



Full wwPDB EM Validation Report ⓘ

Apr 20, 2026 – 05:52 PM JST

PDB ID : 9K5C / pdb_00009k5c
EMDB ID : EMD-62088
Title : Structure of substrate-engaged single-cap human proteasome in state ED1
Authors : Wu, Z.; Chen, E.; Mao, Y.
Deposited on : 2024-10-21
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

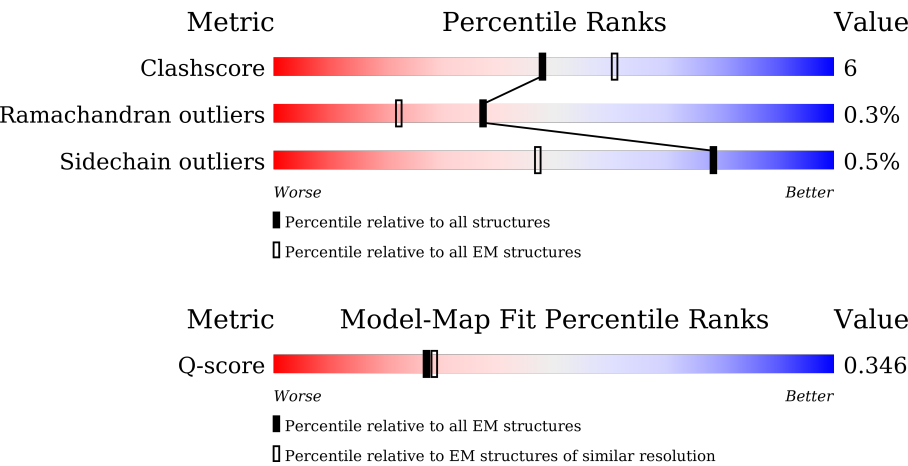
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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

Mol	Chain	Length	Quality of chain
1	A	433	<div><div>43%</div><div><div></div><div>73%</div><div>21%</div><div>5%</div></div></div>
2	B	440	<div><div>24%</div><div><div></div><div>76%</div><div>17%</div><div>7%</div></div></div>
3	C	398	<div><div>10%</div><div><div></div><div>80%</div><div>18%</div><div>...</div></div></div>
4	D	418	<div><div>7%</div><div><div></div><div>74%</div><div>16%</div><div>9%</div></div></div>











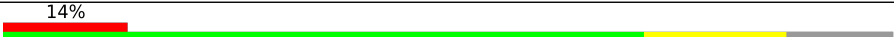

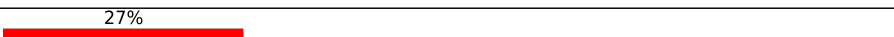
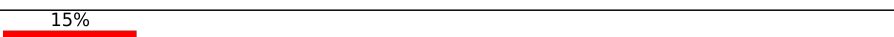
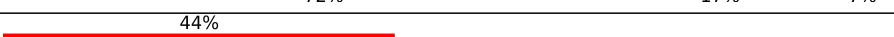
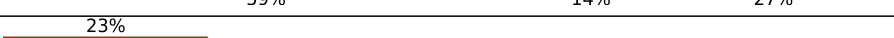

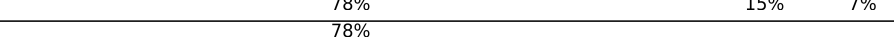
Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 106301 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1578	1012	267	290	9		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	878	Total	C	N	O	S	0	0
			6867	4352	1163	1306	46		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

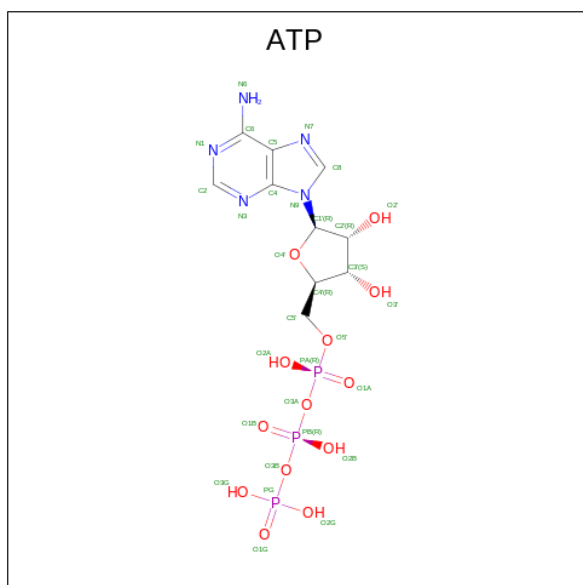
- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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

- Molecule 33 is a protein called Substrate.

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

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



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

Continued on next page...

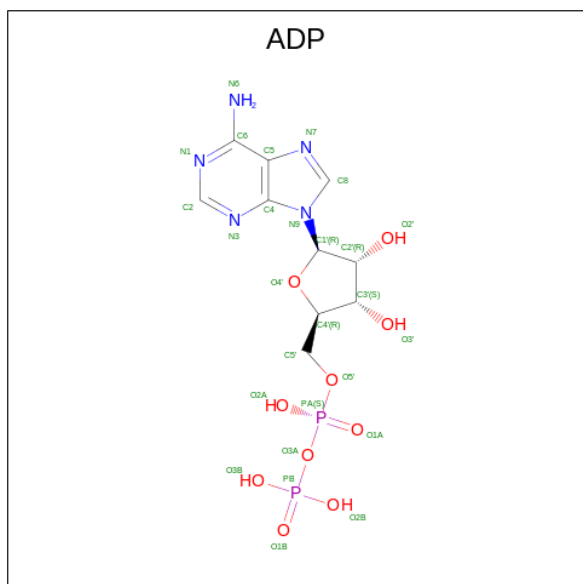
Continued from previous page...

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

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

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

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



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

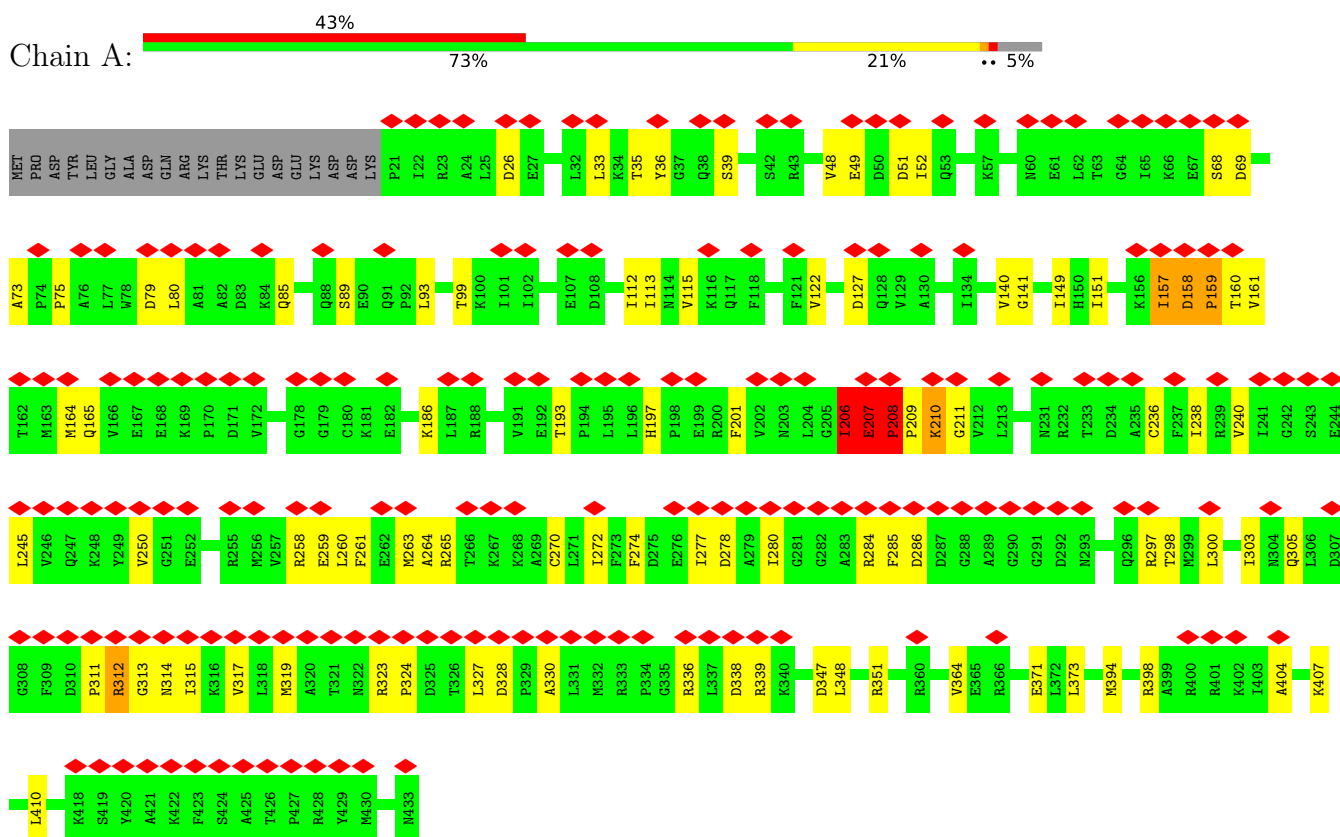
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

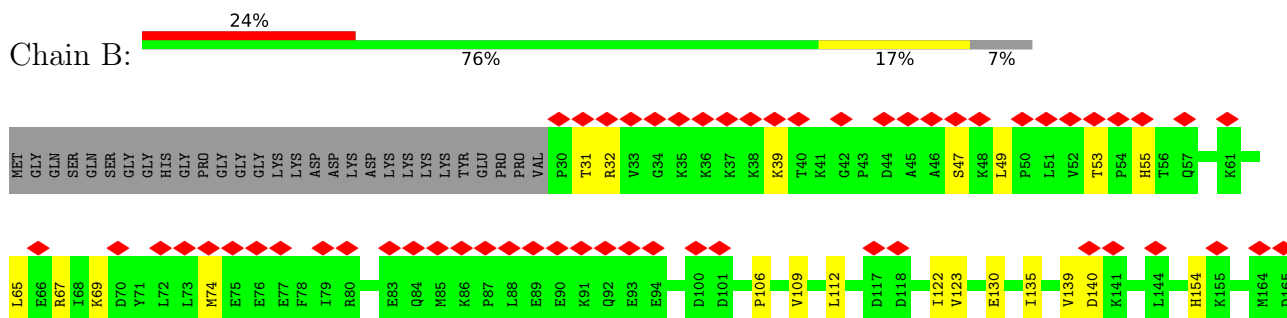
3 Residue-property plots

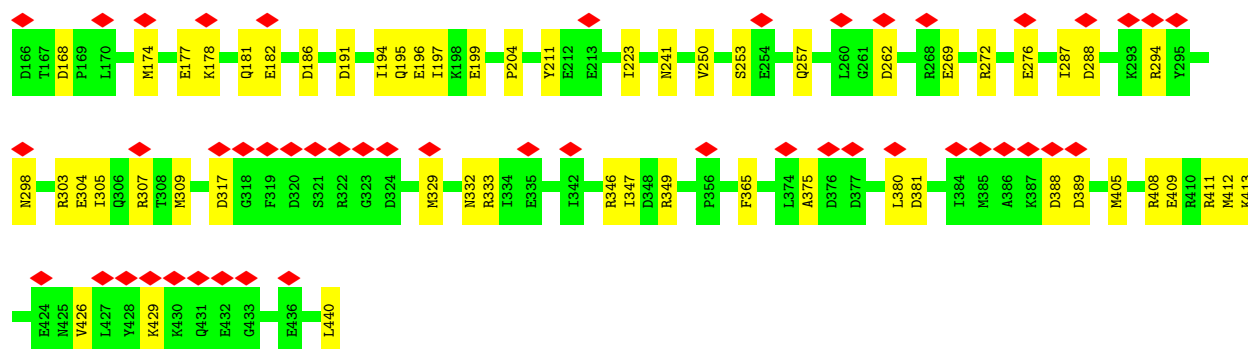
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 26S proteasome regulatory subunit 7

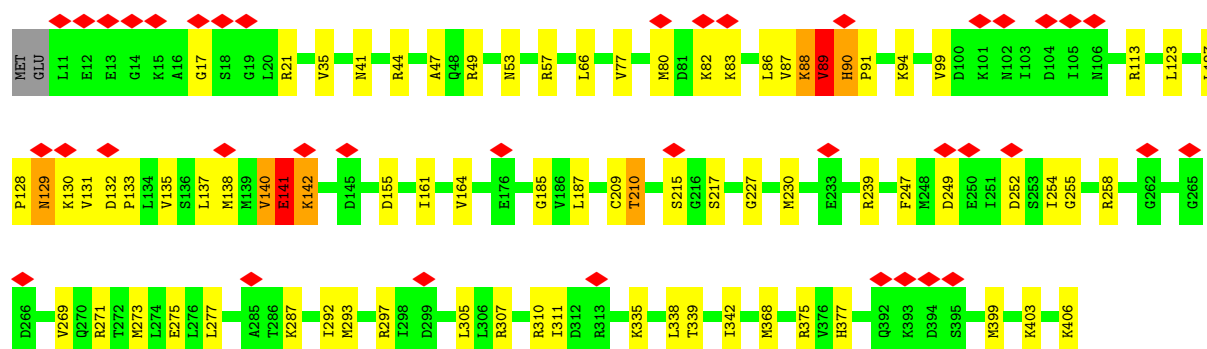


• Molecule 2: 26S proteasome regulatory subunit 4

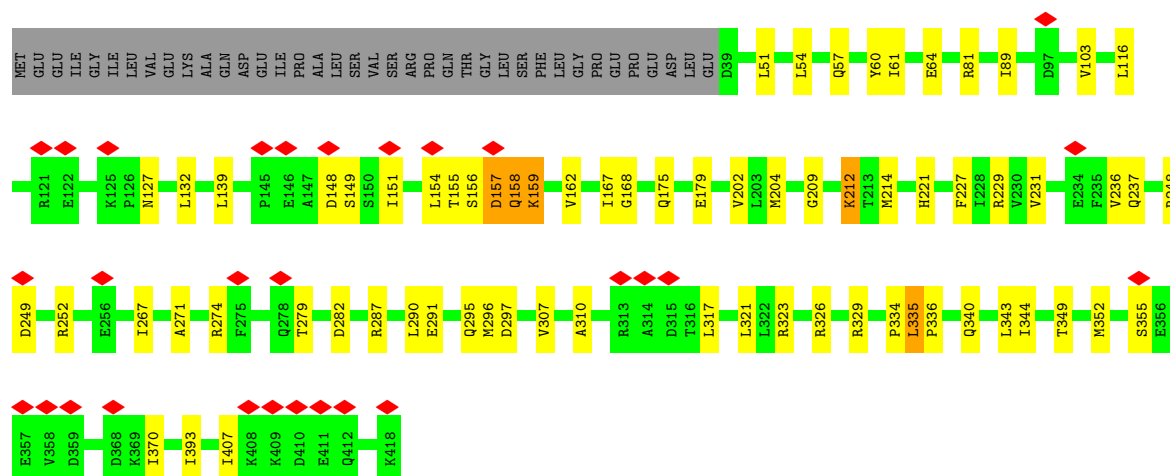
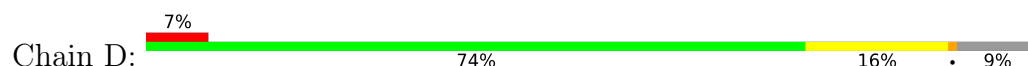




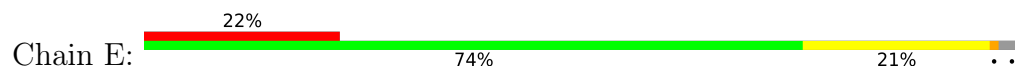
• Molecule 3: 26S proteasome regulatory subunit 8

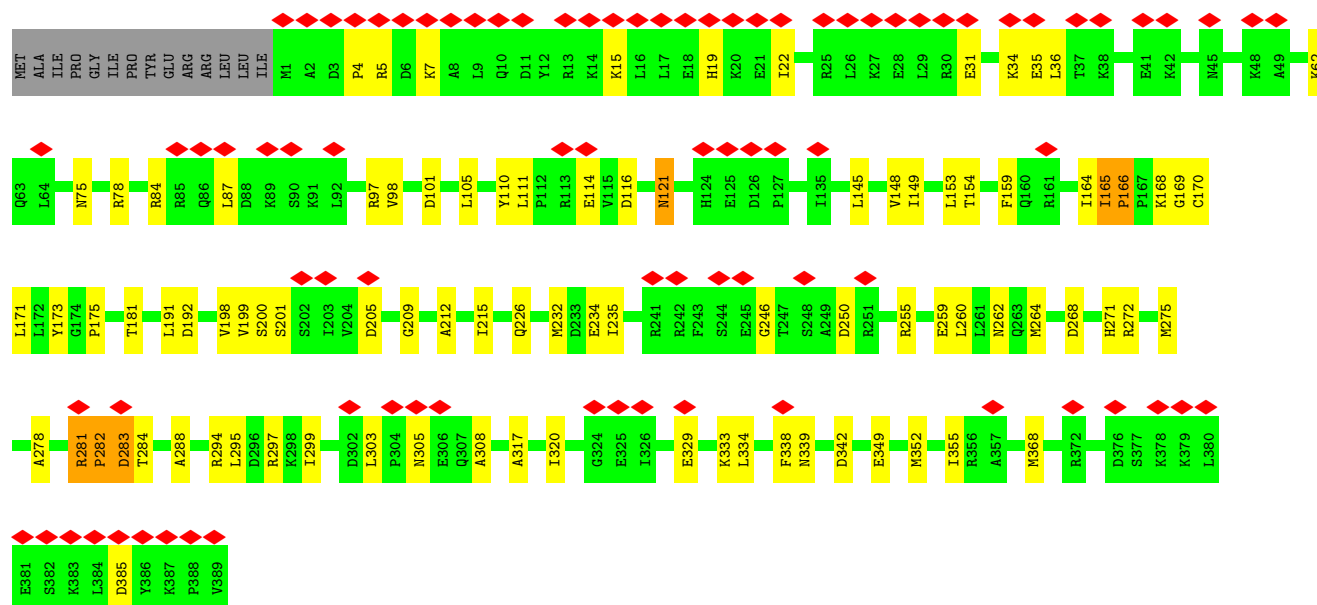


• Molecule 4: 26S proteasome regulatory subunit 6B

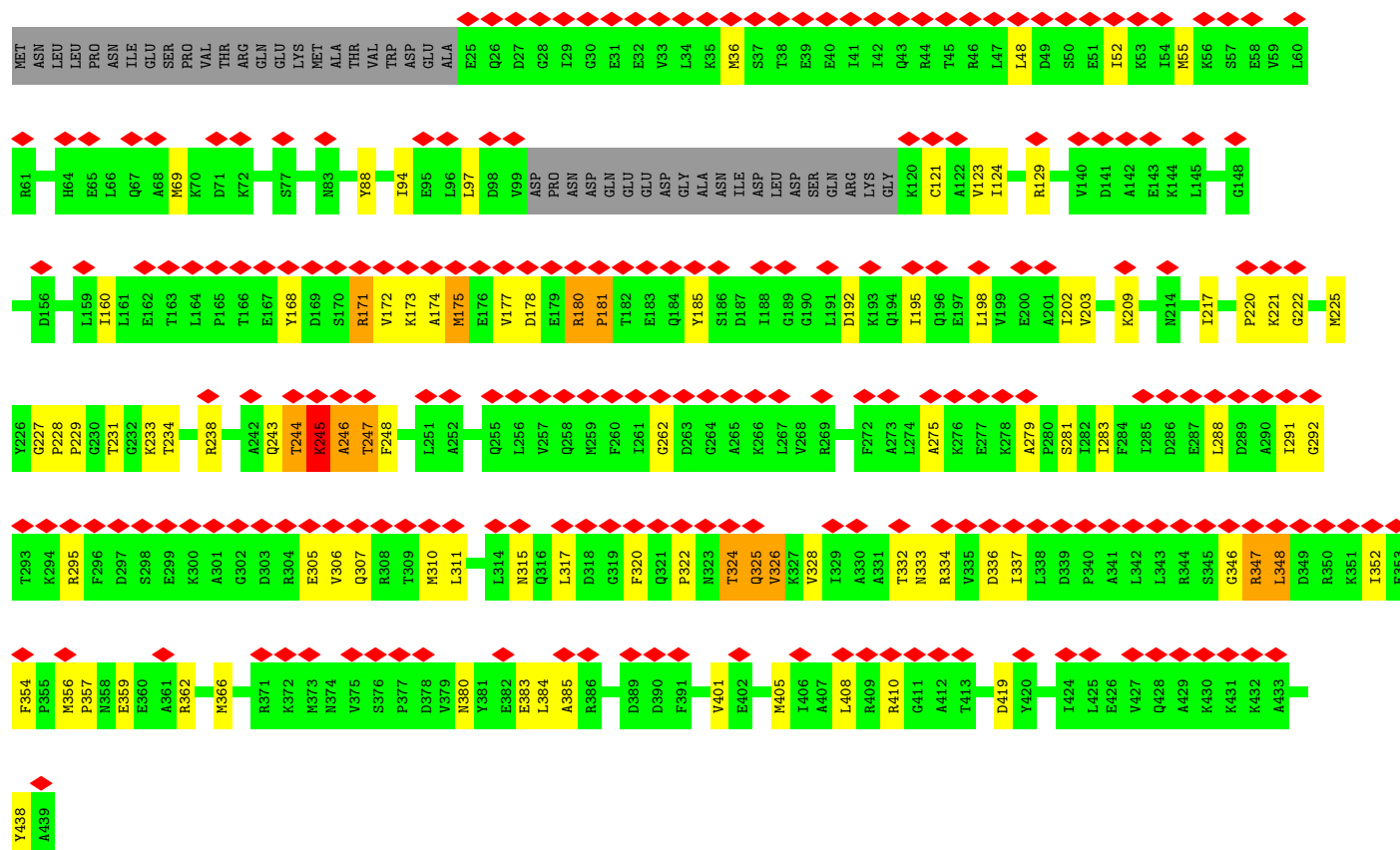


• Molecule 5: Proteasome 26S subunit, ATPase 6

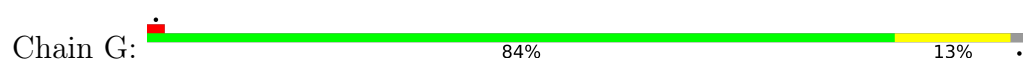


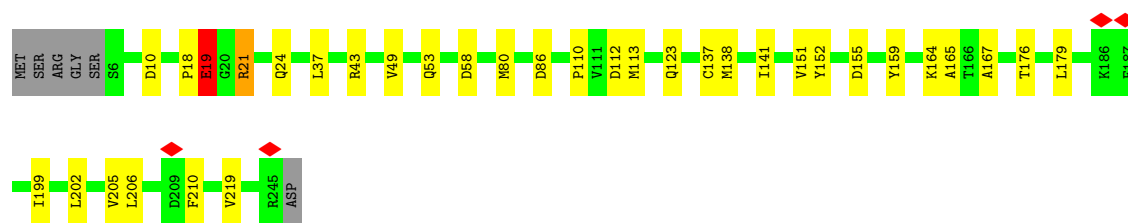


• Molecule 6: 26S proteasome regulatory subunit 6A

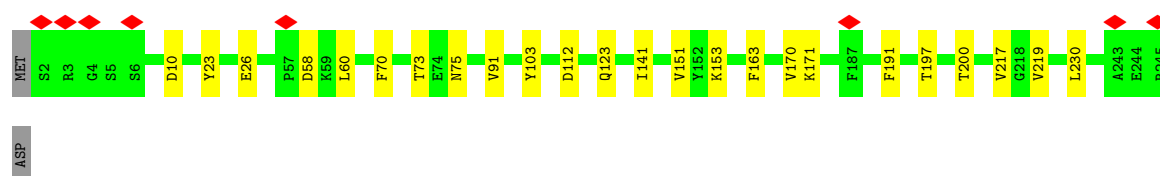
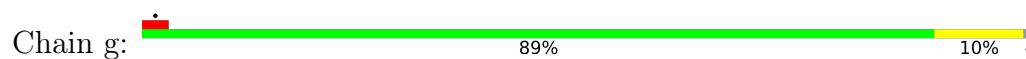


• Molecule 7: Proteasome subunit alpha type-6

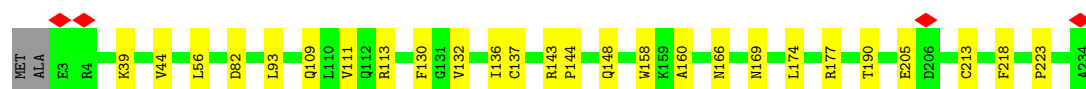
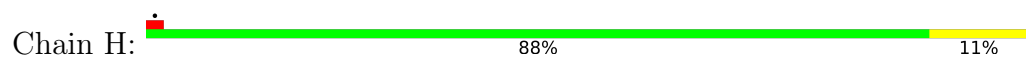




• Molecule 7: Proteasome subunit alpha type-6



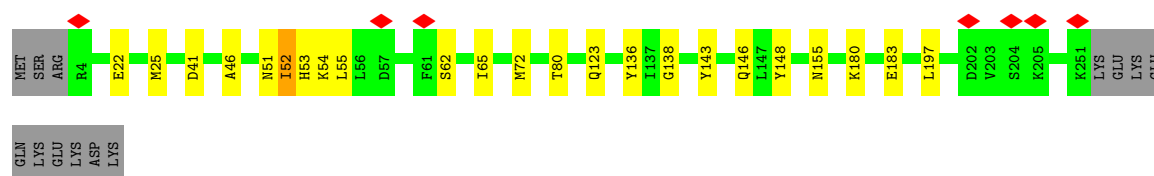
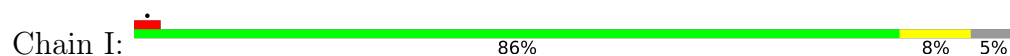
• Molecule 8: Proteasome subunit alpha type-2



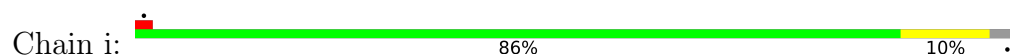
• Molecule 8: Proteasome subunit alpha type-2

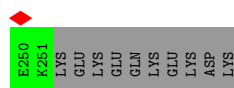


• Molecule 9: Proteasome subunit alpha type-4

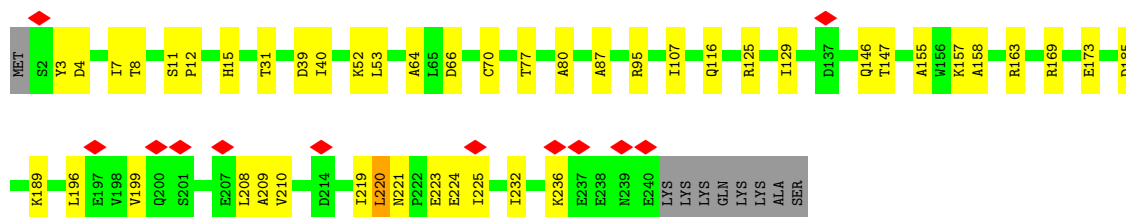
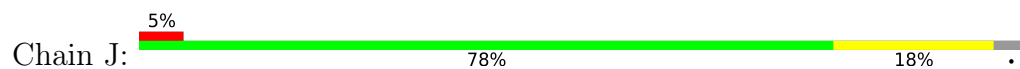


• Molecule 9: Proteasome subunit alpha type-4

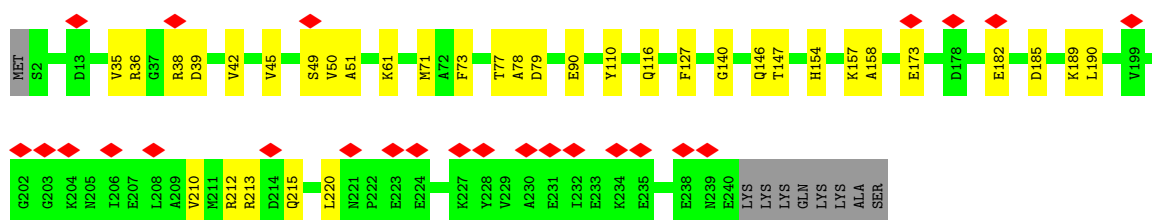
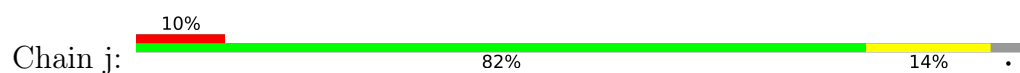




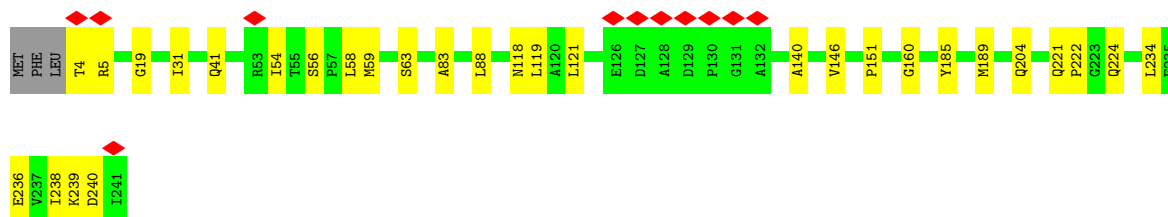
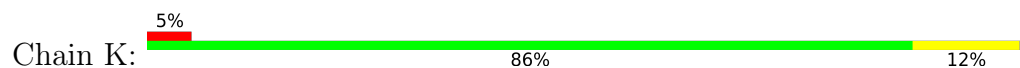
- Molecule 10: Proteasome subunit alpha type-7



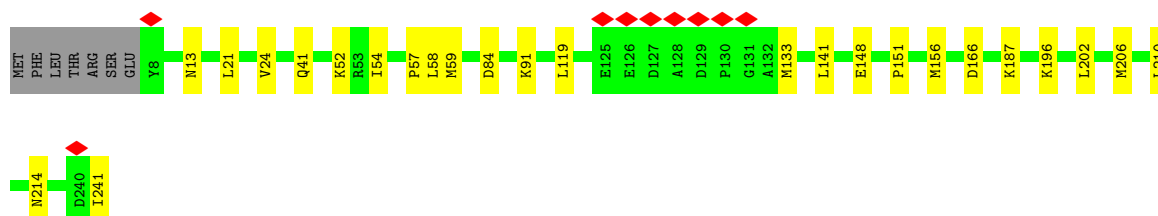
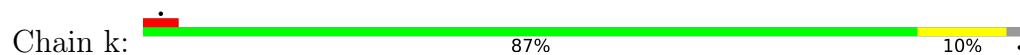
- Molecule 10: Proteasome subunit alpha type-7




