286

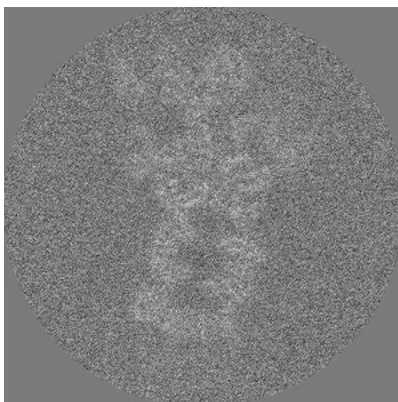


Z Index: 282

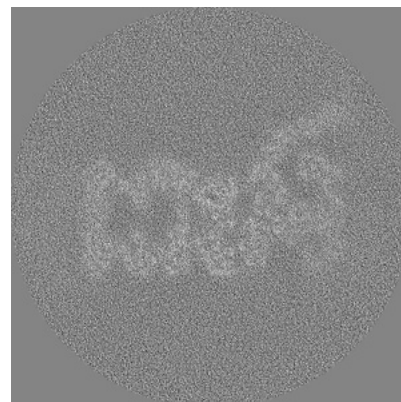
6.3.2 Raw map



X Index: 299



Y Index: 285

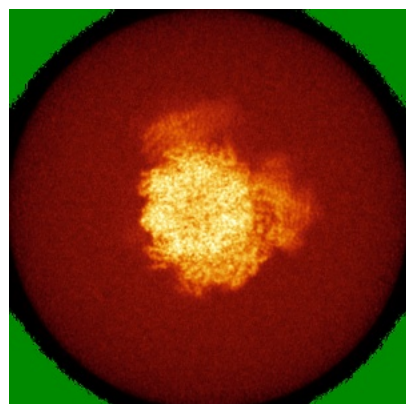


Z Index: 283

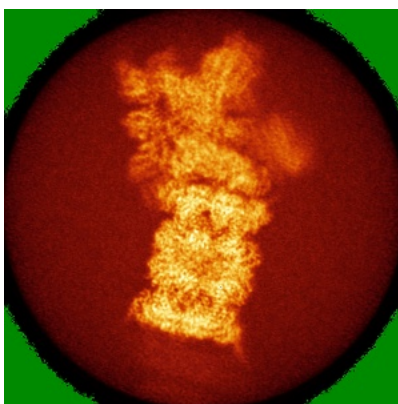
The images above show the largest variance slices of the map in three orthogonal directions.

