



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:44 AM UTC

PDB ID : 7W3H / pdb_00007w3h
EMDB ID : EMD-32280
Title : Structure of USP14-bound human 26S proteasome in substrate-engaged state
ED2.1_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

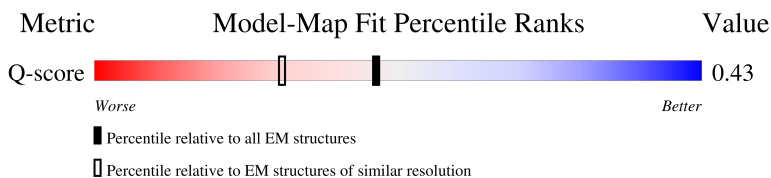
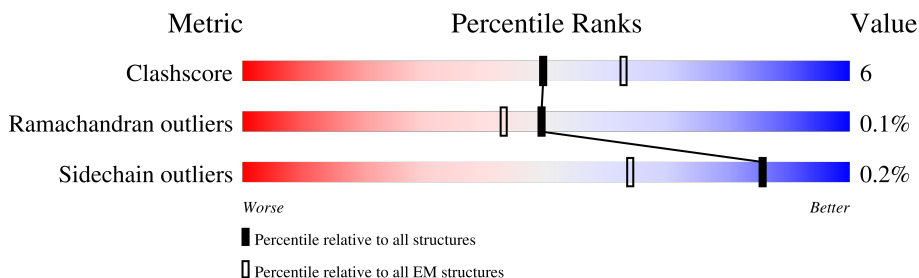
1 Overall quality at a glance

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.



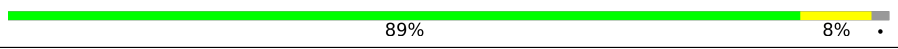
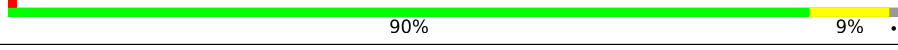
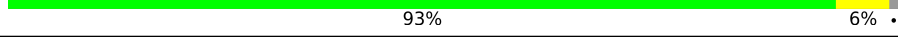
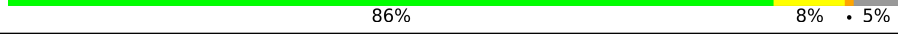
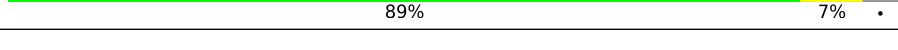
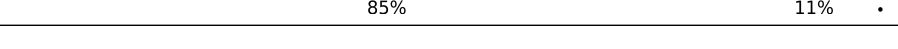
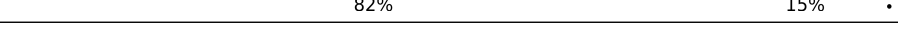
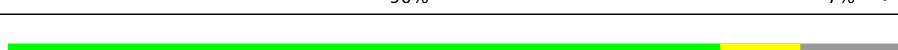
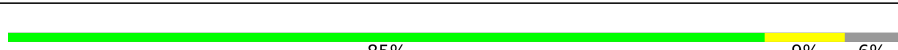
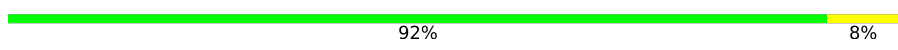
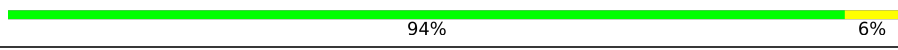
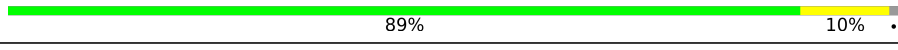
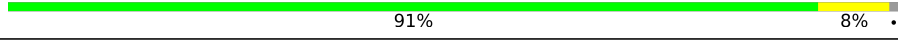
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	
2	B	440	
3	C	398	
4	D	418	

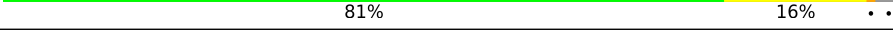
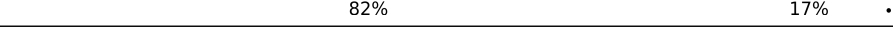
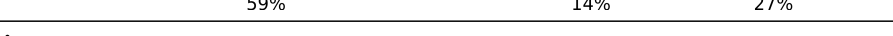
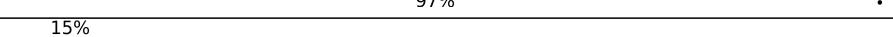
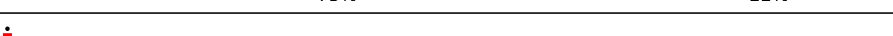
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Mol	Chain	Length	Quality of chain
5	E	403	
6	F	439	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	269	
12	l	269	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	Q	201	
17	q	201	
18	R	263	

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Mol	Chain	Length	Quality of chain
18	r	263	
19	S	241	
19	s	241	
20	T	264	
20	t	264	
21	U	953	 .
22	V	534	 .
23	X	422	
24	Y	389	 . .
25	Z	324	
26	a	376	 .
27	b	377	
28	c	310	
29	d	350	 .
30	f	908	 .
31	v	36	 .
32	x	494	
33	y	76	
34	W	456	 . .
35	e	70	

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 110771 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
			3245	2044	570	613	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 3.

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

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

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

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

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

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

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

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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

- Molecule 31 is a protein called Substrate.

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

- Molecule 32 is a protein called Ubiquitin carboxyl-terminal hydrolase 14.

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

- Molecule 33 is a protein called Ubiquitin.

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

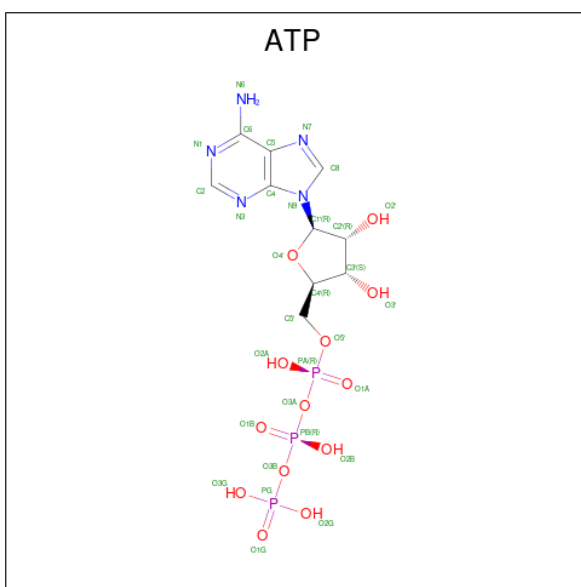
- Molecule 34 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

- 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).

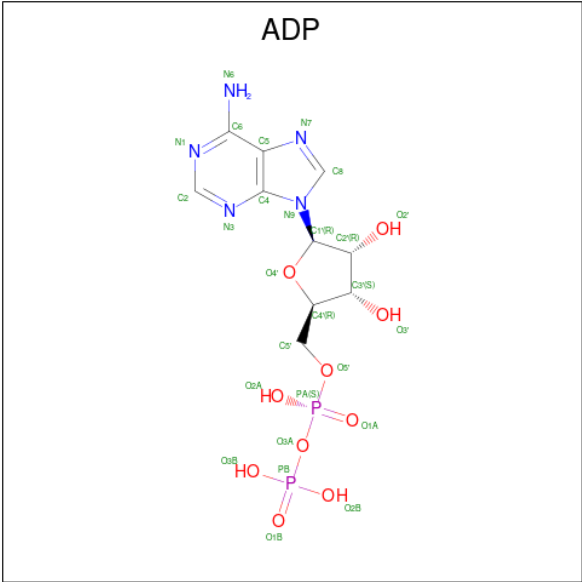


Mol	Chain	Residues	Atoms					AltConf
36	A	1	Total 31	C 10	N 5	O 13	P 3	0
36	B	1	Total 31	C 10	N 5	O 13	P 3	0
36	C	1	Total 31	C 10	N 5	O 13	P 3	0
36	F	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

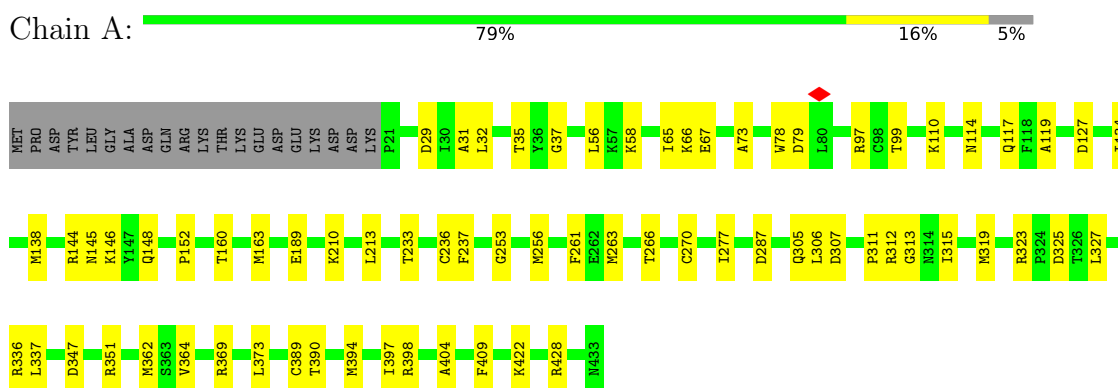
- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



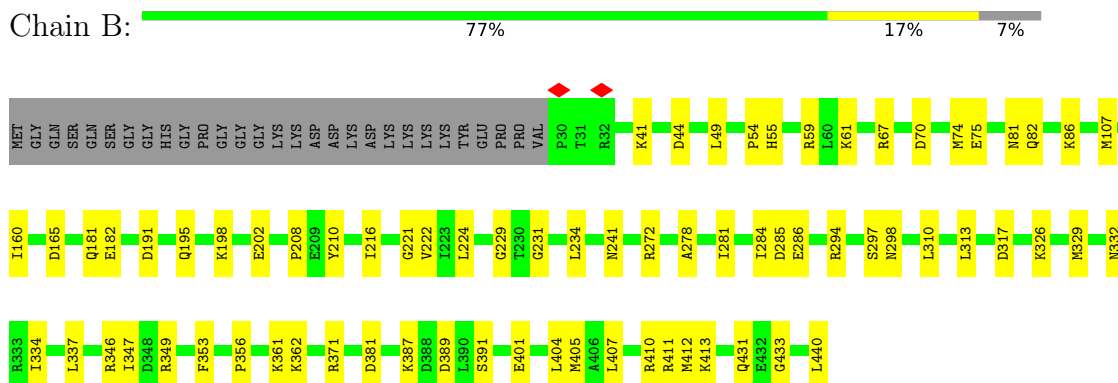
3 Residue-property plots [i](#)

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

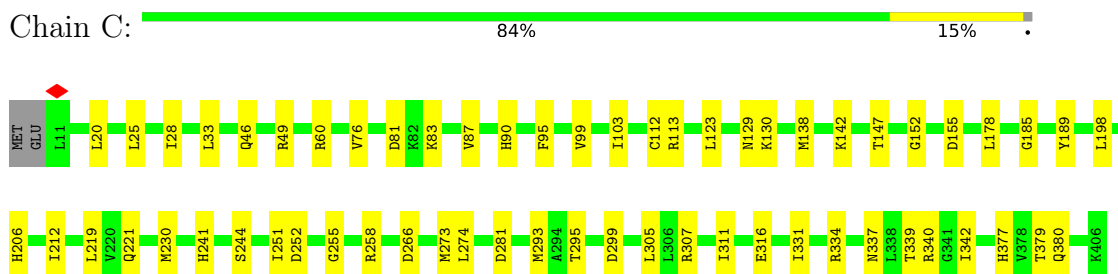
• Molecule 1: 26S protease regulatory subunit 7



• Molecule 2: 26S protease regulatory subunit 4

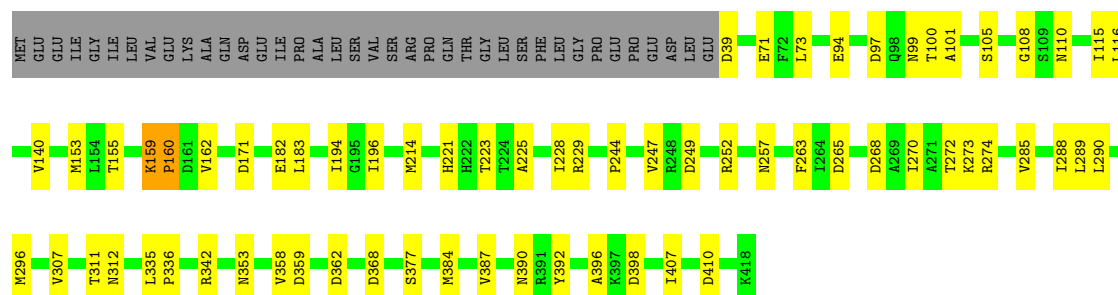


• Molecule 3: Isoform 2 of 26S proteasome regulatory subunit 8



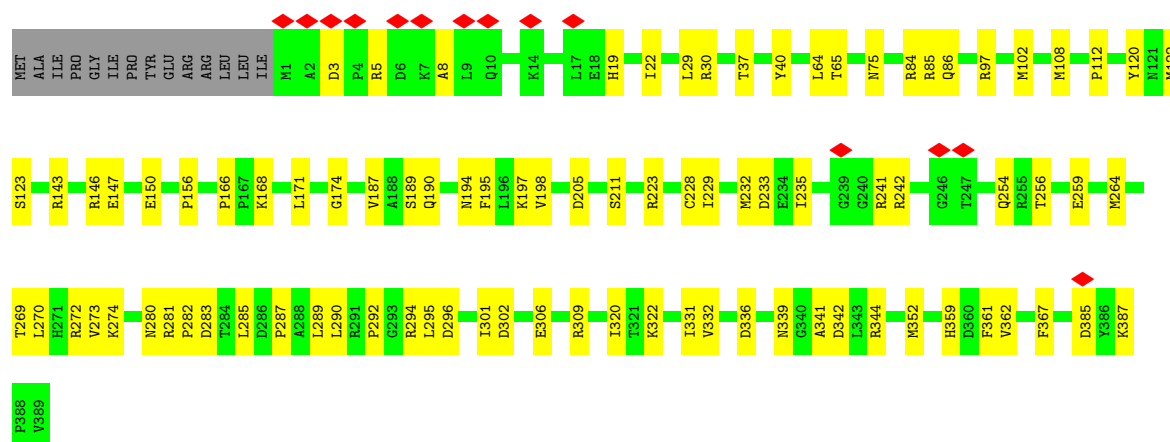
- Molecule 4: 26S protease regulatory subunit 6B

Chain D:  75% 16% 9%



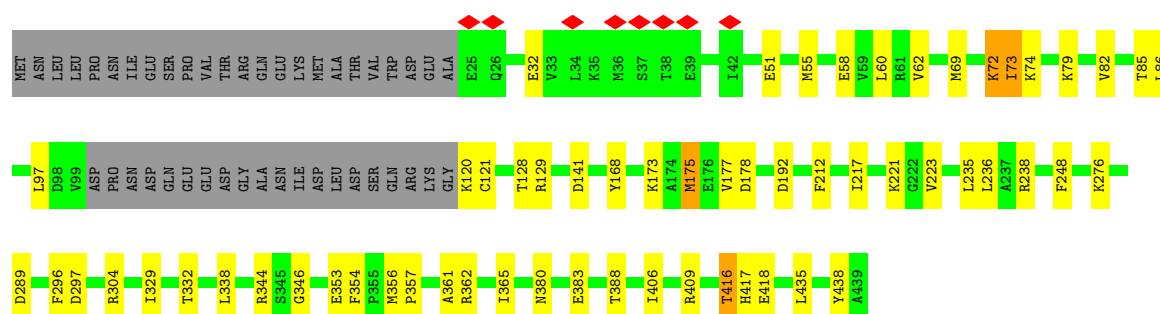
- Molecule 5: 26S proteasome regulatory subunit 10B

Chain E:  74% 22% 4%



- Molecule 6: 26S protease regulatory subunit 6A

Chain F:  76% 13% 10%



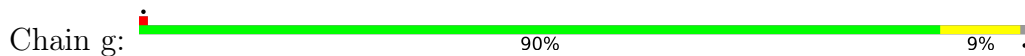
- Molecule 7: Proteasome subunit alpha type-6

Chain G:  89% 8% 3%

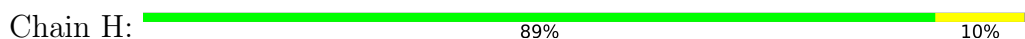




• Molecule 7: Proteasome subunit alpha type-6



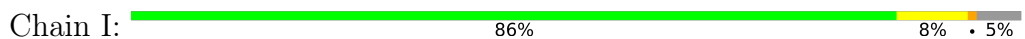
• Molecule 8: Proteasome subunit alpha type-2



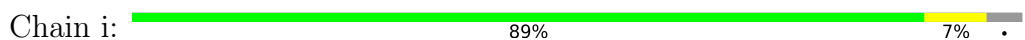
• Molecule 8: Proteasome subunit alpha type-2



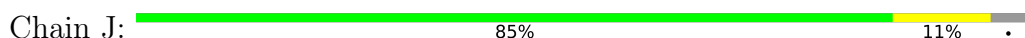
• Molecule 9: Proteasome subunit alpha type-4



• Molecule 9: Proteasome subunit alpha type-4



• Molecule 10: Proteasome subunit alpha type-7



• Molecule 10: Proteasome subunit alpha type-7

Chain j:  82% 15% .



- Molecule 11: Proteasome subunit alpha type-5

Chain K:  90% 8% .



- Molecule 11: Proteasome subunit alpha type-5

Chain k:  90% 7% .



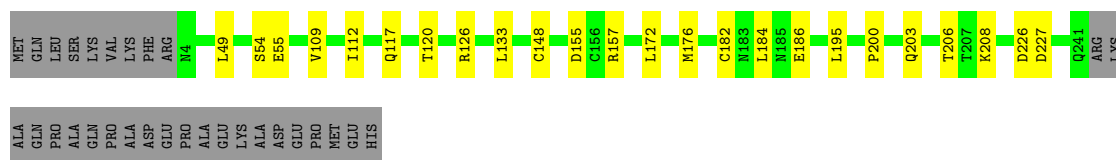
- Molecule 12: Isoform Long of Proteasome subunit alpha type-1

Chain L:  80% 9% 11%



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

Chain l:  80% 9% 12%



- Molecule 13: Proteasome subunit alpha type-3

Chain M:  87% 8% 5%



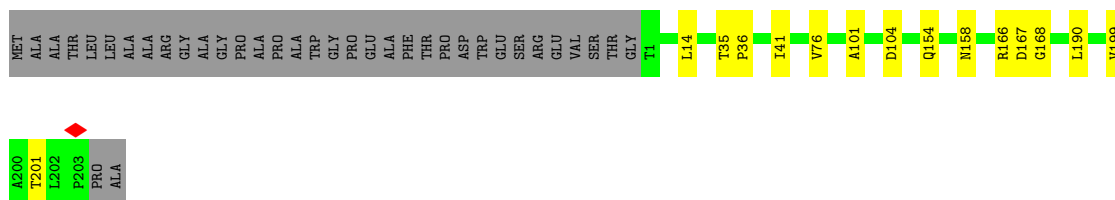
- Molecule 13: Proteasome subunit alpha type-3

Chain m:  85% 9% 6%



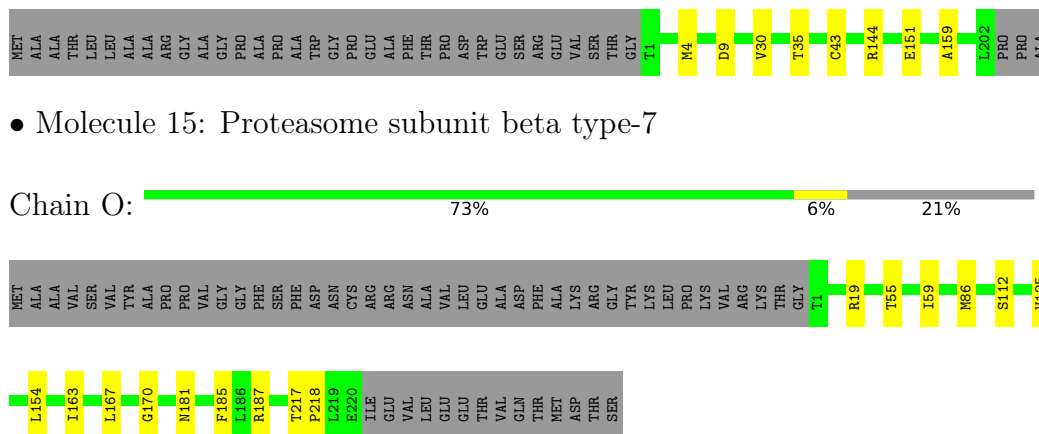
- Molecule 14: Proteasome subunit beta type-6

Chain N:  79% 6% 15%



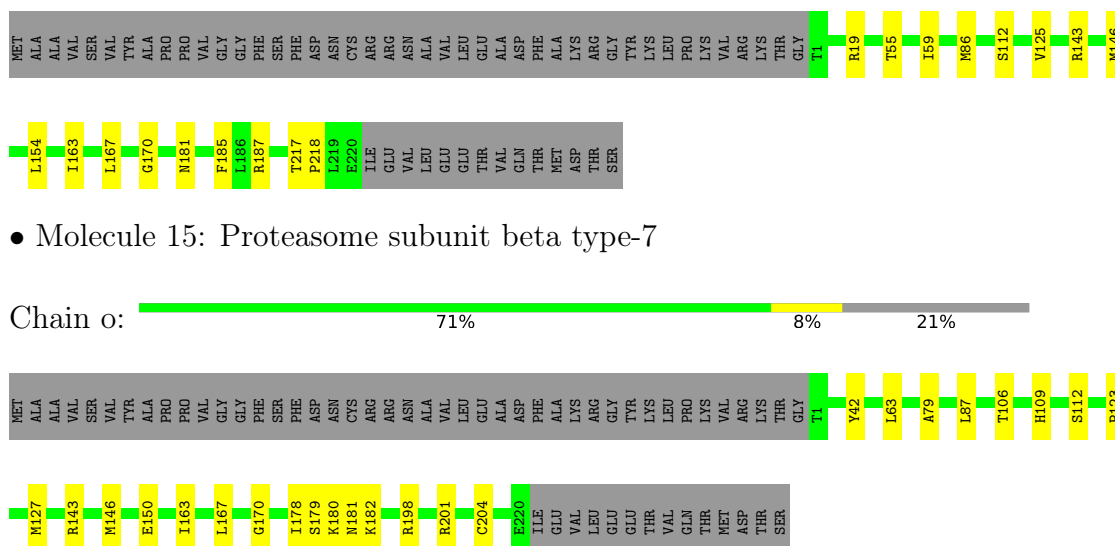
- Molecule 14: Proteasome subunit beta type-6

Chain n:  81% 15%



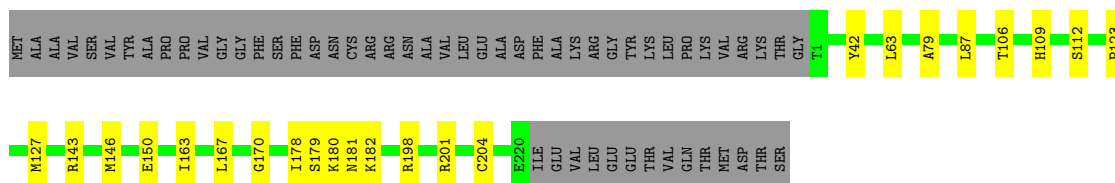
- Molecule 15: Proteasome subunit beta type-7

Chain O:  73% 6% 21%



- Molecule 15: Proteasome subunit beta type-7

Chain o:  71% 8% 21%



- Molecule 16: Proteasome subunit beta type-3

Chain P:  92% 8%



- Molecule 16: Proteasome subunit beta type-3

Chain p: 94% 6%



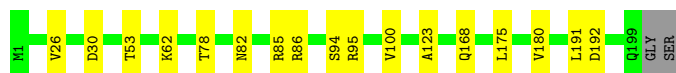
- Molecule 17: Proteasome subunit beta type-2

Chain Q: 89% 10%



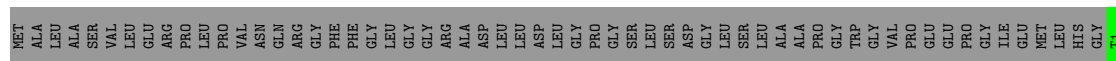
- Molecule 17: Proteasome subunit beta type-2

Chain q: 91% 8%



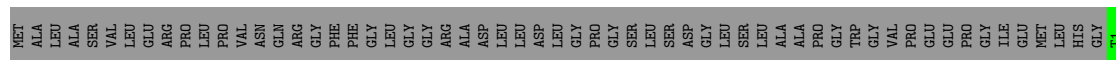
- Molecule 18: Proteasome subunit beta type-5

Chain R: 75% 24%



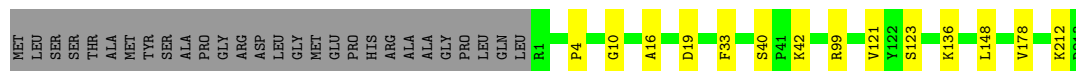
- Molecule 18: Proteasome subunit beta type-5

Chain r: 71% 5% 24%



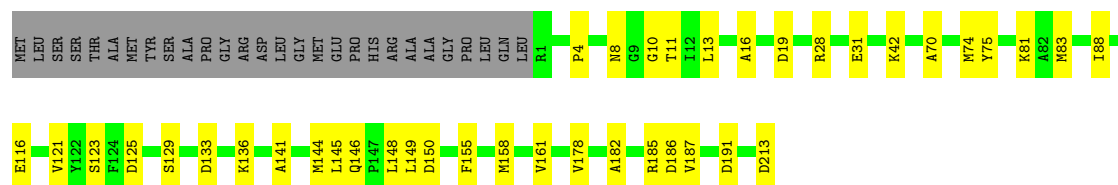
- Molecule 19: Proteasome subunit beta type-1

Chain S: 83% 6% 12%



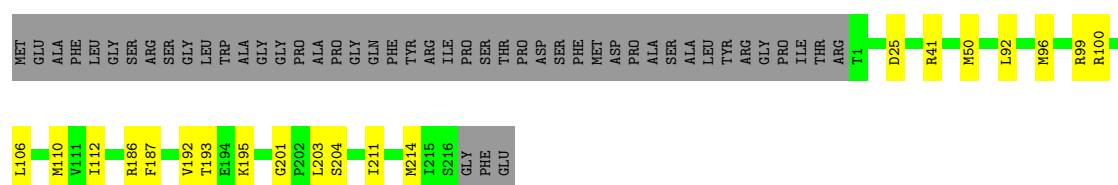
- Molecule 19: Proteasome subunit beta type-1