- Molecule 11: Proteasome subunit alpha type-5

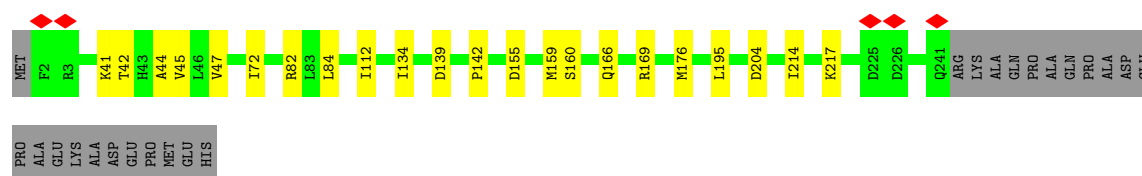


- Molecule 11: Proteasome subunit alpha type-5




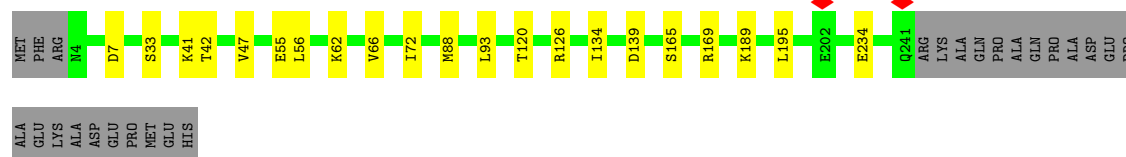
- Molecule 12: Proteasome subunit alpha type-1

Chain L: 




- Molecule 12: Proteasome subunit alpha type-1

Chain l: 




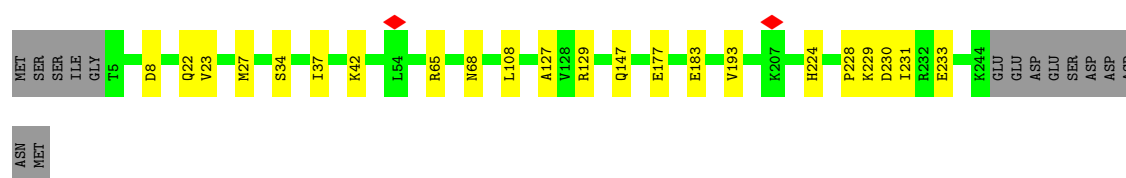
- Molecule 13: Proteasome subunit alpha type-3

Chain M: 




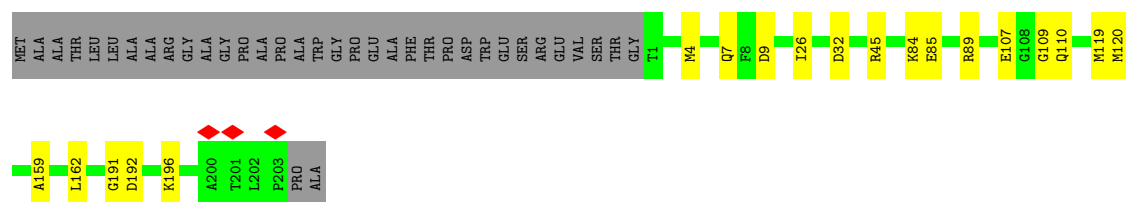
- Molecule 13: Proteasome subunit alpha type-3

Chain m: 




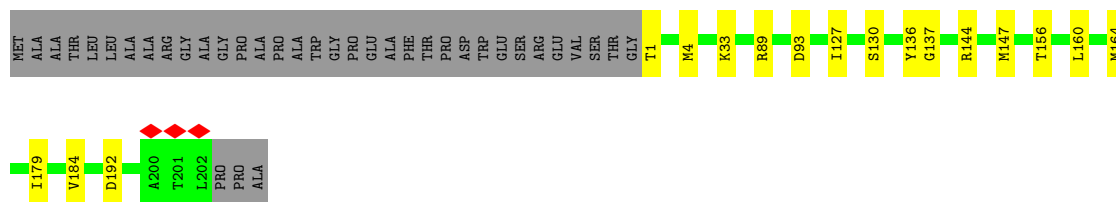
- Molecule 14: Proteasome subunit beta type-6

Chain N: 



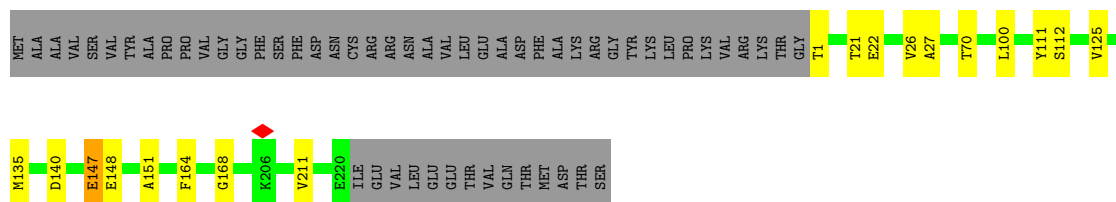
- Molecule 14: Proteasome subunit beta type-6

Chain n: 



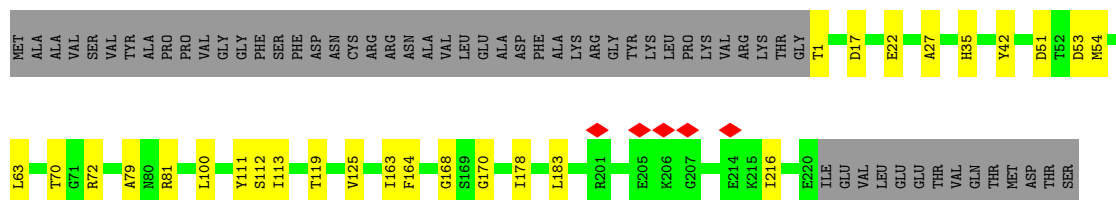
- Molecule 15: Proteasome subunit beta type-7

Chain O: 




- Molecule 15: Proteasome subunit beta type-7

Chain o: 




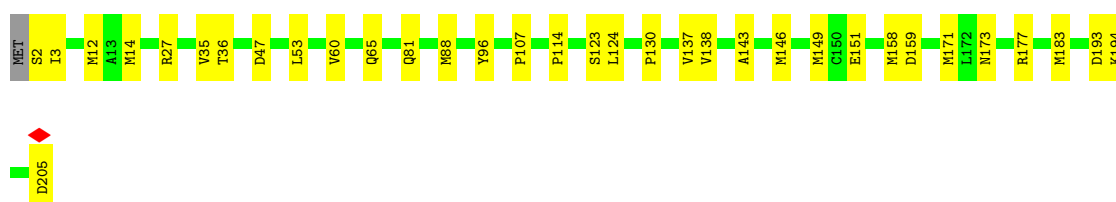
- Molecule 16: Proteasome subunit beta type-3

Chain P: 

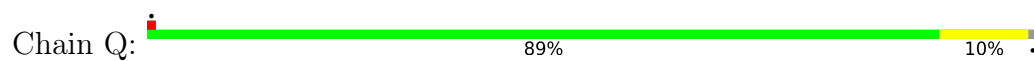


- Molecule 16: Proteasome subunit beta type-3

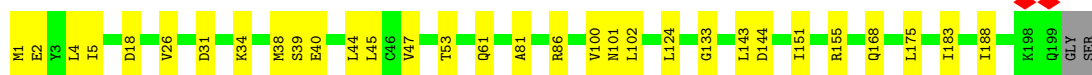
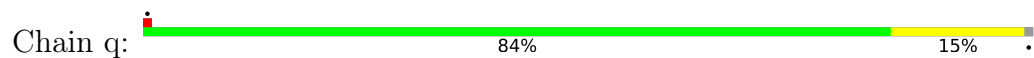
Chain p: 



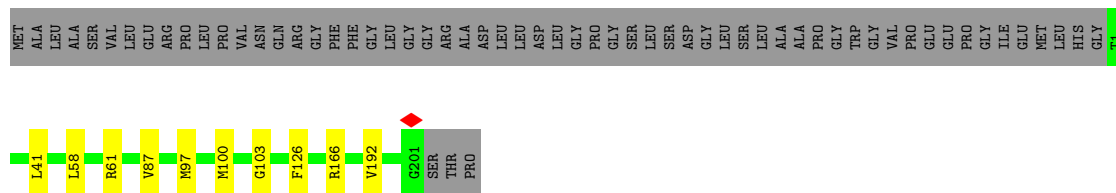
- Molecule 17: Proteasome subunit beta type-2



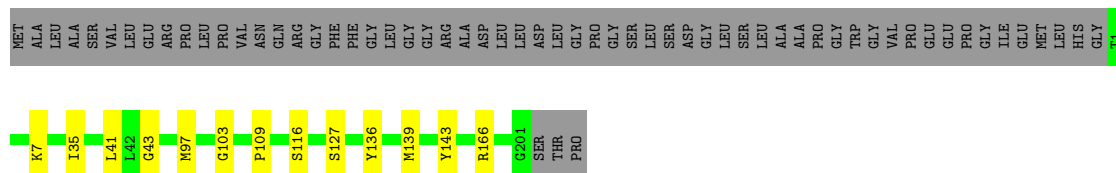
- Molecule 17: Proteasome subunit beta type-2



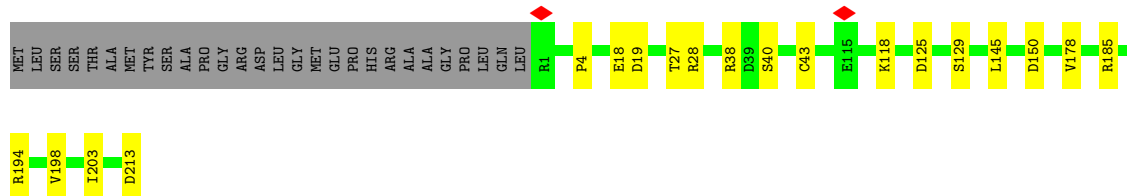
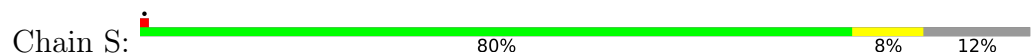
- Molecule 18: Proteasome subunit beta type-5



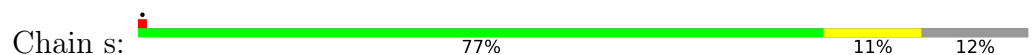
- Molecule 18: Proteasome subunit beta type-5

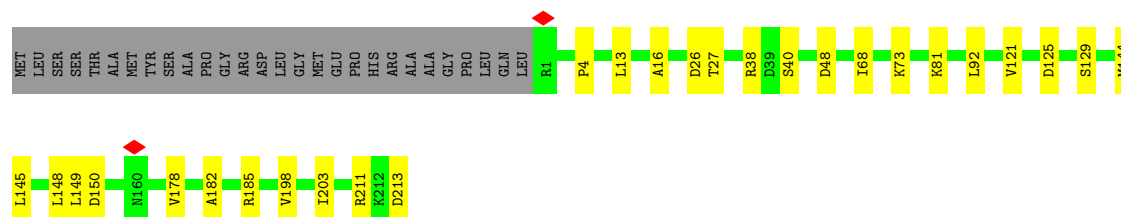


- Molecule 19: Proteasome subunit beta type-1



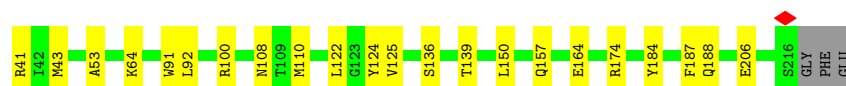
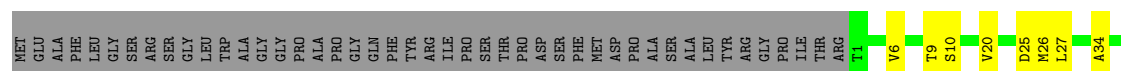
- Molecule 19: Proteasome subunit beta type-1





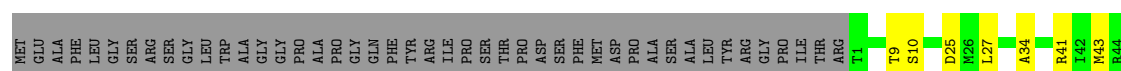
- Molecule 20: Proteasome subunit beta type-4

Chain T:



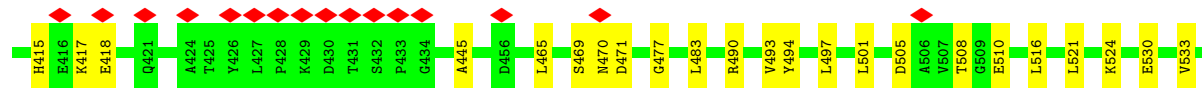
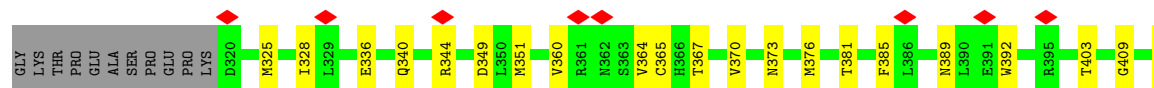
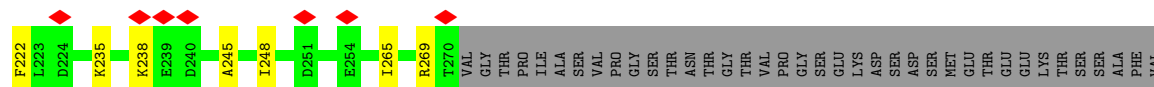
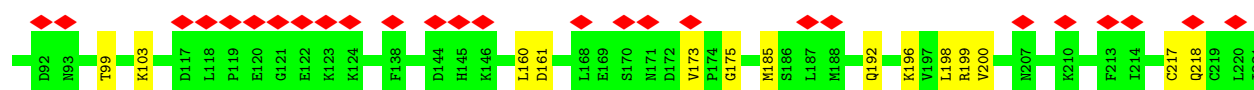
- Molecule 20: Proteasome subunit beta type-4

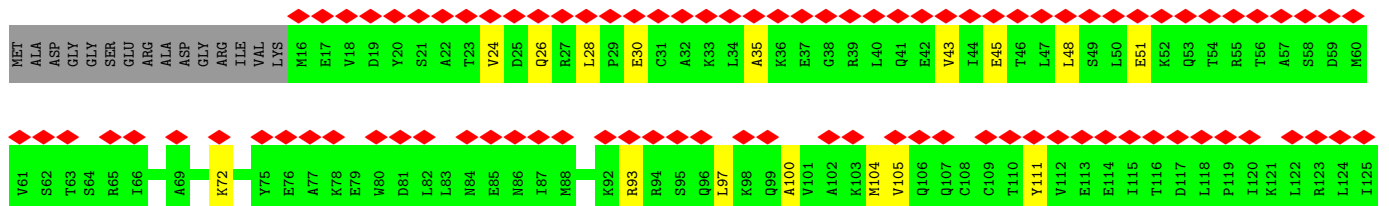
Chain t:

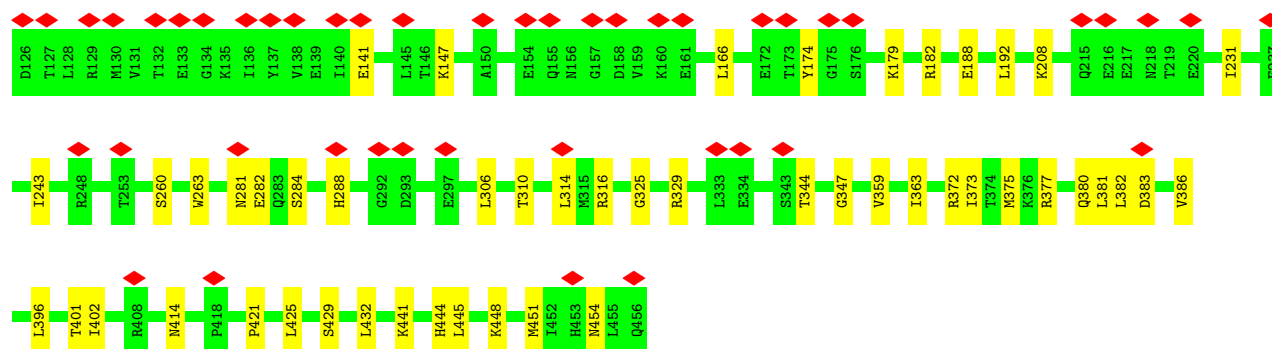


- Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

Chain U:

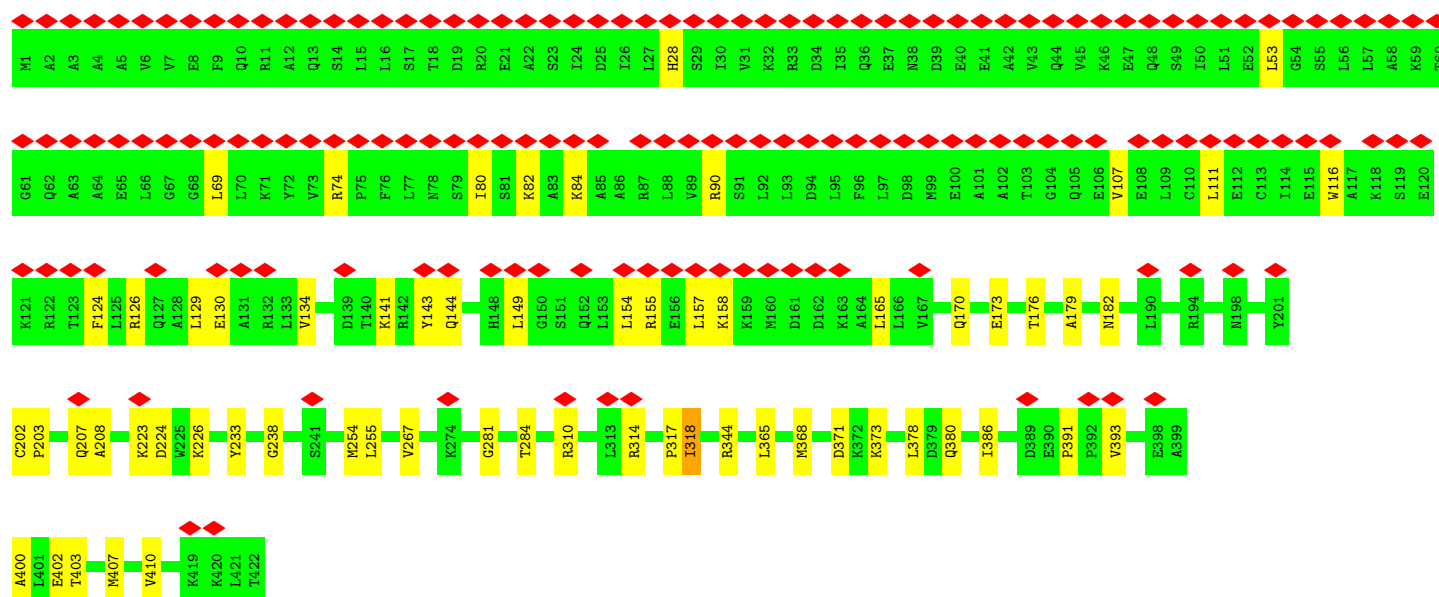






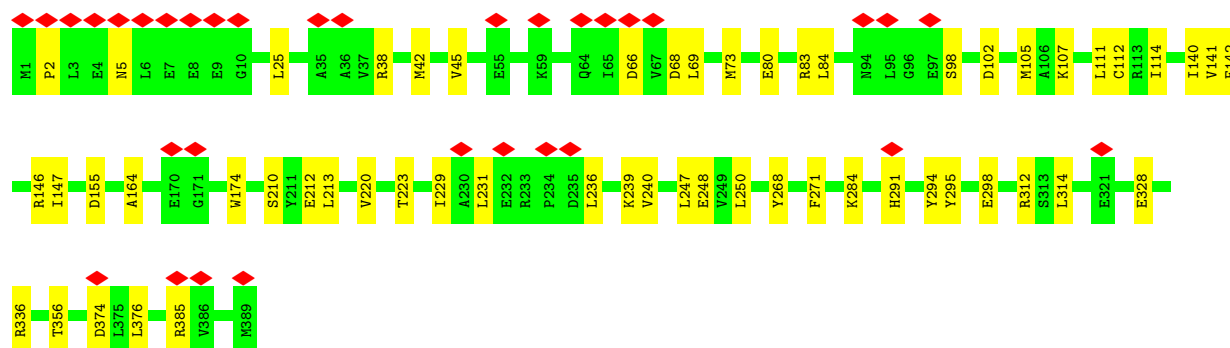
- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

Chain X:

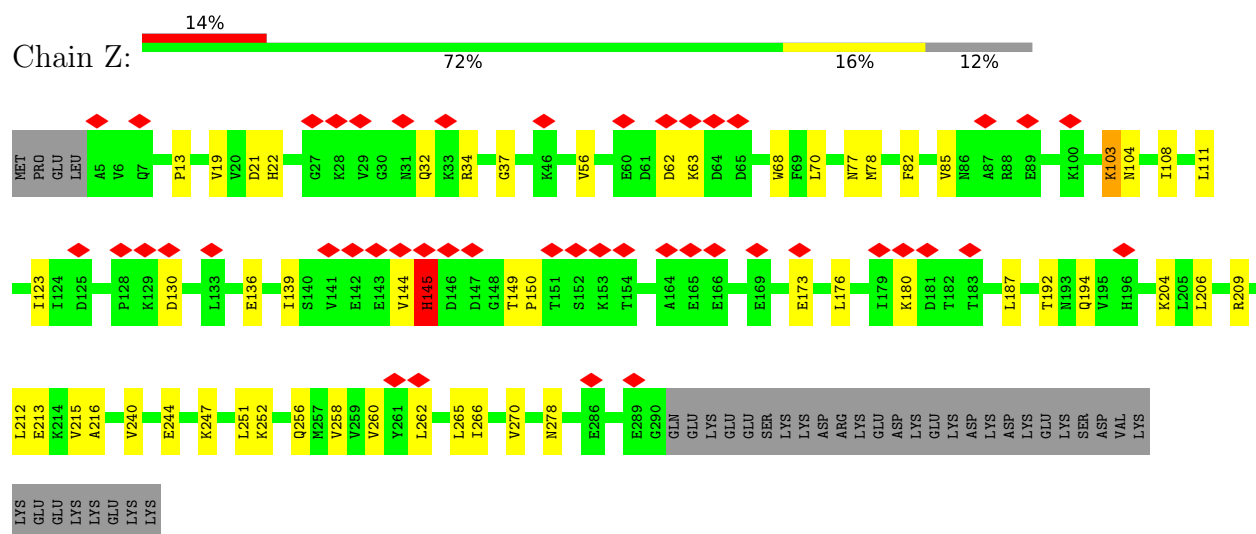


- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

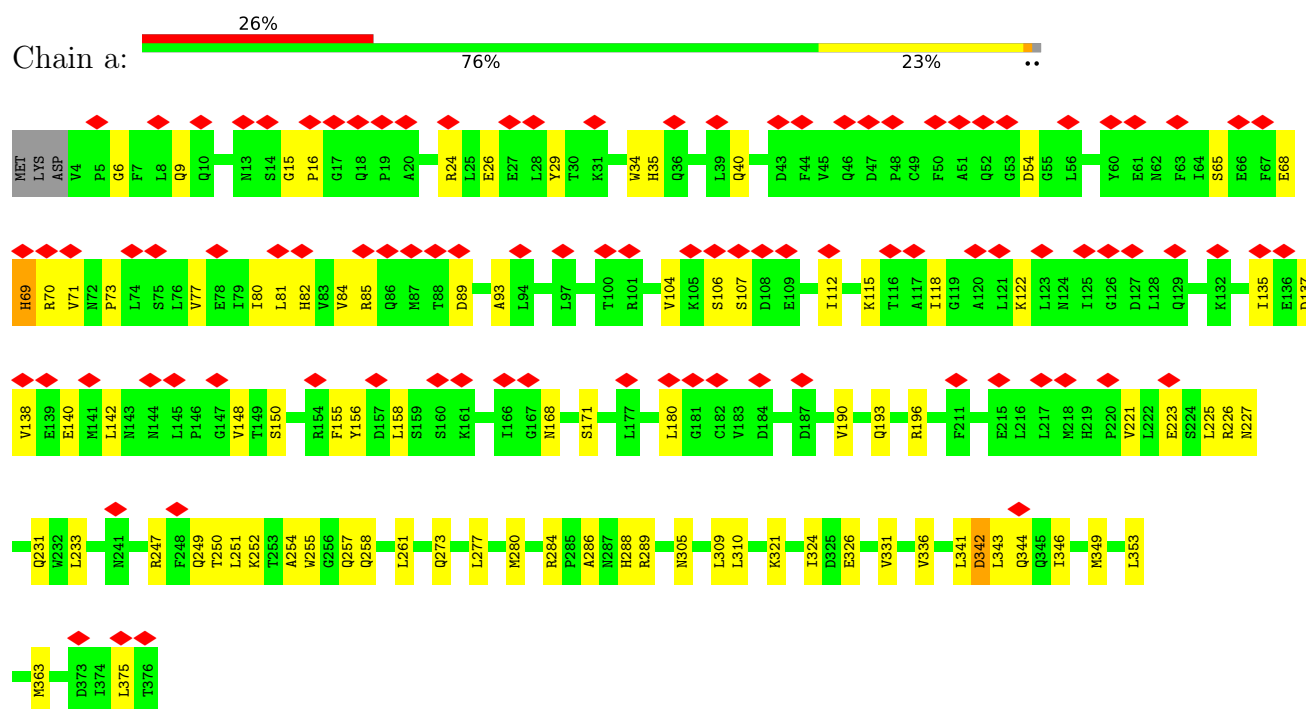
Chain Y:



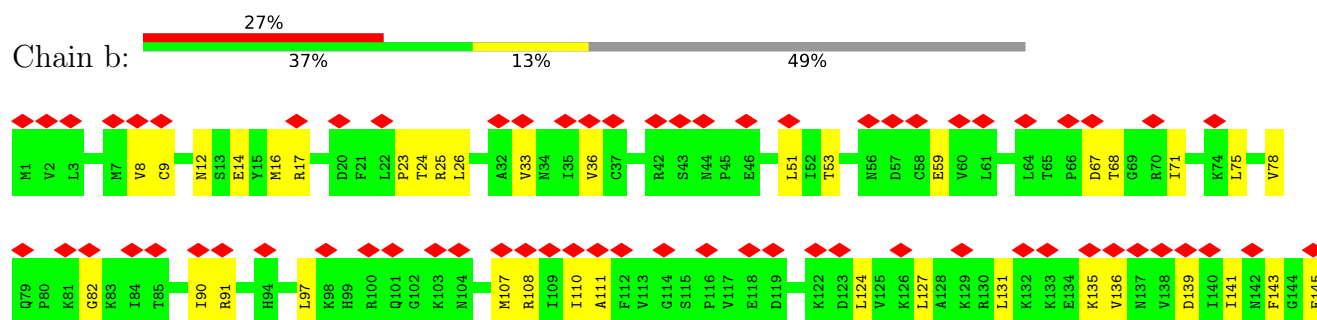
- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7



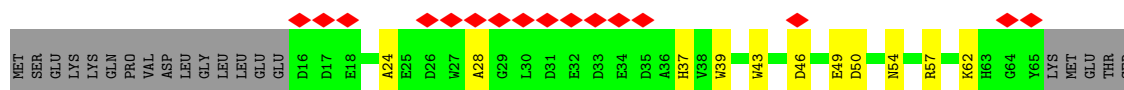
• Molecule 27: 26S proteasome non-ATPase regulatory subunit 13



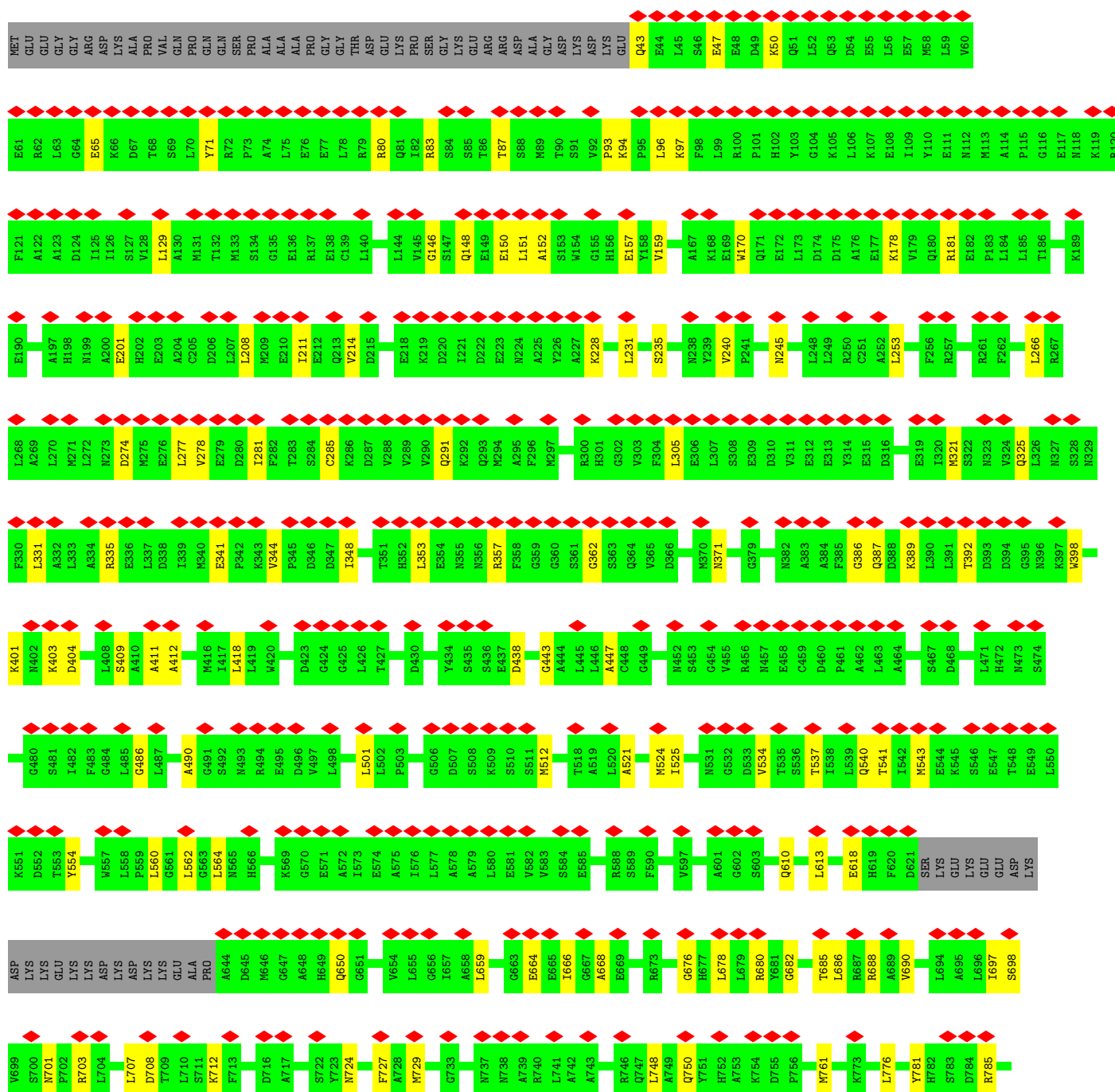
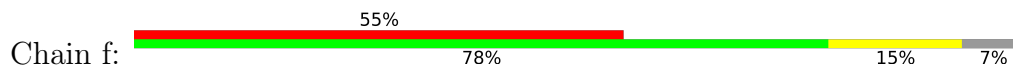
• Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