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

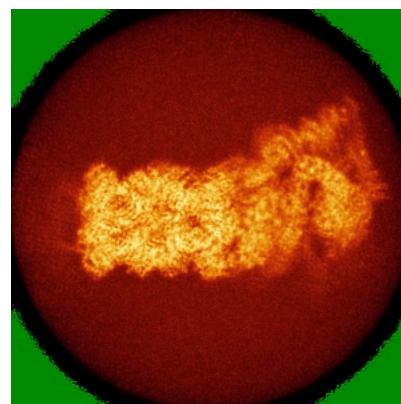
6.4.1 Primary map



X

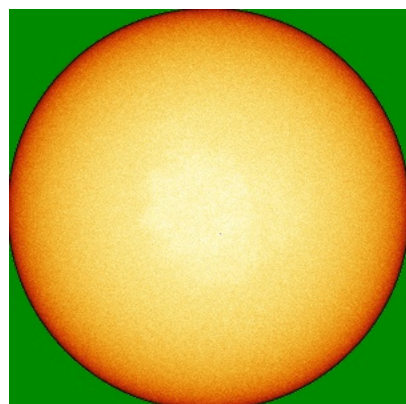


Y

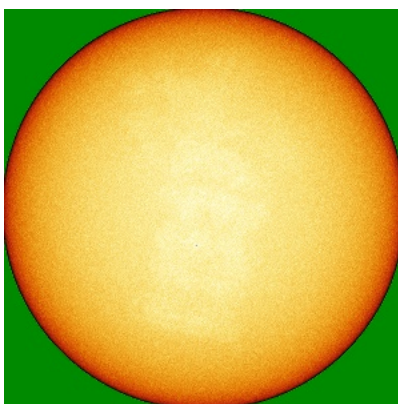


Z

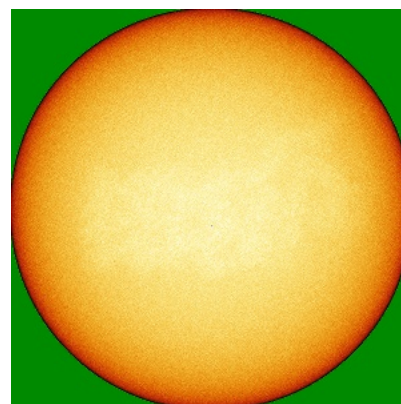
6.4.2 Raw map



X



Y

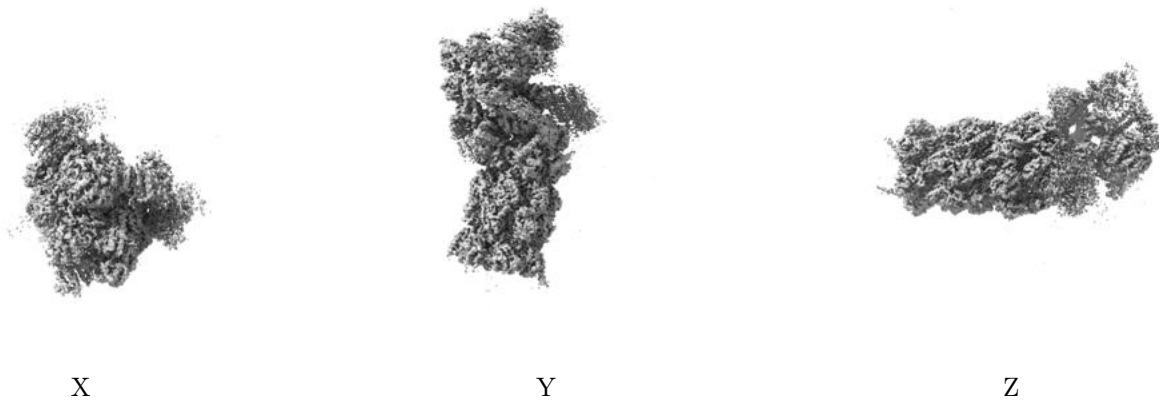


Z

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.

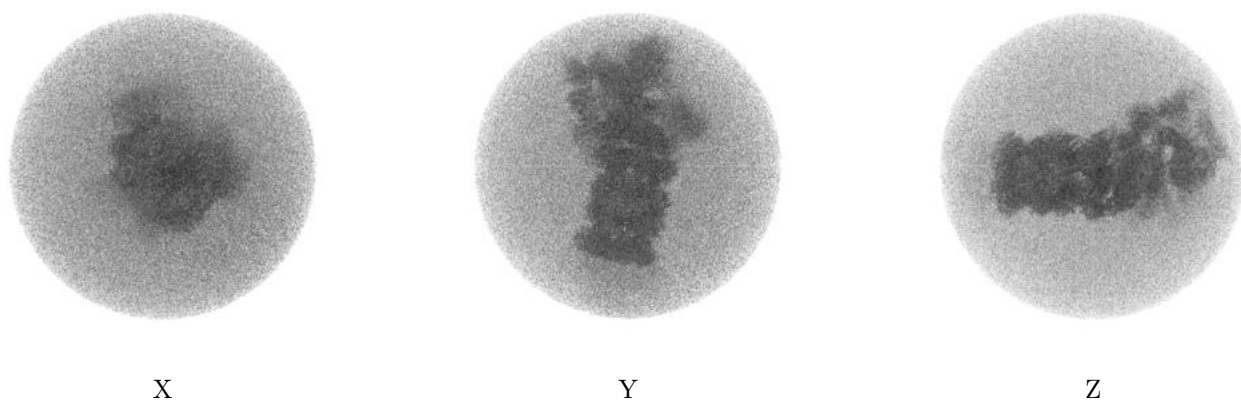
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00589. 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.