Chain s:  72% 17% 12%



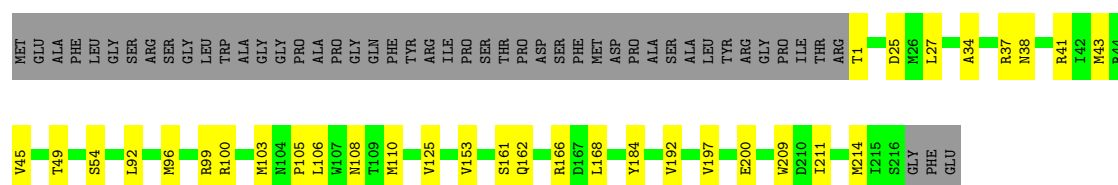
- Molecule 20: Proteasome subunit beta type-4

Chain T:  74% 8% 18%



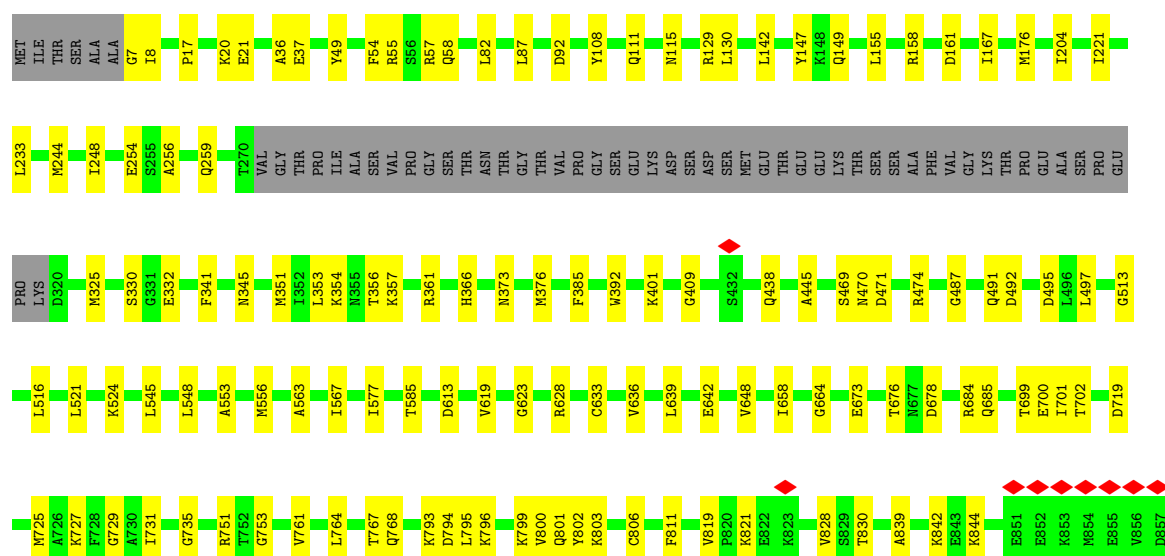
- Molecule 20: Proteasome subunit beta type-4

Chain t:  69% 12% 18%

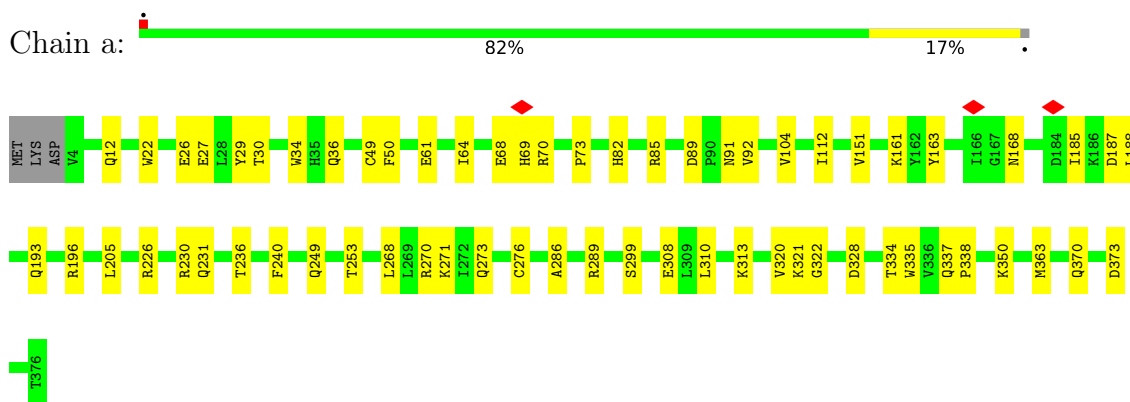


- Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

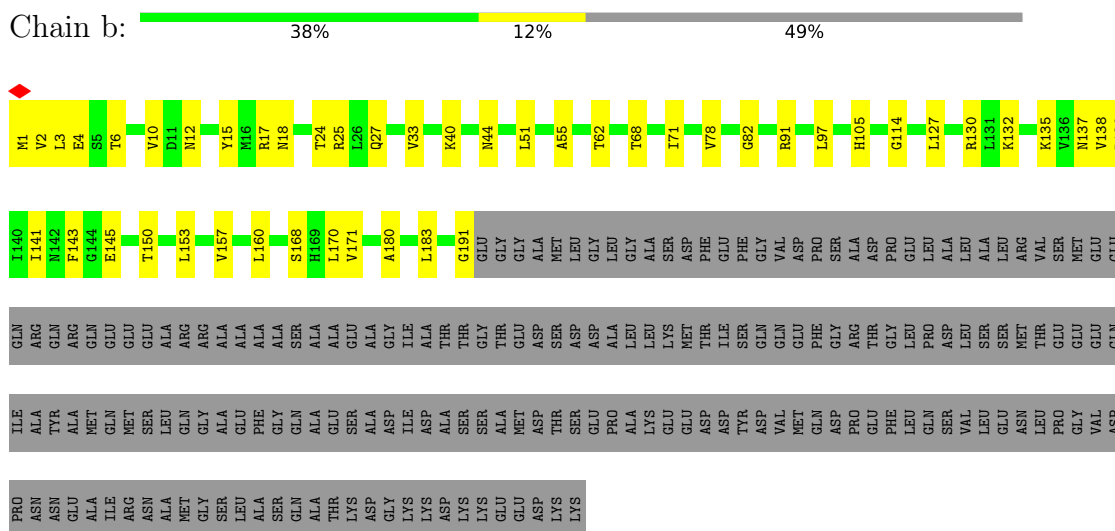
Chain U:  77% 15% 8%



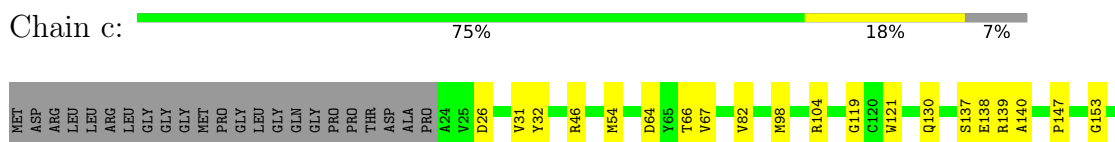
- Molecule 26: 26S proteasome non-ATPase regulatory subunit 13



- Molecule 27: 26S proteasome non-ATPase regulatory subunit 4

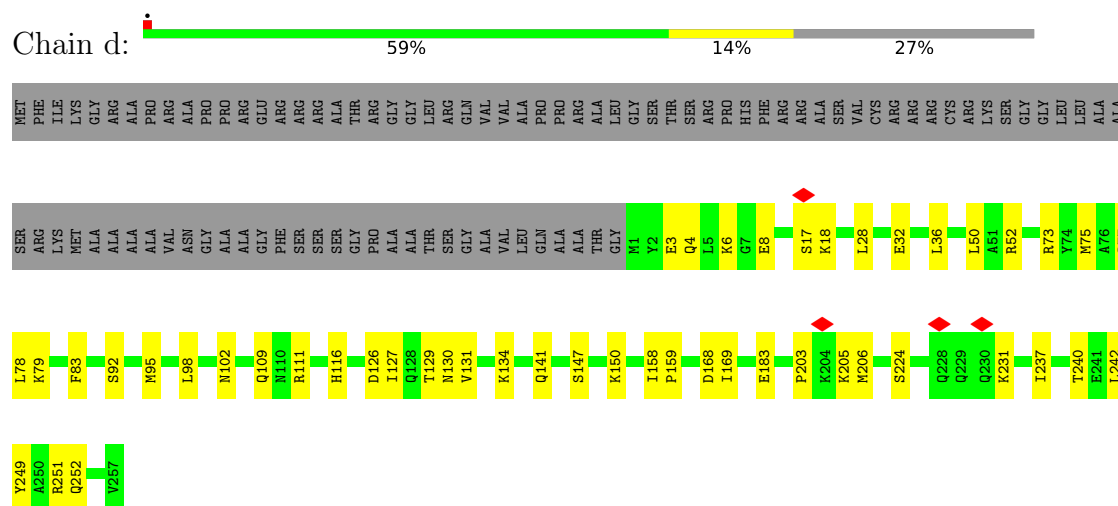


- Molecule 28: 26S proteasome non-ATPase regulatory subunit 14

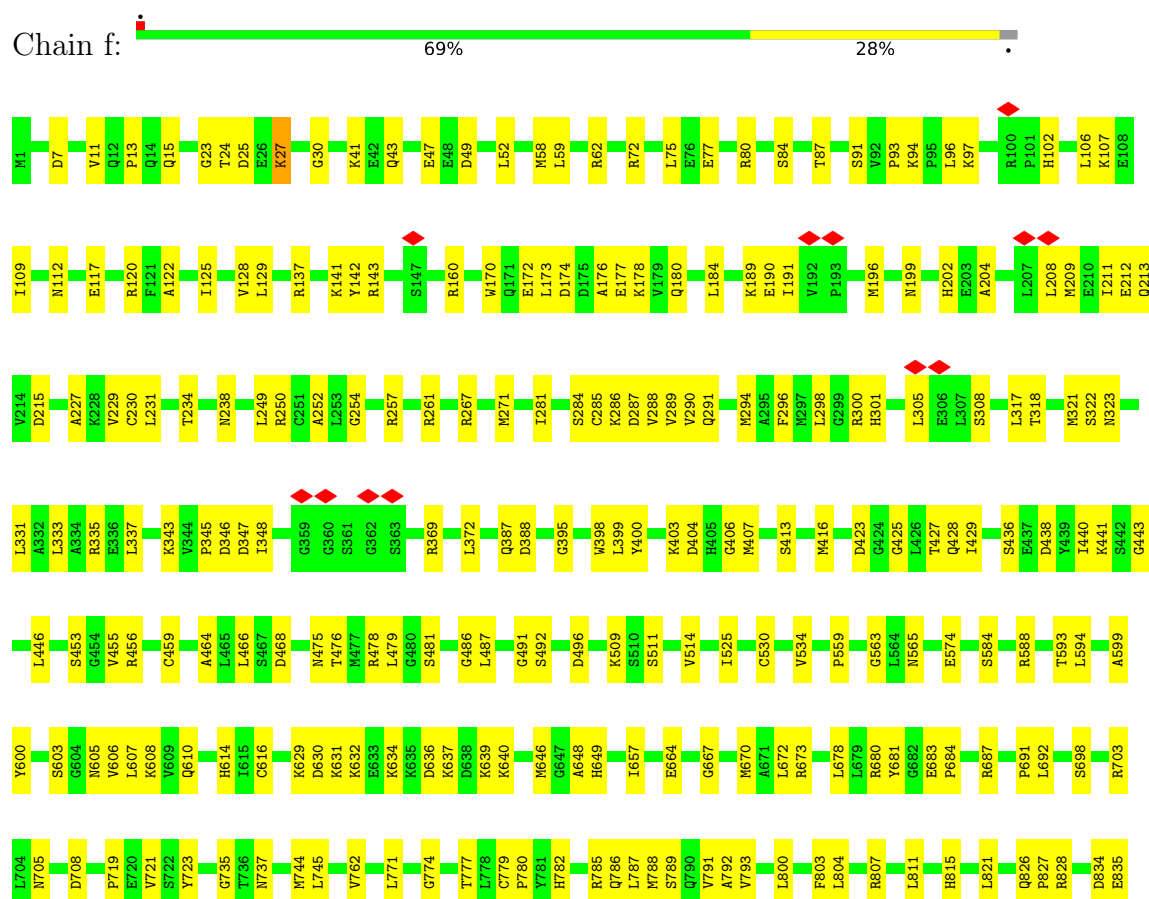




- Molecule 29: 26S proteasome non-ATPase regulatory subunit 8



- Molecule 30: 26S proteasome non-ATPase regulatory subunit 2





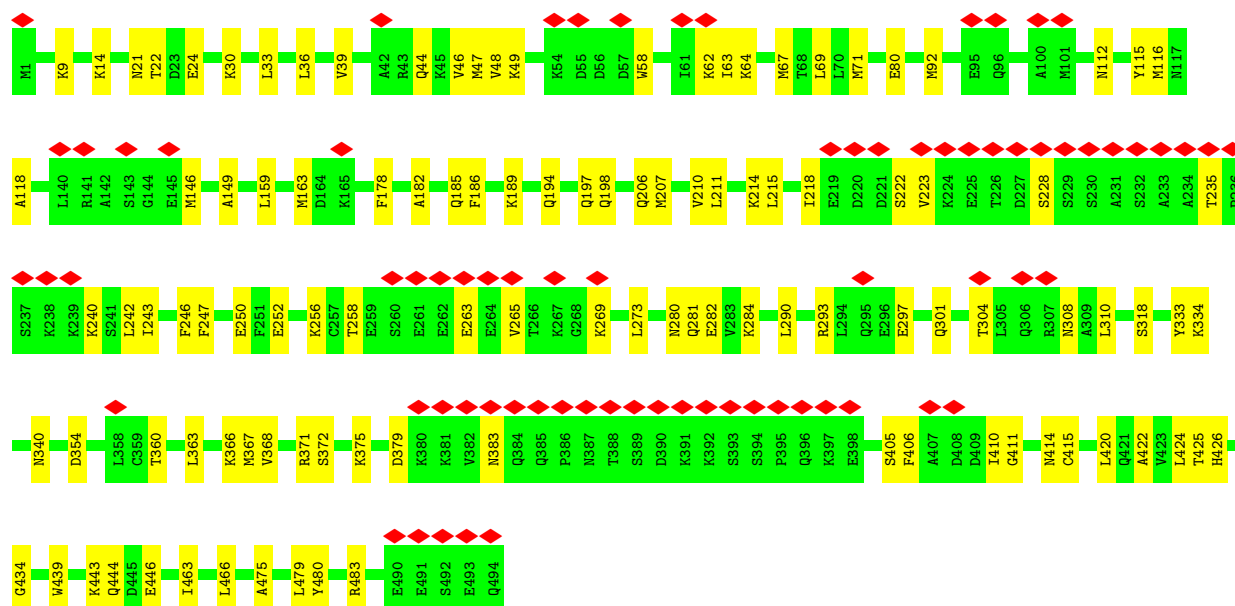
• Molecule 31: Substrate

Chain v: 97%



• Molecule 32: Ubiquitin carboxyl-terminal hydrolase 14

Chain x: 15% 78% 22%



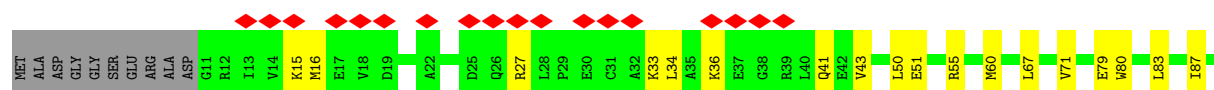
• Molecule 33: Ubiquitin

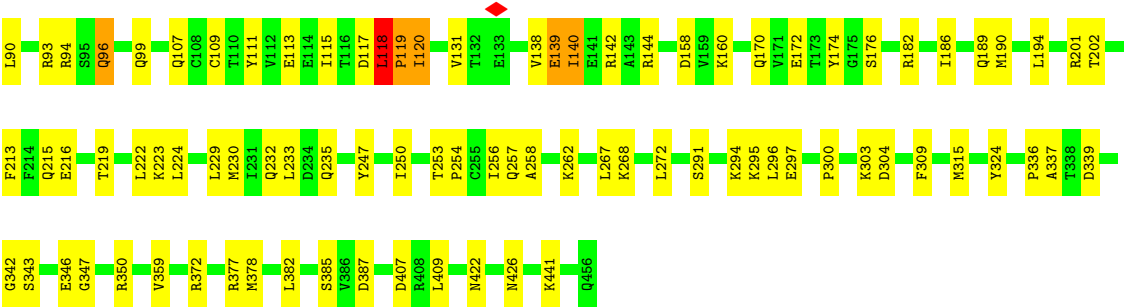
Chain y: 74% 26%



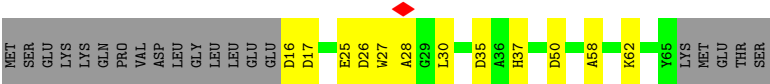
• Molecule 34: 26S proteasome non-ATPase regulatory subunit 12

Chain W: 75% 22%





• 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	283431	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	0.025	Depositor
Minimum map value	-0.003	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	438.4, 438.4, 438.4	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.21	0/3299	0.46	0/4454
2	B	0.23	0/3254	0.47	0/4388
3	C	0.23	0/3146	0.47	0/4226
4	D	0.24	0/3090	0.54	0/4168
5	E	0.17	0/3145	0.47	0/4233
6	F	0.20	0/3137	0.48	2/4223 (0.0%)
7	G	0.24	0/1901	0.40	0/2572
7	g	0.23	0/1913	0.40	0/2589
8	H	0.23	0/1840	0.38	0/2495
8	h	0.21	0/1844	0.39	0/2497
9	I	0.27	0/1963	0.40	0/2650
9	i	0.19	0/1985	0.33	0/2677
10	J	0.21	0/1887	0.39	0/2553
10	j	0.17	0/1887	0.40	0/2549
11	K	0.24	0/1841	0.36	0/2486
11	k	0.19	0/1809	0.33	0/2444
12	L	0.23	0/1911	0.38	0/2584
12	l	0.22	0/1896	0.39	0/2565
13	M	0.22	0/1925	0.38	0/2592
13	m	0.21	0/1916	0.34	0/2580
14	N	0.23	0/1548	0.32	0/2097
14	n	0.23	0/1536	0.34	0/2080
15	O	0.23	0/1672	0.41	0/2267
15	o	0.22	0/1686	0.41	0/2282
16	P	0.23	0/1616	0.38	0/2180
16	p	0.22	0/1620	0.37	0/2184
17	Q	0.23	0/1621	0.38	0/2194
17	q	0.23	0/1611	0.38	0/2182
18	R	0.23	0/1590	0.34	0/2147
18	r	0.23	0/1580	0.33	0/2135
19	S	0.23	0/1671	0.37	0/2252
19	s	0.22	0/1680	0.38	0/2264

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.25	0/1716	0.39	0/2323
20	t	0.23	0/1720	0.37	0/2328
21	U	0.19	0/6945	0.46	0/9382
22	V	0.20	0/3681	0.41	0/4969
23	X	0.21	0/3053	0.43	2/4115 (0.0%)
24	Y	0.25	0/3173	0.50	0/4273
25	Z	0.23	0/2324	0.52	1/3150 (0.0%)
26	a	0.19	0/3053	0.45	0/4133
27	b	0.17	0/1478	0.49	0/2001
28	c	0.23	0/2302	0.52	0/3110
29	d	0.25	1/2162 (0.0%)	0.53	0/2919
30	f	0.23	0/6980	0.56	0/9433
32	x	0.14	0/4002	0.39	0/5390
33	y	0.20	0/607	0.45	0/816
34	W	0.21	0/3683	0.50	3/4952 (0.1%)
35	e	0.24	0/437	0.68	1/595 (0.2%)
All	All	0.22	1/112336 (0.0%)	0.44	9/151678 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	237	ILE	C-N	6.27	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	W	139	GLU	CA-C-N	6.59	133.83	121.97
34	W	139	GLU	C-N-CA	6.59	133.83	121.97
34	W	96	GLN	CB-CA-C	-6.01	109.65	116.63
35	e	28	ALA	CB-CA-C	-5.83	109.83	116.54
6	F	85	THR	CA-C-N	5.70	135.70	121.80
6	F	85	THR	C-N-CA	5.70	135.70	121.80
25	Z	14	LEU	N-CA-C	-5.56	107.14	114.04
23	X	317	PRO	CA-C-N	5.16	131.26	121.97
23	X	317	PRO	C-N-CA	5.16	131.26	121.97

