



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:23 AM UTC

PDB ID : 7W3G / pdb_00007w3g
EMDB ID : EMD-32279
Title : Structure of USP14-bound human 26S proteasome in substrate-engaged state
ED2.0_USP14
Authors : Zhang, S.; Zou, S.; Yin, D.; Wu, Z.; Mao, Y.
Deposited on : 2021-11-25
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

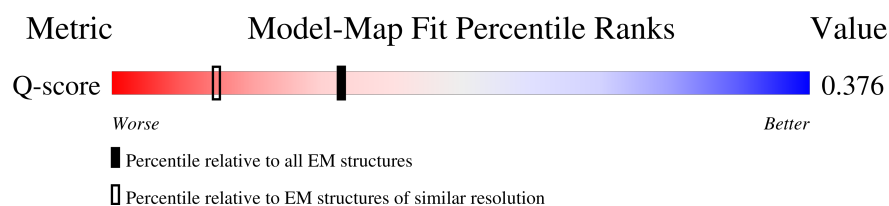
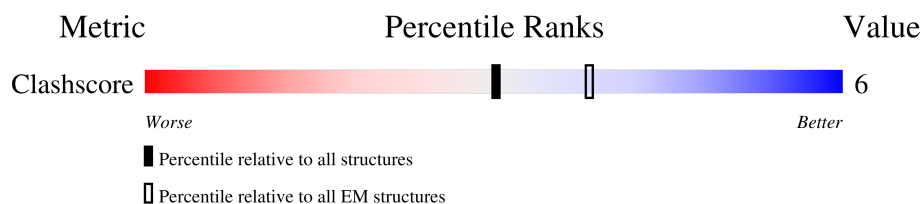
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

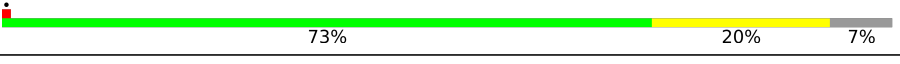
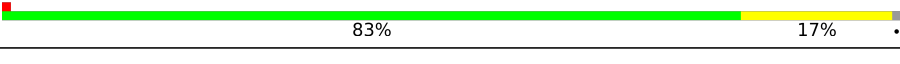
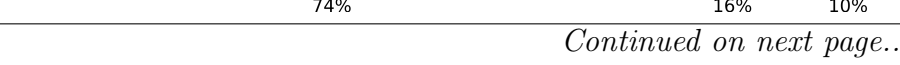
The reported resolution of this entry is 3.20 Å.

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.



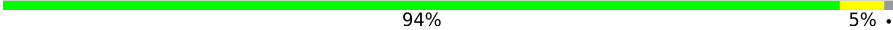
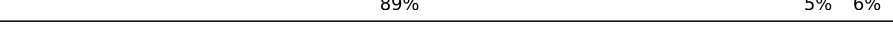
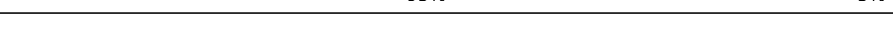
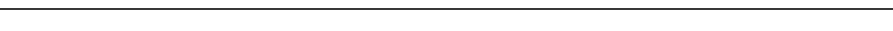
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	 81% 15% 5%
2	B	440	 73% 20% 7%
3	C	398	 83% 17% .
4	D	418	 72% 19% 9%
5	E	403	 9% 77% 19% .
6	F	439	 8% 74% 16% 10%

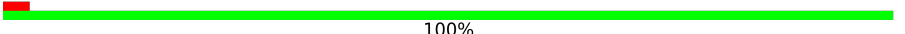
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Mol	Chain	Length	Quality of chain
7	G	246	 89% 9% .
7	g	246	 89% 10% .
8	H	234	 90% 9% .
8	h	234	 94% 5% .
9	I	261	 84% 11% 5%
9	i	261	 89% 7% .
10	J	248	 85% 11% .
10	j	248	 82% 15% .
11	K	241	 86% 13% .
11	k	241	 87% 10% .
12	L	269	 79% 10% 11%
12	l	269	 82% 7% 12%
13	M	255	 84% 11% 5%
13	m	255	 89% 5% 6%
14	N	239	 77% 8% 15%
14	n	239	 79% 6% 15%
15	O	277	 75% . 21%
15	o	277	 72% 7% 21%
16	P	205	 95% 5%
16	p	205	 90% 10%
17	Q	201	 82% 17% .
17	q	201	 86% 13% .
18	R	263	 71% 5% 24%
18	r	263	 69% 8% 24%
19	S	241	 80% 8% 12%

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Mol	Chain	Length	Quality of chain
19	s	241	
20	T	264	
20	t	264	
21	U	953	
22	X	422	
23	Y	389	
24	Z	324	
25	a	376	
26	b	377	
27	c	310	
28	d	350	
29	f	908	
30	x	494	
31	y	76	
32	W	456	
33	v	34	
34	V	534	
35	e	70	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 110741 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 protease regulatory subunit 7.

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

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

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

- Molecule 3 is a protein called Isoform 2 of 26S proteasome regulatory subunit 8.

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

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

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

- Molecule 5 is a protein called 26S proteasome regulatory subunit 10B.

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 protease regulatory subunit 6A.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	242	Total	C	N	O	S	0	0
			1890	1200	323	356	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	203	Total	C	N	O	S	0	0
			1521	954	259	296	12		
14	n	202	Total	C	N	O	S	0	0
			1510	947	258	293	12		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	872	Total	C	N	O	S	0	0
			6828	4328	1157	1298	45		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

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

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

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

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	889	Total	C	N	O	S	0	0
			6866	4315	1174	1331	46		

- Molecule 30 is a protein called Ubiquitin carboxyl-terminal hydrolase 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	x	494	Total	C	N	O	S	0	0
			3929	2485	647	769	28		

- Molecule 31 is a protein called Ubiquitin.

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

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	W	446	Total	C	N	O	S	0	0
			3635	2302	622	687	24		

- Molecule 33 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	v	34	Total	C	N	O	0	0
			170	102	34	34		

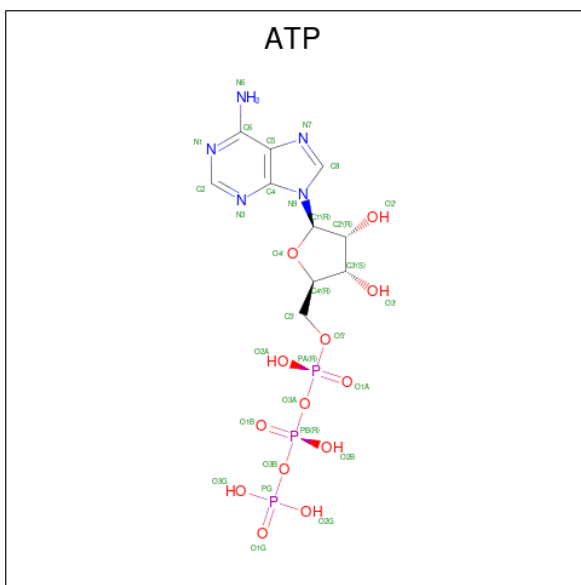
- Molecule 34 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

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

- Molecule 35 is a protein called 26S proteasome complex subunit DSS1.

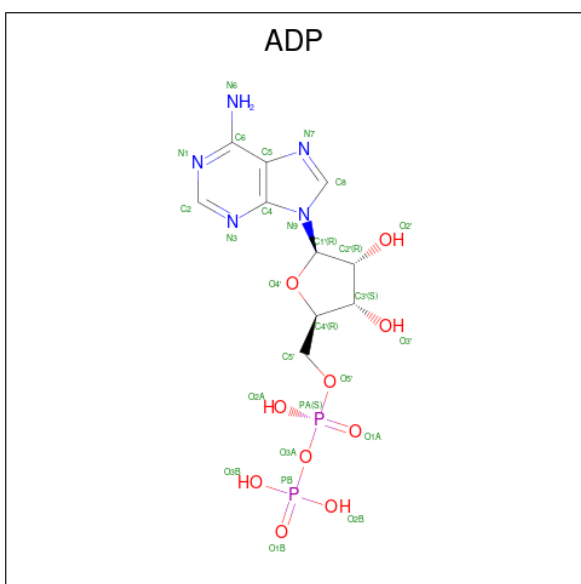
Mol	Chain	Residues	Atoms				AltConf	Trace
35	e	50	Total	C	N	O	0	0
			425	260	65	100		

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



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

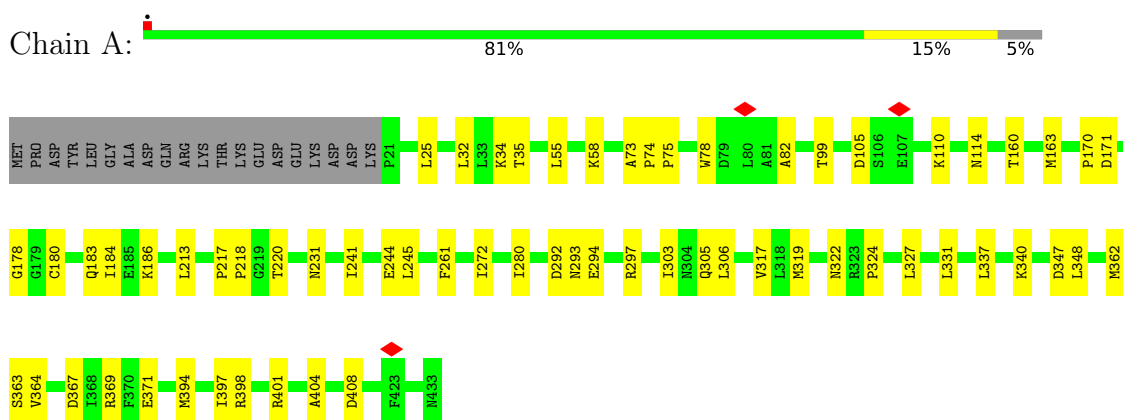
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

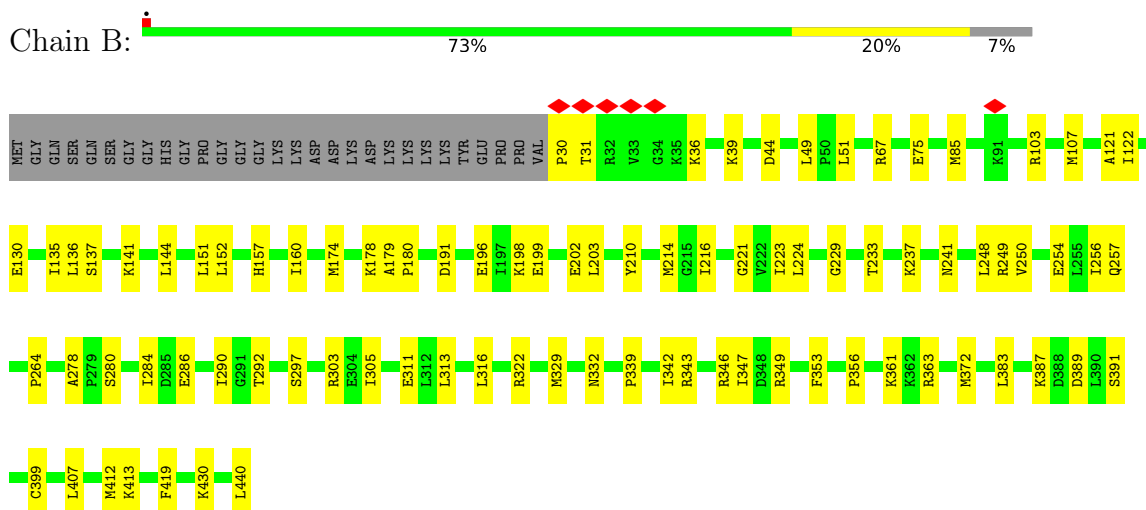
3 Residue-property plots

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

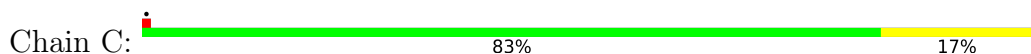
- Molecule 1: 26S protease regulatory subunit 7

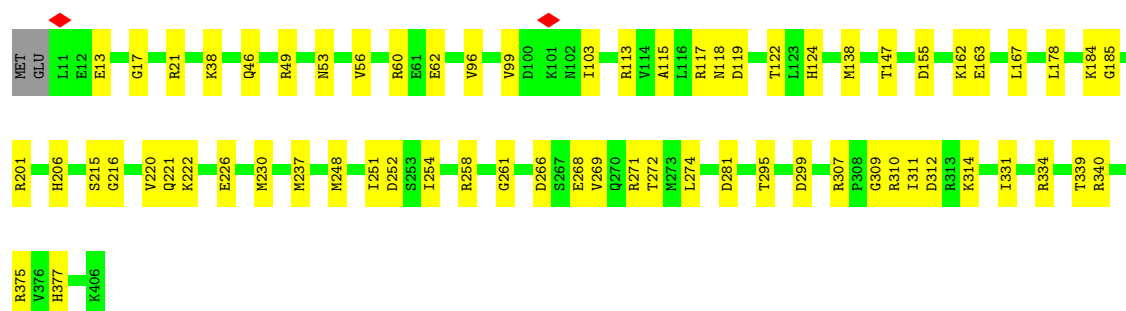


- Molecule 2: 26S protease regulatory subunit 4



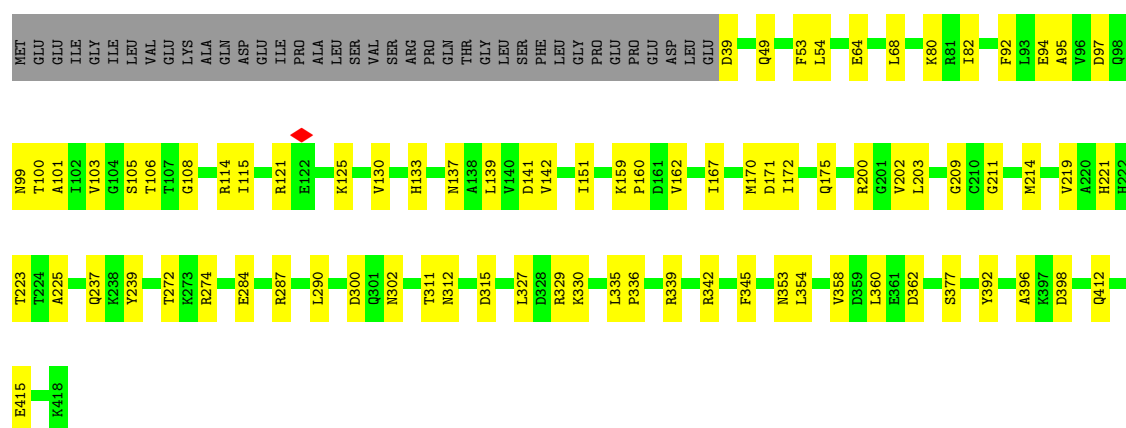
- Molecule 3: Isoform 2 of 26S proteasome regulatory subunit 8





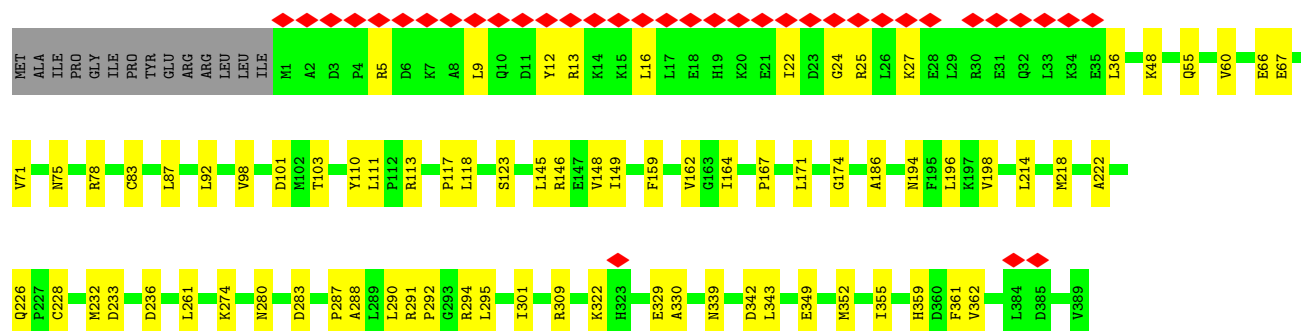
- Molecule 4: 26S protease regulatory subunit 6B

Chain D: 72% 19% 9%



- Molecule 5: 26S proteasome regulatory subunit 10B

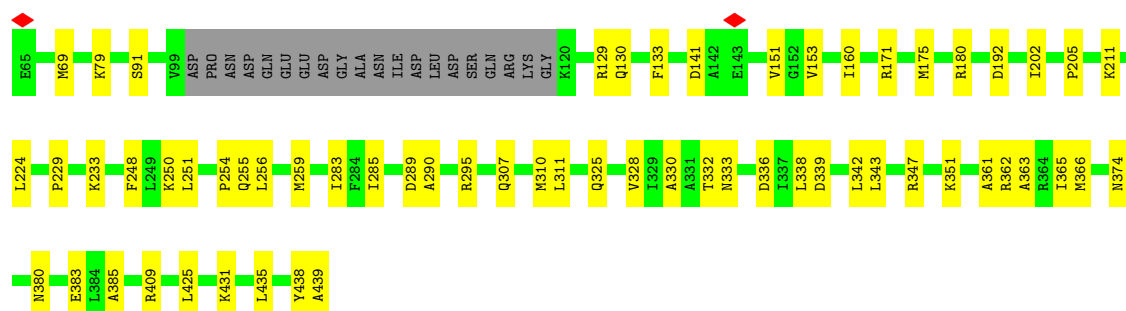
Chain E: 9% 77% 19%



- Molecule 6: 26S protease regulatory subunit 6A

Chain F: 8% 74% 16% 10%





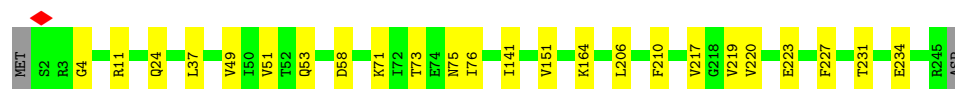
- Molecule 7: Proteasome subunit alpha type-6

Chain G: 89% 9% .



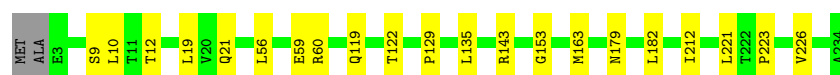
- Molecule 7: Proteasome subunit alpha type-6

Chain g: 89% 10% .



- Molecule 8: Proteasome subunit alpha type-2

Chain H: 90% 9% .



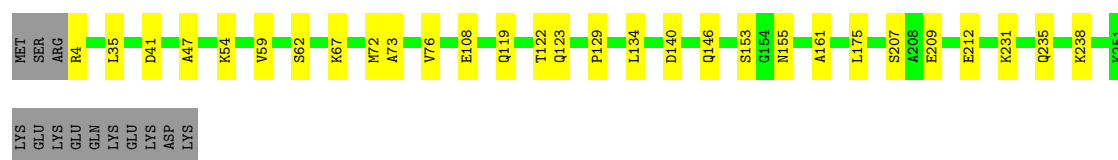
- Molecule 8: Proteasome subunit alpha type-2

Chain h: 94% 5% .



- Molecule 9: Proteasome subunit alpha type-4

Chain I: 84% 11% 5%



- Molecule 9: Proteasome subunit alpha type-4

Chain i:  89% 7%



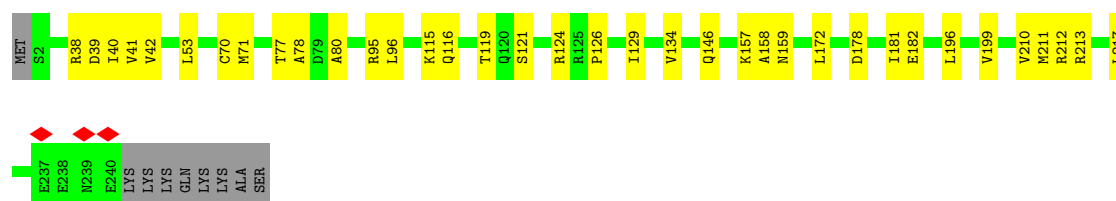
- Molecule 10: Proteasome subunit alpha type-7

Chain J:  85% 11%



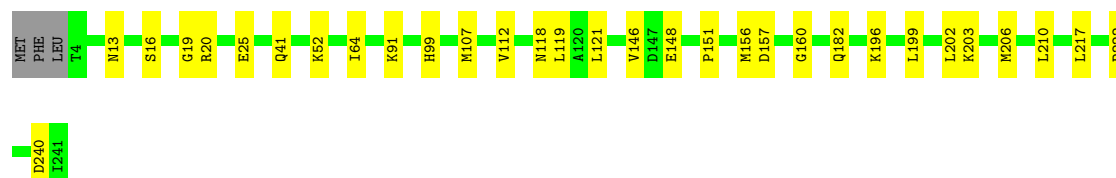
- Molecule 10: Proteasome subunit alpha type-7

Chain j:  82% 15%



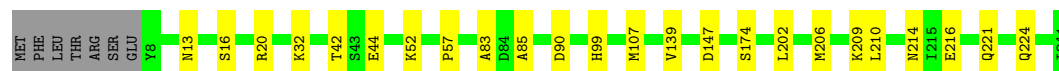
- Molecule 11: Proteasome subunit alpha type-5

Chain K:  86% 13%



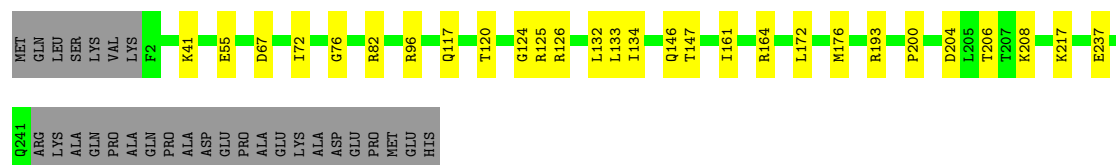
- Molecule 11: Proteasome subunit alpha type-5

Chain k:  87% 10%



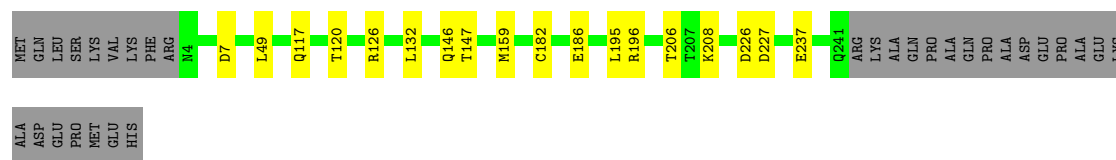
- Molecule 12: Isoform Long of Proteasome subunit alpha type-1

Chain L:  79% 10% 11%



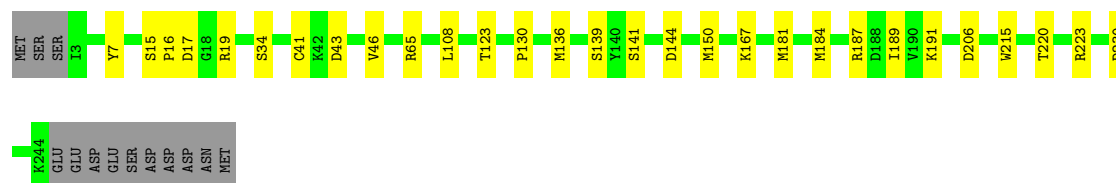
- Molecule 12: Isoform Long of Proteasome subunit alpha type-1

Chain l: 



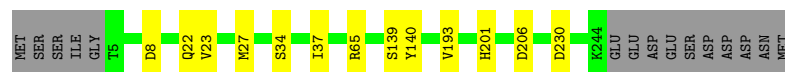
- Molecule 13: Proteasome subunit alpha type-3

Chain M: 



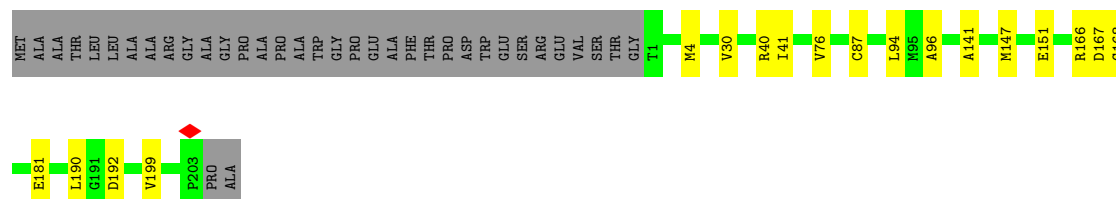
- Molecule 13: Proteasome subunit alpha type-3

