



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:43 PM UTC

PDB ID : 7W3K / pdb_00007w3k
EMDB ID : EMD-32283
Title : Structure of USP14-bound human 26S proteasome in substrate-inhibited state
SD4_USP14
Authors : Zhang, S.; Zou, S.; Yin, D.; Wu, Z.; Mao, Y.
Deposited on : 2021-11-25
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

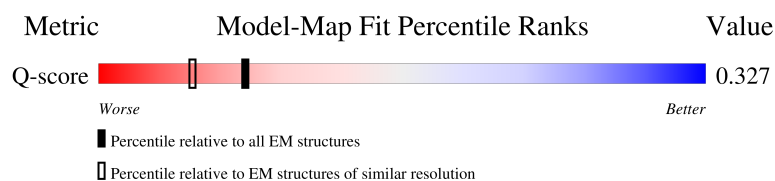
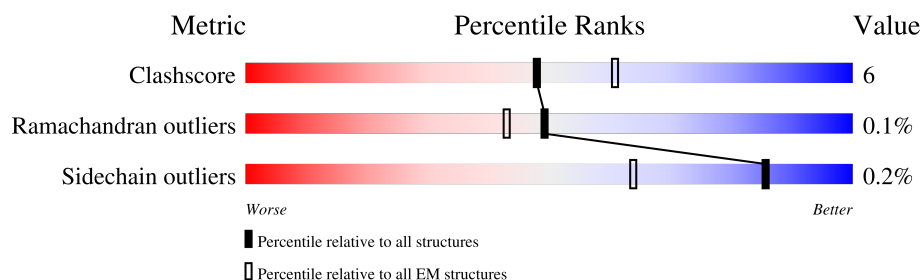
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	 5% 74% 21% 5%
2	B	440	 5% 78% 15% 7%
3	E	403	 5% 77% 19% .
4	F	439	 5% 73% 18% 9%

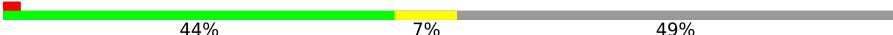
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Mol	Chain	Length	Quality of chain
5	G	246	 88% 10%
5	g	246	 90% 9%
6	H	234	 88% 11%
6	h	234	 87% 12%
7	I	261	 89% 6% 5%
7	i	261	 86% 10%
8	J	248	 84% 12%
8	j	248	 81% 15%
9	K	241	 83% 16%
9	k	241	 85% 12%
10	L	269	 76% 13% 11%
10	l	269	 79% 9% 12%
11	M	255	 87% 8% 5%
11	m	255	 85% 9% 6%
12	N	239	 80% 5% 15%
12	n	239	 80% 5% 15%
13	O	277	 71% 8% 21%
13	o	277	 71% 8% 21%
14	P	205	 91% 9%
14	p	205	 90% 9%
15	Q	201	 92% 7%
15	q	201	 90% 9%
16	R	263	 67% 10% 24%
16	r	263	 68% 8% 24%
17	S	241	 76% 12% 12%

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Mol	Chain	Length	Quality of chain
17	s	241	
18	T	264	
18	t	264	
19	x	494	
20	y	76	
21	C	398	
22	D	418	
23	U	953	
24	W	456	
25	X	422	
26	Y	389	
27	Z	324	
28	a	376	
29	b	377	
30	c	310	
31	d	350	
32	f	908	
33	V	534	
34	e	70	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 110657 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

- Molecule 3 is a protein called 26S proteasome regulatory subunit 10B.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	400	Total	C	N	O	S	0	0
			3133	1972	540	603	18		

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 6 is a protein called Proteasome subunit alpha type-2.

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

- Molecule 7 is a protein called Proteasome subunit alpha type-4.

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

- Molecule 8 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 9 is a protein called Proteasome subunit alpha type-5.

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

- Molecule 10 is a protein called Isoform Long of Proteasome subunit alpha type-1.

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

- Molecule 11 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	242	Total	C	N	O	S	0	0
			1890	1200	323	356	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

- Molecule 12 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	203	Total	C	N	O	S	0	0
			1521	954	259	296	12		
12	n	202	Total	C	N	O	S	0	0
			1510	947	258	293	12		

- Molecule 13 is a protein called Proteasome subunit beta type-7.

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

- Molecule 14 is a protein called Proteasome subunit beta type-3.

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

- Molecule 15 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	199	Total	C	N	O	S	0	0
			1588	1017	270	292	9		
15	q	199	Total	C	N	O	S	0	0
			1578	1012	267	290	9		

- Molecule 16 is a protein called Proteasome subunit beta type-5.

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

- Molecule 17 is a protein called Proteasome subunit beta type-1.

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

- Molecule 18 is a protein called Proteasome subunit beta type-4.

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

- Molecule 19 is a protein called Ubiquitin carboxyl-terminal hydrolase 14.

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

- Molecule 20 is a protein called Ubiquitin.

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

- Molecule 21 is a protein called Isoform 2 of 26S proteasome regulatory subunit 8.

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

- Molecule 22 is a protein called 26S protease regulatory subunit 6B.

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

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

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

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

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

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

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

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

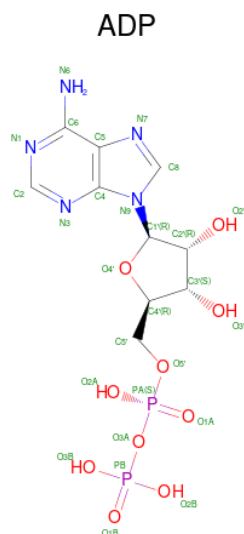
- Molecule 33 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

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

- Molecule 34 is a protein called 26S proteasome complex subunit DSS1.

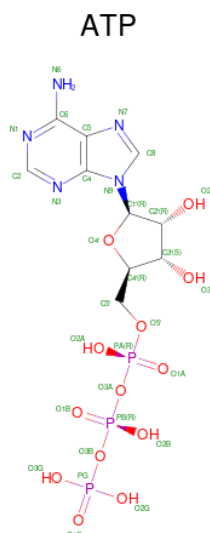
Mol	Chain	Residues	Atoms				AltConf	Trace
34	e	50	Total	C	N	O	0	0
			425	260	65	100		

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total 27	C 10	N 5	O 10	P 2	0
35	B	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



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

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

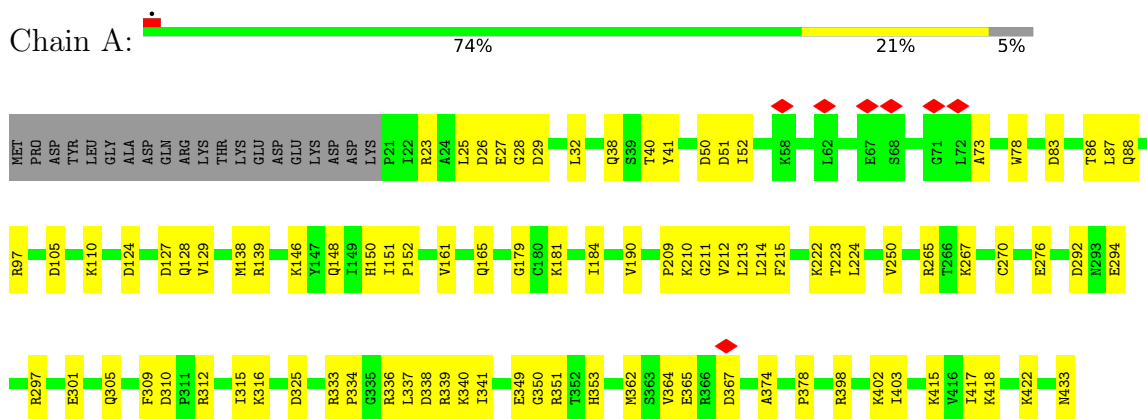
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

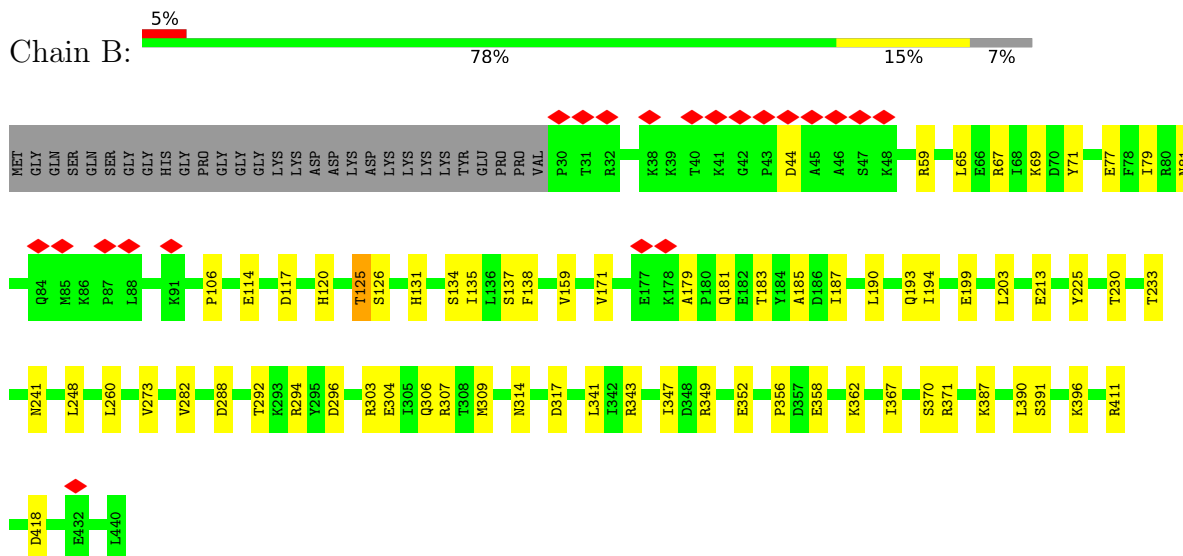
3 Residue-property plots

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.

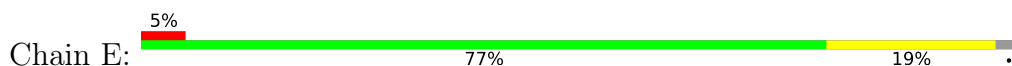
- Molecule 1: 26S protease regulatory subunit 7

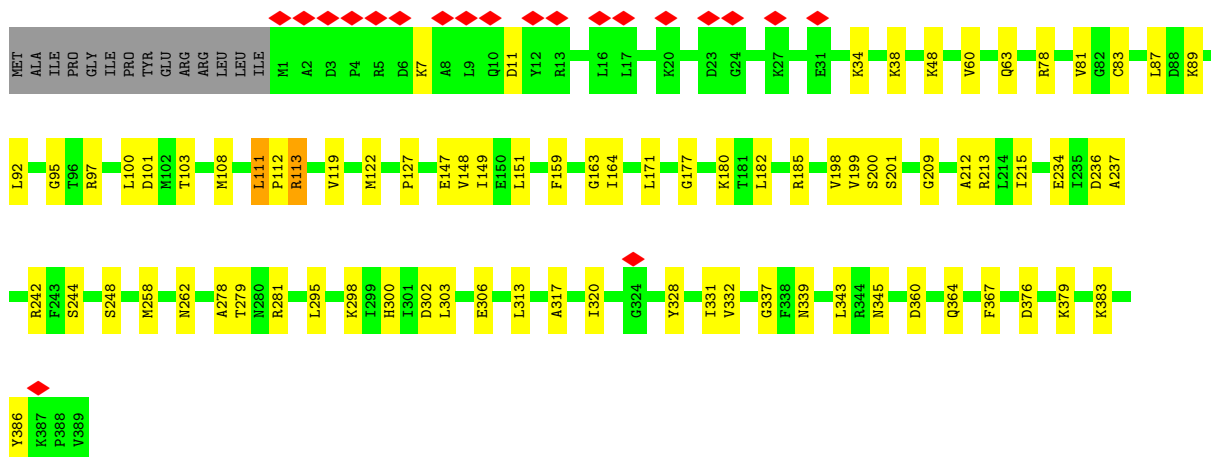


- Molecule 2: 26S protease regulatory subunit 4



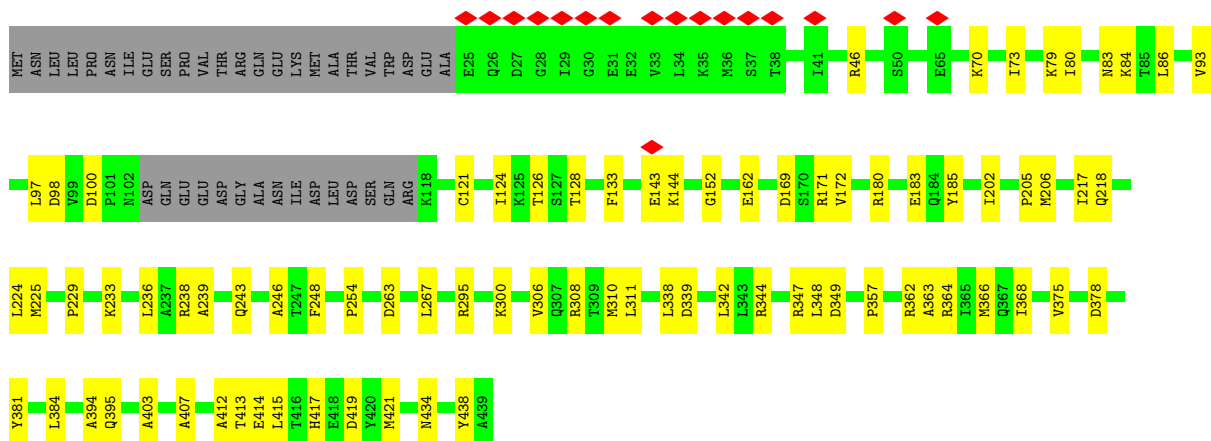
- Molecule 3: 26S proteasome regulatory subunit 10B





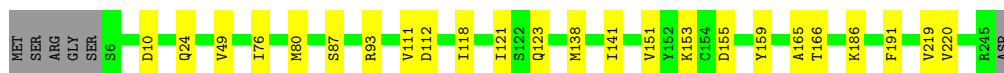
- Molecule 4: 26S protease regulatory subunit 6A

Chain F: 73% 18% 9%



- Molecule 5: Proteasome subunit alpha type-6

Chain G: 88% 10% 2%



- Molecule 5: Proteasome subunit alpha type-6

Chain g: 90% 9% 1%



- Molecule 6: Proteasome subunit alpha type-2

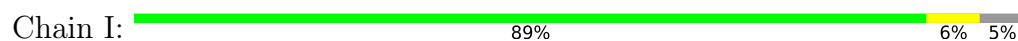
Chain H: 88% 11% 1%



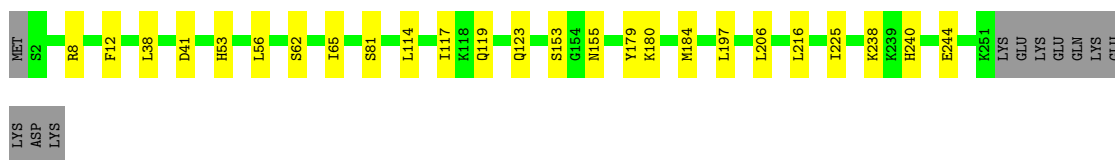
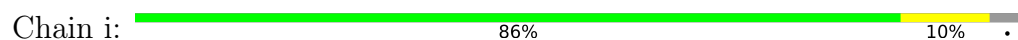
- Molecule 6: Proteasome subunit alpha type-2



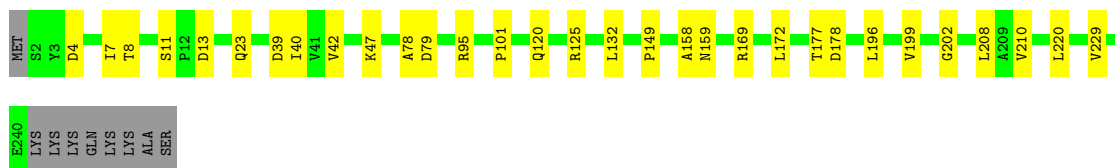
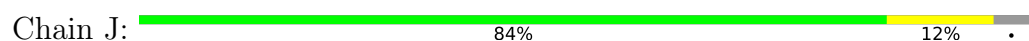
- Molecule 7: Proteasome subunit alpha type-4



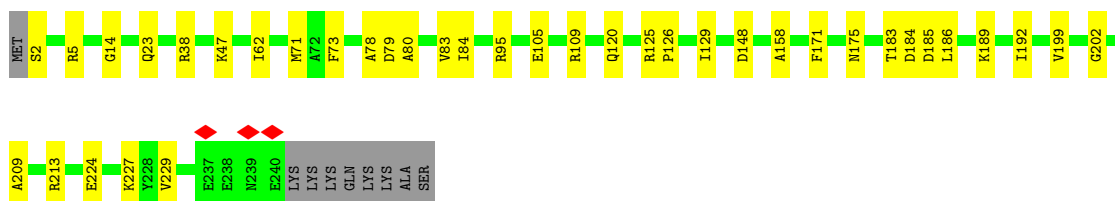
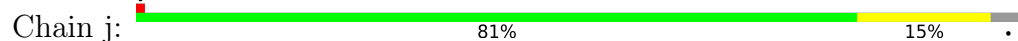
- Molecule 7: Proteasome subunit alpha type-4



- Molecule 8: Proteasome subunit alpha type-7

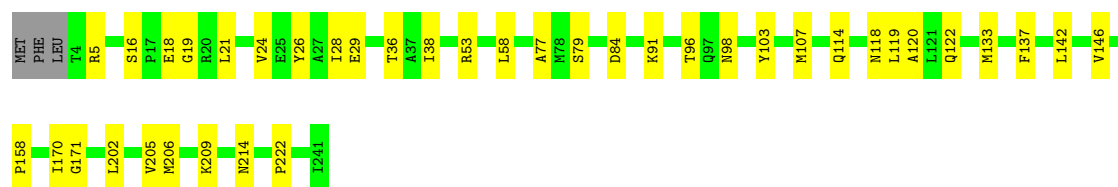


- Molecule 8: Proteasome subunit alpha type-7



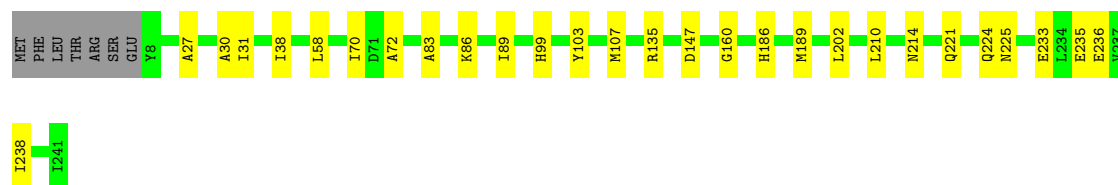
- Molecule 9: Proteasome subunit alpha type-5

Chain K: 



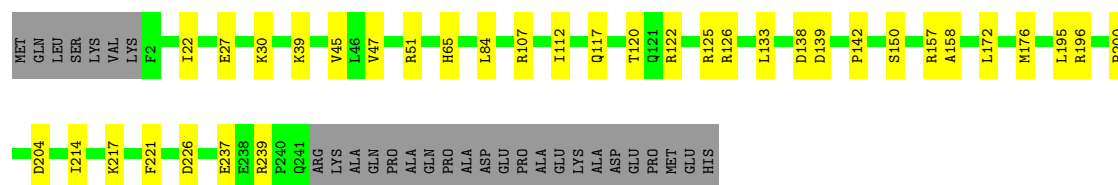
• Molecule 9: Proteasome subunit alpha type-5

Chain k: 



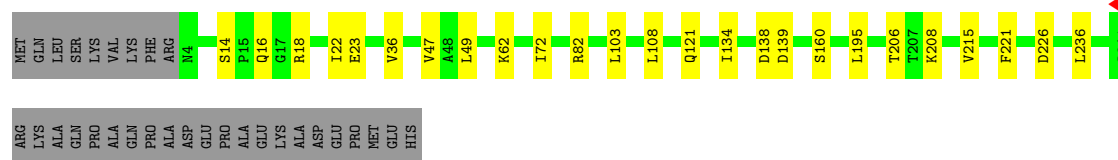
• Molecule 10: Isoform Long of Proteasome subunit alpha type-1

Chain L: 



• Molecule 10: Isoform Long of Proteasome subunit alpha type-1

Chain l: 



• Molecule 11: Proteasome subunit alpha type-3

Chain M: 

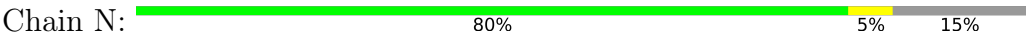


• Molecule 11: Proteasome subunit alpha type-3

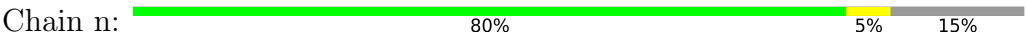
Chain m: 



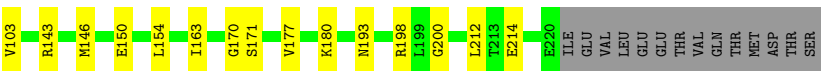
• Molecule 12: Proteasome subunit beta type-6



• Molecule 12: Proteasome subunit beta type-6



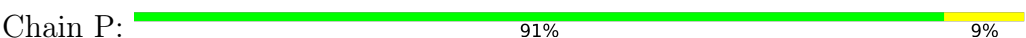
• Molecule 13: Proteasome subunit beta type-7



• Molecule 13: Proteasome subunit beta type-7



• Molecule 14: Proteasome subunit beta type-3



• Molecule 14: Proteasome subunit beta type-3

Chain p:  90% 9%



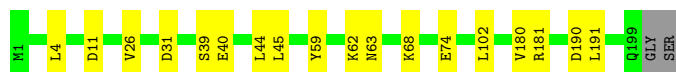
- Molecule 15: Proteasome subunit beta type-2

Chain Q:  92% 7%



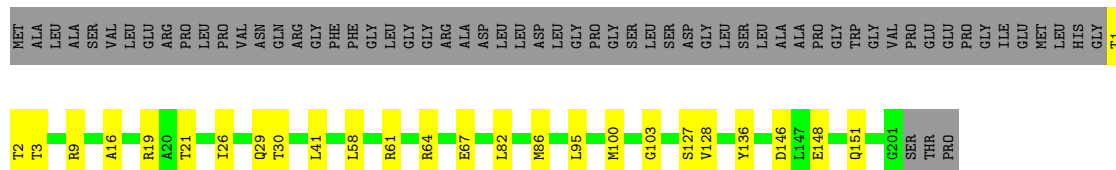
- Molecule 15: Proteasome subunit beta type-2

Chain q:  90% 9%



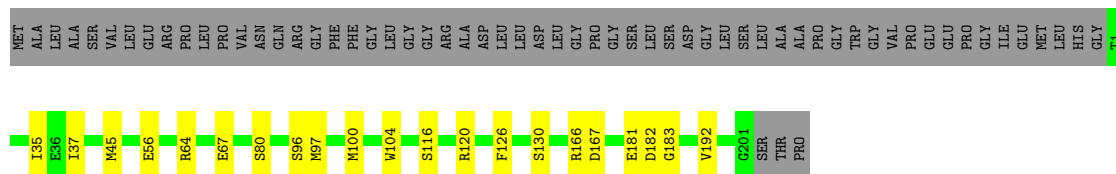
- Molecule 16: Proteasome subunit beta type-5

Chain R:  67% 10% 24%



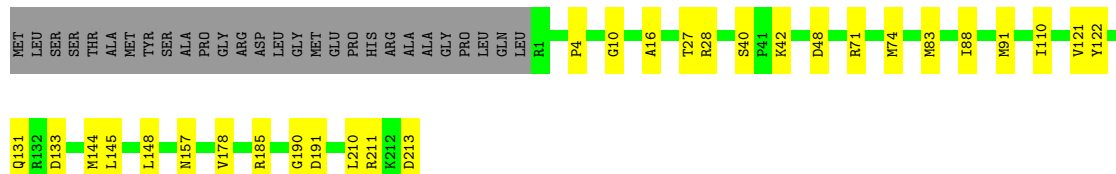
- Molecule 16: Proteasome subunit beta type-5

Chain r:  68% 8% 24%



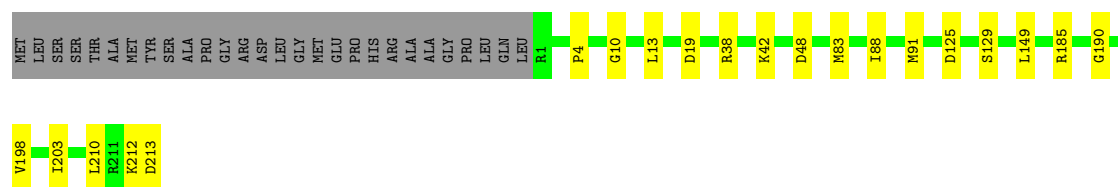
- Molecule 17: Proteasome subunit beta type-1

Chain S:  76% 12% 12%



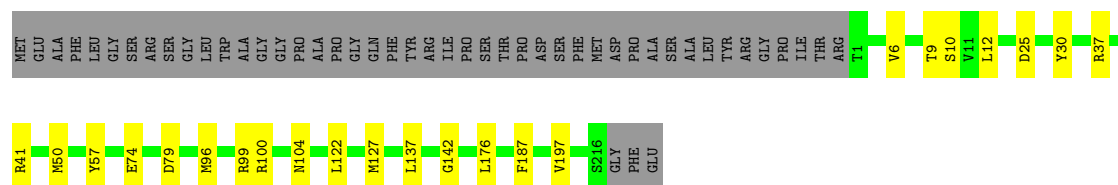
- Molecule 17: Proteasome subunit beta type-1

Chain s:  80% 8% 12%



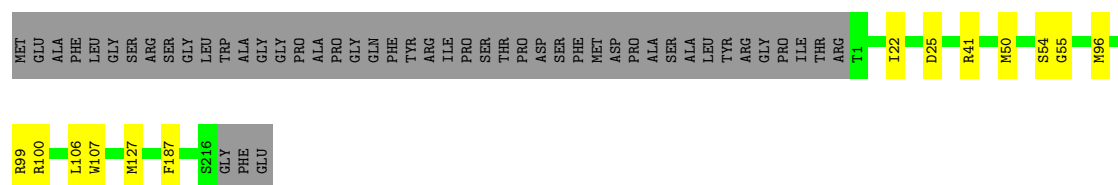
- Molecule 18: Proteasome subunit beta type-4

Chain T:  73% 9% 18%



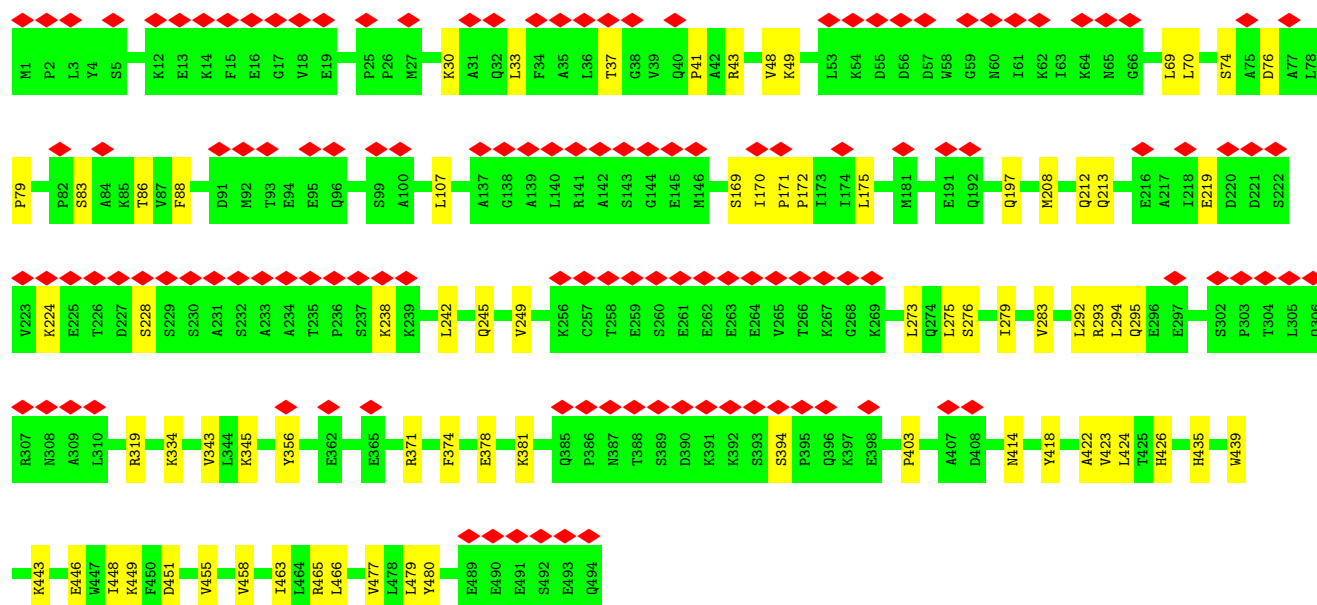
- Molecule 18: Proteasome subunit beta type-4