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	3245	0	3300	51	0
2	B	3207	0	3278	54	0
3	C	3105	0	3219	42	0
4	D	3040	0	3076	48	0
5	E	3097	0	3174	64	0
6	F	3098	0	3186	44	0
7	G	1867	0	1867	13	0
7	g	1879	0	1872	13	0
8	H	1801	0	1773	14	0
8	h	1805	0	1798	10	0
9	I	1933	0	1923	13	0
9	i	1955	0	1955	13	0
10	J	1861	0	1846	19	0
10	j	1861	0	1865	23	0
11	K	1813	0	1796	14	0
11	k	1782	0	1766	12	0
12	L	1876	0	1856	17	0
12	l	1861	0	1839	15	0
13	M	1890	0	1880	11	0
13	m	1881	0	1868	14	0
14	N	1521	0	1494	10	0
14	n	1510	0	1483	5	0
15	O	1645	0	1648	11	0
15	o	1659	0	1681	15	0
16	P	1587	0	1598	11	0
16	p	1591	0	1609	12	0
17	Q	1588	0	1584	13	0
17	q	1578	0	1569	13	0
18	R	1559	0	1523	4	0
18	r	1549	0	1506	10	0
19	S	1641	0	1639	10	0
19	s	1650	0	1645	25	0
20	T	1683	0	1662	14	0
20	t	1687	0	1666	23	0
21	U	6828	0	6884	87	0
22	V	3612	0	3682	46	0
23	X	3009	0	3113	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	Y	3115	0	3120	39	0
25	Z	2281	0	2312	33	0
26	a	2995	0	3012	42	0
27	b	1458	0	1505	32	0
28	c	2260	0	2276	38	0
29	d	2116	0	2146	33	0
30	f	6866	0	6866	176	0
31	v	180	0	42	1	0
32	x	3929	0	3915	73	0
33	y	601	0	629	12	0
34	W	3635	0	3762	68	0
35	e	425	0	328	12	0
36	A	31	0	12	1	0
36	B	31	0	12	3	0
36	C	31	0	12	2	0
36	F	31	0	12	1	0
37	A	1	0	0	0	0
37	B	1	0	0	0	0
37	C	1	0	0	0	0
37	F	1	0	0	0	0
38	D	27	0	12	1	0
39	c	1	0	0	0	0
All	All	110771	0	111096	1254	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 (1254) 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)
6:F:357:PRO:HB2	6:F:362:ARG:HG2	1.64	0.79
28:c:303:MET:HE1	29:d:242:LEU:HB2	1.67	0.76
30:f:789:SER:H	30:f:793:VAL:HB	1.51	0.75
25:Z:223:ASN:HB3	25:Z:227:ILE:HG12	1.69	0.73
22:V:309:MET:HE1	22:V:331:LEU:HB3	1.71	0.73
25:Z:263:ALA:HB1	28:c:288:VAL:HG13	1.71	0.72
30:f:204:ALA:O	30:f:208:LEU:HB2	1.89	0.72
4:D:223:THR:HG22	4:D:225:ALA:H	1.55	0.72
29:d:8:GLU:H	29:d:18:LYS:HD2	1.56	0.71
21:U:800:VAL:H	21:U:880:ASN:HB2	1.55	0.71
30:f:333:LEU:HA	30:f:337:LEU:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:255:GLY:HA2	3:C:273:MET:HG3	1.74	0.69
3:C:221:GLN:NE2	3:C:230:MET:SD	2.66	0.69
34:W:267:LEU:HD22	34:W:295:LYS:HB2	1.75	0.67
10:J:63:CYS:SG	10:J:88:ARG:NH2	2.68	0.66
29:d:147:SER:HB3	29:d:150:LYS:HB2	1.76	0.66
26:a:370:GLN:O	29:d:251:ARG:NH2	2.28	0.66
32:x:112:ASN:HB3	32:x:197:GLN:HB3	1.78	0.66
5:E:228:CYS:HB3	5:E:273:VAL:HG12	1.78	0.66
34:W:219:THR:HG23	34:W:222:LEU:H	1.60	0.66
27:b:91:ARG:HH21	27:b:127:LEU:HD11	1.61	0.66
8:h:77:SER:HB2	8:h:163:MET:HE2	1.76	0.66
30:f:106:LEU:HB3	30:f:137:ARG:HD3	1.79	0.65
32:x:406:PHE:HA	32:x:414:ASN:HB3	1.79	0.65
2:B:49:LEU:HD21	30:f:649:HIS:HB3	1.77	0.65
28:c:130:GLN:NE2	28:c:140:ALA:O	2.27	0.65
13:m:108:LEU:HD12	13:m:139:SER:HB3	1.77	0.64
28:c:224:SER:HB2	28:c:227:GLU:HB3	1.79	0.64
1:A:138:MET:HE1	1:A:152:PRO:HB3	1.80	0.64
28:c:251:LEU:HD13	28:c:283:HIS:HB3	1.80	0.64
32:x:360:THR:HB	32:x:363:LEU:HB2	1.79	0.64
14:N:199:VAL:HG13	20:t:37:ARG:HH21	1.61	0.64
5:E:22:ILE:HG13	6:F:55:MET:HE1	1.79	0.64
30:f:719:PRO:HG2	30:f:721:VAL:HB	1.80	0.64
25:Z:209:ARG:O	26:a:350:LYS:NZ	2.31	0.64
29:d:75:MET:HE2	29:d:102:ASN:HB2	1.80	0.64
30:f:811:LEU:HG	30:f:878:GLU:HA	1.78	0.64
22:V:85:ALA:HB2	22:V:93:PHE:HB2	1.79	0.64
30:f:143:ARG:HG2	30:f:191:ILE:HD11	1.80	0.64
19:s:144:MET:HE1	19:s:186:ASP:HB2	1.80	0.64
21:U:373:ASN:HD22	21:U:385:PHE:HD2	1.46	0.63
19:s:145:LEU:HD21	19:s:182:ALA:HB2	1.79	0.63
27:b:25:ARG:NH2	27:b:114:GLY:O	2.31	0.63
16:p:122:CYS:SG	16:p:123:SER:N	2.71	0.63
17:Q:44:LEU:HD11	17:Q:102:LEU:HD12	1.79	0.63
4:D:353:ASN:ND2	4:D:392:TYR:O	2.32	0.62
5:E:235:ILE:HB	5:E:282:PRO:HG3	1.79	0.62
21:U:806:CYS:HB3	21:U:874:ASN:HB2	1.80	0.62
9:I:140:ASP:OD1	9:I:146:GLN:NE2	2.32	0.62
28:c:217:LEU:O	28:c:221:HIS:HB2	1.99	0.62
20:t:211:ILE:HA	20:t:214:MET:HG3	1.81	0.62
21:U:17:PRO:HA	21:U:20:LYS:HE2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:f:670:MET:O	30:f:673:ARG:NH1	2.31	0.62
26:a:308:GLU:OE2	34:W:377:ARG:NH2	2.33	0.62
30:f:407:MET:HE1	30:f:440:ILE:HG12	1.80	0.62
7:g:141:ILE:HD12	7:g:220:VAL:HG12	1.82	0.62
27:b:6:THR:HG21	27:b:40:LYS:HD2	1.80	0.61
32:x:443:LYS:HB2	32:x:446:GLU:HB3	1.83	0.61
22:V:177:ASN:O	22:V:179:LYS:NZ	2.34	0.61
32:x:64:LYS:NZ	32:x:67:MET:SD	2.74	0.61
20:t:108:ASN:HB3	20:t:110:MET:HE3	1.81	0.61
29:d:78:LEU:HD13	29:d:98:LEU:HD21	1.83	0.61
30:f:281:ILE:HG13	30:f:286:LYS:HB2	1.83	0.61
5:E:322:LYS:HA	5:E:362:VAL:H	1.65	0.61
4:D:229:ARG:NH1	4:D:265:ASP:OD2	2.34	0.60
7:G:155:ASP:OD1	7:G:159:TYR:N	2.34	0.60
23:X:252:LYS:HG3	23:X:287:LEU:HD11	1.83	0.60
32:x:235:THR:HG23	32:x:240:LYS:HE2	1.82	0.60
3:C:113:ARG:NH2	4:D:94:GLU:OE1	2.35	0.60
19:S:148:LEU:HD23	19:S:178:VAL:HG12	1.83	0.60
33:y:1:MET:N	33:y:17:VAL:O	2.35	0.60
34:W:90:LEU:O	34:W:96:GLN:NE2	2.35	0.60
11:k:42:THR:HG23	11:k:44:GLU:H	1.66	0.60
36:A:501:ATP:O1G	2:B:346:ARG:NH2	2.34	0.60
23:X:398:GLU:OE2	24:Y:365:GLN:NE2	2.35	0.60
3:C:293:MET:HE1	3:C:305:LEU:HD21	1.83	0.60
28:c:168:MET:HG2	28:c:169:VAL:HG13	1.84	0.60
10:J:211:MET:HB2	10:J:217:LEU:HD12	1.83	0.60
30:f:593:THR:OG1	30:f:631:LYS:NZ	2.35	0.60
19:s:4:PRO:HB2	20:t:100:ARG:HH11	1.67	0.60
1:A:306:LEU:O	1:A:312:ARG:NH1	2.35	0.60
25:Z:141:VAL:O	25:Z:154:THR:OG1	2.20	0.60
32:x:405:SER:O	32:x:414:ASN:ND2	2.35	0.60
4:D:342:ARG:NH1	23:X:234:GLU:OE2	2.35	0.59
30:f:234:THR:O	30:f:238:ASN:ND2	2.34	0.59
19:s:10:GLY:HA3	19:s:42:LYS:HE3	1.84	0.59
1:A:311:PRO:HD3	6:F:238:ARG:HH22	1.66	0.59
1:A:323:ARG:NH1	2:B:294:ARG:O	2.34	0.59
30:f:416:MET:HE2	30:f:804:LEU:HD22	1.84	0.59
30:f:534:VAL:HG13	30:f:565:ASN:HD22	1.68	0.59
19:S:4:PRO:O	20:T:100:ARG:NH2	2.35	0.59
29:d:73:ARG:O	29:d:77:GLN:NE2	2.35	0.59
29:d:92:SER:H	29:d:95:MET:HE1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:153:SER:OG	9:i:155:ASN:ND2	2.35	0.59
34:W:80:TRP:HA	34:W:83:LEU:HB3	1.85	0.59
3:C:20:LEU:HD13	21:U:149:GLN:HG2	1.84	0.59
30:f:94:LYS:HE3	30:f:106:LEU:HD12	1.83	0.59
10:j:38:ARG:HG3	10:j:181:ILE:HG22	1.83	0.59
32:x:420:LEU:HA	32:x:480:TYR:HA	1.83	0.59
21:U:259:GLN:NE2	21:U:487:GLY:O	2.35	0.59
23:X:363:ARG:NH2	24:Y:266:CYS:O	2.36	0.59
27:b:157:VAL:HG21	27:b:170:LEU:HB3	1.84	0.59
4:D:358:VAL:HG22	4:D:396:ALA:HB2	1.84	0.59
22:V:355:ARG:NH1	35:e:27:TRP:O	2.35	0.59
25:Z:64:ASP:OD2	27:b:91:ARG:NH1	2.35	0.59
21:U:54:PHE:O	21:U:57:ARG:NH2	2.35	0.58
9:I:119:GLN:NE2	10:J:79:ASP:OD1	2.36	0.58
24:Y:233:ARG:HA	24:Y:236:LEU:HD22	1.85	0.58
30:f:464:ALA:HB3	32:x:47:MET:HE3	1.85	0.58
30:f:681:TYR:OH	30:f:687:ARG:NH1	2.36	0.58
32:x:252:GLU:HA	32:x:269:LYS:HA	1.85	0.58
4:D:153:MET:SD	4:D:257:ASN:ND2	2.76	0.58
21:U:628:ARG:NH1	21:U:753:GLY:O	2.36	0.58
28:c:31:VAL:HB	28:c:205:ILE:HG22	1.86	0.58
5:E:30:ARG:NH2	6:F:58:GLU:OE1	2.37	0.58
11:K:121:LEU:HD23	11:K:160:GLY:HA3	1.86	0.58
29:d:52:ARG:HH21	29:d:92:SER:HG	1.48	0.58
11:k:210:LEU:HA	11:k:214:ASN:HD22	1.69	0.58
30:f:387:GLN:NE2	30:f:388:ASP:OD1	2.36	0.58
19:s:158:MET:HE3	19:s:161:VAL:HG11	1.86	0.58
35:e:35:ASP:HB3	35:e:37:HIS:HD2	1.69	0.58
30:f:475:ASN:OD1	30:f:478:ARG:NH2	2.37	0.58
8:h:65:VAL:O	8:h:220:ARG:NH1	2.37	0.58
3:C:185:GLY:HA3	3:C:311:ILE:HA	1.85	0.57
30:f:664:GLU:OE1	30:f:667:GLY:N	2.37	0.57
7:g:49:VAL:HG12	7:g:219:VAL:HG23	1.84	0.57
18:R:19:ARG:NH2	16:p:205:ASP:OD1	2.37	0.57
16:P:125:ASP:OD1	16:P:129:CYS:N	2.36	0.57
27:b:2:VAL:O	27:b:44:ASN:ND2	2.36	0.57
13:M:34:SER:HB2	13:M:65:ARG:HH12	1.69	0.57
21:U:142:LEU:HA	21:U:147:TYR:HE1	1.69	0.57
6:F:97:LEU:O	6:F:120:LYS:N	2.37	0.57
2:B:41:LYS:HA	2:B:278:ALA:HB2	1.87	0.57
21:U:376:MET:HE3	21:U:735:GLY:HA2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:GLU:HB3	3:C:274:LEU:HD23	1.85	0.57
24:Y:81:LEU:HG	24:Y:107:LYS:HG2	1.85	0.57
30:f:672:LEU:HD13	30:f:708:ASP:HB3	1.86	0.57
17:q:168:GLN:NE2	17:q:175:LEU:O	2.38	0.57
21:U:233:LEU:HD22	21:U:325:MET:HE1	1.85	0.57
1:A:347:ASP:O	1:A:351:ARG:NH1	2.37	0.57
20:t:54:SER:O	20:t:108:ASN:ND2	2.37	0.57
33:y:2:GLN:NE2	33:y:16:GLU:OE1	2.38	0.57
34:W:216:GLU:OE1	34:W:223:LYS:NZ	2.36	0.57
2:B:208:PRO:HD2	30:f:723:TYR:HB3	1.87	0.56
5:E:84:ARG:NH1	5:E:108:MET:O	2.35	0.56
20:t:96:MET:HE1	20:t:106:LEU:HD12	1.87	0.56
2:B:181:GLN:O	2:B:241:ASN:ND2	2.37	0.56
12:L:164:ARG:HH12	12:L:200:PRO:HG3	1.70	0.56
25:Z:239:ASP:OD1	25:Z:239:ASP:N	2.39	0.56
1:A:364:VAL:HG12	1:A:404:ALA:HB3	1.86	0.56
15:O:19:ARG:NH2	19:s:213:ASP:OD2	2.38	0.56
21:U:111:GLN:O	21:U:115:ASN:ND2	2.39	0.56
21:U:167:ILE:HG22	21:U:176:MET:HE1	1.87	0.56
22:V:289:LEU:HB3	22:V:312:ALA:HB2	1.86	0.56
23:X:73:VAL:O	23:X:77:LEU:N	2.37	0.56
25:Z:267:ARG:HD3	28:c:292:MET:HE1	1.86	0.56
27:b:1:MET:SD	27:b:1:MET:N	2.78	0.56
4:D:162:VAL:O	4:D:221:HIS:ND1	2.38	0.56
30:f:172:GLU:HG2	30:f:208:LEU:HD11	1.87	0.56
10:j:40:ILE:HG22	10:j:212:ARG:HG3	1.88	0.56
34:W:253:THR:O	34:W:257:GLN:N	2.35	0.56
32:x:62:LYS:NZ	32:x:63:ILE:O	2.37	0.56
34:W:51:GLU:HG3	34:W:67:LEU:HD21	1.87	0.56
5:E:194:ASN:HD21	5:E:228:CYS:HA	1.70	0.56
20:T:25:ASP:OD1	20:T:41:ARG:NH2	2.37	0.56
22:V:121:PHE:O	22:V:128:ARG:NH1	2.39	0.56
30:f:466:LEU:O	30:f:481:SER:OG	2.22	0.56
30:f:600:TYR:HB3	30:f:603:SER:HB2	1.88	0.56
32:x:375:LYS:O	32:x:379:ASP:HB2	2.06	0.56
15:O:55:THR:HG22	15:O:86:MET:HE1	1.86	0.56
23:X:51:LEU:HD11	23:X:88:LEU:HD22	1.87	0.56
30:f:94:LYS:NZ	30:f:106:LEU:O	2.37	0.56
30:f:584:SER:HB2	30:f:588:ARG:HB3	1.88	0.56
5:E:174:GLY:O	5:E:280:ASN:ND2	2.36	0.56
20:t:25:ASP:OD1	20:t:41:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:OE1	6:F:409:ARG:NH1	2.38	0.55
26:a:226:ARG:O	26:a:231:GLN:NE2	2.38	0.55
3:C:112:CYS:SG	3:C:130:LYS:NZ	2.79	0.55
6:F:296:PHE:O	6:F:304:ARG:NH2	2.39	0.55
14:N:154:GLN:O	14:N:158:ASN:ND2	2.36	0.55
22:V:58:ALA:O	22:V:62:HIS:ND1	2.39	0.55
26:a:335:TRP:CD1	26:a:337:GLN:H	2.24	0.55
30:f:261:ARG:HD3	30:f:267:ARG:HH22	1.70	0.55
30:f:478:ARG:NH2	30:f:511:SER:OG	2.39	0.55
8:H:179:ASN:HB3	8:H:182:LEU:HG	1.89	0.55
20:T:186:ARG:NH1	20:T:204:SER:OG	2.40	0.55
34:W:194:LEU:HD13	34:W:202:THR:HG21	1.87	0.55
4:D:274:ARG:HH21	4:D:289:LEU:HD23	1.71	0.55
5:E:146:ARG:NH1	5:E:187:VAL:O	2.39	0.55
13:M:174:THR:O	13:M:178:LYS:NZ	2.39	0.55
21:U:366:HIS:NE2	21:U:392:TRP:O	2.39	0.55
26:a:286:ALA:O	26:a:289:ARG:NH1	2.40	0.55
30:f:80:ARG:O	30:f:80:ARG:NH1	2.36	0.55
20:t:1:THR:N	20:t:105:PRO:O	2.39	0.55
34:W:109:CYS:O	34:W:113:GLU:HB2	2.07	0.55
21:U:82:LEU:O	21:U:129:ARG:NH2	2.39	0.55
30:f:281:ILE:HB	30:f:284:SER:HB2	1.87	0.55
15:o:179:SER:HB3	15:o:182:LYS:HG2	1.88	0.55
22:V:147:PHE:O	22:V:148:ARG:NH1	2.38	0.55
29:d:203:PRO:HD2	29:d:206:MET:HE3	1.89	0.55
30:f:176:ALA:HB3	30:f:178:LYS:HE2	1.89	0.55
2:B:281:ILE:HG22	2:B:326:LYS:HB2	1.88	0.55
6:F:289:ASP:OD1	6:F:289:ASP:N	2.40	0.55
21:U:803:LYS:HB3	21:U:877:LEU:HD23	1.87	0.55
22:V:480:ILE:HD13	25:Z:260:VAL:HA	1.88	0.55
26:a:70:ARG:O	27:b:17:ARG:NE	2.38	0.55
12:l:206:THR:HG23	12:l:208:LYS:H	1.71	0.55
32:x:33:LEU:HD13	32:x:71:MET:HG3	1.88	0.55
8:H:212:ILE:HD12	8:H:221:LEU:HD21	1.88	0.55
30:f:423:ASP:HB3	32:x:9:LYS:HE2	1.88	0.55
30:f:815:HIS:HA	30:f:881:GLU:HG2	1.89	0.55
19:s:125:ASP:OD1	19:s:129:SER:N	2.40	0.55
32:x:218:ILE:HD11	32:x:242:LEU:H	1.71	0.55
21:U:521:LEU:HD11	21:U:761:VAL:HG21	1.89	0.55
30:f:250:ARG:HH11	30:f:252:ALA:HB3	1.71	0.55
10:j:196:LEU:HA	10:j:199:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:W:55:ARG:HD2	34:W:94:ARG:HD2	1.89	0.55
25:Z:30:GLY:O	25:Z:33:LYS:NZ	2.40	0.54
30:f:466:LEU:HD12	30:f:481:SER:HA	1.88	0.54
11:k:210:LEU:HD12	11:k:215:ILE:HD13	1.89	0.54
3:C:113:ARG:NH2	3:C:129:ASN:O	2.41	0.54
14:N:41:ILE:HG12	14:N:76:VAL:HG12	1.90	0.54
32:x:211:LEU:HD22	32:x:215:LEU:HD22	1.88	0.54
11:K:16:SER:HB3	11:K:20:ARG:H	1.71	0.54
21:U:409:GLY:HA3	21:U:445:ALA:HB1	1.87	0.54
25:Z:245:PHE:O	25:Z:249:PHE:HB2	2.07	0.54
30:f:343:LYS:HB3	30:f:388:ASP:HA	1.88	0.54
2:B:440:LEU:O	10:J:61:LYS:NZ	2.39	0.54
4:D:390:ASN:O	34:W:201:ARG:NH2	2.40	0.54
5:E:75:ASN:ND2	6:F:129:ARG:O	2.37	0.54
5:E:120:TYR:HA	5:E:123:SER:HB2	1.89	0.54
26:a:328:ASP:OD2	34:W:372:ARG:NH2	2.40	0.54
30:f:11:VAL:O	30:f:15:GLN:N	2.41	0.54
20:t:153:VAL:HG21	20:t:168:LEU:HD11	1.88	0.54
6:F:223:VAL:HB	6:F:329:ILE:HG22	1.87	0.54
13:M:187:ARG:O	13:M:191:LYS:NZ	2.41	0.54
30:f:459:CYS:HA	32:x:49:LYS:HG2	1.88	0.54
30:f:574:GLU:HG3	30:f:599:ALA:HB2	1.90	0.54
32:x:39:VAL:O	32:x:44:GLN:NE2	2.37	0.54
11:K:118:ASN:OD1	12:L:82:ARG:NH2	2.41	0.54
26:a:270:ARG:HE	26:a:313:LYS:HD3	1.73	0.54
30:f:395:GLY:HA2	30:f:398:TRP:HB3	1.90	0.54
11:k:118:ASN:O	11:k:122:GLN:NE2	2.40	0.54
34:W:33:LYS:HA	34:W:36:LYS:HG2	1.88	0.54
34:W:41:GLN:NE2	34:W:79:GLU:OE2	2.41	0.54
7:G:17:SER:HB3	7:G:21:ARG:H	1.72	0.54
16:p:193:ASP:OD1	16:p:193:ASP:N	2.38	0.54
32:x:63:ILE:HA	32:x:67:MET:HE1	1.90	0.54
5:E:3:ASP:OD2	5:E:8:ALA:N	2.39	0.54
8:H:122:THR:HG22	8:H:129:PRO:HB3	1.89	0.54
21:U:799:LYS:NZ	21:U:801:GLN:OE1	2.40	0.54
19:s:8:ASN:ND2	19:s:31:GLU:OE1	2.39	0.54
20:T:193:THR:HG23	20:T:195:LYS:H	1.72	0.54
27:b:24:THR:HG23	27:b:27:GLN:H	1.73	0.54
15:O:163:ILE:HG12	15:O:170:GLY:HA2	1.90	0.54
21:U:341:PHE:O	21:U:345:ASN:ND2	2.37	0.54
26:a:26:GLU:OE1	26:a:29:TYR:OH	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:GLY:O	2:B:391:SER:OG	2.25	0.53
6:F:406:ILE:HD13	6:F:409:ARG:HE	1.74	0.53
27:b:141:ILE:HA	27:b:171:VAL:HB	1.90	0.53
30:f:122:ALA:HA	30:f:125:ILE:HG22	1.90	0.53
14:n:144:ARG:NH2	14:n:151:GLU:OE2	2.41	0.53
1:A:79:ASP:OD1	1:A:79:ASP:N	2.42	0.53
21:U:7:GLY:N	21:U:37:GLU:OE2	2.41	0.53
28:c:46:ARG:NH2	28:c:147:PRO:O	2.41	0.53
7:g:141:ILE:HG22	7:g:151:VAL:HG22	1.89	0.53
24:Y:23:ARG:O	24:Y:27:SER:HB3	2.08	0.53
17:q:192:ASP:OD1	17:q:192:ASP:N	2.41	0.53
34:W:224:LEU:HD23	34:W:256:ILE:HG13	1.90	0.53
4:D:116:LEU:HD12	4:D:140:VAL:HA	1.89	0.53
22:V:477:HIS:ND1	29:d:249:TYR:OH	2.37	0.53
30:f:229:VAL:HG22	30:f:605:ASN:HB2	1.90	0.53
30:f:403:LYS:HG3	30:f:406:GLY:H	1.72	0.53
30:f:413:SER:HA	30:f:416:MET:HG3	1.90	0.53
30:f:436:SER:H	30:f:441:LYS:HE2	1.71	0.53
30:f:771:LEU:HG	30:f:774:GLY:H	1.74	0.53
30:f:821:LEU:HD13	30:f:882:LEU:HG	1.88	0.53
1:A:99:THR:OG1	1:A:114:ASN:O	2.26	0.53
3:C:339:THR:HG22	3:C:377:HIS:HB2	1.91	0.53
15:O:112:SER:HB3	15:O:125:VAL:HG21	1.89	0.53
25:Z:233:VAL:HB	26:a:338:PRO:HG3	1.89	0.53
30:f:606:VAL:O	30:f:610:GLN:HB2	2.08	0.53
6:F:362:ARG:NH2	6:F:388:THR:O	2.42	0.53
13:M:51:LYS:NZ	13:M:62:SER:O	2.38	0.53
21:U:685:GLN:HG2	21:U:729:GLY:HA3	1.90	0.53
23:X:307:THR:HG22	23:X:314:ARG:HH12	1.73	0.53
23:X:414:LEU:HD11	25:Z:273:HIS:HB2	1.90	0.53
33:y:63:LYS:HG3	33:y:64:GLU:OE1	2.09	0.53
1:A:373:LEU:HD11	1:A:409:PHE:HB3	1.89	0.53
8:H:10:LEU:HD12	8:H:19:LEU:HD12	1.89	0.53
27:b:15:TYR:O	27:b:25:ARG:NH1	2.42	0.53
30:f:703:ARG:NH1	30:f:786:GLN:O	2.42	0.53
32:x:149:ALA:HB1	32:x:210:VAL:HG13	1.91	0.53
4:D:214:MET:HE2	38:D:501:ADP:H2'	1.89	0.53
24:Y:204:THR:HG21	24:Y:246:ILE:HD11	1.90	0.53
10:j:38:ARG:O	10:j:213:ARG:NH2	2.42	0.53
32:x:463:ILE:HA	32:x:466:LEU:HD12	1.90	0.53
27:b:3:LEU:HB3	27:b:105:HIS:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:o:163:ILE:HG12	15:o:170:GLY:HA2	1.90	0.53
2:B:413:LYS:NZ	30:f:49:ASP:O	2.42	0.53
11:K:13:ASN:ND2	12:L:124:GLY:O	2.40	0.53
21:U:469:SER:OG	21:U:470:ASN:N	2.38	0.53
25:Z:19:VAL:HG21	25:Z:124:ILE:HD12	1.91	0.53
10:J:199:VAL:HG12	10:J:202:GLY:H	1.74	0.52
18:R:64:ARG:NH1	18:R:67:GLU:OE1	2.42	0.52
22:V:484:LEU:O	22:V:488:ASN:ND2	2.42	0.52
28:c:284:LEU:O	28:c:286:GLU:N	2.41	0.52
34:W:107:GLN:O	34:W:111:TYR:HB2	2.09	0.52
2:B:387:LYS:HE3	2:B:389:ASP:HB3	1.91	0.52
27:b:12:ASN:HD22	27:b:78:VAL:HB	1.72	0.52
27:b:138:VAL:O	27:b:168:SER:OG	2.24	0.52
9:i:155:ASN:OD1	10:j:77:THR:OG1	2.27	0.52
17:q:78:THR:O	17:q:82:ASN:ND2	2.41	0.52
34:W:422:ASN:O	34:W:426:ASN:ND2	2.42	0.52
7:G:165:ALA:HB3	8:H:56:LEU:HD22	1.91	0.52
11:K:99:HIS:HB2	11:K:107:MET:HE3	1.91	0.52
23:X:344:ARG:HH21	34:W:409:LEU:HB3	1.74	0.52
26:a:68:GLU:HG3	26:a:69:HIS:H	1.75	0.52
17:q:180:VAL:HG23	17:q:191:LEU:HB2	1.92	0.52
18:r:12:VAL:HG22	18:r:179:VAL:HB	1.90	0.52
34:W:27:ARG:HH11	34:W:50:LEU:HD22	1.73	0.52
1:A:119:ALA:HB2	6:F:128:THR:HB	1.92	0.52
2:B:362:LYS:NZ	2:B:381:ASP:OD1	2.42	0.52
30:f:267:ARG:HD2	30:f:300:ARG:HH22	1.74	0.52
30:f:605:ASN:HD21	30:f:608:LYS:HB2	1.74	0.52
11:K:4:THR:OG1	11:K:5:ARG:N	2.42	0.52
21:U:36:ALA:O	22:V:273:LYS:NZ	2.42	0.52
24:Y:189:VAL:HG22	24:Y:287:LEU:HD22	1.92	0.52
25:Z:228:TYR:HA	25:Z:231:GLN:HG3	1.91	0.52
27:b:55:ALA:HB1	27:b:82:GLY:HA3	1.91	0.52
30:f:347:ASP:OD1	30:f:347:ASP:N	2.41	0.52
32:x:281:GLN:O	32:x:284:LYS:NZ	2.43	0.52
3:C:49:ARG:HH12	21:U:642:GLU:HB2	1.74	0.52
6:F:168:TYR:HB2	6:F:173:LYS:HE3	1.91	0.52
10:J:119:THR:HG22	10:J:126:PRO:HB3	1.91	0.52
30:f:399:LEU:HD22	30:f:407:MET:HE2	1.91	0.52
21:U:471:ASP:OD1	21:U:471:ASP:N	2.41	0.52
24:Y:50:MET:HA	24:Y:53:TYR:HB3	1.92	0.52
30:f:637:LYS:HD2	30:f:678:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:208:ALA:HB2	9:i:234:GLU:HG3	1.92	0.52
34:W:247:TYR:HA	34:W:250:ILE:HG12	1.92	0.52
3:C:241:HIS:O	3:C:244:SER:OG	2.28	0.52
4:D:159:LYS:H	4:D:160:PRO:HD3	1.74	0.52
5:E:320:ILE:HD12	6:F:217:ILE:HD11	1.92	0.52
5:E:331:ILE:HD11	5:E:367:PHE:HB3	1.91	0.52
26:a:188:LEU:HB2	26:a:193:GLN:HE21	1.75	0.52
30:f:634:LYS:HB2	30:f:673:ARG:HH21	1.74	0.52
8:h:133:SER:OG	8:h:149:SER:O	2.26	0.52
32:x:280:ASN:ND2	32:x:282:GLU:OE1	2.42	0.52
32:x:379:ASP:OD1	32:x:383:ASN:ND2	2.43	0.52
1:A:29:ASP:OD2	2:B:410:ARG:NH1	2.42	0.52
12:L:148:CYS:SG	12:L:150:SER:OG	2.60	0.52
34:W:55:ARG:NH1	34:W:96:GLN:OE1	2.42	0.52
2:B:411:ARG:HA	30:f:52:LEU:HB2	1.91	0.52
3:C:252:ASP:HB2	4:D:290:LEU:HD11	1.91	0.52
29:d:158:ILE:HD12	29:d:159:PRO:HD2	1.91	0.52
10:j:31:THR:OG1	10:j:163:ARG:O	2.28	0.52
5:E:147:GLU:HA	5:E:150:GLU:HB2	1.91	0.51
17:Q:31:ASP:OD1	17:Q:31:ASP:N	2.43	0.51
23:X:306:LEU:HA	23:X:313:LEU:HD11	1.90	0.51
7:g:112:ASP:OD1	7:g:112:ASP:N	2.41	0.51
12:l:117:GLN:O	12:l:120:THR:OG1	2.28	0.51
34:W:343:SER:OG	34:W:347:GLY:N	2.42	0.51
1:A:66:LYS:O	1:A:67:GLU:C	2.52	0.51
1:A:362:MET:HE1	1:A:389:CYS:HB3	1.91	0.51
4:D:270:ILE:HB	4:D:285:VAL:HG13	1.92	0.51
21:U:353:LEU:HD11	21:U:376:MET:HG3	1.91	0.51
22:V:337:LEU:HD21	22:V:364:THR:HG23	1.91	0.51
24:Y:124:PHE:HA	24:Y:127:THR:HG22	1.90	0.51
28:c:237:HIS:O	28:c:240:HIS:ND1	2.42	0.51
32:x:24:GLU:O	32:x:58:TRP:NE1	2.39	0.51
3:C:337:ASN:HB3	24:Y:174:TRP:HE1	1.76	0.51
12:L:125:ARG:NH1	12:L:126:ARG:O	2.41	0.51
21:U:764:LEU:O	21:U:768:GLN:NE2	2.43	0.51
26:a:82:HIS:HA	26:a:85:ARG:HE	1.75	0.51
30:f:346:ASP:OD1	30:f:346:ASP:N	2.43	0.51
32:x:405:SER:HB3	32:x:410:ILE:HA	1.92	0.51
11:K:203:LYS:HB2	11:K:210:LEU:HD22	1.91	0.51
30:f:453:SER:OG	30:f:487:LEU:O	2.29	0.51
32:x:223:VAL:O	32:x:228:SER:OG	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:19:HIS:ND1	6:F:51:GLU:OE2	2.38	0.51
22:V:99:ARG:NH2	24:Y:389:MET:SD	2.83	0.51
24:Y:23:ARG:HH22	24:Y:52:PRO:HB2	1.76	0.51
30:f:630:ASP:OD2	30:f:785:ARG:NH2	2.38	0.51
12:l:54:SER:OG	12:l:55:GLU:N	2.42	0.51
5:E:223:ARG:HD2	5:E:270:LEU:HB3	1.93	0.51
5:E:264:MET:O	5:E:269:THR:OG1	2.29	0.51
5:E:309:ARG:NH1	5:E:336:ASP:OD1	2.39	0.51
26:a:320:VAL:HG12	26:a:322:GLY:H	1.75	0.51
15:o:63:LEU:HD11	15:o:79:ALA:HB2	1.92	0.51
34:W:55:ARG:HH12	34:W:93:ARG:HD3	1.74	0.51
2:B:191:ASP:N	2:B:191:ASP:OD1	2.41	0.51
7:G:206:LEU:HB3	7:G:208:ILE:HG12	1.93	0.51
9:I:123:GLN:NE2	10:J:125:ARG:O	2.44	0.51
24:Y:235:ASP:O	24:Y:239:LYS:NZ	2.39	0.51
10:j:146:GLN:OE1	10:j:159:ASN:ND2	2.43	0.51
34:W:304:ASP:OD2	34:W:324:TYR:OH	2.28	0.51
3:C:155:ASP:N	3:C:155:ASP:OD1	2.43	0.51
5:E:339:ASN:HB2	5:E:342:ASP:HB2	1.93	0.51
5:E:359:HIS:ND1	5:E:361:PHE:O	2.44	0.51
21:U:819:VAL:O	21:U:821:LYS:NZ	2.43	0.51
30:f:160:ARG:NH1	30:f:196:MET:SD	2.82	0.51
30:f:229:VAL:HG21	30:f:607:LEU:HD23	1.91	0.51
30:f:603:SER:H	30:f:639:LYS:HA	1.76	0.51
30:f:637:LYS:HZ2	30:f:678:LEU:HD22	1.75	0.51
33:y:9:THR:O	33:y:11:LYS:NZ	2.44	0.51
34:W:336:PRO:HA	34:W:339:ASP:HB2	1.93	0.51
2:B:75:GLU:HB3	30:f:657:ILE:HD11	1.92	0.51
5:E:229:ILE:HG22	5:E:274:LYS:HB2	1.92	0.51
11:K:167:ALA:HB3	12:L:56:LEU:HD13	1.92	0.51
10:j:38:ARG:NH2	10:j:182:GLU:O	2.43	0.51
34:W:346:GLU:OE2	34:W:350:ARG:NH2	2.44	0.51
5:E:306:GLU:OE2	5:E:309:ARG:NH1	2.44	0.51
22:V:476:PHE:HB3	25:Z:260:VAL:HG21	1.93	0.51
16:p:135:ASP:OD1	16:p:135:ASP:N	2.44	0.51
1:A:369:ARG:NH1	11:K:204:GLN:O	2.44	0.50
1:A:397:ILE:HD12	2:B:210:TYR:HB3	1.92	0.50
2:B:54:PRO:HA	30:f:835:GLU:HB3	1.93	0.50
5:E:205:ASP:OD1	5:E:205:ASP:N	2.43	0.50
12:L:146:GLN:HG3	12:L:161:ILE:HD11	1.93	0.50
22:V:349:ARG:HH12	35:e:37:HIS:HE1	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:4:MET:HE1	14:n:159:ALA:HB3	1.93	0.50
20:t:27:LEU:HD11	20:t:34:ALA:HB1	1.93	0.50
3:C:252:ASP:OD1	3:C:295:THR:OG1	2.29	0.50
23:X:389:ASP:OD1	23:X:389:ASP:N	2.44	0.50
30:f:257:ARG:HD3	30:f:271:MET:HE1	1.92	0.50
30:f:559:PRO:HB2	30:f:594:LEU:HD22	1.93	0.50
10:j:119:THR:HG22	10:j:126:PRO:HB3	1.94	0.50
19:s:13:LEU:HD11	19:s:149:LEU:HD11	1.93	0.50
2:B:198:LYS:NZ	2:B:202:GLU:OE1	2.44	0.50
10:J:4:ASP:N	10:J:4:ASP:OD1	2.45	0.50
21:U:21:GLU:OE1	21:U:55:ARG:NH1	2.43	0.50
28:c:64:ASP:HA	28:c:139:ARG:HH12	1.77	0.50
9:i:216:LEU:HD13	9:i:225:ILE:HG12	1.94	0.50
13:m:34:SER:HB2	13:m:65:ARG:HH12	1.75	0.50
2:B:313:LEU:O	2:B:346:ARG:NH1	2.44	0.50
5:E:242:ARG:O	5:E:387:LYS:NZ	2.45	0.50
9:I:35:LEU:HD12	9:I:163:CYS:HB2	1.93	0.50
30:f:125:ILE:HG21	30:f:129:LEU:HB2	1.94	0.50
34:W:158:ASP:OD2	34:W:160:LYS:NZ	2.37	0.50
2:B:407:LEU:HD22	3:C:178:LEU:HD11	1.94	0.50
4:D:244:PRO:HD3	4:D:288:ILE:HG12	1.93	0.50
13:M:15:SER:HB3	13:M:19:ARG:H	1.76	0.50
19:S:19:ASP:OD1	19:S:19:ASP:N	2.44	0.50
30:f:117:GLU:O	30:f:120:ARG:N	2.41	0.50
30:f:827:PRO:HB2	30:f:860:LYS:HD2	1.94	0.50
35:e:25:GLU:HG2	35:e:27:TRP:H	1.77	0.50
35:e:50:ASP:OD1	35:e:50:ASP:N	2.41	0.50
2:B:54:PRO:HB2	2:B:61:LYS:HG3	1.94	0.50
6:F:438:TYR:OH	11:K:19:GLY:O	2.28	0.50
27:b:180:ALA:HA	27:b:183:LEU:HD12	1.93	0.50
29:d:109:GLN:O	29:d:111:ARG:NH1	2.45	0.50
16:P:151:GLU:OE2	19:s:185:ARG:NH2	2.44	0.50
25:Z:7:GLN:HG2	25:Z:46:LYS:HB3	1.94	0.50
25:Z:74:TYR:OH	28:c:98:MET:O	2.30	0.50
29:d:6:LYS:NZ	29:d:17:SER:OG	2.43	0.50
30:f:84:SER:HA	30:f:87:THR:HG22	1.94	0.50
4:D:249:ASP:OD1	4:D:252:ARG:NH2	2.44	0.50
22:V:150:ARG:NH1	22:V:157:THR:O	2.45	0.50
24:Y:145:LEU:HD13	24:Y:182:VAL:HG11	1.93	0.50
28:c:31:VAL:HG22	28:c:67:VAL:HB	1.94	0.50
30:f:479:LEU:HD13	30:f:514:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:133:ASP:OD1	19:s:133:ASP:N	2.43	0.50
3:C:299:ASP:OD1	3:C:299:ASP:N	2.43	0.50
23:X:343:SER:OG	34:W:407:ASP:OD1	2.30	0.50
29:d:129:THR:HG22	29:d:130:ASN:H	1.77	0.50
34:W:387:ASP:N	34:W:387:ASP:OD1	2.45	0.50
1:A:390:THR:HA	2:B:216:ILE:HD12	1.93	0.49
11:K:182:GLN:NE2	12:L:55:GLU:OE2	2.45	0.49
30:f:762:VAL:HB	30:f:771:LEU:HB3	1.93	0.49
30:f:777:THR:HG22	30:f:803:PHE:HB2	1.94	0.49
30:f:834:ASP:OD1	30:f:834:ASP:N	2.45	0.49
10:J:39:ASP:OD1	10:J:39:ASP:N	2.44	0.49
30:f:93:PRO:O	30:f:97:LYS:N	2.42	0.49
30:f:254:GLY:HA2	30:f:289:VAL:HG21	1.94	0.49
30:f:850:VAL:HB	30:f:852:VAL:HG12	1.93	0.49
12:l:109:VAL:HA	12:l:112:ILE:HD12	1.93	0.49
14:n:35:THR:OG1	14:n:43:CYS:SG	2.69	0.49
19:s:75:TYR:OH	19:s:81:LYS:NZ	2.45	0.49
2:B:221:GLY:HA3	2:B:347:ILE:HA	1.93	0.49
5:E:341:ALA:HA	5:E:344:ARG:HE	1.77	0.49
21:U:830:THR:HG22	30:f:614:HIS:HE1	1.77	0.49
28:c:217:LEU:O	28:c:221:HIS:CB	2.60	0.49
15:o:143:ARG:NH2	15:o:150:GLU:OE1	2.45	0.49
1:A:127:ASP:O	32:x:334:LYS:NZ	2.43	0.49
18:r:179:VAL:HG22	18:r:184:TRP:HB3	1.94	0.49
32:x:256:LYS:HG2	32:x:265:VAL:HG13	1.94	0.49
34:W:71:VAL:HG22	34:W:87:ILE:HD11	1.94	0.49
34:W:138:VAL:HG22	34:W:139:GLU:HG3	1.92	0.49
3:C:339:THR:OG1	3:C:340:ARG:N	2.46	0.49
14:N:167:ASP:OD1	14:N:168:GLY:N	2.46	0.49
20:T:50:MET:HE2	20:T:192:VAL:HG12	1.94	0.49
21:U:799:LYS:HB3	21:U:923:GLU:HB3	1.94	0.49
23:X:317:PRO:HD2	23:X:319:ILE:HG12	1.93	0.49
30:f:117:GLU:H	30:f:120:ARG:HH21	1.61	0.49
2:B:70:ASP:O	2:B:74:MET:HG2	2.12	0.49
3:C:281:ASP:OD2	3:C:307:ARG:NH2	2.46	0.49
5:E:143:ARG:NH2	5:E:150:GLU:OE1	2.45	0.49
24:Y:184:GLN:NE2	24:Y:196:GLN:O	2.45	0.49
30:f:87:THR:OG1	30:f:109:ILE:O	2.30	0.49
32:x:273:LEU:HB2	33:y:47:GLY:HA3	1.93	0.49
1:A:319:MET:HE3	1:A:337:LEU:HD21	1.94	0.49
5:E:97:ARG:NH2	5:E:112:PRO:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:133:LEU:HG	12:L:161:ILE:HD12	1.94	0.49
16:P:177:ARG:NH2	19:s:150:ASP:OD2	2.31	0.49
25:Z:60:GLU:OE2	25:Z:104:ASN:ND2	2.43	0.49
29:d:3:GLU:HB3	29:d:50:LEU:HG	1.94	0.49
30:f:13:PRO:HB3	30:f:41:LYS:HZ1	1.78	0.49
30:f:227:ALA:HB3	30:f:234:THR:HG22	1.95	0.49
2:B:234:LEU:HD22	36:B:501:ATP:H2'	1.95	0.49
6:F:72:LYS:O	6:F:74:LYS:N	2.46	0.49
30:f:43:GLN:O	30:f:47:GLU:HB2	2.12	0.49
30:f:59:LEU:HD13	30:f:62:ARG:HH12	1.76	0.49
19:s:148:LEU:HD23	19:s:178:VAL:HG22	1.95	0.49
34:W:60:MET:HE1	34:W:99:GLN:HB2	1.95	0.49
3:C:331:ILE:O	3:C:334:ARG:NH1	2.44	0.49
4:D:311:THR:OG1	4:D:312:ASN:N	2.46	0.49
5:E:146:ARG:NH2	5:E:190:GLN:OE1	2.45	0.49
12:l:155:ASP:HB3	13:m:62:SER:HB2	1.94	0.49
16:p:62:THR:HG23	17:q:86:ARG:HH22	1.78	0.49
32:x:333:TYR:HA	32:x:340:ASN:HA	1.95	0.49
13:M:23:VAL:HG12	13:M:27:MET:HE2	1.95	0.49
21:U:673:GLU:O	21:U:676:THR:OG1	2.31	0.49
25:Z:134:PRO:HB3	28:c:220:LEU:HD13	1.95	0.49
27:b:168:SER:HA	27:b:191:GLY:HA2	1.94	0.49
30:f:209:MET:HG3	30:f:211:ILE:H	1.77	0.49
34:W:268:LYS:HB3	34:W:336:PRO:HG3	1.95	0.49
21:U:356:THR:HG21	21:U:731:ILE:HD13	1.95	0.48
26:a:205:LEU:HG	26:a:268:LEU:HD11	1.95	0.48
27:b:150:THR:HB	27:b:153:LEU:HD23	1.94	0.48
30:f:486:GLY:HA2	30:f:525:ILE:HD11	1.95	0.48
30:f:640:LYS:HZ3	30:f:648:ALA:HA	1.78	0.48
34:W:291:SER:HA	34:W:296:LEU:HD21	1.95	0.48
1:A:233:THR:HG21	1:A:237:PHE:HB2	1.95	0.48
2:B:224:LEU:HB3	2:B:353:PHE:HE2	1.78	0.48
21:U:619:VAL:HG11	21:U:648:VAL:HG13	1.95	0.48
27:b:137:ASN:HA	27:b:160:LEU:HD21	1.95	0.48
1:A:428:ARG:NH1	10:J:23:GLN:OE1	2.46	0.48
9:I:4:ARG:O	10:J:5:ARG:NH2	2.47	0.48
22:V:311:ASN:OD1	22:V:314:ARG:NH2	2.46	0.48
29:d:79:LYS:O	29:d:83:PHE:N	2.46	0.48
15:o:143:ARG:HG2	15:o:146:MET:HE2	1.96	0.48
19:s:186:ASP:OD1	19:s:187:VAL:N	2.44	0.48
3:C:251:ILE:H	3:C:295:THR:HB	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:177:ARG:HD2	23:X:201:TYR:HB2	1.93	0.48
10:J:209:ALA:HB1	10:J:217:LEU:HD21	1.95	0.48
13:M:37:ILE:HD11	13:M:193:VAL:HG13	1.94	0.48
21:U:545:LEU:HB3	21:U:577:ILE:HG21	1.95	0.48
24:Y:141:VAL:HG11	24:Y:164:ALA:HB2	1.96	0.48
13:m:139:SER:OG	13:m:140:TYR:N	2.46	0.48
27:b:138:VAL:HG12	27:b:160:LEU:HD13	1.95	0.48
14:n:9:ASP:OD1	14:n:9:ASP:N	2.44	0.48
32:x:9:LYS:HD2	32:x:14:LYS:HE3	1.95	0.48
1:A:213:LEU:HD12	1:A:337:LEU:HD13	1.96	0.48
5:E:143:ARG:HD3	34:W:174:TYR:HB3	1.94	0.48
5:E:292:PRO:HA	5:E:296:ASP:HB3	1.94	0.48
13:M:99:ARG:NH1	13:M:105:ASN:OD1	2.45	0.48
26:a:276:CYS:SG	26:a:299:SER:OG	2.62	0.48
30:f:257:ARG:HH22	30:f:286:LYS:HE2	1.79	0.48
4:D:362:ASP:OD1	4:D:362:ASP:N	2.46	0.48
4:D:410:ASP:OD1	4:D:410:ASP:N	2.45	0.48
5:E:281:ARG:NH1	5:E:385:ASP:O	2.45	0.48
6:F:97:LEU:HB2	6:F:121:CYS:HB2	1.95	0.48
14:N:190:LEU:HD12	20:t:209:TRP:HB2	1.96	0.48
21:U:899:ARG:O	21:U:901:GLN:NE2	2.46	0.48
29:d:4:GLN:OE1	29:d:18:LYS:NZ	2.38	0.48
13:m:134:SER:HB2	13:m:153:PRO:HD3	1.95	0.48
33:y:5:VAL:HG22	33:y:67:LEU:HB3	1.96	0.48
1:A:32:LEU:HD22	30:f:96:LEU:HD23	1.96	0.48
22:V:480:ILE:HB	25:Z:260:VAL:HG22	1.95	0.48
30:f:215:ASP:N	30:f:215:ASP:OD1	2.44	0.48
30:f:305:LEU:HB2	30:f:318:THR:HG21	1.95	0.48
30:f:828:ARG:H	30:f:861:THR:HG22	1.78	0.48
34:W:254:PRO:HA	34:W:258:ALA:HA	1.95	0.48
6:F:297:ASP:HA	6:F:304:ARG:HH21	1.79	0.48
21:U:49:TYR:HA	21:U:57:ARG:HB2	1.95	0.48
21:U:806:CYS:O	21:U:874:ASN:ND2	2.47	0.48
10:j:39:ASP:OD1	10:j:213:ARG:NH1	2.46	0.48
10:j:65:LEU:HB2	10:j:69:VAL:HG13	1.96	0.48
35:e:35:ASP:HB3	35:e:37:HIS:CD2	2.49	0.48
1:A:144:ARG:NH1	31:v:30:UNK:O	2.47	0.48
8:H:223:PRO:HA	8:H:226:VAL:HG12	1.95	0.48
9:i:202:ASP:OD1	9:i:203:VAL:N	2.46	0.48
1:A:312:ARG:HD2	1:A:315:ILE:HB	1.96	0.47
5:E:205:ASP:OD1	5:E:211:SER:OG	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:242:ARG:NH2	5:E:254:GLN:OE1	2.47	0.47
5:E:302:ASP:OD1	5:E:302:ASP:N	2.47	0.47
21:U:58:GLN:HG3	21:U:87:LEU:HD21	1.95	0.47
30:f:7:ASP:N	30:f:7:ASP:OD1	2.43	0.47
30:f:530:CYS:HB3	30:f:565:ASN:HD21	1.79	0.47
3:C:138:MET:HB3	3:C:212:ILE:HG23	1.96	0.47
10:J:31:THR:OG1	10:J:163:ARG:O	2.28	0.47
23:X:310:ARG:HG2	23:X:314:ARG:HE	1.80	0.47
24:Y:155:ASP:N	24:Y:155:ASP:OD1	2.44	0.47
30:f:189:LYS:HG2	30:f:190:GLU:HG3	1.96	0.47
32:x:178:PHE:O	32:x:182:ALA:CB	2.62	0.47
3:C:379:THR:OG1	3:C:380:GLN:N	2.47	0.47
17:Q:39:SER:OG	17:Q:40:GLU:N	2.47	0.47
18:R:192:VAL:HG11	16:p:205:ASP:HB3	1.95	0.47
20:T:96:MET:HE2	20:T:110:MET:HE1	1.97	0.47
22:V:468:SER:HB3	24:Y:363:ASN:HD21	1.79	0.47
22:V:469:THR:HG22	22:V:470:ARG:HG2	1.95	0.47
1:A:394:MET:HG2	2:B:349:ARG:HH22	1.79	0.47
6:F:236:LEU:HD13	6:F:354:PHE:HZ	1.80	0.47
24:Y:113:ARG:HG2	24:Y:114:ILE:HG23	1.94	0.47
26:a:236:THR:OG1	26:a:253:THR:OG1	2.32	0.47
30:f:372:LEU:HD13	30:f:406:GLY:HA2	1.96	0.47
10:j:67:ASP:N	10:j:67:ASP:OD1	2.46	0.47
4:D:153:MET:HG2	4:D:228:ILE:HG12	1.96	0.47
4:D:368:ASP:HB3	4:D:407:ILE:HD11	1.95	0.47
23:X:379:ASP:OD2	24:Y:312:ARG:NH1	2.47	0.47
28:c:163:ILE:HD13	28:c:201:TYR:HE2	1.78	0.47
32:x:189:LYS:HE3	32:x:194:GLN:HB3	1.97	0.47
3:C:46:GLN:HB2	21:U:639:LEU:HD11	1.96	0.47
5:E:287:PRO:HA	5:E:290:LEU:HB2	1.97	0.47
21:U:699:THR:HG22	21:U:700:GLU:H	1.79	0.47
30:f:170:TRP:HA	30:f:173:LEU:HB2	1.96	0.47
7:g:58:ASP:OD1	7:g:58:ASP:N	2.48	0.47
13:m:62:SER:OG	13:m:63:ASN:OD1	2.33	0.47
17:q:30:ASP:OD1	17:q:30:ASP:N	2.47	0.47
1:A:253:GLY:HA2	1:A:256:MET:HE2	1.96	0.47
3:C:83:LYS:HB3	3:C:99:VAL:HG22	1.95	0.47
17:Q:168:GLN:NE2	17:Q:175:LEU:O	2.39	0.47
9:i:8:ARG:HB3	9:i:11:ILE:HD12	1.96	0.47
32:x:290:LEU:HD22	32:x:293:ARG:HH21	1.79	0.47
21:U:553:ALA:HA	21:U:585:THR:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:f:284:SER:HA	30:f:883:ALA:HB2	1.96	0.47
8:h:4:ARG:HH12	11:k:126:GLU:HG3	1.80	0.47
33:y:27:LYS:NZ	33:y:41:GLN:OE1	2.34	0.47
34:W:131:VAL:HG11	34:W:144:ARG:HB2	1.97	0.47
34:W:213:PHE:O	34:W:215:GLN:NE2	2.48	0.47
1:A:325:ASP:OD1	1:A:325:ASP:N	2.43	0.47
3:C:25:LEU:HD23	3:C:28:ILE:HD11	1.96	0.47
8:h:189:HIS:CD2	8:h:233:ILE:HG13	2.50	0.47
32:x:297:GLU:O	33:y:12:THR:OG1	2.33	0.47
34:W:385:SER:OG	34:W:387:ASP:OD1	2.30	0.47
3:C:342:ILE:HG22	3:C:380:GLN:HB2	1.96	0.47
5:E:233:ASP:N	5:E:233:ASP:OD1	2.46	0.47
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.96	0.47
