



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 01:06 AM UTC

PDB ID : 7W3J / pdb_00007w3j
EMDB ID : EMD-32282
Title : Structure of USP14-bound human 26S proteasome in substrate-inhibited state
SC_USP14
Authors : Zhang, S.; Zou, S.; Yin, D.; Wu, Z.; Mao, Y.
Deposited on : 2021-11-25
Resolution : 3.50 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

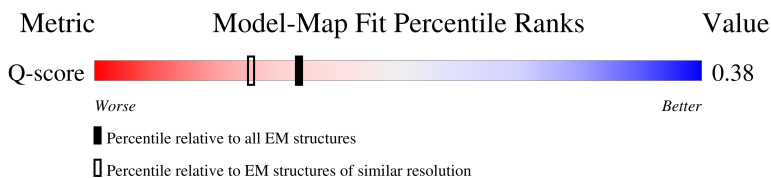
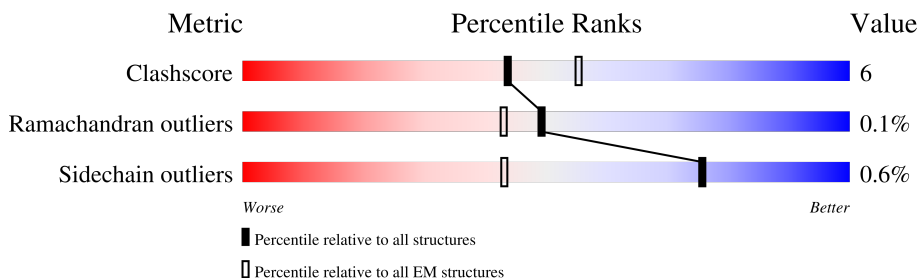
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.



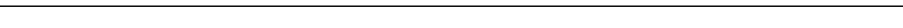
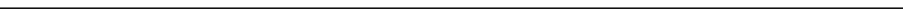
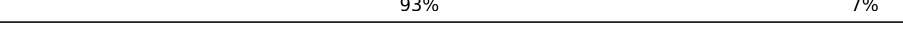
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	E	403	
2	F	439	
3	G	246	
3	g	246	

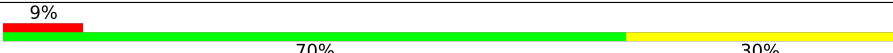
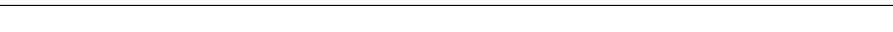
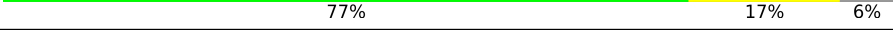
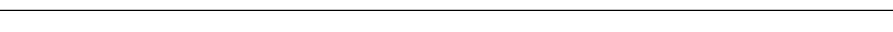
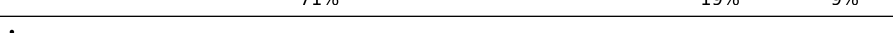
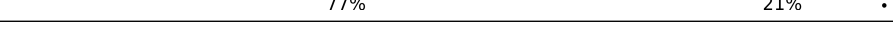
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	H	234	 90% 9% .
4	h	234	 88% 12% .
5	I	261	 90% 5% 5%
5	i	261	 91% 5% .
6	J	248	 82% 14% .
6	j	248	 77% 19% .
7	K	241	 91% 8% .
7	k	241	 87% 10% .
8	L	269	 78% 11% 11%
8	l	269	 79% 9% 12%
9	M	255	 87% 8% 5%
9	m	255	 84% 10% 6%
10	N	239	 85% 15%
10	n	239	 76% 8% 15%
11	O	277	 73% 6% 21%
11	o	277	 73% 7% 21%
12	P	205	 88% 11%
12	p	205	 93% 7%
13	Q	201	 86% 13% .
13	q	201	 90% 9% .
14	R	263	 69% 8% 24%
14	r	263	 71% 6% 24%
15	S	241	 83% 5% 12%
15	s	241	 83% 6% 12%
16	T	264	 73% 9% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	t	264	
17	x	494	
18	y	76	
19	A	433	
20	B	440	
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 [i](#)

There are 37 unique types of molecules in this entry. The entry contains 110559 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 26S proteasome regulatory subunit 10B.

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

- Molecule 2 is a protein called 26S protease regulatory subunit 6A.

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

- Molecule 3 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 4 is a protein called Proteasome subunit alpha type-2.

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

- Molecule 5 is a protein called Proteasome subunit alpha type-4.

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

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

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

- Molecule 7 is a protein called Proteasome subunit alpha type-5.

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

- Molecule 8 is a protein called Isoform Long of Proteasome subunit alpha type-1.

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

- Molecule 9 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	242	Total	C	N	O	S	0	0
			1890	1200	323	356	11		
9	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

- Molecule 10 is a protein called Proteasome subunit beta type-6.

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

- Molecule 11 is a protein called Proteasome subunit beta type-7.

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

- Molecule 12 is a protein called Proteasome subunit beta type-3.

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

- Molecule 13 is a protein called Proteasome subunit beta type-2.

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

- Molecule 14 is a protein called Proteasome subunit beta type-5.

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

- Molecule 15 is a protein called Proteasome subunit beta type-1.

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

- Molecule 16 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	216	Total	C	N	O	S	0	0
			1683	1062	291	318	12		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
16	t	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

- Molecule 17 is a protein called Ubiquitin carboxyl-terminal hydrolase 14.

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

- Molecule 18 is a protein called Ubiquitin.

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

- Molecule 19 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A	406	Total	C	N	O	S	0	0
			3164	1992	555	600	17		

- Molecule 20 is a protein called 26S protease regulatory subunit 4.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	C	395	Total	C	N	O	S	0	0
			3097	1948	557	575	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	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- 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		

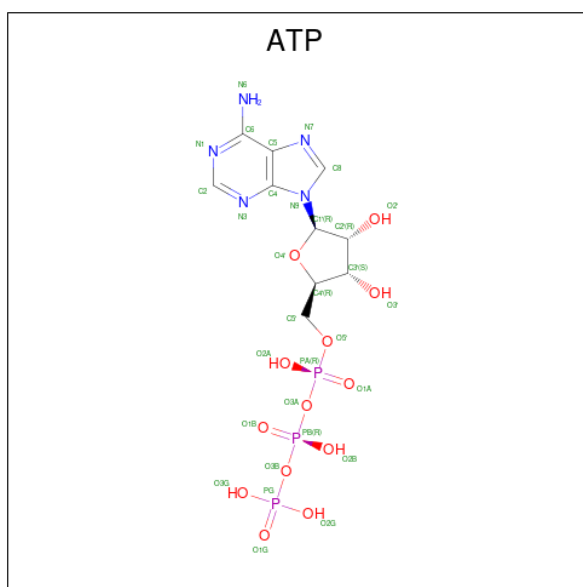
- Molecule 33 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

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.

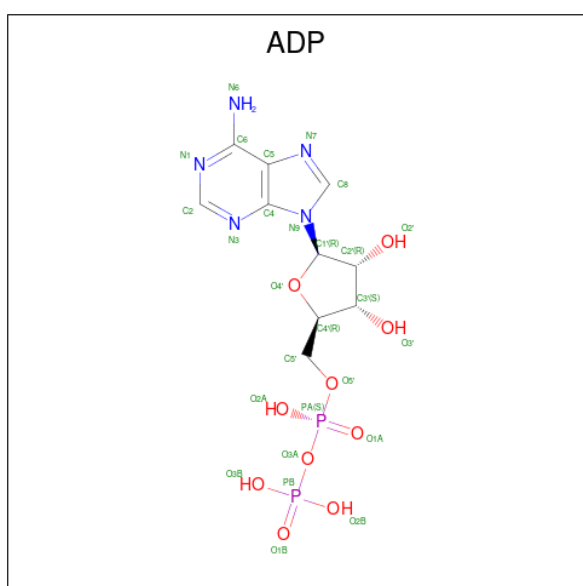
Mol	Chain	Residues	Atoms				AltConf	Trace
34	e	50	Total	C	N	O	0	0
			425	260	65	100		

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



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

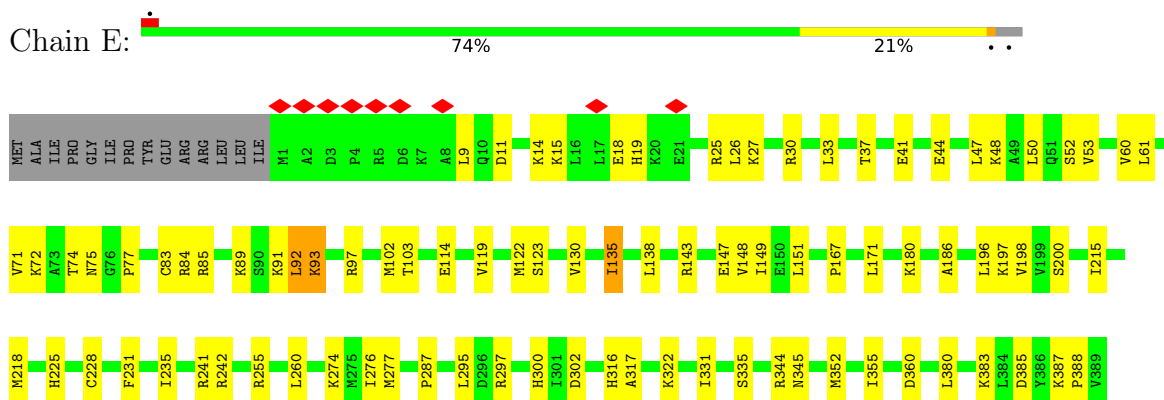
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

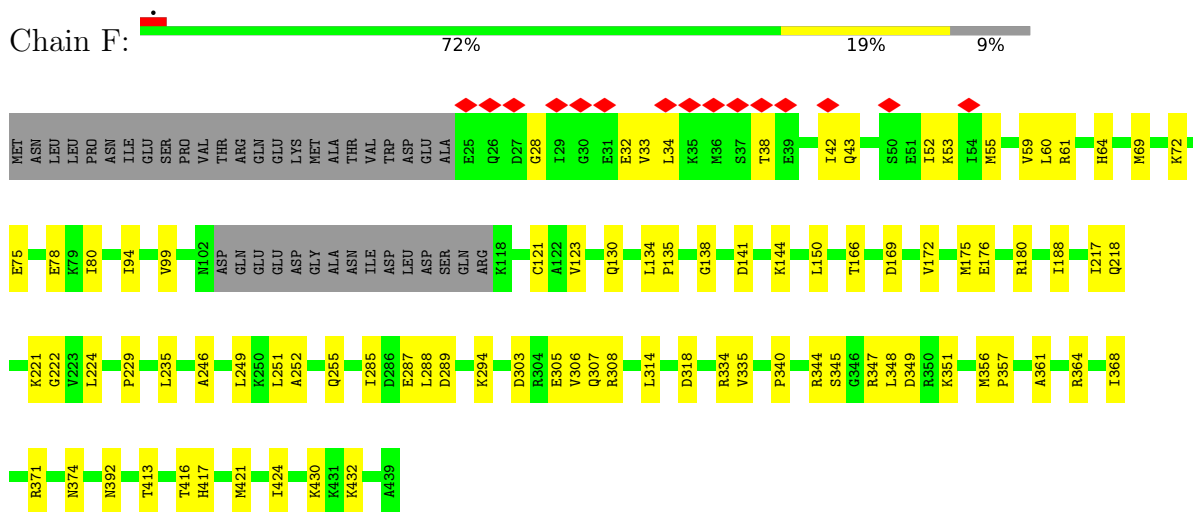
3 Residue-property plots

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.

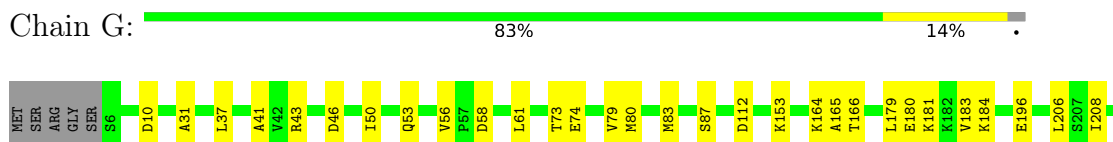
- Molecule 1: 26S proteasome regulatory subunit 10B



- Molecule 2: 26S protease regulatory subunit 6A



- Molecule 3: Proteasome subunit alpha type-6





- Molecule 3: Proteasome subunit alpha type-6

Chain g: 89% 10%



- Molecule 4: Proteasome subunit alpha type-2

Chain H: 90% 9%



- Molecule 4: Proteasome subunit alpha type-2

Chain h: 88% 12%



- Molecule 5: Proteasome subunit alpha type-4

Chain I: 90% 5% 5%



- Molecule 5: Proteasome subunit alpha type-4

Chain i: 91% 5% 5%

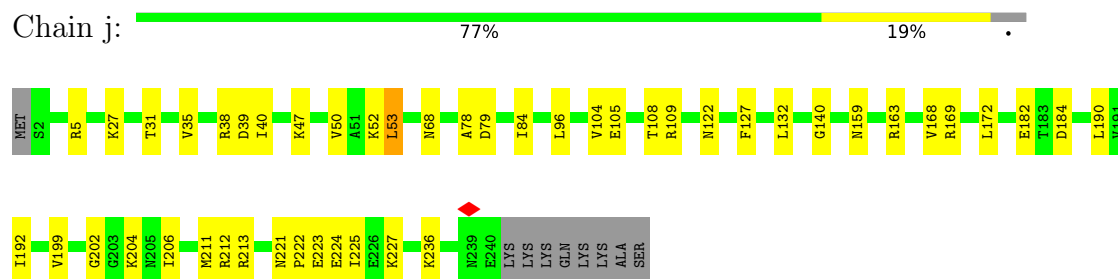


- Molecule 6: Proteasome subunit alpha type-7

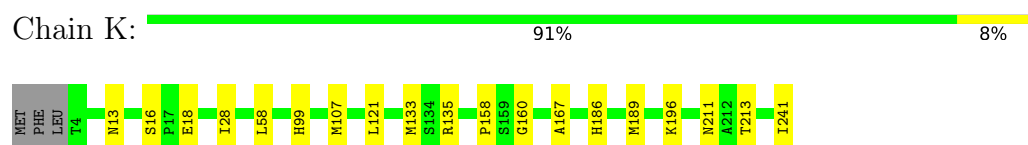
Chain J: 82% 14% 5%



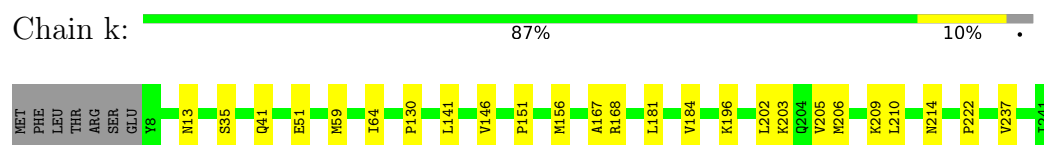
- Molecule 6: Proteasome subunit alpha type-7



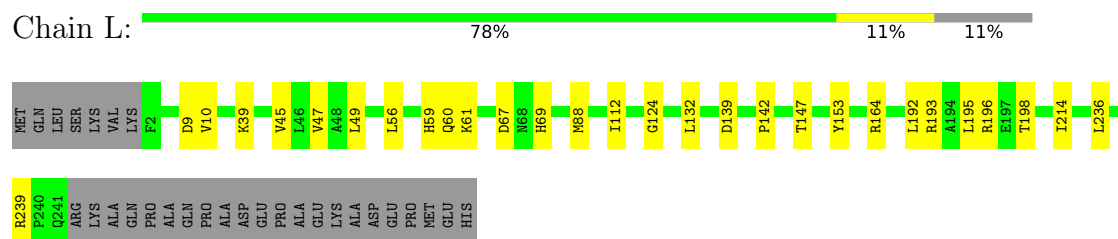
- Molecule 7: Proteasome subunit alpha type-5



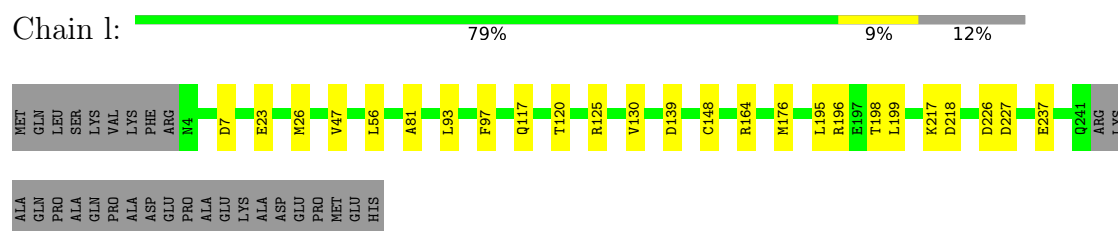
- Molecule 7: Proteasome subunit alpha type-5



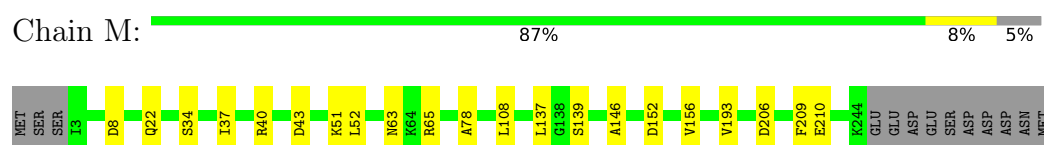
- Molecule 8: Isoform Long of Proteasome subunit alpha type-1



- Molecule 8: Isoform Long of Proteasome subunit alpha type-1

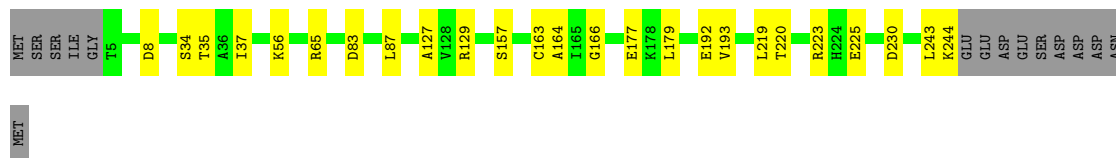


- Molecule 9: Proteasome subunit alpha type-3



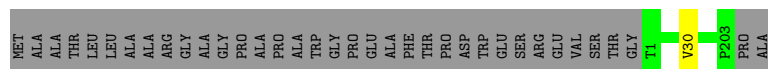
- Molecule 9: Proteasome subunit alpha type-3

Chain m:  84% 10% 6%



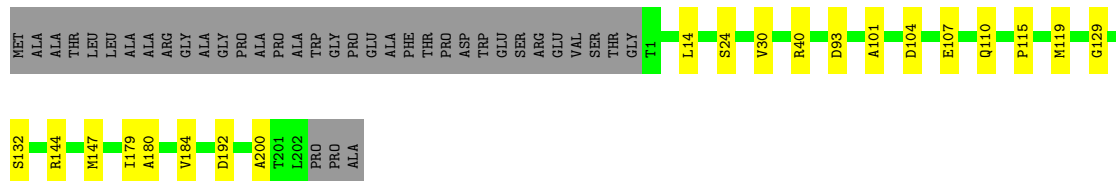
- Molecule 10: Proteasome subunit beta type-6

Chain N:  85% 15%



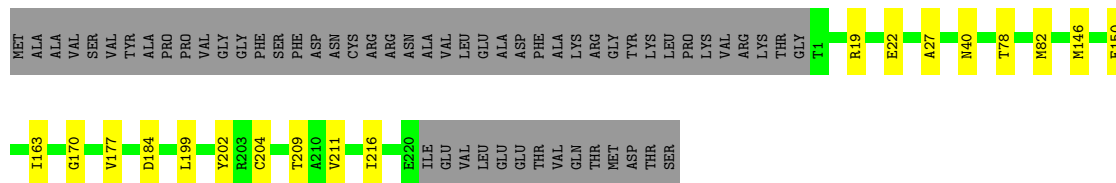
- Molecule 10: Proteasome subunit beta type-6

Chain n:  76% 8% 15%



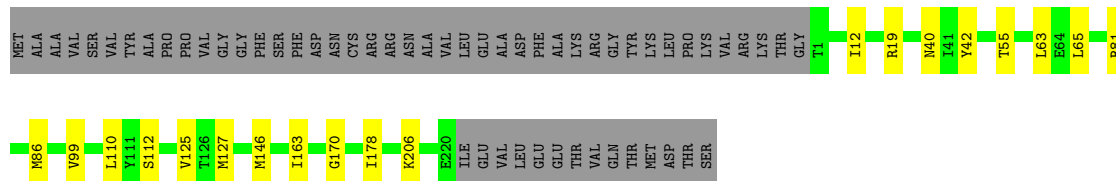
- Molecule 11: Proteasome subunit beta type-7

Chain O:  73% 6% 21%



- Molecule 11: Proteasome subunit beta type-7

Chain o:  73% 7% 21%



- Molecule 12: Proteasome subunit beta type-3

Chain P:  88% 11%



- Molecule 12: Proteasome subunit beta type-3

Chain p: 93% 7%



- Molecule 13: Proteasome subunit beta type-2

Chain Q: 86% 13%



- Molecule 13: Proteasome subunit beta type-2

Chain q: 90% 9%



- Molecule 14: Proteasome subunit beta type-5

Chain R: 69% 8% 24%



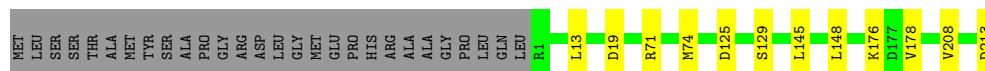
- Molecule 14: Proteasome subunit beta type-5

Chain r: 71% 6% 24%



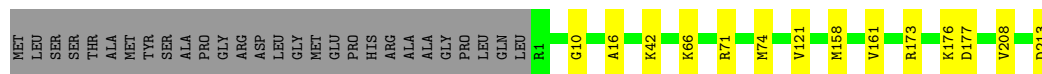
- Molecule 15: Proteasome subunit beta type-1

Chain S: 83% 5% 12%



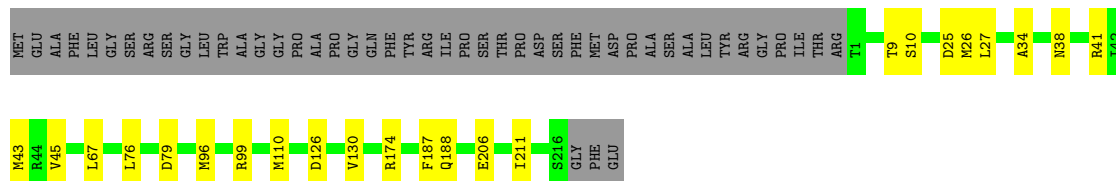
- Molecule 15: Proteasome subunit beta type-1

Chain s:  83% 6% 12%



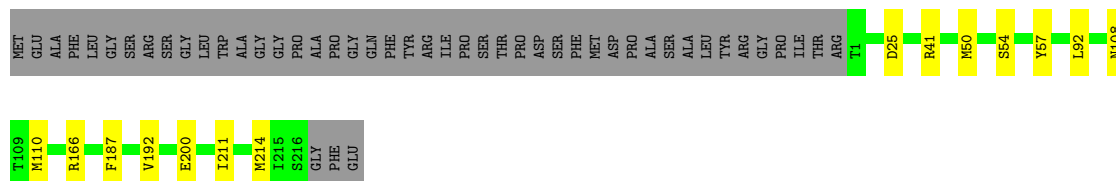
- Molecule 16: Proteasome subunit beta type-4

Chain T:  73% 9% 18%



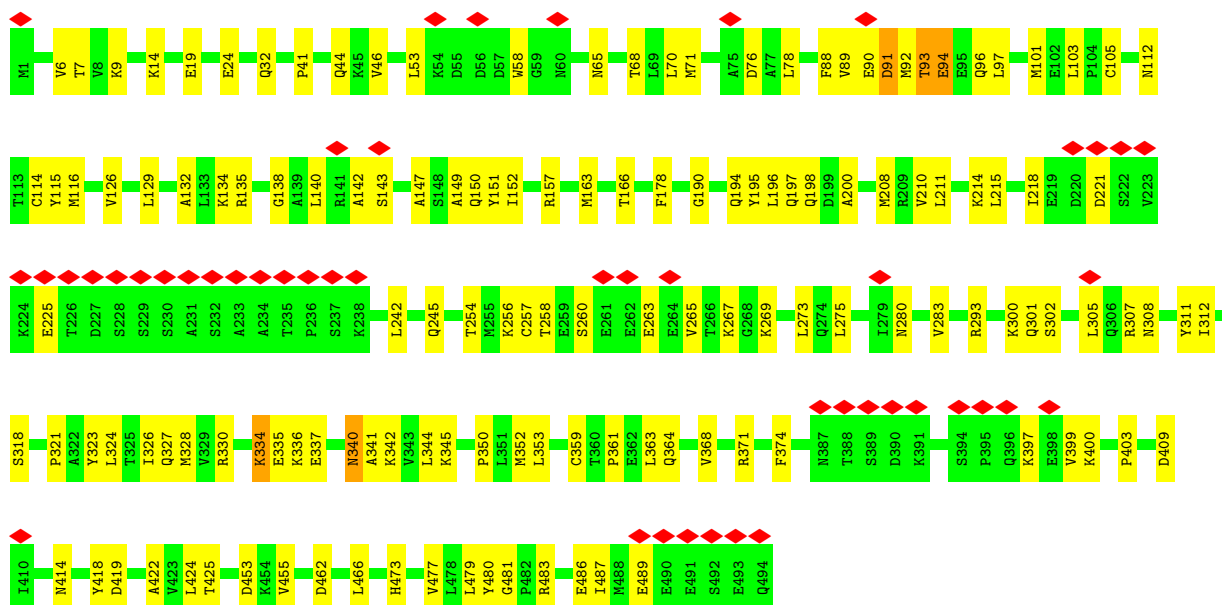
- Molecule 16: Proteasome subunit beta type-4

Chain t:  77% 5% 18%

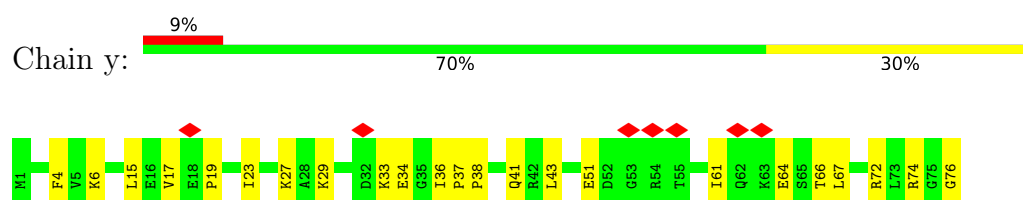


- Molecule 17: Ubiquitin carboxyl-terminal hydrolase 14

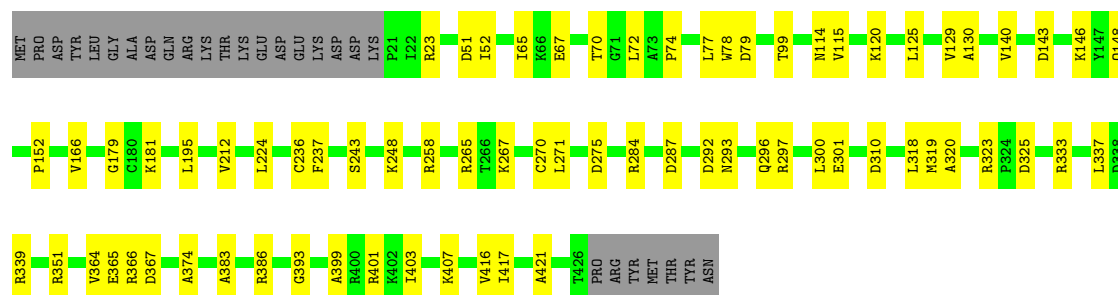
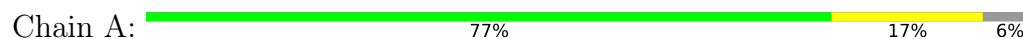
Chain x:  10% 71% 28%



