



## Full wwPDB EM Validation Report ⓘ

Apr 21, 2026 – 06:02 PM JST

PDB ID : 9K4M / pdb\_00009k4m  
EMDB ID : EMD-62064  
Title : Structure of substrate-engaged human 26S proteasome RP-CP subcomplex in state EA2.1  
Authors : Wu, Z.; Chen, E.; Mao, Y.  
Deposited on : 2024-10-21  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

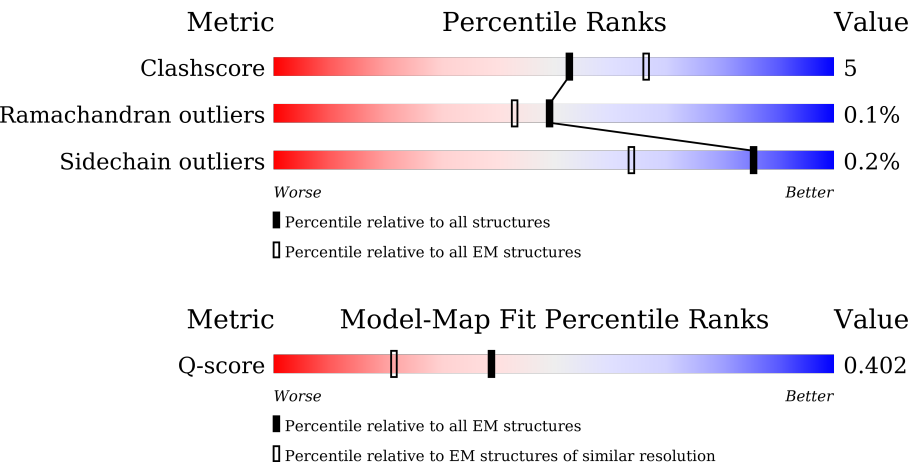
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	440	
3	C	398	
4	D	418	









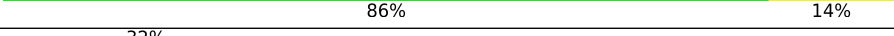


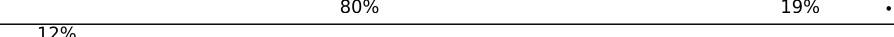

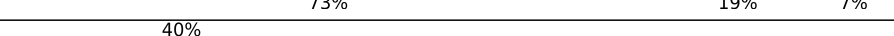


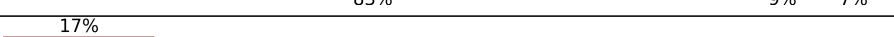
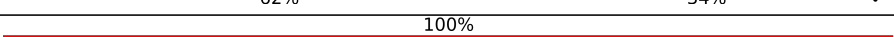
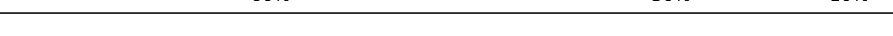
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Mol	Chain	Length	Quality of chain
5	E	403	
6	F	439	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	263	
12	l	263	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17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

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Mol	Chain	Length	Quality of chain
18	r	263	
19	S	241	
19	s	241	
20	T	264	
20	t	264	
21	U	953	
22	V	534	
23	W	456	
24	X	422	
25	Y	389	
26	Z	324	
27	a	376	
28	b	377	
29	c	310	
30	d	350	
31	e	70	
32	f	908	
33	u	76	
34	v	10	

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 105930 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	394	Total	C	N	O	S	0	0
			3096	1951	543	584	18		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	380	Total	C	N	O	S	0	0
			3039	1923	524	579	13		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	415	Total	C	N	O	S	0	0
			3251	2038	561	634	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	244	Total	C	N	O	S	0	0
			1889	1198	316	362	13		
7	g	244	Total	C	N	O	S	0	0
			1880	1193	318	356	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	232	Total	C	N	O	S	0	0
			1805	1152	305	342	6		
8	h	232	Total	C	N	O	S	0	0
			1805	1154	307	338	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	250	Total	C	N	O	S	1	0
			1958	1236	336	376	10		
9	i	250	Total	C	N	O	S	0	0
			1955	1234	336	375	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1880	1179	333	363	5		
10	j	239	Total	C	N	O	S	0	0
			1861	1168	332	356	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	234	Total	C	N	O	S	0	0
			1777	1117	295	354	11		
11	k	234	Total	C	N	O	S	0	0
			1782	1119	295	357	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	238	Total	C	N	O	S	0	0
			1866	1169	336	350	11		
12	l	238	Total	C	N	O	S	0	0
			1861	1165	335	350	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	240	Total	C	N	O	S	0	0
			1876	1191	321	353	11		
13	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		
14	n	202	Total	C	N	O	S	0	0
			1510	947	258	293	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1649	1038	279	320	12		
15	o	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1588	1017	270	292	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1588	1017	270	292	9		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1641	1041	281	309	10		
19	s	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	818	Total	C	N	O	S	0	0
			6373	4047	1084	1197	45		

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

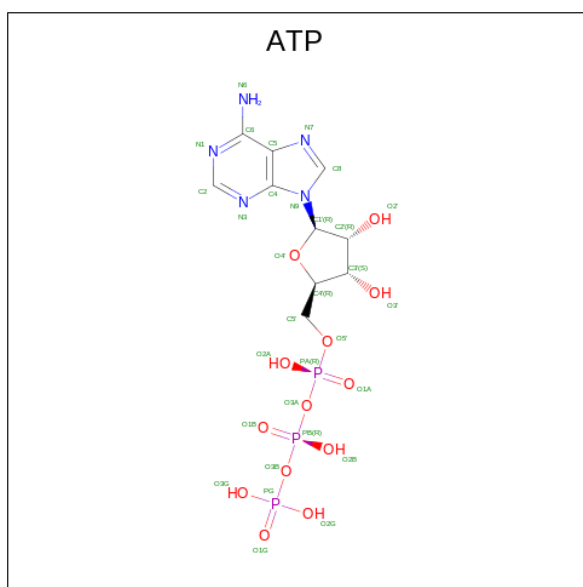
- Molecule 33 is a protein called Ubiquitin.

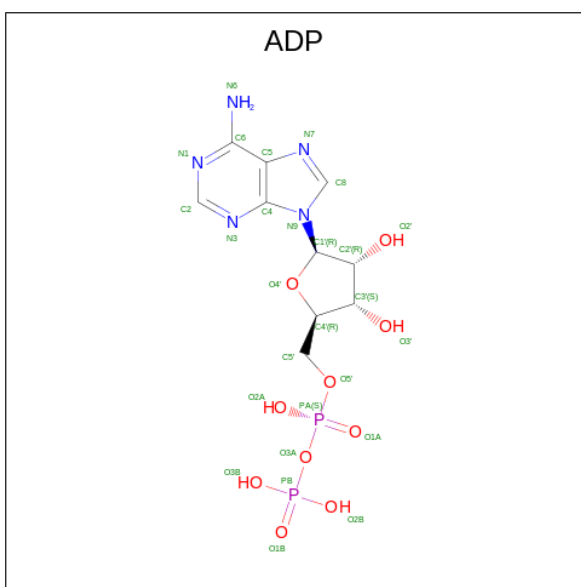
Mol	Chain	Residues	Atoms					AltConf	Trace
33	u	76	Total	C	N	O	S	0	0
			601	378	105	117	1		

- Molecule 34 is a protein called Substrate.

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

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).





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

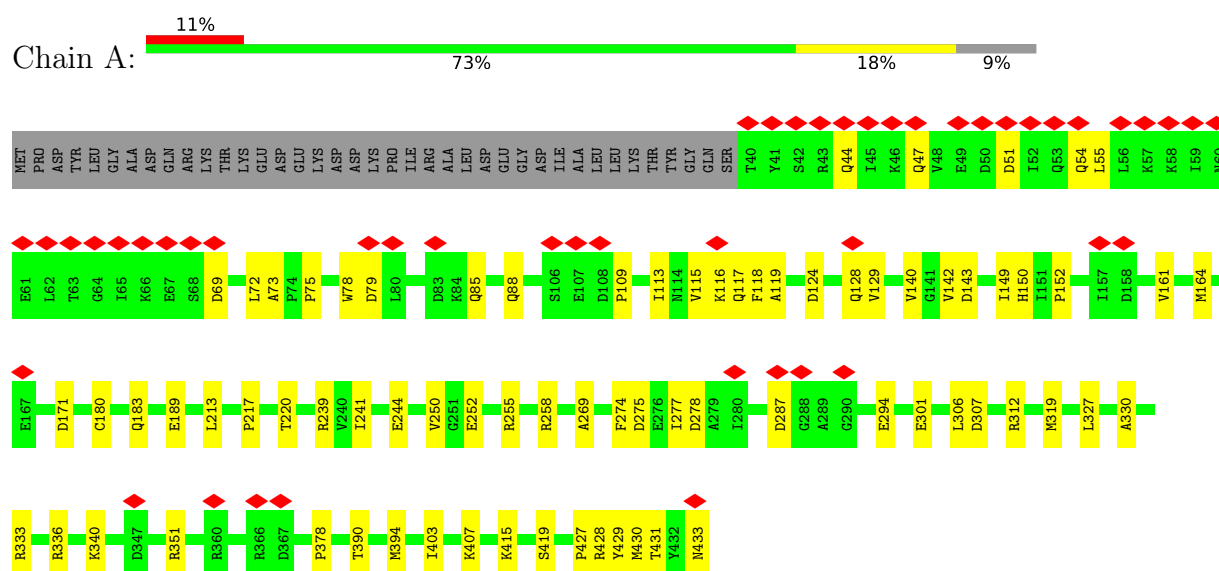
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

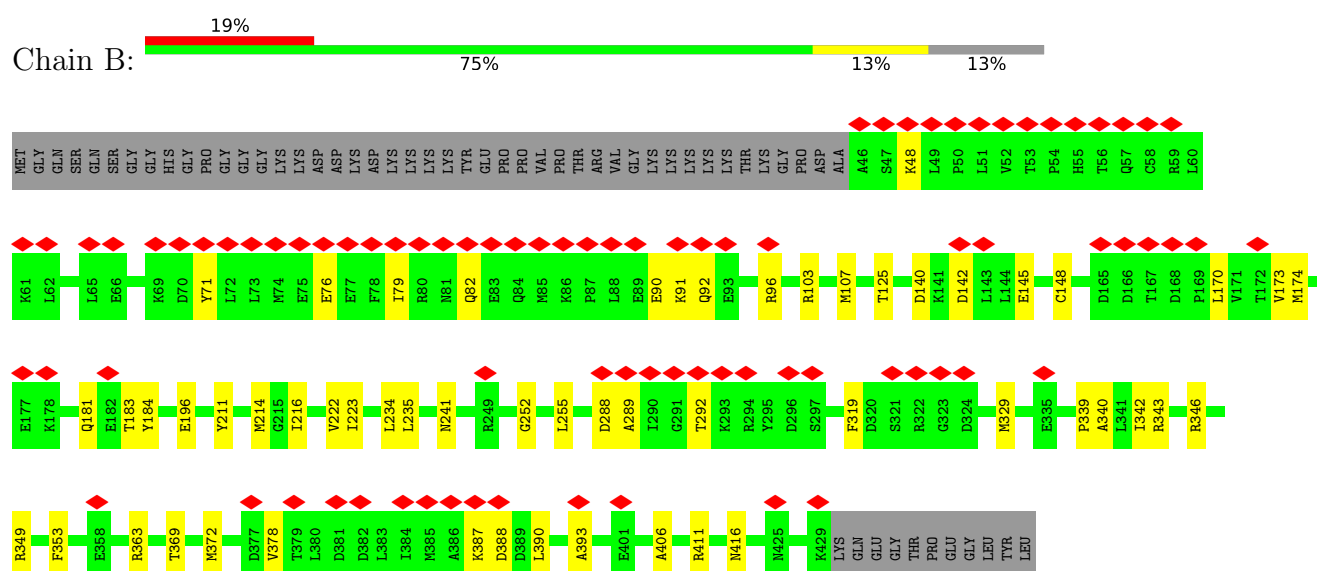
### 3 Residue-property plots

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

#### • Molecule 1: 26S proteasome regulatory subunit 7

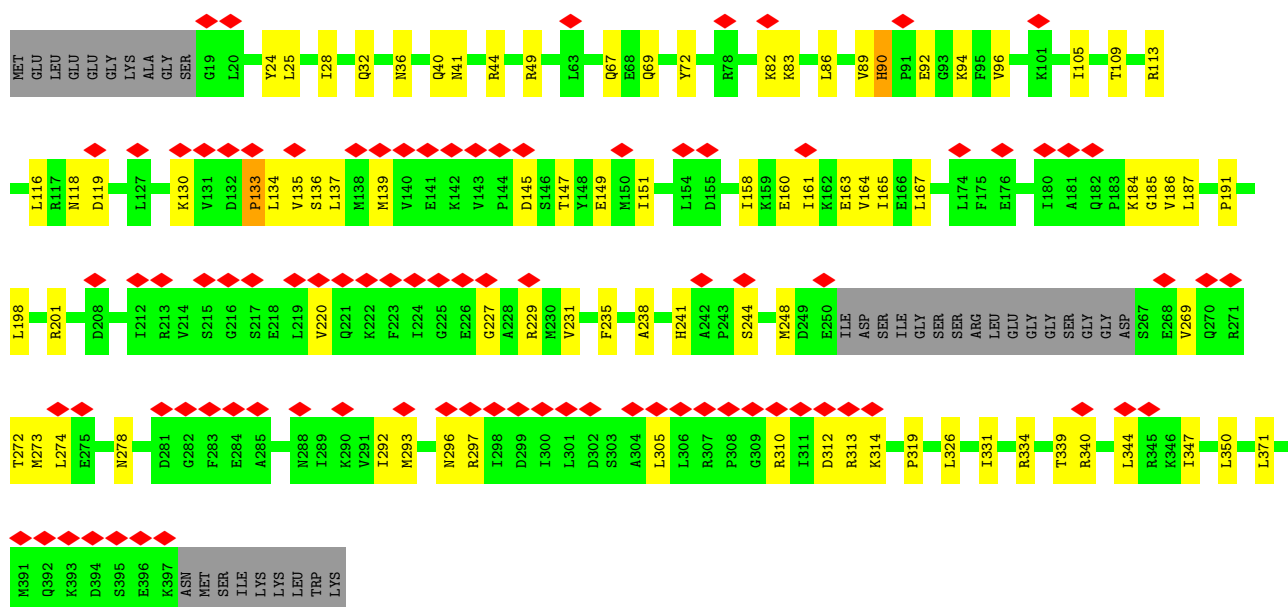


#### • Molecule 2: 26S proteasome regulatory subunit 4



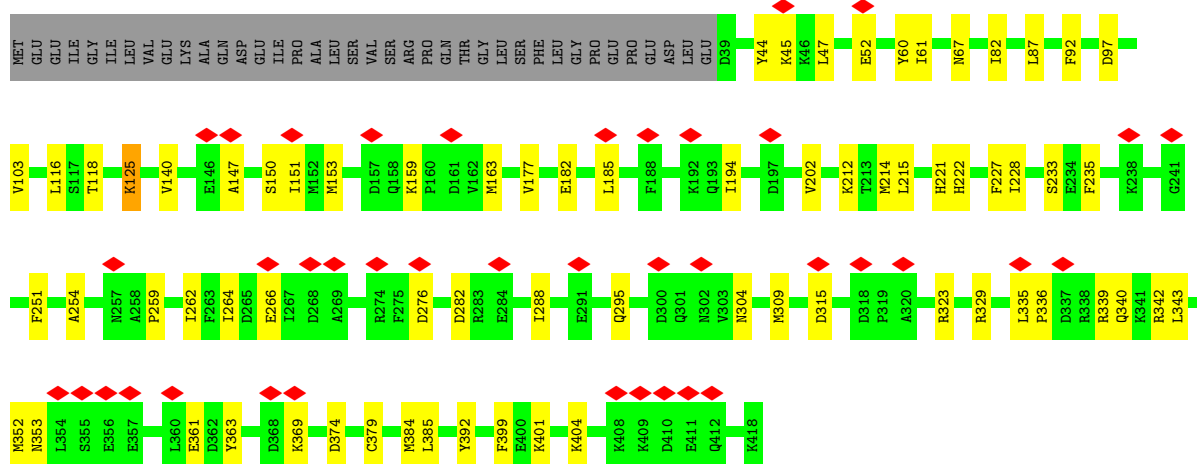
#### • Molecule 3: 26S proteasome regulatory subunit 8

Chain C: 23% 70% 21% 9%



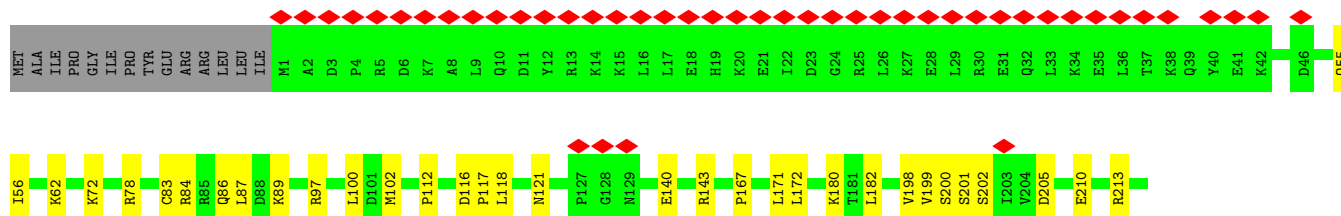
- Molecule 4: 26S proteasome regulatory subunit 6B

Chain D: 10% 74% 17% 9%



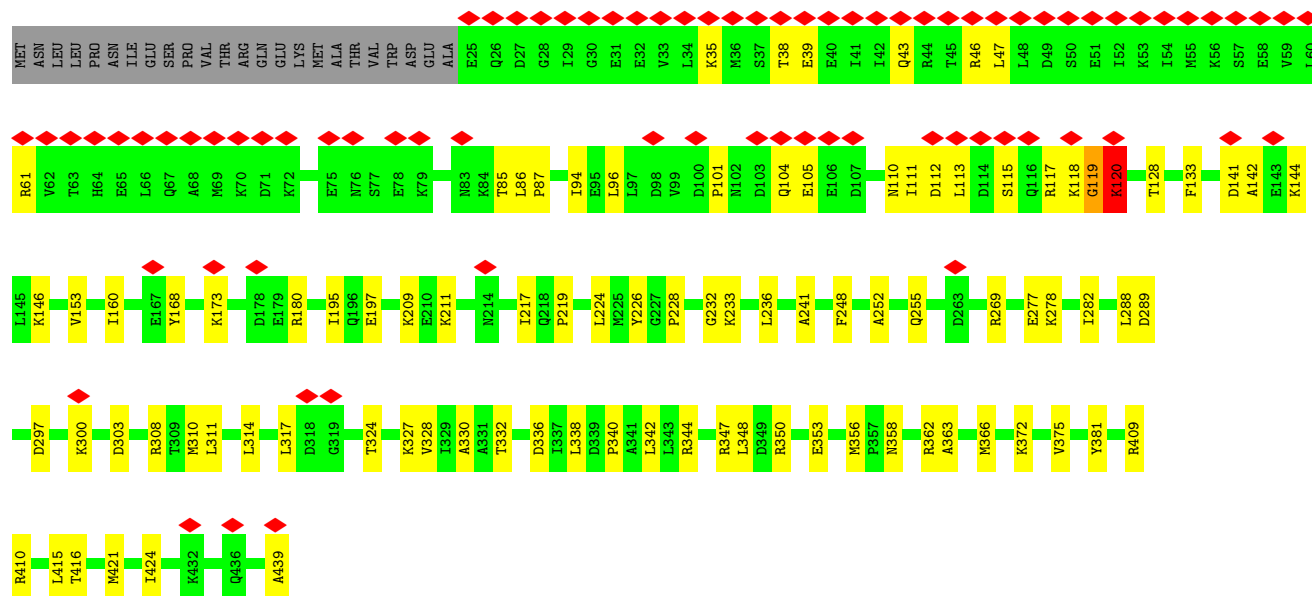
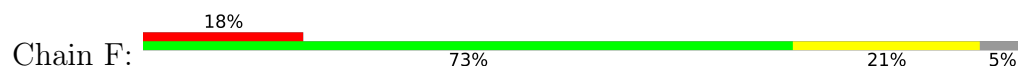
- Molecule 5: Proteasome 26S subunit, ATPase 6

Chain E: 13% 78% 19%





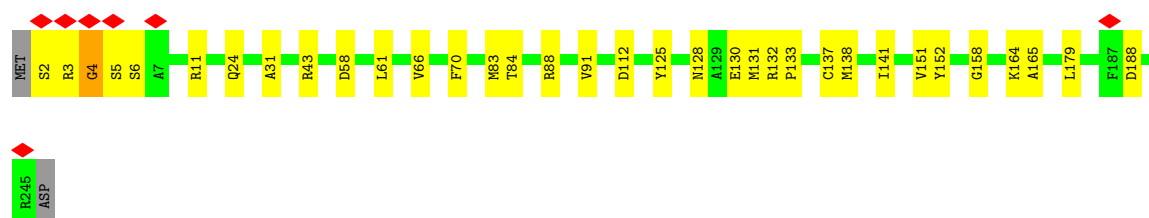
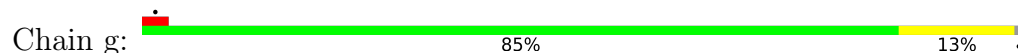
- Molecule 6: 26S proteasome regulatory subunit 6A




- Molecule 7: Proteasome subunit alpha type-6

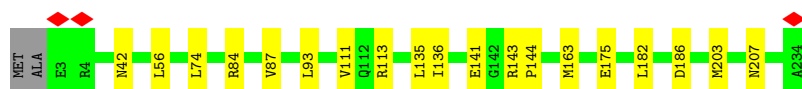


- Molecule 7: Proteasome subunit alpha type-6



- Molecule 8: Proteasome subunit alpha type-2

Chain H:  91% 8%




- Molecule 8: Proteasome subunit alpha type-2

Chain h:  93% 6%




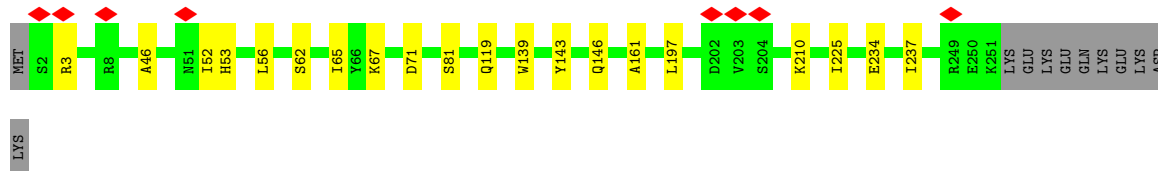
- Molecule 9: Proteasome subunit alpha type-4

Chain I:  88% 8%




- Molecule 9: Proteasome subunit alpha type-4

Chain i:  88% 8%




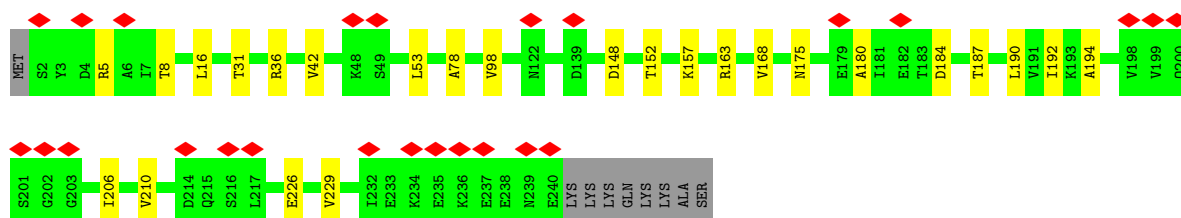
- Molecule 10: Proteasome subunit alpha type-7

Chain J:  88% 8%




- Molecule 10: Proteasome subunit alpha type-7

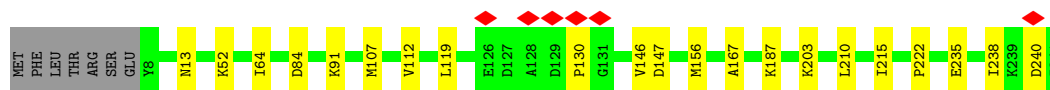
Chain j:  10% 86% 10%






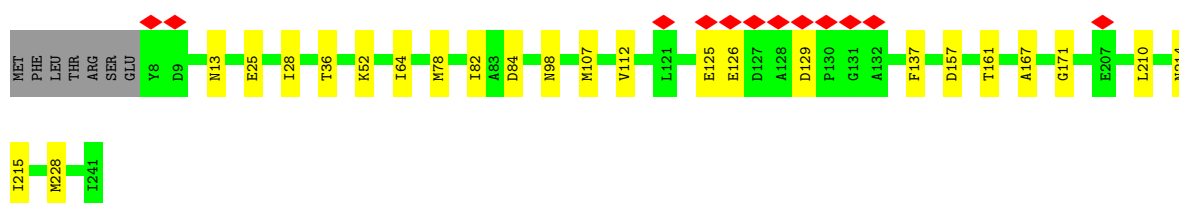
- Molecule 11: Proteasome subunit alpha type-5

Chain K:  88% 9%




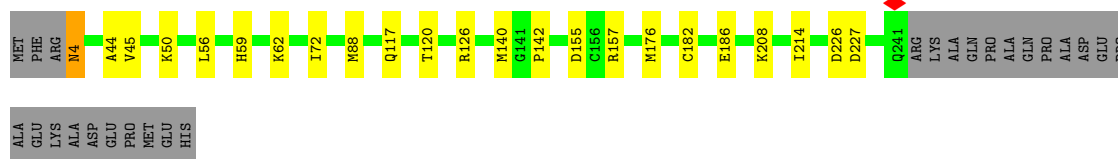
- Molecule 11: Proteasome subunit alpha type-5

Chain k:  5% 87% 10%




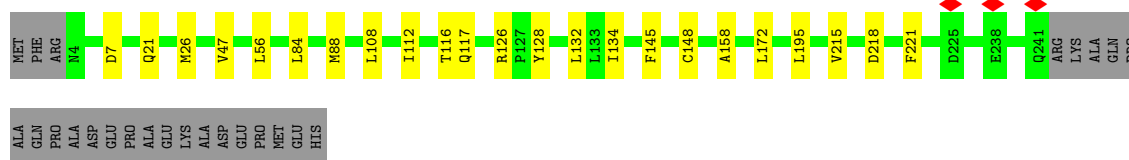
- Molecule 12: Proteasome subunit alpha type-1

Chain L:  82% 8% 10%




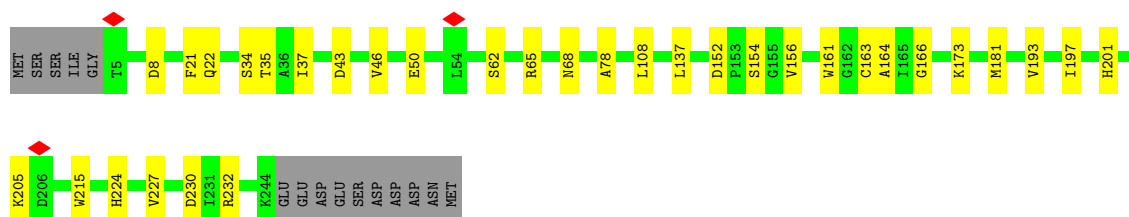
- Molecule 12: Proteasome subunit alpha type-1

Chain l:  82% 9% 10%




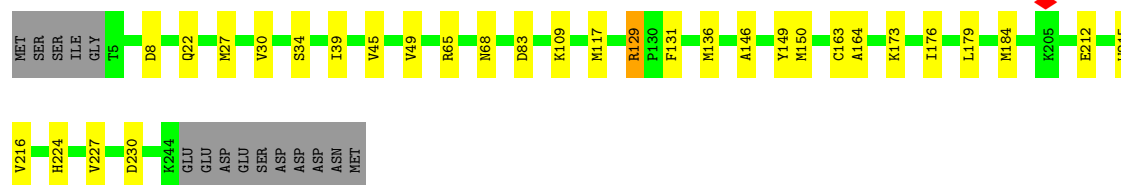
- Molecule 13: Proteasome subunit alpha type-3

Chain M:  81% 13% 6%




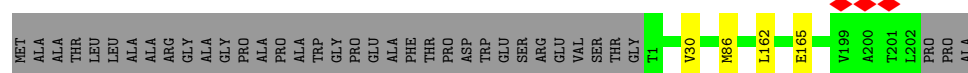
- Molecule 13: Proteasome subunit alpha type-3

Chain m:  82% 12% 6%




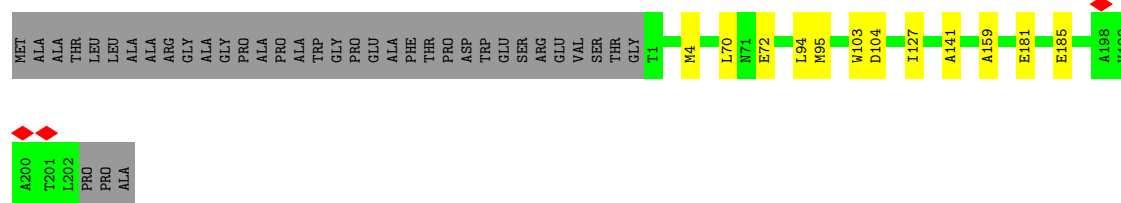
- Molecule 14: Proteasome subunit beta type-6

Chain N:  83% 15%



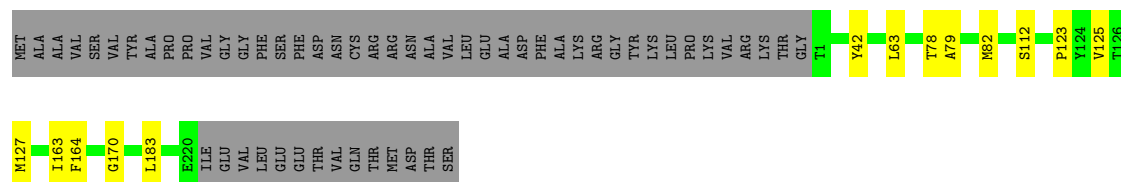
- Molecule 14: Proteasome subunit beta type-6