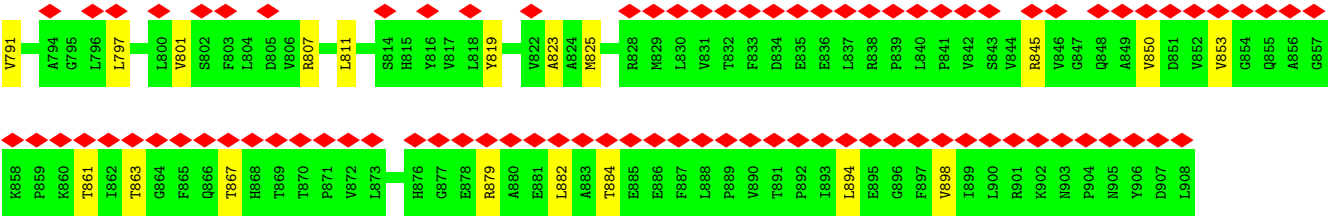


- Molecule 31: 26S proteasome complex subunit SEM1

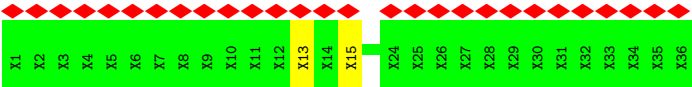
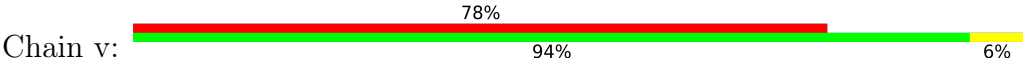


- Molecule 32: 26S proteasome non-ATPase regulatory subunit 2





• Molecule 33: Substrate



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60157	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.022	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00584	Depositor
Map size (Å)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/3283	0.65	1/4433 (0.0%)
2	B	0.21	0/3254	0.56	0/4388
3	C	0.26	0/3146	0.59	0/4226
4	D	0.25	0/3090	0.56	0/4168
5	E	0.25	0/3145	0.61	2/4233 (0.0%)
6	F	0.28	0/3137	0.60	0/4223
7	G	0.21	0/1901	0.47	0/2572
7	g	0.16	0/1913	0.41	0/2589
8	H	0.18	0/1840	0.50	0/2495
8	h	0.16	0/1844	0.42	0/2497
9	I	0.21	0/1963	0.47	0/2650
9	i	0.18	0/1985	0.48	0/2677
10	J	0.20	0/1887	0.47	0/2553
10	j	0.20	0/1887	0.57	2/2549 (0.1%)
11	K	0.16	0/1841	0.41	0/2486
11	k	0.14	0/1809	0.39	0/2444
12	L	0.14	0/1911	0.40	0/2584
12	l	0.14	0/1896	0.40	0/2565
13	M	0.15	0/1925	0.40	0/2592
13	m	0.13	0/1916	0.39	0/2580
14	N	0.13	0/1548	0.31	0/2097
14	n	0.17	0/1536	0.48	1/2080 (0.0%)
15	O	0.20	0/1672	0.51	1/2267 (0.0%)
15	o	0.17	0/1686	0.41	0/2282
16	P	0.16	0/1616	0.42	0/2180
16	p	0.17	0/1620	0.47	0/2184
17	Q	0.17	0/1621	0.44	2/2194 (0.1%)
17	q	0.14	0/1611	0.41	0/2182
18	R	0.15	0/1590	0.38	0/2147
18	r	0.14	0/1580	0.37	0/2135
19	S	0.16	0/1671	0.43	0/2252
19	s	0.16	0/1680	0.42	0/2264