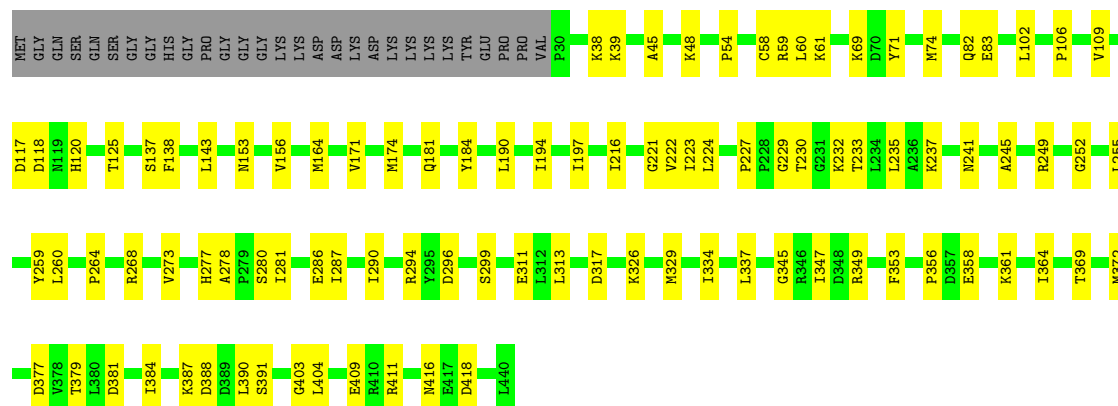
- Molecule 18: Ubiquitin



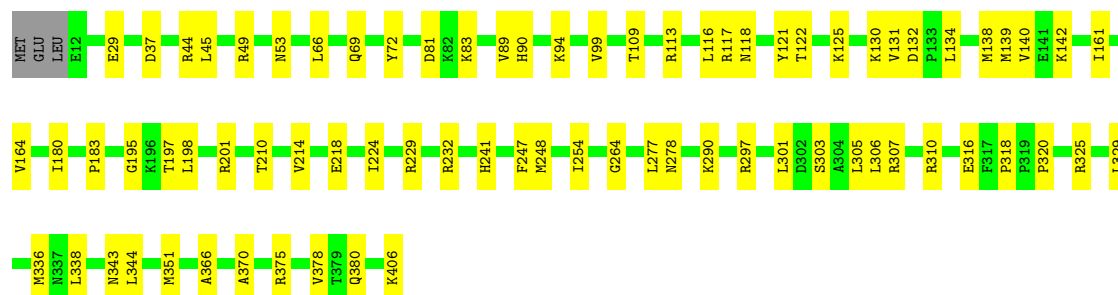
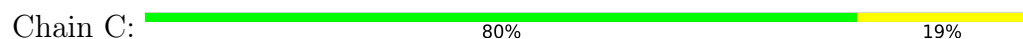
• Molecule 19: 26S protease regulatory subunit 7



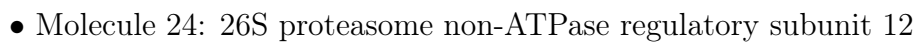
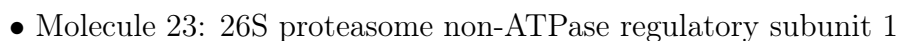
• Molecule 20: 26S protease regulatory subunit 4

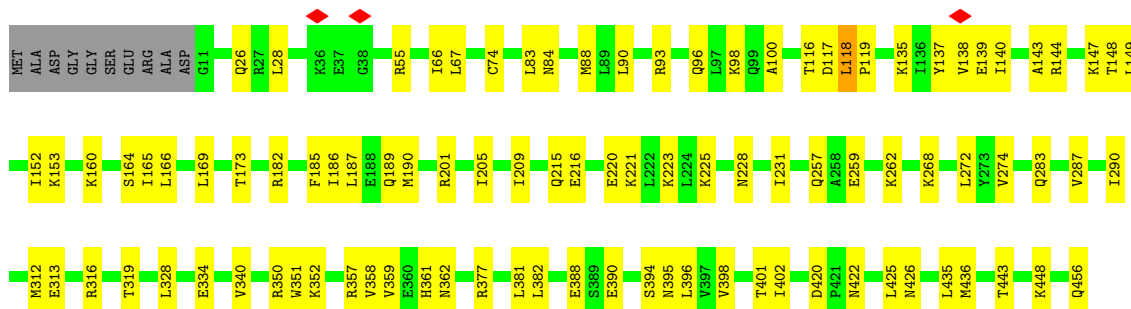


• Molecule 21: Isoform 2 of 26S proteasome regulatory subunit 8



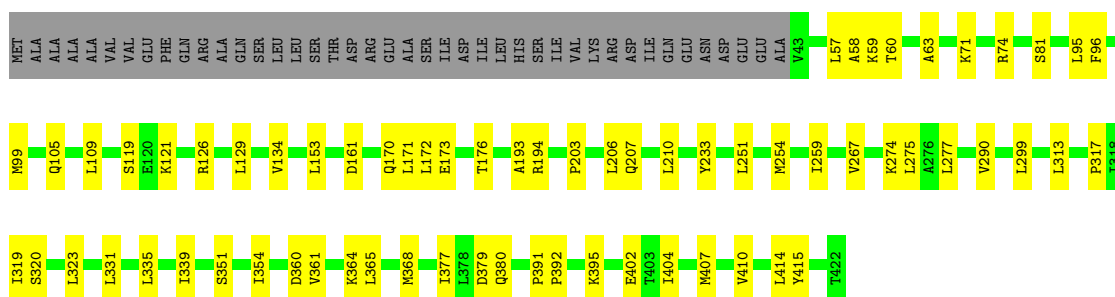
• Molecule 22: 26S protease regulatory subunit 6B





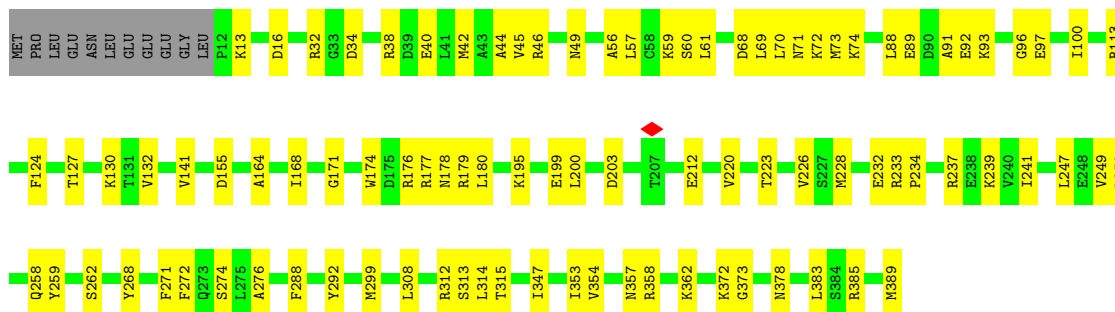
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 11

Chain X: 74% 16% 10%



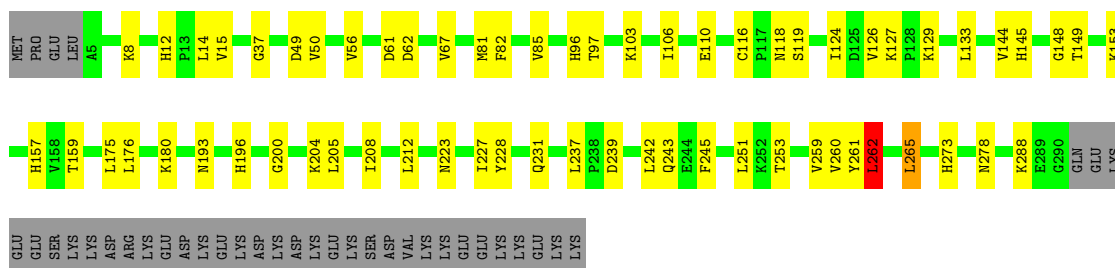
- Molecule 26: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 73% 24% 3%

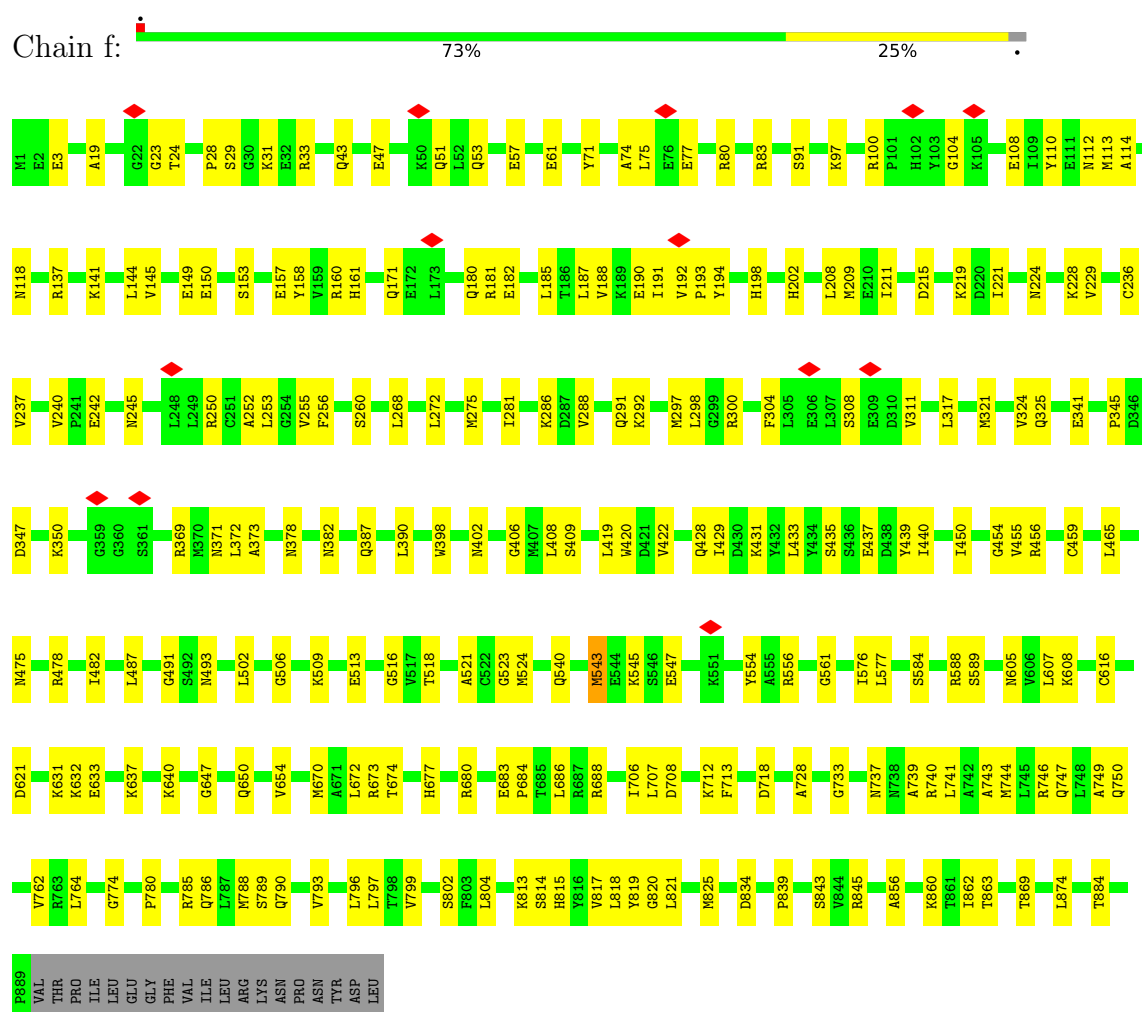


- Molecule 27: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 69% 19% 12%

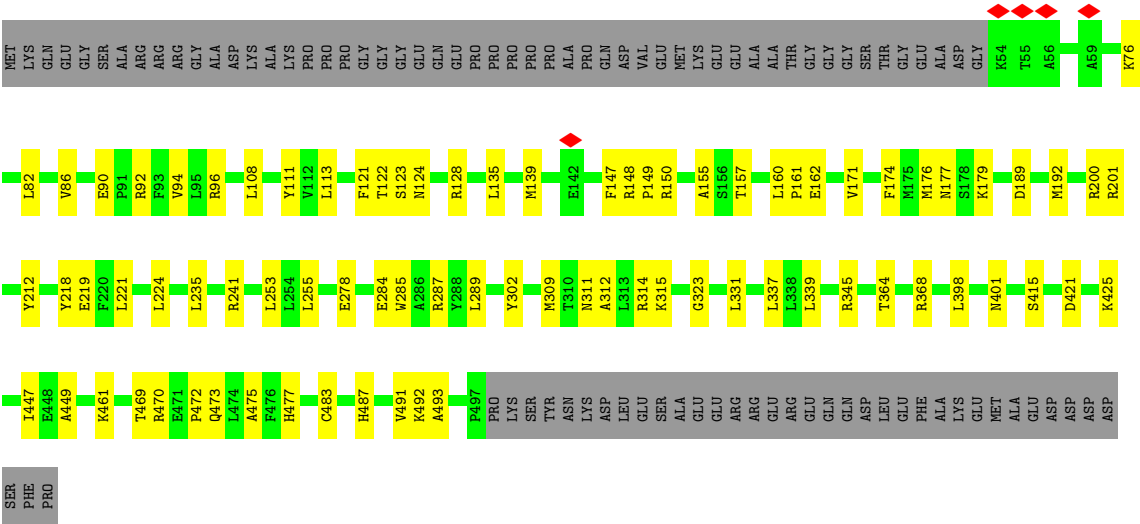


- Molecule 32: 26S proteasome non-ATPase regulatory subunit 2



- Molecule 33: 26S proteasome non-ATPase regulatory subunit 3





● 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	56133	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	0.022	Depositor
Minimum map value	-0.005	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size ($\text{\AA}$)	438.4, 438.4, 438.4	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.685, 0.685, 0.685	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	E	0.20	0/3145	0.52	0/4233
2	F	0.20	0/3173	0.47	0/4273
3	G	0.26	0/1901	0.42	0/2572
3	g	0.25	0/1913	0.45	2/2589 (0.1%)
4	H	0.27	0/1840	0.44	0/2495
4	h	0.25	0/1844	0.39	0/2497
5	I	0.27	0/1963	0.44	0/2650
5	i	0.23	0/1985	0.39	0/2677
6	J	0.23	0/1887	0.43	0/2553
6	j	0.23	0/1887	0.43	0/2549
7	K	0.25	0/1841	0.40	0/2486
7	k	0.24	0/1809	0.39	0/2444
8	L	0.26	0/1911	0.40	0/2584
8	l	0.25	0/1896	0.39	0/2565
9	M	0.26	0/1925	0.41	0/2592
9	m	0.25	0/1916	0.37	0/2580
10	N	0.26	0/1548	0.33	0/2097
10	n	0.26	0/1536	0.36	0/2080
11	O	0.26	0/1672	0.43	0/2267
11	o	0.26	0/1686	0.44	0/2282
12	P	0.27	0/1616	0.45	0/2180
12	p	0.25	0/1620	0.40	0/2184
13	Q	0.27	0/1621	0.40	0/2194
13	q	0.26	0/1611	0.37	0/2182
14	R	0.25	0/1590	0.38	0/2147
14	r	0.26	0/1580	0.38	0/2135
15	S	0.26	0/1671	0.40	0/2252
15	s	0.25	0/1680	0.39	0/2264
16	T	0.26	0/1716	0.40	0/2323
16	t	0.26	0/1720	0.39	0/2328
17	x	0.19	0/4002	0.42	0/5390
18	y	0.16	0/607	0.40	0/816

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	A	0.20	0/3215	0.49	0/4340
20	B	0.19	0/3254	0.48	0/4388
21	C	0.21	0/3138	0.52	2/4215 (0.0%)
22	D	0.21	0/3089	0.48	0/4168
23	U	0.21	0/6945	0.49	0/9382
24	W	0.21	0/3683	0.53	0/4952
25	X	0.20	0/3053	0.46	0/4115
26	Y	0.20	0/3173	0.53	0/4273
27	Z	0.25	0/2324	0.54	0/3150
28	a	0.20	0/3053	0.53	0/4133
29	b	0.20	0/1478	0.52	0/2001
30	c	0.24	0/2302	0.59	0/3110
31	d	0.23	0/2162	0.53	0/2919
32	f	0.23	0/6980	0.56	0/9433
33	V	0.19	0/3681	0.43	0/4969
34	e	0.20	0/437	0.51	0/595
All	All	0.23	0/112279	0.46	4/151603 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	318	PRO	CA-C-N	-8.38	111.75	120.38
21	C	318	PRO	C-N-CA	-8.38	111.75	120.38
3	g	224	ASN	CA-C-N	-6.72	113.97	120.83
3	g	224	ASN	C-N-CA	-6.72	113.97	120.83