Chain n:  79% 5% 15%



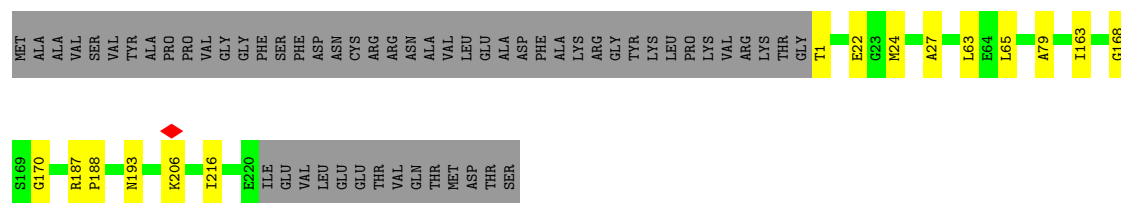
- Molecule 15: Proteasome subunit beta type-7

Chain O:  75% 5% 21%




- Molecule 15: Proteasome subunit beta type-7

Chain o:  74% 5% 21%




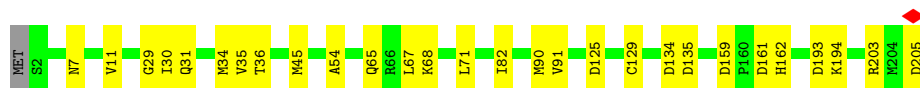
- Molecule 16: Proteasome subunit beta type-3

Chain P:  90% 9%



- Molecule 16: Proteasome subunit beta type-3

Chain p:  86% 14%




- Molecule 17: Proteasome subunit beta type-2

Chain Q:  89% 10%



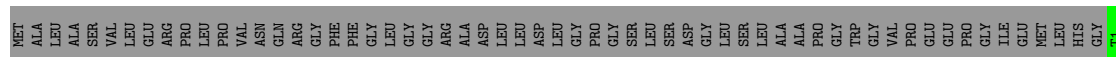
- Molecule 17: Proteasome subunit beta type-2

Chain q:  88% 11%



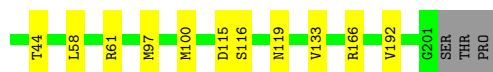
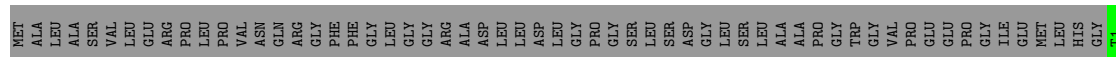
- Molecule 18: Proteasome subunit beta type-5

Chain R:  72% 24%




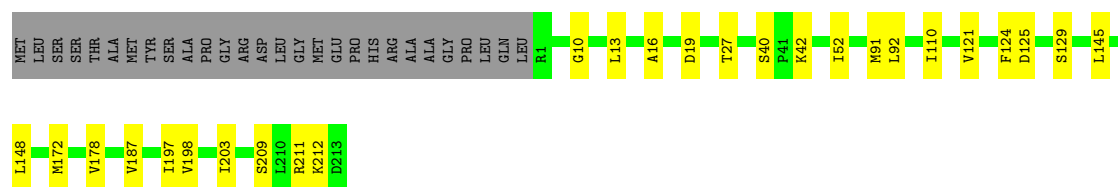
- Molecule 18: Proteasome subunit beta type-5

Chain r:  72% 24%



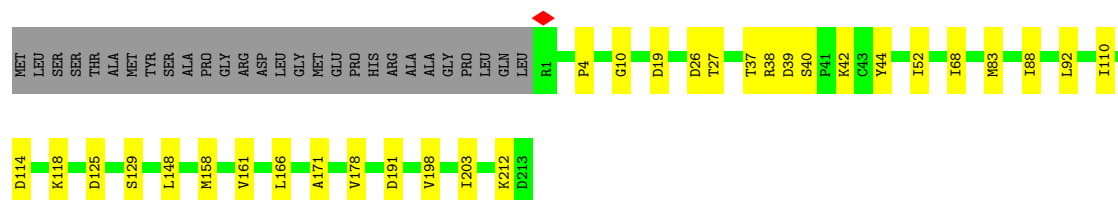
- Molecule 19: Proteasome subunit beta type-1

Chain S:  78% 11% 12%



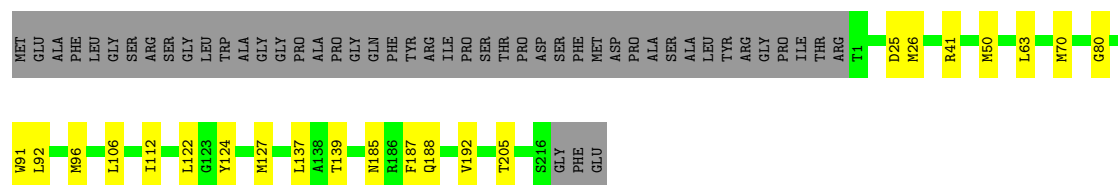
• Molecule 19: Proteasome subunit beta type-1

Chain s:  76% 13% 12%



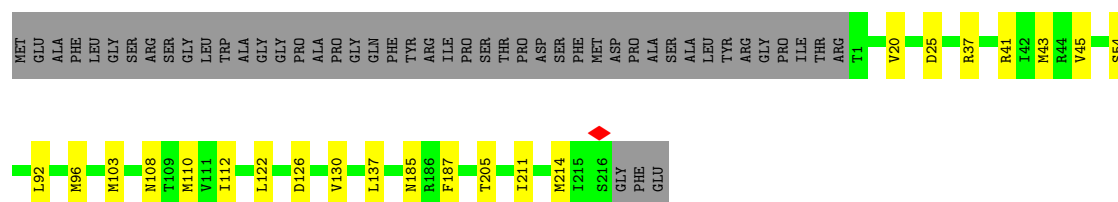
• Molecule 20: Proteasome subunit beta type-4

Chain T:  73% 8% 18%



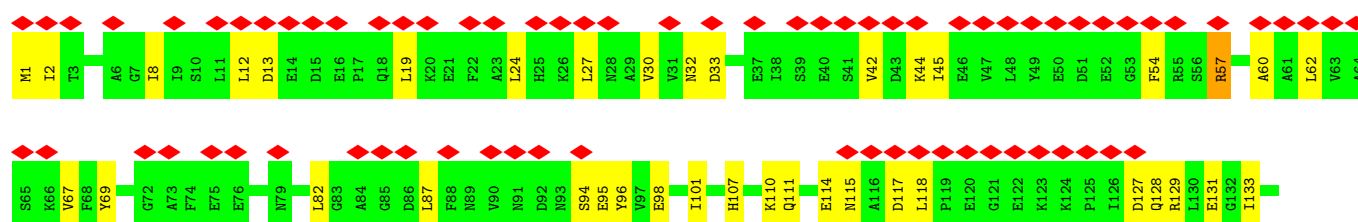
• Molecule 20: Proteasome subunit beta type-4

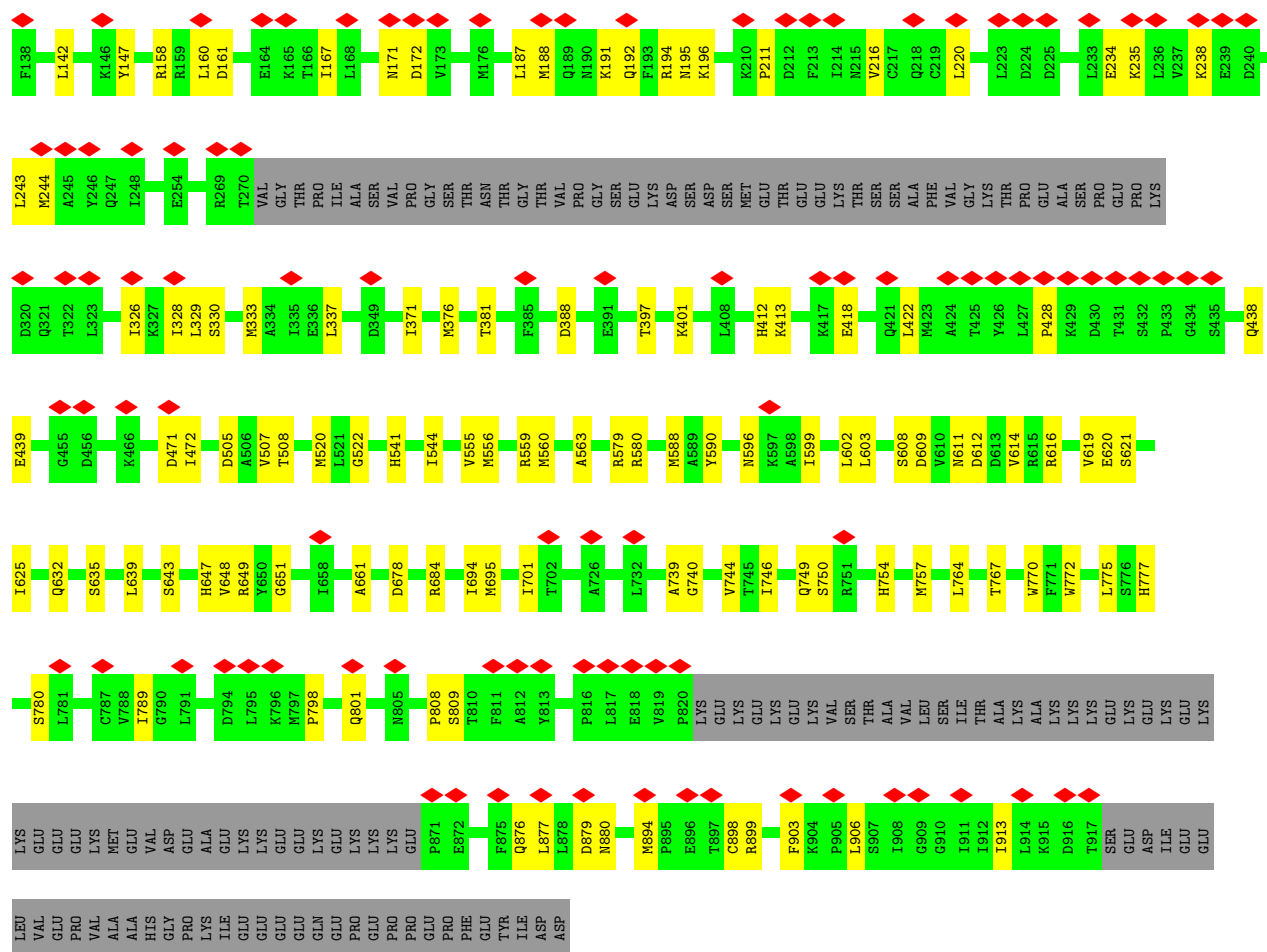
Chain t:  73% 8% 18%



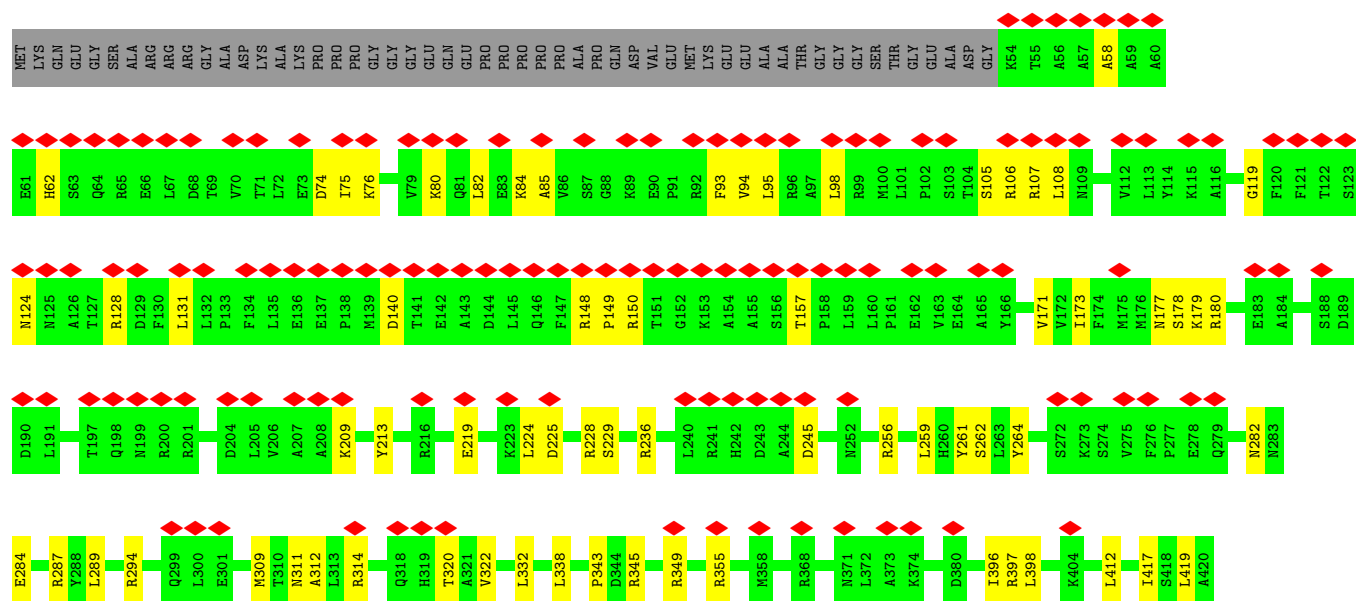
• Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

Chain U:  18% 69% 16% 14%

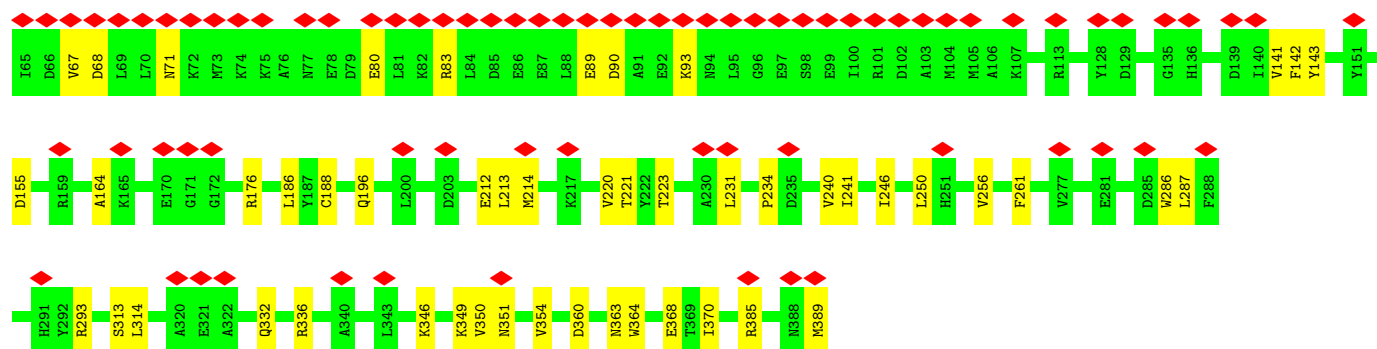




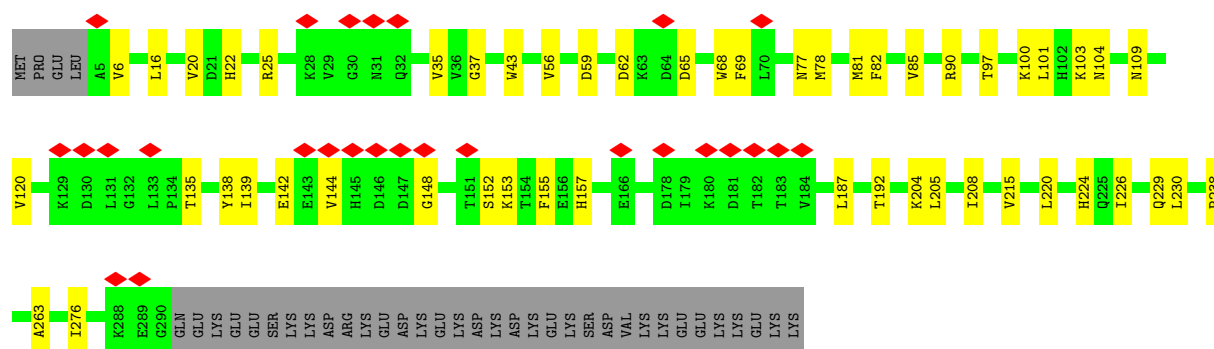
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 3



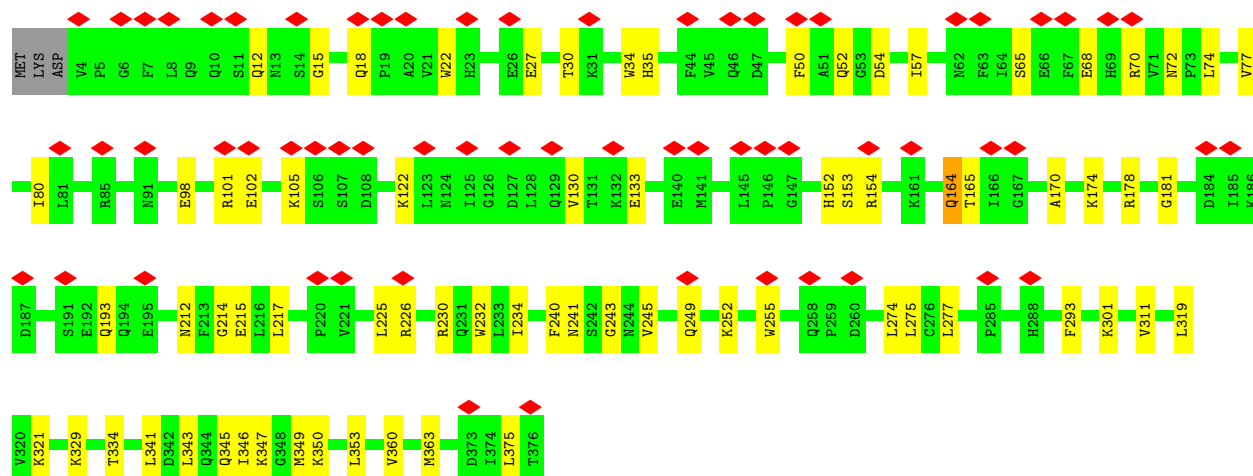
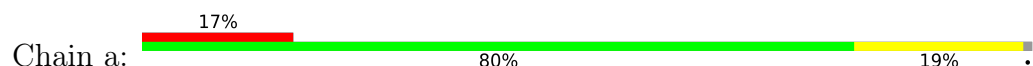




- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

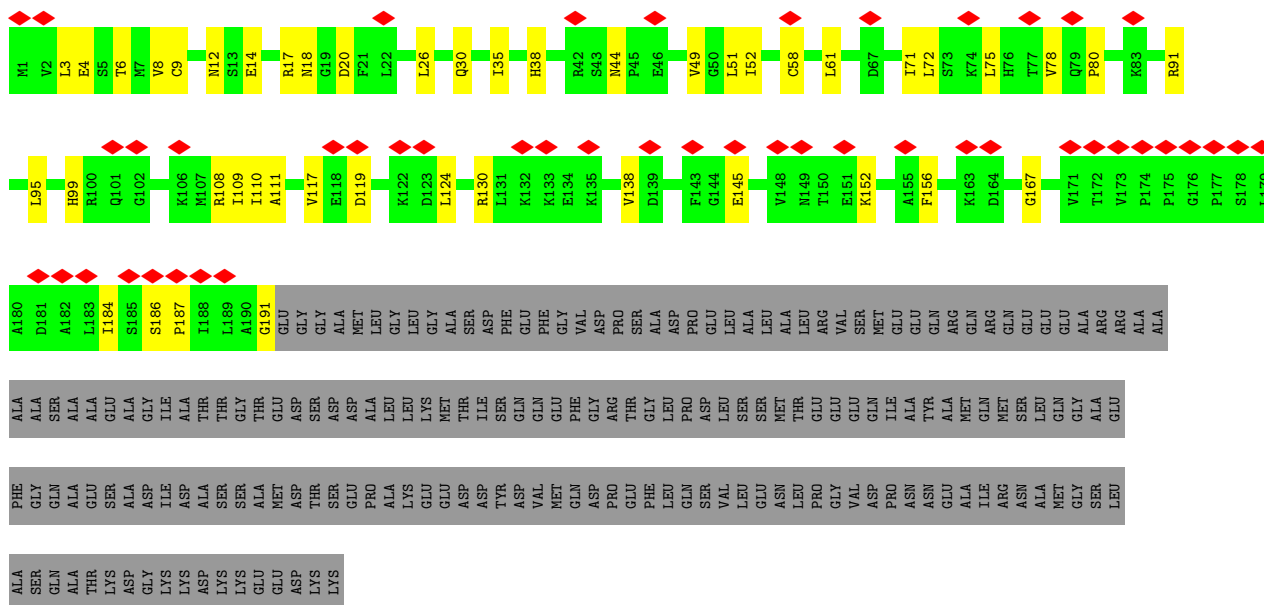


- Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

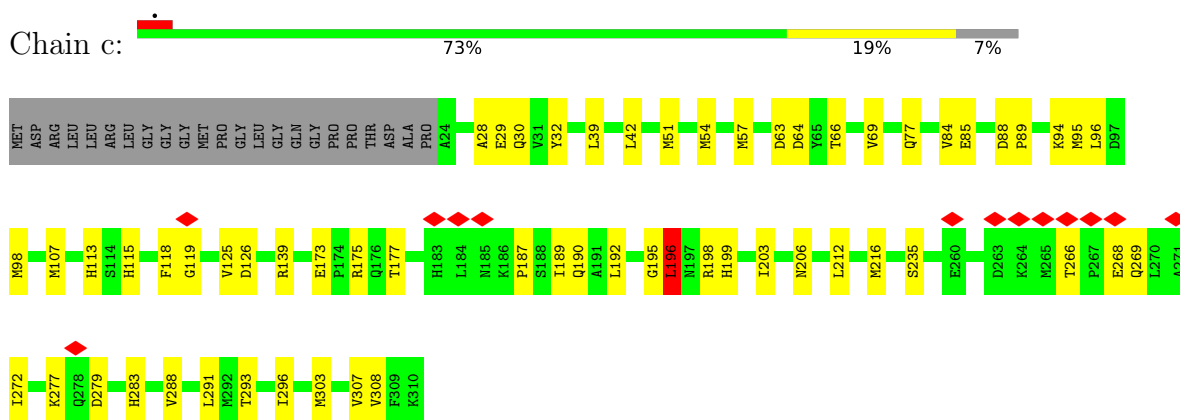


- Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

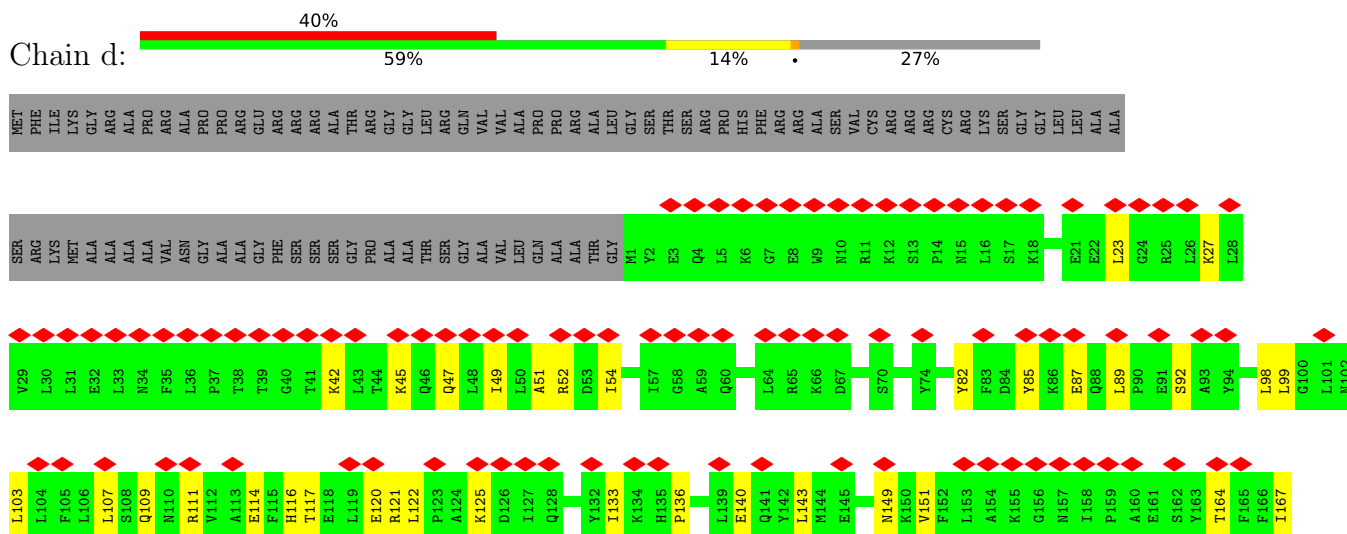




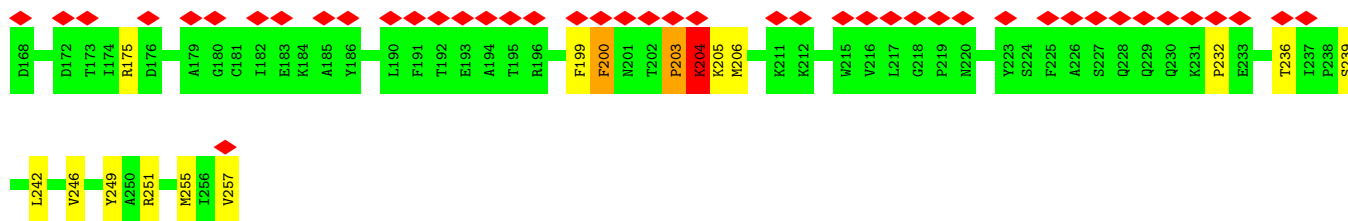
- Molecule 29: 26S proteasome non-ATPase regulatory subunit 14



- Molecule 30: 26S proteasome non-ATPase regulatory subunit 8



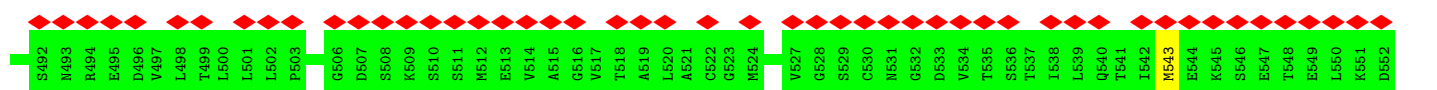
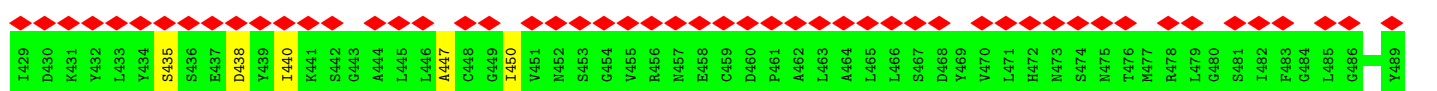
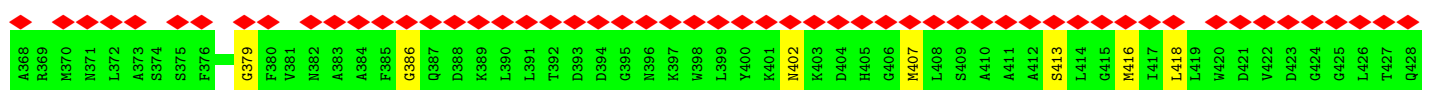
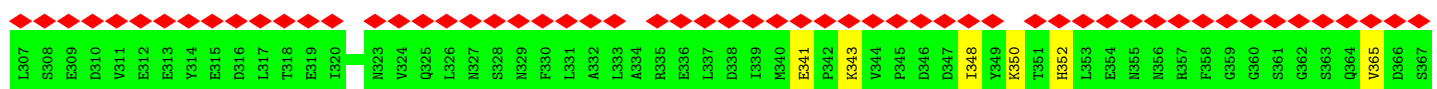
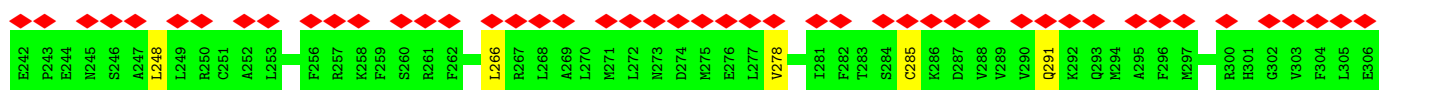
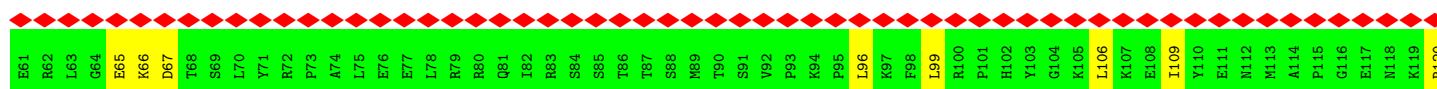
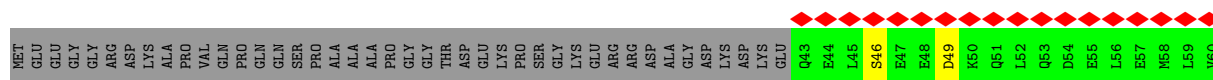
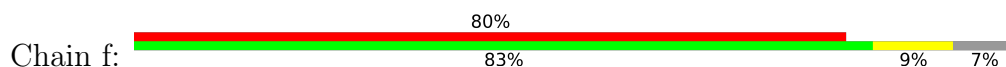