Chain m: 



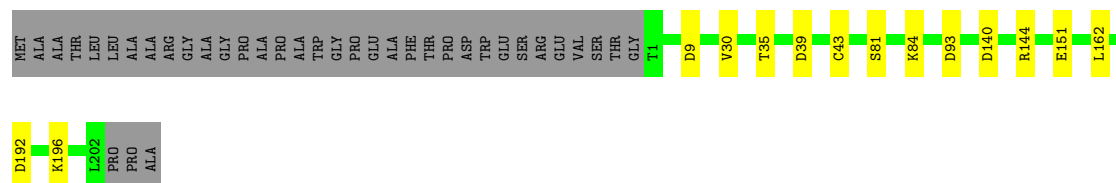
- Molecule 14: Proteasome subunit beta type-6

Chain N: 



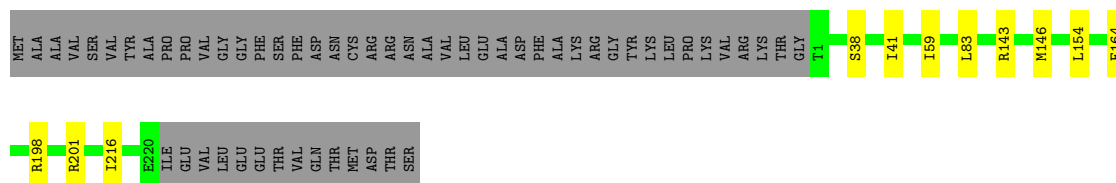
- Molecule 14: Proteasome subunit beta type-6

Chain n: 



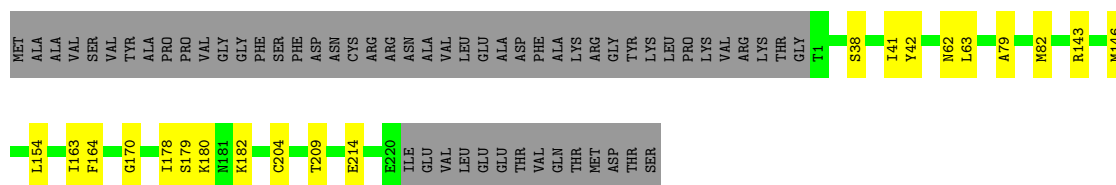
- Molecule 15: Proteasome subunit beta type-7

Chain O:  75% 21%



• Molecule 15: Proteasome subunit beta type-7

Chain o:  72% 7% 21%



• Molecule 16: Proteasome subunit beta type-3

Chain P:  95% 5%



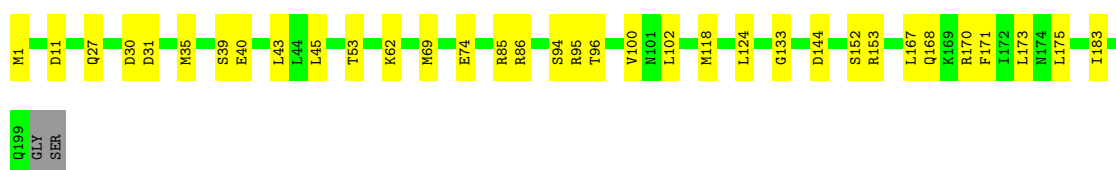
• Molecule 16: Proteasome subunit beta type-3

Chain p:  90% 10%



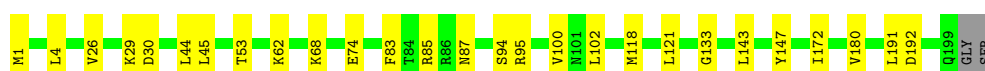
• Molecule 17: Proteasome subunit beta type-2

Chain Q:  82% 17%

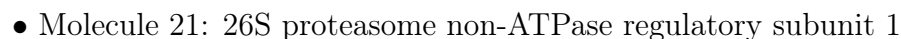


• Molecule 17: Proteasome subunit beta type-2

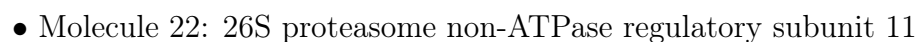
Chain q:  86% 13%



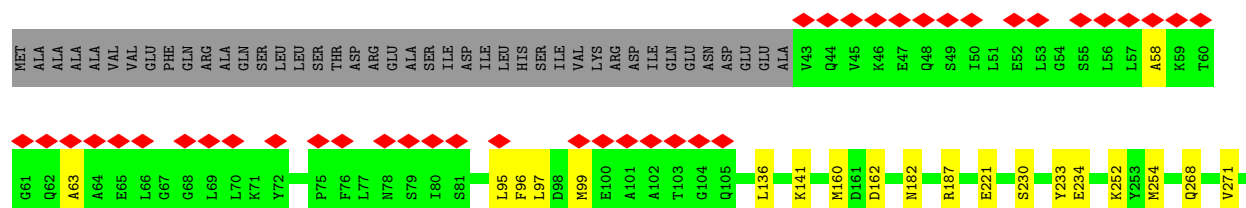
App Type	Percentage
Shopping app	72%
Social media app	9%
Productivity app	18%



Frequency	Percentage
Daily	74%
Weekly	18%
Monthly	8%
Other	7%

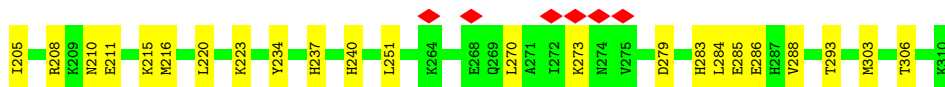
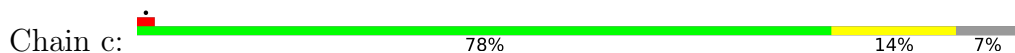


Frequency	Percentage
Daily	10%
Often	82%
Sometimes	8%
Never	10%

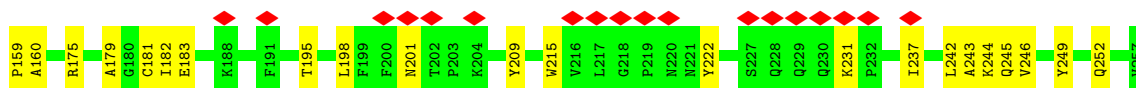
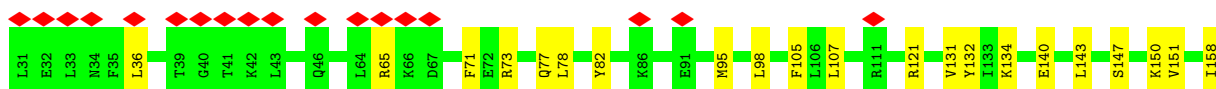
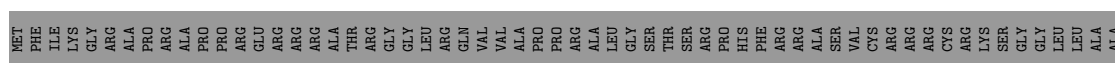




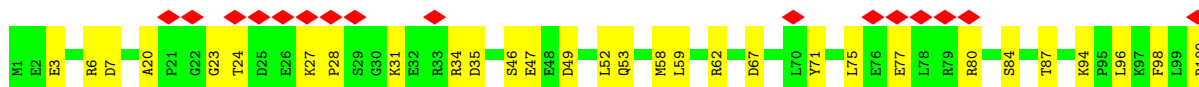
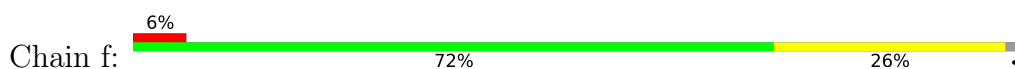
- Molecule 27: 26S proteasome non-ATPase regulatory subunit 14

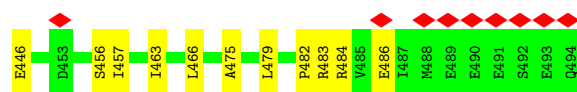


- Molecule 28: 26S proteasome non-ATPase regulatory subunit 8

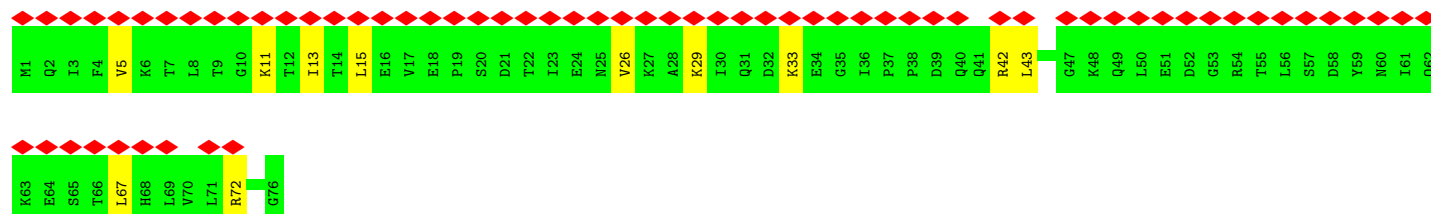
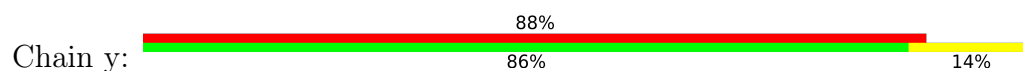


- Molecule 29: 26S proteasome non-ATPase regulatory subunit 2

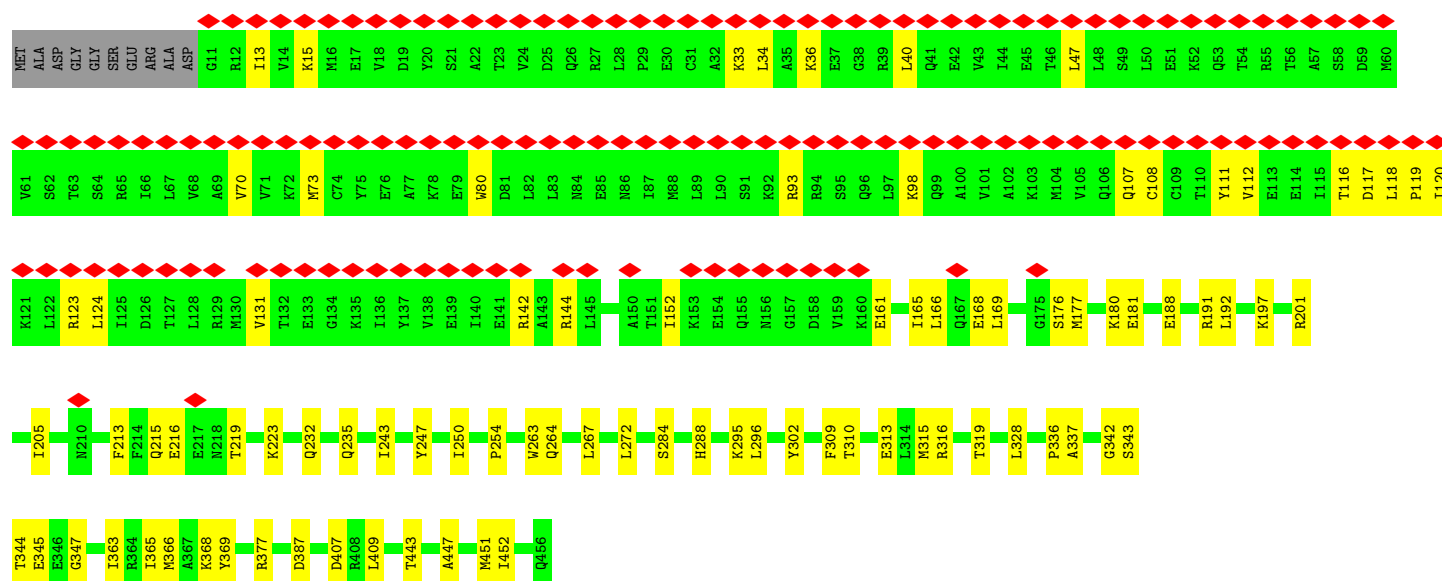
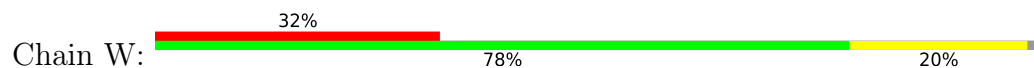




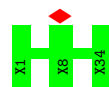
• Molecule 31: Ubiquitin



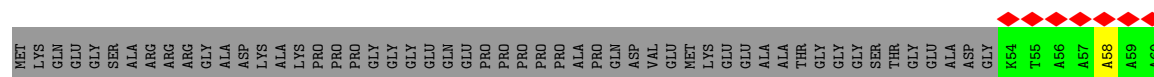
• Molecule 32: 26S proteasome non-ATPase regulatory subunit 12

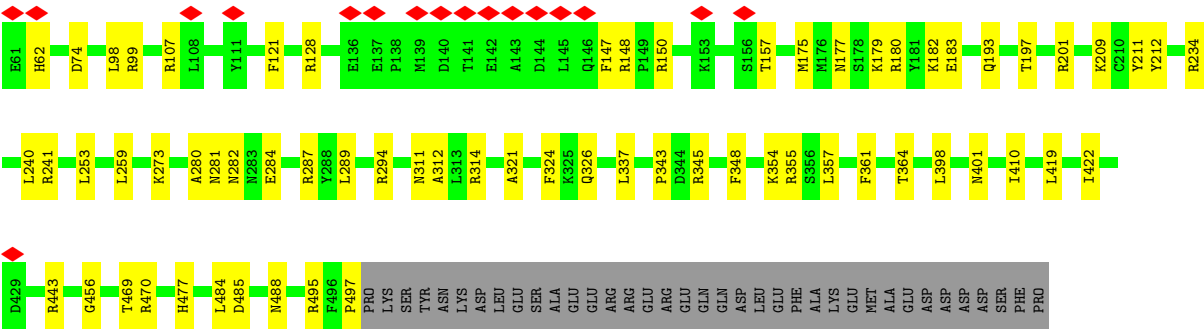


• Molecule 33: Substrate

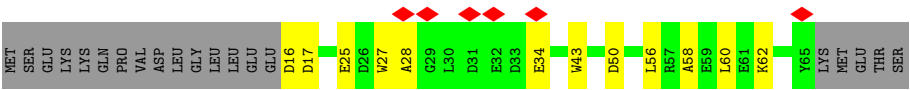


• Molecule 34: 26S proteasome non-ATPase regulatory subunit 3





• Molecule 35: 26S proteasome complex subunit DSS1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	291384	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.018	Depositor
Minimum map value	-0.002	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size ($\text{\AA}$)	438.4, 438.4, 438.4	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.685, 0.685, 0.685	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.18	0/3283	0.44	0/4433
2	B	0.16	0/3254	0.45	0/4388
3	C	0.17	0/3146	0.50	0/4226
4	D	0.20	0/3090	0.48	1/4168 (0.0%)
5	E	0.21	0/3145	0.51	2/4233 (0.0%)
6	F	0.16	0/3137	0.47	0/4223
7	G	0.16	0/1901	0.36	0/2572
7	g	0.16	0/1913	0.41	2/2589 (0.1%)
8	H	0.17	0/1840	0.36	0/2495
8	h	0.20	0/1844	0.40	0/2497
9	I	0.16	0/1963	0.38	0/2650
9	i	0.16	0/1985	0.37	0/2677
10	J	0.15	0/1887	0.38	0/2553
10	j	0.15	0/1887	0.39	0/2549
11	K	0.16	0/1841	0.35	0/2486
11	k	0.14	0/1809	0.31	0/2444
12	L	0.17	0/1911	0.33	0/2584
12	l	0.16	0/1896	0.35	0/2565
13	M	0.16	0/1925	0.36	0/2592
13	m	0.15	0/1916	0.32	0/2580
14	N	0.17	0/1548	0.31	0/2097
14	n	0.16	0/1536	0.32	0/2080
15	O	0.16	0/1672	0.37	0/2267
15	o	0.16	0/1686	0.37	0/2282
16	P	0.16	0/1616	0.36	0/2180
16	p	0.16	0/1620	0.35	0/2184
17	Q	0.17	0/1621	0.37	0/2194
17	q	0.17	0/1611	0.37	0/2182
18	R	0.17	0/1590	0.37	0/2147
18	r	0.15	0/1580	0.30	0/2135
19	S	0.18	0/1671	0.38	0/2252
19	s	0.17	0/1680	0.35	0/2264

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.18	0/1716	0.37	0/2323
20	t	0.16	0/1720	0.33	0/2328
21	U	0.17	0/6945	0.45	0/9382
22	X	0.17	0/3053	0.41	0/4115
23	Y	0.17	0/3173	0.45	0/4273
24	Z	0.22	0/2324	0.49	1/3150 (0.0%)
25	a	0.17	0/3053	0.48	0/4133
26	b	0.18	0/1478	0.49	0/2001
27	c	0.19	0/2302	0.52	0/3110
28	d	0.25	1/2162 (0.0%)	0.50	0/2919
29	f	0.21	0/6980	0.56	1/9433 (0.0%)
30	x	0.13	0/4002	0.37	0/5390
31	y	0.15	0/607	0.39	0/816
32	W	0.21	0/3683	0.50	0/4952
34	V	0.15	0/3681	0.39	0/4969
35	e	0.17	0/437	0.57	1/595 (0.2%)
All	All	0.17	1/112320 (0.0%)	0.43	8/151657 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	d	237	ILE	C-N	6.87	1.39	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	f	24	THR	N-CA-C	-7.75	102.83	111.28
7	g	223	GLU	CA-C-N	7.10	130.07	122.26
7	g	223	GLU	C-N-CA	7.10	130.07	122.26
35	e	28	ALA	CB-CA-C	-5.77	109.90	116.54
5	E	111	LEU	CA-C-N	-5.74	113.64	120.13
5	E	111	LEU	C-N-CA	-5.74	113.64	120.13
24	Z	164	ALA	N-CA-C	5.21	117.19	109.69
4	D	151	ILE	N-CA-C	5.13	115.71	109.30