Chain t:  77% 5% 18%

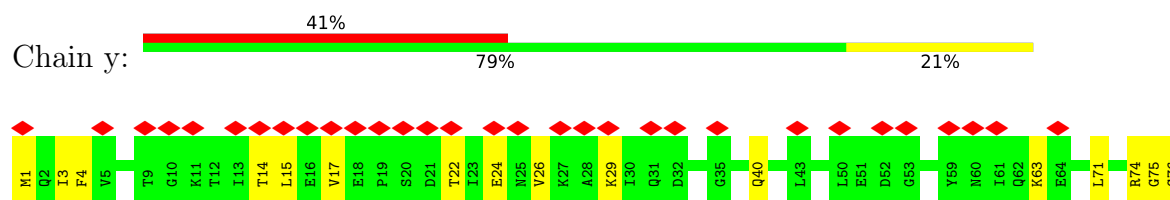


- Molecule 19: Ubiquitin carboxyl-terminal hydrolase 14

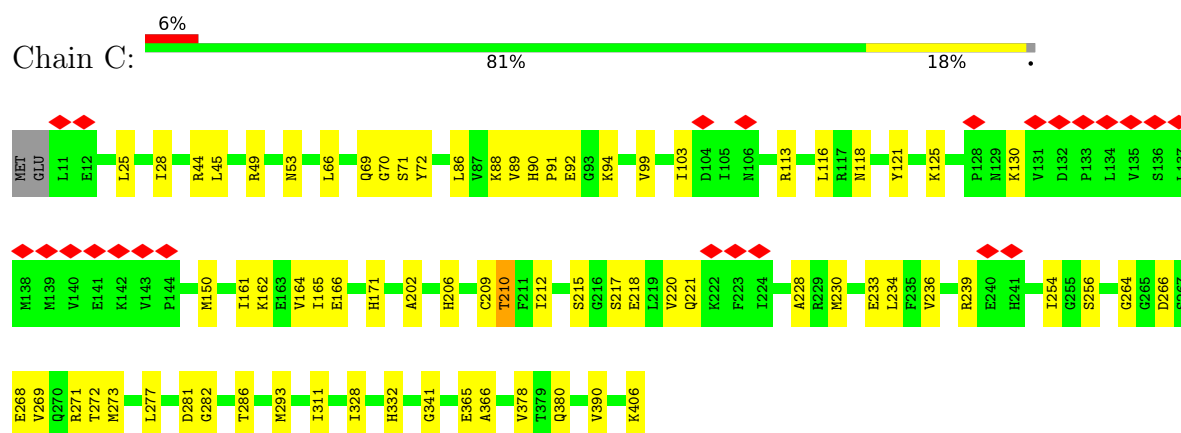
Chain x:  27% 85% 15%



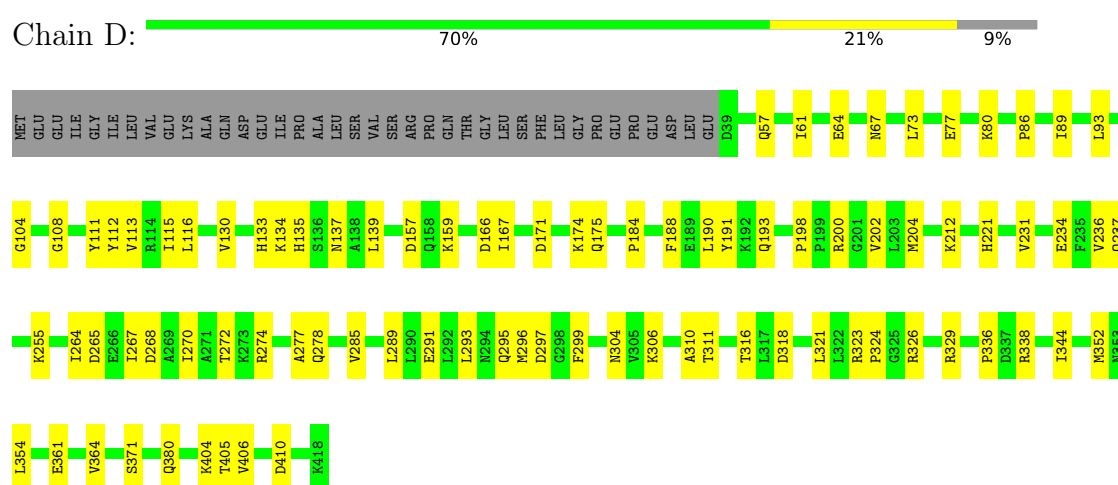
- Molecule 20: Ubiquitin



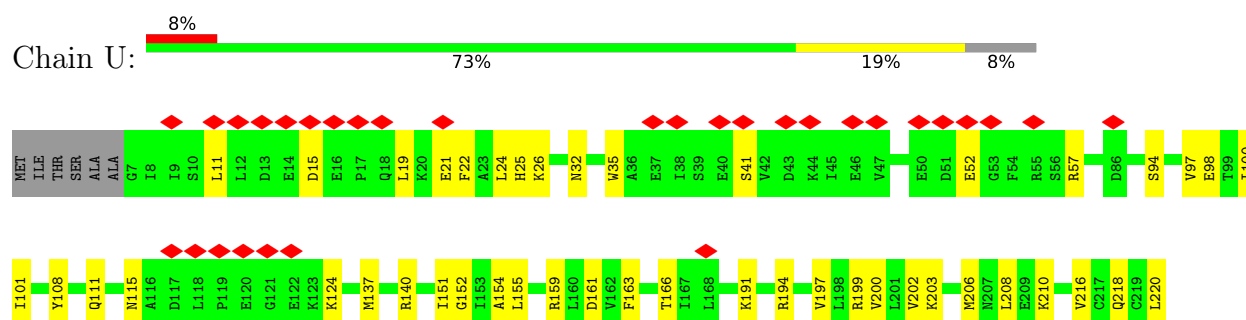
- Molecule 21: Isoform 2 of 26S proteasome regulatory subunit 8

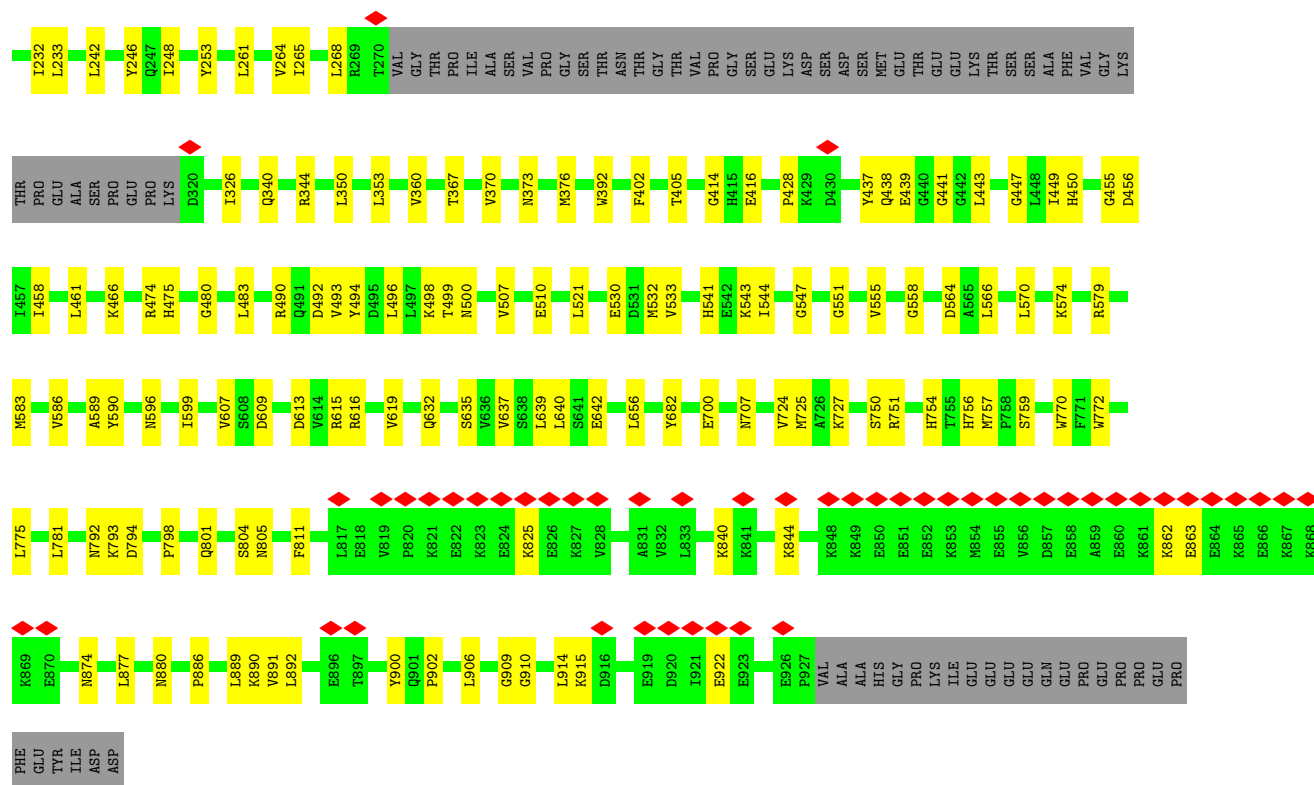


- Molecule 22: 26S protease regulatory subunit 6B

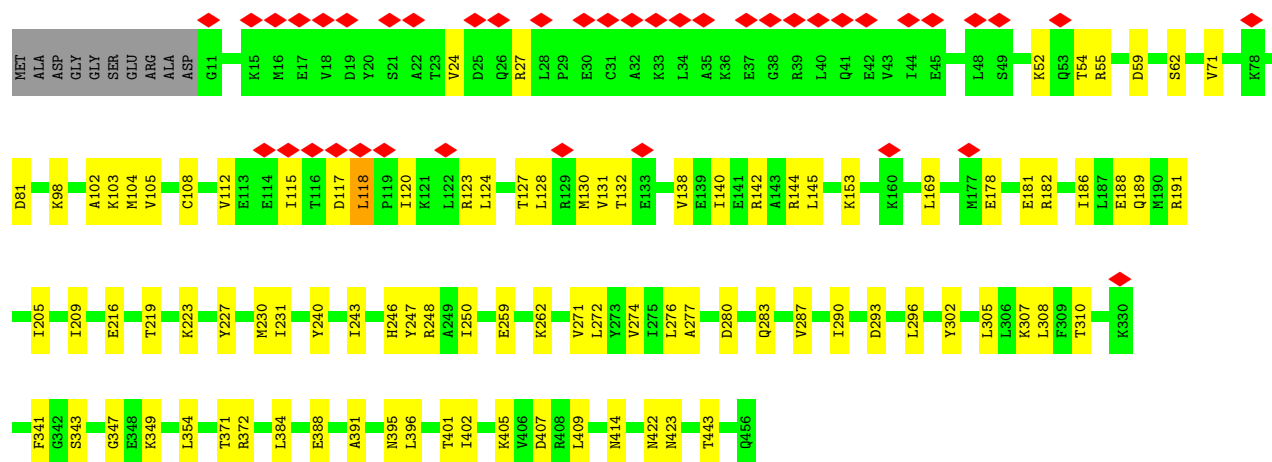
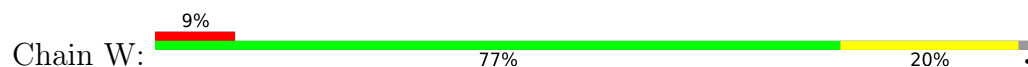


- Molecule 23: 26S proteasome non-ATPase regulatory subunit 1

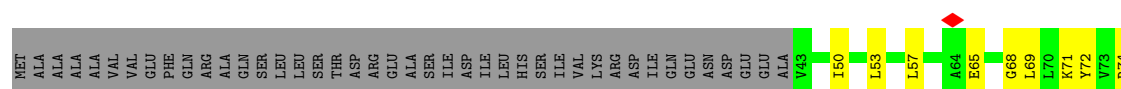
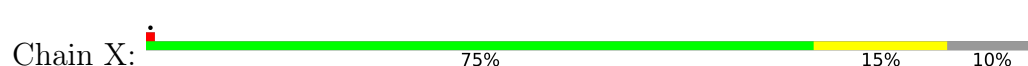


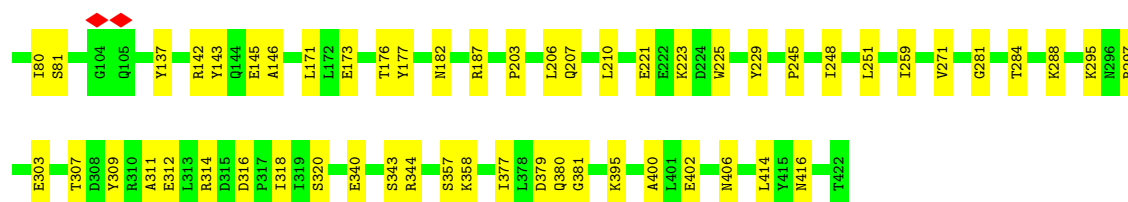


- Molecule 24: 26S proteasome non-ATPase regulatory subunit 12

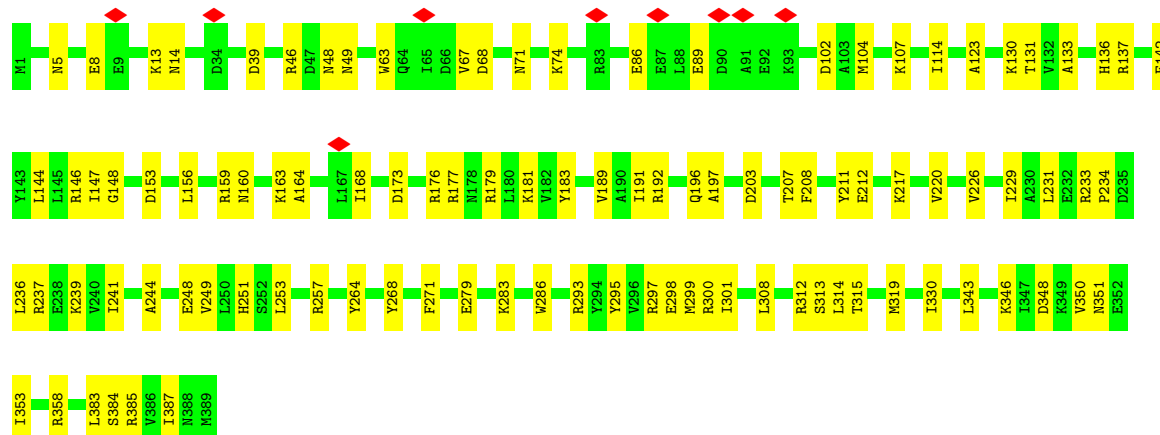


- Molecule 25: 26S proteasome non-ATPase regulatory subunit 11

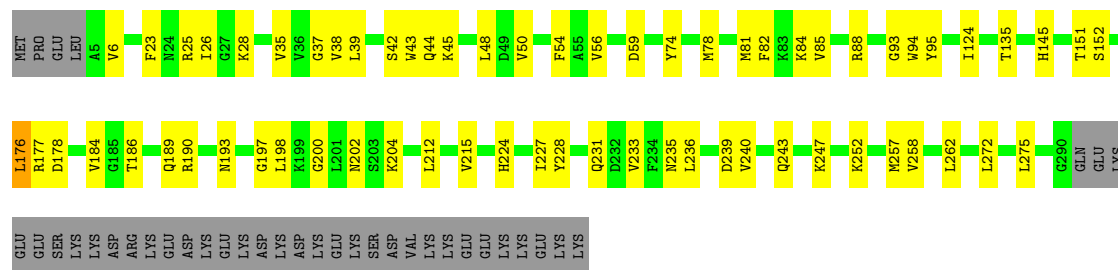




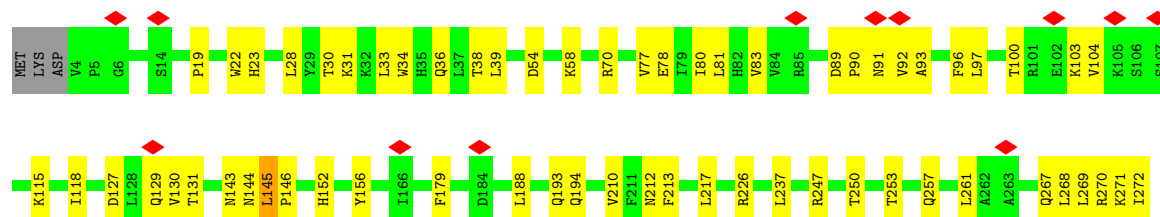
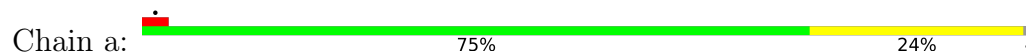
• Molecule 26: 26S proteasome non-ATPase regulatory subunit 6

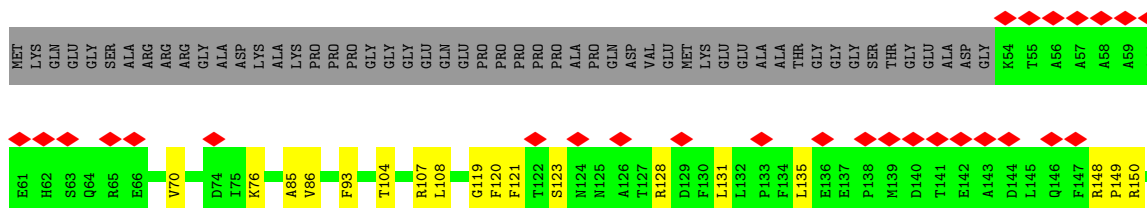
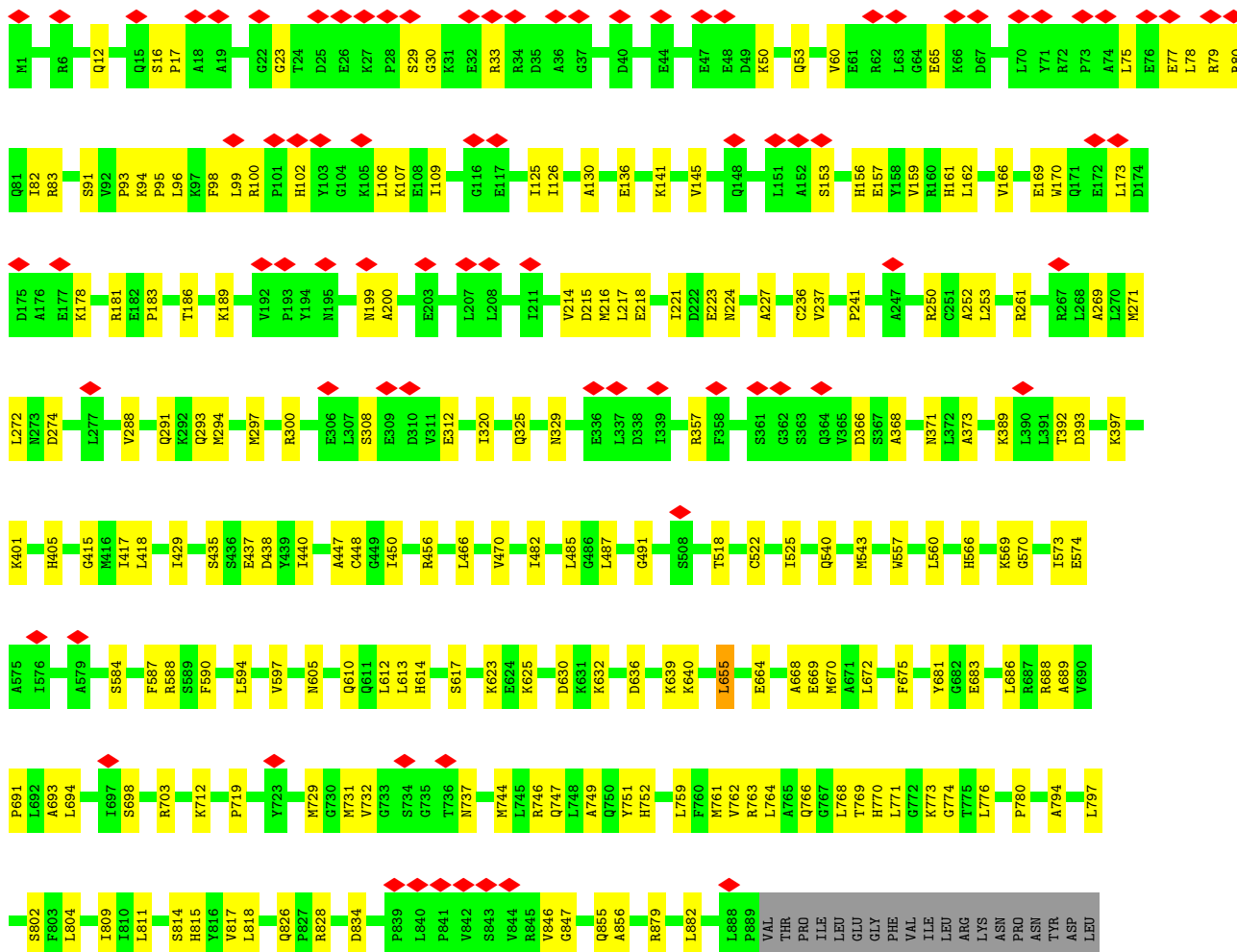


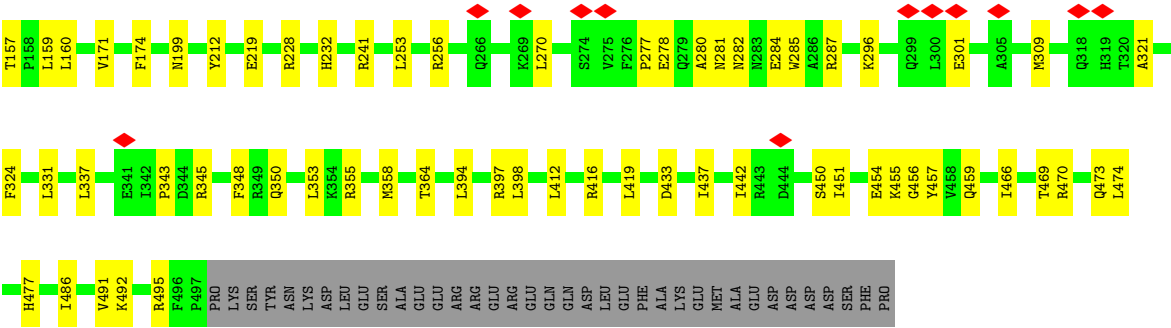
• Molecule 27: 26S proteasome non-ATPase regulatory subunit 7



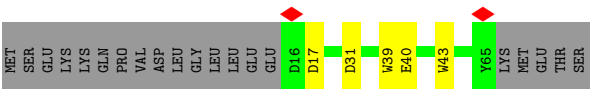
• Molecule 28: 26S proteasome non-ATPase regulatory subunit 13







● Molecule 34: 26S proteasome complex subunit DSS1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74792	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.019	Depositor
Minimum map value	-0.004	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	438.4, 438.4, 438.4	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/3283	0.51	0/4433
2	B	0.18	0/3254	0.49	0/4388
3	E	0.21	0/3145	0.50	1/4233 (0.0%)
4	F	0.16	0/3173	0.45	0/4273
5	G	0.17	0/1901	0.42	0/2572
5	g	0.17	0/1913	0.42	0/2589
6	H	0.19	0/1840	0.42	0/2495
6	h	0.17	0/1844	0.41	0/2497
7	I	0.18	0/1963	0.41	0/2650
7	i	0.18	0/1985	0.42	0/2677
8	J	0.17	0/1887	0.43	0/2553
8	j	0.18	0/1887	0.42	0/2549
9	K	0.19	0/1841	0.39	0/2486
9	k	0.16	0/1809	0.38	0/2444
10	L	0.18	0/1911	0.37	0/2584
10	l	0.19	0/1896	0.37	0/2565
11	M	0.18	0/1925	0.40	0/2592
11	m	0.17	0/1916	0.38	0/2580
12	N	0.16	0/1548	0.31	0/2097
12	n	0.17	0/1536	0.33	0/2080
13	O	0.16	0/1672	0.40	0/2267
13	o	0.17	0/1686	0.40	0/2282
14	P	0.19	0/1616	0.43	0/2180
14	p	0.18	0/1620	0.43	0/2184
15	Q	0.18	0/1621	0.37	0/2194
15	q	0.18	0/1611	0.35	0/2182
16	R	0.17	0/1590	0.35	0/2147
16	r	0.17	0/1580	0.38	0/2135
17	S	0.18	0/1671	0.42	0/2252
17	s	0.19	0/1680	0.42	0/2264
18	T	0.18	0/1716	0.39	0/2323
18	t	0.18	0/1720	0.39	0/2328