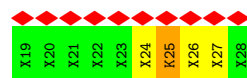


• Molecule 31: 26S proteasome complex subunit SEM1



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





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	147108	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	44	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.024	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00559	Depositor
Map size (Å)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.18	0/3148	0.50	0/4250
2	B	0.17	0/3061	0.48	0/4129
3	C	0.18	0/2902	0.49	0/3904
4	D	0.22	0/3089	0.52	0/4168
5	E	0.18	0/3145	0.47	0/4233
6	F	0.21	0/3292	0.44	0/4435
7	G	0.18	0/1923	0.39	0/2601
7	g	0.21	0/1914	0.42	0/2590
8	H	0.19	0/1844	0.39	0/2499
8	h	0.18	0/1844	0.38	0/2497
9	I	0.18	0/1991	0.42	1/2685 (0.0%)
9	i	0.16	0/1985	0.35	0/2677
10	J	0.17	0/1906	0.38	0/2573
10	j	0.16	0/1887	0.43	1/2549 (0.0%)
11	K	0.17	0/1804	0.36	0/2436
11	k	0.16	0/1809	0.35	0/2444
12	L	0.18	0/1901	0.34	0/2570
12	l	0.16	0/1896	0.35	0/2565
13	M	0.16	0/1911	0.36	0/2573
13	m	0.17	0/1916	0.34	0/2580
14	N	0.17	0/1540	0.31	0/2085
14	n	0.20	0/1536	0.38	0/2080
15	O	0.18	0/1676	0.36	0/2271
15	o	0.17	0/1686	0.34	0/2282
16	P	0.18	0/1616	0.41	0/2180
16	p	0.19	0/1620	0.41	0/2184
17	Q	0.17	0/1621	0.35	0/2194
17	q	0.17	0/1621	0.34	0/2194
18	R	0.18	0/1590	0.38	0/2147
18	r	0.18	0/1590	0.38	0/2147
19	S	0.20	0/1671	0.39	0/2252
19	s	0.18	0/1684	0.41	0/2268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
20	T	0.19	0/1716	0.38	0/2323
20	t	0.17	0/1720	0.35	0/2328
21	U	0.17	0/6488	0.47	3/8782 (0.0%)
22	V	0.15	0/3681	0.38	0/4969
23	W	0.16	0/3644	0.44	1/4901 (0.0%)
24	X	0.18	0/3381	0.47	0/4558
25	Y	0.19	0/3261	0.49	0/4393
26	Z	0.20	0/2324	0.55	1/3150 (0.0%)
27	a	0.19	0/3053	0.54	0/4133
28	b	0.20	0/1478	0.52	0/2001
29	c	0.23	0/2302	0.55	0/3110
30	d	0.27	0/2162	0.60	4/2919 (0.1%)
31	e	0.23	0/437	0.67	1/595 (0.2%)
32	f	0.18	0/6640	0.49	2/8988 (0.0%)
33	u	0.20	0/607	0.40	0/816
34	v	0.16	0/8	0.06	0/8
All	All	0.18	0/107521	0.44	14/145216 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	d	232	PRO	CA-N-CD	-9.35	98.91	112.00
32	f	582	VAL	N-CA-C	-8.09	103.36	111.77
23	W	453	HIS	N-CA-C	7.38	119.33	111.28
21	U	472	ILE	N-CA-C	-7.12	106.55	113.53
10	j	98	VAL	N-CA-C	-6.22	107.07	113.10
30	d	232	PRO	N-CD-CG	-6.09	94.07	103.20
30	d	200	PHE	N-CA-C	5.89	119.24	111.28
32	f	852	VAL	N-CA-C	-5.76	105.77	111.77
31	e	61	GLU	N-CA-CB	5.43	119.25	110.40
26	Z	6	VAL	N-CA-C	-5.18	108.45	113.53
21	U	397	THR	CA-C-N	5.16	131.40	121.54
21	U	397	THR	C-N-CA	5.16	131.40	121.54
30	d	204	LYS	N-CA-C	-5.12	105.92	113.61
9	I	205	LYS	CB-CG-CD	5.04	122.89	111.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3096	0	3139	50	0
2	B	3018	0	3082	43	0
3	C	2864	0	2971	54	0
4	D	3039	0	3075	47	0
5	E	3097	0	3173	51	0
6	F	3251	0	3318	72	0
7	G	1889	0	1885	11	0
7	g	1880	0	1875	24	0
8	H	1805	0	1784	12	0
8	h	1805	0	1798	10	0
9	I	1958	0	1960	13	0
9	i	1955	0	1955	13	0
10	J	1880	0	1892	13	0
10	j	1861	0	1865	14	0
11	K	1777	0	1762	14	0
11	k	1782	0	1766	16	0
12	L	1866	0	1852	16	0
12	l	1861	0	1839	14	0
13	M	1876	0	1861	22	0
13	m	1881	0	1868	22	0
14	N	1514	0	1487	4	0
14	n	1510	0	1483	8	0
15	O	1649	0	1659	8	0
15	o	1659	0	1681	11	0
16	P	1587	0	1598	13	0
16	p	1591	0	1609	21	0
17	Q	1588	0	1584	16	0
17	q	1588	0	1584	16	0
18	R	1559	0	1523	10	0
18	r	1559	0	1523	9	0
19	S	1641	0	1639	16	0
19	s	1654	0	1656	19	0
20	T	1683	0	1662	14	0
20	t	1687	0	1666	14	0
21	U	6373	0	6411	105	0
22	V	3612	0	3682	58	0
23	W	3596	0	3713	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	X	3335	0	3435	37	0
25	Y	3202	0	3204	38	0
26	Z	2281	0	2312	38	0
27	a	2995	0	3012	51	0
28	b	1458	0	1505	29	0
29	c	2260	0	2276	53	0
30	d	2116	0	2146	38	0
31	e	425	0	328	14	0
32	f	6529	0	6541	51	0
33	u	601	0	629	29	0
34	v	53	0	22	5	0
35	A	31	0	12	0	0
35	B	31	0	12	2	0
35	D	31	0	12	2	0
35	E	31	0	12	3	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	D	1	0	0	0	0
36	E	1	0	0	0	0
36	F	1	0	0	0	0
37	C	27	0	12	1	0
37	F	27	0	12	1	0
38	c	1	0	0	0	0
All	All	105930	0	106362	1126	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 5.

