



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:27 PM UTC

PDB ID : 7W38 / pdb_00007w38
EMDB ID : EMD-32273
Title : Structure of USP14-bound human 26S proteasome in state EA2.0_UBL
Authors : Zhang, S.; Zou, S.; Yin, D.; Wu, Z.; Mao, Y.
Deposited on : 2021-11-25
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

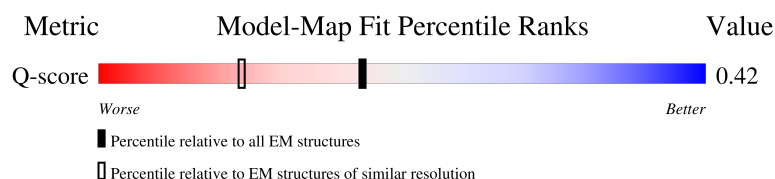
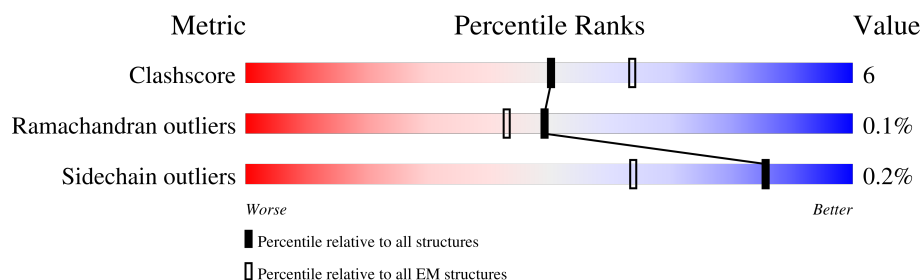
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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.



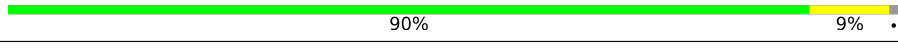
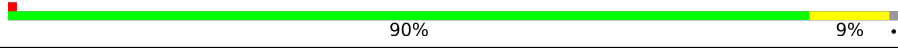
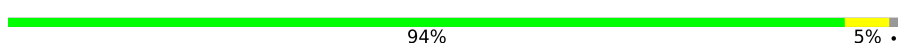
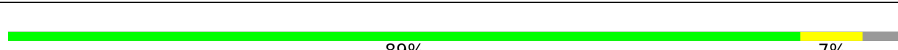
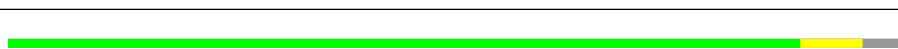
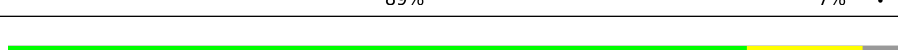
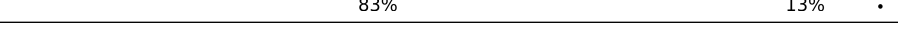
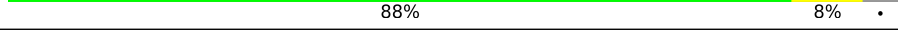
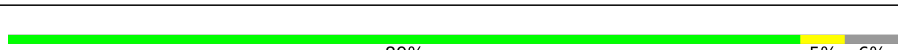
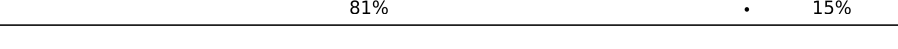
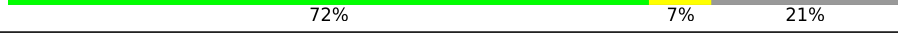
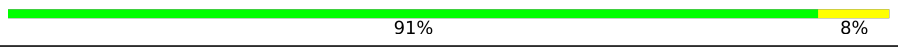
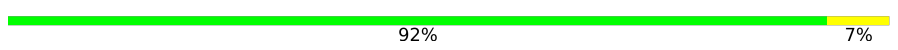
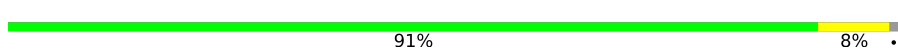
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	403	
6	G	246	
6	g	246	
7	H	234	
7	h	234	
8	I	261	
8	i	261	
9	J	248	
9	j	248	
10	K	241	
10	k	241	
11	L	269	
11	l	269	
12	M	255	
12	m	255	
13	N	239	
13	n	239	
14	O	277	
14	o	277	
15	P	205	
15	p	205	
16	Q	201	
16	q	201	
17	R	263	
17	r	263	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
18	S	241	
18	s	241	
19	T	264	
19	t	264	
20	U	953	
21	V	534	
22	W	456	
23	X	422	
24	Y	389	
25	Z	324	
26	a	376	
27	b	377	
28	d	350	
29	f	908	
30	x	494	
31	c	310	
32	F	439	
33	u	76	
34	e	70	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 106178 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	413	Total	C	N	O	S	0	0
			3240	2042	567	613	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	388	Total	C	N	O	S	0	0
			3042	1915	519	593	15		

- Molecule 3 is a protein called Isoform 2 of 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	379	Total	C	N	O	S	0	0
			2968	1867	534	551	16		

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

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

- Molecule 5 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	375	Total	C	N	O	S	0	0
			2860	1796	512	536	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	244	Total	C	N	O	S	0	0
			1889	1198	316	362	13		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	244	Total	C	N	O	S	0	0
			1880	1193	318	356	13		

- Molecule 7 is a protein called Proteasome subunit alpha type-2.

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

- Molecule 8 is a protein called Proteasome subunit alpha type-4.

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

- Molecule 9 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 10 is a protein called Proteasome subunit alpha type-5.

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

- Molecule 11 is a protein called Isoform Long of Proteasome subunit alpha type-1.

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

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

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

- Molecule 13 is a protein called Proteasome subunit beta type-6.

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

- Molecule 14 is a protein called Proteasome subunit beta type-7.

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

- Molecule 15 is a protein called Proteasome subunit beta type-3.

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

- Molecule 16 is a protein called Proteasome subunit beta type-2.

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

- Molecule 17 is a protein called Proteasome subunit beta type-5.

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

- Molecule 18 is a protein called Proteasome subunit beta type-1.

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

- Molecule 19 is a protein called Proteasome subunit beta type-4.

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

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	764	Total	C	N	O	S	0	0
			5945	3772	1021	1108	44		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	472	Total	C	N	O	S	0	0
			3754	2387	673	681	13		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

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

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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

- Molecule 30 is a protein called Ubiquitin carboxyl-terminal hydrolase 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	x	76	Total	C	N	O	S	0	0
			588	378	96	108	6		

- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 32 is a protein called 26S protease regulatory subunit 6A.

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

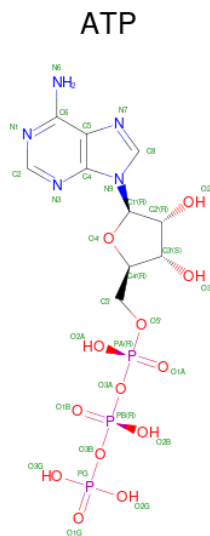
- Molecule 33 is a protein called Ubiquitin.

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

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

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

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

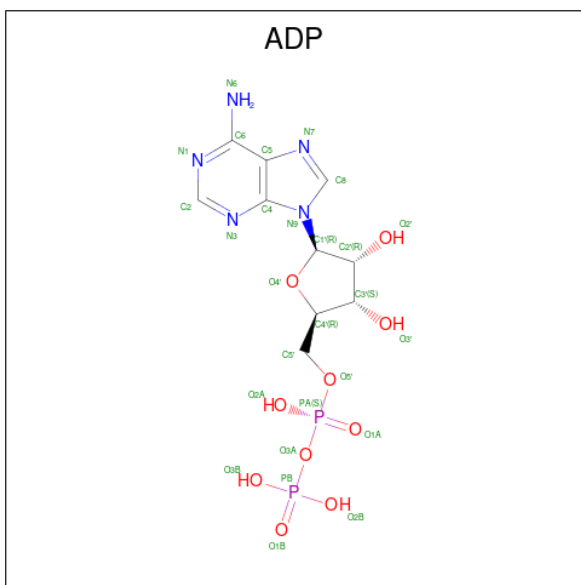


Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total 31	C 10	N 5	O 13	P 3	0
35	B	1	Total 31	C 10	N 5	O 13	P 3	0
35	D	1	Total 31	C 10	N 5	O 13	P 3	0
35	E	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
36	A	1	Total Mg 1 1	0
36	B	1	Total Mg 1 1	0
36	C	1	Total Mg 1 1	0
36	D	1	Total Mg 1 1	0
36	E	1	Total Mg 1 1	0
36	F	1	Total Mg 1 1	0

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



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

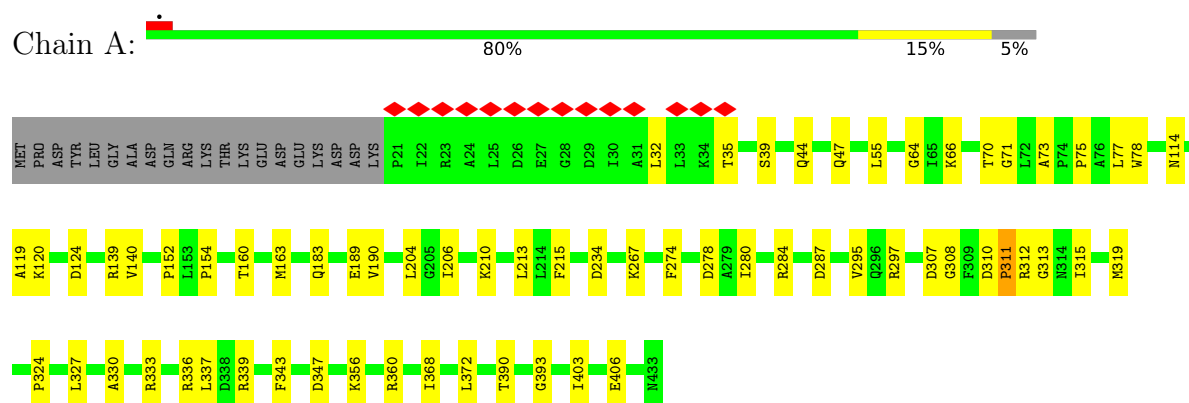
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

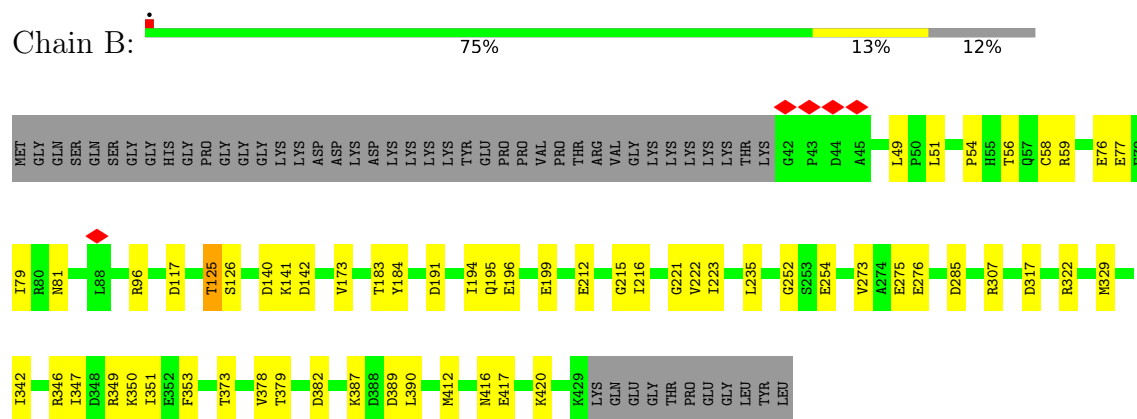
3 Residue-property plots

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

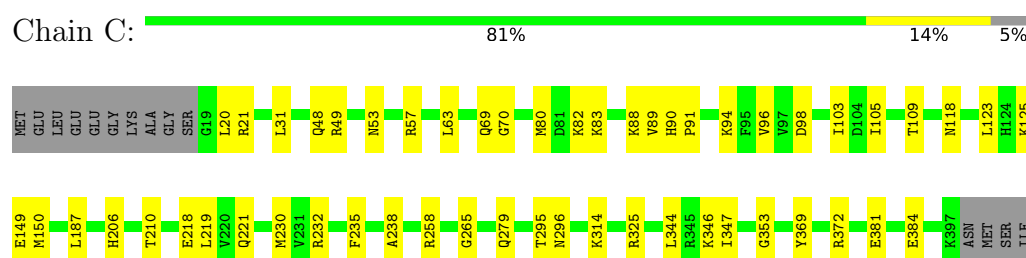
- Molecule 1: 26S protease regulatory subunit 7



- Molecule 2: 26S protease regulatory subunit 4

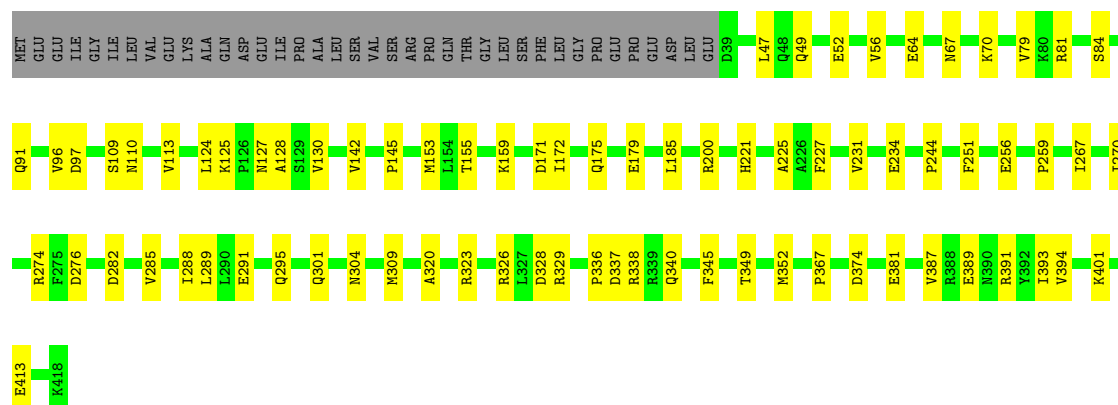


- Molecule 3: Isoform 2 of 26S proteasome regulatory subunit 8



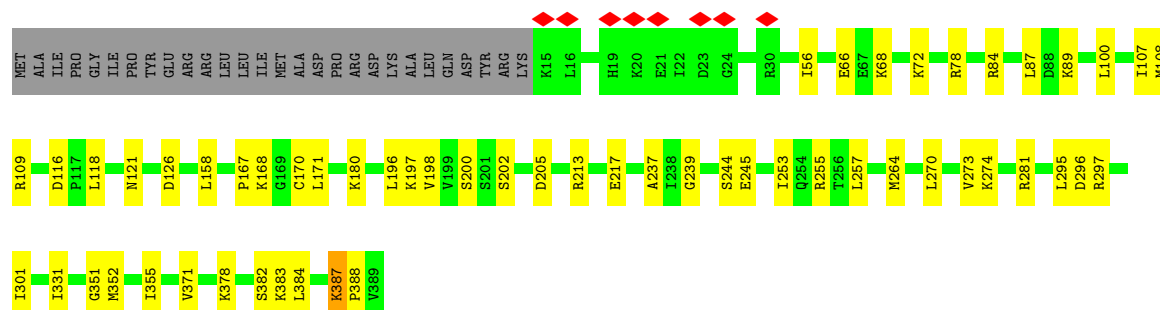
- Molecule 4: 26S protease regulatory subunit 6B

Chain D:  73% 18% 9%



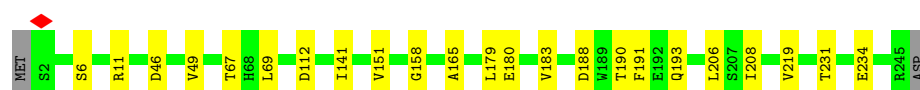
- Molecule 5: 26S proteasome regulatory subunit 10B

Chain E:  79% 14% 7%



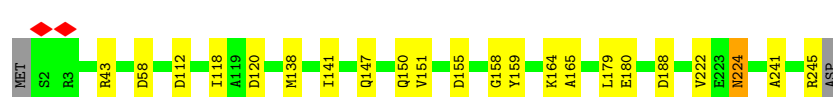
- Molecule 6: Proteasome subunit alpha type-6

Chain G:  90% 9% .



- Molecule 6: Proteasome subunit alpha type-6

Chain g:  90% 9% .



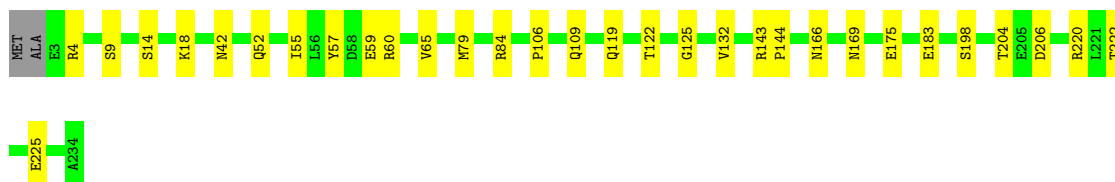
- Molecule 7: Proteasome subunit alpha type-2

Chain H:  94% 5% .



- Molecule 7: Proteasome subunit alpha type-2

Chain h: 86% 13% .



- Molecule 8: Proteasome subunit alpha type-4

Chain I: 89% 7% .



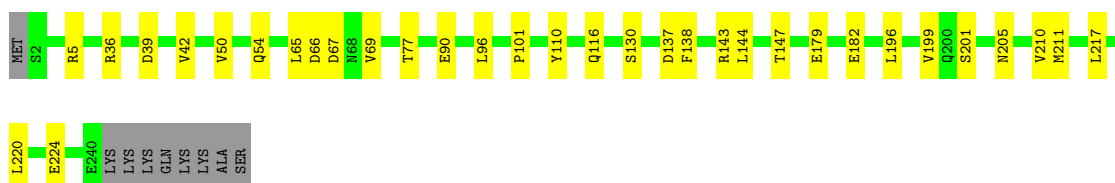
- Molecule 8: Proteasome subunit alpha type-4

Chain i: 89% 7% .



- Molecule 9: Proteasome subunit alpha type-7

Chain J: 83% 13% .



- Molecule 9: Proteasome subunit alpha type-7

Chain j: 88% 8% .



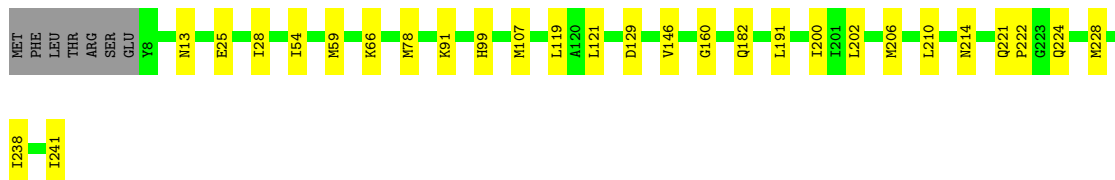
- Molecule 10: Proteasome subunit alpha type-5

Chain K: 88% 9% .