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	3229	0	3261	44	0
2	B	3207	0	3278	60	0
3	C	3105	0	3219	49	0
4	D	3040	0	3076	60	0
5	E	3097	0	3174	56	0
6	F	3098	0	3187	50	0
7	G	1867	0	1867	15	0
7	g	1879	0	1872	14	0
8	H	1801	0	1773	12	0
8	h	1805	0	1798	8	0
9	I	1933	0	1923	21	0
9	i	1955	0	1955	13	0
10	J	1861	0	1846	18	0
10	j	1861	0	1865	23	0
11	K	1813	0	1796	21	0
11	k	1782	0	1766	15	0
12	L	1876	0	1856	17	0
12	l	1861	0	1839	11	0
13	M	1890	0	1880	18	0
13	m	1881	0	1868	8	0
14	N	1521	0	1494	13	0
14	n	1510	0	1483	11	0
15	O	1645	0	1648	7	0
15	o	1659	0	1681	13	0
16	P	1587	0	1598	9	0
16	p	1591	0	1609	18	0
17	Q	1588	0	1584	26	0
17	q	1578	0	1569	19	0
18	R	1559	0	1523	9	0
18	r	1549	0	1506	15	0
19	S	1641	0	1639	14	0
19	s	1650	0	1645	19	0
20	T	1683	0	1662	12	0
20	t	1687	0	1666	17	0
21	U	6828	0	6884	103	0
22	X	3009	0	3113	24	0
23	Y	3115	0	3120	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	Z	2281	0	2312	41	0
25	a	2995	0	3012	35	0
26	b	1458	0	1505	28	0
27	c	2260	0	2276	33	0
28	d	2116	0	2146	30	0
29	f	6866	0	6866	157	0
30	x	3929	0	3915	48	0
31	y	601	0	629	7	0
32	W	3635	0	3762	60	0
33	v	170	0	46	0	0
34	V	3612	0	3682	47	0
35	e	425	0	328	10	0
36	A	31	0	12	1	0
36	B	31	0	12	1	0
36	C	31	0	12	0	0
36	F	31	0	12	0	0
37	D	27	0	12	2	0
38	c	1	0	0	0	0
All	All	110741	0	111062	1246	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 (1246) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:W:116:THR:HG22	32:W:117:ASP:H	1.15	1.12
32:W:116:THR:HG22	32:W:117:ASP:N	1.93	0.83
29:f:748:LEU:O	29:f:752:HIS:HB2	1.79	0.82
35:e:58:ALA:O	35:e:62:LYS:HB2	1.85	0.77
29:f:548:THR:O	29:f:552:ASP:HB2	1.83	0.76
32:W:116:THR:CG2	32:W:117:ASP:H	1.99	0.71
25:a:138:VAL:O	25:a:142:LEU:HB2	1.90	0.71
5:E:146:ARG:HE	32:W:177:MET:HE1	1.57	0.70
21:U:735:GLY:O	21:U:739:ALA:HB2	1.90	0.70
29:f:84:SER:HB3	29:f:115:PRO:HB3	1.72	0.69
2:B:286:GLU:HB3	3:C:274:LEU:HD23	1.73	0.69
28:d:249:TYR:HH	34:V:477:HIS:HD1	1.42	0.68
13:M:34:SER:HB2	13:M:65:ARG:HH12	1.58	0.68
3:C:17:GLY:HA2	3:C:21:ARG:HB3	1.75	0.68
29:f:634:LYS:HD3	29:f:673:ARG:HH21	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:703:ARG:HH12	29:f:788:MET:HE3	1.57	0.67
29:f:180:GLN:HE21	29:f:215:ASP:HB2	1.60	0.67
12:L:146:GLN:HG3	12:L:161:ILE:HD11	1.76	0.66
17:q:44:LEU:HD11	17:q:102:LEU:HD13	1.76	0.66
32:W:165:ILE:HA	32:W:168:GLU:HG2	1.76	0.66
27:c:216:MET:HG3	27:c:220:LEU:HD12	1.77	0.66
19:S:4:PRO:HB2	20:T:100:ARG:HH21	1.59	0.66
2:B:284:ILE:HD12	2:B:329:MET:HE1	1.78	0.66
21:U:17:PRO:HA	21:U:20:LYS:HE2	1.79	0.65
29:f:229:VAL:HG22	29:f:605:ASN:HB2	1.78	0.65
10:J:63:CYS:SG	10:J:88:ARG:NH2	2.70	0.65
30:x:46:VAL:HA	30:x:71:MET:HA	1.78	0.65
2:B:174:MET:HE1	2:B:248:LEU:HB3	1.79	0.65
21:U:409:GLY:HA3	21:U:445:ALA:HB1	1.78	0.64
29:f:229:VAL:HG21	29:f:607:LEU:HD23	1.78	0.64
35:e:56:LEU:O	35:e:60:LEU:HB2	1.97	0.64
28:d:147:SER:HB3	28:d:150:LYS:HB2	1.78	0.64
3:C:254:ILE:HG13	3:C:269:VAL:HG13	1.79	0.64
13:m:34:SER:HB2	13:m:65:ARG:HH12	1.61	0.64
1:A:362:MET:HE1	2:B:216:ILE:HD11	1.79	0.64
5:E:198:VAL:HG11	5:E:232:MET:HA	1.80	0.64
15:O:198:ARG:HH12	15:O:201:ARG:HA	1.63	0.63
19:S:72:LEU:HD13	19:S:83:MET:HE3	1.78	0.63
27:c:113:HIS:NE2	27:c:115:HIS:CE1	2.65	0.63
29:f:313:GLU:HB2	29:f:316:ASP:HB3	1.80	0.63
21:U:701:ILE:HG21	21:U:810:THR:H	1.63	0.63
29:f:453:SER:HA	29:f:488:ALA:HA	1.81	0.63
23:Y:316:LEU:HA	23:Y:319:MET:HG2	1.80	0.63
19:s:145:LEU:HD21	19:s:182:ALA:HB2	1.81	0.62
30:x:172:PRO:HB2	30:x:175:LEU:HB2	1.81	0.62
29:f:111:GLU:HB3	29:f:154:TRP:HH2	1.65	0.62
4:D:272:THR:HG1	4:D:274:ARG:HH11	1.46	0.62
3:C:117:ARG:HE	3:C:122:THR:HB	1.65	0.62
26:b:48:ASN:HB3	26:b:64:LEU:HB3	1.80	0.62
5:E:329:GLU:HG2	32:W:13:ILE:HG12	1.82	0.62
2:B:103:ARG:HG2	2:B:160:ILE:HD12	1.81	0.62
4:D:162:VAL:O	4:D:221:HIS:ND1	2.33	0.62
21:U:616:ARG:HB2	21:U:647:HIS:HB3	1.83	0.61
29:f:631:LYS:HA	29:f:634:LYS:HE2	1.81	0.61
29:f:664:GLU:H	29:f:668:ALA:HB3	1.66	0.61
30:x:322:ALA:HB1	30:x:482:PRO:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:110:TYR:OH	29:f:118:ASN:ND2	2.32	0.61
10:j:196:LEU:HA	10:j:199:VAL:HG12	1.82	0.61
21:U:799:LYS:NZ	21:U:801:GLN:OE1	2.34	0.61
32:W:131:VAL:HG11	32:W:144:ARG:HB2	1.83	0.61
17:Q:35:MET:HG2	17:Q:45:LEU:HG	1.82	0.61
29:f:672:LEU:HD13	29:f:708:ASP:HB3	1.83	0.61
2:B:387:LYS:HE3	2:B:389:ASP:HB3	1.82	0.61
34:V:121:PHE:O	34:V:128:ARG:NH1	2.34	0.61
11:K:91:LYS:HE2	11:K:119:LEU:HB2	1.83	0.60
20:T:193:THR:HG23	20:T:195:LYS:H	1.66	0.60
30:x:442:ARG:HG2	30:x:443:LYS:HG2	1.83	0.60
3:C:46:GLN:HB2	21:U:639:LEU:HD11	1.83	0.60
8:H:122:THR:HG22	8:H:129:PRO:HB3	1.83	0.60
29:f:281:ILE:HG13	29:f:286:LYS:HB2	1.84	0.60
17:q:68:LYS:HD3	17:q:74:GLU:HG2	1.84	0.60
18:R:97:MET:HE3	18:R:98:GLY:H	1.65	0.60
6:F:251:LEU:HD23	6:F:285:ILE:HG12	1.83	0.60
9:I:231:LYS:O	9:I:235:GLN:NE2	2.35	0.60
29:f:407:MET:HE1	29:f:440:ILE:HG12	1.83	0.60
29:f:828:ARG:HD3	29:f:847:GLY:HA3	1.83	0.60
30:x:463:ILE:HA	30:x:466:LEU:HD12	1.83	0.60
21:U:806:CYS:HB2	21:U:874:ASN:HB2	1.84	0.60
22:X:160:MET:HE1	22:X:162:ASP:HB3	1.84	0.60
29:f:260:SER:HB2	29:f:270:LEU:HB3	1.84	0.60
12:l:206:THR:HG23	12:l:208:LYS:H	1.67	0.60
22:X:58:ALA:HA	22:X:99:MET:HE1	1.84	0.60
29:f:811:LEU:HG	29:f:878:GLU:HA	1.83	0.60
5:E:146:ARG:NH1	5:E:186:ALA:O	2.34	0.59
34:V:469:THR:HG22	34:V:470:ARG:HG2	1.83	0.59
11:K:121:LEU:HD23	11:K:160:GLY:HA3	1.84	0.59
21:U:258:GLN:HG2	21:U:488:THR:HG22	1.82	0.59
23:Y:79:ASP:OD2	23:Y:83:ARG:NH1	2.35	0.59
29:f:603:SER:H	29:f:639:LYS:HA	1.66	0.59
7:g:49:VAL:HG12	7:g:219:VAL:HG23	1.84	0.59
10:j:96:LEU:HB2	17:q:62:LYS:HG3	1.84	0.59
6:F:307:GLN:HA	6:F:310:MET:HE3	1.84	0.59
9:I:140:ASP:OD1	9:I:146:GLN:NE2	2.36	0.59
26:b:62:THR:HG21	26:b:71:ILE:HG12	1.84	0.59
6:F:180:ARG:HH12	6:F:248:PHE:H	1.51	0.59
18:R:19:ARG:NH2	16:p:205:ASP:OD2	2.36	0.59
27:c:151:VAL:HG12	27:c:152:LYS:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:ILE:HD12	2:B:305:ILE:HD12	1.85	0.58
27:c:31:VAL:HB	27:c:205:ILE:HG22	1.85	0.58
29:f:425:GLY:HA3	29:f:451:VAL:HG21	1.84	0.58
23:Y:233:ARG:HA	23:Y:236:LEU:HD22	1.85	0.58
25:a:308:GLU:OE2	32:W:377:ARG:NH2	2.36	0.58
15:o:209:THR:HG22	16:p:169:GLN:HE21	1.68	0.58
34:V:201:ARG:NH1	34:V:241:ARG:O	2.35	0.58
26:b:91:ARG:HH21	26:b:127:LEU:HD11	1.68	0.58
2:B:316:LEU:O	2:B:322:ARG:NH1	2.37	0.58
6:F:205:PRO:O	6:F:325:GLN:NE2	2.36	0.58
5:E:194:ASN:HD21	5:E:228:CYS:HA	1.68	0.58
29:f:67:ASP:O	29:f:71:TYR:HB2	2.04	0.58
21:U:362:ASN:OD1	21:U:395:ARG:NH2	2.36	0.58
29:f:28:PRO:HA	29:f:31:LYS:HE3	1.85	0.58
18:r:179:VAL:HG22	18:r:184:TRP:HB3	1.86	0.58
3:C:163:GLU:HA	3:C:167:LEU:HD13	1.86	0.58
10:j:39:ASP:OD1	10:j:213:ARG:NH1	2.37	0.58
11:K:118:ASN:OD1	12:L:82:ARG:NH2	2.37	0.58
11:k:202:LEU:O	11:k:206:MET:HB2	2.03	0.58
2:B:356:PRO:O	2:B:361:LYS:NZ	2.37	0.57
8:H:143:ARG:HH12	9:I:59:VAL:HG21	1.69	0.57
30:x:422:ALA:HB3	30:x:479:LEU:HD23	1.86	0.57
2:B:233:THR:HG22	2:B:237:LYS:HE2	1.87	0.57
29:f:844:VAL:HG12	29:f:845:ARG:HG3	1.86	0.57
30:x:199:ASP:HB3	30:x:202:GLU:HG2	1.87	0.57
1:A:217:PRO:HG2	1:A:220:THR:HG21	1.85	0.57
2:B:180:PRO:O	2:B:241:ASN:ND2	2.37	0.57
5:E:287:PRO:HA	5:E:290:LEU:HB2	1.86	0.57
13:M:167:LYS:NZ	13:M:206:ASP:OD2	2.37	0.57
23:Y:39:ASP:HA	23:Y:42:MET:HG3	1.87	0.57
29:f:284:SER:HB3	29:f:872:VAL:HG11	1.86	0.57
16:p:49:LEU:HD21	16:p:84:PRO:HG3	1.86	0.57
11:K:16:SER:HB3	11:K:20:ARG:H	1.68	0.57
11:K:203:LYS:HB2	11:K:210:LEU:HD22	1.85	0.57
26:b:18:ASN:ND2	26:b:145:GLU:OE1	2.37	0.57
23:Y:67:VAL:O	23:Y:71:ASN:HB2	2.05	0.57
23:Y:315:THR:HG22	23:Y:353:ILE:HG12	1.86	0.57
29:f:635:LYS:HE3	29:f:778:LEU:HB2	1.87	0.57
2:B:196:GLU:OE1	2:B:349:ARG:NH1	2.38	0.57
3:C:266:ASP:HB2	3:C:269:VAL:HB	1.86	0.57
29:f:706:ILE:HG23	29:f:745:LEU:HG	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:x:163:MET:HA	30:x:166:THR:HG22	1.86	0.57
21:U:353:LEU:HD11	21:U:376:MET:HG3	1.86	0.57
1:A:180:CYS:HB3	1:A:183:GLN:HB2	1.87	0.57
20:T:127:MET:HB3	20:T:128:LEU:HD12	1.87	0.57
28:d:73:ARG:O	28:d:77:GLN:NE2	2.38	0.57
29:f:313:GLU:O	29:f:317:LEU:HB2	2.05	0.57
34:V:289:LEU:HB3	34:V:312:ALA:HB2	1.87	0.57
4:D:353:ASN:HD21	5:E:162:VAL:HG22	1.68	0.56
15:o:143:ARG:H	15:o:146:MET:HE3	1.70	0.56
6:F:224:LEU:HD23	6:F:351:LYS:HB3	1.87	0.56
17:Q:168:GLN:NE2	17:Q:175:LEU:O	2.38	0.56
22:X:384:VAL:HG21	32:W:409:LEU:HD22	1.87	0.56
16:p:122:CYS:SG	16:p:123:SER:N	2.78	0.56
2:B:85:MET:HE1	29:f:618:GLU:HG3	1.86	0.56
4:D:342:ARG:NH1	22:X:234:GLU:OE2	2.39	0.56
32:W:169:LEU:HD13	32:W:205:ILE:HG21	1.87	0.56
34:V:175:MET:HE2	34:V:183:GLU:HB2	1.87	0.56
13:M:187:ARG:O	13:M:191:LYS:NZ	2.38	0.56
20:T:25:ASP:OD1	20:T:41:ARG:NH2	2.37	0.56
30:x:217:ALA:HA	30:x:240:LYS:HD3	1.87	0.56
32:W:263:TRP:HH2	32:W:295:LYS:HG2	1.70	0.56
1:A:369:ARG:NH1	11:K:206:MET:O	2.38	0.56
2:B:67:ARG:HB3	29:f:646:MET:HE1	1.87	0.56
5:E:75:ASN:ND2	6:F:129:ARG:O	2.39	0.56
21:U:510:GLU:HG2	21:U:543:LYS:HE3	1.88	0.56
14:n:144:ARG:NH2	14:n:151:GLU:OE1	2.38	0.56
1:A:303:ILE:HA	1:A:306:LEU:HD12	1.87	0.56
29:f:478:ARG:NH2	29:f:509:LYS:O	2.39	0.56
5:E:359:HIS:O	6:F:211:LYS:NZ	2.39	0.56
19:S:148:LEU:HD23	19:S:178:VAL:HG12	1.88	0.56
29:f:387:GLN:NE2	29:f:388:ASP:OD1	2.39	0.56
6:F:233:LYS:NZ	6:F:332:THR:O	2.32	0.56
29:f:294:MET:SD	29:f:807:ARG:NH2	2.79	0.56
11:k:210:LEU:HA	11:k:214:ASN:HD22	1.69	0.56
2:B:332:ASN:HB2	3:C:258:ARG:HH12	1.70	0.55
9:I:119:GLN:NE2	10:J:79:ASP:OD1	2.37	0.55
29:f:475:ASN:OD1	29:f:478:ARG:NH2	2.38	0.55
13:M:15:SER:HB3	13:M:19:ARG:H	1.71	0.55
3:C:113:ARG:NH2	4:D:94:GLU:OE1	2.39	0.55
23:Y:385:ARG:NH2	34:V:280:ALA:O	2.39	0.55
24:Z:12:HIS:ND1	24:Z:50:VAL:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:264:ASN:HB3	25:a:267:GLN:HG2	1.89	0.55
26:b:100:ARG:NH1	26:b:102:GLY:O	2.40	0.55
19:s:4:PRO:HB2	20:t:100:ARG:HH11	1.71	0.55
20:t:166:ARG:NH1	20:t:200:GLU:OE1	2.39	0.55
30:x:215:LEU:O	30:x:240:LYS:NZ	2.40	0.55
28:d:195:THR:HB	28:d:201:ASN:HA	1.86	0.55
29:f:257:ARG:HD3	29:f:289:VAL:HG11	1.87	0.55
31:y:13:ILE:HD11	31:y:33:LYS:HZ2	1.70	0.55
7:G:181:LYS:O	7:G:185:LYS:NZ	2.40	0.55
25:a:26:GLU:OE1	25:a:29:TYR:OH	2.24	0.55
4:D:167:ILE:HG23	4:D:170:MET:HE2	1.88	0.55
4:D:412:GLN:NE2	4:D:415:GLU:OE1	2.40	0.55
27:c:303:MET:HE1	28:d:242:LEU:HB2	1.88	0.55
5:E:149:ILE:O	5:E:274:LYS:NZ	2.39	0.55
3:C:118:ASN:ND2	3:C:119:ASP:OD1	2.40	0.55
21:U:743:ASN:OD1	21:U:883:ARG:NH1	2.39	0.55
23:Y:50:MET:HA	23:Y:53:TYR:HB3	1.88	0.55
23:Y:78:GLU:OE2	23:Y:107:LYS:NZ	2.40	0.55
23:Y:124:PHE:HA	23:Y:127:THR:HG22	1.88	0.55
29:f:23:GLY:HA2	29:f:27:LYS:HB2	1.88	0.55
4:D:200:ARG:NH2	4:D:302:ASN:O	2.40	0.54
8:H:212:ILE:HD12	8:H:221:LEU:HD21	1.88	0.54
11:K:20:ARG:NH2	11:K:25:GLU:OE2	2.41	0.54
12:L:41:LYS:O	12:L:217:LYS:NZ	2.39	0.54
26:b:12:ASN:HA	26:b:16:MET:HG2	1.89	0.54
34:V:287:ARG:NH2	35:e:17:ASP:OD2	2.40	0.54
1:A:213:LEU:HB3	1:A:340:LYS:HA	1.89	0.54
2:B:49:LEU:HD21	29:f:649:HIS:HB3	1.89	0.54
34:V:484:LEU:O	34:V:488:ASN:ND2	2.41	0.54
1:A:272:ILE:HB	1:A:317:VAL:HA	1.89	0.54
3:C:99:VAL:HB	3:C:103:ILE:HD11	1.89	0.54
7:G:165:ALA:HB3	8:H:56:LEU:HD22	1.89	0.54
10:J:52:LYS:HB3	10:J:53:LEU:HD12	1.89	0.54
29:f:176:ALA:HB3	29:f:178:LYS:HE2	1.90	0.54
29:f:531:ASN:HA	29:f:534:VAL:HG22	1.89	0.54
29:f:559:PRO:HB2	29:f:594:LEU:HD22	1.88	0.54
7:g:141:ILE:HG22	7:g:151:VAL:HG22	1.88	0.54
4:D:203:LEU:HB2	4:D:327:LEU:HD22	1.90	0.54
25:a:278:MET:HA	25:a:281:THR:HG22	1.89	0.54
29:f:779:CYS:HA	29:f:782:HIS:CE1	2.43	0.54
32:W:47:LEU:HD21	32:W:70:VAL:HG11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:141:SER:HB3	13:M:144:ASP:HB2	1.89	0.54
21:U:401:LYS:HB3	21:U:438:GLN:HG2	1.90	0.54
29:f:34:ARG:NH1	29:f:35:ASP:OD1	2.41	0.54
29:f:107:LYS:HB3	29:f:137:ARG:HD2	1.89	0.54
29:f:125:ILE:HG12	29:f:129:LEU:HB2	1.89	0.54
1:A:34:LYS:HG3	1:A:35:THR:HG23	1.90	0.54
1:A:170:PRO:O	1:A:231:ASN:ND2	2.35	0.54
1:A:178:GLY:O	36:A:501:ATP:N6	2.40	0.54
9:i:72:MET:HE2	9:i:110:LEU:HD23	1.89	0.54
10:j:211:MET:HG3	10:j:217:LEU:HB3	1.89	0.54
31:y:26:VAL:HA	31:y:29:LYS:HZ1	1.72	0.54
32:W:188:GLU:OE2	32:W:191:ARG:NH2	2.41	0.54
4:D:272:THR:OG1	4:D:274:ARG:NH1	2.38	0.53
29:f:584:SER:HB2	29:f:588:ARG:HB3	1.91	0.53
3:C:248:MET:HG3	3:C:251:ILE:HD11	1.89	0.53
5:E:87:LEU:HB3	5:E:92:LEU:HD11	1.90	0.53
5:E:171:LEU:HD13	5:E:295:LEU:HD21	1.90	0.53
7:G:206:LEU:HB3	7:G:208:ILE:HG12	1.90	0.53
9:I:108:GLU:OE1	10:J:57:ARG:NH2	2.41	0.53
32:W:284:SER:O	32:W:288:HIS:ND1	2.41	0.53
5:E:174:GLY:O	5:E:280:ASN:ND2	2.39	0.53
5:E:352:MET:HA	5:E:355:ILE:HG12	1.91	0.53
7:G:10:ASP:OD1	7:G:10:ASP:N	2.41	0.53
26:b:13:SER:OG	26:b:14:GLU:N	2.42	0.53
29:f:285:CYS:HB3	29:f:872:VAL:HB	1.90	0.53
9:i:119:GLN:HG3	10:j:78:ALA:HB1	1.89	0.53
2:B:254:GLU:O	2:B:257:GLN:NE2	2.39	0.53
3:C:215:SER:OG	3:C:216:GLY:N	2.42	0.53
8:H:59:GLU:OE2	8:H:60:ARG:NH1	2.41	0.53
25:a:61:GLU:HA	25:a:64:ILE:HD12	1.90	0.53
10:j:38:ARG:NH1	10:j:182:GLU:OE1	2.41	0.53
34:V:58:ALA:O	34:V:62:HIS:ND1	2.41	0.53
4:D:203:LEU:HD22	4:D:327:LEU:HD13	1.90	0.53
36:B:501:ATP:O1G	3:C:310:ARG:NH2	2.42	0.53
16:P:205:ASP:HB3	18:r:192:VAL:HG11	1.91	0.53
20:t:54:SER:O	20:t:108:ASN:ND2	2.33	0.53
20:t:153:VAL:HG21	20:t:168:LEU:HD11	1.89	0.53
30:x:30:LYS:HB3	30:x:41:PRO:HB3	1.89	0.53
4:D:327:LEU:O	4:D:330:LYS:NZ	2.39	0.53
24:Z:37:GLY:HA2	24:Z:56:VAL:HG12	1.90	0.53
32:W:235:GLN:HB3	32:W:243:ILE:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:V:74:ASP:OD2	34:V:107:ARG:NH2	2.42	0.53
6:F:362:ARG:NH2	6:F:385:ALA:O	2.38	0.53
21:U:522:GLY:O	21:U:559:ARG:NH2	2.42	0.53
27:c:251:LEU:HD13	27:c:283:HIS:HB3	1.90	0.53
34:V:337:LEU:HD21	34:V:364:THR:HG23	1.89	0.53
4:D:398:ASP:OD1	4:D:398:ASP:N	2.42	0.53
6:F:285:ILE:HB	6:F:330:ALA:HA	1.91	0.53
29:f:291:GLN:NE2	29:f:325:GLN:OE1	2.42	0.53
9:i:18:LEU:HB2	9:i:21:VAL:HG22	1.90	0.53
32:W:247:TYR:HA	32:W:250:ILE:HG12	1.90	0.53
2:B:412:MET:HG2	29:f:52:LEU:HG	1.90	0.53
23:Y:23:ARG:HH22	23:Y:52:PRO:HB2	1.73	0.53
23:Y:268:TYR:HA	23:Y:271:PHE:HB3	1.91	0.53
29:f:464:ALA:HB3	30:x:47:MET:HE3	1.90	0.53
11:k:85:ALA:HB2	11:k:139:VAL:HG11	1.90	0.53
32:W:337:ALA:O	32:W:342:GLY:N	2.42	0.53
13:M:136:MET:HG2	13:M:150:MET:HB2	1.92	0.52
27:c:64:ASP:OD1	27:c:64:ASP:N	2.41	0.52
32:W:254:PRO:HD3	32:W:263:TRP:CD1	2.44	0.52
23:Y:389:MET:SD	34:V:99:ARG:NH2	2.78	0.52
17:q:180:VAL:HG23	17:q:191:LEU:HB2	1.92	0.52
1:A:213:LEU:HD12	1:A:337:LEU:HD13	1.91	0.52
6:F:30:GLY:HA2	6:F:34:LEU:HD13	1.91	0.52
21:U:471:ASP:HB2	21:U:507:VAL:HB	1.90	0.52
28:d:143:LEU:HB3	28:d:151:VAL:HG21	1.92	0.52
29:f:227:ALA:HB3	29:f:234:THR:HG22	1.89	0.52
29:f:680:ARG:HA	29:f:715:HIS:HA	1.91	0.52
2:B:297:SER:O	2:B:303:ARG:NH1	2.42	0.52
7:G:54:LYS:NZ	7:G:216:GLU:OE2	2.41	0.52
7:G:244:GLU:HA	32:W:93:ARG:HD3	1.92	0.52
14:N:166:ARG:NH2	14:n:140:ASP:OD2	2.40	0.52