7:G:165:ALA:HB1	7:G:179:LEU:HD13	1.95	0.47
26:a:27:GLU:O	26:a:30:THR:OG1	2.32	0.47
27:b:68:THR:HA	27:b:71:ILE:HD12	1.97	0.47
32:x:444:GLN:OE1	32:x:483:ARG:NH1	2.46	0.47
34:W:170:GLN:HG2	34:W:174:TYR:HE2	1.79	0.47
4:D:97:ASP:OD1	4:D:97:ASP:N	2.48	0.46
4:D:155:THR:HA	4:D:159:LYS:HD3	1.98	0.46
5:E:289:LEU:HA	5:E:294:ARG:HD2	1.97	0.46
21:U:633:CYS:HA	21:U:636:VAL:HG12	1.96	0.46
24:Y:90:ASP:O	24:Y:93:LYS:NZ	2.47	0.46
30:f:735:GLY:O	30:f:737:ASN:ND2	2.48	0.46
20:t:45:VAL:HB	20:t:49:THR:HG23	1.97	0.46
32:x:92:MET:SD	32:x:92:MET:N	2.88	0.46
32:x:367:MET:HG3	32:x:406:PHE:HE1	1.80	0.46
34:W:262:LYS:HE3	34:W:262:LYS:HB2	1.75	0.46
1:A:261:PHE:HD2	1:A:305:GLN:HB3	1.79	0.46
2:B:431:GLN:OE1	2:B:433:GLY:N	2.48	0.46
4:D:296:MET:HE2	4:D:307:VAL:HG11	1.96	0.46
4:D:359:ASP:OD1	4:D:359:ASP:N	2.49	0.46
8:H:196:LYS:HB3	8:H:203:MET:HE2	1.97	0.46
24:Y:184:GLN:HE22	24:Y:197:ALA:C	2.23	0.46
30:f:27:LYS:HG2	30:f:30:GLY:HA3	1.97	0.46
30:f:608:LYS:HB3	30:f:639:LYS:HE3	1.97	0.46
19:s:19:ASP:OD1	19:s:19:ASP:N	2.48	0.46
2:B:82:GLN:O	2:B:86:LYS:NZ	2.41	0.46
2:B:165:ASP:OD1	2:B:272:ARG:NH1	2.48	0.46
4:D:377:SER:HB3	5:E:292:PRO:HG2	1.98	0.46
5:E:29:LEU:HB3	6:F:62:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:309:ARG:HD2	5:E:332:VAL:HG13	1.97	0.46
6:F:435:LEU:HD12	6:F:438:TYR:HE2	1.80	0.46
12:L:132:LEU:HB2	12:L:147:THR:HB	1.97	0.46
13:M:23:VAL:O	13:M:27:MET:HG2	2.15	0.46
21:U:802:TYR:O	21:U:878:LEU:N	2.47	0.46
24:Y:133:ALA:HB3	24:Y:136:HIS:HB2	1.96	0.46
26:a:236:THR:OG1	26:a:249:GLN:NE2	2.40	0.46
30:f:404:ASP:OD1	30:f:404:ASP:N	2.46	0.46
8:h:51:LYS:NZ	8:h:199:PHE:O	2.48	0.46
16:p:58:THR:O	17:q:85:ARG:NH2	2.48	0.46
6:F:177:VAL:HG21	6:F:248:PHE:HD2	1.79	0.46
19:S:40:SER:O	19:S:40:SER:OG	2.33	0.46
21:U:244:MET:HE3	21:U:248:ILE:HD11	1.98	0.46
24:Y:262:SER:OG	24:Y:267:ARG:O	2.33	0.46
27:b:141:ILE:HG22	27:b:143:PHE:HB2	1.98	0.46
13:m:198:TYR:OH	13:m:236:GLU:OE2	2.33	0.46
34:W:294:LYS:HA	34:W:297:GLU:HB2	1.97	0.46
3:C:266:ASP:OD1	3:C:266:ASP:N	2.47	0.46
11:K:199:LEU:HB3	11:K:241:ILE:HD11	1.96	0.46
22:V:80:LYS:HG2	22:V:84:LYS:HE3	1.97	0.46
23:X:119:SER:O	23:X:121:LYS:NZ	2.49	0.46
30:f:703:ARG:HH12	30:f:788:MET:HG2	1.80	0.46
20:t:161:SER:OG	20:t:162:GLN:N	2.48	0.46
34:W:267:LEU:HB2	34:W:295:LYS:HE3	1.97	0.46
34:W:300:PRO:HA	34:W:303:LYS:HE3	1.96	0.46
5:E:171:LEU:HD12	5:E:295:LEU:HD21	1.97	0.46
7:G:196:GLU:HG3	7:G:242:LEU:HD12	1.96	0.46
21:U:8:ILE:HD13	29:d:36:LEU:HD22	1.97	0.46
21:U:330:SER:OG	21:U:332:GLU:OE2	2.34	0.46
21:U:764:LEU:O	21:U:767:THR:OG1	2.32	0.46
22:V:419:LEU:HD12	22:V:456:GLY:HA2	1.96	0.46
22:V:479:ARG:NH1	24:Y:374:ASP:OD1	2.49	0.46
24:Y:226:VAL:HA	24:Y:229:ILE:HG22	1.97	0.46
30:f:174:ASP:N	30:f:178:LYS:HZ1	2.14	0.46
30:f:322:SER:OG	30:f:455:VAL:O	2.34	0.46
7:g:50:ILE:HD12	7:g:79:VAL:HB	1.98	0.46
34:W:172:GLU:HB2	34:W:182:ARG:HG2	1.97	0.46
3:C:152:GLY:HA3	36:C:501:ATP:HN62	1.80	0.46
5:E:85:ARG:HG3	5:E:86:GLN:HG2	1.98	0.46
15:O:185:PHE:HE2	15:O:187:ARG:HD2	1.80	0.46
21:U:725:MET:HE3	28:c:183:HIS:NE2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:132:LYS:O	27:b:135:LYS:NZ	2.39	0.46
30:f:468:ASP:OD1	30:f:468:ASP:N	2.47	0.46
32:x:22:THR:HG22	32:x:63:ILE:HD12	1.98	0.46
1:A:31:ALA:O	1:A:35:THR:OG1	2.32	0.46
21:U:492:ASP:OD1	21:U:492:ASP:N	2.48	0.46
25:Z:172:VAL:HG13	28:c:217:LEU:HD13	1.98	0.46
26:a:226:ARG:HH12	26:a:230:ARG:HE	1.63	0.46
30:f:744:MET:HE3	30:f:745:LEU:HD22	1.97	0.46
30:f:828:ARG:HD3	30:f:847:GLY:HA3	1.97	0.46
10:j:79:ASP:HB3	10:j:127:PHE:HD1	1.80	0.46
17:q:94:SER:OG	17:q:95:ARG:N	2.48	0.46
32:x:21:ASN:HB3	32:x:24:GLU:HG3	1.97	0.46
32:x:118:ALA:HB1	32:x:424:LEU:HD22	1.97	0.46
32:x:159:LEU:O	32:x:163:MET:HG3	2.15	0.46
1:A:277:ILE:HD11	1:A:327:LEU:HD21	1.96	0.46
4:D:194:ILE:HB	4:D:196:ILE:HG12	1.98	0.46
5:E:146:ARG:HH12	5:E:189:SER:HB3	1.80	0.46
9:I:180:LYS:H	9:I:184:MET:HE3	1.81	0.46
25:Z:49:ASP:OD1	25:Z:49:ASP:N	2.48	0.46
30:f:331:LEU:HB3	30:f:335:ARG:HH21	1.80	0.46
5:E:296:ASP:OD1	5:E:296:ASP:N	2.49	0.46
27:b:51:LEU:H	27:b:62:THR:HB	1.81	0.46
11:k:13:ASN:HB3	12:l:126:ARG:HB3	1.98	0.46
32:x:246:PHE:HE1	32:x:411:GLY:HA2	1.80	0.46
34:W:230:MET:HA	34:W:233:LEU:HB3	1.98	0.46
16:P:138:VAL:HG11	16:P:146:MET:HB3	1.99	0.45
26:a:61:GLU:HA	26:a:64:ILE:HD12	1.98	0.45
30:f:478:ARG:NH1	30:f:509:LYS:O	2.48	0.45
7:g:37:LEU:HD22	7:g:53:GLN:HG3	1.99	0.45
16:p:159:ASP:OD2	16:p:162:HIS:ND1	2.49	0.45
3:C:147:THR:HA	3:C:206:HIS:HE1	1.81	0.45
3:C:258:ARG:HH21	3:C:274:LEU:HD11	1.81	0.45
5:E:242:ARG:HA	5:E:242:ARG:HD2	1.75	0.45
13:M:197:ILE:HG21	13:M:211:LEU:HD13	1.97	0.45
17:Q:118:MET:HE2	17:Q:124:LEU:HD13	1.97	0.45
30:f:400:TYR:HE2	32:x:80:GLU:HB2	1.82	0.45
20:t:43:MET:HE3	20:t:43:MET:HB2	1.85	0.45
34:W:79:GLU:O	34:W:83:LEU:N	2.47	0.45
2:B:356:PRO:O	2:B:361:LYS:NZ	2.49	0.45
19:S:16:ALA:HB2	19:S:121:VAL:HG23	1.98	0.45
21:U:839:ALA:HA	21:U:842:LYS:HZ3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:119:GLY:HA2	22:V:148:ARG:HD3	1.98	0.45
24:Y:95:LEU:O	24:Y:98:SER:OG	2.27	0.45
20:t:166:ARG:NH1	20:t:200:GLU:OE1	2.39	0.45
32:x:263:GLU:OE2	32:x:304:THR:OG1	2.30	0.45
2:B:294:ARG:HH11	2:B:310:LEU:HD21	1.82	0.45
4:D:105:SER:OG	4:D:108:GLY:O	2.34	0.45
21:U:221:ILE:HG12	21:U:256:ALA:HB2	1.99	0.45
26:a:273:GLN:HB3	26:a:310:LEU:HD11	1.98	0.45
30:f:345:PRO:HD2	30:f:348:ILE:HD13	1.98	0.45
10:j:121:SER:HB2	10:j:124:ARG:HD2	1.96	0.45
15:o:112:SER:HB2	15:o:127:MET:HE3	1.99	0.45
17:q:26:VAL:HG11	18:r:136:TYR:HE2	1.82	0.45
1:A:67:GLU:HA	3:C:81:ASP:HB3	1.99	0.45
19:S:99:ARG:HE	19:S:99:ARG:HB3	1.56	0.45
24:Y:58:CYS:SG	24:Y:59:LYS:NZ	2.88	0.45
26:a:91:ASN:OD1	26:a:91:ASN:N	2.49	0.45
10:j:96:LEU:HD12	17:q:62:LYS:HG3	1.99	0.45
16:p:49:LEU:HD21	16:p:84:PRO:HG3	1.97	0.45
34:W:219:THR:HG21	34:W:224:LEU:H	1.81	0.45
22:V:212:TYR:HA	22:V:253:LEU:HD11	1.99	0.45
23:X:187:ARG:NE	23:X:221:GLU:OE2	2.50	0.45
24:Y:287:LEU:O	24:Y:291:HIS:ND1	2.50	0.45
25:Z:96:HIS:ND1	25:Z:97:THR:O	2.50	0.45
28:c:176:GLN:HG3	28:c:177:THR:H	1.81	0.45
30:f:305:LEU:O	30:f:308:SER:OG	2.34	0.45
30:f:680:ARG:NH2	30:f:762:VAL:H	2.15	0.45
30:f:787:LEU:HD23	30:f:791:VAL:HB	1.98	0.45
32:x:30:LYS:NZ	32:x:44:GLN:O	2.50	0.45
32:x:354:ASP:OD2	32:x:371:ARG:NH2	2.42	0.45
1:A:160:THR:HA	1:A:163:MET:HG3	1.99	0.45
2:B:284:ILE:HB	2:B:329:MET:HG2	1.98	0.45
24:Y:34:ASP:OD1	24:Y:35:ALA:N	2.49	0.45
27:b:25:ARG:NH2	27:b:145:GLU:O	2.50	0.45
30:f:209:MET:HB3	30:f:212:GLU:HB2	1.98	0.45
30:f:287:ASP:O	30:f:291:GLN:HB2	2.17	0.45
30:f:779:CYS:HA	30:f:782:HIS:CE1	2.51	0.45
34:W:109:CYS:O	34:W:113:GLU:CB	2.65	0.45
3:C:142:LYS:HA	3:C:142:LYS:HD2	1.84	0.45
22:V:464:ILE:HB	22:V:467:TYR:HE1	1.81	0.45
24:Y:107:LYS:HE3	24:Y:107:LYS:HB3	1.76	0.45
27:b:127:LEU:HG	27:b:130:ARG:HH12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:f:680:ARG:HH21	30:f:762:VAL:HG13	1.82	0.45
2:B:67:ARG:HB3	30:f:646:MET:HE1	1.98	0.45
4:D:183:LEU:HD23	4:D:183:LEU:HA	1.85	0.45
4:D:229:ARG:HG3	4:D:263:PHE:HD2	1.81	0.45
4:D:398:ASP:OD1	4:D:398:ASP:N	2.41	0.45
7:G:180:GLU:HA	7:G:183:VAL:HG12	1.99	0.45
8:H:82:ASP:HB3	8:H:130:PHE:HD1	1.81	0.45
22:V:287:ARG:NH2	35:e:17:ASP:OD2	2.49	0.45
26:a:36:GLN:NE2	27:b:145:GLU:OE2	2.49	0.45
30:f:142:TYR:CG	30:f:189:LYS:HG3	2.52	0.45
30:f:209:MET:O	30:f:213:GLN:NE2	2.47	0.45
5:E:198:VAL:HG11	5:E:232:MET:HA	1.99	0.45
17:Q:67:TYR:O	17:Q:71:ASN:ND2	2.45	0.45
21:U:354:LYS:HA	21:U:357:LYS:HE2	1.99	0.45
30:f:75:LEU:HD12	30:f:77:GLU:H	1.81	0.45
19:s:16:ALA:HB2	19:s:121:VAL:HG23	1.99	0.45
32:x:371:ARG:HG3	32:x:415:CYS:HA	1.99	0.45
2:B:107:MET:HG3	2:B:160:ILE:HD11	1.99	0.44
4:D:182:GLU:OE2	4:D:223:THR:OG1	2.30	0.44
4:D:270:ILE:HD12	4:D:285:VAL:HA	1.99	0.44
9:I:186:LEU:HD12	9:I:186:LEU:HA	1.88	0.44
9:I:238:LYS:HB2	9:I:238:LYS:HE3	1.78	0.44
10:J:7:ILE:HG23	10:J:8:THR:HG23	1.99	0.44
23:X:147:LEU:HD21	23:X:177:TYR:HE1	1.81	0.44
26:a:373:ASP:HB2	29:d:251:ARG:HH12	1.82	0.44
30:f:72:ARG:NH2	30:f:112:ASN:OD1	2.45	0.44
3:C:189:TYR:CZ	3:C:316:GLU:HB3	2.52	0.44
7:G:181:LYS:HA	7:G:184:LYS:HE3	2.00	0.44
10:J:184:ASP:O	10:J:187:THR:OG1	2.28	0.44
30:f:443:GLY:HA2	30:f:446:LEU:HD12	1.99	0.44
13:m:125:TYR:HB2	13:m:128:VAL:HG22	1.98	0.44
32:x:258:THR:HB	32:x:310:LEU:HB2	1.99	0.44
1:A:32:LEU:HD11	30:f:58:MET:HB3	1.99	0.44
2:B:412:MET:H	30:f:52:LEU:HD23	1.82	0.44
2:B:412:MET:HB2	30:f:52:LEU:HG	1.99	0.44
3:C:60:ARG:HH22	4:D:71:GLU:HG3	1.82	0.44
5:E:174:GLY:HA3	5:E:301:ILE:HG13	1.98	0.44
8:H:74:LEU:HD13	8:H:136:ILE:HG12	2.00	0.44
30:f:177:GLU:HG3	30:f:180:GLN:HB2	1.99	0.44
30:f:427:THR:OG1	30:f:428:GLN:OE1	2.35	0.44
10:j:95:ARG:HG2	17:q:62:LYS:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:PHE:CD2	1:A:305:GLN:HB3	2.52	0.44
21:U:794:ASP:OD1	21:U:795:LEU:N	2.48	0.44
25:Z:177:ARG:NH1	28:c:153:GLY:O	2.49	0.44
27:b:139:ASP:OD1	27:b:168:SER:OG	2.36	0.44
6:F:178:ASP:OD1	6:F:178:ASP:N	2.47	0.44
6:F:380:ASN:HB3	6:F:383:GLU:HB3	1.99	0.44
22:V:118:GLN:OE1	22:V:148:ARG:NH2	2.51	0.44
23:X:407:MET:HE3	28:c:252:ALA:HB1	2.00	0.44
24:Y:177:ARG:HH21	24:Y:203:ASP:HB2	1.83	0.44
24:Y:319:MET:HA	24:Y:322:ALA:HB3	1.98	0.44
26:a:49:CYS:SG	26:a:50:PHE:N	2.90	0.44
28:c:304:LEU:HA	28:c:307:VAL:HG12	2.00	0.44
7:g:51:VAL:HG22	7:g:217:VAL:HG22	1.99	0.44
10:j:4:ASP:OD1	10:j:122:ASN:ND2	2.51	0.44
17:q:53:THR:HG22	17:q:100:VAL:HG12	1.99	0.44
4:D:101:ALA:HB2	4:D:115:ILE:HD11	1.99	0.44
4:D:268:ASP:OD1	4:D:311:THR:OG1	2.36	0.44
4:D:335:LEU:HD23	4:D:336:PRO:HD3	2.00	0.44
6:F:418:GLU:OE1	12:L:164:ARG:NH2	2.47	0.44
15:O:146:MET:HE1	15:O:154:LEU:HD22	2.00	0.44
16:P:88:MET:HE2	16:P:88:MET:HB3	1.88	0.44
26:a:89:ASP:HB2	26:a:92:VAL:HB	2.00	0.44
30:f:438:ASP:OD1	30:f:476:THR:OG1	2.34	0.44
7:g:80:MET:SD	7:g:138:MET:HB2	2.58	0.44
34:W:142:ARG:HH21	34:W:176:SER:HB2	1.82	0.44
2:B:59:ARG:HB2	30:f:184:LEU:HG	1.99	0.44
5:E:40:TYR:HB2	6:F:73:ILE:HD11	1.99	0.44
6:F:60:LEU:HD12	6:F:60:LEU:HA	1.82	0.44
20:T:99:ARG:HG2	20:T:106:LEU:HG	1.98	0.44
22:V:123:SER:OG	22:V:155:ALA:O	2.35	0.44
29:d:127:ILE:HA	29:d:134:LYS:HE2	2.00	0.44
30:f:317:LEU:O	30:f:321:MET:HG3	2.17	0.44
10:j:184:ASP:O	10:j:187:THR:OG1	2.28	0.44
18:r:176:LEU:HB3	18:r:187:VAL:HB	2.00	0.44
12:L:203:GLN:O	12:L:239:ARG:NH2	2.51	0.44
19:S:10:GLY:HA3	19:S:42:LYS:HE3	1.99	0.44
21:U:623:GLY:HA3	21:U:658:ILE:HG13	1.99	0.44
21:U:799:LYS:O	21:U:900:TYR:OH	2.35	0.44
22:V:452:ASN:HB3	22:V:457:TYR:HB2	1.99	0.44
12:l:172:LEU:O	12:l:176:MET:HB3	2.18	0.44
15:o:42:TYR:HB2	15:o:178:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:x:301:GLN:HA	32:x:308:ASN:HA	2.00	0.44
34:W:120:ILE:HD13	34:W:120:ILE:HA	1.61	0.44
6:F:416:THR:OG1	6:F:417:HIS:N	2.51	0.44
12:L:172:LEU:O	12:L:176:MET:HB3	2.17	0.44
21:U:491:GLN:NE2	21:U:495:ASP:OD1	2.51	0.44
23:X:166:LEU:HG	23:X:170:GLN:HE21	1.83	0.44
30:f:285:CYS:HB3	30:f:872:VAL:HB	1.99	0.44
12:l:200:PRO:HG2	12:l:203:GLN:HG3	2.00	0.44
34:W:118:LEU:HB3	34:W:119:PRO:HD3	2.00	0.44
34:W:232:GLN:HA	34:W:235:GLN:HG2	2.00	0.44
34:W:441:LYS:HD2	34:W:441:LYS:HA	1.86	0.44
2:B:181:GLN:HG2	2:B:182:GLU:H	1.83	0.43
2:B:297:SER:OG	2:B:298:ASN:N	2.51	0.43
12:L:117:GLN:O	12:L:120:THR:OG1	2.35	0.43
25:Z:212:LEU:HA	25:Z:215:VAL:HG12	1.99	0.43
29:d:131:VAL:HG22	29:d:159:PRO:HG3	2.00	0.43
30:f:102:HIS:O	30:f:106:LEU:N	2.51	0.43
30:f:369:ARG:NH2	30:f:792:ALA:O	2.35	0.43
8:h:119:GLN:HG3	9:i:81:SER:HB2	1.99	0.43
9:i:8:ARG:HD3	10:j:5:ARG:HH22	1.83	0.43
32:x:178:PHE:O	32:x:182:ALA:HB3	2.18	0.43
1:A:37:GLY:HA2	30:f:128:VAL:HG23	1.99	0.43
5:E:283:ASP:OD1	5:E:283:ASP:N	2.51	0.43
23:X:358:LYS:HB2	23:X:358:LYS:HE3	1.81	0.43
25:Z:105:ASP:OD1	25:Z:105:ASP:N	2.52	0.43
26:a:112:ILE:HG13	26:a:151:VAL:HG21	1.99	0.43
30:f:425:GLY:O	30:f:429:ILE:HG12	2.18	0.43
30:f:631:LYS:HE3	30:f:631:LYS:HB3	1.81	0.43
13:m:75:MET:HE1	13:m:88:ALA:HB2	2.00	0.43
20:t:27:LEU:HD22	20:t:184:TYR:HB2	2.00	0.43
1:A:66:LYS:HB2	1:A:66:LYS:HE2	1.81	0.43
2:B:332:ASN:ND2	36:B:501:ATP:O3G	2.51	0.43
20:T:25:ASP:HA	20:T:187:PHE:HA	2.00	0.43
21:U:613:ASP:OD1	21:U:613:ASP:N	2.49	0.43
22:V:419:LEU:HA	22:V:422:ILE:HG22	2.00	0.43
29:d:131:VAL:HA	29:d:134:LYS:HB3	2.00	0.43
7:g:131:MET:HE2	7:g:131:MET:HB2	1.69	0.43
12:l:133:LEU:HD23	12:l:133:LEU:HA	1.90	0.43
12:l:182:CYS:HB3	12:l:186:GLU:HB3	1.99	0.43
34:W:190:MET:HB3	34:W:229:LEU:HD13	2.00	0.43
3:C:87:VAL:O	3:C:95:PHE:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:198:LEU:HD22	36:C:501:ATP:H2'	2.00	0.43
14:N:104:ASP:OD1	14:N:104:ASP:N	2.50	0.43
22:V:469:THR:O	22:V:470:ARG:NE	2.49	0.43
25:Z:251:LEU:HB3	28:c:234:TYR:CZ	2.54	0.43
30:f:294:MET:SD	30:f:807:ARG:NH1	2.92	0.43
30:f:496:ASP:OD1	30:f:496:ASP:N	2.51	0.43
30:f:845:ARG:HG2	30:f:846:VAL:H	1.82	0.43
33:y:25:ASN:O	33:y:29:LYS:HG3	2.19	0.43
34:W:272:LEU:HD23	34:W:272:LEU:HA	1.91	0.43
34:W:337:ALA:O	34:W:342:GLY:N	2.51	0.43
21:U:497:LEU:HB3	21:U:516:LEU:HG	1.99	0.43
26:a:321:LYS:O	26:a:334:THR:OG1	2.36	0.43
30:f:107:LYS:HB3	30:f:137:ARG:HD2	2.00	0.43
30:f:780:PRO:HG3	30:f:803:PHE:CD1	2.53	0.43
1:A:73:ALA:O	1:A:78:TRP:NE1	2.43	0.43
4:D:171:ASP:OD1	4:D:171:ASP:N	2.48	0.43
11:K:202:LEU:HD23	11:K:202:LEU:HA	1.90	0.43
22:V:251:LEU:HD23	22:V:276:PHE:HD1	1.83	0.43
29:d:126:ASP:OD1	29:d:126:ASP:N	2.49	0.43
20:t:110:MET:HB2	20:t:125:VAL:HB	2.01	0.43
32:x:363:LEU:HA	32:x:366:LYS:HE3	2.00	0.43
1:A:263:MET:O	1:A:266:THR:OG1	2.37	0.43
10:J:52:LYS:HB3	10:J:53:LEU:HD12	2.01	0.43
12:L:7:ASP:OD1	12:L:7:ASP:N	2.48	0.43
15:O:143:ARG:H	15:O:146:MET:HE3	1.83	0.43
19:S:123:SER:HB2	19:S:136:LYS:HG2	2.00	0.43
23:X:56:LEU:O	23:X:60:THR:OG1	2.36	0.43
9:i:34:CYS:SG	9:i:75:SER:OG	2.73	0.43
13:m:37:ILE:HD11	13:m:193:VAL:HG13	2.00	0.43
32:x:368:VAL:O	32:x:372:SER:OG	2.33	0.43
32:x:406:PHE:HD1	32:x:414:ASN:HA	1.84	0.43
5:E:256:THR:HA	5:E:259:GLU:HG2	2.01	0.43
26:a:34:TRP:N	27:b:18:ASN:OD1	2.52	0.43
28:c:119:GLY:H	28:c:121:TRP:HE1	1.67	0.43
30:f:230:CYS:SG	30:f:231:LEU:N	2.92	0.43
30:f:288:VAL:HG21	30:f:880:ALA:HA	1.99	0.43
7:g:191:PHE:HE1	7:g:219:VAL:HG21	1.83	0.43
34:W:272:LEU:HD12	34:W:336:PRO:HB2	2.00	0.43
1:A:58:LYS:HE3	1:A:58:LYS:HB2	1.79	0.43
2:B:231:GLY:N	36:B:501:ATP:O2A	2.51	0.43
2:B:334:ILE:HA	2:B:337:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:99:ASN:HA	4:D:115:ILE:HB	2.00	0.43
6:F:221:LYS:NZ	6:F:346:GLY:O	2.34	0.43
6:F:235:LEU:N	36:F:501:ATP:O2A	2.48	0.43
9:I:153:SER:OG	9:I:155:ASN:OD1	2.34	0.43
22:V:124:ASN:HA	22:V:128:ARG:HD3	2.01	0.43
12:l:176:MET:HE1	13:m:57:LEU:HA	2.01	0.43
12:l:184:LEU:HD23	12:l:184:LEU:HA	1.90	0.43
34:W:15:LYS:NZ	34:W:16:MET:O	2.45	0.43
1:A:236:CYS:HB3	1:A:270:CYS:HA	1.99	0.43
17:Q:1:MET:HE1	17:Q:133:GLY:HA2	2.01	0.43
23:X:396:THR:HG22	28:c:242:GLU:HB3	2.00	0.43
24:Y:134:LEU:HD22	24:Y:168:ILE:HG23	1.99	0.43
26:a:161:LYS:HD2	26:a:161:LYS:HA	1.82	0.43
26:a:363:MET:HE1	29:d:240:THR:HG22	2.01	0.43
27:b:4:GLU:HB2	27:b:44:ASN:HD21	1.83	0.43
28:c:26:ASP:OD2	28:c:175:ARG:NE	2.51	0.43
28:c:158:ASP:OD1	28:c:158:ASP:N	2.50	0.43
30:f:323:ASN:HB2	30:f:455:VAL:HG23	2.01	0.43
19:s:70:ALA:O	19:s:74:MET:HG3	2.19	0.43
32:x:48:VAL:HA	32:x:69:LEU:HD22	2.00	0.43
35:e:58:ALA:O	35:e:62:LYS:HB2	2.19	0.43
5:E:64:LEU:HG	5:E:65:THR:HG23	2.01	0.42
5:E:156:PRO:HG3	5:E:272:ARG:HD2	2.00	0.42
6:F:175:MET:HE3	6:F:175:MET:HB3	1.60	0.42
10:J:68:ASN:HA	10:J:211:MET:HE1	2.01	0.42
17:Q:39:SER:OG	17:Q:74:GLU:OE1	2.36	0.42
20:T:201:GLY:HA2	20:T:203:LEU:HD12	2.01	0.42
24:Y:129:ASP:N	24:Y:129:ASP:OD1	2.51	0.42
26:a:185:ILE:HG13	26:a:187:ASP:HB2	2.00	0.42
30:f:199:ASN:HA	30:f:202:HIS:CD2	2.54	0.42
34:W:55:ARG:HD3	34:W:96:GLN:HG3	2.01	0.42
3:C:76:VAL:HA	3:C:87:VAL:HG12	2.02	0.42
6:F:69:MET:HA	6:F:72:LYS:HB2	2.01	0.42
21:U:161:ASP:OD1	21:U:161:ASP:N	2.51	0.42
21:U:678:ASP:O	21:U:684:ARG:NE	2.52	0.42
21:U:830:THR:HG22	30:f:614:HIS:CE1	2.54	0.42
30:f:848:GLN:HG3	30:f:850:VAL:HG13	2.00	0.42
1:A:134:ILE:HD12	1:A:134:ILE:HG23	1.87	0.42
6:F:192:ASP:N	6:F:192:ASP:OD1	2.51	0.42
21:U:811:PHE:CD2	21:U:888:GLN:HG3	2.54	0.42
19:s:11:THR:HG22	19:s:141:ALA:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:155:PHE:HA	19:s:158:MET:HE2	2.01	0.42
32:x:49:LYS:HE3	32:x:67:MET:HB2	2.00	0.42
34:W:309:PHE:HE1	34:W:315:MET:HE1	1.84	0.42
5:E:5:ARG:HD3	6:F:32:GLU:HB3	2.01	0.42
15:O:167:LEU:HG	19:s:187:VAL:HG22	2.02	0.42
15:O:217:THR:HA	15:O:218:PRO:HD3	1.90	0.42
22:V:349:ARG:HH12	35:e:37:HIS:CE1	2.37	0.42
25:Z:198:LEU:HD11	28:c:304:LEU:HD23	2.01	0.42
25:Z:214:LYS:HE2	25:Z:220:LEU:HD12	2.01	0.42
26:a:73:PRO:HB3	26:a:104:VAL:HG11	2.01	0.42
28:c:137:SER:OG	28:c:138:GLU:N	2.53	0.42
30:f:91:SER:HA	30:f:94:LYS:HE2	2.01	0.42
9:i:119:GLN:HG3	10:j:78:ALA:HB1	2.01	0.42
35:e:26:ASP:OD1	35:e:26:ASP:N	2.48	0.42
1:A:146:LYS:NZ	1:A:148:GLN:HB2	2.34	0.42
2:B:285:ASP:HB3	2:B:286:GLU:HG2	2.01	0.42
7:G:10:ASP:OD1	7:G:10:ASP:N	2.50	0.42
23:X:301:ASP:HA	23:X:304:LYS:HG2	2.01	0.42
23:X:406:ASN:C	23:X:406:ASN:HD22	2.27	0.42
28:c:32:TYR:HE2	28:c:66:THR:HG23	1.84	0.42
30:f:811:LEU:N	30:f:854:GLY:O	2.48	0.42
7:g:206:LEU:HB3	7:g:208:ILE:HG13	2.01	0.42
34:W:34:LEU:HD23	34:W:43:VAL:HB	2.01	0.42
9:I:92:LEU:HD23	9:I:92:LEU:HA	1.88	0.42
16:P:205:ASP:HB3	18:r:192:VAL:HG11	2.02	0.42
20:T:214:MET:HE3	15:o:123:PRO:HG3	2.01	0.42
23:X:268:GLN:HA	23:X:271:VAL:HG22	2.01	0.42
25:Z:94:TRP:CD1	25:Z:112:MET:HE1	2.54	0.42
26:a:196:ARG:HA	26:a:196:ARG:HD2	1.84	0.42
30:f:267:ARG:HH21	30:f:296:PHE:HB2	1.84	0.42
30:f:632:LYS:O	30:f:636:ASP:HB2	2.19	0.42
12:l:226:ASP:OD1	12:l:227:ASP:N	2.52	0.42
18:r:127:SER:HB3	18:r:136:TYR:CE1	2.54	0.42
19:s:123:SER:HB2	19:s:136:LYS:HG2	2.01	0.42
20:t:103:MET:HE3	20:t:103:MET:HB3	1.82	0.42
32:x:425:THR:HG22	32:x:475:ALA:HA	2.02	0.42
33:y:22:THR:HG22	33:y:55:THR:HG22	2.02	0.42
34:W:378:MET:HE2	34:W:382:LEU:HG	2.01	0.42
16:P:30:ILE:HG22	16:P:31:GLN:H	1.85	0.42
21:U:108:TYR:HB2	21:U:130:LEU:HD12	2.00	0.42
29:d:183:GLU:HA	29:d:224:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:186:HIS:CE1	11:k:189:MET:HB3	2.55	0.42
32:x:250:GLU:HB2	32:x:318:SER:HB3	2.02	0.42
10:J:184:ASP:O	10:J:188:ILE:HG12	2.19	0.42
14:N:201:THR:HG23	20:t:38:ASN:HD21	1.83	0.42
20:T:99:ARG:HA	20:T:99:ARG:HD3	1.89	0.42
21:U:719:ASP:O	21:U:727:LYS:NZ	2.48	0.42
23:X:132:ARG:HD2	23:X:132:ARG:HA	1.88	0.42
23:X:143:TYR:CD2	23:X:144:GLN:HG2	2.54	0.42
23:X:163:LYS:HD3	23:X:163:LYS:HA	1.82	0.42
28:c:216:MET:HA	28:c:220:LEU:HD12	2.01	0.42
30:f:267:ARG:HA	30:f:271:MET:HB3	2.01	0.42
30:f:559:PRO:O	30:f:563:GLY:N	2.44	0.42
8:h:101:TYR:HE1	16:p:90:MET:HE2	1.85	0.42
15:o:179:SER:OG	15:o:180:LYS:N	2.51	0.42
15:o:204:CYS:HB2	16:p:162:HIS:HD2	1.85	0.42
34:W:253:THR:HG21	34:W:262:LYS:HG2	2.01	0.42
1:A:210:LYS:NZ	1:A:313:GLY:O	2.41	0.42
5:E:37:THR:HA	6:F:69:MET:HE1	2.02	0.42
7:G:112:ASP:OD1	7:G:112:ASP:N	2.50	0.42
20:T:211:ILE:HG13	14:n:30:VAL:HG11	2.01	0.42
21:U:524:LYS:HG3	21:U:556:MET:HE1	2.02	0.42
11:k:221:GLN:OE1	11:k:224:GLN:NE2	2.53	0.42
19:s:116:GLU:N	19:s:116:GLU:OE1	2.52	0.42
20:t:192:VAL:HG23	20:t:197:VAL:HG22	2.02	0.42
32:x:426:HIS:HE1	32:x:434:GLY:HA3	1.85	0.42
2:B:55:HIS:O	2:B:371:ARG:NH1	2.52	0.42
5:E:84:ARG:HG3	5:E:85:ARG:H	1.85	0.42
13:M:41:CYS:HB3	13:M:189:ILE:HG13	2.02	0.42
21:U:167:ILE:HD11	21:U:204:ILE:HD13	2.02	0.42
21:U:563:ALA:O	21:U:567:ILE:HG12	2.20	0.42
21:U:664:GLY:HA3	21:U:702:THR:HB	2.01	0.42
26:a:12:GLN:HA	26:a:22:TRP:CD2	2.55	0.42
26:a:240:PHE:HZ	26:a:271:LYS:HB3	1.85	0.42
28:c:248:MET:HA	28:c:251:LEU:HD12	2.02	0.42
32:x:46:VAL:HA	32:x:71:MET:HA	2.02	0.42
10:J:13:ASP:OD1	10:J:13:ASP:N	2.51	0.41
14:N:166:ARG:HA	14:N:166:ARG:HD3	1.79	0.41
22:V:199:ASN:OD1	22:V:241:ARG:NH2	2.52	0.41
29:d:168:ASP:OD1	29:d:169:ILE:N	2.51	0.41
9:i:53:HIS:CD2	9:i:55:LEU:H	2.37	0.41
35:e:30:LEU:HD23	35:e:30:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:ASP:HB2	2:B:346:ARG:HG2	2.02	0.41
4:D:73:LEU:HD23	4:D:73:LEU:HA	1.88	0.41
5:E:352:MET:HE1	6:F:212:PHE:HE2	1.85	0.41
7:G:202:LEU:HD12	7:G:202:LEU:HA	1.91	0.41
8:H:50:LYS:HB2	8:H:50:LYS:HE3	1.78	0.41
21:U:513:GLY:HA3	21:U:548:LEU:HD22	2.02	0.41
25:Z:25:ARG:HA	25:Z:28:LYS:HE3	2.01	0.41
30:f:298:LEU:HB3	30:f:492:SER:HA	2.02	0.41
30:f:826:GLN:OE1	30:f:864:GLY:HA2	2.19	0.41
9:i:41:ASP:OD1	9:i:41:ASP:N	2.52	0.41
10:j:189:LYS:HE2	10:j:189:LYS:HB3	1.84	0.41
15:o:198:ARG:HD2	15:o:201:ARG:HH22	1.84	0.41
32:x:240:LYS:HB3	32:x:240:LYS:HE3	1.83	0.41
5:E:254:GLN:HE21	5:E:285:LEU:HG	1.85	0.41
21:U:811:PHE:CG	21:U:888:GLN:HG3	2.54	0.41
21:U:844:LYS:HE2	21:U:844:LYS:HB3	1.84	0.41
22:V:400:HIS:NE2	29:d:141:GLN:OE1	2.53	0.41
22:V:485:ASP:OD1	29:d:252:GLN:NE2	2.52	0.41
24:Y:250:LEU:HD23	24:Y:250:LEU:HA	1.92	0.41
26:a:350:LYS:HD2	26:a:350:LYS:HA	1.84	0.41
29:d:203:PRO:HG2	29:d:205:LYS:HB2	2.02	0.41
30:f:683:GLU:HA	30:f:684:PRO:HD3	1.89	0.41
13:m:50:GLU:OE2	13:m:201:HIS:ND1	2.48	0.41
19:s:28:ARG:NH2	19:s:191:ASP:OD1	2.53	0.41
16:P:58:THR:O	17:Q:85:ARG:NH2	2.53	0.41
22:V:219:GLU:HG3	22:V:224:LEU:HD21	2.02	0.41
22:V:340:GLY:HA2	22:V:405:THR:HB	2.03	0.41
30:f:170:TRP:HD1	30:f:173:LEU:HD13	1.85	0.41
30:f:345:PRO:HB2	30:f:348:ILE:HG23	2.03	0.41
30:f:691:PRO:HB2	30:f:692:LEU:HD12	2.03	0.41
30:f:698:SER:O	30:f:705:ASN:ND2	2.48	0.41
7:g:37:LEU:HA	7:g:53:GLN:HE21	1.86	0.41
32:x:206:GLN:HB3	32:x:207:MET:HE2	2.03	0.41
3:C:33:LEU:HD23	3:C:33:LEU:HA	1.90	0.41
14:N:14:LEU:HD21	14:N:101:ALA:HB3	2.01	0.41
16:P:113:ASP:HB3	16:P:118:LYS:H	1.86	0.41
16:P:135:ASP:OD1	16:P:135:ASP:N	2.53	0.41
28:c:257:LYS:O	28:c:257:LYS:NZ	2.41	0.41
11:k:195:ILE:HG23	11:k:217:LEU:HD11	2.02	0.41
13:m:228:PRO:HD2	13:m:231:ILE:HD12	2.02	0.41
1:A:56:LEU:HD12	1:A:56:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LYS:HE2	1:A:110:LYS:HB3	1.80	0.41
17:Q:26:VAL:HG21	18:R:136:TYR:CE2	2.55	0.41
21:U:469:SER:O	21:U:474:ARG:NE	2.54	0.41
21:U:699:THR:HB	21:U:701:ILE:HG22	2.02	0.41
22:V:227:VAL:HG12	22:V:231:LEU:HD13	2.01	0.41
22:V:300:LEU:HD11	29:d:116:HIS:CE1	2.54	0.41
26:a:68:GLU:O	26:a:70:ARG:HG2	2.21	0.41
30:f:249:LEU:HG	30:f:250:ARG:H	1.86	0.41
30:f:616:CYS:HB3	30:f:632:LYS:HD3	2.01	0.41
12:l:49:LEU:HB2	12:l:195:LEU:HD21	2.01	0.41
15:o:181:ASN:OD1	15:o:181:ASN:N	2.53	0.41
20:t:92:LEU:HD12	20:t:92:LEU:HA	1.93	0.41
32:x:422:ALA:HB3	32:x:479:LEU:HD23	2.02	0.41
1:A:398:ARG:NH1	2:B:195:GLN:OE1	2.54	0.41
15:O:181:ASN:OD1	15:O:181:ASN:N	2.53	0.41
16:P:12:MET:HE3	16:P:171:MET:SD	2.60	0.41
17:Q:11:ASP:OD1	17:Q:11:ASP:N	2.54	0.41
21:U:819:VAL:HG22	21:U:821:LYS:H	1.86	0.41
30:f:456:ARG:NH2	30:f:491:GLY:H	2.19	0.41
30:f:866:GLN:HE21	30:f:888:LEU:HD12	1.85	0.41
32:x:146:MET:HB3	32:x:214:LYS:HD3	2.02	0.41
32:x:185:GLN:HG3	32:x:186:PHE:HD1	1.86	0.41
32:x:425:THR:OG1	32:x:439:TRP:NE1	2.40	0.41
34:W:186:ILE:HA	34:W:189:GLN:HG2	2.03	0.41
2:B:222:VAL:HG22	2:B:349:ARG:HB2	2.03	0.41
4:D:39:ASP:N	4:D:39:ASP:OD1	2.52	0.41
4:D:270:ILE:HD11	4:D:288:ILE:HD12	2.03	0.41
5:E:241:ARG:HD2	5:E:281:ARG:HE	1.86	0.41
6:F:332:THR:HG21	6:F:338:LEU:HD11	2.03	0.41
11:K:199:LEU:HD21	11:K:217:LEU:HD11	2.02	0.41
12:L:53:GLN:H	12:L:53:GLN:HG3	1.75	0.41
24:Y:67:VAL:O	24:Y:71:ASN:HB2	2.21	0.41
10:j:23:GLN:NE2	10:j:148:ASP:OD2	2.54	0.41
32:x:243:ILE:HA	32:x:247:PHE:HB2	2.03	0.41
1:A:287:ASP:OD1	1:A:287:ASP:N	2.54	0.41
1:A:307:ASP:HB3	1:A:336:ARG:HH11	1.86	0.41
4:D:244:PRO:HA	4:D:247:VAL:HG12	2.02	0.41
6:F:79:LYS:HA	6:F:82:VAL:HG12	2.03	0.41
7:G:112:ASP:HB3	7:G:152:TYR:CZ	2.55	0.41
8:H:135:LEU:HG	8:H:163:MET:HE2	2.02	0.41
9:I:35:LEU:HD11	9:I:175:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:226:ASP:OD1	12:L:226:ASP:N	2.52	0.41
21:U:92:ASP:OD1	21:U:92:ASP:N	2.51	0.41
21:U:351:MET:HA	21:U:354:LYS:HG2	2.03	0.41
21:U:361:ARG:HH22	21:U:727:LYS:HE2	1.86	0.41
21:U:870:GLU:HA	21:U:875:PHE:HB3	2.02	0.41
22:V:98:LEU:HD22	22:V:209:LYS:HD2	2.02	0.41
22:V:131:LEU:HD13	22:V:171:VAL:HG21	2.03	0.41
27:b:97:LEU:HD23	27:b:97:LEU:HA	1.88	0.41
28:c:104:ARG:HD3	28:c:104:ARG:H	1.86	0.41
29:d:28:LEU:O	29:d:32:GLU:HB2	2.21	0.41
30:f:107:LYS:HD3	30:f:141:LYS:HE2	2.03	0.41
30:f:287:ASP:HA	30:f:290:VAL:HG22	2.02	0.41
11:k:20:ARG:HA	11:k:20:ARG:HD3	1.82	0.41
16:p:58:THR:HG22	17:q:123:ALA:HB2	2.03	0.41
18:r:37:ILE:HD13	18:r:59:LEU:HD22	2.03	0.41
19:s:83:MET:HG2	19:s:88:ILE:HG13	2.03	0.41
1:A:97:ARG:HH22	1:A:117:GLN:HE22	1.68	0.41
2:B:44:ASP:OD1	2:B:44:ASP:N	2.53	0.41
2:B:401:GLU:O	2:B:405:MET:HG2	2.21	0.41
4:D:110:ASN:OD1	4:D:110:ASN:N	2.53	0.41
5:E:194:ASN:OD1	5:E:195:PHE:N	2.50	0.41
8:H:74:LEU:HD11	8:H:134:LEU:HD22	2.02	0.41
17:Q:167:LEU:HD23	17:Q:167:LEU:HA	1.96	0.41
19:S:212:LYS:HE2	19:S:212:LYS:HB3	1.86	0.41
20:T:92:LEU:HD12	20:T:112:ILE:HD11	2.02	0.41
21:U:254:GLU:OE2	21:U:751:ARG:NH1	2.54	0.41
21:U:802:TYR:HE2	21:U:880:ASN:HA	1.86	0.41
21:U:902:PRO:HA	21:U:914:LEU:HD22	2.02	0.41
23:X:115:GLU:HA	23:X:118:LYS:HE3	2.03	0.41
28:c:54:MET:HG3	28:c:82:VAL:HG13	2.02	0.41
29:d:231:LYS:HE2	29:d:231:LYS:HB2	1.89	0.41
8:h:39:LYS:NZ	9:i:57:ASP:OD2	2.51	0.41
2:B:81:ASN:CG	21:U:828:VAL:HG11	2.46	0.40
3:C:219:LEU:HD23	3:C:230:MET:HE2	2.03	0.40
4:D:272:THR:OG1	4:D:273:LYS:N	2.51	0.40
5:E:168:LYS:HD3	5:E:294:ARG:HA	2.04	0.40
6:F:141:ASP:OD1	6:F:141:ASP:N	2.51	0.40
8:H:195:LEU:HD12	8:H:195:LEU:HA	1.89	0.40
9:I:67:LYS:HA	9:I:73:ALA:HA	2.03	0.40
17:Q:5:ILE:HD11	17:Q:143:LEU:HD11	2.03	0.40
27:b:10:VAL:HG12	27:b:33:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:177:ARG:HD3	8:h:177:ARG:HA	1.84	0.40
10:j:41:VAL:HG11	10:j:134:VAL:HB	2.04	0.40
20:t:99:ARG:HA	20:t:99:ARG:HD2	1.91	0.40
32:x:33:LEU:HA	32:x:36:LEU:HD12	2.03	0.40
32:x:115:TYR:CZ	32:x:116:MET:HE1	2.56	0.40
32:x:186:PHE:HA	32:x:198:GLN:HE22	1.85	0.40
35:e:16:ASP:N	35:e:16:ASP:OD1	2.53	0.40
2:B:404:LEU:HA	2:B:404:LEU:HD23	1.87	0.40
3:C:103:ILE:HD13	3:C:123:LEU:HD22	2.03	0.40
14:N:35:THR:HA	14:N:36:PRO:HD3	1.96	0.40
20:T:92:LEU:HD23	20:T:92:LEU:HA	1.90	0.40
21:U:401:LYS:HB3	21:U:438:GLN:HG2	2.02	0.40
21:U:793:LYS:HB2	21:U:796:LYS:HB2	2.02	0.40
22:V:182:LYS:HE2	22:V:182:LYS:HB2	1.92	0.40
23:X:355:LYS:HE2	23:X:355:LYS:HB2	1.90	0.40
30:f:629:LYS:HE3	30:f:629:LYS:HB2	1.93	0.40
11:k:209:LYS:HD3	11:k:209:LYS:HA	1.93	0.40
18:r:58:LEU:HD23	18:r:58:LEU:HA	1.96	0.40
20:t:106:LEU:HD23	20:t:106:LEU:HA	1.93	0.40
4:D:97:ASP:OD1	4:D:100:THR:OG1	2.39	0.40
4:D:384:MET:HA	4:D:387:VAL:HG12	2.03	0.40
6:F:361:ALA:O	6:F:365:ILE:HG12	2.22	0.40
19:S:33:PHE:HD1	15:o:167:LEU:HB2	1.86	0.40
23:X:292:GLN:HA	23:X:295:LYS:HG2	2.03	0.40
24:Y:39:ASP:HA	24:Y:42:MET:HB2	2.03	0.40
25:Z:190:ARG:HA	25:Z:190:ARG:HD2	1.91	0.40
11:k:90:ASP:OD1	18:r:69:ARG:NH1	2.54	0.40
12:l:157:ARG:HD2	12:l:176:MET:HE2	2.03	0.40
15:o:87:LEU:HD23	15:o:87:LEU:HA	1.90	0.40
15:o:106:THR:OG1	15:o:109:HIS:NE2	2.42	0.40
34:W:140:ILE:HD12	34:W:140:ILE:HA	1.97	0.40
1:A:422:LYS:HE2	1:A:422:LYS:HB2	1.97	0.40
5:E:102:MET:HE2	5:E:102:MET:HB2	1.96	0.40
5:E:280:ASN:OD1	5:E:280:ASN:N	2.53	0.40
9:I:118:LYS:O	9:I:122:THR:HG23	2.20	0.40
15:O:59:ILE:HD13	15:O:59:ILE:HA	1.90	0.40
25:Z:43:TRP:HE3	25:Z:48:LEU:HB2	1.87	0.40
26:a:163:TYR:HA	26:a:168:ASN:HB3	2.04	0.40
30:f:791:VAL:HG13	30:f:800:LEU:HD11	2.02	0.40
18:r:177:TYR:CZ	18:r:186:ARG:HG3	2.56	0.40
33:y:23:ILE:HD12	33:y:23:ILE:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:W:359:VAL:HG13	34:W:382:LEU:HD13	2.02	0.40
5:E:122:MET:HA	5:E:197:LYS:HB3	2.01	0.40
6:F:79:LYS:HA	6:F:79:LYS:HD3	1.82	0.40
6:F:276:LYS:HE3	6:F:276:LYS:HB3	1.88	0.40
21:U:155:LEU:O	21:U:158:ARG:NH1	2.54	0.40
23:X:130:GLU:HG2	23:X:153:LEU:HD22	2.04	0.40
24:Y:385:ARG:HD2	24:Y:385:ARG:HA	1.93	0.40
26:a:335:TRP:NE1	26:a:337:GLN:O	2.55	0.40
28:c:209:LYS:HE2	28:c:214:GLN:HB3	2.02	0.40
30:f:301:HIS:CE1	30:f:456:ARG:HD3	2.57	0.40
13:m:23:VAL:HG12	13:m:27:MET:HE2	2.03	0.40
32:x:198:GLN:HA	33:y:74:ARG:HE	1.86	0.40
32:x:222:SER:OG	32:x:410:ILE:O	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/433 (95%)	372 (90%)	38 (9%)	1 (0%)	43	73
2	B	409/440 (93%)	365 (89%)	44 (11%)	0	100	100
3	C	394/398 (99%)	353 (90%)	40 (10%)	1 (0%)	36	68
4	D	378/418 (90%)	323 (85%)	53 (14%)	2 (0%)	24	59
5	E	387/403 (96%)	344 (89%)	42 (11%)	1 (0%)	36	68
6	F	391/439 (89%)	352 (90%)	35 (9%)	4 (1%)	12	45
7	G	238/246 (97%)	225 (94%)	13 (6%)	0	100	100
7	g	242/246 (98%)	232 (96%)	10 (4%)	0	100	100
8	H	230/234 (98%)	217 (94%)	13 (6%)	0	100	100
8	h	230/234 (98%)	219 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	246/261 (94%)	232 (94%)	11 (4%)	3 (1%)	10	42
9	i	248/261 (95%)	241 (97%)	7 (3%)	0	100	100
10	J	237/248 (96%)	224 (94%)	13 (6%)	0	100	100
10	j	237/248 (96%)	230 (97%)	7 (3%)	0	100	100
11	K	236/241 (98%)	225 (95%)	11 (5%)	0	100	100
11	k	232/241 (96%)	223 (96%)	9 (4%)	0	100	100
12	L	238/269 (88%)	229 (96%)	9 (4%)	0	100	100
12	l	236/269 (88%)	229 (97%)	7 (3%)	0	100	100
13	M	240/255 (94%)	231 (96%)	9 (4%)	0	100	100
13	m	238/255 (93%)	235 (99%)	3 (1%)	0	100	100
14	N	201/239 (84%)	196 (98%)	5 (2%)	0	100	100
14	n	200/239 (84%)	196 (98%)	4 (2%)	0	100	100
15	O	218/277 (79%)	212 (97%)	6 (3%)	0	100	100
15	o	218/277 (79%)	211 (97%)	7 (3%)	0	100	100
16	P	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
16	p	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
17	Q	197/201 (98%)	190 (96%)	7 (4%)	0	100	100
17	q	197/201 (98%)	188 (95%)	9 (5%)	0	100	100
18	R	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
18	r	199/263 (76%)	192 (96%)	7 (4%)	0	100	100
19	S	211/241 (88%)	203 (96%)	8 (4%)	0	100	100
19	s	211/241 (88%)	206 (98%)	5 (2%)	0	100	100
20	T	214/264 (81%)	210 (98%)	4 (2%)	0	100	100
20	t	214/264 (81%)	206 (96%)	8 (4%)	0	100	100
21	U	868/953 (91%)	807 (93%)	61 (7%)	0	100	100
22	V	442/534 (83%)	427 (97%)	15 (3%)	0	100	100
23	X	378/422 (90%)	358 (95%)	19 (5%)	1 (0%)	36	68
24	Y	376/389 (97%)	341 (91%)	34 (9%)	1 (0%)	36	68
25	Z	284/324 (88%)	247 (87%)	36 (13%)	1 (0%)	30	62
26	a	371/376 (99%)	335 (90%)	36 (10%)	0	100	100
27	b	189/377 (50%)	170 (90%)	19 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	c	285/310 (92%)	248 (87%)	36 (13%)	1 (0%)	30	62
29	d	255/350 (73%)	212 (83%)	43 (17%)	0	100	100
30	f	887/908 (98%)	770 (87%)	116 (13%)	1 (0%)	48	79
32	x	492/494 (100%)	463 (94%)	29 (6%)	0	100	100
33	y	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
34	W	444/456 (97%)	413 (93%)	28 (6%)	3 (1%)	18	52
35	e	48/70 (69%)	40 (83%)	8 (17%)	0	100	100
All	All	13974/15458 (90%)	12996 (93%)	958 (7%)	20 (0%)	49	79