All (1126) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:569:LYS:HG2	32:f:572:ALA:HB3	1.28	1.09
33:u:1:MET:SD	33:u:1:MET:N	2.35	0.99
21:U:54:PHE:HB3	21:U:57:ARG:HD2	1.45	0.96
30:d:200:PHE:HB3	30:d:203:PRO:HG3	1.47	0.96
29:c:192:LEU:HA	29:c:196:LEU:HB2	1.52	0.89
30:d:149:ASN:HB3	30:d:199:PHE:CZ	2.09	0.88
23:W:451:MET:HE3	23:W:455:LEU:HD11	1.55	0.87
30:d:149:ASN:HB3	30:d:199:PHE:HZ	1.39	0.85
32:f:569:LYS:CG	32:f:572:ALA:HB3	2.06	0.83
29:c:85:GLU:OE1	33:u:74:ARG:HD3	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:203:PRO:HG2	30:d:205:LYS:H	1.48	0.79
33:u:63:LYS:O	33:u:63:LYS:HG2	1.85	0.77
21:U:57:ARG:HH11	21:U:57:ARG:HG2	1.51	0.76
33:u:1:MET:HG3	33:u:63:LYS:CB	2.16	0.76
21:U:328:ILE:HG13	21:U:329:LEU:HG	1.69	0.75
9:I:180:LYS:H	9:I:184:MET:HE3	1.54	0.73
21:U:694:ILE:HG23	21:U:695:MET:HG3	1.70	0.73
1:A:415:LYS:O	1:A:419:SER:HB3	1.89	0.72
29:c:126:ASP:OD1	33:u:76:GLY:N	2.22	0.72
33:u:51:GLU:OE1	33:u:51:GLU:HA	1.91	0.71
21:U:57:ARG:HD3	21:U:57:ARG:H	1.55	0.71
33:u:23:ILE:HB	33:u:52:ASP:HA	1.73	0.70
17:q:85:ARG:HA	17:q:118:MET:HE1	1.72	0.70
5:E:198:VAL:HG12	5:E:200:SER:H	1.57	0.69
23:W:455:LEU:O	23:W:456:GLN:OXT	2.10	0.69
27:a:65:SER:HA	27:a:68:GLU:HB2	1.74	0.69
26:Z:22:HIS:HA	26:Z:25:ARG:HE	1.57	0.69
29:c:28:ALA:HB2	29:c:175:ARG:HH12	1.58	0.69
29:c:303:MET:HE1	30:d:242:LEU:HB2	1.75	0.68
22:V:85:ALA:HB2	22:V:93:PHE:HB2	1.77	0.67
22:V:397:ARG:HH21	30:d:116:HIS:HB3	1.59	0.67
29:c:96:LEU:HD12	33:u:8:LEU:HD22	1.77	0.67
22:V:124:ASN:HA	22:V:128:ARG:HD3	1.78	0.66
12:L:4:ASN:N	12:L:4:ASN:HD22	1.94	0.66
29:c:195:GLY:O	29:c:198:ARG:HB2	1.96	0.66
1:A:394:MET:HG2	2:B:349:ARG:HH22	1.59	0.65
5:E:244:SER:HB2	6:F:300:LYS:HD3	1.78	0.65
27:a:226:ARG:HB3	27:a:234:ILE:HD11	1.77	0.65
2:B:170:LEU:HD23	3:C:229:ARG:HH21	1.62	0.65
26:Z:208:ILE:HG23	27:a:353:LEU:HD21	1.79	0.65
2:B:369:THR:HA	2:B:372:MET:HE3	1.79	0.65
6:F:232:GLY:HA2	37:F:501:ADP:H5'2	1.79	0.65
10:j:192:ILE:HD12	10:j:206:ILE:HD12	1.79	0.64
24:X:218:HIS:NE2	24:X:227:THR:OG1	2.21	0.64
27:a:363:MET:HG3	29:c:307:VAL:HG11	1.78	0.64
1:A:427:PRO:HA	1:A:430:MET:HE2	1.79	0.64
4:D:336:PRO:HB3	4:D:340:GLN:HB2	1.80	0.64
26:Z:192:THR:HG22	27:a:375:LEU:HD12	1.78	0.64
20:T:26:MET:HE2	20:T:188:GLN:HG3	1.80	0.64
2:B:90:GLU:HG3	2:B:92:GLN:H	1.63	0.63
21:U:243:LEU:HG	21:U:913:ILE:HG23	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:129:ARG:HH21	13:m:131:PHE:HA	1.62	0.63
11:k:210:LEU:HA	11:k:214:ASN:HD21	1.62	0.63
21:U:588:MET:HE3	21:U:764:LEU:HD22	1.81	0.63
25:Y:240:VAL:HG23	25:Y:241:ILE:HG13	1.81	0.63
9:I:143:TYR:HB2	9:I:146:GLN:HE21	1.65	0.62
3:C:28:ILE:HB	4:D:44:TYR:HE1	1.65	0.62
7:g:43:ARG:HH21	7:g:164:LYS:HG2	1.65	0.62
33:u:1:MET:HG3	33:u:63:LYS:HB3	1.82	0.62
18:R:35:ILE:HD11	18:R:45:MET:HG3	1.82	0.61
32:f:435:SER:HB3	32:f:440:ILE:HG21	1.82	0.61
29:c:115:HIS:HB3	29:c:118:PHE:HB2	1.83	0.61
17:q:88:LEU:HD23	17:q:118:MET:HE2	1.83	0.61
8:H:111:VAL:HG22	8:H:136:ILE:HD12	1.81	0.61
19:S:148:LEU:HD23	19:S:178:VAL:HG12	1.83	0.61
21:U:505:ASP:HB3	21:U:508:THR:HG22	1.82	0.61
22:V:178:SER:HB3	22:V:180:ARG:HE	1.65	0.61
17:Q:118:MET:HE2	17:Q:124:LEU:HD13	1.81	0.61
32:f:666:ILE:HG22	32:f:670:MET:HE1	1.82	0.61
3:C:136:SER:HA	3:C:139:MET:HE3	1.83	0.61
25:Y:360:ASP:HB2	25:Y:363:ASN:HB2	1.83	0.61
4:D:67:ASN:HD21	21:U:608:SER:HA	1.64	0.61
21:U:57:ARG:H	21:U:57:ARG:CD	2.13	0.60
3:C:293:MET:HE1	3:C:305:LEU:HD21	1.82	0.60
8:h:119:GLN:HG3	9:i:81:SER:HB2	1.83	0.60
3:C:235:PHE:HA	3:C:238:ALA:HB3	1.83	0.60
23:W:373:ILE:HG23	23:W:378:MET:HE2	1.84	0.60
6:F:111:ILE:HB	29:c:51:MET:HE1	1.82	0.60
19:S:27:THR:HB	19:S:40:SER:H	1.67	0.60
23:W:401:THR:HG23	23:W:402:ILE:HD12	1.82	0.60
9:i:143:TYR:HB2	9:i:146:GLN:HE21	1.66	0.60
5:E:202:SER:HA	6:F:269:ARG:HH22	1.66	0.60
27:a:212:ASN:HB3	27:a:240:PHE:HB3	1.84	0.60
28:b:35:ILE:HD12	28:b:184:ILE:HD13	1.84	0.60
28:b:51:LEU:HD23	28:b:71:ILE:HG23	1.84	0.60
15:O:112:SER:HB2	15:O:127:MET:HE3	1.84	0.59
22:V:228:ARG:HH22	22:V:261:TYR:HB2	1.67	0.59
23:W:172:GLU:HA	23:W:182:ARG:HD3	1.83	0.59
17:Q:83:PHE:O	17:Q:87:ASN:ND2	2.35	0.59
20:t:96:MET:HE2	20:t:110:MET:HE1	1.84	0.59
25:Y:90:ASP:HA	25:Y:93:LYS:HB2	1.83	0.59
1:A:430:MET:HE3	10:J:12:PRO:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:265:ASP:OD2	5:E:291:ARG:NH2	2.36	0.59
6:F:38:THR:HG22	6:F:39:GLU:HG2	1.83	0.59
3:C:28:ILE:HD11	4:D:47:LEU:HD12	1.84	0.59
16:p:45:MET:HE1	16:p:68:LYS:HA	1.83	0.59
3:C:296:ASN:OD1	3:C:297:ARG:N	2.36	0.58
21:U:8:ILE:HD12	21:U:27:LEU:HB3	1.85	0.58
21:U:772:TRP:HB3	21:U:775:LEU:HB2	1.84	0.58
33:u:40:GLN:HA	33:u:72:ARG:HB2	1.85	0.58
4:D:353:ASN:ND2	4:D:392:TYR:O	2.37	0.58
27:a:35:HIS:NE2	28:b:14:GLU:O	2.36	0.58
30:d:111:ARG:HB3	30:d:114:GLU:HB2	1.85	0.58
4:D:264:ILE:HD12	4:D:309:MET:HE1	1.85	0.58
30:d:49:ILE:HD12	30:d:52:ARG:HH21	1.68	0.58
10:j:36:ARG:HH21	10:j:157:LYS:HG2	1.68	0.58
17:q:102:LEU:HB2	17:q:118:MET:HB3	1.85	0.58
1:A:55:LEU:HD11	2:B:76:GLU:HG2	1.86	0.58
19:S:187:VAL:HG21	15:o:24:MET:HE3	1.86	0.58
22:V:177:ASN:O	22:V:179:LYS:NZ	2.36	0.58
22:V:338:LEU:HG	22:V:398:LEU:HD12	1.86	0.57
32:f:151:LEU:HB3	32:f:159:VAL:HG22	1.86	0.57
32:f:413:SER:HA	32:f:416:MET:HE2	1.86	0.57
5:E:83:CYS:HB2	5:E:89:LYS:HE2	1.85	0.57
6:F:112:ASP:O	6:F:117:ARG:NH1	2.37	0.57
4:D:92:PHE:HA	4:D:103:VAL:HG12	1.86	0.57
4:D:182:GLU:HA	4:D:185:LEU:HB2	1.85	0.57
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.85	0.57
15:O:78:THR:HG22	15:O:82:MET:HE2	1.86	0.57
23:W:108:CYS:HB3	23:W:128:LEU:HD11	1.87	0.57
24:X:67:GLY:HA2	24:X:109:LEU:HD21	1.85	0.57
20:T:50:MET:HE2	20:T:192:VAL:HG12	1.87	0.57
21:U:57:ARG:HH11	21:U:57:ARG:CG	2.18	0.57
29:c:119:GLY:HA3	29:c:190:GLN:HG3	1.84	0.57
30:d:175:ARG:HH12	30:d:200:PHE:HE2	1.50	0.57
13:M:163:CYS:SG	13:M:173:LYS:NZ	2.78	0.57
24:X:8:GLU:HG2	24:X:11:ARG:HH12	1.69	0.57
21:U:32:ASN:O	22:V:236:ARG:NH1	2.38	0.57
21:U:27:LEU:HA	21:U:30:VAL:HG22	1.87	0.57
22:V:289:LEU:HB3	22:V:312:ALA:HB2	1.87	0.57
21:U:333:MET:SD	21:U:333:MET:N	2.78	0.57
25:Y:349:LYS:O	25:Y:351:ASN:N	2.38	0.57
7:g:137:CYS:SG	7:g:138:MET:N	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ALA:O	32:f:352:HIS:NE2	2.38	0.56
6:F:282:ILE:HG22	6:F:327:LYS:HB2	1.86	0.56
13:M:34:SER:OG	13:M:65:ARG:NH1	2.37	0.56
16:p:65:GLN:OE1	17:q:86:ARG:NH2	2.38	0.56
1:A:79:ASP:OD2	2:B:91:LYS:NZ	2.39	0.56
7:G:165:ALA:HB3	8:H:56:LEU:HD22	1.86	0.56
15:o:216:ILE:HD11	16:p:194:LYS:HD2	1.86	0.56
6:F:358:ASN:O	6:F:362:ARG:NH1	2.38	0.56
25:Y:186:LEU:HD21	25:Y:214:MET:HE1	1.86	0.56
26:Z:148:GLY:HA3	27:a:181:GLY:HA3	1.85	0.56
16:p:71:LEU:HD11	16:p:82:ILE:HG21	1.87	0.56
19:s:148:LEU:HD23	19:s:178:VAL:HG12	1.85	0.56
35:E:401:ATP:O3G	6:F:347:ARG:NH2	2.37	0.56
25:Y:246:ILE:HG22	25:Y:250:LEU:HD23	1.86	0.56
26:Z:226:ILE:O	26:Z:229:GLN:N	2.39	0.56
3:C:83:LYS:HD2	3:C:105:ILE:HD11	1.85	0.56
6:F:228:PRO:O	6:F:233:LYS:NZ	2.38	0.56
32:f:285:CYS:O	32:f:291:GLN:NE2	2.37	0.56
4:D:116:LEU:HD23	4:D:118:THR:H	1.71	0.56
26:Z:215:VAL:HA	26:Z:220:LEU:HB2	1.87	0.56
5:E:56:ILE:HB	5:E:100:LEU:HB2	1.87	0.56
22:V:105:SER:OG	22:V:106:ARG:NH1	2.39	0.56
27:a:341:LEU:HD13	27:a:345:GLN:HB2	1.87	0.56
2:B:103:ARG:HE	2:B:107:MET:HE1	1.70	0.56
3:C:198:LEU:HD23	37:C:501:ADP:H5'2	1.87	0.56
21:U:333:MET:O	21:U:337:LEU:HB2	2.06	0.56
21:U:678:ASP:O	21:U:684:ARG:NH1	2.37	0.56
4:D:374:ASP:HB3	5:E:292:PRO:HG2	1.87	0.55
16:P:65:GLN:OE1	17:Q:86:ARG:NH2	2.39	0.55
29:c:187:PRO:HB3	29:c:196:LEU:HD21	1.88	0.55
12:l:88:MET:HE3	12:l:108:LEU:HD21	1.87	0.55
33:u:1:MET:HG3	33:u:63:LYS:HB2	1.88	0.55
32:f:827:PRO:HB2	32:f:829:MET:HG2	1.88	0.55
5:E:241:ARG:NH2	5:E:283:ASP:O	2.40	0.55
6:F:195:ILE:HG12	6:F:236:LEU:HD21	1.88	0.55
20:T:25:ASP:OD1	20:T:41:ARG:NH2	2.37	0.55
23:W:422:ASN:HD21	29:c:235:SER:HA	1.71	0.55
26:Z:263:ALA:HB1	29:c:288:VAL:HG13	1.88	0.55
7:g:84:THR:OG1	7:g:88:ARG:NH1	2.39	0.55
1:A:307:ASP:OD2	1:A:333:ARG:NH2	2.40	0.55
1:A:431:THR:O	1:A:433:ASN:ND2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:GLN:HB2	3:C:118:ASN:HD21	1.71	0.55
23:W:60:MET:HE2	23:W:99:GLN:HB2	1.89	0.55
23:W:444:HIS:CE1	26:Z:204:LYS:HB3	2.42	0.55
32:f:894:LEU:HA	32:f:898:VAL:HG21	1.87	0.55
2:B:48:LYS:HE3	32:f:673:ARG:HD3	1.89	0.55
6:F:252:ALA:HB3	6:F:255:GLN:HB2	1.89	0.55
1:A:69:ASP:HB2	1:A:72:LEU:H	1.71	0.55
6:F:43:GLN:HG2	6:F:47:LEU:HD23	1.89	0.55
24:X:74:ARG:HH22	24:X:116:TRP:HB2	1.72	0.55
20:t:25:ASP:HA	20:t:187:PHE:HA	1.89	0.55
33:u:39:ASP:O	33:u:42:ARG:NH1	2.40	0.55
6:F:153:VAL:HG22	6:F:160:ILE:HG22	1.88	0.55
23:W:406:VAL:HG23	24:X:342:PHE:HB3	1.89	0.55
5:E:117:PRO:HD3	6:F:94:ILE:HG23	1.89	0.55
8:H:143:ARG:NH1	8:H:144:PRO:O	2.40	0.55
21:U:376:MET:HA	21:U:739:ALA:HA	1.89	0.55
16:p:71:LEU:HB2	16:p:90:MET:HE1	1.89	0.55
19:s:27:THR:HB	19:s:40:SER:H	1.72	0.55
22:V:259:LEU:HD11	22:V:294:ARG:HD3	1.89	0.54
27:a:102:GLU:O	27:a:105:LYS:NZ	2.38	0.54
11:k:13:ASN:HB2	12:l:126:ARG:HG2	1.89	0.54
19:s:4:PRO:HG3	20:t:103:MET:HE1	1.88	0.54
7:G:6:SER:OG	7:G:11:ARG:NH1	2.40	0.54
21:U:13:ASP:OD1	21:U:44:LYS:NZ	2.38	0.54
21:U:798:PRO:O	21:U:880:ASN:ND2	2.40	0.54
28:b:124:LEU:HD13	28:b:156:PHE:HB2	1.88	0.54
29:c:173:GLU:OE1	29:c:175:ARG:NH2	2.39	0.54
7:g:11:ARG:O	7:g:24:GLN:NE2	2.39	0.54
21:U:1:MET:HG2	22:V:225:ASP:HB3	1.89	0.54
25:Y:360:ASP:OD2	25:Y:363:ASN:ND2	2.41	0.54
29:c:30:GLN:HB3	29:c:66:THR:HG22	1.90	0.54
11:k:167:ALA:HB3	12:l:56:LEU:HD13	1.89	0.54
3:C:135:VAL:HG12	3:C:139:MET:HE2	1.87	0.54
7:G:153:LYS:HB3	7:G:163:PHE:HE2	1.73	0.54
25:Y:188:CYS:SG	25:Y:196:GLN:NE2	2.80	0.54
7:G:158:GLY:O	8:H:84:ARG:NH2	2.40	0.54
22:V:477:HIS:ND1	30:d:249:TYR:OH	2.37	0.54
1:A:128:GLN:HG2	1:A:129:VAL:HG13	1.90	0.54
2:B:288:ASP:N	2:B:288:ASP:OD1	2.39	0.54
21:U:401:LYS:HB3	21:U:438:GLN:HB2	1.89	0.54
21:U:520:MET:HG3	21:U:555:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:349:ARG:NH2	31:e:39:TRP:O	2.41	0.54
7:g:2:SER:C	7:g:4:GLY:H	2.14	0.54
11:k:129:ASP:N	11:k:129:ASP:OD1	2.41	0.54
1:A:119:ALA:HB2	6:F:128:THR:HG23	1.89	0.54
4:D:52:GLU:OE2	21:U:596:ASN:ND2	2.40	0.54
17:Q:4:LEU:HD22	17:Q:45:LEU:HD23	1.90	0.54
19:S:10:GLY:HA3	19:S:42:LYS:HE2	1.88	0.54
6:F:310:MET:HE3	6:F:342:LEU:HD23	1.90	0.54
13:M:161:TRP:HB3	13:M:181:MET:HE3	1.90	0.54
23:W:453:HIS:HD1	23:W:453:HIS:C	2.16	0.54
24:X:134:VAL:HG11	24:X:149:LEU:HD22	1.88	0.54
19:s:158:MET:HE2	19:s:161:VAL:HG21	1.90	0.54
1:A:85:GLN:HA	1:A:88:GLN:HB3	1.90	0.53
21:U:619:VAL:HG23	21:U:651:GLY:HA3	1.89	0.53
7:g:158:GLY:O	8:h:84:ARG:NH2	2.41	0.53
3:C:133:PRO:O	3:C:135:VAL:N	2.41	0.53
5:E:355:ILE:HD11	6:F:211:LYS:HG2	1.89	0.53
22:V:343:PRO:O	31:e:43:TRP:NE1	2.41	0.53
10:j:5:ARG:NH1	11:k:126:GLU:OE2	2.42	0.53
6:F:141:ASP:OD1	6:F:144:LYS:NZ	2.40	0.53
10:J:116:GLN:NE2	11:K:84:ASP:OD1	2.42	0.53
24:X:298:SER:HA	24:X:334:ASN:HD21	1.73	0.53
31:e:37:HIS:CD2	31:e:39:TRP:HB2	2.42	0.53
1:A:277:ILE:HD11	1:A:327:LEU:HD21	1.90	0.53
21:U:599:ILE:HD13	21:U:625:ILE:HD11	1.91	0.53
24:X:187:ARG:HH21	24:X:217:ILE:HG22	1.73	0.53
6:F:153:VAL:HA	6:F:160:ILE:HA	1.91	0.53
11:K:52:LYS:NZ	11:K:64:ILE:O	2.41	0.53
21:U:388:ASP:OD1	21:U:388:ASP:N	2.42	0.53
22:V:284:GLU:OE2	22:V:287:ARG:NH1	2.42	0.53
30:d:52:ARG:HH22	30:d:92:SER:HB3	1.73	0.53
1:A:161:VAL:HA	1:A:164:MET:HE3	1.90	0.53
22:V:76:LYS:HE3	22:V:149:PRO:HB3	1.91	0.53
23:W:129:ARG:NH1	23:W:146:THR:OG1	2.41	0.53
1:A:258:ARG:NH2	1:A:301:GLU:OE1	2.41	0.53
3:C:86:LEU:HD21	3:C:94:LYS:HD3	1.91	0.53
3:C:164:VAL:HG12	3:C:165:ILE:HG13	1.90	0.53
10:J:2:SER:OG	10:J:3:TYR:N	2.41	0.53
28:b:51:LEU:HD11	28:b:61:LEU:HB2	1.90	0.53
4:D:212:LYS:NZ	35:D:501:ATP:O1G	2.37	0.53
26:Z:82:PHE:HA	26:Z:85:VAL:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:214:MET:HE1	35:D:501:ATP:C4	2.44	0.53
23:W:453:HIS:O	23:W:453:HIS:ND1	2.33	0.53
19:S:209:SER:OG	19:S:212:LYS:NZ	2.42	0.52
27:a:217:LEU:HD22	27:a:241:ASN:HD22	1.74	0.52
32:f:96:LEU:HD13	32:f:129:LEU:HD13	1.91	0.52
4:D:266:GLU:OE2	5:E:262:ASN:ND2	2.40	0.52
2:B:252:GLY:HA2	2:B:255:LEU:HD23	1.92	0.52
3:C:90:HIS:CE1	3:C:92:GLU:HB2	2.45	0.52
22:V:150:ARG:NH1	22:V:157:THR:O	2.42	0.52
23:W:55:ARG:NH1	23:W:94:ARG:O	2.42	0.52
4:D:45:LYS:HB3	21:U:187:LEU:HG	1.91	0.52
15:o:1:THR:N	15:o:168:GLY:O	2.42	0.52
1:A:306:LEU:O	1:A:312:ARG:NH1	2.43	0.52
5:E:167:PRO:O	5:E:274:LYS:NZ	2.38	0.52
13:M:230:ASP:N	13:M:230:ASP:OD1	2.42	0.52
16:P:203:ARG:NH2	16:P:205:ASP:OD2	2.41	0.52
12:l:215:VAL:HB	12:l:221:PHE:HD1	1.74	0.52
16:P:34:MET:O	18:r:166:ARG:NH1	2.39	0.52
32:f:565:ASN:O	32:f:565:ASN:ND2	2.42	0.52
8:h:95:GLN:HG3	15:o:65:LEU:HG	1.92	0.52
6:F:180:ARG:NH1	6:F:241:ALA:O	2.43	0.52
6:F:289:ASP:OD1	6:F:289:ASP:N	2.43	0.52
21:U:172:ASP:OD1	21:U:172:ASP:N	2.43	0.52
21:U:418:GLU:HG2	21:U:422:LEU:HB2	1.92	0.52
26:Z:20:VAL:HG13	29:c:212:LEU:HD23	1.91	0.52
11:k:84:ASP:HB3	11:k:137:PHE:HD1	1.74	0.52
1:A:189:GLU:OE2	6:F:409:ARG:NH2	2.42	0.52
27:a:50:PHE:HB2	27:a:52:GLN:HG2	1.92	0.52
12:l:158:ALA:HB1	12:l:172:LEU:HD13	1.91	0.52
5:E:237:ALA:HB1	6:F:308:ARG:HG3	1.91	0.52
17:Q:144:ASP:OD2	18:r:166:ARG:NH2	2.42	0.52
18:R:166:ARG:NH1	16:p:34:MET:O	2.43	0.52
27:a:98:GLU:HG2	27:a:101:ARG:HH21	1.75	0.52
32:f:855:GLN:HB2	32:f:859:PRO:HB3	1.92	0.52
13:M:8:ASP:HB3	13:M:21:PHE:HD2	1.74	0.52
13:M:108:LEU:HD11	13:M:137:LEU:HB3	1.92	0.52
22:V:355:ARG:NE	31:e:31:ASP:OD1	2.36	0.52
23:W:140:ILE:HG12	23:W:177:MET:HE2	1.92	0.52
32:f:46:SER:HB3	32:f:49:ASP:HB2	1.90	0.52
21:U:107:HIS:HA	21:U:110:LYS:HE3	1.92	0.51
21:U:471:ASP:HB2	21:U:507:VAL:HG13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:85:THR:HG22	6:F:87:PRO:HD2	1.92	0.51
27:a:347:LYS:HD3	27:a:350:LYS:HZ1	1.75	0.51
31:e:44:ASP:OD1	31:e:47:ASN:ND2	2.39	0.51
7:g:130:GLU:OE1	8:h:3:GLU:HA	2.09	0.51
11:k:52:LYS:NZ	11:k:64:ILE:O	2.43	0.51
3:C:151:ILE:HG21	3:C:158:ILE:HD11	1.91	0.51
5:E:247:THR:O	5:E:251:ARG:NH1	2.42	0.51
27:a:50:PHE:HD1	27:a:52:GLN:H	1.58	0.51
21:U:580:ARG:HB3	21:U:614:VAL:HG23	1.92	0.51
21:U:894:MET:HE1	21:U:906:LEU:HB3	1.92	0.51
25:Y:26:LEU:HD13	25:Y:63:TRP:HH2	1.74	0.51
17:Q:197:PRO:HD2	17:q:199:GLN:H	1.74	0.51
27:a:193:GLN:HB3	27:a:225:LEU:HD13	1.93	0.51
6:F:101:PRO:HA	6:F:115:SER:HB2	1.92	0.51
15:O:63:LEU:HD11	15:O:79:ALA:HB2	1.91	0.51
22:V:309:MET:HE2	22:V:332:LEU:HB2	1.93	0.51
22:V:417:ILE:HD12	22:V:422:ILE:HB	1.92	0.51
29:c:279:ASP:OD1	29:c:279:ASP:N	2.44	0.51
7:g:141:ILE:HG22	7:g:151:VAL:HG22	1.93	0.51
19:s:114:ASP:OD1	19:s:118:LYS:N	2.39	0.51
21:U:211:PRO:HG2	21:U:244:MET:HE1	1.91	0.51
27:a:346:ILE:HG22	27:a:350:LYS:HZ2	1.75	0.51
32:f:670:MET:SD	32:f:673:ARG:NH2	2.84	0.51
13:m:34:SER:OG	13:m:65:ARG:NH1	2.36	0.51
2:B:235:LEU:HD13	2:B:353:PHE:HZ	1.76	0.51
18:R:133:VAL:HG21	17:q:137:PHE:HB3	1.92	0.51
22:V:131:LEU:HD22	22:V:171:VAL:HG11	1.92	0.51
25:Y:80:GLU:OE2	25:Y:83:ARG:NH2	2.44	0.51
7:g:31:ALA:HB1	7:g:83:MET:HE3	1.93	0.51
14:n:185:GLU:N	14:n:185:GLU:OE2	2.43	0.51
2:B:82:GLN:HG2	32:f:681:TYR:HB3	1.93	0.51
5:E:140:GLU:OE1	5:E:143:ARG:NH2	2.44	0.51
5:E:180:LYS:HG2	5:E:301:ILE:HD12	1.92	0.51
5:E:317:ALA:O	5:E:322:LYS:NZ	2.39	0.51
21:U:522:GLY:O	21:U:559:ARG:NH2	2.44	0.51
26:Z:226:ILE:HG22	26:Z:230:LEU:HB2	1.93	0.51
30:d:114:GLU:HA	30:d:117:THR:HG22	1.93	0.51
2:B:196:GLU:OE2	2:B:349:ARG:NH1	2.42	0.51
3:C:137:LEU:HD11	3:C:220:VAL:HG13	1.93	0.51
6:F:120:LYS:NZ	6:F:120:LYS:H	2.09	0.51
26:Z:62:ASP:N	26:Z:62:ASP:OD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:196:LEU:C	29:c:198:ARG:H	2.19	0.51
22:V:282:ASN:HD21	25:Y:385:ARG:HB3	1.76	0.50
25:Y:89:GLU:HG3	25:Y:93:LYS:HE3	1.93	0.50
19:s:198:VAL:HG22	19:s:203:ILE:HG12	1.93	0.50
5:E:172:LEU:HD22	5:E:301:ILE:HD11	1.92	0.50
8:H:141:GLU:OE2	16:P:80:ARG:NH1	2.43	0.50
10:J:189:LYS:HA	10:J:232:ILE:HD11	1.93	0.50
21:U:632:GLN:O	21:U:635:SER:OG	2.28	0.50
24:X:255:LEU:HD12	24:X:287:LEU:HD13	1.94	0.50
28:b:52:ILE:HD11	28:b:58:CYS:HB3	1.94	0.50
30:d:143:LEU:HD12	30:d:151:VAL:HG21	1.93	0.50
13:M:65:ARG:HH21	13:M:78:ALA:HA	1.77	0.50
18:R:19:ARG:NH1	16:p:205:ASP:O	2.43	0.50
15:o:206:LYS:HD3	16:p:161:ASP:HB3	1.93	0.50
17:Q:13:VAL:HG11	17:Q:105:ALA:HB1	1.94	0.50
22:V:95:LEU:HD11	25:Y:389:MET:HG3	1.93	0.50
13:m:163:CYS:SG	13:m:173:LYS:NZ	2.79	0.50
6:F:336:ASP:OD1	6:F:336:ASP:N	2.44	0.50
21:U:216:VAL:HG23	21:U:220:LEU:HD23	1.94	0.50
33:u:1:MET:CG	33:u:63:LYS:HB2	2.41	0.50
33:u:44:ILE:HB	33:u:68:HIS:HB2	1.94	0.50
5:E:348:THR:HA	6:F:217:ILE:HD11	1.94	0.50
11:K:215:ILE:HD11	11:K:238:ILE:HD11	1.93	0.50
19:S:125:ASP:OD1	19:S:129:SER:N	2.45	0.50
28:b:124:LEU:HD21	28:b:152:LYS:HB3	1.92	0.50
1:A:428:ARG:HD3	2:B:339:PRO:HG3	1.93	0.50
3:C:241:HIS:O	3:C:244:SER:OG	2.29	0.50
3:C:278:ASN:OD1	3:C:310:ARG:NH1	2.43	0.50
21:U:142:LEU:HA	21:U:147:TYR:HE1	1.77	0.50
22:V:82:LEU:HD23	22:V:94:VAL:HG22	1.93	0.50
26:Z:144:VAL:HG22	26:Z:152:SER:H	1.77	0.50
33:u:36:ILE:HB	33:u:41:GLN:HE21	1.75	0.50
4:D:342:ARG:NH2	4:D:361:GLU:OE2	2.44	0.50
22:V:74:ASP:OD2	22:V:107:ARG:NH2	2.45	0.50
22:V:491:VAL:HG11	30:d:257:VAL:HG23	1.92	0.50
12:l:218:ASP:OD1	12:l:218:ASP:N	2.44	0.50
1:A:140:VAL:HG12	1:A:152:PRO:HA	1.94	0.50
21:U:94:SER:HA	21:U:98:GLU:HG3	1.93	0.50
21:U:611:ASN:HB3	21:U:614:VAL:HG12	1.94	0.50
21:U:764:LEU:O	21:U:767:THR:OG1	2.30	0.50
23:W:240:TYR:HA	23:W:243:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:406:VAL:HA	23:W:413:ILE:HG22	1.94	0.50
24:X:35:ILE:HD12	24:X:46:LYS:HD2	1.93	0.50
1:A:180:CYS:HB3	1:A:183:GLN:HB2	1.94	0.49
5:E:199:VAL:HG23	5:E:201:SER:H	1.76	0.49
6:F:120:LYS:H	6:F:120:LYS:HZ1	1.59	0.49
21:U:158:ARG:NH2	21:U:192:GLN:OE1	2.45	0.49
21:U:616:ARG:NH1	21:U:620:GLU:OE2	2.44	0.49
27:a:12:GLN:HG3	27:a:22:TRP:HB3	1.94	0.49
29:c:29:GLU:HB2	29:c:203:ILE:HD11	1.94	0.49
15:o:163:ILE:HG12	15:o:170:GLY:HA2	1.93	0.49
2:B:222:VAL:HG22	2:B:349:ARG:HB2	1.93	0.49
3:C:274:LEU:O	3:C:278:ASN:ND2	2.45	0.49
5:E:102:MET:SD	5:E:102:MET:N	2.85	0.49
29:c:196:LEU:C	29:c:198:ARG:N	2.71	0.49
9:i:62:SER:OG	9:i:65:ILE:O	2.29	0.49
3:C:339:THR:O	3:C:340:ARG:NE	2.41	0.49
4:D:163:MET:SD	4:D:222:HIS:NE2	2.77	0.49
5:E:226:GLN:HG2	5:E:272:ARG:HH21	1.78	0.49
5:E:284:THR:HG22	6:F:297:ASP:HB2	1.94	0.49
21:U:770:TRP:O	29:c:177:THR:OG1	2.29	0.49
27:a:77:VAL:HA	27:a:80:ILE:HG22	1.94	0.49
29:c:54:MET:O	29:c:77:GLN:NE2	2.45	0.49
6:F:358:ASN:HD21	13:M:205:LYS:HD2	1.75	0.49
23:W:16:MET:HE1	23:W:60:MET:H	1.76	0.49
16:p:7:ASN:ND2	16:p:29:GLY:O	2.42	0.49
16:p:30:ILE:HG22	16:p:31:GLN:H	1.77	0.49
19:s:44:TYR:HB2	19:s:52:ILE:HG22	1.94	0.49
11:K:91:LYS:HG2	11:K:119:LEU:HD11	1.93	0.49
23:W:452:ILE:HD13	26:Z:101:LEU:HG	1.95	0.49
24:X:414:LEU:HD22	26:Z:276:ILE:HD11	1.93	0.49
21:U:191:LYS:HA	21:U:194:ARG:HB3	1.95	0.49
21:U:556:MET:HE2	21:U:563:ALA:HB2	1.94	0.49
22:V:311:ASN:HA	22:V:314:ARG:HH11	1.77	0.49
26:Z:68:TRP:CD1	26:Z:104:ASN:HD21	2.30	0.49
6:F:224:LEU:HB2	6:F:348:LEU:HD23	1.94	0.49
21:U:33:ASP:OD2	22:V:229:SER:OG	2.28	0.49
27:a:214:GLY:HA2	27:a:217:LEU:HD13	1.95	0.49
3:C:269:VAL:O	3:C:273:MET:HG2	2.13	0.49
4:D:60:TYR:HB2	21:U:603:LEU:HD21	1.94	0.49
4:D:233:SER:OG	5:E:259:GLU:OE1	2.30	0.49
12:L:44:ALA:HB2	12:L:142:PRO:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:122:LEU:HG	20:T:137:LEU:HD12	1.94	0.49
23:W:67:LEU:HB3	23:W:104:MET:SD	2.53	0.49
26:Z:81:MET:HE1	29:c:94:LYS:HB3	1.94	0.49
30:d:164:THR:HA	30:d:167:ILE:HG12	1.94	0.49
7:g:112:ASP:OD1	7:g:112:ASP:N	2.46	0.49
32:f:566:HIS:HB3	32:f:569:LYS:HE2	1.94	0.49
15:o:22:GLU:HG2	15:o:27:ALA:HB2	1.94	0.49
1:A:330:ALA:O	1:A:336:ARG:NH1	2.45	0.49
3:C:347:ILE:HD12	3:C:350:LEU:HD12	1.94	0.49
6:F:43:GLN:HA	6:F:46:ARG:HG2	1.93	0.49
27:a:153:SER:OG	27:a:154:ARG:NH2	2.46	0.49
6:F:317:LEU:HD13	6:F:328:VAL:HG21	1.94	0.48
7:G:46:ASP:OD1	7:G:46:ASP:N	2.46	0.48
8:H:175:GLU:HG2	9:I:54:LYS:HE2	1.95	0.48
21:U:898:CYS:SG	21:U:899:ARG:N	2.86	0.48
25:Y:67:VAL:O	25:Y:71:ASN:ND2	2.41	0.48
8:h:39:LYS:HG3	8:h:44:VAL:HG22	1.94	0.48
16:p:193:ASP:OD1	16:p:193:ASP:N	2.44	0.48
25:Y:241:ILE:HG12	25:Y:261:PHE:HE1	1.78	0.48
27:a:277:LEU:HD11	27:a:311:VAL:HG12	1.95	0.48
28:b:91:ARG:HH12	28:b:130:ARG:HG2	1.78	0.48
9:i:67:LYS:HE3	9:i:225:ILE:HD12	1.94	0.48
22:V:412:LEU:O	25:Y:346:LYS:NZ	2.45	0.48
11:K:240:ASP:N	11:K:240:ASP:OD1	2.44	0.48
16:P:142:CYS:HB2	16:P:145:GLN:HE21	1.77	0.48
29:c:88:ASP:N	29:c:88:ASP:OD1	2.45	0.48
1:A:250:VAL:HA	1:A:294:GLU:HG3	1.95	0.48
1:A:278:ASP:N	1:A:278:ASP:OD1	2.46	0.48
1:A:287:ASP:OD1	1:A:287:ASP:N	2.46	0.48
21:U:326:ILE:O	21:U:330:SER:OG	2.27	0.48
23:W:224:LEU:O	23:W:228:ASN:ND2	2.46	0.48
26:Z:109:ASN:HD22	26:Z:155:PHE:HE1	1.60	0.48
27:a:34:TRP:HD1	28:b:18:ASN:HA	1.78	0.48
28:b:184:ILE:HA	28:b:187:PRO:HD2	1.95	0.48
7:g:188:ASP:OD1	7:g:188:ASP:N	2.46	0.48
9:i:53:HIS:HB3	9:i:56:LEU:HD23	1.95	0.48
9:i:119:GLN:HG3	10:j:78:ALA:HB1	1.94	0.48
2:B:393:ALA:HB2	35:B:501:ATP:H5'1	1.96	0.48
10:J:31:THR:OG1	10:J:163:ARG:O	2.30	0.48
6:F:111:ILE:HG12	6:F:113:LEU:H	1.79	0.48
21:U:111:GLN:O	21:U:115:ASN:ND2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:203:PRO:HD3	30:d:206:MET:HE1	1.95	0.48
8:h:222:THR:HG23	8:h:225:GLU:H	1.78	0.48
14:n:4:MET:HG3	14:n:127:ILE:HG22	1.95	0.48
3:C:147:THR:HG23	3:C:149:GLU:H	1.78	0.48
15:O:123:PRO:HB3	20:t:214:MET:HE2	1.95	0.48
16:P:193:ASP:OD1	16:P:193:ASP:N	2.46	0.48
22:V:58:ALA:O	22:V:62:HIS:ND1	2.46	0.48
24:X:354:ILE:HG23	24:X:356:LEU:HB3	1.96	0.48
29:c:32:TYR:HE1	29:c:206:ASN:HD21	1.61	0.48
13:m:39:ILE:HD11	13:m:176:ILE:HG12	1.95	0.48
6:F:197:GLU:OE1	6:F:350:ARG:NH2	2.44	0.48
9:I:76:VAL:HG12	9:I:134:LEU:HG	1.96	0.48
19:S:172:MET:HE1	19:S:197:ILE:HG12	1.94	0.48
30:d:149:ASN:HB3	30:d:199:PHE:CE2	2.49	0.48
7:g:61:LEU:HD21	7:g:66:VAL:HG11	1.96	0.48
2:B:76:GLU:HA	2:B:79:ILE:HG12	1.96	0.48
4:D:153:MET:HG2	4:D:227:PHE:HB3	1.96	0.48
21:U:235:LYS:HA	21:U:238:LYS:HD2	1.96	0.48
9:i:46:ALA:HB1	9:i:197:LEU:HD11	1.96	0.48
13:m:68:ASN:OD1	13:m:224:HIS:ND1	2.38	0.48
13:m:230:ASP:OD1	13:m:230:ASP:N	2.47	0.48
3:C:163:GLU:HA	3:C:167:LEU:HD13	1.96	0.47
3:C:191:PRO:HG2	3:C:319:PRO:HG3	1.96	0.47
4:D:385:LEU:HD21	4:D:401:LYS:HD2	1.95	0.47
6:F:180:ARG:HH22	6:F:248:PHE:HB3	1.78	0.47
12:L:155:ASP:HB3	13:M:62:SER:HB2	1.94	0.47
19:S:19:ASP:OD1	19:S:19:ASP:N	2.46	0.47
2:B:406:ALA:HA	2:B:411:ARG:HH21	1.79	0.47
3:C:32:GLN:OE1	3:C:36:ASN:ND2	2.44	0.47
3:C:113:ARG:HD3	3:C:130:LYS:HE2	1.96	0.47
13:M:8:ASP:O	13:M:22:GLN:NE2	2.44	0.47
29:c:113:HIS:NE2	29:c:115:HIS:HE1	1.98	0.47
32:f:832:THR:OG1	32:f:840:LEU:O	2.32	0.47
8:h:175:GLU:OE2	9:i:53:HIS:NE2	2.45	0.47
8:h:204:THR:OG1	8:h:206:ASP:OD1	2.28	0.47
33:u:1:MET:CB	33:u:63:LYS:HB2	2.44	0.47
17:Q:1:MET:HE2	17:Q:133:GLY:HA2	1.95	0.47
21:U:160:LEU:HD11	21:U:196:LYS:HB3	1.96	0.47
21:U:234:GLU:HG2	21:U:238:LYS:HE3	1.95	0.47
21:U:337:LEU:HG	21:U:789:ILE:HD13	1.95	0.47
30:d:204:LYS:HA	30:d:204:LYS:HD3	1.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:215:TRP:CD1	13:m:227:VAL:HG22	2.49	0.47
14:n:104:ASP:OD1	14:n:104:ASP:N	2.47	0.47
6:F:363:ALA:HA	6:F:366:MET:HE2	1.95	0.47
21:U:243:LEU:HD22	21:U:903:PHE:HD2	1.79	0.47
19:s:19:ASP:OD1	19:s:19:ASP:N	2.46	0.47
6:F:375:VAL:HG22	6:F:415:LEU:HD12	1.95	0.47
12:L:50:LYS:HB3	12:L:59:HIS:HB3	1.97	0.47
21:U:619:VAL:HG11	21:U:648:VAL:HG13	1.95	0.47
24:X:299:LEU:H	24:X:334:ASN:HD21	1.61	0.47
27:a:347:LYS:HA	27:a:350:LYS:HZ3	1.79	0.47
28:b:8:VAL:HA	28:b:110:ILE:HG13	1.96	0.47
29:c:269:GLN:HA	29:c:272:ILE:HG12	1.96	0.47
30:d:103:LEU:HD23	30:d:136:PRO:HB2	1.95	0.47
30:d:122:LEU:HB3	30:d:125:LYS:HB2	1.96	0.47
13:m:109:LYS:HA	13:m:149:TYR:HE2	1.79	0.47
1:A:142:VAL:HG22	1:A:149:ILE:HA	1.97	0.47
1:A:258:ARG:HH12	6:F:255:GLN:HA	1.78	0.47
3:C:49:ARG:NH1	21:U:639:LEU:O	2.47	0.47
11:K:107:MET:HE3	11:K:112:VAL:HG22	1.95	0.47
17:Q:137:PHE:HB3	18:r:133:VAL:HG21	1.97	0.47
23:W:431:LYS:HD2	26:Z:238:PRO:HG3	1.96	0.47
9:i:234:GLU:HA	9:i:237:ILE:HG12	1.97	0.47
16:p:67:LEU:HD11	16:p:91:VAL:HG22	1.95	0.47
3:C:184:LYS:N	3:C:312:ASP:OD2	2.43	0.47
4:D:97:ASP:OD1	4:D:97:ASP:N	2.47	0.47
4:D:150:SER:HB3	4:D:228:ILE:HG23	1.96	0.47
4:D:335:LEU:HD21	4:D:369:LYS:HB2	1.96	0.47
5:E:72:LYS:HB2	5:E:78:ARG:HG2	1.96	0.47
15:O:164:PHE:O	19:s:38:ARG:NH2	2.48	0.47
20:T:25:ASP:HA	20:T:187:PHE:HA	1.96	0.47
22:V:219:GLU:OE2	22:V:256:ARG:NH1	2.47	0.47
22:V:262:SER:O	30:d:121:ARG:NH1	2.47	0.47
23:W:453:HIS:C	23:W:453:HIS:ND1	2.73	0.47
25:Y:231:LEU:HD12	25:Y:234:PRO:HG2	1.96	0.47
25:Y:314:LEU:O	25:Y:354:VAL:N	2.41	0.47
27:a:27:GLU:O	27:a:30:THR:OG1	2.30	0.47
10:j:31:THR:OG1	10:j:163:ARG:O	2.31	0.47
15:o:63:LEU:HD11	15:o:79:ALA:HB2	1.95	0.47
1:A:44:GLN:OE1	1:A:47:GLN:NE2	2.36	0.47
3:C:248:MET:SD	3:C:248:MET:N	2.88	0.47
6:F:421:MET:HA	6:F:424:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:92:LEU:HD23	19:S:124:PHE:HE2	1.79	0.47
21:U:371:ILE:HD11	21:U:777:HIS:CD2	2.50	0.47
29:c:216:MET:HB3	29:c:216:MET:HE3	1.78	0.47
1:A:113:ILE:HD11	1:A:142:VAL:HG21	1.97	0.47
3:C:185:GLY:N	3:C:312:ASP:OD2	2.39	0.47
17:Q:11:ASP:N	17:Q:11:ASP:OD1	2.48	0.47
19:S:198:VAL:HG22	19:S:203:ILE:HG12	1.97	0.47
23:W:359:VAL:HG23	23:W:382:LEU:HD22	1.96	0.47
23:W:374:THR:HG22	23:W:412:ILE:HG13	1.96	0.47
27:a:15:GLY:O	27:a:18:GLN:NE2	2.37	0.47
27:a:70:ARG:HD3	28:b:17:ARG:HG2	1.97	0.47
7:g:165:ALA:HB1	7:g:179:LEU:HD13	1.97	0.47
1:A:429:TYR:HE2	2:B:340:ALA:HB2	1.80	0.47
5:E:55:GLN:N	6:F:133:PHE:O	2.46	0.47
5:E:84:ARG:HB2	5:E:87:LEU:HD23	1.96	0.47
7:G:49:VAL:HG22	7:G:219:VAL:HG22	1.96	0.47
9:I:72:MET:HE2	9:I:72:MET:HB3	1.80	0.47
14:N:165:GLU:OE2	20:t:37:ARG:NH1	2.48	0.47
20:T:92:LEU:HD12	20:T:112:ILE:HD11	1.95	0.47
11:k:25:GLU:HA	11:k:28:ILE:HD12	1.95	0.47
11:k:157:ASP:OD1	11:k:161:THR:N	2.48	0.47
23:W:445:LEU:HD22	26:Z:157:HIS:HB2	1.97	0.46
24:X:173:GLU:HA	24:X:176:THR:HG22	1.97	0.46
33:u:1:MET:CG	33:u:63:LYS:CB	2.91	0.46
5:E:121:ASN:OD1	6:F:146:LYS:NZ	2.47	0.46
9:I:41:ASP:OD1	9:I:41:ASP:N	2.49	0.46
13:M:35:THR:HA	13:M:166:GLY:HA3	1.97	0.46
13:M:46:VAL:HG22	13:M:215:TRP:HB3	1.97	0.46
13:M:152:ASP:OD1	13:M:156:VAL:N	2.42	0.46
16:P:38:ASP:OD1	16:P:38:ASP:N	2.46	0.46
27:a:54:ASP:N	27:a:54:ASP:OD1	2.46	0.46
27:a:243:GLY:HA2	27:a:275:LEU:HG	1.97	0.46
29:c:189:ILE:HD12	29:c:192:LEU:HD11	1.98	0.46
12:l:7:ASP:O	12:l:21:GLN:NE2	2.42	0.46
17:q:35:MET:HG2	17:q:45:LEU:HG	1.97	0.46
2:B:96:ARG:HH22	3:C:82:LYS:HE2	1.80	0.46
29:c:39:LEU:HD23	29:c:42:LEU:HD21	1.98	0.46
31:e:16:ASP:OD1	31:e:16:ASP:N	2.46	0.46
5:E:116:ASP:O	5:E:118:LEU:N	2.48	0.46
10:J:67:ASP:OD1	10:J:67:ASP:N	2.48	0.46
11:K:167:ALA:HB3	12:L:56:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:161:ASP:OD1	21:U:161:ASP:N	2.47	0.46
21:U:643:SER:O	21:U:649:ARG:NH1	2.47	0.46
25:Y:14:ASN:HB3	25:Y:143:TYR:HE1	1.81	0.46
32:f:438:ASP:OD1	32:f:438:ASP:N	2.48	0.46
12:l:116:THR:HG22	12:l:128:TYR:HD2	1.81	0.46
33:u:54:ARG:NH2	33:u:58:ASP:HB3	2.30	0.46
4:D:87:LEU:HD22	4:D:140:VAL:HG21	1.97	0.46
4:D:159:LYS:HD2	4:D:221:HIS:HA	1.97	0.46
4:D:363:TYR:HE2	4:D:399:PHE:HB3	1.80	0.46
6:F:168:TYR:O	6:F:173:LYS:NZ	2.48	0.46
6:F:303:ASP:N	6:F:303:ASP:OD1	2.49	0.46
12:L:157:ARG:NH1	12:L:176:MET:SD	2.85	0.46
24:X:194:ARG:NH1	24:X:231:TYR:OH	2.41	0.46
31:e:35:ASP:HB3	31:e:37:HIS:ND1	2.30	0.46
13:m:8:ASP:OD1	13:m:8:ASP:N	2.47	0.46
1:A:75:PRO:HA	1:A:78:TRP:HE1	1.80	0.46
11:K:146:VAL:HG11	11:K:222:PRO:HA	1.97	0.46
21:U:54:PHE:CB	21:U:57:ARG:HD2	2.31	0.46
21:U:801:GLN:HB3	21:U:877:LEU:HD22	1.97	0.46
32:f:120:ARG:HG2	32:f:146:GLY:HA2	1.97	0.46
32:f:140:LEU:HD23	32:f:165:GLU:HB3	1.96	0.46
11:k:98:ASN:OD1	18:r:61:ARG:NH2	2.48	0.46
12:l:117:GLN:NE2	13:m:83:ASP:OD1	2.49	0.46
16:p:34:MET:HE3	16:p:34:MET:HB3	1.81	0.46
1:A:171:ASP:N	1:A:171:ASP:OD1	2.47	0.46
3:C:89:VAL:HG23	3:C:92:GLU:HB3	1.97	0.46
6:F:119:GLY:O	6:F:120:LYS:C	2.58	0.46
19:S:13:LEU:HD12	19:S:145:LEU:HD13	1.98	0.46
22:V:140:ASP:OD1	22:V:140:ASP:N	2.46	0.46
26:Z:69:PHE:HE2	28:b:95:LEU:HB3	1.81	0.46
26:Z:142:GLU:OE2	26:Z:153:LYS:NZ	2.49	0.46
1:A:252:GLU:OE2	1:A:255:ARG:NH2	2.48	0.46
1:A:394:MET:HE1	2:B:211:TYR:HE1	1.80	0.46
4:D:254:ALA:HB2	4:D:262:ILE:HD11	1.98	0.46
4:D:339:ARG:HH21	4:D:343:LEU:HD21	1.80	0.46
4:D:384:MET:SD	5:E:297:ARG:NH2	2.89	0.46
19:S:172:MET:HE2	19:S:172:MET:HB2	1.75	0.46
21:U:381:THR:HG22	21:U:412:HIS:HA	1.98	0.46
23:W:267:LEU:HD23	23:W:299:ILE:HD12	1.98	0.46
13:M:43:ASP:OD1	13:M:43:ASP:N	2.49	0.46
24:X:360:ASP:OD1	24:X:360:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:4:GLY:O	7:g:5:SER:HB2	2.15	0.46
9:i:71:ASP:OD1	9:i:139:TRP:N	2.48	0.46
7:G:155:ASP:OD1	7:G:159:TYR:N	2.47	0.45
26:Z:120:VAL:HG22	26:Z:139:ILE:HD13	1.98	0.45
27:a:321:LYS:O	27:a:334:THR:OG1	2.32	0.45
28:b:6:THR:HB	28:b:49:VAL:HG22	1.98	0.45
19:s:10:GLY:HA3	19:s:42:LYS:HE2	1.98	0.45
20:t:54:SER:O	20:t:108:ASN:ND2	2.39	0.45
20:t:126:ASP:OD1	20:t:130:VAL:N	2.49	0.45
5:E:376:ASP:OD1	5:E:376:ASP:N	2.50	0.45
13:M:163:CYS:SG	13:M:164:ALA:N	2.88	0.45
17:Q:44:LEU:HD11	17:Q:102:LEU:HD22	1.98	0.45
21:U:879:ASP:OD1	21:U:879:ASP:N	2.49	0.45
22:V:98:LEU:HD13	22:V:209:LYS:HE2	1.98	0.45
25:Y:286:TRP:HD1	25:Y:287:LEU:HD12	1.81	0.45
25:Y:364:TRP:NE1	25:Y:368:GLU:OE2	2.49	0.45
10:j:168:VAL:HG23	10:j:194:ALA:HB1	1.98	0.45
20:t:25:ASP:OD1	20:t:41:ARG:NH2	2.43	0.45
10:J:182:GLU:HB2	10:J:186:LEU:HD12	1.99	0.45
21:U:596:ASN:HA	21:U:599:ILE:HG22	1.97	0.45
3:C:41:ASN:OD1	3:C:44:ARG:NH2	2.41	0.45
35:E:401:ATP:O2A	6:F:344:ARG:NH1	2.49	0.45
7:G:188:ASP:OD1	7:G:188:ASP:N	2.49	0.45
21:U:111:GLN:NE2	21:U:114:GLU:OE1	2.48	0.45
22:V:95:LEU:HA	22:V:98:LEU:HG	1.98	0.45
28:b:109:ILE:HB	28:b:138:VAL:HG13	1.99	0.45
1:A:213:LEU:HD21	1:A:340:LYS:HG2	1.98	0.45
2:B:214:MET:HB3	2:B:216:ILE:HG22	1.97	0.45
6:F:96:LEU:HD11	6:F:142:ALA:HB1	1.99	0.45
22:V:75:ILE:HD11	22:V:108:LEU:HD21	1.98	0.45
26:Z:65:ASP:OD1	26:Z:65:ASP:N	2.46	0.45
29:c:94:LYS:HG2	29:c:98:MET:HE3	1.98	0.45
29:c:125:VAL:HG21	34:v:25:LYS:HD2	1.98	0.45
2:B:343:ARG:HE	2:B:346:ARG:NH1	2.14	0.45
5:E:223:ARG:NH1	5:E:268:ASP:OD2	2.50	0.45
6:F:410:ARG:NH2	6:F:416:THR:OG1	2.49	0.45
12:L:72:ILE:HD13	12:L:88:MET:HE1	1.98	0.45
21:U:101:ILE:HG22	21:U:133:ILE:HD11	1.98	0.45
21:U:413:LYS:HD2	21:U:780:SER:HB2	1.99	0.45
23:W:444:HIS:HE1	26:Z:204:LYS:HB3	1.80	0.45
24:X:380:GLN:HG3	25:Y:314:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:26:LEU:HD21	28:b:80:PRO:HG3	1.98	0.45
32:f:266:LEU:HD12	32:f:266:LEU:HA	1.83	0.45
11:k:36:THR:HA	11:k:171:GLY:HA3	1.98	0.45
11:k:210:LEU:HD12	11:k:215:ILE:HD13	1.97	0.45
11:k:228:MET:HE2	11:k:228:MET:HB2	1.83	0.45
3:C:25:LEU:HA	3:C:28:ILE:HG22	1.98	0.45
6:F:219:PRO:HG2	6:F:324:THR:HG21	1.98	0.45
6:F:439:ALA:HB1	12:L:62:LYS:HE3	1.99	0.45
9:I:155:ASN:OD1	10:J:77:THR:OG1	2.35	0.45
21:U:42:VAL:HG11	21:U:67:VAL:HG11	1.98	0.45
21:U:428:PRO:HA	21:U:439:GLU:HB2	1.99	0.45
23:W:444:HIS:CD2	26:Z:208:ILE:HD12	2.52	0.45
24:X:334:ASN:O	24:X:338:VAL:HG22	2.17	0.45
16:p:135:ASP:OD1	16:p:135:ASP:N	2.49	0.45
16:p:203:ARG:NH2	16:p:205:ASP:OD2	2.49	0.45
1:A:275:ASP:OD1	1:A:275:ASP:N	2.49	0.45
2:B:339:PRO:HA	2:B:342:ILE:HG12	1.98	0.45
2:B:387:LYS:HB3	2:B:390:LEU:HB3	1.98	0.45
3:C:227:GLY:HA3	3:C:229:ARG:HH11	1.81	0.45
3:C:273:MET:HG3	3:C:293:MET:HE2	1.97	0.45
4:D:147:ALA:HB3	5:E:62:LYS:HD2	1.98	0.45
6:F:366:MET:HE3	6:F:381:TYR:HD1	1.82	0.45
11:K:147:ASP:OD1	11:K:147:ASP:N	2.48	0.45
17:Q:26:VAL:HG21	18:R:136:TYR:HE2	1.81	0.45
25:Y:293:ARG:HH12	31:e:49:GLU:HG2	1.82	0.45
30:d:99:LEU:HB3	30:d:133:ILE:HD11	1.98	0.45
32:f:543:MET:HE1	32:f:582:VAL:HB	1.99	0.45
32:f:809:ILE:HG23	32:f:814:SER:HB2	1.98	0.45
7:g:125:TYR:HA	7:g:131:MET:HE2	1.98	0.45
24:X:251:LEU:HA	24:X:254:MET:HE2	1.99	0.45
26:Z:43:TRP:HB3	26:Z:90:ARG:HH21	1.82	0.45
27:a:245:VAL:HG11	27:a:301:LYS:HD3	1.98	0.45
29:c:89:PRO:HG2	33:u:44:ILE:HD11	1.98	0.45
11:k:78:MET:HE1	11:k:82:ILE:HG22	1.99	0.45
17:q:4:LEU:HD22	17:q:45:LEU:HD23	1.99	0.45
17:q:44:LEU:HD21	17:q:102:LEU:HD22	1.99	0.45
11:K:235:GLU:HA	11:K:238:ILE:HB	1.99	0.45
17:Q:31:ASP:OD1	17:Q:31:ASP:N	2.48	0.45
21:U:187:LEU:O	21:U:188:MET:HE2	2.16	0.45
22:V:131:LEU:HD13	22:V:171:VAL:HG21	1.99	0.45
30:d:23:LEU:O	30:d:27:LYS:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:447:ALA:HA	32:f:450:ILE:HD12	1.99	0.45
1:A:351:ARG:NH1	1:A:378:PRO:O	2.50	0.44
6:F:118:LYS:O	6:F:119:GLY:C	2.59	0.44
12:L:176:MET:HE2	12:L:176:MET:HB3	1.83	0.44
24:X:357:SER:OG	24:X:358:LYS:N	2.50	0.44
24:X:380:GLN:N	25:Y:313:SER:O	2.50	0.44
25:Y:286:TRP:CD1	25:Y:287:LEU:HD12	2.52	0.44
29:c:107:MET:SD	33:u:10:GLY:CA	3.05	0.44
13:m:129:ARG:NH2	13:m:131:PHE:HA	2.31	0.44
19:s:83:MET:HG2	19:s:88:ILE:HG13	1.97	0.44
6:F:39:GLU:HB3	6:F:43:GLN:HB2	1.99	0.44
32:f:175:ASP:N	32:f:175:ASP:OD1	2.50	0.44
32:f:776:LEU:HD13	32:f:825:MET:HE3	1.98	0.44
7:g:128:ASN:HB2	7:g:131:MET:HE1	2.00	0.44
2:B:223:ILE:HA	2:B:329:MET:HB3	1.99	0.44
22:V:80:LYS:HB3	22:V:84:LYS:HZ3	1.81	0.44
26:Z:59:ASP:OD2	28:b:99:HIS:NE2	2.51	0.44
29:c:63:ASP:OD1	29:c:66:THR:OG1	2.27	0.44
30:d:200:PHE:O	30:d:203:PRO:HD3	2.17	0.44
32:f:266:LEU:HD11	32:f:278:VAL:HG13	1.98	0.44
34:v:24:UNK:O	34:v:26:UNK:N	2.50	0.44
21:U:19:LEU:HG	30:d:27:LYS:HZ3	1.82	0.44
22:V:345:ARG:HE	31:e:43:TRP:HA	1.82	0.44
24:X:154:LEU:HB3	24:X:158:LYS:HE3	1.98	0.44
24:X:218:HIS:HD2	24:X:228:ALA:HB2	1.81	0.44
32:f:348:ILE:O	32:f:350:LYS:NZ	2.51	0.44
4:D:352:MET:HE1	4:D:379:CYS:HB3	1.99	0.44
16:P:27:ARG:HB2	16:P:183:MET:HB2	2.00	0.44
19:S:52:ILE:HG13	19:S:110:ILE:HG12	2.00	0.44
22:V:245:ASP:N	22:V:245:ASP:OD1	2.50	0.44
26:Z:37:GLY:HA2	26:Z:56:VAL:HG12	2.00	0.44
30:d:203:PRO:CD	30:d:206:MET:HE1	2.47	0.44
32:f:402:ASN:HB2	32:f:407:MET:HB2	1.99	0.44
16:p:35:VAL:HG12	16:p:36:THR:HG23	1.99	0.44
16:p:125:ASP:OD1	16:p:129:CYS:N	2.37	0.44
33:u:26:VAL:HA	33:u:29:LYS:HE2	1.98	0.44
2:B:107:MET:HG3	3:C:96:VAL:HB	2.00	0.44
3:C:187:LEU:HD23	3:C:314:LYS:HG2	1.98	0.44
4:D:150:SER:O	4:D:151:ILE:C	2.60	0.44
16:P:45:MET:HE3	16:P:67:LEU:HD23	1.99	0.44
21:U:57:ARG:CG	21:U:57:ARG:NH1	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:175:ASN:HB3	10:j:190:LEU:HD22	2.00	0.44
5:E:182:LEU:HD22	35:E:401:ATP:H2'	2.00	0.44
20:T:63:LEU:HD21	20:T:106:LEU:HD13	1.99	0.44
22:V:173:ILE:HD11	22:V:213:TYR:CD2	2.53	0.44
26:Z:205:LEU:HA	26:Z:208:ILE:HG22	1.98	0.44
30:d:82:TYR:HE2	30:d:98:LEU:HD23	1.83	0.44
13:m:8:ASP:O	13:m:22:GLN:NE2	2.41	0.44
13:m:27:MET:HA	13:m:30:VAL:HG12	2.00	0.44
5:E:328:TYR:HA	5:E:331:ILE:HD12	2.00	0.44
10:J:42:VAL:HG11	10:J:191:VAL:HG21	1.99	0.44
21:U:740:GLY:HA3	21:U:744:VAL:HG22	2.00	0.44
32:f:65:GLU:O	32:f:67:ASP:N	2.51	0.44
7:g:88:ARG:HB3	13:m:117:MET:HE1	1.99	0.44
12:l:84:LEU:HD23	12:l:132:LEU:HD11	1.99	0.44
13:m:136:MET:HE3	13:m:150:MET:HG3	2.00	0.44
1:A:124:ASP:HB2	6:F:86:LEU:HD22	2.00	0.44
19:S:91:MET:HE2	19:S:91:MET:HB3	1.93	0.44
20:T:185:ASN:OD1	20:T:205:THR:OG1	2.31	0.44
21:U:82:LEU:HG	21:U:129:ARG:HB2	2.00	0.44
21:U:602:LEU:HD21	21:U:621:SER:HB2	2.00	0.44
29:c:84:VAL:HG12	33:u:75:GLY:O	2.18	0.44
9:I:71:ASP:OD2	9:I:139:TRP:N	2.43	0.43
13:M:50:GLU:OE2	13:M:201:HIS:ND1	2.39	0.43
21:U:191:LYS:HE3	21:U:195:ASN:HB3	2.00	0.43
32:f:341:GLU:HB2	32:f:343:LYS:HZ2	1.82	0.43
32:f:386:GLY:HA2	32:f:418:LEU:HG	2.00	0.43
11:K:156:MET:HE3	11:K:156:MET:HB3	1.95	0.43
12:L:226:ASP:OD1	12:L:227:ASP:N	2.51	0.43
27:a:346:ILE:HA	27:a:349:MET:SD	2.58	0.43
32:f:791:VAL:HG12	32:f:823:ALA:HB1	2.00	0.43
10:j:148:ASP:OD1	10:j:152:THR:N	2.43	0.43
18:r:44:THR:HG21	18:r:100:MET:HE2	2.01	0.43
19:s:37:THR:OG1	19:s:39:ASP:OD1	2.35	0.43
4:D:315:ASP:N	4:D:315:ASP:OD1	2.51	0.43
12:L:117:GLN:O	12:L:120:THR:OG1	2.33	0.43
22:V:119:GLY:HA2	22:V:148:ARG:HD3	2.01	0.43
22:V:467:TYR:OH	24:X:397:TYR:OH	2.29	0.43
24:X:281:GLY:H	24:X:284:THR:HG22	1.84	0.43
25:Y:155:ASP:OD1	25:Y:155:ASP:N	2.50	0.43
27:a:341:LEU:HB2	27:a:345:GLN:HG3	2.00	0.43
28:b:9:CYS:HB3	28:b:111:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:e:37:HIS:HD2	31:e:39:TRP:HB2	1.81	0.43
3:C:49:ARG:HB2	4:D:61:ILE:HG23	2.00	0.43
9:I:119:GLN:HG3	10:J:78:ALA:HB1	2.00	0.43
14:N:86:MET:HE3	14:N:86:MET:HB2	1.79	0.43
27:a:343:LEU:HA	27:a:346:ILE:HD12	2.00	0.43
12:l:88:MET:HG2	12:l:112:ILE:HD11	2.00	0.43
14:n:94:LEU:O	14:n:95:MET:HE2	2.18	0.43
17:q:11:ASP:N	17:q:11:ASP:OD1	2.50	0.43
3:C:40:GLN:OE1	22:V:495:ARG:NH1	2.52	0.43
5:E:171:LEU:HD21	5:E:298:LYS:HG2	2.01	0.43
5:E:360:ASP:OD1	5:E:360:ASP:N	2.52	0.43
8:H:93:LEU:HD13	8:H:113:ARG:HB3	1.99	0.43
26:Z:77:ASN:HB3	29:c:98:MET:HE1	1.99	0.43
27:a:152:HIS:CE1	27:a:178:ARG:HB3	2.53	0.43
30:d:42:LYS:HD2	30:d:45:LYS:HD2	2.01	0.43
32:f:106:LEU:HA	32:f:109:ILE:HB	2.01	0.43
32:f:755:ASP:OD2	32:f:758:ASN:ND2	2.34	0.43
12:l:134:ILE:HB	12:l:145:PHE:HB2	2.01	0.43
33:u:24:GLU:HB3	33:u:52:ASP:HB3	2.00	0.43
2:B:181:GLN:O	2:B:241:ASN:ND2	2.52	0.43
9:I:197:LEU:HA	9:I:200:THR:HG22	1.99	0.43
28:b:38:HIS:HE1	28:b:72:LEU:HD11	1.84	0.43
14:n:103:TRP:CZ2	14:n:181:GLU:HG2	2.54	0.43
16:p:205:ASP:OD1	16:p:205:ASP:N	2.51	0.43
4:D:235:PHE:HB3	4:D:288:ILE:HD12	1.99	0.43
5:E:269:THR:O	5:E:271:HIS:ND1	2.45	0.43
14:N:162:LEU:HD11	14:n:141:ALA:HB2	2.01	0.43
21:U:2:ILE:HA	30:d:85:TYR:CZ	2.53	0.43
25:Y:39:ASP:HA	25:Y:42:MET:HE3	2.01	0.43
28:b:108:ARG:NH2	28:b:167:GLY:O	2.48	0.43
20:t:122:LEU:HG	20:t:137:LEU:HD12	2.01	0.43
33:u:54:ARG:HG2	33:u:54:ARG:HH11	1.83	0.43
18:R:106:LYS:HE3	18:R:106:LYS:HB2	1.70	0.43
21:U:749:GLN:NE2	21:U:750:SER:O	2.42	0.43
24:X:364:LYS:HG3	24:X:368:MET:HE1	2.01	0.43
7:g:132:ARG:HA	7:g:133:PRO:HD3	1.87	0.43
16:p:134:ASP:OD1	16:p:134:ASP:N	2.52	0.43
19:s:166:LEU:HD21	19:s:171:ALA:HB2	2.01	0.43
33:u:31:GLN:OE1	33:u:38:PRO:HD3	2.19	0.43
6:F:314:LEU:HD22	6:F:347:ARG:HD3	1.99	0.43
21:U:69:TYR:OH	22:V:236:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:54:THR:O	23:W:58:SER:N	2.51	0.43
23:W:166:LEU:HD22	23:W:192:LEU:HD12	2.01	0.43
7:g:165:ALA:HB3	8:h:56:LEU:HD22	2.00	0.43
19:s:52:ILE:HG13	19:s:110:ILE:HG12	2.00	0.43
2:B:329:MET:HE2	2:B:329:MET:HB2	1.80	0.43
4:D:202:VAL:HG23	4:D:329:ARG:HB3	2.00	0.43
13:M:227:VAL:O	13:M:232:ARG:NH2	2.52	0.43
23:W:272:LEU:HD23	23:W:272:LEU:HA	1.88	0.43
25:Y:221:THR:HG22	25:Y:256:VAL:HG21	2.01	0.43
7:g:112:ASP:HB3	7:g:152:TYR:CZ	2.54	0.43
7:g:130:GLU:HG2	8:h:5:GLY:HA2	2.00	0.43
11:k:107:MET:HG2	11:k:112:VAL:HG23	1.99	0.43
13:m:49:VAL:HB	13:m:212:GLU:HB3	2.01	0.43
13:m:216:VAL:HB	13:m:224:HIS:HA	2.01	0.43
4:D:177:VAL:HG21	4:D:215:LEU:HD21	2.01	0.42
6:F:105:GLU:OE2	6:F:110:ASN:HA	2.19	0.42
6:F:356:MET:HE3	6:F:356:MET:HB2	1.89	0.42
11:K:203:LYS:HB2	11:K:210:LEU:HD22	2.00	0.42
15:O:163:ILE:HG12	15:O:170:GLY:HA2	2.01	0.42
16:P:205:ASP:HB3	18:r:192:VAL:HG11	2.01	0.42
21:U:560:MET:HE1	21:U:590:TYR:HA	2.01	0.42
22:V:461:LYS:NZ	22:V:462:GLU:O	2.52	0.42
23:W:455:LEU:HB2	23:W:456:GLN:NE2	2.33	0.42
27:a:130:VAL:HA	27:a:133:GLU:HB2	2.01	0.42
32:f:862:ILE:H	32:f:862:ILE:HG13	1.61	0.42
10:j:42:VAL:HG22	10:j:210:VAL:HG22	1.99	0.42
2:B:140:ASP:O	2:B:142:ASP:N	2.46	0.42
2:B:183:THR:OG1	2:B:184:TYR:N	2.48	0.42
3:C:72:TYR:N	3:C:116:LEU:O	2.52	0.42
3:C:145:ASP:HA	3:C:201:ARG:HG2	2.01	0.42
3:C:326:LEU:HD12	3:C:344:LEU:HG	2.00	0.42
3:C:371:LEU:HD12	4:D:194:ILE:HD12	2.01	0.42
4:D:259:PRO:HB3	4:D:304:ASN:HB2	2.00	0.42
7:G:112:ASP:OD1	7:G:113:MET:N	2.52	0.42
9:I:116:ASP:OD1	9:I:117:ILE:N	2.51	0.42
10:J:211:MET:HB2	10:J:217:LEU:HD13	2.01	0.42
12:L:140:MET:HE1	20:T:80:GLY:HA3	2.01	0.42
16:P:7:ASN:ND2	16:P:29:GLY:O	2.43	0.42
17:Q:52:ASP:OD1	18:R:91:LYS:NZ	2.51	0.42
21:U:115:ASN:HA	21:U:118:LEU:HD12	2.01	0.42
21:U:128:GLN:NE2	21:U:131:GLU:OE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:701:ILE:HD12	21:U:809:SER:HB2	2.00	0.42
9:i:161:ALA:HB3	10:j:53:LEU:HD23	2.01	0.42
10:j:8:THR:HG22	10:j:16:LEU:HD22	2.02	0.42
3:C:331:ILE:HA	3:C:334:ARG:HH21	1.84	0.42
4:D:125:LYS:HB3	29:c:277:LYS:HZ2	1.83	0.42
10:J:8:THR:HG22	10:J:16:LEU:HD22	2.02	0.42
15:O:42:TYR:HE1	15:O:183:LEU:HD11	1.84	0.42
22:V:80:LYS:HB3	22:V:84:LYS:NZ	2.34	0.42
22:V:461:LYS:HD2	22:V:461:LYS:HA	1.74	0.42
22:V:463:MET:HG3	22:V:466:ILE:HG23	2.00	0.42
27:a:70:ARG:HG3	28:b:17:ARG:HH11	1.82	0.42
20:t:185:ASN:OD1	20:t:205:THR:OG1	2.34	0.42
1:A:217:PRO:O	1:A:220:THR:OG1	2.33	0.42
9:I:76:VAL:HG11	9:I:83:ALA:HB1	2.01	0.42
13:M:8:ASP:OD1	13:M:8:ASP:N	2.45	0.42
23:W:177:MET:HE2	23:W:177:MET:HB3	1.91	0.42
24:X:143:TYR:HD2	24:X:144:GLN:HG2	1.84	0.42
26:Z:138:TYR:HB3	26:Z:155:PHE:HB3	2.00	0.42
28:b:4:GLU:OE1	28:b:6:THR:OG1	2.36	0.42
19:s:125:ASP:OD1	19:s:129:SER:N	2.52	0.42
3:C:24:TYR:HD1	3:C:24:TYR:HA	1.70	0.42
3:C:231:VAL:HG11	3:C:272:THR:HG23	2.00	0.42
4:D:401:LYS:HA	4:D:404:LYS:HE2	2.01	0.42
5:E:382:SER:HB3	6:F:340:PRO:HG3	2.02	0.42
24:X:255:LEU:HD22	24:X:267:VAL:HG13	2.02	0.42
32:f:170:TRP:CD1	32:f:211:ILE:HA	2.54	0.42
34:v:25:LYS:O	34:v:26:UNK:C	2.67	0.42
1:A:116:LYS:NZ	1:A:117:GLN:HE22	2.18	0.42
2:B:387:LYS:HB3	2:B:390:LEU:HD23	2.02	0.42
3:C:67:GLN:HE21	4:D:82:ILE:HD13	1.84	0.42
12:L:182:CYS:HB3	12:L:186:GLU:HB2	2.02	0.42
13:M:68:ASN:OD1	13:M:224:HIS:ND1	2.52	0.42
20:T:96:MET:HE2	20:T:127:MET:HA	2.01	0.42
28:b:3:LEU:HD23	28:b:44:ASN:HD21	1.85	0.42
32:f:163:ALA:HB1	32:f:207:LEU:HD21	2.02	0.42
15:o:187:ARG:HA	15:o:188:PRO:HA	1.91	0.42
17:q:31:ASP:OD1	17:q:31:ASP:N	2.53	0.42
17:q:153:ARG:NH2	17:q:184:ASP:OD1	2.53	0.42
11:K:13:ASN:HB3	12:L:126:ARG:HB3	2.02	0.42
16:P:153:LEU:HB3	16:P:166:THR:HG23	2.01	0.42
18:R:35:ILE:N	18:R:43:GLY:O	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:82:LEU:HD21	21:U:127:ASP:HB3	2.01	0.42
24:X:365:LEU:HA	24:X:368:MET:HE2	2.02	0.42
27:a:122:LYS:HD2	27:a:130:VAL:HG22	2.02	0.42
29:c:64:ASP:OD1	29:c:64:ASP:N	2.53	0.42
30:d:200:PHE:HB2	30:d:205:LYS:HE2	2.02	0.42
32:f:211:ILE:HG23	32:f:213:GLN:H	1.84	0.42
9:i:52:ILE:HD11	9:i:210:LYS:HE2	2.00	0.42
1:A:390:THR:HA	2:B:216:ILE:HD11	2.02	0.42
6:F:288:LEU:HD23	6:F:330:ALA:HB1	2.01	0.42
18:R:19:ARG:HH21	18:R:29:GLN:HE22	1.67	0.42
19:S:16:ALA:HB2	19:S:121:VAL:HG23	2.00	0.42
19:S:211:ARG:HE	15:o:193:ASN:HB3	1.84	0.42
24:X:190:LEU:HD21	24:X:214:SER:HA	2.00	0.42
27:a:274:LEU:HD13	27:a:319:LEU:HD21	2.00	0.42
32:f:99:LEU:HD22	32:f:106:LEU:HD11	2.00	0.42
9:i:3:ARG:NH2	11:k:125:GLU:OE2	2.53	0.42
5:E:97:ARG:NH2	5:E:112:PRO:O	2.50	0.42
5:E:205:ASP:N	5:E:205:ASP:OD1	2.50	0.42
6:F:226:TYR:CZ	6:F:353:GLU:HB3	2.55	0.42
6:F:314:LEU:HD21	6:F:342:LEU:HB3	2.01	0.42
10:J:146:GLN:NE2	10:J:147:THR:O	2.53	0.42
17:Q:102:LEU:HB2	17:Q:118:MET:HB3	2.01	0.42
20:T:92:LEU:HD23	20:T:92:LEU:HA	1.91	0.42
21:U:808:PRO:HB3	21:U:876:GLN:HE22	1.85	0.42
22:V:322:VAL:HG11	31:e:27:TRP:HZ3	1.84	0.42
23:W:452:ILE:HD11	26:Z:100:LYS:HB3	2.01	0.42
24:X:268:GLN:HA	24:X:271:VAL:HG22	2.01	0.42
25:Y:19:ILE:HG21	25:Y:50:MET:HE1	2.02	0.42
28:b:12:ASN:HB3	28:b:78:VAL:HG22	2.01	0.42
18:r:58:LEU:HD12	18:r:61:ARG:HD3	2.01	0.42
19:s:26:ASP:OD1	19:s:26:ASP:N	2.49	0.42
33:u:27:LYS:HB3	33:u:38:PRO:HB3	2.02	0.42
3:C:186:VAL:HB	3:C:292:ILE:HG12	2.02	0.42
6:F:332:THR:HG21	6:F:338:LEU:HD11	2.01	0.42
13:M:37:ILE:HG12	13:M:197:ILE:HD11	2.02	0.42
21:U:42:VAL:HA	21:U:45:ILE:HD13	2.01	0.42
23:W:112:VAL:HG11	23:W:125:ILE:HD11	2.02	0.42
29:c:266:THR:O	29:c:268:GLU:N	2.53	0.42
29:c:296:ILE:HD12	30:d:246:VAL:HG13	2.02	0.42
31:e:57:ARG:O	31:e:60:LEU:HG	2.19	0.42
13:m:136:MET:HE1	13:m:163:CYS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:q:39:SER:OG	17:q:40:GLU:N	2.53	0.42
18:r:97:MET:H	18:r:116:SER:HB3	1.85	0.42
1:A:73:ALA:HB2	2:B:140:ASP:H	1.85	0.41
4:D:276:ASP:N	4:D:282:ASP:OD2	2.52	0.41
5:E:235:ILE:HD12	5:E:277:MET:SD	2.60	0.41
7:G:190:THR:OG1	7:G:193:GLN:OE1	2.32	0.41
26:Z:35:VAL:H	26:Z:97:THR:HG22	1.85	0.41
27:a:230:ARG:HB3	27:a:232:TRP:CD1	2.56	0.41
29:c:196:LEU:HD13	29:c:196:LEU:HA	1.74	0.41
30:d:107:LEU:HD11	30:d:140:GLU:HB2	2.01	0.41
7:g:2:SER:C	7:g:4:GLY:N	2.76	0.41
10:j:184:ASP:O	10:j:187:THR:OG1	2.29	0.41
17:q:1:MET:HE3	17:q:2:GLU:H	1.84	0.41
20:t:92:LEU:HD12	20:t:112:ILE:HD11	2.01	0.41
9:I:174:MET:HB2	9:I:174:MET:HE3	1.77	0.41
23:W:387:ASP:OD1	23:W:387:ASP:N	2.52	0.41
25:Y:141:VAL:HG11	25:Y:164:ALA:HB2	2.02	0.41
25:Y:220:VAL:HA	25:Y:223:THR:HG22	2.01	0.41
32:f:554:TYR:HA	32:f:557:TRP:CD1	2.55	0.41
12:l:26:MET:HE1	12:l:148:CYS:HB3	2.02	0.41
12:l:47:VAL:HG12	12:l:195:LEU:HD22	2.01	0.41
34:v:25:LYS:C	34:v:27:UNK:N	2.77	0.41
1:A:51:ASP:HA	1:A:54:GLN:HG3	2.02	0.41
13:M:37:ILE:HD11	13:M:193:VAL:HG13	2.02	0.41
21:U:337:LEU:HD21	21:U:789:ILE:HG21	2.02	0.41
22:V:264:TYR:HE2	30:d:120:GLU:HG2	1.85	0.41
22:V:479:ARG:HH12	25:Y:370:ILE:HD12	1.84	0.41
29:c:125:VAL:CG2	34:v:25:LYS:HD2	2.50	0.41
30:d:109:GLN:HB3	30:d:111:ARG:HH11	1.85	0.41
13:m:179:LEU:HD12	13:m:184:MET:HE1	2.02	0.41
4:D:323:ARG:HA	4:D:323:ARG:HD3	1.93	0.41
5:E:210:GLU:OE1	5:E:213:ARG:NE	2.45	0.41
5:E:242:ARG:HD3	5:E:242:ARG:HA	1.88	0.41
8:H:203:MET:HA	8:H:207:ASN:HD21	1.85	0.41
16:P:30:ILE:HG22	16:P:31:GLN:H	1.85	0.41
21:U:62:LEU:HD22	21:U:87:LEU:HG	2.01	0.41
21:U:167:ILE:O	21:U:171:ASN:ND2	2.51	0.41
23:W:48:LEU:HA	23:W:51:GLU:HG3	2.01	0.41
32:f:692:LEU:HB3	32:f:800:LEU:HD22	2.03	0.41
16:p:11:VAL:HG23	16:p:54:ALA:HB2	2.01	0.41
16:p:159:ASP:OD1	16:p:162:HIS:ND1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:191:ASP:HA	19:s:212:LYS:HD3	2.01	0.41
20:t:20:VAL:HG11	20:t:122:LEU:HD13	2.02	0.41
20:t:43:MET:HE2	20:t:45:VAL:HA	2.02	0.41
1:A:143:ASP:OD1	1:A:143:ASP:N	2.54	0.41
2:B:234:LEU:HD22	35:B:501:ATP:H2'	2.01	0.41
5:E:219:PHE:HD2	5:E:263:GLN:HB3	1.85	0.41
6:F:35:LYS:HB2	6:F:38:THR:HB	2.02	0.41
6:F:236:LEU:HD23	6:F:236:LEU:HA	1.81	0.41
8:H:135:LEU:HG	8:H:163:MET:HE3	2.02	0.41
8:H:182:LEU:HD22	8:H:186:ASP:HB3	2.02	0.41
14:N:30:VAL:HG11	20:t:211:ILE:HG23	2.01	0.41
21:U:579:ARG:NH1	21:U:609:ASP:OD1	2.53	0.41
27:a:72:ASN:HD21	27:a:74:LEU:HD12	1.86	0.41
28:b:30:GLN:HE22	28:b:75:LEU:HB3	1.85	0.41
29:c:57:MET:HB3	29:c:69:VAL:HG21	2.02	0.41
29:c:291:LEU:HD23	29:c:291:LEU:HA	1.94	0.41
7:g:70:PHE:HD2	7:g:91:VAL:HG21	1.85	0.41
2:B:289:ALA:HA	2:B:292:THR:HG22	2.01	0.41
6:F:209:LYS:HE2	6:F:209:LYS:HB2	1.86	0.41
13:M:152:ASP:OD2	13:M:154:SER:OG	2.36	0.41
21:U:45:ILE:HG23	21:U:60:ALA:HB1	2.01	0.41
26:Z:16:LEU:HD22	26:Z:135:THR:HG21	2.03	0.41
28:b:117:VAL:HG22	28:b:119:ASP:H	1.86	0.41
30:d:87:GLU:HA	30:d:89:LEU:HD23	2.02	0.41
32:f:188:VAL:HG21	32:f:211:ILE:HD12	2.02	0.41
7:g:58:ASP:OD1	7:g:58:ASP:N	2.53	0.41
13:m:45:VAL:HG23	13:m:146:ALA:HB1	2.02	0.41
14:n:4:MET:HE1	14:n:159:ALA:HB3	2.03	0.41
15:o:63:LEU:HD23	15:o:63:LEU:HA	1.90	0.41
4:D:67:ASN:ND2	21:U:608:SER:HA	2.33	0.41
6:F:277:GLU:OE1	6:F:278:LYS:NZ	2.40	0.41
8:H:42:ASN:N	8:H:42:ASN:OD1	2.52	0.41
21:U:12:LEU:HD11	21:U:27:LEU:HD21	2.03	0.41
22:V:224:LEU:HB2	22:V:261:TYR:HE1	1.85	0.41
22:V:396:ILE:HD13	22:V:396:ILE:HA	1.97	0.41
26:Z:224:HIS:NE2	27:a:215:GLU:HG3	2.36	0.41
27:a:249:GLN:HA	27:a:252:LYS:HB2	2.03	0.41
1:A:407:LYS:HA	1:A:407:LYS:HD3	1.81	0.41
2:B:378:VAL:HG12	2:B:416:ASN:HA	2.03	0.41
25:Y:142:PHE:HE2	25:Y:176:ARG:HD2	1.86	0.41
26:Z:187:LEU:HB3	29:c:293:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:70:ARG:O	28:b:17:ARG:HD2	2.21	0.41
27:a:252:LYS:HA	27:a:255:TRP:HE3	1.85	0.41
27:a:360:VAL:HG22	29:c:308:VAL:HG13	2.02	0.41
1:A:115:VAL:HG21	1:A:118:PHE:HB2	2.02	0.41
2:B:363:ARG:HA	2:B:363:ARG:HD2	1.90	0.41
6:F:61:ARG:NH1	33:u:53:GLY:O	2.54	0.41
11:K:187:LYS:HD2	11:K:187:LYS:HA	1.93	0.41
12:L:45:VAL:HG12	12:L:214:ILE:HG23	2.03	0.41
21:U:95:GLU:HB3	21:U:96:TYR:H	1.76	0.41
21:U:612:ASP:HB3	21:U:647:HIS:CG	2.56	0.41
21:U:757:MET:HB3	21:U:757:MET:HE2	1.82	0.41
22:V:345:ARG:NH1	31:e:46:ASP:OD2	2.36	0.41
22:V:419:LEU:HA	22:V:422:ILE:HG22	2.02	0.41
24:X:208:ALA:HB2	24:X:238:GLY:HA3	2.01	0.41
25:Y:30:GLU:HG3	25:Y:31:HIS:CD2	2.56	0.41
29:c:107:MET:HG3	33:u:10:GLY:HA3	2.03	0.41
29:c:198:ARG:C	29:c:199:HIS:CG	2.98	0.41
30:d:51:ALA:HA	30:d:54:ILE:HG12	2.01	0.41
32:f:711:SER:HB2	32:f:744:MET:HE1	2.02	0.41
10:j:180:ALA:HB1	10:j:190:LEU:HD11	2.03	0.41
13:m:163:CYS:SG	13:m:164:ALA:N	2.94	0.41
13:m:215:TRP:HD1	13:m:227:VAL:HG22	1.84	0.41
17:q:14:LEU:HD13	17:q:182:ILE:HG12	2.02	0.41
19:s:68:ILE:HD11	19:s:92:LEU:HD13	2.02	0.41
1:A:239:ARG:HD3	2:B:319:PHE:CE1	2.56	0.41
2:B:173:VAL:HG12	2:B:174:MET:HE2	2.01	0.41
3:C:160:GLU:OE1	3:C:313:ARG:NH1	2.54	0.41
15:O:112:SER:HB3	15:O:125:VAL:HG11	2.02	0.41
20:T:70:MET:HE1	20:T:91:TRP:CE2	2.56	0.41
25:Y:212:GLU:HG2	25:Y:213:LEU:HD22	2.03	0.41
26:Z:78:MET:HE1	29:c:95:MET:HE1	2.03	0.41
28:b:186:SER:OG	28:b:191:GLY:O	2.38	0.41
30:d:236:THR:O	30:d:239:SER:OG	2.29	0.41
30:d:251:ARG:O	30:d:255:MET:HG3	2.20	0.41
2:B:388:ASP:N	2:B:388:ASP:OD1	2.51	0.40
5:E:232:MET:HE3	5:E:232:MET:HB3	1.87	0.40
5:E:314:LYS:HA	5:E:314:LYS:HD2	1.92	0.40
5:E:352:MET:O	5:E:355:ILE:HG22	2.21	0.40
21:U:24:LEU:HD23	21:U:27:LEU:HD11	2.03	0.40
23:W:109:CYS:HA	23:W:145:LEU:HD21	2.03	0.40
23:W:267:LEU:HD21	23:W:296:LEU:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:391:PRO:HA	24:X:392:PRO:HD3	1.94	0.40
25:Y:332:GLN:HE22	25:Y:336:ARG:HH21	1.69	0.40
29:c:29:GLU:HG2	29:c:139:ARG:HH21	1.86	0.40
29:c:279:ASP:HB2	29:c:283:HIS:HB2	2.03	0.40
10:j:226:GLU:HA	10:j:229:VAL:HG12	2.03	0.40
19:s:39:ASP:OD1	19:s:39:ASP:N	2.54	0.40
1:A:143:ASP:HB3	1:A:150:HIS:CE1	2.56	0.40
1:A:274:PHE:HB2	1:A:319:MET:HG2	2.03	0.40
3:C:161:ILE:HA	3:C:164:VAL:HB	2.02	0.40
6:F:372:LYS:HE2	6:F:372:LYS:HB2	1.94	0.40
21:U:117:ASP:OD1	21:U:117:ASP:N	2.44	0.40
23:W:174:TYR:O	23:W:182:ARG:NH2	2.47	0.40
24:X:407:MET:HA	24:X:410:VAL:HG22	2.03	0.40
25:Y:68:ASP:N	25:Y:68:ASP:OD1	2.53	0.40
27:a:164:GLN:O	27:a:165:THR:C	2.64	0.40
27:a:170:ALA:O	27:a:174:LYS:HB2	2.22	0.40
27:a:293:PHE:HB3	27:a:329:LYS:HB3	2.03	0.40
2:B:145:GLU:HG2	2:B:148:CYS:HB2	2.04	0.40
3:C:119:ASP:N	3:C:119:ASP:OD1	2.53	0.40
4:D:251:PHE:HD2	4:D:295:GLN:HB3	1.87	0.40
5:E:86:GLN:NE2	6:F:104:GLN:O	2.54	0.40
5:E:295:LEU:HD23	5:E:295:LEU:HA	1.89	0.40
20:T:124:TYR:HE1	20:T:139:THR:HG22	1.86	0.40
22:V:320:THR:HG21	31:e:18:GLU:HG2	2.03	0.40
24:X:56:LEU:HD23	24:X:56:LEU:HA	1.95	0.40
27:a:80:ILE:HD12	27:a:80:ILE:HA	1.95	0.40
32:f:379:GLY:HA3	32:f:416:MET:HE3	2.03	0.40
18:r:115:ASP:OD1	18:r:119:ASN:N	2.51	0.40
2:B:71:TYR:HE1	32:f:609:VAL:HG11	1.85	0.40
12:L:208:LYS:HB2	12:L:208:LYS:HE2	1.81	0.40
18:R:138:VAL:HG23	17:q:141:SER:HB3	2.04	0.40
20:T:127:MET:HE3	20:T:127:MET:HB2	1.82	0.40
21:U:541:HIS:HB2	21:U:544:ILE:HG22	2.03	0.40
21:U:750:SER:OG	21:U:754:HIS:O	2.38	0.40
24:X:239:TYR:HB3	24:X:247:ALA:HB2	2.03	0.40
28:b:20:ASP:OD1	28:b:20:ASP:N	2.52	0.40
32:f:828:ARG:HH21	32:f:875:ALA:HA	1.87	0.40
14:n:70:LEU:HB3	14:n:72:GLU:HG3	2.04	0.40
1:A:241:ILE:HB	1:A:244:GLU:HG3	2.03	0.40
5:E:238:ILE:HD12	5:E:253:ILE:HG23	2.03	0.40
6:F:311:LEU:HD23	6:F:314:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:74:LEU:HD12	8:H:87:VAL:HG22	2.04	0.40
17:Q:18:ASP:OD1	17:Q:18:ASP:N	2.50	0.40
21:U:661:ALA:HB1	21:U:746:ILE:HD12	2.04	0.40
24:X:248:ILE:HD12	24:X:251:LEU:HD12	2.03	0.40
25:Y:332:GLN:OE1	25:Y:336:ARG:NE	2.47	0.40
27:a:57:ILE:HD12	27:a:57:ILE:HA	1.97	0.40
32:f:237:VAL:HB	32:f:248:LEU:HD11	2.03	0.40
32:f:585:GLU:OE2	32:f:588:ARG:NH2	2.55	0.40
33:u:18:GLU:HG3	33:u:19:PRO:HD2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/433 (90%)	345 (88%)	46 (12%)	1 (0%)	36	68
2	B	382/440 (87%)	347 (91%)	35 (9%)	0	100	100
3	C	359/398 (90%)	334 (93%)	22 (6%)	3 (1%)	16	50
4	D	378/418 (90%)	335 (89%)	42 (11%)	1 (0%)	36	68
5	E	387/403 (96%)	352 (91%)	35 (9%)	0	100	100
6	F	413/439 (94%)	380 (92%)	31 (8%)	2 (0%)	24	59
7	G	242/246 (98%)	232 (96%)	10 (4%)	0	100	100
7	g	242/246 (98%)	225 (93%)	16 (7%)	1 (0%)	30	62
8	H	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
8	h	230/234 (98%)	217 (94%)	13 (6%)	0	100	100
9	I	249/261 (95%)	240 (96%)	8 (3%)	1 (0%)	30	62
9	i	248/261 (95%)	241 (97%)	7 (3%)	0	100	100
10	J	237/248 (96%)	229 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	j	237/248 (96%)	223 (94%)	14 (6%)	0	100	100
11	K	232/241 (96%)	219 (94%)	12 (5%)	1 (0%)	30	62
11	k	232/241 (96%)	223 (96%)	9 (4%)	0	100	100
12	L	236/263 (90%)	229 (97%)	7 (3%)	0	100	100
12	l	236/263 (90%)	227 (96%)	9 (4%)	0	100	100
13	M	238/255 (93%)	234 (98%)	4 (2%)	0	100	100
13	m	238/255 (93%)	235 (99%)	3 (1%)	0	100	100
14	N	200/239 (84%)	198 (99%)	2 (1%)	0	100	100
14	n	200/239 (84%)	196 (98%)	4 (2%)	0	100	100
15	O	218/277 (79%)	213 (98%)	5 (2%)	0	100	100
15	o	218/277 (79%)	214 (98%)	4 (2%)	0	100	100
16	P	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
16	p	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
17	Q	197/201 (98%)	193 (98%)	4 (2%)	0	100	100
17	q	197/201 (98%)	193 (98%)	4 (2%)	0	100	100
18	R	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
18	r	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
19	S	211/241 (88%)	205 (97%)	6 (3%)	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%)	207 (97%)	7 (3%)	0	100	100
21	U	812/953 (85%)	752 (93%)	60 (7%)	0	100	100
22	V	442/534 (83%)	430 (97%)	11 (2%)	1 (0%)	43	73
23	W	439/456 (96%)	433 (99%)	6 (1%)	0	100	100
24	X	420/422 (100%)	400 (95%)	20 (5%)	0	100	100
25	Y	387/389 (100%)	363 (94%)	23 (6%)	1 (0%)	36	68
26	Z	284/324 (88%)	259 (91%)	25 (9%)	0	100	100
27	a	371/376 (99%)	344 (93%)	27 (7%)	0	100	100
28	b	189/377 (50%)	170 (90%)	19 (10%)	0	100	100
29	c	285/310 (92%)	259 (91%)	25 (9%)	1 (0%)	30	62
30	d	255/350 (73%)	219 (86%)	35 (14%)	1 (0%)	30	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	e	48/70 (69%)	42 (88%)	6 (12%)	0	100	100
32	f	840/908 (92%)	800 (95%)	38 (4%)	2 (0%)	43	73
33	u	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
34	v	1/10 (10%)	0	0	1 (100%)	0	0
All	All	13367/14962 (89%)	12635 (94%)	715 (5%)	17 (0%)	49	79