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	E	3097	0	3174	60	0
2	F	3133	0	3220	60	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1867	0	1867	23	0
3	g	1879	0	1872	17	0
4	H	1801	0	1773	14	0
4	h	1805	0	1798	16	0
5	I	1933	0	1923	10	0
5	i	1955	0	1955	10	0
6	J	1861	0	1846	24	0
6	j	1861	0	1865	31	0
7	K	1813	0	1796	12	0
7	k	1782	0	1766	15	0
8	L	1876	0	1856	18	0
8	l	1861	0	1839	20	0
9	M	1890	0	1880	14	0
9	m	1881	0	1868	17	0
10	N	1521	0	1494	1	0
10	n	1510	0	1483	14	0
11	O	1645	0	1648	13	0
11	o	1659	0	1681	13	0
12	P	1587	0	1598	18	0
12	p	1591	0	1609	11	0
13	Q	1588	0	1584	20	0
13	q	1578	0	1569	13	0
14	R	1559	0	1523	14	0
14	r	1549	0	1506	10	0
15	S	1641	0	1639	7	0
15	s	1650	0	1645	10	0
16	T	1683	0	1662	17	0
16	t	1687	0	1666	9	0
17	x	3929	0	3915	80	0
18	y	601	0	629	16	0
19	A	3164	0	3201	55	0
20	B	3207	0	3278	67	0
21	C	3097	0	3208	55	0
22	D	3039	0	3076	62	0
23	U	6828	0	6884	107	0
24	W	3635	0	3762	65	0
25	X	3009	0	3113	47	0
26	Y	3115	0	3120	65	0
27	Z	2281	0	2312	52	0
28	a	2995	0	3012	59	0
29	b	1458	0	1505	41	0
30	c	2260	0	2276	54	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	d	2116	0	2146	37	0
32	f	6866	0	6866	149	0
33	V	3612	0	3682	57	0
34	e	425	0	328	8	0
35	A	31	0	12	1	0
35	D	31	0	12	1	0
35	E	31	0	12	4	0
35	F	31	0	12	1	0
36	B	27	0	12	4	0
36	C	27	0	12	1	0
37	c	1	0	0	0	0
All	All	110559	0	110990	1434	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 (1434) 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)
17:x:340:ASN:HB2	18:y:74:ARG:HH21	1.44	0.82
27:Z:262:LEU:HD11	30:c:248:MET:CE	2.13	0.79
28:a:70:ARG:HH22	29:b:25:ARG:H	1.30	0.79
32:f:429:ILE:O	32:f:433:LEU:HB2	1.85	0.76
25:X:233:TYR:HA	25:X:254:MET:HE1	1.69	0.75
27:Z:148:GLY:HA2	28:a:181:GLY:CA	2.17	0.74
16:t:50:MET:HE1	16:t:192:VAL:HB	1.70	0.73
2:F:28:GLY:O	2:F:32:GLU:HB2	1.89	0.73
33:V:124:ASN:HA	33:V:128:ARG:HH12	1.56	0.71
5:i:8:ARG:HH21	6:j:5:ARG:HH21	1.38	0.71
24:W:359:VAL:HG23	24:W:382:LEU:HD12	1.73	0.71
11:o:55:THR:HG23	11:o:86:MET:HE1	1.74	0.70
13:Q:197:PRO:HD2	13:q:199:GLN:H	1.56	0.70
27:Z:262:LEU:HD11	30:c:248:MET:HE3	1.74	0.69
32:f:825:MET:HB2	32:f:862:ILE:HD11	1.75	0.68
24:W:268:LYS:HZ2	24:W:334:GLU:H	1.42	0.68
17:x:305:LEU:HD23	17:x:307:ARG:HE	1.59	0.67
1:E:242:ARG:HH22	22:D:312:ASN:HD21	1.43	0.67
20:B:174:MET:SD	21:C:229:ARG:NH1	2.68	0.67
32:f:75:LEU:HD23	32:f:77:GLU:H	1.60	0.67
27:Z:253:THR:HG23	33:V:469:THR:HG21	1.75	0.67
24:W:436:MET:HE1	30:c:226:MET:HA	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:114:ALA:HA	32:f:118:ASN:HB2	1.77	0.67
32:f:762:VAL:HG23	32:f:774:GLY:HA3	1.75	0.67
24:W:401:THR:HG23	24:W:402:ILE:HD12	1.77	0.66
27:Z:262:LEU:HD11	30:c:248:MET:SD	2.36	0.66
31:d:33:LEU:HD23	31:d:41:THR:HG23	1.78	0.66
32:f:297:MET:SD	32:f:300:ARG:NH1	2.69	0.66
7:k:210:LEU:HA	7:k:214:ASN:HD21	1.62	0.65
25:X:95:LEU:O	25:X:99:MET:HB2	1.97	0.65
28:a:15:GLY:O	28:a:18:GLN:NE2	2.29	0.65
17:x:341:ALA:HB1	19:A:130:ALA:HB2	1.77	0.65
6:J:68:ASN:HA	6:J:211:MET:HE1	1.77	0.65
20:B:39:LYS:HG2	20:B:277:HIS:HA	1.78	0.65
23:U:164:GLU:O	23:U:168:LEU:HB2	1.96	0.65
32:f:113:MET:HE3	32:f:114:ALA:H	1.61	0.65
32:f:137:ARG:HE	32:f:141:LYS:HZ3	1.43	0.65
27:Z:262:LEU:CD1	30:c:248:MET:CE	2.74	0.65
26:Y:373:GLY:HA3	27:Z:261:TYR:CE1	2.32	0.64
23:U:437:TYR:HA	23:U:472:ILE:HG21	1.79	0.64
34:e:35:ASP:HB3	34:e:37:HIS:HD2	1.61	0.64
32:f:300:ARG:HD2	32:f:321:MET:HG2	1.80	0.64
27:Z:106:ILE:HG23	27:Z:153:LYS:HD3	1.79	0.64
32:f:450:ILE:HA	32:f:487:LEU:HD22	1.80	0.64
10:n:107:GLU:HB2	10:n:110:GLN:HE21	1.61	0.64
27:Z:148:GLY:HA2	28:a:181:GLY:HA3	1.80	0.64
23:U:198:LEU:HD11	23:U:219:CYS:HB2	1.78	0.64
24:W:189:GLN:HE21	24:W:205:ILE:HD12	1.61	0.64
32:f:813:LYS:HZ2	32:f:825:MET:HG2	1.62	0.64
23:U:799:LYS:HB2	23:U:923:GLU:HB3	1.80	0.63
30:c:163:ILE:HG12	30:c:200:TYR:HA	1.80	0.63
11:O:216:ILE:HD11	12:P:194:LYS:HD2	1.79	0.63
20:B:230:THR:HG21	20:B:353:PHE:HB3	1.81	0.63
7:K:121:LEU:HD23	7:K:160:GLY:HA3	1.79	0.63
17:x:418:TYR:HB3	17:x:480:TYR:HB3	1.81	0.63
18:y:29:LYS:HG2	18:y:33:LYS:HZ3	1.63	0.63
33:V:309:MET:HE1	33:V:331:LEU:HB3	1.81	0.62
5:i:180:LYS:H	5:i:184:MET:HE3	1.64	0.62
32:f:790:GLN:NE2	32:f:796:LEU:O	2.32	0.62
24:W:340:VAL:HG13	24:W:350:ARG:HH11	1.64	0.62
32:f:869:THR:HA	32:f:884:THR:HA	1.82	0.62
32:f:180:GLN:OE1	32:f:181:ARG:NH1	2.32	0.62
10:n:119:MET:HE2	16:t:57:TYR:HB3	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:259:ILE:HD11	25:X:267:VAL:HB	1.81	0.61
32:f:433:LEU:HD11	32:f:465:LEU:HD11	1.81	0.61
3:g:128:ASN:HB2	3:g:131:MET:HE1	1.83	0.61
32:f:371:ASN:OD1	32:f:398:TRP:NE1	2.32	0.61
24:W:98:LYS:O	24:W:135:LYS:NZ	2.33	0.61
32:f:157:GLU:O	32:f:161:HIS:ND1	2.34	0.61
11:o:12:ILE:HD11	11:o:110:LEU:HD13	1.82	0.61
8:l:120:THR:O	9:m:129:ARG:NH1	2.34	0.61
24:W:443:THR:HG21	27:Z:204:LYS:HD2	1.82	0.61
1:E:149:ILE:HD11	1:E:276:ILE:HD11	1.81	0.61
24:W:28:LEU:HD11	24:W:66:ILE:HG22	1.83	0.61
26:Y:88:LEU:HG	26:Y:100:ILE:HG13	1.83	0.61
32:f:242:GLU:O	32:f:245:ASN:ND2	2.34	0.61
3:G:206:LEU:HD23	3:G:208:ILE:HD12	1.82	0.61
21:C:277:LEU:HD21	21:C:310:ARG:HB3	1.83	0.61
33:V:201:ARG:HH12	33:V:241:ARG:HB3	1.65	0.61
32:f:435:SER:HB3	32:f:440:ILE:HG21	1.83	0.61
33:V:311:ASN:OD1	33:V:314:ARG:NH2	2.34	0.60
20:B:109:VAL:HB	21:C:94:LYS:HB2	1.83	0.60
33:V:473:GLN:O	33:V:477:HIS:ND1	2.34	0.60
6:J:199:VAL:HG11	6:J:206:ILE:HD11	1.84	0.60
17:x:46:VAL:HG22	17:x:71:MET:HE1	1.84	0.60
31:d:29:VAL:HA	31:d:32:GLU:HB2	1.82	0.60
26:Y:378:ASN:OD1	33:V:314:ARG:NH1	2.34	0.60
16:t:92:LEU:HD13	16:t:110:MET:HG3	1.84	0.60
23:U:208:LEU:HD23	23:U:210:LYS:H	1.67	0.60
26:Y:32:ARG:O	26:Y:38:ARG:NH1	2.34	0.60
1:E:387:LYS:NZ	1:E:388:PRO:O	2.34	0.60
32:f:728:ALA:HB2	32:f:750:GLN:HB3	1.84	0.60
1:E:97:ARG:HH11	1:E:114:GLU:HG3	1.67	0.60
17:x:41:PRO:HA	17:x:44:GLN:HB2	1.83	0.60
21:C:195:GLY:HA2	21:C:198:LEU:HD13	1.84	0.60
22:D:230:VAL:HB	22:D:264:ILE:HG12	1.82	0.60
32:f:71:TYR:HA	32:f:74:ALA:HB3	1.84	0.60
1:E:345:ASN:HD22	2:F:345:SER:HB2	1.66	0.59
22:D:353:ASN:ND2	22:D:392:TYR:O	2.35	0.59
36:B:501:ADP:O2B	21:C:307:ARG:NH2	2.34	0.59
32:f:108:GLU:O	32:f:112:ASN:ND2	2.35	0.59
32:f:589:SER:O	32:f:632:LYS:NZ	2.35	0.59
33:V:90:GLU:OE2	33:V:92:ARG:NH1	2.35	0.59
6:J:52:LYS:HG3	6:J:53:LEU:HG	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:616:CYS:HB2	32:f:632:LYS:HB3	1.84	0.59
17:x:399:VAL:HG13	17:x:486:GLU:HG3	1.83	0.59
21:C:320:PRO:O	21:C:325:ARG:NH1	2.35	0.59
12:P:65:GLN:OE1	13:Q:86:ARG:NH2	2.35	0.59
16:T:174:ARG:NH1	16:T:206:GLU:O	2.36	0.59
22:D:391:ARG:NE	22:D:393:ILE:O	2.33	0.59
24:W:186:ILE:HD13	24:W:209:ILE:HD11	1.85	0.59
16:T:26:MET:HE2	16:T:188:GLN:HG3	1.83	0.59
20:B:221:GLY:HA3	20:B:347:ILE:HA	1.85	0.59
32:f:190:GLU:HB2	32:f:193:PRO:HD2	1.85	0.59
6:J:50:VAL:HG11	6:J:54:GLN:HB3	1.84	0.59
20:B:313:LEU:O	20:B:317:ASP:HB2	2.03	0.59
31:d:19:CYS:SG	31:d:65:ARG:NH1	2.76	0.59
1:E:352:MET:HA	1:E:355:ILE:HB	1.85	0.59
23:U:216:VAL:HG23	23:U:220:LEU:HD13	1.84	0.59
26:Y:174:TRP:O	26:Y:178:ASN:ND2	2.35	0.59
6:J:120:GLN:NE2	7:K:133:MET:SD	2.71	0.58
20:B:229:GLY:HA2	36:B:501:ADP:H5'1	1.84	0.58
13:Q:25:ILE:HG22	13:Q:26:VAL:HG13	1.84	0.58
13:Q:38:MET:O	13:Q:65:GLN:NE2	2.36	0.58
24:W:187:LEU:HA	24:W:190:MET:HE1	1.84	0.58
30:c:58:LEU:HD11	30:c:106:GLU:H	1.68	0.58
28:a:70:ARG:HH12	29:b:24:THR:HA	1.69	0.58
19:A:417:ILE:HA	19:A:421:ALA:HB3	1.84	0.58
21:C:366:ALA:HB1	21:C:378:VAL:HG11	1.86	0.58
22:D:391:ARG:HG2	22:D:393:ILE:H	1.68	0.58
26:Y:92:GLU:HB3	26:Y:100:ILE:HD11	1.85	0.58
32:f:780:PRO:HB3	32:f:799:VAL:HG22	1.84	0.58
17:x:300:LYS:NZ	18:y:64:GLU:OE2	2.36	0.58
23:U:890:LYS:HG3	23:U:891:VAL:HG13	1.85	0.58
29:b:144:GLY:H	29:b:174:PRO:HG2	1.67	0.58
7:K:28:ILE:HD13	7:K:158:PRO:HG2	1.86	0.58
3:g:180:GLU:HG3	4:h:54:SER:HB2	1.84	0.58
27:Z:37:GLY:HA2	27:Z:56:VAL:HG12	1.85	0.58
32:f:29:SER:HA	32:f:33:ARG:HD3	1.84	0.58
15:s:16:ALA:HB2	15:s:121:VAL:HG23	1.86	0.58
16:t:25:ASP:OD1	16:t:41:ARG:NH2	2.35	0.58
30:c:277:LYS:HE3	30:c:283:HIS:HD2	1.68	0.58
25:X:203:PRO:HB2	25:X:206:LEU:HB2	1.86	0.58
30:c:49:VAL:HG13	30:c:50:PRO:HD3	1.85	0.58
9:M:34:SER:OG	9:M:65:ARG:NH1	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:l:117:GLN:NE2	9:m:83:ASP:OD1	2.36	0.58
20:B:313:LEU:O	20:B:317:ASP:CB	2.52	0.58
25:X:171:LEU:HD21	25:X:210:LEU:HD12	1.86	0.58
31:d:128:GLN:HG3	31:d:129:THR:HG22	1.86	0.58
32:f:29:SER:O	32:f:33:ARG:HB2	2.04	0.58
8:L:196:ARG:O	8:L:239:ARG:NH2	2.37	0.57
17:x:260:SER:OG	17:x:307:ARG:NH2	2.37	0.57
20:B:197:ILE:HG21	20:B:235:LEU:HD21	1.85	0.57
32:f:160:ARG:NH1	32:f:190:GLU:OE1	2.37	0.57
11:O:22:GLU:HG2	11:O:27:ALA:HB2	1.85	0.57
6:j:140:GLY:O	6:j:213:ARG:NH1	2.37	0.57
17:x:19:GLU:O	17:x:32:GLN:NE2	2.38	0.57
20:B:245:ALA:HB1	20:B:280:SER:HA	1.85	0.57
30:c:145:VAL:HG22	30:c:157:ILE:HG22	1.85	0.57
32:f:24:THR:HG23	32:f:31:LYS:HA	1.85	0.57
32:f:297:MET:O	32:f:300:ARG:NH1	2.36	0.57
23:U:800:VAL:HG23	23:U:880:ASN:HD21	1.69	0.57
24:W:274:VAL:O	24:W:283:GLN:NE2	2.37	0.57
32:f:100:ARG:O	32:f:104:GLY:N	2.37	0.57
3:G:80:MET:HG3	3:G:87:SER:HB3	1.87	0.57
22:D:117:SER:O	30:c:282:ARG:NH1	2.37	0.57
33:V:108:LEU:HD23	33:V:174:PHE:HB2	1.86	0.57
6:J:66:ASP:HA	13:Q:69:MET:HE3	1.87	0.57
3:g:4:GLY:HA2	3:g:11:ARG:HH22	1.69	0.57
7:k:181:LEU:HA	7:k:184:VAL:HG12	1.86	0.57
2:F:43:GLN:HG3	28:a:66:GLU:HB3	1.86	0.57
8:L:49:LEU:HB2	8:L:195:LEU:HD21	1.86	0.57
3:g:103:TYR:O	11:o:81:ARG:NH2	2.38	0.57
27:Z:212:LEU:HD21	27:Z:231:GLN:HE22	1.67	0.57
1:E:235:ILE:HG13	1:E:277:MET:HB3	1.87	0.57
2:F:150:LEU:HD12	2:F:166:THR:HA	1.87	0.57
6:J:11:SER:OG	6:J:13:ASP:OD1	2.21	0.57
9:m:37:ILE:HD11	9:m:193:VAL:HG13	1.87	0.57
17:x:163:MET:HA	17:x:166:THR:HG22	1.87	0.57
19:A:248:LYS:HD3	20:B:259:TYR:HB3	1.85	0.57
32:f:780:PRO:HG3	32:f:802:SER:HB2	1.87	0.57
6:J:158:ALA:HB3	7:K:58:LEU:HD21	1.87	0.57
11:O:78:THR:HG22	11:O:82:MET:HE2	1.85	0.57
12:P:14:MET:HG2	12:P:136:PHE:HB3	1.85	0.57
17:x:245:GLN:NE2	17:x:409:ASP:OD1	2.38	0.57
28:a:11:SER:O	28:a:12:GLN:NE2	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:x:70:LEU:HD22	32:f:459:CYS:HB3	1.85	0.57
17:x:352:MET:HE1	17:x:483:ARG:HD2	1.87	0.57
27:Z:96:HIS:ND1	27:Z:97:THR:O	2.38	0.57
2:F:180:ARG:NH2	2:F:246:ALA:O	2.38	0.57
25:X:317:PRO:HD2	25:X:319:ILE:HG12	1.87	0.57
2:F:305:GLU:OE1	2:F:308:ARG:NH1	2.38	0.56
15:S:125:ASP:OD1	15:S:129:SER:N	2.38	0.56
11:o:206:LYS:HD2	12:p:161:ASP:HB3	1.87	0.56
21:C:343:ASN:HB3	21:C:380:GLN:HE22	1.70	0.56
22:D:81:ARG:HH12	30:c:153:GLY:HA3	1.70	0.56
28:a:156:TYR:HB3	28:a:179:PHE:HB2	1.87	0.56
32:f:236:CYS:SG	32:f:237:VAL:N	2.78	0.56
21:C:183:PRO:O	21:C:290:LYS:NZ	2.36	0.56
23:U:580:ARG:NH2	23:U:768:GLN:OE1	2.38	0.56
23:U:751:ARG:NE	23:U:909:GLY:O	2.34	0.56
27:Z:200:GLY:HA3	30:c:225:TRP:HE1	1.70	0.56
29:b:126:LYS:HA	29:b:129:LYS:HE2	1.86	0.56
31:d:106:LEU:HD21	31:d:114:GLU:HB3	1.88	0.56
32:f:378:ASN:OD1	32:f:382:ASN:ND2	2.38	0.56
3:G:226:LYS:O	3:G:228:ARG:NH1	2.38	0.56
15:s:158:MET:HE2	15:s:161:VAL:HG11	1.88	0.56
19:A:65:ILE:HG21	21:C:81:ASP:H	1.70	0.56
27:Z:15:VAL:HG21	27:Z:50:VAL:HG12	1.87	0.56
28:a:24:ARG:HH12	28:a:39:LEU:HD13	1.70	0.56
1:E:89:LYS:HA	1:E:92:LEU:HB2	1.86	0.56
23:U:12:LEU:O	23:U:20:LYS:NZ	2.39	0.56
24:W:435:LEU:HD13	27:Z:237:LEU:HB2	1.88	0.56
25:X:119:SER:O	25:X:121:LYS:NZ	2.38	0.56
31:d:8:GLU:O	31:d:13:SER:OG	2.24	0.56
35:E:501:ATP:O2G	2:F:344:ARG:NH1	2.39	0.56
28:a:247:ARG:HE	28:a:251:LEU:HB2	1.70	0.56
32:f:475:ASN:ND2	32:f:513:GLU:OE2	2.39	0.56
33:V:147:PHE:O	33:V:148:ARG:NH1	2.38	0.56
1:E:15:LYS:HA	1:E:18:GLU:HB2	1.88	0.56
17:x:149:ALA:HA	17:x:152:ILE:HD12	1.87	0.56
5:I:15:GLU:O	6:J:28:LYS:NZ	2.39	0.56
24:W:166:LEU:O	24:W:201:ARG:NH2	2.38	0.56
28:a:66:GLU:O	28:a:69:HIS:NE2	2.39	0.56
26:Y:127:THR:HA	26:Y:130:LYS:HB3	1.88	0.56
33:V:92:ARG:HD2	33:V:96:ARG:HH21	1.71	0.56
1:E:27:LYS:HD3	2:F:59:VAL:HG22	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:x:142:ALA:HB2	17:x:151:TYR:HE2	1.72	0.55
17:x:301:GLN:HA	17:x:308:ASN:HA	1.88	0.55
32:f:83:ARG:HH21	32:f:112:ASN:HB2	1.69	0.55
22:D:129:SER:HB3	22:D:143:LEU:HD11	1.88	0.55
22:D:385:LEU:HD12	22:D:388:ARG:HD2	1.87	0.55
23:U:215:ASN:OD1	23:U:216:VAL:N	2.34	0.55
26:Y:91:ALA:O	26:Y:93:LYS:NZ	2.39	0.55
32:f:61:GLU:HG3	32:f:97:LYS:HD2	1.87	0.55
6:J:140:GLY:O	6:J:213:ARG:NH2	2.39	0.55
19:A:292:ASP:O	19:A:296:GLN:NE2	2.37	0.55
22:D:339:ARG:HA	22:D:342:ARG:HE	1.71	0.55
2:F:303:ASP:OD2	19:A:293:ASN:ND2	2.39	0.55
17:x:9:LYS:HB2	17:x:14:LYS:HG2	1.87	0.55
32:f:347:ASP:HB2	32:f:350:LYS:HB2	1.89	0.55
33:V:177:ASN:O	33:V:179:LYS:NZ	2.39	0.55
2:F:61:ARG:NH1	29:b:73:SER:O	2.40	0.55
7:K:211:ASN:ND2	7:K:213:THR:OG1	2.39	0.55
8:L:164:ARG:NH1	8:L:198:THR:O	2.40	0.55
17:x:152:ILE:HG12	17:x:178:PHE:HB3	1.89	0.55
19:A:23:ARG:NH2	32:f:3:GLU:O	2.40	0.55
25:X:299:LEU:HD13	25:X:331:LEU:HG	1.89	0.55
25:X:380:GLN:HB3	26:Y:314:LEU:HA	1.89	0.55
27:Z:148:GLY:HA2	28:a:181:GLY:HA2	1.88	0.55
1:E:15:LYS:HB3	1:E:19:HIS:CD2	2.42	0.55
11:o:99:VAL:HG23	11:o:127:MET:HE2	1.88	0.55
21:C:375:ARG:HH21	21:C:378:VAL:HA	1.71	0.55
26:Y:49:ASN:ND2	26:Y:113:ARG:O	2.39	0.55
27:Z:278:ASN:ND2	33:V:493:ALA:O	2.36	0.55
28:a:8:LEU:O	28:a:12:GLN:NE2	2.40	0.55
28:a:318:GLY:O	28:a:321:LYS:NZ	2.40	0.55
32:f:260:SER:HA	32:f:268:LEU:HD21	1.88	0.55
33:V:121:PHE:HB3	33:V:128:ARG:HH21	1.71	0.55
2:F:368:ILE:HG23	2:F:371:ARG:HH12	1.71	0.55
17:x:293:ARG:HH22	18:y:6:LYS:HB3	1.72	0.55
19:A:271:LEU:HD11	19:A:318:LEU:HD23	1.88	0.55
22:D:167:ILE:HG21	22:D:214:MET:HE1	1.89	0.55
23:U:242:LEU:O	23:U:246:TYR:HB2	2.07	0.55
26:Y:203:ASP:N	26:Y:203:ASP:OD1	2.37	0.55
29:b:1:MET:HG2	29:b:44:ASN:HB2	1.87	0.55
32:f:51:GLN:NE2	32:f:53:GLN:O	2.40	0.55
32:f:221:ILE:HG21	32:f:255:VAL:HG11	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:856:ALA:HA	32:f:860:LYS:HE2	1.89	0.55
8:l:218:ASP:OD1	8:l:218:ASP:N	2.39	0.54
21:C:113:ARG:NH2	22:D:94:GLU:OE1	2.39	0.54
21:C:370:ALA:HB2	21:C:378:VAL:HG22	1.88	0.54
18:y:23:ILE:HD13	18:y:51:GLU:HA	1.88	0.54
20:B:264:PRO:HB2	20:B:268:ARG:HH21	1.73	0.54
21:C:53:ASN:ND2	23:U:642:GLU:O	2.40	0.54
23:U:521:LEU:HD13	23:U:554:LEU:HG	1.89	0.54
28:a:102:GLU:O	28:a:105:LYS:NZ	2.39	0.54
29:b:15:TYR:O	29:b:18:ASN:ND2	2.39	0.54
8:l:26:MET:HE1	8:l:148:CYS:HB3	1.89	0.54
32:f:224:ASN:ND2	32:f:236:CYS:SG	2.74	0.54
35:E:501:ATP:O3G	2:F:347:ARG:NH2	2.40	0.54
20:B:137:SER:OG	20:B:138:PHE:N	2.40	0.54
25:X:402:GLU:HB3	30:c:249:LEU:HD11	1.89	0.54
25:X:414:LEU:HD11	27:Z:273:HIS:HB2	1.90	0.54
32:f:633:GLU:OE2	32:f:785:ARG:NH2	2.40	0.54
4:H:143:ARG:NH1	4:H:144:PRO:O	2.41	0.54
8:L:88:MET:HE3	8:L:112:ILE:HG13	1.90	0.54
4:h:9:SER:HA	4:h:125:GLY:HA2	1.90	0.54
17:x:129:LEU:HD11	17:x:211:LEU:HD13	1.89	0.54
20:B:171:VAL:HG21	20:B:273:VAL:HG21	1.90	0.54
25:X:379:ASP:OD2	26:Y:312:ARG:NH2	2.41	0.54
28:a:4:VAL:HB	28:a:7:PHE:HB2	1.89	0.54
31:d:56:GLU:HG3	31:d:78:LEU:HD11	1.90	0.54
32:f:674:THR:HA	32:f:677:HIS:HB3	1.88	0.54
20:B:82:GLN:HG2	20:B:83:GLU:HG2	1.89	0.54
26:Y:234:PRO:O	26:Y:239:LYS:NZ	2.37	0.54
32:f:288:VAL:HA	32:f:291:GLN:HB2	1.89	0.54
32:f:670:MET:O	32:f:673:ARG:NH1	2.39	0.54
16:T:96:MET:HE2	16:T:110:MET:HE1	1.89	0.54
6:J:42:VAL:HG13	6:J:210:VAL:HG12	1.89	0.54
19:A:212:VAL:HG22	19:A:339:ARG:HB3	1.89	0.54
23:U:161:ASP:OD1	23:U:161:ASP:N	2.41	0.54
32:f:324:VAL:HG23	32:f:325:GLN:HG2	1.89	0.54
32:f:817:VAL:HG13	32:f:818:LEU:HD23	1.89	0.54
3:G:153:LYS:HD3	3:G:166:THR:HG21	1.90	0.54
4:H:111:VAL:HG22	4:H:136:ILE:HD12	1.90	0.54
4:h:65:VAL:O	4:h:220:ARG:NH1	2.37	0.54
22:D:231:VAL:HB	22:D:234:GLU:HB3	1.89	0.54
28:a:165:THR:HG1	28:a:168:ASN:HD22	1.53	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:GLU:OE1	2:F:72:LYS:NZ	2.40	0.54
1:E:60:VAL:HA	1:E:71:VAL:HG12	1.90	0.54
2:F:61:ARG:HH11	29:b:76:HIS:HB2	1.73	0.54
7:K:13:ASN:ND2	8:L:124:GLY:O	2.41	0.54
15:S:148:LEU:HD23	15:S:178:VAL:HG12	1.90	0.54
23:U:700:GLU:OE1	23:U:707:ASN:ND2	2.41	0.54
24:W:225:LYS:NZ	24:W:257:GLN:OE1	2.42	0.54
31:d:93:ALA:O	31:d:97:GLN:NE2	2.41	0.54
6:J:189:LYS:HA	6:J:232:ILE:HD11	1.90	0.53
9:M:108:LEU:HD22	9:M:139:SER:HB3	1.90	0.53
23:U:843:GLU:HA	23:U:846:LYS:HE3	1.89	0.53
27:Z:253:THR:OG1	33:V:470:ARG:NH1	2.41	0.53
23:U:387:ARG:NH2	23:U:426:TYR:OH	2.40	0.53
24:W:220:GLU:O	24:W:257:GLN:NE2	2.37	0.53
28:a:128:LEU:O	28:a:132:LYS:NZ	2.39	0.53
7:K:167:ALA:HB3	8:L:56:LEU:HD21	1.90	0.53
13:Q:58:GLU:OE1	13:Q:62:LYS:NZ	2.39	0.53
17:x:400:LYS:O	17:x:487:ILE:N	2.40	0.53
20:B:45:ALA:O	20:B:48:LYS:NZ	2.40	0.53
23:U:35:TRP:HB3	23:U:70:HIS:CE1	2.43	0.53
6:j:96:LEU:HD22	13:q:62:LYS:HD2	1.88	0.53
23:U:265:ILE:HD11	23:U:326:ILE:HG23	1.90	0.53
23:U:906:LEU:HD13	23:U:912:ILE:HD13	1.90	0.53
24:W:358:VAL:O	24:W:362:ASN:ND2	2.41	0.53
26:Y:45:VAL:HG23	26:Y:46:ARG:HD3	1.90	0.53
26:Y:60:SER:OG	26:Y:61:LEU:N	2.42	0.53
23:U:792:ASN:HB3	23:U:914:LEU:HB3	1.90	0.53
20:B:379:THR:OG1	20:B:416:ASN:ND2	2.34	0.53
24:W:228:ASN:HA	24:W:231:ILE:HG12	1.91	0.53
29:b:171:VAL:HG11	29:b:184:ILE:HG22	1.90	0.53
6:j:105:GLU:OE2	6:j:109:ARG:NH1	2.42	0.53
26:Y:385:ARG:HA	26:Y:389:MET:HA	1.91	0.53
27:Z:61:ASP:HB2	27:Z:67:VAL:HB	1.90	0.53
27:Z:228:TYR:HA	27:Z:231:GLN:HG2	1.89	0.53
23:U:18:GLN:HA	23:U:55:ARG:HH21	1.73	0.53
27:Z:223:ASN:HB3	27:Z:227:ILE:HB	1.90	0.53
32:f:112:ASN:O	32:f:158:TYR:OH	2.26	0.53
6:j:122:ASN:ND2	7:k:130:PRO:O	2.42	0.53
17:x:6:VAL:HG12	17:x:65:ASN:HA	1.90	0.53
17:x:327:GLN:HG3	17:x:477:VAL:HG22	1.91	0.53
21:C:301:LEU:HD12	21:C:305:LEU:HD21	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:67:VAL:HG12	29:b:95:LEU:HD22	1.91	0.53
6:j:40:ILE:HD12	6:j:184:ASP:HB3	1.90	0.53
20:B:281:ILE:HG22	20:B:326:LYS:HB2	1.90	0.53
30:c:54:MET:HG3	30:c:82:VAL:HG13	1.91	0.53
2:F:94:ILE:HD12	2:F:123:VAL:HG12	1.90	0.52
2:F:303:ASP:HB3	2:F:307:GLN:HE22	1.73	0.52
4:h:93:LEU:HD13	4:h:113:ARG:HB3	1.89	0.52
20:B:153:ASN:HD22	20:B:156:VAL:HG22	1.75	0.52
23:U:210:LYS:HD2	23:U:211:PRO:HD2	1.90	0.52
23:U:373:ASN:HD22	23:U:385:PHE:HD2	1.57	0.52
29:b:148:VAL:HG13	29:b:173:VAL:HG11	1.90	0.52
2:F:221:LYS:H	2:F:349:ASP:HB2	1.74	0.52
3:G:165:ALA:HB3	4:H:56:LEU:HD22	1.91	0.52
20:B:106:PRO:HB3	21:C:121:TYR:HB2	1.91	0.52
25:X:320:SER:HA	25:X:323:LEU:HD12	1.92	0.52
32:f:91:SER:OG	32:f:110:TYR:O	2.23	0.52
24:W:328:LEU:HD21	24:W:351:TRP:HE1	1.74	0.52
18:y:27:LYS:HB3	18:y:38:PRO:HB3	1.91	0.52
22:D:345:PHE:HB3	22:D:360:LEU:HD11	1.90	0.52
26:Y:89:GLU:HA	26:Y:100:ILE:HG12	1.92	0.52
28:a:150:SER:OG	28:a:154:ARG:NH1	2.43	0.52
28:a:227:ASN:O	28:a:231:GLN:NE2	2.43	0.52
30:c:266:THR:O	30:c:269:GLN:NE2	2.42	0.52
16:T:25:ASP:OD1	16:T:41:ARG:NH2	2.39	0.52
19:A:143:ASP:OD2	19:A:146:LYS:N	2.41	0.52
22:D:92:PHE:HA	22:D:103:VAL:HG12	1.91	0.52
26:Y:315:THR:HA	26:Y:353:ILE:HA	1.91	0.52
28:a:62:ASN:OD1	28:a:103:LYS:NZ	2.42	0.52
6:J:235:GLU:O	6:J:239:ASN:ND2	2.42	0.52
12:p:35:VAL:HG12	12:p:36:THR:HG23	1.91	0.52
21:C:214:VAL:HB	21:C:248:MET:HB3	1.92	0.52
24:W:169:LEU:O	24:W:182:ARG:NH2	2.43	0.52
30:c:277:LYS:HG3	30:c:282:ARG:HB3	1.92	0.52
17:x:190:GLY:N	17:x:194:GLN:O	2.41	0.52
18:y:19:PRO:HB3	18:y:61:ILE:HG12	1.92	0.52
24:W:221:LYS:HG2	24:W:225:LYS:HZ2	1.75	0.52
33:V:76:LYS:HE3	33:V:149:PRO:HB3	1.92	0.52
33:V:278:GLU:HA	33:V:285:TRP:HZ2	1.75	0.52
6:j:39:ASP:OD1	6:j:39:ASP:N	2.43	0.52
10:n:192:ASP:OD1	10:n:192:ASP:N	2.42	0.52
14:r:100:MET:HE2	14:r:126:PHE:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:255:LEU:HD21	20:B:290:ILE:HD11	1.91	0.52
22:D:160:PRO:HD2	22:D:221:HIS:HB2	1.91	0.52
22:D:163:MET:HB2	22:D:166:ASP:HB2	1.92	0.52
2:F:38:THR:HB	2:F:42:ILE:HG13	1.91	0.52
3:g:191:PHE:HE1	3:g:219:VAL:HG21	1.75	0.52
17:x:115:TYR:HB2	17:x:200:ALA:HB2	1.92	0.52
20:B:387:LYS:HB3	20:B:390:LEU:HD23	1.92	0.52
23:U:596:ASN:HA	23:U:599:ILE:HG22	1.92	0.52
31:d:200:PHE:HB3	31:d:203:PRO:HG3	1.91	0.52
1:E:9:LEU:HD21	2:F:33:VAL:HB	1.92	0.52
23:U:541:HIS:HB2	23:U:544:ILE:HG22	1.92	0.52
24:W:422:ASN:O	24:W:426:ASN:ND2	2.43	0.52
30:c:182:GLY:O	30:c:186:LYS:NZ	2.43	0.52
33:V:135:LEU:HD21	33:V:171:VAL:HG13	1.92	0.52
3:G:10:ASP:OD1	3:G:10:ASP:N	2.43	0.51
8:L:67:ASP:OD1	8:L:69:HIS:ND1	2.43	0.51
6:j:224:GLU:HA	6:j:227:LYS:HG2	1.92	0.51
17:x:91:ASP:H	17:x:96:GLN:HG2	1.76	0.51
17:x:208:MET:HE2	17:x:273:LEU:HB3	1.92	0.51
27:Z:14:LEU:HD22	30:c:43:LYS:HD3	1.92	0.51
30:c:104:ARG:NE	30:c:105:PRO:O	2.40	0.51
9:M:8:ASP:O	9:M:22:GLN:NE2	2.43	0.51
15:S:213:ASP:OD2	11:o:19:ARG:NH2	2.43	0.51
4:h:66:GLU:OE1	4:h:91:ARG:NH2	2.42	0.51
19:A:236:CYS:SG	19:A:267:LYS:NZ	2.75	0.51
23:U:764:LEU:O	23:U:767:THR:OG1	2.23	0.51
24:W:152:ILE:HG13	24:W:165:ILE:HD12	1.92	0.51
4:H:185:GLU:HA	4:H:188:ILE:HD12	1.91	0.51
21:C:229:ARG:HB3	21:C:232:ARG:HB2	1.92	0.51
28:a:337:GLN:NE2	28:a:338:PRO:O	2.43	0.51
29:b:139:ASP:OD1	29:b:169:HIS:N	2.41	0.51
32:f:402:ASN:HB3	32:f:406:GLY:HA3	1.91	0.51
33:V:212:TYR:HA	33:V:253:LEU:HD11	1.91	0.51
3:g:2:SER:OG	3:g:3:ARG:N	2.38	0.51
6:j:31:THR:OG1	6:j:163:ARG:O	2.27	0.51
6:j:159:ASN:OD1	6:j:169:ARG:NH2	2.44	0.51
14:r:100:MET:HE3	14:r:128:VAL:HG23	1.92	0.51
25:X:404:ILE:HG21	26:Y:372:LYS:HB3	1.92	0.51
32:f:80:ARG:HA	32:f:83:ARG:HG2	1.93	0.51
12:P:2:SER:OG	12:P:3:ILE:N	2.42	0.51
21:C:336:MET:HE1	22:D:194:ILE:HG23	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:274:LYS:HA	25:X:277:LEU:HB2	1.92	0.51
26:Y:276:ALA:HB2	34:e:56:LEU:HD12	1.92	0.51
32:f:683:GLU:HB3	32:f:686:LEU:HD21	1.92	0.51
19:A:51:ASP:OD1	19:A:52:ILE:N	2.44	0.51
19:A:364:VAL:H	19:A:366:ARG:HH12	1.59	0.51
19:A:386:ARG:HH21	20:B:345:GLY:HA2	1.76	0.51
21:C:132:ASP:OD1	21:C:132:ASP:N	2.44	0.51
23:U:741:GLY:O	23:U:743:ASN:ND2	2.43	0.51
26:Y:34:ASP:N	26:Y:34:ASP:OD1	2.43	0.51
27:Z:239:ASP:OD1	27:Z:239:ASP:N	2.40	0.51
28:a:54:ASP:N	28:a:54:ASP:OD1	2.44	0.51
31:d:170:LEU:HA	31:d:173:THR:HG22	1.93	0.51
34:e:16:ASP:OD1	34:e:16:ASP:N	2.44	0.51
5:i:53:HIS:HB3	5:i:56:LEU:HD23	1.93	0.51
13:q:31:ASP:OD1	13:q:31:ASP:N	2.41	0.51
19:A:51:ASP:OD1	20:B:69:LYS:NZ	2.41	0.51
19:A:275:ASP:HA	19:A:320:ALA:HB3	1.92	0.51
25:X:71:LYS:HA	25:X:74:ARG:HD2	1.92	0.51
29:b:90:ILE:HB	29:b:127:LEU:HD21	1.92	0.51
7:k:209:LYS:NZ	7:k:210:LEU:O	2.44	0.51
17:x:134:LYS:HA	17:x:157:ARG:HG3	1.92	0.51
22:D:121:ARG:HA	22:D:124:LEU:HD12	1.93	0.51
15:S:176:LYS:HE2	15:S:208:VAL:HG21	1.93	0.51
14:r:182:ASP:OD1	14:r:182:ASP:N	2.43	0.51
15:s:71:ARG:HA	15:s:74:MET:HE3	1.93	0.51
22:D:204:MET:HE1	22:D:212:LYS:HG3	1.93	0.51
22:D:213:THR:N	35:D:501:ATP:O1B	2.36	0.51
23:U:636:VAL:HG23	23:U:637:VAL:HG23	1.92	0.51
32:f:420:TRP:HA	32:f:454:GLY:HA3	1.93	0.51
2:F:374:ASN:ND2	2:F:413:THR:O	2.43	0.51
3:G:43:ARG:HH21	3:G:164:LYS:HG2	1.76	0.51
9:m:35:THR:HA	9:m:166:GLY:HA3	1.92	0.51
26:Y:308:LEU:O	26:Y:358:ARG:NH2	2.44	0.51
31:d:114:GLU:HA	31:d:117:THR:HG22	1.93	0.51
32:f:345:PRO:HA	32:f:390:LEU:HD11	1.93	0.51
33:V:337:LEU:HD21	33:V:364:THR:HG23	1.93	0.51
4:h:143:ARG:NH1	4:h:144:PRO:O	2.44	0.50
17:x:112:ASN:ND2	17:x:195:TYR:O	2.44	0.50
19:A:143:ASP:HB3	19:A:148:GLN:H	1.75	0.50
19:A:325:ASP:OD1	19:A:325:ASP:N	2.44	0.50
29:b:140:ILE:HG21	29:b:153:LEU:HD23	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:428:GLN:HA	32:f:431:LYS:HG2	1.93	0.50
32:f:733:GLY:N	32:f:737:ASN:OD1	2.42	0.50
12:P:99:ARG:O	12:P:99:ARG:NH1	2.41	0.50
3:g:112:ASP:OD1	3:g:112:ASP:N	2.41	0.50
12:p:62:THR:HG23	13:q:86:ARG:HH22	1.76	0.50
23:U:470:ASN:OD1	23:U:474:ARG:NH2	2.44	0.50
26:Y:68:ASP:OD1	26:Y:69:LEU:N	2.43	0.50
6:J:108:THR:HG22	6:J:133:ILE:HD12	1.93	0.50
13:Q:148:THR:HG22	13:Q:150:THR:H	1.76	0.50
28:a:217:LEU:HA	28:a:222:LEU:HD11	1.91	0.50
29:b:109:ILE:HB	29:b:138:VAL:HG22	1.92	0.50
32:f:419:LEU:HD13	32:f:804:LEU:HD11	1.93	0.50
12:P:159:ASP:N	12:P:159:ASP:OD1	2.44	0.50
23:U:13:ASP:OD1	23:U:44:LYS:NZ	2.43	0.50
28:a:335:TRP:NE1	28:a:337:GLN:O	2.45	0.50
31:d:234:ASP:OD1	31:d:234:ASP:N	2.41	0.50
33:V:86:VAL:HG21	33:V:160:LEU:HD13	1.93	0.50
6:J:8:THR:HG23	7:K:135:ARG:HB3	1.94	0.50
8:L:153:TYR:O	9:M:63:ASN:ND2	2.40	0.50
9:m:243:LEU:HD23	9:m:244:LYS:HE3	1.94	0.50
19:A:364:VAL:O	19:A:366:ARG:NH1	2.44	0.50
27:Z:251:LEU:HB3	30:c:234:TYR:CZ	2.46	0.50
33:V:447:ILE:HG23	33:V:449:ALA:H	1.77	0.50
4:H:212:ILE:HD12	4:H:221:LEU:HD21	1.93	0.50
7:k:141:LEU:HB2	7:k:156:MET:HE2	1.93	0.50
14:r:64:ARG:NH1	14:r:67:GLU:OE1	2.44	0.50
14:r:105:ASP:OD1	14:r:105:ASP:N	2.44	0.50
17:x:256:LYS:HB3	17:x:265:VAL:HG13	1.93	0.50
22:D:81:ARG:HB2	30:c:152:LYS:HE3	1.94	0.50
23:U:456:ASP:N	23:U:456:ASP:OD1	2.43	0.50
23:U:772:TRP:HB3	23:U:775:LEU:HG	1.93	0.50
28:a:81:LEU:HA	28:a:84:VAL:HG12	1.92	0.50
3:G:58:ASP:N	3:G:58:ASP:OD1	2.42	0.50
3:g:141:ILE:HG22	3:g:151:VAL:HG22	1.93	0.50
8:l:139:ASP:N	8:l:139:ASP:OD1	2.44	0.50
24:W:422:ASN:HA	30:c:234:TYR:HD2	1.76	0.50
31:d:43:LEU:HD12	31:d:46:GLN:HE22	1.77	0.50
32:f:298:LEU:HD11	32:f:493:ASN:H	1.76	0.50
8:L:59:HIS:O	8:L:61:LYS:NZ	2.44	0.50
9:M:52:LEU:HD22	9:M:206:ASP:HB2	1.94	0.50
24:W:395:ASN:HA	24:W:398:VAL:HG22	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:232:GLU:HG2	26:Y:233:ARG:H	1.76	0.50
32:f:372:LEU:HD21	32:f:797:LEU:HD11	1.94	0.50
32:f:684:PRO:HA	32:f:688:ARG:HG3	1.94	0.50
3:G:31:ALA:HB1	3:G:83:MET:HE3	1.92	0.50
4:h:4:ARG:HE	9:m:127:ALA:HB2	1.77	0.50
11:o:163:ILE:HG12	11:o:170:GLY:HA2	1.94	0.50
23:U:632:GLN:O	23:U:635:SER:OG	2.29	0.50
34:e:27:TRP:H	34:e:27:TRP:CD1	2.30	0.50
3:G:37:LEU:HD22	3:G:53:GLN:HG3	1.94	0.49
3:G:46:ASP:OD1	3:G:46:ASP:N	2.45	0.49
6:J:67:ASP:OD1	6:J:67:ASP:N	2.44	0.49
6:j:47:LYS:HD2	6:j:50:VAL:HG12	1.92	0.49
19:A:114:ASN:HB3	19:A:120:LYS:HG2	1.93	0.49
21:C:329:LEU:HD11	21:C:344:LEU:HB3	1.93	0.49
22:D:207:PRO:O	22:D:212:LYS:NZ	2.35	0.49
28:a:254:ALA:HA	28:a:261:LEU:HD23	1.94	0.49
31:d:82:TYR:O	31:d:121:ARG:NH2	2.45	0.49
31:d:139:LEU:HD11	31:d:151:VAL:HG13	1.94	0.49
1:E:143:ARG:HH22	22:D:388:ARG:HD3	1.77	0.49
2:F:99:VAL:HG13	2:F:121:CYS:HB2	1.94	0.49
18:y:34:GLU:HB3	18:y:36:ILE:HG12	1.93	0.49
21:C:130:LYS:NZ	21:C:131:VAL:O	2.39	0.49
24:W:215:GLN:HG2	24:W:223:LYS:HE2	1.93	0.49
28:a:68:GLU:HG2	28:a:70:ARG:H	1.78	0.49
30:c:59:GLY:HA3	30:c:69:VAL:HA	1.94	0.49
31:d:140:GLU:HA	31:d:143:LEU:HG	1.94	0.49
1:E:25:ARG:NH1	1:E:26:LEU:HB3	2.27	0.49
23:U:364:VAL:O	23:U:367:THR:OG1	2.27	0.49
32:f:843:SER:HA	32:f:863:THR:HG21	1.94	0.49
1:E:147:GLU:HG3	1:E:151:LEU:HD12	1.94	0.49
11:O:146:MET:HE2	11:O:150:GLU:HB3	1.94	0.49
22:D:268:ASP:OD1	22:D:316:THR:OG1	2.30	0.49
24:W:287:VAL:HA	24:W:290:ILE:HG12	1.94	0.49
1:E:300:HIS:NE2	1:E:302:ASP:OD1	2.45	0.49
20:B:377:ASP:O	20:B:416:ASN:ND2	2.44	0.49
23:U:505:ASP:HB3	23:U:508:THR:HG22	1.93	0.49
9:m:230:ASP:OD1	9:m:230:ASP:N	2.45	0.49
20:B:181:GLN:O	20:B:241:ASN:ND2	2.45	0.49
23:U:447:GLY:HA3	23:U:480:GLY:HA2	1.93	0.49
23:U:522:GLY:O	23:U:559:ARG:NH2	2.45	0.49
23:U:918:SER:OG	23:U:919:GLU:N	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:32:LYS:HD3	29:b:19:GLY:HA3	1.94	0.49
33:V:337:LEU:HB3	33:V:398:LEU:HD11	1.94	0.49
6:J:185:ASP:OD1	6:J:185:ASP:N	2.45	0.49
21:C:134:LEU:HD13	21:C:138:MET:HE3	1.95	0.49
32:f:341:GLU:OE2	32:f:387:GLN:NE2	2.43	0.49
33:V:86:VAL:HG22	33:V:200:ARG:HH22	1.77	0.49
33:V:323:GLY:HA3	34:e:24:ALA:HA	1.94	0.49
28:a:221:VAL:HA	28:a:225:LEU:HD12	1.94	0.49
1:E:241:ARG:HG2	1:E:287:PRO:HD3	1.95	0.49
2:F:188:ILE:HG12	2:F:235:LEU:HD23	1.94	0.49
14:R:33:LYS:HA	14:R:45:MET:HE2	1.95	0.49
3:g:58:ASP:OD1	3:g:58:ASP:N	2.45	0.49
5:i:41:ASP:OD1	5:i:41:ASP:N	2.42	0.49
5:i:119:GLN:NE2	6:j:79:ASP:OD1	2.45	0.49
17:x:422:ALA:HB3	17:x:479:LEU:HB3	1.95	0.49
22:D:191:TYR:HA	22:D:196:ILE:HD12	1.94	0.49
23:U:98:GLU:HA	23:U:101:ILE:HG12	1.95	0.49
23:U:672:LEU:HA	23:U:675:MET:HB2	1.95	0.49
23:U:710:ARG:HG2	23:U:737:LEU:HD21	1.95	0.49
27:Z:116:CYS:O	27:Z:119:SER:OG	2.31	0.49
27:Z:259:VAL:HA	30:c:292:MET:HE1	1.94	0.49
28:a:40:GLN:NE2	28:a:43:ASP:O	2.44	0.49
29:b:24:THR:HG22	29:b:26:LEU:H	1.78	0.49
35:F:501:ATP:O5'	19:A:333:ARG:NH1	2.46	0.49
6:j:168:VAL:O	6:j:172:LEU:HB2	2.13	0.49
21:C:139:MET:HG3	22:D:293:LEU:HD13	1.94	0.49
22:D:323:ARG:HD3	22:D:324:PRO:HD2	1.94	0.49
23:U:701:ILE:HG21	23:U:810:THR:HG23	1.93	0.49
32:f:145:VAL:HG13	32:f:150:GLU:HA	1.95	0.49
7:K:99:HIS:HB2	7:K:107:MET:HE3	1.95	0.48
17:x:341:ALA:HB1	19:A:130:ALA:CB	2.43	0.48
29:b:5:SER:HB3	29:b:64:LEU:HD11	1.95	0.48
4:H:189:HIS:HB3	4:H:233:ILE:HD11	1.94	0.48
15:S:19:ASP:OD1	15:S:19:ASP:N	2.45	0.48
3:g:88:ARG:HH12	9:m:157:SER:H	1.59	0.48
14:r:144:SER:OG	14:r:146:ASP:OD1	2.31	0.48
17:x:269:LYS:NZ	17:x:318:SER:OG	2.46	0.48
20:B:117:ASP:OD1	20:B:117:ASP:N	2.46	0.48
23:U:236:LEU:HD13	23:U:244:MET:HE3	1.94	0.48
23:U:678:ASP:O	23:U:684:ARG:NH1	2.39	0.48
29:b:161:ASN:HB3	29:b:167:GLY:H	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:621:ASP:OD1	32:f:621:ASP:N	2.46	0.48
32:f:706:ILE:HD11	32:f:741:LEU:HD21	1.95	0.48
2:F:52:ILE:HA	2:F:55:MET:HB2	1.95	0.48
3:G:213:SER:OG	3:G:232:GLU:OE2	2.30	0.48
9:m:163:CYS:SG	9:m:164:ALA:N	2.86	0.48
17:x:197:GLN:HB3	18:y:76:GLY:HA2	1.95	0.48
19:A:65:ILE:HG12	21:C:81:ASP:HB3	1.95	0.48
22:D:273:LYS:HB2	22:D:316:THR:HA	1.94	0.48
24:W:215:GLN:HE21	24:W:223:LYS:HG3	1.78	0.48
33:V:284:GLU:OE2	33:V:287:ARG:NH1	2.46	0.48
9:M:52:LEU:HA	9:M:209:PHE:HA	1.93	0.48
20:B:54:PRO:HD2	20:B:61:LYS:HG3	1.95	0.48
28:a:291:LEU:HG	28:a:333:MET:HE1	1.95	0.48
1:E:167:PRO:O	1:E:274:LYS:NZ	2.45	0.48
8:L:45:VAL:HG12	8:L:214:ILE:HG12	1.94	0.48
27:Z:193:ASN:HA	27:Z:196:HIS:CE1	2.48	0.48
29:b:20:ASP:HB3	29:b:25:ARG:HG3	1.95	0.48
1:E:47:LEU:HD23	2:F:80:ILE:HG21	1.95	0.48
2:F:289:ASP:OD1	2:F:289:ASP:N	2.45	0.48
8:L:193:ARG:HG3	8:L:236:LEU:HD11	1.96	0.48
8:L:196:ARG:HG2	8:L:239:ARG:HH21	1.78	0.48
19:A:399:ALA:HB3	19:A:401:ARG:HE	1.79	0.48
20:B:222:VAL:HA	20:B:349:ARG:HB2	1.96	0.48
24:W:216:GLU:OE1	24:W:223:LYS:NZ	2.42	0.48
24:W:259:GLU:HB3	24:W:262:LYS:HE2	1.96	0.48
26:Y:178:ASN:O	26:Y:179:ARG:NH1	2.46	0.48
26:Y:220:VAL:HG21	26:Y:249:VAL:HG21	1.96	0.48
2:F:285:ILE:HG21	2:F:288:LEU:HD13	1.95	0.48
4:H:185:GLU:HG3	25:X:81:SER:HB3	1.95	0.48
6:J:196:LEU:HA	6:J:199:VAL:HG12	1.96	0.48
5:i:79:ILE:HG22	5:i:81:SER:H	1.77	0.48
20:B:249:ARG:HH22	21:C:278:ASN:HB3	1.78	0.48
26:Y:228:MET:HB2	26:Y:299:MET:HE1	1.94	0.48
33:V:162:GLU:OE1	33:V:200:ARG:NH1	2.47	0.48
33:V:302:TYR:HB3	33:V:339:LEU:HD21	1.96	0.48
1:E:360:ASP:N	1:E:360:ASP:OD1	2.45	0.48
3:G:56:VAL:HG23	3:G:61:LEU:HD12	1.96	0.48
5:I:49:ARG:NH2	5:I:211:VAL:O	2.45	0.48
8:l:196:ARG:NH1	8:l:237:GLU:O	2.47	0.48
33:V:82:LEU:HD23	33:V:94:VAL:HG22	1.94	0.48
3:g:11:ARG:O	3:g:24:GLN:NE2	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:l:164:ARG:NH2	8:l:198:THR:O	2.47	0.48
17:x:257:CYS:HA	17:x:311:TYR:HA	1.94	0.48
28:a:281:THR:HG22	28:a:333:MET:HE3	1.94	0.48
30:c:158:ASP:OD1	30:c:158:ASP:N	2.46	0.48
32:f:576:ILE:HG23	32:f:577:LEU:HD12	1.96	0.48
33:V:368:ARG:HH12	34:e:43:TRP:HB3	1.79	0.48
6:j:35:VAL:HG11	6:j:190:LEU:HD11	1.96	0.48
17:x:140:LEU:HA	17:x:151:TYR:HB3	1.96	0.48
27:Z:62:ASP:N	27:Z:62:ASP:OD1	2.47	0.48
30:c:175:ARG:NH2	30:c:202:SER:O	2.46	0.48
30:c:303:MET:O	30:c:306:THR:OG1	2.30	0.48
32:f:372:LEU:HD11	32:f:409:SER:HB2	1.96	0.48
6:J:31:THR:OG1	6:J:163:ARG:O	2.32	0.47
4:h:95:GLN:HG3	11:o:65:LEU:HD22	1.96	0.47
10:n:129:GLY:O	10:n:132:SER:OG	2.31	0.47
17:x:24:GLU:O	17:x:58:TRP:NE1	2.38	0.47
23:U:798:PRO:O	23:U:880:ASN:ND2	2.43	0.47
25:X:194:ARG:HD2	25:X:210:LEU:HD21	1.96	0.47
26:Y:199:GLU:HG3	26:Y:200:LEU:HD22	1.95	0.47
32:f:28:PRO:HA	32:f:31:LYS:HB3	1.95	0.47
2:F:60:LEU:O	2:F:64:HIS:ND1	2.33	0.47
11:O:19:ARG:NH2	15:s:213:ASP:OD2	2.47	0.47
12:P:125:ASP:OD1	12:P:129:CYS:N	2.44	0.47
23:U:901:GLN:O	23:U:915:LYS:N	2.41	0.47
32:f:506:GLY:HA2	32:f:540:GLN:HE21	1.79	0.47
14:R:38:ASN:HD21	14:R:41:LEU:HD12	1.78	0.47
17:x:359:CYS:HB3	17:x:363:LEU:HD23	1.96	0.47
21:C:44:ARG:HE	33:V:491:VAL:HG22	1.80	0.47
23:U:367:THR:HA	23:U:370:VAL:HG12	1.95	0.47
29:b:132:LYS:NZ	29:b:162:GLY:O	2.45	0.47
32:f:28:PRO:HA	32:f:31:LYS:HE2	1.96	0.47
32:f:487:LEU:HD21	32:f:804:LEU:HD22	1.95	0.47
2:F:430:LYS:O	2:F:432:LYS:NZ	2.47	0.47
15:s:10:GLY:HA3	15:s:42:LYS:HE2	1.97	0.47
17:x:138:GLY:HA2	17:x:150:GLN:HG2	1.95	0.47
23:U:510:GLU:HA	23:U:547:GLY:HA3	1.96	0.47
30:c:27:THR:HG22	30:c:28:ALA:H	1.79	0.47
2:F:229:PRO:HB2	19:A:333:ARG:HD3	1.97	0.47
7:k:41:GLN:NE2	7:k:151:PRO:O	2.48	0.47
21:C:72:TYR:N	21:C:116:LEU:O	2.44	0.47
22:D:169:GLY:HA2	22:D:343:LEU:HD13	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D:345:PHE:O	22:D:349:THR:OG1	2.21	0.47
24:W:390:GLU:O	24:W:394:SER:OG	2.27	0.47
26:Y:69:LEU:HA	26:Y:72:LYS:HE2	1.96	0.47
27:Z:245:PHE:HZ	30:c:306:THR:HG22	1.79	0.47
32:f:215:ASP:HB3	32:f:839:PRO:HG3	1.96	0.47
11:O:202:TYR:OH	15:s:177:ASP:OD2	2.30	0.47
13:Q:11:ASP:N	13:Q:11:ASP:OD1	2.46	0.47
7:k:203:LYS:HA	7:k:206:MET:HG2	1.96	0.47
16:t:166:ARG:NH1	16:t:200:GLU:OE1	2.47	0.47
16:t:211:ILE:HA	16:t:214:MET:HE3	1.96	0.47
17:x:321:PRO:O	17:x:418:TYR:OH	2.32	0.47
26:Y:97:GLU:OE2	26:Y:132:VAL:N	2.47	0.47
27:Z:8:LYS:NZ	27:Z:159:THR:OG1	2.38	0.47
32:f:281:ILE:HG13	32:f:286:LYS:HB2	1.95	0.47
32:f:650:GLN:HE21	32:f:654:VAL:HG23	1.79	0.47
33:V:123:SER:H	33:V:150:ARG:NH2	2.12	0.47
1:E:37:THR:HG22	2:F:69:MET:HE1	1.96	0.47
6:J:224:GLU:HA	6:J:227:LYS:HE2	1.95	0.47
9:M:51:LYS:O	9:M:210:GLU:N	2.38	0.47
16:T:43:MET:HE2	16:T:45:VAL:HG22	1.95	0.47
16:T:79:ASP:OD1	16:T:79:ASP:N	2.44	0.47
17:x:280:ASN:HD21	17:x:283:VAL:HG23	1.80	0.47
18:y:36:ILE:O	18:y:41:GLN:NE2	2.48	0.47
20:B:181:GLN:HG3	20:B:237:LYS:HB3	1.97	0.47
21:C:161:ILE:HA	21:C:164:VAL:HG12	1.97	0.47
23:U:599:ILE:HD11	23:U:622:LEU:HD23	1.96	0.47
24:W:137:TYR:HD2	24:W:138:VAL:HG12	1.80	0.47
25:X:351:SER:HA	25:X:354:ILE:HG22	1.97	0.47
31:d:178:ILE:HG21	31:d:198:LEU:HD21	1.95	0.47
32:f:253:LEU:HB3	32:f:256:PHE:HB3	1.97	0.47
32:f:545:LYS:HG3	32:f:547:GLU:HG3	1.96	0.47
32:f:673:ARG:HD2	32:f:707:LEU:HD11	1.96	0.47
32:f:814:SER:HA	32:f:819:TYR:HA	1.97	0.47
33:V:150:ARG:NH1	33:V:157:THR:O	2.48	0.47
8:L:132:LEU:HB2	8:L:147:THR:HB	1.97	0.47
13:Q:38:MET:HE2	13:Q:44:LEU:HB2	1.97	0.47
16:T:126:ASP:OD1	16:T:130:VAL:N	2.48	0.47
4:h:86:LEU:HD13	4:h:134:LEU:HD11	1.97	0.47
30:c:137:SER:OG	30:c:138:GLU:N	2.48	0.47
32:f:373:ALA:HB2	32:f:744:MET:HG2	1.96	0.47
2:F:175:MET:HE2	2:F:251:LEU:HD21	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:41:ASP:N	5:I:41:ASP:OD1	2.47	0.47
13:Q:137:PHE:HB3	14:r:133:VAL:HG21	1.96	0.47
19:A:99:THR:HG22	19:A:115:VAL:HA	1.96	0.47
24:W:153:LYS:HA	24:W:153:LYS:HD3	1.83	0.47
32:f:743:ALA:O	32:f:747:GLN:HB2	2.14	0.47
34:e:35:ASP:HB3	34:e:37:HIS:CD2	2.47	0.47
13:Q:50:ALA:O	14:R:91:LYS:NZ	2.48	0.47
6:j:104:VAL:O	6:j:108:THR:OG1	2.30	0.47
6:j:204:LYS:HA	6:j:204:LYS:HD3	1.74	0.47
17:x:197:GLN:O	18:y:72:ARG:NH2	2.48	0.47
20:B:232:LYS:NZ	36:B:501:ADP:O2B	2.44	0.47