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	90	HIS
6	F	72	LYS
6	F	73	ILE
6	F	86	LEU
9	I	54	LYS
23	X	318	ILE
28	c	285	GLU
34	W	140	ILE
30	f	23	GLY
1	A	145	ASN
4	D	159	LYS
6	F	344	ARG
9	I	63	GLU
34	W	118	LEU
34	W	119	PRO
5	E	166	PRO
25	Z	145	HIS
9	I	52	ILE
24	Y	205	VAL
4	D	160	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	354/372 (95%)	353 (100%)	1 (0%)	86	88
2	B	357/385 (93%)	357 (100%)	0	100	100
3	C	340/346 (98%)	340 (100%)	0	100	100
4	D	333/366 (91%)	333 (100%)	0	100	100
5	E	341/353 (97%)	341 (100%)	0	100	100
6	F	340/379 (90%)	336 (99%)	4 (1%)	63	79
7	G	202/210 (96%)	202 (100%)	0	100	100
7	g	201/210 (96%)	197 (98%)	4 (2%)	48	72
8	H	187/191 (98%)	187 (100%)	0	100	100
8	h	188/191 (98%)	188 (100%)	0	100	100
9	I	202/221 (91%)	199 (98%)	3 (2%)	57	76
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	197/211 (93%)	197 (100%)	0	100	100
10	j	196/211 (93%)	196 (100%)	0	100	100
11	K	197/203 (97%)	197 (100%)	0	100	100
11	k	195/203 (96%)	195 (100%)	0	100	100
12	L	202/230 (88%)	202 (100%)	0	100	100
12	l	201/230 (87%)	200 (100%)	1 (0%)	81	85
13	M	198/212 (93%)	198 (100%)	0	100	100
13	m	198/212 (93%)	198 (100%)	0	100	100
14	N	158/181 (87%)	158 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	178/228 (78%)	178 (100%)	0	100	100
15	o	181/228 (79%)	181 (100%)	0	100	100
16	P	172/174 (99%)	172 (100%)	0	100	100
16	p	173/174 (99%)	173 (100%)	0	100	100
17	Q	168/171 (98%)	168 (100%)	0	100	100
17	q	166/171 (97%)	166 (100%)	0	100	100
18	R	156/202 (77%)	156 (100%)	0	100	100
18	r	154/202 (76%)	154 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	s	177/199 (89%)	176 (99%)	1 (1%)	78	84
20	T	178/215 (83%)	178 (100%)	0	100	100
20	t	179/215 (83%)	179 (100%)	0	100	100
21	U	748/816 (92%)	748 (100%)	0	100	100
22	V	390/460 (85%)	390 (100%)	0	100	100
23	X	327/362 (90%)	327 (100%)	0	100	100
24	Y	334/344 (97%)	332 (99%)	2 (1%)	78	84
25	Z	257/295 (87%)	251 (98%)	6 (2%)	44	70
26	a	333/336 (99%)	333 (100%)	0	100	100
27	b	167/312 (54%)	167 (100%)	0	100	100
28	c	252/268 (94%)	252 (100%)	0	100	100
29	d	231/294 (79%)	231 (100%)	0	100	100
30	f	745/763 (98%)	742 (100%)	3 (0%)	84	86
32	x	439/439 (100%)	439 (100%)	0	100	100
33	y	68/68 (100%)	68 (100%)	0	100	100
34	W	410/416 (99%)	406 (99%)	4 (1%)	68	80
35	e	44/63 (70%)	44 (100%)	0	100	100
All	All	11951/13133 (91%)	11922 (100%)	29 (0%)	85	89