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	x	0.13	0/4002	0.35	0/5390
20	y	0.17	0/607	0.43	0/816
21	C	0.18	0/3146	0.48	0/4226
22	D	0.17	0/3089	0.50	0/4168
23	U	0.18	0/6945	0.48	0/9382
24	W	0.20	0/3683	0.52	2/4952 (0.0%)
25	X	0.17	0/3053	0.46	0/4115
26	Y	0.19	0/3261	0.55	0/4393
27	Z	0.20	0/2324	0.54	1/3150 (0.0%)
28	a	0.19	0/3053	0.53	0/4133
29	b	0.21	0/1478	0.49	0/2001
30	c	0.21	0/2302	0.57	0/3110
31	d	0.22	0/2162	0.56	0/2919
32	f	0.20	0/6980	0.53	0/9433
33	V	0.16	0/3681	0.42	0/4969
34	e	0.19	0/437	0.46	0/595
All	All	0.18	0/112443	0.45	4/151827 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	113	ARG	N-CA-C	8.08	118.63	108.45
24	W	310	THR	CA-C-N	5.17	129.67	122.08
24	W	310	THR	C-N-CA	5.17	129.67	122.08
27	Z	240	VAL	N-CA-C	-5.16	106.41	111.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3229	0	3261	68	0
2	B	3207	0	3278	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	3097	0	3174	50	0
4	F	3133	0	3220	62	0
5	G	1867	0	1867	17	0
5	g	1879	0	1872	15	0
6	H	1801	0	1773	18	0
6	h	1805	0	1798	19	0
7	I	1933	0	1923	12	0
7	i	1955	0	1955	17	0
8	J	1861	0	1846	22	0
8	j	1861	0	1865	26	0
9	K	1813	0	1796	25	0
9	k	1782	0	1766	17	0
10	L	1876	0	1856	25	0
10	l	1861	0	1839	16	0
11	M	1890	0	1880	14	0
11	m	1881	0	1868	14	0
12	N	1521	0	1494	9	0
12	n	1510	0	1483	7	0
13	O	1645	0	1648	15	0
13	o	1659	0	1681	14	0
14	P	1587	0	1598	13	0
14	p	1591	0	1609	14	0
15	Q	1588	0	1584	9	0
15	q	1578	0	1569	12	0
16	R	1559	0	1523	16	0
16	r	1549	0	1506	12	0
17	S	1641	0	1639	19	0
17	s	1650	0	1645	14	0
18	T	1683	0	1662	17	0
18	t	1687	0	1666	8	0
19	x	3929	0	3915	47	0
20	y	601	0	629	10	0
21	C	3105	0	3219	49	0
22	D	3039	0	3076	57	0
23	U	6828	0	6884	106	0
24	W	3635	0	3762	55	0
25	X	3009	0	3113	43	0
26	Y	3202	0	3204	68	0
27	Z	2281	0	2312	45	0
28	a	2995	0	3012	59	0
29	b	1458	0	1505	15	0
30	c	2260	0	2276	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	d	2116	0	2146	27	0
32	f	6866	0	6866	137	0
33	V	3612	0	3682	52	0
34	e	425	0	328	6	0
35	A	27	0	12	4	0
35	B	27	0	12	1	0
36	E	31	0	12	2	0
36	F	31	0	12	1	0
37	c	1	0	0	0	0
All	All	110657	0	111121	1314	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 (1314) 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)
23:U:551:GLY:O	23:U:555:VAL:HB	1.89	0.72
17:s:4:PRO:HB2	18:t:100:ARG:HH21	1.55	0.70
22:D:278:GLN:HG2	22:D:285:VAL:HB	1.75	0.69
23:U:218:GLN:HE22	23:U:754:HIS:HB2	1.55	0.69
19:x:30:LYS:HB3	19:x:41:PRO:HB3	1.75	0.68
23:U:566:LEU:O	23:U:570:LEU:HB2	1.94	0.68
3:E:97:ARG:HE	3:E:111:LEU:HB2	1.57	0.67
30:c:167:MET:HE1	30:c:174:PRO:HG3	1.77	0.67
5:G:123:GLN:HG3	6:H:81:PRO:HB2	1.76	0.66
23:U:414:GLY:H	23:U:449:ILE:HG23	1.59	0.66
1:A:105:ASP:HB2	1:A:110:LYS:HD2	1.78	0.65
22:D:255:LYS:HE2	22:D:299:PHE:HB3	1.79	0.65
21:C:220:VAL:HG22	21:C:268:GLU:HG2	1.77	0.65
1:A:124:ASP:HB3	4:F:86:LEU:HD23	1.79	0.65
1:A:398:ARG:HH22	2:B:349:ARG:HH12	1.42	0.64
33:V:309:MET:HE1	33:V:331:LEU:HB3	1.79	0.64
23:U:510:GLU:HA	23:U:547:GLY:HA3	1.79	0.64
27:Z:228:TYR:HB2	28:a:341:LEU:HD12	1.80	0.64
3:E:258:MET:SD	3:E:262:ASN:ND2	2.70	0.64
25:X:379:ASP:HB3	26:Y:313:SER:HB3	1.78	0.64
33:V:121:PHE:HB3	33:V:128:ARG:HD2	1.80	0.64
32:f:557:TRP:HA	32:f:560:LEU:HD12	1.78	0.64
17:S:148:LEU:HD23	17:S:178:VAL:HG12	1.80	0.64
29:b:18:ASN:HD21	29:b:25:ARG:HH21	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:b:97:LEU:HD23	29:b:107:MET:HB2	1.81	0.63
33:V:416:ARG:HH11	33:V:457:TYR:HB3	1.63	0.63
19:x:172:PRO:HB2	19:x:175:LEU:HB3	1.81	0.63
23:U:242:LEU:O	23:U:246:TYR:HB2	1.99	0.63
25:X:203:PRO:HB2	25:X:206:LEU:HB2	1.80	0.63
19:x:418:TYR:HB3	19:x:480:TYR:HB3	1.79	0.63
14:p:14:MET:HG2	14:p:136:PHE:HB3	1.80	0.63
21:C:341:GLY:O	21:C:380:GLN:NE2	2.32	0.62
1:A:333:ARG:HH12	4:F:394:ALA:HB3	1.64	0.62
23:U:428:PRO:HG3	23:U:439:GLU:HB3	1.82	0.62
33:V:85:ALA:HB2	33:V:93:PHE:HB2	1.81	0.62
6:H:77:SER:HB3	6:H:163:MET:HE2	1.81	0.62
24:W:112:VAL:HG21	24:W:124:LEU:HD21	1.82	0.62
27:Z:37:GLY:HA2	27:Z:56:VAL:HG12	1.82	0.62
22:D:204:MET:HB3	22:D:310:ALA:HA	1.82	0.62
16:r:97:MET:H	16:r:116:SER:HB2	1.64	0.61
28:a:156:TYR:HB3	28:a:179:PHE:HB2	1.82	0.61
23:U:637:VAL:HG22	23:U:656:LEU:HD11	1.83	0.61
1:A:297:ARG:HH22	4:F:306:VAL:HG11	1.65	0.61
5:G:141:ILE:HG22	5:G:151:VAL:HG22	1.82	0.61
23:U:216:VAL:HG23	23:U:220:LEU:HD13	1.83	0.61
33:V:108:LEU:HD23	33:V:174:PHE:HB2	1.82	0.61
33:V:343:PRO:O	34:e:43:TRP:NE1	2.33	0.61
2:B:317:ASP:OD2	2:B:343:ARG:NH2	2.33	0.61
32:f:291:GLN:NE2	32:f:320:ILE:O	2.34	0.61
4:F:126:THR:HG1	4:F:128:THR:HG1	1.49	0.61
23:U:137:MET:HG2	23:U:140:ARG:HE	1.66	0.61
26:Y:385:ARG:NH2	33:V:282:ASN:O	2.34	0.61
6:H:203:MET:HA	6:H:207:ASN:HD21	1.66	0.60
10:L:196:ARG:NH1	10:L:237:GLU:O	2.34	0.60
28:a:28:LEU:HD22	28:a:33:LEU:HD11	1.81	0.60
30:c:277:LYS:HE3	30:c:282:ARG:HG2	1.81	0.60
23:U:52:GLU:HA	23:U:57:ARG:HD3	1.84	0.60
28:a:19:PRO:HA	28:a:22:TRP:HB2	1.82	0.60
32:f:100:ARG:HE	32:f:136:GLU:HB3	1.66	0.60
32:f:731:MET:O	32:f:737:ASN:ND2	2.35	0.60
2:B:190:LEU:HB3	2:B:193:GLN:HB2	1.83	0.60
13:O:22:GLU:HG2	13:O:27:ALA:HB2	1.82	0.60
27:Z:38:VAL:HA	27:Z:94:TRP:HA	1.84	0.60
32:f:749:ALA:O	32:f:752:HIS:ND1	2.33	0.60
7:I:123:GLN:NE2	8:J:125:ARG:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:371:THR:HG22	24:W:372:ARG:HG3	1.84	0.60
26:Y:297:ARG:HA	26:Y:300:ARG:HG2	1.83	0.60
27:Z:78:MET:HA	27:Z:81:MET:HG3	1.84	0.60
28:a:280:MET:HE1	28:a:296:ILE:HG13	1.83	0.60
32:f:744:MET:HA	32:f:747:GLN:HB2	1.84	0.60
3:E:303:LEU:HD21	3:E:337:GLY:HA2	1.83	0.59
29:b:142:ASN:HB2	29:b:173:VAL:HG11	1.83	0.59
32:f:764:LEU:HB2	32:f:769:THR:HB	1.83	0.59
1:A:333:ARG:HB3	1:A:336:ARG:HD3	1.83	0.59
1:A:214:LEU:O	1:A:222:LYS:NZ	2.35	0.59
23:U:541:HIS:HB2	23:U:544:ILE:HG22	1.84	0.59
27:Z:25:ARG:O	27:Z:28:LYS:NZ	2.36	0.59
33:V:321:ALA:HB1	33:V:324:PHE:HB3	1.84	0.59
28:a:58:LYS:HB2	28:a:83:VAL:HG13	1.82	0.59
3:E:127:PRO:HG2	3:E:185:ARG:HD2	1.85	0.59
19:x:219:GLU:OE1	19:x:238:LYS:NZ	2.36	0.59
21:C:53:ASN:ND2	23:U:642:GLU:O	2.35	0.59
22:D:212:LYS:NZ	22:D:311:THR:O	2.33	0.59
9:K:98:ASN:OD1	16:R:61:ARG:NH2	2.36	0.59
19:x:443:LYS:HB2	19:x:446:GLU:HB3	1.85	0.59
32:f:766:GLN:HE22	32:f:768:LEU:HG	1.68	0.59
21:C:45:LEU:HB3	22:D:61:ILE:HG21	1.85	0.59
23:U:490:ARG:HE	23:U:493:VAL:H	1.50	0.59
19:x:208:MET:HE1	19:x:273:LEU:HB3	1.85	0.58
21:C:209:CYS:SG	21:C:210:THR:N	2.76	0.58
3:E:242:ARG:O	4:F:300:LYS:NZ	2.36	0.58
20:y:3:ILE:HB	20:y:15:LEU:HB3	1.85	0.58
1:A:181:LYS:HA	1:A:184:ILE:HB	1.85	0.58
10:L:27:GLU:HA	10:L:30:LYS:HG2	1.85	0.58
15:Q:25:ILE:HG22	15:Q:26:VAL:HG13	1.85	0.58
23:U:11:LEU:HD12	23:U:19:LEU:HD11	1.84	0.58
19:x:371:ARG:HA	19:x:374:PHE:HB2	1.85	0.58
1:A:351:ARG:HH21	1:A:374:ALA:HB1	1.68	0.58
11:M:34:SER:OG	11:M:65:ARG:NH1	2.37	0.58
19:x:422:ALA:HB3	19:x:479:LEU:HB3	1.84	0.58
21:C:90:HIS:ND1	22:D:108:GLY:O	2.36	0.58
1:A:139:ARG:NH2	2:B:114:GLU:OE1	2.37	0.58
21:C:69:GLN:NE2	22:D:135:HIS:O	2.37	0.58
26:Y:144:LEU:HD13	26:Y:147:ILE:HD11	1.85	0.58
32:f:17:PRO:HB2	32:f:60:VAL:HG21	1.85	0.58
32:f:587:PHE:O	32:f:632:LYS:NZ	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:j:95:ARG:HG2	15:q:62:LYS:HE3	1.86	0.58
11:m:35:THR:HA	11:m:166:GLY:HA3	1.84	0.58
10:L:120:THR:HG22	11:M:129:ARG:HH21	1.69	0.57
8:j:120:GLN:OE1	9:k:135:ARG:NH2	2.37	0.57
13:o:143:ARG:H	13:o:146:MET:HE3	1.69	0.57
32:f:817:VAL:HG13	32:f:818:LEU:HD23	1.86	0.57
11:m:34:SER:OG	11:m:65:ARG:NH1	2.38	0.57
19:x:394:SER:O	32:f:357:ARG:NH1	2.37	0.57
21:C:264:GLY:HA3	21:C:269:VAL:HG11	1.87	0.57
22:D:297:ASP:OD2	22:D:326:ARG:NH2	2.37	0.57
24:W:186:ILE:HG12	24:W:209:ILE:HD12	1.86	0.57
21:C:239:ARG:HH12	21:C:286:THR:HA	1.68	0.57
19:x:378:GLU:HA	19:x:381:LYS:HG2	1.86	0.57
22:D:167:ILE:HG12	22:D:344:ILE:HD13	1.87	0.57
26:Y:315:THR:HA	26:Y:353:ILE:HA	1.86	0.57
1:A:29:ASP:OD1	32:f:53:GLN:NE2	2.37	0.57
7:I:31:ALA:O	7:I:50:ARG:NH2	2.37	0.57
5:g:141:ILE:HG22	5:g:151:VAL:HG22	1.87	0.57
29:b:25:ARG:NH1	29:b:143:PHE:O	2.36	0.57
32:f:762:VAL:HG23	32:f:774:GLY:HA3	1.85	0.57
33:V:355:ARG:NH2	34:e:31:ASP:OD1	2.37	0.57
2:B:294:ARG:NH2	2:B:296:ASP:O	2.38	0.57
9:K:28:ILE:HD13	9:K:158:PRO:HG2	1.86	0.57
23:U:886:PRO:HA	23:U:889:LEU:HB2	1.86	0.57
26:Y:233:ARG:NH2	26:Y:264:TYR:O	2.38	0.57
32:f:294:MET:O	32:f:773:LYS:NZ	2.38	0.57
11:M:187:ARG:O	11:M:191:LYS:NZ	2.37	0.57
31:d:5:LEU:HG	31:d:50:LEU:HD13	1.85	0.57
32:f:94:LYS:HG3	32:f:95:PRO:HD3	1.87	0.57
15:q:180:VAL:HG23	15:q:191:LEU:HB2	1.87	0.57
23:U:890:LYS:HG3	23:U:891:VAL:HG13	1.86	0.57
17:S:10:GLY:HA3	17:S:42:LYS:HE2	1.86	0.56
16:r:64:ARG:NH1	16:r:67:GLU:OE1	2.38	0.56
33:V:492:LYS:HA	33:V:495:ARG:HH22	1.70	0.56
7:I:80:THR:HG22	21:C:406:LYS:HB2	1.86	0.56
17:s:38:ARG:NH1	17:s:212:LYS:O	2.38	0.56
20:y:74:ARG:NH1	20:y:75:GLY:O	2.38	0.56
23:U:724:VAL:HA	23:U:727:LYS:HE3	1.86	0.56
32:f:763:ARG:HE	32:f:770:HIS:HA	1.71	0.56
5:G:165:ALA:HB3	6:H:56:LEU:HD22	1.85	0.56
23:U:840:LYS:HG3	23:U:844:LYS:HE2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:250:ARG:HH12	32:f:252:ALA:HB3	1.70	0.56
33:V:150:ARG:NH1	33:V:157:THR:O	2.38	0.56
33:V:454:GLU:HG3	33:V:455:LYS:HG2	1.88	0.56
7:I:119:GLN:NE2	8:J:79:ASP:OD1	2.39	0.56
9:k:221:GLN:HG3	9:k:224:GLN:HE21	1.70	0.56
2:B:193:GLN:NE2	2:B:352:GLU:O	2.38	0.56
27:Z:224:HIS:HA	27:Z:227:ILE:HG22	1.87	0.56
23:U:543:LYS:NZ	30:c:63:ASP:OD2	2.38	0.56
1:A:301:GLU:HB2	4:F:254:PRO:HG2	1.86	0.56
2:B:304:GLU:HA	2:B:307:ARG:HG2	1.87	0.56
9:K:96:THR:HA	9:K:107:MET:HE3	1.87	0.56
2:B:59:ARG:NH2	32:f:223:GLU:OE2	2.33	0.56
3:E:213:ARG:HE	22:D:237:GLN:HE21	1.54	0.56
10:L:157:ARG:HD2	10:L:176:MET:HE2	1.87	0.56
6:h:119:GLN:HG3	7:i:81:SER:HB2	1.87	0.56
8:j:71:MET:HE1	8:j:73:PHE:HB3	1.87	0.56
23:U:191:LYS:HA	23:U:194:ARG:HB3	1.87	0.56
28:a:19:PRO:O	28:a:23:HIS:ND1	2.39	0.56
32:f:814:SER:OG	32:f:879:ARG:NH1	2.39	0.56
6:H:119:GLN:HG3	7:I:81:SER:HB2	1.88	0.56
10:l:49:LEU:O	10:l:62:LYS:NZ	2.38	0.56
21:C:86:LEU:HD21	21:C:94:LYS:HG3	1.88	0.56
23:U:152:GLY:HA2	23:U:155:LEU:HD13	1.87	0.56
23:U:770:TRP:HA	30:c:179:SER:HB3	1.87	0.56
1:A:333:ARG:NH1	1:A:334:PRO:O	2.39	0.56
2:B:135:ILE:HA	2:B:159:VAL:HB	1.87	0.56
7:i:38:LEU:O	7:i:179:TYR:OH	2.23	0.56
18:T:25:ASP:OD1	18:T:41:ARG:NH2	2.40	0.55
11:m:230:ASP:OD1	11:m:230:ASP:N	2.39	0.55
22:D:200:ARG:HE	22:D:304:ASN:HA	1.71	0.55
32:f:522:CYS:HA	32:f:525:ILE:HD12	1.88	0.55
18:T:99:ARG:NH2	18:T:104:ASN:OD1	2.39	0.55
6:h:95:GLN:NE2	13:o:64:GLU:OE1	2.38	0.55
18:t:25:ASP:OD1	18:t:41:ARG:NH2	2.40	0.55
28:a:100:THR:HA	28:a:103:LYS:HG2	1.88	0.55
15:Q:41:LYS:NZ	15:Q:185:LYS:O	2.38	0.55
19:x:394:SER:H	32:f:357:ARG:HD2	1.71	0.55
21:C:254:ILE:HG23	21:C:269:VAL:HG22	1.88	0.55
23:U:798:PRO:O	23:U:880:ASN:ND2	2.38	0.55
29:b:53:THR:HG22	29:b:59:GLU:H	1.69	0.55
9:K:209:LYS:O	9:K:214:ASN:ND2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:x:197:GLN:HA	20:y:74:ARG:HD3	1.89	0.55
21:C:256:SER:OG	21:C:273:MET:SD	2.63	0.55
33:V:135:LEU:HD21	33:V:171:VAL:HG13	1.88	0.55
7:i:197:LEU:HB3	7:i:206:LEU:HD11	1.89	0.55
24:W:401:THR:HG23	24:W:402:ILE:HD12	1.87	0.55
26:Y:133:ALA:HB3	26:Y:136:HIS:HD2	1.71	0.55
30:c:138:GLU:OE1	30:c:139:ARG:NH1	2.40	0.55
33:V:199:ASN:OD1	33:V:241:ARG:NH2	2.40	0.55
4:F:180:ARG:NH2	4:F:246:ALA:O	2.38	0.55
22:D:336:PRO:HG2	22:D:371:SER:HA	1.87	0.55
4:F:46:ARG:NH1	28:a:103:LYS:O	2.39	0.55
22:D:67:ASN:ND2	23:U:607:VAL:O	2.40	0.55
24:W:24:VAL:HG12	24:W:27:ARG:HH12	1.71	0.55
25:X:221:GLU:O	25:X:223:LYS:NZ	2.36	0.55
23:U:405:THR:HG23	23:U:441:GLY:HA3	1.87	0.55
1:A:23:ARG:NH1	1:A:25:LEU:O	2.39	0.55
3:E:78:ARG:HB2	22:D:89:ILE:HB	1.89	0.55
6:h:203:MET:HE3	6:h:208:ILE:HG21	1.89	0.55
23:U:609:ASP:O	23:U:615:ARG:NH1	2.39	0.55
33:V:450:SER:HB3	33:V:459:GLN:HB3	1.89	0.55
7:i:119:GLN:NE2	8:j:79:ASP:OD1	2.40	0.55
23:U:632:GLN:O	23:U:635:SER:OG	2.25	0.55
14:P:71:LEU:HD11	14:P:82:ILE:HG21	1.88	0.54
16:r:80:SER:OG	16:r:120:ARG:NH1	2.40	0.54
23:U:613:ASP:OD1	23:U:616:ARG:NH2	2.40	0.54
33:V:492:LYS:O	33:V:495:ARG:NH1	2.39	0.54
14:p:126:LEU:HD12	14:p:127:ILE:HG23	1.89	0.54
24:W:407:ASP:OD2	25:X:344:ARG:NH2	2.40	0.54
28:a:188:LEU:O	28:a:193:GLN:NE2	2.40	0.54
31:d:21:GLU:OE2	31:d:25:ARG:NH2	2.40	0.54
3:E:237:ALA:O	4:F:308:ARG:NH1	2.41	0.54
20:y:1:MET:N	20:y:17:VAL:O	2.41	0.54
22:D:191:TYR:HB3	22:D:198:PRO:HD3	1.90	0.54
23:U:751:ARG:HE	23:U:910:GLY:HA3	1.72	0.54
26:Y:237:ARG:HA	26:Y:241:ILE:HD12	1.89	0.54
30:c:32:TYR:HB2	30:c:68:ARG:HG2	1.90	0.54
33:V:120:PHE:HB3	33:V:159:LEU:HD11	1.90	0.54
6:H:93:LEU:HD13	6:H:113:ARG:HB3	1.90	0.54
17:S:211:ARG:NH2	17:S:213:ASP:OD2	2.39	0.54
7:i:114:LEU:HD12	7:i:117:ILE:HD11	1.89	0.54
11:m:187:ARG:HH12	11:m:231:ILE:HD13	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:277:LEU:HA	21:C:281:ASP:HB2	1.90	0.54
33:V:287:ARG:NH2	34:e:17:ASP:OD2	2.41	0.54
10:L:125:ARG:NH1	10:L:126:ARG:O	2.41	0.54
26:Y:268:TYR:HA	26:Y:271:PHE:HB3	1.89	0.54
28:a:360:VAL:HA	28:a:363:MET:HE2	1.89	0.54
32:f:794:ALA:HB1	32:f:797:LEU:HD22	1.88	0.54
1:A:213:LEU:HD11	1:A:340:LYS:HG3	1.89	0.54
6:h:196:LYS:NZ	6:h:234:ALA:O	2.41	0.54
22:D:115:ILE:HG22	22:D:139:LEU:HB3	1.88	0.54
1:A:211:GLY:HA3	1:A:337:LEU:HA	1.88	0.54
27:Z:258:VAL:HG23	27:Z:262:LEU:HD13	1.90	0.54
1:A:161:VAL:HG22	1:A:165:GLN:HE22	1.72	0.54
3:E:328:TYR:HA	3:E:331:ILE:HD12	1.90	0.54
8:J:7:ILE:HG23	8:J:8:THR:HG23	1.88	0.54
14:P:2:SER:OG	14:P:3:ILE:N	2.41	0.54
10:l:18:ARG:NH1	10:l:23:GLU:OE1	2.40	0.54
14:p:35:VAL:HG12	14:p:36:THR:HG23	1.89	0.54
26:Y:231:LEU:HG	26:Y:236:LEU:HD12	1.89	0.54
31:d:215:TRP:H	31:d:225:PHE:HE2	1.56	0.54
32:f:300:ARG:NH1	32:f:456:ARG:O	2.41	0.54
13:o:146:MET:HE1	13:o:154:LEU:HD22	1.90	0.54
27:Z:243:GLN:O	27:Z:247:LYS:NZ	2.40	0.54
32:f:183:PRO:O	32:f:186:THR:N	2.34	0.54
3:E:248:SER:HA	22:D:278:GLN:HE22	1.72	0.54
19:x:43:ARG:HH22	19:x:79:PRO:HD3	1.73	0.54
25:X:143:TYR:OH	26:Y:248:GLU:O	2.26	0.54
25:X:295:LYS:O	25:X:297:ARG:NH1	2.41	0.54
27:Z:26:ILE:HD11	27:Z:35:VAL:HG22	1.90	0.54
26:Y:177:ARG:HH12	26:Y:181:LYS:HB3	1.73	0.53
32:f:415:GLY:HA3	32:f:447:ALA:HB1	1.89	0.53
2:B:181:GLN:O	2:B:241:ASN:ND2	2.41	0.53
17:s:125:ASP:OD1	17:s:129:SER:N	2.41	0.53
21:C:89:VAL:HG23	21:C:90:HIS:H	1.74	0.53
23:U:21:GLU:HA	23:U:24:LEU:HG	1.89	0.53
33:V:281:ASN:HB3	33:V:284:GLU:HG2	1.91	0.53
2:B:125:THR:OG1	2:B:126:SER:N	2.40	0.53
7:I:119:GLN:HG3	8:J:78:ALA:HB1	1.90	0.53
18:t:25:ASP:HA	18:t:187:PHE:HA	1.90	0.53
22:D:291:GLU:OE2	22:D:295:GLN:NE2	2.42	0.53
25:X:271:VAL:HG11	25:X:288:LYS:HD3	1.90	0.53
27:Z:198:LEU:HD11	28:a:363:MET:HE3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:664:GLU:H	32:f:668:ALA:HB3	1.71	0.53
1:A:83:ASP:O	1:A:88:GLN:NE2	2.41	0.53
10:L:200:PRO:O	10:L:239:ARG:NH2	2.41	0.53
23:U:700:GLU:OE1	23:U:707:ASN:ND2	2.42	0.53
24:W:108:CYS:SG	24:W:123:ARG:NH1	2.70	0.53
27:Z:176:LEU:HG	30:c:218:LEU:HD12	1.91	0.53
1:A:129:VAL:O	19:x:334:LYS:NZ	2.41	0.53
8:j:224:GLU:HA	8:j:227:LYS:HG2	1.90	0.53
23:U:208:LEU:HD23	23:U:210:LYS:H	1.73	0.53
26:Y:86:GLU:HA	26:Y:89:GLU:HG2	1.90	0.53
26:Y:156:LEU:HD22	26:Y:159:ARG:HH21	1.73	0.53
32:f:613:LEU:HA	32:f:617:SER:HB3	1.89	0.53
6:H:118:MET:HG3	6:H:130:PHE:HD2	1.73	0.53
19:x:449:LYS:HE2	19:x:451:ASP:HB2	1.91	0.53
21:C:277:LEU:O	21:C:282:GLY:N	2.36	0.53
23:U:483:LEU:HD21	23:U:781:LEU:HD11	1.91	0.53
25:X:395:LYS:NZ	30:c:242:GLU:OE1	2.42	0.53
7:i:12:PHE:HE2	8:j:126:PRO:HD2	1.74	0.53
33:V:212:TYR:HD1	33:V:253:LEU:HD21	1.74	0.53
13:o:70:THR:HG23	13:o:72:ARG:H	1.74	0.53
19:x:79:PRO:HG2	32:f:435:SER:HB2	1.91	0.53
23:U:889:LEU:HD13	23:U:909:GLY:HA3	1.89	0.53
2:B:77:GLU:OE1	2:B:81:ASN:ND2	2.42	0.53
3:E:108:MET:SD	3:E:108:MET:N	2.76	0.53
7:i:8:ARG:HE	8:j:5:ARG:HH12	1.57	0.53
23:U:111:GLN:HE22	23:U:124:LYS:HE3	1.74	0.53
23:U:792:ASN:HB3	23:U:914:LEU:HB3	1.90	0.53
11:m:8:ASP:O	11:m:22:GLN:NE2	2.42	0.53
21:C:228:ALA:HB1	21:C:271:ARG:HG2	1.90	0.53
24:W:52:LYS:HG3	24:W:55:ARG:HH21	1.74	0.53
24:W:443:THR:HG21	27:Z:204:LYS:HD2	1.89	0.53
3:E:63:GLN:NE2	3:E:92:LEU:O	2.42	0.52
4:F:169:ASP:HB3	4:F:172:VAL:HG23	1.91	0.52
4:F:375:VAL:HG22	4:F:415:LEU:HB3	1.90	0.52
8:J:95:ARG:HD3	8:J:101:PRO:HA	1.90	0.52
5:g:141:ILE:HD12	5:g:220:VAL:HG12	1.90	0.52
11:m:223:ARG:NH1	11:m:225:GLU:OE2	2.42	0.52
22:D:274:ARG:HB2	22:D:277:ALA:HB2	1.89	0.52
23:U:490:ARG:HH21	23:U:493:VAL:HB	1.74	0.52
11:M:51:LYS:NZ	11:M:210:GLU:OE2	2.38	0.52
22:D:338:ARG:NH1	22:D:364:VAL:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:d:103:LEU:HD23	31:d:136:PRO:HB2	1.91	0.52
31:d:119:LEU:HD21	31:d:137:VAL:HG11	1.91	0.52
6:h:166:ASN:OD1	6:h:169:ASN:ND2	2.39	0.52
18:t:96:MET:HE3	18:t:127:MET:HA	1.92	0.52
23:U:494:TYR:CZ	23:U:498:LYS:HD2	2.45	0.52
1:A:51:ASP:OD1	2:B:69:LYS:NZ	2.42	0.52
4:F:83:ASN:OD1	30:c:77:GLN:NE2	2.42	0.52
9:k:186:HIS:H	9:k:189:MET:HE3	1.75	0.52
21:C:66:LEU:HD11	22:D:116:LEU:HD21	1.90	0.52
32:f:450:ILE:HG13	32:f:804:LEU:HD22	1.91	0.52
4:F:183:GLU:HB2	4:F:239:ALA:HA	1.91	0.52
9:K:202:LEU:O	9:K:206:MET:N	2.39	0.52
24:W:127:THR:HA	24:W:130:MET:HG3	1.92	0.52
24:W:248:ARG:HD3	24:W:290:ILE:HD11	1.92	0.52
5:G:191:PHE:HE1	5:G:219:VAL:HG21	1.74	0.52
6:H:143:ARG:NH1	6:H:144:PRO:O	2.43	0.52
12:n:144:ARG:H	12:n:147:MET:HE3	1.74	0.52
13:o:63:LEU:HD11	13:o:79:ALA:HB2	1.91	0.52
21:C:70:GLY:O	21:C:118:ASN:ND2	2.42	0.52
23:U:756:HIS:HB3	23:U:759:SER:HB3	1.91	0.52
25:X:316:ASP:HA	25:X:320:SER:HB2	1.92	0.52
1:A:250:VAL:HG23	1:A:294:GLU:HB2	1.91	0.52
8:j:183:THR:HB	8:j:186:LEU:HD13	1.92	0.52
21:C:233:GLU:HA	21:C:236:VAL:HG22	1.91	0.52
23:U:521:LEU:HD21	23:U:757:MET:HE3	1.92	0.52
27:Z:6:VAL:HG21	27:Z:48:LEU:HB2	1.90	0.52
27:Z:42:SER:OG	27:Z:88:ARG:O	2.28	0.52
32:f:75:LEU:HD23	32:f:77:GLU:H	1.75	0.52
1:A:215:PHE:HE1	1:A:340:LYS:HB3	1.74	0.52
3:E:177:GLY:HA3	3:E:339:ASN:HD22	1.74	0.52
15:q:44:LEU:HD11	15:q:102:LEU:HD23	1.92	0.52
23:U:900:TYR:OH	23:U:922:GLU:O	2.28	0.52
28:a:30:THR:OG1	28:a:31:LYS:NZ	2.38	0.52
30:c:52:GLU:HA	30:c:114:SER:HB2	1.91	0.52
30:c:244:VAL:HG22	30:c:291:LEU:HD13	1.92	0.52
10:L:158:ALA:HB1	10:L:172:LEU:HD13	1.91	0.52
11:M:141:SER:OG	11:M:144:ASP:OD1	2.28	0.52
6:h:65:VAL:O	6:h:220:ARG:NH1	2.42	0.52
24:W:277:ALA:HB3	24:W:283:GLN:HE22	1.74	0.52
25:X:248:ILE:HD12	25:X:251:LEU:HD21	1.91	0.52
3:E:7:LYS:HA	3:E:11:ASP:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:217:ILE:HG13	4:F:218:GLN:H	1.75	0.52
13:O:198:ARG:NH1	13:O:200:GLY:O	2.43	0.52
19:x:107:LEU:HD23	19:x:169:SER:HB2	1.92	0.52
27:Z:186:THR:HA	27:Z:189:GLN:HE21	1.75	0.52
8:J:208:LEU:HD23	8:J:220:LEU:HG	1.92	0.51
10:l:215:VAL:HB	10:l:221:PHE:HD1	1.74	0.51
22:D:159:LYS:NZ	22:D:221:HIS:O	2.43	0.51
32:f:218:GLU:HA	32:f:221:ILE:HG12	1.91	0.51
1:A:138:MET:SD	1:A:138:MET:N	2.83	0.51
3:E:103:THR:HG21	30:c:49:VAL:HG21	1.92	0.51
9:k:160:GLY:O	10:l:82:ARG:NH2	2.43	0.51
15:q:68:LYS:HG3	15:q:74:GLU:HG2	1.91	0.51
24:W:384:LEU:HD13	24:W:388:GLU:HB2	1.92	0.51
30:c:57:MET:HA	30:c:72:VAL:HG13	1.93	0.51
30:c:100:LYS:HD2	30:c:105:PRO:HG3	1.92	0.51
31:d:241:GLU:OE2	31:d:245:GLN:NE2	2.44	0.51
4:F:225:MET:HE2	4:F:236:LEU:HD21	1.91	0.51
8:J:40:ILE:HD11	8:J:210:VAL:HB	1.92	0.51
13:o:51:ASP:HB3	13:o:94:ILE:HG23	1.92	0.51
23:U:474:ARG:NH1	23:U:500:ASN:OD1	2.43	0.51
23:U:892:LEU:HD21	23:U:906:LEU:HG	1.92	0.51
29:b:55:ALA:HB1	29:b:82:GLY:HA3	1.93	0.51
5:G:10:ASP:O	5:G:24:GLN:NE2	2.44	0.51
18:t:54:SER:OG	18:t:55:GLY:N	2.43	0.51
19:x:423:VAL:HB	19:x:439:TRP:HB2	1.91	0.51
21:C:215:SER:HB2	21:C:218:GLU:HG2	1.93	0.51
23:U:98:GLU:HA	23:U:101:ILE:HG12	1.92	0.51
23:U:108:TYR:OH	23:U:159:ARG:NH2	2.44	0.51
27:Z:252:LYS:HE3	30:c:299:CYS:HA	1.91	0.51
32:f:271:MET:HA	32:f:274:ASP:HB2	1.91	0.51
3:E:244:SER:H	4:F:300:LYS:HZ2	1.57	0.51
8:J:23:GLN:HA	8:J:149:PRO:HG2	1.93	0.51
23:U:15:ASP:OD1	23:U:15:ASP:N	2.42	0.51
26:Y:348:ASP:OD2	26:Y:351:ASN:ND2	2.43	0.51
31:d:12:LYS:HE2	31:d:14:PRO:HB3	1.92	0.51
4:F:93:VAL:HA	4:F:124:ILE:HG12	1.93	0.51
18:T:37:ARG:NH1	12:n:165:GLU:OE2	2.43	0.51
24:W:118:LEU:C	24:W:120:ILE:H	2.17	0.51
28:a:363:MET:HE1	30:c:308:VAL:HA	1.92	0.51
31:d:141:GLN:NE2	31:d:145:GLU:OE2	2.43	0.51
8:J:39:ASP:OD1	8:J:39:ASP:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:88:LYS:HG3	21:C:92:GLU:HB2	1.91	0.51
22:D:323:ARG:NH1	22:D:324:PRO:O	2.44	0.51
32:f:169:GLU:HG2	32:f:173:LEU:HD13	1.92	0.51
10:L:39:LYS:HD2	10:L:142:PRO:HB2	1.92	0.51
10:L:139:ASP:N	10:L:139:ASP:OD1	2.42	0.51
5:g:155:ASP:OD1	5:g:159:TYR:N	2.41	0.51
6:h:9:SER:HA	6:h:125:GLY:HA2	1.93	0.51
26:Y:384:SER:HA	26:Y:387:ILE:HG22	1.93	0.51
29:b:184:ILE:HA	29:b:187:PRO:HD2	1.93	0.51
1:A:336:ARG:NH2	4:F:229:PRO:O	2.44	0.51
3:E:339:ASN:HD21	4:F:344:ARG:HD2	1.76	0.51
16:R:19:ARG:NH2	14:p:205:ASP:O	2.44	0.51
18:t:99:ARG:HG2	18:t:106:LEU:HG	1.93	0.51
24:W:259:GLU:HB2	24:W:262:LYS:HB3	1.93	0.51
25:X:402:GLU:O	25:X:406:ASN:ND2	2.44	0.51
5:G:93:ARG:HE	5:G:121:ILE:HD13	1.75	0.51
6:H:133:SER:HB3	6:H:163:MET:HE1	1.93	0.51
5:g:138:MET:HB3	5:g:154:CYS:HB2	1.92	0.50
19:x:403:PRO:O	19:x:414:ASN:ND2	2.43	0.50
32:f:389:LYS:HE2	32:f:418:LEU:HD11	1.93	0.50
1:A:325:ASP:OD1	1:A:325:ASP:N	2.43	0.50
14:P:65:GLN:OE1	15:Q:86:ARG:NH2	2.40	0.50
18:T:122:LEU:HG	18:T:137:LEU:HD12	1.92	0.50
22:D:111:TYR:HB3	22:D:113:VAL:HG13	1.94	0.50
23:U:22:PHE:O	23:U:26:LYS:NZ	2.42	0.50
32:f:99:LEU:HD23	32:f:102:HIS:HB2	1.92	0.50
1:A:210:LYS:HA	1:A:316:LYS:HD3	1.92	0.50
1:A:417:ILE:HG23	1:A:422:LYS:HD3	1.92	0.50
2:B:370:SER:OG	2:B:371:ARG:NH1	2.44	0.50
19:x:424:LEU:HB3	19:x:477:VAL:HB	1.94	0.50