22:X:63:ALA:HB1	22:X:96:PHE:HD1	1.75	0.52
20:t:25:ASP:OD1	20:t:41:ARG:NH2	2.38	0.52
32:W:118:LEU:HB3	32:W:119:PRO:HD3	1.89	0.52
3:C:115:ALA:O	3:C:124:HIS:N	2.42	0.52
7:G:165:ALA:HB1	7:G:179:LEU:HD13	1.90	0.52
17:Q:102:LEU:HD11	17:Q:118:MET:HE3	1.91	0.52
31:y:42:ARG:HE	31:y:72:ARG:HG2	1.74	0.52
21:U:740:GLY:O	21:U:743:ASN:ND2	2.41	0.52
24:Z:263:ALA:HB1	27:c:288:VAL:HG13	1.92	0.52
2:B:372:MET:HE1	2:B:399:CYS:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:251:ILE:H	3:C:295:THR:HB	1.75	0.52
3:C:339:THR:OG1	3:C:340:ARG:N	2.42	0.52
5:E:196:LEU:HD13	5:E:218:MET:HE2	1.92	0.52
6:F:289:ASP:OD1	6:F:289:ASP:N	2.43	0.52
21:U:847:GLU:O	21:U:851:GLU:HB2	2.09	0.52
1:A:397:ILE:HD12	2:B:210:TYR:HB3	1.92	0.52
6:F:339:ASP:HB3	6:F:342:LEU:HB2	1.92	0.52
19:s:75:TYR:OH	19:s:81:LYS:NZ	2.42	0.52
34:V:150:ARG:NH1	34:V:157:THR:O	2.43	0.52
1:A:32:LEU:HD13	29:f:96:LEU:HD23	1.92	0.52
2:B:122:ILE:HD11	2:B:130:GLU:HB3	1.91	0.52
29:f:190:GLU:HB3	29:f:193:PRO:HG2	1.92	0.52
29:f:407:MET:HA	29:f:410:ALA:HB3	1.92	0.52
4:D:97:ASP:OD1	4:D:100:THR:OG1	2.28	0.52
12:L:67:ASP:OD1	12:L:96:ARG:NH2	2.43	0.52
14:N:199:VAL:HG13	20:t:37:ARG:HH21	1.75	0.52
21:U:78:LEU:HD11	21:U:103:LYS:HG3	1.92	0.52
23:Y:376:LEU:HD23	24:Z:265:LEU:HD21	1.91	0.52
25:a:273:GLN:HB3	25:a:310:LEU:HD11	1.92	0.52
25:a:274:LEU:HB2	25:a:313:LYS:HZ3	1.74	0.52
28:d:7:GLY:HA2	28:d:18:LYS:HE2	1.92	0.52
12:l:132:LEU:HB2	12:l:147:THR:HB	1.90	0.52
1:A:160:THR:HA	1:A:163:MET:HG2	1.92	0.51
2:B:44:ASP:OD1	2:B:44:ASP:N	2.42	0.51
23:Y:132:VAL:HA	23:Y:137:ARG:HH21	1.74	0.51
29:f:353:LEU:HG	29:f:355:ASN:H	1.75	0.51
10:j:40:ILE:HG22	10:j:212:ARG:HG3	1.91	0.51
3:C:222:LYS:HD2	4:D:239:TYR:HD2	1.75	0.51
3:C:266:ASP:OD1	3:C:266:ASP:N	2.43	0.51
4:D:130:VAL:HG12	4:D:142:VAL:HG22	1.93	0.51
16:P:58:THR:O	17:Q:85:ARG:NH2	2.42	0.51
26:b:2:VAL:O	26:b:44:ASN:ND2	2.42	0.51
5:E:83:CYS:HB2	5:E:87:LEU:HB2	1.92	0.51
21:U:49:TYR:HA	21:U:57:ARG:HB2	1.92	0.51
20:t:1:THR:N	20:t:105:PRO:O	2.43	0.51
4:D:92:PHE:HZ	4:D:95:ALA:HB2	1.75	0.51
9:I:4:ARG:HB3	10:J:5:ARG:HH21	1.75	0.51
9:I:123:GLN:NE2	10:J:125:ARG:O	2.43	0.51
21:U:356:THR:HG21	21:U:731:ILE:HD13	1.91	0.51
10:J:146:GLN:OE1	10:J:159:ASN:ND2	2.44	0.51
19:S:123:SER:HB2	19:S:136:LYS:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:366:HIS:NE2	21:U:392:TRP:O	2.42	0.51
32:W:80:TRP:HB3	32:W:123:ARG:HH11	1.74	0.51
34:V:177:ASN:O	34:V:179:LYS:NZ	2.43	0.51
2:B:229:GLY:O	2:B:391:SER:OG	2.27	0.51
4:D:345:PHE:HB3	4:D:360:LEU:HD13	1.90	0.51
9:I:35:LEU:HD11	9:I:175:LEU:HD11	1.93	0.51
12:L:164:ARG:HH12	12:L:200:PRO:HG3	1.76	0.51
21:U:545:LEU:HB3	21:U:577:ILE:HG21	1.92	0.51
24:Z:19:VAL:HG21	24:Z:124:ILE:HD12	1.93	0.51
8:h:205:GLU:HG2	8:h:227:LYS:HD3	1.93	0.51
10:J:96:LEU:HB2	17:Q:62:LYS:HG3	1.92	0.51
21:U:8:ILE:HD13	28:d:36:LEU:HD22	1.92	0.51
21:U:475:HIS:NE2	21:U:510:GLU:OE2	2.37	0.51
21:U:521:LEU:HD11	21:U:761:VAL:HG21	1.92	0.51
23:Y:180:LEU:HA	23:Y:183:TYR:HD2	1.76	0.51
15:o:163:ILE:HG12	15:o:170:GLY:HA2	1.92	0.51
32:W:152:ILE:HD12	32:W:161:GLU:HB3	1.93	0.51
2:B:107:MET:HB3	3:C:96:VAL:HB	1.93	0.51
3:C:281:ASP:HB3	3:C:310:ARG:HE	1.76	0.51
26:b:58:CYS:HB3	26:b:92:VAL:HG21	1.93	0.51
29:f:333:LEU:HG	29:f:337:LEU:HD22	1.92	0.51
29:f:346:ASP:OD1	29:f:346:ASP:N	2.43	0.51
29:f:691:PRO:HB2	29:f:692:LEU:HD12	1.93	0.51
18:r:37:ILE:HD13	18:r:59:LEU:HD22	1.93	0.51
2:B:221:GLY:HA3	2:B:347:ILE:HA	1.92	0.51
13:M:7:TYR:HD2	13:M:16:PRO:HD3	1.75	0.51
21:U:646:PRO:HB3	21:U:680:VAL:HG21	1.93	0.51
29:f:554:TYR:OH	29:f:789:SER:O	2.26	0.51
32:W:343:SER:OG	32:W:347:GLY:N	2.44	0.51
6:F:374:ASN:ND2	6:F:374:ASN:O	2.44	0.50
22:X:344:ARG:HH21	32:W:409:LEU:HB3	1.75	0.50
29:f:281:ILE:HB	29:f:284:SER:HB2	1.93	0.50
32:W:216:GLU:OE1	32:W:223:LYS:NZ	2.42	0.50
3:C:155:ASP:N	3:C:155:ASP:OD1	2.44	0.50
5:E:322:LYS:HA	5:E:362:VAL:H	1.76	0.50
5:E:359:HIS:ND1	5:E:361:PHE:O	2.43	0.50
21:U:890:LYS:HG3	21:U:891:VAL:HG13	1.93	0.50
29:f:511:SER:H	29:f:514:VAL:HB	1.76	0.50
2:B:174:MET:O	2:B:249:ARG:NH1	2.45	0.50
9:I:153:SER:OG	9:I:155:ASN:OD1	2.29	0.50
28:d:175:ARG:HG2	28:d:198:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:347:ASP:HA	29:f:350:LYS:HB2	1.93	0.50
9:i:106:PRO:HB2	9:i:109:GLN:HG3	1.94	0.50
11:k:90:ASP:OD1	18:r:69:ARG:NH1	2.44	0.50
21:U:685:GLN:HG2	21:U:729:GLY:HA3	1.93	0.50
29:f:567:LEU:HA	29:f:599:ALA:HA	1.94	0.50
34:V:284:GLU:OE2	34:V:287:ARG:NH1	2.44	0.50
12:L:72:ILE:HG22	12:L:134:ILE:HG12	1.94	0.50
17:Q:43:LEU:HB2	17:Q:183:ILE:HD11	1.92	0.50
21:U:583:MET:SD	21:U:621:SER:OG	2.64	0.50
21:U:793:LYS:HB2	21:U:796:LYS:HB2	1.93	0.50
15:o:204:CYS:HB2	16:p:162:HIS:HD2	1.77	0.50
17:q:192:ASP:OD1	17:q:192:ASP:N	2.44	0.50
21:U:605:VAL:O	21:U:609:ASP:HB2	2.12	0.50
23:Y:131:THR:O	23:Y:137:ARG:NH2	2.45	0.50
10:j:121:SER:HB2	10:j:124:ARG:HD2	1.94	0.50
16:p:38:ASP:OD1	16:p:38:ASP:N	2.44	0.50
9:I:62:SER:OG	9:I:212:GLU:OE2	2.24	0.50
11:K:182:GLN:NE2	12:L:55:GLU:OE2	2.44	0.50
21:U:85:GLY:HA2	21:U:129:ARG:HG2	1.94	0.50
27:c:210:ASN:ND2	27:c:211:GLU:O	2.45	0.50
34:V:311:ASN:OD1	34:V:314:ARG:NH2	2.45	0.50
15:O:216:ILE:HD11	16:P:194:LYS:HD2	1.94	0.50
21:U:567:ILE:HD12	21:U:586:VAL:HB	1.93	0.50
22:X:63:ALA:HB2	22:X:99:MET:HE3	1.93	0.50
25:a:188:LEU:HB2	25:a:193:GLN:HE21	1.76	0.50
4:D:121:ARG:O	4:D:125:LYS:NZ	2.41	0.50
4:D:223:THR:HG22	4:D:225:ALA:H	1.76	0.50
21:U:233:LEU:HD22	21:U:325:MET:HE1	1.94	0.50
21:U:838:LYS:NZ	29:f:147:SER:OG	2.45	0.50
12:L:133:LEU:HG	12:L:161:ILE:HD12	1.94	0.49
18:R:192:VAL:HG11	16:p:205:ASP:HB3	1.93	0.49
24:Z:134:PRO:HB3	27:c:220:LEU:HB3	1.93	0.49
28:d:107:LEU:HD11	28:d:140:GLU:HB2	1.94	0.49
14:n:35:THR:OG1	14:n:43:CYS:SG	2.70	0.49
18:r:12:VAL:HG21	18:r:102:CYS:HB3	1.94	0.49
30:x:257:CYS:SG	30:x:258:THR:N	2.85	0.49
34:V:259:LEU:HD11	34:V:294:ARG:HD3	1.94	0.49
1:A:293:ASN:O	1:A:297:ARG:NH1	2.46	0.49
3:C:184:LYS:N	3:C:312:ASP:OD2	2.43	0.49
4:D:353:ASN:ND2	4:D:392:TYR:O	2.45	0.49
32:W:33:LYS:HA	32:W:36:LYS:HG2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:LYS:HA	2:B:144:LEU:HD13	1.93	0.49
2:B:339:PRO:HA	2:B:342:ILE:HG12	1.94	0.49
19:S:40:SER:O	19:S:40:SER:OG	2.30	0.49
34:V:147:PHE:O	34:V:148:ARG:NH1	2.46	0.49
3:C:62:GLU:OE1	4:D:114:ARG:NH2	2.45	0.49
4:D:141:ASP:N	4:D:141:ASP:OD1	2.45	0.49
8:H:135:LEU:HG	8:H:163:MET:HE2	1.95	0.49
28:d:252:GLN:HB3	34:V:484:LEU:HD13	1.95	0.49
10:j:146:GLN:OE1	10:j:159:ASN:ND2	2.45	0.49
17:q:102:LEU:HD11	17:q:118:MET:HE2	1.95	0.49
24:Z:111:LEU:O	24:Z:114:ARG:NE	2.44	0.49
29:f:297:MET:O	29:f:301:HIS:ND1	2.45	0.49
7:g:11:ARG:O	7:g:24:GLN:NE2	2.45	0.49
10:j:70:CYS:SG	10:j:71:MET:N	2.85	0.49
15:o:63:LEU:HD11	15:o:79:ALA:HB2	1.94	0.49
30:x:483:ARG:NH1	30:x:484:ARG:O	2.45	0.49
34:V:419:LEU:HD12	34:V:456:GLY:HA2	1.94	0.49
1:A:245:LEU:HD12	1:A:280:ILE:HG21	1.94	0.49
2:B:198:LYS:NZ	2:B:202:GLU:OE1	2.40	0.49
4:D:159:LYS:H	4:D:160:PRO:HD3	1.77	0.49
9:I:41:ASP:OD1	9:I:41:ASP:N	2.45	0.49
10:J:199:VAL:HG12	10:J:202:GLY:H	1.77	0.49
17:Q:118:MET:HE2	17:Q:124:LEU:HD13	1.94	0.49
21:U:78:LEU:HD21	21:U:103:LYS:HB3	1.95	0.49
29:f:53:GLN:HB2	29:f:58:MET:HE1	1.94	0.49
29:f:633:GLU:OE2	29:f:673:ARG:NH1	2.46	0.49
10:j:116:GLN:HG3	11:k:83:ALA:HB1	1.93	0.49
13:m:8:ASP:OD1	13:m:8:ASP:N	2.46	0.49
30:x:97:LEU:HG	30:x:101:MET:HE1	1.94	0.49
4:D:237:GLN:HG2	4:D:239:TYR:H	1.77	0.49
17:Q:31:ASP:OD1	17:Q:31:ASP:N	2.46	0.49
23:Y:138:LEU:HD13	23:Y:168:ILE:HG21	1.93	0.49
23:Y:141:VAL:HG11	23:Y:164:ALA:HB2	1.94	0.49
23:Y:262:SER:OG	23:Y:267:ARG:O	2.31	0.49
7:g:231:THR:OG1	7:g:234:GLU:OE1	2.23	0.49
11:k:99:HIS:HB2	11:k:107:MET:HE3	1.95	0.49
13:m:139:SER:OG	13:m:140:TYR:N	2.45	0.49
19:s:125:ASP:OD1	19:s:129:SER:N	2.45	0.49
1:A:324:PRO:HA	1:A:327:LEU:HD13	1.94	0.49
4:D:115:ILE:HA	4:D:139:LEU:HB3	1.94	0.49
21:U:406:ALA:HA	21:U:445:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:62:ASP:OD1	23:Y:62:ASP:N	2.45	0.49
29:f:7:ASP:N	29:f:7:ASP:OD1	2.45	0.49
29:f:422:VAL:HG22	29:f:455:VAL:HG21	1.94	0.49
30:x:280:ASN:ND2	30:x:282:GLU:OE1	2.45	0.49
5:E:9:LEU:HG	5:E:13:ARG:HH21	1.78	0.49
6:F:336:ASP:OD1	6:F:336:ASP:N	2.43	0.49
14:N:141:ALA:HB2	14:n:162:LEU:HD11	1.95	0.49
20:T:96:MET:HE1	20:T:108:ASN:HB2	1.95	0.49
24:Z:256:GLN:HA	24:Z:259:VAL:HG12	1.95	0.49
25:a:54:ASP:N	25:a:54:ASP:OD1	2.43	0.49
29:f:267:ARG:HA	29:f:271:MET:HB2	1.94	0.49
29:f:398:TRP:HD1	29:f:401:LYS:HE2	1.77	0.49
29:f:834:ASP:OD1	29:f:834:ASP:N	2.46	0.49
1:A:294:GLU:HG2	6:F:259:MET:HE1	1.95	0.49
22:X:343:SER:OG	32:W:407:ASP:OD1	2.31	0.49
23:Y:210:SER:H	23:Y:213:LEU:HD12	1.77	0.49
24:Z:25:ARG:HA	24:Z:28:LYS:HE3	1.95	0.49
32:W:216:GLU:HA	32:W:219:THR:HB	1.94	0.49
21:U:832:VAL:HG21	29:f:610:GLN:HG3	1.95	0.48
22:X:364:LYS:HG3	22:X:368:MET:HE3	1.95	0.48
28:d:252:GLN:NE2	34:V:485:ASP:OD1	2.45	0.48
29:f:288:VAL:HG21	29:f:880:ALA:HA	1.95	0.48
14:n:9:ASP:OD1	14:n:9:ASP:N	2.41	0.48
20:t:89:HIS:HD2	20:t:112:ILE:HD12	1.78	0.48
1:A:261:PHE:HD2	1:A:305:GLN:HG3	1.77	0.48
4:D:358:VAL:HG22	4:D:396:ALA:HB2	1.94	0.48
5:E:22:ILE:HD12	5:E:25:ARG:HH21	1.77	0.48
9:I:207:SER:OG	9:I:209:GLU:OE1	2.31	0.48
26:b:137:ASN:HB2	26:b:168:SER:HB2	1.96	0.48
29:f:106:LEU:HD23	29:f:137:ARG:HD3	1.95	0.48
29:f:713:PHE:HB2	29:f:749:ALA:HB1	1.95	0.48
30:x:48:VAL:HG11	30:x:61:ILE:HG21	1.95	0.48
30:x:307:ARG:HH12	30:x:309:ALA:HB2	1.77	0.48
3:C:375:ARG:NH1	3:C:377:HIS:O	2.47	0.48
21:U:54:PHE:O	21:U:57:ARG:NH2	2.46	0.48
29:f:117:GLU:H	29:f:120:ARG:HH21	1.62	0.48
29:f:555:ALA:HA	29:f:558:LEU:HD23	1.95	0.48
9:i:140:ASP:OD1	9:i:146:GLN:NE2	2.46	0.48
1:A:55:LEU:HA	1:A:58:LYS:HG2	1.95	0.48
19:S:28:ARG:NH2	19:S:213:ASP:OXT	2.46	0.48
21:U:628:ARG:NH1	21:U:753:GLY:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:46:SER:HB3	29:f:129:LEU:HD11	1.95	0.48
12:l:196:ARG:NH1	12:l:237:GLU:O	2.45	0.48
32:W:296:LEU:HD21	32:W:302:TYR:HA	1.95	0.48
1:A:364:VAL:HG12	1:A:404:ALA:HB3	1.96	0.48
1:A:398:ARG:NH2	2:B:196:GLU:OE2	2.45	0.48
2:B:412:MET:H	29:f:52:LEU:HD23	1.78	0.48
3:C:38:LYS:HB3	4:D:54:LEU:HD23	1.95	0.48
21:U:794:ASP:OD1	21:U:794:ASP:N	2.45	0.48
29:f:3:GLU:HB2	29:f:6:ARG:HB2	1.96	0.48
29:f:585:GLU:HG2	29:f:587:PHE:H	1.78	0.48
29:f:690:VAL:HA	29:f:694:LEU:HD13	1.96	0.48
9:i:155:ASN:OD1	10:j:77:THR:OG1	2.31	0.48
32:W:34:LEU:HG	32:W:40:LEU:HD21	1.95	0.48
2:B:413:LYS:NZ	29:f:49:ASP:O	2.43	0.48
6:F:363:ALA:HA	6:F:366:MET:HE2	1.96	0.48
24:Z:69:PHE:HZ	26:b:63:THR:HG23	1.78	0.48
29:f:106:LEU:HD13	29:f:133:MET:HE1	1.95	0.48
19:s:10:GLY:HA3	19:s:42:LYS:HE3	1.94	0.48
30:x:48:VAL:HG11	30:x:61:ILE:HD13	1.95	0.48
2:B:178:LYS:NZ	2:B:179:ALA:O	2.46	0.48
21:U:376:MET:HE3	21:U:735:GLY:HA2	1.95	0.48
24:Z:34:ARG:NH1	24:Z:100:LYS:O	2.41	0.48
30:x:301:GLN:HA	30:x:308:ASN:HA	1.96	0.48
3:C:49:ARG:NH2	4:D:64:GLU:OE2	2.41	0.48
5:E:123:SER:HA	5:E:218:MET:HE1	1.94	0.48
9:I:76:VAL:HG12	9:I:134:LEU:HG	1.95	0.48
24:Z:211:TYR:HA	24:Z:214:LYS:HE3	1.96	0.48
29:f:468:ASP:OD1	29:f:468:ASP:N	2.45	0.48
12:l:182:CYS:HB3	12:l:186:GLU:HB3	1.95	0.48
1:A:218:PRO:HB3	1:A:322:ASN:HD21	1.78	0.48
1:A:292:ASP:OD1	1:A:292:ASP:N	2.45	0.48
4:D:209:GLY:N	37:D:501:ADP:O3B	2.44	0.48
15:O:59:ILE:HG13	15:O:83:LEU:HD23	1.95	0.48
17:Q:95:ARG:HG3	17:Q:96:THR:HG23	1.96	0.48
21:U:201:LEU:O	21:U:205:TYR:HB2	2.14	0.48
25:a:246:GLU:HB3	25:a:249:GLN:HB3	1.95	0.48
29:f:530:CYS:HB3	29:f:565:ASN:HD21	1.78	0.48
29:f:603:SER:HB2	29:f:639:LYS:HB2	1.95	0.48
7:g:164:LYS:NZ	8:h:55:ILE:O	2.44	0.48
17:Q:39:SER:OG	17:Q:40:GLU:N	2.47	0.48
23:Y:133:ALA:HB3	23:Y:136:HIS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:r:12:VAL:HG22	18:r:179:VAL:HB	1.96	0.48
2:B:152:LEU:HD23	2:B:157:HIS:HB3	1.95	0.47
3:C:185:GLY:N	3:C:312:ASP:OD2	2.39	0.47
4:D:82:ILE:HA	27:c:152:LYS:HE3	1.96	0.47
4:D:97:ASP:OD1	4:D:97:ASP:N	2.46	0.47
4:D:171:ASP:OD1	4:D:171:ASP:N	2.47	0.47
21:U:36:ALA:O	34:V:273:LYS:NZ	2.47	0.47
8:H:223:PRO:HA	8:H:226:VAL:HG12	1.96	0.47
11:K:196:LYS:NZ	11:K:240:ASP:OD2	2.47	0.47
21:U:802:TYR:O	21:U:878:LEU:N	2.47	0.47
22:X:274:LYS:HG3	22:X:275:LEU:HD12	1.96	0.47
25:a:292:THR:OG1	25:a:295:GLU:OE1	2.28	0.47
7:g:71:LYS:HG3	7:g:227:PHE:HD2	1.78	0.47
30:x:285:TYR:HE1	30:x:348:LYS:HE2	1.79	0.47
32:W:310:THR:HB	32:W:315:MET:HB3	1.95	0.47
1:A:363:SER:OG	2:B:214:MET:SD	2.72	0.47
12:L:117:GLN:O	12:L:120:THR:OG1	2.30	0.47
21:U:694:ILE:O	21:U:698:GLN:NE2	2.47	0.47
29:f:320:ILE:HA	29:f:324:VAL:HB	1.97	0.47
29:f:771:LEU:HD22	29:f:807:ARG:HE	1.80	0.47
32:W:98:LYS:HA	32:W:98:LYS:HD3	1.80	0.47
9:I:122:THR:HG22	9:I:129:PRO:HB3	1.95	0.47
17:Q:69:MET:HB3	17:Q:69:MET:HE3	1.78	0.47
21:U:206:MET:HE2	21:U:206:MET:HB3	1.73	0.47
21:U:800:VAL:H	21:U:880:ASN:HB2	1.79	0.47
26:b:138:VAL:O	26:b:168:SER:OG	2.31	0.47
27:c:54:MET:HB2	27:c:82:VAL:HG22	1.96	0.47
7:g:51:VAL:HG22	7:g:217:VAL:HG22	1.95	0.47
30:x:328:MET:SD	30:x:328:MET:N	2.85	0.47
5:E:66:GLU:HG2	5:E:67:GLU:HG2	1.96	0.47
6:F:91:SER:N	6:F:151:VAL:O	2.46	0.47
22:X:389:ASP:OD1	22:X:389:ASP:N	2.47	0.47
25:a:70:ARG:HH22	26:b:24:THR:HB	1.79	0.47
26:b:9:CYS:HB3	26:b:54:LEU:HD21	1.96	0.47
12:l:49:LEU:HB2	12:l:195:LEU:HD21	1.96	0.47
16:p:28:PHE:HD2	16:p:36:THR:HG22	1.79	0.47
19:s:68:ILE:HD11	19:s:92:LEU:HD13	1.95	0.47
17:Q:170:ARG:NE	18:r:140:ASP:OD2	2.48	0.47
26:b:109:ILE:HB	26:b:138:VAL:HG23	1.97	0.47
34:V:98:LEU:HD22	34:V:209:LYS:HD2	1.97	0.47
34:V:212:TYR:HA	34:V:253:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:75:ASN:ND2	6:F:130:GLN:OE1	2.47	0.47
6:F:283:ILE:HB	6:F:328:VAL:HG23	1.97	0.47
9:I:67:LYS:HA	9:I:73:ALA:HA	1.97	0.47
10:J:11:SER:OG	10:J:13:ASP:OD1	2.28	0.47
10:J:119:THR:HG22	10:J:126:PRO:HB3	1.96	0.47
11:K:146:VAL:HG11	11:K:222:PRO:HA	1.96	0.47
21:U:486:MET:HB3	21:U:518:LEU:HG	1.96	0.47
17:q:83:PHE:O	17:q:87:ASN:ND2	2.40	0.47
17:q:94:SER:OG	17:q:95:ARG:N	2.46	0.47
32:W:120:ILE:HG22	32:W:124:LEU:HD23	1.96	0.47
1:A:105:ASP:HB2	1:A:110:LYS:HB2	1.97	0.47
2:B:264:PRO:HB3	2:B:311:GLU:HG2	1.97	0.47
4:D:219:VAL:O	4:D:223:THR:OG1	2.33	0.47
13:M:46:VAL:HG22	13:M:215:TRP:HB3	1.97	0.47
29:f:80:ARG:O	29:f:80:ARG:NH1	2.42	0.47
29:f:597:VAL:HG11	29:f:635:LYS:HB3	1.97	0.47
4:D:202:VAL:HG23	4:D:329:ARG:HB2	1.96	0.47
5:E:283:ASP:OD1	5:E:283:ASP:N	2.48	0.47
21:U:330:SER:OG	21:U:332:GLU:OE2	2.32	0.47
16:p:49:LEU:HD23	16:p:111:GLY:HA3	1.96	0.47
30:x:484:ARG:NH1	30:x:486:GLU:OE2	2.41	0.47
4:D:315:ASP:N	4:D:315:ASP:OD1	2.47	0.47
5:E:117:PRO:HB2	6:F:311:LEU:HB3	1.97	0.47
5:E:194:ASN:HB3	5:E:226:GLN:HB2	1.96	0.47
9:I:47:ALA:HB3	9:I:212:GLU:HB3	1.96	0.47
11:K:13:ASN:ND2	12:L:124:GLY:O	2.48	0.47
11:K:156:MET:HE3	11:K:157:ASP:H	1.79	0.47
12:L:132:LEU:HB2	12:L:147:THR:HB	1.97	0.47
23:Y:48:ASN:HB3	23:Y:50:MET:HE1	1.97	0.47
7:g:4:GLY:HA2	7:g:11:ARG:HH21	1.80	0.47