25:X:377:ILE:HG12	26:Y:312:ARG:HB2	1.97	0.47
30:c:36:LEU:HD11	30:c:71:ASP:HA	1.97	0.47
5:i:119:GLN:HG3	6:j:78:ALA:HB1	1.97	0.46
6:j:40:ILE:HG12	6:j:212:ARG:HG2	1.96	0.46
18:y:29:LYS:HG2	18:y:33:LYS:NZ	2.30	0.46
20:B:184:TYR:O	32:f:845:ARG:NH2	2.43	0.46
28:a:33:LEU:HA	29:b:18:ASN:HA	1.98	0.46
29:b:100:ARG:NE	29:b:102:GLY:O	2.48	0.46
3:G:165:ALA:HB1	3:G:179:LEU:HD13	1.96	0.46
3:g:49:VAL:HG22	3:g:219:VAL:HG23	1.97	0.46
4:h:124:SER:OG	4:h:125:GLY:N	2.47	0.46
17:x:453:ASP:OD1	17:x:453:ASP:N	2.42	0.46
20:B:252:GLY:HA2	20:B:286:GLU:HB2	1.96	0.46
22:D:278:GLN:OE1	22:D:283:ARG:NE	2.48	0.46
23:U:845:GLU:O	23:U:849:LYS:NZ	2.48	0.46
25:X:63:ALA:HB1	25:X:96:PHE:HE1	1.80	0.46
25:X:105:GLN:HB3	25:X:109:LEU:HD13	1.98	0.46
25:X:126:ARG:HH22	25:X:153:LEU:HD11	1.79	0.46
25:X:380:GLN:N	26:Y:313:SER:O	2.48	0.46
26:Y:259:TYR:HB2	26:Y:274:SER:HB2	1.97	0.46
27:Z:228:TYR:HE1	28:a:340:VAL:HA	1.79	0.46
29:b:52:ILE:HD12	29:b:60:VAL:HA	1.97	0.46
30:c:80:THR:HB	30:c:86:ALA:HB2	1.97	0.46
31:d:82:TYR:HD1	31:d:89:LEU:HD11	1.80	0.46
32:f:743:ALA:O	32:f:746:ARG:NH1	2.49	0.46
32:f:818:LEU:HG	32:f:820:GLY:H	1.80	0.46
2:F:294:LYS:HE3	2:F:340:PRO:HD3	1.97	0.46
2:F:357:PRO:HB2	2:F:361:ALA:HB3	1.96	0.46
17:x:132:ALA:HA	17:x:135:ARG:HE	1.80	0.46
22:D:263:PHE:HD1	22:D:308:ILE:HG23	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:167:ILE:HD12	23:U:204:ILE:HG21	1.97	0.46
23:U:796:LYS:HE3	23:U:924:LEU:HD11	1.98	0.46
23:U:899:ARG:NH2	23:U:919:GLU:O	2.48	0.46
26:Y:141:VAL:HG11	26:Y:164:ALA:HB2	1.96	0.46
26:Y:168:ILE:O	26:Y:176:ARG:NH2	2.48	0.46
28:a:347:LYS:HA	28:a:350:LYS:HE2	1.97	0.46
30:c:162:LEU:HD12	30:c:200:TYR:HB3	1.97	0.46
30:c:277:LYS:HG2	30:c:283:HIS:HB2	1.96	0.46
32:f:108:GLU:OE2	32:f:112:ASN:ND2	2.44	0.46
12:P:10:ALA:HB1	12:P:146:MET:HE1	1.97	0.46
10:n:93:ASP:N	10:n:93:ASP:OD1	2.48	0.46
17:x:368:VAL:HA	17:x:371:ARG:HB2	1.98	0.46
20:B:294:ARG:NH1	20:B:296:ASP:OD1	2.49	0.46
22:D:303:VAL:HG12	22:D:305:VAL:HG23	1.95	0.46
24:W:67:LEU:HD12	24:W:100:ALA:HB1	1.97	0.46
26:Y:40:GLU:O	26:Y:44:ALA:HB2	2.16	0.46
32:f:739:ALA:O	32:f:743:ALA:N	2.48	0.46
2:F:318:ASP:HB3	2:F:347:ARG:HD3	1.98	0.46
13:Q:31:ASP:OD1	13:Q:31:ASP:N	2.49	0.46
14:R:182:ASP:OD1	14:R:182:ASP:N	2.45	0.46
20:B:278:ALA:O	20:B:280:SER:N	2.49	0.46
22:D:349:THR:HB	22:D:354:LEU:HD12	1.97	0.46
25:X:407:MET:HA	25:X:410:VAL:HG22	1.97	0.46
27:Z:262:LEU:CD1	30:c:248:MET:HE3	2.41	0.46
30:c:186:LYS:HA	30:c:186:LYS:HD3	1.79	0.46
32:f:110:TYR:HD2	32:f:137:ARG:HH11	1.63	0.46
17:x:221:ASP:O	17:x:225:GLU:N	2.43	0.46
17:x:419:ASP:O	17:x:481:GLY:N	2.49	0.46
21:C:49:ARG:HD2	23:U:639:LEU:HD21	1.98	0.46
22:D:410:ASP:OD1	22:D:410:ASP:N	2.47	0.46
23:U:392:TRP:HE3	23:U:393:LEU:HD22	1.80	0.46
29:b:181:ASP:OD1	29:b:181:ASP:N	2.48	0.46
33:V:219:GLU:HA	33:V:224:LEU:HD21	1.97	0.46
1:E:331:ILE:O	1:E:335:SER:OG	2.28	0.46
18:y:43:LEU:HG	18:y:67:LEU:HD12	1.97	0.46
33:V:108:LEU:HD21	33:V:113:LEU:HD21	1.97	0.46
8:l:176:MET:HE1	9:m:56:LYS:HG2	1.98	0.46
19:A:224:LEU:HD22	35:A:501:ATP:H2'	1.97	0.46
20:B:334:ILE:HA	20:B:337:LEU:HD23	1.98	0.46
22:D:170:MET:HB2	22:D:173:GLN:HB2	1.96	0.46
26:Y:258:GLN:O	26:Y:262:SER:OG	2.26	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:149:GLU:OE1	32:f:153:SER:OG	2.23	0.46
32:f:198:HIS:NE2	32:f:236:CYS:O	2.48	0.46
32:f:786:GLN:NE2	32:f:788:MET:SD	2.89	0.46
2:F:368:ILE:HG12	2:F:371:ARG:HH22	1.80	0.46
11:O:211:VAL:HG21	12:P:198:ARG:HD3	1.97	0.46
4:h:230:LEU:HA	4:h:233:ILE:HG12	1.98	0.46
14:r:19:ARG:HH21	14:r:29:GLN:HE22	1.64	0.46
17:x:46:VAL:HB	17:x:53:LEU:HB3	1.98	0.46
17:x:76:ASP:N	17:x:76:ASP:OD1	2.48	0.46
21:C:325:ARG:NH2	21:C:351:MET:O	2.49	0.46
23:U:405:THR:HG23	23:U:441:GLY:HA3	1.98	0.46
30:c:41:MET:HE1	30:c:112:TYR:CD1	2.51	0.46
31:d:131:VAL:HA	31:d:134:LYS:HB3	1.97	0.46
32:f:19:ALA:O	32:f:23:GLY:N	2.44	0.46
32:f:229:VAL:HG21	32:f:607:LEU:HD13	1.97	0.46
32:f:321:MET:SD	32:f:321:MET:N	2.88	0.46
19:A:236:CYS:HB3	19:A:270:CYS:HA	1.98	0.46
19:A:265:ARG:NH2	19:A:310:ASP:O	2.49	0.46
23:U:742:HIS:O	23:U:883:ARG:NE	2.49	0.46
24:W:352:LYS:HA	24:W:352:LYS:HD3	1.78	0.46
31:d:34:ASN:HB3	31:d:41:THR:OG1	2.16	0.46
31:d:107:LEU:HD21	31:d:143:LEU:HD21	1.97	0.46
31:d:235:THR:HA	31:d:238:PRO:HG2	1.97	0.46
32:f:422:VAL:HA	32:f:455:VAL:HG22	1.98	0.46
33:V:469:THR:HB	33:V:470:ARG:HH11	1.81	0.46
14:R:192:VAL:HG11	12:p:205:ASP:HB3	1.98	0.45
9:m:8:ASP:OD1	9:m:8:ASP:N	2.47	0.45
17:x:257:CYS:SG	17:x:258:THR:N	2.89	0.45
19:A:78:TRP:HA	19:A:78:TRP:CE3	2.50	0.45
19:A:78:TRP:CD1	20:B:138:PHE:HA	2.52	0.45
20:B:388:ASP:OD1	20:B:388:ASP:N	2.45	0.45
20:B:409:GLU:HG3	20:B:411:ARG:HB2	1.98	0.45
22:D:92:PHE:HZ	22:D:95:ALA:HB2	1.81	0.45
22:D:358:VAL:HG22	22:D:396:ALA:HA	1.97	0.45
23:U:381:THR:HG21	23:U:415:HIS:HD2	1.81	0.45
27:Z:82:PHE:HA	27:Z:85:VAL:HG12	1.98	0.45
28:a:321:LYS:O	28:a:334:THR:OG1	2.33	0.45
32:f:180:GLN:HE22	32:f:219:LYS:HE3	1.81	0.45
32:f:543:MET:HE2	32:f:543:MET:HB3	1.87	0.45
15:s:158:MET:HE2	15:s:158:MET:HB3	1.87	0.45
17:x:334:LYS:HD3	17:x:337:GLU:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:x:371:ARG:HA	17:x:374:PHE:HB2	1.97	0.45
20:B:227:PRO:O	20:B:230:THR:OG1	2.32	0.45
26:Y:70:LEU:HA	26:Y:73:MET:SD	2.57	0.45
1:E:119:VAL:O	1:E:123:SER:N	2.50	0.45
2:F:314:LEU:HD22	2:F:347:ARG:HD2	1.98	0.45
12:P:135:ASP:OD1	12:P:135:ASP:N	2.49	0.45
20:B:233:THR:OG1	36:B:501:ADP:O1B	2.35	0.45
21:C:83:LYS:HB2	21:C:99:VAL:HG22	1.98	0.45
21:C:89:VAL:HG23	21:C:90:HIS:H	1.81	0.45
23:U:41:SER:O	23:U:41:SER:OG	2.33	0.45
32:f:523:GLY:HA3	32:f:561:GLY:HA2	1.97	0.45
1:E:83:CYS:SG	1:E:84:ARG:N	2.89	0.45
7:K:186:HIS:H	7:K:189:MET:HE2	1.82	0.45
12:P:30:ILE:HG22	12:P:31:GLN:H	1.82	0.45
22:D:235:PHE:HB2	22:D:243:GLY:HA2	1.99	0.45
29:b:16:MET:HE2	29:b:16:MET:HB2	1.80	0.45
2:F:33:VAL:HG23	2:F:34:LEU:HD12	1.98	0.45
10:n:179:ILE:HG12	10:n:184:VAL:HG22	1.99	0.45
19:A:407:LYS:HA	19:A:407:LYS:HD2	1.84	0.45
32:f:43:GLN:O	32:f:47:GLU:HG2	2.17	0.45
1:E:84:ARG:O	1:E:85:ARG:NE	2.50	0.45
9:M:8:ASP:N	9:M:8:ASP:OD1	2.49	0.45
7:k:196:LYS:NZ	7:k:237:VAL:O	2.49	0.45
19:A:365:GLU:HG2	19:A:367:ASP:H	1.82	0.45
20:B:58:CYS:SG	20:B:59:ARG:N	2.89	0.45
23:U:160:LEU:HA	23:U:163:PHE:HB3	1.99	0.45
24:W:456:GLN:HA	27:Z:103:LYS:HD2	1.97	0.45
26:Y:96:GLY:HA2	26:Y:130:LYS:HG2	1.98	0.45
28:a:77:VAL:HA	28:a:80:ILE:HG12	1.98	0.45
31:d:211:LYS:HD3	31:d:211:LYS:HA	1.74	0.45
3:G:181:LYS:HA	3:G:184:LYS:HD2	1.99	0.45
17:x:210:VAL:O	17:x:214:LYS:HB2	2.16	0.45
17:x:425:THR:HB	17:x:473:HIS:HB3	1.99	0.45
21:C:37:ASP:OD1	33:V:492:LYS:NZ	2.48	0.45
26:Y:155:ASP:N	26:Y:155:ASP:OD1	2.48	0.45
27:Z:12:HIS:NE2	27:Z:49:ASP:OD2	2.50	0.45
32:f:215:ASP:OD1	32:f:215:ASP:N	2.50	0.45
9:M:43:ASP:OD1	9:M:43:ASP:N	2.46	0.45
12:P:14:MET:HE2	12:P:167:ILE:HB	1.99	0.45
16:T:110:MET:HE2	16:T:110:MET:HB2	1.88	0.45
9:m:34:SER:OG	9:m:65:ARG:NH1	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:n:104:ASP:OD1	10:n:104:ASP:N	2.50	0.45
23:U:398:ASN:H	23:U:401:LYS:HG3	1.82	0.45
24:W:118:LEU:H	24:W:119:PRO:HD2	1.82	0.45
25:X:59:LYS:HB3	25:X:59:LYS:HE3	1.83	0.45
25:X:203:PRO:O	25:X:207:GLN:N	2.45	0.45
2:F:356:MET:SD	2:F:392:ASN:HA	2.57	0.45
10:n:14:LEU:HD21	10:n:101:ALA:HB3	1.99	0.45
17:x:93:THR:HB	17:x:94:GLU:H	1.63	0.45
17:x:256:LYS:O	17:x:312:ILE:N	2.50	0.45
17:x:403:PRO:O	17:x:414:ASN:ND2	2.40	0.45
22:D:45:LYS:HB3	23:U:187:LEU:HD23	1.98	0.45
24:W:140:ILE:HG13	24:W:143:ALA:HB3	1.98	0.45
24:W:313:GLU:OE2	24:W:361:HIS:NE2	2.49	0.45
26:Y:223:THR:HA	26:Y:226:VAL:HG12	1.98	0.45
31:d:167:ILE:HA	31:d:170:LEU:HG	1.99	0.45
32:f:437:GLU:HG2	32:f:440:ILE:H	1.82	0.45
6:J:109:ARG:NH2	14:R:70:ASN:OD1	2.49	0.45
14:R:97:MET:HB2	14:R:116:SER:N	2.32	0.45
7:k:59:MET:HE2	7:k:64:ILE:HD11	1.99	0.45
7:k:167:ALA:HB3	8:l:56:LEU:HD13	1.99	0.45
12:p:135:ASP:OD1	12:p:136:PHE:N	2.50	0.45
14:r:179:VAL:HG22	14:r:184:TRP:HB3	1.99	0.45
17:x:215:LEU:HD22	17:x:218:ILE:HD12	1.99	0.45
19:A:243:SER:HB3	20:B:311:GLU:HB3	1.98	0.45
20:B:358:GLU:HA	20:B:361:LYS:HD2	1.99	0.45
21:C:125:LYS:HE2	21:C:125:LYS:HB3	1.81	0.45
22:D:230:VAL:N	22:D:263:PHE:O	2.44	0.45
22:D:369:LYS:HD3	22:D:369:LYS:HA	1.83	0.45
24:W:90:LEU:O	24:W:96:GLN:NE2	2.31	0.45
28:a:284:ARG:HA	28:a:284:ARG:HD3	1.79	0.45
31:d:179:ALA:HA	31:d:182:ILE:HG22	1.98	0.45
4:H:203:MET:HA	4:H:207:ASN:HD21	1.82	0.44
19:A:383:ALA:HB1	20:B:345:GLY:HA3	1.99	0.44
21:C:197:THR:OG1	21:C:201:ARG:NH2	2.50	0.44
22:D:125:LYS:HB3	22:D:125:LYS:HE3	1.65	0.44
23:U:62:LEU:HD11	23:U:87:LEU:HB2	1.99	0.44
23:U:455:GLY:H	23:U:458:ILE:HD12	1.82	0.44
28:a:146:PRO:O	28:a:149:THR:OG1	2.30	0.44
29:b:26:LEU:HG	29:b:80:PRO:HG3	1.99	0.44
14:R:81:LYS:HE3	14:R:85:ASN:HD21	1.82	0.44
6:j:192:ILE:HD12	6:j:206:ILE:HD12	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:j:222:PRO:HA	6:j:225:ILE:HD12	1.98	0.44
8:l:81:ALA:HB2	8:l:130:VAL:HG21	1.98	0.44
17:x:7:THR:HB	17:x:68:THR:HA	1.98	0.44
17:x:116:MET:SD	17:x:116:MET:N	2.89	0.44
20:B:403:GLY:HA3	21:C:180:ILE:HG21	1.99	0.44
22:D:167:ILE:O	22:D:174:LYS:NZ	2.37	0.44
23:U:383:ASP:OD2	23:U:387:ARG:NH2	2.45	0.44
24:W:160:LYS:NZ	24:W:164:SER:OG	2.50	0.44
31:d:107:LEU:HD11	31:d:140:GLU:HB2	1.99	0.44
32:f:250:ARG:HD3	32:f:253:LEU:H	1.81	0.44
1:E:171:LEU:HB2	1:E:295:LEU:HD13	1.98	0.44
1:E:198:VAL:HG12	1:E:200:SER:H	1.82	0.44
9:M:37:ILE:HD11	9:M:193:VAL:HG13	2.00	0.44
14:R:122:SER:OG	14:R:123:GLY:N	2.50	0.44
5:i:95:GLN:HG3	12:p:73:LEU:HG	1.98	0.44
13:q:11:ASP:N	13:q:11:ASP:OD1	2.49	0.44
20:B:260:LEU:HG	20:B:299:SER:HB3	1.97	0.44
22:D:201:GLY:HA3	22:D:327:LEU:HA	2.00	0.44
23:U:482:GLY:HA2	23:U:519:VAL:HG13	1.99	0.44
29:b:58:CYS:HB3	29:b:92:VAL:HG11	1.98	0.44
30:c:168:MET:HA	30:c:172:HIS:CE1	2.51	0.44
1:E:74:THR:O	22:D:239:TYR:OH	2.30	0.44
1:E:122:MET:HE1	1:E:198:VAL:HG22	1.98	0.44
2:F:169:ASP:HB3	2:F:172:VAL:HG23	1.99	0.44
12:P:205:ASP:OD1	12:P:205:ASP:N	2.50	0.44
11:o:40:ASN:OD1	11:o:40:ASN:N	2.51	0.44
25:X:290:VAL:HG21	25:X:313:LEU:HD21	1.99	0.44
29:b:157:VAL:HG13	29:b:168:SER:HB2	1.98	0.44
30:c:216:MET:O	30:c:220:LEU:HB2	2.17	0.44
32:f:478:ARG:HH22	32:f:509:LYS:HZ1	1.65	0.44
1:E:215:ILE:HA	1:E:218:MET:SD	2.58	0.44
4:H:177:ARG:HH12	25:X:161:ASP:H	1.65	0.44
3:g:60:LEU:HD21	9:m:177:GLU:HG3	1.99	0.44
17:x:101:MET:HG3	17:x:103:LEU:H	1.83	0.44
21:C:197:THR:HG22	21:C:247:PHE:HE2	1.82	0.44
23:U:474:ARG:NH1	23:U:500:ASN:OD1	2.51	0.44
32:f:300:ARG:HE	32:f:321:MET:HE3	1.83	0.44
32:f:482:ILE:HD12	32:f:518:THR:HB	1.99	0.44
1:E:135:ILE:H	1:E:135:ILE:HG13	1.47	0.44
13:Q:23:SER:HB3	13:Q:28:MET:HE3	2.00	0.44
15:S:71:ARG:HD2	15:S:74:MET:HE3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:n:144:ARG:HG2	10:n:147:MET:HE2	2.00	0.44
17:x:397:LYS:HB3	17:x:489:GLU:HB2	2.00	0.44
25:X:58:ALA:HA	25:X:99:MET:HE3	2.00	0.44
29:b:54:LEU:HD13	29:b:84:ILE:HA	2.00	0.44
32:f:144:LEU:HD13	32:f:149:GLU:HG3	1.99	0.44
32:f:708:ASP:O	32:f:712:LYS:HG2	2.17	0.44
33:V:345:ARG:NH2	34:e:42:ASN:O	2.39	0.44
33:V:421:ASP:HB3	33:V:425:LYS:HE2	1.99	0.44
2:F:141:ASP:HB2	2:F:144:LYS:HB2	1.99	0.44
4:H:86:LEU:HD13	4:H:134:LEU:HD11	1.99	0.44
11:o:146:MET:HE3	11:o:146:MET:HB2	1.80	0.44
20:B:223:ILE:HA	20:B:329:MET:HB2	2.00	0.44
21:C:44:ARG:HG3	33:V:491:VAL:HA	1.99	0.44
21:C:297:ARG:HA	21:C:297:ARG:HD2	1.78	0.44
22:D:395:LEU:HD23	22:D:395:LEU:HA	1.87	0.44
23:U:490:ARG:HB3	23:U:493:VAL:HG12	1.99	0.44
30:c:63:ASP:OD1	30:c:66:THR:OG1	2.32	0.44
32:f:188:VAL:HA	32:f:191:ILE:HD11	1.99	0.44
32:f:311:VAL:HG21	32:f:317:LEU:HD23	1.99	0.44
1:E:380:LEU:HD13	2:F:335:VAL:HG11	2.00	0.44
4:H:185:GLU:O	4:H:189:HIS:ND1	2.51	0.44
15:s:176:LYS:HE2	15:s:208:VAL:HG21	1.99	0.44
17:x:275:LEU:HD12	17:x:324:LEU:HD11	1.99	0.44
24:W:144:ARG:HA	24:W:147:LYS:HZ2	1.82	0.44
32:f:369:ARG:HE	32:f:740:ARG:HD3	1.81	0.44
14:R:38:ASN:OD1	14:R:41:LEU:N	2.50	0.44
4:h:179:ASN:HB3	4:h:182:LEU:HD23	2.00	0.44
19:A:67:GLU:HG2	20:B:164:MET:HG2	1.98	0.44
22:D:297:ASP:OD1	22:D:326:ARG:HG2	2.18	0.44
23:U:245:ALA:HA	23:U:248:ILE:HG22	1.99	0.44
24:W:357:ARG:HA	24:W:357:ARG:HD3	1.85	0.44
26:Y:56:ALA:HA	26:Y:59:LYS:HG2	1.98	0.44
30:c:310:LYS:HD2	30:c:310:LYS:HA	1.77	0.44
32:f:521:ALA:HA	32:f:524:MET:HG2	1.99	0.44
32:f:584:SER:HB2	32:f:588:ARG:HD3	2.00	0.44
32:f:815:HIS:CD2	32:f:821:LEU:HD13	2.53	0.44
1:E:75:ASN:HB2	2:F:130:GLN:HG3	1.99	0.43
2:F:306:VAL:HG21	19:A:297:ARG:HH22	1.81	0.43
9:M:40:ARG:NE	9:M:146:ALA:O	2.51	0.43
11:O:199:LEU:HG	15:s:173:ARG:HD3	2.00	0.43
11:O:204:CYS:SG	12:P:162:HIS:ND1	2.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:7:LYS:HG2	14:R:12:VAL:HG22	1.99	0.43
16:T:99:ARG:HA	16:T:99:ARG:HD2	1.86	0.43
6:j:47:LYS:HE3	6:j:47:LYS:HB2	1.83	0.43
19:A:179:GLY:H	19:A:181:LYS:HE3	1.82	0.43
20:B:364:ILE:HD13	20:B:364:ILE:HA	1.83	0.43
23:U:21:GLU:HG2	23:U:56:SER:HB2	1.99	0.43
25:X:395:LYS:HE3	25:X:395:LYS:HB3	1.85	0.43
26:Y:71:ASN:HA	26:Y:74:LYS:HG2	2.00	0.43
31:d:9:TRP:HE1	31:d:25:ARG:NH2	2.16	0.43
31:d:191:PHE:HB2	31:d:220:ASN:HA	2.00	0.43
32:f:250:ARG:NH1	32:f:252:ALA:HB3	2.33	0.43
32:f:292:LYS:HB3	32:f:764:LEU:HD22	2.00	0.43
1:E:77:PRO:HG3	22:D:107:THR:HG22	2.00	0.43
2:F:314:LEU:HD22	2:F:347:ARG:HH11	1.83	0.43
9:M:65:ARG:HH21	9:M:78:ALA:HA	1.82	0.43
3:g:123:GLN:O	3:g:126:THR:OG1	2.34	0.43
6:j:38:ARG:NH1	6:j:182:GLU:OE1	2.50	0.43
12:p:205:ASP:OD1	12:p:205:ASP:N	2.50	0.43
13:q:5:ILE:HD11	13:q:143:LEU:HD11	2.00	0.43
17:x:114:CYS:SG	17:x:197:GLN:NE2	2.91	0.43
23:U:108:TYR:HE1	23:U:126:ILE:HD13	1.82	0.43
25:X:170:GLN:HB3	25:X:193:ALA:HB2	1.99	0.43
30:c:270:LEU:HA	30:c:273:LYS:HE3	2.00	0.43
1:E:44:GLU:HB3	1:E:48:LYS:NZ	2.32	0.43
16:t:25:ASP:HA	16:t:187:PHE:HA	2.01	0.43
20:B:232:LYS:H	20:B:232:LYS:HG2	1.60	0.43
23:U:376:MET:SD	23:U:376:MET:N	2.90	0.43
24:W:137:TYR:CD2	24:W:138:VAL:HG12	2.53	0.43
25:X:134:VAL:HG13	25:X:172:LEU:HD23	1.99	0.43
27:Z:14:LEU:HG	30:c:39:LEU:HB3	2.01	0.43
28:a:90:PRO:HA	28:a:93:ALA:HB3	2.00	0.43
1:E:14:LYS:HD2	1:E:14:LYS:HA	1.84	0.43
1:E:61:LEU:HD11	1:E:72:LYS:HB2	1.99	0.43
11:O:177:VAL:HB	11:O:184:ASP:HB3	1.99	0.43
21:C:254:ILE:HG13	21:C:264:GLY:H	1.83	0.43
23:U:333:MET:SD	23:U:333:MET:N	2.92	0.43
25:X:172:LEU:HD12	25:X:172:LEU:HA	1.80	0.43
30:c:209:LYS:HB3	30:c:209:LYS:HE2	1.81	0.43
32:f:185:LEU:HB3	32:f:188:VAL:HB	2.00	0.43
32:f:408:LEU:HD23	32:f:439:TYR:HD1	1.84	0.43
32:f:422:VAL:HG23	32:f:455:VAL:HA	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:180:GLU:HA	3:G:183:VAL:HG12	2.00	0.43
13:Q:27:GLN:NE2	13:q:169:LYS:O	2.50	0.43
9:m:219:LEU:HD12	9:m:220:THR:HG23	2.00	0.43
16:t:54:SER:O	16:t:108:ASN:ND2	2.33	0.43
18:y:37:PRO:HA	18:y:38:PRO:HD3	1.81	0.43
23:U:804:SER:OG	23:U:805:ASN:N	2.51	0.43
24:W:74:CYS:HB3	24:W:83:LEU:HD13	2.00	0.43
24:W:448:LYS:HE2	27:Z:157:HIS:HB2	1.99	0.43
26:Y:177:ARG:HA	26:Y:180:LEU:HD13	2.01	0.43
30:c:29:GLU:HB2	30:c:203:ILE:HD11	2.01	0.43
31:d:63:ILE:HD12	31:d:63:ILE:HA	1.93	0.43
2:F:222:GLY:HA3	2:F:348:LEU:HA	1.99	0.43
3:g:141:ILE:HD12	3:g:220:VAL:HG12	2.01	0.43
6:j:132:LEU:HD21	6:j:159:ASN:HB3	1.99	0.43
23:U:573:ASP:OD1	23:U:574:LYS:N	2.52	0.43
28:a:85:ARG:NH1	28:a:86:GLN:OE1	2.42	0.43
32:f:304:PHE:HB3	32:f:308:SER:HA	1.99	0.43
1:E:52:SER:OG	1:E:53:VAL:N	2.51	0.43
5:i:65:ILE:HD13	5:i:75:SER:HB2	2.01	0.43
8:l:125:ARG:HA	8:l:125:ARG:HD2	1.79	0.43
9:m:179:LEU:HD21	9:m:192:GLU:HB3	2.01	0.43
23:U:581:SER:O	23:U:585:THR:OG1	2.26	0.43
23:U:669:ILE:HG21	23:U:705:LYS:HG2	2.00	0.43
26:Y:178:ASN:HB3	26:Y:179:ARG:NH1	2.34	0.43
27:Z:81:MET:HB2	27:Z:81:MET:HE2	1.70	0.43
28:a:371:ALA:O	28:a:375:LEU:HB2	2.18	0.43
29:b:30:GLN:O	29:b:34:ASN:ND2	2.52	0.43
32:f:521:ALA:HA	32:f:524:MET:HE2	2.00	0.43
6:j:79:ASP:HB3	6:j:127:PHE:HD1	1.83	0.43
8:l:227:ASP:OD1	8:l:227:ASP:N	2.49	0.43
20:B:71:TYR:HA	20:B:74:MET:SD	2.59	0.43
21:C:66:LEU:HD23	21:C:66:LEU:HA	1.90	0.43
22:D:170:MET:HG2	22:D:174:LYS:HG3	2.01	0.43
26:Y:234:PRO:HG2	26:Y:239:LYS:HD2	2.01	0.43
30:c:278:GLN:HB3	30:c:281:LYS:HG2	2.00	0.43
32:f:640:LYS:NZ	32:f:647:GLY:O	2.51	0.43
7:K:196:LYS:HE3	7:K:241:ILE:HG13	2.01	0.43
3:g:155:ASP:OD1	3:g:159:TYR:N	2.46	0.43
6:j:53:LEU:HD12	6:j:53:LEU:HA	1.68	0.43
13:q:81:ALA:HB1	13:q:124:LEU:HD11	2.00	0.43
23:U:216:VAL:HG21	23:U:232:ILE:HD11	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:496:LEU:HD12	23:U:497:LEU:HD12	2.01	0.43
26:Y:237:ARG:HG3	26:Y:241:ILE:HD12	2.00	0.43
26:Y:347:ILE:HG13	26:Y:354:VAL:HG22	2.01	0.43
32:f:202:HIS:HB2	32:f:240:VAL:HG22	2.01	0.43
11:O:163:ILE:HG12	11:O:170:GLY:HA2	2.01	0.43
7:k:168:ARG:HA	7:k:168:ARG:HD2	1.83	0.43
10:n:24:SER:O	10:n:24:SER:OG	2.33	0.43
13:q:18:ASP:OD1	13:q:18:ASP:N	2.45	0.43
17:x:143:SER:H	17:x:147:ALA:HB3	1.83	0.43
17:x:323:TYR:HD2	17:x:479:LEU:HD11	1.84	0.43
17:x:361:PRO:HA	17:x:364:GLN:HB2	2.01	0.43
20:B:38:LYS:HE3	20:B:143:LEU:HB3	2.00	0.43
24:W:190:MET:SD	24:W:190:MET:N	2.92	0.43
25:X:275:LEU:HD12	25:X:275:LEU:HA	1.89	0.43
28:a:173:TYR:CZ	28:a:177:LEU:HD11	2.53	0.43
29:b:154:THR:O	29:b:158:ASN:ND2	2.52	0.43
30:c:40:LYS:HD3	30:c:40:LYS:HA	1.86	0.43
14:r:106:LYS:HB3	14:r:106:LYS:HE3	1.76	0.42
17:x:462:ASP:O	17:x:466:LEU:HG	2.19	0.42
21:C:69:GLN:HB3	21:C:118:ASN:HD21	1.84	0.42
22:D:287:ARG:HE	22:D:287:ARG:HB3	1.74	0.42
25:X:57:LEU:O	25:X:60:THR:OG1	2.24	0.42
25:X:365:LEU:HA	25:X:368:MET:HG3	2.01	0.42
26:Y:268:TYR:HA	26:Y:271:PHE:HB3	2.01	0.42
26:Y:373:GLY:HA3	27:Z:261:TYR:CZ	2.54	0.42
29:b:8:VAL:HA	29:b:110:ILE:HG13	2.01	0.42
33:V:122:THR:HG21	33:V:155:ALA:HB1	2.01	0.42
33:V:472:PRO:HA	33:V:475:ALA:HB3	2.00	0.42
1:E:242:ARG:HG3	22:D:313:ARG:NE	2.34	0.42
1:E:317:ALA:O	1:E:322:LYS:NZ	2.37	0.42
6:J:211:MET:HB2	6:J:217:LEU:HD12	2.00	0.42
7:K:16:SER:OG	7:K:18:GLU:OE1	2.37	0.42
11:O:40:ASN:OD1	11:O:40:ASN:N	2.52	0.42
13:Q:13:VAL:HG11	13:Q:105:ALA:HB1	2.01	0.42
17:x:196:LEU:O	17:x:198:GLN:NE2	2.49	0.42
20:B:287:ILE:HG21	20:B:329:MET:HE1	2.02	0.42
22:D:74:HIS:NE2	27:Z:180:LYS:HB2	2.34	0.42
22:D:264:ILE:HD12	22:D:309:MET:HE1	2.01	0.42
23:U:848:LYS:HA	23:U:851:GLU:HG3	2.01	0.42
26:Y:347:ILE:O	33:V:415:SER:N	2.47	0.42
26:Y:362:LYS:HB2	26:Y:362:LYS:HE2	1.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:34:TRP:CD1	28:a:70:ARG:HD3	2.54	0.42
31:d:79:LYS:HA	31:d:79:LYS:HD3	1.79	0.42
32:f:209:MET:HE1	32:f:211:ILE:HB	2.01	0.42
32:f:713:PHE:HB3	32:f:749:ALA:HB1	2.01	0.42
33:V:111:TYR:OH	33:V:139:MET:N	2.52	0.42
5:I:140:ASP:OD1	5:I:140:ASP:N	2.50	0.42
8:L:47:VAL:HG12	8:L:195:LEU:HD22	2.00	0.42
19:A:166:VAL:HG11	19:A:237:PHE:HB3	2.00	0.42
21:C:45:LEU:HD23	21:C:45:LEU:HA	1.91	0.42
21:C:218:GLU:O	22:D:286:GLN:NE2	2.51	0.42
24:W:259:GLU:HB3	24:W:262:LYS:HB3	2.02	0.42
27:Z:205:LEU:HA	27:Z:208:ILE:HG22	2.01	0.42
28:a:226:ARG:NH1	28:a:230:ARG:HH21	2.17	0.42
2:F:417:HIS:O	2:F:421:MET:HG2	2.20	0.42
14:R:127:SER:HB3	14:R:136:TYR:CE1	2.55	0.42
7:k:146:VAL:HG11	7:k:222:PRO:HA	2.02	0.42
17:x:215:LEU:HD23	17:x:215:LEU:HA	1.87	0.42
19:A:416:VAL:HG12	19:A:421:ALA:HB2	2.01	0.42
20:B:190:LEU:O	20:B:194:ILE:N	2.44	0.42
21:C:224:ILE:O	21:C:232:ARG:NH2	2.33	0.42
23:U:128:GLN:NE2	23:U:131:GLU:OE2	2.52	0.42
24:W:55:ARG:HD3	24:W:96:GLN:HA	2.01	0.42
24:W:312:MET:HG2	28:a:316:SER:HB3	2.02	0.42
25:X:364:LYS:HA	25:X:364:LYS:HD2	1.81	0.42
26:Y:171:GLY:O	26:Y:176:ARG:NH2	2.52	0.42
26:Y:195:LYS:O	26:Y:199:GLU:N	2.43	0.42
26:Y:247:LEU:HD12	26:Y:250:LEU:HD11	2.02	0.42
29:b:9:CYS:HB3	29:b:111:ALA:HA	2.01	0.42
32:f:187:LEU:HD21	32:f:228:LYS:HG2	1.99	0.42
32:f:245:ASN:HB3	32:f:275:MET:HE3	2.00	0.42
1:E:123:SER:HB2	1:E:196:LEU:HG	2.00	0.42
5:I:206:LEU:HD22	5:I:237:ILE:HD11	2.02	0.42
13:Q:167:LEU:HD23	13:Q:167:LEU:HA	1.89	0.42
17:x:254:THR:HG22	17:x:267:LYS:HE3	2.02	0.42
19:A:292:ASP:OD1	19:A:292:ASP:N	2.46	0.42
25:X:415:TYR:HD1	26:Y:383:LEU:HD13	1.83	0.42
29:b:16:MET:HG3	29:b:25:ARG:NH1	2.35	0.42
1:E:50:LEU:HD11	2:F:138:GLY:HA2	2.02	0.42
1:E:215:ILE:HD13	1:E:260:LEU:HG	2.02	0.42
2:F:334:ARG:NH1	19:A:284:ARG:O	2.52	0.42
8:L:39:LYS:HD2	8:L:142:PRO:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:q:22:ALA:HA	13:q:27:GLN:HA	2.01	0.42
21:C:142:LYS:HG3	21:C:201:ARG:HD2	2.01	0.42
23:U:219:CYS:HA	23:U:222:PHE:HB2	2.01	0.42
25:X:121:LYS:HE2	25:X:121:LYS:HB2	1.94	0.42
27:Z:261:TYR:O	27:Z:262:LEU:C	2.61	0.42
28:a:174:LYS:HA	28:a:177:LEU:HD12	2.02	0.42
35:E:501:ATP:O2A	35:E:501:ATP:H8	2.03	0.42
10:N:30:VAL:HG11	16:t:211:ILE:HG23	2.02	0.42
11:O:209:THR:HG21	12:P:168:SER:HB2	2.01	0.42
16:T:67:LEU:HD12	16:T:67:LEU:HA	1.90	0.42
23:U:32:ASN:HA	23:U:35:TRP:NE1	2.34	0.42
23:U:793:LYS:HG2	23:U:794:ASP:H	1.85	0.42
24:W:55:ARG:NH2	24:W:93:ARG:HH22	2.18	0.42
25:X:335:LEU:O	25:X:339:ILE:HG12	2.20	0.42
30:c:236:GLU:HA	30:c:239:LYS:HE2	2.01	0.42
32:f:208:LEU:HD23	32:f:209:MET:HG3	2.02	0.42
32:f:272:LEU:HD11	32:f:286:LYS:HE3	2.00	0.42
5:I:197:LEU:HD23	5:I:197:LEU:HA	1.88	0.42
17:x:214:LYS:HA	17:x:214:LYS:HD2	1.88	0.42
20:B:118:ASP:O	20:B:120:HIS:ND1	2.44	0.42
20:B:224:LEU:HD21	20:B:235:LEU:HD22	2.00	0.42
23:U:330:SER:OG	23:U:332:GLU:OE1	2.30	0.42
23:U:825:LYS:HE3	23:U:825:LYS:HB3	1.85	0.42
23:U:889:LEU:HD13	23:U:909:GLY:HA3	2.01	0.42
24:W:148:THR:O	24:W:152:ILE:HG12	2.20	0.42
28:a:220:PRO:O	28:a:224:SER:OG	2.34	0.42
29:b:80:PRO:O	29:b:81:LYS:HE2	2.20	0.42
32:f:171:GLN:NE2	32:f:182:GLU:OE1	2.53	0.42
32:f:516:GLY:HA3	32:f:554:TYR:CE2	2.54	0.42
1:E:316:HIS:CE1	1:E:344:ARG:HB2	2.55	0.42
2:F:252:ALA:HB3	2:F:255:GLN:HG3	2.02	0.42
4:H:68:ILE:HD11	4:H:74:LEU:HD12	2.01	0.42
13:Q:59:TYR:O	13:Q:63:ASN:ND2	2.53	0.42
10:n:115:PRO:HD2	10:n:119:MET:HB3	2.01	0.42
12:p:12:MET:HG3	12:p:138:VAL:HG12	2.02	0.42
12:p:71:LEU:HD11	12:p:82:ILE:HG21	2.02	0.42
23:U:563:ALA:HB1	23:U:567:ILE:HG12	2.02	0.42
23:U:666:LYS:HA	23:U:669:ILE:HD12	2.02	0.42
24:W:377:ARG:O	24:W:381:LEU:HB2	2.20	0.42
26:Y:385:ARG:HB3	33:V:315:LYS:HG2	2.02	0.42
27:Z:288:LYS:HD2	27:Z:288:LYS:HA	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:637:LYS:HD3	32:f:637:LYS:HA	1.93	0.42
33:V:189:ASP:HA	33:V:192:MET:SD	2.60	0.42
1:E:11:ASP:O	1:E:15:LYS:HG2	2.20	0.42
1:E:130:VAL:HG23	1:E:186:ALA:HA	2.02	0.42
2:F:75:GLU:O	2:F:78:GLU:HG3	2.20	0.42
5:I:125:GLY:HA3	5:I:127:LYS:HE3	2.02	0.42
5:I:237:ILE:HD13	5:I:237:ILE:HA	1.90	0.42
19:A:351:ARG:NH2	19:A:374:ALA:O	2.53	0.42
20:B:381:ASP:HA	20:B:384:ILE:HD12	2.02	0.42
20:B:411:ARG:NH2	20:B:418:ASP:OD2	2.53	0.42
23:U:176:MET:HA	23:U:179:TYR:HB3	2.02	0.42
24:W:425:LEU:HA	24:W:425:LEU:HD12	1.74	0.42
26:Y:13:LYS:HG2	26:Y:16:ASP:HB2	2.02	0.42
28:a:245:VAL:HG13	28:a:272:ILE:HD12	2.01	0.42
28:a:302:ILE:HD12	28:a:302:ILE:HA	1.97	0.42
29:b:4:GLU:OE2	29:b:40:LYS:NZ	2.41	0.42
31:d:168:ASP:OD1	31:d:169:ILE:N	2.53	0.42
1:E:30:ARG:HA	1:E:33:LEU:HD12	2.01	0.41
1:E:93:LYS:H	1:E:93:LYS:HG3	1.52	0.41
3:G:196:GLU:HG2	3:G:242:LEU:HD13	2.02	0.41
6:J:227:LYS:HE2	6:J:227:LYS:HB3	1.86	0.41
8:L:139:ASP:OD1	8:L:139:ASP:N	2.52	0.41
16:T:25:ASP:HA	16:T:187:PHE:HA	2.02	0.41
16:T:43:MET:HE1	16:T:67:LEU:HB3	2.02	0.41
6:j:68:ASN:HA	6:j:211:MET:HE1	2.02	0.41
8:l:199:LEU:HD23	8:l:199:LEU:HA	1.86	0.41
8:l:226:ASP:OD1	8:l:227:ASP:N	2.52	0.41
17:x:263:GLU:OE2	17:x:302:SER:OG	2.33	0.41
24:W:173:THR:H	24:W:182:ARG:HH21	1.68	0.41
26:Y:57:LEU:HD12	26:Y:57:LEU:HA	1.92	0.41
26:Y:272:PHE:HD1	26:Y:272:PHE:HA	1.74	0.41
28:a:251:LEU:HG	28:a:255:TRP:HZ3	1.85	0.41
31:d:200:PHE:O	31:d:203:PRO:HD3	2.20	0.41
32:f:456:ARG:HH22	32:f:491:GLY:H	1.67	0.41
32:f:680:ARG:HH22	32:f:762:VAL:HB	1.85	0.41
1:E:180:LYS:NZ	35:E:501:ATP:O2B	2.53	0.41
16:T:9:THR:OG1	16:T:10:SER:N	2.52	0.41
4:h:213:CYS:HB2	4:h:218:PHE:HD1	1.85	0.41
7:k:13:ASN:OD1	7:k:13:ASN:N	2.53	0.41
8:l:47:VAL:HG12	8:l:195:LEU:HD22	2.02	0.41
8:l:217:LYS:HE3	8:l:217:LYS:HB3	1.92	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D:145:PRO:HB2	22:D:256:GLU:HG3	2.02	0.41
23:U:587:ALA:HB2	23:U:621:SER:HB3	2.02	0.41
23:U:861:LYS:HA	23:U:861:LYS:HD3	1.89	0.41
24:W:118:LEU:HD12	24:W:118:LEU:HA	1.92	0.41
28:a:308:GLU:O	28:a:312:MET:HG2	2.20	0.41
33:V:398:LEU:HA	33:V:401:ASN:HB2	2.02	0.41
2:F:176:GLU:HA	2:F:249:LEU:HD12	2.02	0.41
3:G:73:THR:HG22	3:G:74:GLU:H	1.85	0.41
5:I:17:ARG:HH21	5:I:19:TYR:HE1	1.67	0.41
8:L:9:ASP:OD1	8:L:10:VAL:N	2.54	0.41
7:k:35:SER:OG	7:k:51:GLU:HB2	2.20	0.41
9:m:87:LEU:HD23	9:m:87:LEU:HA	1.92	0.41
17:x:218:ILE:O	17:x:242:LEU:HB3	2.20	0.41
17:x:424:LEU:HB3	17:x:477:VAL:HB	2.02	0.41
20:B:60:LEU:HD23	20:B:60:LEU:HA	1.91	0.41
22:D:255:LYS:HE3	22:D:255:LYS:HB3	1.91	0.41
23:U:97:VAL:HA	23:U:100:ILE:HG12	2.02	0.41
33:V:483:CYS:O	33:V:487:HIS:ND1	2.53	0.41
1:E:148:VAL:HB	1:E:297:ARG:HH22	1.85	0.41
19:A:78:TRP:HA	19:A:78:TRP:HE3	1.85	0.41
19:A:79:ASP:OD1	19:A:79:ASP:N	2.53	0.41
25:X:126:ARG:HA	25:X:129:LEU:HB2	2.01	0.41
32:f:100:ARG:NH1	32:f:110:TYR:OH	2.54	0.41
32:f:180:GLN:HG2	32:f:215:ASP:HB2	2.03	0.41
32:f:789:SER:HA	32:f:793:VAL:HG23	2.01	0.41
1:E:276:ILE:C	1:E:277:MET:HE2	2.45	0.41
1:E:383:LYS:HG2	1:E:385:ASP:H	1.86	0.41
2:F:224:LEU:HB3	2:F:351:LYS:HG2	2.02	0.41
2:F:364:ARG:HE	2:F:368:ILE:HG13	1.85	0.41
4:H:119:GLN:HB3	4:H:153:GLY:HA3	2.02	0.41
9:M:108:LEU:HD11	9:M:137:LEU:HB3	2.03	0.41
6:j:84:ILE:HD13	6:j:84:ILE:HA	1.89	0.41
19:A:319:MET:HG2	19:A:337:LEU:HD21	2.01	0.41
23:U:165:LYS:O	23:U:169:GLU:N	2.54	0.41
24:W:316:ARG:O	24:W:319:THR:OG1	2.24	0.41
24:W:316:ARG:HH22	24:W:381:LEU:HA	1.85	0.41
27:Z:243:GLN:HE22	28:a:289:ARG:HH22	1.69	0.41
32:f:192:VAL:HB	32:f:193:PRO:HD3	2.03	0.41
32:f:556:ARG:HE	32:f:631:LYS:HD3	1.86	0.41
33:V:176:MET:HE3	33:V:176:MET:O	2.20	0.41
3:G:79:VAL:O	3:G:80:MET:HE2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:n:40:ARG:NH1	10:n:180:ALA:O	2.54	0.41
11:o:42:TYR:HB2	11:o:178:ILE:HD11	2.01	0.41
24:W:149:LEU:HB2	24:W:185:PHE:HE1	1.86	0.41
24:W:268:LYS:O	24:W:272:LEU:HG	2.20	0.41
32:f:605:ASN:HD21	32:f:608:LYS:HB2	1.86	0.41
32:f:834:ASP:OD1	32:f:834:ASP:N	2.54	0.41
33:V:218:TYR:HA	33:V:221:LEU:HD12	2.03	0.41
9:M:152:ASP:OD1	9:M:156:VAL:N	2.52	0.41
3:g:166:THR:OG1	3:g:167:ALA:N	2.54	0.41
21:C:29:GLU:HG2	33:V:201:ARG:NH2	2.35	0.41
28:a:35:HIS:HE1	29:b:18:ASN:HB3	1.85	0.41
33:V:161:PRO:HD2	33:V:200:ARG:HH11	1.85	0.41
2:F:421:MET:HA	2:F:424:ILE:HD12	2.02	0.41
3:G:41:ALA:HB2	3:G:50:ILE:HD13	2.03	0.41
16:T:76:LEU:HD23	16:T:76:LEU:HA	1.88	0.41
13:q:39:SER:OG	13:q:40:GLU:N	2.53	0.41
13:q:119:ASP:OD1	13:q:119:ASP:N	2.49	0.41
19:A:195:LEU:HD23	19:A:195:LEU:HA	1.93	0.41
19:A:393:GLY:HA3	20:B:216:ILE:HD13	2.03	0.41
21:C:303:SER:HB2	21:C:306:LEU:HD11	2.02	0.41
29:b:161:ASN:HD22	29:b:168:SER:H	1.69	0.41
31:d:176:ASP:OD1	31:d:177:GLU:N	2.53	0.41
33:V:255:LEU:HD23	33:V:255:LEU:HA	1.89	0.41
33:V:491:VAL:HG12	33:V:492:LYS:HE2	2.03	0.41
1:E:102:MET:HG2	1:E:103:THR:HG23	2.03	0.41
1:E:255:ARG:HG2	22:D:269:ALA:HB1	2.03	0.41
2:F:134:LEU:HD12	2:F:135:PRO:HD2	2.02	0.41
2:F:217:ILE:HG13	2:F:218:GLN:N	2.35	0.41
4:H:100:VAL:HG13	12:P:93:ASN:HD22	1.86	0.41
12:P:61:GLN:HB2	13:Q:85:ARG:NH2	2.36	0.41
4:h:52:GLN:HB3	4:h:57:TYR:HD2	1.85	0.41
6:j:27:LYS:HA	6:j:27:LYS:HD3	1.83	0.41
6:j:236:LYS:HA	6:j:236:LYS:HD3	1.84	0.41
8:l:23:GLU:HA	8:l:26:MET:HB2	2.02	0.41
20:B:264:PRO:HB3	20:B:311:GLU:HG2	2.02	0.41
20:B:404:LEU:HD22	21:C:180:ILE:HD12	2.02	0.41
21:C:134:LEU:O	21:C:241:HIS:NE2	2.52	0.41
21:C:338:LEU:HD21	21:C:378:VAL:HB	2.03	0.41
22:D:45:LYS:HA	22:D:45:LYS:HD2	1.91	0.41
23:U:82:LEU:HD22	23:U:129:ARG:HG2	2.03	0.41
23:U:94:SER:HB3	23:U:97:VAL:HG12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:469:SER:OG	23:U:470:ASN:N	2.53	0.41
23:U:645:ASN:OD1	23:U:645:ASN:N	2.54	0.41
24:W:84:ASN:O	24:W:88:MET:HG2	2.21	0.41
24:W:420:ASP:OD1	24:W:420:ASP:N	2.54	0.41
26:Y:357:ASN:HD22	33:V:461:LYS:HE2	1.85	0.41
27:Z:110:GLU:HG2	27:Z:153:LYS:HE2	2.02	0.41
28:a:15:GLY:N	28:a:18:GLN:HE21	2.19	0.41
28:a:113:LEU:HB3	28:a:151:VAL:HG23	2.03	0.41
29:b:12:ASN:HB3	29:b:78:VAL:HG22	2.02	0.41
30:c:200:TYR:HD2	30:c:201:TYR:H	1.67	0.41
33:V:289:LEU:HB3	33:V:312:ALA:HB2	2.02	0.41
1:E:84:ARG:HD2	1:E:85:ARG:N	2.36	0.41
1:E:225:HIS:HB2	1:E:228:CYS:SG	2.61	0.41
4:h:14:SER:HB3	4:h:18:LYS:H	1.86	0.41
4:h:119:GLN:HG3	5:i:81:SER:HB2	2.03	0.41
17:x:88:PHE:HD2	17:x:89:VAL:HG12	1.86	0.41
18:y:4:PHE:HB2	18:y:66:THR:HA	2.01	0.41
22:D:143:LEU:HD13	22:D:147:ALA:HB3	2.02	0.41
23:U:35:TRP:HZ3	33:V:235:LEU:HD23	1.86	0.41
23:U:350:LEU:HD12	23:U:350:LEU:HA	1.88	0.41
24:W:396:LEU:HD23	24:W:396:LEU:HA	1.94	0.41
27:Z:251:LEU:HD21	30:c:238:CYS:HB2	2.02	0.41
31:d:122:LEU:HA	31:d:123:PRO:HD3	1.95	0.41
32:f:790:GLN:HE22	32:f:797:LEU:HA	1.86	0.41
13:Q:5:ILE:HD11	13:Q:143:LEU:HD11	2.03	0.40
15:S:13:LEU:HD12	15:S:145:LEU:HD23	2.02	0.40
8:l:97:PHE:O	15:s:66:LYS:NZ	2.41	0.40
11:o:63:LEU:HD23	11:o:63:LEU:HA	1.91	0.40
17:x:126:VAL:HG13	17:x:323:TYR:CZ	2.55	0.40
17:x:350:PRO:HG2	17:x:353:LEU:HD13	2.02	0.40
19:A:125:LEU:HB2	19:A:129:VAL:HG23	2.03	0.40
19:A:140:VAL:HG12	19:A:152:PRO:HA	2.03	0.40
19:A:323:ARG:HD2	19:A:323:ARG:HA	1.74	0.40
20:B:369:THR:HA	20:B:372:MET:HE3	2.02	0.40
23:U:199:ARG:HB3	23:U:223:LEU:HD21	2.04	0.40
23:U:801:GLN:HB3	23:U:877:LEU:HD22	2.03	0.40
25:X:360:ASP:OD1	25:X:361:VAL:N	2.54	0.40
26:Y:124:PHE:HA	26:Y:127:THR:HG22	2.03	0.40
30:c:113:HIS:CE1	30:c:144:VAL:HG22	2.56	0.40
31:d:12:LYS:HE3	31:d:14:PRO:HB3	2.02	0.40
1:E:30:ARG:NH2	2:F:59:VAL:O	2.45	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:192:LEU:HD23	8:L:192:LEU:HA	1.86	0.40
14:R:46:ALA:HB3	14:R:98:GLY:HA3	2.02	0.40
16:T:211:ILE:HG23	10:n:30:VAL:HG11	2.03	0.40
6:j:199:VAL:HG12	6:j:202:GLY:H	1.86	0.40
13:q:13:VAL:HG21	13:q:105:ALA:HB1	2.04	0.40
19:A:258:ARG:NH2	19:A:301:GLU:OE1	2.48	0.40
21:C:198:LEU:HD11	36:C:501:ADP:H2'	2.04	0.40
25:X:299:LEU:HD22	25:X:331:LEU:HD12	2.03	0.40
26:Y:179:ARG:HH12	26:Y:212:GLU:HB3	1.86	0.40
26:Y:288:PHE:CE1	26:Y:292:TYR:HB3	2.56	0.40
31:d:105:PHE:HB2	31:d:166:PHE:CZ	2.56	0.40
31:d:175:ARG:HH21	31:d:198:LEU:HB3	1.86	0.40
1:E:197:LYS:HZ3	1:E:231:PHE:HE2	1.69	0.40
2:F:287:GLU:HG2	19:A:300:LEU:HD22	2.04	0.40
3:G:37:LEU:HA	3:G:53:GLN:HE21	1.86	0.40
3:G:112:ASP:N	3:G:112:ASP:OD1	2.52	0.40
16:T:27:LEU:HD11	16:T:34:ALA:HB1	2.03	0.40
7:k:202:LEU:HA	7:k:205:VAL:HG22	2.02	0.40
9:m:223:ARG:NE	9:m:225:GLU:OE2	2.41	0.40
12:p:153:LEU:HD23	12:p:153:LEU:HA	1.85	0.40
17:x:105:CYS:HA	17:x:455:VAL:HG21	2.03	0.40
18:y:15:LEU:HB3	18:y:17:VAL:HG13	2.04	0.40
19:A:287:ASP:N	19:A:287:ASP:OD1	2.54	0.40
20:B:356:PRO:HG2	20:B:391:SER:HA	2.03	0.40
23:U:354:LYS:HD2	23:U:354:LYS:HA	1.88	0.40
26:Y:42:MET:SD	26:Y:42:MET:N	2.91	0.40
27:Z:265:LEU:HA	27:Z:265:LEU:HD13	1.83	0.40
28:a:28:LEU:HD22	28:a:36:GLN:HB3	2.03	0.40
28:a:267:GLN:HE22	28:a:271:LYS:HD2	1.86	0.40
32:f:191:ILE:HA	32:f:194:TYR:HB2	2.02	0.40
32:f:672:LEU:HB3	32:f:707:LEU:HD23	2.03	0.40
2:F:72:LYS:HE3	2:F:72:LYS:HB3	1.95	0.40
2:F:134:LEU:HD12	2:F:134:LEU:HA	1.86	0.40
3:G:83:MET:O	3:G:87:SER:OG	2.33	0.40
12:P:58:THR:O	13:Q:85:ARG:NH2	2.55	0.40
8:l:7:ASP:OD1	8:l:7:ASP:N	2.55	0.40
19:A:70:THR:HB	20:B:143:LEU:HD21	2.03	0.40
22:D:81:ARG:CZ	30:c:152:LYS:HG3	2.51	0.40
23:U:811:PHE:HE1	23:U:874:ASN:H	1.69	0.40
25:X:173:GLU:HA	25:X:176:THR:HG22	2.03	0.40
25:X:391:PRO:HA	25:X:392:PRO:HD3	2.00	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:242:LEU:H	27:Z:243:GLN:NE2	2.19	0.40
29:b:33:VAL:HA	29:b:36:VAL:HG22	2.03	0.40
30:c:202:SER:OG	30:c:203:ILE:N	2.53	0.40
32:f:347:ASP:OD1	32:f:347:ASP:N	2.54	0.40
32:f:718:ASP:OD1	32:f:718:ASP:N	2.54	0.40
5:I:64:LYS:NZ	21:C:406:LYS:O	2.50	0.40
6:J:99:GLU:HG2	14:R:81:LYS:HE2	2.03	0.40
16:T:38:ASN:ND2	10:n:200:ALA:O	2.54	0.40
6:j:221:ASN:ND2	6:j:223:GLU:OE2	2.54	0.40
8:l:93:LEU:HD23	8:l:93:LEU:HA	1.92	0.40
11:o:112:SER:HB3	11:o:125:VAL:HG11	2.04	0.40
12:p:159:ASP:OD1	12:p:159:ASP:N	2.53	0.40
21:C:117:ARG:HB2	21:C:122:THR:H	1.86	0.40
24:W:135:LYS:HZ2	24:W:139:GLU:HG2	1.86	0.40
24:W:388:GLU:OE1	24:W:388:GLU:N	2.55	0.40
25:X:251:LEU:O	25:X:254:MET:HB2	2.22	0.40
27:Z:118:ASN:OD1	27:Z:118:ASN:N	2.53	0.40
32:f:57:GLU:HA	32:f:61:GLU:HB3	2.03	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	E	387/403 (96%)	353 (91%)	34 (9%)	0	100	100
2	F	396/439 (90%)	364 (92%)	31 (8%)	1 (0%)	36	67
3	G	238/246 (97%)	226 (95%)	12 (5%)	0	100	100
3	g	242/246 (98%)	232 (96%)	10 (4%)	0	100	100
4	H	230/234 (98%)	220 (96%)	10 (4%)	0	100	100
4	h	230/234 (98%)	221 (96%)	9 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	I	246/261 (94%)	233 (95%)	13 (5%)	0	100	100
5	i	248/261 (95%)	243 (98%)	5 (2%)	0	100	100
6	J	237/248 (96%)	225 (95%)	12 (5%)	0	100	100
6	j	237/248 (96%)	227 (96%)	10 (4%)	0	100	100
7	K	236/241 (98%)	224 (95%)	12 (5%)	0	100	100
7	k	232/241 (96%)	219 (94%)	13 (6%)	0	100	100
8	L	238/269 (88%)	230 (97%)	8 (3%)	0	100	100
8	l	236/269 (88%)	224 (95%)	12 (5%)	0	100	100
9	M	240/255 (94%)	230 (96%)	10 (4%)	0	100	100
9	m	238/255 (93%)	234 (98%)	4 (2%)	0	100	100
10	N	201/239 (84%)	196 (98%)	5 (2%)	0	100	100
10	n	200/239 (84%)	192 (96%)	8 (4%)	0	100	100
11	O	218/277 (79%)	210 (96%)	8 (4%)	0	100	100
11	o	218/277 (79%)	207 (95%)	11 (5%)	0	100	100
12	P	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
12	p	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
13	Q	197/201 (98%)	195 (99%)	2 (1%)	0	100	100
13	q	197/201 (98%)	194 (98%)	3 (2%)	0	100	100
14	R	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
14	r	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
15	S	211/241 (88%)	204 (97%)	7 (3%)	0	100	100
15	s	211/241 (88%)	202 (96%)	9 (4%)	0	100	100
16	T	214/264 (81%)	207 (97%)	7 (3%)	0	100	100
16	t	214/264 (81%)	205 (96%)	9 (4%)	0	100	100
17	x	492/494 (100%)	461 (94%)	31 (6%)	0	100	100
18	y	74/76 (97%)	67 (90%)	7 (10%)	0	100	100
19	A	404/433 (93%)	368 (91%)	34 (8%)	2 (0%)	24	57
20	B	409/440 (93%)	375 (92%)	34 (8%)	0	100	100
21	C	393/398 (99%)	348 (88%)	44 (11%)	1 (0%)	36	67
22	D	378/418 (90%)	341 (90%)	37 (10%)	0	100	100
23	U	868/953 (91%)	800 (92%)	68 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	W	444/456 (97%)	411 (93%)	32 (7%)	1 (0%)	43	74
25	X	378/422 (90%)	357 (94%)	21 (6%)	0	100	100
26	Y	376/389 (97%)	332 (88%)	44 (12%)	0	100	100
27	Z	284/324 (88%)	249 (88%)	33 (12%)	2 (1%)	18	51
28	a	371/376 (99%)	338 (91%)	33 (9%)	0	100	100
29	b	189/377 (50%)	164 (87%)	25 (13%)	0	100	100
30	c	285/310 (92%)	244 (86%)	41 (14%)	0	100	100
31	d	255/350 (73%)	210 (82%)	45 (18%)	0	100	100
32	f	887/908 (98%)	765 (86%)	122 (14%)	0	100	100
33	V	442/534 (83%)	430 (97%)	12 (3%)	0	100	100
34	e	48/70 (69%)	42 (88%)	6 (12%)	0	100	100
All	All	13971/15458 (90%)	12998 (93%)	966 (7%)	7 (0%)	49	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	53	LYS
27	Z	262	LEU
27	Z	145	HIS
24	W	118	LEU
19	A	72	LEU
19	A	74	PRO
21	C	140	VAL