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ILE
6	F	175	MET
6	F	353	GLU
6	F	356	MET
6	F	416	THR
9	I	50	ARG
9	I	52	ILE
9	I	54	LYS
24	Y	204	THR
24	Y	205	VAL
25	Z	144	VAL
25	Z	146	ASP
25	Z	147	ASP
25	Z	149	THR

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Mol	Chain	Res	Type
25	Z	161	GLU
25	Z	165	GLU
30	f	24	THR
30	f	25	ASP
30	f	27	LYS
7	g	130	GLU
7	g	131	MET
7	g	134	LEU
7	g	224	ASN
12	l	148	CYS
19	s	146	GLN
34	W	115	ILE
34	W	117	ASP
34	W	118	LEU
34	W	120	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
2	B	207	HIS
2	B	241	ASN
2	B	368	HIS
3	C	102	ASN
3	C	205	HIS
3	C	270	GLN
4	D	187	HIS
4	D	237	GLN
5	E	307	GLN
5	E	339	ASN
6	F	76	ASN
6	F	243	GLN
6	F	369	HIS
7	G	68	HIS
7	G	75	ASN
9	I	40	ASN
9	I	84	ASN
10	J	85	ASN
10	J	239	ASN
11	K	122	GLN
11	K	211	ASN
11	K	227	HIS