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	90	HIS
3	C	134	LEU
4	D	125	LYS
25	Y	350	VAL
29	c	196	LEU
30	d	203	PRO
32	f	66	LYS
7	g	4	GLY
34	v	25	LYS
6	F	119	GLY
22	V	496	PHE
3	C	133	PRO
6	F	120	LYS
9	I	53	HIS
32	f	365	VAL
11	K	130	PRO
1	A	109	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	337/372 (91%)	336 (100%)	1 (0%)	86	88
2	B	339/385 (88%)	338 (100%)	1 (0%)	86	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	314/346 (91%)	313 (100%)	1 (0%)	86	88
4	D	333/366 (91%)	333 (100%)	0	100	100
5	E	341/353 (97%)	341 (100%)	0	100	100
6	F	357/379 (94%)	356 (100%)	1 (0%)	86	88
7	G	205/210 (98%)	205 (100%)	0	100	100
7	g	202/210 (96%)	200 (99%)	2 (1%)	68	80
8	H	188/191 (98%)	188 (100%)	0	100	100
8	h	188/191 (98%)	186 (99%)	2 (1%)	65	79
9	I	207/221 (94%)	207 (100%)	0	100	100
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	201/211 (95%)	201 (100%)	0	100	100
10	j	196/211 (93%)	196 (100%)	0	100	100
11	K	193/203 (95%)	193 (100%)	0	100	100
11	k	195/203 (96%)	195 (100%)	0	100	100
12	L	202/224 (90%)	201 (100%)	1 (0%)	81	85
12	l	201/224 (90%)	201 (100%)	0	100	100
13	M	196/212 (92%)	196 (100%)	0	100	100
13	m	198/212 (93%)	197 (100%)	1 (0%)	81	85
14	N	157/181 (87%)	157 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	179/228 (78%)	179 (100%)	0	100	100
15	o	181/228 (79%)	181 (100%)	0	100	100
16	P	172/174 (99%)	172 (100%)	0	100	100
16	p	173/174 (99%)	173 (100%)	0	100	100
17	Q	168/171 (98%)	168 (100%)	0	100	100
17	q	168/171 (98%)	168 (100%)	0	100	100
18	R	156/202 (77%)	156 (100%)	0	100	100
18	r	156/202 (77%)	156 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	178/199 (89%)	178 (100%)	0	100	100
20	T	178/215 (83%)	178 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	t	179/215 (83%)	179 (100%)	0	100	100
21	U	696/816 (85%)	695 (100%)	1 (0%)	88	91
22	V	390/460 (85%)	390 (100%)	0	100	100
23	W	406/416 (98%)	404 (100%)	2 (0%)	81	85
24	X	362/362 (100%)	361 (100%)	1 (0%)	86	88
25	Y	344/344 (100%)	344 (100%)	0	100	100
26	Z	257/295 (87%)	256 (100%)	1 (0%)	84	86
27	a	333/336 (99%)	332 (100%)	1 (0%)	86	88
28	b	167/312 (54%)	166 (99%)	1 (1%)	78	84
29	c	252/268 (94%)	251 (100%)	1 (0%)	84	86
30	d	231/294 (79%)	229 (99%)	2 (1%)	70	81
31	e	44/63 (70%)	44 (100%)	0	100	100
32	f	711/763 (93%)	710 (100%)	1 (0%)	88	91
33	u	68/68 (100%)	65 (96%)	3 (4%)	25	59
34	v	1/1 (100%)	1 (100%)	0	100	100
All	All	11437/12683 (90%)	11413 (100%)	24 (0%)	85	89