• Molecule 10: Proteasome subunit alpha type-5

Chain k: 85% 12%



• Molecule 11: Isoform Long of Proteasome subunit alpha type-1

Chain L: 81% 7% 12%



• Molecule 11: Isoform Long of Proteasome subunit alpha type-1

Chain l: 80% 9% 12%



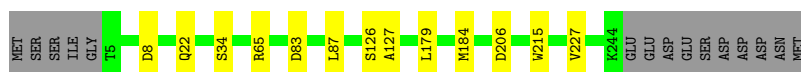
• Molecule 12: Proteasome subunit alpha type-3

Chain M: 87% 7% 6%



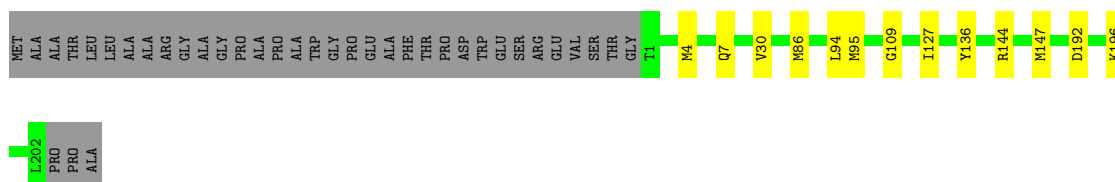
• Molecule 12: Proteasome subunit alpha type-3

Chain m: 89% 5% 6%



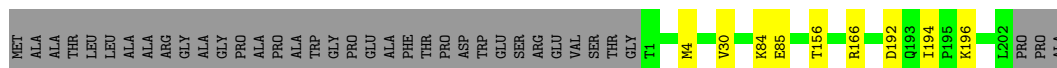
• Molecule 13: Proteasome subunit beta type-6

Chain N: 79% 5% 15%



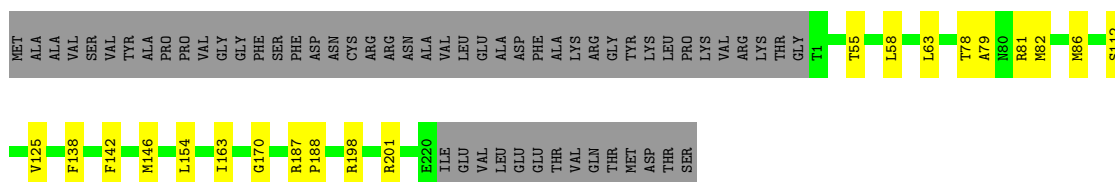
- Molecule 13: Proteasome subunit beta type-6

Chain n: 81% 15%



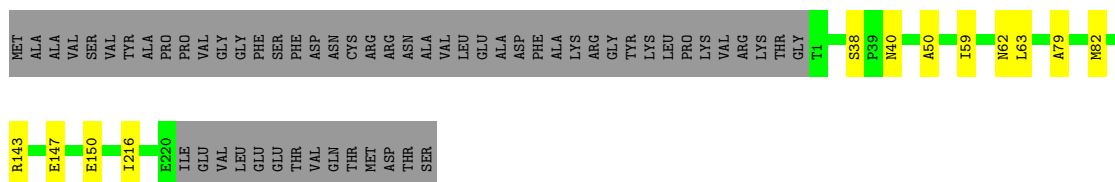
- Molecule 14: Proteasome subunit beta type-7

Chain O: 72% 7% 21%



- Molecule 14: Proteasome subunit beta type-7

Chain o: 75% 21%



- Molecule 15: Proteasome subunit beta type-3

Chain P: 91% 8%



- Molecule 15: Proteasome subunit beta type-3

Chain p: 92% 7%



- Molecule 16: Proteasome subunit beta type-2

Chain Q:  91% 8%



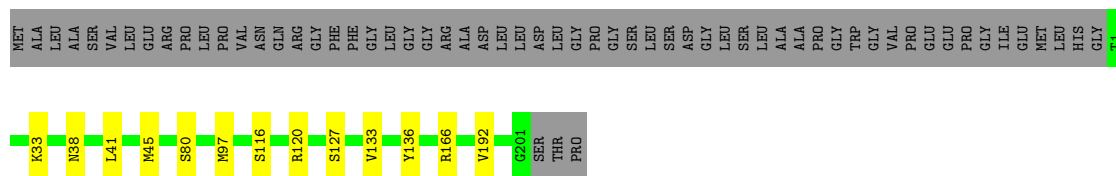
- Molecule 16: Proteasome subunit beta type-2

Chain q:  88% 11%



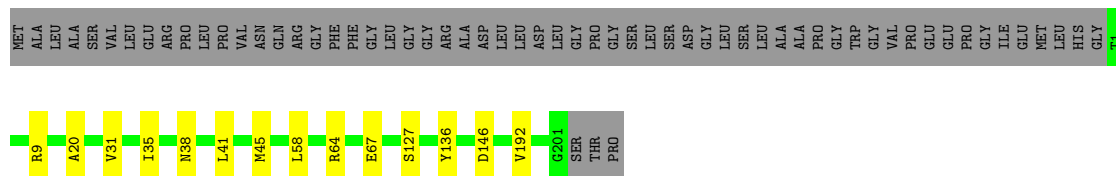
- Molecule 17: Proteasome subunit beta type-5

Chain R:  71% 5% 24%



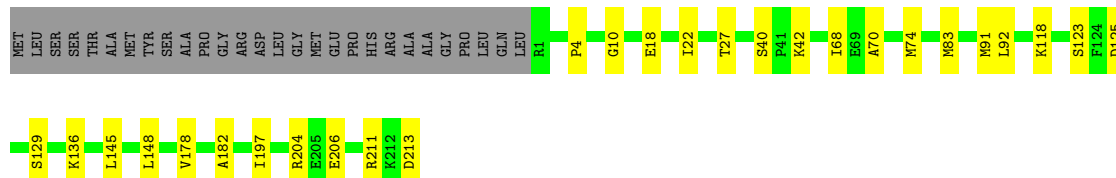
- Molecule 17: Proteasome subunit beta type-5

Chain r:  71% 5% 24%



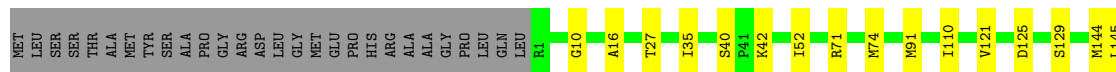
- Molecule 18: Proteasome subunit beta type-1

Chain S:  77% 11% 12%



- Molecule 18: Proteasome subunit beta type-1

Chain s:  78% 10% 12%





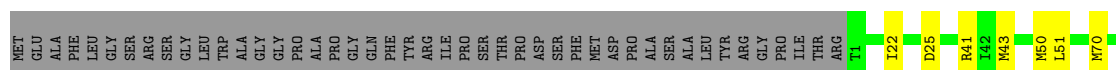
• Molecule 19: Proteasome subunit beta type-4

Chain T: 74% 8% 18%



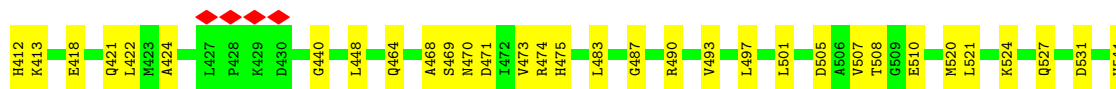
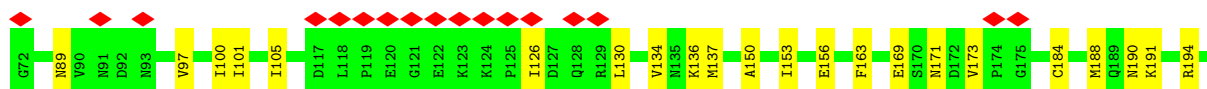
• Molecule 19: Proteasome subunit beta type-4

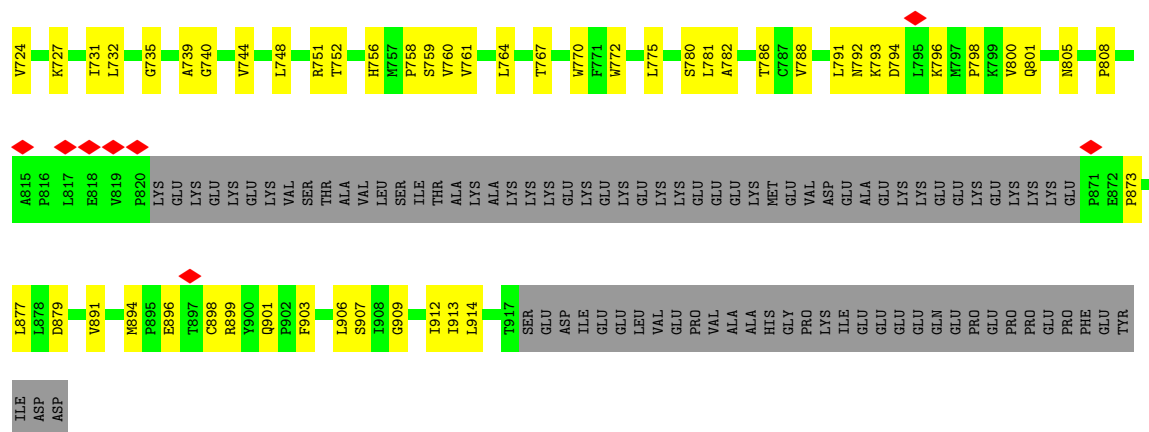
Chain t: 75% 7% 18%



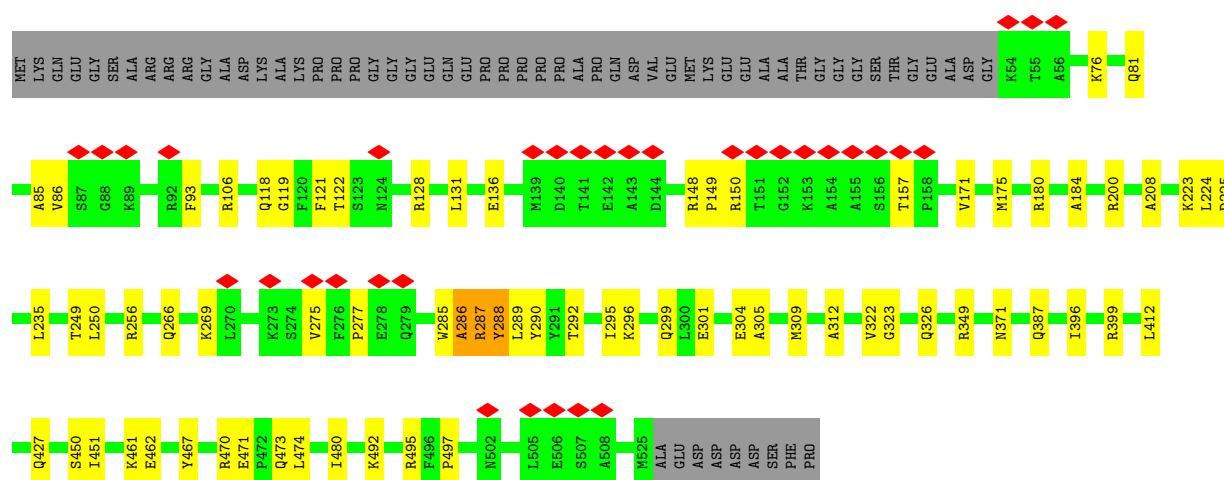
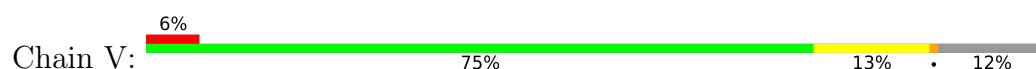
• Molecule 20: 26S proteasome non-ATPase regulatory subunit 1

Chain U: 62% 18% 20%

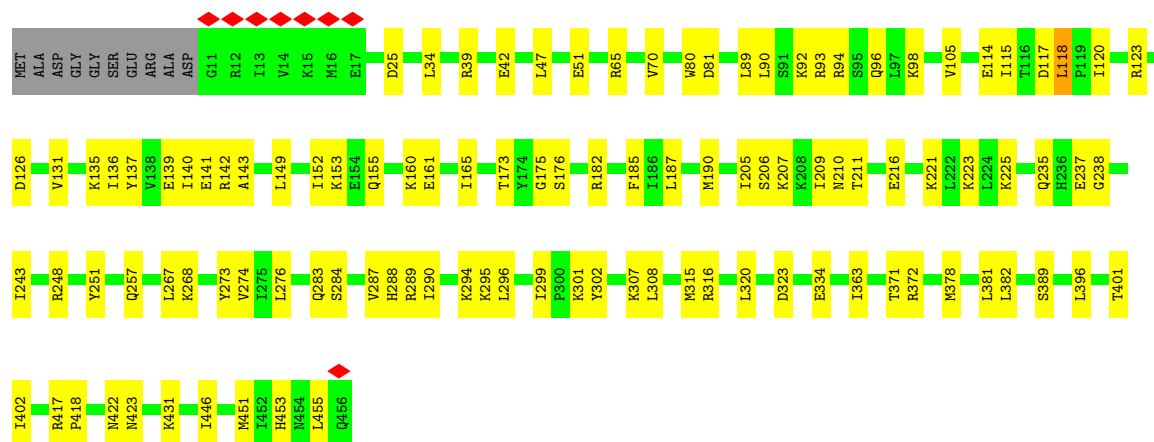
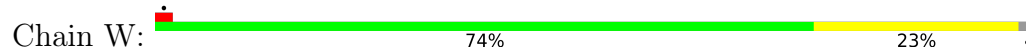




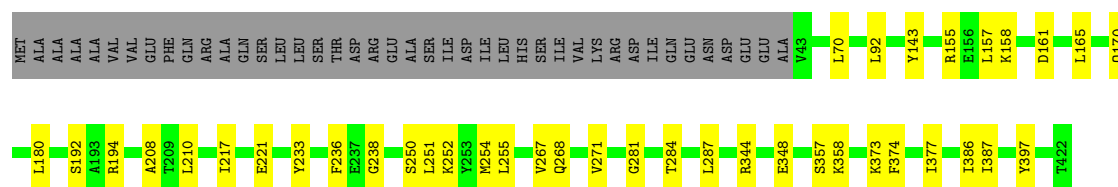
• Molecule 21: 26S proteasome non-ATPase regulatory subunit 3



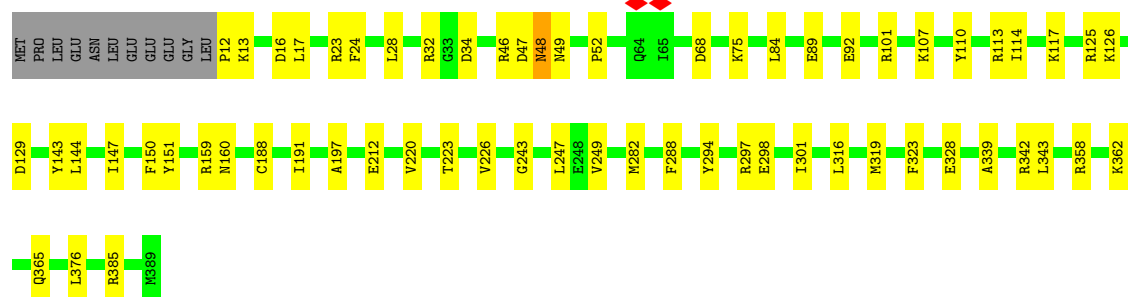
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 12



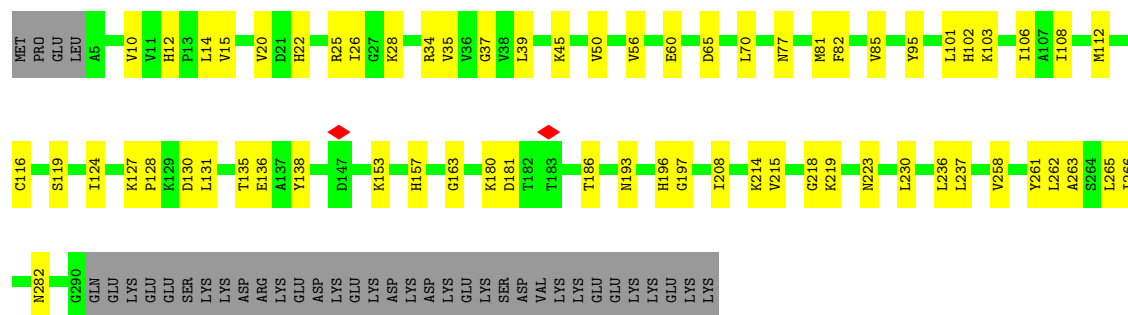
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 11



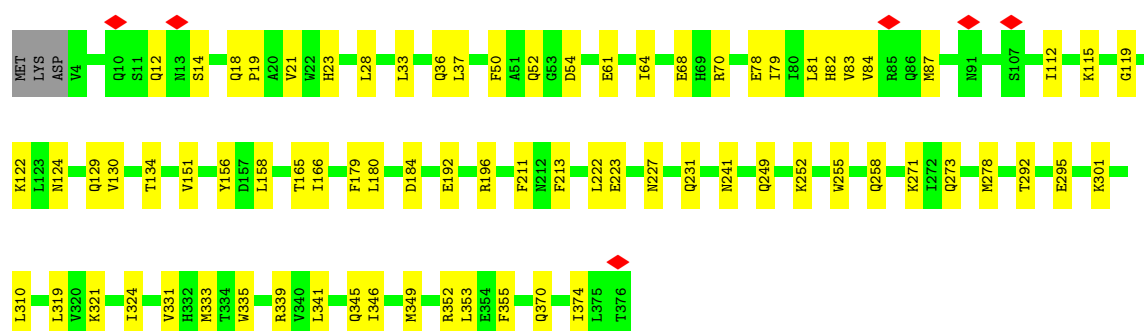
Chain Y: 81% 16%



Chain Z: 68% 20% 12%



Chain a: 79% 20%



Chain b:

Sequence logo for Chain b. The y-axis represents amino acid frequency. The x-axis shows positions 1 to 126. The logo is divided into three segments: 39% (positions 1-49), 12% (positions 50-61), and 49% (positions 62-126). Amino acids are color-coded: red for high frequency, yellow for medium, and green for low. A red diamond is present at position 1.

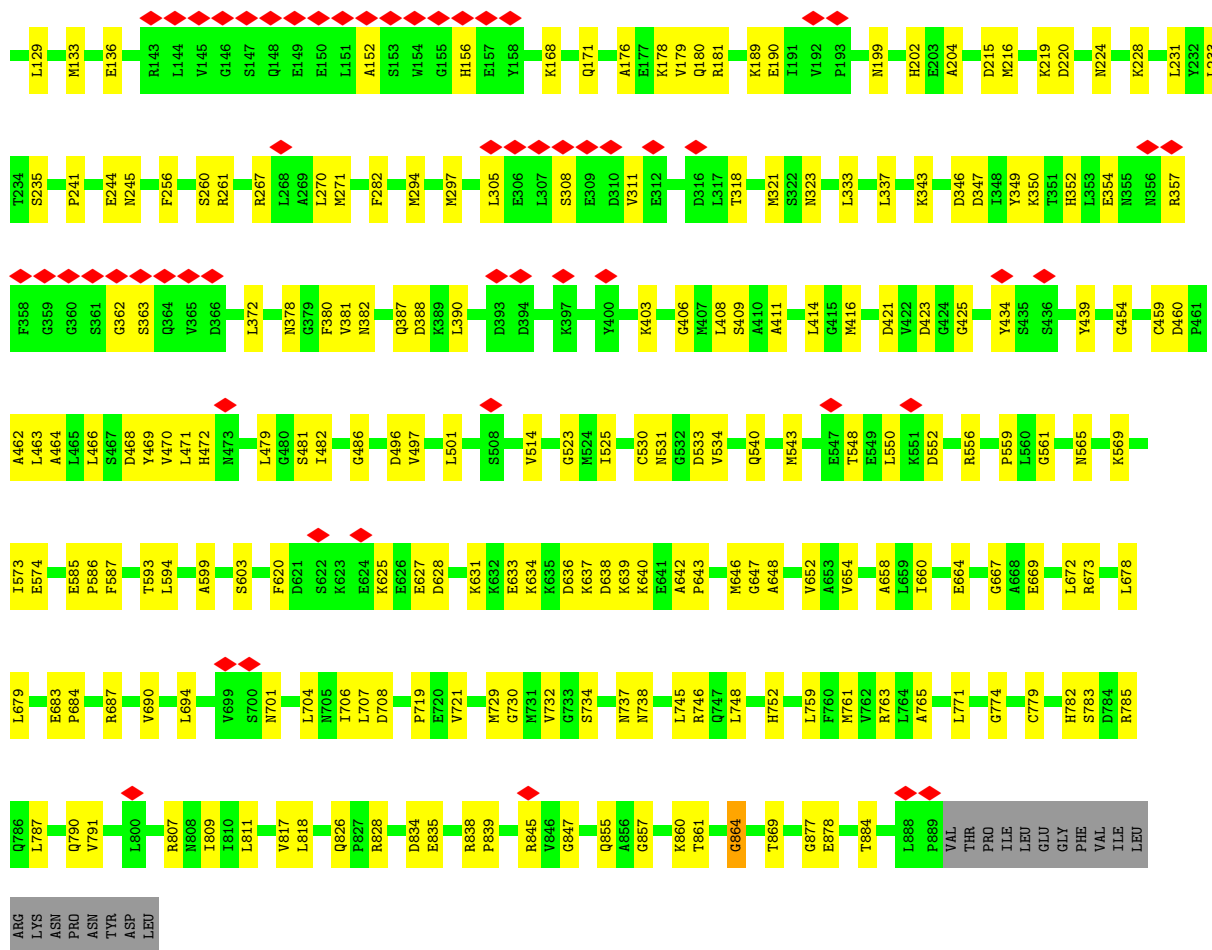
Position	Amino Acid	Frequency (%)
1	M1	39%
2	V2	39%
3	L3	39%
4	E4	39%
5	V8	39%
6	C9	39%
7	M12	39%
8	S13	39%
9	E14	39%
10	Y15	39%
11	M16	39%
12	R17	39%
13	L22	39%
14	P23	39%
15	T24	39%
16	R25	39%
17	Q30	39%
18	N34	39%
19	H38	39%
20	R42	39%
21	S43	39%
22	M44	39%
23	P45	39%
24	E46	39%
25	T53	39%
26	T62	39%
27	T63	39%
28	L64	39%
29	T65	39%
30	R70	39%
31	I71	39%
32	L75	39%
33	Q79	39%
34	L97	39%
35	R100	39%
36	K106	39%
37	M107	39%
38	I110	39%
39	A111	39%
40	L124	39%
41	V125	39%
42	K126	39%