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.16	0/1716	0.43	0/2323
20	t	0.16	0/1720	0.44	0/2328
21	U	0.18	0/6984	0.49	1/9435 (0.0%)
22	V	0.17	0/3681	0.45	0/4969
23	W	0.16	0/3644	0.44	0/4901
24	X	0.18	0/3381	0.46	0/4558
25	Y	0.16	0/3261	0.46	2/4393 (0.0%)
26	Z	0.22	0/2324	0.60	1/3150 (0.0%)
27	a	0.21	0/3053	0.56	0/4133
28	b	0.20	0/1478	0.55	0/2001
29	c	0.34	1/2302 (0.0%)	0.69	2/3110 (0.1%)
30	d	0.24	0/2162	0.59	1/2919 (0.0%)
31	e	0.27	0/437	0.65	0/595
32	f	0.18	0/6640	0.47	0/8988
All	All	0.20	1/107787 (0.0%)	0.49	16/145571 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	284	LEU	N-CA	5.21	1.49	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	j	220	LEU	CA-C-N	11.01	141.87	120.94
10	j	220	LEU	C-N-CA	11.01	141.87	120.94
21	U	364	VAL	N-CA-C	-6.90	105.77	111.91
30	d	144	MET	N-CA-C	6.45	118.00	110.97
14	n	89	ARG	CB-CG-CD	6.26	125.70	111.30
1	A	208	PRO	N-CA-C	6.02	118.05	110.70
17	Q	23	SER	CA-C-N	5.92	132.85	121.54
17	Q	23	SER	C-N-CA	5.92	132.85	121.54
26	Z	19	VAL	N-CA-C	-5.84	107.17	111.90
15	O	148	GLU	N-CA-C	5.51	117.09	111.14
5	E	35	GLU	N-CA-CB	5.51	119.38	110.40
29	c	211	GLU	CA-C-N	5.16	131.39	121.54
29	c	211	GLU	C-N-CA	5.16	131.39	121.54
5	E	283	ASP	N-CA-C	-5.07	107.65	113.88
25	Y	291	HIS	CA-C-N	5.02	131.13	121.54
25	Y	291	HIS	C-N-CA	5.02	131.13	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3229	0	3261	65	0
2	B	3207	0	3278	55	0
3	C	3105	0	3219	60	0
4	D	3040	0	3076	57	0
5	E	3097	0	3174	68	0
6	F	3098	0	3187	86	0
7	G	1867	0	1867	25	0
7	g	1879	0	1872	15	0
8	H	1801	0	1773	16	0
8	h	1805	0	1798	11	0
9	I	1933	0	1923	18	0
9	i	1955	0	1955	16	0
10	J	1861	0	1846	35	0
10	j	1861	0	1865	22	0
11	K	1813	0	1796	21	0
11	k	1782	0	1766	17	0
12	L	1876	0	1856	15	0
12	l	1861	0	1839	13	0
13	M	1890	0	1880	16	0
13	m	1881	0	1868	13	0
14	N	1521	0	1494	13	0
14	n	1510	0	1483	13	0
15	O	1645	0	1648	11	0
15	o	1659	0	1681	18	0
16	P	1587	0	1598	15	0
16	p	1591	0	1609	23	0
17	Q	1588	0	1584	12	0
17	q	1578	0	1569	18	0
18	R	1559	0	1523	6	0
18	r	1549	0	1506	8	0
19	S	1641	0	1639	12	0
19	s	1650	0	1645	18	0
20	T	1683	0	1662	19	0
20	t	1687	0	1666	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	U	6867	0	6929	93	0
22	V	3612	0	3682	43	0
23	W	3596	0	3713	44	0
24	X	3335	0	3435	36	0
25	Y	3202	0	3204	35	0
26	Z	2281	0	2312	48	0
27	a	2995	0	3012	61	0
28	b	1458	0	1505	32	0
29	c	2260	0	2276	55	0
30	d	2116	0	2146	29	0
31	e	425	0	328	12	0
32	f	6529	0	6541	78	0
33	v	180	0	44	1	0
34	A	31	0	12	0	0
34	B	31	0	12	2	0
34	C	31	0	12	1	0
34	D	31	0	12	5	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
36	E	27	0	12	1	0
37	c	1	0	0	0	0
All	All	106301	0	106593	1256	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 (1256) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:180:ARG:HB2	6:F:181:PRO:HD2	1.37	1.07
1:A:210:LYS:HD2	1:A:336:ARG:HG3	1.61	0.81
6:F:221:LYS:H	6:F:348:LEU:HD13	1.47	0.80
10:J:221:ASN:HD21	10:J:223:GLU:HB3	1.48	0.79
6:F:221:LYS:HD2	6:F:322:PRO:HA	1.66	0.76
6:F:177:VAL:HG13	6:F:180:ARG:HD2	1.67	0.75
6:F:178:ASP:H	6:F:180:ARG:HE	1.35	0.75
10:J:208:LEU:HD22	10:J:220:LEU:HG	1.68	0.74
23:W:425:LEU:HB2	26:Z:247:LYS:HD3	1.69	0.74
29:c:192:LEU:HA	29:c:196:LEU:HB2	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:168:TYR:CD1	6:F:171:ARG:HD3	2.21	0.74
19:s:4:PRO:HB2	20:t:100:ARG:HH21	1.52	0.73
6:F:347:ARG:NH1	6:F:347:ARG:HA	2.03	0.73
21:U:773:PHE:HB2	29:c:177:THR:HB	1.73	0.71
19:S:4:PRO:HB2	20:T:100:ARG:HH21	1.56	0.70
3:C:88:LYS:HG2	3:C:94:LYS:HG2	1.73	0.70
7:G:18:PRO:O	7:G:19:GLU:HB2	1.89	0.70
9:I:53:HIS:CG	9:I:54:LYS:H	2.08	0.70
9:i:143:TYR:HB2	9:i:146:GLN:HE21	1.57	0.70
5:E:281:ARG:HH22	5:E:284:THR:HG22	1.57	0.69
6:F:283:ILE:HD12	6:F:328:VAL:HG22	1.74	0.69
6:F:246:ALA:O	6:F:247:THR:C	2.36	0.69
23:W:401:THR:HG23	23:W:402:ILE:HD12	1.74	0.69
29:c:278:GLN:HB2	29:c:280:PRO:HD2	1.74	0.69
10:j:154:HIS:HB3	11:k:59:MET:HE1	1.74	0.69
3:C:90:HIS:HB2	3:C:91:PRO:HD3	1.75	0.68
6:F:317:LEU:HD21	6:F:347:ARG:HE	1.57	0.68
23:W:377:ARG:O	23:W:381:LEU:HB2	1.92	0.68
23:W:445:LEU:HG	23:W:448:LYS:HE2	1.74	0.68
7:G:21:ARG:HB2	7:G:21:ARG:HH11	1.58	0.68
1:A:240:VAL:HB	1:A:274:PHE:HA	1.76	0.67
6:F:279:ALA:O	6:F:325:GLN:HB3	1.95	0.67
21:U:344:ARG:HD3	21:U:881:PRO:HG3	1.76	0.67
6:F:244:THR:HB	6:F:245:LYS:HE3	1.76	0.67
21:U:821:LYS:HD2	21:U:823:LYS:HE3	1.77	0.66
12:L:176:MET:HE1	13:M:57:LEU:HA	1.76	0.66
20:t:110:MET:HB2	20:t:125:VAL:HB	1.78	0.66
28:b:9:CYS:HB2	28:b:111:ALA:HA	1.77	0.65
6:F:359:GLU:HB2	6:F:385:ALA:HB1	1.79	0.65
24:X:233:TYR:HA	24:X:254:MET:HE1	1.77	0.65
9:I:143:TYR:HB2	9:I:146:GLN:HE21	1.62	0.65
27:a:112:ILE:HD11	27:a:138:VAL:HA	1.78	0.64
6:F:220:PRO:HB3	6:F:348:LEU:HD22	1.78	0.64
9:I:53:HIS:NE2	9:I:55:LEU:HB2	2.12	0.64
3:C:77:VAL:HG11	3:C:88:LYS:HE2	1.79	0.64
32:f:698:SER:HB2	32:f:703:ARG:HH21	1.63	0.64
19:s:148:LEU:HD23	19:s:178:VAL:HG12	1.79	0.64
2:B:49:LEU:HD11	32:f:666:ILE:HG12	1.79	0.64
10:J:52:LYS:HG3	10:J:53:LEU:HG	1.78	0.64
6:F:317:LEU:HD21	6:F:347:ARG:NE	2.12	0.64
29:c:251:LEU:HD11	29:c:283:HIS:O	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:292:GLY:HA2	6:F:295:ARG:HH21	1.63	0.63
21:U:583:MET:HA	21:U:586:VAL:HG12	1.80	0.63
27:a:69:HIS:O	27:a:70:ARG:HD2	1.97	0.63
5:E:145:LEU:HA	5:E:297:ARG:HH22	1.62	0.63
21:U:344:ARG:HH22	21:U:925:VAL:HG13	1.64	0.63
6:F:366:MET:HE2	6:F:384:LEU:HD12	1.81	0.63
27:a:70:ARG:HH21	28:b:17:ARG:HA	1.63	0.63
8:h:77:SER:HB2	8:h:163:MET:HE2	1.80	0.63
6:F:324:THR:O	6:F:325:GLN:HB2	1.98	0.62
22:V:85:ALA:HB2	22:V:93:PHE:HB2	1.80	0.62
19:s:68:ILE:HD11	19:s:92:LEU:HD13	1.81	0.62
27:a:82:HIS:HD2	27:a:85:ARG:HH21	1.48	0.62
22:V:355:ARG:HG3	22:V:358:MET:HE2	1.82	0.62
22:V:343:PRO:O	31:e:43:TRP:NE1	2.33	0.61
10:j:173:GLU:HG2	11:k:57:PRO:HG2	1.81	0.61
30:d:188:LYS:HD2	30:d:221:ASN:HD21	1.65	0.61
7:G:165:ALA:HB3	8:H:56:LEU:HD22	1.81	0.61
15:o:51:ASP:HA	15:o:54:MET:HE2	1.82	0.61
23:W:325:GLY:O	23:W:329:ARG:HB2	2.00	0.61
6:F:180:ARG:HB2	6:F:181:PRO:CD	2.22	0.61
6:F:380:ASN:HB3	6:F:383:GLU:HB2	1.82	0.61
27:a:223:GLU:O	27:a:227:ASN:HB2	2.01	0.61
11:k:202:LEU:O	11:k:206:MET:HB2	2.00	0.61
26:Z:192:THR:HG22	27:a:375:LEU:HG	1.83	0.61
32:f:240:VAL:O	32:f:245:ASN:ND2	2.34	0.61
3:C:269:VAL:HG11	4:D:287:ARG:HH12	1.66	0.60
9:I:180:LYS:NZ	9:I:183:GLU:OE2	2.34	0.60
21:U:803:LYS:HB2	21:U:875:PHE:HB2	1.83	0.60
6:F:168:TYR:HD1	6:F:171:ARG:HD3	1.67	0.60
27:a:193:GLN:HB3	27:a:225:LEU:HD13	1.83	0.60
4:D:355:SER:HB2	4:D:393:ILE:HD11	1.83	0.60
11:K:121:LEU:HD23	11:K:160:GLY:HA3	1.83	0.60
21:U:742:HIS:HB3	21:U:883:ARG:HH21	1.66	0.60
1:A:157:ILE:O	1:A:158:ASP:C	2.44	0.60
2:B:317:ASP:OD2	2:B:346:ARG:NH1	2.34	0.60
14:N:107:GLU:OE1	14:N:110:GLN:NE2	2.35	0.60
14:N:119:MET:HE1	20:T:6:VAL:HB	1.83	0.60
10:J:158:ALA:HB3	11:K:58:LEU:HD21	1.84	0.60
21:U:58:GLN:HB2	21:U:87:LEU:HD12	1.84	0.60
30:d:44:THR:OG1	30:d:47:GLN:NE2	2.35	0.60
16:p:81:GLN:HE21	16:p:114:PRO:HB2	1.65	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:HA	1:A:280:ILE:HG12	1.84	0.60
6:F:347:ARG:HA	6:F:347:ARG:HH11	1.67	0.60
23:W:147:LYS:HE3	23:W:188:GLU:HG3	1.82	0.60
29:c:283:HIS:HD2	29:c:287:HIS:CE1	2.20	0.59
2:B:294:ARG:HE	2:B:309:MET:HE1	1.67	0.59
3:C:215:SER:HA	3:C:249:ASP:HB2	1.83	0.59
21:U:14:GLU:OE2	30:d:73:ARG:NH1	2.35	0.59
14:n:144:ARG:H	14:n:147:MET:HE3	1.67	0.59
21:U:483:LEU:HD11	21:U:781:LEU:HD11	1.85	0.59
27:a:342:ASP:HB2	27:a:344:GLN:CD	2.27	0.59
20:t:27:LEU:HD11	20:t:34:ALA:HB1	1.84	0.59
4:D:267:ILE:O	4:D:271:ALA:HB2	2.03	0.59
4:D:335:LEU:HB3	4:D:336:PRO:HD2	1.84	0.59
14:n:4:MET:HE1	14:n:156:THR:HA	1.83	0.59
1:A:122:VAL:HB	6:F:88:TYR:HB2	1.84	0.59
26:Z:173:GLU:O	26:Z:180:LYS:NZ	2.36	0.59
29:c:209:LYS:HG3	29:c:214:GLN:HE21	1.68	0.59
10:j:212:ARG:HB2	10:j:215:GLN:HG3	1.84	0.59
2:B:47:SER:OG	2:B:241:ASN:OD1	2.20	0.59
3:C:227:GLY:HA2	3:C:230:MET:HE3	1.84	0.59
6:F:229:PRO:HB3	6:F:333:ASN:HD21	1.68	0.59
7:G:202:LEU:HA	7:G:205:VAL:HG12	1.85	0.59
32:f:83:ARG:O	32:f:87:THR:OG1	2.20	0.59
5:E:148:VAL:HG13	5:E:149:ILE:HG13	1.83	0.58
6:F:288:LEU:HB2	6:F:332:THR:HG22	1.85	0.58
32:f:151:LEU:HB3	32:f:159:VAL:HG22	1.85	0.58
28:b:131:LEU:HD22	28:b:136:VAL:HB	1.84	0.58
1:A:317:VAL:HB	1:A:336:ARG:HH22	1.68	0.58
6:F:228:PRO:O	6:F:233:LYS:NZ	2.37	0.58
6:F:203:VAL:HG13	6:F:245:LYS:NZ	2.18	0.58
22:V:397:ARG:HH21	30:d:116:HIS:HB3	1.67	0.58
24:X:255:LEU:HD22	24:X:267:VAL:HG13	1.84	0.58
29:c:145:VAL:HG22	29:c:157:ILE:HA	1.86	0.58
9:i:22:GLU:HG2	9:i:25:MET:HE2	1.84	0.58
6:F:203:VAL:HG13	6:F:245:LYS:HZ2	1.69	0.58
22:V:473:GLN:HA	26:Z:256:GLN:HE22	1.66	0.58
32:f:512:MET:HE1	32:f:554:TYR:HB3	1.86	0.58
2:B:223:ILE:HA	2:B:329:MET:HB2	1.86	0.58
29:c:115:HIS:ND1	29:c:118:PHE:HE1	2.01	0.58
5:E:75:ASN:ND2	6:F:129:ARG:O	2.37	0.58
10:J:221:ASN:ND2	10:J:223:GLU:HB3	2.16	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:231:LEU:HG	25:Y:236:LEU:HD12	1.85	0.58
28:b:108:ARG:NH2	28:b:139:ASP:OD2	2.37	0.58
30:d:61:TRP:HB3	30:d:65:ARG:HH21	1.69	0.58
32:f:357:ARG:HH21	32:f:362:GLY:HA2	1.69	0.58
2:B:223:ILE:HG13	2:B:347:ILE:HG21	1.86	0.57
6:F:178:ASP:N	6:F:180:ARG:HE	2.02	0.57
6:F:198:LEU:HG	6:F:202:ILE:HD12	1.86	0.57
27:a:227:ASN:O	27:a:231:GLN:NE2	2.36	0.57
6:F:357:PRO:O	6:F:362:ARG:NH1	2.37	0.57
21:U:559:ARG:HB3	21:U:562:GLU:HB2	1.85	0.57
28:b:53:THR:HG22	28:b:59:GLU:H	1.69	0.57
13:m:23:VAL:HG12	13:m:27:MET:HE2	1.85	0.57
2:B:204:PRO:HG3	2:B:211:TYR:HE2	1.70	0.57
26:Z:270:VAL:HG13	29:c:281:LYS:HD3	1.85	0.57
3:C:49:ARG:NH1	21:U:639:LEU:O	2.37	0.57
4:D:162:VAL:O	4:D:221:HIS:ND1	2.38	0.57
5:E:166:PRO:C	5:E:168:LYS:H	2.12	0.57
5:E:352:MET:HA	5:E:355:ILE:HD12	1.85	0.57
27:a:249:GLN:HA	27:a:252:LYS:HB2	1.86	0.57
1:A:398:ARG:NH1	2:B:195:GLN:OE1	2.37	0.57
10:J:209:ALA:HB2	10:J:219:ILE:HD12	1.86	0.57
26:Z:216:ALA:HB1	27:a:343:LEU:HD21	1.86	0.57
15:O:164:PHE:O	19:s:38:ARG:NH2	2.36	0.57
26:Z:212:LEU:HA	26:Z:215:VAL:HG12	1.85	0.57
1:A:112:ILE:HG12	1:A:122:VAL:HG22	1.87	0.57
20:T:110:MET:HB2	20:T:125:VAL:HB	1.86	0.57
10:j:36:ARG:HH21	10:j:157:LYS:HG2	1.70	0.57
11:k:52:LYS:HE3	11:k:54:ILE:HD11	1.86	0.57
2:B:177:GLU:HG2	2:B:178:LYS:HG2	1.85	0.57
16:P:65:GLN:OE1	17:Q:86:ARG:NH2	2.36	0.57
21:U:697:GLN:NE2	21:U:744:VAL:O	2.38	0.57
21:U:906:LEU:HD13	21:U:912:ILE:HD13	1.86	0.57
29:c:279:ASP:N	29:c:280:PRO:HD2	2.19	0.57
30:d:19:CYS:SG	30:d:65:ARG:NH2	2.78	0.57
3:C:87:VAL:HG12	3:C:89:VAL:H	1.70	0.56
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.87	0.56
9:I:54:LYS:HG3	9:I:55:LEU:HD12	1.86	0.56
10:J:66:ASP:OD2	10:J:95:ARG:NH2	2.37	0.56
17:Q:4:LEU:HD22	17:Q:45:LEU:HD23	1.86	0.56
28:b:161:ASN:HB2	28:b:165:GLY:HA3	1.87	0.56
29:c:46:ARG:HH21	29:c:147:PRO:HB2	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:68:ASN:OD1	13:m:224:HIS:ND1	2.38	0.56
1:A:398:ARG:NH2	2:B:196:GLU:OE2	2.37	0.56
2:B:409:GLU:OE2	2:B:411:ARG:NH2	2.37	0.56
3:C:141:GLU:O	3:C:142:LYS:C	2.47	0.56
5:E:199:VAL:HG13	5:E:201:SER:H	1.71	0.56
8:H:148:GLN:OE1	8:H:158:TRP:NE1	2.35	0.56
23:W:284:SER:O	23:W:288:HIS:ND1	2.34	0.56
25:Y:239:LYS:HG3	25:Y:240:VAL:HG13	1.87	0.56
27:a:135:ILE:HG12	27:a:158:LEU:HD13	1.87	0.56
30:d:47:GLN:HA	30:d:50:LEU:HG	1.86	0.56
11:k:141:LEU:HB2	11:k:156:MET:HE3	1.87	0.56
13:m:34:SER:OG	13:m:65:ARG:NH1	2.38	0.56
3:C:217:SER:OG	4:D:248:ARG:NH2	2.37	0.56
7:G:80:MET:HE1	7:G:138:MET:HG3	1.86	0.56
19:S:198:VAL:HG22	19:S:203:ILE:HG12	1.87	0.56
32:f:96:LEU:HD13	32:f:129:LEU:HD13	1.87	0.56
9:i:119:GLN:NE2	10:j:79:ASP:OD1	2.38	0.56
16:p:88:MET:HE2	16:p:130:PRO:HB2	1.87	0.56
2:B:122:ILE:HD11	2:B:130:GLU:HB3	1.87	0.56
5:E:281:ARG:NH2	5:E:283:ASP:HB2	2.21	0.56
5:E:175:PRO:HB2	5:E:303:LEU:HD21	1.87	0.56
9:I:53:HIS:CG	9:I:54:LYS:N	2.74	0.56
7:g:73:THR:HG23	7:g:75:ASN:H	1.71	0.56
3:C:80:MET:HE1	3:C:86:LEU:HB2	1.87	0.56
32:f:47:GLU:HA	32:f:50:LYS:HE2	1.87	0.56
2:B:74:MET:HG3	32:f:613:LEU:HD23	1.86	0.56
3:C:99:VAL:HG12	3:C:123:LEU:HD12	1.88	0.56
6:F:180:ARG:CB	6:F:181:PRO:HD2	2.23	0.56
21:U:922:GLU:HG2	21:U:923:GLU:HG2	1.88	0.56
23:W:174:TYR:O	23:W:182:ARG:NH2	2.39	0.56
4:D:249:ASP:OD1	4:D:252:ARG:NH2	2.38	0.56
11:K:236:GLU:HA	11:K:239:LYS:HE3	1.88	0.56
12:L:44:ALA:HB2	12:L:142:PRO:HB3	1.87	0.56
14:N:84:LYS:HG3	14:N:120:MET:HG2	1.86	0.56
24:X:203:PRO:HB2	24:X:207:GLN:HB2	1.88	0.56
8:h:133:SER:OG	8:h:149:SER:O	2.22	0.56
6:F:178:ASP:H	6:F:180:ARG:NE	2.02	0.56
10:J:157:LYS:HE2	11:K:58:LEU:HD12	1.87	0.56
26:Z:37:GLY:HA2	26:Z:56:VAL:HG12	1.87	0.56
11:k:21:LEU:HB2	11:k:24:VAL:HG22	1.88	0.56
13:M:68:ASN:OD1	13:M:224:HIS:ND1	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:27:LEU:HD11	20:T:34:ALA:HB1	1.88	0.55
21:U:235:LYS:HA	21:U:238:LYS:HD2	1.87	0.55
30:d:125:LYS:HE3	30:d:130:ASN:HB2	1.88	0.55
32:f:371:ASN:ND2	32:f:401:LYS:O	2.39	0.55
9:i:155:ASN:ND2	10:j:77:THR:OG1	2.39	0.55
16:p:35:VAL:HG12	16:p:36:THR:HG23	1.86	0.55
5:E:159:PHE:HB3	5:E:164:ILE:O	2.07	0.55
26:Z:252:LYS:NZ	26:Z:256:GLN:OE1	2.39	0.55
6:F:185:TYR:HB3	6:F:195:ILE:HD13	1.88	0.55
27:a:180:LEU:HD11	27:a:221:VAL:HG21	1.87	0.55
29:c:283:HIS:HD2	29:c:287:HIS:HE1	1.54	0.55
32:f:560:LEU:O	32:f:564:LEU:HB3	2.05	0.55
4:D:237:GLN:HA	5:E:209:GLY:HA3	1.89	0.55
4:D:349:THR:HA	4:D:352:MET:HG2	1.89	0.55
5:E:170:CYS:SG	5:E:171:LEU:N	2.79	0.55
30:d:87:GLU:HA	30:d:89:LEU:HD23	1.87	0.55
11:k:210:LEU:HA	11:k:214:ASN:HD21	1.71	0.55
3:C:41:ASN:OD1	3:C:44:ARG:NH2	2.40	0.55
12:l:72:ILE:HG22	12:l:134:ILE:HG12	1.88	0.55
12:l:189:LYS:NZ	12:l:234:GLU:O	2.40	0.55
15:o:1:THR:N	15:o:168:GLY:O	2.40	0.55
2:B:365:PHE:HB3	2:B:380:LEU:HD13	1.88	0.55
3:C:35:VAL:HG22	4:D:54:LEU:HD21	1.88	0.55
3:C:297:ARG:NH1	4:D:274:ARG:O	2.39	0.55
6:F:346:GLY:O	6:F:347:ARG:C	2.50	0.55
24:X:380:GLN:HB2	25:Y:314:LEU:HA	1.88	0.55
32:f:534:VAL:HG13	32:f:562:LEU:HD11	1.89	0.55
17:q:168:GLN:NE2	17:q:175:LEU:O	2.40	0.55
2:B:375:ALA:HB2	2:B:413:LYS:HB3	1.87	0.55
5:E:305:ASN:HB3	5:E:308:ALA:H	1.71	0.55
21:U:772:TRP:HB3	21:U:775:LEU:HG	1.89	0.55
25:Y:247:LEU:HD12	25:Y:250:LEU:HD11	1.88	0.55
32:f:676:GLY:O	32:f:680:ARG:NH1	2.40	0.55
9:I:72:MET:HG3	9:I:138:GLY:HA3	1.89	0.55
12:L:41:LYS:O	12:L:217:LYS:NZ	2.40	0.55
25:Y:84:LEU:HD13	25:Y:107:LYS:HA	1.89	0.55
32:f:285:CYS:O	32:f:291:GLN:NE2	2.38	0.55
16:p:65:GLN:OE1	17:q:86:ARG:NH2	2.40	0.55
17:q:1:MET:HE1	17:q:133:GLY:HA2	1.89	0.55
13:M:211:LEU:O	13:M:232:ARG:NH2	2.40	0.55
20:T:41:ARG:NH1	20:T:53:ALA:O	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:770:TRP:HA	29:c:179:SER:HB3	1.88	0.55
7:g:191:PHE:HE1	7:g:219:VAL:HG21	1.72	0.55
12:l:55:GLU:HG2	12:l:56:LEU:HG	1.88	0.55
7:G:10:ASP:O	7:G:24:GLN:NE2	2.40	0.54
21:U:580:ARG:NH2	21:U:768:GLN:OE1	2.40	0.54
29:c:113:HIS:HE2	29:c:115:HIS:CD2	2.23	0.54
1:A:261:PHE:O	1:A:265:ARG:NH1	2.41	0.54
6:F:222:GLY:HA3	6:F:347:ARG:HD3	1.87	0.54
24:X:182:ASN:ND2	25:Y:248:GLU:OE2	2.40	0.54
26:Z:144:VAL:O	26:Z:145:HIS:HB2	2.07	0.54
29:c:270:LEU:HA	29:c:273:LYS:HG2	1.88	0.54
5:E:4:PRO:HG2	5:E:7:LYS:HB3	1.89	0.54
21:U:336:GLU:OE2	21:U:417:LYS:NZ	2.39	0.54
21:U:900:TYR:HB3	21:U:914:LEU:HD11	1.89	0.54
32:f:353:LEU:HD11	32:f:750:GLN:HE22	1.72	0.54
12:l:120:THR:O	13:m:129:ARG:NH1	2.41	0.54
1:A:347:ASP:O	1:A:351:ARG:NH2	2.41	0.54
2:B:196:GLU:OE1	2:B:349:ARG:NH1	2.40	0.54
32:f:781:TYR:O	32:f:785:ARG:NH1	2.40	0.54
1:A:35:THR:O	1:A:39:SER:OG	2.26	0.54
3:C:53:ASN:ND2	21:U:642:GLU:O	2.41	0.54
4:D:209:GLY:HA2	34:D:501:ATP:H5'1	1.89	0.54
6:F:275:ALA:O	6:F:281:SER:OG	2.25	0.54
1:A:26:ASP:OD1	32:f:43:GLN:N	2.41	0.54
1:A:51:ASP:OD1	2:B:69:LYS:NZ	2.39	0.54
1:A:68:SER:HB3	3:C:80:MET:HB2	1.89	0.54
1:A:278:ASP:HB2	1:A:319:MET:HE2	1.90	0.54
2:B:332:ASN:HB2	3:C:258:ARG:HH12	1.72	0.54
3:C:305:LEU:HA	3:C:310:ARG:HD2	1.90	0.54
14:N:32:ASP:O	14:N:45:ARG:NH2	2.41	0.54
27:a:118:ILE:O	27:a:122:LYS:HB2	2.08	0.54
1:A:260:LEU:O	1:A:264:ALA:HB2	2.07	0.54
3:C:209:CYS:SG	3:C:210:THR:N	2.80	0.54
5:E:5:ARG:HB3	6:F:36:MET:HE1	1.90	0.54
5:E:198:VAL:HG12	5:E:200:SER:H	1.72	0.54
18:R:166:ARG:NH2	17:q:144:ASP:OD2	2.41	0.54
21:U:693:LEU:HD22	21:U:736:ILE:HG21	1.88	0.54
27:a:284:ARG:HH11	27:a:288:HIS:HB2	1.73	0.54
22:V:476:PHE:HD2	26:Z:256:GLN:HE21	1.54	0.54
24:X:53:LEU:HD22	24:X:69:LEU:HD22	1.90	0.54
10:j:35:VAL:HG11	10:j:190:LEU:HD11	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:13:LEU:HD11	19:s:149:LEU:HD11	1.90	0.53
21:U:373:ASN:HD22	21:U:385:PHE:HD2	1.56	0.53
22:V:228:ARG:HH22	22:V:261:TYR:HB2	1.72	0.53
27:a:324:ILE:HG13	27:a:331:VAL:HG13	1.88	0.53
10:j:116:GLN:NE2	11:k:84:ASP:OD1	2.41	0.53
16:p:159:ASP:OD1	16:p:159:ASP:N	2.41	0.53
2:B:411:ARG:NH1	2:B:413:LYS:O	2.42	0.53
32:f:560:LEU:HD11	32:f:801:VAL:HG21	1.91	0.53
14:n:192:ASP:OD1	14:n:192:ASP:N	2.41	0.53
7:g:60:LEU:HD21	13:m:177:GLU:HG3	1.90	0.53
10:j:140:GLY:O	10:j:213:ARG:NH1	2.40	0.53
15:o:112:SER:HB3	15:o:125:VAL:HG11	1.90	0.53
22:V:285:TRP:CD1	25:Y:385:ARG:HH22	2.27	0.53
27:a:273:GLN:HB3	27:a:310:LEU:HD11	1.90	0.53
31:e:54:ASN:OD1	31:e:57:ARG:NH2	2.42	0.53
5:E:173:TYR:HB2	5:E:282:PRO:HG3	1.89	0.53
14:N:26:ILE:O	20:t:179:ARG:NH1	2.40	0.53
17:Q:151:ILE:HD11	17:Q:155:ARG:HD2	1.90	0.53
29:c:251:LEU:HD21	29:c:284:LEU:HD22	1.90	0.53
1:A:364:VAL:HG12	1:A:404:ALA:HB3	1.91	0.53
11:K:221:GLN:HB2	11:K:224:GLN:HG2	1.89	0.53
22:V:177:ASN:O	22:V:179:LYS:NZ	2.42	0.53
6:F:244:THR:O	6:F:245:LYS:HB2	2.08	0.53
3:C:277:LEU:O	3:C:310:ARG:NH1	2.42	0.53
5:E:226:GLN:NE2	5:E:271:HIS:O	2.42	0.53
7:G:86:ASP:OD1	13:M:120:HIS:NE2	2.39	0.53
7:G:113:MET:HE3	15:O:70:THR:HA	1.90	0.53
32:f:398:TRP:HA	32:f:401:LYS:HD3	1.89	0.53
5:E:36:LEU:HG	6:F:69:MET:HE2	1.90	0.53
6:F:177:VAL:HG13	6:F:180:ARG:CD	2.37	0.53
24:X:402:GLU:HB3	29:c:249:LEU:HD11	1.91	0.53
2:B:194:ILE:HA	2:B:197:ILE:HG22	1.90	0.52
2:B:304:GLU:HG3	2:B:307:ARG:HH21	1.74	0.52
24:X:310:ARG:O	24:X:314:ARG:NE	2.39	0.52
27:a:254:ALA:HA	27:a:261:LEU:HD23	1.90	0.52
27:a:255:TRP:O	27:a:258:GLN:NE2	2.42	0.52
19:s:125:ASP:OD1	19:s:129:SER:N	2.43	0.52
3:C:130:LYS:HB3	3:C:131:VAL:HG23	1.90	0.52
27:a:81:LEU:HA	27:a:84:VAL:HG12	1.91	0.52
10:j:146:GLN:NE2	10:j:147:THR:O	2.42	0.52
1:A:48:VAL:HG11	2:B:65:LEU:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:142:PHE:HB3	25:Y:146:ARG:HH21	1.73	0.52
17:q:44:LEU:HD11	17:q:102:LEU:HD23	1.90	0.52
10:J:64:ALA:HA	10:J:70:CYS:HA	1.91	0.52
20:T:43:MET:HG3	20:T:64:LYS:HG3	1.92	0.52
21:U:99:THR:HG22	21:U:103:LYS:HE2	1.90	0.52
21:U:524:LYS:HA	21:U:556:MET:HE1	1.91	0.52
22:V:337:LEU:HD21	22:V:364:THR:HG23	1.91	0.52
27:a:35:HIS:NE2	28:b:14:GLU:O	2.43	0.52
29:c:58:LEU:HB3	29:c:71:ASP:HB3	1.91	0.52
11:k:41:GLN:NE2	11:k:151:PRO:O	2.43	0.52
4:D:168:GLY:O	34:D:501:ATP:N6	2.42	0.52
5:E:153:LEU:HD12	5:E:154:THR:HG23	1.92	0.52
7:G:155:ASP:OD1	7:G:159:TYR:N	2.38	0.52
15:O:140:ASP:OD2	20:t:171:ARG:NH2	2.41	0.52
24:X:407:MET:HA	24:X:410:VAL:HG22	1.90	0.52
25:Y:69:LEU:O	25:Y:73:MET:HB2	2.10	0.52
13:m:229:LYS:NZ	13:m:233:GLU:OE2	2.38	0.52
5:E:97:ARG:NH1	5:E:114:GLU:OE1	2.42	0.52
15:O:21:THR:HG22	15:O:26:VAL:HA	1.91	0.52
19:S:38:ARG:NH2	15:o:164:PHE:O	2.43	0.52
20:T:174:ARG:NH1	20:T:206:GLU:O	2.42	0.52
22:V:92:ARG:HA	22:V:95:LEU:HD12	1.91	0.52
25:Y:25:LEU:HD11	25:Y:284:LYS:HZ2	1.74	0.52
28:b:153:LEU:HD23	28:b:170:LEU:HD11	1.90	0.52
32:f:650:GLN:HB3	32:f:686:LEU:HD13	1.90	0.52
6:F:225:MET:HA	6:F:352:ILE:HB	1.90	0.52
9:I:53:HIS:CE1	9:I:55:LEU:H	2.28	0.52
22:V:76:LYS:HE3	22:V:149:PRO:HB3	1.92	0.52
27:a:257:GLN:HB3	27:a:261:LEU:HD22	1.92	0.52
29:c:279:ASP:O	29:c:280:PRO:C	2.52	0.52
32:f:618:GLU:O	32:f:650:GLN:NE2	2.42	0.52
10:j:45:VAL:HG21	10:j:61:LYS:HD2	1.90	0.52
20:t:27:LEU:HD22	20:t:184:TYR:HB2	1.92	0.52
21:U:185:MET:HE1	21:U:222:PHE:HE2	1.74	0.52
27:a:70:ARG:O	28:b:17:ARG:NH1	2.43	0.52
29:c:234:TYR:O	29:c:235:SER:C	2.53	0.52
7:g:170:VAL:HG13	7:g:171:LYS:HG2	1.92	0.52
9:i:119:GLN:HG3	10:j:78:ALA:HB1	1.92	0.52
20:t:25:ASP:OD1	20:t:41:ARG:NH2	2.40	0.52
1:A:193:THR:HA	1:A:197:HIS:HB2	1.92	0.52
12:L:84:LEU:HD22	12:L:112:ILE:HD11	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:100:LEU:HB3	15:O:111:TYR:HB2	1.92	0.52
19:S:27:THR:HB	19:S:40:SER:H	1.74	0.52
25:Y:231:LEU:HD21	25:Y:239:LYS:HZ1	1.75	0.52
16:p:12:MET:HE3	16:p:171:MET:HG2	1.92	0.52
2:B:74:MET:SD	32:f:610:GLN:NE2	2.83	0.52
3:C:127:LEU:HB3	3:C:128:PRO:HD2	1.92	0.52
5:E:84:ARG:H	5:E:87:LEU:HD23	1.76	0.52
10:J:232:ILE:HG22	10:J:236:LYS:HE2	1.91	0.52
22:V:289:LEU:HB3	22:V:312:ALA:HB2	1.92	0.52
25:Y:336:ARG:NH1	31:e:49:GLU:OE2	2.43	0.52
30:d:8:GLU:HB2	30:d:18:LYS:HD2	1.92	0.52
21:U:792:ASN:HB3	21:U:914:LEU:H	1.75	0.51
22:V:213:TYR:HA	22:V:216:ARG:HG2	1.93	0.51
29:c:283:HIS:CD2	29:c:287:HIS:CE1	2.98	0.51
7:g:123:GLN:NE2	8:h:82:ASP:OD1	2.43	0.51
5:E:246:GLY:HA3	5:E:250:ASP:HB2	1.92	0.51
6:F:438:TYR:OH	11:K:19:GLY:O	2.28	0.51
16:P:142:CYS:HB2	16:P:145:GLN:HE21	1.76	0.51
28:b:8:VAL:HA	28:b:110:ILE:HG13	1.92	0.51
28:b:24:THR:HG22	28:b:26:LEU:H	1.76	0.51
29:c:231:LEU:HD21	29:c:305:ASP:OD2	2.09	0.51
10:j:79:ASP:HB3	10:j:127:PHE:HD1	1.74	0.51
10:j:158:ALA:HB3	11:k:58:LEU:HD21	1.92	0.51
8:H:177:ARG:NH1	24:X:202:CYS:SG	2.83	0.51
21:U:804:SER:HA	21:U:892:LEU:HA	1.92	0.51
23:W:314:LEU:HD12	27:a:309:LEU:HG	1.92	0.51
26:Z:21:ASP:OD1	26:Z:22:HIS:N	2.43	0.51
15:o:63:LEU:HD11	15:o:79:ALA:HB2	1.91	0.51
5:E:281:ARG:C	5:E:281:ARG:HD2	2.35	0.51
21:U:494:TYR:HD1	21:U:516:LEU:HD11	1.74	0.51
26:Z:78:MET:HE2	29:c:98:MET:HE2	1.92	0.51
15:o:22:GLU:HG2	15:o:27:ALA:HB2	1.92	0.51
4:D:231:VAL:HG13	5:E:262:ASN:HD22	1.75	0.51
6:F:94:ILE:HD12	6:F:123:VAL:HG12	1.91	0.51
8:H:213:CYS:HB2	8:H:218:PHE:HD1	1.75	0.51
15:O:22:GLU:HG2	15:O:27:ALA:HB2	1.91	0.51
30:d:200:PHE:HB3	30:d:203:PRO:HG3	1.91	0.51
32:f:850:VAL:HG21	32:f:863:THR:HG23	1.92	0.51
19:s:198:VAL:HG22	19:s:203:ILE:HG12	1.93	0.51
2:B:253:SER:N	3:C:275:GLU:OE2	2.43	0.51
5:E:215:ILE:HD13	5:E:260:LEU:HB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:35:VAL:HG12	16:P:36:THR:HG23	1.91	0.51
19:s:16:ALA:HB2	19:s:121:VAL:HG23	1.93	0.51
20:t:99:ARG:NH1	20:t:104:ASN:O	2.44	0.51
34:D:501:ATP:O1G	5:E:294:ARG:NH2	2.41	0.51
29:c:174:PRO:O	29:c:176:GLN:NE2	2.44	0.51
29:c:251:LEU:HD12	29:c:283:HIS:CE1	2.46	0.51
29:c:285:GLU:HA	29:c:288:VAL:HB	1.91	0.51
10:J:7:ILE:HG13	10:J:8:THR:HG23	1.92	0.51
24:X:154:LEU:HD11	24:X:170:GLN:HE21	1.74	0.51
27:a:77:VAL:HA	27:a:80:ILE:HG22	1.93	0.51
10:j:71:MET:HE1	10:j:73:PHE:HB3	1.92	0.51
19:s:27:THR:HB	19:s:40:SER:H	1.74	0.51
6:F:347:ARG:C	6:F:347:ARG:HD3	2.34	0.51
20:T:157:GLN:NE2	20:T:164:GLU:OE1	2.43	0.51
21:U:217:CYS:O	21:U:754:HIS:NE2	2.44	0.51
26:Z:13:PRO:HG2	29:c:221:HIS:HD2	1.76	0.51
29:c:162:LEU:HD12	29:c:200:TYR:HB3	1.93	0.51
16:p:143:ALA:HA	16:p:146:MET:HE2	1.93	0.51
8:H:166:ASN:OD1	8:H:169:ASN:ND2	2.44	0.50
17:Q:83:PHE:O	17:Q:87:ASN:ND2	2.44	0.50
1:A:245:LEU:HD11	1:A:298:THR:HG21	1.91	0.50
3:C:399:MET:HE3	3:C:403:LYS:HD3	1.93	0.50
9:I:46:ALA:HB1	9:I:197:LEU:HD11	1.94	0.50
10:J:87:ALA:HB1	10:J:107:ILE:HD11	1.93	0.50
12:L:166:GLN:OE1	12:L:169:ARG:NH2	2.34	0.50
23:W:429:SER:OG	29:c:233:ASP:HB2	2.11	0.50
9:i:175:LEU:O	9:i:179:TYR:HB2	2.10	0.50
1:A:80:LEU:O	1:A:85:GLN:NE2	2.45	0.50
3:C:82:LYS:HD2	3:C:83:LYS:HG3	1.94	0.50
5:E:288:ALA:O	5:E:294:ARG:NH1	2.43	0.50
20:T:25:ASP:OD1	20:T:41:ARG:NH2	2.36	0.50
32:f:65:GLU:O	32:f:71:TYR:OH	2.29	0.50
12:l:33:SER:OG	12:l:62:LYS:NZ	2.35	0.50
10:J:196:LEU:HA	10:J:199:VAL:HG12	1.94	0.50
32:f:682:GLY:HA3	32:f:686:LEU:HD23	1.93	0.50
9:i:46:ALA:HB1	9:i:197:LEU:HD11	1.93	0.50
1:A:160:THR:OG1	1:A:161:VAL:N	2.44	0.50
19:S:125:ASP:OD1	19:S:129:SER:N	2.44	0.50
21:U:160:LEU:HD12	21:U:200:VAL:HG21	1.92	0.50
5:E:329:GLU:OE2	5:E:333:LYS:NZ	2.40	0.50
9:i:53:HIS:HB3	9:i:56:LEU:HD23	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:93:LEU:HD21	19:s:73:LYS:HD2	1.93	0.50
14:n:1:THR:N	14:n:130:SER:OG	2.44	0.50
19:s:211:ARG:NH2	19:s:213:ASP:OD2	2.43	0.50
5:E:148:VAL:HG22	5:E:169:GLY:H	1.77	0.50
29:c:63:ASP:OD1	29:c:66:THR:OG1	2.27	0.50
30:d:25:ARG:HA	30:d:28:LEU:HG	1.93	0.50
32:f:412:ALA:HA	32:f:447:ALA:HB2	1.93	0.50
14:n:93:ASP:N	14:n:93:ASP:OD1	2.43	0.50
5:E:205:ASP:OD1	5:E:205:ASP:N	2.45	0.50
6:F:317:LEU:HD11	6:F:328:VAL:HG21	1.93	0.50
7:G:165:ALA:HB1	7:G:179:LEU:HD13	1.94	0.50
16:P:138:VAL:HG11	16:P:146:MET:HB3	1.94	0.50
20:T:108:ASN:HB3	20:T:110:MET:HE3	1.94	0.50
21:U:505:ASP:HB3	21:U:508:THR:HG22	1.92	0.50
22:V:406:GLY:HA2	22:V:409:MET:HE2	1.94	0.50
4:D:202:VAL:HA	4:D:329:ARG:HB2	1.93	0.50
6:F:347:ARG:HA	6:F:347:ARG:CZ	2.41	0.50
26:Z:63:LYS:O	28:b:91:ARG:NH2	2.43	0.50
16:P:34:MET:O	18:r:166:ARG:NH1	2.44	0.49
21:U:470:ASN:OD1	21:U:471:ASP:N	2.45	0.49
22:V:209:LYS:HE2	22:V:213:TYR:CE1	2.47	0.49
30:d:234:ASP:HB3	30:d:237:ILE:HG12	1.94	0.49
32:f:146:GLY:O	32:f:148:GLN:NE2	2.45	0.49
13:m:42:LYS:HE2	13:m:183:GLU:HA	1.94	0.49
1:A:164:MET:HE2	1:A:238:ILE:HA	1.94	0.49
21:U:894:MET:HG3	21:U:902:PRO:HD3	1.94	0.49
26:Z:32:GLN:HE22	26:Z:34:ARG:HD2	1.78	0.49
26:Z:145:HIS:HB3	26:Z:149:THR:OG1	2.12	0.49
30:d:78:LEU:HD13	30:d:98:LEU:HD21	1.94	0.49
11:k:148:GLU:OE2	19:s:81:LYS:NZ	2.43	0.49
17:q:26:VAL:HG11	18:r:136:TYR:HE2	1.76	0.49
5:E:264:MET:HG3	5:E:275:MET:HE2	1.93	0.49
6:F:124:ILE:HD11	6:F:160:ILE:HD11	1.93	0.49
6:F:227:GLY:HA3	6:F:354:PHE:HB2	1.93	0.49
13:M:37:ILE:HD11	13:M:193:VAL:HG13	1.94	0.49
25:Y:328:GLU:OE2	31:e:62:LYS:NZ	2.40	0.49
26:Z:130:ASP:OD1	26:Z:130:ASP:N	2.43	0.49
32:f:274:ASP:HB3	32:f:277:LEU:HB2	1.94	0.49
20:T:9:THR:OG1	20:T:10:SER:N	2.45	0.49
27:a:137:ASP:HA	27:a:140:GLU:HG2	1.94	0.49
27:a:138:VAL:HG11	27:a:155:PHE:HB2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:68:LYS:HD3	17:Q:74:GLU:HG2	1.95	0.49
24:X:223:LYS:HD2	24:X:224:ASP:HB2	1.95	0.49
27:a:252:LYS:HA	27:a:255:TRP:HE3	1.77	0.49
32:f:178:LYS:HD2	32:f:181:ARG:HD2	1.94	0.49
2:B:191:ASP:HA	2:B:194:ILE:HG22	1.94	0.49
2:B:195:GLN:NE2	2:B:199:GLU:OE2	2.46	0.49
6:F:209:LYS:HB3	6:F:324:THR:HG21	1.95	0.49
9:I:136:TYR:HB2	9:I:148:TYR:HB2	1.95	0.49
16:P:203:ARG:NH2	16:P:205:ASP:OD2	2.45	0.49
23:W:26:GLN:NE2	23:W:30:GLU:OE2	2.45	0.49
23:W:363:ILE:HD11	23:W:382:LEU:HD11	1.94	0.49
32:f:331:LEU:HG	32:f:335:ARG:HE	1.77	0.49
20:t:43:MET:HE3	20:t:45:VAL:HG22	1.95	0.49
3:C:185:GLY:HA3	3:C:311:ILE:HA	1.93	0.49
4:D:57:GLN:HA	4:D:60:TYR:CE1	2.47	0.49
29:c:230:THR:O	29:c:231:LEU:HD13	2.13	0.49
3:C:254:ILE:HG13	3:C:273:MET:HB2	1.95	0.49
6:F:221:LYS:HE2	6:F:320:PHE:HE2	1.78	0.49
14:n:1:THR:OG1	14:n:33:LYS:NZ	2.46	0.49
1:A:371:GLU:OE2	11:K:204:GLN:NE2	2.46	0.49
3:C:161:ILE:HA	3:C:164:VAL:HG12	1.94	0.49
5:E:15:LYS:HB3	6:F:48:LEU:HD13	1.94	0.49
22:V:58:ALA:O	22:V:62:HIS:ND1	2.43	0.49
23:W:100:ALA:O	23:W:104:MET:HG2	2.12	0.49
1:A:272:ILE:HG12	1:A:315:ILE:HG21	1.95	0.48
4:D:156:SER:O	4:D:158:GLN:HG2	2.13	0.48
5:E:98:VAL:HA	5:E:110:TYR:HA	1.94	0.48
5:E:121:ASN:CG	6:F:311:LEU:HD12	2.38	0.48
7:G:205:VAL:HG13	7:G:206:LEU:HD12	1.95	0.48
9:I:41:ASP:N	9:I:41:ASP:OD1	2.45	0.48
10:J:221:ASN:O	10:J:224:GLU:HG2	2.13	0.48
14:N:191:GLY:O	14:N:196:LYS:NZ	2.46	0.48
21:U:521:LEU:HD11	21:U:757:MET:HE2	1.94	0.48
19:s:145:LEU:HD21	19:s:182:ALA:HB2	1.93	0.48
20:t:25:ASP:HA	20:t:187:PHE:HA	1.95	0.48
34:B:501:ATP:O1G	3:C:310:ARG:NH2	2.46	0.48
13:M:197:ILE:HG21	13:M:211:LEU:HD13	1.94	0.48
21:U:792:ASN:HB3	21:U:914:LEU:HB3	1.95	0.48
22:V:121:PHE:O	22:V:128:ARG:NH1	2.46	0.48
24:X:157:LEU:HD11	24:X:165:LEU:HD23	1.94	0.48
26:Z:145:HIS:HB2	26:Z:150:PRO:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:212:LEU:HD21	27:a:353:LEU:HD22	1.95	0.48
32:f:325:GLN:H	32:f:325:GLN:CD	2.20	0.48
1:A:89:SER:HA	1:A:93:LEU:HD23	1.94	0.48
2:B:426:VAL:O	2:B:429:LYS:NZ	2.42	0.48
4:D:154:LEU:HD12	4:D:227:PHE:HD2	1.78	0.48
5:E:153:LEU:HD13	5:E:191:LEU:HD22	1.95	0.48
8:H:111:VAL:HG22	8:H:136:ILE:HD12	1.95	0.48
13:M:163:CYS:SG	13:M:164:ALA:N	2.86	0.48
23:W:281:ASN:OD1	23:W:282:GLU:N	2.46	0.48
27:a:342:ASP:HB2	27:a:344:GLN:NE2	2.28	0.48
30:d:92:SER:H	30:d:95:MET:HE3	1.77	0.48
32:f:228:LYS:HA	32:f:231:LEU:HG	1.96	0.48
17:q:39:SER:OG	17:q:40:GLU:N	2.47	0.48
1:A:211:GLY:O	1:A:338:ASP:N	2.45	0.48
1:A:258:ARG:NH2	1:A:305:GLN:OE1	2.45	0.48
2:B:181:GLN:O	2:B:241:ASN:ND2	2.46	0.48
5:E:349:GLU:HA	5:E:352:MET:HG3	1.96	0.48
7:G:123:GLN:NE2	8:H:82:ASP:OD1	2.46	0.48
23:W:45:GLU:HA	23:W:48:LEU:HG	1.94	0.48
23:W:425:LEU:HD23	26:Z:251:LEU:HD23	1.96	0.48
23:W:451:MET:HE2	23:W:454:ASN:HD22	1.78	0.48
1:A:236:CYS:HB3	1:A:270:CYS:HA	1.95	0.48
19:S:185:ARG:NE	16:p:151:GLU:OE2	2.45	0.48
20:T:27:LEU:HD22	20:T:184:TYR:HB2	1.93	0.48
24:X:208:ALA:HB2	24:X:238:GLY:HA3	1.95	0.48
26:Z:206:LEU:HA	26:Z:209:ARG:HB3	1.95	0.48
27:a:321:LYS:HE2	27:a:336:VAL:HG21	1.95	0.48
28:b:157:VAL:HG21	28:b:170:LEU:HB2	1.96	0.48
17:q:47:VAL:HG13	17:q:101:ASN:HB2	1.95	0.48
4:D:370:ILE:HD11	4:D:407:ILE:HD13	1.96	0.48
5:E:15:LYS:O	5:E:19:HIS:ND1	2.45	0.48
9:I:123:GLN:NE2	10:J:125:ARG:O	2.46	0.48
13:M:34:SER:HG	13:M:65:ARG:HH12	1.57	0.48
24:X:80:ILE:HB	24:X:84:LYS:HD2	1.95	0.48
10:j:49:SER:O	10:j:51:ALA:N	2.47	0.48
11:K:185:TYR:HA	11:K:189:MET:HE3	1.96	0.48
27:a:89:ASP:O	27:a:93:ALA:HB2	2.13	0.48
27:a:286:ALA:HA	27:a:289:ARG:HB3	1.94	0.48
28:b:169:HIS:CE1	28:b:187:PRO:HB3	2.49	0.48
18:r:7:LYS:HD2	18:r:109:PRO:HB2	1.94	0.48
21:U:409:GLY:HA3	21:U:445:ALA:HB1	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:294:TYR:O	25:Y:298:GLU:HB2	2.13	0.48
28:b:97:LEU:HD23	28:b:107:MET:HG3	1.94	0.48
20:t:92:LEU:HD12	20:t:112:ILE:HD11	1.96	0.48
19:S:18:GLU:OE2	19:S:118:LYS:NZ	2.46	0.48
26:Z:212:LEU:HD22	27:a:349:MET:HE1	1.94	0.48
29:c:278:GLN:C	29:c:280:PRO:HD2	2.39	0.48
16:p:14:MET:HE3	16:p:158:MET:HE1	1.95	0.48
5:E:116:ASP:N	5:E:116:ASP:OD1	2.47	0.48
11:K:56:SER:HB3	11:K:59:MET:HB2	1.95	0.48
21:U:381:THR:HG22	21:U:412:HIS:HA	1.95	0.48
23:W:432:LEU:HD11	29:c:305:ASP:HB3	1.95	0.48
1:A:49:GLU:HA	1:A:52:ILE:HG22	1.96	0.47
1:A:141:GLY:N	1:A:151:ILE:O	2.41	0.47
3:C:57:ARG:NH2	21:U:643:SER:O	2.45	0.47
21:U:678:ASP:O	21:U:684:ARG:NH1	2.40	0.47
22:V:294:ARG:NH2	22:V:390:GLY:O	2.47	0.47
24:X:90:ARG:HH22	24:X:129:LEU:HD22	1.78	0.47
26:Z:82:PHE:HA	26:Z:85:VAL:HG12	1.96	0.47
26:Z:240:VAL:HG23	26:Z:244:GLU:HG2	1.95	0.47
28:b:14:GLU:N	28:b:82:GLY:O	2.47	0.47
29:c:195:GLY:O	29:c:198:ARG:HG2	2.14	0.47
17:q:4:LEU:HD22	17:q:45:LEU:HD23	1.95	0.47
2:B:298:ASN:OD1	2:B:303:ARG:NH2	2.47	0.47
3:C:128:PRO:O	3:C:129:ASN:C	2.57	0.47
5:E:297:ARG:HE	5:E:299:ILE:HG23	1.78	0.47
21:U:681:ASN:ND2	21:U:723:ASP:OD2	2.48	0.47
23:W:444:HIS:CE1	26:Z:204:LYS:HD2	2.49	0.47
24:X:74:ARG:HH21	24:X:116:TRP:HB3	1.80	0.47
26:Z:187:LEU:HG	29:c:293:THR:HG22	1.96	0.47
27:a:138:VAL:O	27:a:142:LEU:HB2	2.14	0.47
17:Q:44:LEU:HD11	17:Q:102:LEU:HD22	1.96	0.47
23:W:316:ARG:NH1	23:W:383:ASP:OD1	2.47	0.47
32:f:698:SER:OG	32:f:701:ASN:O	2.31	0.47
19:s:48:ASP:OD1	19:s:48:ASP:N	2.47	0.47
1:A:394:MET:HE1	1:A:398:ARG:HH21	1.79	0.47
4:D:148:ASP:HB3	5:E:62:LYS:HD2	1.97	0.47
18:R:100:MET:HE3	18:R:126:PHE:HB2	1.95	0.47
21:U:161:ASP:OD1	21:U:161:ASP:N	2.47	0.47
22:V:349:ARG:HH22	31:e:37:HIS:CE1	2.32	0.47
32:f:150:GLU:HG3	32:f:152:ALA:H	1.80	0.47
32:f:861:THR:HB	32:f:879:ARG:HH11	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:108:LEU:HD22	13:m:147:GLN:HB3	1.95	0.47
5:E:171:LEU:HB2	5:E:295:LEU:HD22	1.96	0.47
5:E:281:ARG:NH1	5:E:283:ASP:H	2.13	0.47
5:E:303:LEU:HB3	5:E:338:PHE:HB3	1.96	0.47
29:c:116:PRO:HA	29:c:146:ASP:OD1	2.14	0.47
32:f:659:LEU:HD13	32:f:797:LEU:HD21	1.97	0.47
11:k:196:LYS:HG3	11:k:241:ILE:HD11	1.96	0.47
20:t:180:ASP:HB3	20:t:183:SER:HB3	1.97	0.47
1:A:407:LYS:HA	1:A:410:LEU:HB2	1.96	0.47
3:C:17:GLY:HA2	3:C:21:ARG:HB2	1.97	0.47
4:D:279:THR:OG1	4:D:282:ASP:OD2	2.31	0.47
10:J:116:GLN:NE2	11:K:83:ALA:O	2.47	0.47
13:M:108:LEU:HD11	13:M:137:LEU:HB3	1.97	0.47
16:P:53:LEU:HG	16:P:107:PRO:HB3	1.96	0.47
21:U:792:ASN:OD1	21:U:793:LYS:N	2.47	0.47
27:a:148:VAL:HG12	27:a:150:SER:H	1.80	0.47
27:a:190:VAL:HA	27:a:193:GLN:HB2	1.97	0.47
7:g:153:LYS:HD3	7:g:163:PHE:HE2	1.79	0.47
11:k:166:ASP:OD2	11:k:187:LYS:NZ	2.48	0.47
1:A:300:LEU:HD23	1:A:303:ILE:HD11	1.97	0.47
2:B:106:PRO:O	2:B:154:HIS:NE2	2.48	0.47
2:B:388:ASP:OD1	2:B:388:ASP:N	2.47	0.47
6:F:52:ILE:HA	6:F:55:MET:HG3	1.96	0.47
8:H:93:LEU:HD13	8:H:113:ARG:HB3	1.97	0.47
18:R:58:LEU:HD12	18:R:61:ARG:HD3	1.96	0.47
21:U:740:GLY:HA3	21:U:744:VAL:HG22	1.97	0.47
21:U:806:CYS:O	21:U:874:ASN:ND2	2.48	0.47
22:V:350:GLN:HB2	22:V:353:LEU:HB3	1.97	0.47
24:X:141:LYS:HE2	24:X:179:ALA:HB1	1.96	0.47
24:X:391:PRO:HB2	24:X:393:VAL:HG12	1.96	0.47
32:f:776:LEU:HD13	32:f:825:MET:HG2	1.96	0.47
9:i:66:TYR:HD2	9:i:87:THR:HG21	1.79	0.47
14:n:179:ILE:HG12	14:n:184:VAL:HG22	1.96	0.47
16:p:47:ASP:OD1	16:p:47:ASP:N	2.48	0.47
16:p:123:SER:HB3	16:p:137:VAL:HB	1.97	0.47
2:B:31:THR:HG23	2:B:32:ARG:HG2	1.97	0.47
2:B:405:MET:HA	2:B:408:ARG:HD3	1.96	0.47
4:D:175:GLN:NE2	4:D:179:GLU:OE2	2.48	0.47
5:E:339:ASN:HB3	5:E:342:ASP:HB2	1.96	0.47
21:U:469:SER:OG	21:U:470:ASN:N	2.48	0.47
22:V:368:ARG:HH22	31:e:46:ASP:HB2	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:e:50:ASP:OD1	31:e:50:ASP:N	2.45	0.47
15:o:17:ASP:OD1	15:o:17:ASP:N	2.48	0.47
17:q:18:ASP:O	17:q:34:LYS:NZ	2.44	0.47
10:J:11:SER:OG	10:J:15:HIS:N	2.46	0.47
19:S:28:ARG:NH2	19:S:213:ASP:OXT	2.43	0.47
23:W:35:ALA:HB2	23:W:43:VAL:HG21	1.97	0.47
30:d:155:LYS:HD3	30:d:171:LEU:HD11	1.96	0.47
20:t:96:MET:HE1	20:t:106:LEU:HD12	1.96	0.47
6:F:317:LEU:CD2	6:F:347:ARG:HG2	2.44	0.47
10:J:220:LEU:HD12	10:J:225:ILE:HG12	1.97	0.47
13:M:204:VAL:HG13	13:M:205:LYS:HG2	1.97	0.47
21:U:541:HIS:HB2	21:U:544:ILE:HG22	1.96	0.47
29:c:97:ASP:HA	29:c:100:LYS:HG2	1.96	0.47
10:j:90:GLU:HG3	10:j:110:TYR:CZ	2.50	0.47
19:S:145:LEU:HD22	19:S:178:VAL:HB	1.96	0.46
21:U:490:ARG:HB3	21:U:493:VAL:HG12	1.97	0.46
28:b:155:ALA:O	28:b:159:THR:OG1	2.24	0.46
1:A:250:VAL:HG12	1:A:297:ARG:HD3	1.97	0.46
1:A:300:LEU:HD13	6:F:173:LYS:HG2	1.96	0.46
5:E:153:LEU:HA	5:E:272:ARG:HH12	1.80	0.46
5:E:212:ALA:HB1	5:E:259:GLU:HG2	1.97	0.46
6:F:246:ALA:O	6:F:248:PHE:N	2.49	0.46
6:F:401:VAL:HG12	6:F:405:MET:HE3	1.97	0.46
10:J:40:ILE:HD11	10:J:210:VAL:HB	1.98	0.46
21:U:389:ASN:HB2	21:U:392:TRP:HB3	1.97	0.46
27:a:277:LEU:HA	27:a:280:MET:HG2	1.96	0.46
32:f:707:LEU:HA	32:f:729:MET:HE1	1.97	0.46
10:j:173:GLU:HG3	11:k:58:LEU:HB2	1.98	0.46
20:t:99:ARG:HD3	20:t:106:LEU:HG	1.98	0.46
2:B:440:LEU:HB2	10:J:77:THR:HG22	1.97	0.46
4:D:158:GLN:O	4:D:159:LYS:C	2.58	0.46
19:S:150:ASP:OD2	16:p:177:ARG:NH2	2.40	0.46
9:i:72:MET:HG3	9:i:138:GLY:HA3	1.97	0.46
13:m:228:PRO:HD2	13:m:231:ILE:HD12	1.96	0.46
1:A:312:ARG:HH11	1:A:312:ARG:HB3	1.80	0.46
4:D:154:LEU:HA	4:D:158:GLN:HG3	1.98	0.46
4:D:229:ARG:NH2	5:E:268:ASP:OD2	2.49	0.46
6:F:336:ASP:OD1	6:F:336:ASP:N	2.48	0.46
9:I:52:ILE:O	9:I:53:HIS:C	2.58	0.46
11:K:118:ASN:OD1	12:L:82:ARG:NH2	2.49	0.46
12:L:139:ASP:N	12:L:139:ASP:OD1	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:67:PHE:HB2	13:M:75:MET:HB3	1.97	0.46
15:O:1:THR:N	15:O:168:GLY:O	2.47	0.46
30:d:23:LEU:O	30:d:27:LYS:HG2	2.16	0.46
19:s:145:LEU:HD22	19:s:178:VAL:HB	1.96	0.46
2:B:305:ILE:HG21	3:C:271:ARG:HH21	1.80	0.46
20:T:91:TRP:HE3	20:T:92:LEU:HD12	1.80	0.46
24:X:373:LYS:HB2	24:X:373:LYS:HE3	1.68	0.46
25:Y:66:ASP:HB3	25:Y:69:LEU:HB3	1.97	0.46
27:a:34:TRP:HB3	27:a:71:VAL:HG22	1.96	0.46
27:a:342:ASP:HB2	27:a:344:GLN:OE1	2.15	0.46
30:d:168:ASP:OD1	30:d:169:ILE:N	2.49	0.46
3:C:47:ALA:HB2	22:V:495:ARG:HH21	1.80	0.46
4:D:154:LEU:HA	4:D:158:GLN:CD	2.41	0.46
6:F:279:ALA:O	6:F:325:GLN:CB	2.63	0.46
23:W:373:ILE:HA	27:a:326:GLU:HB2	1.98	0.46
25:Y:155:ASP:OD1	25:Y:155:ASP:N	2.49	0.46
26:Z:77:ASN:HB2	29:c:98:MET:HE1	1.98	0.46
12:l:165:SER:OG	12:l:169:ARG:NH1	2.49	0.46
3:C:247:PHE:HD1	3:C:292:ILE:HB	1.81	0.46
5:E:181:THR:OG1	36:E:401:ADP:O2A	2.28	0.46
6:F:243:GLN:O	6:F:244:THR:C	2.59	0.46
10:J:80:ALA:HA	10:J:129:ILE:HD13	1.98	0.46
13:M:51:LYS:NZ	13:M:62:SER:O	2.46	0.46
21:U:22:PHE:O	21:U:26:LYS:NZ	2.48	0.46
17:q:151:ILE:HG13	17:q:155:ARG:HG3	1.96	0.46
18:r:41:LEU:HD23	18:r:103:GLY:HA3	1.97	0.46
2:B:182:GLU:OE2	2:B:186:ASP:N	2.48	0.46
10:J:155:ALA:HB3	11:K:63:SER:HB2	1.97	0.46
14:N:9:ASP:OD1	14:N:9:ASP:N	2.47	0.46
22:V:349:ARG:HH12	31:e:37:HIS:HE1	1.62	0.46
29:c:94:LYS:O	29:c:98:MET:HB3	2.15	0.46
32:f:521:ALA:HA	32:f:524:MET:HE2	1.98	0.46
1:A:323:ARG:HD3	1:A:324:PRO:HD2	1.98	0.46
3:C:155:ASP:N	3:C:155:ASP:OD1	2.48	0.46
25:Y:220:VAL:HA	25:Y:223:THR:HG22	1.98	0.46
2:B:381:ASP:OD1	2:B:381:ASP:N	2.49	0.46
3:C:368:MET:HG2	4:D:329:ARG:HH22	1.81	0.46
6:F:180:ARG:O	6:F:181:PRO:C	2.59	0.46
8:H:143:ARG:NH1	8:H:144:PRO:O	2.49	0.46
11:K:41:GLN:NE2	11:K:151:PRO:O	2.49	0.46
15:O:147:GLU:O	15:O:151:ALA:HB2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:210:SER:HB3	25:Y:213:LEU:HD23	1.98	0.46
28:b:33:VAL:HA	28:b:36:VAL:HG12	1.97	0.46
32:f:698:SER:OG	32:f:698:SER:O	2.33	0.46
1:A:158:ASP:O	1:A:159:PRO:C	2.59	0.45
10:J:3:TYR:HD2	10:J:12:PRO:HD3	1.81	0.45
12:L:42:THR:HA	12:L:217:LYS:HZ3	1.81	0.45
17:Q:47:VAL:HG23	17:Q:101:ASN:HB2	1.98	0.45
21:U:78:LEU:HD22	21:U:103:LYS:HB3	1.98	0.45
28:b:149:ASN:OD1	28:b:154:THR:OG1	2.35	0.45
10:J:208:LEU:HD22	10:J:220:LEU:CG	2.44	0.45
21:U:796:LYS:HA	21:U:924:LEU:HD11	1.97	0.45
26:Z:209:ARG:HH21	26:Z:213:GLU:HG3	1.81	0.45
26:Z:258:VAL:HG13	26:Z:262:LEU:HD23	1.98	0.45
27:a:24:ARG:NH1	27:a:40:GLN:OE1	2.50	0.45
28:b:51:LEU:HD23	28:b:71:ILE:HG23	1.98	0.45
32:f:201:GLU:HB2	32:f:228:LYS:NZ	2.32	0.45
1:A:328:ASP:O	1:A:330:ALA:N	2.47	0.45
1:A:347:ASP:OD1	1:A:348:LEU:N	2.45	0.45
7:G:199:ILE:HG23	7:G:210:PHE:HZ	1.82	0.45
16:P:38:ASP:OD1	16:P:38:ASP:N	2.48	0.45
21:U:340:GLN:HG3	21:U:344:ARG:HE	1.81	0.45
22:V:477:HIS:CG	30:d:245:GLN:HE21	2.34	0.45
26:Z:103:LYS:NZ	26:Z:103:LYS:H	2.14	0.45
32:f:688:ARG:O	32:f:724:ASN:ND2	2.36	0.45
7:g:70:PHE:HD2	7:g:91:VAL:HG21	1.80	0.45
3:C:49:ARG:NH2	4:D:64:GLU:OE2	2.50	0.45
4:D:317:LEU:HD13	4:D:321:LEU:HD23	1.98	0.45
4:D:336:PRO:HB3	4:D:344:ILE:HD12	1.97	0.45
5:E:334:LEU:HD22	5:E:368:MET:HE1	1.99	0.45
7:G:21:ARG:HB2	7:G:21:ARG:NH1	2.28	0.45
14:N:4:MET:HE1	14:N:159:ALA:HB3	1.97	0.45
23:W:396:LEU:HD13	23:W:402:ILE:HD13	1.98	0.45
25:Y:80:GLU:HA	25:Y:83:ARG:HG2	1.99	0.45
25:Y:268:TYR:HA	25:Y:271:PHE:HB3	1.98	0.45
12:l:139:ASP:N	12:l:139:ASP:OD1	2.49	0.45
2:B:168:ASP:OD1	2:B:168:ASP:N	2.49	0.45
8:H:205:GLU:HG2	8:H:223:PRO:HB3	1.99	0.45
15:O:211:VAL:HG21	16:P:198:ARG:HD3	1.99	0.45
21:U:751:ARG:HH22	21:U:904:LYS:HD3	1.82	0.45
22:V:103:SER:O	22:V:107:ARG:NH2	2.49	0.45
24:X:143:TYR:HD2	24:X:144:GLN:HG2	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:141:VAL:HG11	25:Y:164:ALA:HB2	1.99	0.45
29:c:189:ILE:HA	29:c:192:LEU:HG	1.98	0.45
32:f:341:GLU:OE2	32:f:387:GLN:NE2	2.49	0.45
32:f:438:ASP:OD1	32:f:438:ASP:N	2.47	0.45
32:f:894:LEU:HA	32:f:898:VAL:HG21	1.98	0.45
5:E:22:ILE:HG23	6:F:55:MET:HE3	1.98	0.45
21:U:756:HIS:CE1	21:U:758:PRO:HD2	2.52	0.45
29:c:195:GLY:O	29:c:196:LEU:C	2.60	0.45
1:A:284:ARG:HH22	2:B:307:ARG:HD3	1.82	0.45
2:B:109:VAL:HB	3:C:94:LYS:HB2	1.99	0.45
4:D:156:SER:O	4:D:158:GLN:N	2.50	0.45
12:L:42:THR:HA	12:L:217:LYS:NZ	2.32	0.45
21:U:799:LYS:HB2	21:U:923:GLU:HB3	1.98	0.45
22:V:476:PHE:CG	26:Z:260:VAL:HG11	2.52	0.45
24:X:281:GLY:H	24:X:284:THR:HG22	1.81	0.45
27:a:65:SER:HA	27:a:68:GLU:HB2	1.99	0.45
30:d:190:LEU:HD22	30:d:192:THR:HG22	1.98	0.45
8:h:203:MET:HE1	8:h:208:ILE:HG21	1.98	0.45
1:A:33:LEU:HD12	2:B:412:MET:HE3	1.97	0.45
3:C:133:PRO:HB2	3:C:135:VAL:HG12	1.98	0.45
6:F:324:THR:O	6:F:325:GLN:CB	2.64	0.45
8:H:44:VAL:HG21	8:H:137:CYS:HB2	1.99	0.45
27:a:73:PRO:HB3	27:a:104:VAL:HG11	1.99	0.45
30:d:98:LEU:HA	30:d:101:LEU:HD12	1.99	0.45
32:f:386:GLY:HA2	32:f:418:LEU:HG	1.97	0.45
32:f:791:VAL:HG12	32:f:823:ALA:HB1	1.98	0.45
12:l:7:ASP:OD1	12:l:7:ASP:N	2.50	0.45
5:E:192:ASP:OD1	5:E:192:ASP:N	2.46	0.45
6:F:178:ASP:H	6:F:180:ARG:HH21	1.64	0.45
7:G:112:ASP:N	7:G:112:ASP:OD1	2.49	0.45
10:J:185:ASP:OD1	10:J:185:ASP:N	2.49	0.45
13:M:65:ARG:HH21	13:M:78:ALA:HA	1.82	0.45
16:P:177:ARG:NH2	19:s:150:ASP:OD2	2.41	0.45
22:V:309:MET:HE1	22:V:331:LEU:HB3	1.99	0.45
22:V:349:ARG:NH2	31:e:39:TRP:O	2.50	0.45
23:W:51:GLU:OE1	23:W:93:ARG:NH1	2.43	0.45
27:a:346:ILE:HA	27:a:349:MET:HG3	1.99	0.45
29:c:114:SER:O	29:c:116:PRO:HD3	2.17	0.45
29:c:283:HIS:CD2	29:c:287:HIS:HE1	2.32	0.45
32:f:253:LEU:HD21	32:f:281:ILE:HD11	1.98	0.45
11:k:13:ASN:HB2	12:l:126:ARG:HD3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:41:LYS:HG3	12:l:42:THR:HG23	1.99	0.45
18:r:127:SER:HB3	18:r:136:TYR:CE1	2.52	0.45
2:B:112:LEU:HD23	2:B:123:VAL:HG12	1.99	0.45
6:F:172:VAL:HB	6:F:175:MET:HE2	1.98	0.45
7:G:43:ARG:HH21	7:G:164:LYS:HG2	1.82	0.45
10:J:169:ARG:O	10:J:173:GLU:HG2	2.17	0.45
21:U:10:SER:HB2	30:d:73:ARG:HG3	2.00	0.45
21:U:196:LYS:HA	21:U:199:ARG:HG2	1.98	0.45
21:U:530:GLU:HA	21:U:533:VAL:HG12	1.98	0.45
22:V:228:ARG:HH21	22:V:258:TYR:HA	1.82	0.45
23:W:97:LEU:HG	23:W:100:ALA:H	1.81	0.45
24:X:126:ARG:O	24:X:130:GLU:HG2	2.17	0.45
32:f:409:SER:O	32:f:819:TYR:OH	2.34	0.45
18:r:35:ILE:N	18:r:43:GLY:O	2.48	0.45
2:B:287:ILE:HG21	2:B:329:MET:SD	2.57	0.44
4:D:159:LYS:HD2	4:D:159:LYS:HA	1.69	0.44
4:D:340:GLN:HG2	4:D:343:LEU:HD12	1.99	0.44
17:Q:148:THR:HG22	17:Q:150:THR:H	1.82	0.44
30:d:114:GLU:HA	30:d:117:THR:HG22	1.99	0.44
1:A:207:GLU:C	1:A:209:PRO:HD3	2.42	0.44
4:D:297:ASP:OD2	4:D:323:ARG:NH2	2.48	0.44
5:E:97:ARG:HH21	5:E:111:LEU:HB3	1.82	0.44
5:E:200:SER:HB2	5:E:232:MET:HE3	1.99	0.44
9:I:53:HIS:CD2	9:I:54:LYS:H	2.33	0.44
12:L:155:ASP:HB3	13:M:62:SER:HB2	1.98	0.44
25:Y:68:ASP:OD1	25:Y:68:ASP:N	2.48	0.44
27:a:168:ASN:OD1	27:a:171:SER:OG	2.35	0.44
2:B:333:ARG:NH1	3:C:258:ARG:O	2.51	0.44
20:T:25:ASP:HA	20:T:187:PHE:HA	2.00	0.44
21:U:501:LEU:HD11	21:U:548:LEU:HD11	1.99	0.44
25:Y:111:LEU:HD23	25:Y:114:ILE:HD11	1.98	0.44
25:Y:312:ARG:HA	25:Y:356:THR:HG22	1.98	0.44
27:a:54:ASP:N	27:a:54:ASP:OD1	2.45	0.44
27:a:247:ARG:HA	27:a:250:THR:HG22	1.98	0.44
29:c:284:LEU:HB3	29:c:285:GLU:H	1.60	0.44
8:h:3:GLU:HB2	13:m:127:ALA:HB3	1.99	0.44
15:o:42:TYR:HB2	15:o:178:ILE:HD11	1.98	0.44
15:o:163:ILE:HG12	15:o:170:GLY:HA2	1.99	0.44
2:B:269:GLU:OE1	2:B:272:ARG:NH2	2.51	0.44
3:C:239:ARG:HH12	3:C:287:LYS:H	1.66	0.44
11:K:31:ILE:HD13	11:K:140:ALA:HB2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:26:MET:SD	20:T:188:GLN:NE2	2.90	0.44
25:Y:42:MET:HA	25:Y:45:VAL:HB	1.99	0.44
25:Y:105:MET:HE1	25:Y:140:ILE:HD11	1.98	0.44
28:b:124:LEU:HD13	28:b:156:PHE:HB2	1.98	0.44
10:j:42:VAL:HG22	10:j:210:VAL:HG22	1.99	0.44
13:m:230:ASP:OD1	13:m:230:ASP:N	2.50	0.44
20:t:51:LEU:HD21	20:t:110:MET:HE1	1.99	0.44
2:B:174:MET:HE2	2:B:250:VAL:HG13	2.00	0.44
3:C:252:ASP:HB3	4:D:290:LEU:HD11	2.00	0.44
10:J:31:THR:OG1	10:J:163:ARG:O	2.33	0.44
21:U:510:GLU:HA	21:U:547:GLY:HA3	1.99	0.44
21:U:805:ASN:OD1	21:U:893:THR:OG1	2.29	0.44
22:V:212:TYR:HA	22:V:253:LEU:HD11	2.00	0.44
3:C:132:ASP:HB3	3:C:137:LEU:HD21	2.00	0.44
6:F:192:ASP:HA	6:F:195:ILE:HD12	1.99	0.44
22:V:323:GLY:HA3	31:e:24:ALA:HA	1.98	0.44
32:f:540:GLN:HG3	32:f:543:MET:HE2	1.99	0.44
11:k:133:MET:SD	11:k:133:MET:N	2.89	0.44
15:o:42:TYR:HE2	15:o:183:LEU:HD21	1.81	0.44
20:t:152:GLU:HG2	20:t:156:LYS:NZ	2.32	0.44
1:A:207:GLU:O	1:A:208:PRO:C	2.61	0.44
14:N:119:MET:HE3	14:N:119:MET:HB2	1.77	0.44
20:T:26:MET:HE2	20:T:26:MET:HB3	1.86	0.44
21:U:641:SER:HB2	21:U:675:MET:HE3	2.00	0.44
32:f:93:PRO:HB2	32:f:96:LEU:HD23	2.00	0.44
32:f:678:LEU:HB3	32:f:690:VAL:HG21	1.98	0.44
16:p:27:ARG:HB2	16:p:183:MET:HB2	2.00	0.44
17:q:31:ASP:OD1	17:q:31:ASP:N	2.51	0.44
4:D:89:ILE:HB	5:E:78:ARG:HB2	2.00	0.44
4:D:148:ASP:HB2	4:D:151:ILE:CG2	2.48	0.44
12:L:159:MET:HE3	12:L:160:SER:H	1.83	0.44
18:R:41:LEU:HD23	18:R:103:GLY:HA3	1.98	0.44
25:Y:376:LEU:HD23	26:Z:265:LEU:HD23	1.98	0.44
26:Z:216:ALA:HA	27:a:343:LEU:HD11	1.99	0.44
27:a:6:GLY:HA2	27:a:9:GLN:HB2	1.99	0.44
28:b:12:ASN:HD22	28:b:78:VAL:HG22	1.83	0.44
28:b:33:VAL:HG11	28:b:75:LEU:HD21	1.99	0.44
29:c:113:HIS:NE2	29:c:115:HIS:CD2	2.86	0.44
16:p:107:PRO:HG2	16:p:124:LEU:HD12	1.98	0.44
16:p:138:VAL:HG11	16:p:146:MET:HB3	1.99	0.44
11:K:88:LEU:HD23	11:K:119:LEU:HD23	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:192:ASP:OD1	14:N:192:ASP:N	2.51	0.44
21:U:906:LEU:HD13	21:U:912:ILE:HG21	2.00	0.44
29:c:176:GLN:HB3	29:c:177:THR:H	1.57	0.44
17:q:81:ALA:HB1	17:q:124:LEU:HD11	2.00	0.44
21:U:360:VAL:HG13	21:U:365:CYS:HB3	1.99	0.43
21:U:403:THR:HG23	21:U:777:HIS:HE1	1.83	0.43
22:V:494:MET:HE3	26:Z:278:ASN:HD22	1.83	0.43
24:X:371:ASP:HB2	24:X:373:LYS:HE2	1.98	0.43
28:b:25:ARG:NH1	28:b:145:GLU:OE1	2.45	0.43
7:g:103:TYR:O	15:o:81:ARG:NH2	2.51	0.43
15:o:70:THR:HG23	15:o:72:ARG:H	1.82	0.43
3:C:338:LEU:HD22	3:C:342:ILE:HD13	2.00	0.43
7:G:49:VAL:HG13	7:G:219:VAL:HG12	2.00	0.43
21:U:12:LEU:HD21	21:U:24:LEU:HG	2.00	0.43
21:U:465:LEU:HD11	21:U:477:GLY:HA3	2.00	0.43
22:V:495:ARG:HB3	26:Z:278:ASN:ND2	2.33	0.43
25:Y:2:PRO:HG2	25:Y:5:ASN:HB2	1.99	0.43
26:Z:123:ILE:HB	26:Z:136:GLU:HB3	1.99	0.43
6:F:168:TYR:O	6:F:171:ARG:HG3	2.17	0.43
11:K:41:GLN:HE21	11:K:151:PRO:HB2	1.83	0.43
14:N:85:GLU:OE2	14:N:89:ARG:NH2	2.49	0.43
18:R:192:VAL:HG11	16:p:205:ASP:HB3	2.01	0.43
21:U:611:ASN:HB3	21:U:614:VAL:HG12	1.99	0.43
22:V:479:ARG:NH1	25:Y:374:ASP:OD1	2.51	0.43
26:Z:103:LYS:HE2	26:Z:103:LYS:HB2	1.75	0.43
26:Z:176:LEU:HD13	26:Z:180:LYS:HA	1.99	0.43
7:g:141:ILE:HG22	7:g:151:VAL:HG22	1.99	0.43
10:j:39:ASP:OD1	10:j:39:ASP:N	2.50	0.43
1:A:285:PHE:HA	1:A:327:LEU:HD11	2.01	0.43
1:A:339:ARG:HH22	6:F:405:MET:HB3	1.84	0.43
4:D:296:MET:HE2	4:D:307:VAL:HG11	2.01	0.43
7:G:18:PRO:O	7:G:19:GLU:CB	2.63	0.43
12:L:45:VAL:HG12	12:L:214:ILE:HG12	2.00	0.43
17:Q:8:GLN:HG3	17:Q:128:PRO:O	2.18	0.43
21:U:415:HIS:CD2	21:U:418:GLU:HB3	2.54	0.43
23:W:344:THR:HG23	23:W:347:GLY:H	1.83	0.43
24:X:226:LYS:HA	24:X:226:LYS:HD2	1.83	0.43
27:a:226:ARG:HH12	27:a:233:LEU:HB3	1.84	0.43
28:b:67:ASP:OD1	28:b:68:THR:N	2.51	0.43
15:o:100:LEU:HB3	15:o:111:TYR:HB2	2.00	0.43
1:A:127:ASP:OD1	1:A:127:ASP:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ASP:O	1:A:160:THR:N	2.52	0.43
4:D:155:THR:HA	4:D:159:LYS:HZ2	1.83	0.43
23:W:48:LEU:HD13	23:W:93:ARG:HH22	1.84	0.43
23:W:425:LEU:HG	29:c:233:ASP:OD1	2.19	0.43
3:C:375:ARG:HG2	3:C:377:HIS:H	1.83	0.43
15:o:216:ILE:HD11	16:p:194:LYS:HD2	2.00	0.43
5:E:166:PRO:C	5:E:168:LYS:N	2.74	0.43
10:J:220:LEU:HD22	10:J:220:LEU:HA	1.82	0.43
28:b:16:MET:HE1	28:b:143:PHE:HE2	1.82	0.43
4:D:248:ARG:HA	4:D:295:GLN:HE22	1.84	0.43
10:J:39:ASP:OD1	10:J:39:ASP:N	2.51	0.43
21:U:265:ILE:O	21:U:269:ARG:NH1	2.52	0.43
24:X:82:LYS:HB3	24:X:124:PHE:HZ	1.83	0.43
31:e:37:HIS:CE1	31:e:39:TRP:HB2	2.53	0.43
32:f:266:LEU:HD11	32:f:278:VAL:HG13	2.00	0.43
12:l:47:VAL:HG12	12:l:195:LEU:HD22	1.99	0.43
5:E:281:ARG:C	5:E:281:ARG:HH11	2.26	0.43
21:U:198:LEU:HD21	21:U:218:GLN:HE21	1.84	0.43
24:X:365:LEU:HB3	24:X:378:LEU:HD21	2.01	0.43
27:a:363:MET:HE1	29:c:307:VAL:HB	2.01	0.43
32:f:486:GLY:HA2	32:f:525:ILE:HD11	2.00	0.43
7:g:58:ASP:OD1	7:g:58:ASP:N	2.52	0.43
3:C:339:THR:HG23	25:Y:174:TRP:HZ3	1.84	0.43
5:E:385:ASP:OD1	5:E:385:ASP:N	2.52	0.43
6:F:317:LEU:HD23	6:F:347:ARG:HG2	2.01	0.43
10:J:4:ASP:OD1	10:J:4:ASP:N	2.52	0.43
21:U:325:MET:HA	21:U:328:ILE:HG12	2.01	0.43
26:Z:62:ASP:N	26:Z:62:ASP:OD1	2.51	0.43
28:b:90:ILE:HD12	28:b:156:PHE:HZ	1.84	0.43
17:q:38:MET:HG2	17:q:61:GLN:HA	2.01	0.43
1:A:99:THR:HG21	1:A:115:VAL:HG22	2.01	0.42
34:B:501:ATP:H5'1	3:C:307:ARG:HH12	1.84	0.42
3:C:66:LEU:HD21	4:D:116:LEU:HG	2.00	0.42
5:E:101:ASP:HB3	5:E:105:LEU:H	1.84	0.42
5:E:159:PHE:O	5:E:164:ILE:N	2.52	0.42
6:F:347:ARG:O	6:F:348:LEU:C	2.62	0.42
7:G:58:ASP:OD1	7:G:58:ASP:N	2.49	0.42
22:V:240:LEU:HD12	22:V:241:ARG:HG3	1.99	0.42
22:V:419:LEU:HD12	22:V:456:GLY:HA2	2.00	0.42
27:a:106:SER:OG	27:a:107:SER:N	2.52	0.42
32:f:305:LEU:H	32:f:321:MET:HE1	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:49:GLU:HA	8:h:208:ILE:HG22	2.01	0.42
10:j:38:ARG:NH2	10:j:182:GLU:O	2.52	0.42
3:C:217:SER:OG	4:D:291:GLU:OE1	2.34	0.42
6:F:97:LEU:HB2	6:F:121:CYS:HB2	2.01	0.42
20:T:20:VAL:HG11	20:T:122:LEU:HD13	2.01	0.42
24:X:107:VAL:HG12	24:X:111:LEU:HD23	2.01	0.42
24:X:365:LEU:HA	24:X:368:MET:HE2	2.01	0.42
7:g:112:ASP:OD1	7:g:112:ASP:N	2.51	0.42
12:l:66:VAL:HG11	12:l:88:MET:HE2	2.00	0.42
20:t:122:LEU:HG	20:t:137:LEU:HD12	2.01	0.42
2:B:257:GLN:HB2	2:B:262:ASP:HB3	2.02	0.42
4:D:51:LEU:HA	4:D:54:LEU:HG	2.00	0.42
4:D:167:ILE:HG12	4:D:214:MET:HE1	2.01	0.42
10:J:189:LYS:HA	10:J:232:ILE:HD11	2.01	0.42
12:L:47:VAL:HG12	12:L:195:LEU:HD22	2.00	0.42
16:P:159:ASP:OD1	16:P:159:ASP:N	2.53	0.42
13:m:8:ASP:O	13:m:22:GLN:NE2	2.45	0.42
13:m:37:ILE:HD11	13:m:193:VAL:HG13	2.01	0.42
18:r:139:MET:O	18:r:143:TYR:HB2	2.19	0.42
1:A:161:VAL:O	1:A:165:GLN:HB2	2.20	0.42
1:A:165:GLN:HG3	1:A:236:CYS:HB2	2.02	0.42
5:E:317:ALA:HA	5:E:320:ILE:HD12	2.00	0.42
7:G:137:CYS:SG	7:G:138:MET:N	2.92	0.42
8:H:39:LYS:HA	8:H:44:VAL:HG12	2.02	0.42
12:L:204:ASP:OD1	12:L:204:ASP:N	2.52	0.42
13:M:45:VAL:HG23	13:M:146:ALA:HB1	2.01	0.42
16:P:14:MET:HE3	16:P:154:TRP:HD1	1.85	0.42
19:S:43:CYS:H	19:S:194:ARG:HH21	1.67	0.42
22:V:76:LYS:HB2	22:V:147:PHE:HZ	1.84	0.42
23:W:359:VAL:HG23	23:W:382:LEU:HD22	2.01	0.42
25:Y:112:CYS:HB2	25:Y:147:ILE:HD11	2.01	0.42
30:d:139:LEU:HD11	30:d:151:VAL:HG13	2.01	0.42
3:C:86:LEU:HD21	3:C:94:LYS:HB3	2.01	0.42
3:C:187:LEU:HA	3:C:293:MET:HB2	2.01	0.42
16:P:125:ASP:OD1	16:P:129:CYS:N	2.39	0.42
21:U:31:VAL:HG23	21:U:38:ILE:HD11	2.02	0.42
23:W:260:SER:HA	23:W:263:TRP:NE1	2.34	0.42
24:X:344:ARG:HG3	24:X:386:ILE:HG12	2.00	0.42
28:b:131:LEU:O	28:b:135:LYS:N	2.49	0.42
32:f:537:THR:O	32:f:541:THR:OG1	2.34	0.42
7:g:23:TYR:HA	7:g:26:GLU:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:14:SER:HB3	8:h:18:LYS:H	1.84	0.42
16:p:193:ASP:OD1	16:p:193:ASP:N	2.52	0.42
20:t:147:GLN:HE21	20:t:147:GLN:HB3	1.69	0.42
5:E:232:MET:HG3	5:E:235:ILE:HG22	2.02	0.42
21:U:376:MET:HA	21:U:739:ALA:HA	2.01	0.42
23:W:179:LYS:HD2	23:W:182:ARG:HH11	1.84	0.42
25:Y:38:ARG:HG2	25:Y:42:MET:HE1	2.02	0.42
32:f:411:ALA:HB3	32:f:443:GLY:HA3	2.02	0.42
16:p:53:LEU:HG	16:p:107:PRO:HB3	2.01	0.42
18:r:97:MET:HB3	18:r:116:SER:HB2	2.00	0.42
20:t:69:GLN:HA	20:t:72:ILE:HG22	2.02	0.42
1:A:259:GLU:O	1:A:263:MET:HG3	2.19	0.42
3:C:113:ARG:NE	3:C:130:LYS:O	2.48	0.42
4:D:204:MET:HE3	4:D:310:ALA:HB2	2.02	0.42
5:E:164:ILE:C	5:E:165:ILE:HG13	2.42	0.42
8:H:177:ARG:HD2	8:H:190:THR:HG23	2.02	0.42
24:X:155:ARG:HA	24:X:158:LYS:HG2	2.02	0.42
1:A:201:PHE:HE1	6:F:408:LEU:HD11	1.84	0.42
6:F:221:LYS:HD2	6:F:322:PRO:CA	2.45	0.42
14:N:162:LEU:HD22	14:n:137:GLY:HA2	2.01	0.42
21:U:802:TYR:HA	21:U:895:PRO:HD3	2.01	0.42
21:U:852:GLU:HG3	21:U:853:LYS:HE3	2.02	0.42
22:V:470:ARG:CZ	30:d:242:LEU:HD21	2.50	0.42
26:Z:63:LYS:HG3	28:b:91:ARG:HH22	1.84	0.42
9:i:62:SER:OG	9:i:65:ILE:O	2.26	0.42
9:i:136:TYR:HB2	9:i:148:TYR:HB2	2.02	0.42
15:o:35:HIS:NE2	15:o:53:ASP:OD1	2.52	0.42
16:p:53:LEU:HB3	16:p:60:VAL:HG22	2.00	0.42
1:A:113:ILE:HD11	1:A:149:ILE:HD11	2.02	0.42
1:A:206:ILE:C	1:A:207:GLU:HG2	2.45	0.42
11:K:54:ILE:HD11	11:K:59:MET:HB3	2.00	0.42
19:S:19:ASP:OD1	19:S:19:ASP:N	2.52	0.42
21:U:245:ALA:HA	21:U:248:ILE:HG12	2.01	0.42
21:U:712:LEU:HA	21:U:715:LYS:HG2	2.01	0.42
22:V:119:GLY:HA2	22:V:148:ARG:HD3	2.02	0.42
26:Z:139:ILE:HD12	26:Z:139:ILE:HA	1.96	0.42
32:f:668:ALA:HA	32:f:697:ILE:HD11	2.02	0.42
3:C:138:MET:HE2	4:D:127:ASN:HB2	2.02	0.42
3:C:141:GLU:HB3	3:C:142:LYS:H	1.68	0.42
4:D:103:VAL:HG11	4:D:132:LEU:HD21	2.00	0.42
6:F:244:THR:CB	6:F:245:LYS:HE3	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:220:LEU:HD12	10:J:225:ILE:CG1	2.50	0.42
15:O:135:MET:HE2	20:t:179:ARG:CZ	2.50	0.42
21:U:639:LEU:HD12	21:U:639:LEU:HA	1.86	0.42
21:U:720:LYS:HA	21:U:720:LYS:HD3	1.83	0.42
7:g:217:VAL:HG12	7:g:230:LEU:HD13	2.02	0.42
16:p:2:SER:OG	16:p:3:ILE:N	2.53	0.42
1:A:69:ASP:OD1	1:A:69:ASP:N	2.52	0.41
1:A:73:ALA:HB2	2:B:140:ASP:HA	2.01	0.41
1:A:140:VAL:HB	1:A:149:ILE:HG23	2.02	0.41
1:A:186:LYS:HA	1:A:186:LYS:HD2	1.84	0.41
6:F:234:THR:O	6:F:238:ARG:HG2	2.19	0.41
7:G:167:ALA:HB3	7:G:176:THR:HG23	2.01	0.41
20:T:136:SER:HB2	20:T:150:LEU:HD13	2.02	0.41
23:W:166:LEU:HD22	23:W:192:LEU:HD12	2.01	0.41
28:b:90:ILE:HD11	28:b:131:LEU:HD11	2.02	0.41
9:i:33:THR:H	9:i:48:GLU:HB3	1.85	0.41
16:p:149:MET:HE2	16:p:173:ASN:HB2	2.01	0.41
2:B:67:ARG:NH2	32:f:664:GLU:OE2	2.54	0.41
4:D:214:MET:HG2	34:D:501:ATP:H2'	2.00	0.41
17:Q:38:MET:HG2	17:Q:44:LEU:HB2	2.01	0.41
21:U:805:ASN:N	21:U:891:VAL:O	2.53	0.41
22:V:346:LEU:HD23	22:V:349:ARG:HD3	2.02	0.41
23:W:208:LYS:HB2	23:W:208:LYS:HE2	1.94	0.41
23:W:377:ARG:HA	23:W:380:GLN:HG2	2.01	0.41
29:c:282:ARG:HH11	29:c:283:HIS:HB2	1.85	0.41
8:h:119:GLN:HG3	9:i:81:SER:HB2	2.02	0.41
17:q:5:ILE:HD11	17:q:143:LEU:HD21	2.02	0.41
2:B:287:ILE:HD13	2:B:329:MET:SD	2.60	0.41
4:D:61:ILE:HD12	21:U:639:LEU:HD23	2.02	0.41
4:D:139:LEU:HA	4:D:139:LEU:HD23	1.81	0.41
6:F:334:ARG:HD3	6:F:337:ILE:HD12	2.01	0.41
7:G:37:LEU:HD12	7:G:53:GLN:HG3	2.02	0.41
11:K:240:ASP:OD1	11:K:240:ASP:N	2.52	0.41
21:U:173:VAL:O	21:U:175:GLY:N	2.53	0.41
23:W:306:LEU:O	23:W:310:THR:OG1	2.35	0.41
24:X:407:MET:HE2	26:Z:266:ILE:HG22	2.02	0.41
27:a:115:LYS:HD3	27:a:118:ILE:HD12	2.02	0.41
27:a:138:VAL:HG21	27:a:158:LEU:HD21	2.03	0.41
32:f:80:ARG:HH11	32:f:83:ARG:HB2	1.85	0.41
32:f:708:ASP:O	32:f:712:LYS:HG2	2.21	0.41
11:k:91:LYS:HG2	11:k:119:LEU:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:t:50:MET:HE2	20:t:197:VAL:HG13	2.03	0.41
4:D:297:ASP:HB3	4:D:326:ARG:HH21	1.86	0.41
9:I:62:SER:OG	9:I:65:ILE:O	2.29	0.41
21:U:367:THR:HA	21:U:370:VAL:HG22	2.01	0.41
23:W:105:VAL:HG23	23:W:141:GLU:HG3	2.03	0.41
4:D:267:ILE:O	4:D:271:ALA:CB	2.67	0.41
5:E:355:ILE:HD11	6:F:217:ILE:HD11	2.03	0.41
11:K:146:VAL:HG11	11:K:222:PRO:HA	2.02	0.41
21:U:73:ALA:HB1	21:U:76:GLU:HB2	2.02	0.41
24:X:400:ALA:O	24:X:403:THR:OG1	2.34	0.41
26:Z:68:TRP:CD1	26:Z:104:ASN:HD21	2.38	0.41
26:Z:70:LEU:HD11	26:Z:108:ILE:HG23	2.02	0.41
32:f:882:LEU:HD23	32:f:884:THR:H	1.85	0.41
8:h:4:ARG:HH22	8:h:7:SER:N	2.18	0.41
14:n:160:LEU:O	14:n:164:MET:HG2	2.21	0.41
17:q:2:GLU:HG3	17:q:47:VAL:HG23	2.01	0.41
17:q:53:THR:HG22	17:q:100:VAL:HG12	2.03	0.41
33:v:13:UNK:O	33:v:15:UNK:N	2.54	0.41
2:B:53:THR:HA	2:B:55:HIS:CE1	2.56	0.41
5:E:234:GLU:N	5:E:278:ALA:O	2.53	0.41
11:K:4:THR:OG1	11:K:5:ARG:N	2.54	0.41
27:a:343:LEU:O	27:a:346:ILE:N	2.54	0.41
29:c:247:GLU:O	29:c:251:LEU:HB2	2.21	0.41
32:f:389:LYS:HB2	32:f:392:THR:HB	2.01	0.41
32:f:845:ARG:HG2	32:f:867:THR:HG22	2.03	0.41
15:o:113:ILE:HG12	15:o:119:THR:HG22	2.02	0.41
9:I:22:GLU:HA	9:I:25:MET:HB2	2.02	0.41
10:J:146:GLN:NE2	10:J:147:THR:O	2.54	0.41
14:N:7:GLN:NE2	14:N:109:GLY:O	2.53	0.41
16:P:135:ASP:OD1	16:P:136:PHE:N	2.53	0.41
16:P:143:ALA:HA	16:P:146:MET:HE2	2.02	0.41
23:W:24:VAL:O	23:W:28:LEU:HG	2.20	0.41
24:X:317:PRO:C	24:X:318:ILE:HG12	2.46	0.41
25:Y:98:SER:O	25:Y:102:ASP:N	2.52	0.41
30:d:8:GLU:O	30:d:13:SER:OG	2.32	0.41
15:o:54:MET:HE1	16:p:96:TYR:OH	2.21	0.41
20:t:146:ALA:HB1	20:t:172:CYS:HB3	2.02	0.41
1:A:36:TYR:HE1	32:f:157:GLU:HG3	1.86	0.41
3:C:406:LYS:HB2	9:I:80:THR:HG22	2.01	0.41
6:F:291:ILE:HB	6:F:306:VAL:HG13	2.03	0.41
6:F:356:MET:HA	6:F:357:PRO:HD3	1.91	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:524:LYS:NZ	21:U:562:GLU:O	2.37	0.41
23:W:441:LYS:HG3	23:W:445:LEU:HD13	2.02	0.41
27:a:26:GLU:HA	27:a:29:TYR:CE2	2.56	0.41
29:c:46:ARG:HH22	29:c:148:ILE:HG22	1.84	0.41
29:c:234:TYR:C	29:c:236:GLU:N	2.76	0.41
32:f:235:SER:HB3	32:f:853:VAL:HG21	2.02	0.41
32:f:490:ALA:HA	32:f:525:ILE:HA	2.03	0.41
14:n:4:MET:HG2	14:n:127:ILE:HG22	2.02	0.41
17:q:183:ILE:HG12	17:q:188:ILE:HG12	2.03	0.41
1:A:201:PHE:CD2	1:A:207:GLU:HB3	2.55	0.41
1:A:286:ASP:OD1	1:A:286:ASP:N	2.48	0.41
2:B:135:ILE:HD11	2:B:139:VAL:HG21	2.03	0.41
3:C:88:LYS:O	3:C:89:VAL:C	2.63	0.41
3:C:254:ILE:HD12	3:C:255:GLY:H	1.86	0.41
3:C:335:LYS:HB2	3:C:335:LYS:HE2	1.91	0.41
5:E:31:GLU:HA	5:E:34:LYS:HG2	2.03	0.41
6:F:410:ARG:NH2	6:F:419:ASP:OD2	2.42	0.41
7:G:110:PRO:HG2	7:G:113:MET:HB2	2.02	0.41
8:H:130:PHE:HB3	8:H:132:VAL:HG22	2.03	0.41
8:H:160:ALA:HB1	8:H:174:LEU:HD13	2.01	0.41
13:M:125:TYR:HB2	13:M:128:VAL:HG22	2.02	0.41
21:U:497:LEU:HB2	21:U:516:LEU:HD13	2.03	0.41
22:V:355:ARG:NH1	31:e:28:ALA:HB3	2.36	0.41
23:W:231:ILE:HG12	23:W:243:ILE:HG23	2.02	0.41
23:W:375:MET:HE1	23:W:386:VAL:HB	2.02	0.41
23:W:377:ARG:NH2	27:a:305:ASN:O	2.53	0.41
26:Z:68:TRP:HH2	26:Z:111:LEU:HD13	1.85	0.41
28:b:90:ILE:HG21	28:b:127:LEU:HD13	2.02	0.41
32:f:208:LEU:HB3	32:f:214:VAL:HG12	2.03	0.41
7:g:10:ASP:OD1	7:g:10:ASP:N	2.52	0.41
9:i:53:HIS:HE1	9:i:55:LEU:HD12	1.86	0.41
14:n:127:ILE:HD11	14:n:136:TYR:CE1	2.56	0.41
15:o:63:LEU:HD23	15:o:63:LEU:HA	1.96	0.41
19:s:26:ASP:OD1	19:s:26:ASP:N	2.53	0.41
19:s:144:MET:HE1	19:s:185:ARG:HB2	2.01	0.41
34:C:501:ATP:O3B	4:D:323:ARG:NH1	2.54	0.41
4:D:212:LYS:N	34:D:501:ATP:O1A	2.54	0.41
7:G:112:ASP:HB3	7:G:152:TYR:CZ	2.56	0.41
9:I:155:ASN:OD1	10:J:77:THR:OG1	2.39	0.41
12:L:72:ILE:HG22	12:L:134:ILE:HG12	2.02	0.41
20:T:124:TYR:HE1	20:T:139:THR:HG22	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:844:LYS:O	21:U:848:LYS:HG2	2.21	0.41
26:Z:194:GLN:NE2	29:c:301:ALA:HB2	2.36	0.41
27:a:156:TYR:HE2	27:a:196:ARG:HH22	1.69	0.41
32:f:170:TRP:CD1	32:f:211:ILE:HA	2.56	0.41
32:f:727:PHE:HB2	32:f:761:MET:HE2	2.02	0.41
8:h:74:LEU:HD12	8:h:134:LEU:HD22	2.02	0.41
2:B:288:ASP:OD1	2:B:288:ASP:N	2.54	0.40
4:D:236:VAL:HG11	5:E:255:ARG:HD2	2.02	0.40
5:E:297:ARG:HE	5:E:299:ILE:CG2	2.34	0.40
6:F:225:MET:HE1	6:F:233:LYS:HB3	2.03	0.40
6:F:262:GLY:N	6:F:305:GLU:OE2	2.40	0.40
6:F:307:GLN:HA	6:F:310:MET:HG2	2.03	0.40
8:H:109:GLN:HB3	8:H:113:ARG:HH12	1.87	0.40
10:J:221:ASN:HB3	10:J:224:GLU:HG2	2.02	0.40
15:O:112:SER:HB3	15:O:125:VAL:HG11	2.03	0.40
21:U:751:ARG:NH1	21:U:909:GLY:O	2.50	0.40
23:W:372:ARG:HG2	23:W:414:ASN:HB3	2.03	0.40
32:f:344:VAL:HG13	32:f:348:ILE:HG21	2.02	0.40
32:f:807:ARG:HA	32:f:811:LEU:HD12	2.02	0.40
9:i:241:GLU:HA	9:i:244:GLU:HG3	2.03	0.40
2:B:389:ASP:N	2:B:389:ASP:OD1	2.54	0.40
4:D:81:ARG:HH12	29:c:152:LYS:C	2.29	0.40
6:F:228:PRO:HG2	6:F:231:THR:HG21	2.02	0.40
11:K:234:LEU:O	11:K:238:ILE:HG12	2.21	0.40
17:Q:31:ASP:OD1	17:Q:31:ASP:N	2.54	0.40
18:R:87:VAL:HG11	18:R:97:MET:HE2	2.02	0.40
25:Y:212:GLU:HG2	25:Y:213:LEU:HD22	2.02	0.40
25:Y:229:ILE:HD11	25:Y:295:TYR:HE1	1.85	0.40
28:b:141:ILE:HG12	28:b:171:VAL:HB	2.02	0.40
32:f:94:LYS:HA	32:f:97:LYS:HE2	2.03	0.40
8:h:148:GLN:NE2	8:h:149:SER:O	2.54	0.40
14:n:127:ILE:HD11	14:n:136:TYR:CD1	2.56	0.40
2:B:39:LYS:HD2	2:B:276:GLU:HB3	2.04	0.40
4:D:61:ILE:HD13	4:D:61:ILE:HA	1.95	0.40
22:V:358:MET:HG3	22:V:359:PRO:HD3	2.02	0.40
27:a:15:GLY:HA2	27:a:16:PRO:HD3	1.97	0.40
30:d:183:GLU:OE2	30:d:215:TRP:NE1	2.54	0.40
14:n:127:ILE:HG21	14:n:127:ILE:HD13	1.89	0.40
23:W:72:LYS:NZ	23:W:111:TYR:OH	2.46	0.40
23:W:421:PRO:HB3	26:Z:247:LYS:HG2	2.04	0.40
30:d:122:LEU:HD12	30:d:133:ILE:HG21	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:129:THR:OG1	30:d:130:ASN:N	2.55	0.40
32:f:403:LYS:HG2	32:f:404:ASP:H	1.86	0.40
32:f:501:LEU:HD23	32:f:501:LEU:HA	1.94	0.40
32:f:685:THR:HA	32:f:688:ARG:HD2	2.04	0.40
32:f:748:LEU:HD23	32:f:748:LEU:HA	1.91	0.40
7:g:197:THR:HA	7:g:200:THR:HG22	2.04	0.40
10:j:185:ASP:O	10:j:189:LYS:HG2	2.22	0.40
1:A:75:PRO:O	1:A:79:ASP:HB2	2.21	0.40
17:Q:11:ASP:N	17:Q:11:ASP:OD1	2.54	0.40
21:U:192:GLN:O	21:U:196:LYS:NZ	2.55	0.40
21:U:349:ASP:OD2	21:U:351:MET:HE3	2.22	0.40
24:X:134:VAL:HB	24:X:149:LEU:HD23	2.03	0.40
24:X:173:GLU:HA	24:X:176:THR:HG22	2.03	0.40
27:a:251:LEU:HD12	27:a:254:ALA:HB3	2.04	0.40
29:c:248:MET:HA	29:c:251:LEU:HD13	2.03	0.40
20:t:9:THR:OG1	20:t:10:SER:N	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/433 (95%)	361 (88%)	43 (10%)	7 (2%)	7	34
2	B	409/440 (93%)	365 (89%)	44 (11%)	0	100	100
3	C	394/398 (99%)	349 (89%)	40 (10%)	5 (1%)	9	38
4	D	378/418 (90%)	322 (85%)	53 (14%)	3 (1%)	16	48
5	E	387/403 (96%)	349 (90%)	36 (9%)	2 (0%)	24	57
6	F	391/439 (89%)	350 (90%)	30 (8%)	11 (3%)	4	26
7	G	238/246 (97%)	228 (96%)	9 (4%)	1 (0%)	30	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	g	242/246 (98%)	229 (95%)	13 (5%)	0	100	100
8	H	230/234 (98%)	215 (94%)	15 (6%)	0	100	100
8	h	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
9	I	246/261 (94%)	237 (96%)	9 (4%)	0	100	100
9	i	248/261 (95%)	243 (98%)	5 (2%)	0	100	100
10	J	237/248 (96%)	221 (93%)	16 (7%)	0	100	100
10	j	237/248 (96%)	225 (95%)	11 (5%)	1 (0%)	30	62
11	K	236/241 (98%)	225 (95%)	11 (5%)	0	100	100
11	k	232/241 (96%)	221 (95%)	11 (5%)	0	100	100
12	L	238/263 (90%)	228 (96%)	10 (4%)	0	100	100
12	l	236/263 (90%)	230 (98%)	6 (2%)	0	100	100
13	M	240/255 (94%)	231 (96%)	9 (4%)	0	100	100
13	m	238/255 (93%)	232 (98%)	6 (2%)	0	100	100
14	N	201/239 (84%)	196 (98%)	5 (2%)	0	100	100
14	n	200/239 (84%)	194 (97%)	6 (3%)	0	100	100
15	O	218/277 (79%)	214 (98%)	4 (2%)	0	100	100
15	o	218/277 (79%)	211 (97%)	7 (3%)	0	100	100
16	P	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
16	p	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
17	Q	197/201 (98%)	190 (96%)	7 (4%)	0	100	100
17	q	197/201 (98%)	192 (98%)	5 (2%)	0	100	100
18	R	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
18	r	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
19	S	211/241 (88%)	203 (96%)	8 (4%)	0	100	100
19	s	211/241 (88%)	205 (97%)	6 (3%)	0	100	100
20	T	214/264 (81%)	207 (97%)	7 (3%)	0	100	100
20	t	214/264 (81%)	206 (96%)	8 (4%)	0	100	100
21	U	874/953 (92%)	806 (92%)	68 (8%)	0	100	100
22	V	442/534 (83%)	422 (96%)	20 (4%)	0	100	100
23	W	439/456 (96%)	430 (98%)	9 (2%)	0	100	100
24	X	420/422 (100%)	404 (96%)	15 (4%)	1 (0%)	43	73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Y	387/389 (100%)	368 (95%)	19 (5%)	0	100	100
26	Z	284/324 (88%)	254 (89%)	29 (10%)	1 (0%)	30	62
27	a	371/376 (99%)	343 (92%)	27 (7%)	1 (0%)	36	67
28	b	189/377 (50%)	168 (89%)	20 (11%)	1 (0%)	24	57
29	c	285/310 (92%)	242 (85%)	39 (14%)	4 (1%)	9	37
30	d	255/350 (73%)	213 (84%)	42 (16%)	0	100	100
31	e	48/70 (69%)	43 (90%)	5 (10%)	0	100	100
32	f	840/908 (92%)	808 (96%)	32 (4%)	0	100	100
All	All	13415/14876 (90%)	12574 (94%)	803 (6%)	38 (0%)	37	67

