



Full wwPDB EM Validation Report ⓘ

Apr 21, 2026 – 03:35 PM JST

PDB ID : 9K4V / pdb_00009k4v
EMDB ID : EMD-62071
Title : Structure of substrate-engaged human 26S proteasome RP-CP subcomplex in state EC2
Authors : Wu, Z.; Chen, E.; Mao, Y.
Deposited on : 2024-10-21
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

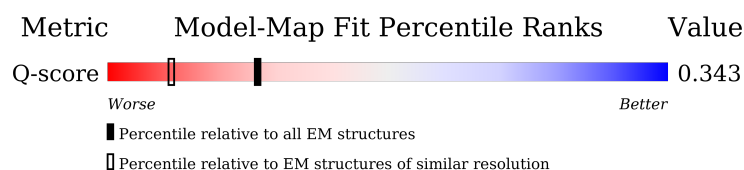
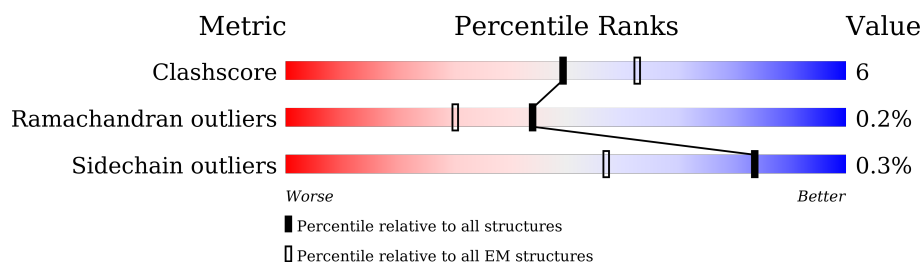
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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

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
















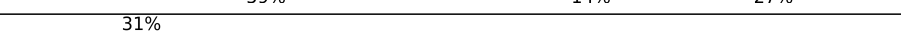


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Mol	Chain	Length	Quality of chain
5	E	403	
6	F	439	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	263	
12	l	263	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17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

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

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 106109 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	402	Total	C	N	O	S	0	0
			3135	1973	551	594	17		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	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
			1954	1233	335	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
			1858	1165	327	361	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
			1773	1115	295	352	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	1	0
			1879	1193	321	353	12		
13	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	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	1	0
			1591	1019	270	292	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			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
			1555	980	273	293	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1641	1041	281	309	10		
19	s	213	Total	C	N	O	S	0	0
			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	878	Total	C	N	O	S	0	0
			6867	4352	1163	1306	46		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

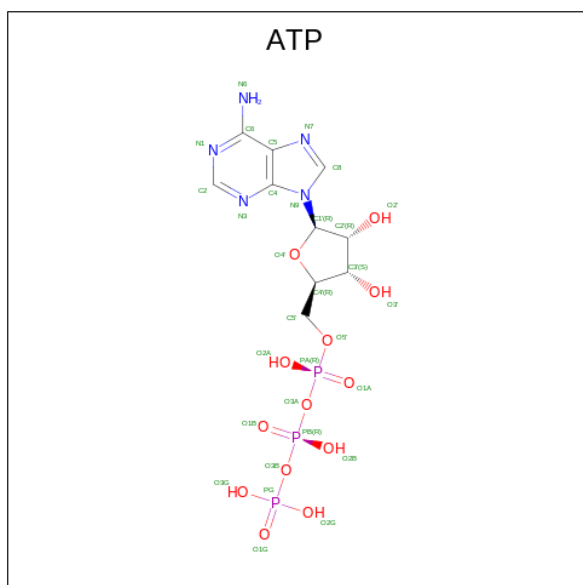
- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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

- Molecule 33 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	v	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



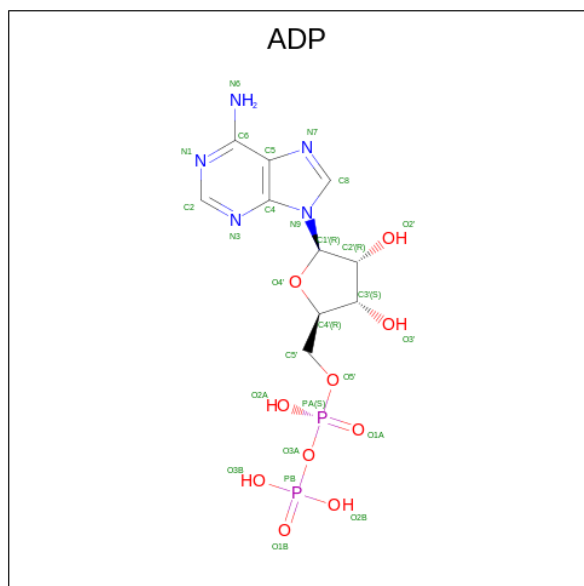
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Mol	Chain	Residues	Atoms					AltConf
34	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
35	C	1	Total	Mg	0
			1	1	
35	D	1	Total	Mg	0
			1	1	
35	E	1	Total	Mg	0
			1	1	

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

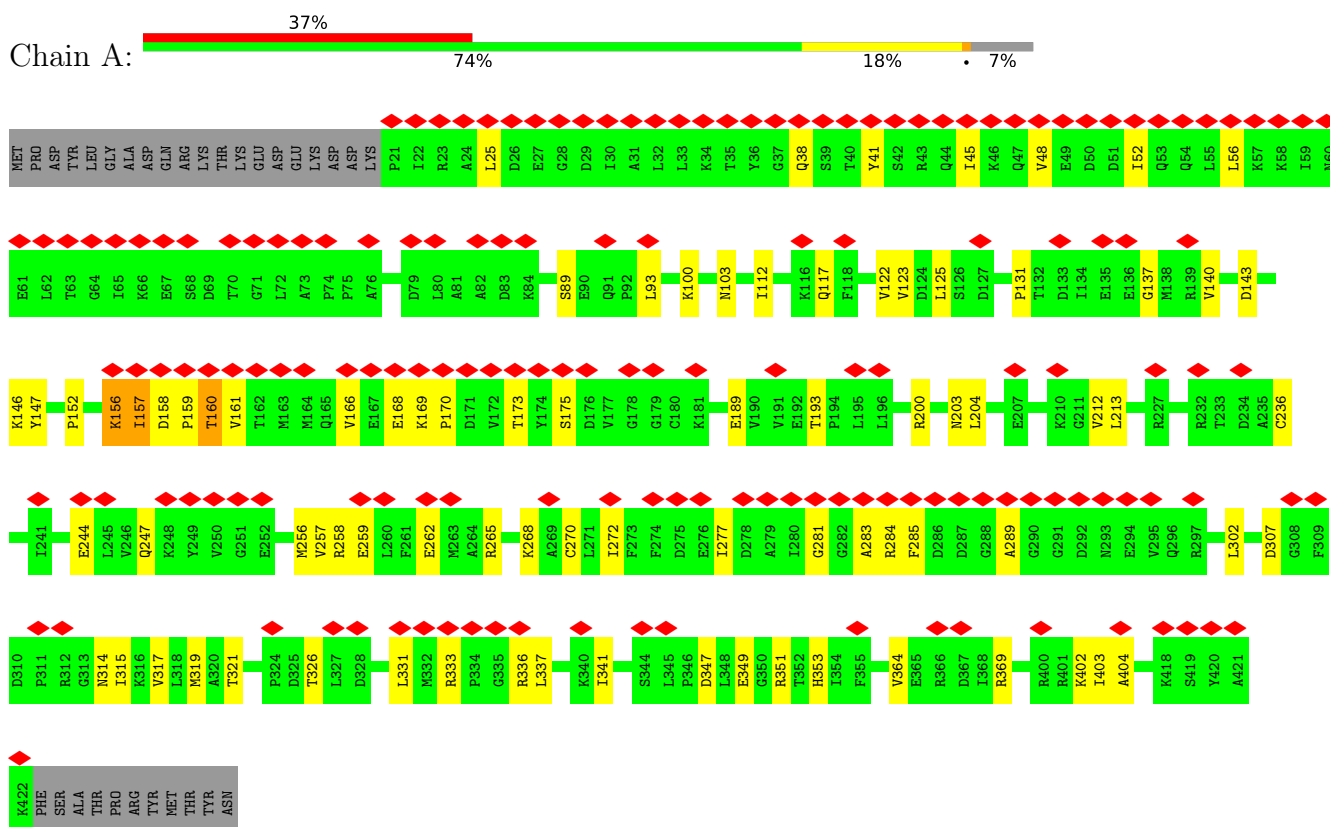
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

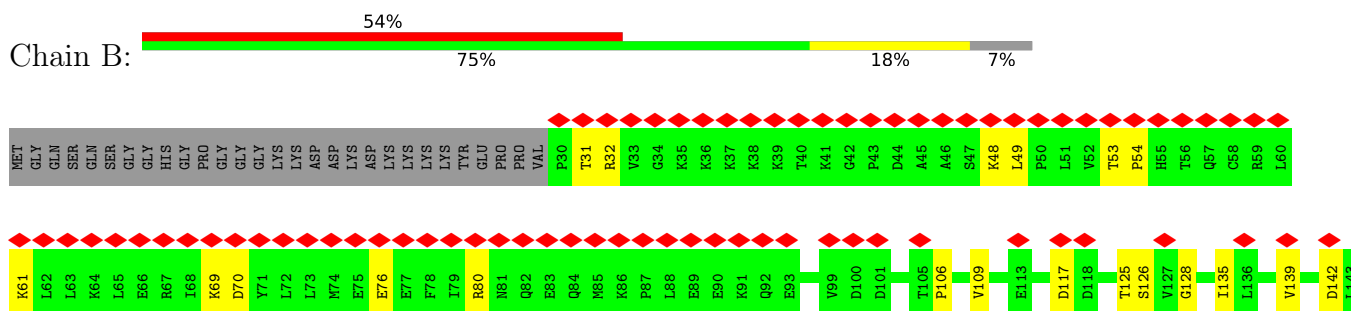
3 Residue-property plots

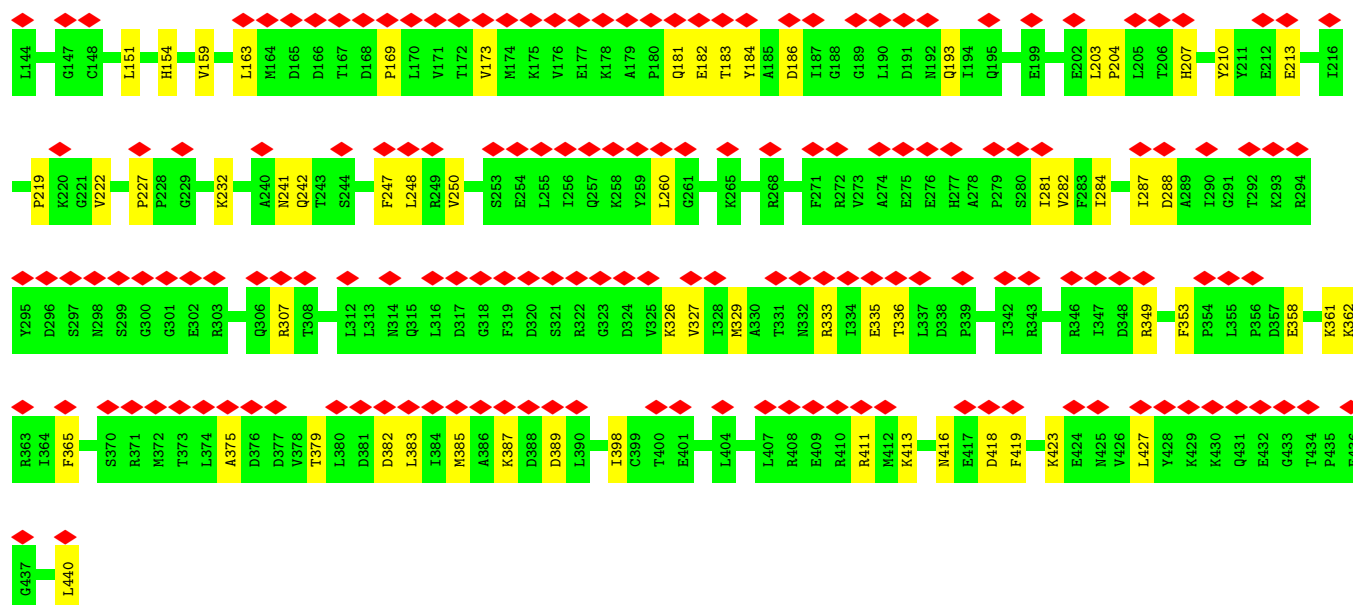
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 26S proteasome regulatory subunit 7

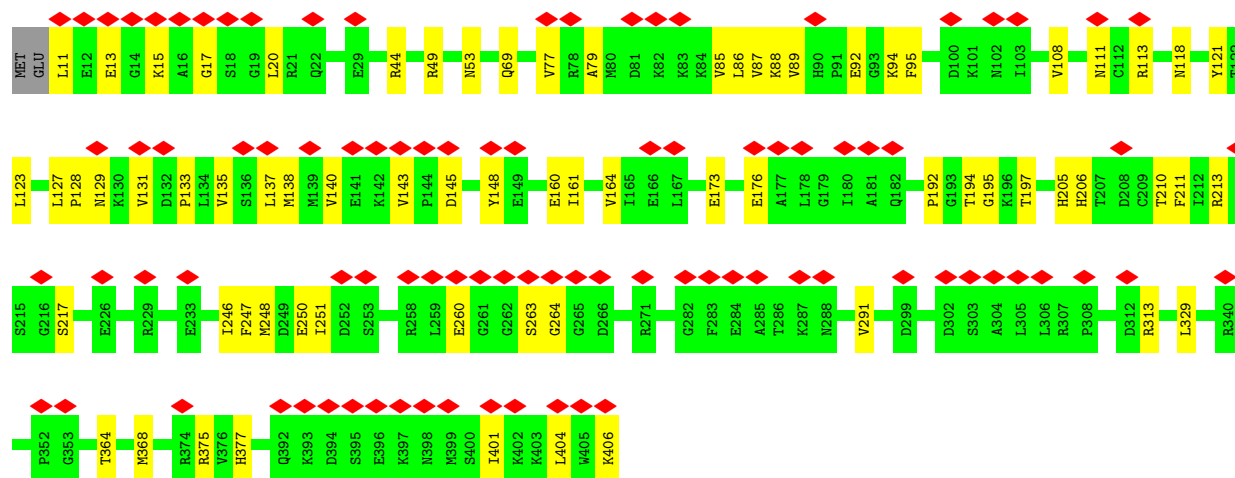
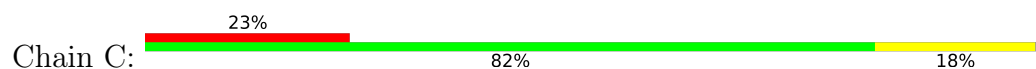


• Molecule 2: 26S proteasome regulatory subunit 4

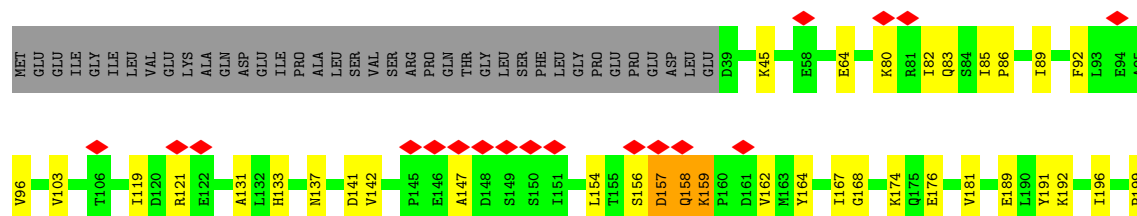


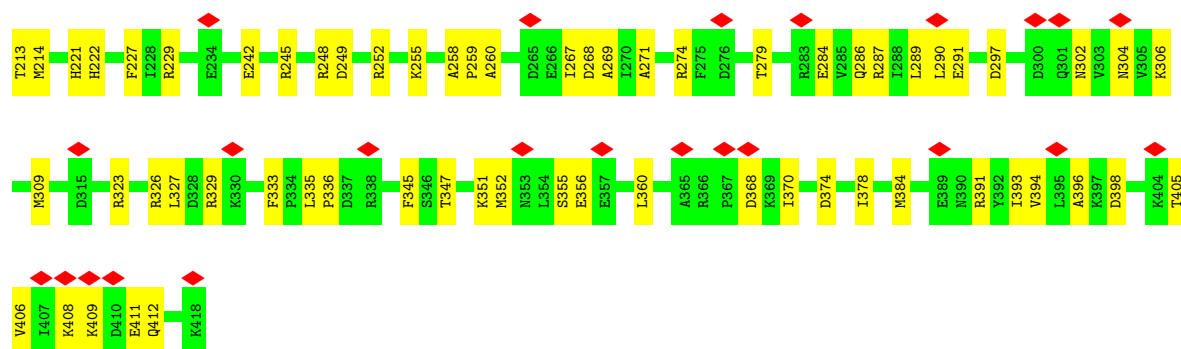


• Molecule 3: 26S proteasome regulatory subunit 8

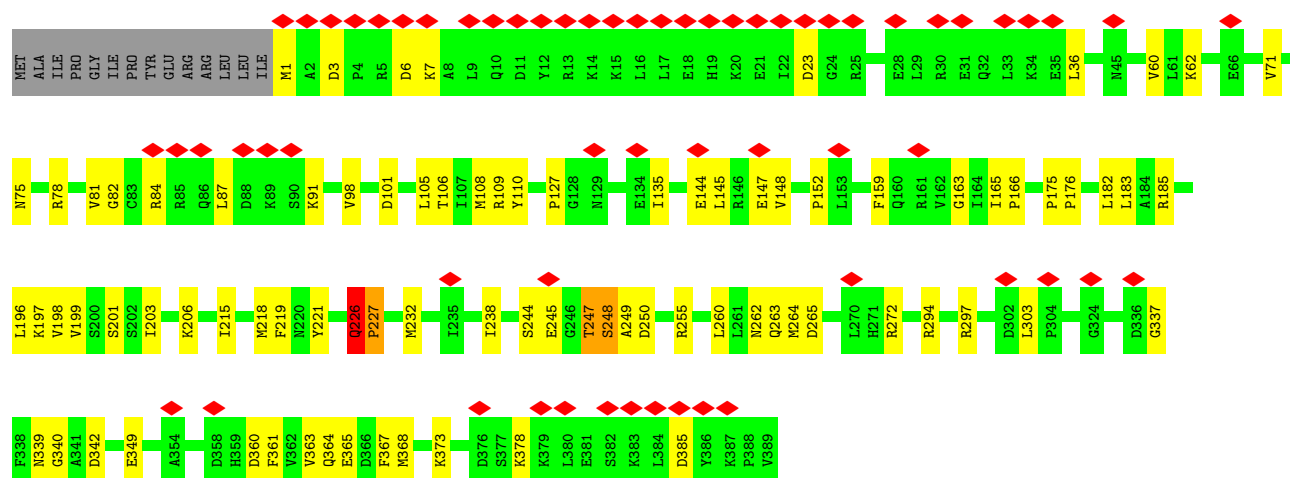
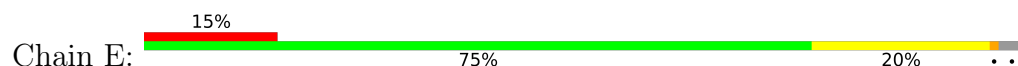


• Molecule 4: 26S proteasome regulatory subunit 6B

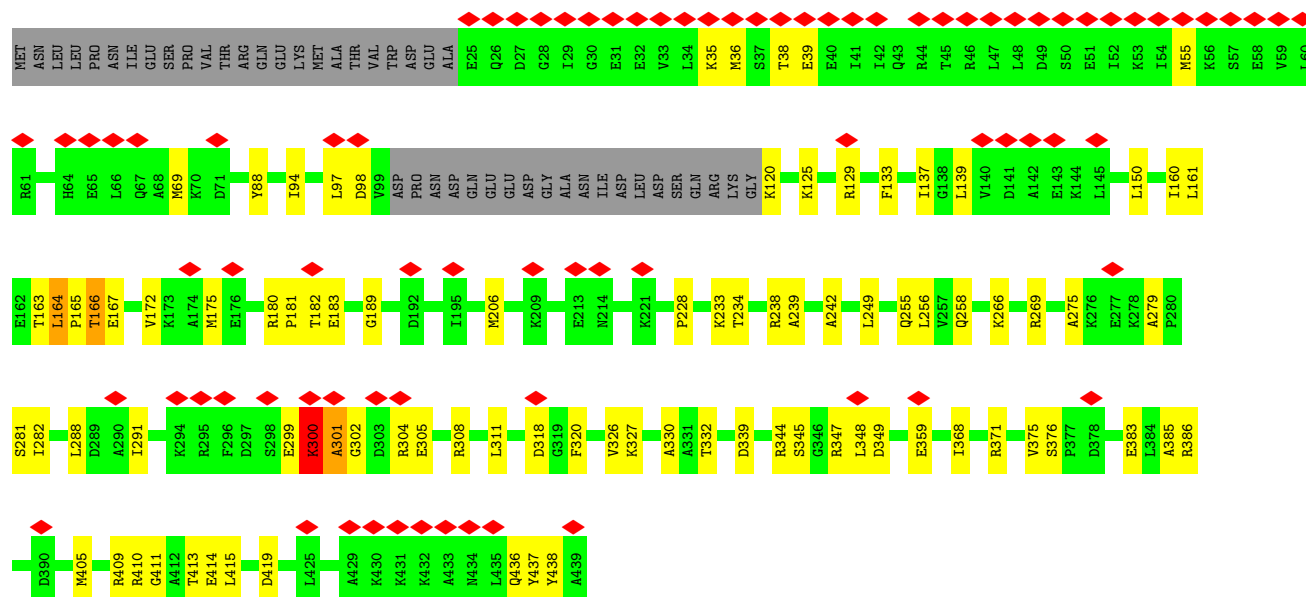




• Molecule 5: Proteasome 26S subunit, ATPase 6



• Molecule 6: 26S proteasome regulatory subunit 6A




- Molecule 7: Proteasome subunit alpha type-6

Chain G:  92% 7%




- Molecule 7: Proteasome subunit alpha type-6

Chain g:  89% 10%




- Molecule 8: Proteasome subunit alpha type-2

Chain H:  91% 8%




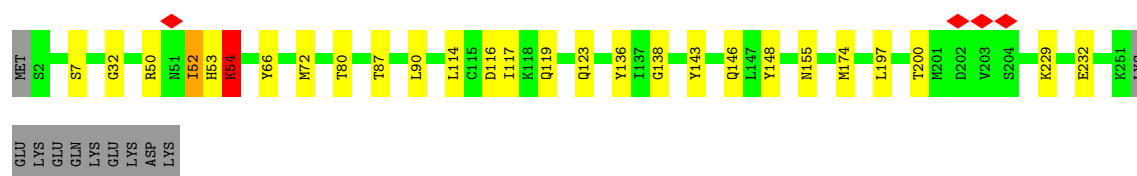
- Molecule 8: Proteasome subunit alpha type-2

Chain h:  89% 9%




- Molecule 9: Proteasome subunit alpha type-4

Chain I:  85% 10%




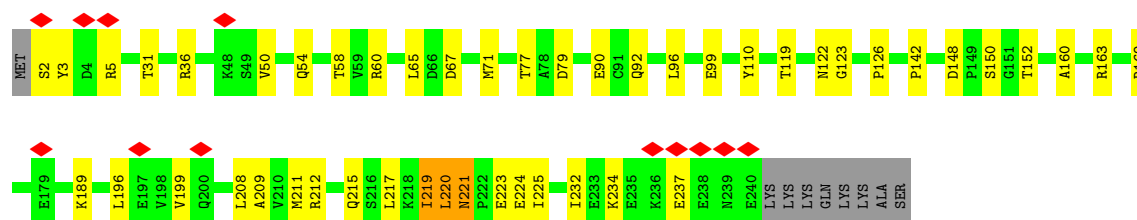
- Molecule 9: Proteasome subunit alpha type-4

Chain i:  89% 7%




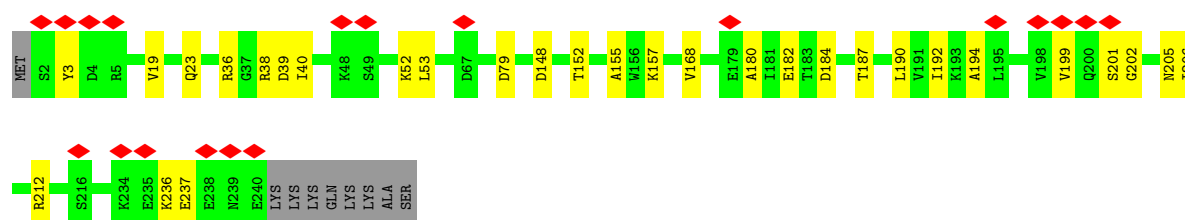
- Molecule 10: Proteasome subunit alpha type-7

Chain J:  5% 77% 18% . .



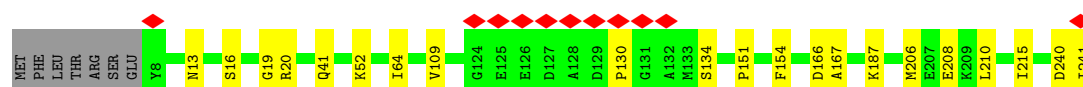
- Molecule 10: Proteasome subunit alpha type-7

Chain j:  8% 84% 12% .




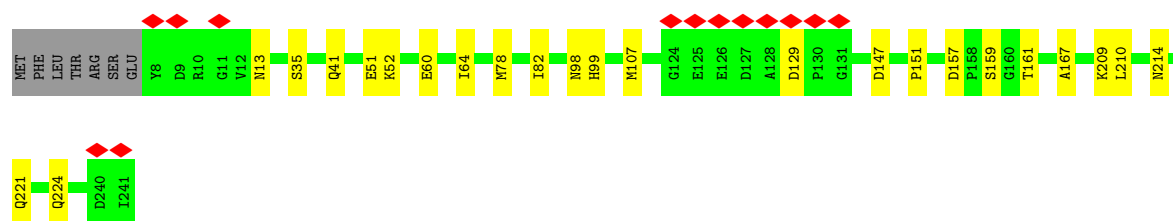
- Molecule 11: Proteasome subunit alpha type-5

Chain K:  5% 88% 9% .




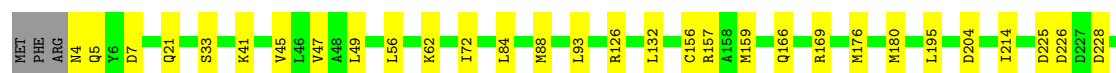
- Molecule 11: Proteasome subunit alpha type-5

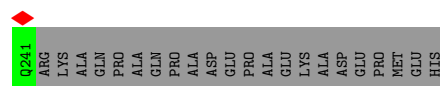
Chain k:  5% 87% 10% .