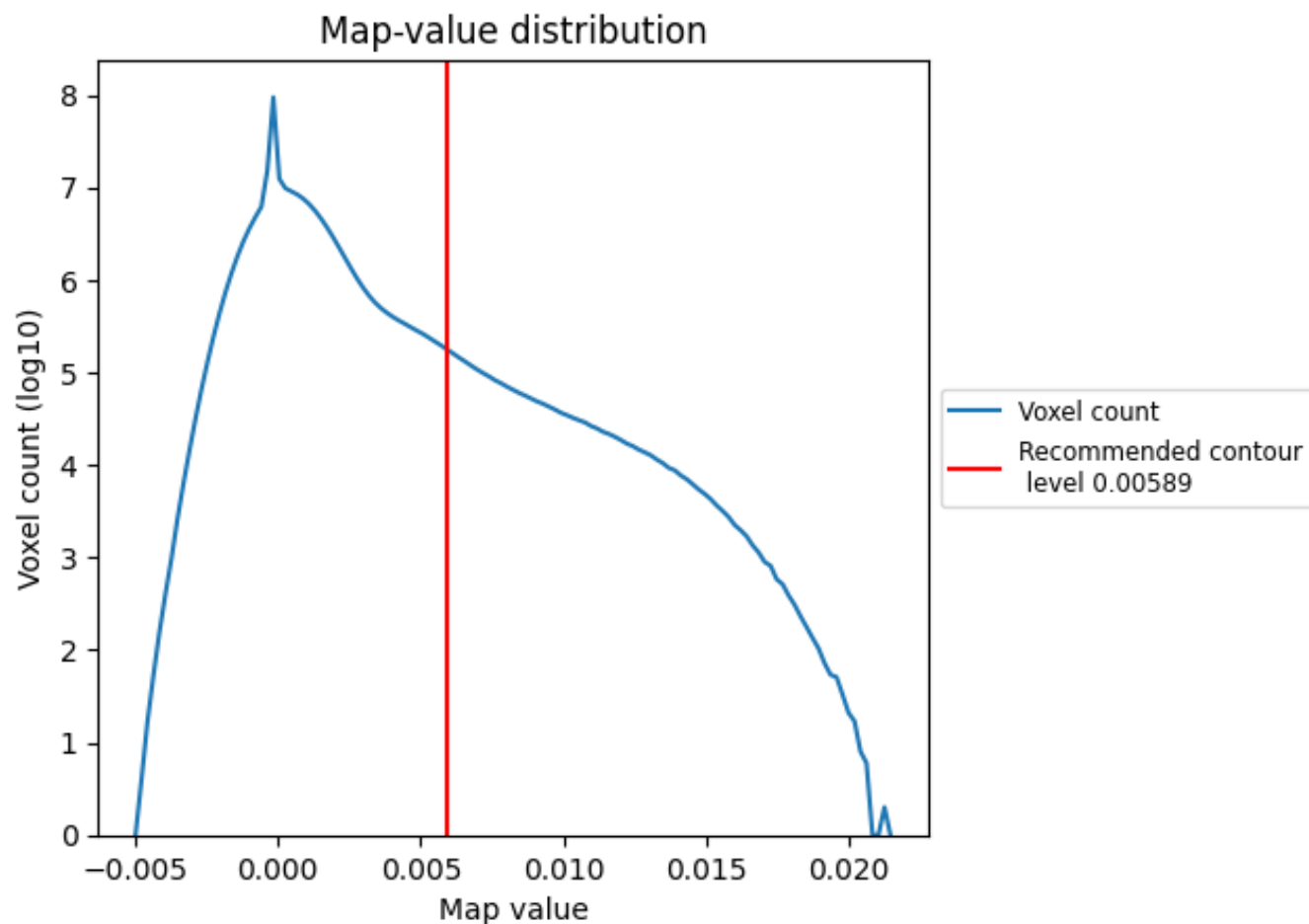
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