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	PRO
3	C	141	GLU
5	E	166	PRO
5	E	282	PRO
6	F	246	ALA
26	Z	145	HIS
29	c	280	PRO
1	A	314	ASN
4	D	157	ASP
6	F	181	PRO
6	F	247	THR
6	F	326	VAL
6	F	348	LEU
7	G	19	GLU
27	a	69	HIS
10	j	50	VAL
1	A	159	PRO
1	A	207	GLU
3	C	89	VAL
3	C	90	HIS
3	C	129	ASN
3	C	140	VAL
6	F	174	ALA
6	F	244	THR
28	b	23	PRO
29	c	198	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	c	285	GLU
4	D	335	LEU
6	F	180	ARG
6	F	245	LYS
6	F	324	THR
24	X	318	ILE
29	c	116	PRO
1	A	206	ILE
1	A	313	GLY
6	F	325	GLN
4	D	334	PRO
1	A	311	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/372 (94%)	341 (98%)	8 (2%)	44	63
2	B	357/385 (93%)	357 (100%)	0	100	100
3	C	340/346 (98%)	334 (98%)	6 (2%)	51	67
4	D	333/366 (91%)	328 (98%)	5 (2%)	57	69
5	E	341/353 (97%)	338 (99%)	3 (1%)	70	74
6	F	340/379 (90%)	334 (98%)	6 (2%)	51	67
7	G	202/210 (96%)	200 (99%)	2 (1%)	68	74
7	g	201/210 (96%)	201 (100%)	0	100	100
8	H	187/191 (98%)	187 (100%)	0	100	100
8	h	188/191 (98%)	187 (100%)	1 (0%)	81	81
9	I	202/221 (91%)	200 (99%)	2 (1%)	68	74
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	197/211 (93%)	196 (100%)	1 (0%)	81	81
10	j	196/211 (93%)	196 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	197/203 (97%)	197 (100%)	0	100	100
11	k	195/203 (96%)	195 (100%)	0	100	100
12	L	202/224 (90%)	202 (100%)	0	100	100
12	l	201/224 (90%)	201 (100%)	0	100	100
13	M	198/212 (93%)	198 (100%)	0	100	100
13	m	198/212 (93%)	198 (100%)	0	100	100
14	N	158/181 (87%)	158 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	178/228 (78%)	177 (99%)	1 (1%)	78	79
15	o	181/228 (79%)	181 (100%)	0	100	100
16	P	172/174 (99%)	172 (100%)	0	100	100
16	p	173/174 (99%)	173 (100%)	0	100	100
17	Q	168/171 (98%)	167 (99%)	1 (1%)	78	79
17	q	166/171 (97%)	166 (100%)	0	100	100
18	R	156/202 (77%)	156 (100%)	0	100	100
18	r	154/202 (76%)	154 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	177/199 (89%)	177 (100%)	0	100	100
20	T	178/215 (83%)	178 (100%)	0	100	100
20	t	179/215 (83%)	178 (99%)	1 (1%)	78	79
21	U	752/816 (92%)	752 (100%)	0	100	100
22	V	390/460 (85%)	389 (100%)	1 (0%)	86	84
23	W	406/416 (98%)	406 (100%)	0	100	100
24	X	362/362 (100%)	361 (100%)	1 (0%)	86	84
25	Y	344/344 (100%)	344 (100%)	0	100	100
26	Z	257/295 (87%)	255 (99%)	2 (1%)	73	76
27	a	333/336 (99%)	331 (99%)	2 (1%)	78	79
28	b	167/312 (54%)	166 (99%)	1 (1%)	78	79
29	c	252/268 (94%)	241 (96%)	11 (4%)	25	49
30	d	231/294 (79%)	229 (99%)	2 (1%)	70	74
31	e	44/63 (70%)	44 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	f	711/763 (93%)	711 (100%)	0	100	100
All	All	11450/12614 (91%)	11393 (100%)	57 (0%)	78	81