- Molecule 12: Proteasome subunit alpha type-1

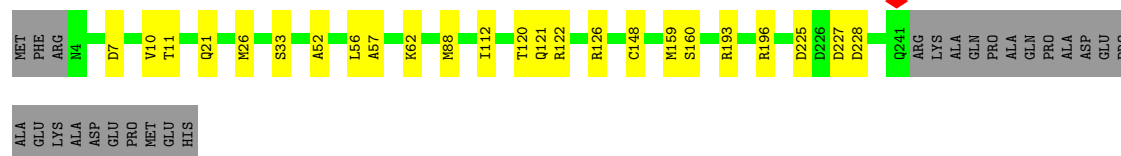
Chain L:  79% 11% 10%





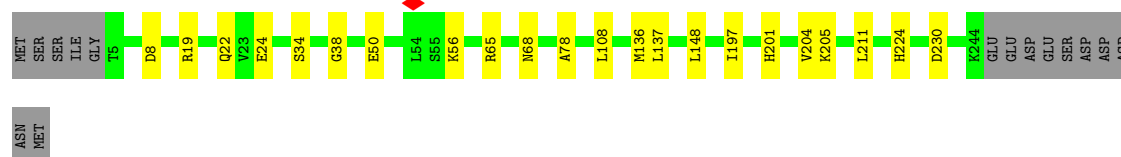
• Molecule 12: Proteasome subunit alpha type-1

Chain l: 81% 9% 10%



• Molecule 13: Proteasome subunit alpha type-3

Chain M: 85% 9% 6%



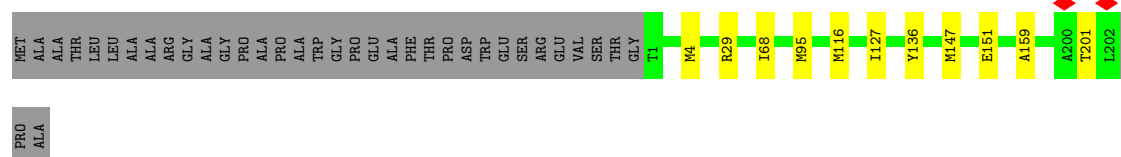
• Molecule 13: Proteasome subunit alpha type-3

Chain m: 80% 14% 6%



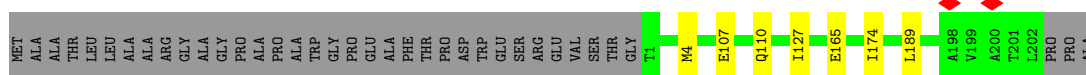
• Molecule 14: Proteasome subunit beta type-6

Chain N: 80% 5% 15%

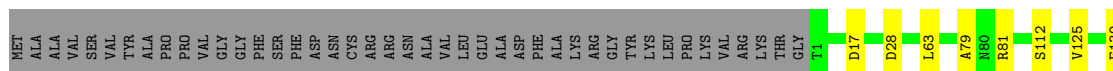


• Molecule 14: Proteasome subunit beta type-6

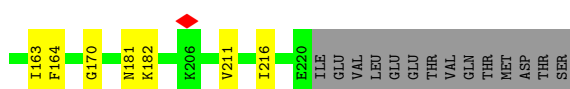
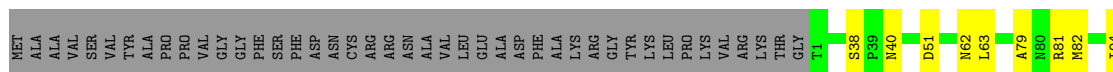
Chain n: 82% 15%



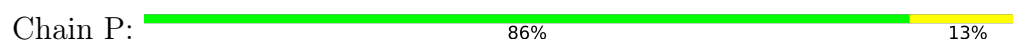
• Molecule 15: Proteasome subunit beta type-7



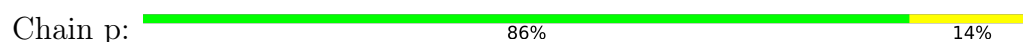
• Molecule 15: Proteasome subunit beta type-7



• Molecule 16: Proteasome subunit beta type-3



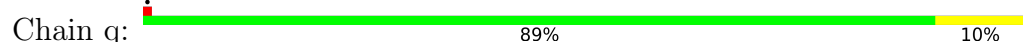
• Molecule 16: Proteasome subunit beta type-3



• Molecule 17: Proteasome subunit beta type-2



• Molecule 17: Proteasome subunit beta type-2





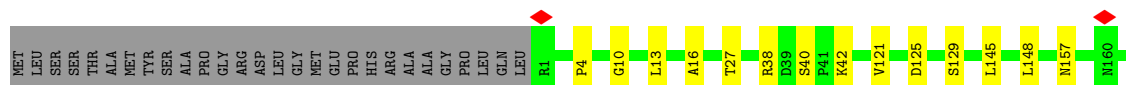
- Molecule 18: Proteasome subunit beta type-5



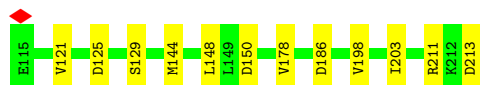
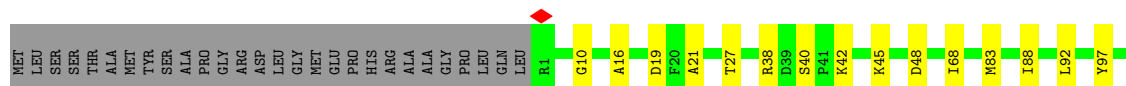
- Molecule 18: Proteasome subunit beta type-5



- Molecule 19: Proteasome subunit beta type-1



- Molecule 19: Proteasome subunit beta type-1

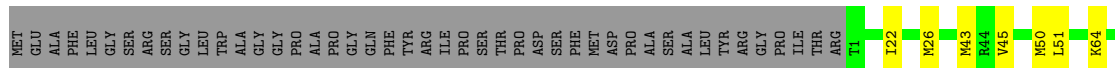


- Molecule 20: Proteasome subunit beta type-4

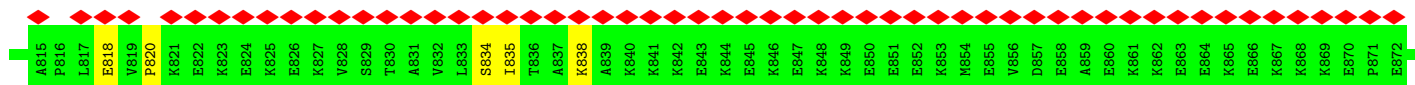
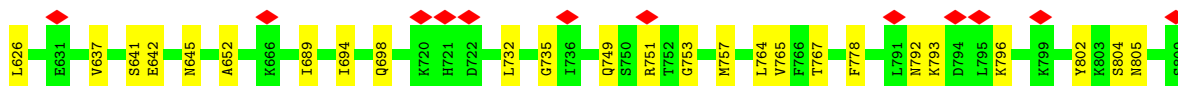
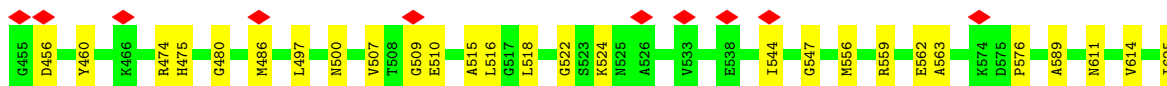
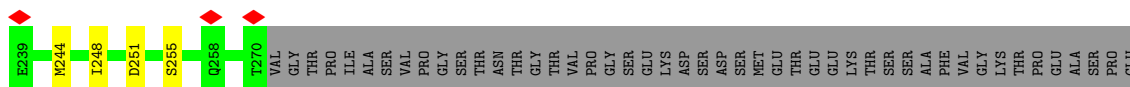
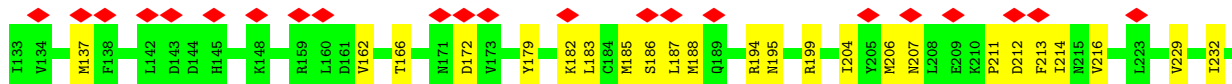
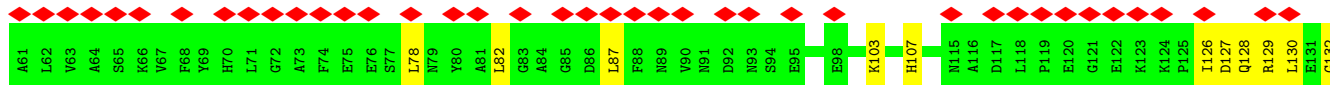
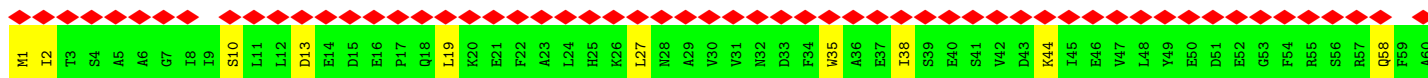
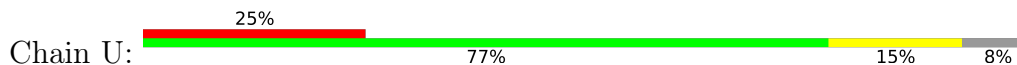


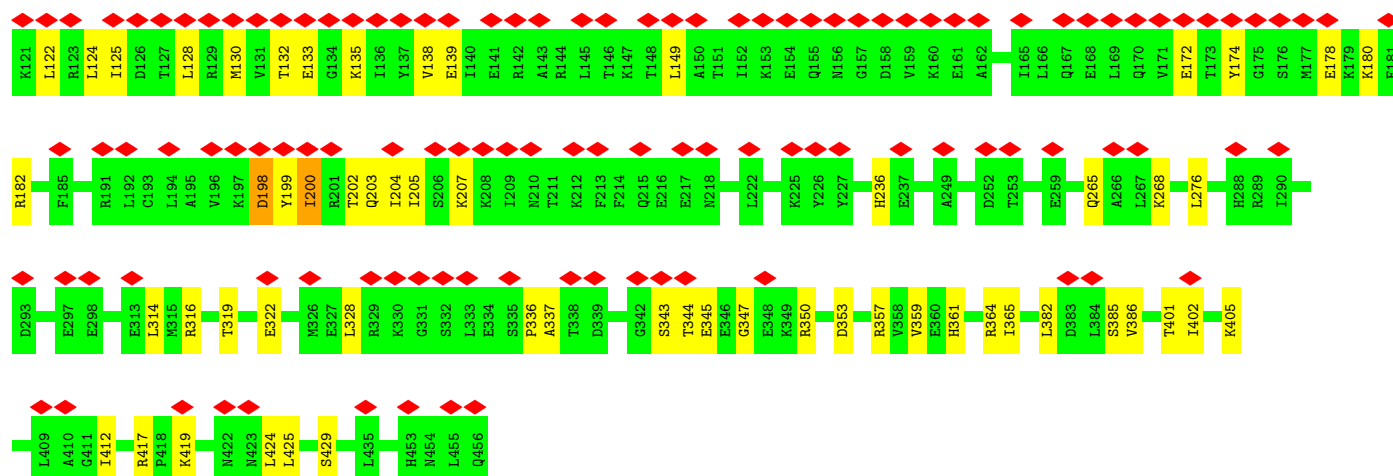


- Molecule 20: Proteasome subunit beta type-4

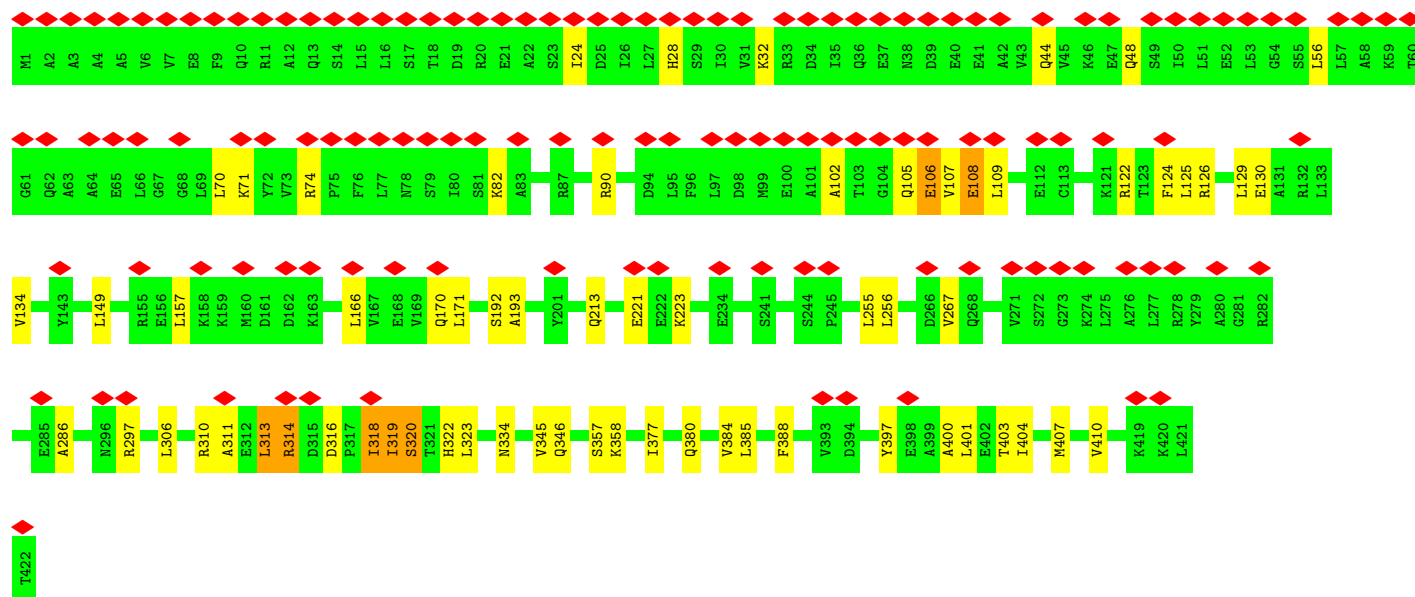
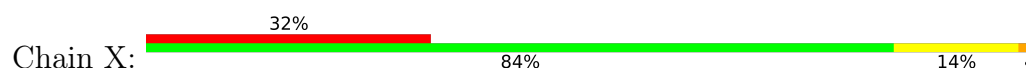


- Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

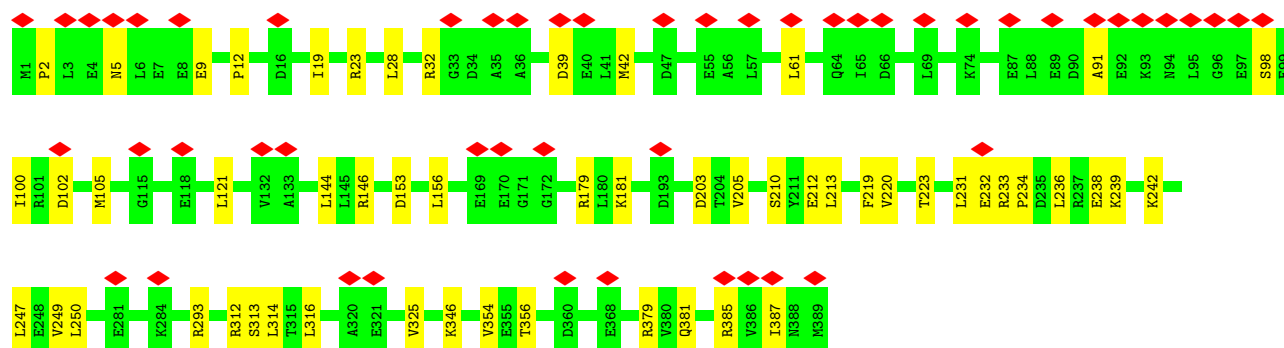
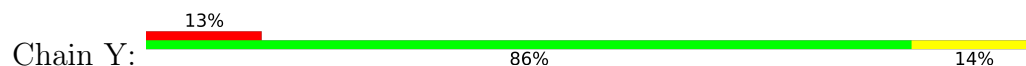




- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

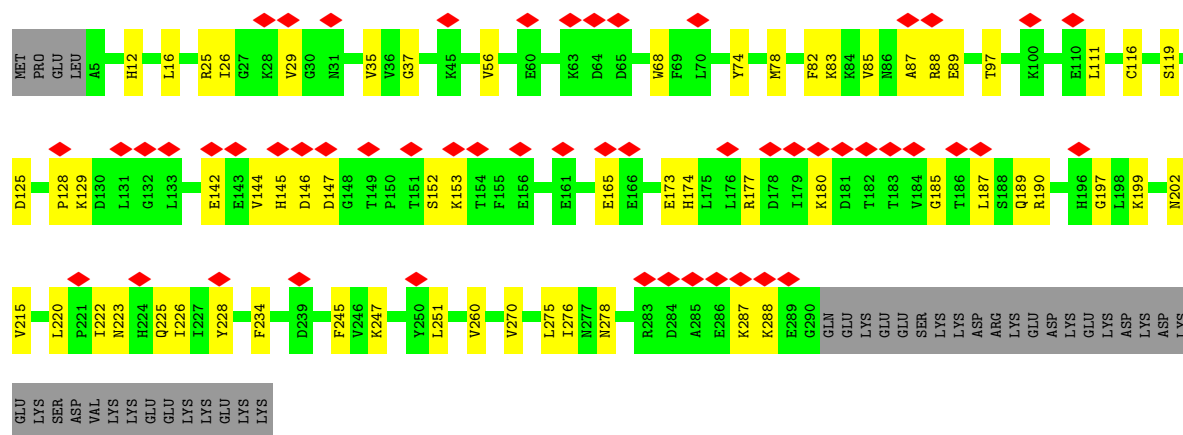


- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6




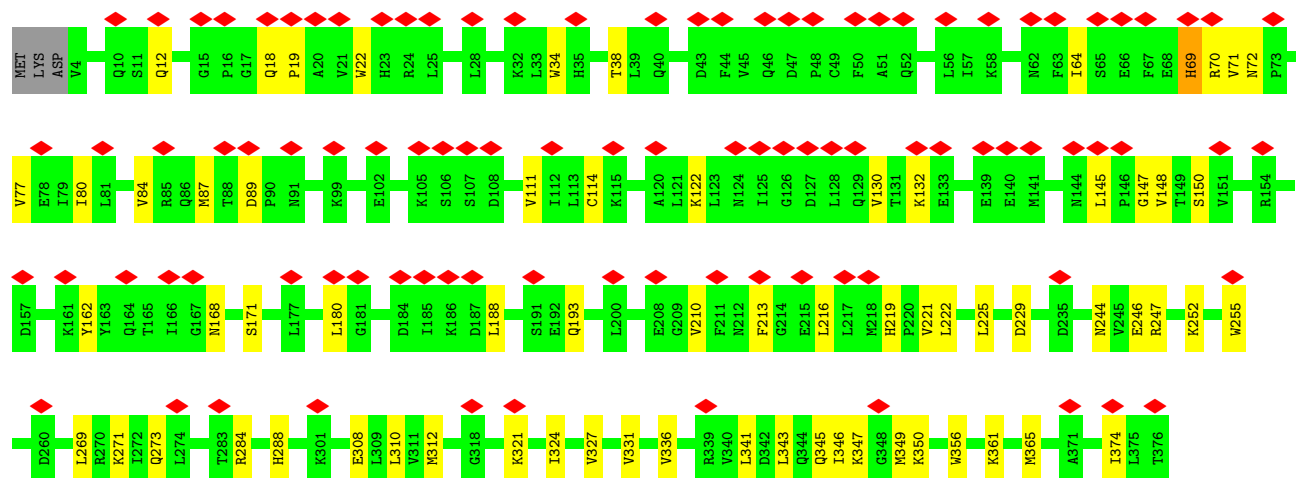
• Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 



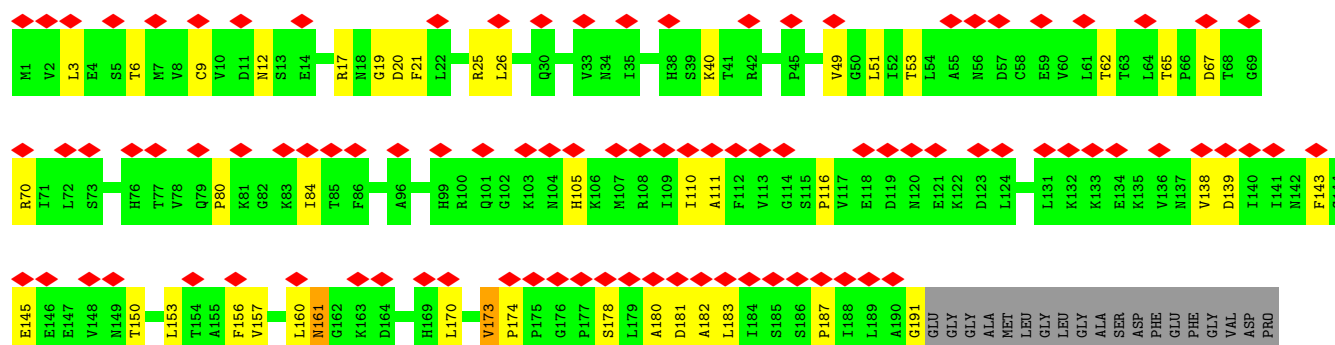
• Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

Chain a: 

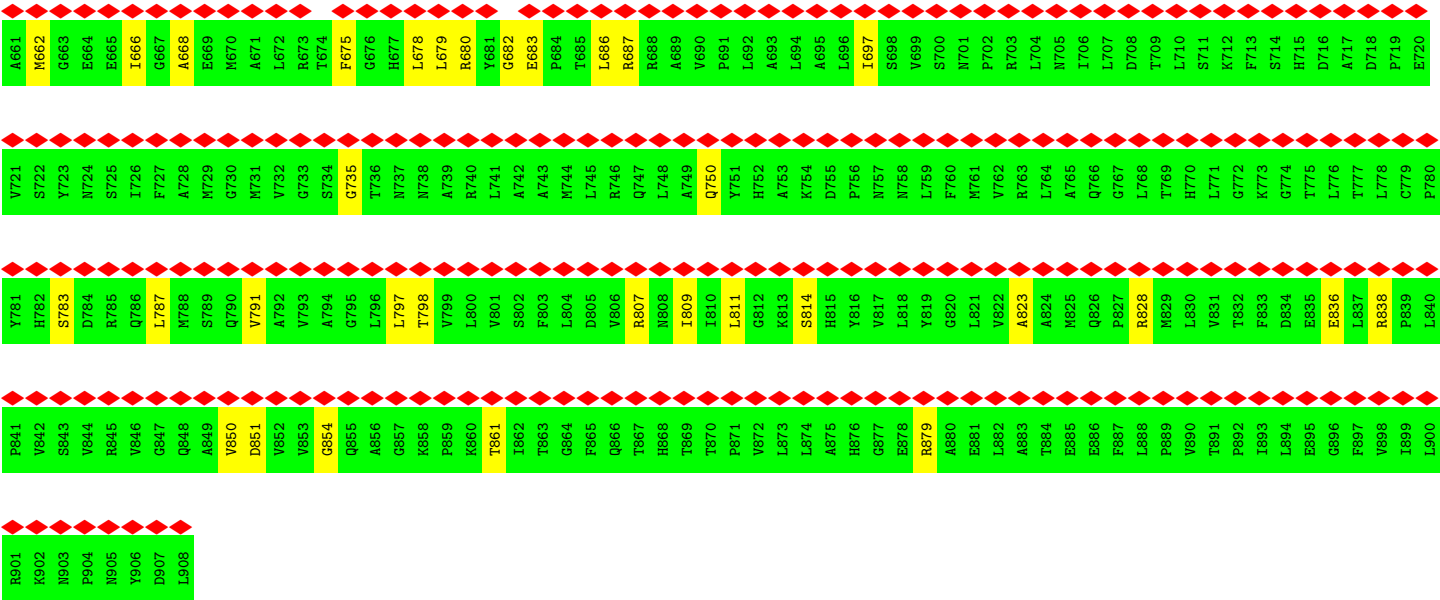


• Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

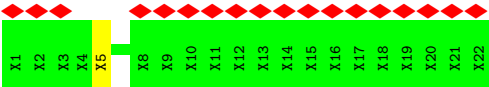
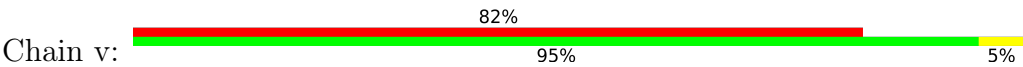
Chain b: 







● Molecule 33: Substrate



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77545	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	0.021	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00556	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: MG, ZN, ATP, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.22	0/3185	0.52	0/4299
2	B	0.17	0/3254	0.46	0/4388
3	C	0.18	0/3146	0.49	0/4226
4	D	0.21	0/3090	0.52	0/4168
5	E	0.22	0/3145	0.52	2/4233 (0.0%)
6	F	0.21	0/3137	0.52	0/4223
7	G	0.19	0/1923	0.44	0/2601
7	g	0.21	0/1914	0.42	0/2590
8	H	0.20	0/1844	0.42	0/2499
8	h	0.19	0/1844	0.40	0/2497
9	I	0.19	0/1987	0.44	0/2681
9	i	0.18	0/1985	0.42	0/2677
10	J	0.22	0/1884	0.44	0/2549
10	j	0.18	0/1887	0.44	0/2549
11	K	0.18	0/1800	0.40	0/2431
11	k	0.16	0/1809	0.36	0/2444
12	L	0.18	0/1901	0.36	0/2570
12	l	0.18	0/1896	0.39	0/2565
13	M	0.18	0/1917	0.40	0/2581
13	m	0.18	0/1916	0.37	0/2580
14	N	0.19	0/1540	0.35	0/2085
14	n	0.18	0/1536	0.37	0/2080
15	O	0.19	0/1676	0.41	0/2271
15	o	0.18	0/1686	0.40	0/2282
16	P	0.20	0/1616	0.45	0/2180
16	p	0.20	0/1620	0.45	0/2184
17	Q	0.20	0/1627	0.39	0/2202
17	q	0.19	0/1621	0.37	0/2194
18	R	0.20	0/1590	0.38	0/2147
18	r	0.21	0/1586	0.39	0/2142
19	S	0.20	0/1671	0.44	0/2252
19	s	0.20	0/1684	0.47	0/2268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.18	0/1716	0.37	0/2323
20	t	0.20	0/1720	0.42	0/2328
21	U	0.18	0/6984	0.49	0/9435
22	V	0.18	0/3681	0.47	0/4969
23	W	0.18	0/3644	0.52	0/4901
24	X	0.20	0/3381	0.49	1/4558 (0.0%)
25	Y	0.17	0/3261	0.47	0/4393
26	Z	0.22	0/2324	0.59	2/3150 (0.1%)
27	a	0.22	0/3053	0.54	0/4133
28	b	0.22	0/1478	0.55	2/2001 (0.1%)
29	c	0.23	0/2302	0.59	0/3110
30	d	0.24	0/2162	0.58	0/2919
31	e	0.23	0/437	0.56	0/595
32	f	0.17	0/6640	0.46	1/8988 (0.0%)
All	All	0.19	0/107700	0.47	8/145441 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	319	ILE	N-CA-C	8.87	118.63	111.62
32	f	582	VAL	N-CA-C	-8.45	104.15	112.17
5	E	226	GLN	CA-C-N	6.91	128.48	119.84
5	E	226	GLN	C-N-CA	6.91	128.48	119.84
26	Z	144	VAL	N-CA-C	-6.14	105.74	111.45
26	Z	29	VAL	N-CA-C	-5.91	107.53	113.20
28	b	173	VAL	CA-C-N	5.70	126.25	120.38
28	b	173	VAL	C-N-CA	5.70	126.25	120.38