30:x:8:VAL:HA	30:x:71:MET:HE1	1.97	0.47
3:C:56:VAL:HG22	3:C:60:ARG:HE	1.80	0.46
3:C:185:GLY:HA3	3:C:311:ILE:HA	1.97	0.46
9:I:54:LYS:H	9:I:54:LYS:HG3	1.57	0.46
23:Y:385:ARG:HA	23:Y:385:ARG:HD2	1.75	0.46
29:f:110:TYR:HD2	29:f:137:ARG:HH12	1.63	0.46
29:f:664:GLU:OE1	29:f:667:GLY:N	2.40	0.46
20:t:45:VAL:HB	20:t:49:THR:HG23	1.97	0.46
32:W:107:GLN:NE2	32:W:111:TYR:OH	2.48	0.46
32:W:387:ASP:N	32:W:387:ASP:OD1	2.46	0.46
2:B:313:LEU:O	2:B:346:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:802:TYR:HE2	21:U:880:ASN:HD22	1.64	0.46
23:Y:113:ARG:HG2	23:Y:114:ILE:HG23	1.96	0.46
26:b:137:ASN:HB3	26:b:166:THR:HG21	1.98	0.46
9:i:161:ALA:HB3	10:j:53:LEU:HD23	1.96	0.46
32:W:316:ARG:NH1	32:W:319:THR:OG1	2.48	0.46
4:D:49:GLN:OE1	21:U:596:ASN:ND2	2.45	0.46
4:D:99:ASN:HA	4:D:115:ILE:HB	1.97	0.46
24:Z:239:ASP:OD1	24:Z:239:ASP:N	2.47	0.46
29:f:127:SER:HB2	29:f:178:LYS:HD3	1.98	0.46
29:f:383:ALA:HA	29:f:417:ILE:HA	1.97	0.46
7:g:58:ASP:OD1	7:g:58:ASP:N	2.48	0.46
15:o:146:MET:HE1	15:o:154:LEU:HD22	1.96	0.46
5:E:12:TYR:OH	6:F:40:GLU:O	2.32	0.46
10:J:7:ILE:HG23	10:J:8:THR:HG23	1.98	0.46
21:U:613:ASP:OD1	21:U:613:ASP:N	2.45	0.46
21:U:806:CYS:O	21:U:874:ASN:ND2	2.49	0.46
23:Y:104:MET:HE1	23:Y:127:THR:HB	1.98	0.46
29:f:682:GLY:N	29:f:715:HIS:O	2.48	0.46
10:j:38:ARG:HG3	10:j:181:ILE:HG22	1.98	0.46
10:j:115:LYS:NZ	10:j:129:ILE:O	2.49	0.46
17:q:26:VAL:HG11	18:r:136:TYR:HE2	1.80	0.46
34:V:343:PRO:O	35:e:43:TRP:NE1	2.48	0.46
10:J:80:ALA:HA	10:J:129:ILE:HD13	1.98	0.46
21:U:236:LEU:HD11	21:U:248:ILE:HD12	1.97	0.46
26:b:6:THR:HG22	26:b:108:ARG:HB3	1.98	0.46
28:d:95:MET:SD	28:d:95:MET:N	2.88	0.46
29:f:94:LYS:HD2	29:f:106:LEU:HD12	1.98	0.46
13:m:23:VAL:O	13:m:27:MET:HG2	2.16	0.46
17:q:29:LYS:NZ	18:r:122:SER:O	2.40	0.46
1:A:401:ARG:NH1	1:A:408:ASP:OD2	2.49	0.46
16:P:61:GLN:HB2	17:Q:85:ARG:NH2	2.31	0.46
21:U:847:GLU:HA	21:U:851:GLU:HG3	1.98	0.46
28:d:215:TRP:HB3	28:d:222:TYR:HB3	1.97	0.46
29:f:250:ARG:HH11	29:f:252:ALA:HB3	1.81	0.46
29:f:537:THR:O	29:f:541:THR:OG1	2.23	0.46
19:s:91:MET:HE2	19:s:91:MET:HB3	1.86	0.46
34:V:398:LEU:HA	34:V:401:ASN:HB2	1.97	0.46
4:D:106:THR:HG21	5:E:78:ARG:H	1.80	0.46
22:X:397:TYR:HE2	23:Y:362:LYS:HG3	1.81	0.46
34:V:321:ALA:HB1	34:V:324:PHE:HB3	1.96	0.46
1:A:171:ASP:OD1	1:A:171:ASP:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LYS:HE2	6:F:409:ARG:HH22	1.81	0.46
2:B:223:ILE:HA	2:B:329:MET:HB2	1.97	0.46
4:D:92:PHE:HA	4:D:103:VAL:HG12	1.98	0.46
5:E:349:GLU:HA	5:E:352:MET:HE2	1.97	0.46
21:U:161:ASP:OD1	21:U:162:VAL:N	2.49	0.46
16:p:135:ASP:OD1	16:p:135:ASP:N	2.49	0.46
30:x:384:GLN:NE2	30:x:385:GLN:OE1	2.47	0.46
21:U:260:PHE:O	21:U:264:VAL:HG23	2.16	0.46
32:W:116:THR:O	32:W:117:ASP:HB2	2.14	0.46
34:V:419:LEU:HA	34:V:422:ILE:HG22	1.98	0.46
2:B:30:PRO:HB2	2:B:31:THR:H	1.61	0.45
18:R:91:LYS:NZ	18:R:117:GLU:O	2.47	0.45
21:U:717:ILE:O	21:U:727:LYS:NZ	2.49	0.45
22:X:97:LEU:HD22	22:X:136:LEU:HD21	1.97	0.45
24:Z:39:LEU:HB2	24:Z:50:VAL:HG21	1.97	0.45
24:Z:253:THR:HA	24:Z:256:GLN:HB2	1.97	0.45
29:f:218:GLU:HA	29:f:221:ILE:HD12	1.98	0.45
9:i:21:VAL:O	9:i:25:MET:HG2	2.16	0.45
13:m:8:ASP:O	13:m:22:GLN:NE2	2.48	0.45
3:C:307:ARG:HG2	3:C:309:GLY:H	1.81	0.45
4:D:200:ARG:HE	4:D:302:ASN:HB3	1.81	0.45
5:E:330:ALA:HB2	32:W:15:LYS:HB3	1.97	0.45
6:F:39:GLU:HG2	6:F:43:GLN:HB2	1.98	0.45
15:O:38:SER:HB2	15:O:41:ILE:HB	1.97	0.45
19:S:57:PHE:HZ	20:T:128:LEU:HB3	1.80	0.45
21:U:24:LEU:HD22	21:U:63:VAL:HG21	1.98	0.45
21:U:798:PRO:HB3	21:U:924:LEU:HD23	1.98	0.45
24:Z:129:LYS:HD2	27:c:215:LYS:HE2	1.97	0.45
25:a:229:ASP:OD1	25:a:229:ASP:N	2.50	0.45
29:f:143:ARG:HG2	29:f:191:ILE:HD11	1.98	0.45
29:f:637:LYS:HD2	29:f:678:LEU:HD13	1.97	0.45
11:k:221:GLN:OE1	11:k:224:GLN:NE2	2.47	0.45
30:x:364:GLN:O	30:x:368:VAL:HB	2.16	0.45
5:E:118:LEU:HD11	6:F:295:ARG:HH22	1.81	0.45
17:Q:144:ASP:OD2	18:r:166:ARG:NH2	2.44	0.45
25:a:87:MET:SD	25:a:88:THR:N	2.89	0.45
29:f:189:LYS:HG2	29:f:190:GLU:HG3	1.97	0.45
29:f:433:LEU:O	29:f:441:LYS:NZ	2.40	0.45
29:f:703:ARG:HD3	29:f:785:ARG:HH12	1.81	0.45
8:h:204:THR:HG23	8:h:206:ASP:H	1.82	0.45
19:s:133:ASP:OD1	19:s:133:ASP:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:57:SER:HA	26:b:76:HIS:CE1	2.51	0.45
8:H:179:ASN:HB3	8:H:182:LEU:HG	1.98	0.45
9:I:72:MET:HE3	9:I:72:MET:HB3	1.79	0.45
27:c:279:ASP:HA	27:c:283:HIS:HD2	1.81	0.45
29:f:59:LEU:HD13	29:f:62:ARG:HH12	1.82	0.45
29:f:408:LEU:HB2	29:f:439:TYR:HD1	1.81	0.45
29:f:426:LEU:HA	29:f:429:ILE:HB	1.99	0.45
29:f:762:VAL:HB	29:f:771:LEU:HB3	1.98	0.45
2:B:224:LEU:HB3	2:B:353:PHE:HE2	1.81	0.45
5:E:5:ARG:NH1	6:F:32:GLU:OE1	2.50	0.45
5:E:36:LEU:HB3	6:F:69:MET:HE1	1.97	0.45
22:X:95:LEU:O	22:X:99:MET:HG2	2.16	0.45
23:Y:173:ASP:OD1	23:Y:173:ASP:N	2.49	0.45
23:Y:235:ASP:O	23:Y:239:LYS:NZ	2.43	0.45
24:Z:141:VAL:O	24:Z:154:THR:OG1	2.34	0.45
25:a:243:GLY:HA3	25:a:279:GLU:HG3	1.99	0.45
27:c:137:SER:HB3	27:c:140:ALA:HB2	1.98	0.45
29:f:771:LEU:HD13	29:f:807:ARG:HH21	1.80	0.45
11:k:42:THR:HG23	11:k:44:GLU:H	1.81	0.45
13:m:201:HIS:HE1	13:m:206:ASP:HB2	1.82	0.45
19:s:148:LEU:HD23	19:s:178:VAL:HG22	1.99	0.45
32:W:180:LYS:NZ	32:W:181:GLU:OE2	2.50	0.45
32:W:447:ALA:O	32:W:451:MET:HB2	2.16	0.45
3:C:201:ARG:NH1	4:D:300:ASP:OD2	2.50	0.45
4:D:101:ALA:HB2	4:D:115:ILE:HD11	1.98	0.45
5:E:164:ILE:HG22	5:E:167:PRO:HD3	1.98	0.45
6:F:192:ASP:N	6:F:192:ASP:OD1	2.49	0.45
16:P:62:THR:HG23	17:Q:86:ARG:HH22	1.81	0.45
18:R:139:MET:O	18:R:143:TYR:HB2	2.16	0.45
21:U:7:GLY:N	21:U:37:GLU:OE2	2.49	0.45
21:U:43:ASP:N	21:U:43:ASP:OD1	2.47	0.45
19:s:186:ASP:OD1	19:s:187:VAL:N	2.46	0.45
30:x:7:THR:HB	30:x:68:THR:HA	1.98	0.45
32:W:165:ILE:HD13	32:W:192:LEU:HG	1.98	0.45
3:C:268:GLU:HA	3:C:271:ARG:HG2	1.98	0.45
5:E:261:LEU:HD23	5:E:294:ARG:HH11	1.81	0.45
12:L:172:LEU:O	12:L:176:MET:HB3	2.16	0.45
22:X:320:SER:HA	22:X:323:LEU:HD12	1.98	0.45
26:b:107:MET:HG3	26:b:136:VAL:HG22	1.99	0.45
14:n:93:ASP:N	14:n:93:ASP:OD1	2.49	0.45
30:x:89:VAL:HG23	30:x:90:GLU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:GLU:HB3	29:f:657:ILE:HD11	1.98	0.45
2:B:191:ASP:N	2:B:191:ASP:OD1	2.49	0.45
2:B:440:LEU:O	10:J:61:LYS:NZ	2.50	0.45
3:C:311:ILE:HD11	3:C:314:LYS:HE3	1.99	0.45
4:D:339:ARG:HG2	22:X:230:SER:HB2	1.99	0.45
5:E:339:ASN:HB2	5:E:342:ASP:HB2	1.98	0.45
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.99	0.45
13:M:123:THR:HG22	13:M:130:PRO:HB3	1.98	0.45
19:S:38:ARG:NH2	15:o:164:PHE:O	2.50	0.45
7:g:73:THR:HG23	7:g:75:ASN:H	1.82	0.45
13:M:181:MET:HA	13:M:184:MET:HG2	1.99	0.45
22:X:182:ASN:HA	23:Y:244:ALA:HB1	1.98	0.45
8:h:119:GLN:HG3	9:i:81:SER:HB2	1.98	0.45
30:x:406:PHE:HA	30:x:414:ASN:HB3	1.99	0.45
2:B:36:LYS:NZ	2:B:39:LYS:O	2.50	0.45
5:E:171:LEU:HB2	5:E:295:LEU:HD11	1.98	0.45
6:F:229:PRO:HG3	6:F:333:ASN:HB2	1.99	0.45
14:N:190:LEU:HD12	20:t:209:TRP:HB2	1.99	0.45
29:f:298:LEU:HA	29:f:301:HIS:CE1	2.52	0.45
10:j:80:ALA:HA	10:j:129:ILE:HD13	1.99	0.45
30:x:6:VAL:HG11	30:x:20:LEU:HD13	1.98	0.45
1:A:73:ALA:O	1:A:78:TRP:NE1	2.47	0.44
8:H:10:LEU:HD12	8:H:19:LEU:HD12	1.98	0.44
21:U:193:PHE:HA	21:U:196:LYS:HE3	1.98	0.44
26:b:106:LYS:HE2	26:b:106:LYS:HB3	1.86	0.44
29:f:174:ASP:N	29:f:178:LYS:HZ1	2.15	0.44
29:f:466:LEU:HD12	29:f:481:SER:HA	1.97	0.44
11:k:32:LYS:NZ	11:k:174:SER:OG	2.49	0.44
30:x:249:VAL:HB	30:x:321:PRO:HG3	1.97	0.44
6:F:435:LEU:HD12	6:F:438:TYR:HE2	1.82	0.44
11:K:199:LEU:HD21	11:K:217:LEU:HD11	1.99	0.44
27:c:113:HIS:NE2	27:c:115:HIS:CD2	2.86	0.44
28:d:131:VAL:HA	28:d:134:LYS:HB3	1.99	0.44
29:f:117:GLU:O	29:f:120:ARG:N	2.47	0.44
34:V:495:ARG:NH1	34:V:497:PRO:O	2.42	0.44
1:A:303:ILE:HD11	1:A:331:LEU:HB2	1.99	0.44
1:A:367:ASP:OD1	1:A:367:ASP:N	2.49	0.44
2:B:107:MET:HG3	2:B:151:LEU:HD22	1.99	0.44
7:G:211:LYS:H	7:G:211:LYS:HG2	1.55	0.44
24:Z:123:ILE:O	24:Z:135:THR:OG1	2.27	0.44
28:d:78:LEU:HD13	28:d:98:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:301:HIS:HA	29:f:305:LEU:HB2	2.00	0.44
20:t:122:LEU:HG	20:t:137:LEU:HD12	1.99	0.44
30:x:456:SER:OG	30:x:457:ILE:N	2.50	0.44
2:B:343:ARG:HE	2:B:346:ARG:HE	1.65	0.44
4:D:311:THR:OG1	4:D:312:ASN:N	2.50	0.44
9:I:238:LYS:HB2	9:I:238:LYS:HE3	1.85	0.44
21:U:790:GLY:O	21:U:792:ASN:ND2	2.50	0.44
25:a:240:PHE:HZ	25:a:271:LYS:HB3	1.82	0.44
29:f:148:GLN:HG2	29:f:149:GLU:HG2	1.99	0.44
9:i:8:ARG:HB3	9:i:11:ILE:HD12	2.00	0.44
11:k:209:LYS:O	11:k:214:ASN:ND2	2.51	0.44
4:D:211:GLY:HA2	4:D:214:MET:HE2	1.99	0.44
15:O:146:MET:HE1	15:O:154:LEU:HD22	1.99	0.44
24:Z:212:LEU:HA	24:Z:215:VAL:HG12	2.00	0.44
29:f:403:LYS:HG3	29:f:406:GLY:H	1.82	0.44
15:o:38:SER:HB3	15:o:41:ILE:HB	1.99	0.44
30:x:235:THR:HG23	30:x:240:LYS:HZ1	1.83	0.44
3:C:53:ASN:ND2	21:U:642:GLU:O	2.51	0.44
21:U:188:MET:HE1	21:U:194:ARG:HB2	2.00	0.44
24:Z:236:LEU:HD23	25:a:335:TRP:HB3	2.00	0.44
3:C:252:ASP:HB2	4:D:290:LEU:HD11	2.00	0.44
4:D:105:SER:OG	4:D:108:GLY:O	2.36	0.44
6:F:79:LYS:HA	6:F:79:LYS:HD3	1.74	0.44
8:H:10:LEU:HD13	8:H:21:GLN:HB2	1.98	0.44
22:X:315:ASP:OD1	22:X:315:ASP:N	2.51	0.44
24:Z:54:PHE:HB3	24:Z:82:PHE:HE2	1.82	0.44
27:c:75:MET:HE3	27:c:76:PRO:HD2	2.00	0.44
18:r:127:SER:HB3	18:r:136:TYR:CE1	2.53	0.44
1:A:394:MET:HE2	1:A:394:MET:HB2	1.85	0.44
3:C:340:ARG:HD3	3:C:340:ARG:HA	1.87	0.44
6:F:438:TYR:OH	11:K:19:GLY:O	2.32	0.44
13:M:7:TYR:CD2	13:M:16:PRO:HD3	2.52	0.44
13:M:15:SER:OG	13:M:17:ASP:OD1	2.32	0.44
13:M:230:ASP:N	13:M:230:ASP:OD1	2.50	0.44
14:N:167:ASP:OD1	14:N:168:GLY:N	2.51	0.44
15:O:164:PHE:O	19:s:38:ARG:NH2	2.50	0.44
18:R:127:SER:HB3	18:R:136:TYR:CE1	2.53	0.44
21:U:128:GLN:HG3	21:U:129:ARG:HD3	2.00	0.44
21:U:150:ALA:HA	21:U:153:ILE:HG12	1.99	0.44
23:Y:226:VAL:HA	23:Y:229:ILE:HG22	1.99	0.44
24:Z:251:LEU:HB3	27:c:234:TYR:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:205:LEU:HG	25:a:268:LEU:HD11	1.98	0.44
8:h:14:SER:HB2	8:h:18:LYS:H	1.82	0.44
17:q:143:LEU:O	17:q:147:TYR:HB2	2.18	0.44
32:W:36:LYS:HB3	32:W:73:MET:HE1	2.00	0.44
34:V:175:MET:HE3	34:V:180:ARG:HB2	1.99	0.44
18:R:182:ASP:OD1	18:R:182:ASP:N	2.41	0.44
21:U:524:LYS:HG3	21:U:556:MET:HE1	2.00	0.44
22:X:233:TYR:HD1	22:X:254:MET:HE2	1.82	0.44
24:Z:134:PRO:HD3	27:c:223:LYS:HE2	1.99	0.44
24:Z:213:GLU:HG3	25:a:350:LYS:HE2	2.00	0.44
25:a:308:GLU:HG3	25:a:309:LEU:HD12	2.00	0.44
27:c:237:HIS:O	27:c:240:HIS:ND1	2.51	0.44
28:d:15:ASN:HB2	28:d:18:LYS:HB2	2.00	0.44
10:j:95:ARG:HG2	17:q:62:LYS:HE3	2.00	0.44
20:t:25:ASP:HA	20:t:187:PHE:HA	1.98	0.44
2:B:256:ILE:HD11	2:B:290:ILE:HG13	1.99	0.43
6:F:153:VAL:HG12	6:F:160:ILE:HG12	2.00	0.43
14:N:192:ASP:OD1	14:N:192:ASP:N	2.49	0.43
17:Q:53:THR:HG22	17:Q:100:VAL:HG12	2.00	0.43
20:T:211:ILE:HG13	14:n:30:VAL:HG11	2.00	0.43
21:U:575:ASP:HB3	21:U:578:LEU:HB2	1.99	0.43
23:Y:50:MET:SD	23:Y:50:MET:N	2.91	0.43
29:f:369:ARG:NH2	29:f:792:ALA:O	2.48	0.43
7:g:141:ILE:HD12	7:g:220:VAL:HG12	2.00	0.43
10:j:157:LYS:NZ	11:k:57:PRO:O	2.40	0.43
1:A:241:ILE:HG22	1:A:244:GLU:H	1.84	0.43
4:D:335:LEU:HD23	4:D:336:PRO:HD3	1.98	0.43
4:D:362:ASP:OD1	4:D:362:ASP:N	2.50	0.43
5:E:48:LYS:HB3	5:E:48:LYS:HE2	1.85	0.43
10:J:4:ASP:OD1	10:J:4:ASP:N	2.42	0.43
16:P:135:ASP:OD1	16:P:135:ASP:N	2.45	0.43
23:Y:45:VAL:HA	23:Y:70:LEU:HD21	1.99	0.43
14:n:196:LYS:HE2	14:n:196:LYS:HB2	1.86	0.43
16:p:193:ASP:OD1	16:p:193:ASP:N	2.50	0.43
17:q:53:THR:HG22	17:q:100:VAL:HG12	2.00	0.43
31:y:43:LEU:HD12	31:y:67:LEU:HG	2.00	0.43
32:W:166:LEU:HD13	32:W:169:LEU:HD11	2.00	0.43
1:A:82:ALA:HB2	2:B:137:SER:HB3	1.99	0.43
1:A:213:LEU:HA	1:A:319:MET:HB3	2.01	0.43
5:E:113:ARG:H	5:E:113:ARG:HG3	1.51	0.43
6:F:343:LEU:HB2	6:F:347:ARG:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:172:MET:HE3	19:S:172:MET:HB3	1.75	0.43
26:b:7:MET:HE3	26:b:64:LEU:HD21	2.00	0.43
10:j:119:THR:HG22	10:j:126:PRO:HB3	2.00	0.43
14:n:81:SER:HA	14:n:84:LYS:HG2	1.98	0.43
15:o:179:SER:OG	15:o:180:LYS:N	2.51	0.43
17:q:4:LEU:HD22	17:q:45:LEU:HB3	1.99	0.43
34:V:354:LYS:HZ3	35:e:34:GLU:H	1.66	0.43
35:e:16:ASP:OD1	35:e:16:ASP:N	2.52	0.43
3:C:162:LYS:HE3	3:C:162:LYS:HB2	1.90	0.43
6:F:57:SER:HA	26:b:76:HIS:HE1	1.83	0.43
11:K:41:GLN:NE2	11:K:151:PRO:O	2.51	0.43
21:U:466:LYS:HB2	21:U:466:LYS:HE3	1.77	0.43
29:f:215:ASP:OD1	29:f:216:MET:N	2.50	0.43
29:f:267:ARG:HH11	29:f:271:MET:HG3	1.83	0.43
12:l:226:ASP:OD1	12:l:227:ASP:N	2.51	0.43
15:o:42:TYR:HB2	15:o:178:ILE:HD11	1.99	0.43
19:s:11:THR:HG22	19:s:141:ALA:H	1.83	0.43
10:J:39:ASP:OD1	10:J:39:ASP:N	2.52	0.43
21:U:401:LYS:HD2	21:U:438:GLN:HE21	1.83	0.43
25:a:331:VAL:HG12	25:a:333:MET:HE3	2.00	0.43
29:f:144:LEU:O	29:f:148:GLN:NE2	2.52	0.43
19:s:144:MET:HE1	19:s:185:ARG:HB3	2.00	0.43
32:W:112:VAL:HG12	32:W:120:ILE:HG23	2.00	0.43
3:C:299:ASP:OD1	3:C:299:ASP:N	2.51	0.43
9:I:161:ALA:HB1	9:I:175:LEU:HD13	1.99	0.43
12:L:204:ASP:N	12:L:204:ASP:OD1	2.50	0.43
14:N:4:MET:HE3	14:N:4:MET:HB2	1.86	0.43
22:X:268:GLN:HA	22:X:271:VAL:HG22	2.01	0.43
13:m:37:ILE:HD11	13:m:193:VAL:HG13	1.99	0.43
7:G:17:SER:HB3	7:G:21:ARG:H	1.82	0.43
7:G:202:LEU:HD12	7:G:202:LEU:HA	1.88	0.43
22:X:187:ARG:NE	22:X:221:GLU:OE2	2.51	0.43
23:Y:319:MET:HA	23:Y:322:ALA:HB3	2.00	0.43
24:Z:204:LYS:HD2	32:W:443:THR:HG21	2.00	0.43
28:d:82:TYR:O	28:d:121:ARG:NH2	2.48	0.43
28:d:231:LYS:HE2	28:d:231:LYS:HB2	1.88	0.43
29:f:785:ARG:O	29:f:785:ARG:NH1	2.45	0.43
19:s:27:THR:HB	19:s:40:SER:H	1.84	0.43
32:W:328:LEU:HD23	32:W:328:LEU:HA	1.89	0.43
1:A:58:LYS:HE3	1:A:58:LYS:HB2	1.83	0.43
1:A:348:LEU:HD21	1:A:371:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:159:PHE:HA	5:E:164:ILE:HD13	2.01	0.43
14:N:41:ILE:HG12	14:N:76:VAL:HG12	2.01	0.43
23:Y:177:ARG:NH1	23:Y:205:VAL:O	2.34	0.43
29:f:198:HIS:CD2	29:f:240:VAL:HB	2.54	0.43
34:V:281:ASN:OD1	34:V:282:ASN:N	2.52	0.43
2:B:292:THR:HG21	3:C:261:GLY:HA3	2.00	0.43
3:C:254:ILE:HD11	3:C:272:THR:HB	2.01	0.43
10:J:154:HIS:HD1	11:K:64:ILE:HG22	1.84	0.43
16:P:113:ASP:HB3	16:P:118:LYS:H	1.84	0.43
17:Q:152:SER:OG	17:Q:153:ARG:N	2.51	0.43
24:Z:35:VAL:H	24:Z:97:THR:HG22	1.84	0.43
27:c:32:TYR:HB3	27:c:208:ARG:HG2	2.01	0.43
28:d:243:ALA:HA	28:d:246:VAL:HG22	2.00	0.43
10:j:41:VAL:HG11	10:j:134:VAL:HB	2.01	0.43
1:A:99:THR:OG1	1:A:114:ASN:O	2.29	0.43
5:E:174:GLY:HA3	5:E:301:ILE:HG13	2.01	0.43
17:Q:171:PHE:CE2	17:Q:173:LEU:HB2	2.54	0.43
25:a:293:PHE:HE2	25:a:304:VAL:HG13	1.84	0.43
29:f:404:ASP:OD1	29:f:404:ASP:N	2.51	0.43
29:f:411:ALA:HB3	29:f:443:GLY:HA3	2.00	0.43
29:f:780:PRO:HG3	29:f:803:PHE:HD2	1.84	0.43
21:U:368:ALA:HB2	21:U:728:PHE:HD1	1.84	0.42
22:X:338:VAL:HG23	22:X:339:ILE:HG23	2.00	0.42
23:Y:334:LEU:HD23	23:Y:347:ILE:HD12	2.01	0.42
28:d:245:GLN:OE1	34:V:477:HIS:ND1	2.52	0.42
29:f:423:ASP:OD1	29:f:423:ASP:N	2.52	0.42
16:p:58:THR:O	17:q:85:ARG:NH2	2.51	0.42
19:s:16:ALA:HB2	19:s:121:VAL:HG23	2.00	0.42
32:W:272:LEU:HD12	32:W:336:PRO:HB2	2.00	0.42