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Mol	Chain	Res	Type
14	N	154	GLN
14	N	193	GLN
15	O	91	GLN
16	P	65	GLN
16	P	93	ASN
16	P	169	GLN
17	Q	27	GLN
17	Q	82	ASN
17	Q	132	HIS
19	S	36	HIS
19	S	131	GLN
19	S	152	GLN
20	T	147	GLN
20	T	213	HIS
21	U	149	GLN
21	U	195	ASN
21	U	227	GLN
21	U	718	ASN
21	U	721	HIS
21	U	743	ASN
23	X	170	GLN
23	X	367	GLN
24	Y	48	ASN
24	Y	184	GLN
24	Y	280	GLN
24	Y	351	ASN
25	Z	145	HIS
25	Z	202	ASN
25	Z	256	GLN
25	Z	274	ASN
26	a	164	GLN
26	a	193	GLN
26	a	273	GLN
26	a	344	GLN
26	a	345	GLN
27	b	48	ASN
28	c	219	ASN
28	c	256	ASN
28	c	298	GLN
30	f	195	ASN
30	f	291	GLN
30	f	565	ASN

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Mol	Chain	Res	Type
30	f	605	ASN
30	f	614	HIS
30	f	737	ASN
7	g	53	GLN
7	g	68	HIS
7	g	75	ASN
7	g	127	GLN
7	g	128	ASN
8	h	88	HIS
8	h	109	GLN
9	i	20	GLN
9	i	40	ASN
9	i	146	GLN
9	i	198	ASN
10	j	68	ASN
10	j	154	HIS
10	j	215	GLN
11	k	152	GLN
11	k	214	ASN
12	l	43	HIS
12	l	90	GLN
14	n	123	GLN
14	n	193	GLN
15	o	193	ASN
16	p	7	ASN
16	p	65	GLN
17	q	24	ASN
17	q	27	GLN
17	q	61	GLN
17	q	101	ASN
17	q	174	ASN
18	r	162	GLN
19	s	108	ASN
20	t	147	GLN
32	x	112	ASN
32	x	197	GLN
32	x	306	GLN
32	x	413	ASN
34	W	41	GLN
34	W	232	GLN
34	W	257	GLN
34	W	399	ASN

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Mol	Chain	Res	Type
34	W	456	GLN
35	e	63	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	ADP	D	501	-	28,29,29	1.38	5 (17%)	43,45,45	1.84	8 (18%)
36	ATP	F	501	37	32,33,33	0.63	2 (6%)	48,52,52	0.34	0
36	ATP	B	501	37	32,33,33	0.98	2 (6%)	48,52,52	0.41	0
36	ATP	A	501	37	32,33,33	0.56	0	48,52,52	0.39	0
36	ATP	C	501	37	32,33,33	0.68	2 (6%)	48,52,52	0.33	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
38	ADP	D	501	-	-	3/16/32/32	0/3/3/3
36	ATP	F	501	37	-	5/22/38/38	0/3/3/3
36	ATP	B	501	37	-	2/22/38/38	0/3/3/3
36	ATP	A	501	37	-	6/22/38/38	0/3/3/3
36	ATP	C	501	37	-	0/22/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	D	501	ADP	C5-C4	4.48	1.47	1.39
36	B	501	ATP	PA-O3A	-4.10	1.55	1.59
36	B	501	ATP	PB-O3B	-3.22	1.56	1.59
38	D	501	ADP	C5-N7	-2.58	1.34	1.39
36	C	501	ATP	PB-O3B	-2.48	1.56	1.59
38	D	501	ADP	C5-C6	2.42	1.47	1.41
38	D	501	ADP	C8-N7	2.29	1.36	1.31
36	F	501	ATP	PA-O3A	-2.27	1.57	1.59
36	C	501	ATP	PA-O3A	-2.20	1.57	1.59
38	D	501	ADP	C4-N9	-2.20	1.33	1.37
36	F	501	ATP	PB-O3B	-2.08	1.57	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	D	501	ADP	C5-C4-N3	-5.95	118.53	126.72
38	D	501	ADP	N3-C4-N9	4.64	135.06	127.17
38	D	501	ADP	C2-N3-C4	3.71	120.88	111.83
38	D	501	ADP	C4-C5-N7	-3.30	106.81	110.58
38	D	501	ADP	N3-C2-N1	-3.24	123.67	128.58
38	D	501	ADP	C3'-C2'-C1'	2.63	106.44	101.46
38	D	501	ADP	C4-N9-C8	2.58	108.44	105.74
38	D	501	ADP	C5-N7-C8	2.35	107.14	103.45

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	A	501	ATP	PB-O3B-PG-O2G
36	B	501	ATP	C5'-O5'-PA-O2A
36	B	501	ATP	C5'-O5'-PA-O3A
36	F	501	ATP	C5'-O5'-PA-O2A

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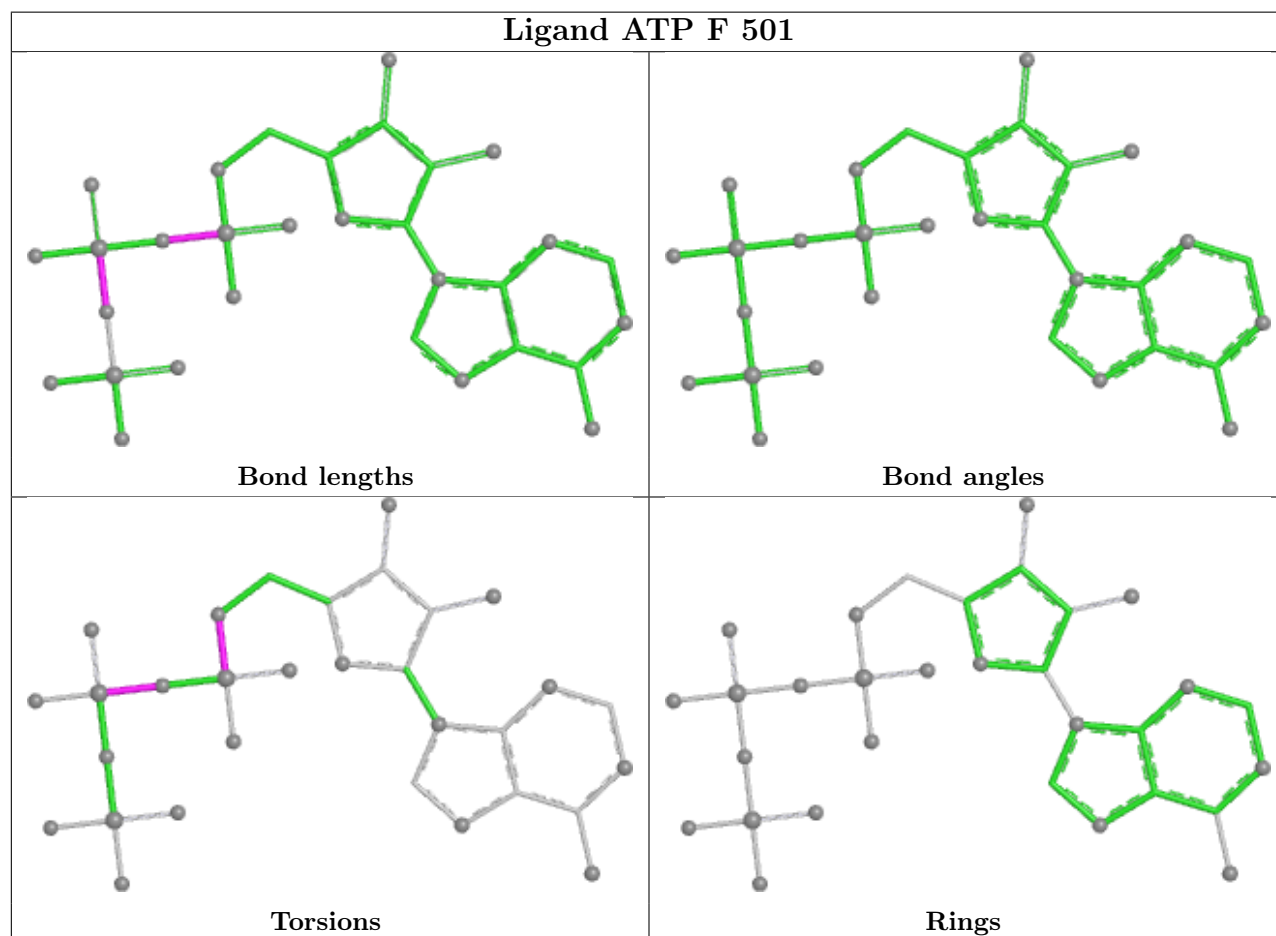
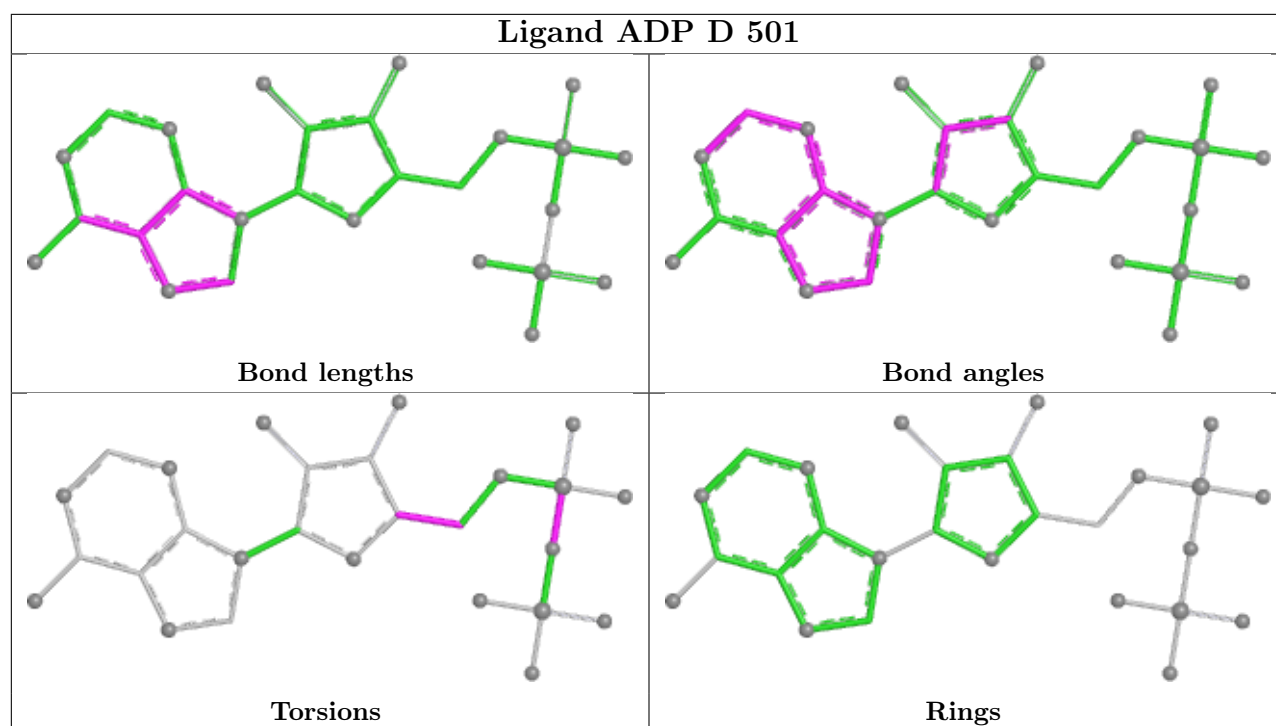
Mol	Chain	Res	Type	Atoms
36	A	501	ATP	C3'-C4'-C5'-O5'
36	A	501	ATP	O4'-C4'-C5'-O5'
38	D	501	ADP	O4'-C4'-C5'-O5'
36	A	501	ATP	PB-O3B-PG-O1G
38	D	501	ADP	C3'-C4'-C5'-O5'
36	F	501	ATP	PA-O3A-PB-O1B
36	F	501	ATP	C5'-O5'-PA-O1A
36	F	501	ATP	C5'-O5'-PA-O3A
36	A	501	ATP	C4'-C5'-O5'-PA
38	D	501	ADP	PB-O3A-PA-O2A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

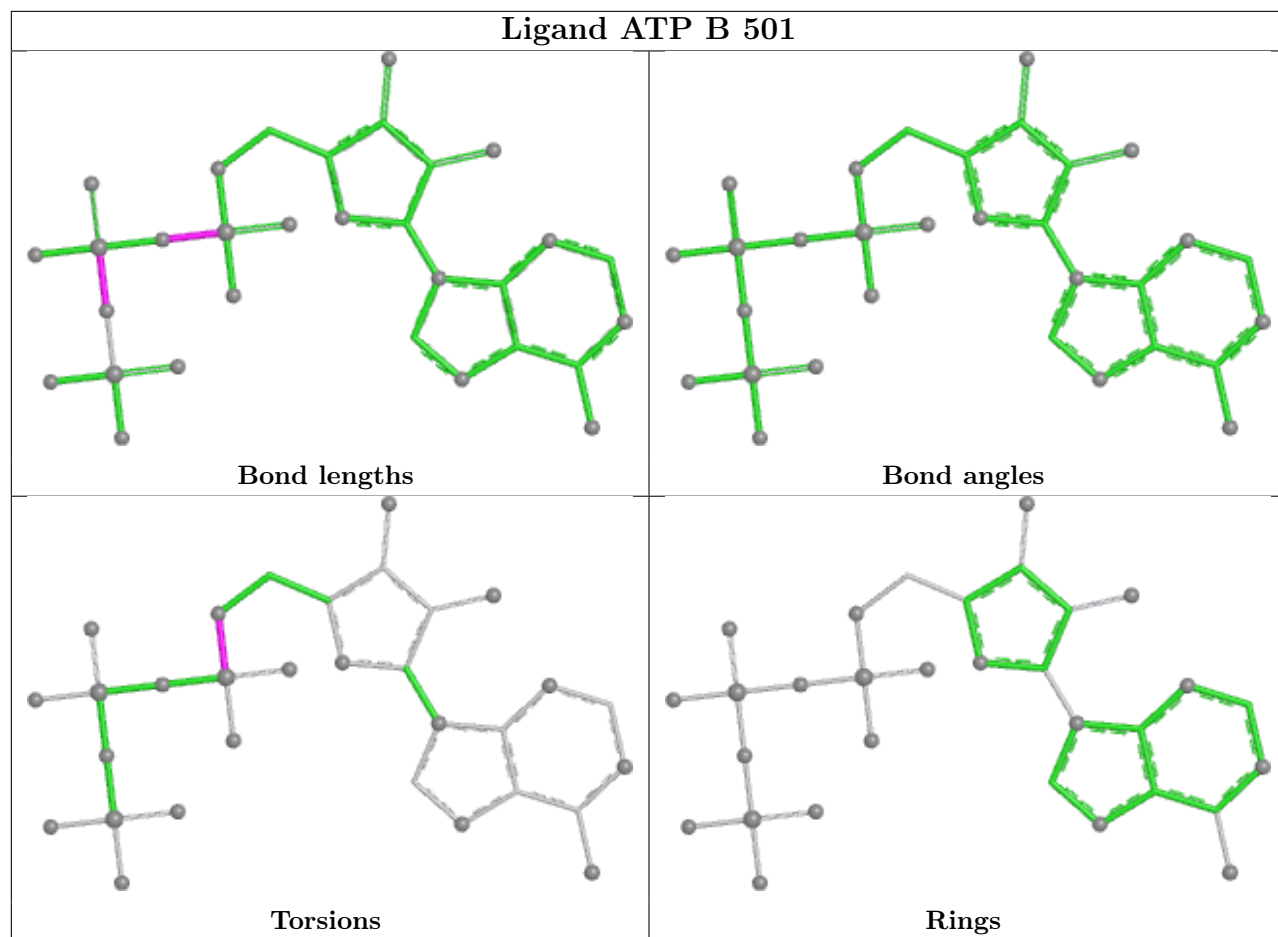
There are no ring outliers.

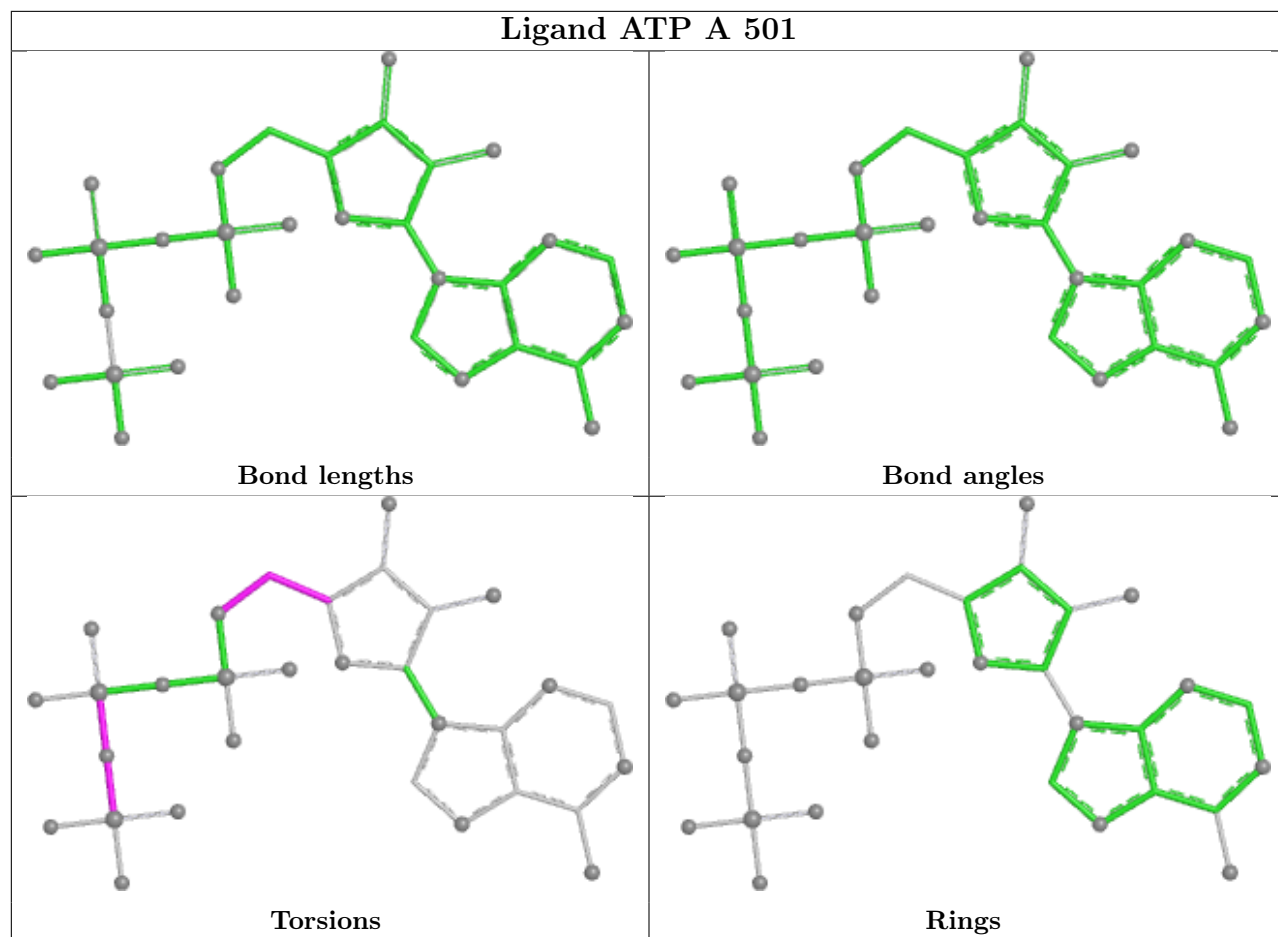
5 monomers are involved in 8 short contacts:

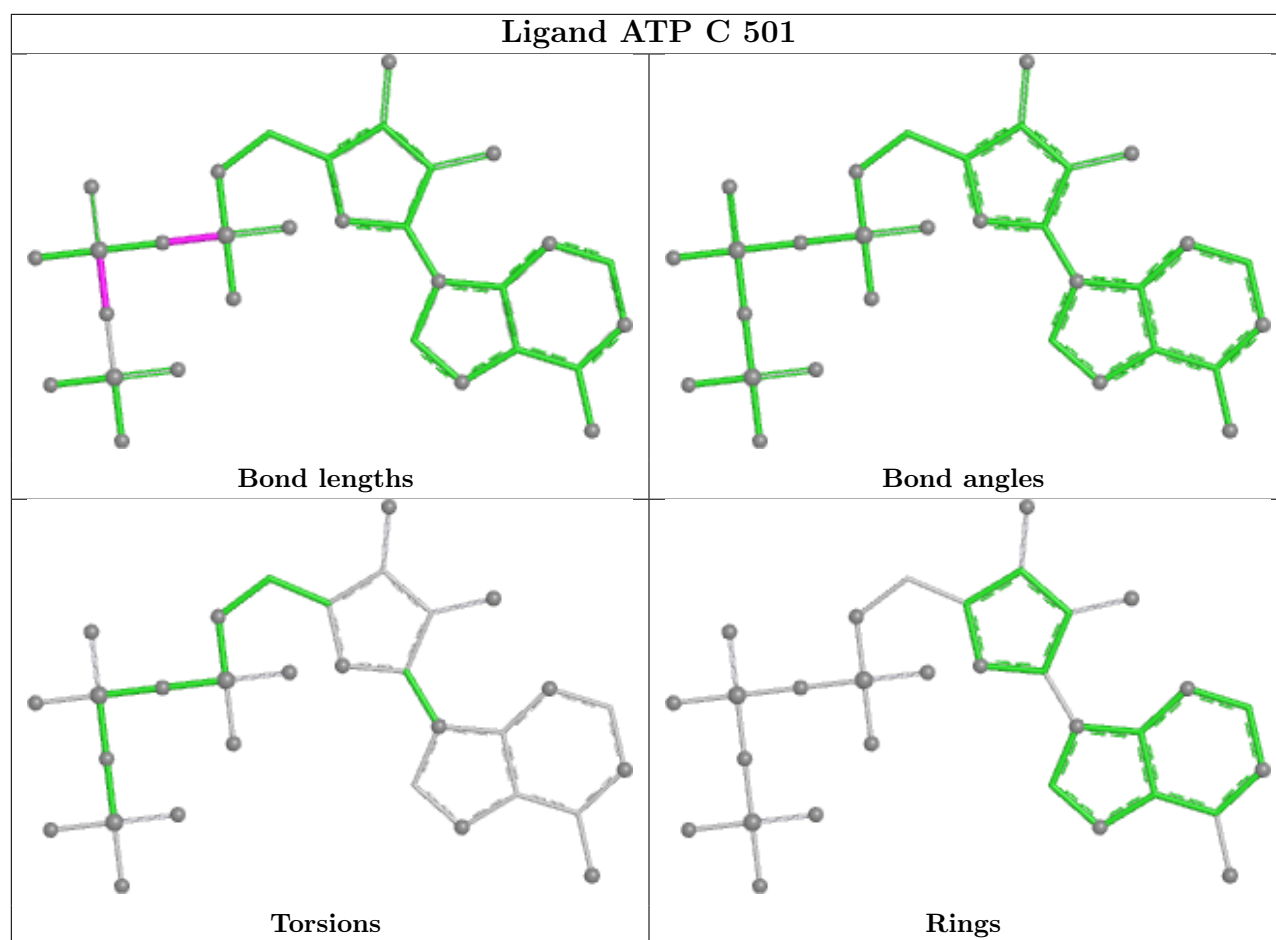
Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	D	501	ADP	1	0
36	F	501	ATP	1	0
36	B	501	ATP	3	0
36	A	501	ATP	1	0
36	C	501	ATP	2	0

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.









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.

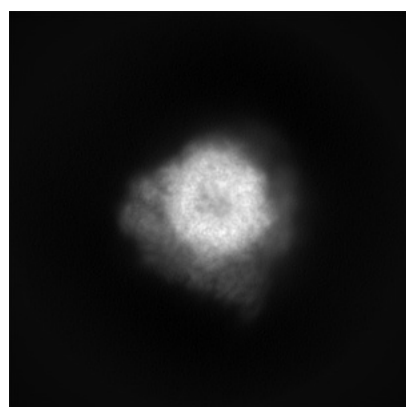
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32280. These allow visual inspection of the internal detail of the map and identification of artifacts.