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	3135	0	3175	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3207	0	3278	53	0
3	C	3105	0	3219	49	0
4	D	3040	0	3076	70	0
5	E	3097	0	3174	60	0
6	F	3098	0	3187	62	0
7	G	1889	0	1885	13	0
7	g	1880	0	1875	18	0
8	H	1805	0	1784	15	0
8	h	1805	0	1798	15	0
9	I	1954	0	1949	19	0
9	i	1955	0	1955	12	0
10	J	1858	0	1844	36	0
10	j	1861	0	1865	17	0
11	K	1773	0	1758	13	0
11	k	1782	0	1766	16	0
12	L	1866	0	1852	21	0
12	l	1861	0	1839	15	0
13	M	1879	0	1866	14	0
13	m	1881	0	1868	23	0
14	N	1514	0	1487	8	0
14	n	1510	0	1483	4	0
15	O	1649	0	1659	13	0
15	o	1659	0	1681	10	0
16	P	1587	0	1598	20	0
16	p	1591	0	1609	20	0
17	Q	1591	0	1589	14	0
17	q	1588	0	1584	14	0
18	R	1559	0	1523	9	0
18	r	1555	0	1517	8	0
19	S	1641	0	1639	12	0
19	s	1654	0	1656	17	0
20	T	1683	0	1662	16	0
20	t	1687	0	1666	13	0
21	U	6867	0	6929	88	0
22	V	3612	0	3682	47	0
23	W	3596	0	3713	51	0
24	X	3335	0	3435	44	0
25	Y	3202	0	3204	43	0
26	Z	2281	0	2312	42	0
27	a	2995	0	3012	51	0
28	b	1458	0	1505	36	0
29	c	2260	0	2276	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	d	2116	0	2146	35	0
31	e	425	0	328	11	0
32	f	6529	0	6541	83	0
33	v	110	0	29	1	0
34	C	31	0	12	3	0
34	D	31	0	12	1	0
34	E	31	0	12	1	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	E	1	0	0	0	0
36	F	27	0	12	1	0
37	c	1	0	0	0	0
All	All	106109	0	106526	1204	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1204) 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:566:HIS:CD2	32:f:576:ILE:CD1	2.25	1.20
24:X:256:LEU:HD13	24:X:319:ILE:HG22	1.26	1.09
29:c:192:LEU:HA	29:c:196:LEU:HB2	1.40	1.02
32:f:566:HIS:NE2	32:f:576:ILE:HD11	1.74	1.01
32:f:566:HIS:CD2	32:f:576:ILE:HD11	1.92	1.00
32:f:566:HIS:HD2	32:f:576:ILE:CD1	1.68	1.00
1:A:156:LYS:HE2	1:A:256:MET:HE1	1.49	0.94
25:Y:312:ARG:HA	25:Y:356:THR:CG2	1.97	0.94
24:X:256:LEU:HD13	24:X:319:ILE:CG2	2.05	0.86
5:E:226:GLN:HB3	5:E:227:PRO:HD2	1.57	0.86
25:Y:312:ARG:HA	25:Y:356:THR:HG22	1.56	0.85
1:A:284:ARG:NH2	1:A:289:ALA:HB2	1.92	0.84
10:J:221:ASN:HD21	10:J:223:GLU:HB3	1.41	0.83
32:f:566:HIS:HE2	32:f:576:ILE:HD11	1.38	0.83
28:b:116:PRO:HD3	28:b:145:GLU:OE2	1.79	0.82
1:A:158:ASP:HB3	1:A:259:GLU:HG3	1.64	0.80
29:c:279:ASP:HB3	29:c:280:PRO:HD3	1.64	0.79
32:f:566:HIS:CD2	32:f:576:ILE:HD12	2.14	0.78
5:E:226:GLN:CB	5:E:227:PRO:HD2	2.13	0.78
1:A:284:ARG:HH22	1:A:289:ALA:HB2	1.50	0.77
8:H:175:GLU:HA	9:I:54:LYS:NZ	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ARG:NH2	1:A:289:ALA:CB	2.48	0.76
24:X:318:ILE:HG13	24:X:322:HIS:CE1	2.19	0.76
1:A:158:ASP:N	1:A:159:PRO:HD2	2.02	0.75
23:W:343:SER:HB3	23:W:347:GLY:H	1.51	0.74
23:W:200:ILE:HD12	23:W:200:ILE:H	1.53	0.74
25:Y:312:ARG:HA	25:Y:356:THR:HG21	1.70	0.73
10:J:208:LEU:HD22	10:J:220:LEU:HG	1.69	0.73
21:U:792:ASN:HB3	21:U:914:LEU:H	1.55	0.71
9:I:143:TYR:HB2	9:I:146:GLN:HE21	1.56	0.70
27:a:69:HIS:O	27:a:70:ARG:HD2	1.91	0.70
28:b:173:VAL:HG22	28:b:174:PRO:HD2	1.74	0.70
10:J:96:LEU:HB2	17:Q:62:LYS:HD3	1.74	0.69
25:Y:312:ARG:CA	25:Y:356:THR:HG22	2.23	0.69
4:D:167:ILE:HG12	4:D:214:MET:HE2	1.74	0.69
30:d:203:PRO:HD2	30:d:206:MET:HG2	1.72	0.69
1:A:158:ASP:HB3	1:A:259:GLU:CG	2.22	0.69
4:D:394:VAL:HG12	4:D:396:ALA:H	1.57	0.68
25:Y:102:ASP:HA	25:Y:105:MET:HG2	1.75	0.68
29:c:75:MET:HE3	29:c:76:PRO:HD2	1.75	0.68
23:W:101:VAL:HA	23:W:104:MET:HG3	1.75	0.68
23:W:200:ILE:HD12	23:W:200:ILE:N	2.07	0.68
5:E:23:ASP:HA	6:F:55:MET:HE3	1.76	0.68
22:V:476:PHE:HB3	26:Z:260:VAL:HG21	1.74	0.68
32:f:566:HIS:O	32:f:569:LYS:HG2	1.94	0.67
4:D:154:LEU:HB3	4:D:159:LYS:HZ3	1.58	0.67
19:s:68:ILE:HD11	19:s:92:LEU:HD13	1.75	0.67
23:W:401:THR:HG23	23:W:402:ILE:HD12	1.74	0.67
24:X:319:ILE:O	24:X:323:LEU:HG	1.95	0.67
13:M:38:GLY:HA3	13:M:136:MET:HE1	1.77	0.66
21:U:58:GLN:HB2	21:U:87:LEU:HD12	1.77	0.66
3:C:406:LYS:HG3	9:I:80:THR:HG22	1.78	0.66
23:W:172:GLU:HA	23:W:182:ARG:HE	1.61	0.65
26:Z:199:LYS:HD2	26:Z:202:ASN:HD21	1.61	0.65
24:X:102:ALA:O	24:X:106:GLU:HB2	1.97	0.65
16:p:149:MET:HE1	16:p:173:ASN:HD22	1.61	0.65
26:Z:26:ILE:HD11	26:Z:35:VAL:HG22	1.78	0.65
11:k:210:LEU:HA	11:k:214:ASN:HD21	1.62	0.65
6:F:376:SER:HB3	6:F:414:GLU:HB2	1.79	0.64
19:S:148:LEU:HD23	19:S:178:VAL:HG12	1.78	0.64
1:A:158:ASP:H	1:A:159:PRO:HD2	1.62	0.64
29:c:248:MET:HE1	29:c:284:LEU:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:238:GLU:HA	25:Y:242:LYS:HB2	1.79	0.63
32:f:566:HIS:HD2	32:f:576:ILE:HD13	1.56	0.63
28:b:173:VAL:CG2	28:b:174:PRO:HD2	2.28	0.63
1:A:140:VAL:HG12	1:A:152:PRO:HB3	1.79	0.63
26:Z:209:ARG:HD2	26:Z:212:LEU:HD11	1.80	0.62
32:f:96:LEU:HD13	32:f:129:LEU:HD13	1.81	0.62
19:S:38:ARG:NH2	15:o:164:PHE:O	2.32	0.62
2:B:398:ILE:HD11	2:B:427:LEU:HD11	1.80	0.62
6:F:228:PRO:O	6:F:233:LYS:NZ	2.33	0.62
22:V:221:LEU:HD13	22:V:223:LYS:HZ1	1.64	0.62
3:C:69:GLN:HG3	3:C:118:ASN:HD21	1.63	0.62
24:X:44:GLN:O	24:X:48:GLN:NE2	2.32	0.62
1:A:173:THR:HG22	1:A:175:SER:H	1.63	0.62
1:A:277:ILE:HD11	1:A:321:THR:HB	1.82	0.62
22:V:117:VAL:HG13	22:V:128:ARG:HB2	1.81	0.62
23:W:112:VAL:HG22	23:W:124:LEU:HD13	1.82	0.62
32:f:150:GLU:HG3	32:f:152:ALA:H	1.65	0.62
13:M:65:ARG:HH21	13:M:78:ALA:HA	1.65	0.62
19:s:83:MET:HE3	19:s:88:ILE:HG12	1.82	0.62
23:W:200:ILE:H	23:W:200:ILE:CD1	2.12	0.62
6:F:405:MET:HE3	6:F:409:ARG:HG2	1.81	0.61
14:N:147:MET:HE2	14:N:151:GLU:HB3	1.82	0.61
21:U:213:PHE:HE1	21:U:244:MET:HG3	1.65	0.61
20:t:110:MET:HB3	20:t:125:VAL:HB	1.82	0.61
18:R:100:MET:HE3	18:R:126:PHE:HB2	1.81	0.61
30:d:87:GLU:HA	30:d:89:LEU:HD23	1.82	0.61
32:f:807:ARG:HA	32:f:811:LEU:HD12	1.83	0.61
26:Z:187:LEU:HG	29:c:293:THR:HG22	1.83	0.61
3:C:137:LEU:O	3:C:213:ARG:NH1	2.34	0.61
1:A:122:VAL:HB	6:F:88:TYR:HB2	1.82	0.61
23:W:90:LEU:HB3	23:W:104:MET:HE1	1.82	0.61
8:H:175:GLU:HA	9:I:54:LYS:HZ3	1.65	0.60
24:X:108:GLU:OE2	24:X:108:GLU:HA	2.00	0.60
5:E:364:GLN:NE2	5:E:368:MET:SD	2.74	0.60
10:J:221:ASN:HD22	10:J:224:GLU:HG3	1.66	0.60
24:X:318:ILE:HG23	24:X:318:ILE:O	2.01	0.60
1:A:284:ARG:HH21	1:A:289:ALA:CB	2.13	0.60
1:A:369:ARG:NH2	11:K:206:MET:O	2.34	0.60
20:T:174:ARG:NH1	20:T:206:GLU:O	2.34	0.60
6:F:302:GLY:HA2	6:F:305:GLU:OE2	2.01	0.60
23:W:319:THR:O	23:W:322:GLU:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:162:VAL:O	4:D:221:HIS:ND1	2.34	0.60
27:a:374:ILE:HG21	30:d:251:ARG:HA	1.82	0.60
28:b:84:ILE:HD13	28:b:116:PRO:O	2.01	0.60
21:U:522:GLY:O	21:U:559:ARG:NH2	2.34	0.60
16:P:177:ARG:NH2	19:s:150:ASP:OD2	2.33	0.60
29:c:145:VAL:HG22	29:c:157:ILE:HG12	1.84	0.60
1:A:156:LYS:CE	1:A:256:MET:HE1	2.29	0.60
2:B:54:PRO:HA	32:f:854:GLY:HA3	1.84	0.59
32:f:659:LEU:HA	32:f:662:MET:HE3	1.83	0.59
22:V:494:MET:O	26:Z:278:ASN:ND2	2.35	0.59
23:W:199:TYR:HE2	23:W:236:HIS:CE1	2.20	0.59
32:f:240:VAL:O	32:f:245:ASN:ND2	2.33	0.59
4:D:384:MET:HE2	5:E:147:GLU:HG2	1.83	0.59
3:C:53:ASN:ND2	21:U:642:GLU:O	2.36	0.59
8:H:175:GLU:HA	9:I:54:LYS:HZ1	1.65	0.59
32:f:566:HIS:HD2	32:f:576:ILE:HD12	1.59	0.59
1:A:158:ASP:N	1:A:159:PRO:CD	2.65	0.59
24:X:256:LEU:CD1	24:X:319:ILE:HG22	2.18	0.59
6:F:234:THR:O	6:F:238:ARG:NH2	2.35	0.59
26:Z:129:LYS:HZ3	29:c:215:LYS:HE3	1.67	0.59
24:X:122:ARG:HD2	24:X:125:LEU:HB2	1.84	0.59
27:a:180:LEU:HD21	27:a:221:VAL:HG11	1.83	0.59
27:a:219:HIS:HB3	27:a:221:VAL:HG22	1.85	0.59
32:f:379:GLY:HA3	32:f:416:MET:HE3	1.85	0.59
21:U:818:GLU:HG2	21:U:820:PRO:HD3	1.85	0.59
22:V:397:ARG:HH21	30:d:116:HIS:HB3	1.67	0.59
27:a:70:ARG:O	28:b:17:ARG:NH1	2.36	0.59
32:f:442:SER:HB2	32:f:477:MET:HA	1.85	0.59
2:B:375:ALA:HB2	2:B:413:LYS:HB3	1.85	0.59
4:D:297:ASP:OD2	4:D:323:ARG:NH2	2.36	0.59
2:B:181:GLN:O	2:B:241:ASN:ND2	2.36	0.58
10:J:50:VAL:HB	10:J:54:GLN:HB2	1.85	0.58
21:U:10:SER:HB2	30:d:73:ARG:HG3	1.85	0.58
27:a:34:TRP:HB3	27:a:71:VAL:HG22	1.84	0.58
27:a:361:LYS:HG2	27:a:365:MET:HE2	1.83	0.58
2:B:411:ARG:NH2	2:B:418:ASP:OD2	2.36	0.58
22:V:282:ASN:ND2	25:Y:385:ARG:O	2.34	0.58
29:c:139:ARG:HB2	29:c:161:ARG:HE	1.68	0.58
15:O:164:PHE:O	19:s:38:ARG:NH2	2.37	0.58
21:U:793:LYS:HE3	21:U:796:LYS:HB2	1.86	0.58
29:c:149:GLN:HB3	29:c:156:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:34:SER:OG	13:m:65:ARG:NH1	2.36	0.58
22:V:289:LEU:HB3	22:V:312:ALA:HB2	1.85	0.58
27:a:18:GLN:HB3	27:a:22:TRP:CD1	2.39	0.58
27:a:188:LEU:O	27:a:193:GLN:NE2	2.37	0.58
29:c:270:LEU:HA	29:c:273:LYS:HG2	1.85	0.58
2:B:109:VAL:HG21	3:C:94:LYS:HE2	1.85	0.58
21:U:510:GLU:HA	21:U:547:GLY:HA3	1.85	0.58
6:F:94:ILE:HD11	6:F:125:LYS:HB2	1.85	0.58
23:W:105:VAL:HG21	23:W:138:VAL:HG21	1.85	0.58
32:f:570:GLY:H	32:f:599:ALA:HB1	1.69	0.58
12:l:225:ASP:H	12:l:228:ASP:HB2	1.68	0.58
2:B:219:PRO:O	2:B:326:LYS:NZ	2.37	0.58
1:A:158:ASP:HB3	1:A:259:GLU:CD	2.29	0.58
18:R:64:ARG:NH1	18:R:67:GLU:OE1	2.36	0.58
19:S:27:THR:HB	19:S:40:SER:H	1.69	0.58
23:W:425:LEU:HB2	26:Z:247:LYS:HD3	1.86	0.58
32:f:836:GLU:HB3	32:f:838:ARG:HG3	1.86	0.58
4:D:411:GLU:CD	4:D:412:GLN:H	2.11	0.57
17:Q:68:LYS:HD3	17:Q:74:GLU:HG2	1.86	0.57
10:J:212:ARG:HB2	10:J:215:GLN:HE22	1.68	0.57
28:b:138:VAL:H	28:b:160:LEU:HD21	1.70	0.57
1:A:100:LYS:HG3	1:A:137:GLY:HA2	1.86	0.57
4:D:351:LYS:NZ	5:E:163:GLY:O	2.35	0.57
16:P:61:GLN:HB2	17:Q:85:ARG:HH21	1.70	0.57
5:E:144:GLU:O	5:E:297:ARG:NH2	2.38	0.57
16:P:35:VAL:HG12	16:P:36:THR:HG23	1.86	0.57
25:Y:220:VAL:HG21	25:Y:249:VAL:HG21	1.87	0.57
8:h:3:GLU:N	13:m:125:TYR:HB3	2.19	0.57
17:q:151:ILE:HA	17:q:155:ARG:HH21	1.69	0.57
3:C:368:MET:HE1	4:D:199:PRO:HD3	1.87	0.57
27:a:72:ASN:HB2	28:b:17:ARG:HH22	1.69	0.57
28:b:174:PRO:HG2	28:b:178:SER:HB2	1.87	0.57
2:B:106:PRO:O	2:B:154:HIS:NE2	2.36	0.57
4:D:45:LYS:HG2	21:U:187:LEU:HB2	1.86	0.57
22:V:219:GLU:HA	22:V:224:LEU:HD11	1.87	0.57
24:X:286:ALA:HB1	24:X:313:LEU:HD21	1.85	0.57
30:d:248:GLU:HG2	30:d:249:TYR:N	2.20	0.57
9:i:119:GLN:NE2	10:j:79:ASP:OD1	2.38	0.57
9:i:174:MET:SD	9:i:195:LYS:NZ	2.77	0.57
12:l:120:THR:O	13:m:129:ARG:NH1	2.38	0.57
19:s:148:LEU:HD23	19:s:178:VAL:HG12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:HB	1:A:281:GLY:HA3	1.85	0.56
2:B:382:ASP:HA	2:B:385:MET:HG2	1.85	0.56
6:F:165:PRO:O	6:F:166:THR:C	2.48	0.56
5:E:265:ASP:O	5:E:294:ARG:NH2	2.38	0.56
6:F:282:ILE:HG22	6:F:327:LYS:HB2	1.86	0.56
18:R:125:THR:HB	18:R:139:MET:HE3	1.85	0.56
23:W:115:ILE:HG21	23:W:124:LEU:HD21	1.87	0.56
8:h:14:SER:HB3	8:h:18:LYS:H	1.70	0.56
2:B:53:THR:HG21	32:f:851:ASP:HB3	1.86	0.56
9:I:32:GLY:HA2	9:I:50:ARG:HH21	1.71	0.56
20:t:43:MET:HE2	20:t:51:LEU:HD23	1.86	0.56
5:E:75:ASN:ND2	6:F:129:ARG:O	2.38	0.56
5:E:82:GLY:H	5:E:106:THR:HG22	1.71	0.56
1:A:268:LYS:HD2	1:A:314:ASN:HD22	1.69	0.56
20:T:37:ARG:NH1	14:n:165:GLU:OE2	2.37	0.56
30:d:161:GLU:HG2	30:d:162:SER:H	1.69	0.56
32:f:560:LEU:HD21	32:f:798:THR:HA	1.87	0.56
5:E:337:GLY:O	5:E:378:LYS:NZ	2.39	0.56
5:E:339:ASN:HB3	5:E:342:ASP:HB2	1.87	0.56
21:U:637:VAL:HG13	21:U:652:ALA:HB1	1.88	0.56
32:f:282:PHE:HZ	32:f:317:LEU:HD21	1.71	0.56
7:g:70:PHE:HD2	7:g:91:VAL:HG21	1.71	0.56
13:M:136:MET:HE3	13:M:148:LEU:HD11	1.87	0.56
23:W:405:LYS:HB2	23:W:417:ARG:HH12	1.70	0.56
14:n:174:ILE:HB	14:n:189:LEU:HB2	1.87	0.56
1:A:156:LYS:HE3	1:A:156:LYS:H	1.71	0.56
24:X:70:LEU:HD12	24:X:109:LEU:HD21	1.88	0.56
5:E:197:LYS:HE3	6:F:320:PHE:HB2	1.87	0.56
25:Y:210:SER:HB3	25:Y:213:LEU:HD23	1.88	0.56
21:U:179:TYR:HA	21:U:182:LYS:HE2	1.88	0.55
26:Z:215:VAL:HG22	26:Z:222:ILE:HG22	1.87	0.55
17:q:168:GLN:NE2	17:q:175:LEU:O	2.37	0.55
1:A:307:ASP:OD2	1:A:333:ARG:NH2	2.38	0.55
4:D:154:LEU:HB3	4:D:159:LYS:NZ	2.21	0.55
8:H:74:LEU:HD22	8:H:136:ILE:HG12	1.87	0.55
11:K:167:ALA:HB3	12:L:56:LEU:HD13	1.88	0.55
25:Y:231:LEU:HG	25:Y:236:LEU:HD12	1.89	0.55
24:X:90:ARG:HH22	24:X:129:LEU:HD12	1.71	0.55
19:s:27:THR:HB	19:s:40:SER:H	1.71	0.55
6:F:255:GLN:O	6:F:258:GLN:NE2	2.37	0.55
25:Y:293:ARG:NH1	31:e:45:ASP:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:165:ALA:HB1	7:g:179:LEU:HD13	1.89	0.55
13:m:8:ASP:O	13:m:22:GLN:NE2	2.39	0.55
4:D:156:SER:O	4:D:157:ASP:HB2	2.06	0.55
4:D:168:GLY:HA3	4:D:347:THR:HG21	1.89	0.55
11:K:13:ASN:HB3	12:L:126:ARG:HB3	1.89	0.55
17:Q:169:LYS:O	17:q:27:GLN:NE2	2.40	0.55
24:X:407:MET:HA	24:X:410:VAL:HG22	1.87	0.55
5:E:98:VAL:HA	5:E:110:TYR:HA	1.88	0.55
3:C:264:GLY:HA3	4:D:279:THR:HA	1.87	0.55
17:Q:170:ARG:HA	17:q:27:GLN:HE21	1.72	0.55
21:U:486:MET:HE1	21:U:757:MET:HE1	1.87	0.55
26:Z:174:HIS:O	26:Z:177:ARG:NH2	2.39	0.55
13:m:93:GLU:OE2	13:m:97:ASN:ND2	2.40	0.55
13:M:50:GLU:OE2	13:M:201:HIS:ND1	2.36	0.55
7:G:103:TYR:O	15:O:81:ARG:NH2	2.40	0.55
10:J:148:ASP:OD1	10:J:152:THR:N	2.39	0.55
15:O:206:LYS:HD2	16:P:161:ASP:HB3	1.88	0.55
8:h:119:GLN:HG3	9:i:81:SER:HB2	1.89	0.55
17:q:25:ILE:HG22	17:q:26:VAL:HG13	1.89	0.55
16:P:65:GLN:OE1	17:Q:86:ARG:NH2	2.40	0.55
21:U:204:ILE:HA	21:U:207:ASN:HB2	1.89	0.54
24:X:255:LEU:HD22	24:X:267:VAL:HG13	1.89	0.54
27:a:87:MET:HE1	27:a:89:ASP:HB2	1.89	0.54
12:l:7:ASP:O	12:l:21:GLN:NE2	2.36	0.54
1:A:117:GLN:HE22	2:B:128:GLY:HA3	1.71	0.54
1:A:283:ALA:HA	1:A:326:THR:HB	1.89	0.54
3:C:195:GLY:N	34:C:501:ATP:O1A	2.38	0.54
29:c:264:LYS:HA	29:c:267:PRO:HB3	1.89	0.54
15:o:163:ILE:HG12	15:o:170:GLY:HA2	1.88	0.54
29:c:167:MET:HG3	29:c:170:LEU:HB3	1.89	0.54
10:j:236:LYS:NZ	10:j:237:GLU:OE2	2.40	0.54
1:A:200:ARG:HD3	6:F:411:GLY:HA2	1.90	0.54
4:D:85:ILE:HG21	29:c:152:LYS:HE2	1.88	0.54
8:h:148:GLN:OE1	8:h:158:TRP:NE1	2.41	0.54
20:t:26:MET:HE1	20:t:202:PRO:HB3	1.88	0.54
3:C:192:PRO:HG2	3:C:194:THR:HG23	1.90	0.54
21:U:611:ASN:HB3	21:U:614:VAL:HG22	1.90	0.54
32:f:548:THR:O	32:f:551:LYS:NZ	2.40	0.54
21:U:13:ASP:OD1	21:U:44:LYS:NZ	2.40	0.54
21:U:419:ALA:HB1	21:U:449:ILE:HD13	1.90	0.54
8:h:42:ASN:ND2	8:h:183:GLU:OE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:375:ARG:HG2	3:C:377:HIS:H	1.73	0.54
19:S:211:ARG:NH2	19:S:213:ASP:OD2	2.41	0.54
21:U:889:LEU:HD13	21:U:908:ILE:HA	1.90	0.54
22:V:150:ARG:NH1	22:V:157:THR:O	2.41	0.54
28:b:180:ALA:HA	28:b:183:LEU:HD13	1.90	0.54
32:f:270:LEU:HD12	32:f:297:MET:HE1	1.90	0.54
16:p:159:ASP:OD1	16:p:159:ASP:N	2.41	0.54
3:C:113:ARG:NH2	3:C:129:ASN:O	2.39	0.54
3:C:260:GLU:HB2	3:C:263:SER:HB3	1.90	0.54
6:F:330:ALA:HB3	6:F:348:LEU:HD21	1.89	0.54
21:U:474:ARG:NH2	21:U:500:ASN:OD1	2.37	0.54
22:V:287:ARG:NH2	31:e:17:ASP:OD2	2.41	0.54
23:W:203:GLN:OE1	23:W:207:LYS:NZ	2.36	0.54
32:f:735:GLY:O	32:f:828:ARG:NH1	2.41	0.54
7:g:103:TYR:O	15:o:81:ARG:NH2	2.41	0.54
18:r:75:SER:HB2	18:r:107:ARG:HH22	1.72	0.54
6:F:376:SER:OG	6:F:415:LEU:O	2.26	0.54
9:I:66:TYR:HD2	9:I:87:THR:HG21	1.73	0.54
10:J:65:LEU:HD21	10:J:71:MET:HE2	1.90	0.54
21:U:162:VAL:O	21:U:166:THR:OG1	2.23	0.54
32:f:120:ARG:HB3	32:f:147:SER:H	1.72	0.54
11:k:98:ASN:OD1	18:r:61:ARG:NH2	2.41	0.54
5:E:364:GLN:HA	5:E:367:PHE:HD2	1.72	0.54
2:B:182:GLU:HB2	2:B:186:ASP:HB2	1.90	0.53
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.90	0.53
12:L:157:ARG:NH1	12:L:176:MET:SD	2.82	0.53
21:U:486:MET:HG2	21:U:518:LEU:HD22	1.90	0.53
1:A:189:GLU:O	1:A:193:THR:OG1	2.24	0.53
3:C:250:GLU:HB3	4:D:290:LEU:HD22	1.91	0.53
25:Y:312:ARG:CA	25:Y:356:THR:CG2	2.78	0.53
7:g:141:ILE:HG22	7:g:151:VAL:HG22	1.90	0.53
17:q:1:MET:HE3	17:q:133:GLY:HA2	1.90	0.53
19:s:10:GLY:HA3	19:s:42:LYS:HE2	1.88	0.53
4:D:335:LEU:HD12	4:D:336:PRO:HD2	1.91	0.53
5:E:87:LEU:O	5:E:91:LYS:NZ	2.40	0.53
6:F:345:SER:HA	6:F:349:ASP:HB3	1.91	0.53
13:M:8:ASP:O	13:M:22:GLN:NE2	2.39	0.53
10:J:160:ALA:O	10:J:169:ARG:NH2	2.41	0.53
22:V:467:TYR:HH	24:X:397:TYR:HH	1.57	0.53
23:W:419:LYS:HG3	23:W:424:LEU:HD12	1.89	0.53
6:F:150:LEU:O	6:F:164:LEU:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:25:ARG:NH1	28:b:145:GLU:OE1	2.40	0.53
32:f:320:ILE:HA	32:f:325:GLN:HE22	1.73	0.53
11:k:221:GLN:HB2	11:k:224:GLN:HG2	1.89	0.53
1:A:156:LYS:HE3	1:A:156:LYS:N	2.24	0.53
4:D:398:ASP:OD1	4:D:398:ASP:N	2.41	0.53
6:F:359:GLU:HB3	6:F:385:ALA:HB1	1.91	0.53
9:I:50:ARG:O	9:I:52:ILE:HG13	2.09	0.53
21:U:694:ILE:O	21:U:698:GLN:NE2	2.42	0.53
26:Z:88:ARG:NH1	26:Z:89:GLU:OE1	2.41	0.53
27:a:321:LYS:HE2	27:a:336:VAL:HG21	1.89	0.53
12:l:159:MET:HE3	12:l:160:SER:H	1.73	0.53
12:L:226:ASP:OD1	12:L:226:ASP:N	2.40	0.53
22:V:208:ALA:HB1	22:V:249:THR:HG21	1.90	0.53
28:b:138:VAL:HB	28:b:160:LEU:HD11	1.91	0.53
32:f:675:PHE:HD1	32:f:678:LEU:HD12	1.74	0.53
4:D:92:PHE:HA	4:D:103:VAL:HG12	1.90	0.53
21:U:515:ALA:HA	21:U:518:LEU:HD12	1.90	0.53
21:U:556:MET:HE1	21:U:589:ALA:HB2	1.91	0.53
15:O:63:LEU:HD11	15:O:79:ALA:HB2	1.91	0.53
27:a:148:VAL:HG12	27:a:150:SER:H	1.74	0.53
32:f:142:TYR:HA	32:f:145:VAL:HG22	1.91	0.53
4:D:157:ASP:O	4:D:158:GLN:HB3	2.09	0.53
10:J:221:ASN:ND2	10:J:224:GLU:HG3	2.24	0.53
14:N:95:MET:HG3	14:N:116:MET:HE1	1.91	0.53
16:P:88:MET:HE3	16:P:122:CYS:HB2	1.91	0.53
7:g:158:GLY:O	8:h:84:ARG:NH2	2.42	0.53
19:s:211:ARG:NH2	19:s:213:ASP:OD2	2.41	0.53
21:U:402:PHE:HB2	21:U:437:TYR:HB3	1.92	0.52
26:Z:270:VAL:HG13	29:c:281:LYS:HE2	1.90	0.52
29:c:195:GLY:O	29:c:198:ARG:HG2	2.09	0.52
30:d:47:GLN:HA	30:d:50:LEU:HG	1.89	0.52
32:f:568:GLY:H	32:f:599:ALA:HA	1.73	0.52
4:D:86:PRO:HB3	5:E:81:VAL:HG12	1.92	0.52
4:D:249:ASP:OD1	4:D:252:ARG:NH2	2.42	0.52
5:E:101:ASP:HB3	5:E:105:LEU:H	1.73	0.52
20:T:193:THR:OG1	20:T:195:LYS:NZ	2.43	0.52
4:D:89:ILE:HD12	5:E:78:ARG:HB3	1.90	0.52
10:J:221:ASN:ND2	10:J:223:GLU:HB3	2.18	0.52
22:V:321:ALA:HB1	22:V:324:PHE:HB3	1.90	0.52
32:f:417:ILE:HG22	32:f:418:LEU:HD12	1.91	0.52
5:E:247:THR:O	5:E:249:ALA:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:192:ILE:HG23	8:H:203:MET:HE1	1.91	0.52
27:a:347:LYS:HD2	27:a:350:LYS:HE2	1.91	0.52
29:c:52:GLU:HG3	29:c:82:VAL:HG23	1.91	0.52
29:c:54:MET:H	29:c:77:GLN:HE21	1.57	0.52
29:c:161:ARG:NH1	29:c:162:LEU:O	2.41	0.52
32:f:566:HIS:CD2	32:f:576:ILE:HD13	2.34	0.52
19:s:198:VAL:HG22	19:s:203:ILE:HG12	1.90	0.52
1:A:89:SER:HA	1:A:93:LEU:HD23	1.92	0.52
14:N:4:MET:HE1	14:N:159:ALA:HB3	1.90	0.52
22:V:314:ARG:NH1	25:Y:381:GLN:OE1	2.43	0.52
24:X:134:VAL:HB	24:X:149:LEU:HD23	1.91	0.52
25:Y:19:ILE:O	25:Y:23:ARG:N	2.41	0.52
10:J:90:GLU:HG3	10:J:110:TYR:CZ	2.44	0.52
16:P:159:ASP:N	16:P:159:ASP:OD1	2.42	0.52
20:T:25:ASP:HA	20:T:187:PHE:HA	1.91	0.52
28:b:9:CYS:HB3	28:b:111:ALA:HA	1.92	0.52
28:b:156:PHE:O	28:b:160:LEU:HB2	2.10	0.52
32:f:650:GLN:HB3	32:f:686:LEU:HD13	1.92	0.52
7:g:241:ALA:O	7:g:245:ARG:NH1	2.43	0.52
9:I:155:ASN:OD1	10:J:77:THR:OG1	2.26	0.52
21:U:216:VAL:HG11	21:U:248:ILE:HB	1.91	0.52
24:X:157:LEU:HG	24:X:166:LEU:HD22	1.92	0.52
28:b:6:THR:HG21	28:b:40:LYS:HG3	1.92	0.52
32:f:850:VAL:O	32:f:879:ARG:NH1	2.43	0.52
6:F:438:TYR:OH	11:K:19:GLY:O	2.27	0.52
17:Q:4:LEU:HD22	17:Q:45:LEU:HD23	1.91	0.52
21:U:749:GLN:NE2	21:U:753:GLY:O	2.42	0.52
27:a:216:LEU:HB2	27:a:222:LEU:HD21	1.92	0.52
29:c:46:ARG:NH2	29:c:147:PRO:O	2.42	0.52
32:f:267:ARG:HG3	32:f:787:LEU:HD21	1.91	0.52
30:d:111:ARG:HH12	30:d:113:ALA:H	1.58	0.52
18:r:179:VAL:HG22	18:r:184:TRP:HB3	1.92	0.52
1:A:349:GLU:O	1:A:353:HIS:ND1	2.39	0.52
23:W:344:THR:OG1	23:W:345:GLU:OE1	2.23	0.52
27:a:210:VAL:HG13	27:a:213:PHE:HB2	1.92	0.52
18:R:166:ARG:NH1	16:p:34:MET:O	2.43	0.51
22:V:113:LEU:HB3	22:V:135:LEU:HD22	1.92	0.51
22:V:480:ILE:HD11	26:Z:260:VAL:HA	1.92	0.51
32:f:344:VAL:HG13	32:f:347:ASP:H	1.75	0.51
1:A:284:ARG:NH2	1:A:289:ALA:N	2.58	0.51
21:U:360:VAL:HG13	21:U:365:CYS:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:199:TYR:N	23:W:199:TYR:CD1	2.73	0.51
7:g:164:LYS:NZ	8:h:55:ILE:O	2.41	0.51
3:C:161:ILE:HA	3:C:164:VAL:HG12	1.92	0.51
6:F:150:LEU:HB2	6:F:166:THR:HG22	1.92	0.51
12:L:72:ILE:HD13	12:L:88:MET:HE1	1.92	0.51