22:D:318:ASP:HB3	22:D:321:LEU:HG	1.92	0.50
23:U:111:GLN:HE21	23:U:115:ASN:HD21	1.58	0.50
31:d:86:LYS:HB2	31:d:89:LEU:HG	1.92	0.50
15:q:39:SER:OG	15:q:40:GLU:N	2.42	0.50
23:U:455:GLY:H	23:U:458:ILE:HD12	1.76	0.50
24:W:422:ASN:OD1	24:W:423:ASN:N	2.45	0.50
22:D:190:LEU:HA	22:D:193:GLN:HG2	1.93	0.50
23:U:801:GLN:HG2	23:U:877:LEU:HB3	1.94	0.50
26:Y:191:ILE:HD12	34:e:40:GLU:H	1.77	0.50
32:f:29:SER:HB2	32:f:33:ARG:HE	1.75	0.50
1:A:349:GLU:O	1:A:353:HIS:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ARG:NH1	1:A:378:PRO:O	2.45	0.50
19:x:74:SER:OG	19:x:76:ASP:OD1	2.27	0.50
28:a:77:VAL:HA	28:a:80:ILE:HG12	1.93	0.50
1:A:32:LEU:HD21	32:f:96:LEU:HD23	1.93	0.50
4:F:97:LEU:O	4:F:121:CYS:N	2.44	0.50
5:g:10:ASP:OD1	5:g:10:ASP:N	2.44	0.50
16:r:130:SER:OG	16:r:167:ASP:OD2	2.28	0.50
19:x:219:GLU:HA	19:x:242:LEU:HB3	1.94	0.50
22:D:57:GLN:O	22:D:61:ILE:HG12	2.11	0.50
23:U:751:ARG:NE	23:U:909:GLY:O	2.44	0.50
27:Z:200:GLY:HA3	30:c:225:TRP:HE1	1.76	0.50
33:V:337:LEU:HD21	33:V:364:THR:HG23	1.93	0.50
1:A:52:ILE:HG22	2:B:69:LYS:HZ2	1.77	0.50
24:W:188:GLU:HB2	24:W:191:ARG:HH21	1.76	0.50
24:W:276:LEU:HD22	24:W:354:LEU:HD13	1.94	0.50
3:E:376:ASP:HA	3:E:379:LYS:HD3	1.94	0.49
6:h:14:SER:HB3	6:h:18:LYS:H	1.77	0.49
20:y:40:GLN:HE21	20:y:71:LEU:HB3	1.77	0.49
26:Y:217:LYS:HD3	26:Y:253:LEU:HD21	1.94	0.49
32:f:91:SER:HA	32:f:94:LYS:HE3	1.94	0.49
32:f:371:ASN:ND2	32:f:401:LYS:O	2.39	0.49
32:f:566:HIS:ND1	32:f:574:GLU:OE2	2.45	0.49
32:f:780:PRO:HG3	32:f:802:SER:HB2	1.94	0.49
1:A:179:GLY:HA3	1:A:350:GLY:HA2	1.93	0.49
3:E:60:VAL:O	3:E:95:GLY:N	2.43	0.49
3:E:83:CYS:HB3	3:E:87:LEU:HB2	1.93	0.49
7:I:51:ASN:OD1	7:I:53:HIS:ND1	2.45	0.49
31:d:126:ASP:OD1	31:d:126:ASP:N	2.45	0.49
32:f:466:LEU:O	32:f:470:VAL:HB	2.11	0.49
4:F:238:ARG:NH2	36:F:501:ATP:O3'	2.45	0.49
8:J:11:SER:OG	8:J:13:ASP:OD1	2.27	0.49
9:K:114:GLN:O	9:K:118:ASN:ND2	2.45	0.49
24:W:227:TYR:HA	24:W:230:MET:HG3	1.95	0.49
25:X:187:ARG:HH21	25:X:221:GLU:HG3	1.76	0.49
25:X:203:PRO:O	25:X:207:GLN:N	2.45	0.49
27:Z:124:ILE:HA	27:Z:135:THR:HG22	1.95	0.49
28:a:321:LYS:HE3	28:a:336:VAL:HG21	1.95	0.49
4:F:357:PRO:O	4:F:362:ARG:NH1	2.45	0.49
16:R:30:THR:O	17:S:131:GLN:NE2	2.44	0.49
16:R:58:LEU:HD12	16:R:61:ARG:HD3	1.94	0.49
21:C:72:TYR:HB2	21:C:116:LEU:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:583:MET:HA	23:U:586:VAL:HG12	1.93	0.49
24:W:178:GLU:HG3	24:W:181:GLU:HB3	1.94	0.49
32:f:429:ILE:HG21	32:f:448:CYS:HB2	1.95	0.49
23:U:490:ARG:HB3	23:U:493:VAL:HG12	1.95	0.49
31:d:151:VAL:O	31:d:155:LYS:HB2	2.13	0.49
32:f:828:ARG:HH11	32:f:847:GLY:HA3	1.76	0.49
11:M:230:ASP:N	11:M:230:ASP:OD1	2.46	0.49
17:S:71:ARG:HA	17:S:74:MET:HE3	1.94	0.49
16:r:35:ILE:HD11	16:r:45:MET:HG3	1.95	0.49
26:Y:63:TRP:HE1	26:Y:67:VAL:HB	1.78	0.49
31:d:250:ALA:O	31:d:254:GLU:N	2.44	0.49
3:E:236:ASP:OD2	3:E:279:THR:OG1	2.29	0.49
4:F:143:GLU:OE2	4:F:144:LYS:NZ	2.46	0.49
22:D:157:ASP:OD1	22:D:157:ASP:N	2.45	0.49
23:U:151:ILE:HD12	23:U:154:ALA:HB3	1.94	0.49
24:W:128:LEU:HA	24:W:131:VAL:HG12	1.95	0.49
25:X:381:GLY:N	26:Y:313:SER:O	2.38	0.49
26:Y:229:ILE:HD11	26:Y:299:MET:HE2	1.94	0.49
32:f:12:GLN:O	32:f:16:SER:HB2	2.12	0.49
33:V:337:LEU:HB3	33:V:398:LEU:HD11	1.95	0.49
5:G:112:ASP:N	5:G:112:ASP:OD1	2.46	0.49
7:I:62:SER:OG	7:I:65:ILE:O	2.31	0.49
10:L:84:LEU:HD13	10:L:112:ILE:HD11	1.95	0.49
19:x:86:THR:HG21	32:f:401:LYS:HE3	1.95	0.49
22:D:272:THR:HB	22:D:277:ALA:HB3	1.95	0.49
23:U:21:GLU:O	23:U:25:HIS:ND1	2.46	0.49
26:Y:308:LEU:O	26:Y:358:ARG:NH1	2.45	0.49
33:V:470:ARG:O	33:V:473:GLN:NE2	2.46	0.49
1:A:50:ASP:N	1:A:50:ASP:OD1	2.46	0.49
10:L:117:GLN:HG3	11:M:82:ALA:HB1	1.93	0.49
9:k:210:LEU:HA	9:k:214:ASN:HD21	1.77	0.49
19:x:292:LEU:O	19:x:295:GLN:NE2	2.45	0.49
21:C:217:SER:OG	21:C:218:GLU:OE1	2.26	0.49
28:a:90:PRO:HA	28:a:93:ALA:HB3	1.94	0.49
32:f:80:ARG:HD2	32:f:83:ARG:HE	1.78	0.49
9:K:5:ARG:NH1	9:K:26:TYR:OH	2.45	0.49
6:h:101:TYR:HE1	14:p:90:MET:HE2	1.78	0.49
14:p:138:VAL:HG11	14:p:146:MET:HB3	1.94	0.49
22:D:86:PRO:HB2	22:D:134:LYS:HD2	1.94	0.49
26:Y:48:ASN:HB3	26:Y:114:ILE:HG12	1.95	0.49
32:f:125:ILE:HG23	32:f:130:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:V:355:ARG:HA	33:V:358:MET:HE2	1.95	0.49
2:B:367:ILE:O	2:B:370:SER:OG	2.30	0.48
4:F:438:TYR:OH	9:K:19:GLY:O	2.31	0.48
11:M:236:GLU:OE1	11:M:240:LYS:NZ	2.46	0.48
10:l:121:GLN:HG3	11:m:129:ARG:HG2	1.95	0.48
21:C:161:ILE:HA	21:C:164:VAL:HG12	1.95	0.48
25:X:309:TYR:HB3	25:X:312:GLU:HB2	1.95	0.48
26:Y:173:ASP:HA	26:Y:176:ARG:HH21	1.78	0.48
28:a:257:GLN:HB3	28:a:261:LEU:HD22	1.94	0.48
28:a:309:LEU:HA	28:a:312:MET:HE2	1.94	0.48
4:F:79:LYS:O	4:F:83:ASN:ND2	2.43	0.48
17:S:4:PRO:O	18:T:100:ARG:NH1	2.46	0.48
10:l:226:ASP:OD1	10:l:226:ASP:N	2.45	0.48
23:U:216:VAL:HG21	23:U:232:ILE:HD11	1.95	0.48
23:U:350:LEU:HA	23:U:353:LEU:HD12	1.94	0.48
24:W:271:VAL:HG23	24:W:305:LEU:HD22	1.94	0.48
25:X:50:ILE:HD13	25:X:53:LEU:HD21	1.96	0.48
5:G:112:ASP:OD2	13:O:72:ARG:NH2	2.46	0.48
9:K:84:ASP:HB3	9:K:137:PHE:HD2	1.78	0.48
19:x:33:LEU:O	19:x:37:THR:N	2.40	0.48
24:W:343:SER:HB2	24:W:347:GLY:H	1.79	0.48
27:Z:39:LEU:HD22	27:Z:50:VAL:HG11	1.95	0.48
27:Z:82:PHE:HA	27:Z:85:VAL:HG12	1.95	0.48
32:f:540:GLN:HA	32:f:543:MET:HG3	1.96	0.48
34:e:31:ASP:OD1	34:e:31:ASP:N	2.46	0.48
2:B:230:THR:HG1	2:B:391:SER:HG	1.60	0.48
5:G:153:LYS:HD2	5:G:166:THR:HG21	1.94	0.48
13:O:193:ASN:ND2	17:s:213:ASP:OD2	2.44	0.48
13:O:214:GLU:HG3	14:P:198:ARG:HG2	1.94	0.48
5:g:123:GLN:O	5:g:126:THR:OG1	2.31	0.48
22:D:171:ASP:O	22:D:175:GLN:HB2	2.12	0.48
27:Z:228:TYR:HA	27:Z:231:GLN:HG3	1.96	0.48
28:a:346:ILE:HA	28:a:349:MET:HE2	1.95	0.48
30:c:190:GLN:O	30:c:194:HIS:ND1	2.37	0.48
32:f:597:VAL:HA	32:f:639:LYS:HE2	1.95	0.48
12:N:9:ASP:OD1	12:N:9:ASP:N	2.45	0.48
21:C:91:PRO:HD2	21:C:92:GLU:HG2	1.95	0.48
28:a:343:LEU:HG	28:a:346:ILE:HD11	1.95	0.48
4:F:338:LEU:HD22	4:F:342:LEU:HD11	1.95	0.48
19:x:224:LYS:HA	19:x:228:SER:HB3	1.93	0.48
21:C:202:ALA:O	21:C:206:HIS:ND1	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:240:TYR:OH	24:W:349:LYS:NZ	2.46	0.48
7:I:41:ASP:N	7:I:41:ASP:OD1	2.46	0.48
16:R:64:ARG:NH1	16:R:67:GLU:OE1	2.47	0.48
28:a:347:LYS:HG3	28:a:350:LYS:HE2	1.95	0.48
32:f:261:ARG:NH1	32:f:293:GLN:OE1	2.38	0.48
32:f:456:ARG:NH2	32:f:487:LEU:O	2.36	0.48
23:U:750:SER:HA	23:U:756:HIS:CE1	2.49	0.48
24:W:396:LEU:HD13	24:W:402:ILE:HD13	1.95	0.48
30:c:150:SER:HB2	30:c:155:VAL:HA	1.96	0.48
32:f:153:SER:H	32:f:156:HIS:HB3	1.79	0.48
32:f:482:ILE:HD12	32:f:518:THR:HB	1.96	0.48
1:A:151:ILE:HD12	1:A:152:PRO:HD2	1.95	0.48
7:I:7:SER:OG	7:I:8:ARG:N	2.45	0.48
10:L:226:ASP:OD1	10:L:226:ASP:N	2.46	0.48
19:x:426:HIS:ND1	19:x:435:HIS:O	2.46	0.48
26:Y:102:ASP:N	26:Y:102:ASP:OD1	2.42	0.48
33:V:277:PRO:HG2	33:V:280:ALA:HB2	1.94	0.48
3:E:295:LEU:O	3:E:298:LYS:NZ	2.47	0.48
5:G:155:ASP:OD1	5:G:159:TYR:N	2.44	0.48
10:l:14:SER:OG	10:l:16:GLN:OE1	2.29	0.48
17:s:13:LEU:HD11	17:s:149:LEU:HD11	1.95	0.48
28:a:250:THR:HA	28:a:253:THR:HG22	1.96	0.48
29:b:157:VAL:HG21	29:b:170:LEU:HD22	1.96	0.48
33:V:394:LEU:HA	33:V:397:ARG:HD2	1.95	0.48
3:E:313:LEU:HG	3:E:343:LEU:HD13	1.96	0.47
5:g:47:CYS:HB2	5:g:221:THR:HG22	1.95	0.47
22:D:184:PRO:HA	22:D:188:PHE:HB3	1.95	0.47
23:U:405:THR:HG21	23:U:438:GLN:HA	1.96	0.47
23:U:456:ASP:N	23:U:456:ASP:OD1	2.47	0.47
5:g:112:ASP:OD1	5:g:112:ASP:N	2.45	0.47
7:i:62:SER:OG	7:i:65:ILE:O	2.29	0.47
9:k:72:ALA:HB1	9:k:225:ASN:HD21	1.79	0.47
24:W:205:ILE:O	24:W:209:ILE:HG12	2.14	0.47
25:X:137:TYR:HB3	25:X:146:ALA:HB2	1.96	0.47
27:Z:84:LYS:HG2	30:c:76:PRO:HG3	1.94	0.47
32:f:732:VAL:HG11	32:f:746:ARG:HH21	1.78	0.47
33:V:474:LEU:HD23	33:V:477:HIS:HD2	1.78	0.47
3:E:360:ASP:N	3:E:360:ASP:OD1	2.44	0.47
4:F:403:ALA:HB1	4:F:419:ASP:HB3	1.96	0.47
24:W:296:LEU:HB3	24:W:302:TYR:CG	2.50	0.47
26:Y:67:VAL:O	26:Y:71:ASN:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:203:ASP:N	26:Y:203:ASP:OD1	2.45	0.47
26:Y:297:ARG:NH1	26:Y:298:GLU:OE2	2.46	0.47
28:a:291:LEU:HB2	28:a:331:VAL:HB	1.96	0.47
1:A:224:LEU:N	35:A:501:ADP:O2A	2.47	0.47
1:A:309:PHE:HE1	4:F:238:ARG:HG2	1.80	0.47
1:A:312:ARG:HB3	1:A:315:ILE:HD13	1.95	0.47
21:C:165:ILE:HG13	21:C:166:GLU:HG3	1.97	0.47
24:W:182:ARG:O	24:W:186:ILE:HB	2.15	0.47
28:a:145:LEU:HD12	28:a:152:HIS:CE1	2.49	0.47
2:B:387:LYS:HG2	2:B:390:LEU:HD13	1.97	0.47
7:I:201:MET:HB3	7:I:203:VAL:HG22	1.96	0.47
8:J:158:ALA:HB3	9:K:58:LEU:HD21	1.97	0.47
13:O:13:VAL:HG22	13:O:177:VAL:HG22	1.96	0.47
8:j:23:GLN:NE2	8:j:148:ASP:OD1	2.47	0.47
11:m:175:GLU:HB3	11:m:196:ILE:HD12	1.97	0.47
19:x:435:HIS:HA	20:y:76:GLY:H	1.78	0.47
21:C:366:ALA:HB1	21:C:378:VAL:HG11	1.97	0.47
23:U:574:LYS:O	23:U:579:ARG:NH2	2.47	0.47
25:X:281:GLY:H	25:X:284:THR:HG22	1.80	0.47
25:X:380:GLN:HB3	26:Y:314:LEU:HA	1.97	0.47
28:a:324:ILE:HG13	28:a:331:VAL:HG13	1.96	0.47
32:f:417:ILE:HG22	32:f:418:LEU:HD12	1.96	0.47
1:A:209:PRO:HB3	1:A:338:ASP:HB2	1.96	0.47
1:A:276:GLU:OE2	2:B:314:ASN:ND2	2.48	0.47
18:T:25:ASP:HA	18:T:187:PHE:HA	1.97	0.47
6:h:69:THR:HG22	6:h:70:LYS:H	1.78	0.47
20:y:26:VAL:HA	20:y:29:LYS:HG2	1.97	0.47
23:U:490:ARG:HD2	23:U:492:ASP:H	1.80	0.47
28:a:91:ASN:OD1	28:a:92:VAL:N	2.48	0.47
33:V:104:THR:HG22	33:V:107:ARG:HH21	1.78	0.47
2:B:288:ASP:HA	2:B:292:THR:HB	1.96	0.47
3:E:182:LEU:HD11	36:E:501:ATP:H2'	1.95	0.47
3:E:199:VAL:HG23	3:E:201:SER:H	1.80	0.47
4:F:357:PRO:HB2	4:F:362:ARG:HG3	1.97	0.47
9:K:16:SER:OG	9:K:18:GLU:OE1	2.32	0.47
10:L:65:HIS:HD2	10:L:221:PHE:HD2	1.61	0.47
17:S:145:LEU:HD22	17:S:178:VAL:HB	1.96	0.47
8:j:62:ILE:HD13	8:j:209:ALA:HB3	1.97	0.47
21:C:150:MET:HE1	21:C:332:HIS:HE1	1.79	0.47
26:Y:5:ASN:ND2	26:Y:207:THR:O	2.48	0.47
28:a:210:VAL:O	28:a:271:LYS:NZ	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:438:ASP:OD1	32:f:438:ASP:N	2.48	0.47
32:f:689:ALA:O	32:f:693:ALA:N	2.42	0.47
33:V:345:ARG:HA	33:V:348:PHE:HD2	1.79	0.47
2:B:183:THR:HG23	2:B:185:ALA:H	1.80	0.47
10:L:27:GLU:HA	10:L:30:LYS:HE3	1.97	0.47
14:P:36:THR:OG1	14:P:38:ASP:OD1	2.32	0.47
7:i:216:LEU:HD12	7:i:225:ILE:HG12	1.97	0.47
22:D:167:ILE:O	22:D:174:LYS:NZ	2.47	0.47
25:X:311:ALA:HA	25:X:314:ARG:HG2	1.96	0.47
28:a:349:MET:SD	28:a:352:ARG:NH1	2.88	0.47
33:V:350:GLN:HB2	33:V:353:LEU:HB3	1.96	0.47
2:B:306:GLN:HA	2:B:309:MET:HE3	1.96	0.47
4:F:295:ARG:H	4:F:339:ASP:HB3	1.79	0.47
16:R:3:THR:HG23	16:R:16:ALA:HB2	1.97	0.47
17:S:133:ASP:N	17:S:133:ASP:OD1	2.48	0.47
17:S:185:ARG:HA	13:o:26:VAL:HB	1.97	0.47
5:g:80:MET:HE2	5:g:87:SER:HA	1.97	0.47
6:h:4:ARG:NH2	8:j:2:SER:O	2.48	0.47
25:X:50:ILE:HD12	25:X:69:LEU:HD11	1.97	0.47
26:Y:189:VAL:HB	26:Y:286:TRP:HZ3	1.79	0.47
27:Z:145:HIS:HB2	27:Z:151:THR:HA	1.97	0.47
29:b:4:GLU:HA	29:b:106:LYS:H	1.80	0.47
32:f:157:GLU:O	32:f:161:HIS:ND1	2.39	0.47
32:f:393:ASP:OD1	32:f:393:ASP:N	2.46	0.47
32:f:630:ASP:OD1	32:f:630:ASP:N	2.45	0.47
2:B:358:GLU:HG3	2:B:362:LYS:HZ2	1.80	0.47
3:E:34:LYS:NZ	3:E:38:LYS:HE3	2.31	0.47
9:K:120:ALA:O	9:K:122:GLN:HG2	2.15	0.47
18:T:79:ASP:OD1	18:T:79:ASP:N	2.45	0.47
1:A:127:ASP:OD1	1:A:127:ASP:N	2.46	0.46
1:A:267:LYS:HD2	1:A:270:CYS:HB2	1.97	0.46
2:B:187:ILE:HG21	2:B:194:ILE:HD11	1.96	0.46
3:E:345:ASN:ND2	4:F:349:ASP:OD1	2.40	0.46
13:O:163:ILE:HG12	13:O:170:GLY:HA2	1.97	0.46
21:C:268:GLU:OE2	21:C:272:THR:OG1	2.34	0.46
24:W:216:GLU:HA	24:W:219:THR:HB	1.98	0.46
24:W:274:VAL:O	24:W:283:GLN:NE2	2.48	0.46
26:Y:319:MET:HE1	26:Y:330:ILE:HG21	1.97	0.46
28:a:261:LEU:HD11	28:a:268:LEU:HD11	1.97	0.46
32:f:145:VAL:HG21	32:f:159:VAL:HG21	1.97	0.46
3:E:159:PHE:O	3:E:163:GLY:N	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:413:THR:HG23	4:F:414:GLU:HG2	1.97	0.46
10:L:122:ARG:NH1	11:M:122:TYR:OH	2.48	0.46
19:x:245:GLN:OE1	19:x:319:ARG:NH2	2.49	0.46
19:x:463:ILE:HA	19:x:466:LEU:HD12	1.97	0.46
21:C:49:ARG:HD2	23:U:639:LEU:HD11	1.97	0.46
23:U:41:SER:O	23:U:41:SER:OG	2.30	0.46
25:X:400:ALA:HB1	27:Z:262:LEU:HD11	1.97	0.46
4:F:183:GLU:HG3	4:F:238:ARG:HB3	1.96	0.46
16:r:104:TRP:NE1	16:r:181:GLU:OE2	2.48	0.46
19:x:356:TYR:HB2	19:x:371:ARG:HH12	1.79	0.46
21:C:99:VAL:HB	21:C:103:ILE:HD11	1.96	0.46
25:X:80:ILE:HG22	25:X:81:SER:H	1.80	0.46
26:Y:13:LYS:HB3	26:Y:146:ARG:HB3	1.96	0.46
30:c:49:VAL:HG23	30:c:50:PRO:HD3	1.97	0.46
32:f:215:ASP:OD1	32:f:216:MET:N	2.48	0.46
2:B:120:HIS:HA	2:B:134:SER:HA	1.97	0.46
7:i:180:LYS:H	7:i:184:MET:HE2	1.80	0.46
10:l:138:ASP:OD1	10:l:138:ASP:N	2.47	0.46
21:C:365:GLU:HG3	21:C:390:VAL:HG11	1.96	0.46
30:c:75:MET:SD	30:c:75:MET:N	2.89	0.46
32:f:729:MET:SD	32:f:751:TYR:OH	2.67	0.46
1:A:146:LYS:HB3	1:A:148:GLN:HG3	1.96	0.46
1:A:415:LYS:HG2	1:A:418:LYS:HE3	1.98	0.46
6:H:143:ARG:HD2	6:H:144:PRO:HD2	1.97	0.46
8:J:177:THR:OG1	8:J:178:ASP:N	2.49	0.46
22:D:265:ASP:N	22:D:265:ASP:OD1	2.48	0.46
25:X:221:GLU:HB3	25:X:223:LYS:HG2	1.97	0.46
27:Z:45:LYS:HA	27:Z:45:LYS:HD3	1.77	0.46
32:f:166:VAL:HA	32:f:170:TRP:HD1	1.81	0.46
1:A:212:VAL:HA	1:A:339:ARG:HB3	1.97	0.46
2:B:117:ASP:OD1	2:B:117:ASP:N	2.48	0.46
4:F:100:ASP:N	4:F:100:ASP:OD1	2.48	0.46
15:q:31:ASP:OD1	15:q:31:ASP:N	2.45	0.46
26:Y:71:ASN:HA	26:Y:74:LYS:HG2	1.97	0.46
30:c:56:LEU:HG	30:c:75:MET:HE1	1.98	0.46
33:V:433:ASP:OD1	33:V:433:ASP:N	2.48	0.46
4:F:339:ASP:N	4:F:339:ASP:OD1	2.48	0.46
18:T:96:MET:HE2	18:T:127:MET:HA	1.98	0.46
23:U:682:TYR:HA	23:U:725:MET:HE1	1.98	0.46
25:X:357:SER:OG	25:X:358:LYS:N	2.48	0.46
26:Y:130:LYS:HG2	26:Y:131:THR:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:V:119:GLY:HA2	33:V:148:ARG:HD3	1.97	0.46
2:B:171:VAL:HG11	2:B:273:VAL:HG21	1.98	0.46
4:F:366:MET:HE3	4:F:381:TYR:HD1	1.80	0.46
13:O:26:VAL:O	17:s:185:ARG:NH1	2.49	0.46
17:S:190:GLY:HA2	17:S:210:LEU:HD23	1.97	0.46
5:g:86:ASP:OD1	11:m:120:HIS:NE2	2.42	0.46
12:n:164:MET:HE3	12:n:171:GLY:HA2	1.96	0.46
21:C:44:ARG:HD3	33:V:491:VAL:HG22	1.97	0.46
23:U:265:ILE:HD11	23:U:326:ILE:HD13	1.98	0.46
33:V:76:LYS:HE3	33:V:149:PRO:HB3	1.96	0.46
2:B:341:LEU:HD23	2:B:347:ILE:HD13	1.97	0.46
3:E:317:ALA:HA	3:E:320:ILE:HD12	1.98	0.46
14:p:47:ASP:OD1	14:p:47:ASP:N	2.47	0.46
19:x:83:SER:OG	32:f:397:LYS:NZ	2.49	0.46
19:x:343:VAL:HG12	19:x:345:LYS:H	1.81	0.46
24:W:81:ASP:N	24:W:81:ASP:OD1	2.48	0.46
1:A:28:GLY:HA3	32:f:53:GLN:HG3	1.98	0.46
11:M:136:MET:HE1	11:M:163:CYS:HB3	1.96	0.46
17:S:110:ILE:HB	17:S:122:TYR:HB2	1.96	0.46
14:p:205:ASP:OD1	14:p:205:ASP:N	2.45	0.46
20:y:63:LYS:HA	20:y:63:LYS:HD2	1.76	0.46
23:U:233:LEU:HD22	23:U:268:LEU:HD21	1.96	0.46
23:U:619:VAL:HG13	23:U:640:LEU:HD13	1.98	0.46
32:f:366:ASP:N	32:f:366:ASP:OD1	2.48	0.46
3:E:81:VAL:HG11	3:E:100:LEU:HD22	1.98	0.45
10:L:138:ASP:OD1	10:L:138:ASP:N	2.48	0.45
17:S:16:ALA:HB2	17:S:121:VAL:HG23	1.98	0.45
19:x:49:LYS:HE3	19:x:70:LEU:HB3	1.98	0.45
26:Y:46:ARG:NH1	26:Y:49:ASN:OD1	2.49	0.45
31:d:44:THR:HA	31:d:47:GLN:HG3	1.98	0.45
32:f:681:TYR:HB3	32:f:761:MET:HB3	1.97	0.45
13:O:143:ARG:NH2	13:O:150:GLU:OE1	2.49	0.45
5:g:205:VAL:HG12	5:g:206:LEU:HD12	1.99	0.45
9:k:38:ILE:HD12	9:k:202:LEU:HG	1.98	0.45
22:D:202:VAL:HA	22:D:329:ARG:HB2	1.98	0.45
26:Y:179:ARG:O	26:Y:183:TYR:N	2.47	0.45
30:c:27:THR:HG22	30:c:28:ALA:H	1.82	0.45
1:A:292:ASP:OD2	2:B:303:ARG:NE	2.40	0.45
8:J:196:LEU:HD11	8:J:229:VAL:HG23	1.97	0.45
14:p:53:LEU:HD23	14:p:107:PRO:HB3	1.98	0.45
17:s:48:ASP:OD1	17:s:48:ASP:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:212:ILE:HD13	21:C:234:LEU:HD13	1.98	0.45
23:U:564:ASP:OD1	23:U:590:TYR:OH	2.33	0.45
32:f:683:GLU:HB3	32:f:686:LEU:HD21	1.98	0.45
8:J:120:GLN:HB2	9:K:133:MET:HE1	1.97	0.45
12:N:138:TYR:O	12:N:142:THR:OG1	2.25	0.45
14:P:159:ASP:OD1	14:P:159:ASP:N	2.49	0.45
16:R:82:LEU:HD23	16:R:86:MET:HE2	1.98	0.45
16:r:37:ILE:HD11	16:r:56:GLU:HB3	1.99	0.45
19:x:170:ILE:HD12	19:x:171:PRO:HD2	1.97	0.45
24:W:405:LYS:HB3	25:X:343:SER:HB3	1.98	0.45
25:X:57:LEU:HD13	25:X:65:GLU:HB3	1.98	0.45
28:a:97:LEU:HD11	28:a:118:ILE:HG23	1.98	0.45
32:f:170:TRP:HA	32:f:178:LYS:HD2	1.98	0.45
32:f:389:LYS:HZ2	32:f:393:ASP:HB3	1.82	0.45
2:B:179:ALA:HB3	2:B:241:ASN:HA	1.99	0.45
4:F:364:ARG:HE	4:F:368:ILE:HG13	1.82	0.45
15:Q:53:THR:HG22	15:Q:100:VAL:HG12	1.97	0.45
8:j:185:ASP:O	8:j:189:LYS:HG2	2.16	0.45
9:k:103:TYR:HE1	17:s:91:MET:HE2	1.81	0.45
19:x:293:ARG:HD3	19:x:294:LEU:HD22	1.98	0.45
23:U:199:ARG:HA	23:U:202:VAL:HG22	1.97	0.45
28:a:78:GLU:HA	28:a:81:LEU:HD23	1.99	0.45
28:a:80:ILE:HD12	28:a:96:PHE:HZ	1.82	0.45
30:c:36:LEU:HD11	30:c:71:ASP:HA	1.99	0.45
4:F:225:MET:HE1	4:F:233:LYS:HB3	1.99	0.45
8:J:159:ASN:OD1	8:J:169:ARG:NH2	2.50	0.45
9:K:91:LYS:HE3	9:K:119:LEU:HD13	1.99	0.45
5:g:206:LEU:HB3	5:g:208:ILE:HG12	1.98	0.45
23:U:889:LEU:HA	23:U:892:LEU:HD23	1.97	0.45
24:W:243:ILE:HA	24:W:246:HIS:CE1	2.52	0.45
32:f:664:GLU:O	32:f:669:GLU:N	2.40	0.45
15:Q:38:MET:HE1	15:Q:61:GLN:HA	1.99	0.45
16:R:41:LEU:HD23	16:R:103:GLY:HA3	1.98	0.45
13:o:214:GLU:HG2	14:p:198:ARG:HG2	1.98	0.45
23:U:558:GLY:H	23:U:589:ALA:HA	1.80	0.45
32:f:308:SER:HB3	32:f:312:GLU:HA	1.98	0.45
32:f:694:LEU:O	32:f:698:SER:N	2.50	0.45
32:f:815:HIS:CE1	32:f:882:LEU:HB2	2.52	0.45
3:E:234:GLU:HG2	4:F:311:LEU:HG	1.98	0.45
3:E:300:HIS:ND1	3:E:302:ASP:OD1	2.49	0.45
5:G:49:VAL:HG22	5:G:219:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:138:VAL:HB	14:P:146:MET:HE2	1.98	0.45
17:S:157:ASN:ND2	14:p:173:ASN:OD1	2.49	0.45
9:k:235:GLU:HA	9:k:238:ILE:HG22	1.99	0.45
13:o:58:LEU:HD23	13:o:86:MET:HE1	1.98	0.45
28:a:269:LEU:HD23	28:a:272:ILE:HD11	1.99	0.45
32:f:79:ARG:HB3	32:f:82:ILE:HG12	1.98	0.45
32:f:106:LEU:HD13	32:f:109:ILE:HD12	1.99	0.45
32:f:214:VAL:HA	32:f:217:LEU:HG	1.99	0.45
32:f:655:LEU:HD21	32:f:675:PHE:HB2	1.98	0.45
33:V:228:ARG:O	33:V:232:HIS:ND1	2.50	0.45
3:E:148:VAL:HG13	3:E:149:ILE:HG13	1.98	0.45
4:F:224:LEU:HB2	4:F:348:LEU:HD22	1.98	0.45
8:J:158:ALA:HB1	8:J:172:LEU:HD13	1.99	0.45
13:O:171:SER:HA	13:O:193:ASN:HD22	1.82	0.45
23:U:416:GLU:OE1	23:U:450:HIS:NE2	2.50	0.45
32:f:236:CYS:SG	32:f:237:VAL:N	2.90	0.45
33:V:442:ILE:HG21	33:V:451:ILE:HD11	1.98	0.45
1:A:26:ASP:OD1	1:A:26:ASP:N	2.49	0.45
2:B:65:LEU:O	2:B:69:LYS:HG2	2.17	0.45
36:E:501:ATP:O1G	4:F:347:ARG:NH2	2.42	0.45
9:K:36:THR:HA	9:K:171:GLY:HA3	1.97	0.45
8:j:171:PHE:O	8:j:175:ASN:ND2	2.34	0.45
8:j:192:ILE:HG12	8:j:229:VAL:HG12	1.98	0.45
10:l:103:LEU:HD23	10:l:108:LEU:HD12	1.99	0.45
19:x:279:ILE:HA	19:x:283:VAL:HG21	1.98	0.45
21:C:293:MET:SD	21:C:293:MET:N	2.90	0.45
22:D:268:ASP:OD2	22:D:316:THR:OG1	2.33	0.45
23:U:475:HIS:NE2	23:U:507:VAL:O	2.50	0.45
23:U:596:ASN:HA	23:U:599:ILE:HG22	1.98	0.45
23:U:902:PRO:HA	23:U:915:LYS:H	1.81	0.45
24:W:305:LEU:HA	24:W:308:LEU:HD12	1.99	0.45
26:Y:197:ALA:HB3	26:Y:226:VAL:HG21	1.99	0.45
26:Y:279:GLU:HA	26:Y:295:TYR:HE1	1.81	0.45
28:a:115:LYS:HD3	28:a:118:ILE:HD12	1.98	0.45
28:a:217:LEU:HD23	28:a:237:LEU:HB3	1.99	0.45
32:f:156:HIS:ND1	32:f:157:GLU:OE2	2.44	0.45
33:V:219:GLU:OE2	33:V:256:ARG:NH1	2.50	0.45
1:A:402:LYS:HE3	2:B:213:GLU:HB3	1.98	0.44
16:R:1:THR:OG1	16:R:2:THR:N	2.50	0.44
18:T:9:THR:OG1	18:T:10:SER:N	2.49	0.44
8:j:158:ALA:HB3	9:k:58:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:72:TYR:O	21:C:116:LEU:N	2.41	0.44
26:Y:192:ARG:HD2	26:Y:192:ARG:HA	1.77	0.44
27:Z:39:LEU:N	27:Z:93:GLY:O	2.48	0.44
28:a:194:GLN:HB2	28:a:226:ARG:HG3	1.99	0.44
32:f:224:ASN:HA	32:f:227:ALA:HB2	1.98	0.44
33:V:419:LEU:HB3	33:V:456:GLY:HA3	1.98	0.44
8:j:105:GLU:OE1	8:j:109:ARG:NH1	2.50	0.44
24:W:280:ASP:HB3	24:W:283:GLN:HB3	1.99	0.44
2:B:71:TYR:OH	32:f:640:LYS:NZ	2.33	0.44
4:F:79:LYS:HB2	4:F:79:LYS:HE2	1.79	0.44
6:H:195:LEU:HD23	6:H:195:LEU:HA	1.84	0.44
13:O:58:LEU:HD23	13:O:86:MET:HE2	1.97	0.44
14:P:53:LEU:HD13	14:P:107:PRO:HB3	2.00	0.44
9:k:83:ALA:O	9:k:86:LYS:NZ	2.49	0.44
21:C:125:LYS:NZ	22:D:112:TYR:OH	2.39	0.44
23:U:360:VAL:HG11	23:U:392:TRP:HE1	1.82	0.44
27:Z:275:LEU:HD13	33:V:486:ILE:HG23	1.99	0.44
32:f:241:PRO:HB3	32:f:253:LEU:HD11	1.98	0.44
32:f:811:LEU:HB2	32:f:856:ALA:HB2	1.99	0.44
8:J:4:ASP:N	8:J:4:ASP:OD1	2.49	0.44
5:g:170:VAL:HG13	5:g:171:LYS:HG2	1.97	0.44
8:j:199:VAL:HG12	8:j:202:GLY:H	1.83	0.44
15:q:11:ASP:N	15:q:11:ASP:OD1	2.48	0.44
28:a:210:VAL:HG23	28:a:213:PHE:CG	2.53	0.44
4:F:80:ILE:O	4:F:84:LYS:N	2.48	0.44
4:F:407:ALA:HB1	4:F:412:ALA:HB3	2.00	0.44
6:H:213:CYS:HB2	6:H:218:PHE:HD1	1.83	0.44
14:P:205:ASP:HB3	16:r:192:VAL:HG11	1.98	0.44
17:S:28:ARG:NE	17:S:191:ASP:OD2	2.39	0.44
18:T:142:GLY:HA2	18:T:176:LEU:HD21	1.99	0.44
15:q:39:SER:OG	15:q:74:GLU:OE1	2.36	0.44
28:a:127:ASP:HA	28:a:131:THR:HG21	1.98	0.44
32:f:107:LYS:HD2	32:f:107:LYS:HA	1.77	0.44
32:f:170:TRP:HE3	32:f:178:LYS:HB2	1.83	0.44
3:E:281:ARG:HE	3:E:386:TYR:HE2	1.65	0.44
3:E:383:LYS:HE2	11:M:3:ILE:HB	1.99	0.44
13:O:212:LEU:HG	14:P:201:LYS:HB3	2.00	0.44
30:c:137:SER:HB3	30:c:140:ALA:HB2	1.98	0.44
32:f:141:LYS:HZ3	32:f:162:LEU:HD22	1.83	0.44
8:J:199:VAL:HG12	8:J:202:GLY:H	1.82	0.44
16:R:21:THR:HG22	16:R:26:ILE:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:s:190:GLY:HA2	17:s:210:LEU:HD23	1.99	0.44
22:D:270:ILE:HG22	22:D:289:LEU:HD21	1.99	0.44
23:U:532:MET:HE1	23:U:555:VAL:HG11	1.99	0.44
30:c:29:GLU:HG2	30:c:65:TYR:HB2	1.99	0.44
32:f:809:ILE:HG23	32:f:855:GLN:HB3	1.99	0.44
32:f:834:ASP:OD1	32:f:834:ASP:N	2.50	0.44
9:K:38:ILE:HD12	9:K:202:LEU:HD22	2.00	0.44
21:C:49:ARG:NH2	22:D:64:GLU:OE2	2.41	0.44
24:W:169:LEU:HD11	24:W:189:GLN:HG3	2.00	0.44
24:W:287:VAL:HA	24:W:290:ILE:HD12	2.00	0.44
25:X:71:LYS:HA	25:X:74:ARG:HH11	1.81	0.44
28:a:34:TRP:O	28:a:38:THR:OG1	2.34	0.44
28:a:143:ASN:O	28:a:145:LEU:HD23	2.18	0.44