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	E	341/353 (97%)	336 (98%)	5 (2%)	57	71
2	F	344/379 (91%)	343 (100%)	1 (0%)	86	83
3	G	202/210 (96%)	202 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	g	201/210 (96%)	200 (100%)	1 (0%)	81	80
4	H	187/191 (98%)	187 (100%)	0	100	100
4	h	188/191 (98%)	188 (100%)	0	100	100
5	I	202/221 (91%)	201 (100%)	1 (0%)	81	80
5	i	206/221 (93%)	206 (100%)	0	100	100
6	J	197/211 (93%)	197 (100%)	0	100	100
6	j	196/211 (93%)	194 (99%)	2 (1%)	68	75
7	K	197/203 (97%)	197 (100%)	0	100	100
7	k	195/203 (96%)	195 (100%)	0	100	100
8	L	202/230 (88%)	201 (100%)	1 (0%)	81	80
8	l	201/230 (87%)	201 (100%)	0	100	100
9	M	198/212 (93%)	198 (100%)	0	100	100
9	m	198/212 (93%)	198 (100%)	0	100	100
10	N	158/181 (87%)	158 (100%)	0	100	100
10	n	156/181 (86%)	156 (100%)	0	100	100
11	O	178/228 (78%)	178 (100%)	0	100	100
11	o	181/228 (79%)	181 (100%)	0	100	100
12	P	172/174 (99%)	172 (100%)	0	100	100
12	p	173/174 (99%)	173 (100%)	0	100	100
13	Q	168/171 (98%)	168 (100%)	0	100	100
13	q	166/171 (97%)	166 (100%)	0	100	100
14	R	156/202 (77%)	156 (100%)	0	100	100
14	r	154/202 (76%)	154 (100%)	0	100	100
15	S	175/199 (88%)	175 (100%)	0	100	100
15	s	177/199 (89%)	177 (100%)	0	100	100
16	T	178/215 (83%)	178 (100%)	0	100	100
16	t	179/215 (83%)	179 (100%)	0	100	100
17	x	439/439 (100%)	422 (96%)	17 (4%)	28	54
18	y	68/68 (100%)	68 (100%)	0	100	100
19	A	341/372 (92%)	339 (99%)	2 (1%)	78	79
20	B	357/385 (93%)	355 (99%)	2 (1%)	78	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	C	339/346 (98%)	336 (99%)	3 (1%)	70	76
22	D	333/366 (91%)	330 (99%)	3 (1%)	70	76
23	U	748/816 (92%)	746 (100%)	2 (0%)	86	83
24	W	410/416 (99%)	407 (99%)	3 (1%)	76	78
25	X	327/362 (90%)	327 (100%)	0	100	100
26	Y	334/344 (97%)	334 (100%)	0	100	100
27	Z	257/295 (87%)	245 (95%)	12 (5%)	23	49
28	a	333/336 (99%)	329 (99%)	4 (1%)	63	73
29	b	167/312 (54%)	167 (100%)	0	100	100
30	c	252/268 (94%)	249 (99%)	3 (1%)	63	73
31	d	231/294 (79%)	230 (100%)	1 (0%)	84	81
32	f	745/763 (98%)	742 (100%)	3 (0%)	84	81
33	V	390/460 (85%)	390 (100%)	0	100	100
34	e	44/63 (70%)	44 (100%)	0	100	100
All	All	11941/13133 (91%)	11875 (99%)	66 (1%)	76	79