19:S:125:ASP:OD1	19:S:129:SER:N	2.44	0.51
24:X:377:ILE:HG12	25:Y:312:ARG:HB3	1.92	0.51
32:f:226:TYR:OH	32:f:261:ARG:NH2	2.43	0.51
1:A:213:LEU:HA	1:A:319:MET:HB3	1.92	0.51
27:a:111:VAL:HA	27:a:114:CYS:HB2	1.93	0.51
15:o:51:ASP:HB3	15:o:94:ILE:HG23	1.92	0.51
10:J:211:MET:HB2	10:J:217:LEU:HD13	1.92	0.51
21:U:764:LEU:O	21:U:767:THR:OG1	2.28	0.51
26:Z:35:VAL:H	26:Z:97:THR:HG22	1.74	0.51
27:a:252:LYS:HA	27:a:255:TRP:HE3	1.76	0.51
4:D:370:ILE:HG23	4:D:374:ASP:HB2	1.92	0.51
19:S:4:PRO:HG3	20:T:103:MET:HE1	1.93	0.51
20:T:86:ARG:NH1	20:T:133:GLU:OE2	2.43	0.51
21:U:397:THR:OG1	21:U:401:LYS:NZ	2.43	0.51
3:C:86:LEU:HD21	3:C:94:LYS:HD2	1.93	0.51
16:p:65:GLN:OE1	17:q:86:ARG:NH2	2.43	0.51
9:I:229:LYS:N	9:I:232:GLU:OE2	2.44	0.51
10:J:212:ARG:HB2	10:J:215:GLN:NE2	2.25	0.51
26:Z:185:GLY:HA3	26:Z:189:GLN:HB2	1.92	0.51
27:a:284:ARG:HD3	27:a:288:HIS:HB2	1.92	0.51
32:f:261:ARG:HG3	32:f:264:GLU:HB2	1.92	0.51
2:B:49:LEU:HD11	32:f:666:ILE:HG12	1.93	0.51
3:C:135:VAL:HA	3:C:138:MET:HE2	1.92	0.51
4:D:274:ARG:HD2	4:D:286:GLN:HG3	1.93	0.51
3:C:88:LYS:HB3	3:C:94:LYS:HG2	1.92	0.51
4:D:212:LYS:HG2	4:D:333:PHE:HD2	1.75	0.51
21:U:188:MET:HE1	21:U:194:ARG:HB2	1.92	0.51
27:a:341:LEU:HD12	27:a:345:GLN:HB2	1.93	0.51
1:A:284:ARG:HH21	1:A:289:ALA:HB3	1.76	0.50
27:a:193:GLN:HB3	27:a:225:LEU:HD13	1.93	0.50
28:b:20:ASP:H	28:b:25:ARG:HE	1.59	0.50
32:f:368:ALA:HB1	32:f:403:LYS:HB2	1.94	0.50
8:h:204:THR:OG1	8:h:206:ASP:OD2	2.27	0.50
21:U:19:LEU:HD22	30:d:27:LYS:HZ3	1.75	0.50
22:V:494:MET:SD	22:V:495:ARG:HG2	2.52	0.50
27:a:168:ASN:OD1	27:a:171:SER:OG	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:174:PRO:HD2	28:b:178:SER:OG	2.11	0.50
8:h:175:GLU:OE2	9:i:53:HIS:NE2	2.34	0.50
10:j:52:LYS:HG3	10:j:53:LEU:HD12	1.93	0.50
14:n:4:MET:HG3	14:n:127:ILE:HG22	1.92	0.50
15:o:216:ILE:HD11	16:p:194:LYS:HD2	1.93	0.50
1:A:169:LYS:HD2	1:A:170:PRO:HD2	1.93	0.50
6:F:165:PRO:HG2	6:F:167:GLU:OE1	2.12	0.50
8:H:222:THR:OG1	8:H:225:GLU:OE1	2.23	0.50
23:W:361:HIS:HA	23:W:364:ARG:HH21	1.75	0.50
4:D:405:THR:O	4:D:408:LYS:NZ	2.40	0.50
9:I:119:GLN:HE22	9:I:123:GLN:HE21	1.60	0.50
25:Y:220:VAL:HA	25:Y:223:THR:HG22	1.93	0.50
32:f:783:SER:HB2	32:f:787:LEU:HD13	1.94	0.50
10:j:201:SER:OG	10:j:205:ASN:OD1	2.30	0.50
1:A:158:ASP:H	1:A:159:PRO:CD	2.23	0.50
21:U:78:LEU:HD21	21:U:107:HIS:HB2	1.93	0.50
22:V:338:LEU:HG	22:V:398:LEU:HD12	1.93	0.50
11:k:13:ASN:HB2	12:l:126:ARG:HD3	1.93	0.50
19:s:48:ASP:OD1	19:s:48:ASP:N	2.42	0.50
7:G:165:ALA:HB3	8:H:56:LEU:HD22	1.93	0.50
8:H:175:GLU:CA	9:I:54:LYS:HZ3	2.23	0.50
18:R:133:VAL:HG21	17:q:137:PHE:HB3	1.94	0.50
28:b:110:ILE:HG22	28:b:139:ASP:HB2	1.93	0.50
10:j:40:ILE:HG22	10:j:212:ARG:HG2	1.93	0.50
12:l:122:ARG:HE	13:m:128:VAL:HG12	1.76	0.50
19:s:144:MET:HE1	19:s:186:ASP:HB2	1.92	0.50
15:O:143:ARG:NH2	15:O:150:GLU:OE1	2.45	0.50
15:O:148:GLU:OE2	15:O:182:LYS:NZ	2.44	0.50
24:X:310:ARG:HB3	24:X:314:ARG:CZ	2.42	0.50
24:X:318:ILE:HG13	24:X:322:HIS:HE1	1.71	0.50
24:X:320:SER:HA	24:X:323:LEU:HD12	1.94	0.50
26:Z:223:ASN:HB3	26:Z:226:ILE:HG22	1.94	0.50
13:m:167:LYS:NZ	13:m:206:ASP:OD2	2.44	0.50
2:B:106:PRO:HB3	3:C:121:TYR:HB2	1.93	0.50
10:J:2:SER:OG	10:J:3:TYR:N	2.45	0.50
14:N:201:THR:HG21	20:t:186:ARG:HH22	1.76	0.50
21:U:35:TRP:CD1	22:V:273:LYS:HZ1	2.30	0.50
10:j:148:ASP:OD1	10:j:152:THR:N	2.43	0.50
1:A:212:VAL:HG11	1:A:341:ILE:HD12	1.93	0.49
2:B:387:LYS:HB2	2:B:423:LYS:HE2	1.94	0.49
4:D:181:VAL:HG22	4:D:306:LYS:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:84:ARG:HD2	5:E:108:MET:HA	1.94	0.49
13:M:34:SER:OG	13:M:65:ARG:NH1	2.34	0.49
22:V:412:LEU:O	25:Y:346:LYS:NZ	2.44	0.49
28:b:19:GLY:HA2	28:b:25:ARG:HG3	1.94	0.49
13:m:35:THR:HA	13:m:166:GLY:HA3	1.93	0.49
19:s:125:ASP:OD1	19:s:129:SER:N	2.45	0.49
4:D:271:ALA:HA	4:D:289:LEU:HD21	1.93	0.49
24:X:297:ARG:NH1	24:X:334:ASN:OD1	2.39	0.49
27:a:229:ASP:OD1	27:a:229:ASP:N	2.44	0.49
32:f:278:VAL:HG12	32:f:305:LEU:HD11	1.94	0.49
32:f:618:GLU:O	32:f:650:GLN:NE2	2.45	0.49
7:g:3:ARG:O	7:g:4:GLY:C	2.55	0.49
1:A:25:LEU:O	32:f:43:GLN:N	2.45	0.49
9:I:136:TYR:HB2	9:I:148:TYR:HB2	1.95	0.49
12:L:176:MET:HE1	13:M:56:LYS:HB3	1.95	0.49
23:W:328:LEU:HD13	23:W:337:ALA:HB1	1.95	0.49
12:l:52:ALA:HB1	12:l:57:ALA:HB3	1.93	0.49
3:C:217:SER:OG	4:D:291:GLU:OE1	2.31	0.49
7:G:158:GLY:O	8:H:84:ARG:NH2	2.45	0.49
17:Q:137:PHE:HB3	18:r:133:VAL:HG21	1.93	0.49
21:U:128:GLN:O	21:U:132:GLY:N	2.44	0.49
24:X:306:LEU:HD12	24:X:313:LEU:HD12	1.95	0.49
25:Y:387:ILE:HD12	26:Z:275:LEU:HD22	1.93	0.49
27:a:132:LYS:NZ	27:a:162:TYR:OH	2.33	0.49
29:c:194:HIS:C	29:c:198:ARG:HH21	2.20	0.49
30:d:75:MET:HE1	30:d:98:LEU:HG	1.94	0.49
1:A:265:ARG:HG2	1:A:315:ILE:HD13	1.94	0.49
4:D:213:THR:N	34:D:501:ATP:O1A	2.45	0.49
4:D:297:ASP:HB3	4:D:326:ARG:HH21	1.77	0.49
27:a:324:ILE:HG13	27:a:331:VAL:HG13	1.93	0.49
32:f:213:GLN:HB3	32:f:216:MET:HE1	1.94	0.49
21:U:183:LEU:HA	21:U:186:SER:HB3	1.95	0.49
21:U:415:HIS:HB3	21:U:418:GLU:HB3	1.93	0.49
7:g:11:ARG:O	7:g:24:GLN:NE2	2.40	0.49
8:h:9:SER:OG	8:h:123:GLN:O	2.30	0.49
12:l:193:ARG:HG2	12:l:196:ARG:HH12	1.78	0.49
3:C:145:ASP:OD1	3:C:145:ASP:N	2.45	0.49
4:D:167:ILE:O	4:D:174:LYS:NZ	2.45	0.49
5:E:165:ILE:HD12	5:E:166:PRO:HD2	1.94	0.49
6:F:436:GLN:HG2	6:F:437:TYR:H	1.77	0.49
8:H:213:CYS:HB2	8:H:218:PHE:HD1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:68:ASN:OD1	13:M:224:HIS:ND1	2.45	0.49
22:V:438:VAL:O	22:V:439:ALA:C	2.56	0.49
16:p:7:ASN:ND2	16:p:29:GLY:O	2.41	0.49
1:A:257:VAL:HG21	1:A:302:LEU:HD11	1.94	0.49
3:C:87:VAL:O	3:C:95:PHE:N	2.43	0.49
11:k:99:HIS:HB2	11:k:107:MET:HE3	1.93	0.49
1:A:112:ILE:HG12	1:A:122:VAL:HG22	1.95	0.49
3:C:11:LEU:HB2	3:C:15:LYS:HG2	1.95	0.49
6:F:163:THR:O	6:F:164:LEU:HB2	2.13	0.49
23:W:130:MET:HA	23:W:133:GLU:HG2	1.93	0.49
24:X:170:GLN:OE1	24:X:192:SER:OG	2.29	0.49
29:c:198:ARG:HG3	29:c:199:HIS:CG	2.47	0.49
26:Z:287:LYS:HG3	26:Z:288:LYS:HG2	1.94	0.48
29:c:55:GLY:HA2	29:c:75:MET:HG2	1.95	0.48
30:d:1:MET:N	30:d:3:GLU:OE2	2.44	0.48
16:p:35:VAL:HG12	16:p:36:THR:HG23	1.95	0.48
17:q:44:LEU:HD11	17:q:102:LEU:HD22	1.93	0.48
3:C:85:VAL:HG21	3:C:123:LEU:HD11	1.95	0.48
4:D:147:ALA:HB1	5:E:62:LYS:HD3	1.95	0.48
6:F:375:VAL:HG22	6:F:415:LEU:HD12	1.96	0.48
22:V:225:ASP:OD2	22:V:225:ASP:N	2.44	0.48
26:Z:234:PHE:HE1	27:a:349:MET:HB3	1.79	0.48
32:f:162:LEU:HD21	32:f:187:LEU:HD21	1.94	0.48
32:f:170:TRP:NE1	32:f:211:ILE:O	2.46	0.48
7:g:61:LEU:HD21	7:g:66:VAL:HG11	1.95	0.48
12:l:88:MET:HG2	12:l:112:ILE:HD11	1.95	0.48
3:C:79:ALA:HB3	3:C:108:VAL:HG22	1.95	0.48
5:E:198:VAL:HB	5:E:232:MET:HG3	1.94	0.48
28:b:157:VAL:HG21	28:b:170:LEU:HB2	1.94	0.48
5:E:215:ILE:HD13	5:E:260:LEU:HB2	1.96	0.48
5:E:264:MET:HE1	5:E:294:ARG:HB2	1.95	0.48
10:J:208:LEU:O	10:J:220:LEU:HB2	2.13	0.48
26:Z:173:GLU:HB3	26:Z:180:LYS:HE2	1.95	0.48
1:A:204:LEU:HD12	6:F:413:THR:HA	1.95	0.48
3:C:11:LEU:HD12	3:C:15:LYS:HE3	1.96	0.48
5:E:81:VAL:HB	5:E:106:THR:HA	1.95	0.48
24:X:71:LYS:HA	24:X:74:ARG:HE	1.77	0.48
29:c:257:LYS:HA	29:c:260:GLU:HG3	1.95	0.48
9:i:53:HIS:HB3	9:i:56:LEU:HD23	1.95	0.48
5:E:175:PRO:HG2	5:E:303:LEU:HD13	1.94	0.48
15:O:28:ASP:HB2	16:P:131:MET:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:18:GLN:HB3	27:a:22:TRP:HD1	1.77	0.48
28:b:26:LEU:HD11	28:b:80:PRO:HG3	1.95	0.48
29:c:279:ASP:HB3	29:c:280:PRO:CD	2.40	0.48
18:r:97:MET:H	18:r:116:SER:HB3	1.79	0.48
4:D:268:ASP:OD1	4:D:268:ASP:N	2.45	0.48
5:E:215:ILE:HG12	5:E:218:MET:HE2	1.96	0.48
25:Y:181:LYS:NZ	25:Y:203:ASP:OD2	2.45	0.48
10:j:184:ASP:O	10:j:187:THR:OG1	2.29	0.48
3:C:143:VAL:O	3:C:205:HIS:ND1	2.38	0.48
3:C:197:THR:OG1	34:C:501:ATP:O1B	2.27	0.48
21:U:126:ILE:HB	21:U:130:LEU:HD11	1.96	0.48
21:U:206:MET:HE1	21:U:232:ILE:HG21	1.96	0.48
21:U:765:VAL:HG11	21:U:778:PHE:HD2	1.78	0.48
25:Y:32:ARG:NH2	25:Y:61:LEU:O	2.47	0.48
28:b:65:THR:O	28:b:70:ARG:NH2	2.46	0.48
32:f:475:ASN:ND2	32:f:513:GLU:OE2	2.46	0.48
32:f:668:ALA:HA	32:f:697:ILE:HD11	1.95	0.48
11:K:166:ASP:OD2	11:K:187:LYS:NZ	2.47	0.48
11:K:240:ASP:OD1	11:K:241:ILE:N	2.44	0.48
22:V:296:LYS:HA	22:V:299:GLN:HG2	1.96	0.48
24:X:377:ILE:HB	24:X:388:PHE:HE1	1.77	0.48
32:f:861:THR:HB	32:f:879:ARG:HH11	1.79	0.48
18:r:35:ILE:N	18:r:43:GLY:O	2.43	0.48
4:D:158:GLN:HE21	4:D:229:ARG:HH21	1.61	0.48
10:J:122:ASN:OD1	11:K:134:SER:OG	2.31	0.48
22:V:303:SER:OG	22:V:304:GLU:OE1	2.32	0.48
22:V:337:LEU:HD21	22:V:364:THR:HG23	1.95	0.48
26:Z:190:ARG:HG2	29:c:297:VAL:HG11	1.95	0.48
30:d:114:GLU:HA	30:d:117:THR:HG22	1.96	0.48
11:k:41:GLN:NE2	11:k:151:PRO:O	2.47	0.48
13:m:230:ASP:OD1	13:m:230:ASP:N	2.47	0.48
2:B:31:THR:HG23	2:B:32:ARG:HG2	1.95	0.47
21:U:211:PRO:HB2	21:U:244:MET:HE1	1.96	0.47
23:W:49:SER:HA	23:W:52:LYS:HE3	1.96	0.47
24:X:400:ALA:O	24:X:403:THR:OG1	2.30	0.47
32:f:573:ILE:HG22	32:f:577:LEU:HG	1.96	0.47
32:f:682:GLY:HA3	32:f:686:LEU:HD23	1.96	0.47
16:p:193:ASP:OD1	16:p:193:ASP:N	2.47	0.47
2:B:362:LYS:HA	2:B:365:PHE:HD2	1.79	0.47
5:E:135:ILE:HD13	5:E:182:LEU:HD23	1.96	0.47
5:E:196:LEU:HD11	5:E:221:TYR:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:148:GLN:OE1	8:H:158:TRP:NE1	2.46	0.47
10:J:209:ALA:HB2	10:J:219:ILE:HD12	1.96	0.47
19:S:157:ASN:ND2	16:p:173:ASN:OD1	2.41	0.47
20:T:126:ASP:OD1	20:T:130:VAL:N	2.47	0.47
25:Y:12:PRO:O	25:Y:146:ARG:NH1	2.47	0.47
4:D:259:PRO:HB3	4:D:304:ASN:HB3	1.96	0.47
5:E:250:ASP:OD2	6:F:304:ARG:NH1	2.47	0.47
6:F:436:GLN:HG2	6:F:437:TYR:CD1	2.49	0.47
12:L:41:LYS:HG3	12:L:180:MET:HG3	1.96	0.47
20:T:44:ARG:NH2	20:T:47:ASN:OD1	2.47	0.47
21:U:475:HIS:HE1	21:U:507:VAL:HG22	1.79	0.47
21:U:805:ASN:OD1	21:U:893:THR:OG1	2.26	0.47
30:d:111:ARG:HA	30:d:111:ARG:HD2	1.71	0.47
5:E:176:PRO:HB2	6:F:344:ARG:HH22	1.78	0.47
26:Z:142:GLU:OE2	26:Z:153:LYS:NZ	2.47	0.47
9:i:90:LEU:HD21	9:i:114:LEU:HB2	1.96	0.47
20:t:122:LEU:HG	20:t:137:LEU:HD12	1.94	0.47
2:B:135:ILE:HG13	2:B:159:VAL:HB	1.95	0.47
20:T:63:LEU:HD21	20:T:106:LEU:HD13	1.97	0.47
28:b:3:LEU:HB3	28:b:105:HIS:CD2	2.50	0.47
28:b:21:PHE:HD2	28:b:25:ARG:HG2	1.78	0.47
32:f:78:LEU:HD23	32:f:125:ILE:HD13	1.97	0.47
9:i:143:TYR:HB2	9:i:146:GLN:HE21	1.79	0.47
13:m:50:GLU:OE2	13:m:201:HIS:ND1	2.36	0.47
13:m:68:ASN:OD1	13:m:224:HIS:ND1	2.43	0.47
3:C:248:MET:HB3	3:C:251:ILE:HD11	1.96	0.47
4:D:141:ASP:OD1	4:D:142:VAL:N	2.47	0.47
6:F:234:THR:HG22	6:F:238:ARG:HH22	1.79	0.47
22:V:315:LYS:HE2	25:Y:385:ARG:HE	1.79	0.47
1:A:402:LYS:NZ	2:B:213:GLU:OE1	2.36	0.47
2:B:335:GLU:HG2	2:B:336:THR:HG23	1.97	0.47
3:C:20:LEU:HB2	21:U:137:MET:HE3	1.97	0.47
15:O:17:ASP:OD1	15:O:17:ASP:N	2.42	0.47
16:P:190:ILE:HG12	16:P:195:ILE:HD12	1.95	0.47
21:U:251:ASP:O	21:U:255:SER:CB	2.63	0.47
21:U:576:PRO:HB3	21:U:611:ASN:HD22	1.80	0.47
22:V:309:MET:HE1	22:V:332:LEU:HB2	1.97	0.47
22:V:345:ARG:HE	31:e:43:TRP:HA	1.80	0.47
32:f:367:SER:O	32:f:371:ASN:ND2	2.48	0.47
32:f:574:GLU:HA	32:f:577:LEU:HB2	1.96	0.47
13:m:5:THR:OG1	13:m:6:GLY:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:p:135:ASP:OD1	16:p:136:PHE:N	2.48	0.47
2:B:379:THR:OG1	2:B:416:ASN:ND2	2.45	0.47
5:E:185:ARG:NE	6:F:320:PHE:O	2.47	0.47
13:M:108:LEU:HD11	13:M:137:LEU:HB3	1.97	0.47
17:Q:102:LEU:HB2	17:Q:118:MET:HB2	1.96	0.47
18:R:7:LYS:HG2	18:R:12:VAL:HG22	1.97	0.47
21:U:414:GLY:H	21:U:449:ILE:HG23	1.80	0.47
24:X:221:GLU:O	24:X:223:LYS:NZ	2.41	0.47
25:Y:231:LEU:HD21	25:Y:239:LYS:HZ1	1.80	0.47
4:D:345:PHE:HB3	4:D:360:LEU:HD22	1.96	0.47
15:O:163:ILE:HG12	15:O:170:GLY:HA2	1.96	0.47
31:e:50:ASP:OD1	31:e:50:ASP:N	2.43	0.47
32:f:466:LEU:HB3	32:f:485:LEU:HD12	1.96	0.47
2:B:287:ILE:HD13	2:B:329:MET:HG2	1.96	0.47
2:B:440:LEU:HD13	10:J:77:THR:HG21	1.97	0.47
21:U:802:TYR:HB3	21:U:895:PRO:HD3	1.96	0.47
21:U:885:MET:HG2	21:U:887:ALA:H	1.79	0.47
29:c:41:MET:HE1	29:c:112:TYR:CG	2.50	0.47
9:i:25:MET:HE2	9:i:151:ASP:HB2	1.97	0.47
10:j:192:ILE:HD12	10:j:206:ILE:HD12	1.97	0.47
20:t:51:LEU:HD11	20:t:110:MET:SD	2.54	0.47
4:D:164:TYR:HB2	4:D:222:HIS:CD2	2.50	0.46
26:Z:125:ASP:HB3	26:Z:128:PRO:HD2	1.97	0.46
31:e:16:ASP:OD1	31:e:16:ASP:N	2.46	0.46
7:g:56:VAL:HG23	7:g:61:LEU:HD22	1.98	0.46
8:H:81:PRO:HA	8:H:84:ARG:HE	1.79	0.46
9:I:72:MET:HG2	9:I:138:GLY:HA3	1.97	0.46
20:T:1:THR:N	20:T:104:ASN:OD1	2.48	0.46
21:U:212:ASP:HB3	21:U:214:ILE:HG22	1.95	0.46
23:W:43:VAL:HG23	23:W:73:MET:HE1	1.98	0.46
28:b:67:ASP:HB3	28:b:70:ARG:HE	1.80	0.46
10:j:155:ALA:HB3	11:k:60:GLU:HB3	1.96	0.46
1:A:272:ILE:HB	1:A:317:VAL:HG22	1.97	0.46
11:K:206:MET:HG2	11:K:208:GLU:H	1.80	0.46
21:U:900:TYR:HB3	21:U:914:LEU:HD21	1.97	0.46
27:a:122:LYS:HZ2	27:a:130:VAL:HG13	1.79	0.46
27:a:308:GLU:O	27:a:312:MET:HG2	2.14	0.46
30:d:75:MET:HE2	30:d:102:ASN:HB2	1.97	0.46
9:i:234:GLU:HA	9:i:237:ILE:HG12	1.97	0.46
4:D:355:SER:OG	4:D:356:GLU:N	2.49	0.46
5:E:247:THR:O	5:E:248:SER:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:112:ASP:N	7:G:112:ASP:OD1	2.48	0.46
19:S:198:VAL:HG22	19:S:203:ILE:HG12	1.96	0.46
24:X:310:ARG:C	24:X:314:ARG:HD2	2.40	0.46
27:a:34:TRP:HZ3	27:a:64:ILE:HG23	1.80	0.46
28:b:143:PHE:HZ	28:b:183:LEU:HD21	1.80	0.46
1:A:143:ASP:OD2	1:A:146:LYS:N	2.48	0.46
6:F:35:LYS:HD3	6:F:38:THR:HB	1.97	0.46
6:F:183:GLU:HB2	6:F:239:ALA:HA	1.97	0.46
17:Q:44:LEU:HD11	17:Q:102:LEU:HD22	1.97	0.46
24:X:380:GLN:HB2	25:Y:314:LEU:HA	1.97	0.46
5:E:203:ILE:HD11	5:E:238:ILE:HG13	1.98	0.46
24:X:24:ILE:HG12	24:X:56:LEU:HD13	1.97	0.46
25:Y:121:LEU:HD23	25:Y:144:LEU:HD22	1.97	0.46
28:b:12:ASN:OD1	28:b:53:THR:OG1	2.34	0.46
29:c:104:ARG:HH12	29:c:106:GLU:HB3	1.80	0.46
30:d:111:ARG:HH22	30:d:113:ALA:HB3	1.79	0.46
12:l:33:SER:OG	12:l:62:LYS:NZ	2.36	0.46
1:A:258:ARG:O	1:A:262:GLU:HG2	2.15	0.46
5:E:206:LYS:O	33:v:5:UNK:N	2.49	0.46
21:U:78:LEU:HD22	21:U:103:LYS:HB3	1.98	0.46
27:a:84:VAL:HA	27:a:87:MET:HG3	1.97	0.46
32:f:654:VAL:HA	32:f:657:ILE:HD12	1.97	0.46
6:F:368:ILE:O	6:F:371:ARG:NE	2.49	0.46
14:N:4:MET:HG3	14:N:127:ILE:HG22	1.97	0.46
21:U:524:LYS:NZ	21:U:562:GLU:O	2.40	0.46
25:Y:247:LEU:HD12	25:Y:250:LEU:HD11	1.96	0.46
16:p:45:MET:HE3	16:p:71:LEU:HD13	1.98	0.46
19:s:45:LYS:HE3	19:s:203:ILE:HD12	1.98	0.46
1:A:45:ILE:HD11	2:B:61:LYS:HE2	1.98	0.46
10:J:220:LEU:HD12	10:J:225:ILE:HG13	1.98	0.46
13:M:204:VAL:HG23	13:M:205:LYS:HE2	1.98	0.46
16:P:14:MET:HE1	16:P:166:THR:HG22	1.97	0.46
23:W:200:ILE:N	23:W:200:ILE:CD1	2.74	0.46
28:b:51:LEU:N	28:b:62:THR:OG1	2.46	0.46
10:j:168:VAL:HG23	10:j:194:ALA:HB1	1.98	0.46
12:l:227:ASP:OD1	12:l:227:ASP:N	2.47	0.46
15:o:63:LEU:HD11	15:o:79:ALA:HB2	1.97	0.46
6:F:189:GLY:H	36:F:501:ADP:HN62	1.64	0.46
21:U:229:VAL:HA	21:U:232:ILE:HG12	1.98	0.46
29:c:198:ARG:HG3	29:c:199:HIS:ND1	2.30	0.46
20:t:96:MET:HE3	20:t:106:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:PHE:HD1	2:B:281:ILE:HB	1.82	0.45
5:E:244:SER:OG	5:E:245:GLU:N	2.48	0.45
15:O:112:SER:HB3	15:O:125:VAL:HG11	1.99	0.45
22:V:204:ASP:OD1	22:V:204:ASP:N	2.49	0.45
24:X:82:LYS:HB3	24:X:124:PHE:HZ	1.80	0.45
8:h:130:PHE:HB3	8:h:132:VAL:HG22	1.98	0.45
10:j:19:VAL:O	10:j:23:GLN:HG2	2.16	0.45
2:B:260:LEU:O	2:B:307:ARG:NH2	2.42	0.45
3:C:131:VAL:HG12	3:C:133:PRO:HD3	1.97	0.45
5:E:227:PRO:HD3	5:E:272:ARG:HB3	1.98	0.45
5:E:349:GLU:OE1	5:E:373:LYS:NZ	2.39	0.45
21:U:509:GLY:HA3	21:U:544:ILE:HA	1.98	0.45
27:a:12:GLN:HG2	27:a:18:GLN:HB3	1.97	0.45
8:h:93:LEU:HD13	8:h:113:ARG:HB3	1.98	0.45
11:k:35:SER:HB2	11:k:51:GLU:HG3	1.98	0.45
3:C:329:LEU:HD23	3:C:344:LEU:HB3	1.97	0.45
4:D:391:ARG:NH2	4:D:393:ILE:O	2.48	0.45
6:F:256:LEU:HD12	6:F:291:ILE:HD13	1.97	0.45
15:O:211:VAL:HG21	16:P:198:ARG:HD3	1.98	0.45
21:U:82:LEU:O	21:U:129:ARG:NH2	2.48	0.45
21:U:835:ILE:HB	21:U:838:LYS:HE3	1.98	0.45
22:V:268:GLU:HA	22:V:271:VAL:HG12	1.97	0.45
21:U:388:ASP:OD1	21:U:388:ASP:N	2.49	0.45
26:Z:116:CYS:O	26:Z:119:SER:OG	2.31	0.45
7:g:147:GLN:OE1	7:g:150:GLN:NE2	2.50	0.45
15:o:181:ASN:OD1	15:o:182:LYS:N	2.49	0.45
2:B:248:LEU:HD12	2:B:282:VAL:HG22	1.97	0.45
3:C:148:TYR:CZ	3:C:206:HIS:HB2	2.52	0.45
4:D:248:ARG:NH2	4:D:291:GLU:OE1	2.49	0.45
11:K:16:SER:OG	11:K:20:ARG:N	2.48	0.45
23:W:125:ILE:HG21	23:W:149:LEU:HB2	1.97	0.45
23:W:350:ARG:HA	23:W:353:ASP:HB2	1.98	0.45
3:C:49:ARG:NH2	4:D:64:GLU:OE2	2.49	0.45
5:E:145:LEU:HD13	5:E:183:LEU:HD23	1.99	0.45
21:U:637:VAL:O	21:U:641:SER:N	2.47	0.45
24:X:126:ARG:NH2	24:X:130:GLU:OE1	2.50	0.45
24:X:345:VAL:O	24:X:385:LEU:N	2.47	0.45
32:f:120:ARG:HD3	32:f:147:SER:HB3	1.99	0.45
16:p:71:LEU:O	16:p:75:GLU:HG2	2.17	0.45
18:r:105:ASP:OD1	18:r:105:ASP:N	2.49	0.45
19:s:16:ALA:HB2	19:s:121:VAL:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:300:LYS:HA	6:F:300:LYS:HD3	1.42	0.45
6:F:304:ARG:O	6:F:308:ARG:NH1	2.49	0.45
21:U:895:PRO:HB2	21:U:898:CYS:HB3	1.98	0.45
29:c:134:GLU:OE1	29:c:161:ARG:NH1	2.50	0.45
11:k:52:LYS:NZ	11:k:64:ILE:O	2.50	0.45
20:t:126:ASP:OD1	20:t:130:VAL:N	2.50	0.45
19:S:10:GLY:HA3	19:S:42:LYS:HE2	1.99	0.45
29:c:63:ASP:OD1	29:c:66:THR:OG1	2.26	0.45
30:d:75:MET:HE3	30:d:79:LYS:HE3	1.99	0.45
32:f:267:ARG:HD3	32:f:787:LEU:HD11	1.98	0.45
4:D:133:HIS:HB3	4:D:137:ASN:H	1.82	0.45
6:F:275:ALA:HB1	6:F:326:VAL:HG21	1.99	0.45
9:I:90:LEU:HD21	9:I:114:LEU:HB2	1.98	0.45
23:W:359:VAL:HG23	23:W:382:LEU:HD22	1.98	0.45
24:X:401:LEU:HA	24:X:404:ILE:HD12	1.99	0.45
26:Z:68:TRP:HH2	26:Z:111:LEU:HD13	1.80	0.45
20:t:43:MET:HE3	20:t:45:VAL:HG22	1.99	0.45
1:A:331:LEU:HD23	1:A:336:ARG:HD3	1.99	0.45
4:D:352:MET:SD	4:D:352:MET:N	2.90	0.45
5:E:219:PHE:HD2	5:E:263:GLN:HB3	1.81	0.45
12:L:84:LEU:HD23	12:L:132:LEU:HD11	1.99	0.45
17:Q:62:LYS:HB3	17:Q:62:LYS:HE2	1.76	0.45
29:c:32:TYR:HE1	29:c:206:ASN:HD21	1.65	0.45
8:h:3:GLU:OE2	13:m:127:ALA:HB3	2.17	0.45
11:k:157:ASP:OD2	11:k:159:SER:OG	2.35	0.45
16:p:53:LEU:HB3	16:p:60:VAL:HG22	1.99	0.45
16:p:67:LEU:HD11	16:p:91:VAL:HG22	1.97	0.45
13:M:197:ILE:HG21	13:M:211:LEU:HD13	1.99	0.44
25:Y:379:ARG:O	25:Y:379:ARG:NH1	2.50	0.44
26:Z:37:GLY:HA2	26:Z:56:VAL:HG12	1.99	0.44
26:Z:215:VAL:HG23	26:Z:220:LEU:HD11	1.98	0.44
27:a:12:GLN:O	27:a:22:TRP:NE1	2.50	0.44
27:a:145:LEU:HD23	27:a:147:GLY:H	1.82	0.44
2:B:135:ILE:HG12	2:B:139:VAL:HG21	2.00	0.44
3:C:205:HIS:HD2	3:C:206:HIS:CE1	2.34	0.44
6:F:318:ASP:OD2	6:F:347:ARG:NH1	2.51	0.44
12:L:7:ASP:OD1	12:L:7:ASP:N	2.49	0.44
18:R:148:GLU:HG3	18:R:151:GLN:HG3	1.99	0.44
25:Y:231:LEU:HB2	25:Y:234:PRO:HG2	1.98	0.44
30:d:131:VAL:HA	30:d:134:LYS:HB3	1.99	0.44
7:g:43:ARG:HH21	7:g:164:LYS:HG2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:39:ILE:HD11	13:m:176:ILE:HG12	1.99	0.44
4:D:267:ILE:HD13	4:D:309:MET:HG2	1.98	0.44
6:F:339:ASP:OD1	6:F:339:ASP:N	2.50	0.44
6:F:383:GLU:HG2	6:F:386:ARG:HH12	1.82	0.44
10:J:5:ARG:O	10:J:123:GLY:N	2.49	0.44
22:V:322:VAL:HG11	31:e:27:TRP:HZ3	1.82	0.44
32:f:679:LEU:HD23	32:f:680:ARG:HE	1.83	0.44
10:j:36:ARG:HH21	10:j:157:LYS:HG2	1.82	0.44
16:p:30:ILE:HG22	16:p:31:GLN:H	1.82	0.44
4:D:406:VAL:O	4:D:409:LYS:NZ	2.36	0.44
21:U:179:TYR:CZ	21:U:183:LEU:HD11	2.53	0.44
22:V:309:MET:SD	22:V:328:VAL:HG13	2.57	0.44
23:W:265:GLN:HA	23:W:336:PRO:HG3	2.00	0.44
24:X:171:LEU:HD13	24:X:213:GLN:HE22	1.81	0.44
24:X:380:GLN:N	25:Y:313:SER:O	2.44	0.44
10:j:180:ALA:HB1	10:j:190:LEU:HD11	1.99	0.44
15:o:62:ASN:HB3	15:o:82:MET:HE1	2.00	0.44
6:F:137:ILE:HG23	6:F:160:ILE:HD13	2.00	0.44
6:F:288:LEU:HG	6:F:332:THR:HG22	1.99	0.44
10:J:196:LEU:HA	10:J:199:VAL:HG12	1.98	0.44
12:L:47:VAL:HG12	12:L:195:LEU:HD22	1.99	0.44
19:S:213:ASP:OD1	19:S:213:ASP:N	2.51	0.44
22:V:355:ARG:HD2	31:e:27:TRP:HB2	1.99	0.44
23:W:314:LEU:HD23	23:W:365:ILE:HD11	1.99	0.44
25:Y:28:LEU:O	25:Y:32:ARG:N	2.50	0.44