31:d:30:LEU:HD11	31:d:54:ILE:HD11	1.99	0.44
1:A:265:ARG:NH2	1:A:305:GLN:O	2.51	0.44
4:F:180:ARG:HH21	4:F:248:PHE:H	1.64	0.44
6:h:70:LYS:HA	6:h:70:LYS:HD2	1.91	0.44
8:j:38:ARG:O	8:j:213:ARG:NH2	2.50	0.44
15:q:181:ARG:NE	15:q:190:ASP:OD1	2.50	0.44
25:X:414:LEU:HD22	30:c:260:GLU:HG2	2.00	0.44
28:a:103:LYS:HG3	28:a:104:VAL:HG23	2.00	0.44
28:a:335:TRP:NE1	28:a:337:GLN:O	2.50	0.44
31:d:158:ILE:HG23	31:d:162:SER:HA	2.00	0.44
32:f:759:LEU:HG	32:f:761:MET:HG3	2.00	0.44
2:B:199:GLU:HA	2:B:203:LEU:HD13	2.00	0.43
4:F:310:MET:SD	4:F:311:LEU:HD22	2.59	0.43
5:g:60:LEU:HD21	11:m:177:GLU:HG3	2.00	0.43
6:h:59:GLU:HG2	6:h:60:ARG:HG3	1.99	0.43
10:l:47:VAL:HG12	10:l:195:LEU:HD22	2.00	0.43
22:D:73:LEU:HD12	27:Z:184:VAL:HG13	2.00	0.43
23:U:161:ASP:OD1	23:U:161:ASP:N	2.51	0.43
24:W:391:ALA:O	24:W:395:ASN:ND2	2.50	0.43
28:a:70:ARG:O	29:b:17:ARG:NH1	2.52	0.43
28:a:247:ARG:HA	28:a:250:THR:HG22	2.00	0.43
2:B:233:THR:N	35:B:501:ADP:O1A	2.51	0.43
16:R:100:MET:HE2	16:R:128:VAL:HG22	2.00	0.43
7:i:153:SER:OG	7:i:155:ASN:OD1	2.36	0.43
19:x:439:TRP:HZ3	19:x:458:VAL:HG21	1.82	0.43
22:D:264:ILE:HD12	22:D:267:ILE:HG21	2.00	0.43
26:Y:144:LEU:HB3	26:Y:160:ASN:HD22	1.83	0.43
32:f:612:LEU:HD21	32:f:636:ASP:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:m:23:VAL:O	11:m:27:MET:HG2	2.17	0.43
19:x:279:ILE:HG12	19:x:283:VAL:HG11	1.99	0.43
22:D:200:ARG:HA	22:D:304:ASN:HB3	1.98	0.43
24:W:142:ARG:HA	24:W:145:LEU:HD12	2.01	0.43
26:Y:220:VAL:HG21	26:Y:249:VAL:HG21	2.00	0.43
26:Y:301:ILE:HG13	26:Y:343:LEU:HD12	2.00	0.43
27:Z:197:GLY:HA2	30:c:225:TRP:CD1	2.53	0.43
27:Z:212:LEU:HA	27:Z:215:VAL:HG12	1.99	0.43
1:A:38:GLN:OE1	1:A:40:THR:OG1	2.36	0.43
9:K:202:LEU:HA	9:K:205:VAL:HG22	2.00	0.43
23:U:94:SER:HB3	23:U:97:VAL:HG12	2.00	0.43
28:a:212:ASN:OD1	28:a:213:PHE:N	2.48	0.43
29:b:131:LEU:HB3	29:b:136:VAL:HB	1.99	0.43
32:f:297:MET:HA	32:f:300:ARG:HG3	2.01	0.43
32:f:815:HIS:HE1	32:f:882:LEU:HB2	1.83	0.43
23:U:163:PHE:O	23:U:166:THR:OG1	2.34	0.43
23:U:367:THR:HA	23:U:370:VAL:HG12	2.00	0.43
24:W:103:LYS:HA	24:W:103:LYS:HD3	1.78	0.43
24:W:219:THR:HG21	24:W:223:LYS:H	1.83	0.43
27:Z:74:TYR:CZ	30:c:98:MET:HG3	2.54	0.43
32:f:466:LEU:HB3	32:f:485:LEU:HD12	2.00	0.43
32:f:773:LYS:HA	32:f:776:LEU:HD23	2.00	0.43
16:R:9:ARG:HE	16:R:146:ASP:HA	1.83	0.43
14:p:68:LYS:HD2	14:p:68:LYS:HA	1.80	0.43
18:t:107:TRP:CE3	18:t:127:MET:HE1	2.54	0.43
28:a:278:MET:HE3	28:a:339:ARG:HE	1.84	0.43
29:b:5:SER:HB2	29:b:107:MET:HA	2.00	0.43
31:d:49:ILE:HD12	31:d:52:ARG:HH21	1.83	0.43
31:d:140:GLU:O	31:d:144:MET:HG2	2.19	0.43
31:d:162:SER:OG	31:d:163:TYR:N	2.52	0.43
4:F:121:CYS:HA	4:F:133:PHE:HE1	1.83	0.43
10:L:47:VAL:HG12	10:L:195:LEU:HD22	2.01	0.43
10:L:107:ARG:NH2	18:T:74:GLU:OE2	2.36	0.43
17:S:83:MET:HE3	17:S:88:ILE:HG12	2.00	0.43
7:i:119:GLN:HG3	8:j:78:ALA:HB1	2.00	0.43
10:l:36:VAL:HG22	10:l:160:SER:HB2	1.99	0.43
15:q:59:TYR:O	15:q:63:ASN:ND2	2.52	0.43
19:x:212:GLN:HG2	19:x:213:GLN:HG3	2.00	0.43
19:x:448:ILE:HG23	19:x:455:VAL:HG13	2.01	0.43
22:D:404:LYS:HZ3	22:D:410:ASP:HB3	1.83	0.43
26:Y:191:ILE:HB	34:e:39:TRP:HD1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:231:LEU:HD11	26:Y:239:LYS:HD2	2.00	0.43
27:Z:43:TRP:HB3	27:Z:48:LEU:HD13	2.00	0.43
28:a:325:ASP:OD1	28:a:326:GLU:N	2.52	0.43
32:f:560:LEU:HD23	32:f:594:LEU:HD21	2.00	0.43
32:f:569:LYS:HB2	32:f:573:ILE:HD12	2.01	0.43
1:A:27:GLU:OE2	21:C:171:HIS:NE2	2.40	0.43
1:A:365:GLU:HG2	1:A:367:ASP:H	1.83	0.43
2:B:137:SER:OG	2:B:138:PHE:N	2.52	0.43
10:L:217:LYS:HA	10:L:217:LYS:HD3	1.93	0.43
18:T:99:ARG:HD2	18:T:99:ARG:HA	1.88	0.43
23:U:97:VAL:HA	23:U:100:ILE:HG12	2.01	0.43
28:a:89:ASP:OD1	28:a:89:ASP:N	2.49	0.43
28:a:372:HIS:HA	28:a:375:LEU:HG	2.01	0.43
29:b:40:LYS:HD3	29:b:40:LYS:HA	1.81	0.43
29:b:61:LEU:HD23	29:b:74:LYS:HE3	2.01	0.43
31:d:52:ARG:HH12	31:d:94:TYR:HE1	1.66	0.43
32:f:65:GLU:HG2	32:f:98:PHE:HE2	1.84	0.43
32:f:320:ILE:HG22	32:f:325:GLN:HG3	1.99	0.43
33:V:466:ILE:O	33:V:470:ARG:HD3	2.19	0.43
1:A:38:GLN:HG3	1:A:41:TYR:HB2	2.00	0.43
1:A:433:ASN:HB3	9:K:53:ARG:HH21	1.83	0.43
2:B:44:ASP:OD1	2:B:44:ASP:N	2.48	0.43
2:B:67:ARG:HH12	32:f:605:ASN:HA	1.84	0.43
14:P:28:PHE:HD2	14:P:36:THR:HG22	1.84	0.43
16:R:127:SER:HB3	16:R:136:TYR:CE1	2.54	0.43
16:r:96:SER:O	16:r:96:SER:OG	2.36	0.43
22:D:77:GLU:HG2	22:D:80:LYS:HE3	2.00	0.43
23:U:466:LYS:HA	23:U:466:LYS:HD3	1.81	0.43
33:V:70:VAL:HG12	33:V:107:ARG:HH12	1.84	0.43
1:A:292:ASP:HB2	2:B:303:ARG:HH21	1.84	0.43
2:B:411:ARG:NH1	2:B:418:ASP:OD2	2.43	0.43
9:K:146:VAL:HG11	9:K:222:PRO:HA	2.01	0.43
15:Q:11:ASP:N	15:Q:11:ASP:OD1	2.50	0.43
17:s:19:ASP:OD1	17:s:19:ASP:N	2.52	0.43
21:C:266:ASP:HB2	21:C:269:VAL:HG23	2.01	0.43
23:U:197:VAL:HA	23:U:200:VAL:HG12	2.01	0.43
25:X:182:ASN:HA	26:Y:244:ALA:HB1	2.00	0.43
25:X:245:PRO:HA	25:X:248:ILE:HG22	2.00	0.43
32:f:186:THR:HA	32:f:189:LYS:HG2	2.00	0.43
3:E:147:GLU:HG3	3:E:151:LEU:HG	2.01	0.42
5:G:76:ILE:HD12	5:G:111:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:26:ILE:HG21	16:R:29:GLN:HE21	1.84	0.42
16:r:182:ASP:OD1	16:r:183:GLY:N	2.52	0.42
17:s:198:VAL:HG22	17:s:203:ILE:HG12	2.02	0.42
22:D:304:ASN:O	22:D:306:LYS:NZ	2.51	0.42
23:U:261:LEU:HA	23:U:264:VAL:HG12	2.00	0.42
23:U:811:PHE:HE1	23:U:874:ASN:HA	1.84	0.42
25:X:303:GLU:O	25:X:307:THR:OG1	2.29	0.42
33:V:131:LEU:HD22	33:V:171:VAL:HG11	2.01	0.42
33:V:278:GLU:HA	33:V:285:TRP:HZ2	1.84	0.42
2:B:230:THR:HG21	2:B:356:PRO:HG3	2.01	0.42
2:B:396:LYS:HE3	2:B:396:LYS:HB3	1.85	0.42
3:E:48:LYS:HG2	27:Z:88:ARG:HH12	1.84	0.42
4:F:363:ALA:HA	4:F:366:MET:HE2	2.01	0.42
8:J:42:VAL:HG13	8:J:210:VAL:HG12	2.01	0.42
7:i:41:ASP:OD1	7:i:41:ASP:N	2.52	0.42
23:U:35:TRP:HZ3	33:V:270:LEU:HD12	1.82	0.42
23:U:447:GLY:HA3	23:U:480:GLY:HA2	2.01	0.42
24:W:54:THR:HB	24:W:59:ASP:HB3	2.01	0.42
26:Y:293:ARG:O	26:Y:297:ARG:NE	2.52	0.42
28:a:309:LEU:HG	28:a:312:MET:HE2	2.01	0.42
10:L:204:ASP:N	10:L:204:ASP:OD1	2.50	0.42
16:R:148:GLU:HB3	16:R:151:GLN:HG3	2.01	0.42
17:S:144:MET:HE1	17:S:185:ARG:HB2	2.02	0.42
7:i:123:GLN:HA	8:j:125:ARG:HE	1.84	0.42
23:U:32:ASN:O	23:U:35:TRP:NE1	2.52	0.42
24:W:71:VAL:HG21	24:W:104:MET:SD	2.59	0.42
27:Z:177:ARG:HD2	27:Z:177:ARG:HA	1.82	0.42
28:a:333:MET:SD	28:a:333:MET:N	2.92	0.42
31:d:19:CYS:SG	31:d:20:GLY:N	2.91	0.42
32:f:199:ASN:OD1	32:f:200:ALA:N	2.53	0.42
32:f:729:MET:SD	32:f:729:MET:N	2.93	0.42
33:V:296:LYS:HB3	33:V:301:GLU:HB3	2.01	0.42
3:E:364:GLN:HA	3:E:367:PHE:HD2	1.83	0.42
12:N:162:LEU:HD11	12:n:141:ALA:HB2	2.01	0.42
7:i:53:HIS:HB3	7:i:56:LEU:HD23	2.00	0.42
11:m:37:ILE:HD11	11:m:193:VAL:HG13	2.01	0.42
23:U:248:ILE:HD12	23:U:248:ILE:HA	1.81	0.42
25:X:377:ILE:HG12	26:Y:312:ARG:HB2	2.02	0.42
25:X:416:ASN:HB3	26:Y:383:LEU:HD13	2.01	0.42
30:c:240:HIS:O	30:c:244:VAL:HG23	2.20	0.42
30:c:253:LYS:HD2	30:c:253:LYS:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:405:HIS:HB3	32:f:797:LEU:HD21	2.02	0.42
3:E:101:ASP:OD2	3:E:103:THR:OG1	2.36	0.42
4:F:434:ASN:OD1	10:L:51:ARG:NH2	2.53	0.42
8:J:210:VAL:HG13	8:J:220:LEU:HD21	2.02	0.42
12:N:68:ILE:HD12	12:N:68:ILE:HA	1.93	0.42
12:N:119:MET:HE1	18:T:6:VAL:HB	2.02	0.42
6:h:189:HIS:HA	6:h:233:ILE:HD11	2.02	0.42
19:x:48:VAL:HA	19:x:69:LEU:HD22	2.01	0.42
25:X:142:ARG:HB3	25:X:145:GLU:HG2	2.01	0.42
26:Y:39:ASP:OD1	26:Y:39:ASP:N	2.51	0.42
1:A:222:LYS:H	35:A:501:ADP:PA	2.42	0.42
1:A:334:PRO:HG2	4:F:395:GLN:HE21	1.84	0.42
3:E:209:GLY:HA2	22:D:236:VAL:HG23	2.01	0.42
9:K:26:TYR:HA	9:K:29:GLU:HG3	2.01	0.42
12:N:119:MET:HE2	18:T:57:TYR:HB3	2.00	0.42
6:h:133:SER:OG	6:h:149:SER:O	2.36	0.42
11:m:8:ASP:N	11:m:8:ASP:OD1	2.52	0.42
24:W:247:TYR:HA	24:W:250:ILE:HG12	2.01	0.42
26:Y:283:LYS:HB2	26:Y:283:LYS:HE3	1.79	0.42
27:Z:145:HIS:CD2	27:Z:152:SER:HB3	2.54	0.42
32:f:75:LEU:HD22	32:f:78:LEU:HD22	2.00	0.42
32:f:93:PRO:HA	32:f:96:LEU:HD13	2.02	0.42
3:E:180:LYS:HD2	3:E:278:ALA:HB1	2.00	0.42
9:K:21:LEU:HB2	9:K:24:VAL:HG12	2.01	0.42
20:y:22:THR:HG22	20:y:24:GLU:H	1.85	0.42
21:C:162:LYS:HE3	21:C:206:HIS:HD2	1.85	0.42
28:a:270:ARG:HD2	28:a:270:ARG:HA	1.78	0.42
1:A:128:GLN:HE22	1:A:150:HIS:CD2	2.38	0.42
3:E:171:LEU:HD23	3:E:298:LYS:HG3	2.01	0.42
3:E:212:ALA:HA	3:E:215:ILE:HD12	2.02	0.42
6:H:99:LEU:HD23	6:H:99:LEU:HA	1.89	0.42
9:k:147:ASP:N	9:k:147:ASP:OD1	2.53	0.42
19:x:465:ARG:HA	19:x:465:ARG:HD2	1.90	0.42
22:D:133:HIS:HB3	22:D:137:ASN:H	1.85	0.42
25:X:340:GLU:OE1	25:X:340:GLU:N	2.44	0.42
26:Y:142:PHE:HB3	26:Y:146:ARG:HH21	1.85	0.42
28:a:129:GLN:HG2	28:a:130:VAL:H	1.85	0.42
31:d:52:ARG:HH11	31:d:82:TYR:HE1	1.68	0.42
31:d:151:VAL:O	31:d:155:LYS:CB	2.68	0.42
32:f:181:ARG:HA	32:f:181:ARG:HD3	1.80	0.42
1:A:265:ARG:HH11	1:A:310:ASP:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:LEU:HD22	2:B:304:GLU:HG2	2.01	0.42
3:E:119:VAL:HA	3:E:122:MET:HG3	2.02	0.42
4:F:98:ASP:OD1	4:F:98:ASP:N	2.52	0.42
4:F:152:GLY:N	4:F:162:GLU:O	2.40	0.42
4:F:378:ASP:N	4:F:378:ASP:OD1	2.52	0.42
6:H:9:SER:HB3	6:H:12:THR:HG22	2.01	0.42
12:N:103:TRP:CZ2	12:N:181:GLU:HG2	2.55	0.42
14:P:172:LEU:HD23	14:P:172:LEU:HA	1.92	0.42
14:p:71:LEU:HD11	14:p:82:ILE:HG21	2.02	0.42
18:t:22:ILE:HG23	18:t:50:MET:HE3	2.02	0.42
19:x:49:LYS:H	19:x:69:LEU:HD22	1.85	0.42
19:x:88:PHE:HD1	32:f:368:ALA:H	1.68	0.42
23:U:772:TRP:HB3	23:U:775:LEU:HG	2.02	0.42
23:U:862:LYS:HG2	23:U:863:GLU:H	1.85	0.42
26:Y:208:PHE:CD2	26:Y:211:TYR:HB2	2.55	0.42
31:d:193:GLU:HA	31:d:197:ILE:HD13	2.01	0.42
32:f:325:GLN:OE1	32:f:329:ASN:ND2	2.52	0.42
32:f:826:GLN:HG3	32:f:846:VAL:HG13	2.02	0.42
33:V:123:SER:OG	33:V:155:ALA:O	2.38	0.42
6:H:39:LYS:NZ	6:H:143:ARG:HH12	2.18	0.42
14:P:34:MET:O	16:r:166:ARG:NH1	2.53	0.42
8:j:14:GLY:HA3	9:k:30:ALA:HB2	2.02	0.42
17:s:83:MET:HG2	17:s:88:ILE:HG13	2.02	0.42
23:U:530:GLU:HA	23:U:533:VAL:HG12	2.02	0.42
32:f:269:ALA:HA	32:f:272:LEU:HB3	2.01	0.42
3:E:306:GLU:HB2	3:E:332:VAL:HG13	2.02	0.41
4:F:169:ASP:OD2	4:F:171:ARG:NE	2.43	0.41
4:F:417:HIS:NE2	4:F:421:MET:SD	2.93	0.41
9:K:24:VAL:O	9:K:28:ILE:HG12	2.20	0.41
10:L:117:GLN:NE2	11:M:83:ASP:OD1	2.53	0.41
14:p:10:ALA:HB1	14:p:146:MET:HE1	2.02	0.41
22:D:93:LEU:HG	22:D:104:GLY:H	1.84	0.41
22:D:231:VAL:HB	22:D:234:GLU:HB3	2.02	0.41
23:U:203:LYS:HA	23:U:206:MET:HE2	2.00	0.41
24:W:24:VAL:HG11	24:W:62:SER:HB3	2.02	0.41
24:W:372:ARG:HG2	24:W:414:ASN:HB3	2.03	0.41
25:X:259:ILE:HD13	25:X:259:ILE:HA	1.87	0.41
26:Y:68:ASP:OD1	26:Y:68:ASP:N	2.53	0.41
27:Z:202:ASN:HD21	28:a:360:VAL:HG12	1.84	0.41
27:Z:257:MET:HE3	33:V:469:THR:HG22	2.02	0.41
7:I:54:LYS:HA	7:I:54:LYS:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:163:ILE:HG12	13:o:170:GLY:HA2	2.02	0.41
28:a:370:GLN:HG3	31:d:247:ILE:HG21	2.01	0.41
32:f:590:PHE:HB3	32:f:632:LYS:HA	2.02	0.41
32:f:672:LEU:HD11	32:f:694:LEU:HD13	2.02	0.41
32:f:691:PRO:HB2	32:f:712:LYS:HE3	2.02	0.41
4:F:381:TYR:HA	4:F:384:LEU:HB2	2.02	0.41
5:G:80:MET:HG3	5:G:87:SER:HB3	2.02	0.41
6:H:86:LEU:HD23	6:H:86:LEU:HA	1.86	0.41
11:M:77:VAL:HG11	11:M:84:ALA:HB1	2.02	0.41
18:T:6:VAL:HG22	18:T:30:TYR:HB2	2.02	0.41
23:U:253:TYR:HA	23:U:261:LEU:HD11	2.03	0.41
23:U:825:LYS:HE3	23:U:825:LYS:HB3	1.87	0.41
24:W:153:LYS:HA	24:W:153:LYS:HD3	1.74	0.41
24:W:409:LEU:HD21	25:X:344:ARG:HG2	2.01	0.41
25:X:225:TRP:O	25:X:229:TYR:N	2.46	0.41
26:Y:164:ALA:HA	26:Y:168:ILE:HB	2.01	0.41
26:Y:251:HIS:HA	26:Y:257:ARG:HE	1.85	0.41
31:d:221:ASN:OD1	31:d:222:TYR:N	2.54	0.41
31:d:227:SER:OG	31:d:228:GLN:OE1	2.34	0.41
32:f:584:SER:HB2	32:f:588:ARG:HD3	2.02	0.41
1:A:362:MET:HB3	1:A:364:VAL:HG13	2.02	0.41
6:h:133:SER:OG	6:h:148:GLN:NE2	2.53	0.41
9:k:99:HIS:HB2	9:k:107:MET:HE2	2.03	0.41
13:o:78:THR:O	13:o:82:MET:HG3	2.20	0.41
19:x:249:VAL:HG11	19:x:275:LEU:HD21	2.01	0.41
21:C:221:GLN:NE2	21:C:230:MET:SD	2.93	0.41
22:D:405:THR:OG1	22:D:406:VAL:N	2.54	0.41
23:U:340:GLN:OE1	23:U:344:ARG:NH2	2.53	0.41
24:W:132:THR:HA	24:W:144:ARG:HH12	1.85	0.41
26:Y:160:ASN:HA	26:Y:163:LYS:HG2	2.02	0.41
27:Z:239:ASP:HB2	30:c:309:PHE:HB3	2.01	0.41
28:a:36:GLN:HA	28:a:39:LEU:HD12	2.02	0.41
28:a:54:ASP:OD1	28:a:54:ASP:N	2.53	0.41
32:f:23:GLY:HA3	32:f:30:GLY:HA3	2.02	0.41
32:f:437:GLU:HB3	32:f:440:ILE:HB	2.03	0.41
3:E:383:LYS:HE3	3:E:386:TYR:HD1	1.85	0.41
4:F:172:VAL:HG22	4:F:267:LEU:HD12	2.03	0.41
4:F:185:TYR:CZ	4:F:243:GLN:HG3	2.56	0.41
9:K:79:SER:HB3	9:K:170:ILE:HD12	2.03	0.41
13:O:55:THR:HG23	13:O:86:MET:HE1	2.03	0.41
13:O:146:MET:HE1	13:O:154:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:170:ARG:HG3	15:q:26:VAL:HG23	2.02	0.41
16:R:95:LEU:HD23	16:R:95:LEU:HA	1.92	0.41
17:S:27:THR:HB	17:S:40:SER:H	1.86	0.41
17:S:48:ASP:N	17:S:48:ASP:OD1	2.50	0.41
5:g:59:LYS:HD3	5:g:59:LYS:HA	1.84	0.41
7:i:238:LYS:HB2	7:i:238:LYS:HE2	1.79	0.41
22:D:352:MET:HB3	22:D:354:LEU:HD23	2.02	0.41
24:W:227:TYR:O	24:W:231:ILE:HG23	2.19	0.41
26:Y:346:LYS:NZ	33:V:412:LEU:O	2.49	0.41
27:Z:44:GLN:N	27:Z:44:GLN:OE1	2.53	0.41
1:A:128:GLN:HE22	1:A:150:HIS:HD2	1.68	0.41
2:B:225:TYR:OH	2:B:352:GLU:OE2	2.32	0.41
12:N:4:MET:HG3	12:N:127:ILE:HG22	2.03	0.41
15:Q:29:LYS:HE3	15:Q:32:HIS:HA	2.02	0.41
6:h:44:VAL:HG23	6:h:144:PRO:HB2	2.02	0.41
8:j:47:LYS:HB2	8:j:47:LYS:HE3	1.88	0.41
21:C:113:ARG:HG3	21:C:130:LYS:HZ3	1.85	0.41
22:D:293:LEU:HA	22:D:296:MET:HG3	2.02	0.41
23:U:443:LEU:HD22	23:U:461:LEU:HG	2.02	0.41
24:W:98:LYS:HE2	24:W:138:VAL:HB	2.02	0.41
32:f:29:SER:O	32:f:33:ARG:HG3	2.20	0.41
32:f:80:ARG:O	32:f:80:ARG:NH1	2.54	0.41
32:f:688:ARG:HH22	32:f:719:PRO:HB3	1.84	0.41
32:f:764:LEU:HD23	32:f:764:LEU:HA	1.93	0.41
32:f:771:LEU:HD23	32:f:773:LYS:H	1.86	0.41
33:V:355:ARG:HG3	33:V:358:MET:HE2	2.02	0.41
4:F:263:ASP:HB3	4:F:267:LEU:HB3	2.01	0.41
6:H:49:GLU:HA	6:H:208:ILE:HG22	2.03	0.41
9:K:103:TYR:HE1	17:S:91:MET:HE2	1.85	0.41
6:h:213:CYS:HB3	6:h:218:PHE:HD1	1.85	0.41
8:j:80:ALA:O	8:j:84:ILE:HG12	2.21	0.41
8:j:83:VAL:HG21	8:j:129:ILE:HD11	2.01	0.41
9:k:70:ILE:HD11	9:k:89:ILE:HD12	2.02	0.41
10:l:139:ASP:N	10:l:139:ASP:OD1	2.53	0.41
10:l:206:THR:HG23	10:l:208:LYS:H	1.84	0.41
16:r:100:MET:HE2	16:r:126:PHE:HB3	2.02	0.41
19:x:276:SER:O	19:x:293:ARG:NE	2.53	0.41
23:U:402:PHE:HB2	23:U:437:TYR:HB3	2.02	0.41
25:X:68:GLY:O	25:X:72:TYR:HB3	2.21	0.41
26:Y:104:MET:HE1	26:Y:123:ALA:O	2.21	0.41
26:Y:133:ALA:HB3	26:Y:136:HIS:CD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:c:196:LEU:HA	30:c:199:HIS:CD2	2.55	0.41
32:f:297:MET:HG3	32:f:491:GLY:HA3	2.03	0.41
32:f:670:MET:SD	32:f:703:ARG:NE	2.93	0.41
1:A:97:ARG:HE	2:B:131:HIS:CE1	2.38	0.41
1:A:223:THR:N	35:A:501:ADP:O2A	2.53	0.41
5:G:80:MET:HE1	5:G:138:MET:HB2	2.03	0.41
13:o:84:LYS:HB2	13:o:84:LYS:HE3	1.91	0.41
20:y:4:PHE:HE1	20:y:14:THR:HG22	1.85	0.41
23:U:804:SER:OG	23:U:805:ASN:N	2.53	0.41
26:Y:137:ARG:HB3	26:Y:168:ILE:HD13	2.03	0.41
26:Y:192:ARG:HG3	26:Y:196:GLN:HB2	2.02	0.41
26:Y:383:LEU:HD21	27:Z:272:LEU:HD13	2.02	0.41
32:f:809:ILE:O	32:f:856:ALA:N	2.49	0.41
1:A:224:LEU:HB2	35:A:501:ADP:H3'	2.03	0.41
2:B:79:ILE:HD13	2:B:79:ILE:HA	1.95	0.41
3:E:83:CYS:HB2	3:E:89:LYS:HD3	2.03	0.41
3:E:198:VAL:HG12	3:E:200:SER:H	1.85	0.41
4:F:70:LYS:HA	4:F:73:ILE:HG22	2.03	0.41
5:G:141:ILE:HD12	5:G:220:VAL:HG12	2.03	0.41
6:H:135:LEU:HD23	6:H:135:LEU:HA	1.96	0.41
10:L:133:LEU:HD23	10:L:133:LEU:HA	1.93	0.41
11:M:198:TYR:OH	11:M:236:GLU:OE1	2.39	0.41
13:O:103:VAL:HG11	13:O:180:LYS:HA	2.02	0.41
8:j:189:LYS:HA	8:j:192:ILE:HG22	2.01	0.41
11:m:191:LYS:HB3	11:m:238:TYR:CD2	2.56	0.41
21:C:71:SER:OG	21:C:116:LEU:O	2.34	0.41
22:D:166:ASP:OD1	22:D:166:ASP:N	2.54	0.41
22:D:361:GLU:HA	22:D:364:VAL:HB	2.03	0.41
22:D:410:ASP:OD1	22:D:410:ASP:N	2.47	0.41
26:Y:148:GLY:HA2	26:Y:153:ASP:HB2	2.03	0.41
26:Y:231:LEU:HD12	26:Y:234:PRO:HG2	2.03	0.41
27:Z:38:VAL:HB	27:Z:54:PHE:CE1	2.56	0.41
28:a:267:GLN:O	28:a:271:LYS:HG2	2.21	0.41
31:d:146:GLY:HA3	33:V:437:ILE:HG13	2.03	0.41
32:f:766:GLN:OE1	32:f:769:THR:OG1	2.34	0.41
4:F:202:ILE:O	4:F:205:PRO:HD2	2.21	0.41
8:J:47:LYS:HE3	8:J:47:LYS:HB3	1.92	0.41
9:K:77:ALA:HB3	9:K:142:LEU:HB2	2.03	0.41
10:L:45:VAL:HG12	10:L:214:ILE:HG12	2.02	0.41
8:j:184:ASP:OD1	8:j:185:ASP:N	2.54	0.41
12:n:45:ARG:HD2	12:n:52:THR:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:496:LEU:HA	23:U:499:THR:HG22	2.03	0.41
25:X:177:TYR:HB3	25:X:182:ASN:HB3	2.03	0.41
26:Y:104:MET:HA	26:Y:107:LYS:HB3	2.03	0.41
27:Z:23:PHE:HA	27:Z:35:VAL:HG21	2.01	0.41
27:Z:54:PHE:O	27:Z:95:TYR:OH	2.26	0.41
27:Z:59:ASP:HB3	29:b:95:LEU:HD11	2.03	0.41
32:f:392:THR:HG21	32:f:417:ILE:HG21	2.03	0.41
32:f:623:LYS:HG3	32:f:625:LYS:H	1.86	0.41
1:A:86:THR:OG1	1:A:87:LEU:N	2.54	0.40
2:B:248:LEU:HB2	2:B:282:VAL:HG22	2.03	0.40
5:G:186:LYS:HA	5:G:186:LYS:HD3	1.78	0.40
17:s:10:GLY:HA3	17:s:42:LYS:HE2	2.03	0.40
21:C:328:ILE:HG23	21:C:332:HIS:CE1	2.56	0.40
24:W:102:ALA:HA	24:W:105:VAL:HG22	2.02	0.40
24:W:272:LEU:HD22	24:W:341:PHE:HE2	1.85	0.40
25:X:173:GLU:HA	25:X:176:THR:HG22	2.03	0.40
32:f:610:GLN:HG3	32:f:614:HIS:CE1	2.57	0.40
1:A:73:ALA:HB3	1:A:78:TRP:HE1	1.86	0.40
1:A:214:LEU:HA	1:A:341:ILE:HB	2.03	0.40
5:G:118:ILE:HD13	5:G:118:ILE:HA	1.94	0.40
10:L:22:ILE:HG21	10:L:150:SER:HB3	2.03	0.40
9:k:233:GLU:HA	9:k:236:GLU:HB3	2.04	0.40
10:l:236:LEU:HD12	10:l:236:LEU:HA	1.95	0.40
12:n:84:LYS:HD3	12:n:120:MET:HE3	2.02	0.40
17:s:212:LYS:H	17:s:212:LYS:HG2	1.68	0.40
23:U:792:ASN:OD1	23:U:793:LYS:N	2.53	0.40
25:X:171:LEU:HD21	25:X:210:LEU:HD22	2.03	0.40
26:Y:350:VAL:HG11	33:V:457:TYR:HE1	1.87	0.40
30:c:300:LEU:HA	30:c:303:MET:SD	2.61	0.40
2:B:106:PRO:HB3	21:C:121:TYR:HD2	1.86	0.40
4:F:206:MET:N	4:F:206:MET:SD	2.95	0.40
8:J:132:LEU:HD21	8:J:159:ASN:HB3	2.04	0.40
6:h:95:GLN:HG3	13:o:65:LEU:HD22	2.04	0.40
7:i:240:HIS:O	7:i:244:GLU:HB2	2.21	0.40
9:k:27:ALA:O	9:k:31:ILE:HG12	2.21	0.40
10:l:22:ILE:HD13	10:l:22:ILE:HA	1.96	0.40
10:l:72:ILE:HG22	10:l:134:ILE:HG12	2.02	0.40
32:f:570:GLY:O	32:f:574:GLU:N	2.45	0.40
33:V:86:VAL:HG21	33:V:160:LEU:HD13	2.03	0.40
2:B:411:ARG:HG3	32:f:50:LYS:HG3	2.03	0.40
12:N:40:ARG:NH2	12:N:181:GLU:O	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:196:PHE:HA	15:Q:197:PRO:HD3	1.95	0.40
18:T:12:LEU:HD21	18:T:176:LEU:HD11	2.04	0.40
13:o:106:THR:OG1	13:o:109:HIS:NE2	2.36	0.40
21:C:25:LEU:HA	21:C:28:ILE:HG12	2.04	0.40
22:D:130:VAL:HB	22:D:139:LEU:HD13	2.03	0.40
23:U:373:ASN:HA	23:U:376:MET:HG2	2.04	0.40
24:W:293:ASP:H	24:W:296:LEU:HD12	1.87	0.40
24:W:307:LYS:HE3	24:W:307:LYS:HB3	1.98	0.40
26:Y:48:ASN:ND2	26:Y:74:LYS:HB3	2.36	0.40
32:f:126:ILE:HG23	32:f:178:LYS:HD3	2.02	0.40
32:f:288:VAL:HA	32:f:291:GLN:HB2	2.03	0.40
32:f:373:ALA:HB2	32:f:744:MET:HE1	2.03	0.40
1:A:190:VAL:HG21	1:A:341:ILE:HD11	2.02	0.40
3:E:164:ILE:HG12	22:D:380:GLN:HG3	2.03	0.40
18:T:50:MET:HB3	18:T:197:VAL:HG21	2.04	0.40
12:n:104:ASP:OD1	12:n:104:ASP:N	2.55	0.40
15:q:4:LEU:HD22	15:q:45:LEU:HD23	2.04	0.40
23:U:794:ASP:OD1	23:U:794:ASP:N	2.55	0.40
27:Z:190:ARG:NH2	27:Z:193:ASN:ND2	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/433 (95%)	375 (91%)	36 (9%)	0	100	100
2	B	409/440 (93%)	367 (90%)	42 (10%)	0	100	100
3	E	387/403 (96%)	359 (93%)	27 (7%)	1 (0%)	36	65
4	F	396/439 (90%)	373 (94%)	23 (6%)	0	100	100
5	G	238/246 (97%)	226 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	g	242/246 (98%)	232 (96%)	10 (4%)	0	100	100
6	H	230/234 (98%)	220 (96%)	10 (4%)	0	100	100
6	h	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
7	I	246/261 (94%)	235 (96%)	11 (4%)	0	100	100
7	i	248/261 (95%)	238 (96%)	10 (4%)	0	100	100
8	J	237/248 (96%)	222 (94%)	15 (6%)	0	100	100
8	j	237/248 (96%)	229 (97%)	8 (3%)	0	100	100
9	K	236/241 (98%)	224 (95%)	12 (5%)	0	100	100
9	k	232/241 (96%)	223 (96%)	9 (4%)	0	100	100
10	L	238/269 (88%)	227 (95%)	11 (5%)	0	100	100
10	l	236/269 (88%)	230 (98%)	6 (2%)	0	100	100
11	M	240/255 (94%)	233 (97%)	7 (3%)	0	100	100
11	m	238/255 (93%)	234 (98%)	4 (2%)	0	100	100
12	N	201/239 (84%)	194 (96%)	7 (4%)	0	100	100
12	n	200/239 (84%)	196 (98%)	4 (2%)	0	100	100
13	O	218/277 (79%)	209 (96%)	9 (4%)	0	100	100
13	o	218/277 (79%)	208 (95%)	10 (5%)	0	100	100
14	P	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
14	p	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
15	Q	197/201 (98%)	191 (97%)	6 (3%)	0	100	100
15	q	197/201 (98%)	190 (96%)	7 (4%)	0	100	100
16	R	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
16	r	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
17	S	211/241 (88%)	201 (95%)	10 (5%)	0	100	100
17	s	211/241 (88%)	205 (97%)	6 (3%)	0	100	100
18	T	214/264 (81%)	205 (96%)	9 (4%)	0	100	100
18	t	214/264 (81%)	206 (96%)	8 (4%)	0	100	100
19	x	492/494 (100%)	477 (97%)	15 (3%)	0	100	100
20	y	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
21	C	394/398 (99%)	353 (90%)	40 (10%)	1 (0%)	36	65
22	D	378/418 (90%)	337 (89%)	41 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	U	868/953 (91%)	828 (95%)	40 (5%)	0	100	100
24	W	444/456 (97%)	420 (95%)	22 (5%)	2 (0%)	24	57
25	X	378/422 (90%)	355 (94%)	22 (6%)	1 (0%)	36	65
26	Y	387/389 (100%)	349 (90%)	35 (9%)	3 (1%)	16	49
27	Z	284/324 (88%)	251 (88%)	33 (12%)	0	100	100
28	a	371/376 (99%)	340 (92%)	30 (8%)	1 (0%)	36	65
29	b	189/377 (50%)	179 (95%)	10 (5%)	0	100	100
30	c	285/310 (92%)	251 (88%)	34 (12%)	0	100	100
31	d	255/350 (73%)	217 (85%)	35 (14%)	3 (1%)	10	41
32	f	887/908 (98%)	795 (90%)	92 (10%)	0	100	100
33	V	442/534 (83%)	433 (98%)	9 (2%)	0	100	100
34	e	48/70 (69%)	41 (85%)	7 (15%)	0	100	100
All	All	13990/15458 (90%)	13141 (94%)	837 (6%)	12 (0%)	49	79