34:V:234:ARG:HD2	34:V:234:ARG:HA	1.70	0.42
3:C:331:ILE:O	3:C:334:ARG:NH1	2.51	0.42
21:U:744:VAL:HG12	21:U:785:PRO:HA	2.00	0.42
22:X:252:LYS:HG3	22:X:287:LEU:HD11	2.01	0.42
24:Z:264:SER:HA	24:Z:267:ARG:HG2	2.01	0.42
8:h:186:ASP:N	8:h:186:ASP:OD1	2.48	0.42
30:x:443:LYS:HB2	30:x:446:GLU:HB3	2.00	0.42
4:D:39:ASP:N	4:D:39:ASP:OD1	2.51	0.42
8:H:9:SER:HG	8:H:12:THR:HG1	1.58	0.42
23:Y:116:ASP:OD1	23:Y:116:ASP:N	2.52	0.42
28:d:175:ARG:NH1	28:d:209:TYR:OH	2.52	0.42
7:g:37:LEU:HD22	7:g:53:GLN:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:p:158:MET:HE3	16:p:158:MET:HB2	1.88	0.42
18:r:97:MET:HE3	18:r:99:THR:HG22	2.01	0.42
30:x:298:ILE:HD13	30:x:313:LYS:HD3	2.01	0.42
30:x:370:PHE:HE2	30:x:414:ASN:HB2	1.84	0.42
34:V:193:GLN:O	34:V:197:THR:OG1	2.29	0.42
35:e:50:ASP:N	35:e:50:ASP:OD1	2.47	0.42
1:A:74:PRO:HA	1:A:75:PRO:HD3	1.90	0.42
2:B:383:LEU:HD21	2:B:419:PHE:HB3	2.01	0.42
5:E:24:GLY:HA2	5:E:27:LYS:HE2	2.01	0.42
6:F:289:ASP:HA	6:F:338:LEU:HD21	2.00	0.42
13:M:108:LEU:HD22	13:M:139:SER:HB3	2.01	0.42
17:Q:94:SER:OG	17:Q:95:ARG:N	2.51	0.42
21:U:186:SER:O	21:U:189:GLN:NE2	2.46	0.42
23:Y:384:SER:HA	23:Y:387:ILE:HG22	2.02	0.42
24:Z:187:LEU:HB2	27:c:293:THR:HG22	2.00	0.42
29:f:47:GLU:HB3	29:f:124:ASP:HB3	2.00	0.42
9:i:34:CYS:SG	9:i:75:SER:OG	2.77	0.42
15:o:62:ASN:HB3	15:o:82:MET:HE1	2.01	0.42
19:s:2:PHE:HZ	20:t:100:ARG:HG2	1.84	0.42
30:x:64:LYS:HG2	30:x:67:MET:HB2	2.01	0.42
4:D:377:SER:HB3	5:E:292:PRO:HG2	2.01	0.42
5:E:222:ALA:HB1	5:E:228:CYS:HB2	2.00	0.42
6:F:256:LEU:HD23	6:F:256:LEU:HA	1.91	0.42
9:I:54:LYS:HE2	9:I:54:LYS:HB2	1.73	0.42
23:Y:203:ASP:OD1	23:Y:203:ASP:N	2.52	0.42
24:Z:96:HIS:ND1	24:Z:97:THR:O	2.47	0.42
29:f:75:LEU:HD12	29:f:77:GLU:H	1.84	0.42
11:k:13:ASN:HB3	12:l:126:ARG:HB3	2.01	0.42
14:n:39:ASP:OD1	14:n:39:ASP:N	2.52	0.42
30:x:91:ASP:C	30:x:92:MET:HE2	2.44	0.42
31:y:15:LEU:HD23	31:y:29:LYS:NZ	2.34	0.42
11:K:99:HIS:CG	11:K:107:MET:HB2	2.54	0.42
14:N:94:LEU:HD13	14:N:96:ALA:HB3	2.01	0.42
16:P:159:ASP:OD1	16:P:159:ASP:N	2.51	0.42
21:U:759:SER:HA	21:U:782:ALA:HA	2.02	0.42
23:Y:290:PRO:HG2	23:Y:291:HIS:CE1	2.55	0.42
24:Z:105:ASP:OD1	24:Z:105:ASP:N	2.53	0.42
11:k:16:SER:OG	11:k:20:ARG:N	2.51	0.42
19:s:123:SER:HB2	19:s:136:LYS:HG2	2.01	0.42
34:V:410:ILE:HG21	34:V:422:ILE:HG13	2.02	0.42
5:E:309:ARG:HB2	5:E:343:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:49:ASP:HA	6:F:52:ILE:HG12	2.02	0.42
11:K:202:LEU:O	11:K:206:MET:HG2	2.20	0.42
21:U:536:ALA:HA	21:U:539:THR:HG22	2.01	0.42
25:a:83:VAL:O	25:a:87:MET:HG3	2.20	0.42
27:c:31:VAL:HG22	27:c:67:VAL:HB	2.02	0.42
29:f:94:LYS:HA	29:f:98:PHE:HB2	2.01	0.42
29:f:679:LEU:HD13	29:f:687:ARG:HD2	2.01	0.42
29:f:828:ARG:HB2	29:f:843:SER:HB2	2.01	0.42
30:x:400:LYS:NZ	30:x:401:TYR:O	2.42	0.42
31:y:5:VAL:HG21	31:y:15:LEU:HD22	2.01	0.42
34:V:355:ARG:NH1	35:e:27:TRP:O	2.51	0.42
2:B:51:LEU:HD12	29:f:646:MET:HG2	2.01	0.42
3:C:13:GLU:OE1	3:C:21:ARG:NH1	2.53	0.42
5:E:16:LEU:HD23	5:E:16:LEU:HA	1.94	0.42
5:E:214:LEU:HD23	5:E:214:LEU:HA	1.91	0.42
6:F:380:ASN:HB3	6:F:383:GLU:HB3	2.01	0.42
13:M:41:CYS:HB3	13:M:189:ILE:HG13	2.01	0.42
19:S:145:LEU:HD22	19:S:178:VAL:HB	2.01	0.42
22:X:141:LYS:HD2	22:X:141:LYS:HA	1.74	0.42
25:a:70:ARG:HD3	26:b:17:ARG:O	2.20	0.42
26:b:3:LEU:HB3	26:b:105:HIS:HA	2.02	0.42
28:d:158:ILE:HD12	28:d:159:PRO:HD2	2.01	0.42
29:f:442:SER:HB2	29:f:477:MET:HA	2.00	0.42
29:f:593:THR:OG1	29:f:631:LYS:NZ	2.53	0.42
9:i:190:LEU:HB3	9:i:236:LEU:HD21	2.02	0.42
18:r:113:TYR:OH	18:r:115:ASP:OD2	2.31	0.42
30:x:122:CYS:HB3	30:x:424:LEU:HD21	2.02	0.42
35:e:58:ALA:O	35:e:62:LYS:CB	2.62	0.42
5:E:288:ALA:O	5:E:291:ARG:NE	2.52	0.42
6:F:425:LEU:HD23	6:F:425:LEU:HA	1.95	0.42
10:J:158:ALA:HB1	10:J:172:LEU:HD13	2.02	0.42
21:U:619:VAL:HG23	21:U:651:GLY:HA3	2.01	0.42
26:b:14:GLU:N	26:b:82:GLY:O	2.52	0.42
16:p:183:MET:HE3	16:p:183:MET:HB3	1.90	0.42
18:r:32:LYS:HE2	18:r:32:LYS:HB3	1.89	0.42
32:W:309:PHE:HB2	32:W:313:GLU:HA	2.01	0.42
34:V:240:LEU:HD12	34:V:241:ARG:HG3	2.02	0.42
34:V:326:GLN:HE22	35:e:25:GLU:HG2	1.85	0.42
2:B:136:LEU:HB2	2:B:160:ILE:HG22	2.00	0.42
5:E:98:VAL:HA	5:E:110:TYR:HA	2.01	0.42
14:N:30:VAL:HG11	20:t:211:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:456:ASP:OD1	21:U:456:ASP:N	2.50	0.42
21:U:838:LYS:HB3	29:f:228:LYS:HZ1	1.85	0.42
25:a:312:MET:HE1	32:W:369:TYR:CG	2.55	0.42
28:d:132:TYR:HD1	28:d:160:ALA:HB2	1.85	0.42
13:m:230:ASP:OD1	13:m:230:ASP:N	2.52	0.42
15:o:179:SER:HB3	15:o:182:LYS:HG3	2.01	0.42
5:E:60:VAL:HA	5:E:71:VAL:HG22	2.03	0.41
6:F:171:ARG:O	6:F:175:MET:HG2	2.19	0.41
6:F:439:ALA:N	12:L:76:GLY:O	2.50	0.41
17:Q:39:SER:OG	17:Q:74:GLU:OE1	2.38	0.41
20:T:12:LEU:HD12	20:T:150:LEU:HD11	2.02	0.41
20:T:27:LEU:HD11	20:T:34:ALA:HB1	2.01	0.41
21:U:428:PRO:HB3	21:U:438:GLN:HB2	2.02	0.41
23:Y:12:PRO:HB2	23:Y:13:LYS:H	1.63	0.41
24:Z:155:PHE:HB3	32:W:452:ILE:HD11	2.01	0.41
25:a:329:LYS:HD2	25:a:329:LYS:HA	1.75	0.41
8:h:100:VAL:HG13	16:p:93:ASN:HD22	1.85	0.41
9:i:72:MET:HE3	9:i:72:MET:HB3	1.98	0.41
16:p:58:THR:HG21	17:q:121:LEU:HG	2.02	0.41
30:x:40:GLN:O	30:x:44:GLN:N	2.53	0.41
32:W:142:ARG:HH21	32:W:176:SER:HB2	1.85	0.41
32:W:197:LYS:HE2	32:W:197:LYS:HB2	1.94	0.41
4:D:53:PHE:HZ	21:U:636:VAL:HB	1.84	0.41
5:E:145:LEU:HD12	5:E:148:VAL:HB	2.02	0.41
5:E:236:ASP:OD1	5:E:236:ASP:N	2.44	0.41
5:E:359:HIS:HD1	5:E:361:PHE:H	1.67	0.41
7:G:180:GLU:HA	7:G:183:VAL:HG12	2.02	0.41
12:L:193:ARG:NE	12:L:237:GLU:OE2	2.40	0.41
17:Q:30:ASP:OD1	17:Q:30:ASP:N	2.51	0.41
21:U:789:ILE:HB	21:U:911:ILE:HA	2.02	0.41
24:Z:20:VAL:HG11	27:c:216:MET:HE1	2.01	0.41
29:f:664:GLU:HB3	29:f:668:ALA:H	1.85	0.41
16:p:11:VAL:HG21	16:p:52:GLY:HA3	2.02	0.41
30:x:328:MET:HG2	30:x:330:ARG:HG3	2.01	0.41
32:W:213:PHE:O	32:W:215:GLN:NE2	2.50	0.41
1:A:25:LEU:HD22	1:A:25:LEU:HA	1.82	0.41
2:B:430:LYS:HA	2:B:430:LYS:HD3	1.86	0.41
5:E:55:GLN:HB2	6:F:133:PHE:HD2	1.84	0.41
11:K:148:GLU:OE2	19:S:81:LYS:NZ	2.44	0.41
13:M:43:ASP:OD1	13:M:43:ASP:N	2.52	0.41
23:Y:145:LEU:HD13	23:Y:182:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:293:PHE:HB2	25:a:307:VAL:HG11	2.01	0.41
26:b:83:LYS:HE3	26:b:83:LYS:HB2	1.85	0.41
29:f:198:HIS:NE2	29:f:244:GLU:OE2	2.52	0.41
29:f:249:LEU:HG	29:f:250:ARG:H	1.86	0.41
32:W:232:GLN:HA	32:W:235:GLN:HG2	2.01	0.41
34:V:357:LEU:O	34:V:361:PHE:N	2.52	0.41
6:F:141:ASP:OD1	6:F:141:ASP:N	2.49	0.41
6:F:202:ILE:HD13	6:F:202:ILE:HA	1.94	0.41
14:N:40:ARG:NH2	14:N:181:GLU:O	2.53	0.41
21:U:172:ASP:OD1	21:U:172:ASP:N	2.53	0.41
21:U:183:LEU:HG	21:U:187:LEU:HD12	2.02	0.41
23:Y:279:GLU:HG3	23:Y:296:VAL:HG21	2.03	0.41
24:Z:219:LYS:H	24:Z:219:LYS:HG2	1.72	0.41
25:a:322:GLY:HA3	25:a:333:MET:HA	2.02	0.41
26:b:33:VAL:HA	26:b:36:VAL:HG22	2.03	0.41
27:c:137:SER:OG	27:c:138:GLU:N	2.54	0.41
11:k:52:LYS:HD3	11:k:216:GLU:HB2	2.03	0.41
2:B:363:ARG:HA	2:B:363:ARG:HD3	1.84	0.41
3:C:56:VAL:HG11	4:D:68:LEU:HD22	2.03	0.41
13:M:220:THR:OG1	13:M:223:ARG:O	2.29	0.41
23:Y:111:LEU:HD23	23:Y:111:LEU:HA	1.89	0.41
24:Z:77:ASN:HB3	24:Z:81:MET:HE1	2.02	0.41
27:c:284:LEU:O	27:c:286:GLU:N	2.54	0.41
28:d:179:ALA:HA	28:d:182:ILE:HG22	2.02	0.41
29:f:87:THR:OG1	29:f:109:ILE:O	2.39	0.41
29:f:242:GLU:HB3	29:f:256:PHE:HE1	1.85	0.41
29:f:375:SER:HA	29:f:398:TRP:HH2	1.85	0.41
29:f:456:ARG:HH21	29:f:491:GLY:H	1.67	0.41
29:f:548:THR:O	29:f:552:ASP:CB	2.62	0.41
30:x:110:LEU:HD21	30:x:171:PRO:HB3	2.03	0.41
32:W:264:GLN:HA	32:W:267:LEU:HG	2.03	0.41
18:R:166:ARG:HD2	18:R:166:ARG:HA	1.82	0.41
21:U:354:LYS:HA	21:U:357:LYS:HE2	2.02	0.41
25:a:370:GLN:HE22	28:d:244:LYS:HA	1.85	0.41
10:j:42:VAL:HG22	10:j:210:VAL:HG22	2.01	0.41
17:q:1:MET:HE3	17:q:133:GLY:HA2	2.01	0.41
20:t:76:LEU:HD23	20:t:76:LEU:HA	1.88	0.41
2:B:250:VAL:HG23	2:B:284:ILE:HG23	2.02	0.41
20:T:5:MET:HE3	20:T:5:MET:HB3	1.92	0.41
21:U:563:ALA:O	21:U:567:ILE:HG12	2.21	0.41
21:U:584:TYR:HE1	21:U:617:ALA:HB1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:40:LEU:HD21	24:Z:54:PHE:HE1	1.86	0.41
24:Z:223:ASN:ND2	24:Z:225:GLN:OE1	2.54	0.41
7:g:206:LEU:HD12	7:g:210:PHE:HZ	1.86	0.41
8:h:177:ARG:HA	8:h:177:ARG:HD3	1.89	0.41
10:j:178:ASP:O	10:j:182:GLU:HG2	2.20	0.41
1:A:347:ASP:OD1	1:A:348:LEU:N	2.49	0.41
4:D:209:GLY:HA2	37:D:501:ADP:H5'1	2.02	0.41
7:G:80:MET:HE2	7:G:87:SER:HA	2.03	0.41
21:U:532:MET:HE3	21:U:552:ILE:HG13	2.02	0.41
21:U:749:GLN:HA	21:U:755:THR:HA	2.02	0.41
25:a:236:THR:HG21	25:a:253:THR:HG21	2.02	0.41
25:a:321:LYS:HZ3	25:a:321:LYS:HG2	1.73	0.41
27:c:270:LEU:HA	27:c:273:LYS:HE3	2.03	0.41
29:f:538:ILE:HG13	29:f:562:LEU:HD21	2.02	0.41
29:f:679:LEU:HD13	29:f:687:ARG:HH11	1.86	0.41
11:k:147:ASP:OD1	11:k:147:ASP:N	2.54	0.41
15:o:214:GLU:OE2	16:p:198:ARG:NE	2.42	0.41
17:q:30:ASP:OD1	17:q:30:ASP:N	2.53	0.41
30:x:8:VAL:HB	30:x:15:PHE:HB2	2.03	0.41
30:x:425:THR:HG22	30:x:475:ALA:HA	2.03	0.41
32:W:344:THR:OG1	32:W:345:GLU:N	2.54	0.41
32:W:365:ILE:HA	32:W:368:LYS:HE2	2.02	0.41
2:B:121:ALA:HB2	2:B:135:ILE:HD11	2.03	0.41
3:C:147:THR:HA	3:C:206:HIS:HE1	1.86	0.41
3:C:220:VAL:HG23	3:C:221:GLN:H	1.84	0.41
3:C:226:GLU:HB2	3:C:230:MET:HE2	2.03	0.41
4:D:80:LYS:HE2	4:D:80:LYS:HB3	1.88	0.41
15:O:143:ARG:H	15:O:146:MET:HE3	1.85	0.41
17:Q:153:ARG:HE	17:Q:153:ARG:HB2	1.71	0.41
19:S:63:THR:HG21	20:T:97:TYR:CZ	2.56	0.41
21:U:164:GLU:HA	21:U:167:ILE:HG12	2.03	0.41
21:U:499:THR:O	21:U:503:GLN:NE2	2.39	0.41
21:U:623:GLY:O	21:U:627:PHE:HB3	2.21	0.41
23:Y:372:LYS:HA	23:Y:372:LYS:HD3	1.93	0.41
23:Y:385:ARG:HB3	34:V:282:ASN:HD21	1.85	0.41
24:Z:108:ILE:O	24:Z:112:MET:HG2	2.20	0.41
24:Z:138:TYR:HD1	24:Z:157:HIS:HA	1.85	0.41
24:Z:209:ARG:HH21	25:a:354:GLU:HA	1.86	0.41
26:b:91:ARG:HA	26:b:94:HIS:CD2	2.56	0.41
27:c:34:SER:HA	27:c:208:ARG:HB2	2.02	0.41
27:c:139:ARG:HH21	27:c:161:ARG:HH12	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:285:GLU:HA	27:c:288:VAL:HB	2.02	0.41
29:f:456:ARG:HD3	29:f:494:ARG:HH22	1.85	0.41
29:f:523:GLY:HA3	29:f:561:GLY:HA2	2.03	0.41
7:g:73:THR:HG22	7:g:76:ILE:HB	2.03	0.41
10:j:158:ALA:HB1	10:j:172:LEU:HD21	2.02	0.41
19:s:145:LEU:HD22	19:s:178:VAL:HG13	2.02	0.41
30:x:409:ASP:OD1	30:x:409:ASP:N	2.52	0.41
32:W:201:ARG:O	32:W:205:ILE:HG12	2.21	0.41
34:V:345:ARG:HA	34:V:348:PHE:HD2	1.85	0.41
1:A:35:THR:HB	29:f:100:ARG:HD2	2.03	0.41
2:B:199:GLU:HA	2:B:203:LEU:HB2	2.03	0.41
4:D:172:ILE:O	4:D:175:GLN:HG2	2.21	0.41
5:E:233:ASP:OD1	5:E:233:ASP:N	2.47	0.41
7:G:138:MET:HG2	7:G:140:LEU:HD22	2.03	0.41
11:K:52:LYS:HG2	11:K:64:ILE:HD11	2.03	0.41
17:Q:11:ASP:N	17:Q:11:ASP:OD1	2.54	0.41
21:U:351:MET:HA	21:U:354:LYS:HG2	2.03	0.41
29:f:746:ARG:HA	29:f:749:ALA:HB3	2.03	0.41
12:l:146:GLN:HB2	12:l:159:MET:HE1	2.02	0.41
18:r:148:GLU:HB2	18:r:151:GLN:HG3	2.03	0.41
32:W:363:ILE:HA	32:W:366:MET:HG2	2.03	0.41
2:B:407:LEU:HD22	3:C:178:LEU:HD11	2.03	0.40
4:D:354:LEU:HD12	4:D:358:VAL:HG21	2.03	0.40
8:H:119:GLN:HB3	8:H:153:GLY:HA3	2.03	0.40
11:K:107:MET:HE3	11:K:112:VAL:HG22	2.03	0.40
14:N:147:MET:HE2	14:N:151:GLU:HB3	2.02	0.40
17:Q:27:GLN:HG3	17:q:172:ILE:HG22	2.02	0.40
24:Z:25:ARG:HH11	27:c:104:ARG:HD3	1.86	0.40
24:Z:198:LEU:HD23	24:Z:198:LEU:HA	1.96	0.40
29:f:178:LYS:H	29:f:178:LYS:HG3	1.61	0.40
29:f:789:SER:H	29:f:793:VAL:HB	1.86	0.40
34:V:121:PHE:HB3	34:V:128:ARG:HD2	2.02	0.40
34:V:182:LYS:HE2	34:V:182:LYS:HB2	1.86	0.40
34:V:211:TYR:OH	34:V:234:ARG:NE	2.50	0.40
1:A:184:ILE:HD13	1:A:184:ILE:HA	1.99	0.40
5:E:101:ASP:OD2	5:E:103:THR:OG1	2.35	0.40
6:F:431:LYS:HD3	6:F:431:LYS:HA	1.94	0.40
7:G:10:ASP:OD2	13:M:7:TYR:OH	2.28	0.40
17:Q:1:MET:HE3	17:Q:133:GLY:HA2	2.03	0.40
21:U:329:LEU:HD23	21:U:329:LEU:HA	1.95	0.40
21:U:644:TYR:O	21:U:649:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:844:LYS:HE2	21:U:844:LYS:HB3	1.77	0.40
27:c:160:PHE:HB3	27:c:200:TYR:HE2	1.86	0.40
27:c:303:MET:O	27:c:306:THR:OG1	2.32	0.40
28:d:65:ARG:HE	28:d:65:ARG:HB2	1.68	0.40
28:d:181:CYS:HB2	34:V:443:ARG:HH21	1.86	0.40
20:t:70:MET:HE1	20:t:91:TRP:CE2	2.55	0.40
20:t:100:ARG:HG3	20:t:128:LEU:HA	2.03	0.40
30:x:133:LEU:HD23	30:x:133:LEU:HA	1.96	0.40
4:D:133:HIS:HB3	4:D:137:ASN:H	1.86	0.40
6:F:250:LYS:HD2	6:F:255:GLN:HE22	1.87	0.40
20:T:15:LYS:HA	20:T:20:VAL:HA	2.03	0.40
21:U:504:ASP:OD1	21:U:535:TYR:OH	2.31	0.40
21:U:664:GLY:HA2	21:U:695:MET:HE1	2.02	0.40
25:a:68:GLU:HG3	25:a:69:HIS:H	1.86	0.40
29:f:741:LEU:HD12	29:f:792:ALA:HB1	2.03	0.40
12:l:7:ASP:OD1	12:l:7:ASP:N	2.52	0.40
3:C:138:MET:HB2	3:C:237:MET:HE1	2.04	0.40
6:F:254:PRO:HD3	6:F:290:ALA:HB3	2.03	0.40
6:F:361:ALA:O	6:F:365:ILE:HG12	2.22	0.40
12:L:125:ARG:NH1	12:L:126:ARG:O	2.50	0.40
17:Q:167:LEU:HD23	17:Q:167:LEU:HA	1.95	0.40
18:R:71:LYS:HE2	18:R:71:LYS:HB2	1.96	0.40
19:S:26:ASP:OD1	19:S:190:GLY:N	2.44	0.40
19:S:27:THR:HG21	19:S:192:ALA:HB3	2.03	0.40
21:U:69:TYR:OH	21:U:95:GLU:OE1	2.27	0.40
25:a:72:ASN:HA	25:a:73:PRO:HD3	1.99	0.40
28:d:183:GLU:OE2	28:d:215:TRP:NE1	2.55	0.40
29:f:20:ALA:HA	29:f:23:GLY:HA3	2.04	0.40
14:n:192:ASP:OD1	14:n:192:ASP:N	2.54	0.40
19:s:99:ARG:HD3	19:s:104:TYR:CE2	2.57	0.40
30:x:126:VAL:HG12	30:x:129:LEU:H	1.86	0.40
2:B:278:ALA:O	2:B:280:SER:N	2.54	0.40
4:D:284:GLU:HA	4:D:287:ARG:HB2	2.03	0.40
12:L:206:THR:HG23	12:L:208:LYS:H	1.86	0.40
14:N:87:CYS:HA	14:N:94:LEU:HD21	2.04	0.40
16:P:4:MET:HE3	16:P:4:MET:HB3	1.82	0.40
21:U:669:ILE:HG23	21:U:709:PHE:HE2	1.86	0.40
28:d:71:PHE:HE2	28:d:105:PHE:CG	2.40	0.40
12:l:117:GLN:O	12:l:120:THR:OG1	2.38	0.40
12:l:159:MET:HE2	12:l:159:MET:HB3	1.86	0.40
31:y:11:LYS:HA	31:y:11:LYS:HD3	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:W:108:CYS:HA	32:W:111:TYR:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	ADP	D	501	-	28,29,29	1.45	5 (17%)	43,45,45	1.84	8 (18%)
36	ATP	A	501	-	32,33,33	0.33	0	48,52,52	0.27	0
36	ATP	B	501	-	32,33,33	0.34	0	48,52,52	0.28	0
36	ATP	F	501	-	32,33,33	0.27	0	48,52,52	0.28	0
36	ATP	C	501	-	32,33,33	0.37	0	48,52,52	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	ADP	D	501	-	-	2/16/32/32	0/3/3/3
36	ATP	A	501	-	-	4/22/38/38	0/3/3/3
36	ATP	B	501	-	-	7/22/38/38	0/3/3/3
36	ATP	F	501	-	-	7/22/38/38	0/3/3/3
36	ATP	C	501	-	-	7/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D	501	ADP	C5-C4	4.74	1.47	1.39
37	D	501	ADP	C5-C6	2.70	1.48	1.41
37	D	501	ADP	C5-N7	-2.38	1.34	1.39
37	D	501	ADP	PA-O3A	2.33	1.62	1.59
37	D	501	ADP	C8-N7	2.29	1.36	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D	501	ADP	C5-C4-N3	-5.96	118.51	126.72
37	D	501	ADP	N3-C4-N9	4.74	135.23	127.17
37	D	501	ADP	C2-N3-C4	3.71	120.90	111.83
37	D	501	ADP	C4-C5-N7	-3.37	106.73	110.58
37	D	501	ADP	N3-C2-N1	-3.19	123.75	128.58
37	D	501	ADP	C3'-C2'-C1'	2.53	106.24	101.46
37	D	501	ADP	C5-N7-C8	2.46	107.32	103.45
37	D	501	ADP	C4-N9-C8	2.46	108.32	105.74