12:l:121:GLN:HG3	13:m:129:ARG:HG2	2.00	0.44
1:A:236:CYS:HB3	1:A:270:CYS:HA	1.99	0.44
3:C:401:ILE:HA	3:C:404:LEU:HG	1.98	0.44
4:D:368:ASP:HA	4:D:411:GLU:HG2	1.99	0.44
19:S:16:ALA:HB2	19:S:121:VAL:HG23	2.00	0.44
21:U:351:MET:HG2	21:U:818:GLU:HG3	2.00	0.44
22:V:439:ALA:HB1	30:d:181:CYS:SG	2.57	0.44
23:W:276:LEU:HA	23:W:357:ARG:HG3	2.00	0.44
24:X:316:ASP:HB2	24:X:320:SER:HB3	1.99	0.44
32:f:446:LEU:HD12	32:f:480:GLY:HA2	1.99	0.44
1:A:48:VAL:HG13	2:B:69:LYS:HE2	2.00	0.44
12:L:156:CYS:HB3	12:L:159:MET:HE3	2.00	0.44
12:L:204:ASP:N	12:L:204:ASP:OD1	2.49	0.44
12:L:225:ASP:H	12:L:228:ASP:HB2	1.83	0.44
16:P:142:CYS:HB2	16:P:145:GLN:HE21	1.83	0.44
18:R:27:ALA:O	16:p:177:ARG:NH1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:804:SER:HA	21:U:892:LEU:HA	2.00	0.44
2:B:204:PRO:HG2	2:B:326:LYS:HE3	1.99	0.44
4:D:158:GLN:HE21	4:D:229:ARG:NH2	2.16	0.44
10:J:220:LEU:HD13	10:J:224:GLU:HB2	1.98	0.44
21:U:127:ASP:H	21:U:130:LEU:HD21	1.83	0.44
23:W:385:SER:OG	23:W:386:VAL:N	2.51	0.44
24:X:28:HIS:O	24:X:32:LYS:HB2	2.18	0.44
25:Y:231:LEU:HD12	25:Y:234:PRO:HD2	1.99	0.44
28:b:181:ASP:OD1	28:b:182:ALA:N	2.51	0.44
29:c:244:VAL:HB	29:c:291:LEU:HD11	1.98	0.44
32:f:83:ARG:O	32:f:87:THR:OG1	2.34	0.44
13:m:39:ILE:HD12	13:m:193:VAL:HG12	1.99	0.44
1:A:123:VAL:HG11	1:A:147:TYR:HB3	2.00	0.44
1:A:213:LEU:HB2	1:A:337:LEU:HD13	2.00	0.44
4:D:159:LYS:HD2	4:D:159:LYS:HA	1.68	0.44
4:D:269:ALA:HB1	5:E:255:ARG:HG2	2.00	0.44
9:I:197:LEU:HA	9:I:200:THR:HG22	1.99	0.44
11:K:109:VAL:HG12	11:K:154:PHE:HD2	1.83	0.44
21:U:185:MET:HE2	21:U:185:MET:HB2	1.89	0.44
23:W:199:TYR:CE2	23:W:236:HIS:CE1	3.05	0.44
26:Z:25:ARG:HB3	29:c:103:GLY:HA2	2.00	0.44
26:Z:197:GLY:HA2	29:c:225:TRP:HD1	1.82	0.44
32:f:173:LEU:HD11	32:f:181:ARG:HE	1.82	0.44
3:C:364:THR:O	3:C:368:MET:HG2	2.18	0.43
4:D:131:ALA:HB3	4:D:141:ASP:H	1.83	0.43
4:D:156:SER:O	4:D:157:ASP:CB	2.65	0.43
6:F:410:ARG:NH1	6:F:419:ASP:OD1	2.51	0.43
7:G:188:ASP:OD1	7:G:188:ASP:N	2.49	0.43
10:J:119:THR:HG22	10:J:126:PRO:HB3	2.00	0.43
20:T:12:LEU:HD12	20:T:173:MET:HE2	2.00	0.43
21:U:367:THR:HA	21:U:370:VAL:HG22	2.00	0.43
21:U:751:ARG:HH21	21:U:904:LYS:HD3	1.82	0.43
27:a:210:VAL:O	27:a:271:LYS:NZ	2.39	0.43
7:g:133:PRO:HD2	13:m:14:PHE:HE2	1.83	0.43
1:A:103:ASN:OD1	1:A:103:ASN:N	2.51	0.43
2:B:125:THR:OG1	2:B:126:SER:N	2.51	0.43
2:B:282:VAL:HB	2:B:327:VAL:HA	2.00	0.43
7:G:10:ASP:OD1	7:G:10:ASP:N	2.49	0.43
32:f:67:ASP:N	32:f:67:ASP:OD1	2.51	0.43
11:k:209:LYS:HA	11:k:209:LYS:HD2	1.84	0.43
17:q:11:ASP:N	17:q:11:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ASP:O	1:A:351:ARG:NH2	2.51	0.43
2:B:183:THR:HG22	2:B:184:TYR:CD1	2.54	0.43
2:B:288:ASP:OD2	2:B:333:ARG:NH1	2.51	0.43
5:E:3:ASP:HB2	6:F:36:MET:HB3	2.00	0.43
6:F:175:MET:HG3	6:F:249:LEU:HD11	1.99	0.43
7:G:13:ILE:HG13	7:G:15:ILE:HG12	2.00	0.43
11:K:41:GLN:NE2	11:K:151:PRO:O	2.52	0.43
16:P:53:LEU:HB3	16:P:60:VAL:HG22	1.99	0.43
22:V:278:GLU:HA	22:V:285:TRP:HZ2	1.82	0.43
22:V:437:ILE:HG12	30:d:146:GLY:HA3	1.98	0.43
32:f:407:MET:HE1	32:f:440:ILE:HG12	1.99	0.43
10:j:199:VAL:HG12	10:j:202:GLY:H	1.84	0.43
11:k:147:ASP:OD1	11:k:147:ASP:N	2.50	0.43
13:m:136:MET:HE3	13:m:165:ILE:HG12	2.01	0.43
1:A:364:VAL:HA	1:A:404:ALA:HB3	2.01	0.43
3:C:213:ARG:HA	3:C:247:PHE:HB3	2.00	0.43
11:K:52:LYS:NZ	11:K:64:ILE:O	2.52	0.43
21:U:103:LYS:HB2	21:U:103:LYS:HE3	1.79	0.43
26:Z:74:TYR:O	26:Z:78:MET:HG2	2.19	0.43
30:d:8:GLU:O	30:d:13:SER:OG	2.28	0.43
15:o:211:VAL:HG21	16:p:198:ARG:HD3	2.01	0.43
16:p:47:ASP:OD1	16:p:47:ASP:N	2.48	0.43
4:D:80:LYS:O	4:D:83:GLN:NE2	2.50	0.43
4:D:176:GLU:OE2	4:D:329:ARG:NH1	2.52	0.43
5:E:109:ARG:HH11	6:F:133:PHE:HE2	1.67	0.43
11:K:210:LEU:HD11	11:K:215:ILE:HD13	2.00	0.43
12:L:49:LEU:HB2	12:L:195:LEU:HD21	2.01	0.43
21:U:689:ILE:HG12	21:U:732:LEU:HD22	2.00	0.43
27:a:18:GLN:HB2	27:a:19:PRO:HD3	1.99	0.43
27:a:247:ARG:HH12	27:a:269:LEU:HD11	1.83	0.43
2:B:383:LEU:HD11	2:B:419:PHE:HB3	2.00	0.43
17:Q:35:MET:SD	17:Q:181:ARG:NH1	2.86	0.43
21:U:645:ASN:OD1	21:U:645:ASN:N	2.51	0.43
22:V:175:MET:HE3	22:V:175:MET:HB2	1.76	0.43
23:W:45:GLU:HA	23:W:48:LEU:HG	1.99	0.43
23:W:119:PRO:HA	23:W:122:LEU:HG	1.99	0.43
27:a:18:GLN:H	27:a:18:GLN:NE2	2.16	0.43
12:l:26:MET:HE1	12:l:148:CYS:HB3	2.01	0.43
5:E:60:VAL:HG22	5:E:71:VAL:HG12	2.00	0.43
23:W:108:CYS:HB3	23:W:128:LEU:HD11	2.01	0.43
23:W:132:THR:HA	23:W:135:LYS:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:213:ARG:HH21	30:d:215:TRP:HE1	1.66	0.43
1:A:159:PRO:O	1:A:160:THR:C	2.61	0.43
1:A:160:THR:O	1:A:161:VAL:C	2.62	0.43
2:B:288:ASP:N	2:B:288:ASP:OD1	2.51	0.43
10:J:58:THR:HA	10:J:60:ARG:HH11	1.84	0.43
12:L:166:GLN:OE1	12:L:169:ARG:NH2	2.45	0.43
21:U:27:LEU:HD11	21:U:38:ILE:HG23	2.00	0.43
21:U:350:LEU:HG	21:U:354:LYS:HG2	2.00	0.43
21:U:432:SER:HB3	21:U:435:SER:HB3	2.01	0.43
23:W:198:ASP:O	23:W:202:THR:N	2.37	0.43
32:f:566:HIS:O	32:f:569:LYS:CG	2.66	0.43
20:t:185:ASN:OD1	20:t:205:THR:OG1	2.37	0.43
3:C:77:VAL:HA	3:C:111:ASN:H	1.84	0.43
27:a:145:LEU:HD22	27:a:148:VAL:HG23	2.00	0.43
30:d:49:ILE:HD12	30:d:52:ARG:HH21	1.84	0.43
1:A:200:ARG:HA	1:A:203:ASN:HB2	2.01	0.43
4:D:242:GLU:OE1	4:D:245:ARG:NH2	2.35	0.43
4:D:309:MET:HE1	4:D:327:LEU:HD11	2.00	0.43
16:P:153:LEU:HB3	16:P:166:THR:HG23	2.01	0.43
21:U:376:MET:HE3	21:U:735:GLY:HA2	2.01	0.43
23:W:39:ARG:NH1	23:W:42:GLU:OE2	2.47	0.43
26:Z:225:GLN:HA	26:Z:228:TYR:CE1	2.54	0.43
27:a:244:ASN:ND2	27:a:246:GLU:OE1	2.51	0.43
29:c:303:MET:SD	30:d:242:LEU:HB3	2.59	0.43
30:d:245:GLN:HA	30:d:248:GLU:OE1	2.18	0.43
3:C:140:VAL:HG11	3:C:211:PHE:HD2	1.83	0.42
4:D:284:GLU:OE2	4:D:287:ARG:NH1	2.52	0.42
6:F:98:ASP:HA	6:F:120:LYS:HB2	2.01	0.42
10:J:31:THR:OG1	10:J:163:ARG:O	2.27	0.42
12:L:33:SER:OG	12:L:62:LYS:NZ	2.35	0.42
21:U:172:ASP:OD1	21:U:172:ASP:N	2.51	0.42
21:U:451:ALA:O	21:U:453:HIS:ND1	2.50	0.42
23:W:139:GLU:HB3	23:W:174:TYR:HE1	1.83	0.42
23:W:174:TYR:O	23:W:182:ARG:NH2	2.51	0.42
23:W:268:LYS:HD2	23:W:336:PRO:HG2	2.01	0.42
7:g:165:ALA:HB3	8:h:56:LEU:HD22	2.01	0.42
12:l:10:VAL:HG13	12:l:11:THR:HG23	2.00	0.42
17:q:13:VAL:HG13	17:q:113:PRO:HB2	2.01	0.42
2:B:32:ARG:HG3	32:f:750:GLN:HG3	2.01	0.42
3:C:89:VAL:HG23	3:C:92:GLU:H	1.83	0.42
3:C:246:ILE:HB	3:C:291:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:189:GLU:HA	4:D:192:LYS:HG2	2.00	0.42
20:T:69:GLN:NE2	20:T:73:ASP:OD1	2.53	0.42
25:Y:98:SER:O	25:Y:102:ASP:N	2.46	0.42
30:d:99:LEU:O	30:d:103:LEU:HB2	2.19	0.42
3:C:69:GLN:HG3	3:C:118:ASN:ND2	2.33	0.42
5:E:340:GLY:HA3	34:E:401:ATP:C4	2.54	0.42
6:F:349:ASP:OD1	6:F:349:ASP:N	2.48	0.42
7:G:57:PRO:HD2	7:G:61:LEU:HD11	2.00	0.42
12:L:4:ASN:OD1	12:L:5:GLN:NE2	2.53	0.42
21:U:625:ILE:HG13	21:U:626:LEU:HG	2.01	0.42
24:X:357:SER:OG	24:X:358:LYS:N	2.53	0.42
25:Y:2:PRO:HG2	25:Y:5:ASN:HB2	2.01	0.42
26:Z:251:LEU:HD12	26:Z:251:LEU:HA	1.79	0.42
2:B:250:VAL:HB	2:B:284:ILE:HA	2.01	0.42
5:E:360:ASP:N	5:E:360:ASP:OD1	2.52	0.42
14:N:68:ILE:HD12	14:N:68:ILE:HA	1.92	0.42
25:Y:9:GLU:O	25:Y:179:ARG:NH2	2.47	0.42
32:f:348:ILE:HD13	32:f:381:VAL:HG21	2.00	0.42
32:f:791:VAL:HG12	32:f:823:ALA:HB1	2.01	0.42
7:g:58:ASP:OD1	7:g:58:ASP:N	2.52	0.42
16:p:58:THR:O	17:q:85:ARG:NH2	2.53	0.42
2:B:227:PRO:O	2:B:232:LYS:NZ	2.52	0.42
3:C:173:GLU:HA	3:C:176:GLU:HB2	2.01	0.42
4:D:154:LEU:HD12	4:D:227:PHE:HB3	2.01	0.42
4:D:191:TYR:HD1	4:D:196:ILE:HD12	1.84	0.42
5:E:361:PHE:HE2	5:E:363:VAL:HB	1.83	0.42
6:F:139:LEU:HD12	6:F:161:LEU:HB2	2.02	0.42
22:V:150:ARG:NH1	22:V:154:ALA:O	2.53	0.42
25:Y:153:ASP:HB3	25:Y:156:LEU:HB3	2.02	0.42
30:d:111:ARG:NH1	30:d:113:ALA:H	2.17	0.42
31:e:35:ASP:HB3	31:e:37:HIS:HD1	1.84	0.42
32:f:535:THR:HG23	32:f:562:LEU:HG	2.01	0.42
2:B:151:LEU:HD21	2:B:163:LEU:HD13	2.02	0.42
5:E:6:ASP:OD1	5:E:7:LYS:N	2.52	0.42
12:L:33:SER:HG	12:L:62:LYS:HZ2	1.60	0.42
13:M:19:ARG:NH2	13:M:24:GLU:OE1	2.51	0.42
24:X:170:GLN:HB3	24:X:193:ALA:HB2	2.00	0.42
26:Z:212:LEU:HA	26:Z:215:VAL:HG12	2.01	0.42
29:c:163:ILE:HD13	29:c:201:TYR:HE1	1.85	0.42
32:f:478:ARG:O	32:f:482:ILE:HG12	2.19	0.42
11:k:129:ASP:N	11:k:129:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ASN:HD21	1:A:112:ILE:HD12	1.85	0.42
5:E:148:VAL:HB	5:E:297:ARG:HH22	1.84	0.42
5:E:199:VAL:HG23	5:E:201:SER:H	1.85	0.42
10:J:67:ASP:OD1	10:J:67:ASP:N	2.52	0.42
12:L:93:LEU:HD23	12:L:93:LEU:HA	1.92	0.42
13:M:230:ASP:N	13:M:230:ASP:OD1	2.52	0.42
20:T:135:PRO:HB2	20:T:154:LEU:HD13	2.01	0.42
21:U:792:ASN:HD21	21:U:796:LYS:NZ	2.17	0.42
25:Y:232:GLU:HG2	25:Y:233:ARG:H	1.85	0.42
25:Y:325:VAL:HG23	31:e:59:GLU:HG2	2.02	0.42
28:b:173:VAL:HG22	28:b:174:PRO:CD	2.45	0.42
1:A:402:LYS:HZ1	2:B:210:TYR:HD2	1.67	0.42
7:G:131:MET:SD	7:G:131:MET:N	2.90	0.42
20:T:79:ASP:OD1	20:T:79:ASP:N	2.49	0.42
24:X:346:GLN:HA	24:X:384:VAL:HA	2.01	0.42
13:m:52:LEU:HD23	13:m:209:PHE:HB3	2.01	0.42
1:A:56:LEU:HD11	2:B:48:LYS:HE3	2.02	0.42
3:C:128:PRO:HG2	4:D:96:VAL:HG13	2.01	0.42
6:F:182:THR:HA	6:F:242:ALA:HB1	2.01	0.42
6:F:266:LYS:HD2	6:F:269:ARG:HH22	1.85	0.42
26:Z:245:PHE:CZ	30:d:235:THR:HB	2.55	0.42
30:d:23:LEU:O	30:d:27:LYS:HG2	2.19	0.42
32:f:683:GLU:O	32:f:687:ARG:HG2	2.20	0.42
7:g:61:LEU:HA	13:m:160:TYR:HD1	1.85	0.42
13:m:237:LYS:NZ	13:m:241:GLU:OE2	2.42	0.42
9:I:174:MET:HE2	9:I:174:MET:HB3	1.84	0.42
10:J:148:ASP:OD2	10:J:150:SER:OG	2.31	0.42
12:L:7:ASP:O	12:L:21:GLN:NE2	2.53	0.42
23:W:316:ARG:HB3	23:W:319:THR:HG23	2.01	0.42
28:b:161:ASN:C	28:b:161:ASN:HD22	2.28	0.42
11:k:78:MET:HE1	11:k:82:ILE:HG22	2.02	0.42
2:B:70:ASP:OD1	21:U:834:SER:OG	2.36	0.41
3:C:13:GLU:O	3:C:17:GLY:N	2.53	0.41
3:C:113:ARG:HB3	3:C:127:LEU:HD12	2.00	0.41
13:M:68:ASN:HB3	20:T:76:LEU:HD22	2.02	0.41
22:V:132:LEU:HD23	22:V:132:LEU:HA	1.93	0.41
25:Y:312:ARG:HB2	25:Y:356:THR:CG2	2.50	0.41
32:f:211:ILE:HG23	32:f:213:GLN:H	1.84	0.41
10:j:38:ARG:HH22	10:j:182:GLU:HG3	1.85	0.41
2:B:117:ASP:OD1	2:B:117:ASP:N	2.52	0.41
2:B:142:ASP:OD1	2:B:142:ASP:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:85:ILE:HD13	29:c:152:LYS:HE2	2.02	0.41
6:F:180:ARG:HD3	6:F:181:PRO:HD2	2.02	0.41
6:F:311:LEU:HA	6:F:311:LEU:HD23	1.84	0.41
10:J:99:GLU:OE2	18:R:81:LYS:HE2	2.20	0.41
14:N:29:ARG:NH2	15:O:139:GLU:OE2	2.53	0.41
14:N:127:ILE:HD11	14:N:136:TYR:CE1	2.54	0.41
21:U:556:MET:HE2	21:U:563:ALA:HB3	2.01	0.41
23:W:26:GLN:NE2	23:W:30:GLU:OE2	2.53	0.41
23:W:276:LEU:O	23:W:357:ARG:NE	2.51	0.41
27:a:343:LEU:HA	27:a:346:ILE:HD12	2.02	0.41
29:c:280:PRO:HB2	29:c:281:LYS:H	1.64	0.41
18:r:51:ASP:OD1	19:s:97:TYR:OH	2.32	0.41
19:s:21:ALA:HB3	19:s:198:VAL:HB	2.02	0.41
2:B:183:THR:HG23	2:B:242:GLN:HB2	2.02	0.41
2:B:222:VAL:HA	2:B:349:ARG:HB2	2.02	0.41
24:X:311:ALA:HA	24:X:314:ARG:HB2	2.00	0.41
27:a:72:ASN:N	28:b:17:ARG:HH12	2.19	0.41
30:d:44:THR:HA	30:d:47:GLN:HG2	2.02	0.41
9:i:6:ASP:OD2	10:j:3:TYR:OH	2.38	0.41
20:t:22:ILE:HG12	20:t:50:MET:HE2	2.02	0.41
4:D:255:LYS:HD3	4:D:302:ASN:HB3	2.02	0.41
7:G:165:ALA:HB1	7:G:179:LEU:HD13	2.03	0.41
19:S:13:LEU:HD12	19:S:145:LEU:HD13	2.01	0.41
22:V:99:ARG:HD3	22:V:99:ARG:HA	1.91	0.41
23:W:429:SER:OG	29:c:233:ASP:OD1	2.30	0.41
25:Y:205:VAL:HA	25:Y:219:PHE:HE2	1.85	0.41
10:J:36:ARG:HG3	10:J:142:PRO:HB2	2.02	0.41
12:L:45:VAL:HG12	12:L:214:ILE:HG12	2.01	0.41
21:U:559:ARG:HB3	21:U:562:GLU:HB2	2.02	0.41
22:V:349:ARG:HH22	31:e:37:HIS:CD2	2.39	0.41
27:a:34:TRP:O	27:a:38:THR:OG1	2.30	0.41
27:a:273:GLN:HB3	27:a:310:LEU:HD11	2.01	0.41
13:m:43:ASP:OD1	13:m:43:ASP:N	2.54	0.41
13:m:219:LEU:HD12	13:m:220:THR:HG23	2.03	0.41
1:A:156:LYS:HB2	1:A:157:ILE:H	1.62	0.41
5:E:385:ASP:OD1	5:E:385:ASP:N	2.46	0.41
6:F:279:ALA:O	6:F:281:SER:N	2.53	0.41
7:G:38:THR:HG21	7:G:206:LEU:HD21	2.03	0.41
21:U:195:ASN:HB2	21:U:199:ARG:HH21	1.85	0.41
21:U:751:ARG:NH1	21:U:908:ILE:O	2.52	0.41
22:V:440:LYS:O	22:V:443:ARG:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:314:LEU:HG	27:a:312:MET:HE1	2.01	0.41
26:Z:276:ILE:HD13	26:Z:276:ILE:HA	1.97	0.41
28:b:6:THR:HB	28:b:49:VAL:HG22	2.02	0.41
29:c:198:ARG:HG3	29:c:199:HIS:CE1	2.55	0.41
2:B:389:ASP:OD1	2:B:389:ASP:N	2.54	0.41
3:C:197:THR:N	34:C:501:ATP:O2A	2.41	0.41
5:E:215:ILE:HA	5:E:218:MET:HE2	2.03	0.41
16:P:193:ASP:OD1	16:P:193:ASP:N	2.52	0.41
21:U:456:ASP:O	21:U:460:TYR:N	2.47	0.41
23:W:20:TYR:HD2	23:W:54:THR:HA	1.86	0.41
25:Y:39:ASP:HA	25:Y:42:MET:HG3	2.02	0.41
26:Z:83:LYS:HD3	26:Z:87:ALA:HA	2.02	0.41
27:a:70:ARG:HH21	28:b:17:ARG:HG2	1.86	0.41
28:b:150:THR:OG1	28:b:153:LEU:HB2	2.21	0.41
28:b:187:PRO:HA	28:b:191:GLY:HA2	2.03	0.41
29:c:163:ILE:HD12	29:c:163:ILE:HA	1.95	0.41
30:d:65:ARG:HG3	30:d:67:ASP:HB2	2.03	0.41
32:f:94:LYS:HA	32:f:97:LYS:HE2	2.01	0.41
11:k:167:ALA:HB3	12:l:56:LEU:HD13	2.02	0.41
2:B:76:GLU:O	2:B:80:ARG:HG2	2.20	0.41
2:B:193:GLN:HG2	2:B:353:PHE:HE1	1.85	0.41
5:E:87:LEU:HD12	5:E:87:LEU:HA	1.91	0.41
6:F:38:THR:HG22	6:F:39:GLU:HG2	2.02	0.41
8:H:11:THR:HG22	8:H:19:LEU:HD22	2.02	0.41
26:Z:209:ARG:NH1	27:a:350:LYS:O	2.54	0.41
27:a:356:TRP:HH2	29:c:309:PHE:HA	1.86	0.41
16:p:74:TYR:CZ	16:p:78:GLU:HG3	2.56	0.41
1:A:52:ILE:HD12	1:A:52:ILE:HA	1.96	0.41
2:B:169:PRO:HB2	2:B:173:VAL:HG23	2.01	0.41
2:B:203:LEU:HD12	2:B:207:HIS:HB2	2.02	0.41
3:C:44:ARG:HG3	22:V:495:ARG:HB2	2.03	0.41
4:D:258:ALA:O	4:D:260:ALA:N	2.54	0.41
5:E:36:LEU:HB3	6:F:69:MET:HE1	2.03	0.41
5:E:365:GLU:HA	5:E:368:MET:HE2	2.01	0.41
10:J:92:GLN:HB3	17:Q:62:LYS:HE3	2.03	0.41
15:O:209:THR:HG22	16:P:169:GLN:HE21	1.86	0.41
21:U:182:LYS:O	21:U:186:SER:HB2	2.21	0.41
22:V:131:LEU:HD22	22:V:171:VAL:HG11	2.02	0.41
22:V:167:LEU:HD23	22:V:170:LEU:HD21	2.02	0.41
26:Z:12:HIS:HE1	26:Z:165:GLU:HB2	1.85	0.41
26:Z:82:PHE:HA	26:Z:85:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:94:LYS:O	29:c:98:MET:HG2	2.21	0.41
30:d:129:THR:OG1	30:d:130:ASN:N	2.53	0.41
32:f:72:ARG:HE	32:f:118:ASN:ND2	2.19	0.41
32:f:93:PRO:HG2	32:f:96:LEU:HB2	2.03	0.41
32:f:189:LYS:HD2	32:f:189:LYS:HA	1.75	0.41
32:f:208:LEU:HD13	32:f:217:LEU:HD12	2.02	0.41
32:f:266:LEU:HD11	32:f:278:VAL:HG13	2.03	0.41
32:f:797:LEU:HD23	32:f:797:LEU:HA	1.96	0.41
19:s:19:ASP:OD1	19:s:19:ASP:N	2.52	0.41
20:t:110:MET:HE2	20:t:110:MET:HB2	1.98	0.41
4:D:378:ILE:HD11	4:D:406:VAL:HG11	2.03	0.41
5:E:262:ASN:C	5:E:262:ASN:HD22	2.29	0.41
8:H:93:LEU:HD13	8:H:113:ARG:HB3	2.03	0.41
10:J:234:LYS:HA	10:J:237:GLU:HG2	2.03	0.41
16:P:15:LYS:HE3	16:P:121:ILE:HG12	2.03	0.41
16:P:158:MET:HE2	16:P:158:MET:HB3	1.95	0.41
25:Y:91:ALA:HB1	25:Y:100:ILE:HG22	2.03	0.41
25:Y:212:GLU:HG2	25:Y:213:LEU:HD22	2.02	0.41
29:c:57:MET:HB2	29:c:57:MET:HE3	1.86	0.41
30:d:188:LYS:HD2	30:d:221:ASN:HD21	1.85	0.41
9:i:72:MET:HG2	9:i:138:GLY:HA3	2.03	0.41
14:n:107:GLU:HG2	14:n:110:GLN:HE21	1.86	0.41
1:A:166:VAL:HG22	1:A:168:GLU:HB2	2.04	0.40
4:D:82:ILE:HD12	29:c:152:LYS:HZ2	1.86	0.40
17:Q:31:ASP:OD1	17:Q:31:ASP:N	2.54	0.40
23:W:178:GLU:HG2	23:W:180:LYS:H	1.86	0.40
23:W:412:ILE:HG21	27:a:327:VAL:HB	2.02	0.40
29:c:167:MET:HE1	29:c:174:PRO:HG3	2.02	0.40
32:f:573:ILE:HD12	32:f:595:VAL:HG12	2.03	0.40
7:g:10:ASP:OD1	7:g:10:ASP:N	2.54	0.40
10:j:39:ASP:OD1	10:j:39:ASP:N	2.50	0.40
11:k:157:ASP:OD1	11:k:161:THR:N	2.55	0.40
1:A:244:GLU:O	1:A:247:GLN:NE2	2.53	0.40
2:B:358:GLU:HA	2:B:361:LYS:HB2	2.03	0.40
5:E:1:MET:HE2	5:E:1:MET:HB3	1.85	0.40
7:G:93:ARG:HA	7:G:93:ARG:HD2	1.89	0.40
10:J:189:LYS:HA	10:J:232:ILE:HD11	2.02	0.40
21:U:1:MET:HB2	21:U:2:ILE:H	1.67	0.40
21:U:447:GLY:HA3	21:U:480:GLY:HA2	2.02	0.40
22:V:480:ILE:HG21	30:d:249:TYR:CZ	2.56	0.40
26:Z:212:LEU:HD13	27:a:350:LYS:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:77:VAL:HA	27:a:80:ILE:HG22	2.03	0.40
30:d:45:LYS:HE2	30:d:88:GLN:HB2	2.03	0.40
32:f:418:LEU:HD23	32:f:425:GLY:HA2	2.02	0.40
32:f:809:ILE:HG23	32:f:814:SER:HB2	2.03	0.40
9:i:184:MET:HB3	9:i:184:MET:HE3	1.84	0.40
15:o:38:SER:OG	15:o:40:ASN:OD1	2.32	0.40
6:F:97:LEU:O	6:F:120:LYS:N	2.54	0.40
8:H:163:MET:HE2	8:H:163:MET:HB3	1.80	0.40
9:I:119:GLN:NE2	10:J:79:ASP:OD1	2.54	0.40
25:Y:316:LEU:HB3	25:Y:354:VAL:HG23	2.03	0.40
26:Z:16:LEU:HG	29:c:216:MET:HE1	2.03	0.40
1:A:125:LEU:HD21	1:A:131:PRO:HB3	2.02	0.40
3:C:160:GLU:OE1	3:C:313:ARG:NH2	2.54	0.40
4:D:119:ILE:O	4:D:121:ARG:NH1	2.54	0.40
4:D:154:LEU:HD23	4:D:154:LEU:HA	1.96	0.40
5:E:152:PRO:HG3	5:E:159:PHE:HE2	1.86	0.40
10:J:220:LEU:HD22	10:J:220:LEU:HA	1.76	0.40
16:P:88:MET:HG3	16:P:122:CYS:SG	2.61	0.40
21:U:497:LEU:HB3	21:U:516:LEU:HD13	2.04	0.40
23:W:204:ILE:HG23	23:W:205:ILE:HG13	2.04	0.40
26:Z:152:SER:OG	26:Z:153:LYS:N	2.53	0.40
31:e:42:ASN:OD1	31:e:43:TRP:N	2.53	0.40
17:q:39:SER:OG	17:q:40:GLU:N	2.52	0.40
20:t:43:MET:SD	20:t:64:LYS:HG3	2.62	0.40
1:A:38:GLN:HG3	1:A:41:TYR:HB2	2.03	0.40
6:F:172:VAL:HA	6:F:175:MET:HE3	2.04	0.40
6:F:206:MET:HE2	6:F:206:MET:HB2	1.99	0.40
6:F:299:GLU:O	6:F:301:ALA:N	2.55	0.40
9:I:116:ASP:OD1	9:I:117:ILE:N	2.55	0.40
16:P:12:MET:HE2	16:P:167:ILE:HG13	2.02	0.40
20:T:9:THR:OG1	20:T:10:SER:N	2.54	0.40
22:V:337:LEU:HB3	22:V:398:LEU:HD11	2.03	0.40
28:b:161:ASN:ND2	28:b:161:ASN:O	2.54	0.40
8:h:40:ALA:HA	8:h:182:LEU:HD21	2.03	0.40
17:q:140:LEU:HD23	17:q:140:LEU:HA	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	400/433 (92%)	347 (87%)	52 (13%)	1 (0%)	36	65
2	B	409/440 (93%)	366 (90%)	43 (10%)	0	100	100
3	C	394/398 (99%)	349 (89%)	45 (11%)	0	100	100
4	D	378/418 (90%)	346 (92%)	31 (8%)	1 (0%)	36	65
5	E	387/403 (96%)	348 (90%)	35 (9%)	4 (1%)	12	40
6	F	391/439 (89%)	357 (91%)	30 (8%)	4 (1%)	12	40
7	G	242/246 (98%)	230 (95%)	12 (5%)	0	100	100
7	g	242/246 (98%)	223 (92%)	17 (7%)	2 (1%)	16	45
8	H	230/234 (98%)	221 (96%)	9 (4%)	0	100	100
8	h	230/234 (98%)	218 (95%)	12 (5%)	0	100	100
9	I	249/261 (95%)	240 (96%)	7 (3%)	2 (1%)	16	45
9	i	248/261 (95%)	242 (98%)	6 (2%)	0	100	100
10	J	237/248 (96%)	225 (95%)	12 (5%)	0	100	100
10	j	237/248 (96%)	224 (94%)	13 (6%)	0	100	100
11	K	232/241 (96%)	219 (94%)	12 (5%)	1 (0%)	30	60
11	k	232/241 (96%)	223 (96%)	9 (4%)	0	100	100
12	L	236/263 (90%)	228 (97%)	8 (3%)	0	100	100
12	l	236/263 (90%)	225 (95%)	11 (5%)	0	100	100
13	M	239/255 (94%)	233 (98%)	6 (2%)	0	100	100
13	m	238/255 (93%)	235 (99%)	3 (1%)	0	100	100
14	N	200/239 (84%)	196 (98%)	4 (2%)	0	100	100
14	n	200/239 (84%)	195 (98%)	5 (2%)	0	100	100
15	O	218/277 (79%)	211 (97%)	7 (3%)	0	100	100
15	o	218/277 (79%)	213 (98%)	5 (2%)	0	100	100
16	P	202/205 (98%)	195 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	p	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
17	Q	198/201 (98%)	192 (97%)	6 (3%)	0	100	100
17	q	197/201 (98%)	192 (98%)	5 (2%)	0	100	100
18	R	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
18	r	199/263 (76%)	191 (96%)	8 (4%)	0	100	100
19	S	211/241 (88%)	202 (96%)	9 (4%)	0	100	100
19	s	211/241 (88%)	204 (97%)	7 (3%)	0	100	100
20	T	214/264 (81%)	207 (97%)	7 (3%)	0	100	100
20	t	214/264 (81%)	207 (97%)	7 (3%)	0	100	100
21	U	874/953 (92%)	804 (92%)	70 (8%)	0	100	100
22	V	442/534 (83%)	430 (97%)	12 (3%)	0	100	100
23	W	439/456 (96%)	423 (96%)	16 (4%)	0	100	100
24	X	420/422 (100%)	395 (94%)	24 (6%)	1 (0%)	43	71
25	Y	387/389 (100%)	361 (93%)	26 (7%)	0	100	100
26	Z	284/324 (88%)	252 (89%)	29 (10%)	3 (1%)	11	39
27	a	371/376 (99%)	339 (91%)	31 (8%)	1 (0%)	36	65
28	b	189/377 (50%)	166 (88%)	23 (12%)	0	100	100
29	c	285/310 (92%)	247 (87%)	35 (12%)	3 (1%)	11	39
30	d	255/350 (73%)	223 (88%)	31 (12%)	1 (0%)	30	60
31	e	48/70 (69%)	42 (88%)	6 (12%)	0	100	100
32	f	840/908 (92%)	810 (96%)	30 (4%)	0	100	100
All	All	13404/14876 (90%)	12585 (94%)	795 (6%)	24 (0%)	44	71