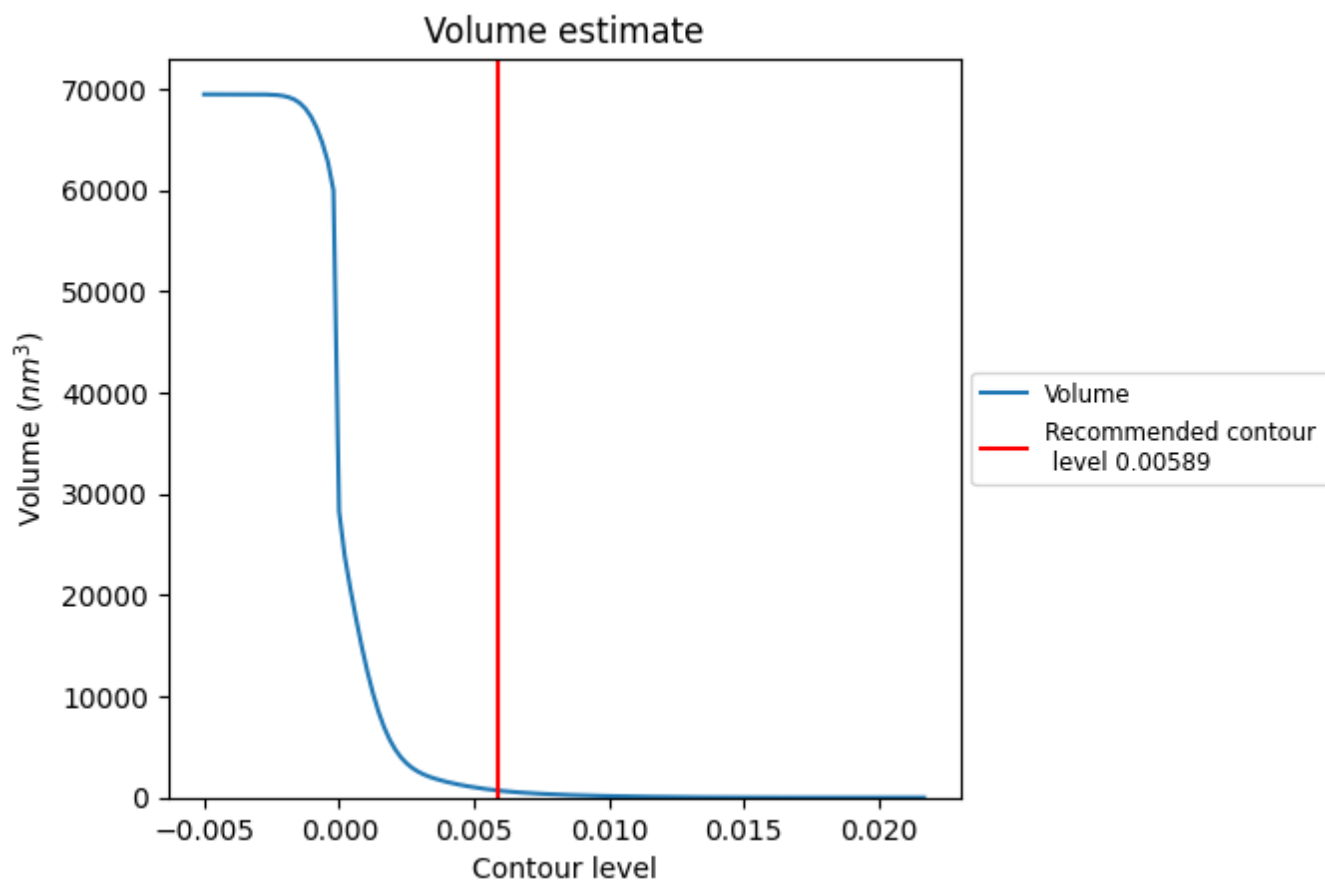
This section contains the results of statistical analysis of the map.

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.