Chain d:

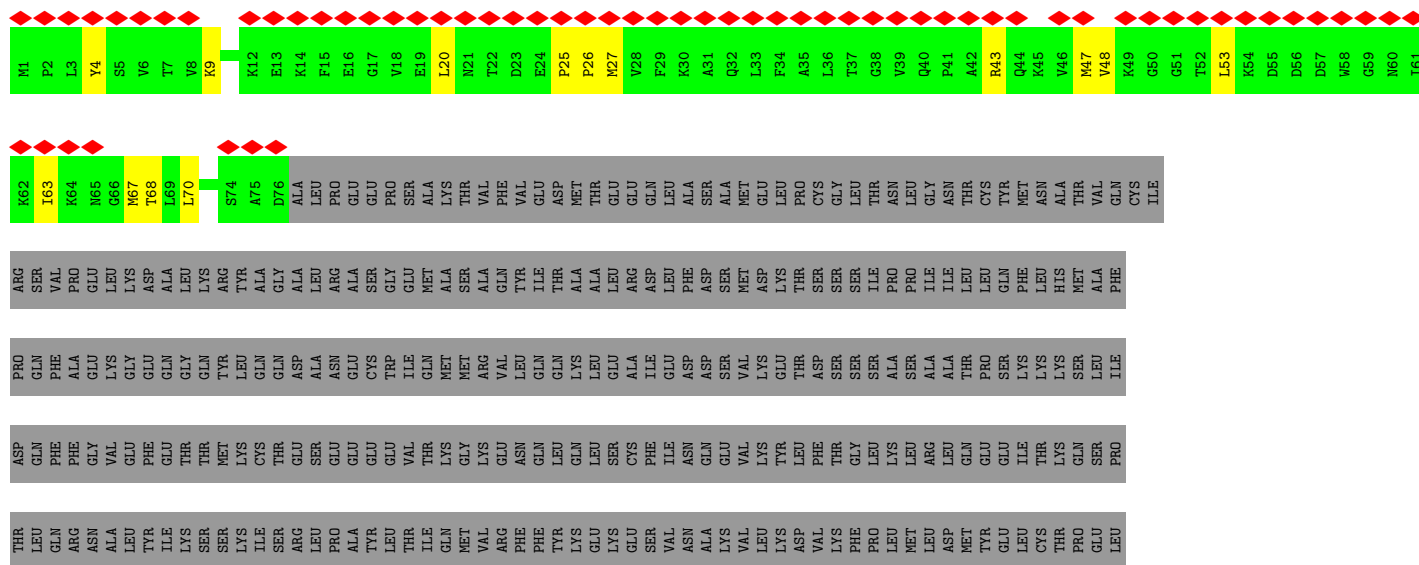
Sequence logo for Chain d. The y-axis represents the frequency of amino acids in bits. The x-axis represents the position in the chain (1 to 237). The legend indicates the following amino acid frequencies: MET (16%), PHE (57%), LYS (16%), and ARG (27%).

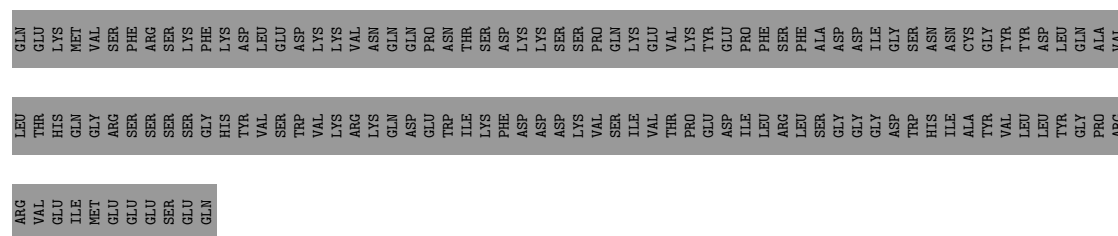
Position	Amino Acid	Frequency (bits)
1	LYS	0.16
2	LYS	0.16
3	LYS	0.16
4	LYS	0.16
5	LYS	0.16
6	LYS	0.16
7	LYS	0.16
8	LYS	0.16
9	LYS	0.16
10	LYS	0.16
11	LYS	0.16
12	LYS	0.16
13	LYS	0.16
14	LYS	0.16
15	LYS	0.16
16	LYS	0.16
17	LYS	0.16
18	LYS	0.16
19	LYS	0.16
20	LYS	0.16
21	LYS	0.16
22	LYS	0.16
23	LYS	0.16
24	LYS	0.16
25	LYS	0.16
26	LYS	0.16
27	LYS	0.16
28	LYS	0.16
29	LYS	0.16
30	LYS	0.16
31	LYS	0.16
32	LYS	0.16
33	LYS	0.16
34	LYS	0.16
35	LYS	0.16
36	LYS	0.16
37	LYS	0.16
38	LYS	0.16
39	LYS	0.16
40	LYS	0.16
41	LYS	0.16
42	LYS	0.16
43	LYS	0.16
44	LYS	0.16
45	LYS	0.16
46	LYS	0.16
47	LYS	0.16
48	LYS	0.16
49	LYS	0.16
50	LYS	0.16
51	LYS	0.16
52	LYS	0.16
53	LYS	0.16
54	LYS	0.16
55	LYS	0.16
56	LYS	0.16
57	LYS	0.16
58	LYS	0.16
59	LYS	0.16
60	LYS	0.16
61	LYS	0.16
62	LYS	0.16
63	LYS	0.16
64	LYS	0.16
65	LYS	0.16
66	LYS	0.16
67	LYS	0.16
68	LYS	0.16
69	LYS	0.16
70	LYS	0.16
71	LYS	0.16
72	LYS	0.16
73	LYS	0.16
74	LYS	0.16
75	LYS	0.16
76	LYS	0.16
77	LYS	0.16
78	LYS	0.16
79	LYS	0.16
80	LYS	0.16
81	LYS	0.16
82	LYS	0.16
83	LYS	0.16
84	LYS	0.16
85	LYS	0.16
86	LYS	0.16
87	LYS	0.16
88	LYS	0.16
89	LYS	0.16
90	LYS	0.16
91	LYS	0.16
92	LYS	0.16
93	LYS	0.16
94	LYS	0.16
95	LYS	0.16
96	LYS	0.16
97	LYS	0.16
98	LYS	0.16
99	LYS	0.16
100	LYS	0.16
101	LYS	0.16
102	LYS	0.16
103	LYS	0.16
104	LYS	0.16
105	LYS	0.16
106	LYS	0.16
107	LYS	0.16
108	LYS	0.16
109	LYS	0.16
110	LYS	0.16
111	LYS	0.16
112	LYS	0.16
113	LYS	0.16
114	LYS	0.16
115	LYS	0.16
116	LYS	0.16
117	LYS	0.16
118	LYS	0.16
119	LYS	0.16
120	LYS	0.16
121	LYS	0.16
122	LYS	0.16
123	LYS	0.16
124	LYS	0.16
125	LYS	0.16
126	LYS	0.16
127	LYS	0.16
128	LYS	0.16
129	LYS	0.16
130	LYS	0.16
131	LYS	0.16
132	LYS	0.16
133	LYS	0.16
134	LYS	0.16
135	LYS	0.16
136	LYS	0.16
137	LYS	0.16
138	LYS	0.16
139	LYS	0.16
140	LYS	0.16
141	LYS	0.16
142	LYS	0.16
143	LYS	0.16
144		

Chain f:



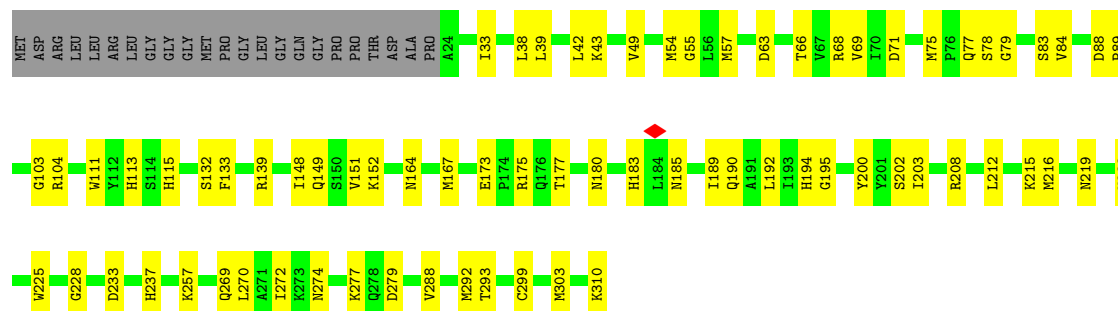
• Molecule 30: Ubiquitin carboxyl-terminal hydrolase 14





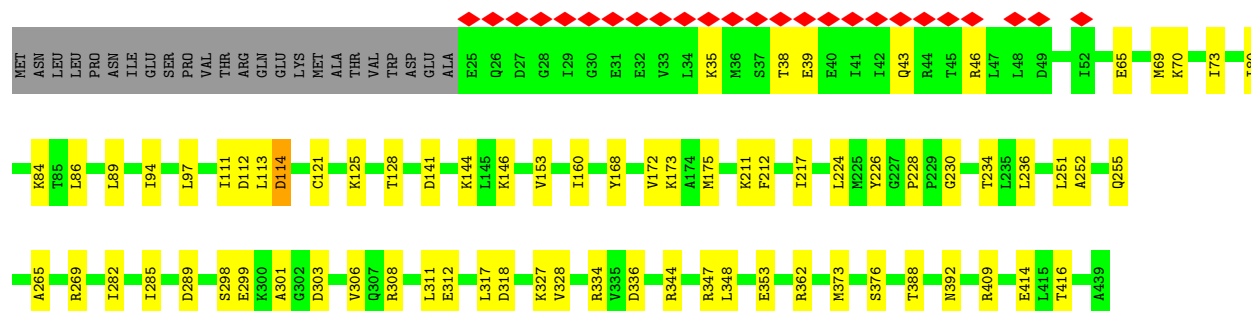
• Molecule 31: 26S proteasome non-ATPase regulatory subunit 14

Chain c: 69% 24% 7%



• Molecule 32: 26S protease regulatory subunit 6A

Chain F: 6% 78% 17% 5%



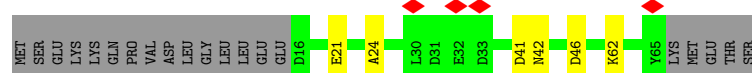
• Molecule 33: Ubiquitin

Chain u: 71% 29%



• Molecule 34: 26S proteasome complex subunit DSS1

Chain e: 6% 63% 9% 29%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	284997	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.029	Depositor
Minimum map value	-0.003	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	438.4, 438.4, 438.4	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/3294	0.50	0/4447
2	B	0.18	0/3086	0.46	0/4164
3	C	0.18	0/3007	0.46	0/4045
4	D	0.20	0/3089	0.50	0/4168
5	E	0.19	0/2904	0.51	3/3924 (0.1%)
6	G	0.18	0/1923	0.40	0/2601
6	g	0.18	0/1914	0.44	2/2590 (0.1%)
7	H	0.18	0/1844	0.38	0/2499
7	h	0.16	0/1844	0.37	0/2497
8	I	0.17	0/1991	0.37	0/2685
8	i	0.18	0/1985	0.40	0/2677
9	J	0.18	0/1906	0.43	0/2573
9	j	0.16	0/1887	0.41	0/2549
10	K	0.16	0/1804	0.35	0/2436
10	k	0.16	0/1809	0.37	0/2444
11	L	0.16	0/1901	0.34	0/2570
11	l	0.17	0/1896	0.38	0/2565
12	M	0.17	0/1911	0.35	0/2573
12	m	0.15	0/1916	0.33	0/2580
13	N	0.16	0/1540	0.31	0/2085
13	n	0.16	0/1536	0.32	0/2080
14	O	0.16	0/1676	0.39	0/2271
14	o	0.16	0/1686	0.35	0/2282
15	P	0.16	0/1616	0.38	0/2180
15	p	0.17	0/1620	0.38	0/2184
16	Q	0.17	0/1621	0.34	0/2194
16	q	0.16	0/1621	0.37	0/2194
17	R	0.17	0/1590	0.34	0/2147
17	r	0.16	0/1590	0.32	0/2147
18	S	0.17	0/1671	0.39	0/2252
18	s	0.18	0/1684	0.40	0/2268
19	T	0.18	0/1716	0.38	0/2323

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	t	0.17	0/1720	0.37	0/2328
20	U	0.17	0/6052	0.45	0/8190
21	V	0.18	0/3824	0.48	4/5170 (0.1%)
22	W	0.21	0/3683	0.55	0/4952
23	X	0.17	0/3053	0.43	0/4115
24	Y	0.22	0/3173	0.51	0/4273
25	Z	0.19	0/2324	0.49	0/3150
26	a	0.19	0/3053	0.52	0/4133
27	b	0.21	0/1478	0.52	0/2001
28	d	0.20	0/2162	0.49	0/2919
29	f	0.21	0/6980	0.56	1/9433 (0.0%)
30	x	0.14	0/599	0.38	0/805
31	c	0.20	0/2302	0.52	0/3110
32	F	0.21	0/3292	0.49	2/4435 (0.0%)
33	u	0.14	0/607	0.38	0/816
34	e	0.21	0/437	0.55	0/595
All	All	0.18	0/107817	0.45	12/145619 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	382	SER	N-CA-C	-5.90	101.46	109.54
29	f	864	GLY	N-CA-C	5.66	121.21	111.98
6	g	224	ASN	CA-C-N	-5.46	115.27	120.83
6	g	224	ASN	C-N-CA	-5.46	115.27	120.83
32	F	228	PRO	CA-C-N	-5.33	114.20	120.12
32	F	228	PRO	C-N-CA	-5.33	114.20	120.12
21	V	277	PRO	CA-C-N	5.31	131.67	121.54
21	V	277	PRO	C-N-CA	5.31	131.67	121.54
21	V	286	ALA	CA-C-N	5.21	131.50	121.54
21	V	286	ALA	C-N-CA	5.21	131.50	121.54
5	E	281	ARG	CA-C-N	-5.21	113.33	119.84
5	E	281	ARG	C-N-CA	-5.21	113.33	119.84