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	157	ASP
5	E	227	PRO
5	E	248	SER
24	X	318	ILE
7	g	4	GLY
5	E	127	PRO
6	F	166	THR
6	F	300	LYS
6	F	301	ALA

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Mol	Chain	Res	Type
26	Z	145	HIS
27	a	69	HIS
29	c	198	ARG
29	c	280	PRO
1	A	285	PHE
5	E	247	THR
26	Z	146	ASP
9	I	54	LYS
6	F	164	LEU
9	I	53	HIS
26	Z	147	ASP
30	d	200	PHE
7	g	7	ALA
11	K	130	PRO
29	c	279	ASP

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	338/372 (91%)	334 (99%)	4 (1%)	63	75
2	B	357/385 (93%)	357 (100%)	0	100	100
3	C	340/346 (98%)	339 (100%)	1 (0%)	86	86
4	D	333/366 (91%)	331 (99%)	2 (1%)	78	81
5	E	341/353 (97%)	340 (100%)	1 (0%)	86	86
6	F	340/379 (90%)	339 (100%)	1 (0%)	86	86
7	G	205/210 (98%)	205 (100%)	0	100	100
7	g	202/210 (96%)	201 (100%)	1 (0%)	81	83
8	H	188/191 (98%)	188 (100%)	0	100	100
8	h	188/191 (98%)	186 (99%)	2 (1%)	65	76
9	I	206/221 (93%)	202 (98%)	4 (2%)	50	68
9	i	206/221 (93%)	206 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	196/211 (93%)	193 (98%)	3 (2%)	57	72
10	j	196/211 (93%)	196 (100%)	0	100	100
11	K	192/203 (95%)	192 (100%)	0	100	100
11	k	195/203 (96%)	195 (100%)	0	100	100
12	L	202/224 (90%)	202 (100%)	0	100	100
12	l	201/224 (90%)	201 (100%)	0	100	100
13	M	197/212 (93%)	197 (100%)	0	100	100
13	m	198/212 (93%)	198 (100%)	0	100	100
14	N	157/181 (87%)	157 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	179/228 (78%)	179 (100%)	0	100	100
15	o	181/228 (79%)	181 (100%)	0	100	100
16	P	172/174 (99%)	172 (100%)	0	100	100
16	p	173/174 (99%)	173 (100%)	0	100	100
17	Q	169/171 (99%)	169 (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	155/202 (77%)	155 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	178/199 (89%)	178 (100%)	0	100	100
20	T	178/215 (83%)	178 (100%)	0	100	100
20	t	179/215 (83%)	179 (100%)	0	100	100
21	U	752/816 (92%)	752 (100%)	0	100	100
22	V	390/460 (85%)	390 (100%)	0	100	100
23	W	406/416 (98%)	404 (100%)	2 (0%)	81	83
24	X	362/362 (100%)	355 (98%)	7 (2%)	50	68
25	Y	344/344 (100%)	344 (100%)	0	100	100
26	Z	257/295 (87%)	257 (100%)	0	100	100
27	a	333/336 (99%)	333 (100%)	0	100	100
28	b	167/312 (54%)	166 (99%)	1 (1%)	78	81
29	c	252/268 (94%)	250 (99%)	2 (1%)	73	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	d	231/294 (79%)	230 (100%)	1 (0%)	84	84
31	e	44/63 (70%)	44 (100%)	0	100	100
32	f	711/763 (93%)	709 (100%)	2 (0%)	86	86
All	All	11446/12614 (91%)	11412 (100%)	34 (0%)	84	86

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	LYS
1	A	157	ILE
1	A	160	THR
1	A	403	ILE
3	C	210	THR
4	D	158	GLN
4	D	159	LYS
5	E	226	GLN
6	F	300	LYS
9	I	7[A]	SER
9	I	7[B]	SER
9	I	52	ILE
9	I	54	LYS
10	J	219	ILE
10	J	220	LEU
10	J	221	ASN
23	W	198	ASP
23	W	200	ILE
24	X	105	GLN
24	X	106	GLU
24	X	107	VAL
24	X	108	GLU
24	X	313	LEU
24	X	314	ARG
24	X	320	SER
28	b	161	ASN
29	c	175	ARG
29	c	197	ASN
30	d	248	GLU
32	f	565	ASN
32	f	566	HIS
7	g	6	SER
8	h	3	GLU

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Mol	Chain	Res	Type
8	h	4	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	145	ASN
1	A	203	ASN
1	A	296	GLN
1	A	314	ASN
1	A	414	ASN
3	C	90	HIS
3	C	124	HIS
3	C	129	ASN
3	C	221	GLN
4	D	99	ASN
4	D	127	ASN
4	D	158	GLN
4	D	294	ASN
4	D	304	ASN
4	D	340	GLN
4	D	414	HIS
5	E	45	ASN
5	E	271	HIS
6	F	184	GLN
6	F	436	GLN
7	G	75	ASN
7	G	128	ASN
7	G	172	GLN
8	H	71	HIS
8	H	88	HIS
8	H	102	GLN
9	I	53	HIS
9	I	84	ASN
9	I	102	GLN
9	I	123	GLN
9	I	146	GLN
10	J	154	HIS
10	J	221	ASN
11	K	97	GLN
12	L	5	GLN
12	L	86	ASN

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Mol	Chain	Res	Type
12	L	143	HIS
14	N	106	GLN
16	P	7	ASN
16	P	145	GLN
17	Q	87	ASN
17	Q	101	ASN
17	Q	168	GLN
18	R	89	GLN
18	R	162	GLN
19	S	77	HIS
20	T	81	HIS
20	T	108	ASN
20	T	213	HIS
21	U	32	ASN
21	U	145	HIS
21	U	340	GLN
21	U	355	ASN
21	U	438	GLN
21	U	491	GLN
21	U	527	GLN
21	U	541	HIS
21	U	632	GLN
21	U	647	HIS
21	U	670	ASN
21	U	743	ASN
21	U	777	HIS
21	U	888	GLN
24	X	48	GLN
24	X	213	GLN
25	Y	64	GLN
25	Y	136	HIS
25	Y	378	ASN
26	Z	77	ASN
26	Z	109	ASN
27	a	18	GLN
27	a	86	GLN
27	a	124	ASN
27	a	143	ASN
27	a	193	GLN
27	a	231	GLN
27	a	257	GLN
27	a	287	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	b	34	ASN
28	b	105	HIS
28	b	149	ASN
29	c	77	GLN
29	c	115	HIS
29	c	128	ASN
29	c	197	ASN
30	d	221	ASN
32	f	198	HIS
32	f	323	ASN
32	f	371	ASN
32	f	472	HIS
32	f	565	ASN
32	f	566	HIS
32	f	782	HIS
32	f	786	GLN
32	f	815	HIS
32	f	876	HIS
7	g	33	ASN
8	h	21	GLN
8	h	95	GLN
9	i	40	ASN
9	i	142	HIS
9	i	177	GLN
10	j	175	ASN
11	k	41	GLN
11	k	99	HIS
11	k	118	ASN
14	n	77	HIS
14	n	123	GLN
15	o	193	ASN
16	p	61	GLN
16	p	81	GLN
17	q	27	GLN
17	q	99	HIS
18	r	85	ASN
18	r	162	GLN
19	s	108	ASN
20	t	147	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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$
34	ATP	D	501	35	29,33,33	0.29	0	44,52,52	0.48	1 (2%)
36	ADP	F	501	-	27,29,29	1.35	4 (14%)	42,45,45	1.99	9 (21%)
34	ATP	E	401	35	29,33,33	0.32	0	44,52,52	0.48	1 (2%)
34	ATP	C	501	35	29,33,33	0.33	0	44,52,52	0.53	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
34	ATP	D	501	35	-	7/22/38/38	0/3/3/3
36	ADP	F	501	-	-	2/16/32/32	0/3/3/3
34	ATP	E	401	35	-	5/22/38/38	0/3/3/3
34	ATP	C	501	35	-	1/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	F	501	ADP	C5-C4	4.41	1.47	1.39
36	F	501	ADP	C5-C6	2.57	1.48	1.41
36	F	501	ADP	C5-N7	-2.35	1.34	1.39
36	F	501	ADP	C8-N7	2.33	1.36	1.31

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	F	501	ADP	C5-C4-N3	-6.29	118.54	126.75
36	F	501	ADP	N3-C4-N9	5.04	135.38	127.08
36	F	501	ADP	C2-N3-C4	3.91	120.99	111.75
36	F	501	ADP	PA-O3A-PB	-3.78	119.84	132.83
36	F	501	ADP	N3-C2-N1	-3.10	123.75	128.60
36	F	501	ADP	C4-C5-N7	-3.00	106.96	110.62
36	F	501	ADP	C5-N7-C8	2.56	107.15	103.51
36	F	501	ADP	C4-N9-C8	2.52	108.46	105.73
36	F	501	ADP	C3'-C2'-C1'	2.52	106.21	101.43
34	C	501	ATP	PB-O3B-PG	2.03	139.80	132.83
34	D	501	ATP	PB-O3B-PG	2.01	139.73	132.83
34	E	401	ATP	PB-O3B-PG	2.00	139.70	132.83

There are no chirality outliers.