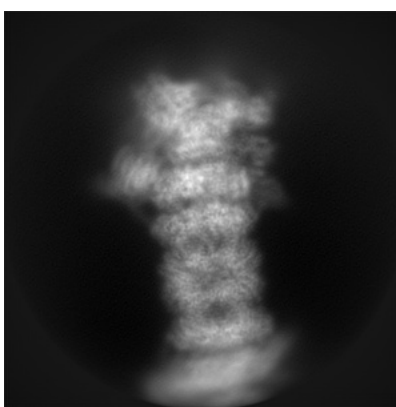
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

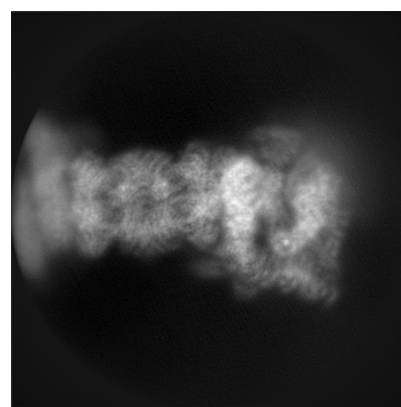
6.1.1 Primary map



X



Y

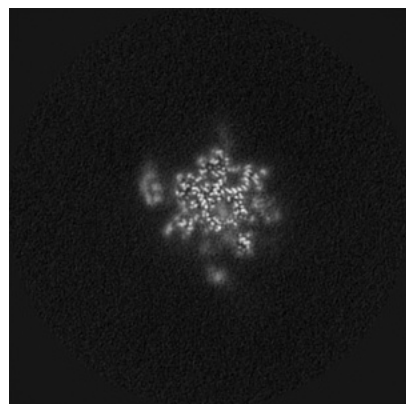


Z

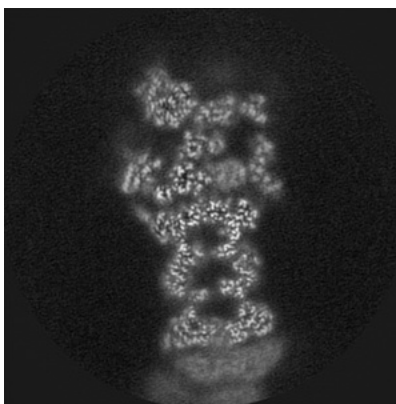
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

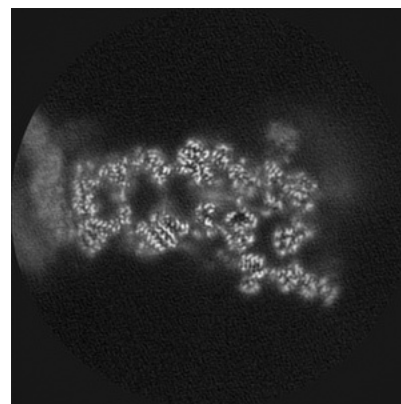
6.2.1 Primary map



X Index: 320



Y Index: 320

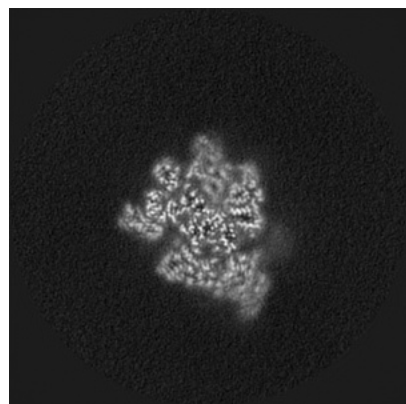


Z Index: 320

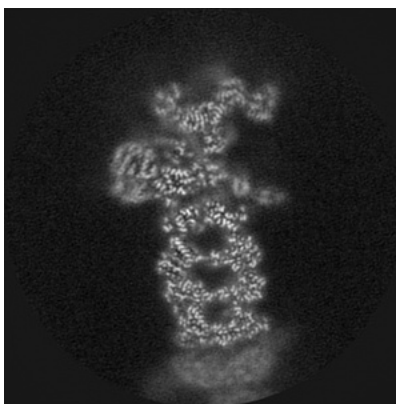
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

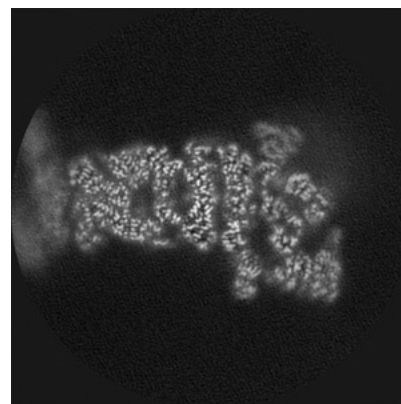
6.3.1 Primary map



X Index: 371



Y Index: 357

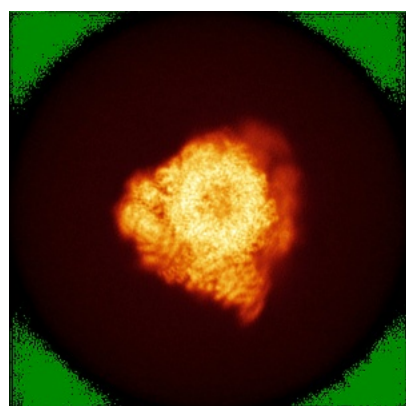


Z Index: 300

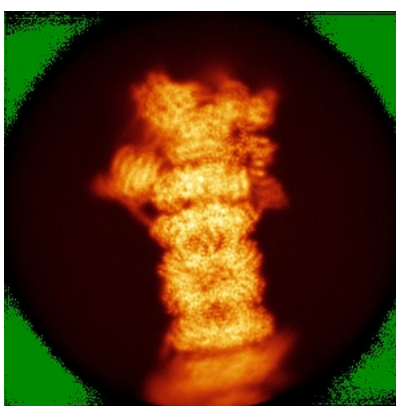
The images above show the largest variance slices of the map in three orthogonal directions.

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

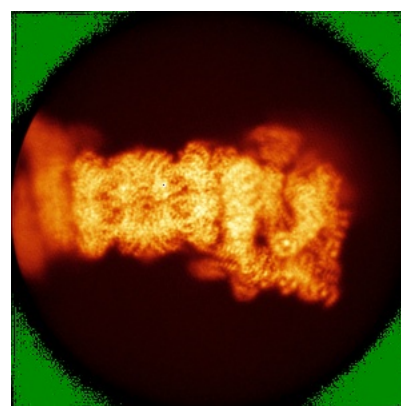
6.4.1 Primary map



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

This section was not generated.

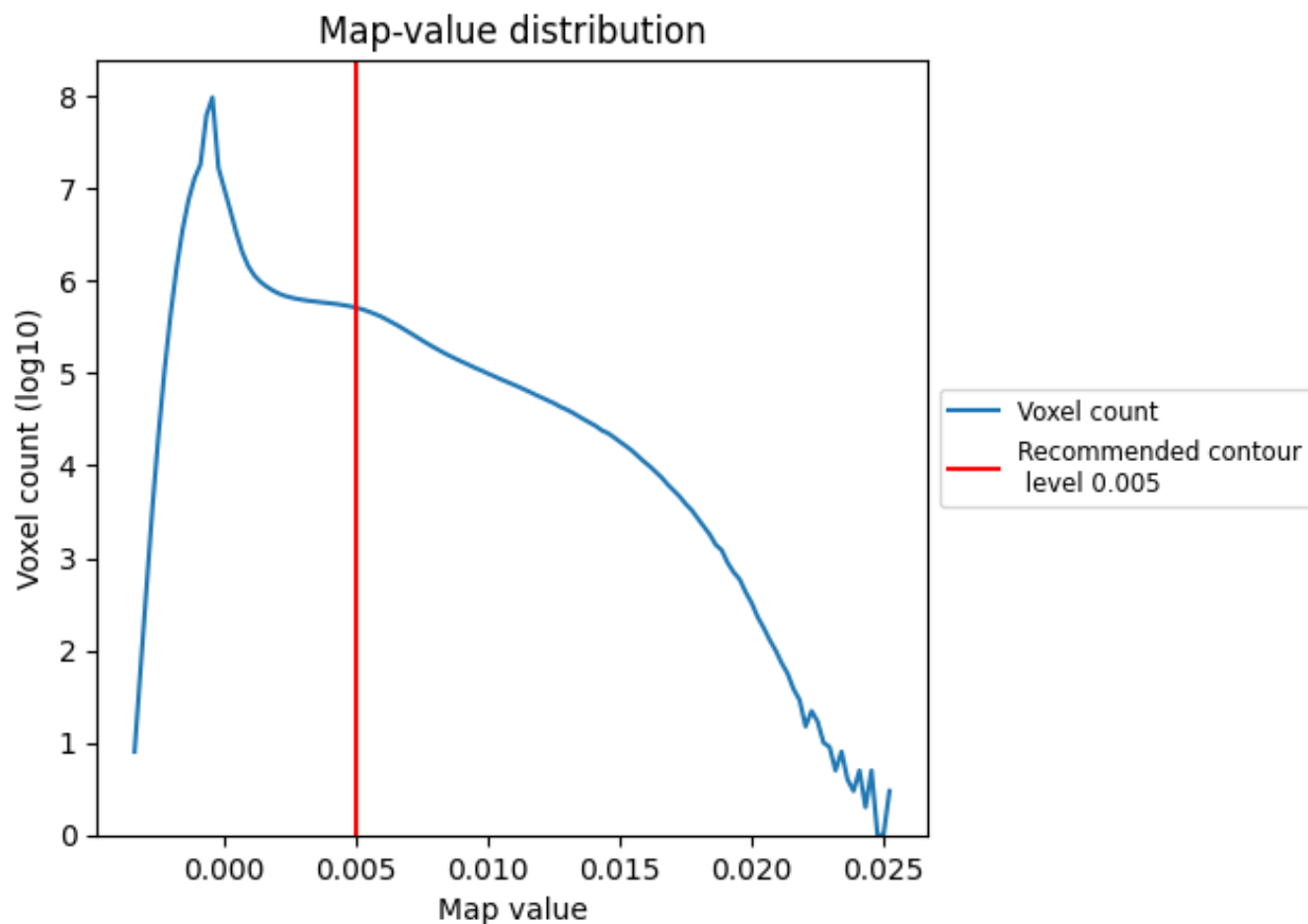
6.6 Mask visualisation

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

7 Map analysis [i](#)

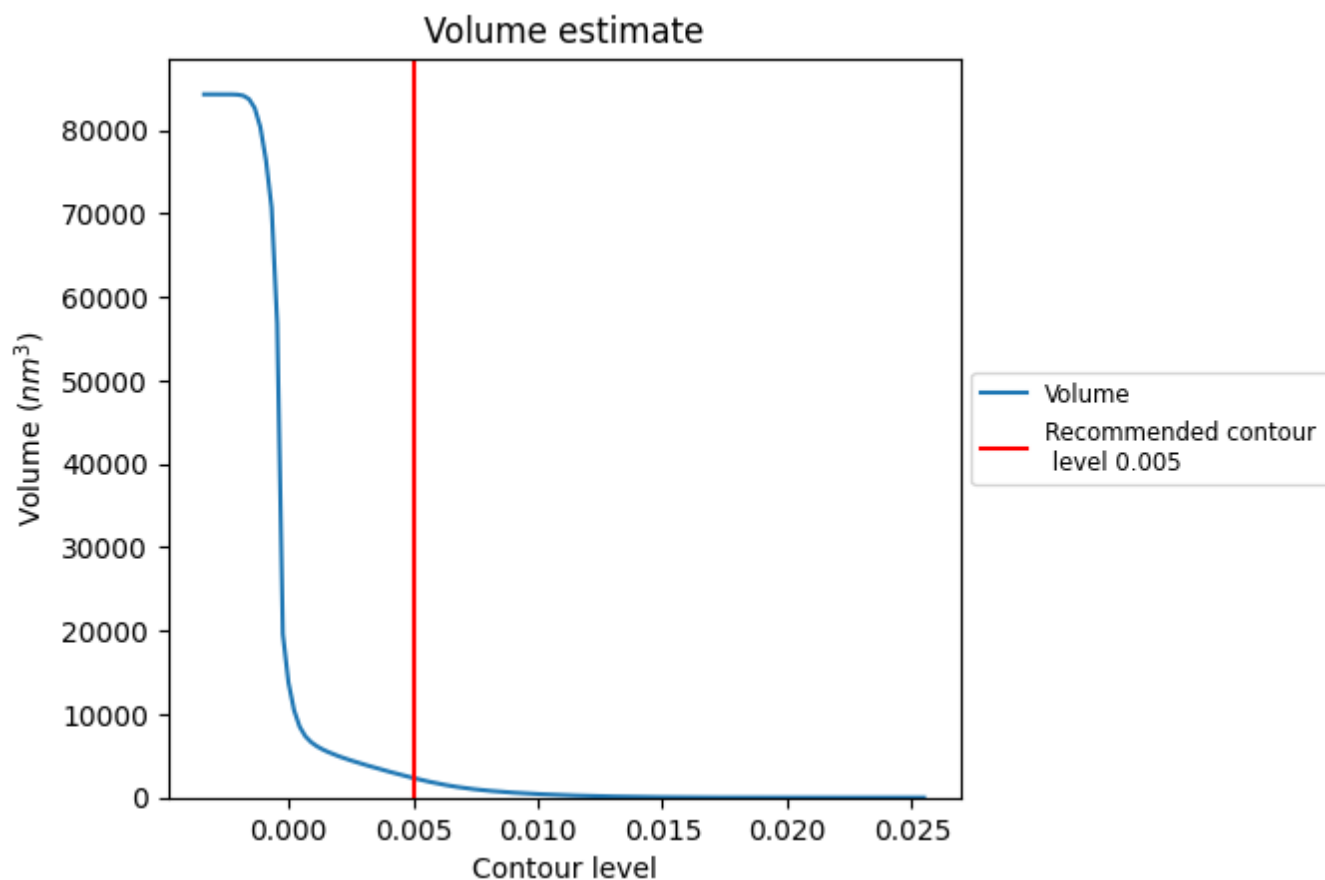
This section contains the results of statistical analysis of the map.

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.

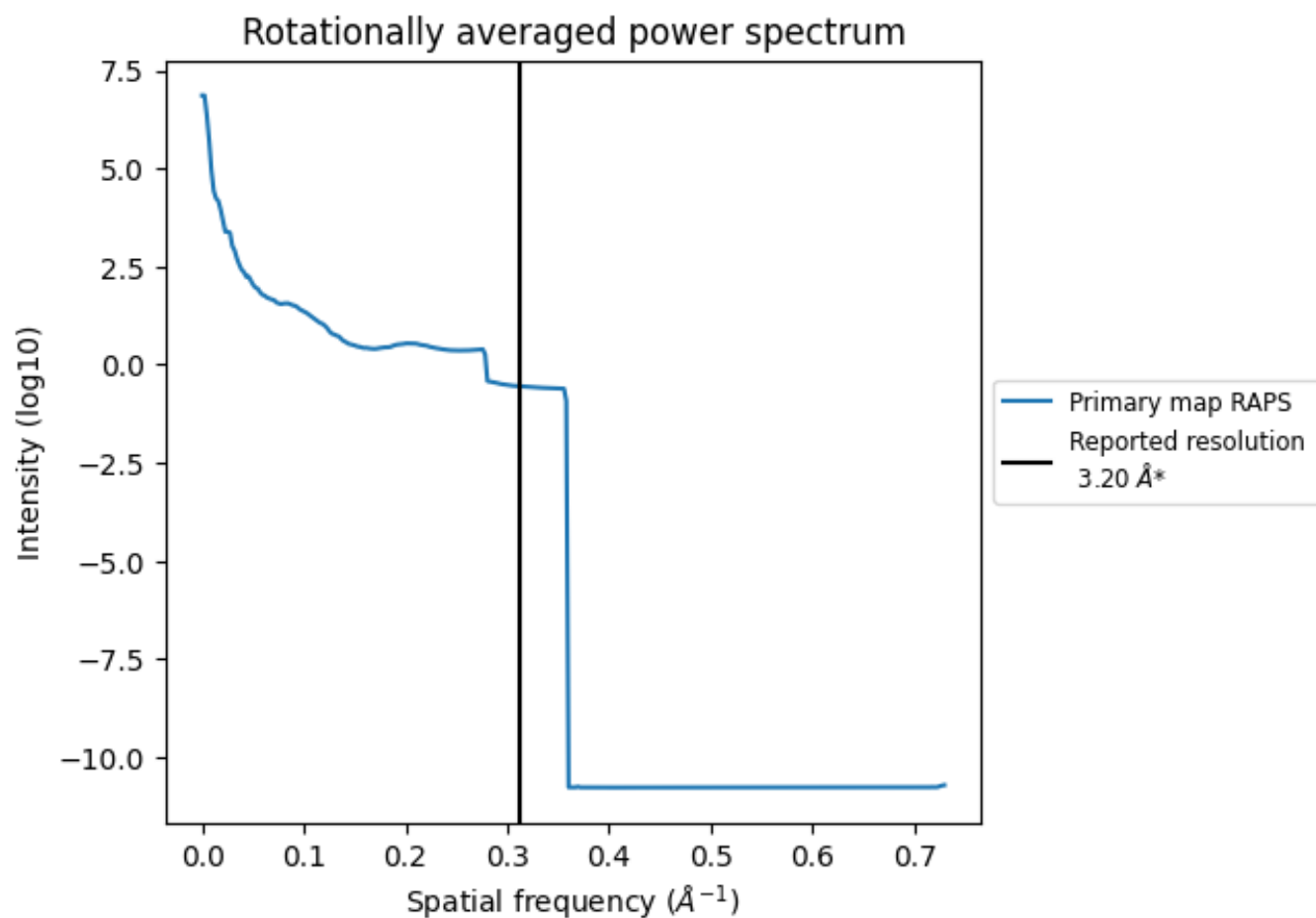
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2352 nm³; this corresponds to an approximate mass of 2124 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

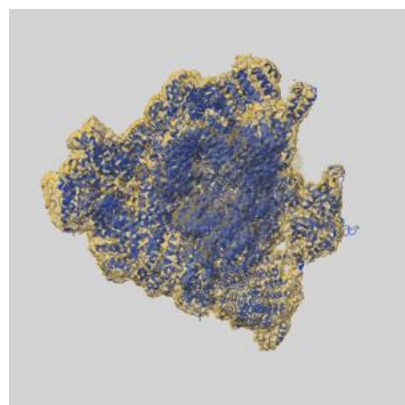
8 Fourier-Shell correlation ⓘ

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

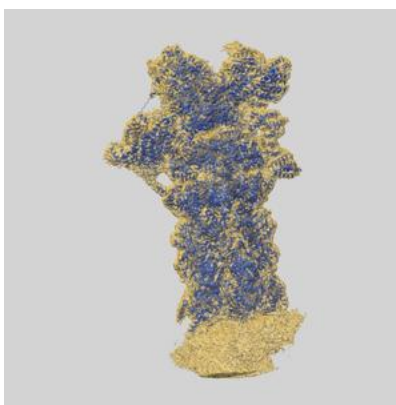
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32280 and PDB model 7W3H. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

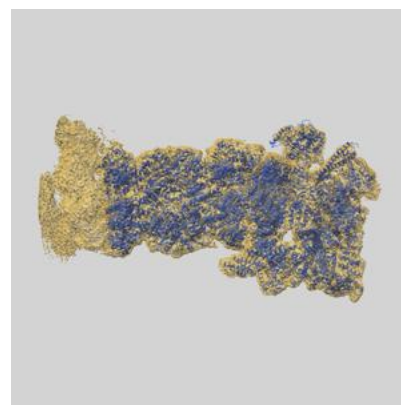
9.1 Map-model overlay [i](#)



X



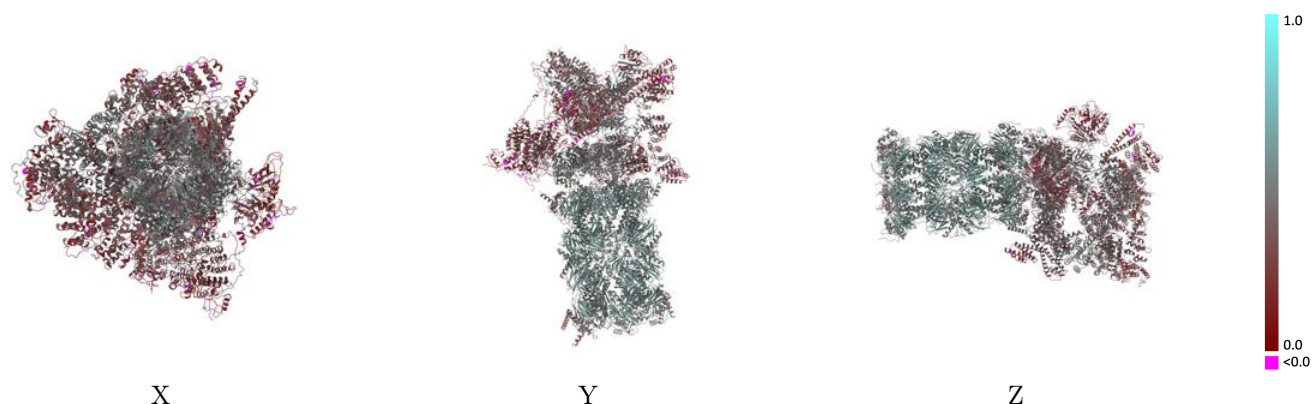
Y



Z

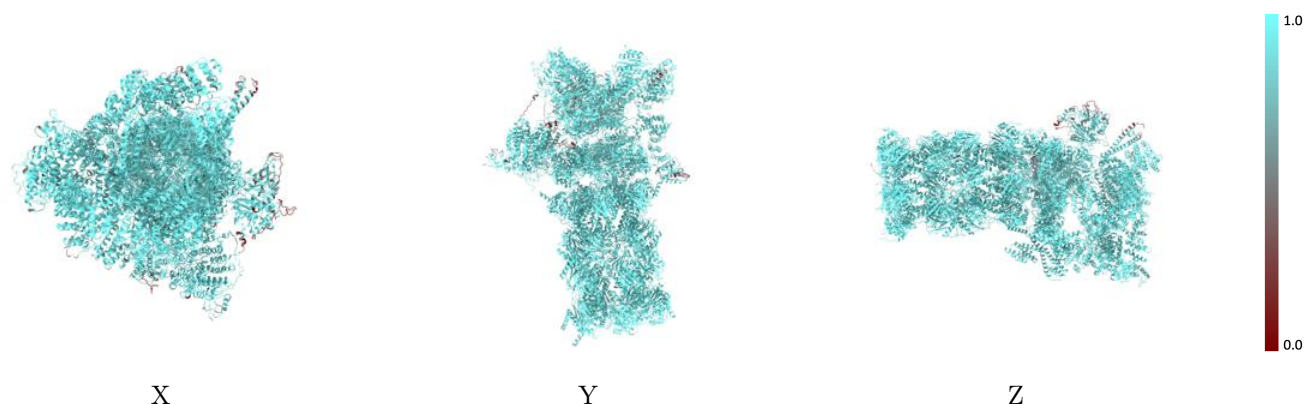
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



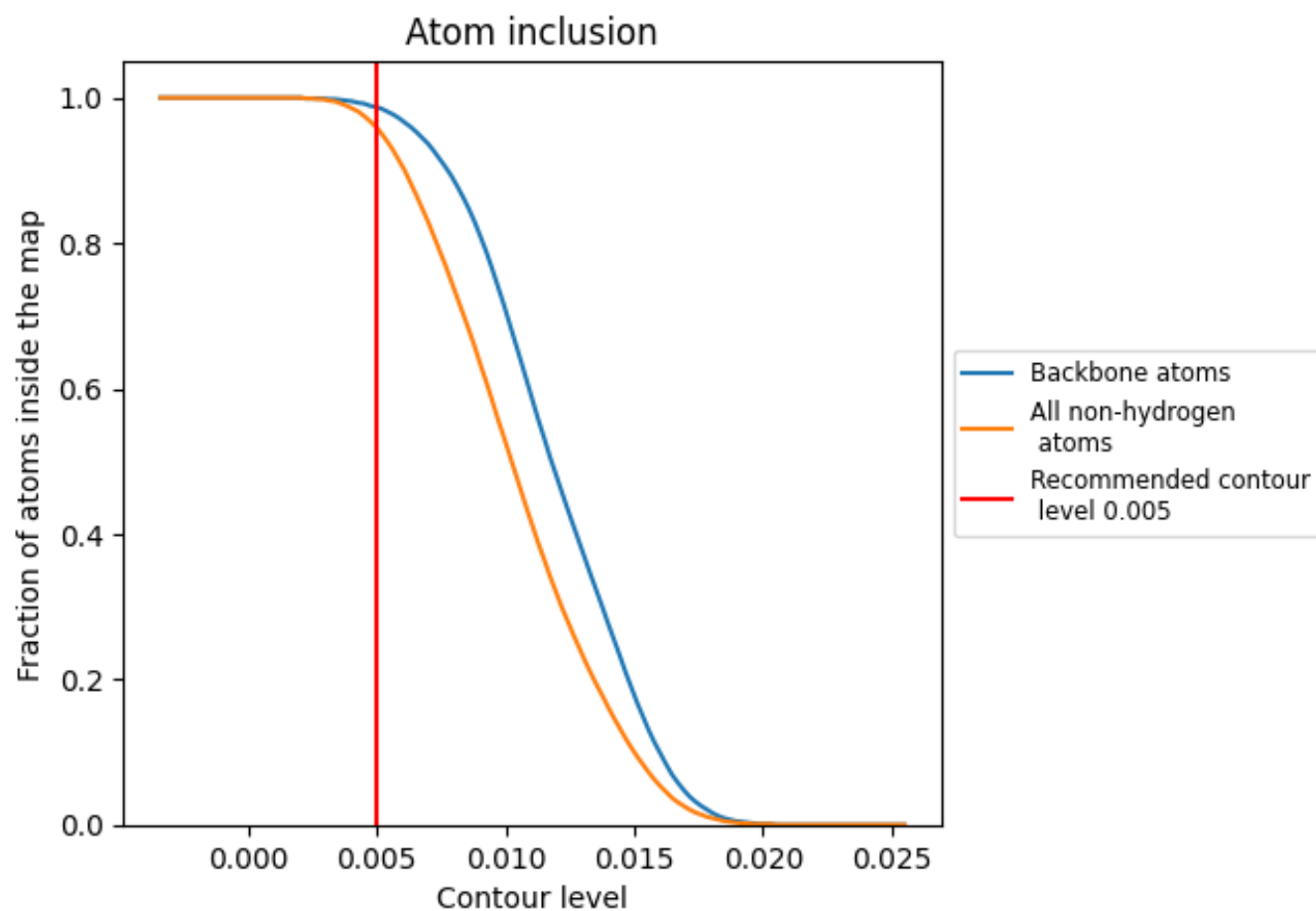
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 99% of all backbone atoms, 96% 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	 0.9590	 0.4300
A	 0.9780	 0.4280
B	 0.9680	 0.4330
C	 0.9800	 0.4470
D	 0.9790	 0.4330
E	 0.9390	 0.2890
F	 0.9530	 0.4040
G	 0.9820	 0.5200
H	 0.9890	 0.5260
I	 0.9760	 0.5080
J	 0.9820	 0.5060
K	 0.9830	 0.5170
L	 0.9900	 0.5340
M	 0.9850	 0.5220
N	 0.9850	 0.5470
O	 0.9900	 0.5400
P	 0.9940	 0.5490
Q	 0.9900	 0.5470
R	 0.9970	 0.5440
S	 0.9930	 0.5390
T	 0.9890	 0.5440
U	 0.9440	 0.3650
V	 0.9560	 0.3680
W	 0.8980	 0.3330
X	 0.9630	 0.3870
Y	 0.9620	 0.3940
Z	 0.9720	 0.3920
a	 0.9410	 0.3290
b	 0.9620	 0.3420
c	 0.9690	 0.3870
d	 0.9160	 0.2840
e	 0.9190	 0.3710
f	 0.9340	 0.2580
g	 0.9760	 0.5140
h	 0.9850	 0.5230



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Chain	Atom inclusion	Q-score
i	 0.9710	 0.4970
j	 0.9700	 0.4670
k	 0.9760	 0.5050
l	 0.9860	 0.5270
m	 0.9770	 0.5150
n	 0.9950	 0.5530
o	 0.9920	 0.5430
p	 0.9940	 0.5490
q	 0.9960	 0.5510
r	 0.9990	 0.5530
s	 0.9920	 0.5420
t	 0.9880	 0.5510
v	 1.0000	 0.3400
x	 0.7570	 0.2310
y	 0.8210	 0.2490