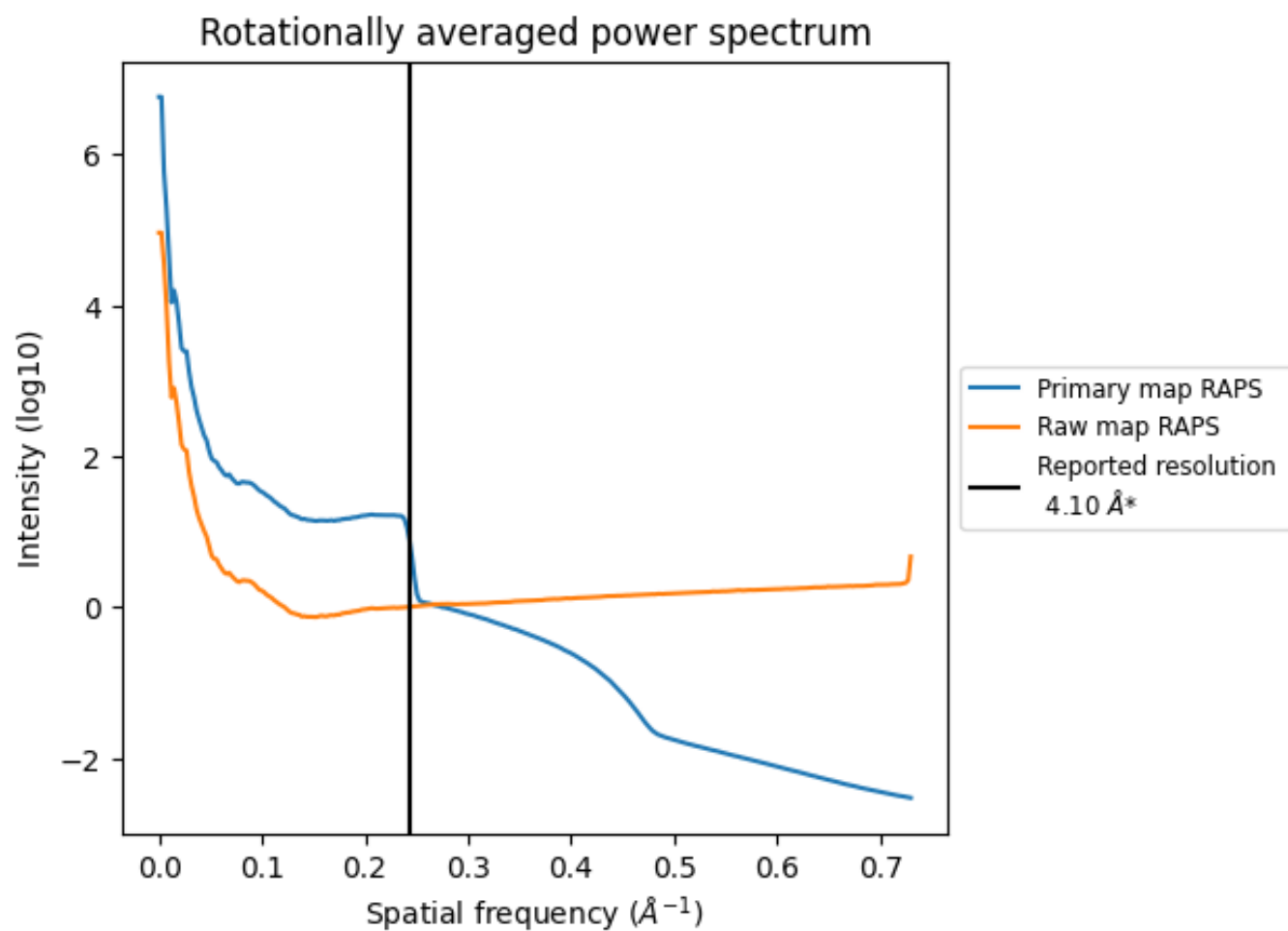
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 699 nm³; this corresponds to an approximate mass of 632 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 [i](#)