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	112	PRO
31	d	93	ALA
26	Y	8	GLU
26	Y	14	ASN
31	d	110	ASN
31	d	255	MET
21	C	311	ILE
24	W	118	LEU
26	Y	212	GLU
28	a	146	PRO
24	W	140	ILE
25	X	318	ILE

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	348/372 (94%)	347 (100%)	1 (0%)	86	83
2	B	357/385 (93%)	356 (100%)	1 (0%)	86	83
3	E	341/353 (97%)	339 (99%)	2 (1%)	78	79
4	F	344/379 (91%)	344 (100%)	0	100	100
5	G	202/210 (96%)	202 (100%)	0	100	100
5	g	201/210 (96%)	201 (100%)	0	100	100
6	H	187/191 (98%)	187 (100%)	0	100	100
6	h	188/191 (98%)	188 (100%)	0	100	100
7	I	202/221 (91%)	202 (100%)	0	100	100
7	i	206/221 (93%)	206 (100%)	0	100	100
8	J	197/211 (93%)	197 (100%)	0	100	100
8	j	196/211 (93%)	196 (100%)	0	100	100
9	K	197/203 (97%)	197 (100%)	0	100	100
9	k	195/203 (96%)	195 (100%)	0	100	100
10	L	202/230 (88%)	202 (100%)	0	100	100
10	l	201/230 (87%)	201 (100%)	0	100	100
11	M	198/212 (93%)	198 (100%)	0	100	100
11	m	198/212 (93%)	198 (100%)	0	100	100
12	N	158/181 (87%)	158 (100%)	0	100	100
12	n	156/181 (86%)	156 (100%)	0	100	100
13	O	178/228 (78%)	178 (100%)	0	100	100
13	o	181/228 (79%)	181 (100%)	0	100	100
14	P	172/174 (99%)	172 (100%)	0	100	100
14	p	173/174 (99%)	173 (100%)	0	100	100
15	Q	168/171 (98%)	168 (100%)	0	100	100
15	q	166/171 (97%)	166 (100%)	0	100	100
16	R	156/202 (77%)	156 (100%)	0	100	100
16	r	154/202 (76%)	154 (100%)	0	100	100
17	S	175/199 (88%)	175 (100%)	0	100	100
17	s	177/199 (89%)	177 (100%)	0	100	100
18	T	178/215 (83%)	178 (100%)	0	100	100
18	t	179/215 (83%)	179 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	x	439/439 (100%)	439 (100%)	0	100	100
20	y	68/68 (100%)	68 (100%)	0	100	100
21	C	340/346 (98%)	339 (100%)	1 (0%)	86	83
22	D	333/366 (91%)	333 (100%)	0	100	100
23	U	748/816 (92%)	748 (100%)	0	100	100
24	W	410/416 (99%)	408 (100%)	2 (0%)	81	80
25	X	327/362 (90%)	327 (100%)	0	100	100
26	Y	344/344 (100%)	344 (100%)	0	100	100
27	Z	257/295 (87%)	252 (98%)	5 (2%)	50	67
28	a	333/336 (99%)	331 (99%)	2 (1%)	78	79
29	b	167/312 (54%)	167 (100%)	0	100	100
30	c	252/268 (94%)	248 (98%)	4 (2%)	55	69
31	d	231/294 (79%)	229 (99%)	2 (1%)	70	76
32	f	745/763 (98%)	744 (100%)	1 (0%)	88	87
33	V	390/460 (85%)	390 (100%)	0	100	100
34	e	44/63 (70%)	44 (100%)	0	100	100
All	All	11959/13133 (91%)	11938 (100%)	21 (0%)	85	85