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	91	LYS
1	E	92	LEU
1	E	93	LYS
1	E	135	ILE
1	E	138	LEU
2	F	416	THR
5	I	155	ASN
8	L	60	GLN
3	g	224	ASN
6	j	52	LYS
6	j	53	LEU
17	x	78	LEU
17	x	90	GLU
17	x	91	ASP
17	x	92	MET
17	x	93	THR
17	x	94	GLU
17	x	97	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	x	326	ILE
17	x	328	MET
17	x	330	ARG
17	x	334	LYS
17	x	335	GLU
17	x	336	LYS
17	x	340	ASN
17	x	342	LYS
17	x	344	LEU
17	x	345	LYS
19	A	77	LEU
19	A	403	ILE
20	B	102	LEU
20	B	125	THR
21	C	109	THR
21	C	210	THR
21	C	316	GLU
22	D	125	LYS
22	D	129	SER
22	D	329	ARG
23	U	465	LEU
23	U	520	MET
24	W	26	GLN
24	W	116	THR
24	W	117	ASP
27	Z	124	ILE
27	Z	126	VAL
27	Z	127	LYS
27	Z	129	LYS
27	Z	133	LEU
27	Z	144	VAL
27	Z	149	THR
27	Z	175	LEU
27	Z	176	LEU
27	Z	260	VAL
27	Z	262	LEU
27	Z	265	LEU
28	a	180	LEU
28	a	340	VAL
28	a	341	LEU
28	a	342	ASP
30	c	114	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	c	123	SER
30	c	125	VAL
31	d	189	ILE
32	f	502	LEU
32	f	543	MET
32	f	874	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	45	ASN
1	E	280	ASN
1	E	345	ASN
2	F	76	ASN
2	F	333	ASN
3	G	68	HIS
3	G	75	ASN
4	H	88	HIS
5	I	95	GLN
5	I	142	HIS
5	I	230	GLN
6	J	94	HIS
6	J	200	GLN
6	J	239	ASN
7	K	73	HIS
8	L	5	GLN
8	L	90	GLN
9	M	32	ASN
9	M	180	GLN
10	N	53	GLN
10	N	106	GLN
10	N	110	GLN
10	N	193	GLN
11	O	91	GLN
11	O	193	ASN
12	P	93	ASN
12	P	145	GLN
12	P	173	ASN
12	P	188	HIS
13	Q	82	ASN
14	R	85	ASN
14	R	162	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	S	8	ASN
15	S	146	GLN
15	S	151	ASN
16	T	3	ASN
3	g	75	ASN
3	g	224	ASN
4	h	109	GLN
4	h	140	ASN
5	i	20	GLN
5	i	102	GLN
5	i	109	GLN
5	i	167	ASN
6	j	54	GLN
6	j	175	ASN
7	k	41	GLN
7	k	98	ASN
7	k	186	HIS
9	m	110	HIS
9	m	143	ASN
9	m	201	HIS
10	n	66	HIS
10	n	110	GLN
10	n	123	GLN
11	o	35	HIS
12	p	81	GLN
12	p	169	GLN
13	q	82	ASN
13	q	132	HIS
13	q	168	GLN
13	q	189	HIS
14	r	175	ASN
15	s	36	HIS
15	s	151	ASN
16	t	3	ASN
16	t	147	GLN
17	x	32	GLN
17	x	40	GLN
17	x	44	GLN
17	x	112	ASN
17	x	201	ASN
18	y	68	HIS
19	A	44	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	A	94	GLN
19	A	231	ASN
19	A	322	ASN
19	A	414	ASN
20	B	57	GLN
20	B	154	HIS
20	B	315	GLN
20	B	332	ASN
20	B	416	ASN
21	C	171	HIS
21	C	205	HIS
21	C	221	GLN
22	D	173	GLN
22	D	187	HIS
22	D	390	ASN
23	U	18	GLN
23	U	107	HIS
23	U	115	ASN
23	U	355	ASN
23	U	670	ASN
23	U	685	GLN
23	U	874	ASN
24	W	218	ASN
24	W	235	GLN
24	W	362	ASN
24	W	444	HIS
25	X	48	GLN
25	X	170	GLN
25	X	218	HIS
25	X	292	GLN
25	X	333	GLN
25	X	405	GLN
25	X	406	ASN
26	Y	154	ASN
26	Y	280	GLN
26	Y	302	HIS
26	Y	367	GLN
27	Z	31	ASN
27	Z	86	ASN
27	Z	145	HIS
27	Z	189	GLN
28	a	18	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	a	143	ASN
28	a	193	GLN
28	a	231	GLN
28	a	241	ASN
28	a	264	ASN
29	b	44	ASN
29	b	158	ASN
30	c	128	ASN
30	c	166	ASN
30	c	221	HIS
30	c	278	GLN
30	c	283	HIS
31	d	34	ASN
31	d	46	GLN
31	d	60	GLN
31	d	96	HIS
31	d	102	ASN
31	d	135	HIS
31	d	252	GLN
32	f	112	ASN
32	f	323	ASN
32	f	352	HIS
32	f	475	ASN
32	f	493	ASN
32	f	790	GLN
33	V	146	GLN
33	V	257	ASN
33	V	347	GLN
34	e	47	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	ADP	C	501	-	28,29,29	1.41	4 (14%)	43,45,45	1.84	8 (18%)
35	ATP	D	501	-	32,33,33	0.54	0	48,52,52	0.31	0
35	ATP	A	501	-	32,33,33	0.54	0	48,52,52	0.32	0
36	ADP	B	501	-	28,29,29	1.38	5 (17%)	43,45,45	1.85	10 (23%)
35	ATP	E	501	-	32,33,33	0.74	2 (6%)	48,52,52	0.41	0
35	ATP	F	501	-	32,33,33	0.54	0	48,52,52	0.32	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
36	ADP	C	501	-	-	0/16/32/32	0/3/3/3
35	ATP	D	501	-	-	8/22/38/38	0/3/3/3
35	ATP	A	501	-	-	8/22/38/38	0/3/3/3
36	ADP	B	501	-	-	3/16/32/32	0/3/3/3
35	ATP	E	501	-	-	6/22/38/38	0/3/3/3
35	ATP	F	501	-	-	7/22/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	501	ADP	C5-C4	4.79	1.47	1.39
36	B	501	ADP	C5-C4	4.54	1.47	1.39
35	E	501	ATP	PB-O3B	-2.71	1.56	1.59
36	C	501	ADP	C5-C6	2.69	1.48	1.41
36	B	501	ADP	C5-N7	-2.56	1.34	1.39
35	E	501	ATP	PA-O3A	-2.44	1.56	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	501	ADP	C5-N7	-2.40	1.34	1.39
36	B	501	ADP	C5-C6	2.35	1.47	1.41
36	B	501	ADP	C8-N7	2.19	1.35	1.31
36	C	501	ADP	C8-N7	2.14	1.35	1.31
36	B	501	ADP	C4-N9	-2.07	1.33	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	501	ADP	C5-C4-N3	-6.08	118.34	126.72
36	B	501	ADP	C5-C4-N3	-5.51	119.14	126.72
36	C	501	ADP	N3-C4-N9	4.94	135.56	127.17
36	B	501	ADP	N3-C4-N9	4.54	134.89	127.17
36	C	501	ADP	C2-N3-C4	3.69	120.85	111.83
36	B	501	ADP	C2-N3-C4	3.56	120.52	111.83
36	B	501	ADP	N3-C2-N1	-3.55	123.21	128.58
36	C	501	ADP	C4-C5-N7	-3.44	106.65	110.58
36	B	501	ADP	C4-C5-N7	-3.15	106.98	110.58
36	C	501	ADP	N3-C2-N1	-3.04	123.99	128.58
36	B	501	ADP	C4-N9-C8	2.83	108.71	105.74
36	B	501	ADP	C3'-C2'-C1'	2.71	106.59	101.46
36	C	501	ADP	C4-N9-C8	2.57	108.44	105.74
36	C	501	ADP	C5-N7-C8	2.54	107.45	103.45
36	C	501	ADP	C3'-C2'-C1'	2.54	106.26	101.46
36	B	501	ADP	C2'-C1'-N9	-2.50	107.08	113.30
36	B	501	ADP	C5-N7-C8	2.37	107.18	103.45
36	B	501	ADP	C2-N1-C6	2.37	122.62	118.73