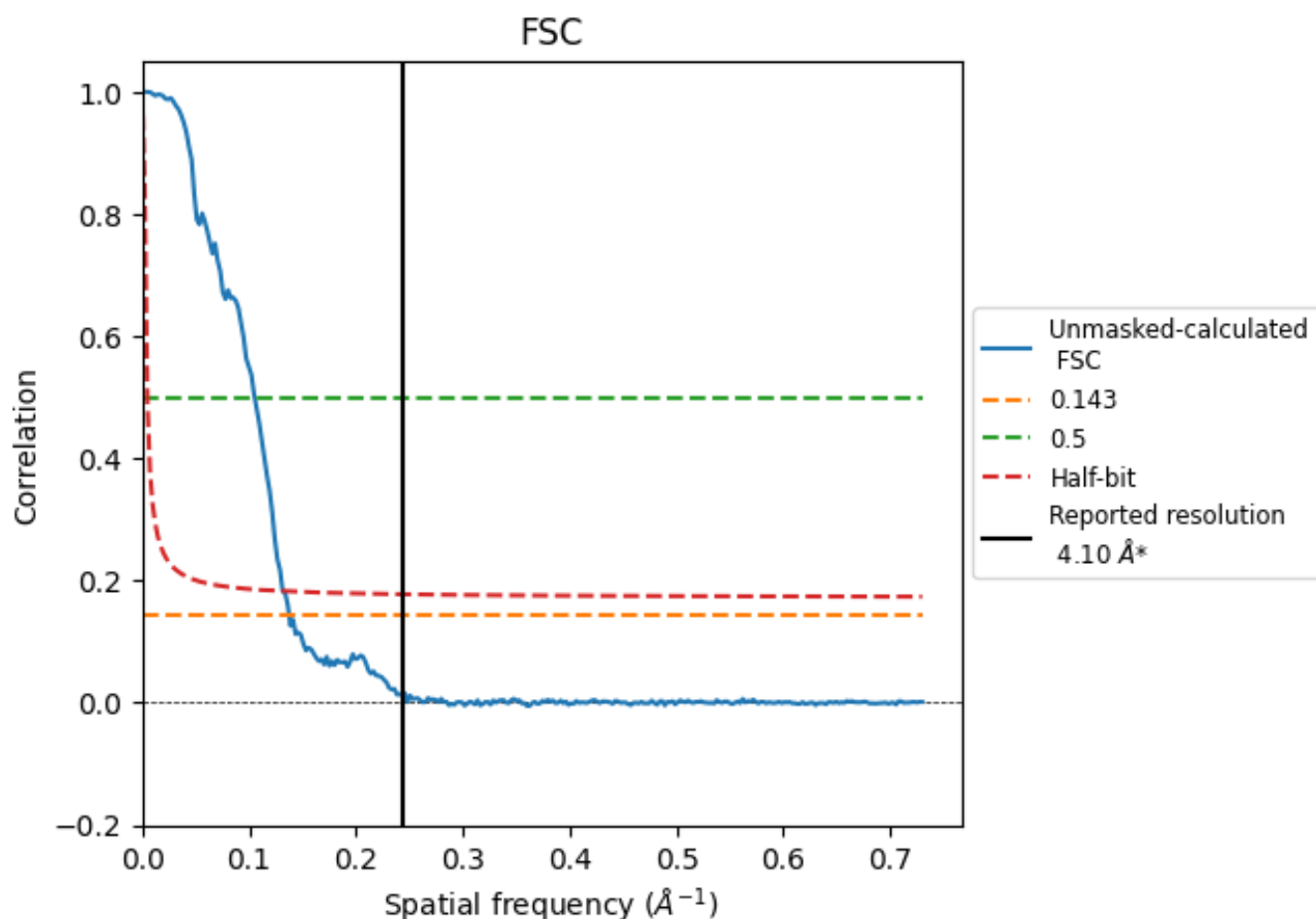


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 \AA^{-1}

8.2 Resolution estimates [i](#)

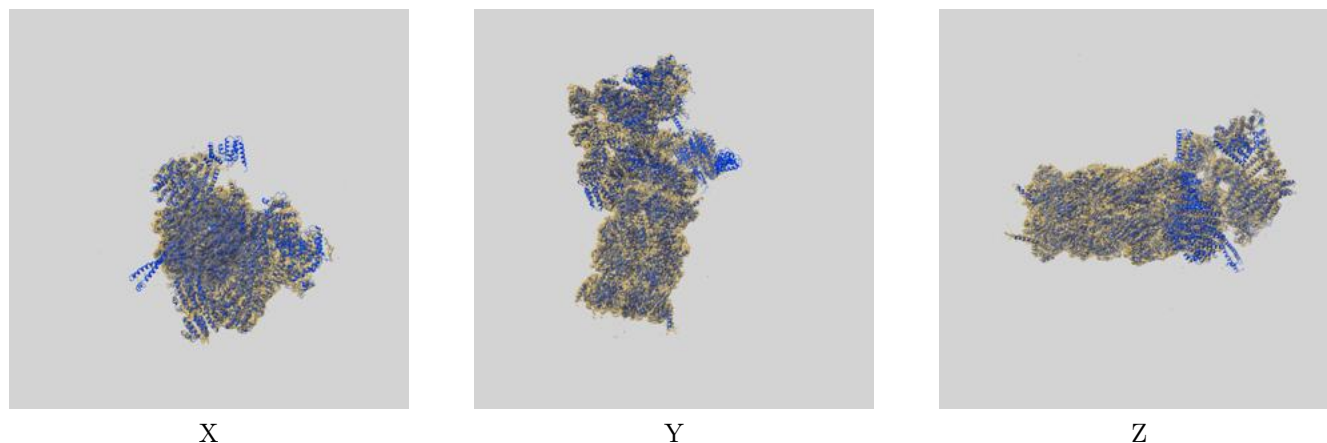
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.28	9.51	7.60

*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 7.28 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