There are no chirality outliers.

All (27) torsion outliers are listed below:

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

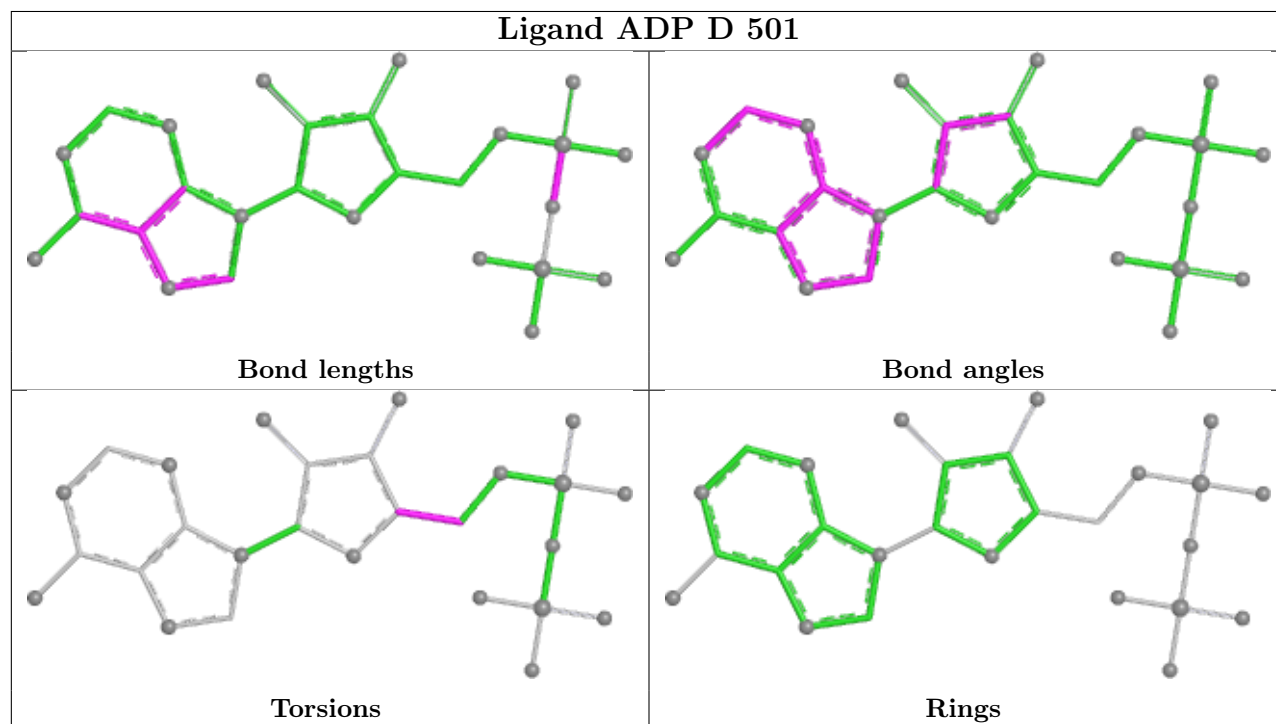
There are no ring outliers.

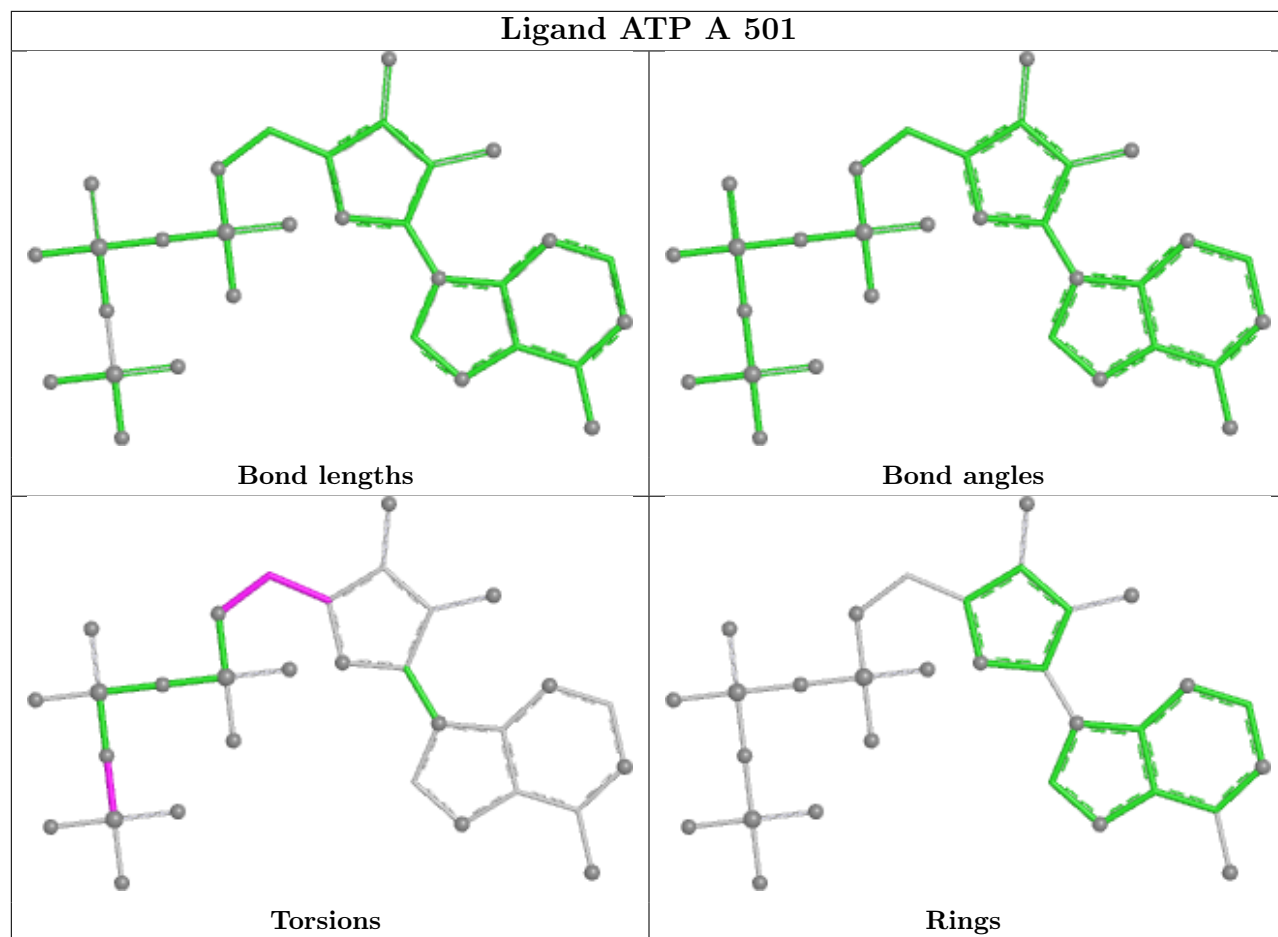
3 monomers are involved in 4 short contacts:

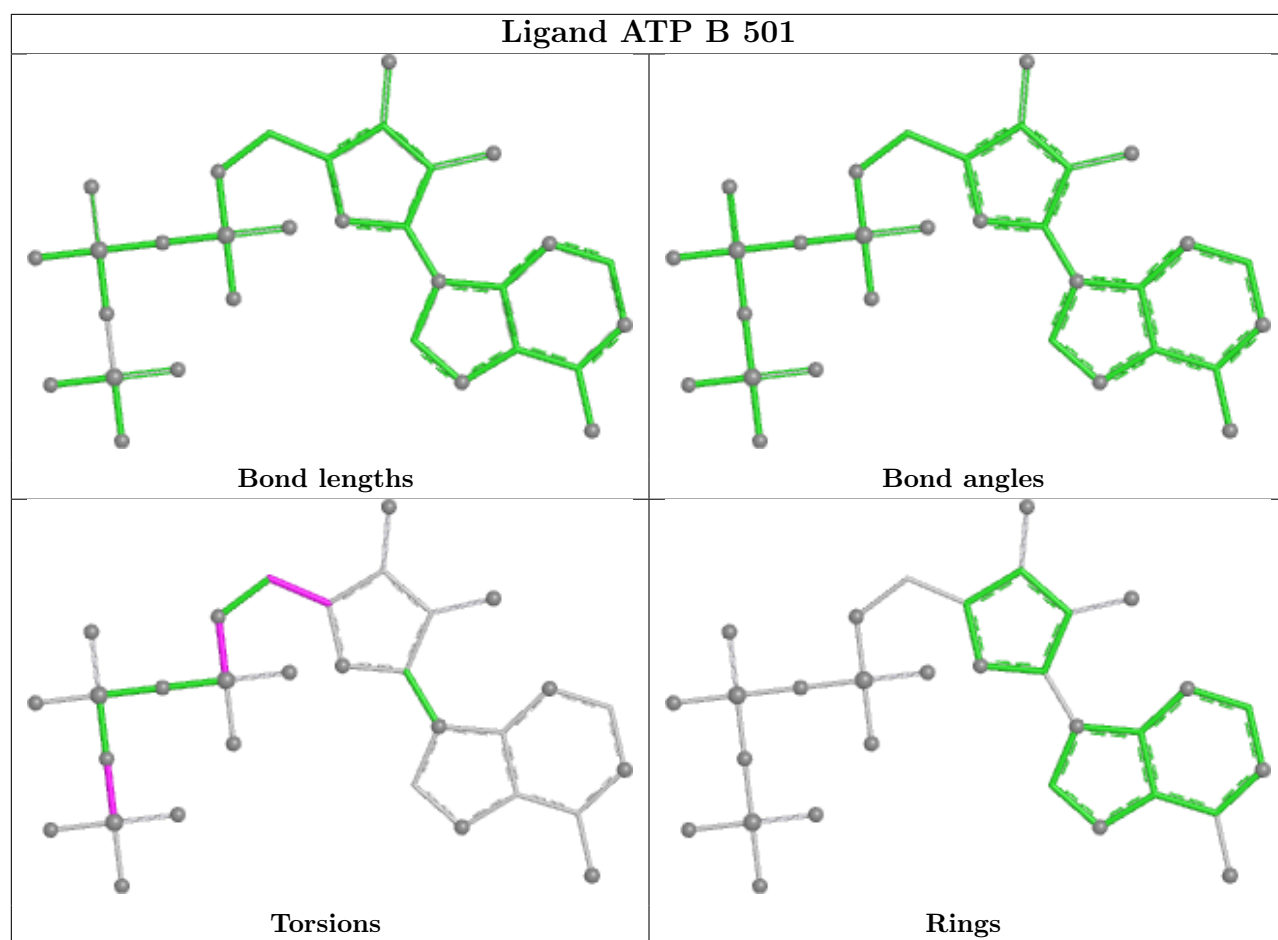
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	D	501	ADP	2	0
36	A	501	ATP	1	0
36	B	501	ATP	1	0

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.

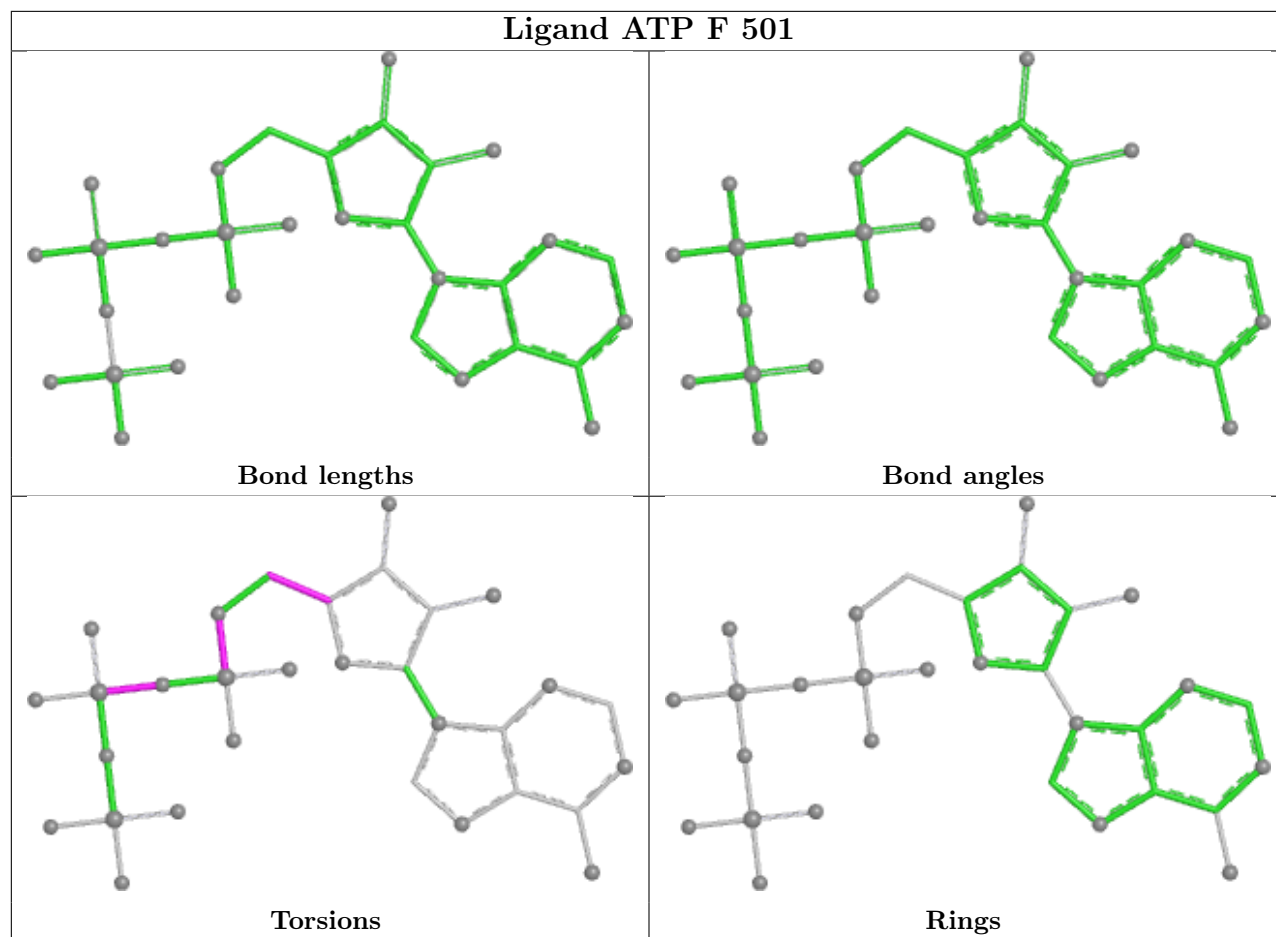
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

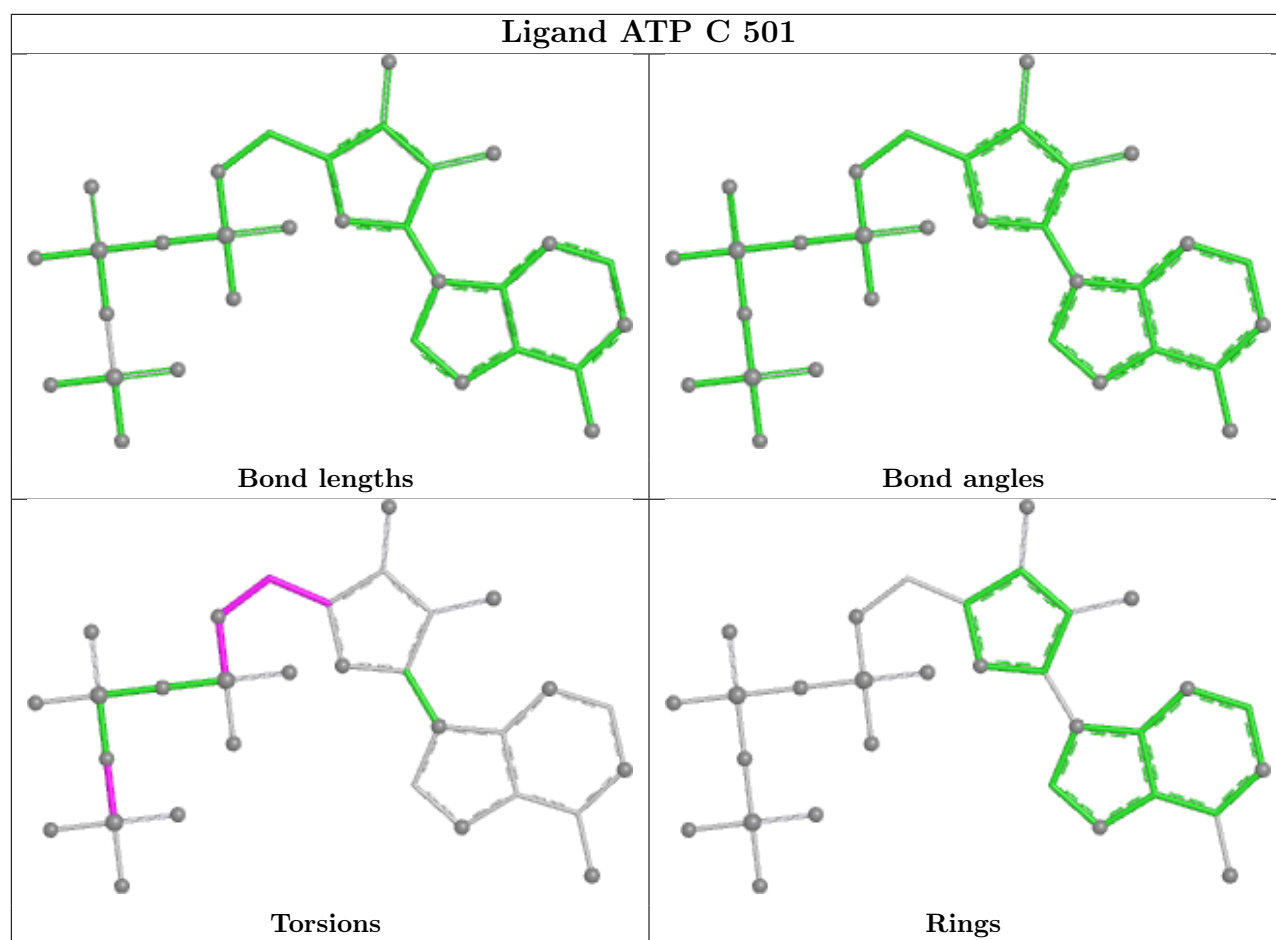






Ligand ATP F 501





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.