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	3240	0	3286	45	0
2	B	3042	0	3100	42	0
3	C	2968	0	3067	40	0
4	D	3039	0	3075	58	0
5	E	2860	0	2828	42	0
6	G	1889	0	1885	15	0
6	g	1880	0	1875	14	0
7	H	1805	0	1784	8	0
7	h	1805	0	1798	20	0
8	I	1958	0	1960	11	0
8	i	1955	0	1955	12	0
9	J	1880	0	1892	21	0
9	j	1861	0	1865	13	0
10	K	1777	0	1762	14	0
10	k	1782	0	1766	18	0
11	L	1866	0	1852	14	0
11	l	1861	0	1839	18	0
12	M	1876	0	1861	13	0
12	m	1881	0	1868	9	0
13	N	1514	0	1487	10	0
13	n	1510	0	1483	6	0
14	O	1649	0	1659	11	0
14	o	1659	0	1681	8	0
15	P	1587	0	1598	13	0
15	p	1591	0	1609	12	0
16	Q	1588	0	1584	12	0
16	q	1588	0	1584	16	0
17	R	1559	0	1523	9	0
17	r	1559	0	1523	8	0
18	S	1641	0	1639	15	0
18	s	1654	0	1656	15	0
19	T	1683	0	1662	14	0
19	t	1687	0	1666	13	0
20	U	5945	0	5995	106	0
21	V	3754	0	3749	47	0
22	W	3635	0	3762	67	0
23	X	3009	0	3113	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	Y	3115	0	3120	39	0
25	Z	2281	0	2312	53	0
26	a	2995	0	3012	50	0
27	b	1458	0	1505	29	0
28	d	2116	0	2146	38	0
29	f	6866	0	6866	157	0
30	x	588	0	607	11	0
31	c	2260	0	2276	53	0
32	F	3251	0	3318	53	0
33	u	601	0	629	15	0
34	e	425	0	328	6	0
35	A	31	0	12	0	0
35	B	31	0	12	0	0
35	D	31	0	12	0	0
35	E	31	0	12	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
36	E	1	0	0	0	0
36	F	1	0	0	0	0
37	C	27	0	12	0	0
37	F	27	0	12	0	0
38	c	1	0	0	0	0
All	All	106178	0	106482	1180	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 (1180) 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)
29:f:548:THR:O	29:f:552:ASP:HB2	1.64	0.97
20:U:342:LEU:O	20:U:346:ASN:HB2	1.69	0.93
20:U:464:GLN:O	20:U:468:ALA:HB2	1.75	0.85
21:V:285:TRP:O	21:V:289:LEU:HB2	1.80	0.81
31:c:113:HIS:NE2	31:c:115:HIS:CD2	2.59	0.71
22:W:417:ARG:HE	22:W:418:PRO:HD2	1.55	0.70
26:a:64:ILE:O	26:a:68:GLU:HB2	1.90	0.70
26:a:70:ARG:HG3	27:b:17:ARG:HB3	1.73	0.70
13:N:4:MET:HG3	13:N:127:ILE:HG22	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:134:VAL:HA	20:U:137:MET:HE2	1.75	0.69
5:E:198:VAL:HG12	5:E:200:SER:H	1.58	0.68
28:d:63:ILE:HG12	28:d:101:LEU:HD21	1.75	0.68
22:W:51:GLU:OE2	22:W:94:ARG:NH2	2.26	0.68
19:t:96:MET:HE2	19:t:110:MET:HE1	1.74	0.68
29:f:176:ALA:HB3	29:f:178:LYS:HE2	1.77	0.67
20:U:894:MET:HE1	20:U:906:LEU:HB3	1.77	0.67
9:J:96:LEU:HD22	16:Q:62:LYS:HD3	1.76	0.67
3:C:89:VAL:HG12	3:C:91:PRO:HD2	1.77	0.67
29:f:828:ARG:HG2	29:f:845:ARG:H	1.60	0.66
9:J:96:LEU:HD11	16:Q:58:GLU:HB3	1.76	0.66
20:U:666:LYS:HA	20:U:669:ILE:HD12	1.77	0.66
25:Z:193:ASN:HB2	31:c:228:GLY:HA2	1.76	0.66
4:D:67:ASN:ND2	20:U:607:VAL:O	2.29	0.66
18:s:172:MET:HE1	18:s:195:ILE:HG21	1.77	0.65
29:f:642:ALA:HB2	29:f:763:ARG:HH21	1.60	0.65
4:D:159:LYS:HD3	4:D:221:HIS:HA	1.76	0.65
1:A:55:LEU:HD11	2:B:76:GLU:HG2	1.79	0.65
32:F:111:ILE:HB	32:F:114:ASP:HB2	1.79	0.65
28:d:215:TRP:HE3	28:d:222:TYR:HB3	1.62	0.64
31:c:71:ASP:HB2	31:c:104:ARG:HH22	1.62	0.64
7:h:4:ARG:NH2	12:m:126:SER:OG	2.31	0.64
27:b:100:ARG:NH2	27:b:107:MET:SD	2.70	0.64
31:c:57:MET:HB3	31:c:69:VAL:HG21	1.79	0.64
29:f:845:ARG:HD3	29:f:847:GLY:H	1.63	0.64
18:s:148:LEU:HD23	18:s:178:VAL:HG12	1.79	0.64
29:f:464:ALA:HB2	30:x:47:MET:HE2	1.80	0.64
32:F:282:ILE:HG22	32:F:327:LYS:HB2	1.80	0.64
20:U:184:CYS:O	20:U:188:MET:HB3	1.98	0.63
20:U:505:ASP:HB3	20:U:508:THR:HG22	1.80	0.63
25:Z:223:ASN:ND2	26:a:341:LEU:O	2.31	0.63
33:u:8:LEU:HD11	33:u:70:VAL:HG13	1.80	0.63
22:W:135:LYS:HG3	22:W:139:GLU:HG2	1.80	0.63
5:E:202:SER:HA	32:F:269:ARG:HH22	1.64	0.62
20:U:191:LYS:HB3	20:U:194:ARG:HH21	1.64	0.62
22:W:90:LEU:HD23	22:W:93:ARG:HE	1.63	0.62
26:a:112:ILE:HD12	26:a:151:VAL:HG11	1.82	0.62
3:C:258:ARG:HG2	3:C:265:GLY:H	1.63	0.62
4:D:155:THR:HG23	4:D:159:LYS:HE3	1.82	0.62
29:f:95:PRO:HG2	29:f:96:LEU:HD12	1.82	0.62
29:f:706:ILE:HG23	29:f:745:LEU:HG	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ARG:HH12	32:F:306:VAL:HG21	1.63	0.61
23:X:194:ARG:HG2	23:X:210:LEU:HD21	1.83	0.61
26:a:33:LEU:HD13	26:a:36:GLN:HB2	1.81	0.61
29:f:117:GLU:H	29:f:120:ARG:HH21	1.49	0.61
2:B:49:LEU:HD21	29:f:646:MET:HB2	1.83	0.61
6:g:158:GLY:O	7:h:84:ARG:NH2	2.34	0.61
26:a:331:VAL:HB	26:a:333:MET:HE3	1.83	0.61
17:R:192:VAL:HG11	15:p:205:ASP:HB3	1.83	0.60
2:B:173:VAL:HG11	3:C:230:MET:HG2	1.82	0.60
29:f:294:MET:HA	29:f:297:MET:HE2	1.83	0.60
33:u:23:ILE:HB	33:u:52:ASP:HA	1.83	0.60
32:F:318:ASP:HB3	32:F:347:ARG:HG2	1.83	0.60
12:m:34:SER:OG	12:m:65:ARG:NH1	2.33	0.60
22:W:142:ARG:HH22	22:W:182:ARG:HD3	1.67	0.60
26:a:341:LEU:HD13	26:a:345:GLN:HB2	1.83	0.60
29:f:403:LYS:HG3	29:f:406:GLY:H	1.67	0.60
25:Z:214:LYS:HG2	25:Z:218:GLY:HA3	1.83	0.60
27:b:157:VAL:HG21	27:b:170:LEU:HB2	1.84	0.60
3:C:49:ARG:HH21	20:U:639:LEU:HG	1.67	0.59
6:G:158:GLY:O	7:H:84:ARG:NH2	2.34	0.59
16:Q:1:MET:HE3	16:Q:133:GLY:HA2	1.83	0.59
20:U:759:SER:HA	20:U:782:ALA:HA	1.84	0.59
25:Z:263:ALA:HB1	31:c:288:VAL:HG13	1.84	0.59
7:h:4:ARG:HD3	12:m:127:ALA:HB2	1.84	0.59
1:A:390:THR:HA	2:B:216:ILE:HD11	1.85	0.59
20:U:469:SER:OG	20:U:470:ASN:N	2.34	0.59
27:b:15:TYR:O	27:b:25:ARG:NH1	2.35	0.59
10:K:91:LYS:HG2	10:K:119:LEU:HD11	1.83	0.59
32:F:224:LEU:HB2	32:F:348:LEU:HD23	1.83	0.59
4:D:81:ARG:HH21	31:c:149:GLN:HB3	1.66	0.59
20:U:898:CYS:SG	20:U:899:ARG:N	2.71	0.59
25:Z:131:LEU:O	25:Z:196:HIS:NE2	2.36	0.59
20:U:555:VAL:HG13	20:U:556:MET:HG3	1.85	0.59
22:W:307:LYS:NZ	22:W:315:MET:SD	2.76	0.59
23:X:255:LEU:HD22	23:X:267:VAL:HG13	1.85	0.59
29:f:652:VAL:HG11	29:f:687:ARG:HD3	1.85	0.59
27:b:25:ARG:NH2	27:b:145:GLU:OE1	2.36	0.58
19:T:26:MET:HE2	19:T:188:GLN:HG3	1.85	0.58
2:B:49:LEU:HG	2:B:51:LEU:HD23	1.86	0.58
12:M:204:VAL:HG13	12:M:205:LYS:HG3	1.85	0.58
20:U:770:TRP:O	31:c:177:THR:OG1	2.21	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:363:ILE:HD11	22:W:382:LEU:HD11	1.83	0.58
27:b:124:LEU:HD13	27:b:156:PHE:HB2	1.86	0.58
5:E:355:ILE:HD11	32:F:211:LYS:HG2	1.85	0.58
22:W:296:LEU:HB3	22:W:302:TYR:HB2	1.86	0.58
21:V:85:ALA:HB2	21:V:93:PHE:HB2	1.86	0.58
29:f:701:ASN:HB3	29:f:704:LEU:HB2	1.85	0.58
29:f:189:LYS:HG2	29:f:190:GLU:HG3	1.84	0.58
24:Y:125:ARG:HH21	24:Y:159:ARG:HH22	1.52	0.58
25:Z:12:HIS:ND1	25:Z:50:VAL:O	2.36	0.58
29:f:748:LEU:O	29:f:752:HIS:HB2	2.04	0.58
20:U:418:GLU:HG2	20:U:422:LEU:HB2	1.85	0.57
1:A:330:ALA:O	1:A:336:ARG:NH1	2.37	0.57
16:Q:68:LYS:HG3	16:Q:74:GLU:HG2	1.86	0.57
18:S:211:ARG:NH2	18:S:213:ASP:OD2	2.38	0.57
29:f:333:LEU:HA	29:f:337:LEU:HB2	1.86	0.57
29:f:748:LEU:O	29:f:752:HIS:CB	2.52	0.57
31:c:79:GLY:HA3	31:c:84:VAL:HA	1.85	0.57
1:A:274:PHE:HB2	1:A:319:MET:HG2	1.86	0.57
3:C:63:LEU:HD12	4:D:79:VAL:HA	1.84	0.57
4:D:320:ALA:O	4:D:326:ARG:NH1	2.37	0.57
15:P:177:ARG:NH2	18:s:150:ASP:OD2	2.31	0.57
24:Y:101:ARG:NH2	24:Y:126:LYS:O	2.34	0.57
29:f:125:ILE:HG12	29:f:129:LEU:HB2	1.86	0.57
31:c:49:VAL:HG23	31:c:148:ILE:HD11	1.86	0.57
18:S:148:LEU:HD23	18:S:178:VAL:HG12	1.86	0.57
29:f:231:LEU:HD22	29:f:235:SER:HB2	1.86	0.57
6:g:147:GLN:OE1	6:g:150:GLN:NE2	2.38	0.57
1:A:324:PRO:HA	1:A:327:LEU:HD13	1.87	0.57
3:C:20:LEU:HD12	3:C:21:ARG:HE	1.69	0.57
25:Z:37:GLY:HA2	25:Z:56:VAL:HG12	1.86	0.57
7:h:175:GLU:OE2	8:i:53:HIS:NE2	2.31	0.57
9:j:215:GLN:HE22	9:j:218:LYS:HG2	1.69	0.57
20:U:793:LYS:HB2	20:U:796:LYS:HB3	1.87	0.57
18:s:145:LEU:HD22	18:s:178:VAL:HB	1.86	0.57
26:a:115:LYS:HB3	26:a:134:THR:HG23	1.85	0.57
27:b:30:GLN:HG3	27:b:75:LEU:HB3	1.86	0.57
26:a:19:PRO:O	26:a:23:HIS:ND1	2.36	0.57
6:G:67:THR:HG22	6:G:69:LEU:H	1.70	0.57
11:L:157:ARG:NH2	12:M:60:GLU:OE1	2.38	0.57
6:g:141:ILE:HG22	6:g:151:VAL:HG22	1.85	0.57
20:U:153:ILE:HA	20:U:156:GLU:HB2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:413:LYS:HD2	20:U:780:SER:HB2	1.86	0.56
10:k:66:LYS:HA	10:k:78:MET:HE2	1.87	0.56
1:A:204:LEU:HD23	1:A:206:ILE:HD13	1.87	0.56
5:E:253:ILE:HG13	32:F:308:ARG:HH22	1.70	0.56
22:W:105:VAL:HG21	22:W:140:ILE:HG12	1.87	0.56
23:X:397:TYR:HE1	25:Z:258:VAL:HG21	1.70	0.56
4:D:91:GLN:NE2	4:D:127:ASN:OD1	2.39	0.56
24:Y:144:LEU:HB3	24:Y:160:ASN:HD22	1.70	0.56
25:Z:70:LEU:HD11	25:Z:108:ILE:HG23	1.87	0.56
25:Z:127:LYS:HG2	31:c:212:LEU:HD11	1.87	0.56
26:a:78:GLU:O	26:a:82:HIS:ND1	2.38	0.56
26:a:249:GLN:OE1	26:a:301:LYS:NZ	2.38	0.56
16:q:168:GLN:NE2	16:q:175:LEU:O	2.38	0.56
21:V:287:ARG:O	21:V:290:TYR:N	2.39	0.56
21:V:371:ASN:OD1	21:V:427:GLN:NE2	2.38	0.56
6:G:6:SER:OG	6:G:11:ARG:NH1	2.39	0.56
26:a:278:MET:HE1	26:a:319:LEU:HB2	1.86	0.56
27:b:151:GLU:OE1	27:b:152:LYS:NZ	2.34	0.56
4:D:200:ARG:HH22	4:D:301:GLN:HA	1.70	0.56
4:D:391:ARG:HG2	4:D:393:ILE:H	1.69	0.56
21:V:461:LYS:NZ	21:V:462:GLU:O	2.33	0.56
27:b:2:VAL:O	27:b:44:ASN:ND2	2.38	0.56
3:C:232:ARG:NH1	3:C:279:GLN:OE1	2.37	0.56
20:U:669:ILE:HG21	20:U:705:LYS:HG3	1.87	0.56
22:W:80:TRP:HB3	22:W:123:ARG:HE	1.69	0.56
29:f:387:GLN:NE2	29:f:388:ASP:OD1	2.38	0.56
12:M:34:SER:OG	12:M:65:ARG:NH1	2.34	0.56
19:T:44:ARG:NH2	19:T:47:ASN:OD1	2.39	0.56
23:X:374:PHE:HZ	23:X:387:ILE:HG12	1.69	0.56
29:f:323:ASN:ND2	29:f:454:GLY:O	2.39	0.56
29:f:470:VAL:HG12	29:f:471:LEU:HG	1.88	0.56
14:o:143:ARG:NH2	14:o:150:GLU:OE1	2.39	0.56
20:U:173:VAL:HB	20:U:208:LEU:HD11	1.88	0.56
29:f:643:PRO:HG2	29:f:647:GLY:H	1.70	0.56
17:r:64:ARG:NH1	17:r:67:GLU:OE1	2.39	0.56
5:E:84:ARG:NH1	32:F:114:ASP:OD1	2.39	0.56
20:U:801:GLN:HB3	20:U:877:LEU:HD22	1.89	0.56
21:V:296:LYS:HB3	21:V:301:GLU:HB3	1.88	0.56
12:m:8:ASP:O	12:m:22:GLN:NE2	2.39	0.56
12:m:179:LEU:HD12	12:m:184:MET:HE1	1.88	0.56
5:E:237:ALA:HB1	32:F:308:ARG:HG3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:10:GLY:HA3	18:S:42:LYS:HE2	1.87	0.55
24:Y:32:ARG:NH1	24:Y:34:ASP:OD1	2.39	0.55
29:f:482:ILE:HG22	29:f:501:LEU:HD11	1.86	0.55
8:I:48:GLU:HG3	8:I:201:MET:HE1	1.87	0.55
8:i:106:PRO:HB2	8:i:109:GLN:HG3	1.88	0.55
32:F:376:SER:HB3	32:F:414:GLU:HG3	1.88	0.55
3:C:48:GLN:HB2	21:V:495:ARG:HD3	1.88	0.55
4:D:49:GLN:NE2	4:D:52:GLU:OE1	2.39	0.55
9:J:116:GLN:NE2	10:K:84:ASP:OD1	2.39	0.55
20:U:208:LEU:HD23	20:U:210:LYS:H	1.71	0.55
20:U:356:THR:HG21	20:U:731:ILE:HD13	1.89	0.55
22:W:90:LEU:O	22:W:96:GLN:NE2	2.39	0.55
22:W:274:VAL:O	22:W:283:GLN:NE2	2.39	0.55
29:f:783:SER:HB2	29:f:790:GLN:HG2	1.88	0.55
7:h:59:GLU:HG2	7:h:60:ARG:HD3	1.89	0.55
33:u:14:THR:O	33:u:33:LYS:NZ	2.39	0.55
2:B:317:ASP:HB2	2:B:346:ARG:HG2	1.89	0.55
20:U:527:GLN:NE2	20:U:531:ASP:OD2	2.39	0.55
24:Y:12:PRO:O	24:Y:113:ARG:NH1	2.38	0.55
19:t:25:ASP:OD1	19:t:41:ARG:NH2	2.37	0.55
31:c:63:ASP:O	31:c:139:ARG:NH1	2.39	0.55
1:A:70:THR:OG1	1:A:71:GLY:N	2.39	0.55
8:I:106:PRO:HB2	8:I:109:GLN:HG3	1.89	0.55
20:U:229:VAL:HA	20:U:232:ILE:HG12	1.88	0.55
32:F:38:THR:HG22	32:F:39:GLU:HG2	1.89	0.55
7:h:143:ARG:NH1	7:h:144:PRO:O	2.40	0.55
21:V:131:LEU:HD22	21:V:171:VAL:HG11	1.87	0.55
27:b:97:LEU:HA	27:b:100:ARG:HE	1.71	0.55
3:C:80:MET:HE1	3:C:96:VAL:HG13	1.88	0.55
28:d:36:LEU:HD23	28:d:38:THR:H	1.71	0.55
29:f:869:THR:HA	29:f:884:THR:HA	1.89	0.55
16:q:118:MET:HE2	16:q:124:LEU:HD13	1.89	0.55
21:V:266:GLN:HE21	21:V:295:ILE:HG23	1.72	0.54
24:Y:101:ARG:HH22	24:Y:129:ASP:HB2	1.72	0.54
20:U:772:TRP:HB3	20:U:775:LEU:HB2	1.89	0.54
22:W:187:LEU:HA	22:W:190:MET:HE1	1.90	0.54
31:c:132:SER:OG	33:u:40:GLN:OE1	2.23	0.54
2:B:215:GLY:HA2	29:f:845:ARG:HH12	1.71	0.54
4:D:231:VAL:HG12	4:D:234:GLU:HG2	1.90	0.54
20:U:126:ILE:HG23	20:U:130:LEU:HD23	1.89	0.54
25:Z:20:VAL:HG21	31:c:216:MET:HG3	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:n:84:LYS:NZ	13:n:85:GLU:OE2	2.40	0.54
29:f:168:LYS:HG2	29:f:204:ALA:HB2	1.90	0.54
7:h:42:ASN:ND2	7:h:183:GLU:OE2	2.41	0.54
7:h:166:ASN:OD1	7:h:169:ASN:ND2	2.41	0.54
10:k:99:HIS:HB2	10:k:107:MET:HE3	1.90	0.54
1:A:213:LEU:HD22	1:A:337:LEU:HD23	1.89	0.54
11:L:41:LYS:NZ	11:L:180:MET:O	2.33	0.54