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	ILE
1	A	158	ASP
1	A	206	ILE
1	A	207	GLU
1	A	208	PRO
1	A	210	LYS
1	A	312	ARG
1	A	373	LEU
3	C	88	LYS
3	C	89	VAL
3	C	140	VAL
3	C	141	GLU
3	C	142	LYS
3	C	210	THR
4	D	149	SER
4	D	157	ASP
4	D	158	GLN
4	D	159	LYS
4	D	212	LYS
5	E	121	ASN
5	E	165	ILE
5	E	281	ARG
6	F	171	ARG
6	F	175	MET
6	F	245	LYS
6	F	315	ASN
6	F	326	VAL
6	F	347	ARG
7	G	19	GLU
7	G	21	ARG
9	I	51	ASN
9	I	52	ILE
10	J	220	LEU
15	O	147	GLU
17	Q	8	GLN
22	V	106	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	X	28	HIS
26	Z	103	LYS
26	Z	145	HIS
27	a	341	LEU
27	a	342	ASP
28	b	161	ASN
29	c	114	SER
29	c	196	LEU
29	c	197	ASN
29	c	198	ARG
29	c	278	GLN
29	c	279	ASP
29	c	280	PRO
29	c	281	LYS
29	c	282	ARG
29	c	285	GLU
29	c	286	GLU
30	d	201	ASN
30	d	202	THR
8	h	3	GLU
20	t	100	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	358	HIS
1	A	414	ASN
2	B	81	ASN
2	B	193	GLN
3	C	48	GLN
3	C	221	GLN
3	C	278	ASN
3	C	332	HIS
4	D	65	GLN
4	D	187	HIS
4	D	257	ASN
4	D	295	GLN
4	D	302	ASN
4	D	390	ASN
4	D	414	HIS
5	E	307	GLN
5	E	359	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	43	GLN
6	F	83	ASN
6	F	208	HIS
6	F	325	GLN
6	F	333	ASN
7	G	12	HIS
7	G	33	ASN
7	G	53	GLN
7	G	75	ASN
7	G	147	GLN
8	H	88	HIS
9	I	53	HIS
9	I	142	HIS
10	J	92	GLN
10	J	120	GLN
10	J	154	HIS
11	K	41	GLN
11	K	97	GLN
11	K	98	ASN
11	K	178	GLN
13	M	32	ASN
14	N	7	GLN
15	O	91	GLN
15	O	116	HIS
16	P	7	ASN
16	P	72	ASN
17	Q	101	ASN
17	Q	110	HIS
18	R	162	GLN
20	T	213	HIS
21	U	258	GLN
21	U	340	GLN
21	U	452	ASN
21	U	632	GLN
21	U	718	ASN
22	V	177	ASN
23	W	155	GLN
23	W	399	ASN
24	X	44	GLN
24	X	213	GLN
24	X	405	GLN
25	Y	160	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	Y	302	HIS
26	Z	77	ASN
26	Z	109	ASN
26	Z	174	HIS
26	Z	189	GLN
26	Z	194	GLN
26	Z	278	ASN
27	a	288	HIS
28	b	161	ASN
29	c	128	ASN
29	c	172	HIS
29	c	240	HIS
29	c	283	HIS
29	c	287	HIS
30	d	15	ASN
30	d	77	GLN
30	d	116	HIS
30	d	149	ASN
30	d	221	ASN
30	d	245	GLN
32	f	325	GLN
32	f	356	ASN
32	f	750	GLN
32	f	876	HIS
7	g	75	ASN
8	h	21	GLN
8	h	95	GLN
8	h	102	GLN
9	i	95	GLN
9	i	167	ASN
10	j	154	HIS
10	j	175	ASN
11	k	23	GLN
11	k	41	GLN
11	k	122	GLN
11	k	182	GLN
11	k	204	GLN
12	l	69	HIS
14	n	123	GLN
15	o	165	ASN
16	p	72	ASN
17	q	82	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	s	157	ASN
19	s	159	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	ATP	B	501	35	29,33,33	0.29	0	44,52,52	0.47	1 (2%)
36	ADP	E	401	-	27,29,29	1.36	4 (14%)	42,45,45	2.07	9 (21%)
34	ATP	C	501	35	29,33,33	0.30	0	44,52,52	0.48	1 (2%)
34	ATP	A	501	35	29,33,33	0.28	0	44,52,52	0.47	1 (2%)
34	ATP	D	501	35	29,33,33	0.28	0	44,52,52	0.46	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	ATP	B	501	35	-	8/22/38/38	0/3/3/3
36	ADP	E	401	-	-	5/16/32/32	0/3/3/3
34	ATP	C	501	35	-	0/22/38/38	0/3/3/3
34	ATP	A	501	35	-	6/22/38/38	0/3/3/3
34	ATP	D	501	35	-	0/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	E	401	ADP	C5-C4	4.54	1.47	1.39
36	E	401	ADP	C5-C6	2.57	1.48	1.41
36	E	401	ADP	C5-N7	-2.48	1.34	1.39
36	E	401	ADP	C8-N7	2.23	1.35	1.31