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	403	ILE
2	B	125	THR
3	C	109	THR
6	F	120	LYS
12	L	4	ASN
21	U	57	ARG
23	W	455	LEU
23	W	456	GLN
24	X	227	THR
26	Z	103	LYS
27	a	164	GLN
28	b	145	GLU
29	c	196	LEU
30	d	47	GLN
30	d	204	LYS
32	f	571	GLU
7	g	3	ARG

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Mol	Chain	Res	Type
7	g	6	SER
8	h	3	GLU
8	h	4	ARG
13	m	129	ARG
33	u	1	MET
33	u	51	GLU
33	u	63	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	117	GLN
1	A	203	ASN
1	A	247	GLN
1	A	358	HIS
2	B	242	GLN
2	B	425	ASN
3	C	53	ASN
3	C	124	HIS
3	C	171	HIS
4	D	67	ASN
4	D	110	ASN
4	D	237	GLN
5	E	45	ASN
5	E	75	ASN
5	E	226	GLN
6	F	102	ASN
6	F	116	GLN
6	F	208	HIS
6	F	321	GLN
7	G	75	ASN
8	H	71	HIS
9	I	142	HIS
9	I	198	ASN
10	J	146	GLN
11	K	41	GLN
11	K	204	GLN
12	L	20	HIS
12	L	86	ASN
12	L	90	GLN
12	L	143	HIS

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Mol	Chain	Res	Type
14	N	77	HIS
16	P	145	GLN
17	Q	65	GLN
17	Q	82	ASN
17	Q	168	GLN
18	R	70	ASN
18	R	151	GLN
18	R	162	GLN
19	S	8	ASN
19	S	152	GLN
20	T	69	GLN
20	T	147	GLN
20	T	157	GLN
20	T	213	HIS
21	U	115	ASN
21	U	128	GLN
21	U	338	HIS
21	U	362	ASN
21	U	647	HIS
21	U	698	GLN
21	U	718	ASN
21	U	805	ASN
22	V	124	ASN
22	V	347	GLN
23	W	228	ASN
23	W	288	HIS
23	W	422	ASN
24	X	292	GLN
24	X	296	ASN
24	X	334	ASN
24	X	405	GLN
24	X	406	ASN
25	Y	31	HIS
25	Y	160	ASN
25	Y	280	GLN
26	Z	77	ASN
26	Z	109	ASN
26	Z	193	ASN
27	a	86	GLN
27	a	241	ASN
27	a	288	HIS
27	a	332	HIS

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Mol	Chain	Res	Type
28	b	142	ASN
29	c	77	GLN
29	c	115	HIS
30	d	47	GLN
30	d	135	HIS
30	d	149	ASN
30	d	201	ASN
32	f	171	GLN
32	f	198	HIS
32	f	238	ASN
32	f	565	ASN
32	f	614	HIS
8	h	95	GLN
9	i	95	GLN
9	i	177	GLN
9	i	235	GLN
10	j	205	ASN
11	k	118	ASN
11	k	224	GLN
12	l	60	GLN
12	l	175	HIS
13	m	97	ASN
14	n	66	HIS
14	n	158	ASN
17	q	82	ASN
17	q	186	ASN
18	r	85	ASN
18	r	162	GLN
18	r	196	HIS
19	s	8	ASN
20	t	81	HIS
33	u	41	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	ADP	C	501	-	27,29,29	1.35	4 (14%)	42,45,45	2.06	9 (21%)
35	ATP	A	501	36	29,33,33	0.28	0	44,52,52	0.47	1 (2%)
35	ATP	D	501	36	29,33,33	0.31	0	44,52,52	0.47	1 (2%)
35	ATP	E	401	36	29,33,33	0.31	0	44,52,52	0.45	1 (2%)
37	ADP	F	501	36	27,29,29	1.34	4 (14%)	42,45,45	1.94	11 (26%)
35	ATP	B	501	36	29,33,33	0.28	0	44,52,52	0.45	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	ADP	C	501	-	-	3/16/32/32	0/3/3/3
35	ATP	A	501	36	-	5/22/38/38	0/3/3/3
35	ATP	D	501	36	-	5/22/38/38	0/3/3/3
35	ATP	E	401	36	-	6/22/38/38	0/3/3/3
37	ADP	F	501	36	-	9/16/32/32	0/3/3/3
35	ATP	B	501	36	-	6/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C	501	ADP	C5-C4	4.64	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	F	501	ADP	C5-C4	4.38	1.47	1.39
37	C	501	ADP	C5-C6	2.61	1.48	1.41
37	F	501	ADP	C5-C6	2.56	1.48	1.41
37	F	501	ADP	C8-N7	2.38	1.36	1.31
37	C	501	ADP	C5-N7	-2.28	1.34	1.39
37	F	501	ADP	C5-N7	-2.22	1.34	1.39
37	C	501	ADP	C8-N7	2.22	1.35	1.31

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	501	ADP	C5-C4-N3	-6.93	117.70	126.75
37	F	501	ADP	C5-C4-N3	-6.13	118.75	126.75
37	C	501	ADP	N3-C4-N9	5.56	136.24	127.08
37	F	501	ADP	N3-C4-N9	4.77	134.94	127.08
37	C	501	ADP	C2-N3-C4	4.14	121.53	111.75
37	F	501	ADP	C2-N3-C4	3.72	120.53	111.75
37	F	501	ADP	PA-O3A-PB	-3.49	120.86	132.83
37	F	501	ADP	C4-C5-N7	-3.30	106.60	110.62
37	C	501	ADP	N3-C2-N1	-3.19	123.61	128.60
37	C	501	ADP	PA-O3A-PB	-3.07	122.30	132.83
37	C	501	ADP	C4-C5-N7	-2.96	107.01	110.62
37	F	501	ADP	N3-C2-N1	-2.96	123.98	128.60
37	C	501	ADP	C3'-C2'-C1'	2.81	106.77	101.43
37	F	501	ADP	C5-N7-C8	2.73	107.39	103.51
37	F	501	ADP	C4-N9-C8	2.64	108.59	105.73
37	C	501	ADP	C5-N7-C8	2.57	107.16	103.51
37	F	501	ADP	C3'-C2'-C1'	2.19	105.59	101.43
37	F	501	ADP	C6-C5-N7	2.13	135.99	132.02
37	C	501	ADP	C4-N9-C8	2.06	107.97	105.73
37	F	501	ADP	N9-C8-N7	-2.05	111.11	113.91
35	D	501	ATP	PB-O3B-PG	2.03	139.79	132.83
35	B	501	ATP	PB-O3B-PG	2.03	139.79	132.83
35	E	401	ATP	PB-O3B-PG	2.02	139.76	132.83
35	A	501	ATP	PB-O3B-PG	2.01	139.73	132.83

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	B	501	ATP	C5'-O5'-PA-O1A
35	B	501	ATP	C5'-O5'-PA-O2A

*Continued on next page...*

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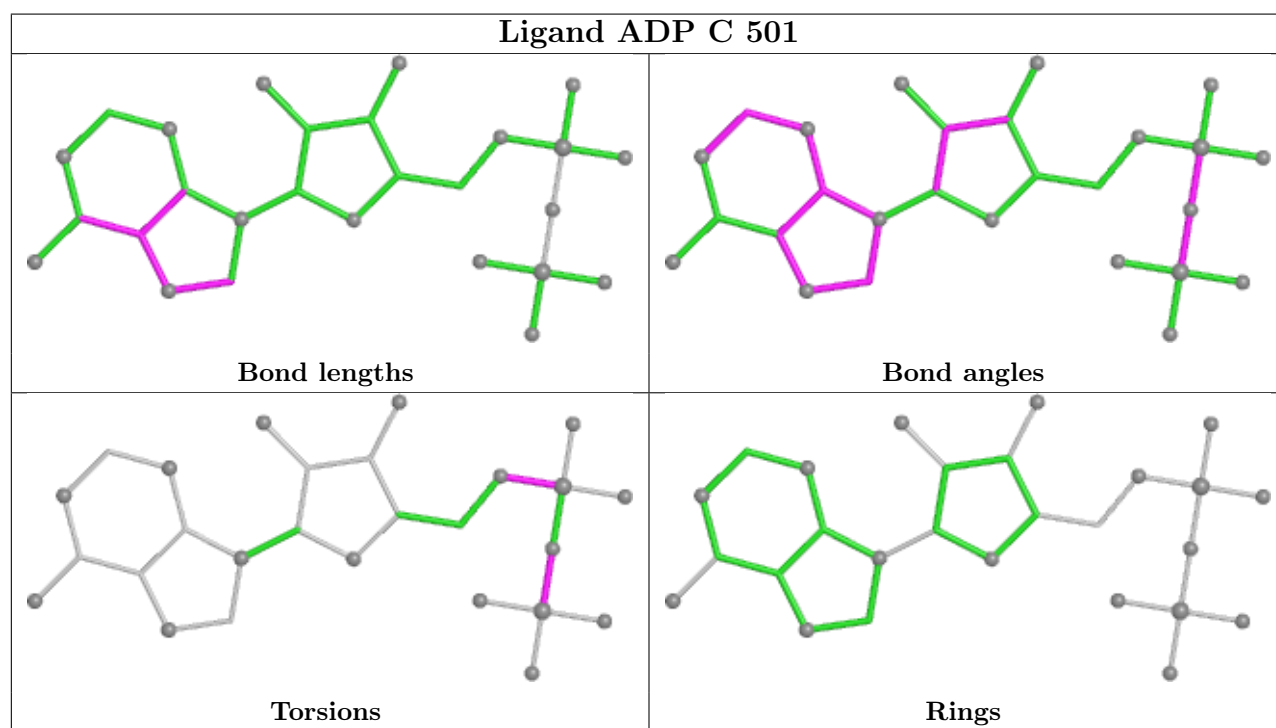
Mol	Chain	Res	Type	Atoms
35	D	501	ATP	C5'-O5'-PA-O2A
35	E	401	ATP	PB-O3B-PG-O2G
35	E	401	ATP	C5'-O5'-PA-O1A
35	E	401	ATP	C5'-O5'-PA-O2A
37	C	501	ADP	C5'-O5'-PA-O2A
37	C	501	ADP	C5'-O5'-PA-O3A
37	F	501	ADP	PA-O3A-PB-O2B
37	F	501	ADP	C5'-O5'-PA-O1A
37	F	501	ADP	O4'-C4'-C5'-O5'
37	F	501	ADP	C3'-C4'-C5'-O5'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

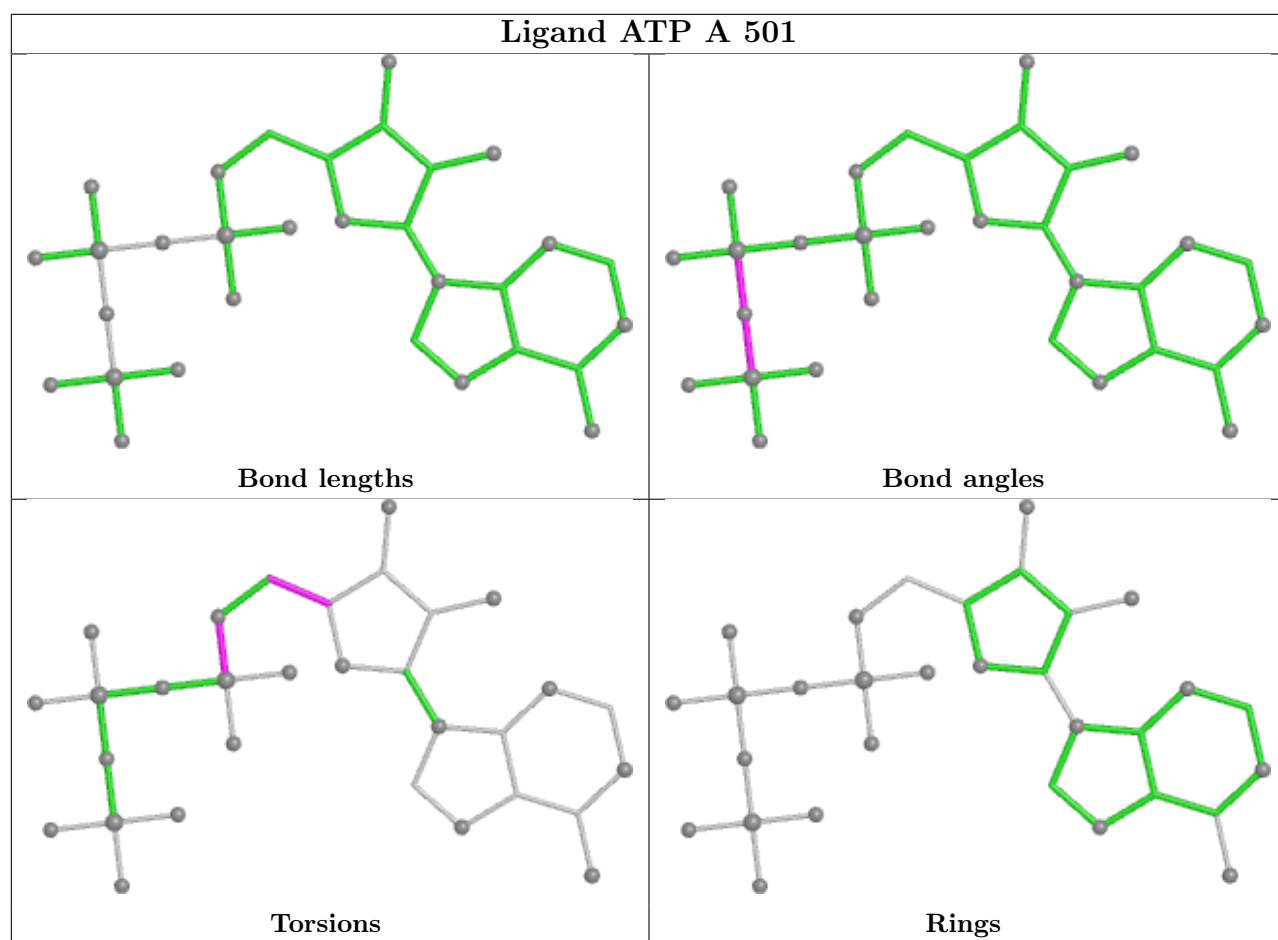
There are no ring outliers.