20:U:440:GLY:HA2	20:U:473:VAL:HG13	1.88	0.54
31:c:164:ASN:HB2	31:c:167:MET:HB2	1.89	0.54
30:x:9:LYS:HB3	30:x:68:THR:HA	1.89	0.54
20:U:350:LEU:HD13	20:U:385:PHE:HD1	1.73	0.54
22:W:160:LYS:NZ	22:W:161:GLU:OE2	2.41	0.54
29:f:45:LEU:HD22	29:f:56:LEU:HD12	1.90	0.54
4:D:274:ARG:N	5:E:245:GLU:OE2	2.40	0.54
16:Q:26:VAL:HG21	17:R:136:TYR:HE2	1.73	0.54
3:C:57:ARG:NH2	20:U:643:SER:O	2.41	0.54
8:I:38:LEU:HD23	8:I:160:LYS:HG2	1.90	0.54
22:W:216:GLU:OE1	22:W:223:LYS:NZ	2.40	0.54
29:f:530:CYS:HB3	29:f:565:ASN:HD21	1.73	0.54
29:f:672:LEU:HD13	29:f:708:ASP:HB3	1.90	0.54
33:u:8:LEU:HD21	33:u:70:VAL:HG22	1.90	0.54
15:P:58:THR:O	16:Q:85:ARG:NH2	2.42	0.53
33:u:16:GLU:O	33:u:29:LYS:NZ	2.39	0.53
4:D:244:PRO:HB3	4:D:291:GLU:HG3	1.90	0.53
22:W:89:LEU:HA	22:W:92:LYS:HG2	1.90	0.53
29:f:50:LYS:HG3	29:f:51:GLN:HG3	1.90	0.53
29:f:633:GLU:HA	29:f:636:ASP:HB2	1.90	0.53
18:S:4:PRO:HB2	19:T:100:ARG:HH21	1.73	0.53
19:T:25:ASP:OD1	19:T:41:ARG:NH2	2.37	0.53
20:U:381:THR:HG22	20:U:412:HIS:HA	1.88	0.53
20:U:896:GLU:HA	20:U:901:GLN:HG2	1.89	0.53
22:W:316:ARG:HH12	22:W:381:LEU:HA	1.74	0.53
26:a:84:VAL:HA	26:a:87:MET:HG3	1.90	0.53
29:f:305:LEU:O	29:f:308:SER:OG	2.26	0.53
18:s:71:ARG:HD2	18:s:74:MET:HE3	1.91	0.53
18:s:211:ARG:NH2	18:s:213:ASP:OD2	2.41	0.53
18:S:125:ASP:OD1	18:S:129:SER:N	2.42	0.53
9:j:116:GLN:NE2	9:j:120:GLN:OE1	2.39	0.53
9:j:146:GLN:OE1	9:j:159:ASN:ND2	2.41	0.53
2:B:387:LYS:HB3	2:B:390:LEU:HD23	1.90	0.53
24:Y:17:LEU:HD13	24:Y:212:GLU:HA	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:301:ILE:HG13	24:Y:343:LEU:HD12	1.91	0.53
29:f:586:PRO:HB2	29:f:625:LYS:HE3	1.91	0.53
18:s:125:ASP:OD1	18:s:129:SER:N	2.42	0.53
3:C:147:THR:OG1	3:C:206:HIS:NE2	2.39	0.53
9:J:220:LEU:HD13	9:J:224:GLU:HB2	1.91	0.53
31:c:88:ASP:N	31:c:88:ASP:OD1	2.42	0.53
31:c:270:LEU:O	31:c:274:ASN:ND2	2.42	0.53
20:U:571:CYS:SG	20:U:601:ARG:NH2	2.82	0.53
26:a:278:MET:HB3	26:a:339:ARG:HH22	1.74	0.53
10:K:235:GLU:HA	10:K:238:ILE:HG22	1.91	0.53
9:j:115:LYS:NZ	9:j:129:ILE:O	2.41	0.53
2:B:56:THR:OG1	29:f:181:ARG:NH2	2.42	0.52
5:E:352:MET:HE1	32:F:212:PHE:HE1	1.74	0.52
9:J:196:LEU:HA	9:J:199:VAL:HG12	1.89	0.52
13:N:144:ARG:HG2	13:N:147:MET:HE3	1.91	0.52
22:W:248:ARG:HG3	22:W:289:ARG:HH22	1.74	0.52
29:f:809:ILE:HD11	29:f:857:GLY:HA2	1.91	0.52
32:F:153:VAL:HG22	32:F:160:ILE:HG22	1.91	0.52
7:H:166:ASN:OD1	7:H:169:ASN:ND2	2.37	0.52
20:U:362:ASN:O	31:c:175:ARG:NH1	2.42	0.52
21:V:399:ARG:NH2	28:d:145:GLU:OE2	2.42	0.52
25:Z:39:LEU:HD13	25:Z:95:TYR:HB3	1.91	0.52
26:a:165:THR:HG22	26:a:166:ILE:H	1.74	0.52
1:A:234:ASP:O	29:f:352:HIS:NE2	2.42	0.52
2:B:196:GLU:OE2	2:B:349:ARG:NH1	2.42	0.52
7:h:65:VAL:O	7:h:220:ARG:NH1	2.41	0.52
3:C:53:ASN:ND2	20:U:642:GLU:O	2.42	0.52
20:U:490:ARG:HB2	20:U:493:VAL:HG12	1.92	0.52
25:Z:65:ASP:OD1	25:Z:65:ASP:N	2.43	0.52
29:f:199:ASN:HA	29:f:202:HIS:CD2	2.44	0.52
29:f:75:LEU:HD12	29:f:77:GLU:H	1.73	0.52
5:E:387:LYS:HE2	5:E:388:PRO:HD2	1.91	0.52
6:G:190:THR:OG1	6:G:193:GLN:OE1	2.27	0.52
22:W:315:MET:HB3	22:W:320:LEU:HD11	1.91	0.52
9:j:96:LEU:HB2	16:q:62:LYS:HD2	1.92	0.52
31:c:89:PRO:HG2	33:u:44:ILE:HD11	1.90	0.52
17:R:80:SER:OG	17:R:120:ARG:NH1	2.40	0.52
10:k:13:ASN:HB2	11:l:126:ARG:HG2	1.90	0.52
10:K:20:ARG:NH1	10:K:25:GLU:OE1	2.44	0.51
21:V:349:ARG:NH1	34:e:41:ASP:OD2	2.44	0.51
25:Z:28:LYS:NZ	31:c:103:GLY:O	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:14:GLN:HG2	29:f:63:LEU:HD11	1.92	0.51
6:g:165:ALA:HB1	6:g:179:LEU:HD13	1.92	0.51
20:U:324:LYS:HA	20:U:327:LYS:HE3	1.90	0.51
21:V:467:TYR:HE2	24:Y:362:LYS:HE2	1.75	0.51
22:W:221:LYS:NZ	22:W:257:GLN:OE1	2.43	0.51
26:a:50:PHE:HD2	26:a:52:GLN:HB3	1.75	0.51
3:C:83:LYS:HA	3:C:105:ILE:HD11	1.91	0.51
6:G:188:ASP:OD1	6:G:188:ASP:N	2.43	0.51
29:f:62:ARG:O	29:f:66:LYS:NZ	2.37	0.51
17:r:38:ASN:HD21	17:r:41:LEU:HD12	1.75	0.51
3:C:187:LEU:HD23	3:C:314:LYS:HG2	1.92	0.51
5:E:84:ARG:HB2	5:E:87:LEU:HD23	1.93	0.51
25:Z:25:ARG:HB2	31:c:104:ARG:HD2	1.91	0.51
29:f:244:GLU:OE1	29:f:244:GLU:N	2.40	0.51
29:f:357:ARG:NH1	29:f:362:GLY:O	2.44	0.51
29:f:664:GLU:OE1	29:f:667:GLY:N	2.44	0.51
1:A:44:GLN:OE1	1:A:47:GLN:NE2	2.36	0.51
22:W:98:LYS:HG3	22:W:139:GLU:HG3	1.92	0.51
22:W:422:ASN:OD1	22:W:423:ASN:N	2.43	0.51
23:X:357:SER:OG	23:X:358:LYS:N	2.43	0.51
27:b:34:ASN:O	27:b:38:HIS:ND1	2.39	0.51
29:f:260:SER:HB2	29:f:270:LEU:HB3	1.93	0.51
29:f:408:LEU:HB2	29:f:439:TYR:HD2	1.74	0.51
7:h:9:SER:HA	7:h:125:GLY:HA2	1.92	0.51
11:L:226:ASP:OD1	11:L:226:ASP:N	2.43	0.51
22:W:131:VAL:HG13	22:W:140:ILE:HG21	1.92	0.51
29:f:468:ASP:OD1	29:f:468:ASP:N	2.43	0.51
29:f:559:PRO:HB2	29:f:594:LEU:HD22	1.92	0.51
32:F:43:GLN:HA	32:F:46:ARG:HG2	1.92	0.51
29:f:75:LEU:HD13	29:f:77:GLU:HG3	1.93	0.51
29:f:531:ASN:HA	29:f:534:VAL:HG22	1.93	0.51
8:i:48:GLU:HG3	8:i:201:MET:HE1	1.93	0.51
8:i:143:TYR:HB2	8:i:146:GLN:HE21	1.75	0.51
11:l:226:ASP:OD1	11:l:226:ASP:N	2.43	0.51
12:M:230:ASP:N	12:M:230:ASP:OD1	2.44	0.51
22:W:284:SER:O	22:W:288:HIS:ND1	2.44	0.51
27:b:4:GLU:HA	27:b:106:LYS:H	1.74	0.51
3:C:147:THR:HG22	3:C:150:MET:HE3	1.92	0.51
3:C:372:ARG:NH1	4:D:179:GLU:OE2	2.43	0.51
10:K:210:LEU:HG	10:K:238:ILE:HD11	1.93	0.51
25:Z:128:PRO:O	31:c:215:LYS:NZ	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:81:LEU:HA	26:a:84:VAL:HG12	1.93	0.51
6:g:120:ASP:OD1	7:h:84:ARG:NH1	2.44	0.51
3:C:69:GLN:HG3	3:C:118:ASN:HD21	1.76	0.51
29:f:690:VAL:HA	29:f:694:LEU:HD13	1.92	0.51
1:A:190:VAL:HG21	1:A:339:ARG:HG3	1.94	0.50
2:B:275:GLU:OE1	2:B:322:ARG:NH2	2.45	0.50
21:V:136:GLU:OE2	21:V:180:ARG:NH1	2.43	0.50
12:m:215:TRP:CD1	12:m:227:VAL:HG22	2.46	0.50
31:c:54:MET:HB3	31:c:77:GLN:HE22	1.75	0.50
5:E:56:ILE:HB	5:E:100:LEU:HB2	1.92	0.50
20:U:233:LEU:HA	20:U:236:LEU:HD12	1.92	0.50
22:W:268:LYS:HZ2	22:W:334:GLU:H	1.60	0.50
29:f:585:GLU:HG2	29:f:587:PHE:H	1.75	0.50
30:x:20:LEU:HD21	30:x:63:ILE:HD12	1.93	0.50
31:c:83:SER:HA	33:u:76:GLY:HA3	1.93	0.50
7:H:177:ARG:NH1	23:X:161:ASP:O	2.43	0.50
12:M:68:ASN:OD1	12:M:224:HIS:ND1	2.38	0.50
24:Y:117:LYS:HB2	24:Y:147:ILE:HD11	1.93	0.50
29:f:423:ASP:OD1	29:f:423:ASP:N	2.44	0.50
11:l:41:LYS:NZ	11:l:180:MET:HB3	2.26	0.50
5:E:244:SER:OG	32:F:299:GLU:OE2	2.22	0.50
8:I:197:LEU:HA	8:I:200:THR:HG22	1.92	0.50
11:L:203:GLN:O	11:L:239:ARG:NH2	2.42	0.50
15:P:205:ASP:HB3	17:r:192:VAL:HG11	1.93	0.50
23:X:348:GLU:OE2	23:X:358:LYS:NZ	2.42	0.50
28:d:212:LYS:HD2	28:d:213:ARG:HG2	1.94	0.50
19:t:122:LEU:HG	19:t:137:LEU:HD12	1.93	0.50
3:C:325:ARG:HD3	3:C:353:GLY:HA2	1.93	0.50
7:H:51:LYS:NZ	7:H:200:GLU:O	2.45	0.50
12:M:43:ASP:OD1	12:M:43:ASP:N	2.43	0.50
27:b:63:THR:O	27:b:70:ARG:NH2	2.44	0.50
29:f:245:ASN:HB3	29:f:256:PHE:HB2	1.94	0.50
9:J:90:GLU:HG3	9:J:110:TYR:CZ	2.46	0.50
20:U:191:LYS:HA	20:U:194:ARG:HE	1.77	0.50
29:f:282:PHE:HE1	29:f:311:VAL:HG12	1.76	0.50
4:D:125:LYS:HB2	4:D:128:ALA:HB2	1.93	0.50
8:I:178:ASP:OD2	8:I:195:LYS:NZ	2.45	0.50
29:f:220:ASP:O	29:f:224:ASN:ND2	2.45	0.50
29:f:574:GLU:HG3	29:f:599:ALA:HB2	1.92	0.50
7:h:79:MET:H	7:h:132:VAL:HG12	1.77	0.50
5:E:331:ILE:HG23	5:E:371:VAL:HG21	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:141:ILE:HG22	6:G:151:VAL:HG22	1.93	0.50
20:U:169:GLU:HG3	20:U:171:ASN:H	1.77	0.50
20:U:249:CYS:HB3	20:U:328:ILE:HG21	1.93	0.50
22:W:446:ILE:HD11	25:Z:208:ILE:HG22	1.93	0.50
22:W:453:HIS:O	25:Z:219:LYS:NZ	2.36	0.50
24:Y:297:ARG:HH12	34:e:42:ASN:HD21	1.60	0.50
29:f:556:ARG:HH21	29:f:627:GLU:HG2	1.77	0.50
11:l:88:MET:HG2	11:l:112:ILE:HD11	1.94	0.50
2:B:373:THR:OG1	2:B:412:MET:O	2.30	0.50
8:I:140:ASP:OD1	8:I:146:GLN:NE2	2.45	0.50
29:f:378:ASN:OD1	29:f:382:ASN:ND2	2.45	0.50
2:B:58:CYS:SG	29:f:219:LYS:NZ	2.77	0.49
20:U:510:GLU:HA	20:U:547:GLY:HA3	1.93	0.49
21:V:497:PRO:HB3	25:Z:282:ASN:HB2	1.93	0.49
29:f:486:GLY:HA2	29:f:525:ILE:HD11	1.94	0.49
28:d:62:SER:HB3	28:d:67:ASP:HB3	1.95	0.49
29:f:80:ARG:O	29:f:80:ARG:NH1	2.41	0.49
8:i:140:ASP:OD1	8:i:146:GLN:NE2	2.44	0.49
31:c:202:SER:OG	31:c:203:ILE:N	2.46	0.49
32:F:298:SER:OG	32:F:301:ALA:O	2.29	0.49
5:E:109:ARG:NH2	32:F:114:ASP:O	2.38	0.49
15:P:126:LEU:HG	15:P:127:ILE:HG23	1.94	0.49
27:b:8:VAL:HA	27:b:110:ILE:HG13	1.94	0.49
27:b:12:ASN:ND2	27:b:53:THR:OG1	2.45	0.49
32:F:80:ILE:O	32:F:84:LYS:HB2	2.12	0.49
21:V:131:LEU:HD13	21:V:171:VAL:HG21	1.94	0.49
25:Z:197:GLY:HA2	31:c:225:TRP:HB2	1.95	0.49
28:d:2:TYR:O	28:d:25:ARG:NH2	2.45	0.49
29:f:42:GLU:OE2	29:f:46:SER:OG	2.29	0.49
11:L:47:VAL:HG12	11:L:195:LEU:HD22	1.95	0.49
19:T:63:LEU:HD21	19:T:106:LEU:HD13	1.95	0.49
20:U:788:VAL:HG12	20:U:909:GLY:HA2	1.94	0.49
22:W:34:LEU:HB3	22:W:39:ARG:HB3	1.95	0.49
22:W:237:GLU:HG2	22:W:238:GLY:H	1.78	0.49
28:d:103:LEU:HD23	28:d:136:PRO:HB2	1.94	0.49
28:d:235:THR:O	28:d:239:SER:N	2.43	0.49
29:f:13:PRO:HG2	29:f:56:LEU:HD22	1.95	0.49
29:f:779:CYS:HA	29:f:782:HIS:CE1	2.48	0.49
32:F:141:ASP:OD1	32:F:144:LYS:NZ	2.42	0.49
5:E:167:PRO:O	5:E:274:LYS:NZ	2.42	0.49
10:K:167:ALA:HB3	11:L:56:LEU:HD13	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:751:ARG:NE	20:U:907:SER:O	2.43	0.49
21:V:81:GLN:HB3	21:V:93:PHE:HB3	1.95	0.49
21:V:396:ILE:O	28:d:141:GLN:NE2	2.46	0.49
23:X:377:ILE:HB	24:Y:358:ARG:HH12	1.77	0.49
24:Y:117:LYS:HD3	24:Y:151:TYR:HD2	1.78	0.49
26:a:213:PHE:O	26:a:241:ASN:ND2	2.35	0.49
31:c:33:ILE:HD11	31:c:38:LEU:HD12	1.94	0.49
2:B:221:GLY:HA3	2:B:347:ILE:HA	1.93	0.49
22:W:320:LEU:HA	22:W:323:ASP:HB2	1.93	0.49
26:a:70:ARG:O	27:b:17:ARG:NH1	2.46	0.49
26:a:211:PHE:HD1	26:a:271:LYS:HE3	1.77	0.49
10:k:182:GLN:HE22	11:l:55:GLU:HB3	1.78	0.49
31:c:183:HIS:ND1	31:c:185:ASN:OD1	2.34	0.49
1:A:160:THR:HA	1:A:163:MET:HE3	1.94	0.49
6:G:46:ASP:OD1	6:G:46:ASP:N	2.45	0.49
16:Q:31:ASP:OD1	16:Q:31:ASP:N	2.44	0.49
19:T:50:MET:HE2	19:T:192:VAL:HG12	1.95	0.49
20:U:376:MET:HA	20:U:739:ALA:HA	1.95	0.49
22:W:371:THR:HG22	22:W:372:ARG:HG3	1.95	0.49
24:Y:243:GLY:O	24:Y:247:LEU:HB2	2.13	0.49
6:g:241:ALA:O	6:g:245:ARG:NH1	2.45	0.49
14:o:63:LEU:HD11	14:o:79:ALA:HB2	1.95	0.49
2:B:222:VAL:HG13	2:B:351:ILE:HD13	1.95	0.49
17:R:166:ARG:NH1	15:p:34:MET:O	2.46	0.49
18:S:145:LEU:HD22	18:S:178:VAL:HB	1.95	0.49
20:U:475:HIS:CE1	20:U:507:VAL:HG22	2.48	0.49
20:U:805:ASN:ND2	20:U:891:VAL:O	2.46	0.49
26:a:28:LEU:HG	26:a:33:LEU:HD11	1.95	0.49
29:f:241:PRO:O	29:f:245:ASN:ND2	2.44	0.49
1:A:73:ALA:HB2	2:B:140:ASP:H	1.78	0.49
1:A:307:ASP:OD2	1:A:333:ARG:NH2	2.46	0.49
9:J:211:MET:HG2	9:J:217:LEU:HB2	1.94	0.49
29:f:834:ASP:OD1	29:f:834:ASP:N	2.46	0.49
6:g:188:ASP:OD1	6:g:188:ASP:N	2.45	0.49
9:j:212:ARG:HB2	9:j:215:GLN:HG2	1.94	0.49
33:u:18:GLU:HG3	33:u:20:SER:H	1.78	0.49
5:E:180:LYS:HG2	5:E:301:ILE:HD12	1.93	0.48
11:L:200:PRO:O	11:L:239:ARG:NH2	2.37	0.48
15:P:193:ASP:OD1	15:P:193:ASP:N	2.45	0.48
22:W:451:MET:HE1	25:Z:101:LEU:HB3	1.95	0.48
29:f:411:ALA:HA	29:f:414:LEU:HG	1.93	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:121:ASN:OD1	32:F:146:LYS:NZ	2.38	0.48
14:O:138:PHE:O	14:O:142:PHE:HB2	2.12	0.48
20:U:623:GLY:O	20:U:627:PHE:HB3	2.13	0.48
25:Z:230:LEU:HB3	26:a:349:MET:HE1	1.95	0.48
26:a:192:GLU:OE2	26:a:196:ARG:NH2	2.44	0.48
33:u:39:ASP:O	33:u:42:ARG:NH1	2.46	0.48
13:N:192:ASP:OD1	13:N:192:ASP:N	2.44	0.48
22:W:114:GLU:HG3	22:W:115:ILE:HG12	1.96	0.48
10:K:240:ASP:N	10:K:240:ASP:OD1	2.41	0.48
21:V:119:GLY:HA2	21:V:148:ARG:HD3	1.95	0.48
24:Y:319:MET:O	24:Y:323:PHE:HB3	2.13	0.48
25:Z:130:ASP:OD1	25:Z:130:ASP:N	2.46	0.48
28:d:2:TYR:HB2	28:d:25:ARG:HH12	1.78	0.48
19:t:22:ILE:HG23	19:t:50:MET:HE3	1.94	0.48
3:C:295:THR:OG1	3:C:296:ASN:N	2.46	0.48
4:D:267:ILE:HD11	4:D:309:MET:HB3	1.93	0.48
6:G:112:ASP:N	6:G:112:ASP:OD1	2.46	0.48
22:W:273:TYR:HB2	22:W:276:LEU:HB2	1.94	0.48