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	E	401	ADP	C5-C4-N3	-6.90	117.75	126.75
36	E	401	ADP	N3-C4-N9	5.48	136.12	127.08
36	E	401	ADP	C2-N3-C4	4.04	121.30	111.75
36	E	401	ADP	PA-O3A-PB	-3.46	120.95	132.83
36	E	401	ADP	C4-C5-N7	-3.27	106.64	110.62
36	E	401	ADP	N3-C2-N1	-3.17	123.64	128.60
36	E	401	ADP	C5-N7-C8	2.95	107.70	103.51
36	E	401	ADP	C3'-C2'-C1'	2.44	106.07	101.43
36	E	401	ADP	C4-N9-C8	2.35	108.27	105.73
34	A	501	ATP	PB-O3B-PG	2.05	139.85	132.83
34	B	501	ATP	PB-O3B-PG	2.04	139.84	132.83
34	C	501	ATP	PB-O3B-PG	2.03	139.80	132.83
34	D	501	ATP	PB-O3B-PG	2.01	139.73	132.83

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	501	ATP	C5'-O5'-PA-O1A
34	A	501	ATP	O4'-C4'-C5'-O5'
34	B	501	ATP	C5'-O5'-PA-O1A
36	E	401	ADP	C5'-O5'-PA-O2A
36	E	401	ADP	O4'-C4'-C5'-O5'
34	A	501	ATP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	E	401	ADP	C3'-C4'-C5'-O5'
34	B	501	ATP	O4'-C4'-C5'-O5'
34	B	501	ATP	C3'-C4'-C5'-O5'
34	A	501	ATP	C5'-O5'-PA-O3A
36	E	401	ADP	C5'-O5'-PA-O3A
34	B	501	ATP	PA-O3A-PB-O1B
34	A	501	ATP	C5'-O5'-PA-O2A
34	B	501	ATP	C5'-O5'-PA-O2A
36	E	401	ADP	C5'-O5'-PA-O1A
34	A	501	ATP	C4'-C5'-O5'-PA
34	B	501	ATP	C5'-O5'-PA-O3A
34	B	501	ATP	PG-O3B-PB-O1B
34	B	501	ATP	PA-O3A-PB-O2B

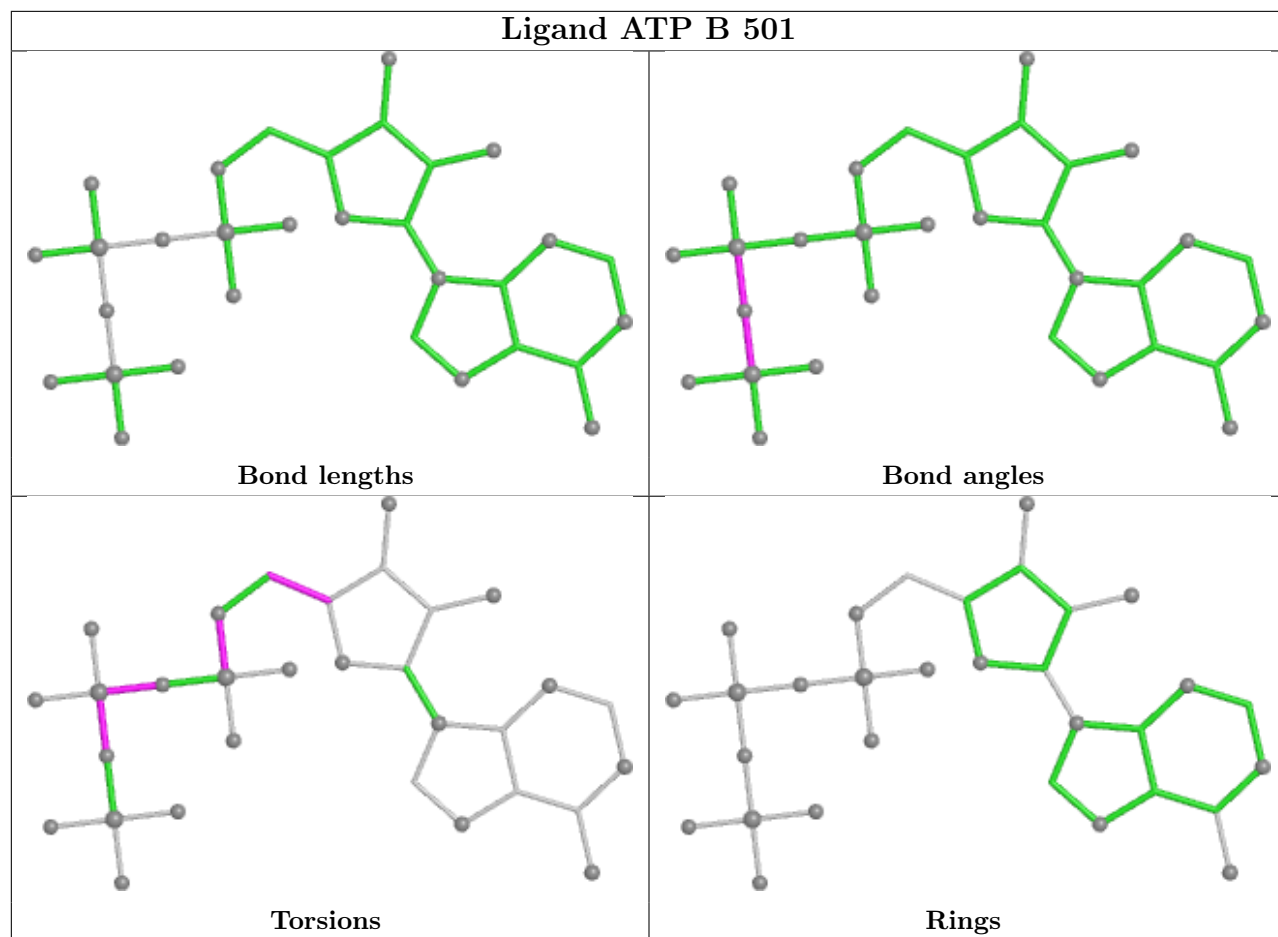
There are no ring outliers.

4 monomers are involved in 9 short contacts:

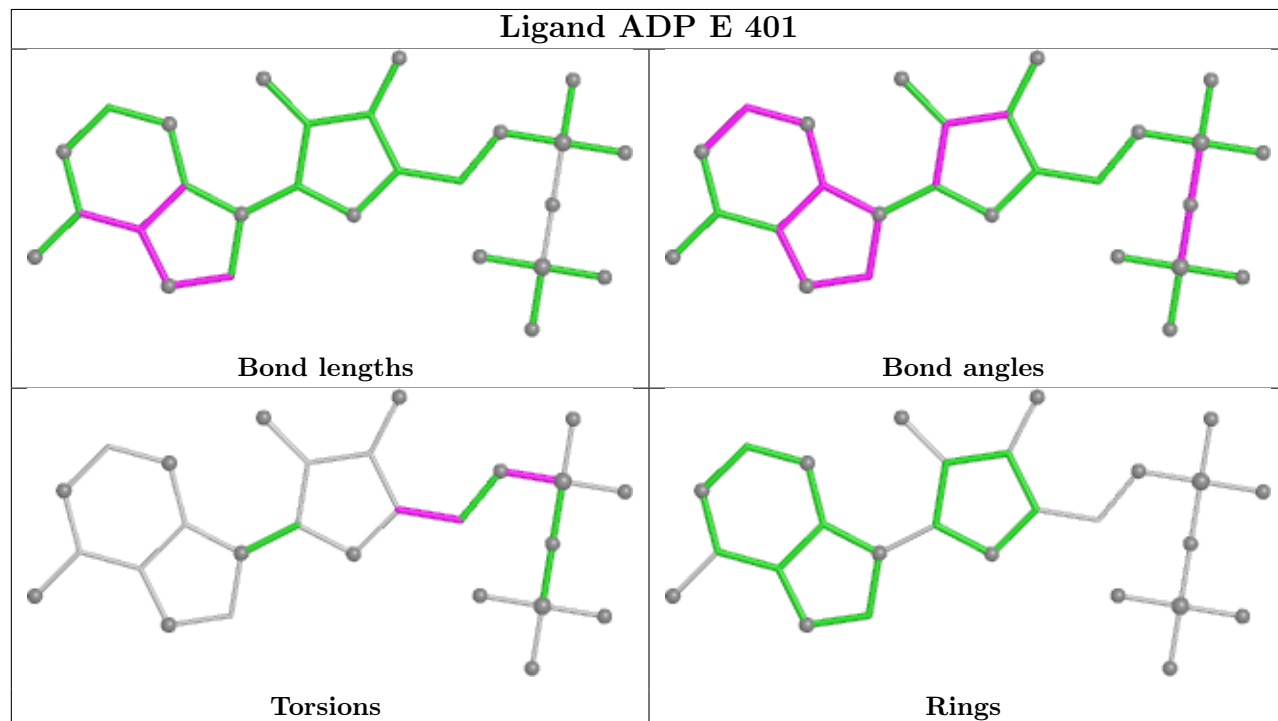
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	B	501	ATP	2	0
36	E	401	ADP	1	0
34	C	501	ATP	1	0
34	D	501	ATP	5	0

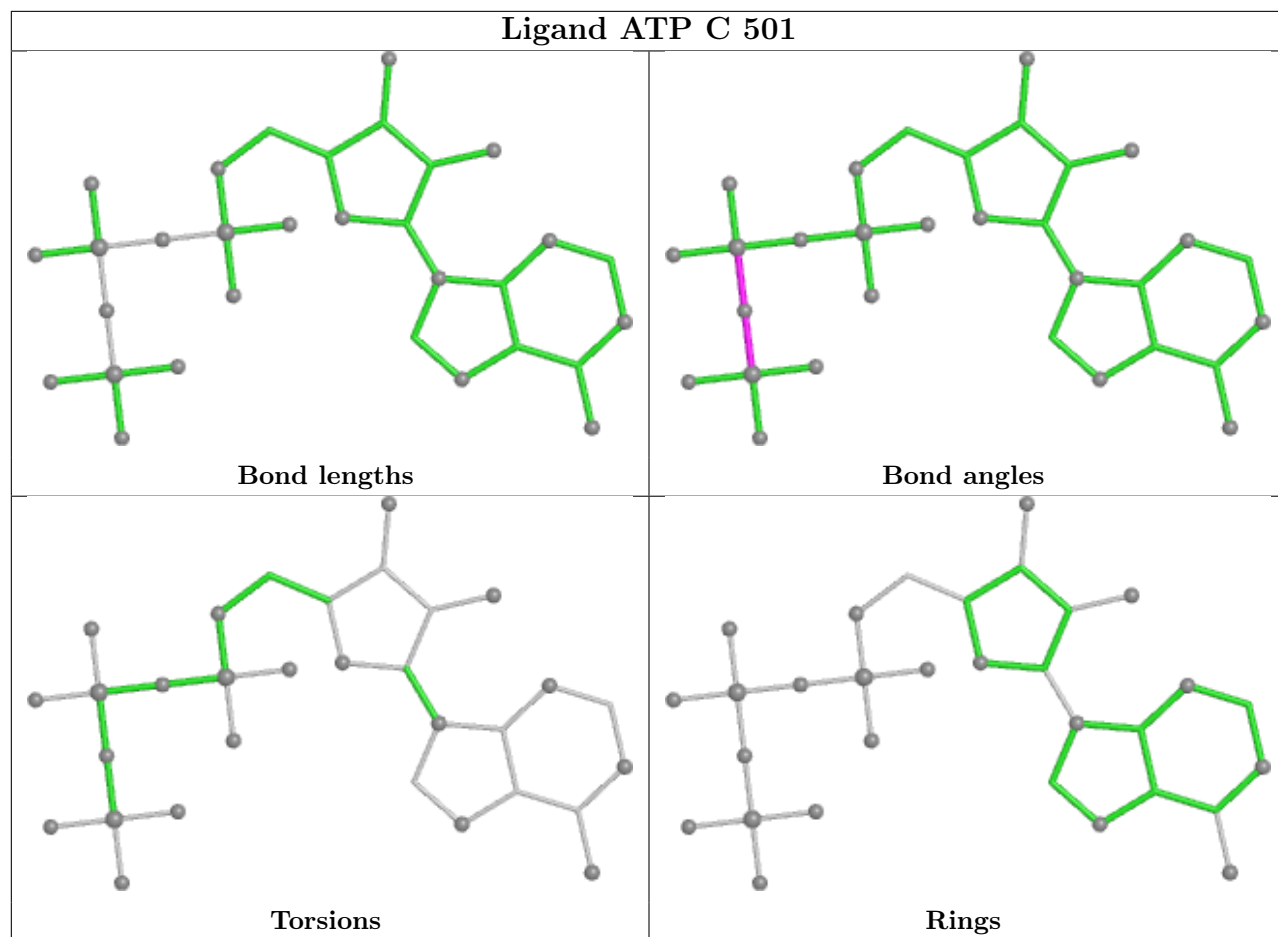
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

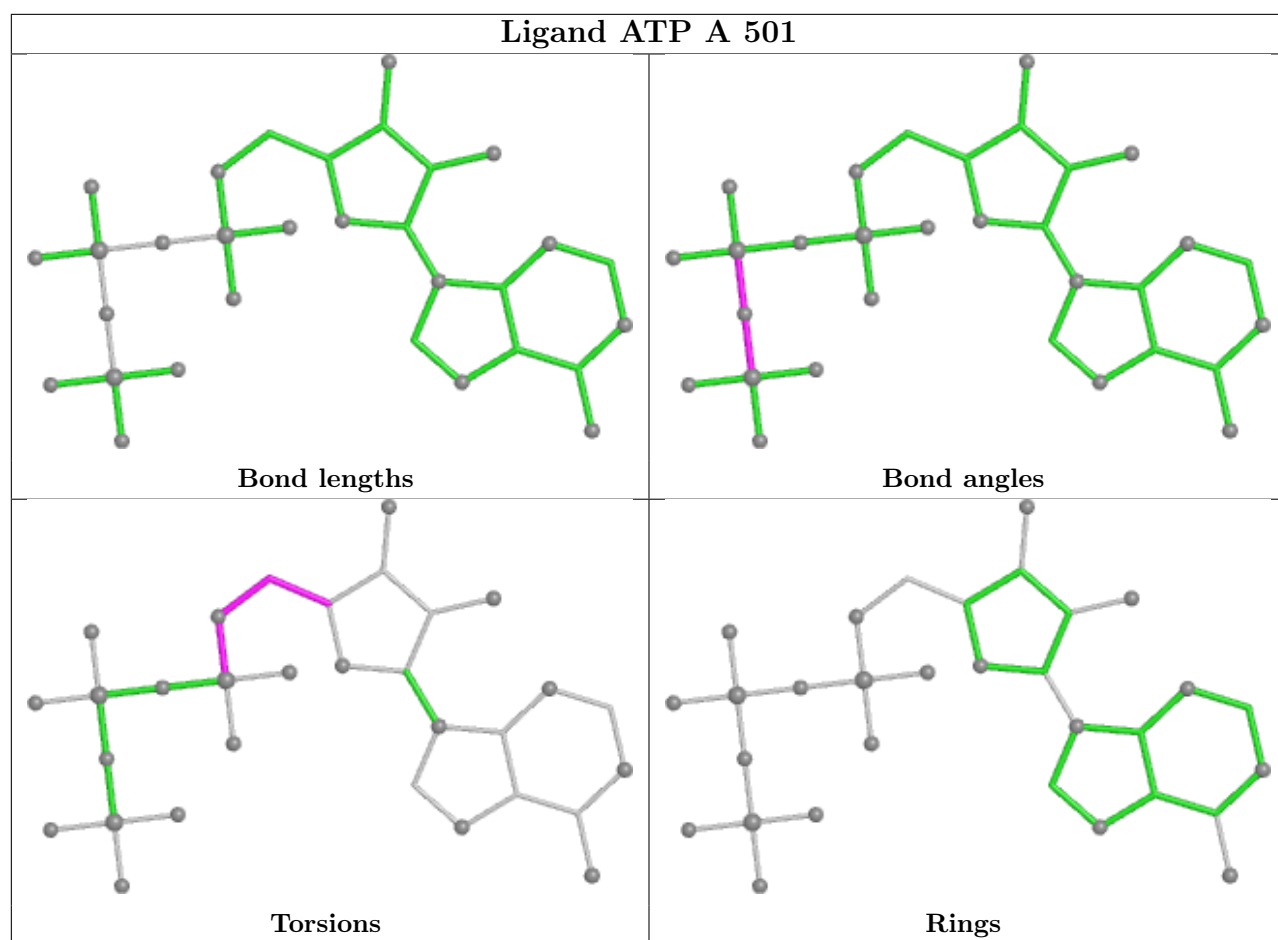
Ligand ATP B 501

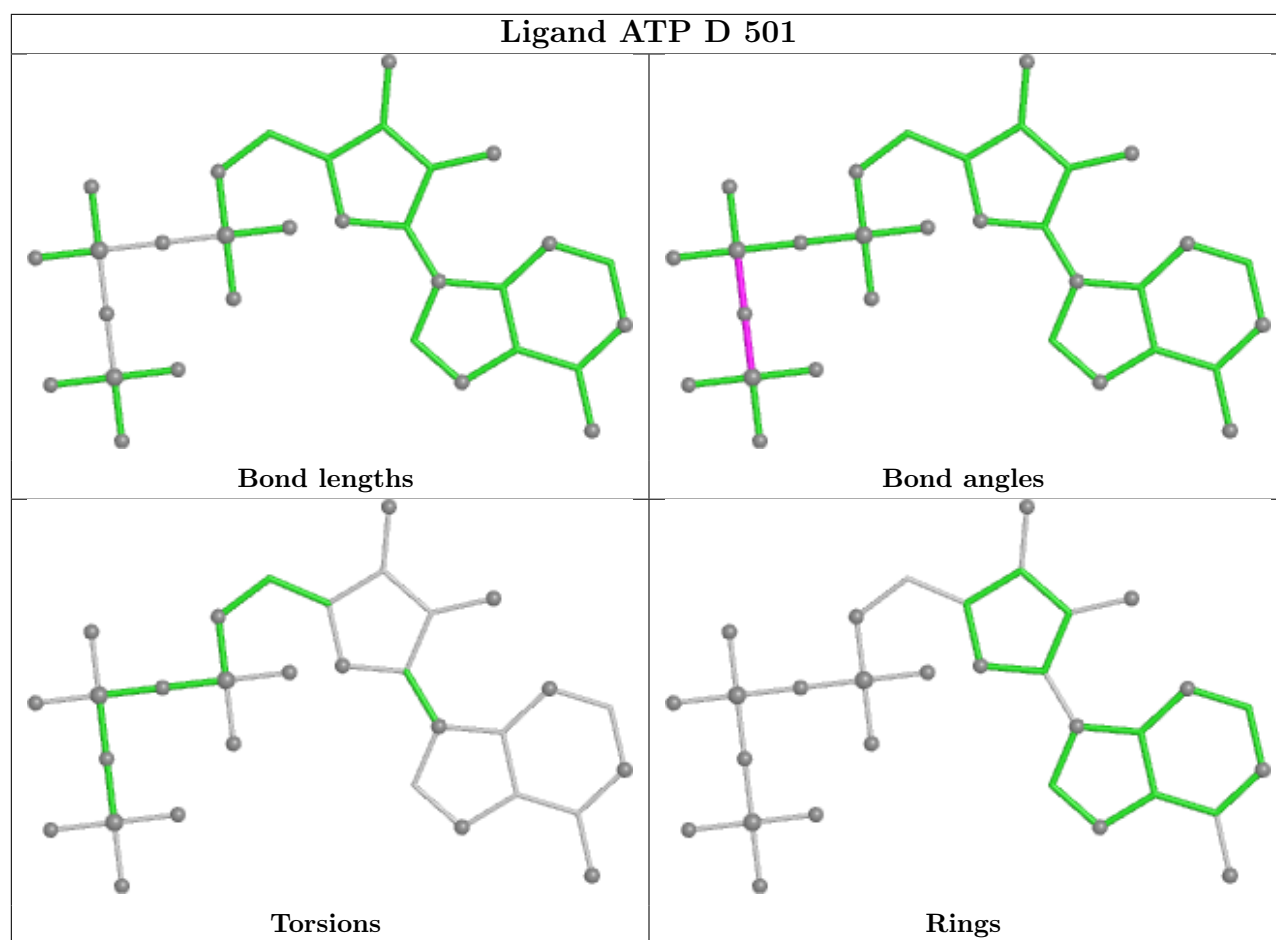


Ligand ADP E 401









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.

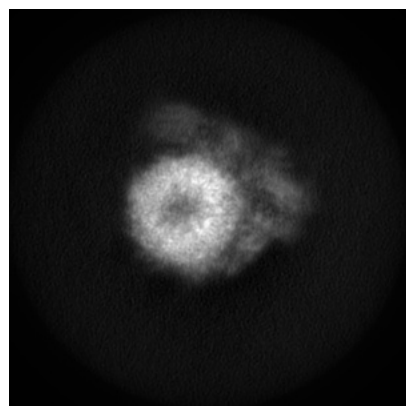
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62088. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

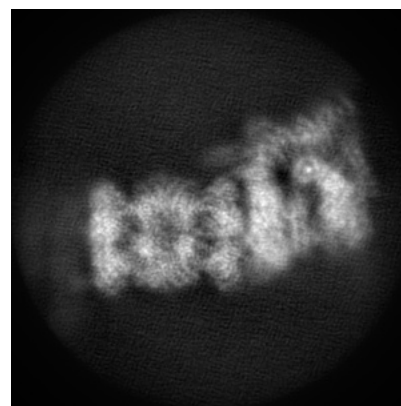
6.1.1 Primary map



X

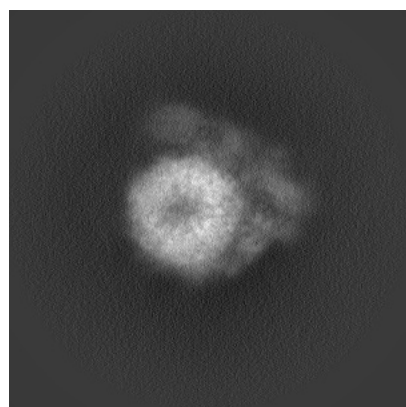


Y

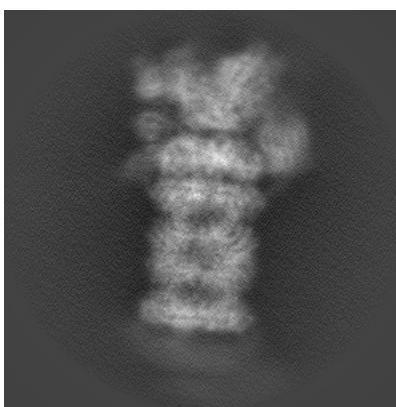


Z

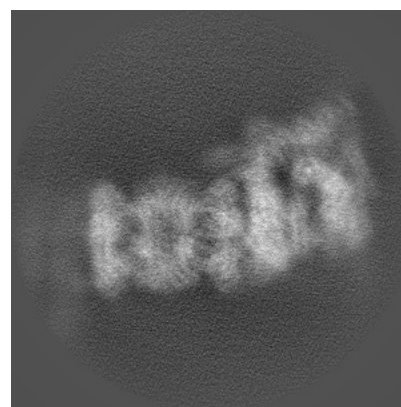
6.1.2 Raw map



X



Y

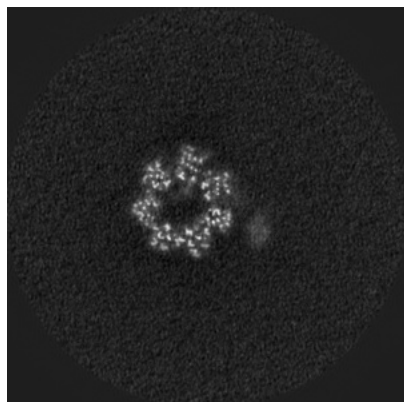


Z

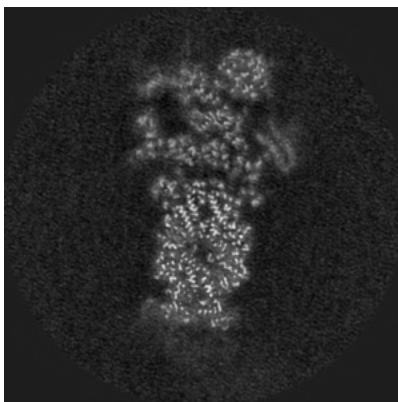
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

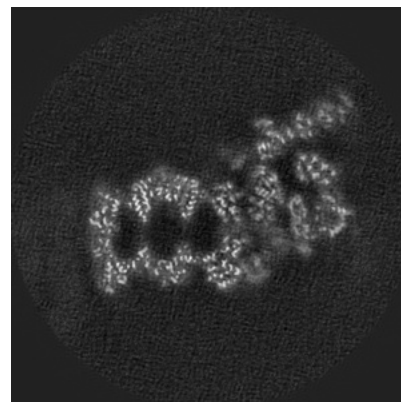
6.2.1 Primary map



X Index: 300

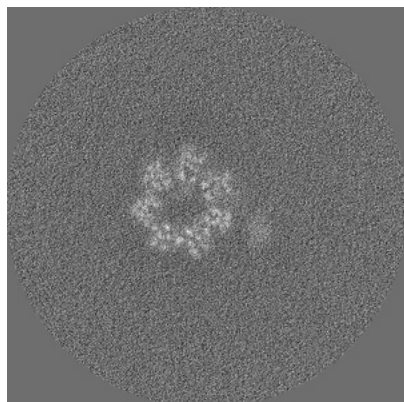


Y Index: 300

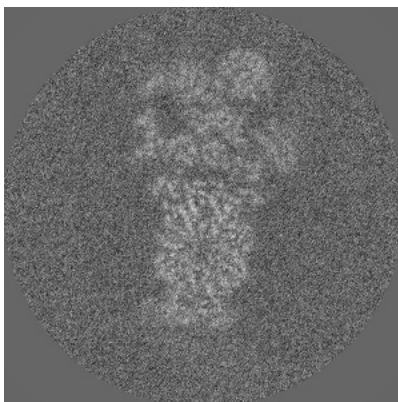


Z Index: 300

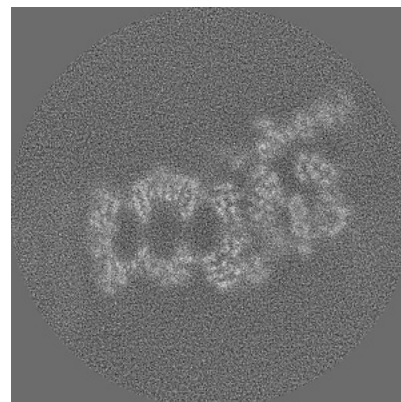
6.2.2 Raw map



X Index: 300



Y Index: 300

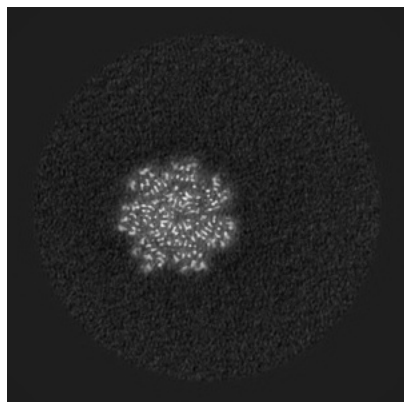


Z Index: 300

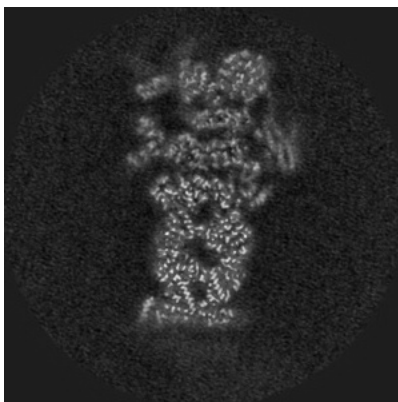
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

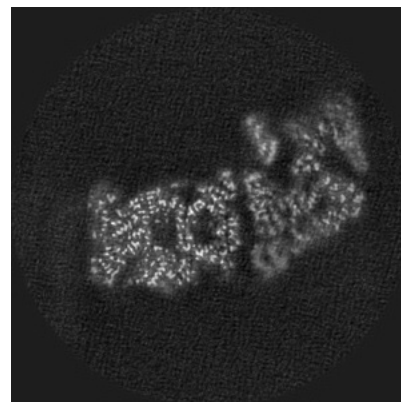
6.3.1 Primary map



X Index: 146

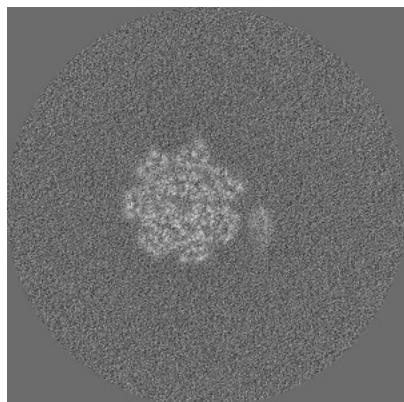


Y Index: 294

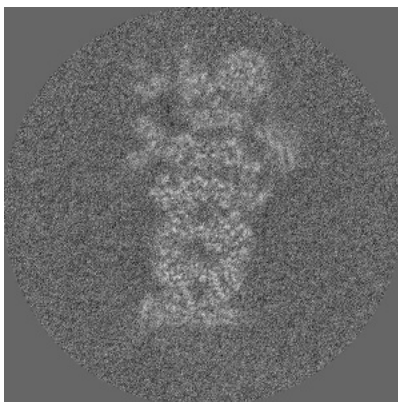


Z Index: 332

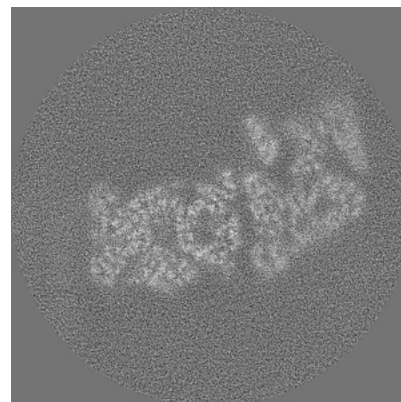
6.3.2 Raw map



X Index: 320



Y Index: 293

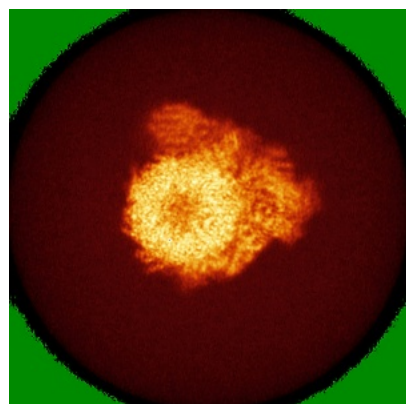


Z Index: 333

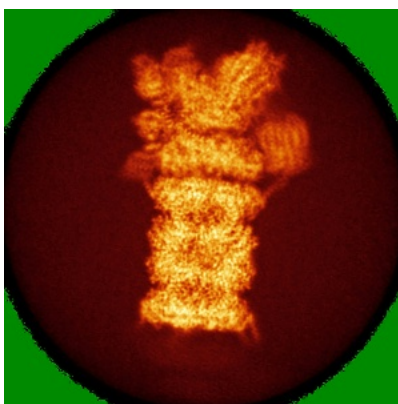
The images above show the largest variance slices of the map in three orthogonal directions.