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	E	501	ATP	C5'-O5'-PA-O1A
35	E	501	ATP	C5'-O5'-PA-O2A
35	E	501	ATP	C5'-O5'-PA-O3A
35	E	501	ATP	O4'-C4'-C5'-O5'
35	F	501	ATP	C5'-O5'-PA-O1A
35	A	501	ATP	PB-O3B-PG-O3G
35	A	501	ATP	C5'-O5'-PA-O1A
35	A	501	ATP	C5'-O5'-PA-O2A
35	A	501	ATP	C5'-O5'-PA-O3A
35	D	501	ATP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

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

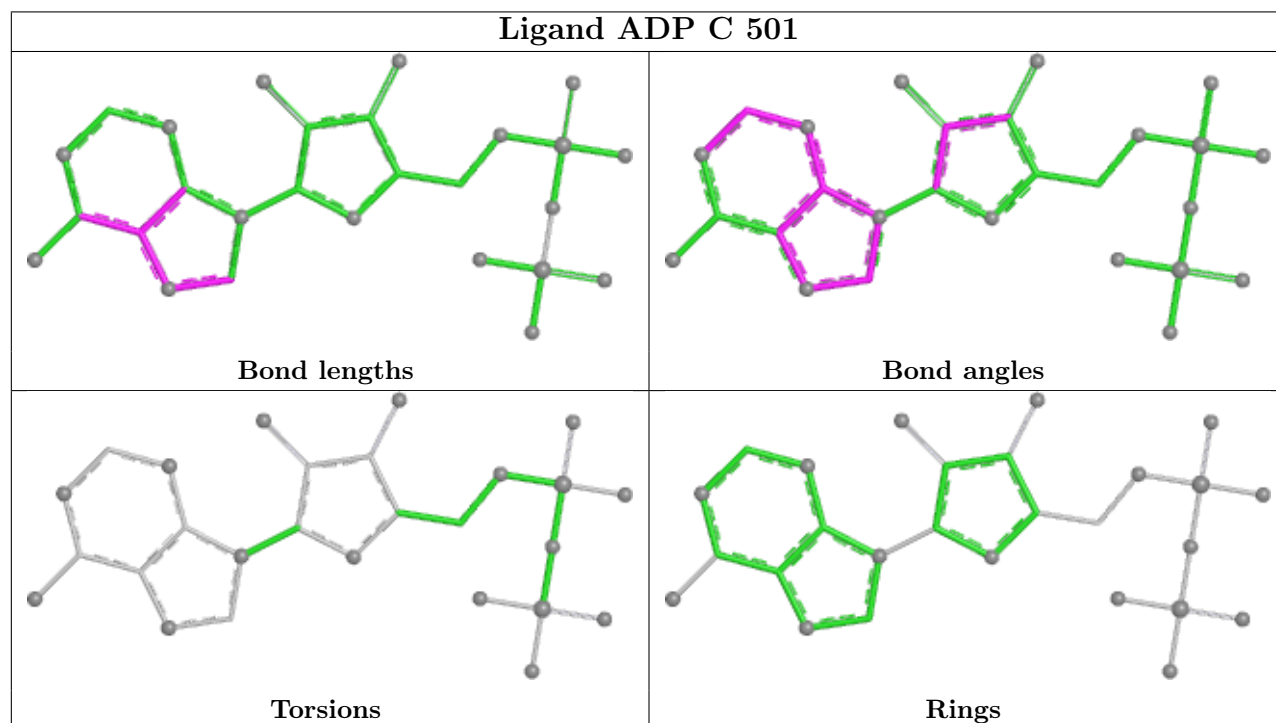
There are no ring outliers.

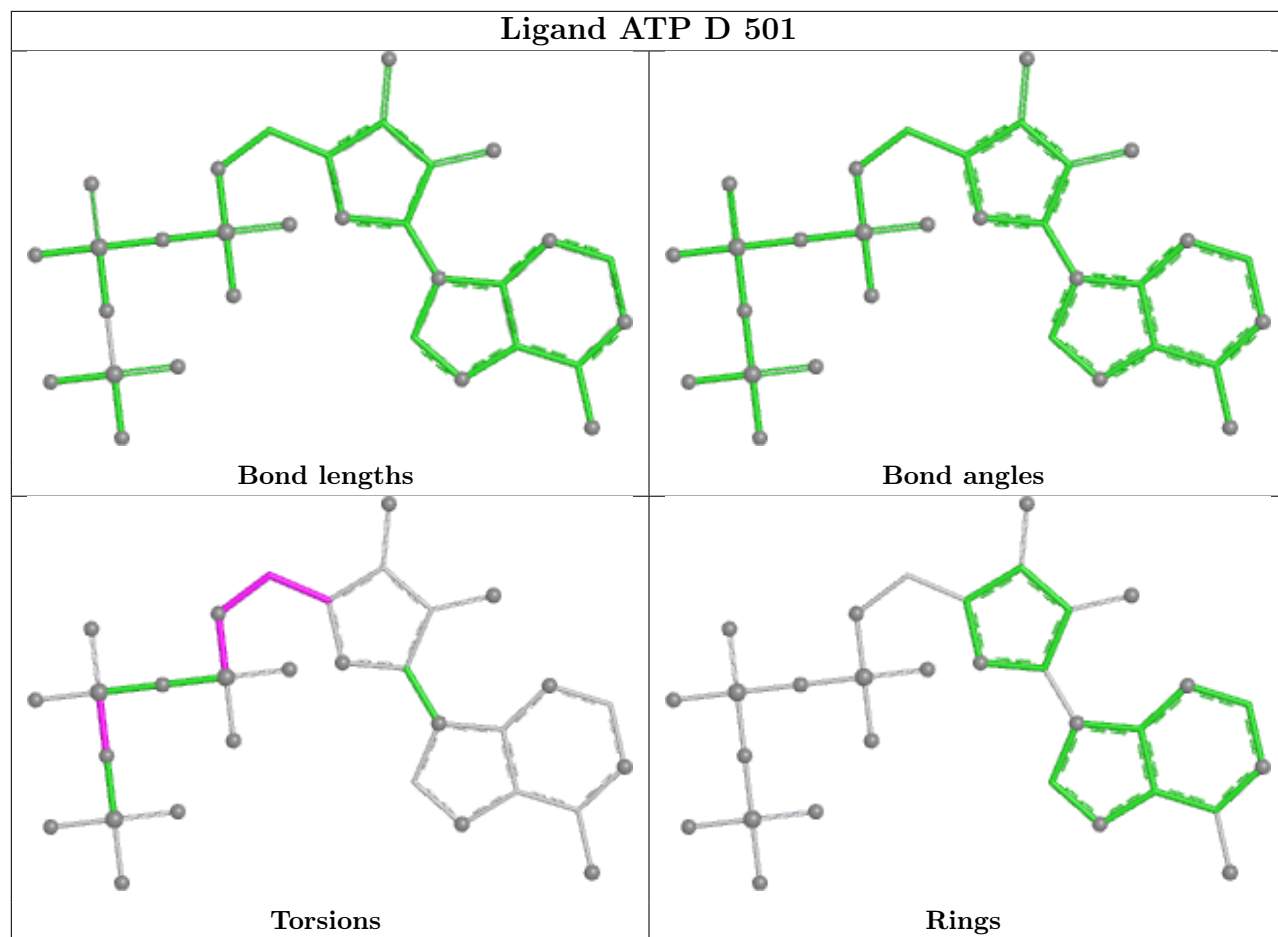
6 monomers are involved in 12 short contacts:

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

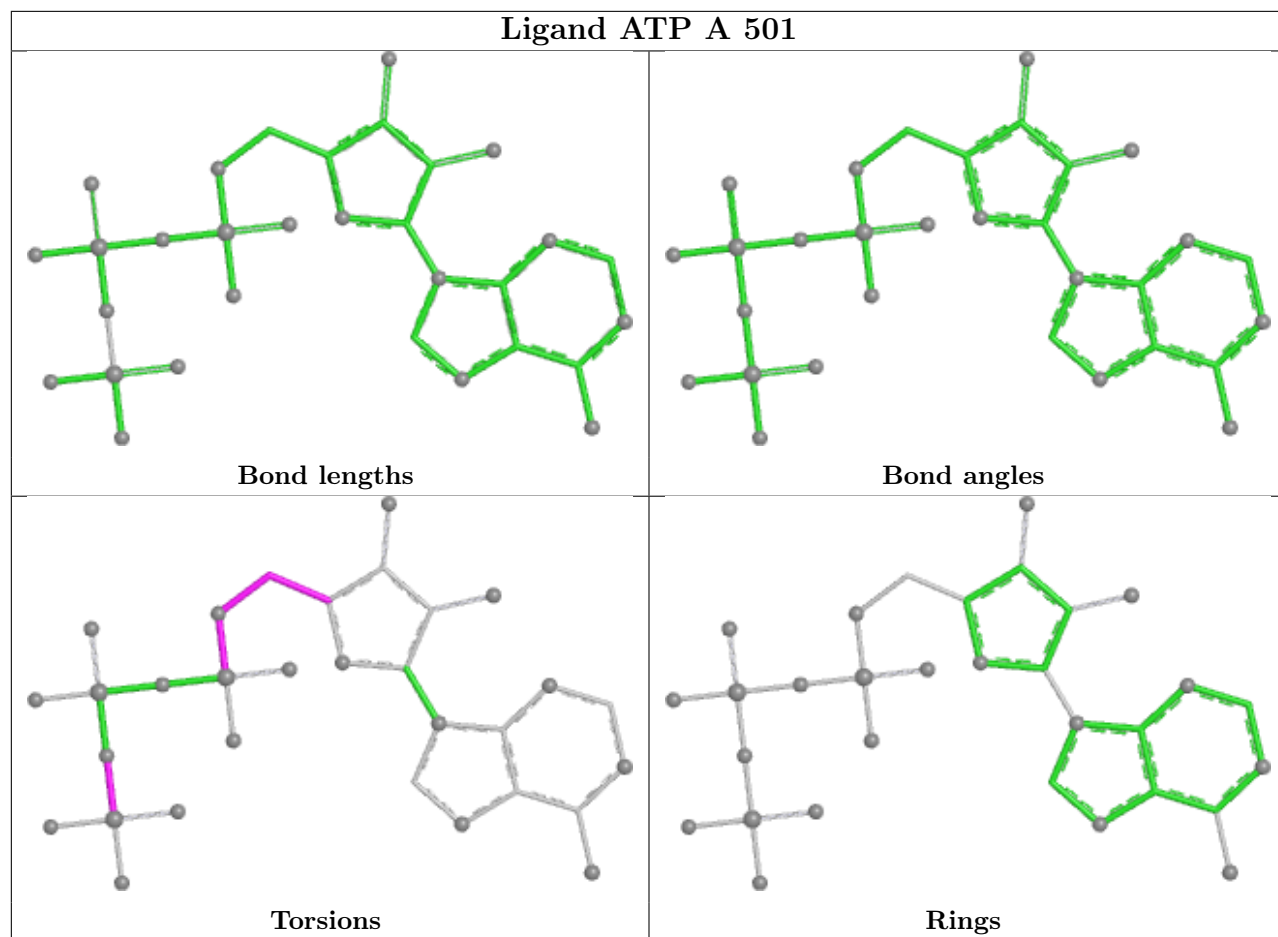
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

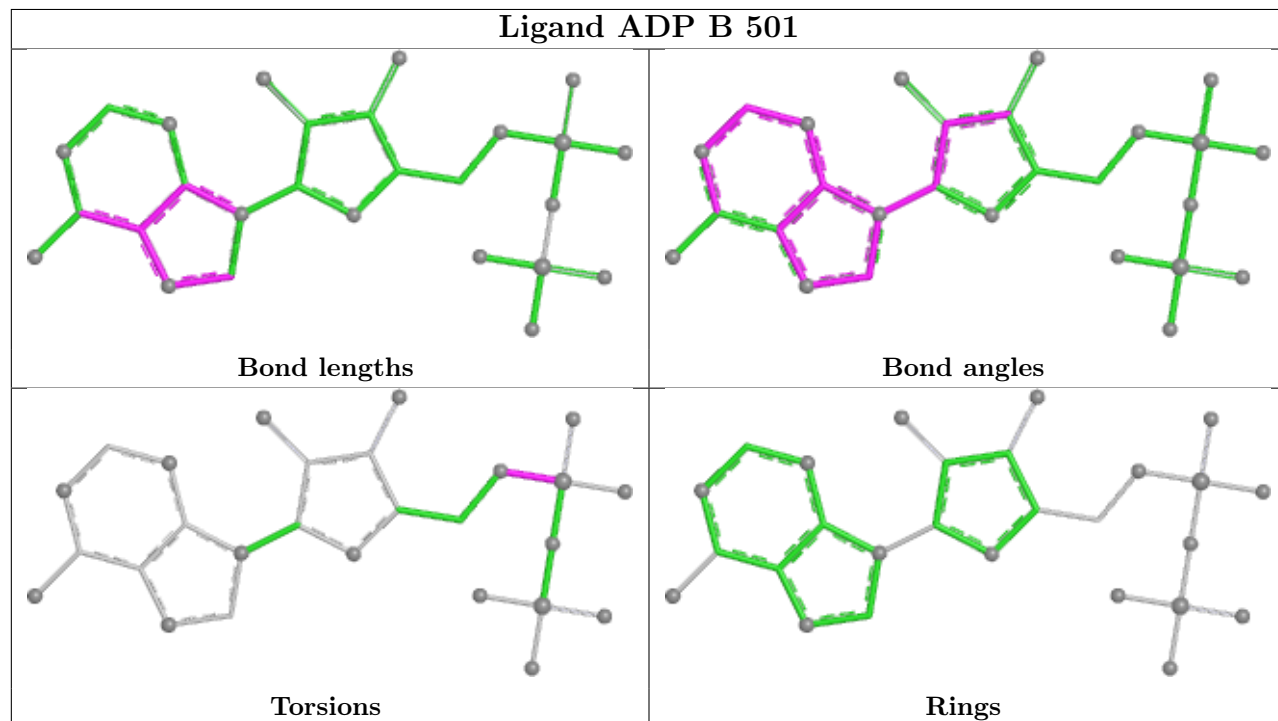




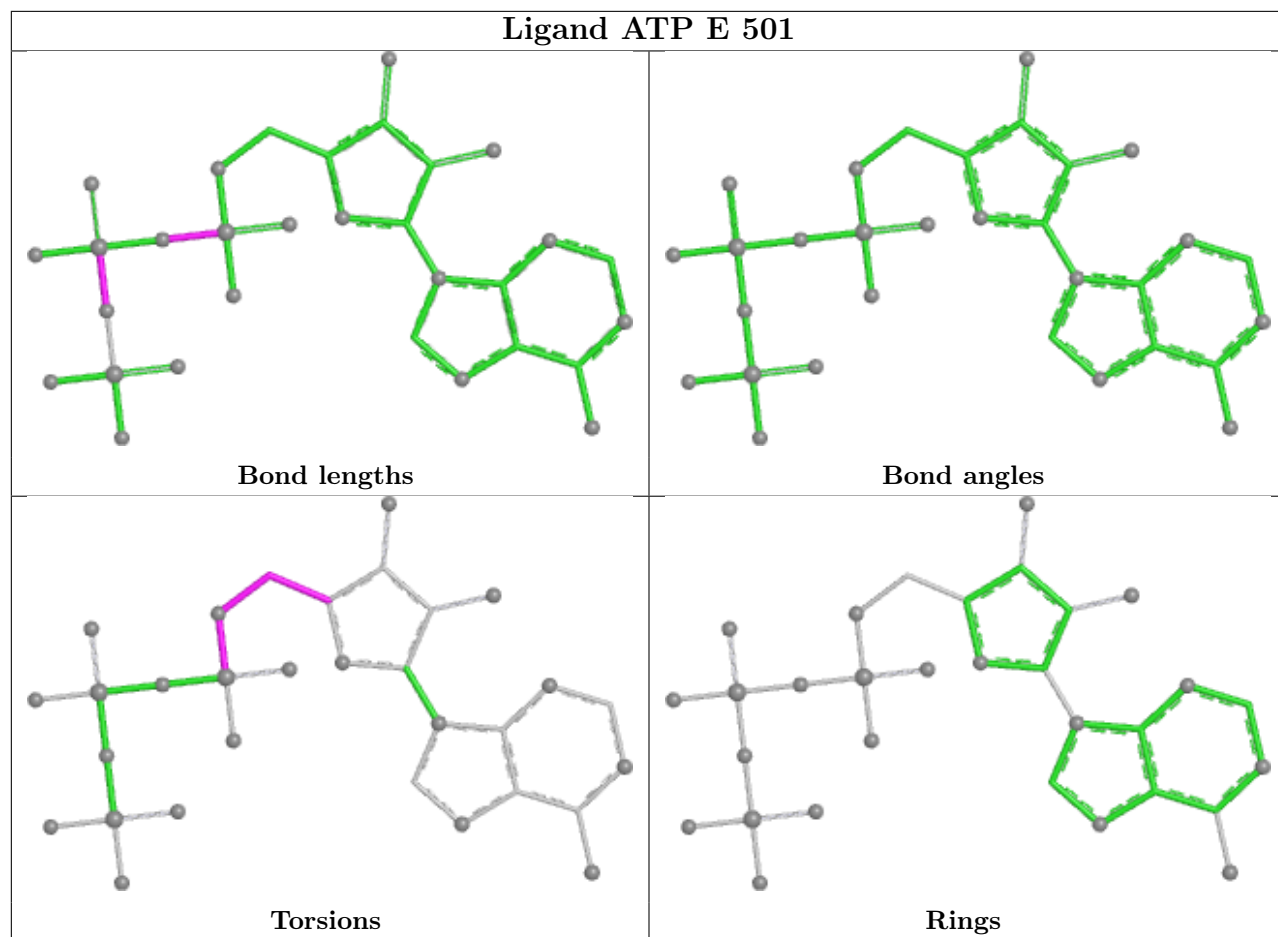
Ligand ATP A 501

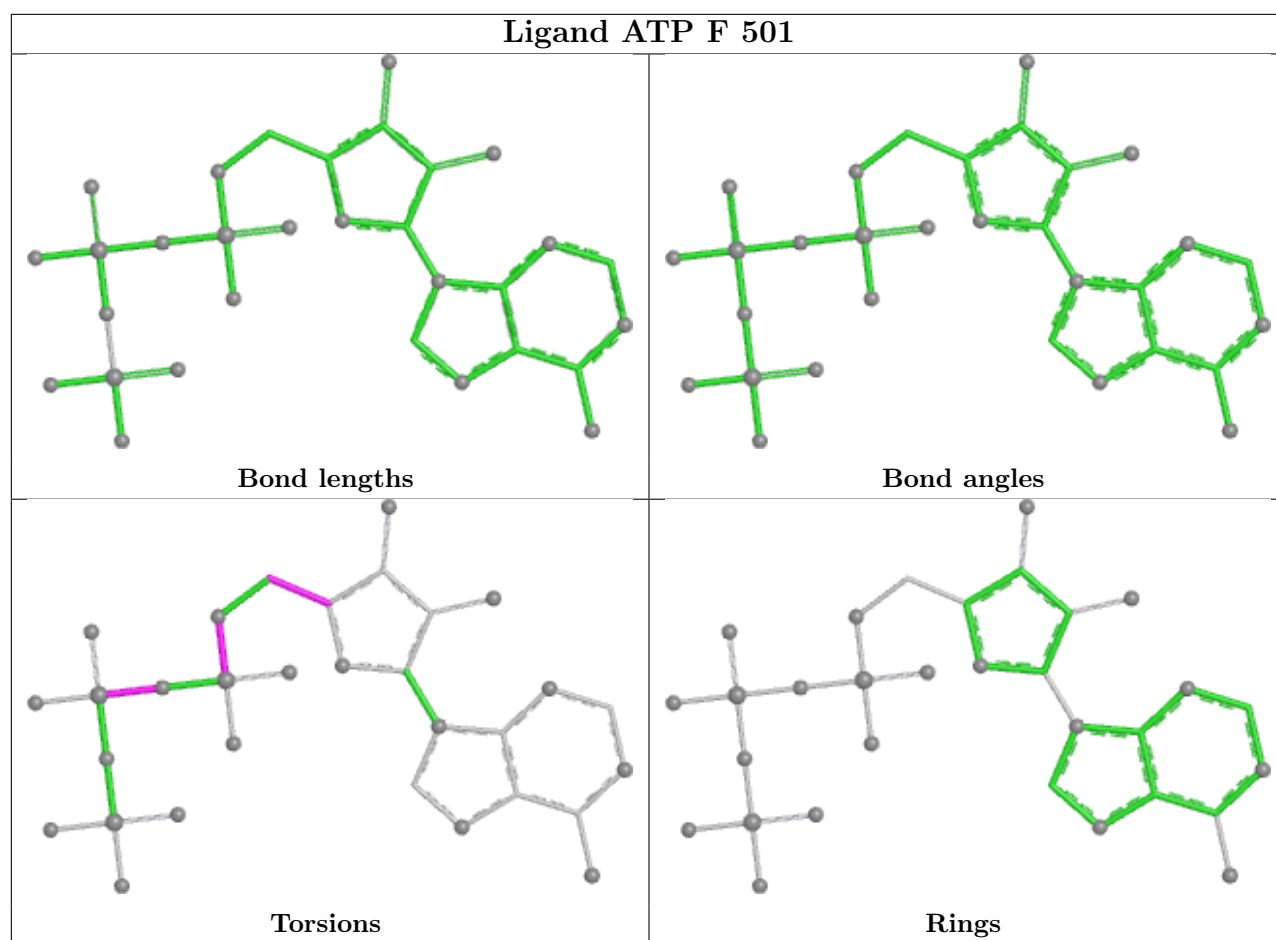


Ligand ADP B 501



Ligand ATP E 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

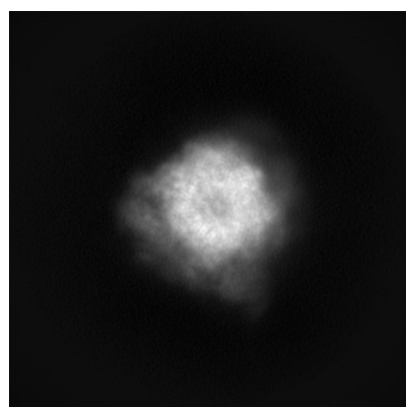
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32282. 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](#)