25:Z:14:LEU:HD22	31:c:43:LYS:HD3	1.95	0.48
11:l:218:ASP:OD1	11:l:218:ASP:N	2.45	0.48
18:s:10:GLY:HA3	18:s:42:LYS:HE2	1.95	0.48
29:f:108:GLU:O	29:f:112:ASN:ND2	2.46	0.48
29:f:719:PRO:HB2	29:f:721:VAL:HG23	1.95	0.48
11:l:239:ARG:HD2	11:l:240:PRO:HD2	1.95	0.48
24:Y:316:LEU:HA	24:Y:319:MET:HG2	1.94	0.48
29:f:104:GLY:O	29:f:107:LYS:NZ	2.38	0.48
16:q:39:SER:OG	16:q:40:GLU:N	2.46	0.48
18:s:144:MET:HE1	18:s:185:ARG:HB2	1.96	0.48
1:A:278:ASP:N	1:A:278:ASP:OD1	2.46	0.48
9:J:66:ASP:HA	16:Q:69:MET:HE3	1.96	0.48
10:k:91:LYS:HG2	10:k:119:LEU:HD11	1.96	0.48
4:D:389:GLU:OE1	4:D:391:ARG:NH2	2.47	0.48
20:U:246:TYR:HE1	20:U:327:LYS:HD2	1.79	0.48
29:f:110:TYR:OH	29:f:118:ASN:ND2	2.38	0.48
8:i:234:GLU:HA	8:i:237:ILE:HG12	1.96	0.48
34:e:46:ASP:OD1	34:e:46:ASP:N	2.47	0.48
4:D:155:THR:HA	4:D:159:LYS:HG3	1.95	0.48
23:X:170:GLN:NE2	23:X:192:SER:OG	2.42	0.48
23:X:397:TYR:HB2	24:Y:365:GLN:NE2	2.29	0.48
29:f:7:ASP:N	29:f:7:ASP:OD1	2.46	0.48
29:f:347:ASP:HA	29:f:350:LYS:HB2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:145:PRO:HG2	4:D:256:GLU:HG3	1.96	0.47
26:a:180:LEU:HD21	26:a:222:LEU:HD21	1.95	0.47
28:d:207:THR:HG23	28:d:217:LEU:HD22	1.95	0.47
9:j:204:LYS:NZ	9:j:222:PRO:O	2.46	0.47
19:t:157:GLN:NE2	19:t:159:VAL:O	2.46	0.47
2:B:223:ILE:HB	2:B:347:ILE:HD13	1.96	0.47
14:O:55:THR:HG23	14:O:86:MET:HE1	1.96	0.47
20:U:383:ASP:OD2	20:U:412:HIS:NE2	2.40	0.47
25:Z:112:MET:HE1	25:Z:119:SER:HB3	1.95	0.47
28:d:170:LEU:HA	28:d:173:THR:HG22	1.95	0.47
29:f:343:LYS:HB2	29:f:390:LEU:HD11	1.95	0.47
29:f:346:ASP:OD1	29:f:346:ASP:N	2.44	0.47
1:A:308:GLY:HA2	32:F:234:THR:HG21	1.96	0.47
4:D:387:VAL:HG13	5:E:158:LEU:HD23	1.96	0.47
5:E:72:LYS:HB2	5:E:78:ARG:HG2	1.96	0.47
18:S:145:LEU:HD21	18:S:182:ALA:HB2	1.95	0.47
28:d:103:LEU:HD21	28:d:119:LEU:HD21	1.96	0.47
2:B:54:PRO:HA	29:f:835:GLU:HB3	1.96	0.47
5:E:213:ARG:NH1	5:E:217:GLU:OE2	2.47	0.47
28:d:62:SER:HA	28:d:65:ARG:HG2	1.96	0.47
29:f:679:LEU:HD13	29:f:687:ARG:HH11	1.79	0.47
4:D:274:ARG:NE	5:E:245:GLU:O	2.48	0.47
14:O:63:LEU:HD11	14:O:79:ALA:HB2	1.96	0.47
15:P:125:ASP:OD1	15:P:129:CYS:N	2.37	0.47
29:f:421:ASP:HB3	29:f:425:GLY:H	1.79	0.47
29:f:707:LEU:HD21	29:f:787:LEU:HD11	1.97	0.47
9:J:67:ASP:OD1	9:J:67:ASP:N	2.46	0.47
29:f:372:LEU:HD11	29:f:409:SER:HB2	1.96	0.47
11:l:49:LEU:HG	11:l:195:LEU:HD21	1.97	0.47
32:F:252:ALA:HB3	32:F:255:GLN:HB2	1.96	0.47
32:F:318:ASP:OD2	32:F:344:ARG:NH2	2.40	0.47
2:B:58:CYS:HG	29:f:219:LYS:HZ1	1.62	0.47
5:E:351:GLY:HA3	32:F:217:ILE:HD12	1.96	0.47
6:G:165:ALA:HB3	7:H:56:LEU:HD22	1.96	0.47
20:U:89:ASN:O	20:U:136:LYS:NZ	2.47	0.47
20:U:906:LEU:HD13	20:U:912:ILE:HD13	1.96	0.47
22:W:294:LYS:HG3	22:W:295:LYS:HD3	1.96	0.47
29:f:318:THR:HA	29:f:321:MET:HG3	1.95	0.47
29:f:460:ASP:HB3	29:f:463:LEU:HB3	1.97	0.47
29:f:603:SER:HB2	29:f:639:LYS:HB2	1.95	0.47
30:x:26:PRO:HB2	30:x:27:MET:HE2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c:173:GLU:OE1	31:c:180:ASN:ND2	2.47	0.47
31:c:219:ASN:HB2	31:c:222:LYS:HZ2	1.78	0.47
5:E:239:GLY:HA2	5:E:257:LEU:HD12	1.96	0.47
20:U:694:ILE:HG23	20:U:695:MET:HG2	1.96	0.47
29:f:654:VAL:O	29:f:658:ALA:HB3	2.14	0.47
10:k:202:LEU:O	10:k:206:MET:HB2	2.15	0.47
19:t:110:MET:HE2	19:t:110:MET:HB2	1.79	0.47
31:c:39:LEU:HD23	31:c:42:LEU:HD21	1.97	0.47
32:F:168:TYR:O	32:F:173:LYS:NZ	2.47	0.47
4:D:130:VAL:HG12	4:D:142:VAL:HG12	1.97	0.47
20:U:493:VAL:HG22	20:U:497:LEU:HD13	1.96	0.47
26:a:156:TYR:HB3	26:a:179:PHE:HB2	1.96	0.47
29:f:133:MET:SD	29:f:133:MET:N	2.82	0.47
29:f:593:THR:OG1	29:f:631:LYS:NZ	2.48	0.47
7:h:52:GLN:HB3	7:h:57:TYR:HD2	1.79	0.47
8:i:155:ASN:ND2	9:j:77:THR:OG1	2.48	0.47
1:A:284:ARG:O	32:F:334:ARG:NH1	2.48	0.47
18:S:204:ARG:NH1	18:S:206:GLU:OE2	2.47	0.47
20:U:554:LEU:HD11	20:U:761:VAL:HG13	1.96	0.47
22:W:378:MET:HE1	22:W:389:SER:HB3	1.96	0.47
27:b:44:ASN:HD21	27:b:46:GLU:HB2	1.80	0.47
28:d:8:GLU:OE1	28:d:13:SER:OG	2.32	0.47
29:f:267:ARG:HD2	29:f:271:MET:HE2	1.97	0.47
29:f:826:GLN:OE1	29:f:864:GLY:HA2	2.15	0.47
32:F:35:LYS:HD3	32:F:39:GLU:HB2	1.97	0.47
1:A:183:GLN:HB3	1:A:343:PHE:HE1	1.80	0.46
1:A:312:ARG:HB2	1:A:315:ILE:HB	1.96	0.46
3:C:98:ASP:OD1	3:C:98:ASP:N	2.46	0.46
14:O:198:ARG:HD2	14:O:201:ARG:HH22	1.79	0.46
15:P:138:VAL:HG11	15:P:146:MET:HB3	1.97	0.46
9:j:137:ASP:OD2	9:j:143:ARG:NE	2.43	0.46
14:o:38:SER:OG	14:o:40:ASN:OD1	2.30	0.46
23:X:281:GLY:H	23:X:284:THR:HG22	1.81	0.46
25:Z:124:ILE:HG22	25:Z:135:THR:HA	1.98	0.46
8:i:41:ASP:OD1	8:i:41:ASP:N	2.49	0.46
14:o:147:GLU:HB2	14:o:150:GLU:HG3	1.96	0.46
15:p:30:ILE:HG22	15:p:31:GLN:H	1.80	0.46
8:I:41:ASP:OD1	8:I:41:ASP:N	2.45	0.46
8:I:201:MET:HG3	8:I:206:LEU:HD11	1.97	0.46
9:J:65:LEU:HD12	9:J:69:VAL:HG12	1.97	0.46
20:U:689:ILE:HD12	20:U:732:LEU:HD22	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:480:ILE:HD11	25:Z:261:TYR:HA	1.98	0.46
26:a:28:LEU:HD23	26:a:37:LEU:HA	1.97	0.46
13:n:4:MET:HG2	13:n:156:THR:HG23	1.96	0.46
10:K:146:VAL:HG11	10:K:222:PRO:HA	1.97	0.46
13:N:30:VAL:HG11	19:t:211:ILE:HG23	1.96	0.46
16:Q:169:LYS:O	16:q:27:GLN:NE2	2.45	0.46
21:V:266:GLN:NE2	21:V:299:GLN:OE1	2.48	0.46
22:W:396:LEU:HD13	22:W:402:ILE:HD13	1.96	0.46
23:X:377:ILE:HG22	23:X:386:ILE:HB	1.97	0.46
10:K:52:LYS:NZ	10:K:64:ILE:O	2.48	0.46
22:W:251:TYR:HE1	22:W:267:LEU:HD22	1.80	0.46
27:b:65:THR:HG21	27:b:70:ARG:HE	1.80	0.46
29:f:215:ASP:OD1	29:f:215:ASP:N	2.48	0.46
29:f:357:ARG:NH1	29:f:363:SER:O	2.45	0.46
10:k:210:LEU:HA	10:k:214:ASN:HD21	1.81	0.46
33:u:51:GLU:OE2	33:u:59:TYR:OH	2.33	0.46
2:B:76:GLU:HA	2:B:79:ILE:HG22	1.96	0.46
13:N:86:MET:HE2	13:N:86:MET:HB3	1.83	0.46
21:V:208:ALA:HB1	21:V:249:THR:HG21	1.97	0.46
26:a:12:GLN:HG2	26:a:19:PRO:HA	1.98	0.46
28:d:155:LYS:HZ3	28:d:171:LEU:HG	1.81	0.46
29:f:119:LYS:HG2	29:f:123:ALA:HB2	1.96	0.46
16:q:30:ASP:OD1	16:q:30:ASP:N	2.45	0.46
31:c:299:CYS:HB3	31:c:303:MET:HE1	1.97	0.46
9:J:36:ARG:HB2	9:J:144:LEU:HD23	1.98	0.46
23:X:208:ALA:HB2	23:X:238:GLY:HA3	1.97	0.46
23:X:344:ARG:HG2	23:X:386:ILE:HG13	1.98	0.46
8:I:9:THR:HB	8:I:20:GLN:HG3	1.97	0.46
14:O:146:MET:HE1	14:O:154:LEU:HD22	1.96	0.46
20:U:541:HIS:HB2	20:U:544:ILE:HG22	1.98	0.46
29:f:787:LEU:HG	29:f:791:VAL:HB	1.98	0.46
29:f:811:LEU:HG	29:f:878:GLU:HA	1.97	0.46
10:k:200:ILE:HG13	10:k:241:ILE:HD12	1.97	0.46
16:q:44:LEU:HD11	16:q:102:LEU:HD22	1.98	0.46
2:B:140:ASP:O	2:B:142:ASP:N	2.46	0.46
20:U:101:ILE:O	20:U:105:ILE:HG12	2.16	0.46
22:W:152:ILE:HG13	22:W:165:ILE:HD12	1.97	0.46
25:Z:106:ILE:HG13	25:Z:153:LYS:HD2	1.97	0.46
29:f:730:GLY:O	29:f:734:SER:OG	2.30	0.46
29:f:737:ASN:OD1	29:f:738:ASN:N	2.49	0.46
2:B:191:ASP:H	2:B:194:ILE:HD12	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:GLU:O	4:D:323:ARG:NH1	2.47	0.46
4:D:70:LYS:NZ	25:Z:180:LYS:O	2.49	0.46
22:W:123:ARG:HA	22:W:126:ASP:HB2	1.98	0.46
26:a:227:ASN:O	26:a:231:GLN:NE2	2.46	0.46
5:E:126:ASP:HB2	5:E:197:LYS:HE2	1.98	0.45
16:Q:35:MET:SD	16:Q:181:ARG:NH1	2.82	0.45
19:T:25:ASP:HA	19:T:187:PHE:HA	1.98	0.45
20:U:578:LEU:HA	20:U:578:LEU:HD12	1.83	0.45
29:f:133:MET:HA	29:f:136:GLU:HB3	1.98	0.45
29:f:860:LYS:HA	29:f:860:LYS:HD3	1.78	0.45
1:A:267:LYS:HA	29:f:354:GLU:HB2	1.98	0.45
1:A:287:ASP:OD1	1:A:287:ASP:N	2.47	0.45
11:L:7:ASP:OD1	11:L:7:ASP:N	2.49	0.45
17:R:38:ASN:HD21	17:R:41:LEU:HD12	1.82	0.45
20:U:691:SER:HA	20:U:694:ILE:HG22	1.98	0.45
20:U:756:HIS:CE1	20:U:758:PRO:HG2	2.51	0.45
21:V:289:LEU:HA	21:V:292:THR:HG22	1.98	0.45
24:Y:197:ALA:HB3	24:Y:226:VAL:HG21	1.97	0.45
29:f:569:LYS:HG2	29:f:573:ILE:HG13	1.98	0.45
7:h:119:GLN:HA	7:h:122:THR:HG22	1.97	0.45
15:p:159:ASP:OD1	15:p:159:ASP:N	2.46	0.45
1:A:210:LYS:NZ	1:A:313:GLY:O	2.39	0.45
3:C:381:GLU:HA	3:C:384:GLU:HG2	1.98	0.45
15:P:135:ASP:OD1	15:P:135:ASP:N	2.49	0.45
20:U:570:LEU:HD22	20:U:578:LEU:HG	1.99	0.45
21:V:285:TRP:HA	21:V:289:LEU:HD13	1.99	0.45
24:Y:328:GLU:OE2	34:e:62:LYS:NZ	2.49	0.45
26:a:324:ILE:HG23	26:a:331:VAL:HG12	1.98	0.45
29:f:637:LYS:HG3	29:f:678:LEU:HB2	1.98	0.45
7:H:208:ILE:HD11	7:H:230:LEU:HD21	1.97	0.45
15:P:159:ASP:N	15:P:159:ASP:OD1	2.47	0.45
19:T:211:ILE:HG13	13:n:30:VAL:HG11	1.99	0.45
28:d:181:CYS:O	28:d:184:LYS:NZ	2.40	0.45
30:x:4:TYR:HB2	30:x:20:LEU:HB3	1.98	0.45
1:A:35:THR:O	1:A:39:SER:OG	2.32	0.45
1:A:368:ILE:HG22	1:A:406:GLU:HB2	1.99	0.45
4:D:185:LEU:HD21	4:D:225:ALA:HB2	1.97	0.45
17:R:133:VAL:HG21	16:q:137:PHE:HB3	1.98	0.45
18:S:68:ILE:HD11	18:S:92:LEU:HD13	1.99	0.45
20:U:501:LEU:HD11	20:U:548:LEU:HD11	1.98	0.45
22:W:153:LYS:HA	22:W:153:LYS:HD3	1.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:186:THR:HB	31:c:293:THR:HG22	1.98	0.45
27:b:14:GLU:HB2	27:b:17:ARG:HH21	1.81	0.45
27:b:161:ASN:HD22	27:b:168:SER:HB2	1.80	0.45
31:c:111:TRP:HB3	31:c:133:PHE:HE2	1.82	0.45
2:B:183:THR:OG1	2:B:184:TYR:N	2.50	0.45
2:B:342:ILE:HG22	2:B:350:LYS:HE3	1.98	0.45
4:D:337:ASP:OD1	4:D:338:ARG:N	2.46	0.45
4:D:381:GLU:OE2	5:E:297:ARG:NH2	2.49	0.45
20:U:475:HIS:HE1	20:U:507:VAL:HG22	1.82	0.45
22:W:142:ARG:HD2	22:W:176:SER:HB2	1.97	0.45
26:a:352:ARG:HA	26:a:355:PHE:CE2	2.51	0.45
29:f:99:LEU:HB3	29:f:101:PRO:HD2	1.98	0.45
29:f:838:ARG:NH1	29:f:839:PRO:O	2.49	0.45
6:g:58:ASP:OD1	6:g:58:ASP:N	2.48	0.45
10:k:146:VAL:HG11	10:k:222:PRO:HA	1.97	0.45
17:R:97:MET:HB2	17:R:116:SER:N	2.32	0.45
20:U:266:GLN:HA	20:U:269:ARG:HG2	1.99	0.45
21:V:175:MET:HB3	21:V:184:ALA:HB2	1.98	0.45
26:a:61:GLU:HG3	26:a:79:ILE:HD13	1.99	0.45
29:f:479:LEU:HD13	29:f:514:VAL:HG22	1.98	0.45
2:B:117:ASP:O	2:B:141:LYS:NZ	2.50	0.45
5:E:171:LEU:HD22	5:E:295:LEU:HD13	1.99	0.45
5:E:237:ALA:HB2	32:F:311:LEU:HD12	1.99	0.45
6:G:165:ALA:HB1	6:G:179:LEU:HD13	1.99	0.45
6:G:191:PHE:HE1	6:G:219:VAL:HG11	1.82	0.45
26:a:70:ARG:NH2	27:b:79:GLN:OE1	2.49	0.45
11:l:47:VAL:HG12	11:l:195:LEU:HD22	1.99	0.45
32:F:94:ILE:HD11	32:F:125:LYS:HB2	1.98	0.45
2:B:329:MET:HE2	2:B:329:MET:HB3	1.80	0.45
11:l:81:ALA:HB2	11:l:130:VAL:HG21	1.98	0.45
31:c:132:SER:HB3	33:u:71:LEU:HD13	1.98	0.45
9:J:101:PRO:HG2	9:J:138:PHE:HE1	1.82	0.45
10:K:99:HIS:CG	10:K:107:MET:HB2	2.52	0.45
10:K:184:VAL:HG11	10:K:197:SER:HB3	1.99	0.45
14:O:112:SER:HB3	14:O:125:VAL:HG11	1.99	0.45
21:V:275:VAL:HG13	21:V:288:TYR:HE2	1.82	0.45
23:X:233:TYR:HA	23:X:254:MET:HE1	1.99	0.45
24:Y:220:VAL:HA	24:Y:223:THR:HG22	1.99	0.45
32:F:317:LEU:HD13	32:F:328:VAL:HG21	1.97	0.45
1:A:347:ASP:OD1	1:A:347:ASP:N	2.48	0.44
3:C:218:GLU:HA	3:C:221:GLN:HG2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:205:ASP:OD1	5:E:205:ASP:N	2.50	0.44
25:Z:208:ILE:HG13	26:a:353:LEU:HD11	1.99	0.44
28:d:114:GLU:O	28:d:118:GLU:HB2	2.17	0.44
28:d:162:SER:HG	28:d:164:THR:HG1	1.65	0.44
29:f:11:VAL:O	29:f:15:GLN:N	2.49	0.44
29:f:640:LYS:HZ3	29:f:648:ALA:HA	1.82	0.44
7:h:166:ASN:HD22	7:h:198:SER:HB3	1.82	0.44
15:p:135:ASP:OD1	15:p:135:ASP:N	2.47	0.44
17:r:35:ILE:HD11	17:r:45:MET:HE2	1.99	0.44
2:B:125:THR:OG1	2:B:126:SER:N	2.50	0.44
20:U:792:ASN:HB3	20:U:914:LEU:H	1.82	0.44
21:V:286:ALA:HA	21:V:312:ALA:HB1	1.99	0.44
27:b:126:LYS:HA	27:b:129:LYS:HG2	1.97	0.44
32:F:230:GLY:HA3	32:F:392:ASN:ND2	2.31	0.44
1:A:124:ASP:HB2	32:F:86:LEU:HD22	1.99	0.44
1:A:139:ARG:NH1	1:A:154:PRO:O	2.49	0.44
11:L:88:MET:HG3	11:L:112:ILE:HD11	1.99	0.44
21:V:150:ARG:NH1	21:V:157:THR:O	2.50	0.44
23:X:268:GLN:HA	23:X:271:VAL:HG22	2.00	0.44
24:Y:68:ASP:OD1	24:Y:68:ASP:N	2.51	0.44
28:d:189:ILE:HB	28:d:222:TYR:HB2	1.98	0.44
29:f:180:GLN:HA	29:f:216:MET:HE1	1.99	0.44
29:f:496:ASP:OD1	29:f:497:VAL:N	2.49	0.44
29:f:817:VAL:HG23	29:f:818:LEU:HG	1.98	0.44
7:h:204:THR:OG1	7:h:206:ASP:OD1	2.33	0.44
14:o:216:ILE:HD11	15:p:194:LYS:HD2	1.98	0.44
16:q:11:ASP:N	16:q:11:ASP:OD1	2.50	0.44
9:J:137:ASP:OD2	9:J:143:ARG:NE	2.41	0.44