All (15) torsion outliers are listed below:

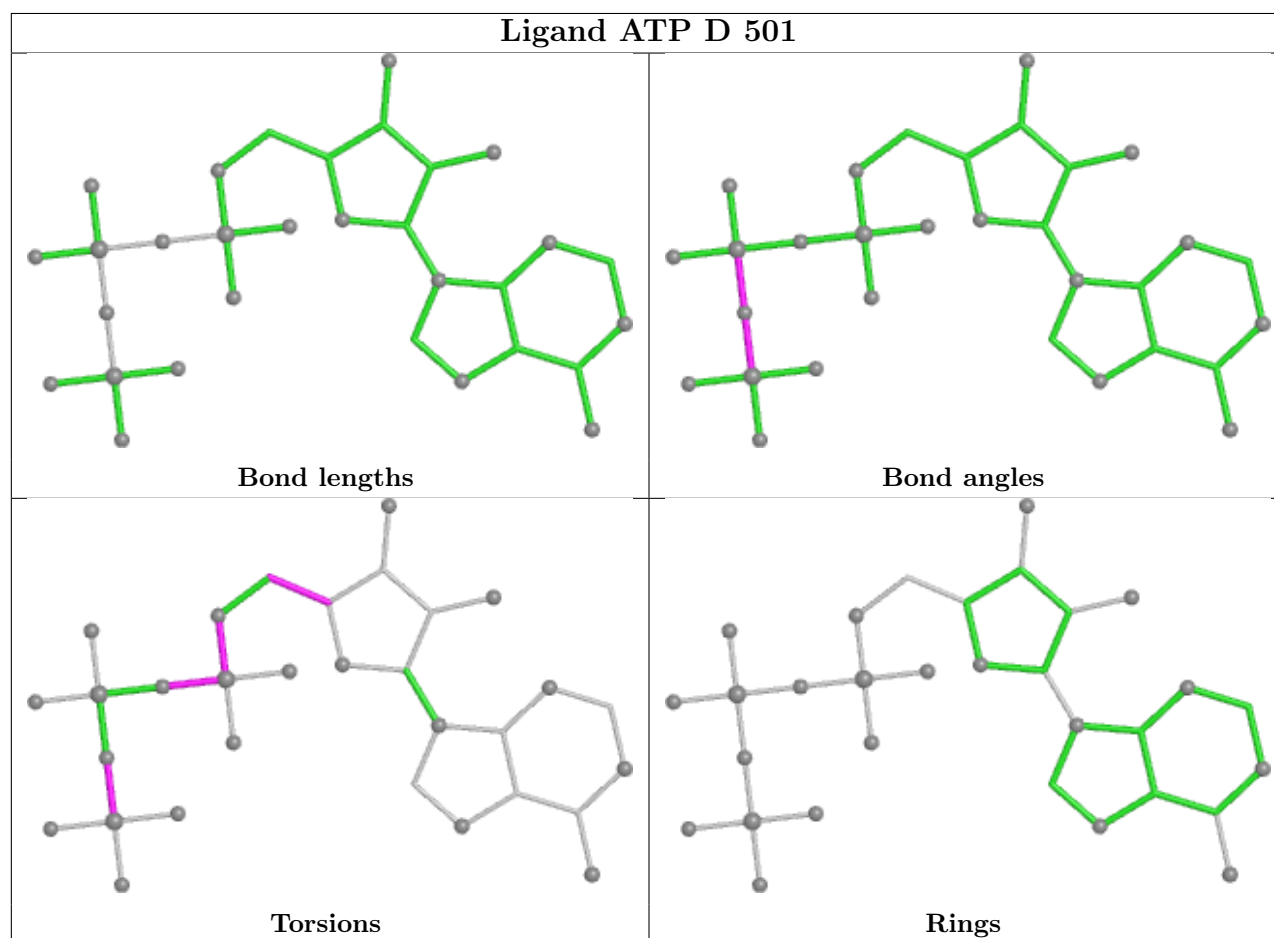
Mol	Chain	Res	Type	Atoms
34	D	501	ATP	PB-O3B-PG-O3G
34	D	501	ATP	C5'-O5'-PA-O3A
34	E	401	ATP	C5'-O5'-PA-O1A
34	E	401	ATP	C5'-O5'-PA-O2A
36	F	501	ADP	C5'-O5'-PA-O3A
34	E	401	ATP	O4'-C4'-C5'-O5'
34	E	401	ATP	C3'-C4'-C5'-O5'
34	D	501	ATP	PB-O3B-PG-O2G
34	D	501	ATP	C5'-O5'-PA-O1A
34	D	501	ATP	C5'-O5'-PA-O2A
36	F	501	ADP	C5'-O5'-PA-O1A
34	C	501	ATP	C4'-C5'-O5'-PA
34	D	501	ATP	PB-O3A-PA-O1A
34	D	501	ATP	O4'-C4'-C5'-O5'
34	E	401	ATP	C5'-O5'-PA-O3A

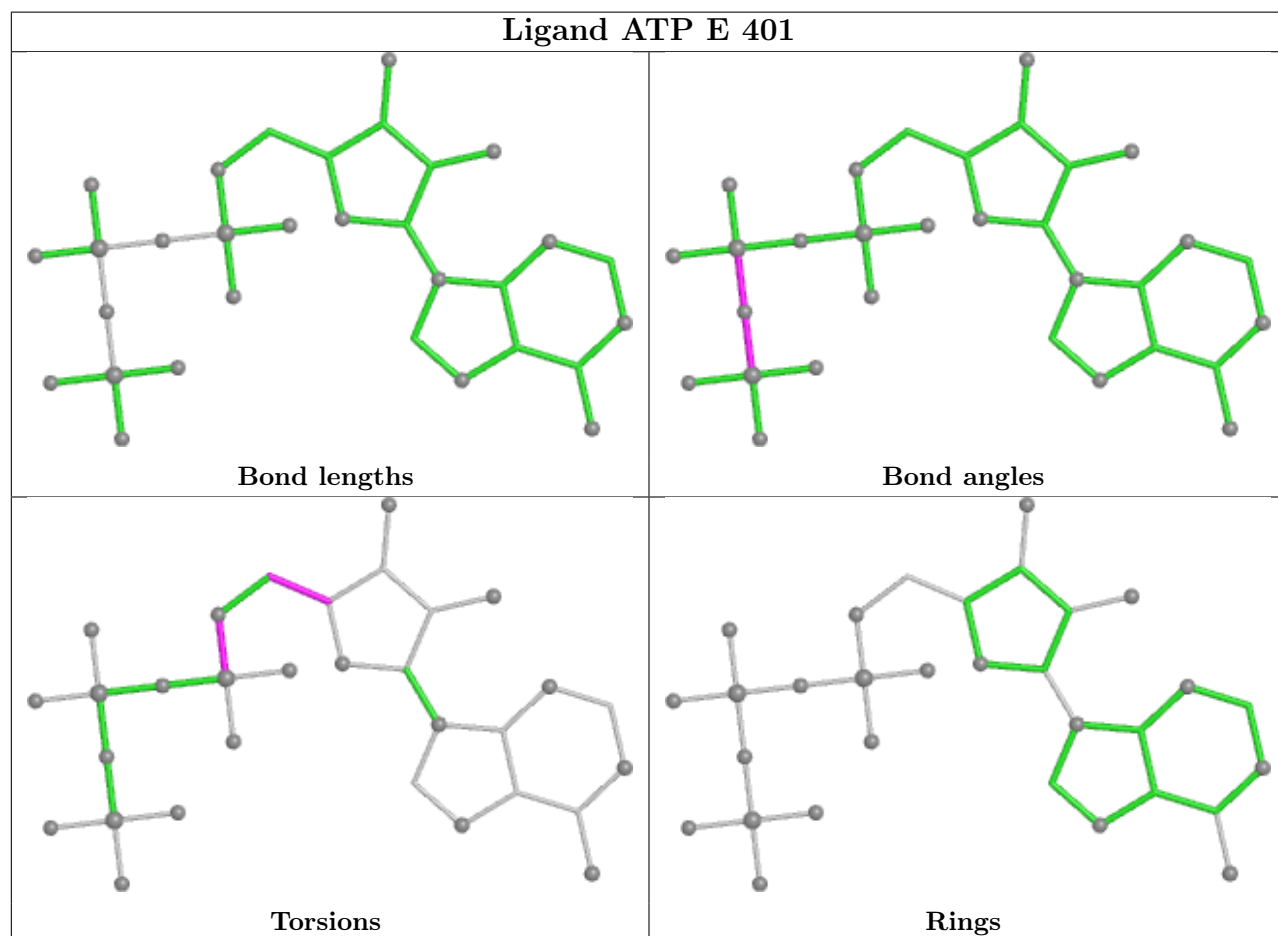
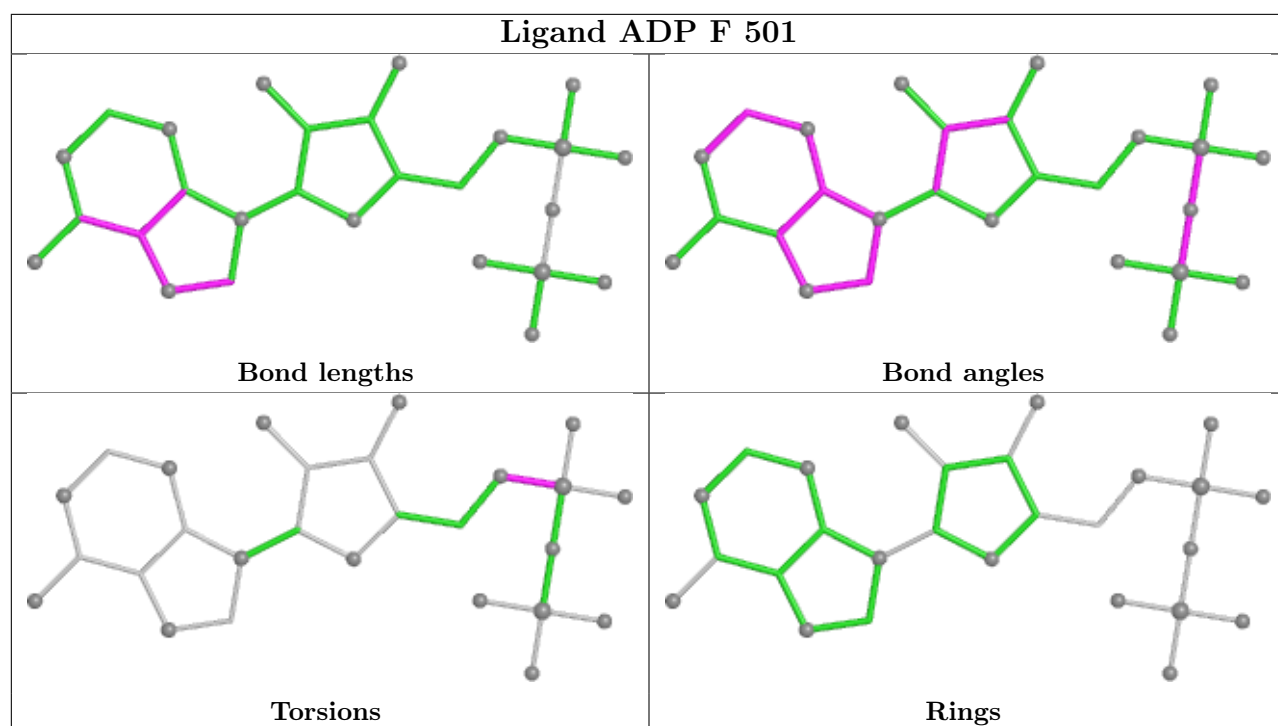
There are no ring outliers.

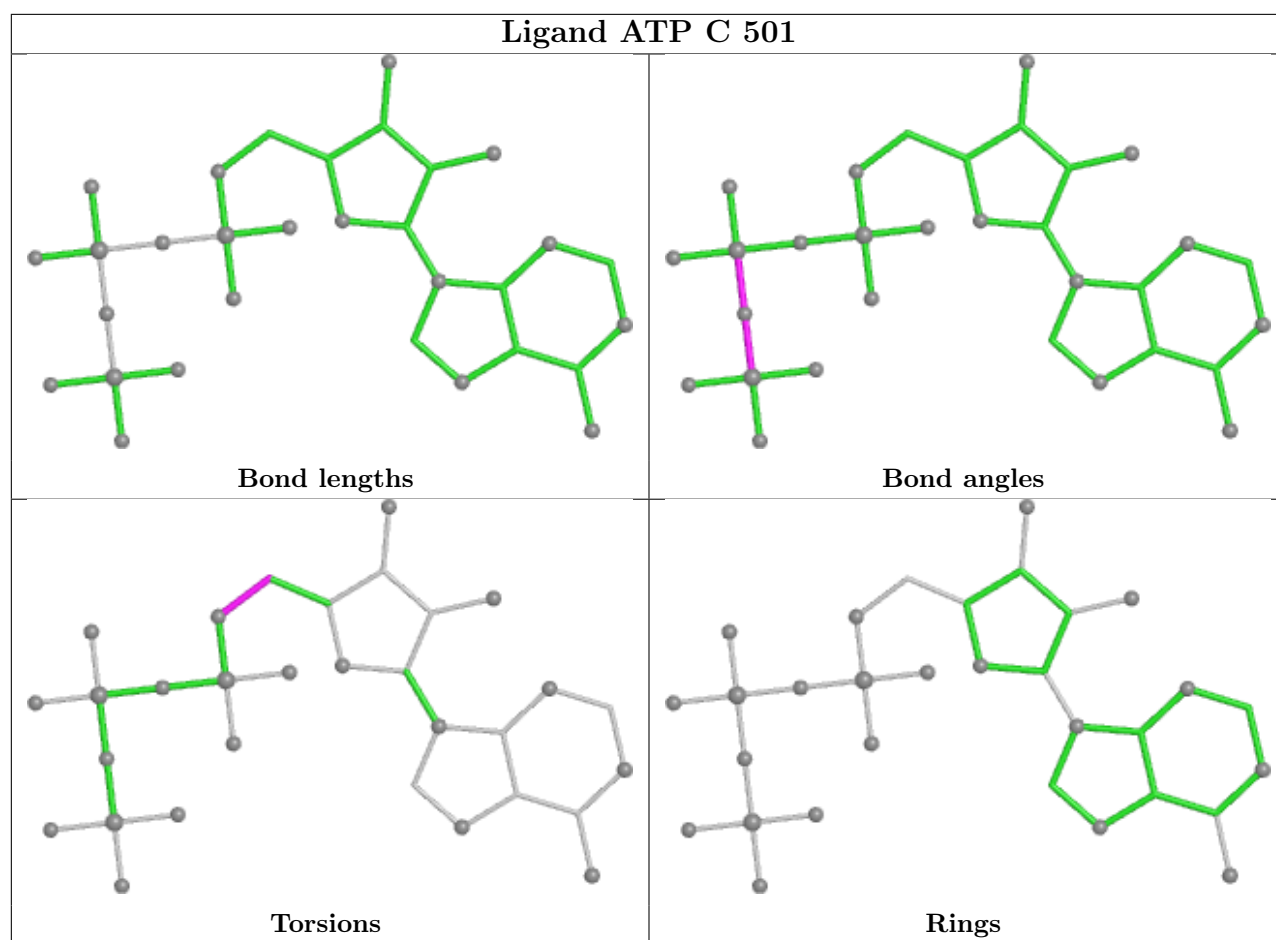
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	D	501	ATP	1	0
36	F	501	ADP	1	0
34	E	401	ATP	1	0
34	C	501	ATP	3	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

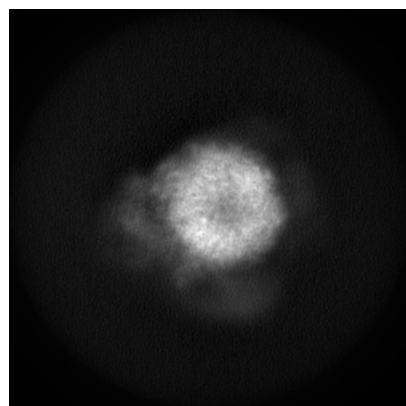
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62071. 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](#)

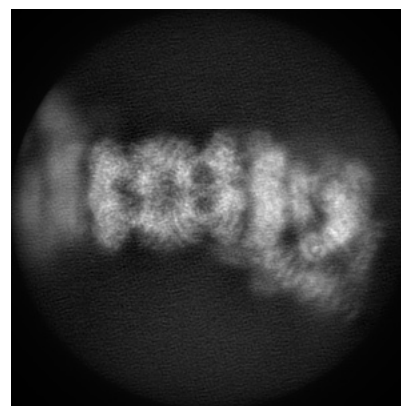
6.1.1 Primary map



X

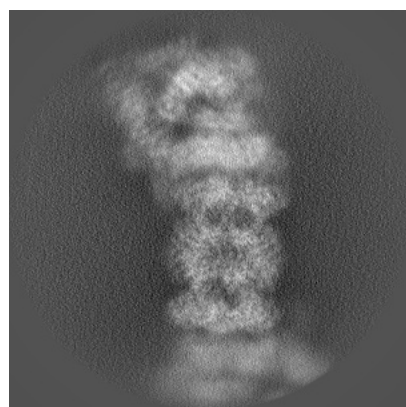


Y

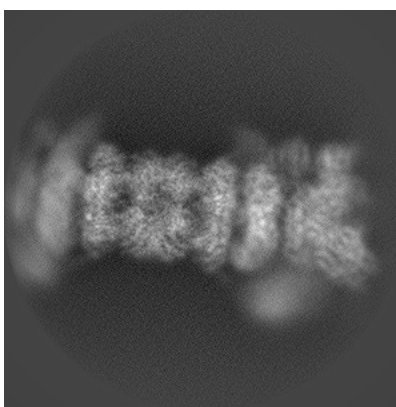


Z

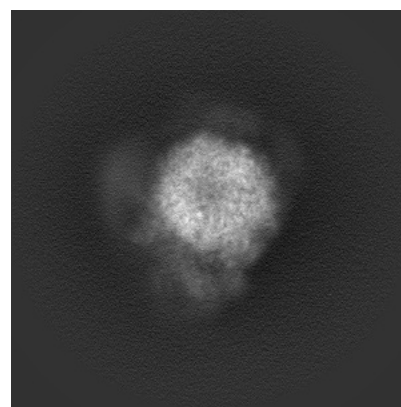
6.1.2 Raw map



X



Y

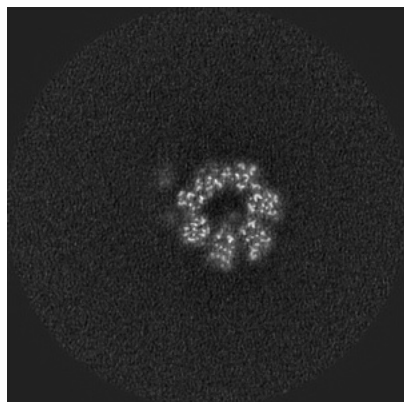


Z

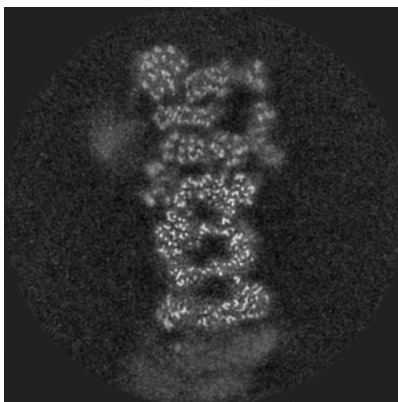
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

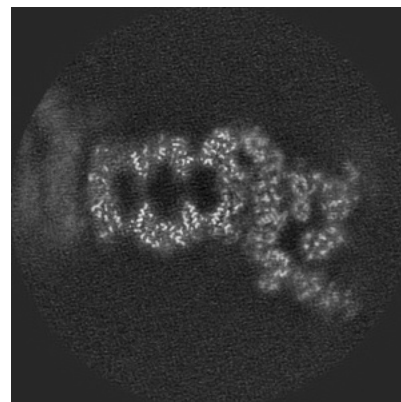
6.2.1 Primary map



X Index: 300

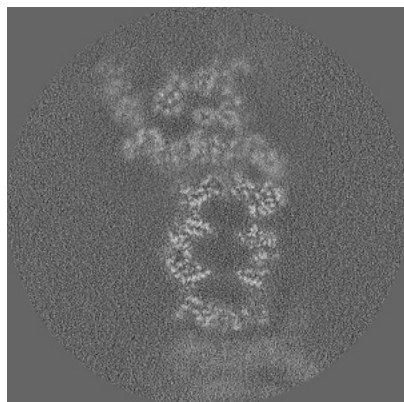


Y Index: 300

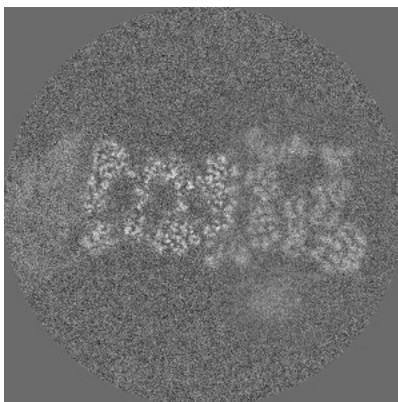


Z Index: 300

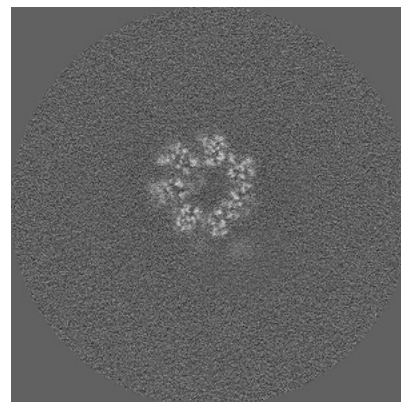
6.2.2 Raw map



X Index: 300



Y Index: 300

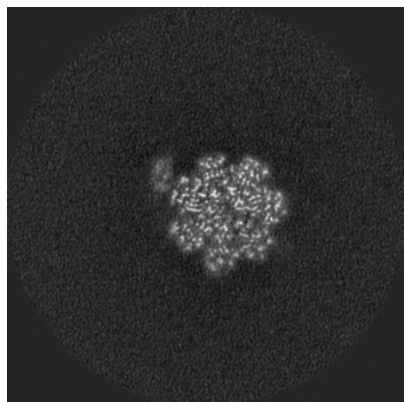


Z Index: 300

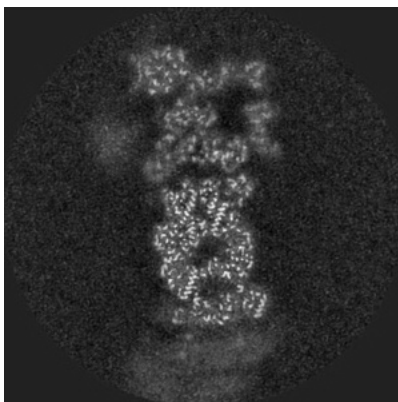
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

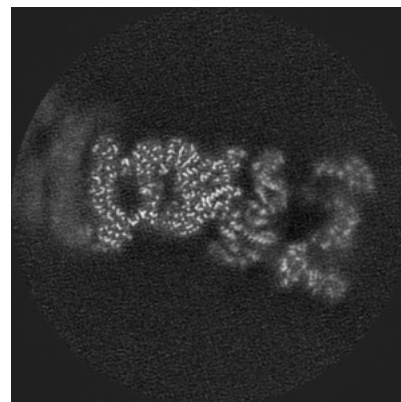
6.3.1 Primary map



X Index: 319

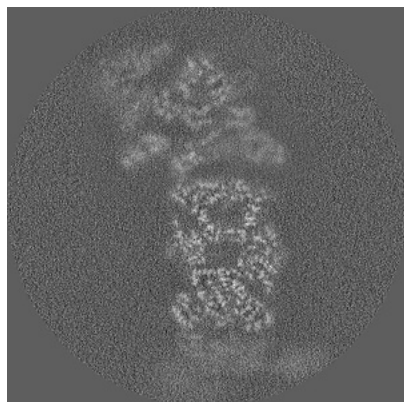


Y Index: 291

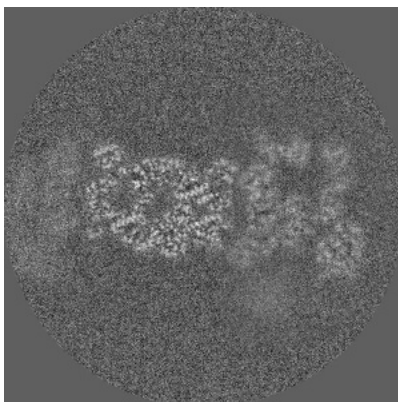


Z Index: 336

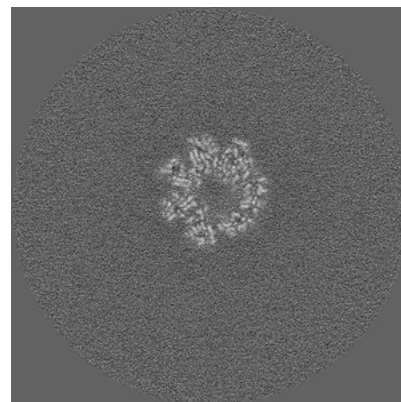
6.3.2 Raw map



X Index: 271



Y Index: 291

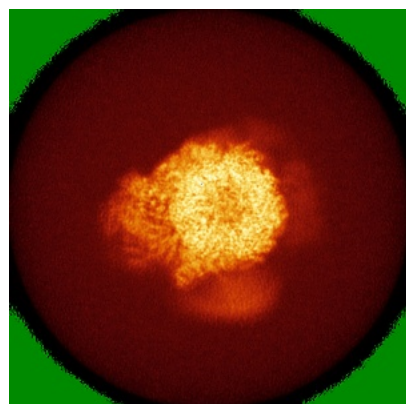


Z Index: 254

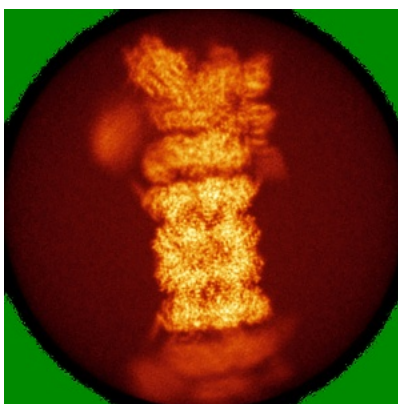
The images above show the largest variance slices of the map in three orthogonal directions.

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

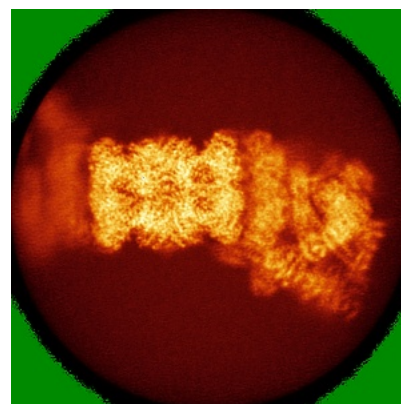
6.4.1 Primary map



X

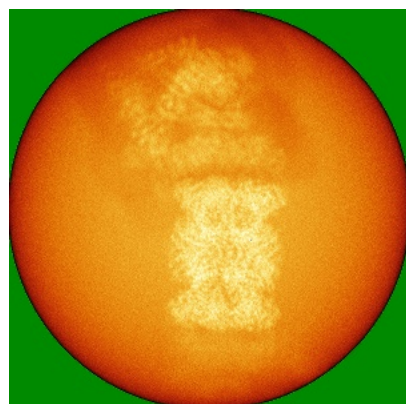


Y

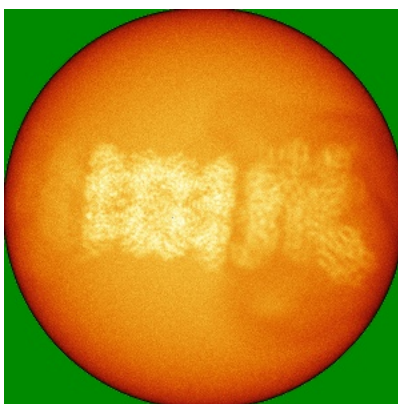


Z

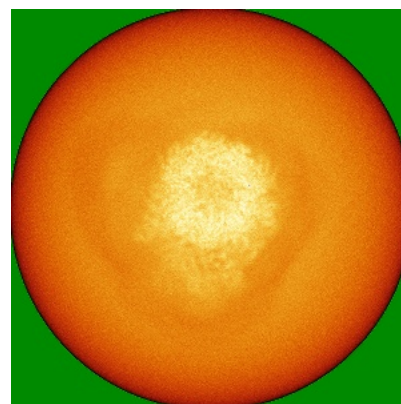
6.4.2 Raw map



X



Y

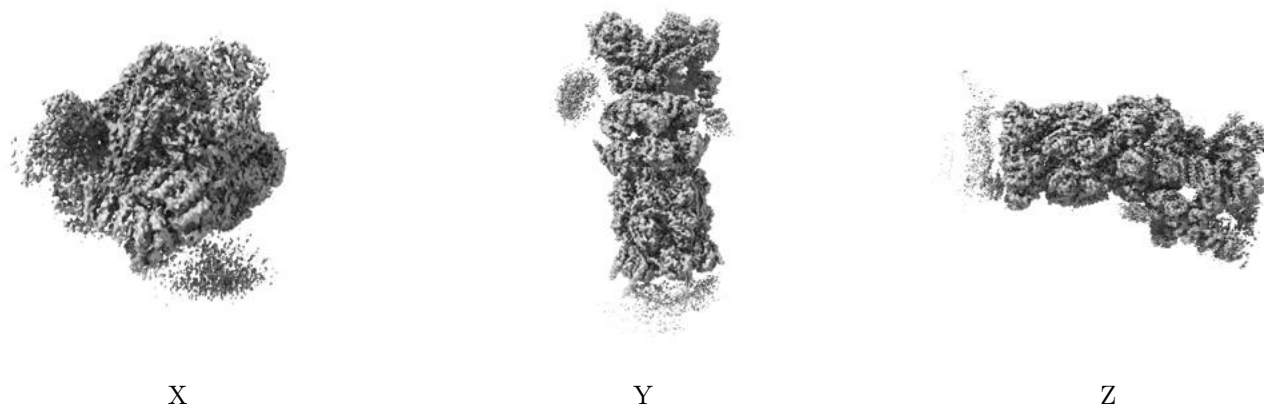


Z

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.