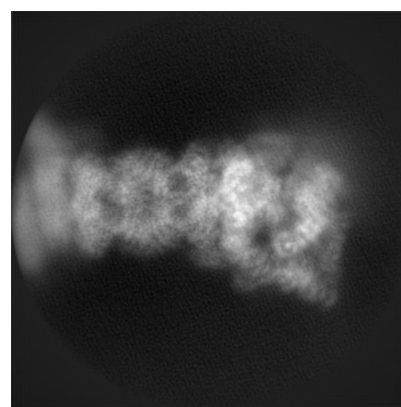
6.1.1 Primary map



X



Y

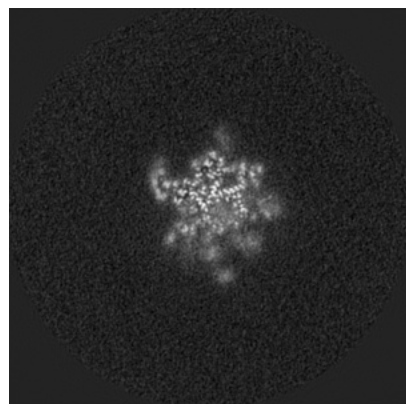


Z

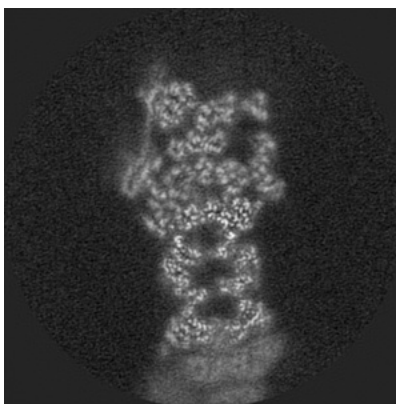
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

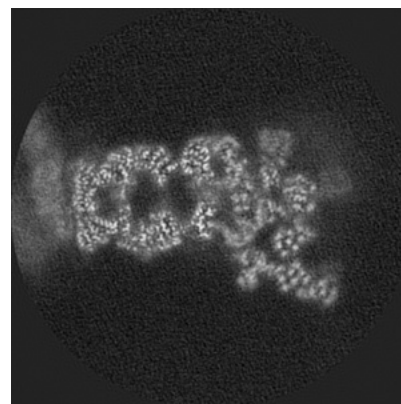
6.2.1 Primary map



X Index: 320



Y Index: 320

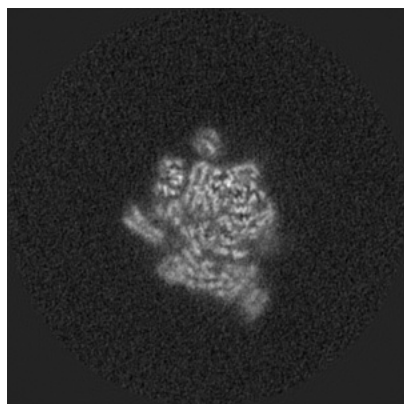


Z Index: 320

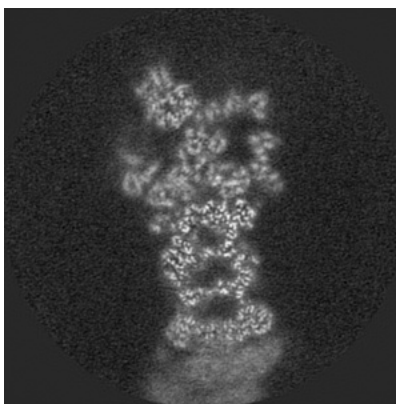
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

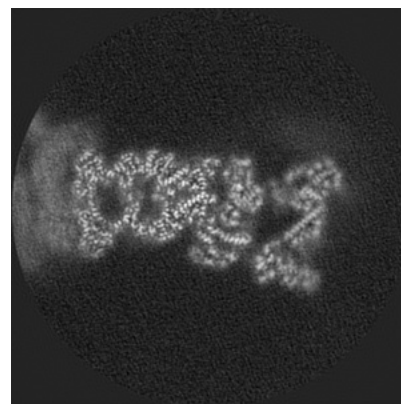
6.3.1 Primary map



X Index: 363



Y Index: 312

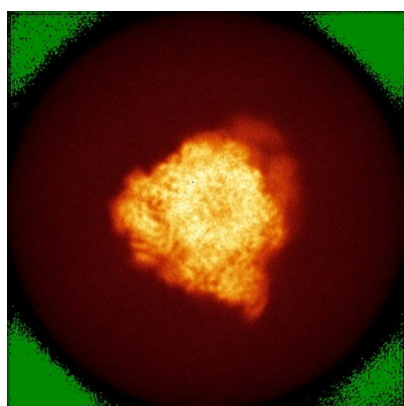


Z Index: 360

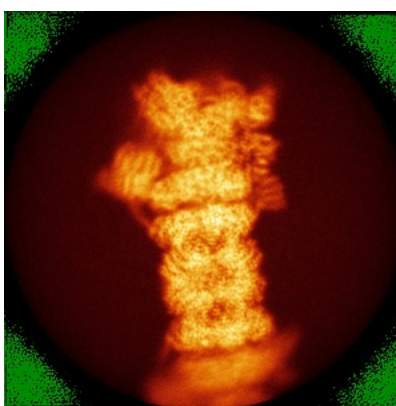
The images above show the largest variance slices of the map in three orthogonal directions.

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

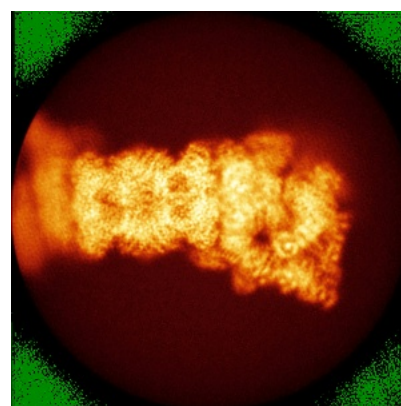
6.4.1 Primary map



X



Y

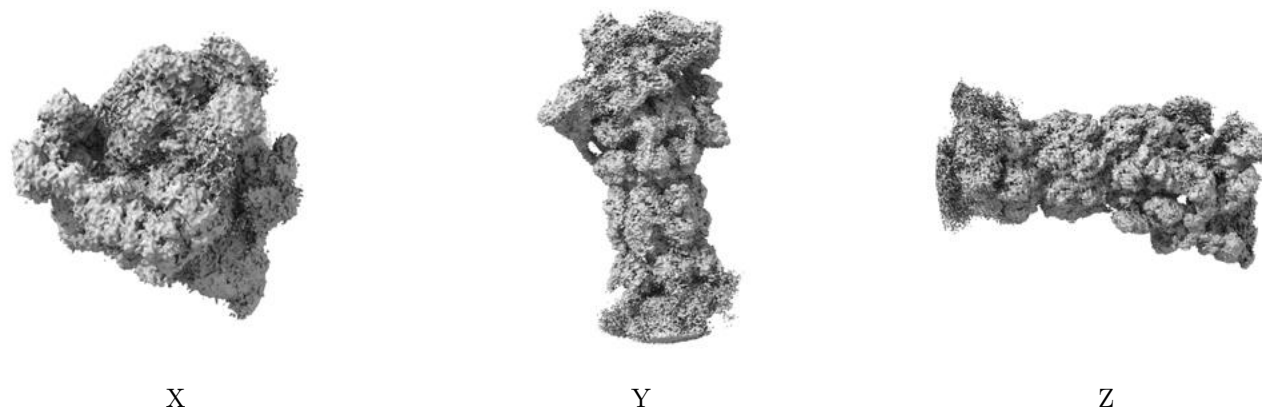


Z

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.

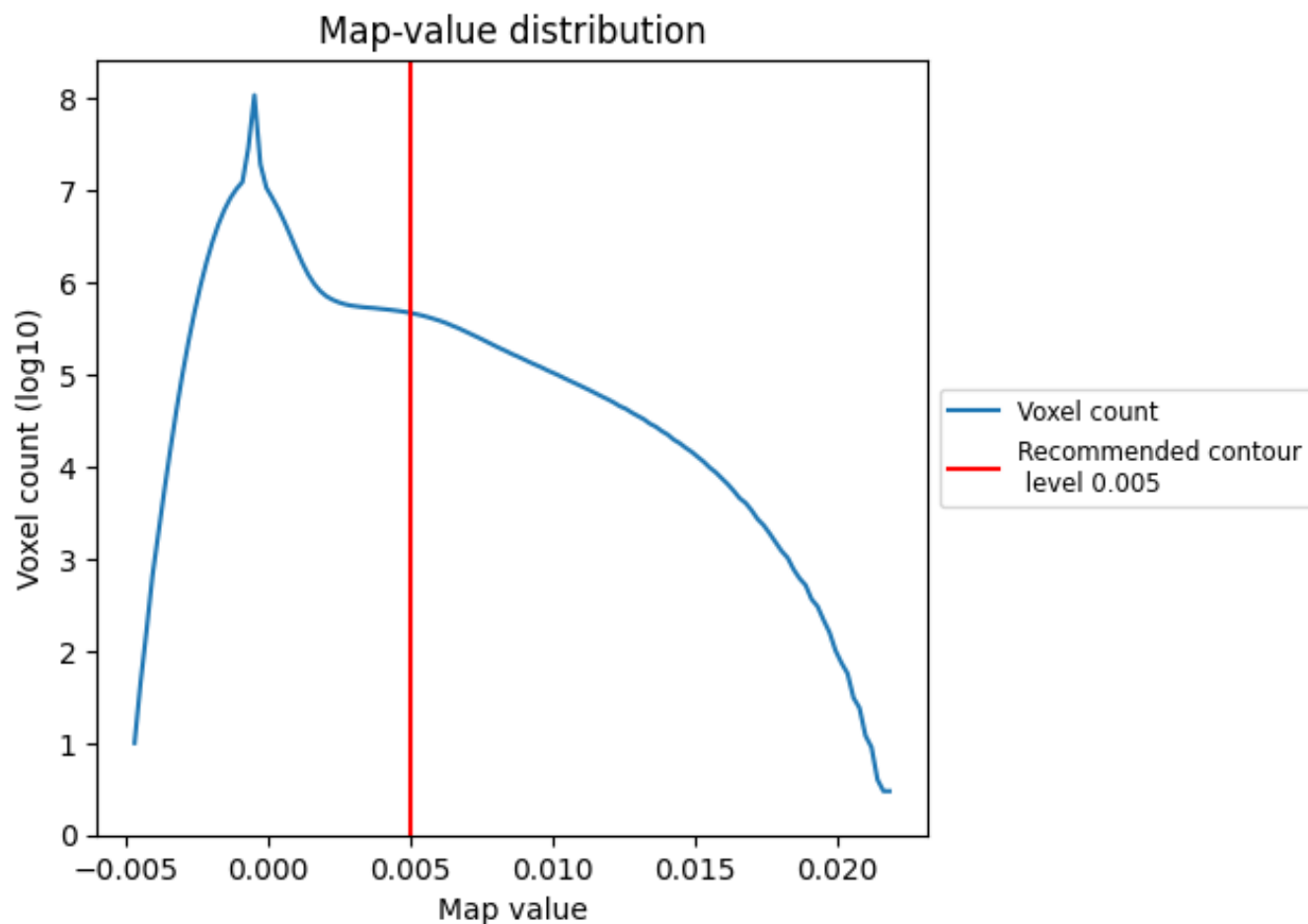
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

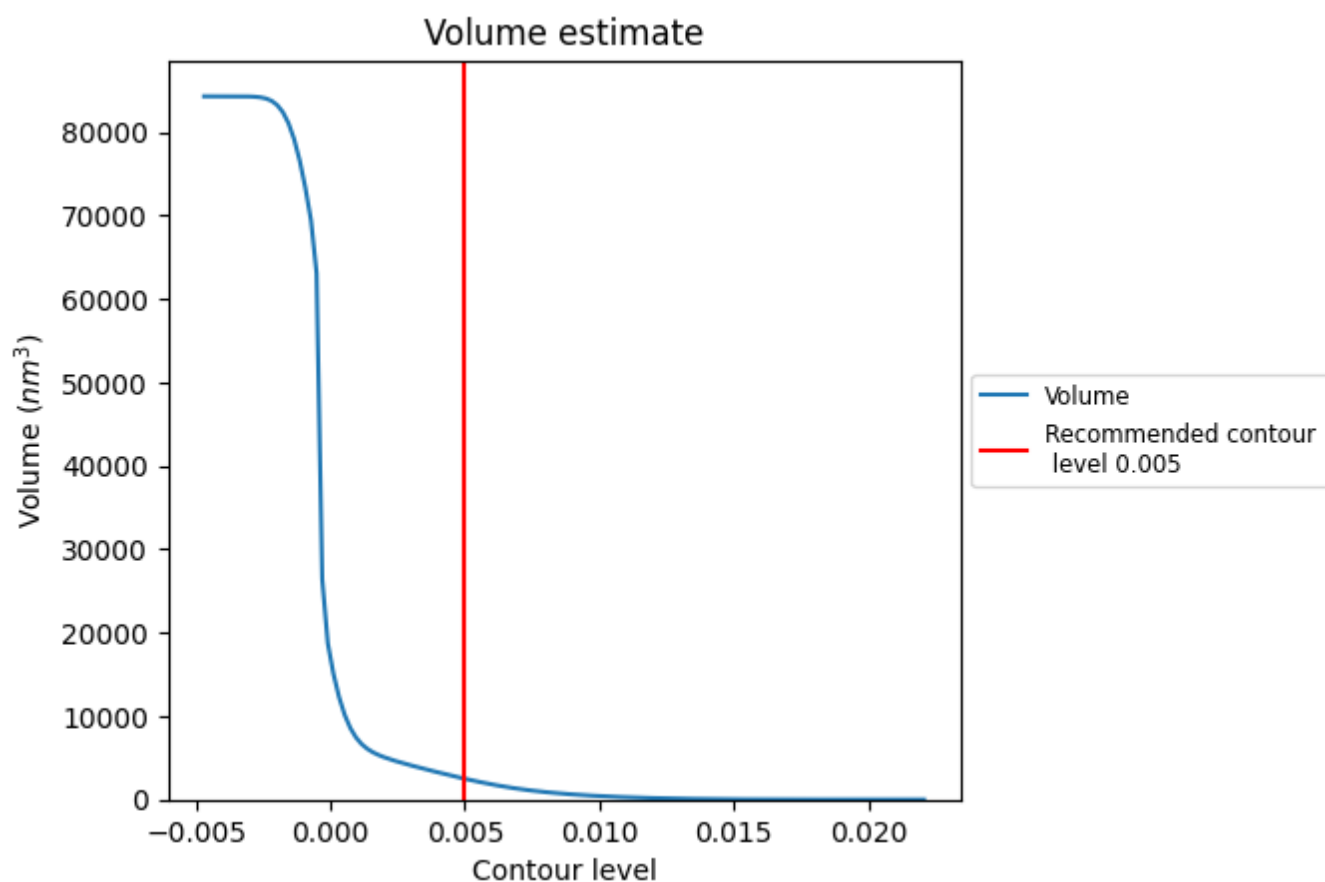
This section contains the results of statistical analysis of the map.

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.

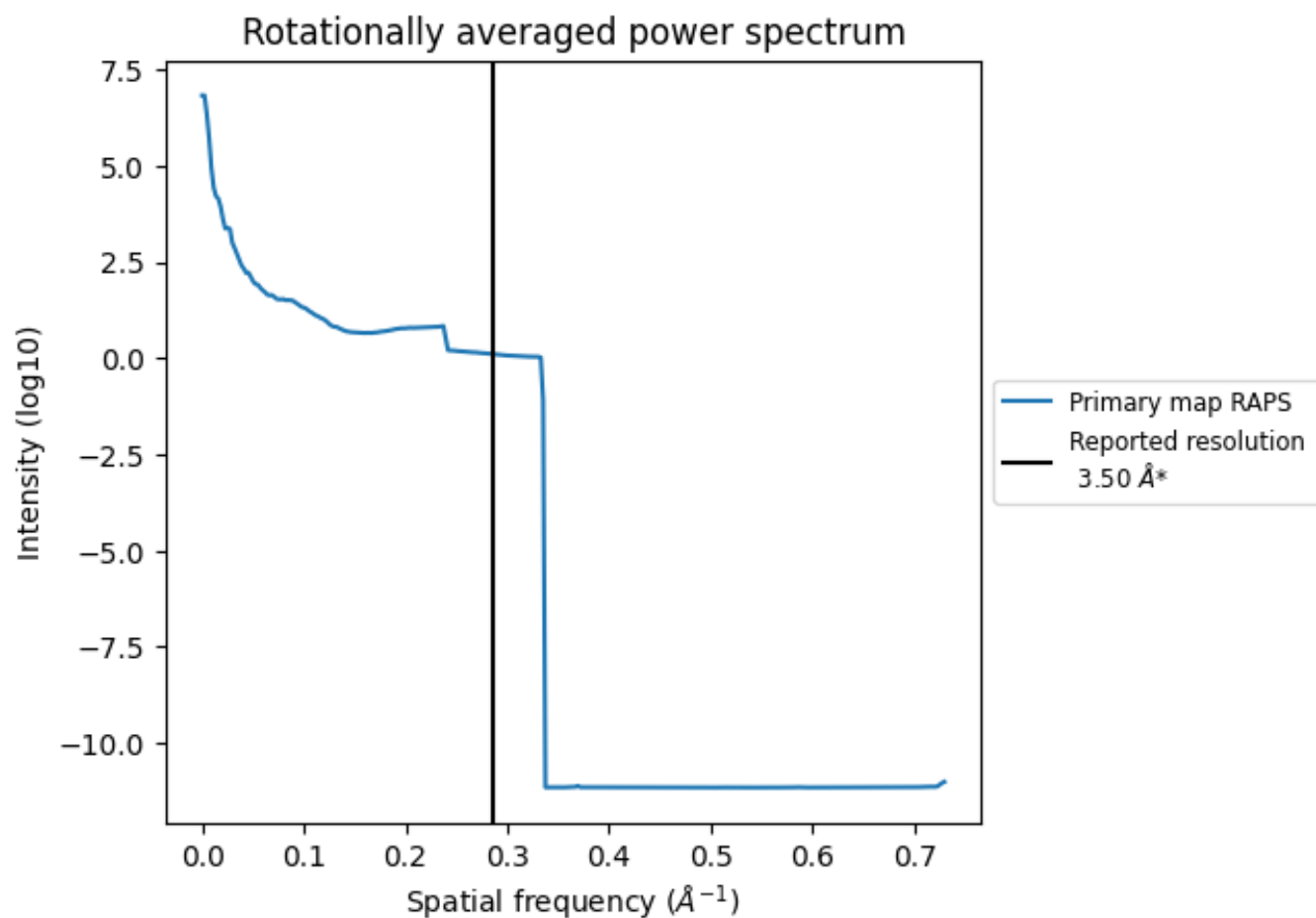
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2497 nm³; this corresponds to an approximate mass of 2255 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 0.286 Å⁻¹

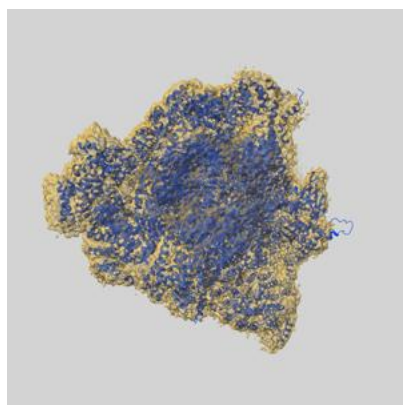
8 Fourier-Shell correlation

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

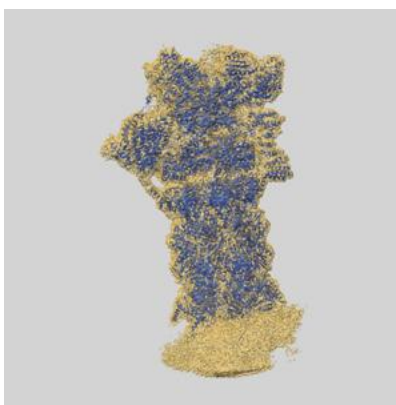
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32282 and PDB model 7W3J. Per-residue inclusion information can be found in section 3 on page 13.

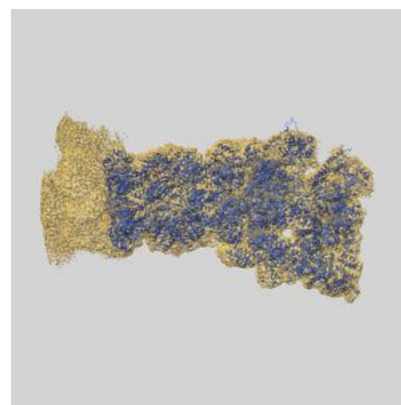
9.1 Map-model overlay [i](#)



X



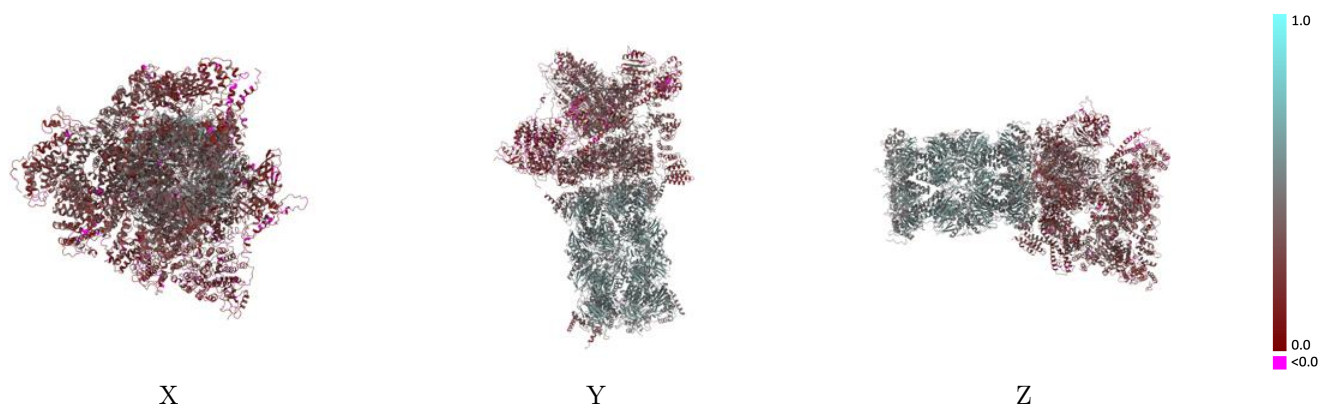
Y



Z

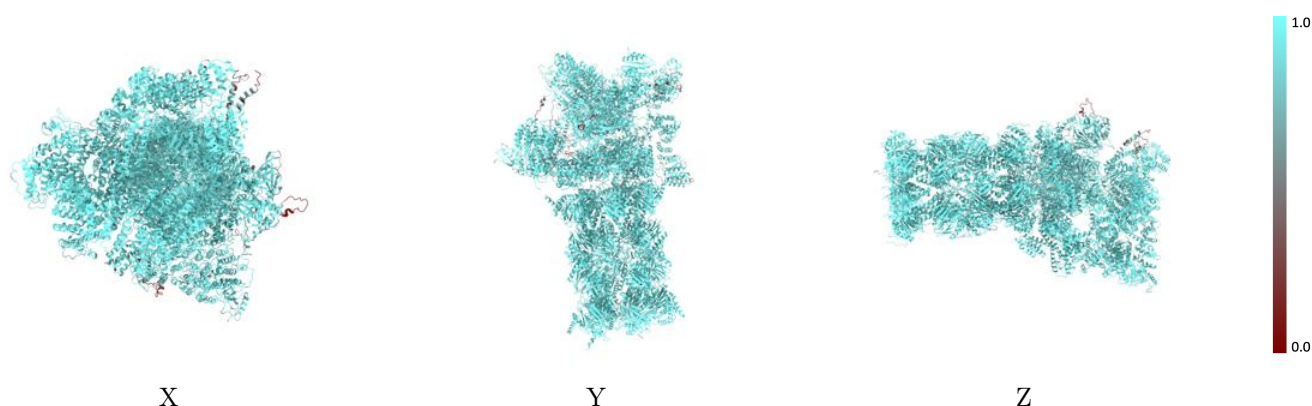
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



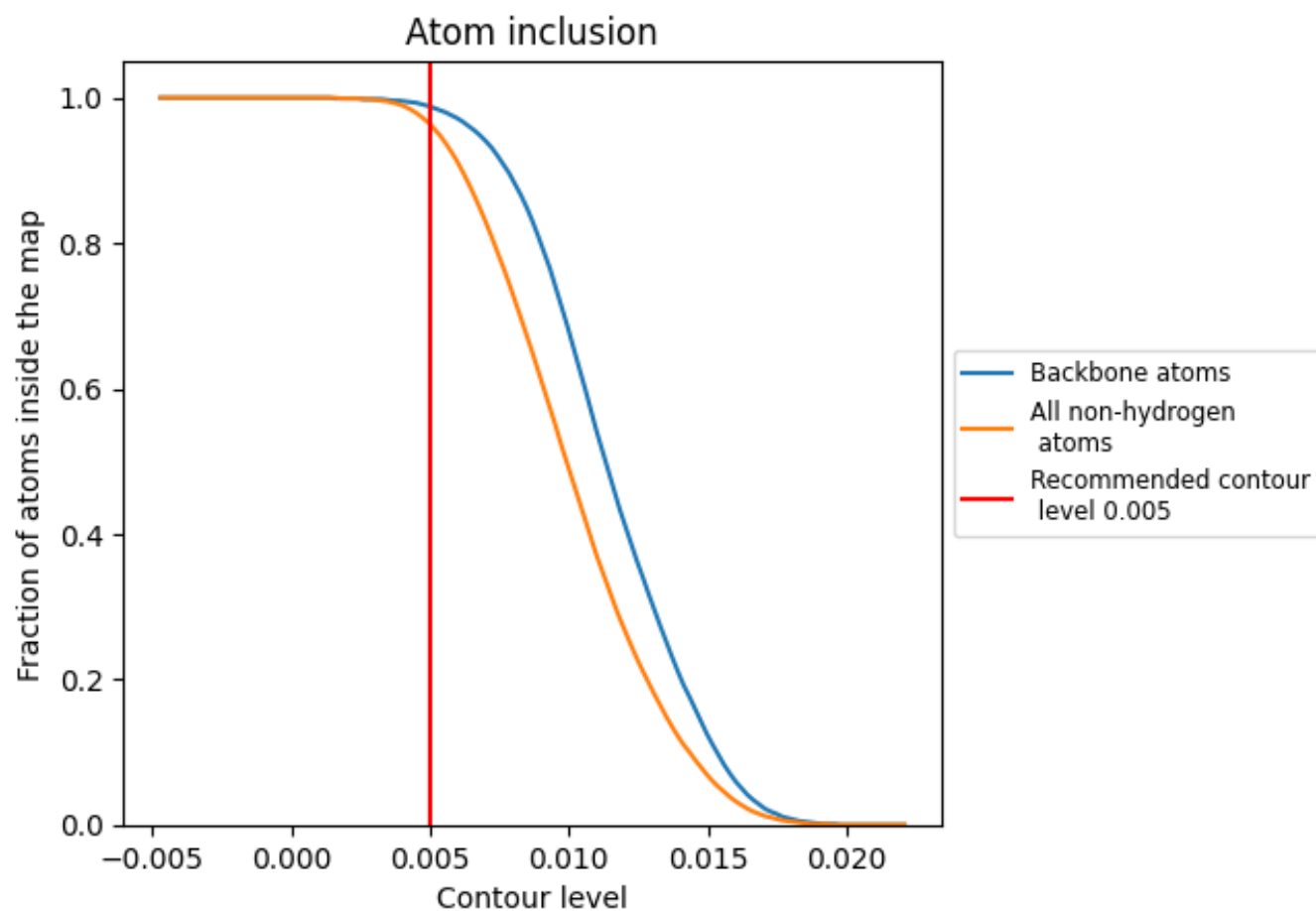
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.9640	 0.3800
A	 0.9760	 0.3150
B	 0.9730	 0.2950
C	 0.9710	 0.2780
D	 0.9760	 0.3140
E	 0.9380	 0.3240
F	 0.9320	 0.3300
G	 0.9860	 0.4960
H	 0.9950	 0.4960
I	 0.9830	 0.4780
J	 0.9840	 0.4560
K	 0.9830	 0.4800
L	 0.9930	 0.5070
M	 0.9820	 0.4970
N	 0.9890	 0.5330
O	 0.9930	 0.5170
P	 0.9950	 0.5320
Q	 0.9940	 0.5170
R	 0.9970	 0.5220
S	 0.9940	 0.5230
T	 0.9880	 0.5350
U	 0.9370	 0.3100
V	 0.9550	 0.2930
W	 0.9200	 0.2590
X	 0.9650	 0.3200
Y	 0.9710	 0.2770
Z	 0.9730	 0.3210
a	 0.9390	 0.2490
b	 0.9600	 0.2750
c	 0.9820	 0.3310
d	 0.9280	 0.2430
e	 0.9360	 0.2790
f	 0.9430	 0.1920
g	 0.9880	 0.5080
h	 0.9880	 0.5140



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.9750	 0.4850
j	 0.9750	 0.4430
k	 0.9760	 0.4840
l	 0.9880	 0.5150
m	 0.9900	 0.5090
n	 0.9940	 0.5370
o	 0.9950	 0.5290
p	 0.9970	 0.5400
q	 0.9960	 0.5290
r	 0.9950	 0.5380
s	 0.9900	 0.5290
t	 0.9930	 0.5340
x	 0.8430	 0.2140
y	 0.8330	 0.2250