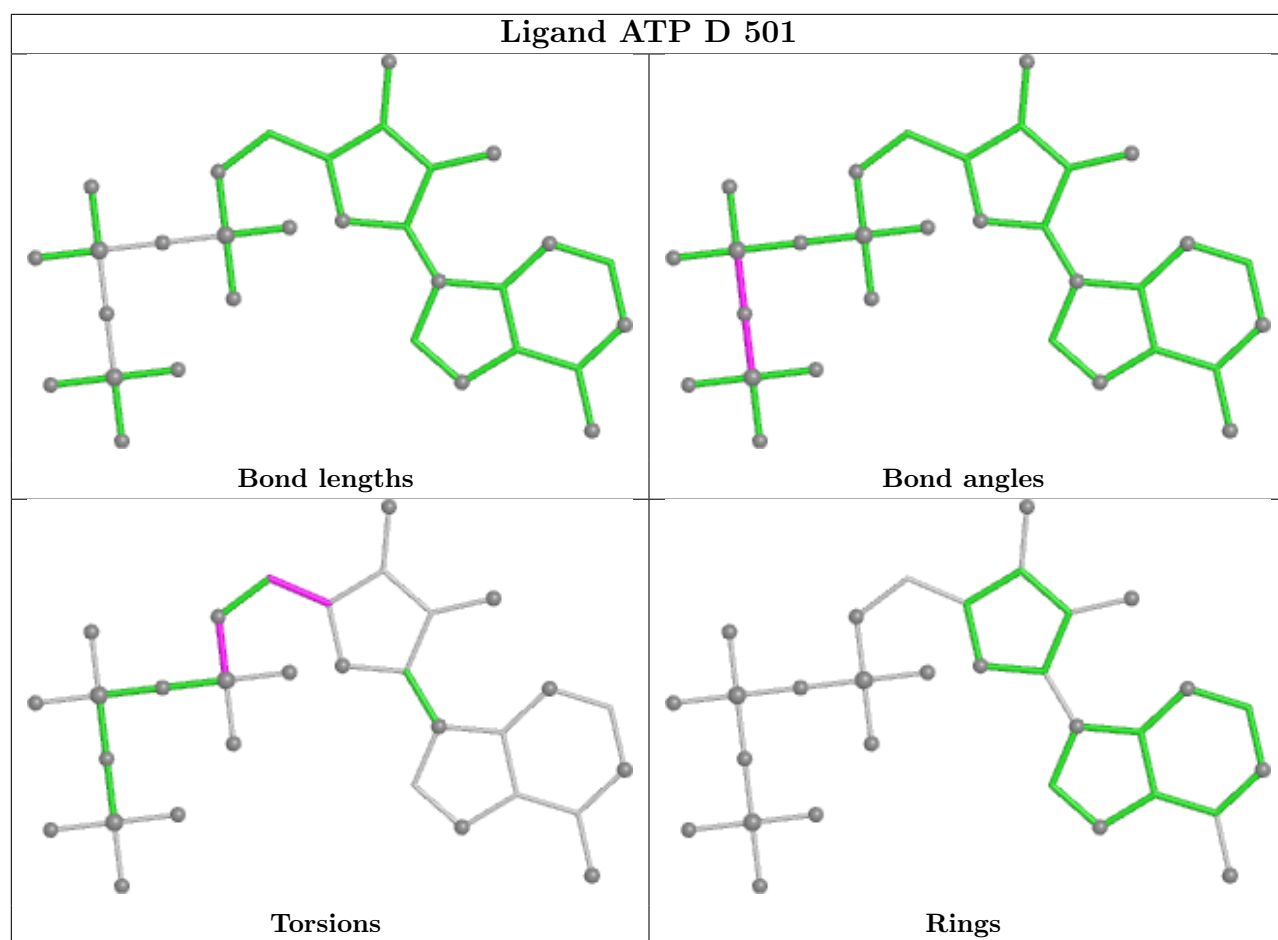
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	C	501	ADP	1	0
35	D	501	ATP	2	0
35	E	401	ATP	3	0
37	F	501	ADP	1	0
35	B	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.

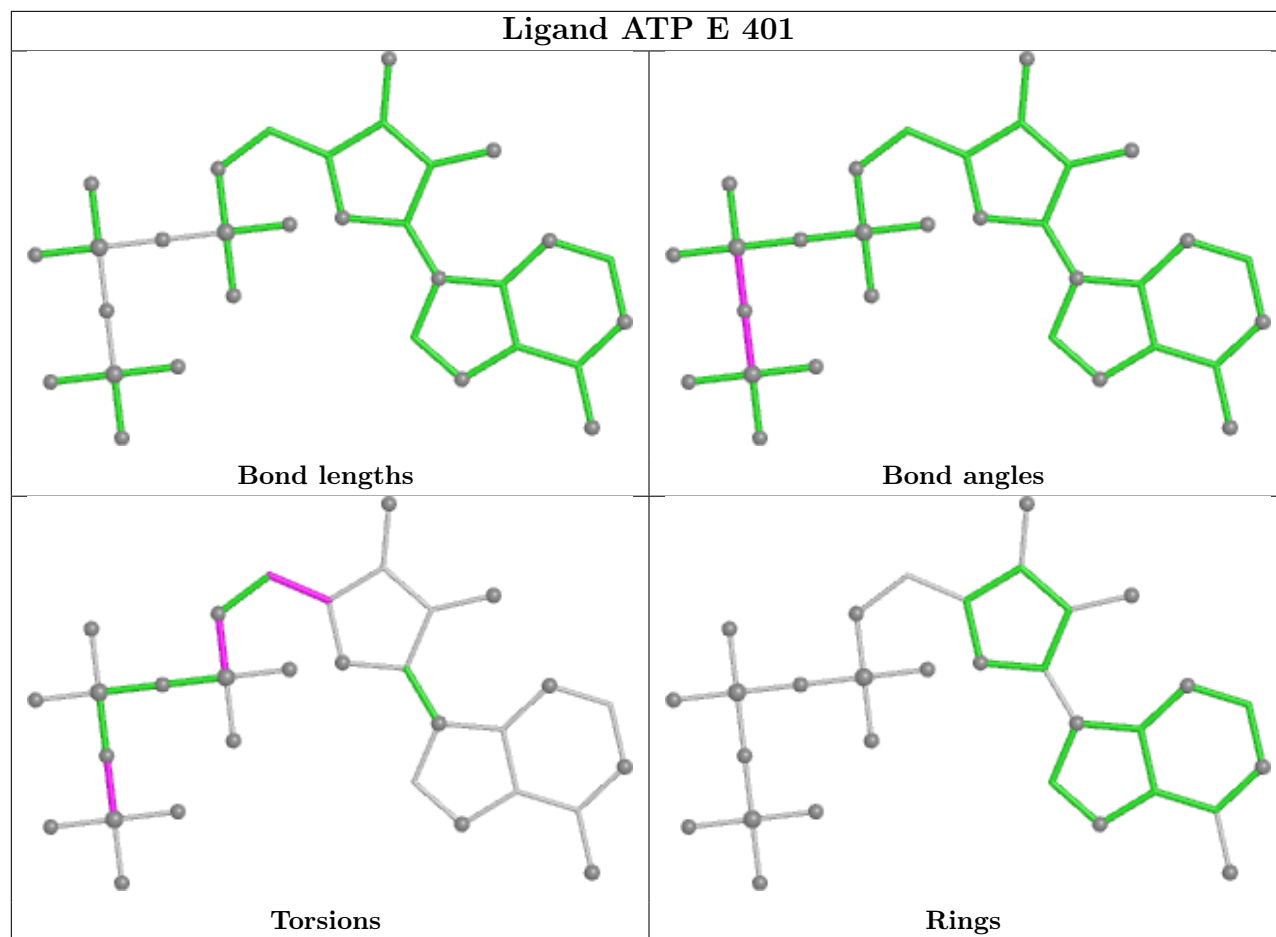




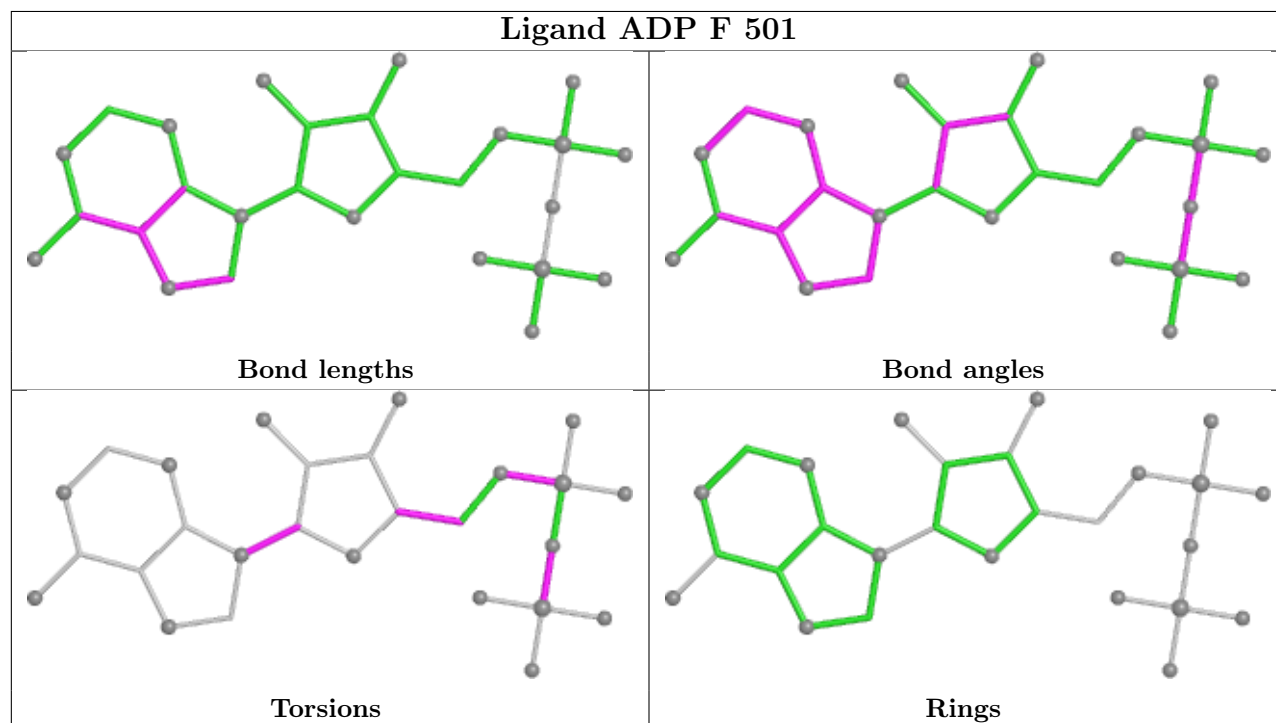


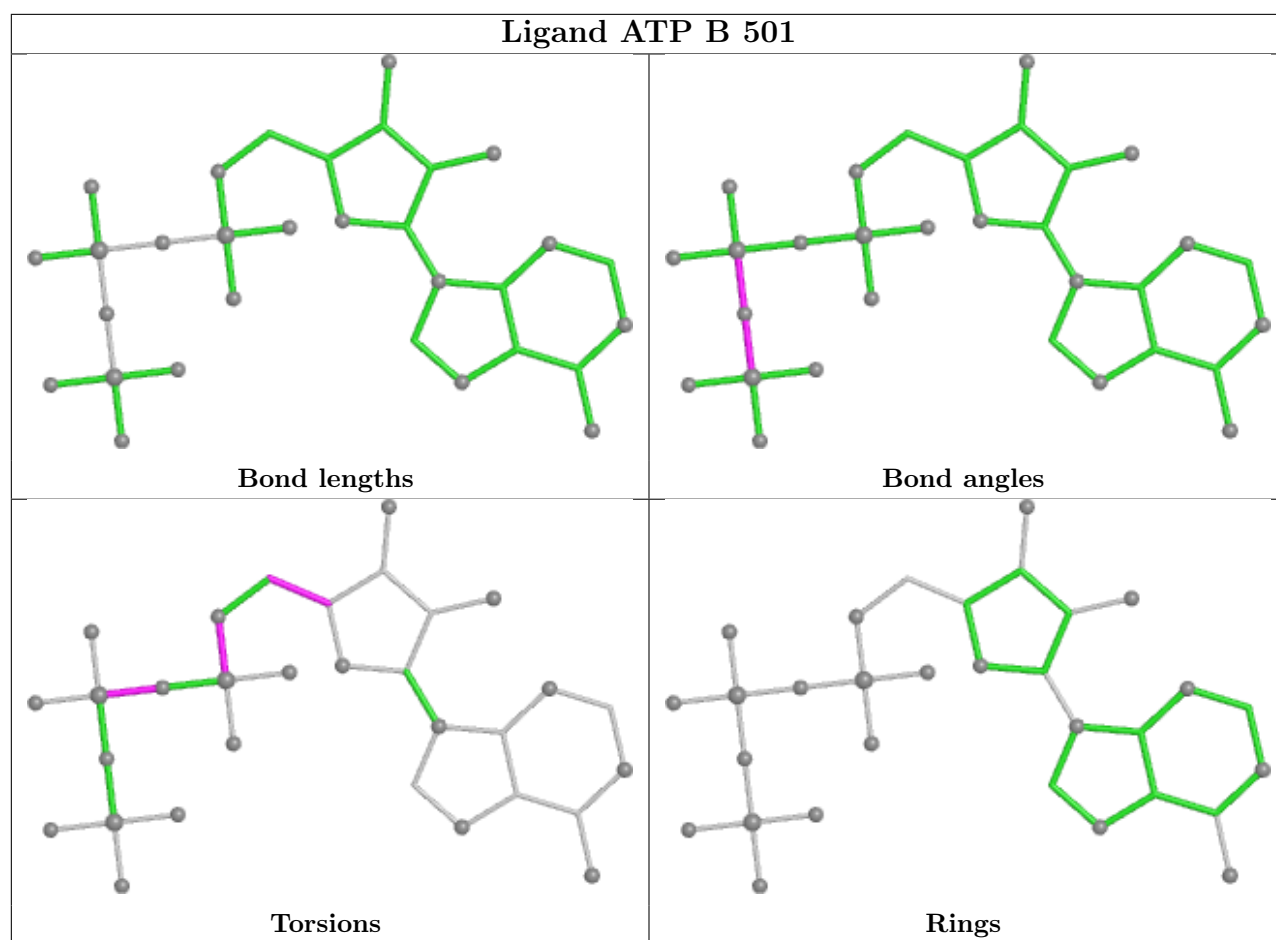


## Ligand ATP E 401



## Ligand ADP F 501





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

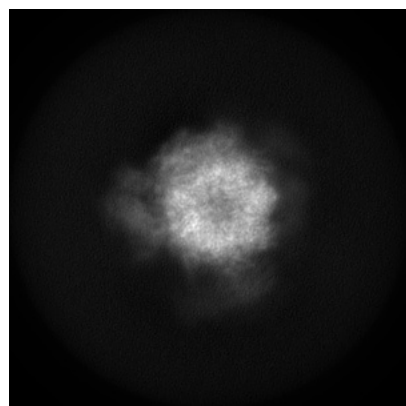
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62064. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections [i](#)

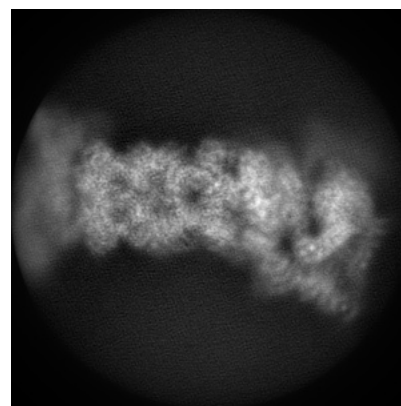
#### 6.1.1 Primary map



X

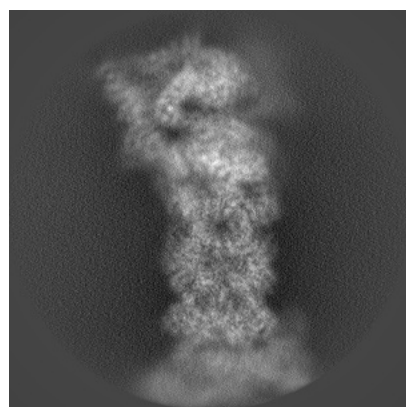


Y

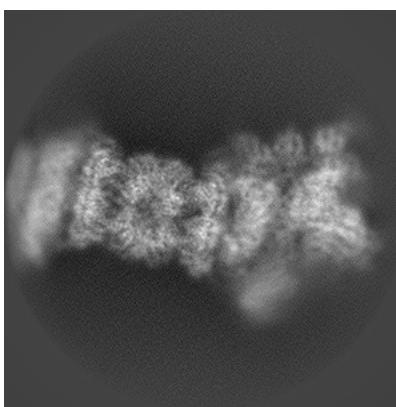


Z

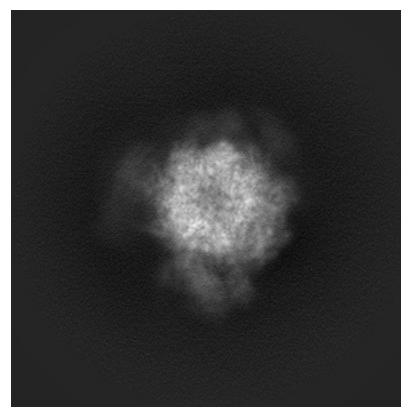
#### 6.1.2 Raw map



X



Y

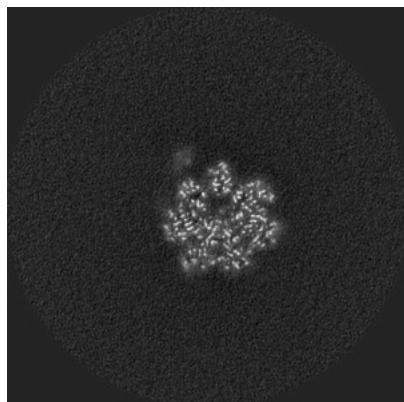


Z

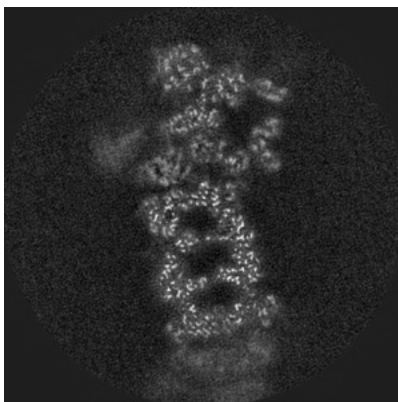
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

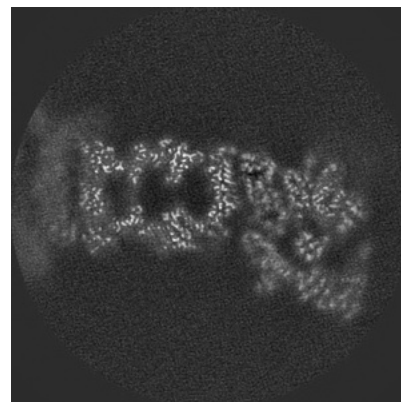
### 6.2.1 Primary map



X Index: 300

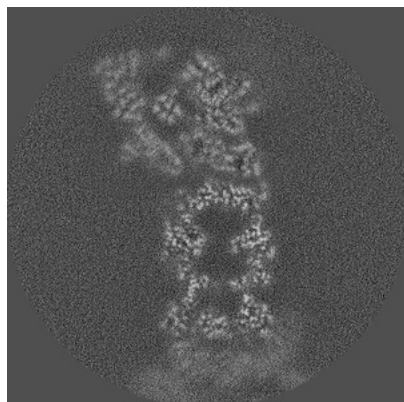


Y Index: 300

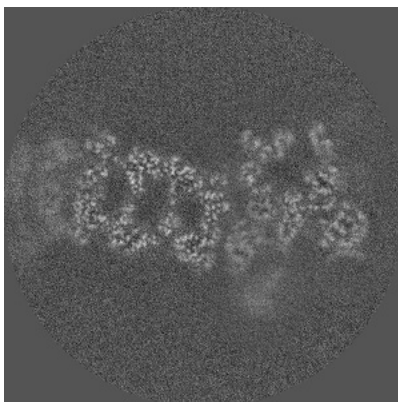


Z Index: 300

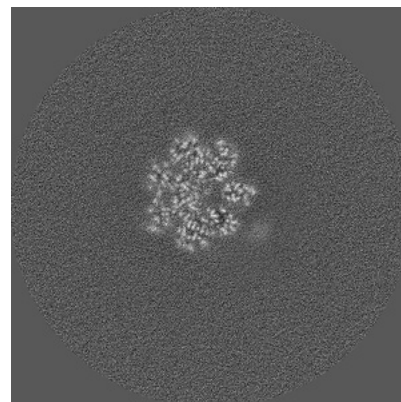
### 6.2.2 Raw map



X Index: 300



Y Index: 300

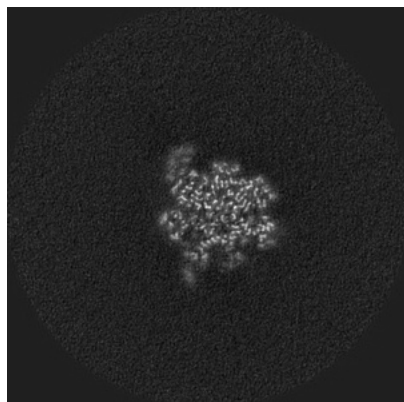


Z Index: 300

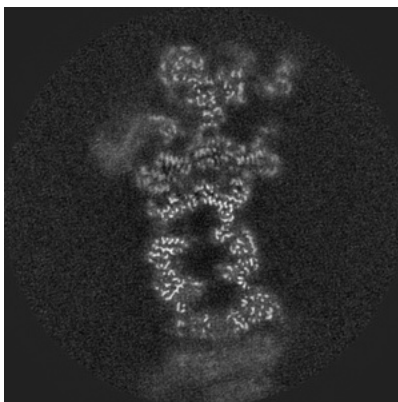
The images above show central slices of the map in three orthogonal directions.

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

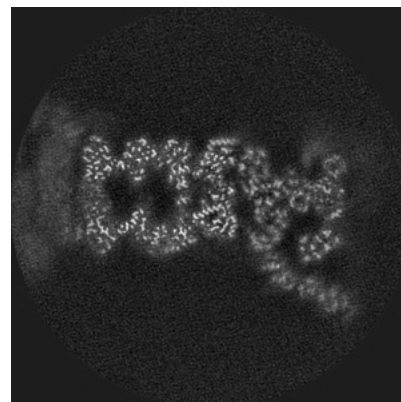
### 6.3.1 Primary map



X Index: 313

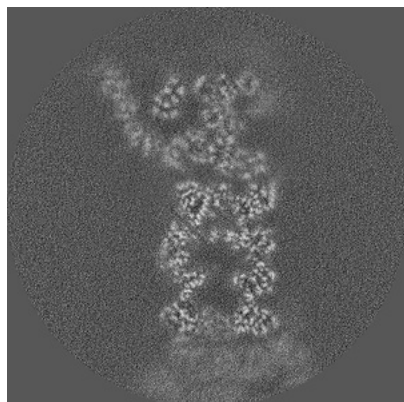


Y Index: 313

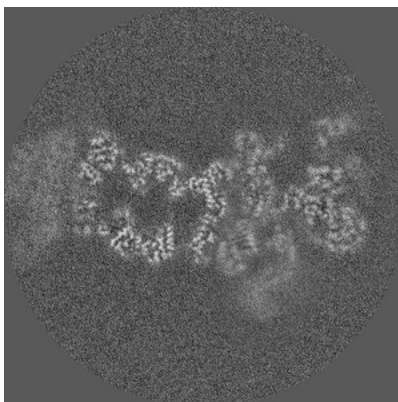


Z Index: 317

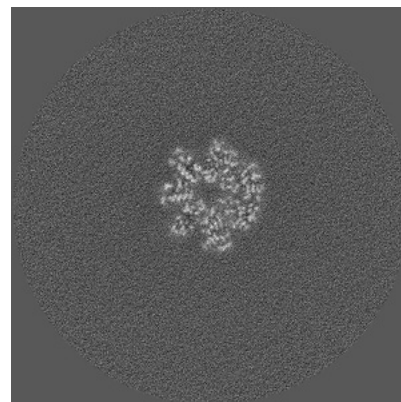
### 6.3.2 Raw map



X Index: 317



Y Index: 313



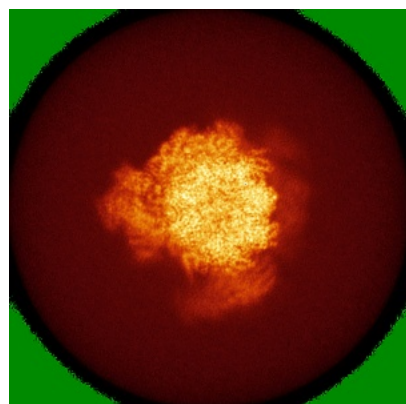
Z Index: 249

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

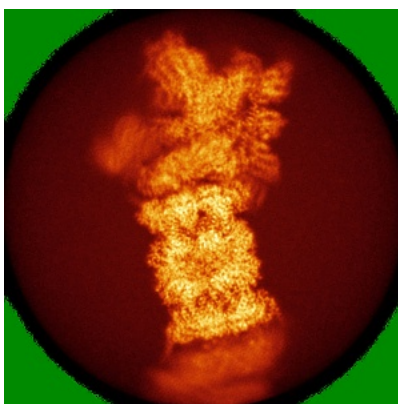


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

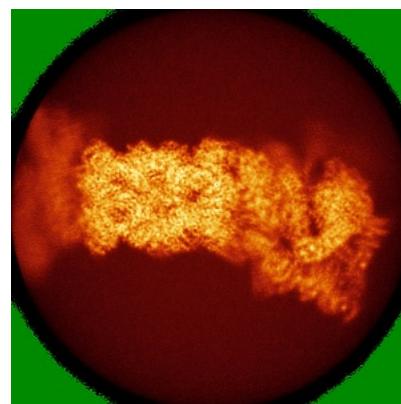
### 6.4.1 Primary map



X

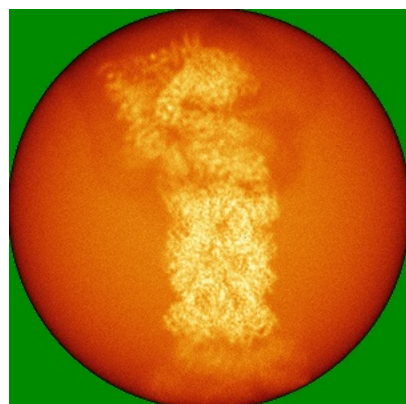


Y

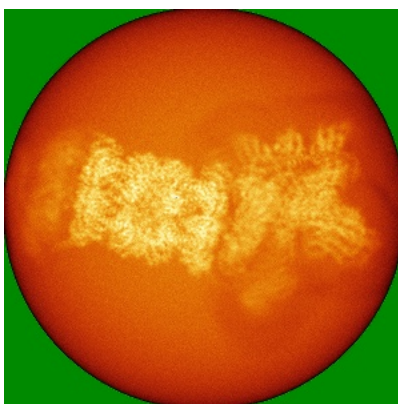


Z

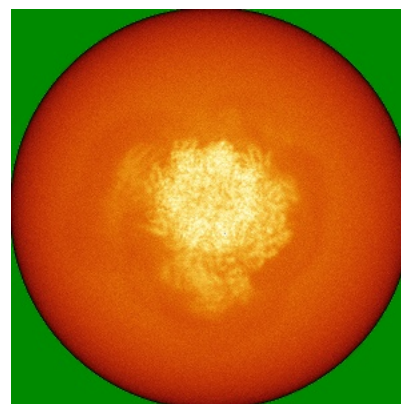
### 6.4.2 Raw map



X



Y

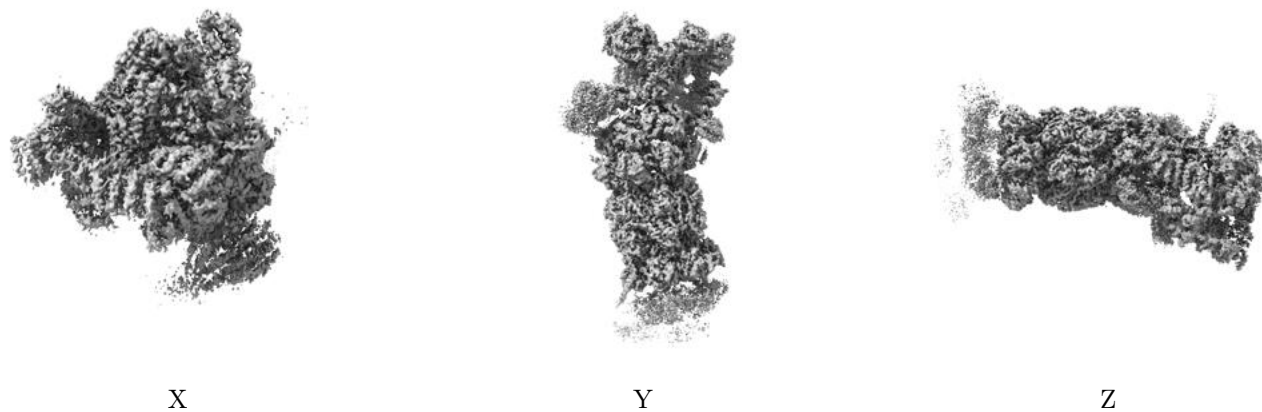


Z

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

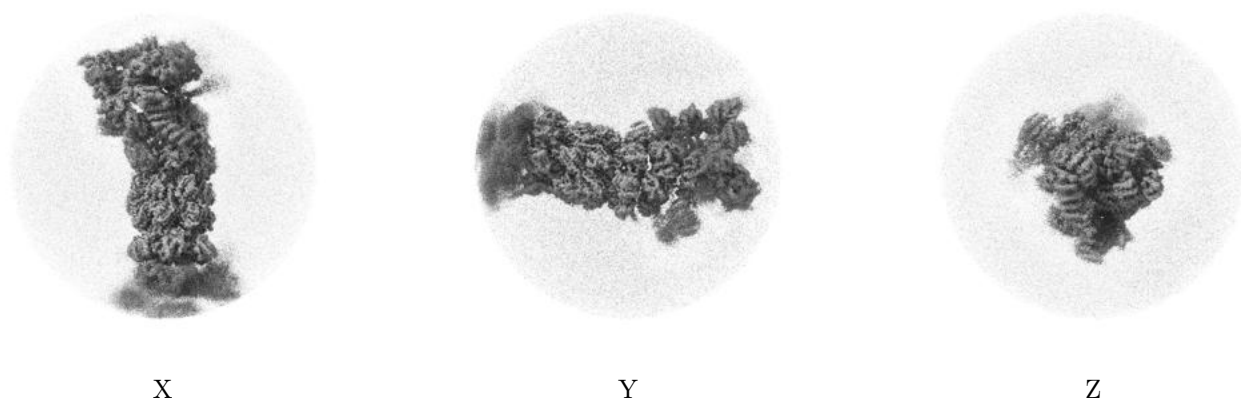
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00559. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