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

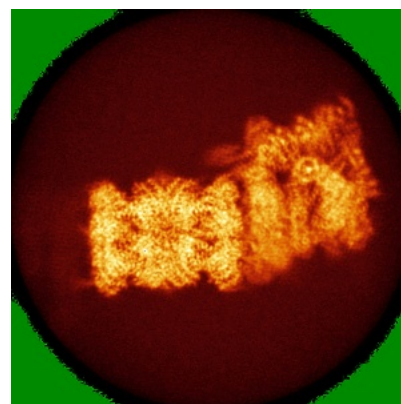
6.4.1 Primary map



X

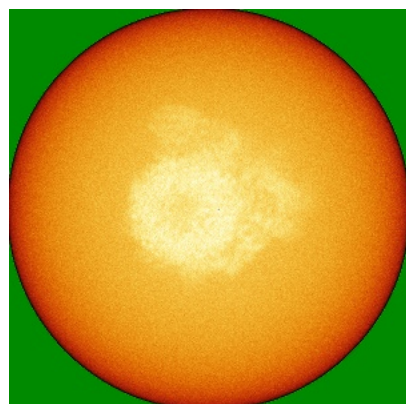


Y

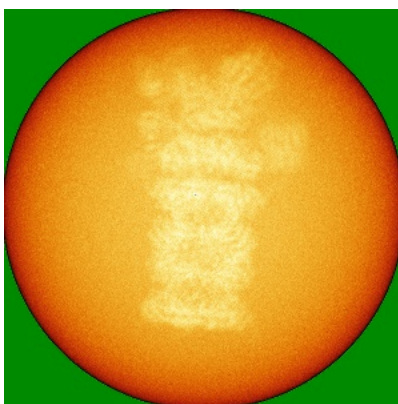


Z

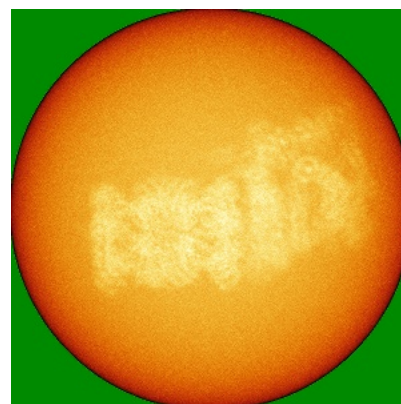
6.4.2 Raw map



X



Y

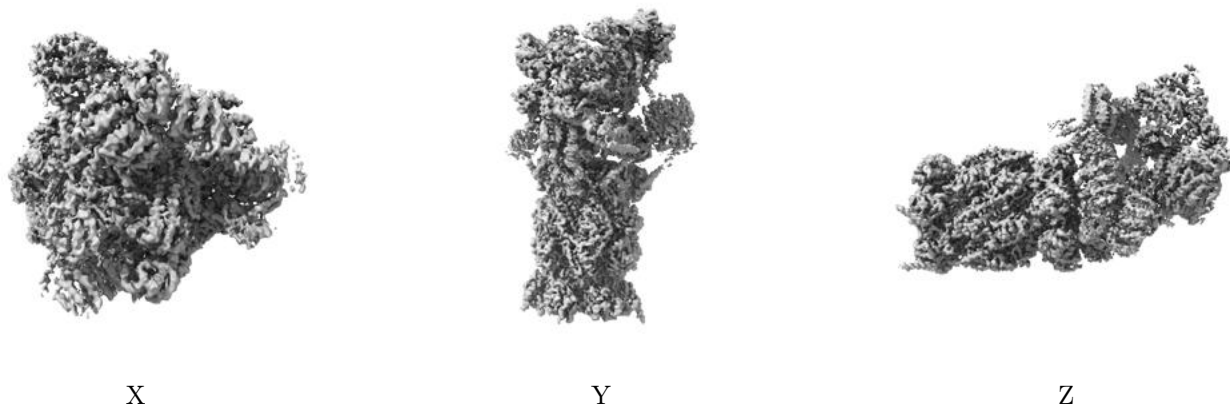


Z

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

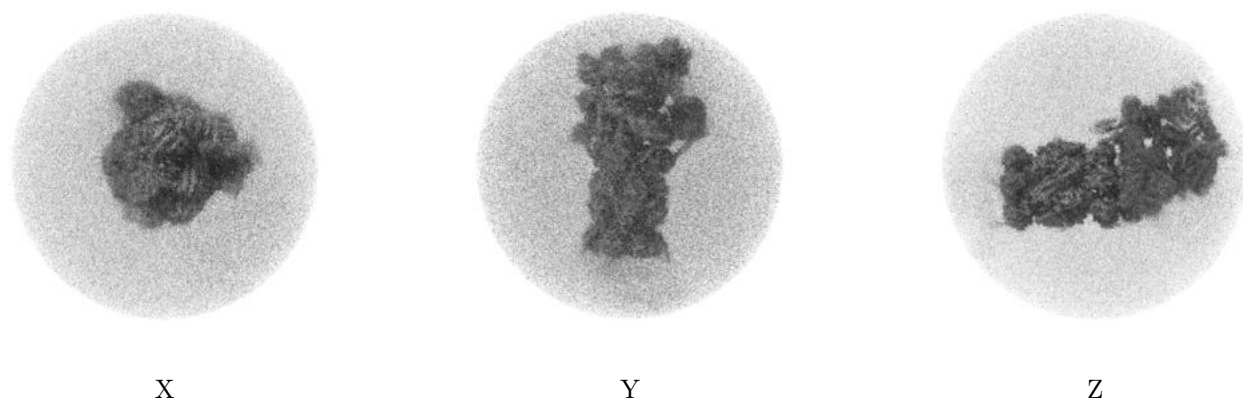
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00584. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

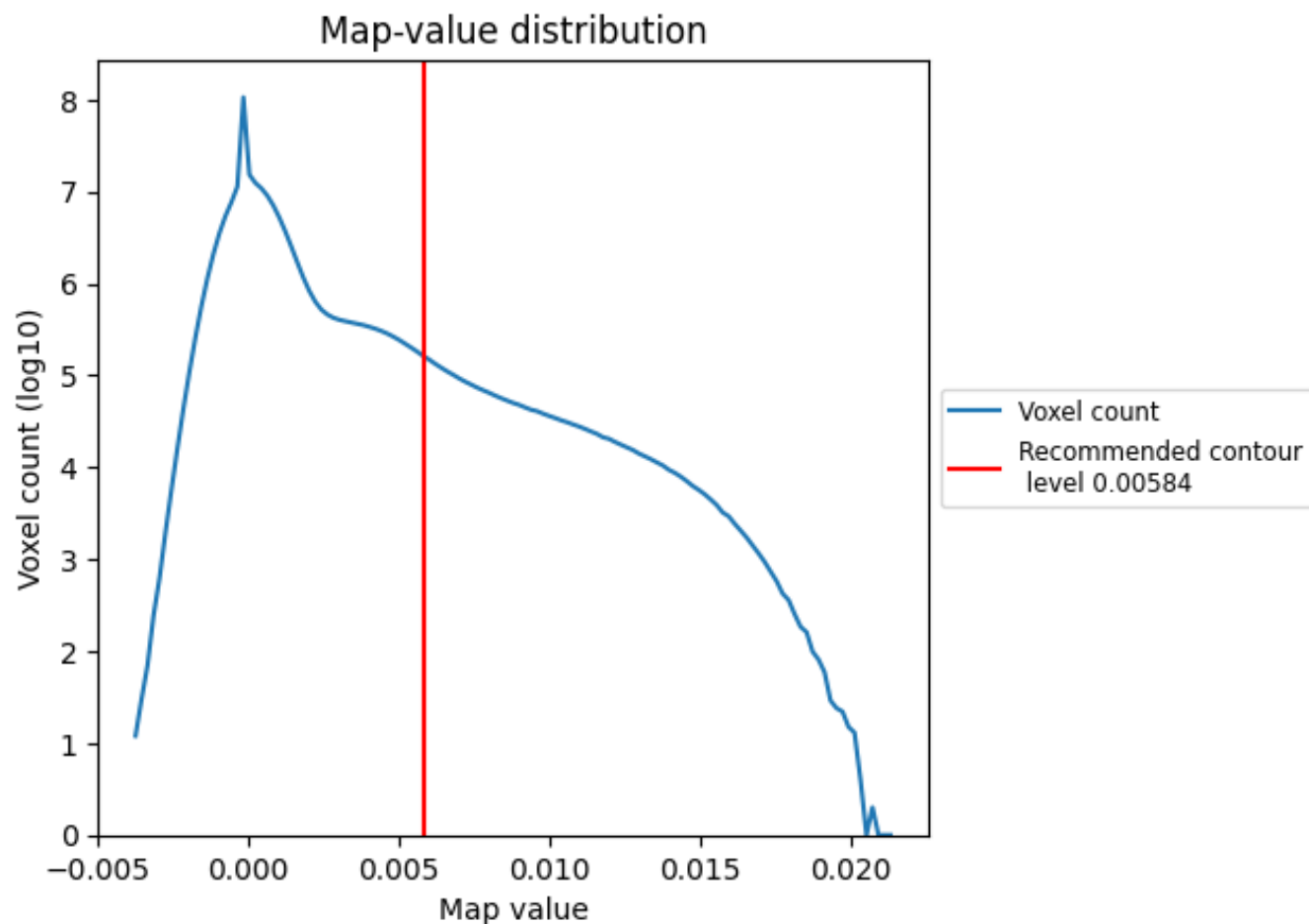
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

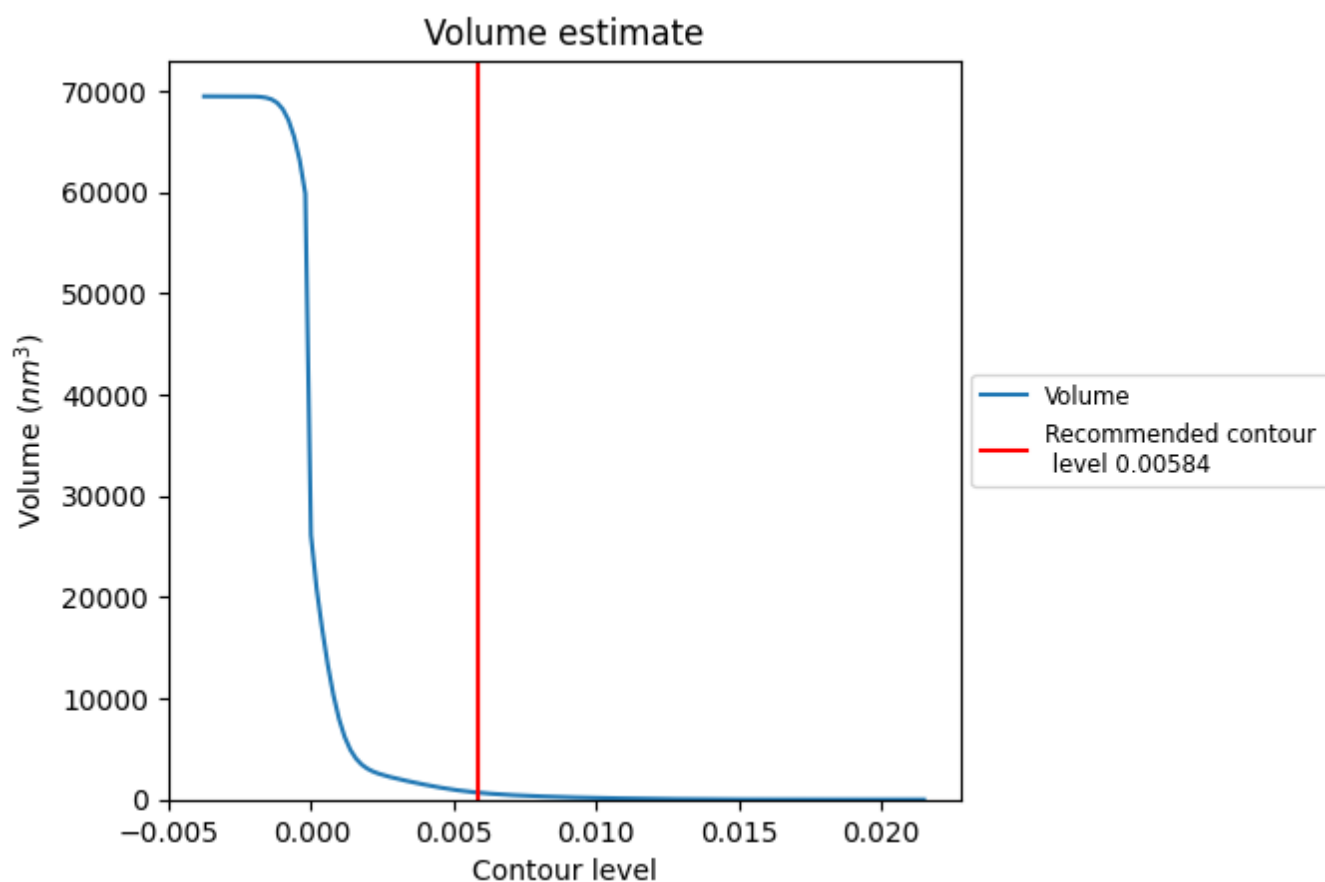
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

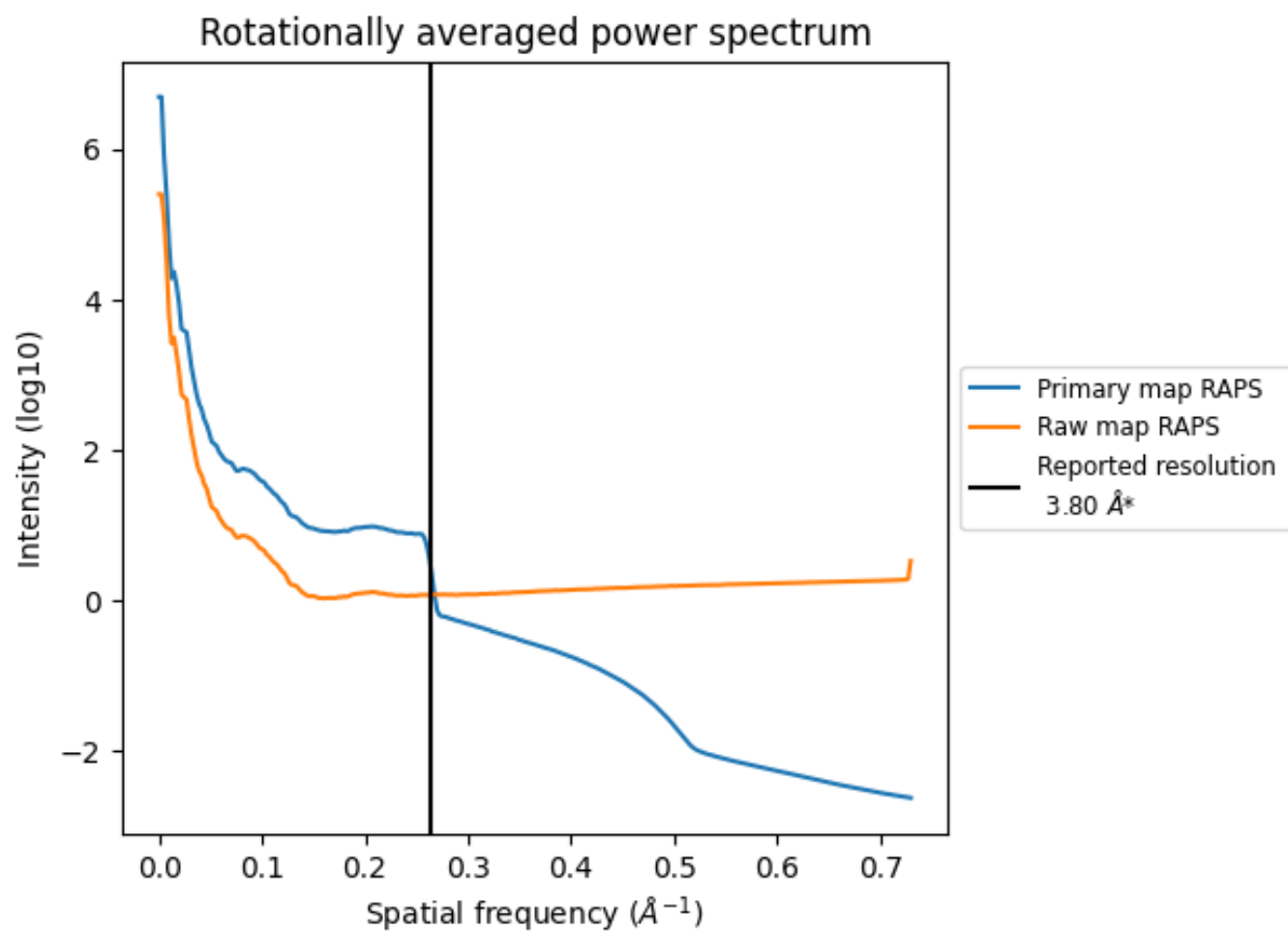
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 693 nm³; this corresponds to an approximate mass of 626 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 ⓘ

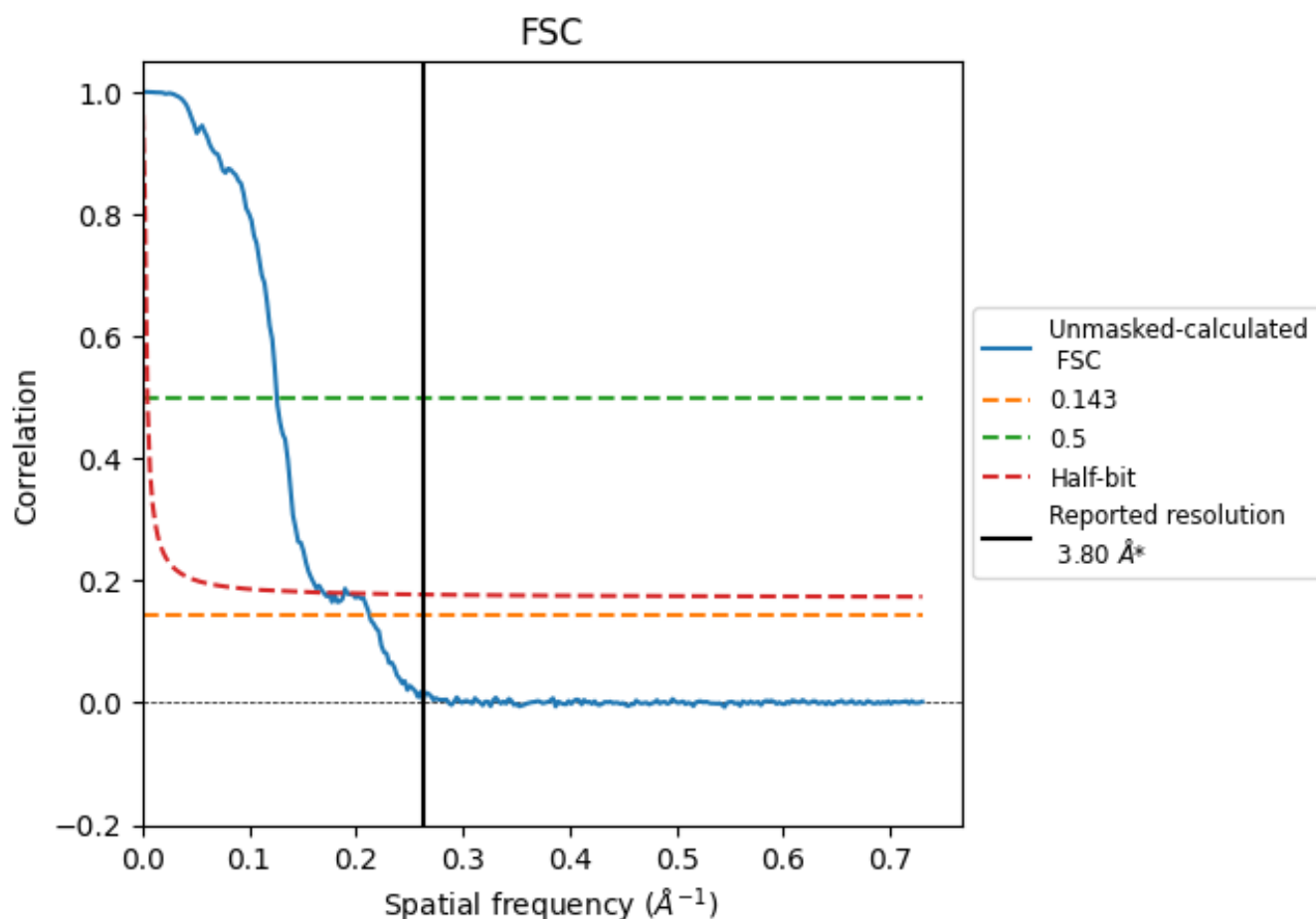


*Reported resolution corresponds to spatial frequency of 0.263 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 \AA^{-1}

8.2 Resolution estimates [i](#)

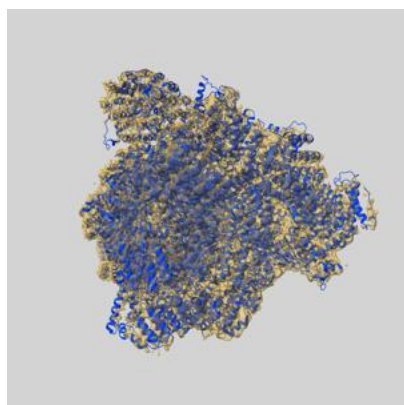
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.70	7.94	5.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.70 differs from the reported value 3.8 by more than 10 %

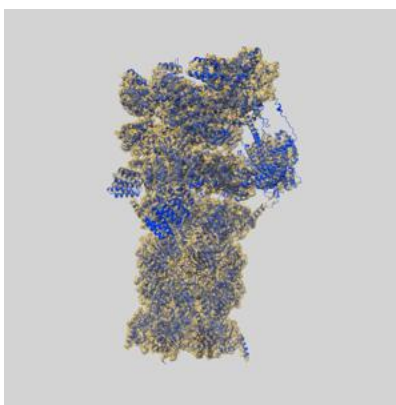
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62088 and PDB model 9K5C. Per-residue inclusion information can be found in section 3 on page 13.

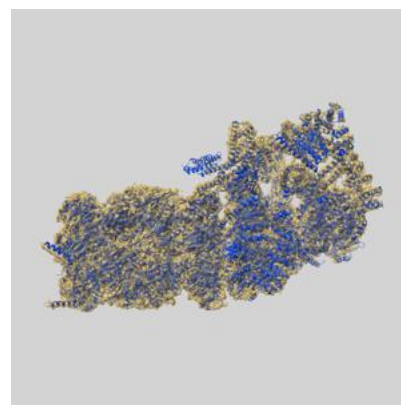
9.1 Map-model overlay [i](#)



X



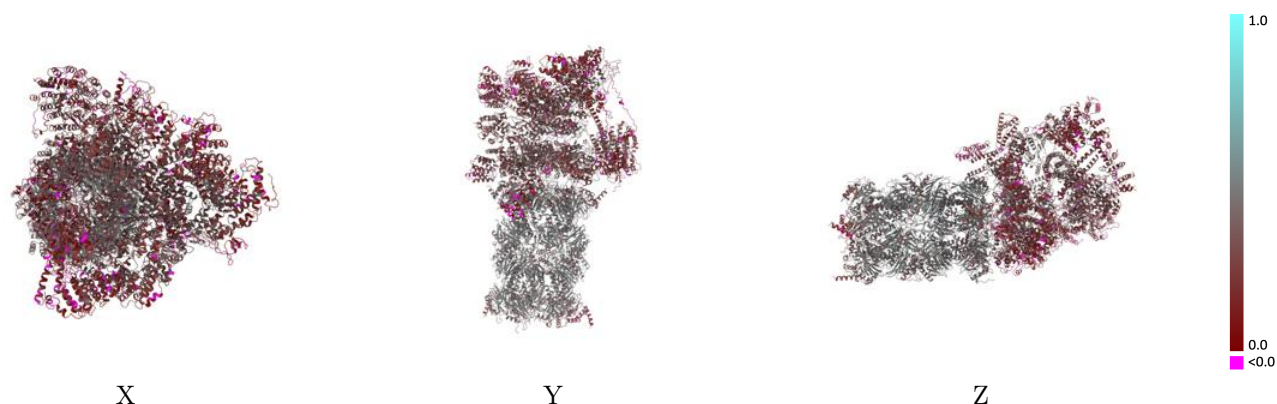
Y



Z

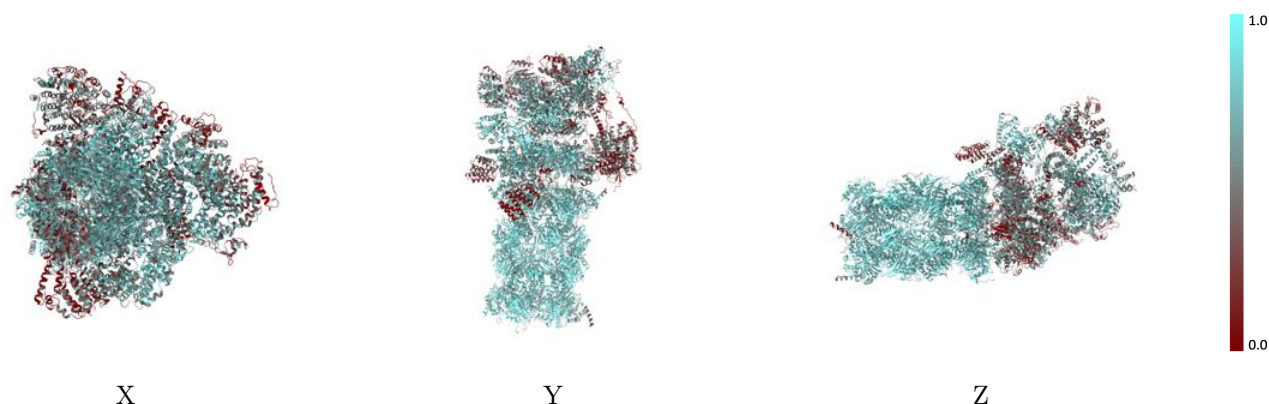
The images above show the 3D surface view of the map at the recommended contour level 0.00584 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



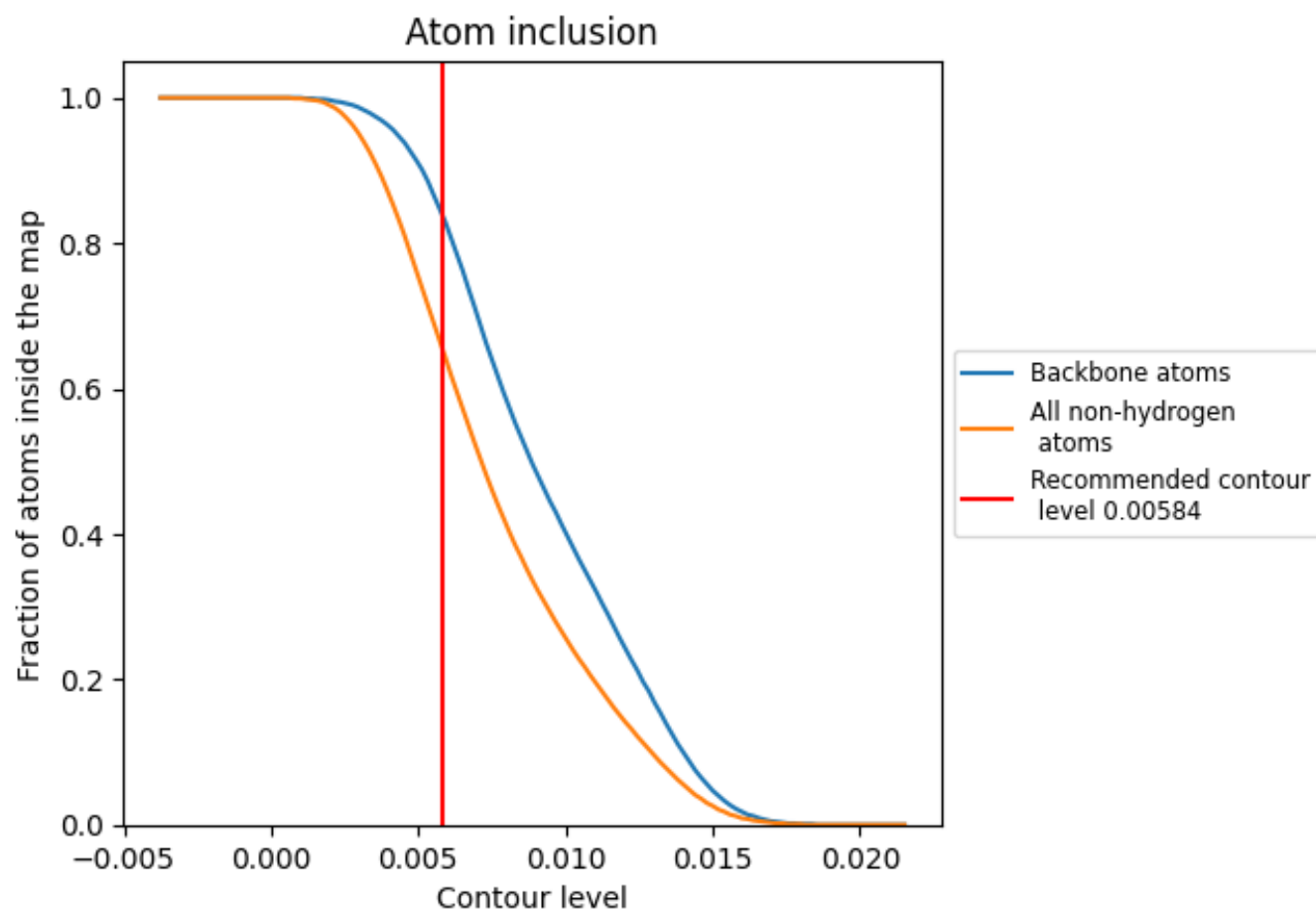
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00584).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 65% 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 (0.00584) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6520	 0.3460
A	 0.4260	 0.2270
B	 0.5350	 0.3100
C	 0.6500	 0.3380
D	 0.6690	 0.3450
E	 0.5550	 0.3040
F	 0.3490	 0.1960
G	 0.7990	 0.4410
H	 0.8150	 0.4400
I	 0.7820	 0.4290
J	 0.7640	 0.4080
K	 0.7630	 0.4220
L	 0.8060	 0.4390
M	 0.7990	 0.4310
N	 0.8550	 0.4640
O	 0.8500	 0.4510
P	 0.8610	 0.4580
Q	 0.8490	 0.4560
R	 0.8520	 0.4510
S	 0.8280	 0.4550
T	 0.8600	 0.4650
U	 0.5810	 0.2750
V	 0.5040	 0.2670
W	 0.5130	 0.2780
X	 0.4650	 0.2680
Y	 0.7210	 0.3260
Z	 0.6070	 0.3000
a	 0.5420	 0.2270
b	 0.3920	 0.1980
c	 0.6100	 0.3040
d	 0.3450	 0.1890
e	 0.5200	 0.3090
f	 0.3330	 0.2210
g	 0.8120	 0.4280
h	 0.8140	 0.4320



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.7740	 0.4060
j	 0.7230	 0.3400
k	 0.7770	 0.4100
l	 0.8320	 0.4320
m	 0.8150	 0.4300
n	 0.8520	 0.4520
o	 0.8330	 0.4470
p	 0.8500	 0.4550
q	 0.8580	 0.4500
r	 0.8710	 0.4600
s	 0.8220	 0.4480
t	 0.8660	 0.4590
v	 0.1830	 0.2400