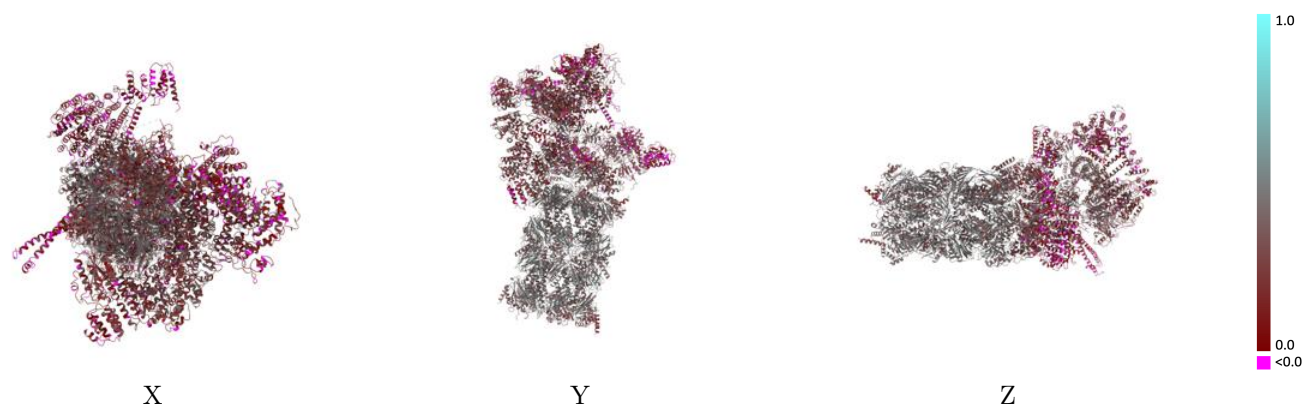
This section contains information regarding the fit between EMDB map EMD-62083 and PDB model 9K57. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



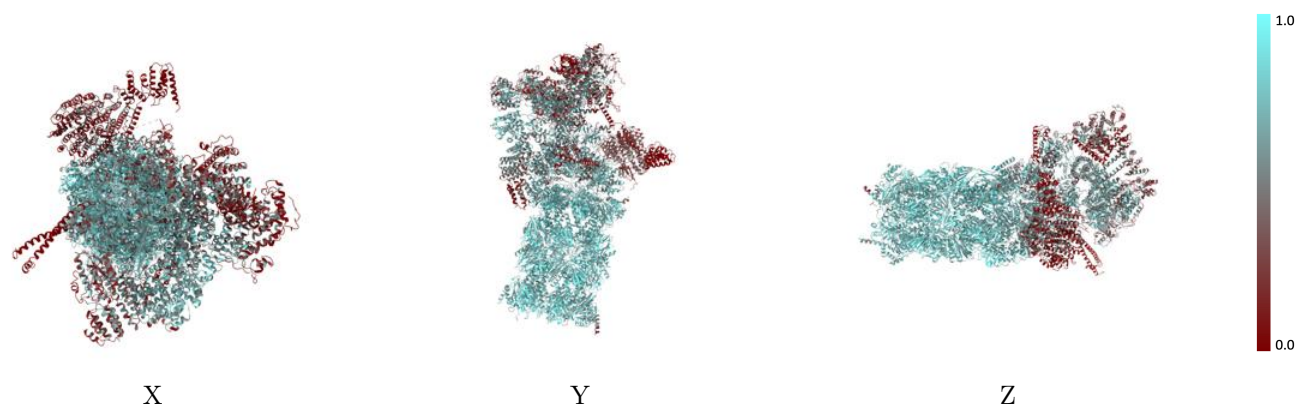
The images above show the 3D surface view of the map at the recommended contour level 0.00589 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