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	403	ILE
2	B	125	THR
3	E	111	LEU
3	E	113	ARG
21	C	210	THR
24	W	115	ILE
24	W	117	ASP
27	Z	176	LEU
27	Z	178	ASP
27	Z	233	VAL
27	Z	235	ASN
27	Z	236	LEU
28	a	144	ASN
28	a	145	LEU
30	c	123	SER

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Mol	Chain	Res	Type
30	c	125	VAL
30	c	217	LEU
30	c	218	LEU
31	d	111	ARG
31	d	112	VAL
32	f	655	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (137) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	150	HIS
1	A	247	GLN
1	A	414	ASN
1	A	433	ASN
3	E	39	GLN
3	E	45	ASN
3	E	220	ASN
3	E	262	ASN
3	E	280	ASN
3	E	359	HIS
4	F	76	ASN
4	F	243	GLN
4	F	358	ASN
5	G	33	ASN
5	G	34	GLN
5	G	68	HIS
6	H	102	GLN
6	H	202	GLN
6	H	207	ASN
7	I	95	GLN
8	J	92	GLN
8	J	154	HIS
9	K	97	GLN
9	K	221	GLN
10	L	21	GLN
10	L	60	GLN
12	N	7	GLN
12	N	158	ASN
13	O	35	HIS
13	O	66	HIS
13	O	172	ASN

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Mol	Chain	Res	Type
13	O	193	ASN
14	P	7	ASN
15	Q	101	ASN
17	S	8	ASN
17	S	152	GLN
17	S	160	ASN
5	g	75	ASN
5	g	172	GLN
6	h	21	GLN
6	h	52	GLN
7	i	40	ASN
8	j	18	GLN
8	j	200	GLN
9	k	13	ASN
9	k	178	GLN
10	l	59	HIS
10	l	166	GLN
11	m	101	ASN
11	m	105	ASN
12	n	158	ASN
12	n	187	GLN
12	n	193	GLN
13	o	35	HIS
14	p	72	ASN
14	p	93	ASN
15	q	101	ASN
16	r	85	ASN
16	r	162	GLN
17	s	151	ASN
18	t	3	ASN
18	t	157	GLN
18	t	185	ASN
19	x	198	GLN
19	x	201	ASN
19	x	274	GLN
19	x	385	GLN
19	x	396	GLN
20	y	68	HIS
21	C	50	ASN
21	C	64	GLN
21	C	241	HIS
22	D	65	GLN

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Mol	Chain	Res	Type
22	D	76	GLN
22	D	173	GLN
22	D	278	GLN
22	D	301	GLN
22	D	304	ASN
22	D	353	ASN
23	U	89	ASN
23	U	111	GLN
23	U	128	GLN
23	U	189	GLN
23	U	192	GLN
23	U	267	ASN
23	U	345	ASN
23	U	355	ASN
23	U	527	GLN
23	U	596	ASN
24	W	96	GLN
24	W	210	ASN
24	W	218	ASN
24	W	228	ASN
24	W	283	GLN
24	W	395	ASN
24	W	426	ASN
24	W	430	GLN
25	X	292	GLN
25	X	296	ASN
25	X	380	GLN
26	Y	154	ASN
26	Y	178	ASN
26	Y	251	HIS
26	Y	273	GLN
26	Y	306	GLN
26	Y	365	GLN
26	Y	367	GLN
26	Y	388	ASN
27	Z	32	GLN
27	Z	189	GLN
27	Z	229	GLN
27	Z	231	GLN
27	Z	235	ASN
28	a	82	HIS
28	a	264	ASN

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Mol	Chain	Res	Type
28	a	332	HIS
28	a	370	GLN
29	b	47	ASN
29	b	158	ASN
30	c	101	GLN
30	c	254	ASN
30	c	287	HIS
31	d	77	GLN
31	d	128	GLN
31	d	229	GLN
32	f	378	ASN
32	f	396	ASN
32	f	402	ASN
32	f	428	GLN
32	f	531	ASN
32	f	724	ASN
32	f	770	HIS
32	f	790	GLN
32	f	848	GLN
32	f	855	GLN
33	V	78	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is 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
35	ADP	A	501	-	28,29,29	1.40	4 (14%)	43,45,45	1.78	8 (18%)
35	ADP	B	501	-	28,29,29	1.42	4 (14%)	43,45,45	1.90	8 (18%)
36	ATP	E	501	-	32,33,33	0.35	0	48,52,52	0.33	0
36	ATP	F	501	-	32,33,33	0.32	0	48,52,52	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ADP	A	501	-	-	5/16/32/32	0/3/3/3
35	ADP	B	501	-	-	2/16/32/32	0/3/3/3
36	ATP	E	501	-	-	7/22/38/38	0/3/3/3
36	ATP	F	501	-	-	9/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	B	501	ADP	C5-C4	4.75	1.47	1.39
35	A	501	ADP	C5-C4	4.65	1.47	1.39
35	B	501	ADP	C5-C6	2.71	1.48	1.41
35	A	501	ADP	C5-C6	2.69	1.48	1.41
35	B	501	ADP	C5-N7	-2.39	1.34	1.39
35	A	501	ADP	C8-N7	2.35	1.36	1.31
35	A	501	ADP	C5-N7	-2.23	1.35	1.39
35	B	501	ADP	C8-N7	2.21	1.35	1.31

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B	501	ADP	C5-C4-N3	-6.39	117.92	126.72
35	A	501	ADP	C5-C4-N3	-5.64	118.95	126.72
35	B	501	ADP	N3-C4-N9	5.13	135.89	127.17
35	A	501	ADP	N3-C4-N9	4.50	134.82	127.17
35	B	501	ADP	C2-N3-C4	3.83	121.19	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	501	ADP	C2-N3-C4	3.66	120.78	111.83
35	B	501	ADP	C4-C5-N7	-3.42	106.67	110.58
35	A	501	ADP	C4-C5-N7	-3.34	106.76	110.58
35	A	501	ADP	N3-C2-N1	-3.29	123.59	128.58
35	B	501	ADP	N3-C2-N1	-3.07	123.94	128.58
35	B	501	ADP	C3'-C2'-C1'	2.93	107.01	101.46
35	A	501	ADP	C4-N9-C8	2.72	108.59	105.74
35	B	501	ADP	C5-N7-C8	2.55	107.46	103.45
35	A	501	ADP	C5-N7-C8	2.42	107.26	103.45
35	B	501	ADP	C4-N9-C8	2.40	108.26	105.74
35	A	501	ADP	C6-C5-N7	2.13	136.19	132.09

There are no chirality outliers.

All (23) torsion outliers are listed below:

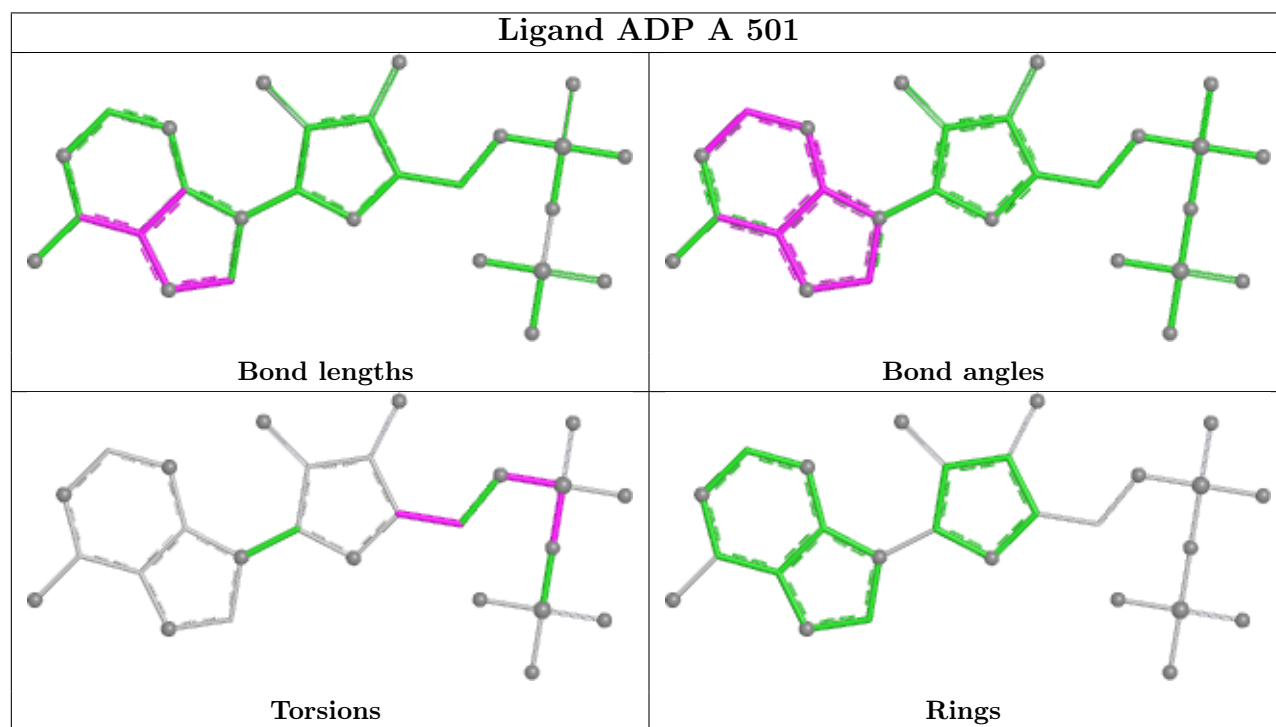
Mol	Chain	Res	Type	Atoms
35	A	501	ADP	C5'-O5'-PA-O1A
36	E	501	ATP	PB-O3B-PG-O3G
36	E	501	ATP	C5'-O5'-PA-O1A
36	E	501	ATP	C5'-O5'-PA-O3A
36	F	501	ATP	PB-O3B-PG-O3G
36	F	501	ATP	C5'-O5'-PA-O1A
36	F	501	ATP	C5'-O5'-PA-O3A
36	E	501	ATP	O4'-C4'-C5'-O5'
36	E	501	ATP	C3'-C4'-C5'-O5'
35	A	501	ADP	O4'-C4'-C5'-O5'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

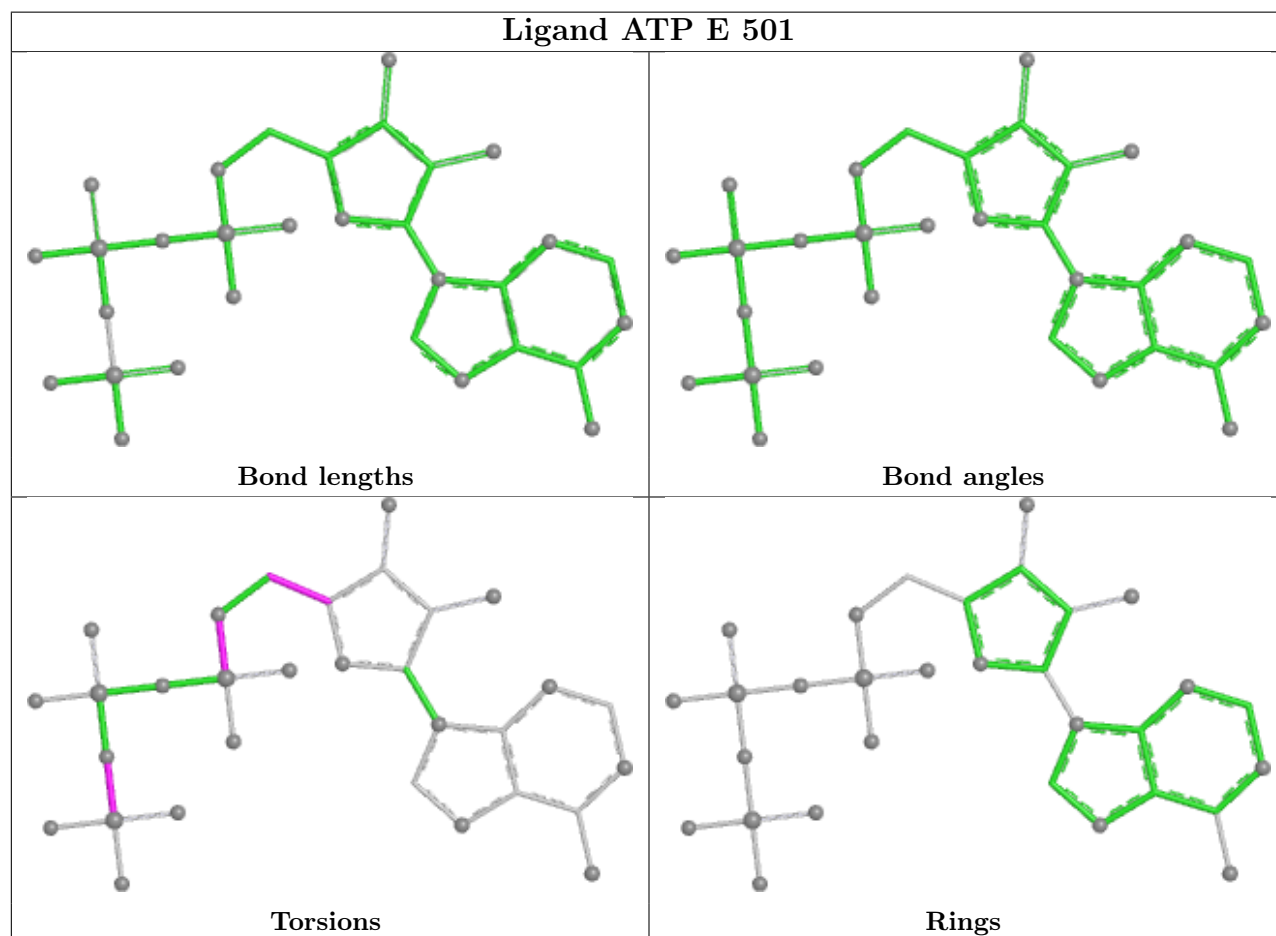
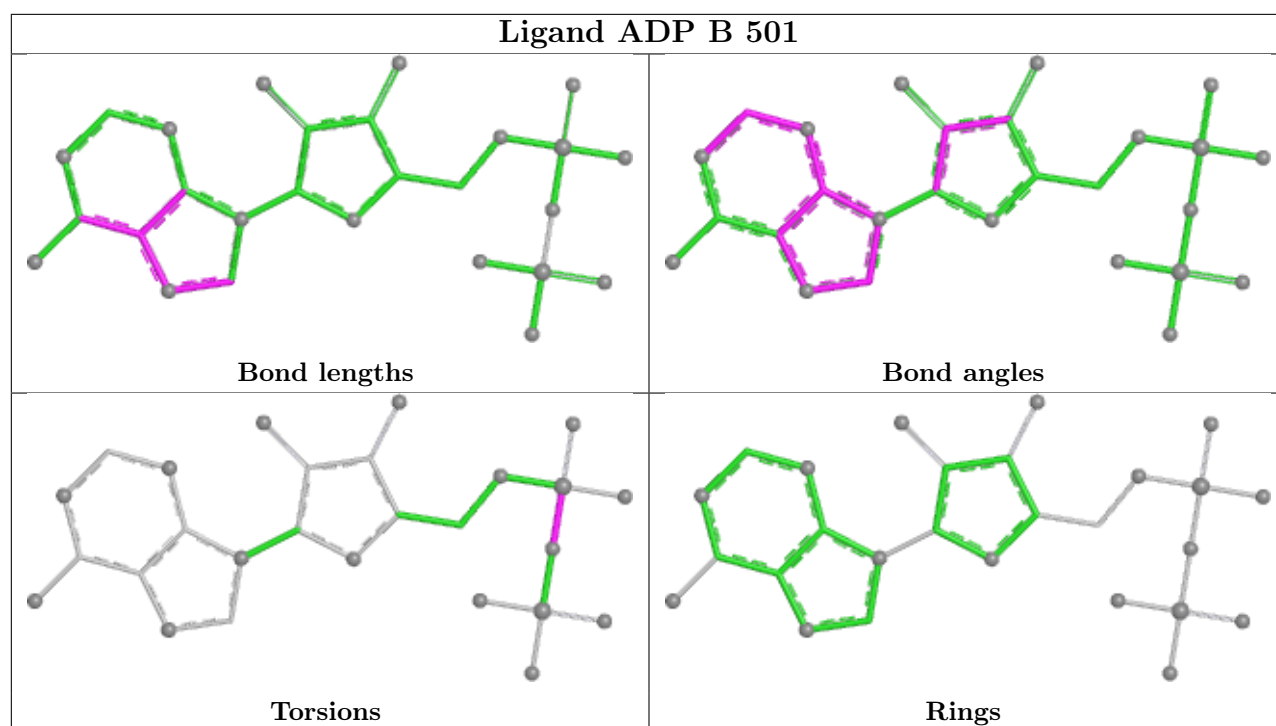
There are no ring outliers.

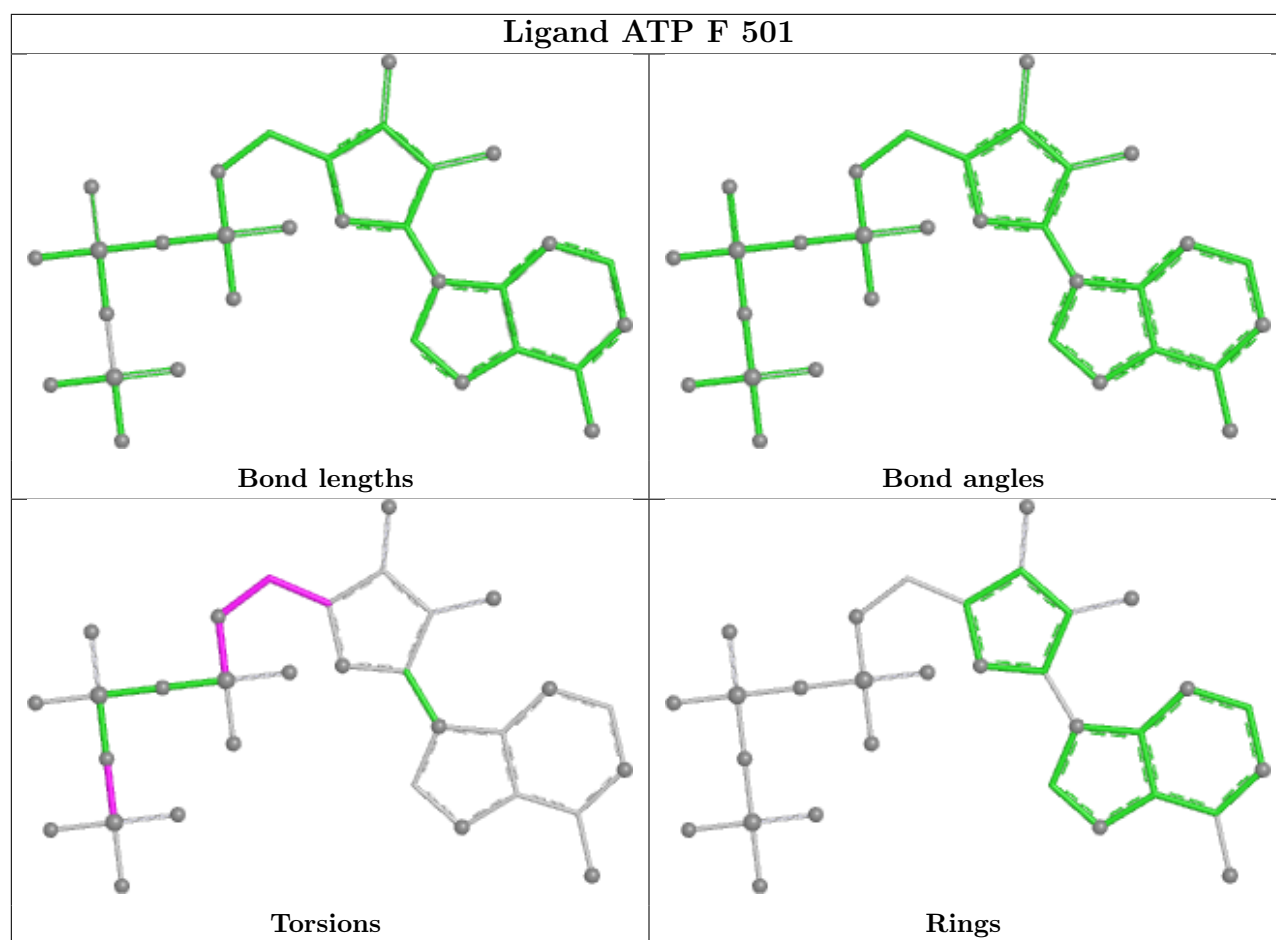
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	501	ADP	4	0
35	B	501	ADP	1	0
36	E	501	ATP	2	0
36	F	501	ATP	1	0

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







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.