15:P:38:ASP:OD1	15:P:38:ASP:N	2.49	0.44
25:Z:82:PHE:HA	25:Z:85:VAL:HG12	2.00	0.44
29:f:765:ALA:HB2	29:f:877:GLY:HA2	1.99	0.44
29:f:771:LEU:HG	29:f:774:GLY:H	1.83	0.44
14:o:62:ASN:HB3	14:o:82:MET:HE1	1.99	0.44
1:A:206:ILE:HG22	32:F:373:MET:HE2	1.98	0.44
20:U:333:MET:SD	20:U:333:MET:N	2.89	0.44
23:X:252:LYS:HG2	23:X:287:LEU:HD11	1.98	0.44
24:Y:376:LEU:HD22	25:Z:265:LEU:HD21	1.99	0.44
26:a:129:GLN:HG2	26:a:130:VAL:HG23	1.99	0.44
28:d:106:LEU:HD11	28:d:114:GLU:HB3	1.99	0.44
10:k:221:GLN:HB2	10:k:224:GLN:HG2	1.98	0.44
1:A:73:ALA:HB1	1:A:77:LEU:HD22	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:25:ARG:HH21	31:c:104:ARG:H	1.64	0.44
26:a:54:ASP:HB2	26:a:83:VAL:HG22	1.99	0.44
27:b:38:HIS:HB3	27:b:42:ARG:NH2	2.33	0.44
29:f:548:THR:O	29:f:552:ASP:CB	2.52	0.44
9:j:39:ASP:OD1	9:j:39:ASP:N	2.51	0.44
15:p:7:ASN:ND2	15:p:29:GLY:O	2.50	0.44
3:C:235:PHE:HE2	3:C:279:GLN:HG2	1.82	0.44
12:M:8:ASP:OD1	12:M:8:ASP:N	2.47	0.44
22:W:118:LEU:HD13	22:W:118:LEU:HA	1.79	0.44
24:Y:84:LEU:HD21	24:Y:107:LYS:HG2	2.00	0.44
25:Z:215:VAL:HG22	26:a:346:ILE:HD12	1.99	0.44
2:B:77:GLU:OE2	2:B:81:ASN:ND2	2.51	0.44
4:D:328:ASP:OD1	4:D:328:ASP:N	2.43	0.44
17:R:127:SER:HB3	17:R:136:TYR:CE1	2.53	0.44
20:U:163:PHE:HE2	20:U:201:LEU:HD11	1.82	0.44
20:U:611:ASN:HB3	20:U:614:VAL:HG12	1.99	0.44
27:b:38:HIS:HB3	27:b:42:ARG:HH22	1.82	0.44
10:k:25:GLU:HA	10:k:28:ILE:HD12	2.00	0.44
10:k:238:ILE:HD12	10:k:238:ILE:HA	1.88	0.44
11:l:80:ASP:OD2	11:l:126:ARG:NH1	2.45	0.44
12:m:206:ASP:OD1	12:m:206:ASP:N	2.50	0.44
18:s:27:THR:HB	18:s:40:SER:H	1.82	0.44
31:c:63:ASP:OD1	31:c:66:THR:OG1	2.30	0.44
33:u:5:VAL:HG22	33:u:67:LEU:HB2	1.99	0.44
4:D:124:LEU:HD23	4:D:124:LEU:HA	1.90	0.44
6:G:231:THR:OG1	6:G:234:GLU:OE1	2.26	0.44
14:O:163:ILE:HG12	14:O:170:GLY:HA2	2.00	0.44
20:U:524:LYS:HA	20:U:556:MET:HG2	2.00	0.44
22:W:431:LYS:NZ	25:Z:236:LEU:O	2.48	0.44
29:f:550:LEU:HD11	29:f:625:LYS:HE2	2.00	0.44
2:B:58:CYS:SG	2:B:59:ARG:N	2.91	0.43
3:C:103:ILE:HG21	3:C:123:LEU:HD23	1.99	0.43
4:D:259:PRO:HB3	4:D:304:ASN:HB2	1.99	0.43
15:P:30:ILE:HG22	15:P:31:GLN:H	1.83	0.43
21:V:121:PHE:HB3	21:V:128:ARG:HD2	2.00	0.43
22:W:287:VAL:HA	22:W:290:ILE:HG12	2.00	0.43
22:W:455:LEU:HD22	25:Z:103:LYS:HB2	1.99	0.43
23:X:251:LEU:HA	23:X:254:MET:HG3	2.00	0.43
26:a:370:GLN:HB3	28:d:247:ILE:HG21	1.99	0.43
28:d:45:LYS:HA	28:d:48:LEU:HD12	2.00	0.43
10:k:121:LEU:HD12	11:l:79:ALA:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:191:LEU:HD12	10:k:191:LEU:HA	1.87	0.43
17:r:9:ARG:NH2	17:r:146:ASP:OD1	2.43	0.43
4:D:391:ARG:HG3	22:W:136:ILE:HD11	2.00	0.43
22:W:173:THR:HG23	22:W:182:ARG:HH21	1.83	0.43
24:Y:13:LYS:HD3	24:Y:143:TYR:HD1	1.83	0.43
26:a:70:ARG:HD2	26:a:70:ARG:HA	1.78	0.43
26:a:252:LYS:HG3	26:a:255:TRP:HE1	1.83	0.43
29:f:469:TYR:HA	29:f:472:HIS:ND1	2.33	0.43
6:g:118:ILE:HG13	6:g:138:MET:HE1	2.00	0.43
18:s:200:LYS:HB3	18:s:200:LYS:HE2	1.79	0.43
31:c:195:GLY:HA3	31:c:200:TYR:CZ	2.52	0.43
3:C:344:LEU:HA	3:C:347:ILE:HD12	2.01	0.43
4:D:345:PHE:O	4:D:349:THR:OG1	2.25	0.43
8:I:72:MET:HE2	8:I:72:MET:HB3	1.93	0.43
20:U:327:LYS:HD3	20:U:794:ASP:HB3	1.98	0.43
21:V:119:GLY:O	21:V:122:THR:OG1	2.36	0.43
22:W:235:GLN:O	22:W:235:GLN:NE2	2.51	0.43
23:X:236:PHE:HB2	23:X:250:SER:HB3	2.01	0.43
25:Z:263:ALA:HB3	31:c:292:MET:HE3	2.00	0.43
26:a:119:GLY:HA3	26:a:158:LEU:HD11	2.01	0.43
26:a:223:GLU:O	26:a:227:ASN:HB2	2.17	0.43
27:b:62:THR:HG21	27:b:71:ILE:HD13	1.99	0.43
29:f:152:ALA:HB3	29:f:156:HIS:HB2	2.00	0.43
3:C:90:HIS:NE2	4:D:110:ASN:OD1	2.52	0.43
20:U:191:LYS:HA	20:U:194:ARG:HB3	2.00	0.43
20:U:548:LEU:O	20:U:552:ILE:HG12	2.19	0.43
21:V:223:LYS:O	21:V:225:ASP:N	2.51	0.43
22:W:47:LEU:HD13	22:W:70:VAL:HG22	2.00	0.43
24:Y:23:ARG:HH22	24:Y:52:PRO:HB2	1.83	0.43
7:h:14:SER:HB3	7:h:18:LYS:H	1.84	0.43
9:j:211:MET:HA	9:j:215:GLN:HE21	1.83	0.43
1:A:114:ASN:HA	1:A:120:LYS:HG3	2.00	0.43
1:A:311:PRO:HB2	1:A:312:ARG:H	1.71	0.43
13:N:127:ILE:HD11	13:N:136:TYR:CD1	2.53	0.43
20:U:214:ILE:HD11	20:U:752:THR:HA	1.99	0.43
24:Y:24:PHE:HE1	24:Y:28:LEU:HD22	1.83	0.43
26:a:14:SER:HB2	26:a:18:GLN:HG2	2.01	0.43
29:f:347:ASP:OD1	29:f:347:ASP:N	2.51	0.43
16:q:103:LEU:HG	16:q:132:HIS:HD2	1.82	0.43
3:C:147:THR:HG23	3:C:149:GLU:H	1.82	0.43
8:I:155:ASN:OD1	9:J:77:THR:OG1	2.37	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:86:ARG:NH1	19:T:133:GLU:OE2	2.52	0.43
22:W:39:ARG:HG3	22:W:42:GLU:HB3	1.99	0.43
22:W:221:LYS:HD3	22:W:225:LYS:HD3	2.00	0.43
24:Y:385:ARG:HD3	24:Y:385:ARG:HA	1.80	0.43
29:f:523:GLY:HA3	29:f:561:GLY:HA2	1.99	0.43
14:o:50:ALA:HB2	15:p:129:CYS:HB2	1.99	0.43
1:A:284:ARG:HH21	32:F:334:ARG:HG3	1.84	0.43
2:B:195:GLN:O	2:B:199:GLU:HB2	2.19	0.43
4:D:274:ARG:H	5:E:245:GLU:CD	2.26	0.43
20:U:97:VAL:HA	20:U:100:ILE:HG12	1.99	0.43
24:Y:220:VAL:HG21	24:Y:249:VAL:HG11	2.00	0.43
10:k:160:GLY:O	11:l:82:ARG:NH2	2.51	0.43
1:A:295:VAL:HG21	2:B:307:ARG:HH22	1.83	0.43
3:C:31:LEU:HD22	4:D:47:LEU:HB3	2.00	0.43
4:D:153:MET:HG2	4:D:227:PHE:HB3	2.01	0.43
9:J:130:SER:OG	9:J:147:THR:O	2.33	0.43
9:J:201:SER:HB2	9:J:205:ASN:HD21	1.83	0.43
11:L:49:LEU:HB2	11:L:195:LEU:HD21	2.01	0.43
18:S:22:ILE:HG12	18:S:197:ILE:HG13	2.00	0.43
22:W:149:LEU:HB2	22:W:185:PHE:HE2	1.84	0.43
24:Y:16:ASP:HB3	24:Y:150:PHE:CZ	2.53	0.43
24:Y:282:MET:HG3	24:Y:288:PHE:HD2	1.84	0.43
26:a:252:LYS:HA	26:a:255:TRP:CE2	2.53	0.43
29:f:352:HIS:HB3	29:f:729:MET:HE2	2.00	0.43
2:B:378:VAL:HG12	2:B:416:ASN:HA	2.00	0.43
20:U:471:ASP:HA	20:U:474:ARG:HG3	2.01	0.43
20:U:791:LEU:HD12	20:U:798:PRO:HD2	1.99	0.43
21:V:305:ALA:O	21:V:309:MET:HG2	2.18	0.43
28:d:217:LEU:HA	28:d:222:TYR:HE1	1.84	0.43
18:s:35:ILE:O	19:t:151:ARG:NH2	2.40	0.43
32:F:65:GLU:O	32:F:69:MET:HG2	2.18	0.43
1:A:215:PHE:CD2	1:A:324:PRO:HG3	2.53	0.43
1:A:372:LEU:HD11	10:K:207:GLU:HA	2.01	0.43
2:B:417:GLU:HA	2:B:420:LYS:HB2	2.01	0.43
9:J:5:ARG:HD3	9:J:5:ARG:HA	1.86	0.43
20:U:808:PRO:HG3	20:U:873:PRO:HD2	2.00	0.43
27:b:16:MET:HA	27:b:25:ARG:HH11	1.84	0.43
29:f:759:LEU:HG	29:f:761:MET:H	1.84	0.43
11:l:41:LYS:HZ2	11:l:180:MET:HB3	1.84	0.43
1:A:140:VAL:HG12	1:A:152:PRO:HA	2.01	0.42
13:N:7:GLN:NE2	13:N:109:GLY:O	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:4:MET:HE3	15:P:4:MET:HB3	1.88	0.42
20:U:190:ASN:OD1	20:U:190:ASN:N	2.52	0.42
20:U:197:VAL:HA	20:U:200:VAL:HG12	2.00	0.42
23:X:348:GLU:HG3	23:X:358:LYS:HD3	2.01	0.42
29:f:12:GLN:HA	29:f:15:GLN:HB2	2.01	0.42
6:g:112:ASP:OD1	6:g:112:ASP:N	2.52	0.42
8:i:202:ASP:OD1	8:i:203:VAL:N	2.52	0.42
11:l:117:GLN:NE2	12:m:83:ASP:OD1	2.51	0.42
19:t:70:MET:HE1	19:t:91:TRP:CE2	2.54	0.42
30:x:48:VAL:HA	30:x:67:MET:HE1	2.01	0.42
32:F:172:VAL:HA	32:F:175:MET:HG2	2.01	0.42
9:J:39:ASP:OD1	9:J:39:ASP:N	2.51	0.42
16:Q:43:LEU:HB2	16:Q:183:ILE:HD11	2.01	0.42
21:V:450:SER:OG	21:V:451:ILE:N	2.49	0.42
23:X:255:LEU:HB2	23:X:287:LEU:HD22	2.01	0.42
24:Y:188:CYS:HA	24:Y:191:ILE:HG22	2.02	0.42
25:Z:101:LEU:HD11	25:Z:138:TYR:HE2	1.84	0.42
26:a:374:ILE:HD11	28:d:251:ARG:HG2	2.00	0.42
29:f:459:CYS:HB2	30:x:70:LEU:HD22	2.00	0.42
29:f:620:PHE:HE2	29:f:628:ASP:HB3	1.83	0.42
19:t:79:ASP:OD1	19:t:79:ASP:N	2.51	0.42
1:A:393:GLY:HA3	2:B:216:ILE:HD12	2.01	0.42
5:E:196:LEU:HD23	5:E:196:LEU:HA	1.89	0.42
9:J:42:VAL:HG22	9:J:210:VAL:HG12	2.00	0.42
11:L:122:ARG:HB2	11:L:125:ARG:HG3	2.00	0.42
17:R:33:LYS:HA	17:R:45:MET:HE2	2.01	0.42
21:V:387:GLN:HE22	28:d:128:GLN:HE22	1.68	0.42
28:d:211:LYS:HD3	28:d:211:LYS:HA	1.77	0.42
19:t:43:MET:HE2	19:t:51:LEU:HD23	2.01	0.42
31:c:189:ILE:HD12	31:c:192:LEU:HD11	2.01	0.42
4:D:251:PHE:HD2	4:D:295:GLN:HB3	1.84	0.42
5:E:378:LYS:HB2	5:E:378:LYS:HE3	1.76	0.42
9:J:50:VAL:HB	9:J:54:GLN:HB2	2.01	0.42
13:N:196:LYS:HD2	13:N:196:LYS:HA	1.93	0.42
20:U:724:VAL:HA	20:U:727:LYS:HG2	2.01	0.42
20:U:735:GLY:O	20:U:739:ALA:HB2	2.20	0.42
25:Z:26:ILE:HD11	25:Z:35:VAL:HG22	2.00	0.42
28:d:139:LEU:HD11	28:d:151:VAL:HG13	2.00	0.42
8:i:175:LEU:O	8:i:179:TYR:HB2	2.19	0.42
32:F:89:LEU:N	32:F:153:VAL:O	2.50	0.42
32:F:336:ASP:OD1	32:F:336:ASP:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:VAL:HA	2:B:276:GLU:HG2	2.02	0.42
23:X:217:ILE:O	23:X:221:GLU:HG2	2.19	0.42
25:Z:15:VAL:HG11	25:Z:50:VAL:HG12	2.01	0.42
29:f:434:TYR:OH	30:x:43:ARG:NH1	2.53	0.42
13:n:194:ILE:O	13:n:196:LYS:NZ	2.49	0.42
2:B:254:GLU:CD	3:C:230:MET:HE1	2.44	0.42
10:K:202:LEU:O	10:K:206:MET:HG3	2.19	0.42
14:O:78:THR:O	14:O:82:MET:HG3	2.19	0.42
19:T:122:LEU:HG	19:T:137:LEU:HD12	2.02	0.42
26:a:273:GLN:HB3	26:a:310:LEU:HD11	2.02	0.42
27:b:147:GLU:HG2	27:b:151:GLU:HB2	2.02	0.42
28:d:188:LYS:NZ	28:d:220:ASN:O	2.44	0.42
29:f:462:ALA:O	29:f:466:LEU:HB2	2.20	0.42
29:f:631:LYS:HA	29:f:634:LYS:HB3	2.00	0.42
15:p:65:GLN:OE1	16:q:86:ARG:NH2	2.53	0.42
16:q:31:ASP:OD1	16:q:31:ASP:N	2.52	0.42
2:B:379:THR:OG1	2:B:382:ASP:OD2	2.38	0.42
5:E:116:ASP:O	5:E:118:LEU:N	2.53	0.42
12:M:46:VAL:HG22	12:M:215:TRP:HB3	2.01	0.42
12:M:215:TRP:CE3	12:M:227:VAL:HG22	2.55	0.42
20:U:740:GLY:HA3	20:U:744:VAL:HG22	2.02	0.42
21:V:470:ARG:O	21:V:473:GLN:HG3	2.19	0.42
28:d:114:GLU:HA	28:d:117:THR:HG22	2.00	0.42
28:d:164:THR:HA	28:d:167:ILE:HG12	2.02	0.42
29:f:828:ARG:H	29:f:861:THR:HG22	1.84	0.42
31:c:68:ARG:HD3	31:c:208:ARG:HH11	1.85	0.42
33:u:1:MET:HE3	33:u:3:ILE:HD11	2.02	0.42
20:U:421:GLN:HA	20:U:424:ALA:HB2	2.02	0.42
25:Z:136:GLU:OE2	25:Z:157:HIS:ND1	2.48	0.42
26:a:292:THR:HG23	26:a:295:GLU:H	1.84	0.42
29:f:171:GLN:HB2	29:f:179:VAL:HG22	2.01	0.42
6:g:155:ASP:OD1	6:g:159:TYR:N	2.46	0.42
13:n:192:ASP:OD1	13:n:192:ASP:N	2.53	0.42
4:D:413:GLU:HB3	7:H:53:LYS:HE3	2.01	0.42
5:E:270:LEU:HG	5:E:273:VAL:HB	2.01	0.42
20:U:483:LEU:HD11	20:U:781:LEU:HD11	2.02	0.42
20:U:524:LYS:HE3	20:U:524:LYS:HB2	1.90	0.42
20:U:619:VAL:HG23	20:U:651:GLY:HA3	2.00	0.42
20:U:764:LEU:O	20:U:767:THR:OG1	2.38	0.42
22:W:81:ASP:OD1	22:W:81:ASP:N	2.51	0.42
22:W:206:SER:O	22:W:210:ASN:ND2	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:299:ILE:HG22	22:W:301:LYS:H	1.85	0.42
22:W:308:LEU:HD23	22:W:308:LEU:HA	1.91	0.42
24:Y:294:TYR:HA	24:Y:297:ARG:HG2	2.02	0.42
26:a:184:ASP:OD1	26:a:184:ASP:N	2.52	0.42
26:a:321:LYS:HB2	26:a:335:TRP:HB3	2.02	0.42
29:f:540:GLN:HA	29:f:543:MET:HG3	2.01	0.42
16:q:38:MET:HE1	16:q:61:GLN:HA	2.02	0.42
30:x:48:VAL:HG23	30:x:53:LEU:HB2	2.02	0.42
32:F:111:ILE:HG22	32:F:113:LEU:H	1.84	0.42
1:A:189:GLU:OE2	32:F:409:ARG:NH2	2.35	0.42
2:B:252:GLY:N	2:B:285:ASP:O	2.49	0.42
4:D:175:GLN:NE2	4:D:179:GLU:OE2	2.47	0.42
20:U:596:ASN:HA	20:U:599:ILE:HG22	2.02	0.42
21:V:235:LEU:HA	21:V:250:LEU:HD13	2.01	0.42
21:V:412:LEU:HD22	24:Y:339:ALA:HA	2.01	0.42
21:V:471:GLU:HA	21:V:474:LEU:HD12	2.02	0.42
23:X:143:TYR:HD1	23:X:180:LEU:HD22	1.85	0.42
25:Z:77:ASN:O	25:Z:81:MET:HG3	2.19	0.42
27:b:174:PRO:HA	27:b:175:PRO:HD3	1.89	0.42
28:d:129:THR:OG1	28:d:130:ASN:N	2.52	0.42
29:f:349:TYR:HA	29:f:352:HIS:HB2	2.01	0.42
18:s:16:ALA:HB2	18:s:121:VAL:HG23	2.02	0.42
3:C:49:ARG:HD3	4:D:64:GLU:HB3	2.00	0.41
3:C:346:LYS:HE2	3:C:346:LYS:HB3	1.93	0.41
4:D:336:PRO:HB3	4:D:340:GLN:HB2	2.01	0.41
19:T:76:LEU:HD23	19:T:76:LEU:HA	1.87	0.41
20:U:261:LEU:HA	20:U:264:VAL:HG12	2.02	0.41
20:U:786:THR:O	20:U:786:THR:OG1	2.37	0.41
21:V:467:TYR:CE2	24:Y:362:LYS:HE2	2.53	0.41
22:W:401:THR:HG23	22:W:402:ILE:HD12	2.02	0.41
25:Z:22:HIS:HA	25:Z:25:ARG:HG2	2.02	0.41
25:Z:45:LYS:HD3	25:Z:45:LYS:HA	1.86	0.41
29:f:530:CYS:SG	29:f:533:ASP:HB2	2.60	0.41
29:f:569:LYS:HE2	29:f:569:LYS:HB2	1.88	0.41
29:f:654:VAL:O	29:f:658:ALA:CB	2.68	0.41
29:f:660:ILE:HA	29:f:669:GLU:HG3	2.02	0.41
11:l:72:ILE:HG22	11:l:134:ILE:HG12	2.02	0.41
31:c:233:ASP:O	31:c:237:HIS:HB3	2.20	0.41