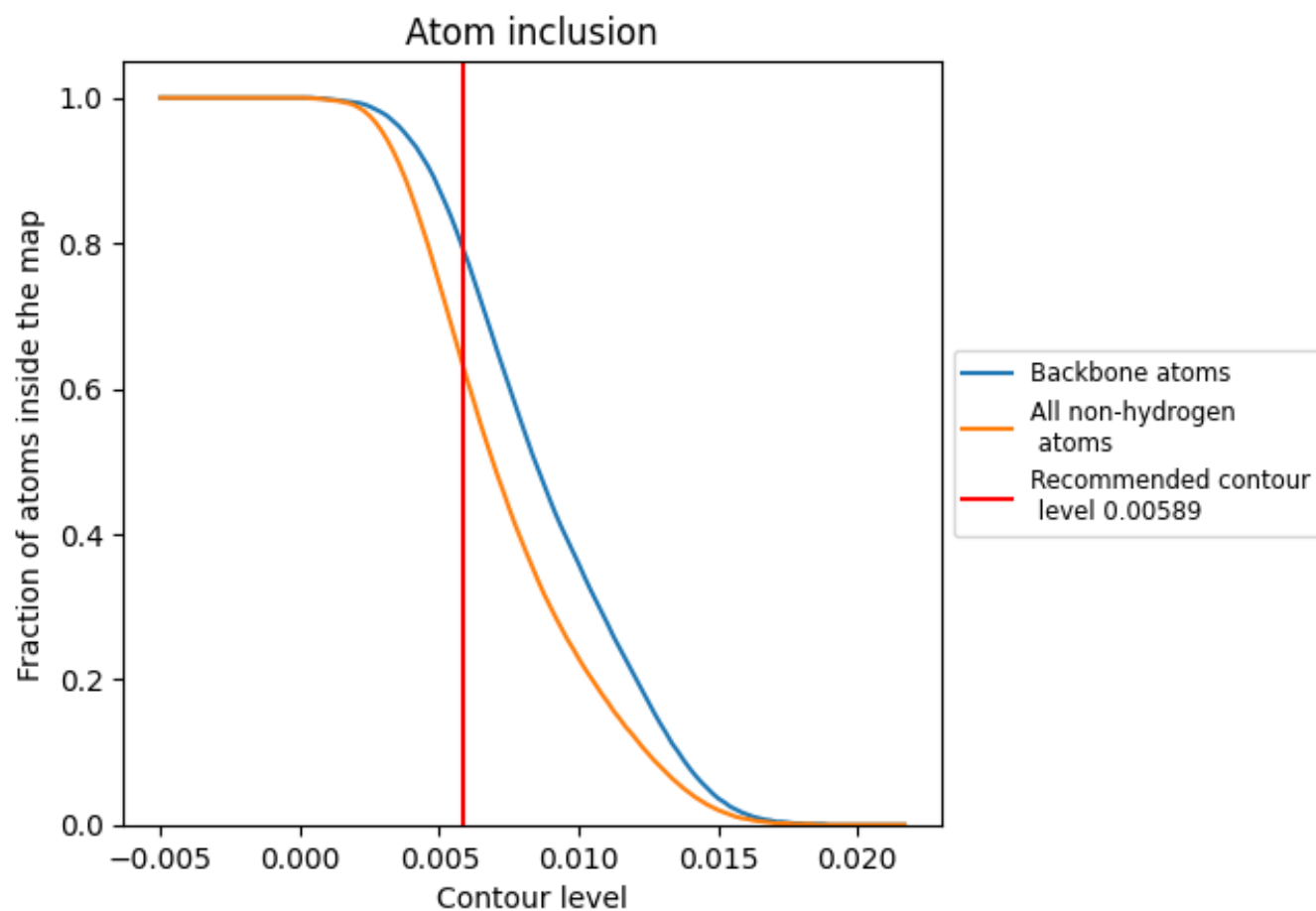
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00589).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 63% 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 (0.00589) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6260	 0.3300
A	 0.6520	 0.3340
B	 0.5740	 0.2930
C	 0.5990	 0.2950
D	 0.6190	 0.3170
E	 0.6040	 0.3160
F	 0.5880	 0.3150
G	 0.7800	 0.4100
H	 0.8180	 0.4290
I	 0.7900	 0.4020
J	 0.7530	 0.3840
K	 0.7740	 0.4140
L	 0.8260	 0.4300
M	 0.8020	 0.4190
N	 0.8380	 0.4340
O	 0.8380	 0.4340
P	 0.8370	 0.4350
Q	 0.8370	 0.4290
R	 0.8520	 0.4330
S	 0.8330	 0.4290
T	 0.8430	 0.4380
U	 0.4390	 0.2340
V	 0.3450	 0.2210
W	 0.5720	 0.2870
X	 0.4840	 0.2470
Y	 0.4680	 0.2180
Z	 0.6020	 0.3120
a	 0.4900	 0.2300
b	 0.3480	 0.2320
c	 0.6260	 0.3270
d	 0.2350	 0.1740
e	 0.3320	 0.2180
f	 0.1340	 0.1500
g	 0.8050	 0.4120
h	 0.8090	 0.4110



Continued on next page...

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Chain	Atom inclusion	Q-score
i	 0.7620	 0.3990
j	 0.7110	 0.3620
k	 0.7860	 0.4040
l	 0.8210	 0.4220
m	 0.8120	 0.4130
n	 0.8380	 0.4270
o	 0.8320	 0.4300
p	 0.8500	 0.4250
q	 0.8210	 0.4210
r	 0.8620	 0.4370
s	 0.8190	 0.4160
t	 0.8320	 0.4340
u	 0.4020	 0.2390
v	 0.0190	 0.0930