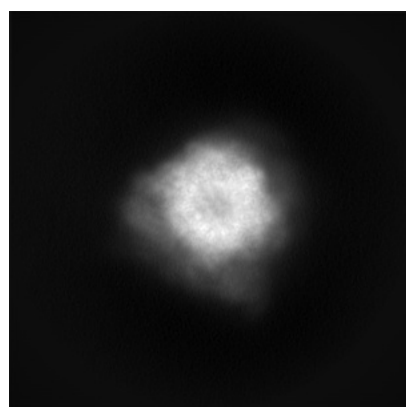
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32283. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

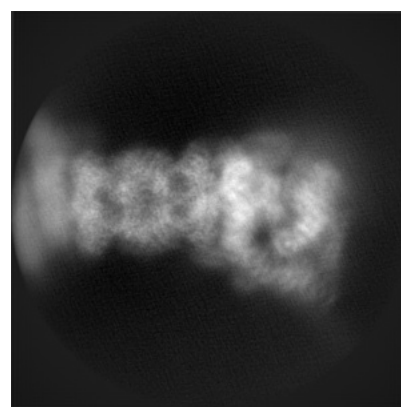
6.1.1 Primary map



X



Y

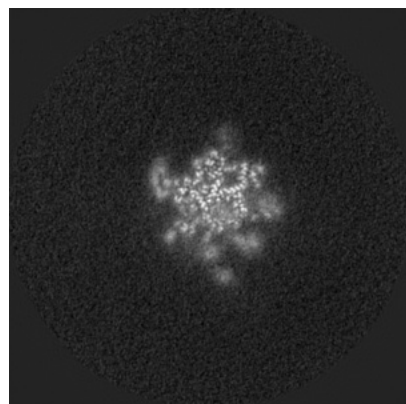


Z

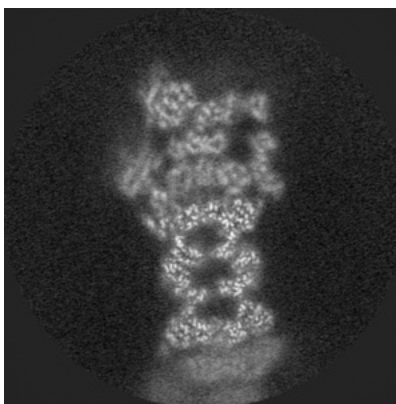
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

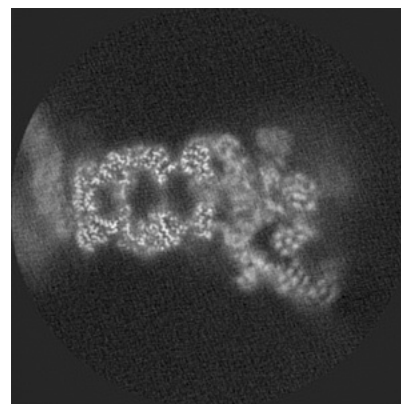
6.2.1 Primary map



X Index: 320



Y Index: 320

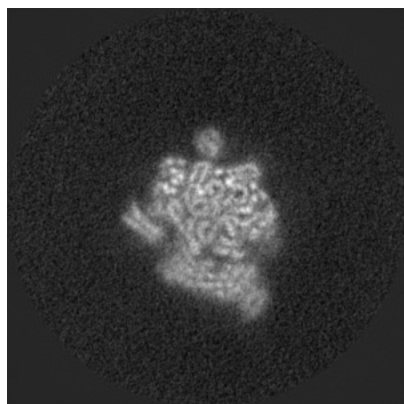


Z Index: 320

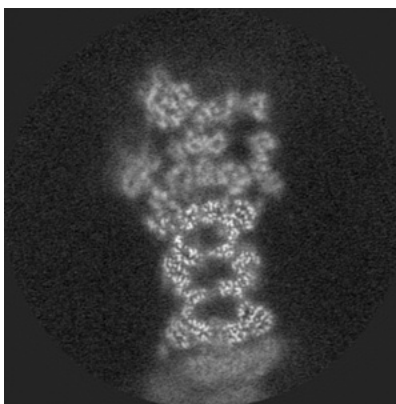
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

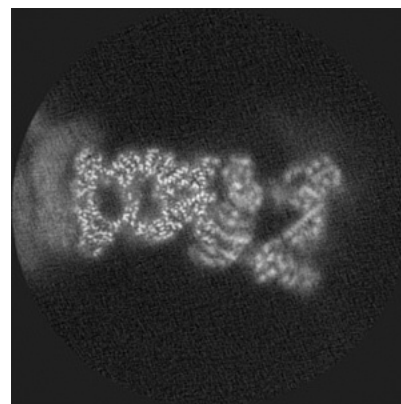
6.3.1 Primary map



X Index: 363



Y Index: 318

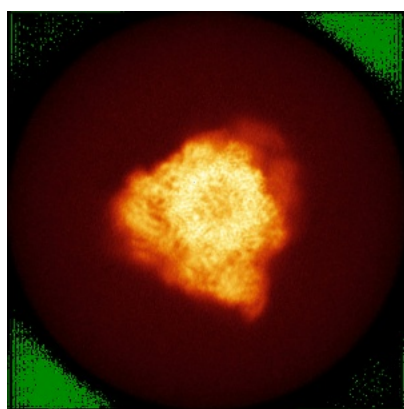


Z Index: 360

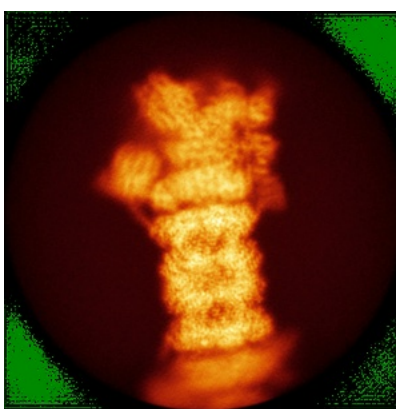
The images above show the largest variance slices of the map in three orthogonal directions.

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

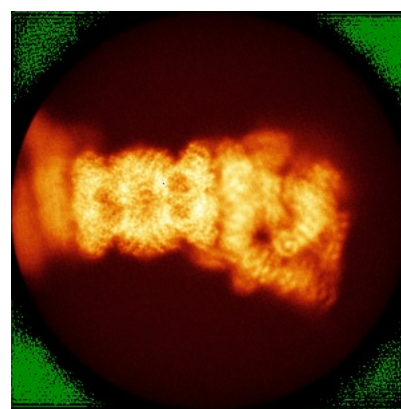
6.4.1 Primary map



X



Y

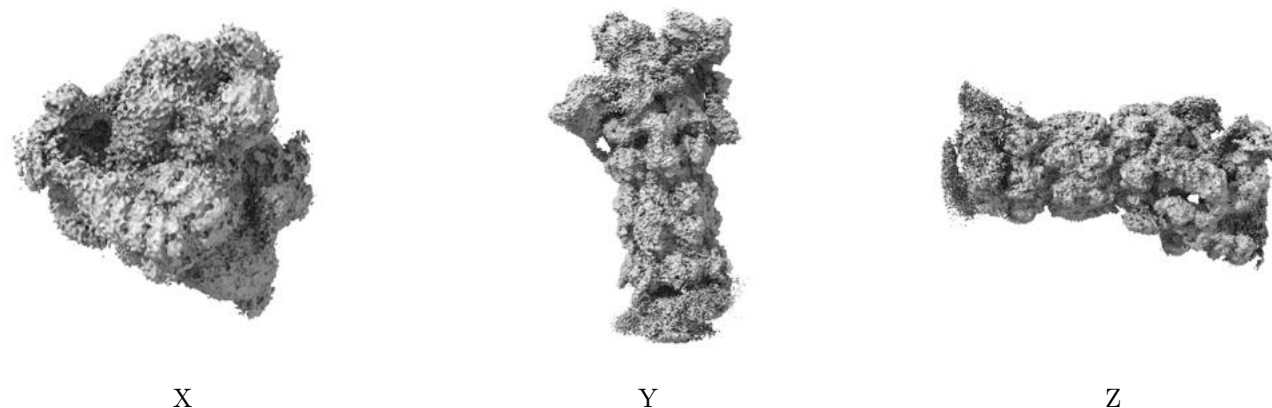


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

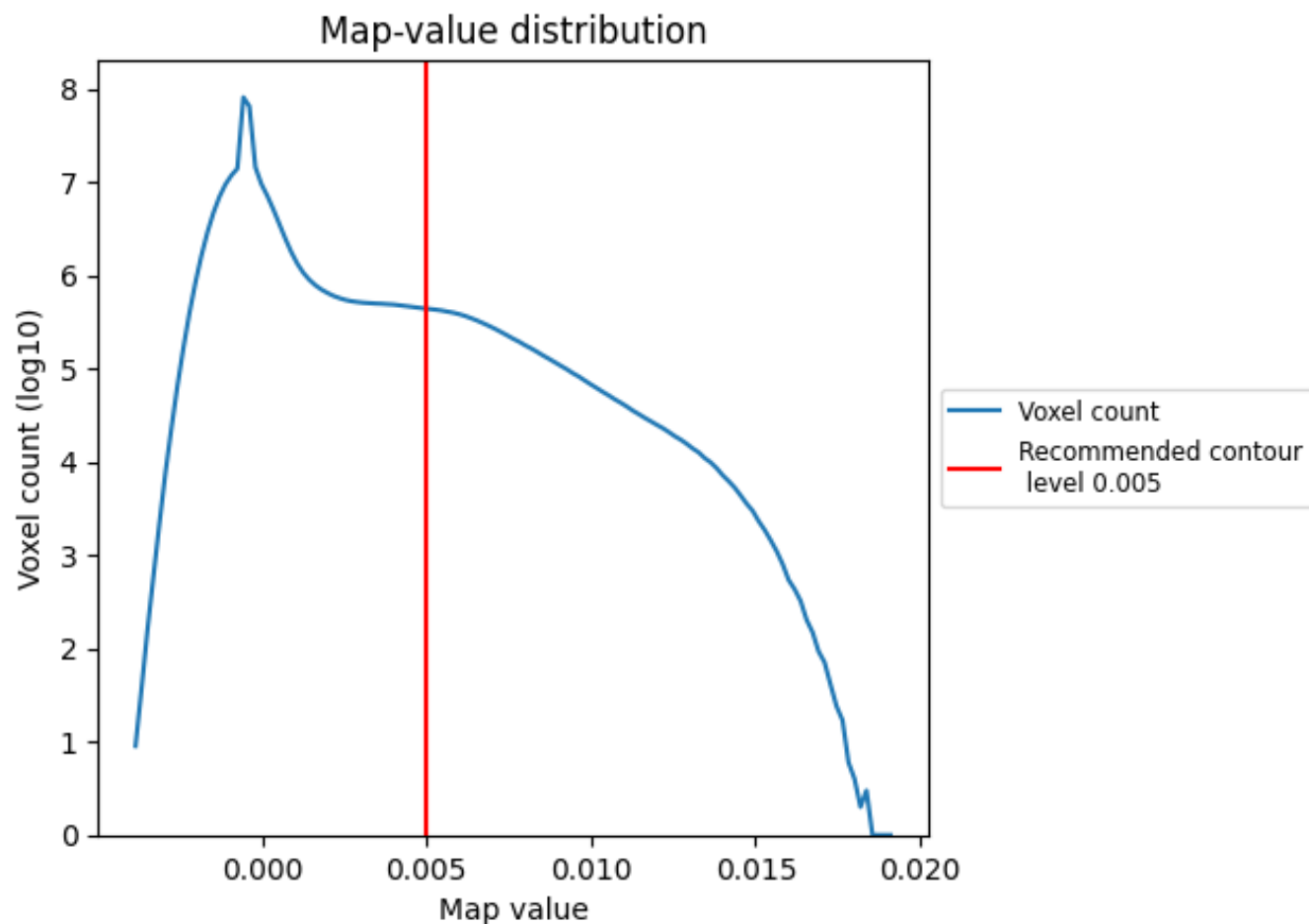
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

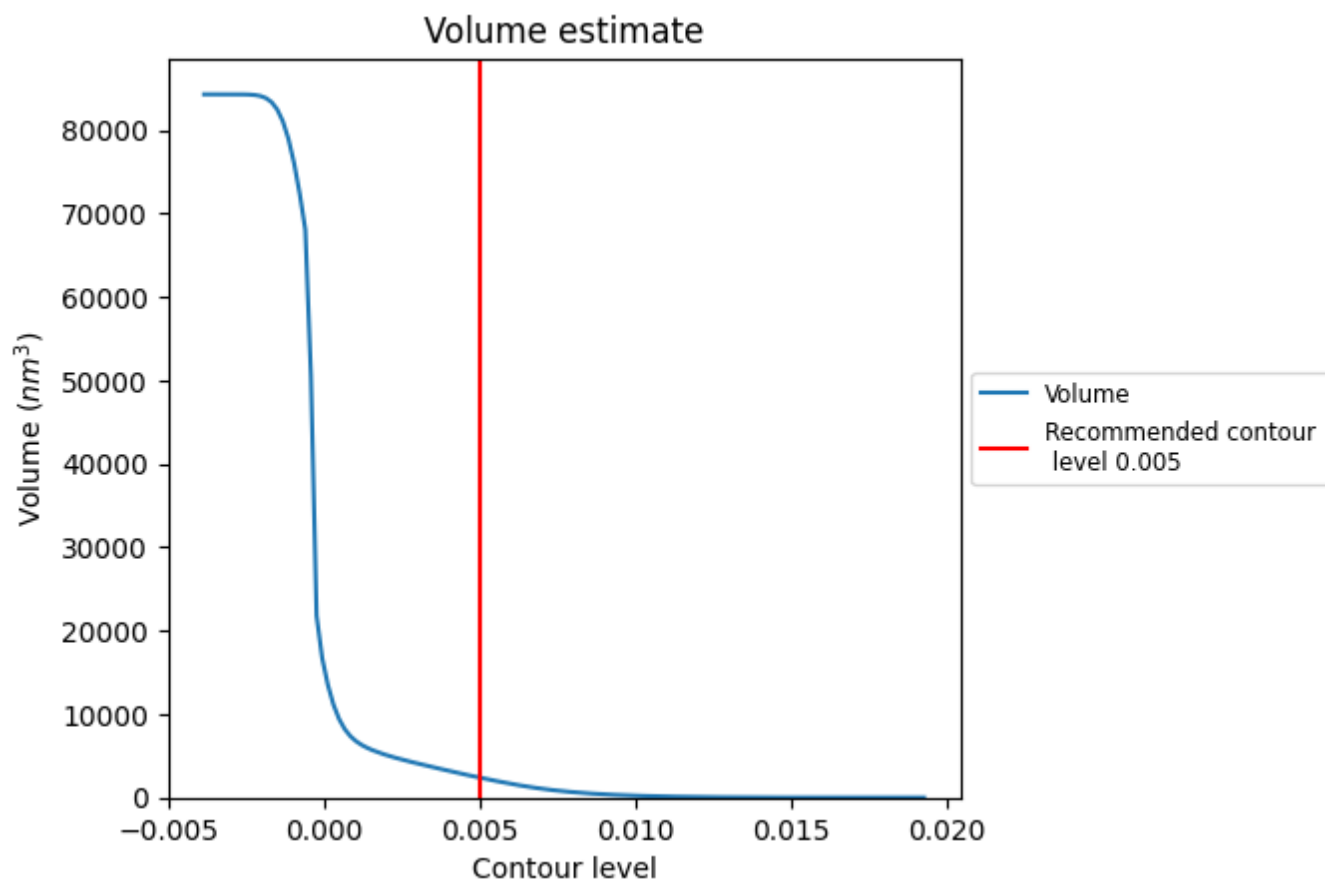
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

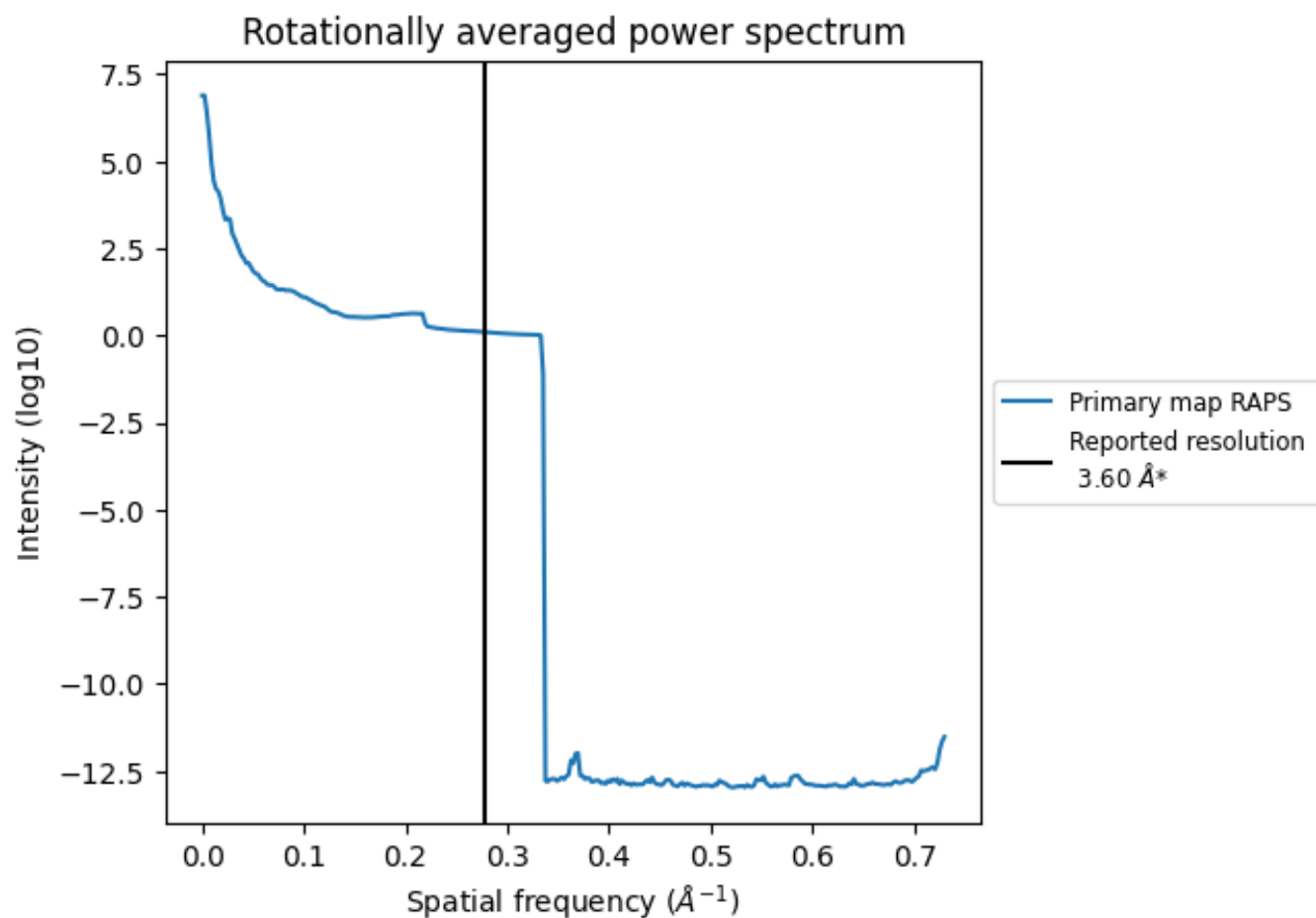
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2395 nm³; this corresponds to an approximate mass of 2164 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

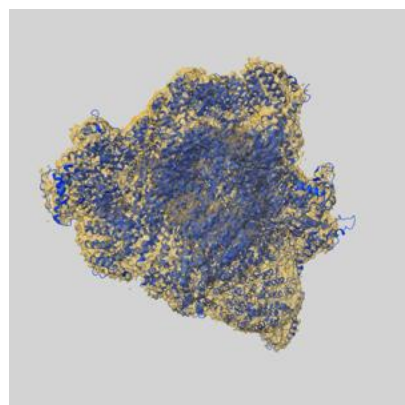
8 Fourier-Shell correlation ⓘ

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

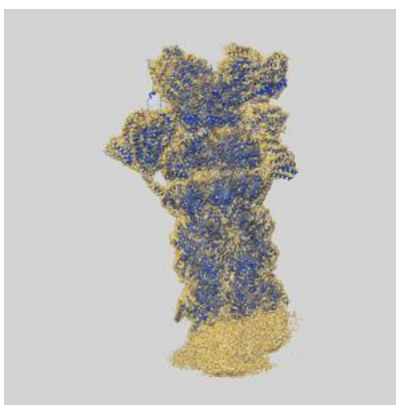
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32283 and PDB model 7W3K. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

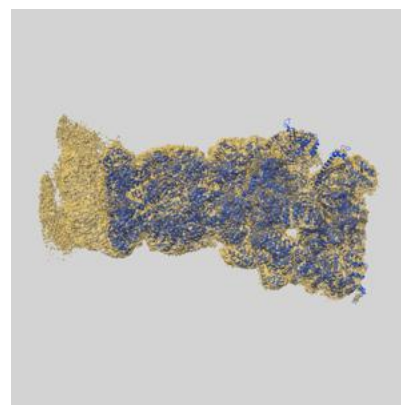
9.1 Map-model overlay [i](#)



X



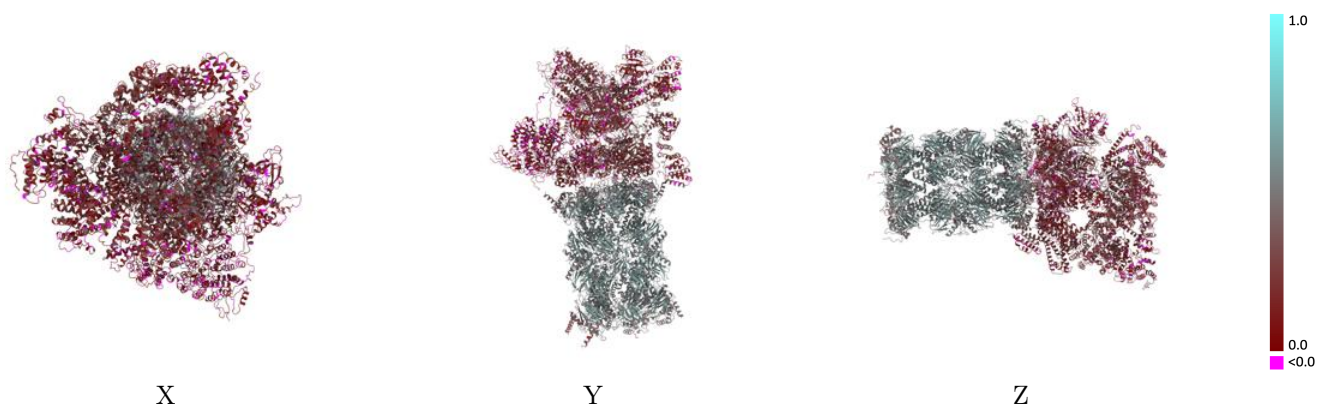
Y



Z

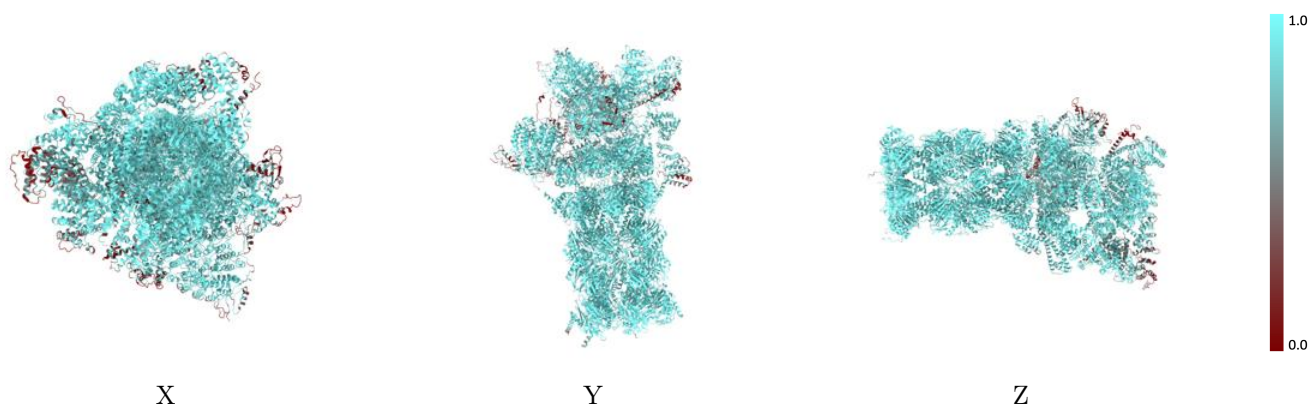
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



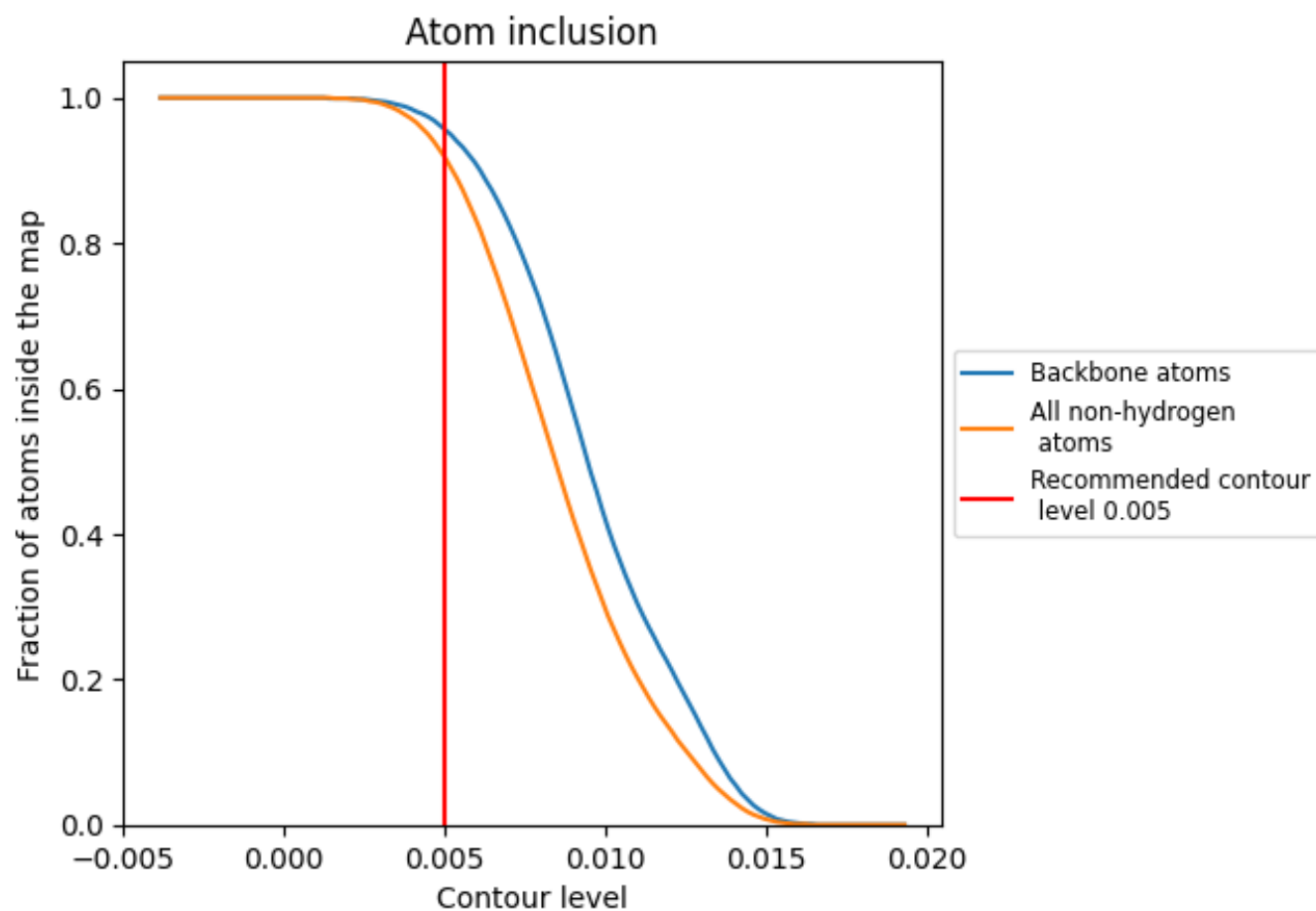
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9170	 0.3270
A	 0.9490	 0.1940
B	 0.9150	 0.1870
C	 0.8930	 0.1740
D	 0.9590	 0.1900
E	 0.9070	 0.2230
F	 0.9120	 0.2260
G	 0.9820	 0.4880
H	 0.9920	 0.4860
I	 0.9860	 0.4700
J	 0.9850	 0.4630
K	 0.9830	 0.4750
L	 0.9910	 0.4980
M	 0.9870	 0.4930
N	 0.9920	 0.5230
O	 0.9900	 0.5150
P	 0.9960	 0.5240
Q	 0.9910	 0.5170
R	 0.9930	 0.5180
S	 0.9900	 0.5200
T	 0.9880	 0.5290
U	 0.8530	 0.2040
V	 0.7970	 0.1900
W	 0.8240	 0.1880
X	 0.9490	 0.2290
Y	 0.9380	 0.2020
Z	 0.9710	 0.2330
a	 0.8730	 0.2050
b	 0.8920	 0.1780
c	 0.9490	 0.2450
d	 0.5910	 0.1610
e	 0.9210	 0.2010
f	 0.8590	 0.1340
g	 0.9660	 0.4920
h	 0.9840	 0.4970



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Chain	Atom inclusion	Q-score
i	 0.9590	 0.4750
j	 0.9600	 0.4480
k	 0.9740	 0.4840
l	 0.9810	 0.5070
m	 0.9730	 0.4940
n	 0.9930	 0.5310
o	 0.9910	 0.5270
p	 0.9930	 0.5240
q	 0.9940	 0.5230
r	 0.9950	 0.5250
s	 0.9900	 0.5170
t	 0.9830	 0.5240
x	 0.6730	 0.1490
y	 0.4900	 0.1130