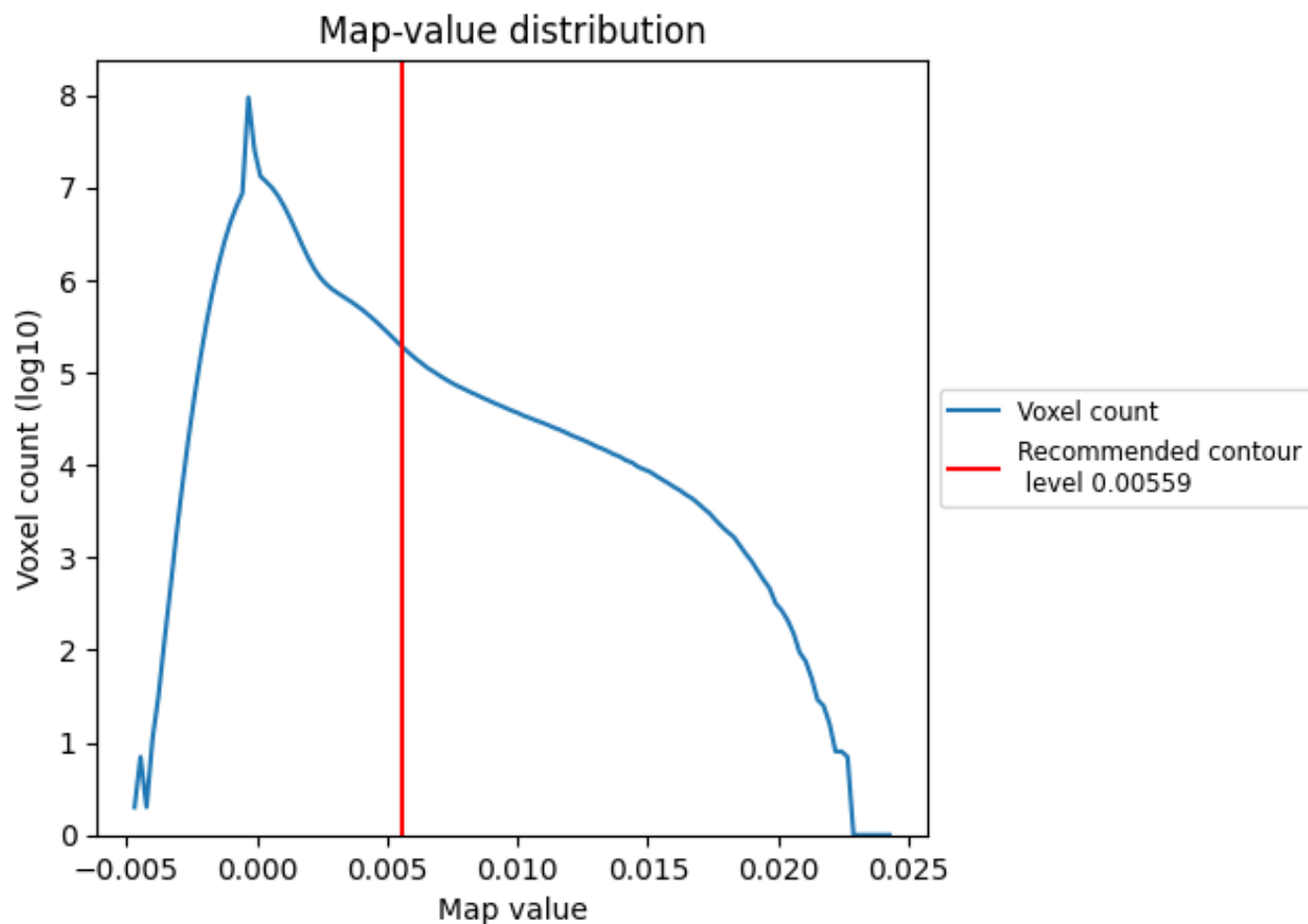
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

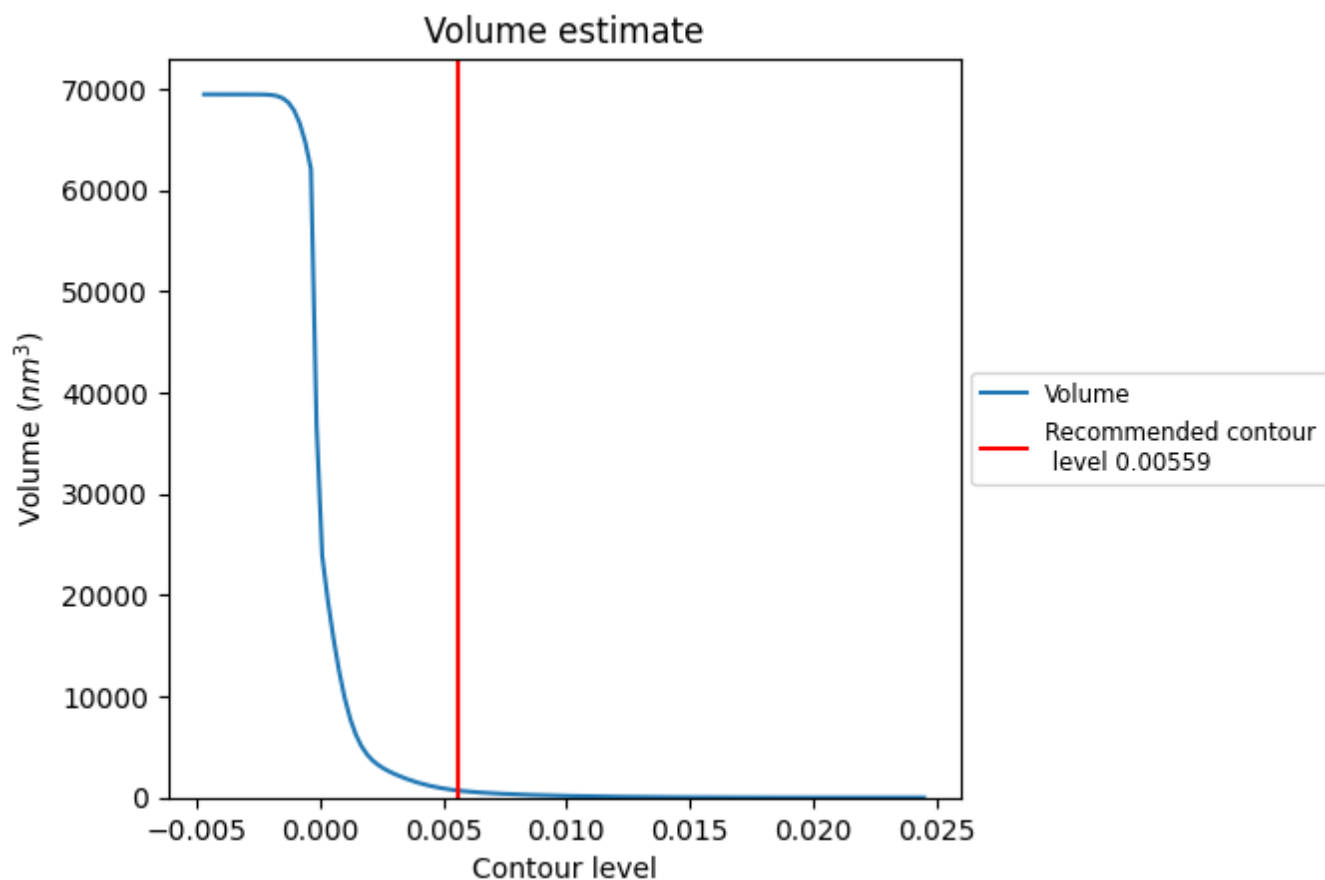
### 7.1 Map-value distribution [i](#)



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



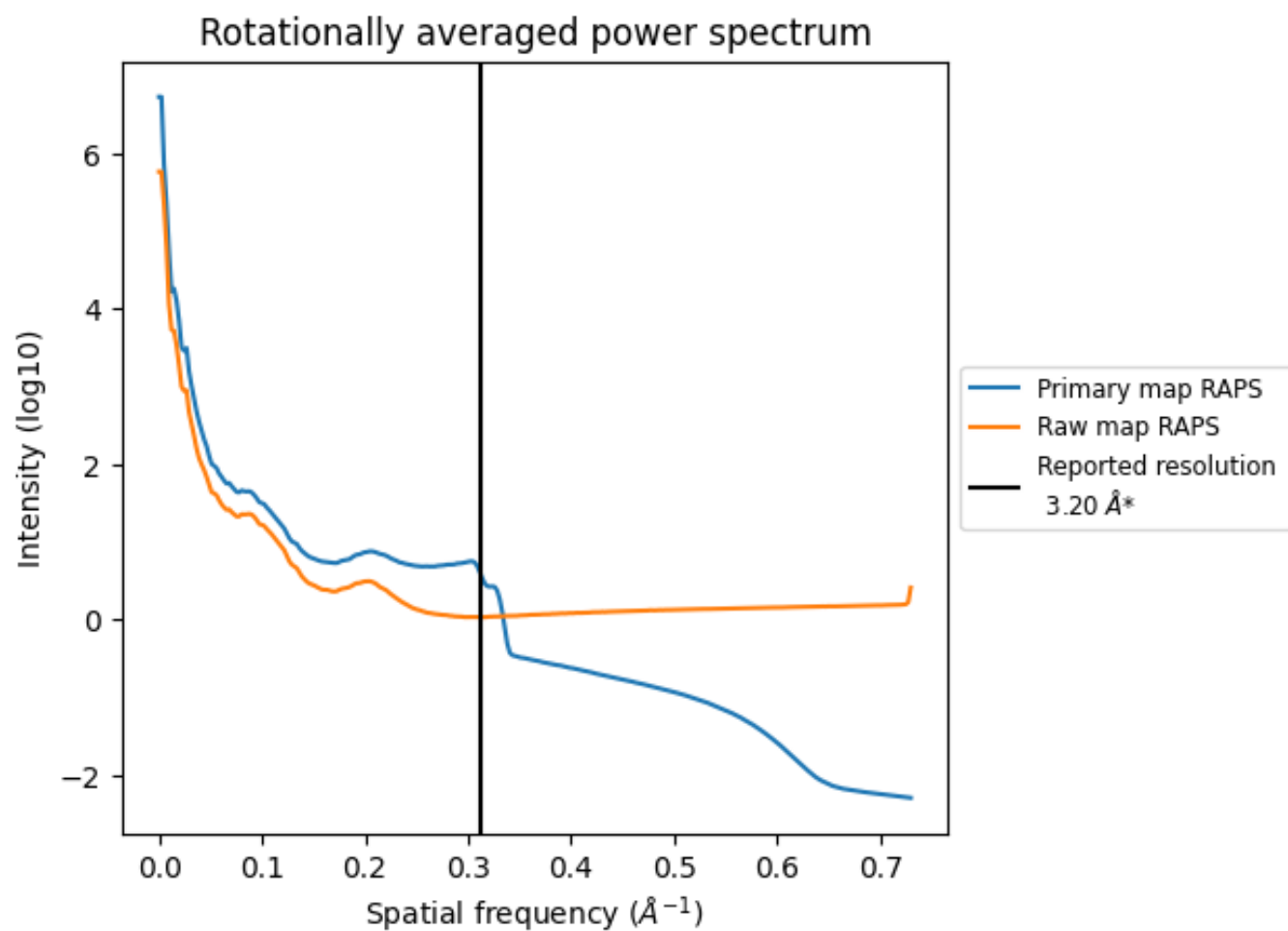
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 700 nm<sup>3</sup>; this corresponds to an approximate mass of 632 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)

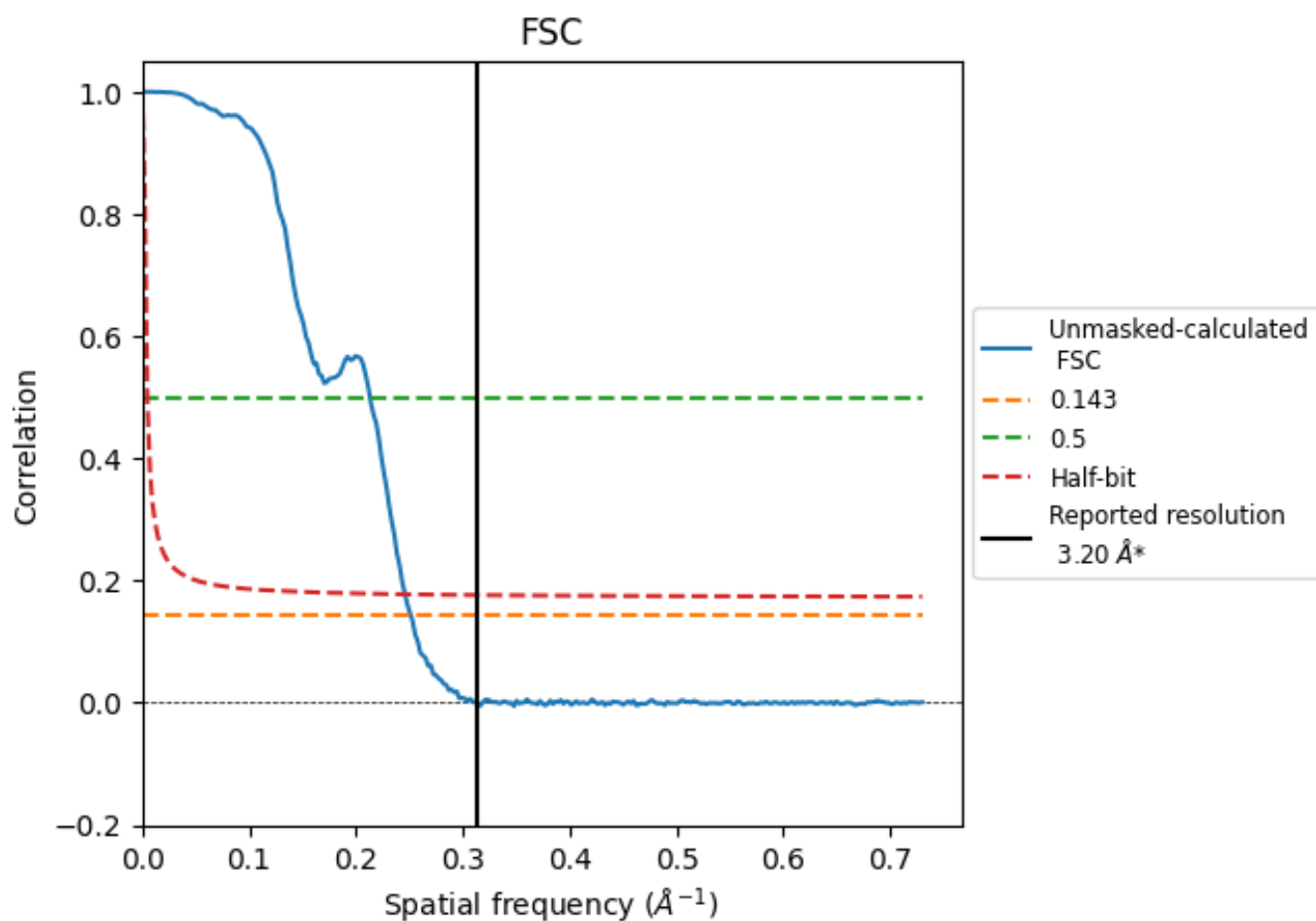


\*Reported resolution corresponds to spatial frequency of  $0.312 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

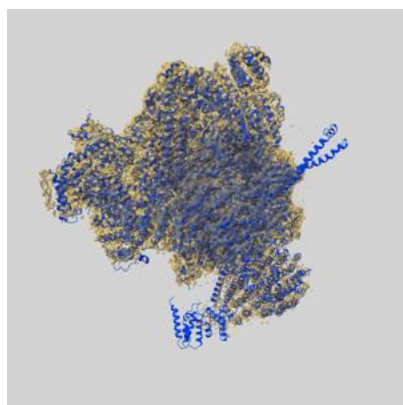
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.98	4.69	4.06

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 3.2 by more than 10 %

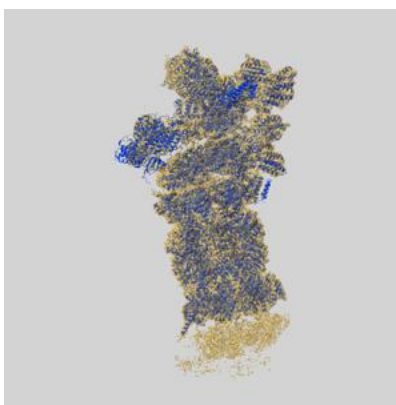
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62064 and PDB model 9K4M. Per-residue inclusion information can be found in section [3](#) on page [13](#).

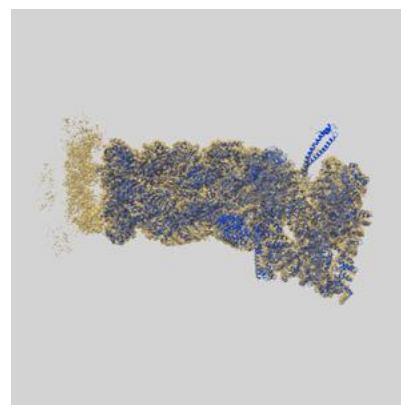
### 9.1 Map-model overlay [i](#)



X



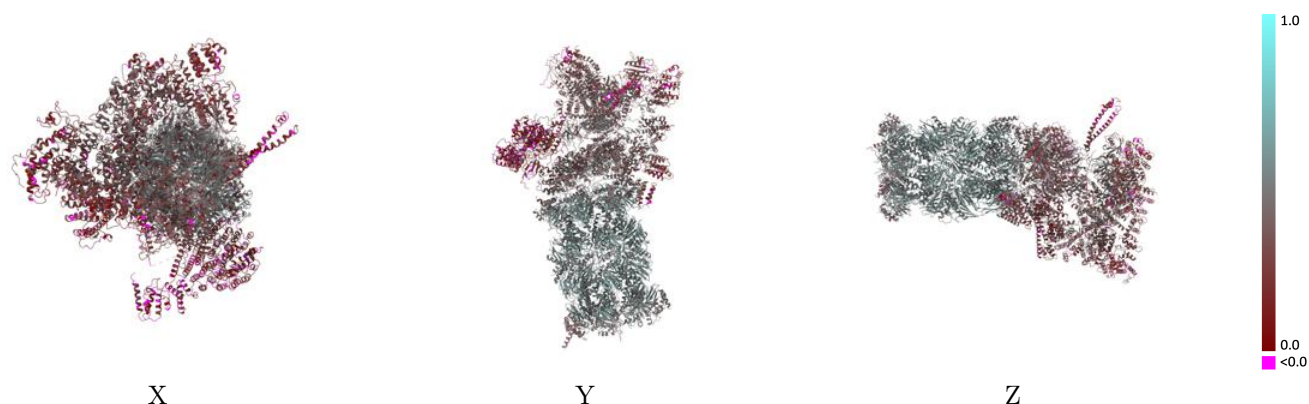
Y



Z

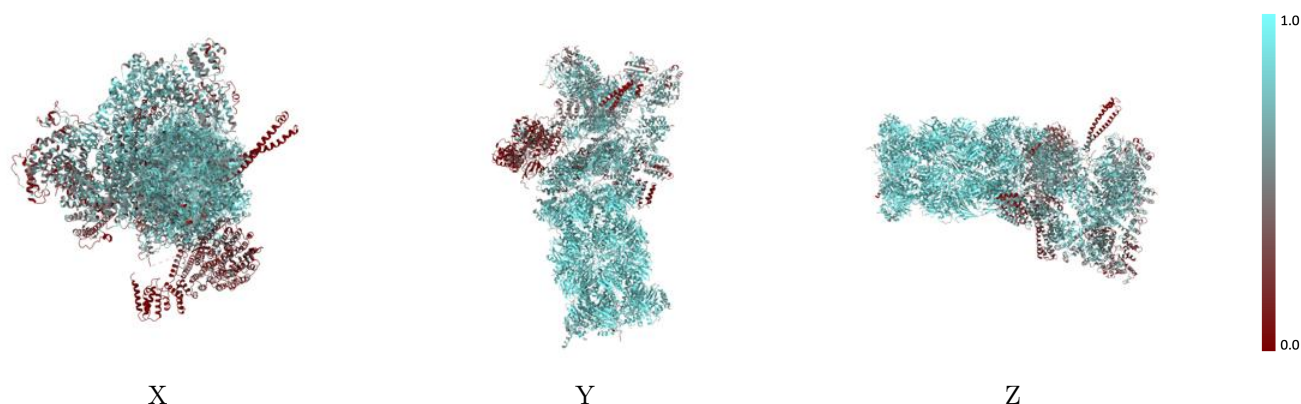
The images above show the 3D surface view of the map at the recommended contour level 0.00559 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



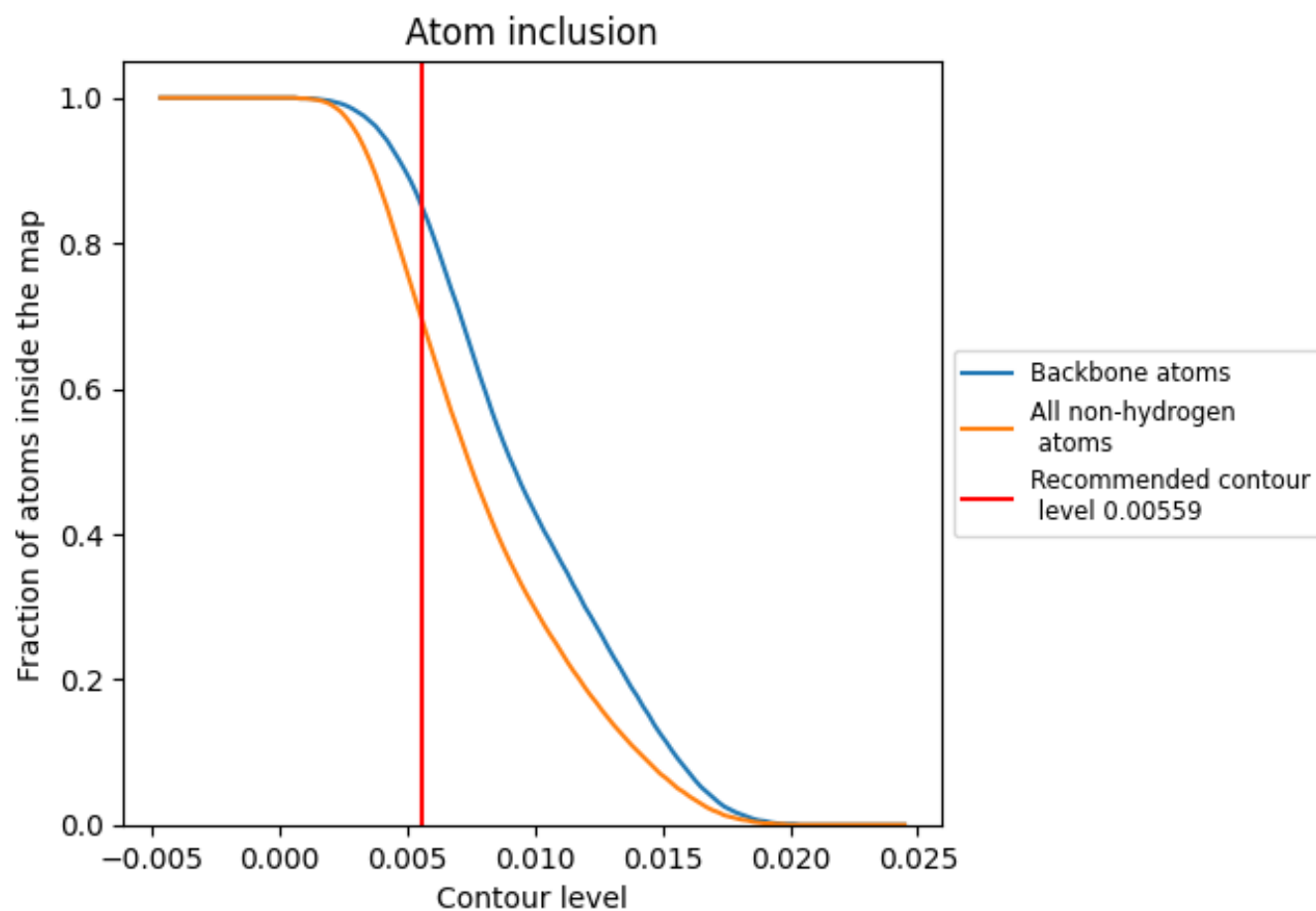
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00559).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.00559) and Q-score for the entire model and for each chain.





























Chain	Atom inclusion	Q-score
All	 0.6920	 0.4020
A	 0.6810	 0.3870
B	 0.5960	 0.3360
C	 0.5850	 0.3360
D	 0.6650	 0.3690
E	 0.6600	 0.3860
F	 0.6350	 0.3700
G	 0.8590	 0.5100
H	 0.8650	 0.5170
I	 0.8430	 0.4950
J	 0.8140	 0.4680
K	 0.8340	 0.5020
L	 0.8710	 0.5200
M	 0.8580	 0.5030
N	 0.8970	 0.5320
O	 0.9070	 0.5280
P	 0.9110	 0.5410
Q	 0.8980	 0.5340
R	 0.9100	 0.5350
S	 0.8860	 0.5310
T	 0.9060	 0.5400
U	 0.5920	 0.3010
V	 0.5170	 0.3000
W	 0.6530	 0.3350
X	 0.5120	 0.3060
Y	 0.5450	 0.2700
Z	 0.6960	 0.3740
a	 0.6070	 0.2770
b	 0.5380	 0.3080
c	 0.7180	 0.4030
d	 0.3830	 0.2240
e	 0.4340	 0.2720
f	 0.1670	 0.1690
g	 0.8260	 0.4900
h	 0.8270	 0.4960



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Chain	Atom inclusion	Q-score
i	 0.7890	 0.4720
j	 0.7310	 0.4290
k	 0.7770	 0.4760
l	 0.8550	 0.5050
m	 0.8330	 0.4960
n	 0.8950	 0.5380
o	 0.9000	 0.5360
p	 0.8960	 0.5310
q	 0.8940	 0.5240
r	 0.9050	 0.5310
s	 0.8730	 0.5200
t	 0.9110	 0.5410
u	 0.5730	 0.3590
v	 0.0190	 0.2660