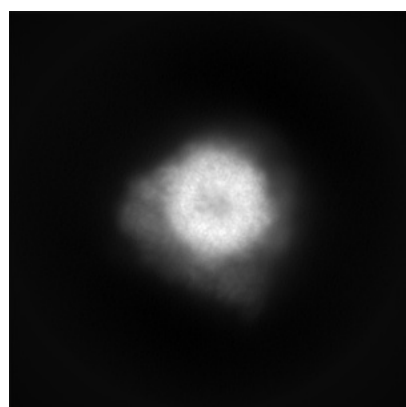
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32279. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

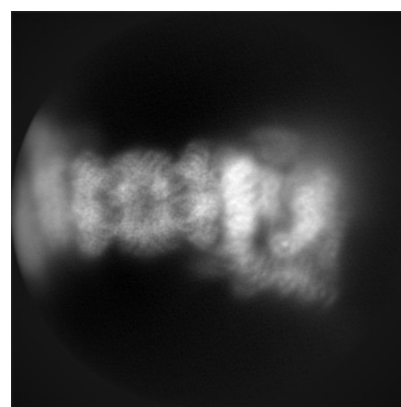
6.1.1 Primary map



X



Y

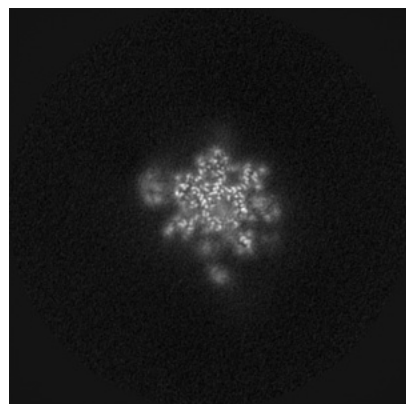


Z

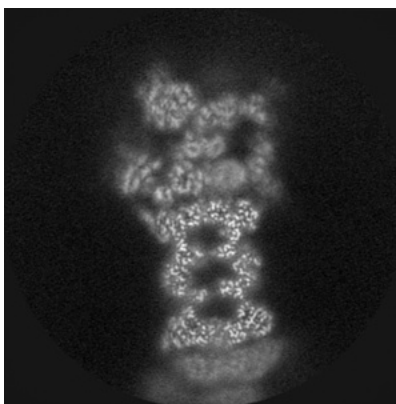
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

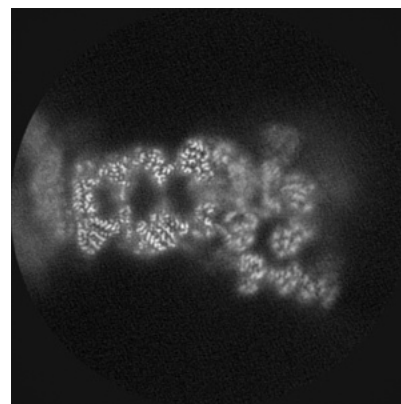
6.2.1 Primary map



X Index: 320



Y Index: 320

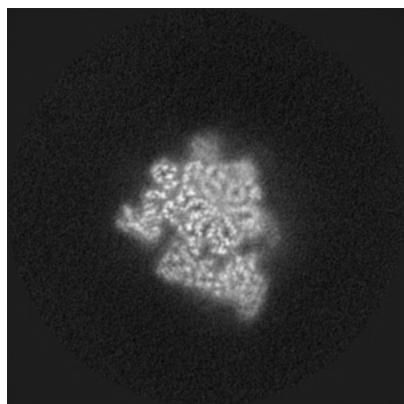


Z Index: 320

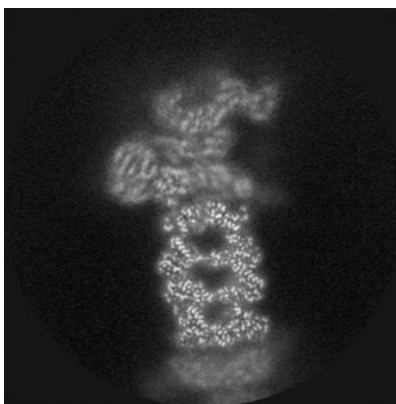
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

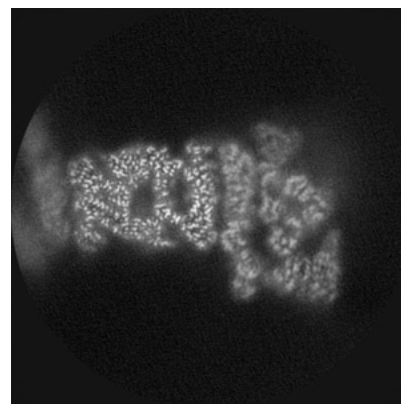
6.3.1 Primary map



X Index: 367



Y Index: 358

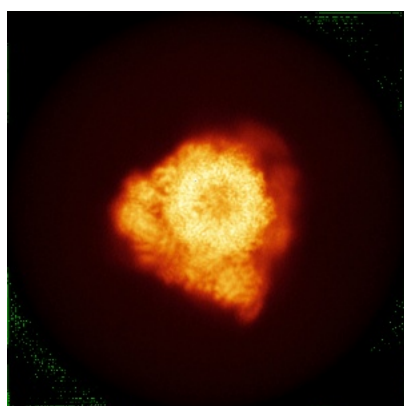


Z Index: 301

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

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

6.4.1 Primary map



X



Y

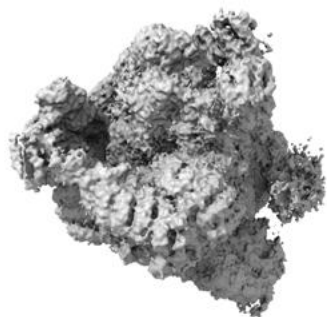


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

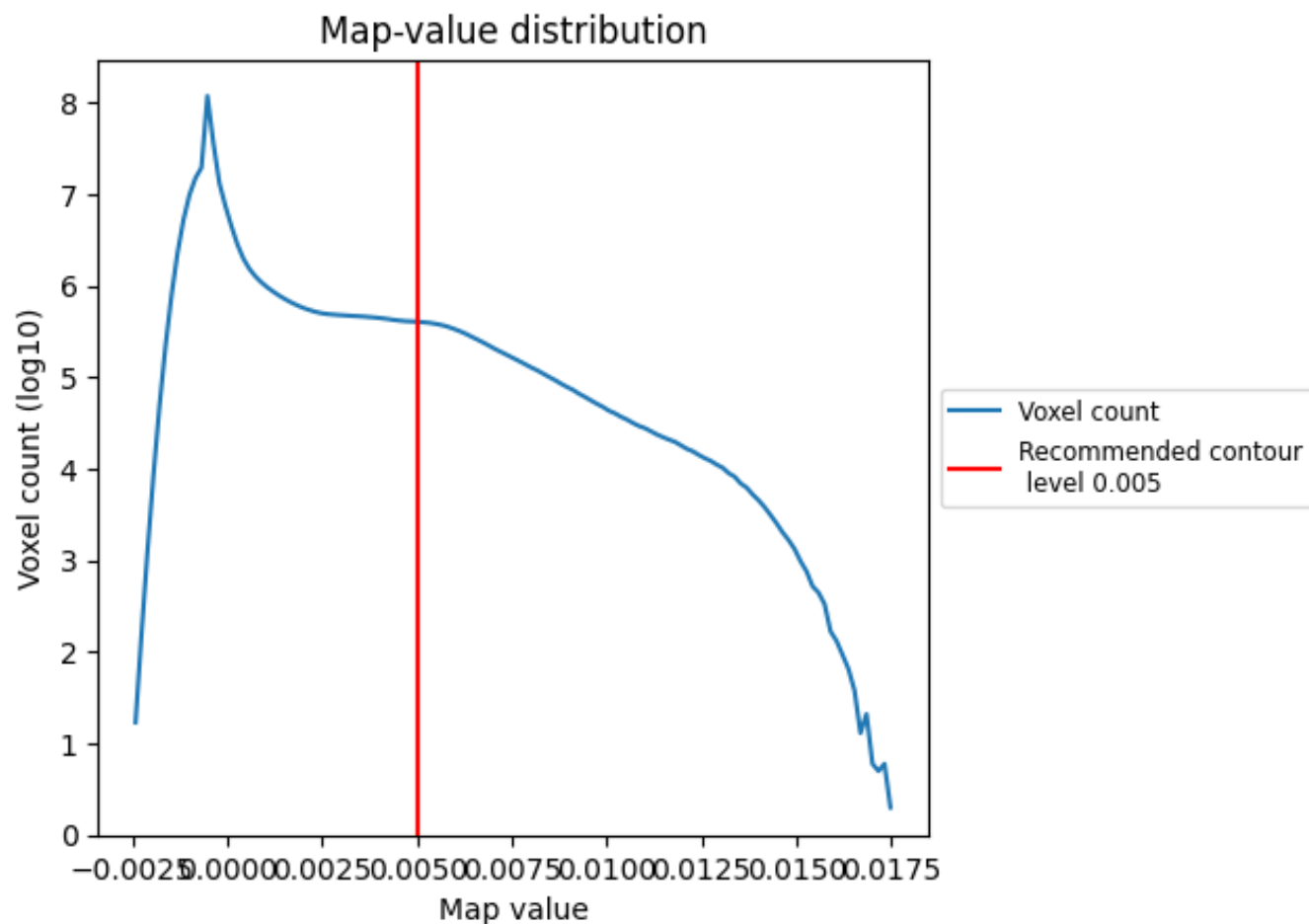
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

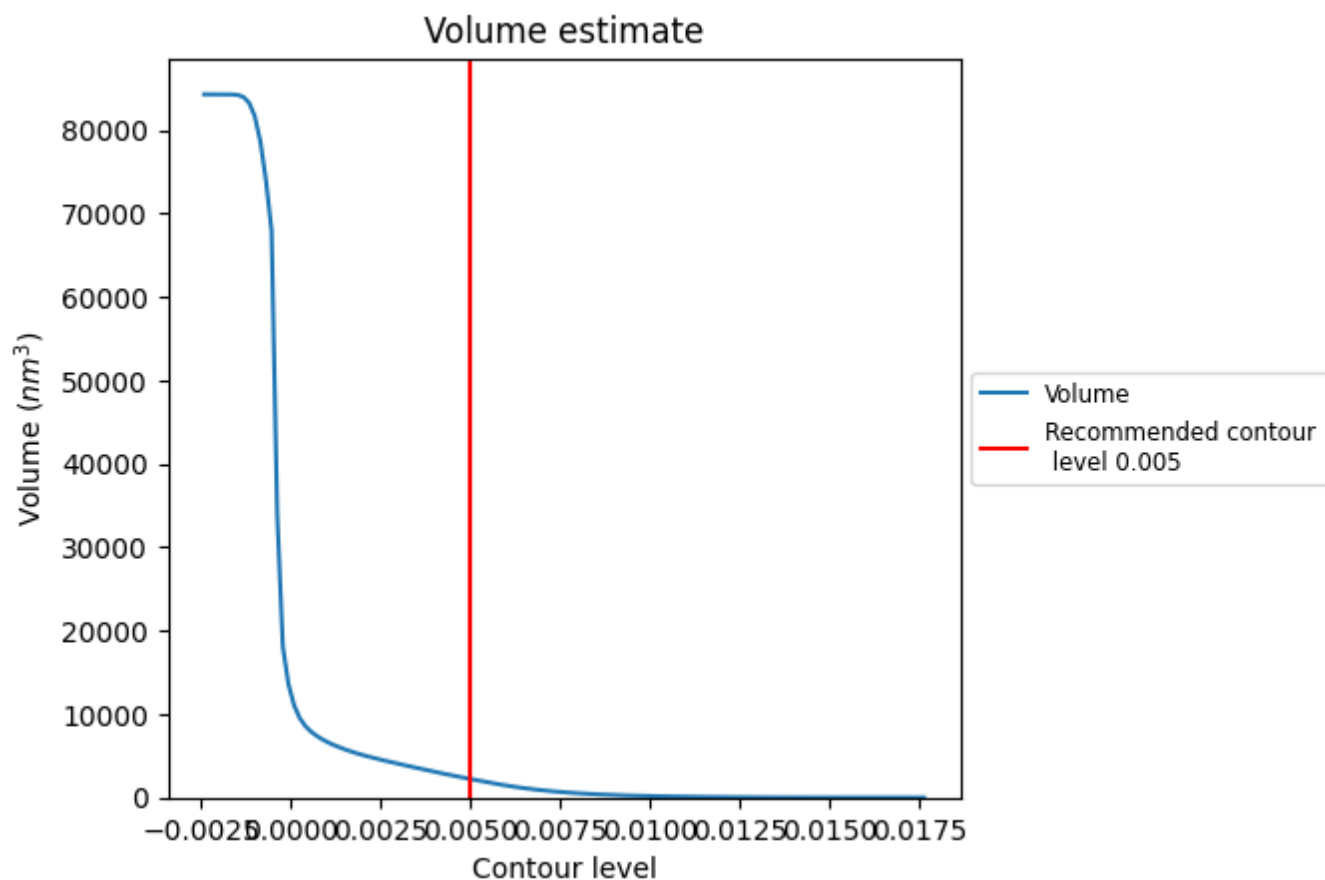
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

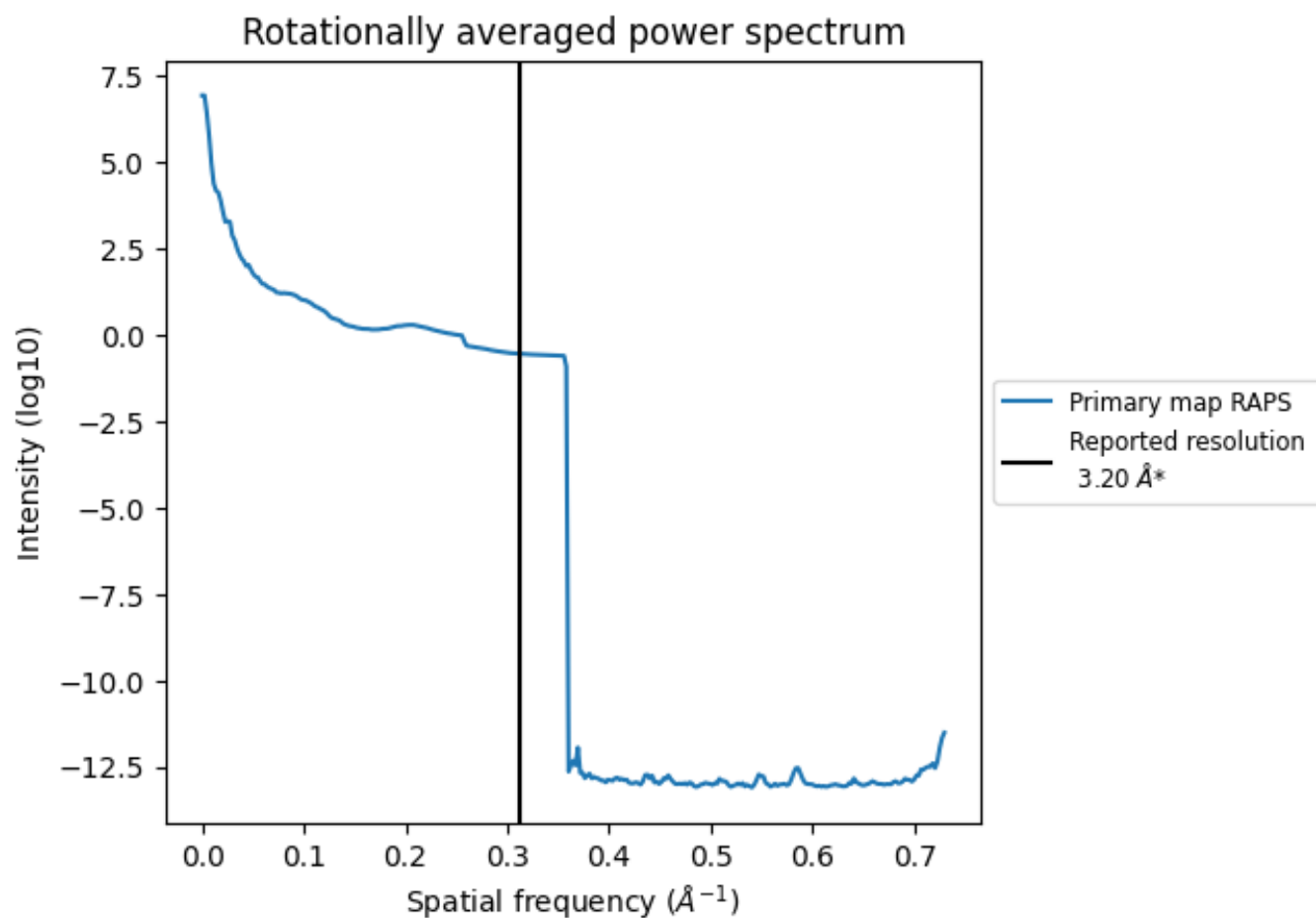
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2224 nm³; this corresponds to an approximate mass of 2009 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

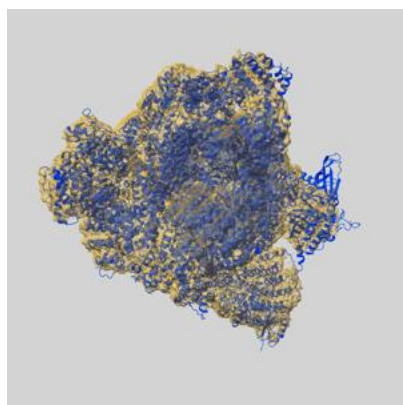
8 Fourier-Shell correlation ⓘ

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

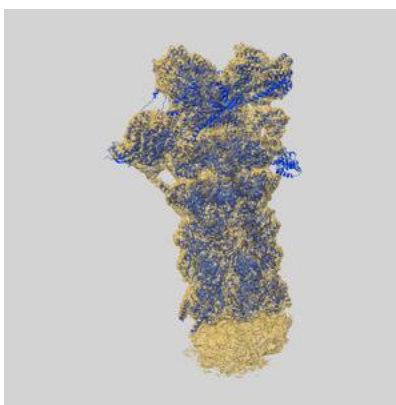
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32279 and PDB model 7W3G. Per-residue inclusion information can be found in section [3](#) on page [13](#).

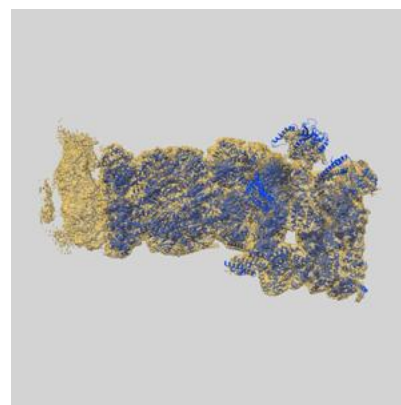
9.1 Map-model overlay [i](#)



X



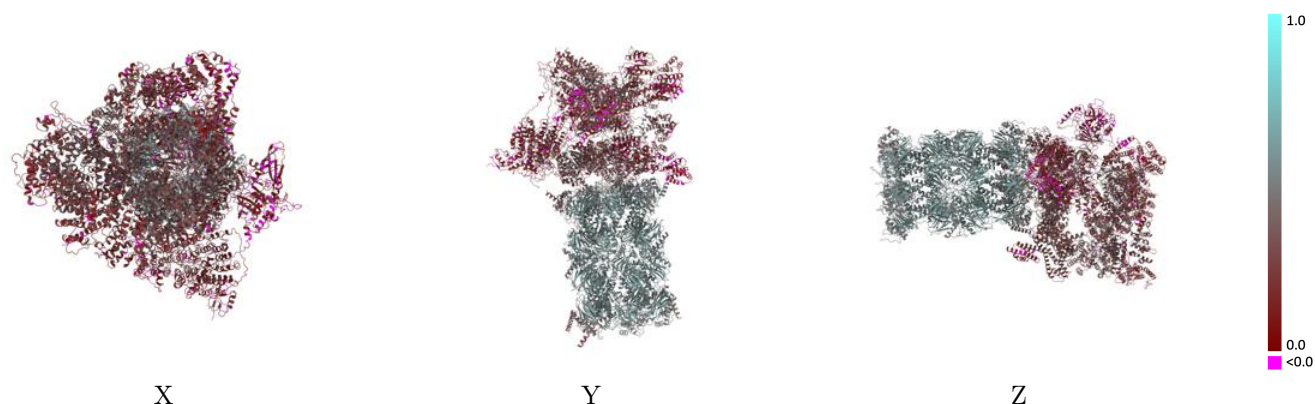
Y



Z

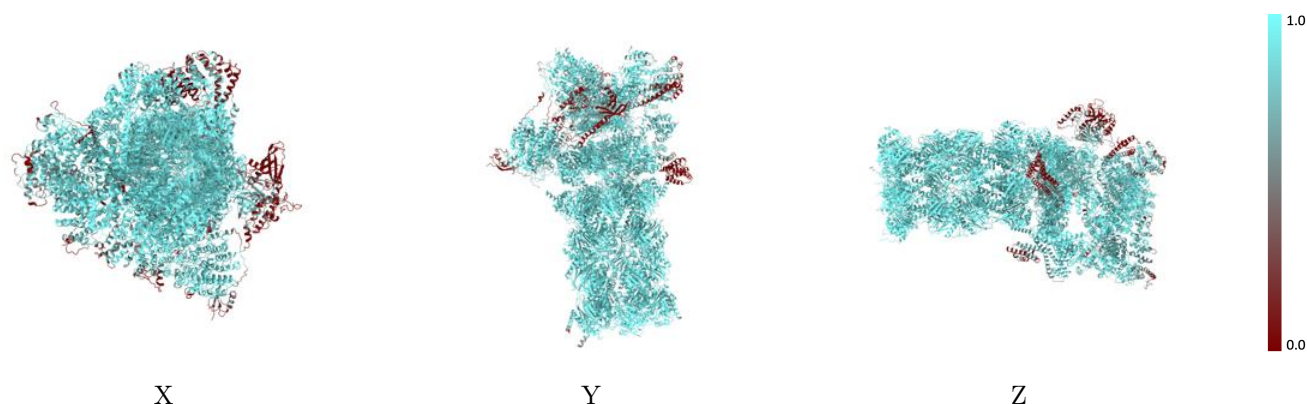
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



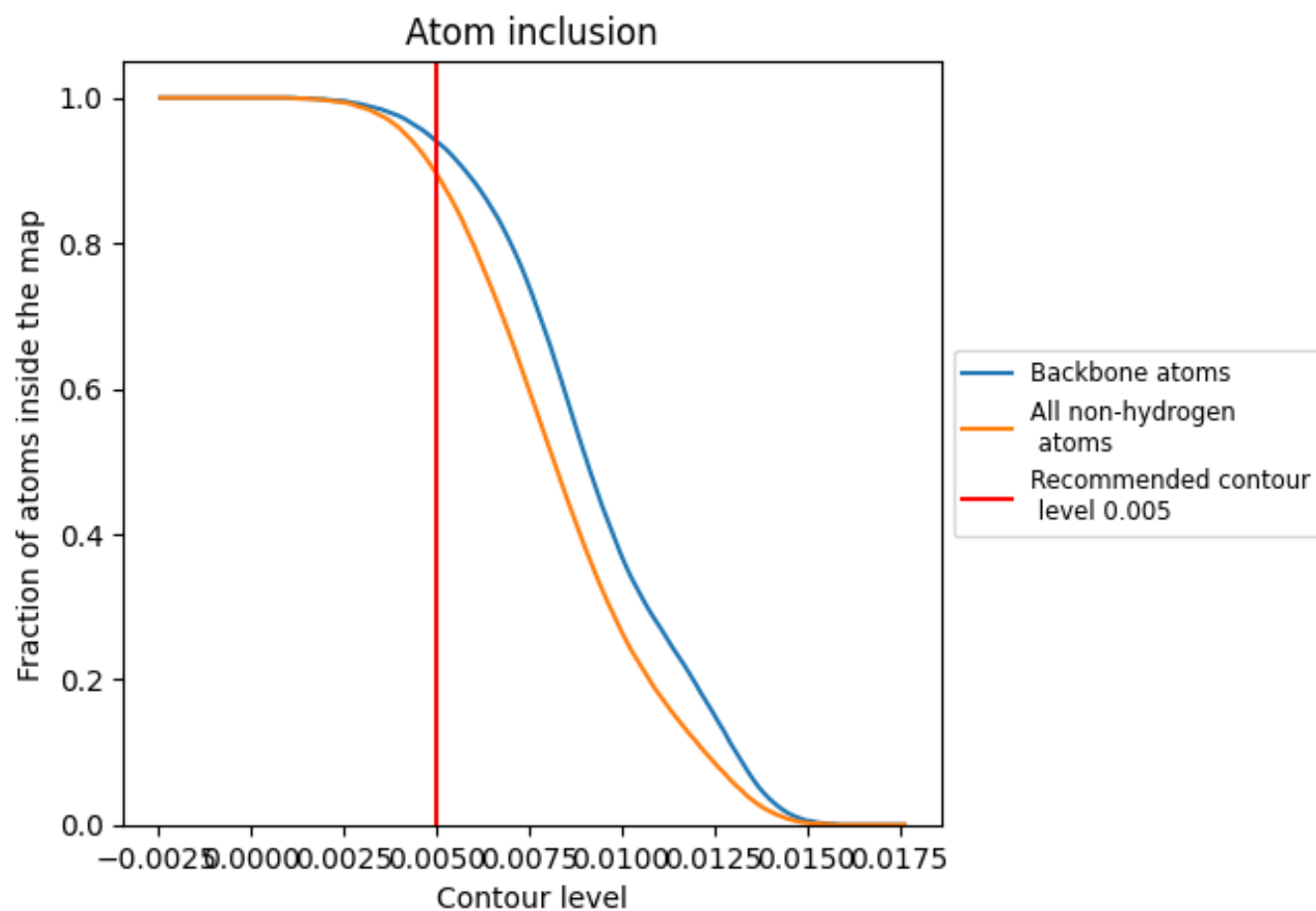
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8970	 0.3760
A	 0.9570	 0.2820
B	 0.9520	 0.3130
C	 0.9740	 0.3390
D	 0.9750	 0.3230
E	 0.8620	 0.1750
F	 0.8810	 0.2150
G	 0.9800	 0.5150
H	 0.9930	 0.5220
I	 0.9770	 0.5080
J	 0.9730	 0.4850
K	 0.9740	 0.5030
L	 0.9870	 0.5330
M	 0.9790	 0.5230
N	 0.9810	 0.5510
O	 0.9930	 0.5460
P	 0.9970	 0.5580
Q	 0.9940	 0.5470
R	 0.9900	 0.5480
S	 0.9850	 0.5510
T	 0.9820	 0.5540
U	 0.8700	 0.2830
V	 0.8570	 0.2980
W	 0.6340	 0.2010
X	 0.8450	 0.2960
Y	 0.9300	 0.3150
Z	 0.9600	 0.2980
a	 0.8120	 0.2470
b	 0.8450	 0.2120
c	 0.9360	 0.2970
d	 0.6850	 0.2300
e	 0.8570	 0.2890
f	 0.8620	 0.1970
g	 0.9640	 0.5220
h	 0.9800	 0.5270



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Chain	Atom inclusion	Q-score
i	 0.9550	 0.5080
j	 0.9590	 0.4730
k	 0.9720	 0.5200
l	 0.9820	 0.5350
m	 0.9610	 0.5220
n	 0.9850	 0.5560
o	 0.9820	 0.5480
p	 0.9920	 0.5530
q	 0.9940	 0.5510
r	 0.9950	 0.5540
s	 0.9890	 0.5490
t	 0.9810	 0.5550
v	 0.9770	 0.2240
x	 0.3590	 0.1410
y	 0.1250	 0.1620