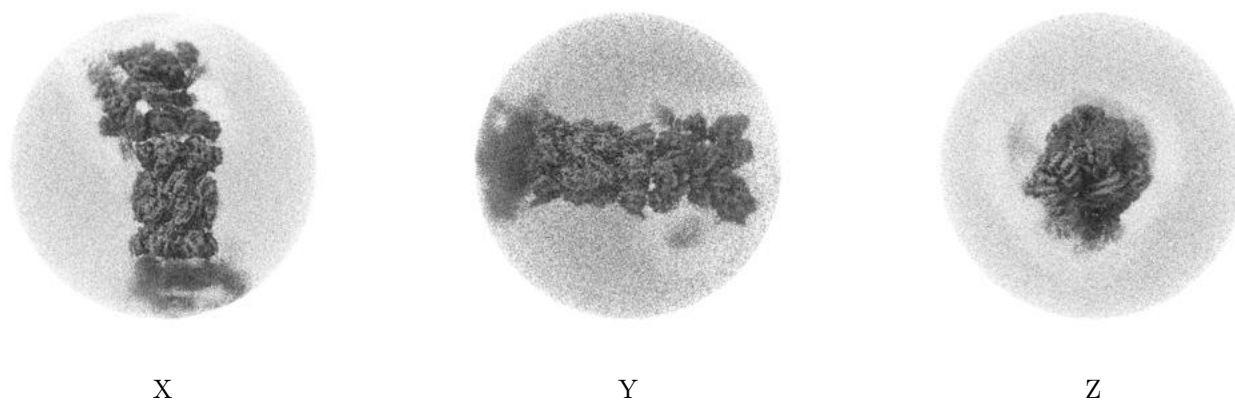
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00556. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

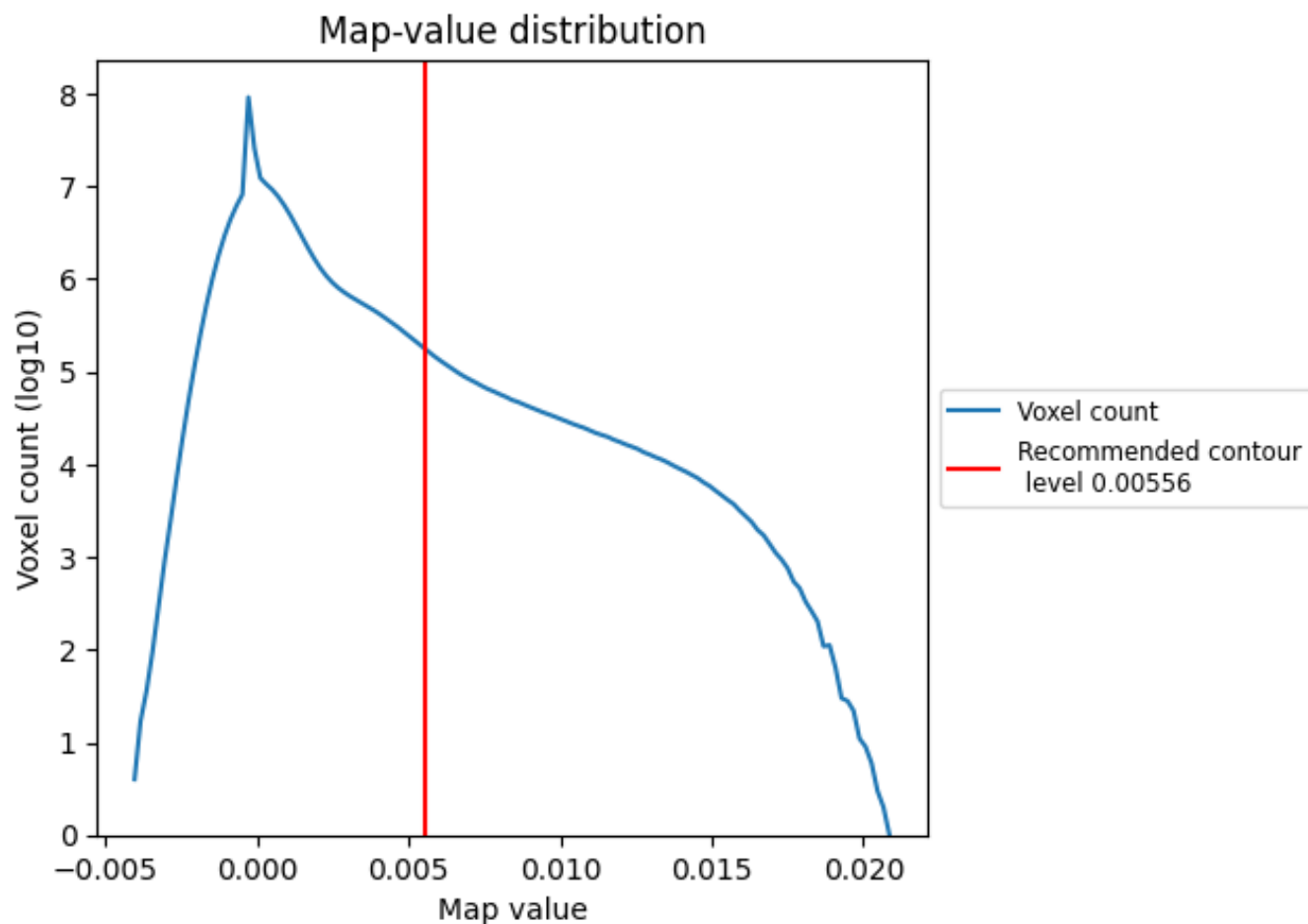
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

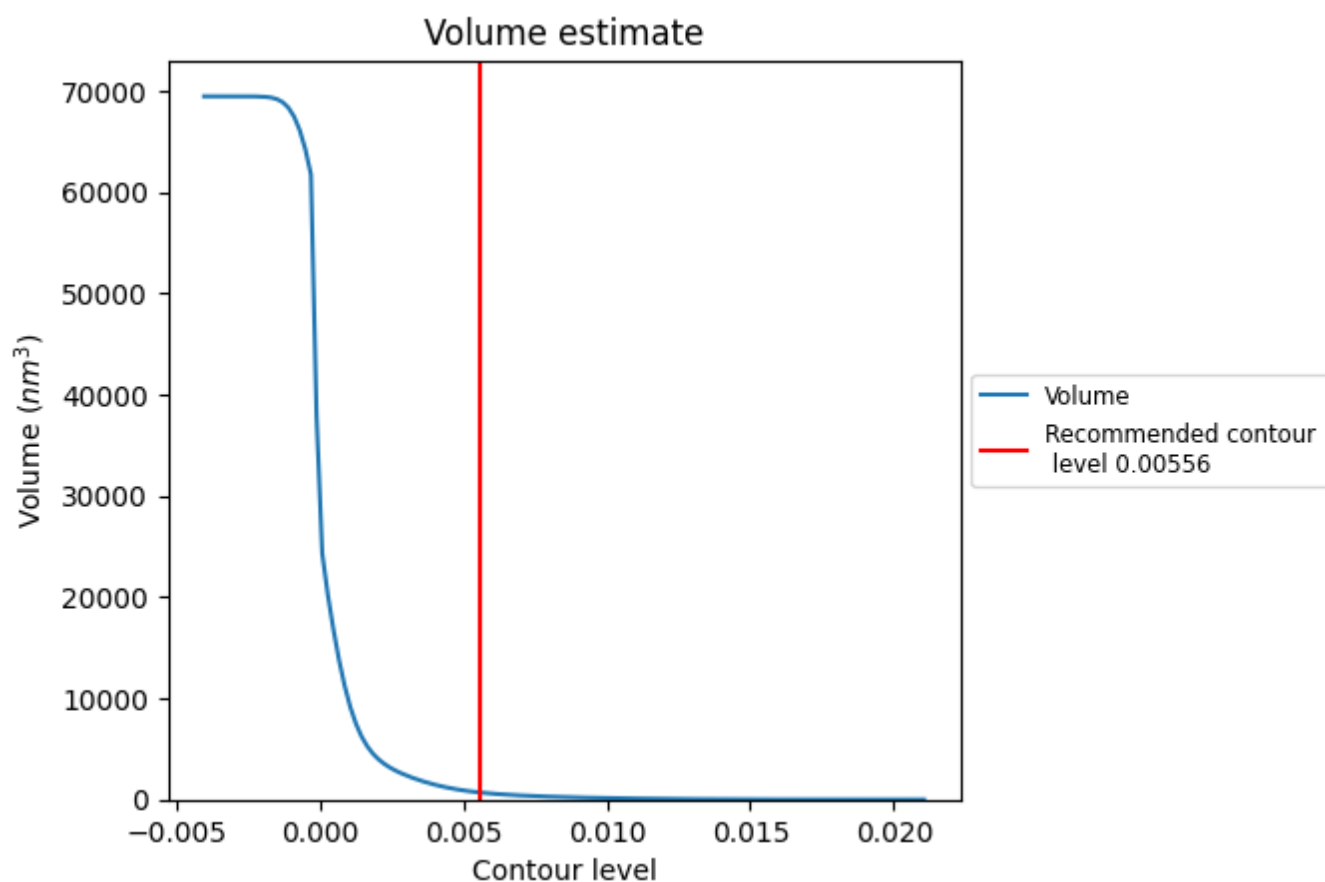
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

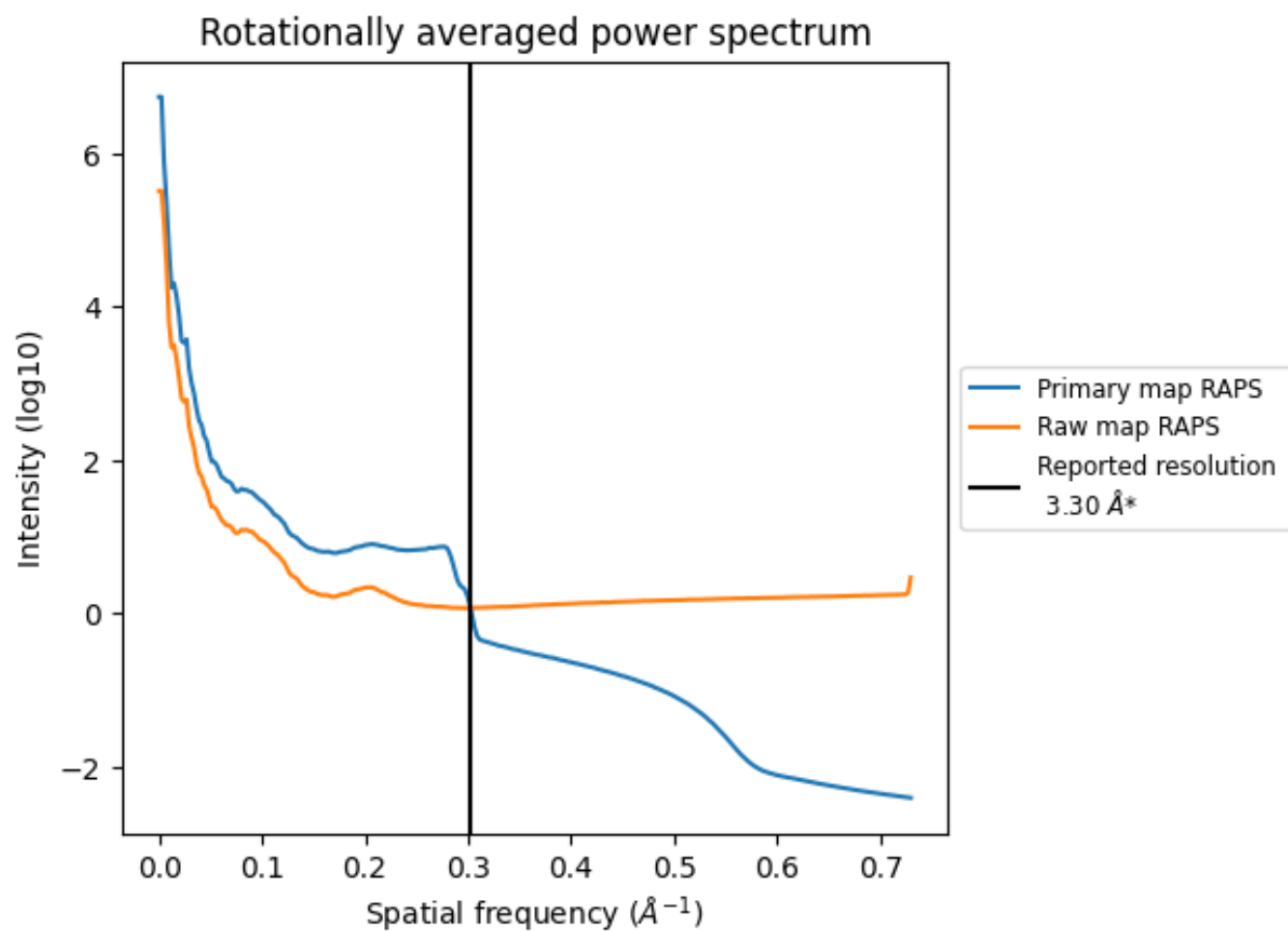
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 699 nm³; this corresponds to an approximate mass of 631 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](#)

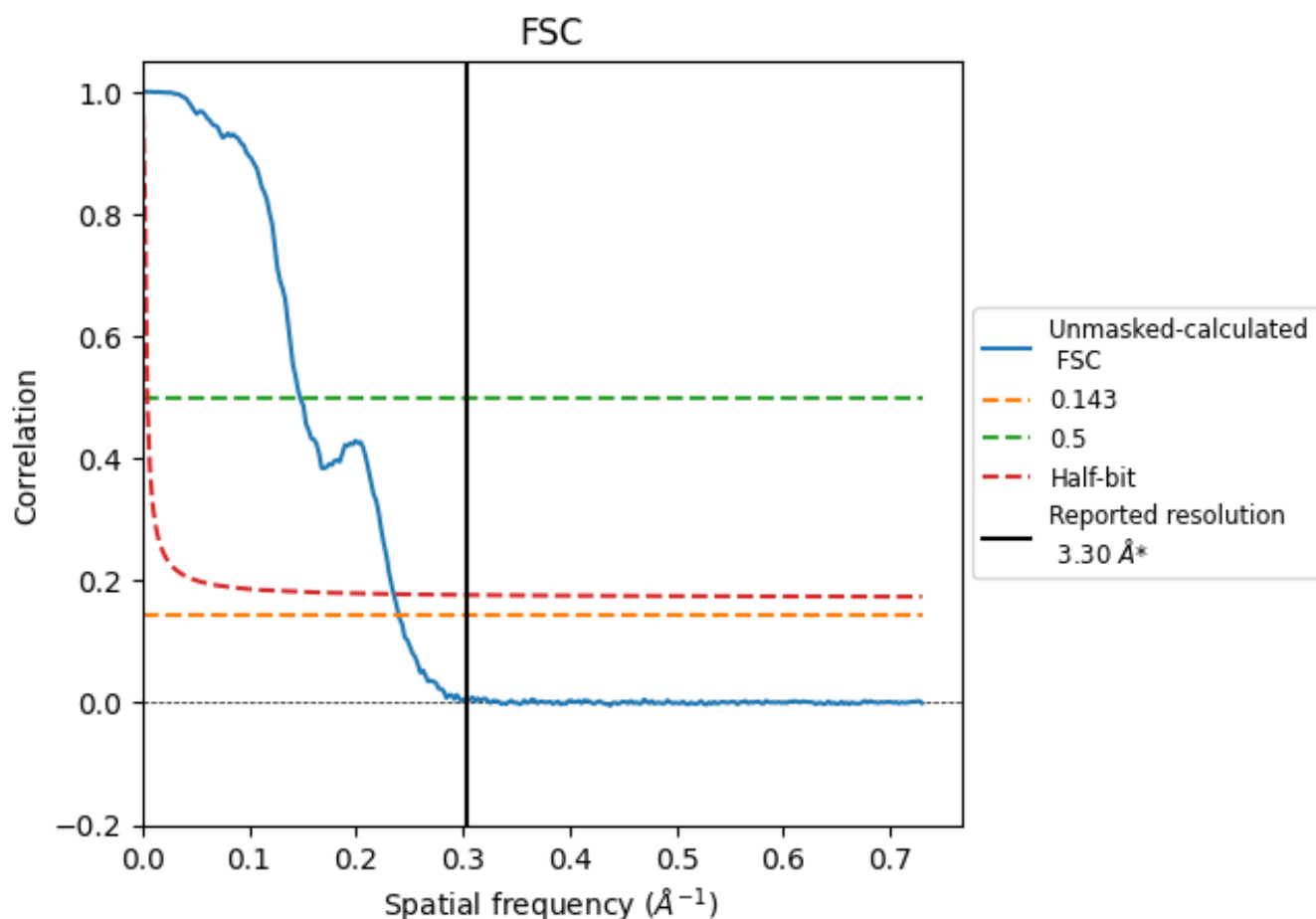


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

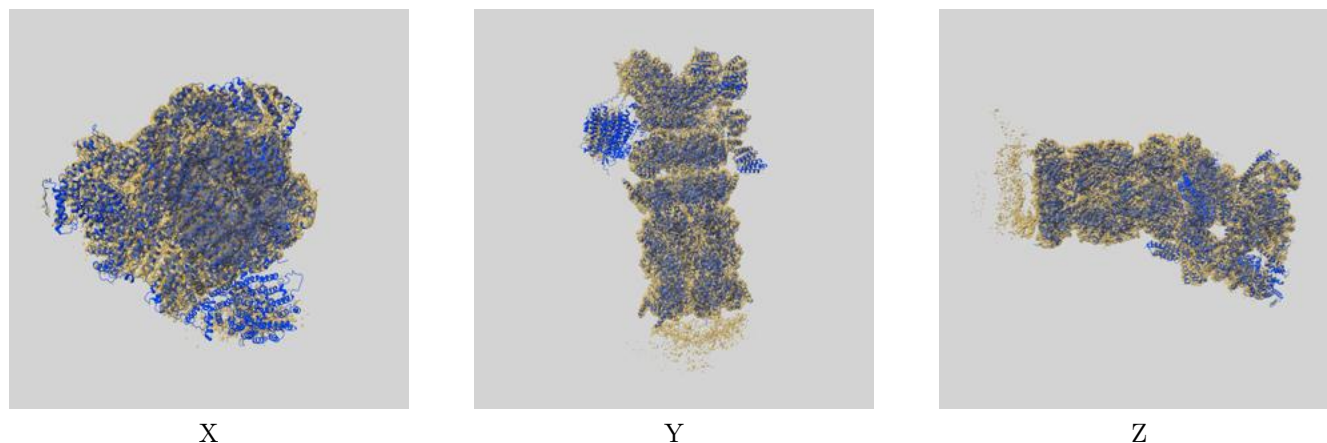
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.16	6.77	4.25

*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 4.16 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

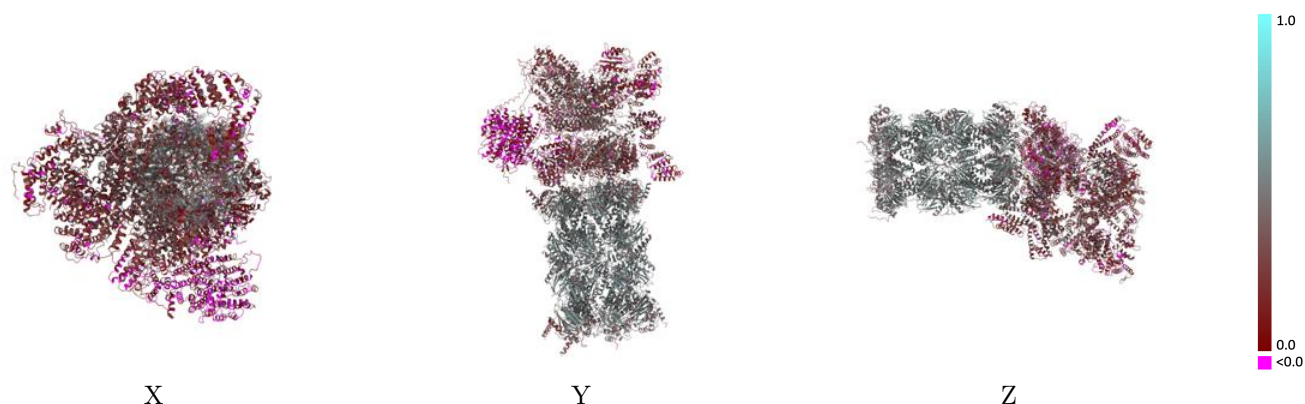
This section contains information regarding the fit between EMDB map EMD-62071 and PDB model 9K4V. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



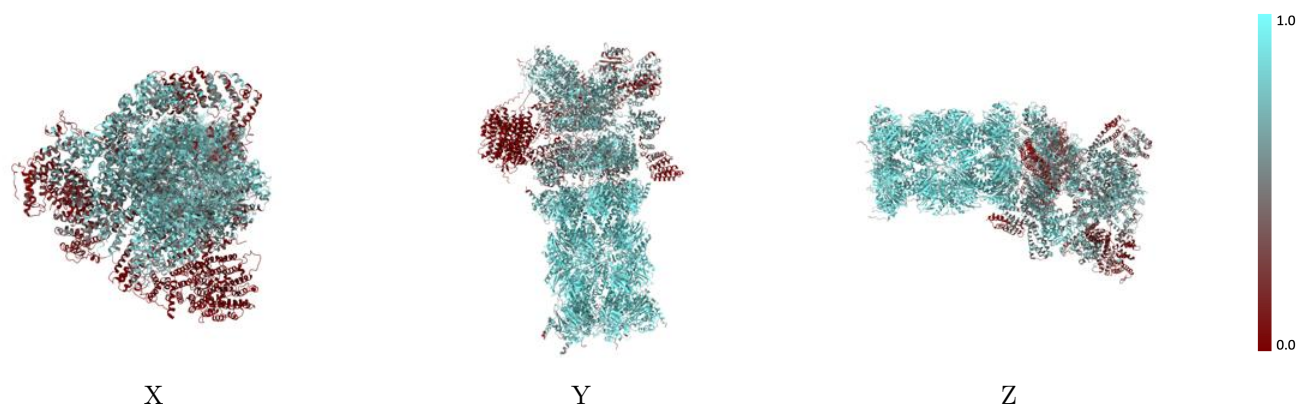
The images above show the 3D surface view of the map at the recommended contour level 0.00556 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



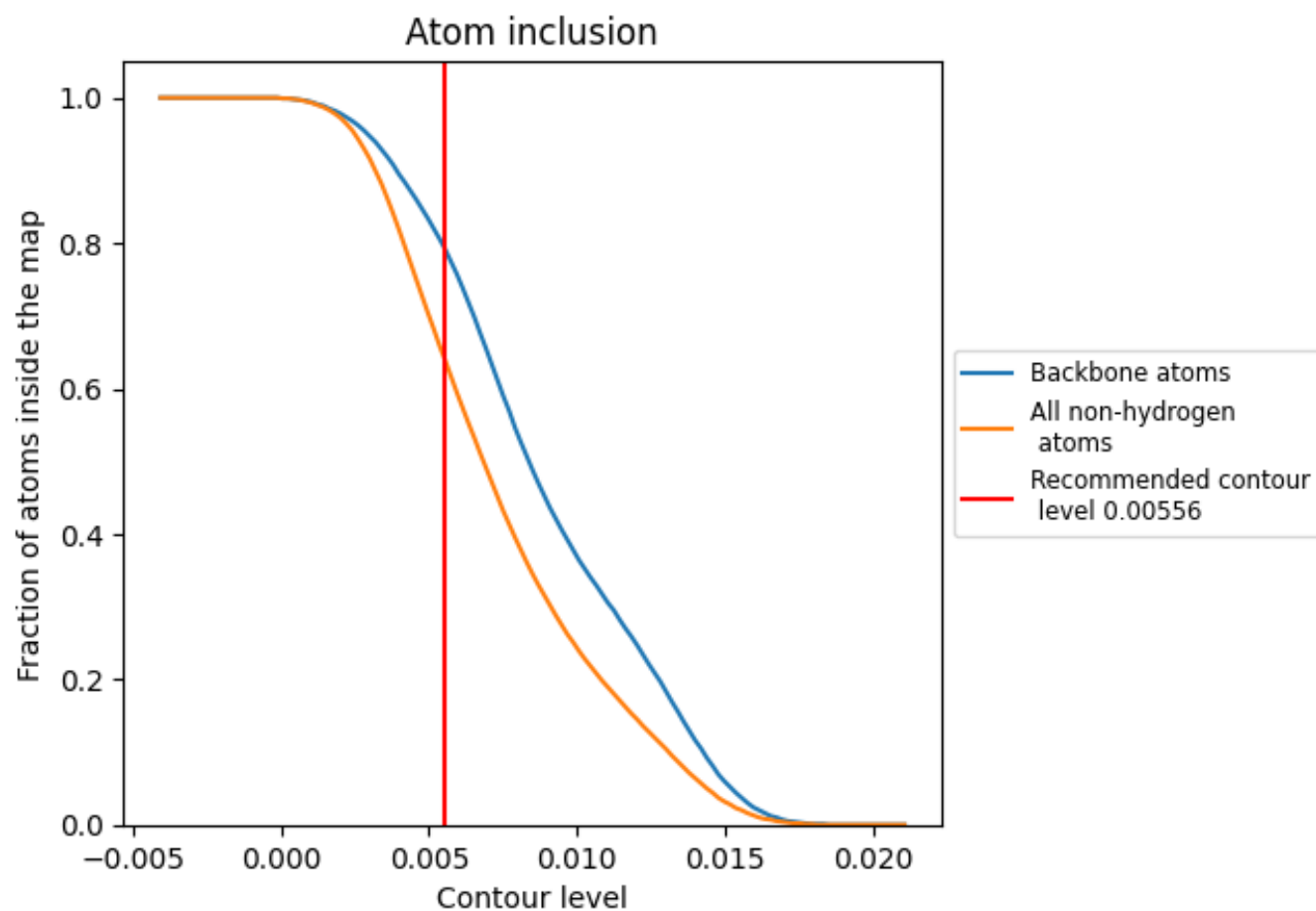
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00556).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 64% 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 (0.00556) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6380	 0.3430
A	 0.4520	 0.1980
B	 0.3400	 0.1770
C	 0.5860	 0.2950
D	 0.6540	 0.3290
E	 0.6260	 0.3070
F	 0.5990	 0.2800
G	 0.8370	 0.4680
H	 0.8500	 0.4830
I	 0.8120	 0.4520
J	 0.7650	 0.4120
K	 0.8040	 0.4560
L	 0.8670	 0.4790
M	 0.8550	 0.4670
N	 0.8880	 0.5050
O	 0.8980	 0.5010
P	 0.8930	 0.5010
Q	 0.8830	 0.5000
R	 0.9010	 0.5050
S	 0.8720	 0.4940
T	 0.8990	 0.5050
U	 0.5510	 0.2590
V	 0.3320	 0.2330
W	 0.4080	 0.1920
X	 0.5290	 0.2760
Y	 0.6920	 0.2710
Z	 0.6070	 0.2770
a	 0.5480	 0.2310
b	 0.3930	 0.1960
c	 0.6170	 0.3060
d	 0.2370	 0.1830
e	 0.4650	 0.2260
f	 0.0310	 0.0540
g	 0.8080	 0.4590
h	 0.8310	 0.4710



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.7790	 0.4460
j	 0.7280	 0.4080
k	 0.7760	 0.4550
l	 0.8530	 0.4800
m	 0.8350	 0.4700
n	 0.8900	 0.5060
o	 0.8830	 0.5000
p	 0.8870	 0.4980
q	 0.8810	 0.4930
r	 0.8980	 0.5010
s	 0.8700	 0.4950
t	 0.8970	 0.5010
v	 0.2000	 0.2440