5:E:66:GLU:O	5:E:89:LYS:NZ	2.42	0.41
12:M:34:SER:HG	12:M:65:ARG:HH12	1.66	0.41
12:M:108:LEU:HD11	12:M:137:LEU:HB3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:81:ARG:HA	14:O:81:ARG:HD2	1.90	0.41
15:P:88:MET:HE2	15:P:88:MET:HB3	1.89	0.41
21:V:492:LYS:HD2	21:V:492:LYS:HA	1.90	0.41
25:Z:116:CYS:O	25:Z:119:SER:OG	2.35	0.41
25:Z:262:LEU:O	25:Z:266:ILE:HG12	2.20	0.41
29:f:634:LYS:HB2	29:f:673:ARG:HH21	1.85	0.41
10:k:54:ILE:HG23	10:k:59:MET:HE3	2.02	0.41
19:t:179:ARG:HD3	19:t:179:ARG:HA	1.88	0.41
31:c:78:SER:OG	32:F:112:ASP:OD1	2.28	0.41
18:S:123:SER:HB3	18:S:136:LYS:HG2	2.02	0.41
20:U:150:ALA:HA	20:U:153:ILE:HG22	2.01	0.41
20:U:646:PRO:HA	20:U:649:ARG:HB2	2.01	0.41
20:U:748:LEU:HD23	20:U:760:VAL:HG22	2.01	0.41
21:V:256:ARG:HH12	34:e:21:GLU:HB2	1.85	0.41
21:V:269:LYS:HE3	21:V:269:LYS:HB2	1.88	0.41
23:X:155:ARG:HA	23:X:158:LYS:HG2	2.01	0.41
24:Y:89:GLU:HA	24:Y:92:GLU:HG2	2.02	0.41
12:m:87:LEU:HD23	12:m:87:LEU:HA	1.93	0.41
21:V:86:VAL:HG22	21:V:200:ARG:HH22	1.86	0.41
21:V:322:VAL:O	21:V:326:GLN:HG2	2.21	0.41
22:W:141:GLU:HG2	22:W:175:GLY:HA3	2.02	0.41
25:Z:34:ARG:HH12	25:Z:60:GLU:HB3	1.85	0.41
28:d:63:ILE:HD13	28:d:71:PHE:HB2	2.01	0.41
28:d:101:LEU:HG	28:d:166:PHE:CE2	2.55	0.41
29:f:631:LYS:HA	29:f:634:LYS:HE2	2.03	0.41
29:f:683:GLU:HA	29:f:684:PRO:HD3	1.94	0.41
6:g:43:ARG:HH21	6:g:164:LYS:HG2	1.85	0.41
8:i:161:ALA:HB1	8:i:175:LEU:HD13	2.02	0.41
18:s:91:MET:HE2	18:s:91:MET:HB3	1.88	0.41
31:c:190:GLN:O	31:c:194:HIS:ND1	2.45	0.41
5:E:170:CYS:HB3	5:E:297:ARG:HB3	2.01	0.41
6:G:206:LEU:HB3	6:G:208:ILE:HG13	2.02	0.41
9:J:179:GLU:HA	9:J:182:GLU:HG2	2.03	0.41
13:N:127:ILE:HD11	13:N:136:TYR:HD1	1.86	0.41
14:O:58:LEU:HD23	14:O:86:MET:HE2	2.02	0.41
18:S:18:GLU:OE2	18:S:118:LYS:NZ	2.51	0.41
28:d:118:GLU:HA	28:d:121:ARG:HH11	1.85	0.41
28:d:176:ASP:OD1	28:d:177:GLU:N	2.54	0.41
8:i:53:HIS:HB3	8:i:56:LEU:HD23	2.02	0.41
16:q:121:LEU:HD23	16:q:121:LEU:HA	1.91	0.41
31:c:54:MET:HB3	31:c:77:GLN:NE2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLY:HA2	1:A:66:LYS:NZ	2.36	0.41
1:A:356:LYS:O	1:A:360:ARG:HB3	2.20	0.41
4:D:171:ASP:OD1	4:D:172:ILE:N	2.54	0.41
4:D:285:VAL:HG21	5:E:255:ARG:NH2	2.35	0.41
4:D:374:ASP:OD1	4:D:374:ASP:N	2.52	0.41
5:E:253:ILE:HG21	32:F:308:ARG:NH2	2.36	0.41
6:G:180:GLU:HA	6:G:183:VAL:HG12	2.02	0.41
18:S:27:THR:HB	18:S:40:SER:H	1.85	0.41
24:Y:107:LYS:HE2	24:Y:107:LYS:HB2	1.94	0.41
25:Z:181:ASP:OD1	25:Z:181:ASP:N	2.51	0.41
25:Z:214:LYS:HE3	25:Z:214:LYS:HB3	1.88	0.41
29:f:466:LEU:HD12	29:f:481:SER:HA	2.02	0.41
11:l:93:LEU:HD23	11:l:93:LEU:HA	1.92	0.41
32:F:289:ASP:OD1	32:F:289:ASP:N	2.51	0.41
1:A:32:LEU:HA	1:A:35:THR:HG22	2.03	0.41
1:A:119:ALA:HB2	32:F:128:THR:HG23	2.03	0.41
2:B:96:ARG:HH22	3:C:82:LYS:HE2	1.85	0.41
4:D:401:LYS:HE2	4:D:401:LYS:HB2	1.87	0.41
16:Q:197:PRO:HD2	16:q:199:GLN:HA	2.03	0.41
20:U:448:LEU:HA	20:U:483:LEU:HD23	2.03	0.41
20:U:664:GLY:HA2	20:U:694:ILE:HG13	2.03	0.41
24:Y:110:TYR:CZ	24:Y:114:ILE:HG13	2.55	0.41
28:d:6:LYS:HA	28:d:9:TRP:HB3	2.02	0.41
29:f:261:ARG:HD2	29:f:267:ARG:HH12	1.85	0.41
29:f:634:LYS:HD3	29:f:673:ARG:HH21	1.84	0.41
9:j:42:VAL:HG22	9:j:210:VAL:HG22	2.02	0.41
31:c:89:PRO:HG3	33:u:42:ARG:HB3	2.03	0.41
31:c:151:VAL:HG22	31:c:152:LYS:H	1.84	0.41
32:F:362:ARG:NE	32:F:388:THR:O	2.54	0.41
3:C:70:GLY:HA3	4:D:113:VAL:HG12	2.01	0.41
11:L:166:GLN:OE1	11:L:169:ARG:NH2	2.45	0.41
14:O:187:ARG:HA	14:O:188:PRO:HA	1.89	0.41
20:U:374:SER:HB3	20:U:407:SER:HB3	2.02	0.41
20:U:487:GLY:HA2	20:U:521:LEU:HB3	2.01	0.41
23:X:70:LEU:HD11	23:X:92:LEU:HB3	2.01	0.41
23:X:157:LEU:HD21	23:X:165:LEU:HD23	2.03	0.41
25:Z:34:ARG:HE	25:Z:102:HIS:CE1	2.38	0.41
29:f:380:PHE:HA	29:f:416:MET:HE1	2.03	0.41
15:p:143:ALA:HA	15:p:146:MET:HE3	2.03	0.41
17:r:127:SER:HB3	17:r:136:TYR:CE1	2.55	0.41
32:F:303:ASP:OD1	32:F:303:ASP:N	2.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:LYS:HG3	2:B:389:ASP:H	1.86	0.41
3:C:219:LEU:HD11	4:D:289:LEU:HD22	2.02	0.41
3:C:235:PHE:HA	3:C:238:ALA:HB3	2.03	0.41
4:D:84:SER:O	5:E:68:LYS:NZ	2.52	0.41
5:E:264:MET:HA	5:E:270:LEU:HD22	2.03	0.41
11:L:56:LEU:HD23	11:L:56:LEU:HA	1.93	0.41
19:T:79:ASP:OD1	19:T:79:ASP:N	2.47	0.41
19:T:215:ILE:HD13	19:T:215:ILE:HA	1.90	0.41
21:V:296:LYS:HE3	21:V:304:GLU:HG2	2.03	0.41
21:V:323:GLY:HA2	34:e:24:ALA:HA	2.02	0.41
22:W:140:ILE:HG23	22:W:143:ALA:HB3	2.03	0.41
22:W:243:ILE:HG13	22:W:273:TYR:HE2	1.86	0.41
22:W:268:LYS:NZ	22:W:334:GLU:H	2.19	0.41
24:Y:298:GLU:OE2	24:Y:342:ARG:NH2	2.50	0.41
27:b:9:CYS:HB3	27:b:111:ALA:HA	2.02	0.41
29:f:771:LEU:HD22	29:f:807:ARG:HE	1.86	0.41
6:g:118:ILE:HD13	6:g:118:ILE:HA	1.95	0.41
15:p:193:ASP:OD1	15:p:193:ASP:N	2.53	0.41
17:r:20:ALA:HB2	17:r:31:VAL:HG21	2.02	0.41
31:c:269:GLN:HA	31:c:272:ILE:HG22	2.02	0.41
32:F:97:LEU:HB2	32:F:121:CYS:HB2	2.03	0.41
2:B:235:LEU:HD13	2:B:353:PHE:HZ	1.86	0.41
4:D:97:ASP:OD1	4:D:97:ASP:N	2.52	0.41
5:E:107:ILE:C	5:E:108:MET:HE2	2.46	0.41
12:M:229:LYS:HA	12:M:232:ARG:HG2	2.03	0.41
20:U:520:MET:HB3	20:U:555:VAL:HG23	2.02	0.41
21:V:76:LYS:HE3	21:V:149:PRO:HB3	2.03	0.41
29:f:45:LEU:HD12	29:f:45:LEU:HA	1.94	0.41
29:f:638:ASP:O	29:f:639:LYS:HG2	2.21	0.41
29:f:673:ARG:NH2	29:f:785:ARG:HD3	2.36	0.41
29:f:732:VAL:HG22	29:f:746:ARG:CZ	2.51	0.41
7:h:222:THR:HG23	7:h:225:GLU:H	1.85	0.41
10:k:228:MET:HE2	10:k:228:MET:HB2	1.98	0.41
31:c:55:GLY:HA2	31:c:75:MET:SD	2.61	0.41
1:A:75:PRO:HA	1:A:78:TRP:CE2	2.56	0.40
1:A:280:ILE:HD12	1:A:280:ILE:HA	1.93	0.40
3:C:88:LYS:HB3	3:C:94:LYS:HG2	2.03	0.40
3:C:125:LYS:HZ1	4:D:96:VAL:HG11	1.86	0.40
4:D:185:LEU:HD11	4:D:259:PRO:HB2	2.03	0.40
4:D:329:ARG:HD3	4:D:329:ARG:HA	1.95	0.40
20:U:213:PHE:HB3	20:U:248:ILE:HD13	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:205:ILE:O	22:W:209:ILE:HG12	2.20	0.40
24:Y:75:LYS:HA	24:Y:75:LYS:HD2	1.79	0.40
26:a:255:TRP:O	26:a:258:GLN:NE2	2.54	0.40
29:f:25:ASP:N	29:f:25:ASP:OD1	2.53	0.40
29:f:228:LYS:HG2	29:f:233:LEU:HD12	2.02	0.40
29:f:748:LEU:O	29:f:752:HIS:HB3	2.21	0.40
6:g:180:GLU:HG2	7:h:55:ILE:HG22	2.04	0.40
7:h:106:PRO:HB2	7:h:109:GLN:HG2	2.03	0.40
10:k:129:ASP:OD1	10:k:129:ASP:N	2.53	0.40
18:s:52:ILE:HG13	18:s:110:ILE:HG12	2.03	0.40
31:c:279:ASP:OD1	31:c:279:ASP:N	2.54	0.40
32:F:226:TYR:CZ	32:F:353:GLU:HB3	2.56	0.40
4:D:125:LYS:NZ	31:c:277:LYS:HG2	2.35	0.40
7:H:39:LYS:HG3	7:H:44:VAL:HG22	2.03	0.40
12:M:87:LEU:HD23	12:M:87:LEU:HA	1.91	0.40
18:S:83:MET:HE1	18:S:91:MET:SD	2.61	0.40
22:W:207:LYS:O	22:W:211:THR:HG23	2.21	0.40
23:X:373:LYS:HE3	23:X:373:LYS:HB2	1.85	0.40
25:Z:237:LEU:HD21	31:c:310:LYS:HB2	2.02	0.40
11:l:52:ALA:HB1	11:l:57:ALA:HB3	2.04	0.40
13:n:166:ARG:HA	13:n:166:ARG:HD3	1.90	0.40
30:x:43:ARG:HA	30:x:43:ARG:HD2	1.83	0.40
2:B:212:GLU:HG3	29:f:845:ARG:HG3	2.02	0.40
4:D:56:VAL:HA	20:U:600:ARG:HE	1.85	0.40
4:D:270:ILE:HD12	4:D:288:ILE:HG21	2.02	0.40
4:D:352:MET:HE2	4:D:394:VAL:HG21	2.04	0.40
5:E:168:LYS:N	5:E:296:ASP:OD2	2.42	0.40
5:E:295:LEU:HD23	5:E:295:LEU:HA	1.87	0.40
10:K:147:ASP:OD1	10:K:147:ASP:N	2.54	0.40
13:N:94:LEU:C	13:N:95:MET:HE2	2.47	0.40
20:U:367:THR:HA	20:U:370:VAL:HG22	2.03	0.40
20:U:879:ASP:OD1	20:U:879:ASP:N	2.45	0.40
20:U:903:PHE:HB3	20:U:913:ILE:HD11	2.02	0.40
22:W:25:ASP:OD1	22:W:65:ARG:NH2	2.47	0.40
22:W:155:GLN:HG2	22:W:160:LYS:HE3	2.04	0.40
25:Z:10:VAL:HG13	25:Z:163:GLY:HA3	2.01	0.40
29:f:133:MET:HE3	29:f:133:MET:HB3	1.97	0.40
16:q:43:LEU:HB2	16:q:183:ILE:HD11	2.02	0.40
19:t:99:ARG:HD2	19:t:99:ARG:HA	1.88	0.40
30:x:25:PRO:HA	30:x:26:PRO:HD3	1.97	0.40
31:c:257:LYS:HA	31:c:257:LYS:HD2	1.96	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:F:236:LEU:HD23	32:F:236:LEU:HA	1.88	0.40
3:C:91:PRO:HG3	4:D:109:SER:HB3	2.03	0.40
6:G:49:VAL:HG22	6:G:219:VAL:HG22	2.02	0.40
18:S:70:ALA:O	18:S:74:MET:HG3	2.22	0.40
19:T:179:ARG:HA	19:T:179:ARG:HD3	1.91	0.40
17:r:58:LEU:HD12	17:r:58:LEU:HA	1.95	0.40
32:F:251:LEU:HD12	32:F:285:ILE:HG12	2.02	0.40
32:F:265:ALA:HB1	32:F:312:GLU:OE1	2.22	0.40
3:C:369:TYR:HA	3:C:372:ARG:HE	1.86	0.40
4:D:276:ASP:N	4:D:282:ASP:OD2	2.49	0.40
11:L:199:LEU:HD23	11:L:199:LEU:HA	1.96	0.40
20:U:800:VAL:HB	20:U:914:LEU:HD21	2.02	0.40
21:V:118:GLN:OE1	21:V:148:ARG:NH2	2.54	0.40
22:W:142:ARG:HH12	22:W:182:ARG:HB2	1.86	0.40
26:a:18:GLN:HA	26:a:21:VAL:HG22	2.04	0.40
29:f:93:PRO:HB2	29:f:96:LEU:HB2	2.03	0.40
29:f:178:LYS:HE3	29:f:178:LYS:HB2	1.86	0.40
29:f:378:ASN:HA	29:f:381:VAL:HG12	2.03	0.40
29:f:809:ILE:HG23	29:f:855:GLN:HB2	2.02	0.40
9:j:36:ARG:HH21	9:j:157:LYS:HG2	1.86	0.40
14:o:59:ILE:HD13	14:o:59:ILE:HA	1.91	0.40
15:p:38:ASP:N	15:p:38:ASP:OD1	2.54	0.40
32:F:70:LYS:HA	32:F:73:ILE:HG22	2.04	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%)	365 (89%)	45 (11%)	1 (0%)	43	73
2	B	386/440 (88%)	363 (94%)	23 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	377/398 (95%)	341 (90%)	36 (10%)	0	100	100
4	D	378/418 (90%)	346 (92%)	31 (8%)	1 (0%)	36	67
5	E	373/403 (93%)	343 (92%)	30 (8%)	0	100	100
6	G	242/246 (98%)	231 (96%)	11 (4%)	0	100	100
6	g	242/246 (98%)	230 (95%)	12 (5%)	0	100	100
7	H	230/234 (98%)	220 (96%)	10 (4%)	0	100	100
7	h	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
8	I	249/261 (95%)	243 (98%)	6 (2%)	0	100	100
8	i	248/261 (95%)	242 (98%)	6 (2%)	0	100	100
9	J	237/248 (96%)	230 (97%)	7 (3%)	0	100	100
9	j	237/248 (96%)	225 (95%)	12 (5%)	0	100	100
10	K	232/241 (96%)	223 (96%)	9 (4%)	0	100	100
10	k	232/241 (96%)	224 (97%)	8 (3%)	0	100	100
11	L	236/269 (88%)	232 (98%)	4 (2%)	0	100	100
11	l	236/269 (88%)	229 (97%)	7 (3%)	0	100	100
12	M	238/255 (93%)	234 (98%)	4 (2%)	0	100	100
12	m	238/255 (93%)	235 (99%)	3 (1%)	0	100	100
13	N	200/239 (84%)	196 (98%)	4 (2%)	0	100	100
13	n	200/239 (84%)	195 (98%)	5 (2%)	0	100	100
14	O	218/277 (79%)	212 (97%)	6 (3%)	0	100	100
14	o	218/277 (79%)	212 (97%)	6 (3%)	0	100	100
15	P	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
15	p	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
16	Q	197/201 (98%)	190 (96%)	7 (4%)	0	100	100
16	q	197/201 (98%)	192 (98%)	5 (2%)	0	100	100
17	R	199/263 (76%)	196 (98%)	3 (2%)	0	100	100
17	r	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
18	S	211/241 (88%)	204 (97%)	7 (3%)	0	100	100
18	s	211/241 (88%)	202 (96%)	9 (4%)	0	100	100
19	T	214/264 (81%)	207 (97%)	7 (3%)	0	100	100
19	t	214/264 (81%)	206 (96%)	8 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	U	758/953 (80%)	713 (94%)	45 (6%)	0	100	100
21	V	470/534 (88%)	444 (94%)	23 (5%)	3 (1%)	21	52
22	W	444/456 (97%)	416 (94%)	27 (6%)	1 (0%)	43	73
23	X	378/422 (90%)	359 (95%)	19 (5%)	0	100	100
24	Y	376/389 (97%)	349 (93%)	25 (7%)	2 (0%)	24	57
25	Z	284/324 (88%)	261 (92%)	23 (8%)	0	100	100
26	a	371/376 (99%)	342 (92%)	29 (8%)	0	100	100
27	b	189/377 (50%)	174 (92%)	14 (7%)	1 (0%)	24	57
28	d	255/350 (73%)	222 (87%)	33 (13%)	0	100	100
29	f	887/908 (98%)	790 (89%)	97 (11%)	0	100	100
30	x	74/494 (15%)	72 (97%)	2 (3%)	0	100	100
31	c	285/310 (92%)	263 (92%)	22 (8%)	0	100	100
32	F	413/439 (94%)	383 (93%)	29 (7%)	1 (0%)	43	73
33	u	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
34	e	48/70 (69%)	40 (83%)	8 (17%)	0	100	100
All	All	13440/15458 (87%)	12665 (94%)	765 (6%)	10 (0%)	49	78

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	PRO
21	V	287	ARG
21	V	288	TYR
22	W	137	TYR
32	F	114	ASP
24	Y	48	ASN
4	D	367	PRO
21	V	224	LEU
24	Y	49	ASN
27	b	23	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	352/372 (95%)	350 (99%)	2 (1%)	78	83
2	B	341/385 (89%)	340 (100%)	1 (0%)	86	87
3	C	325/346 (94%)	323 (99%)	2 (1%)	78	83
4	D	333/366 (91%)	333 (100%)	0	100	100
5	E	298/353 (84%)	295 (99%)	3 (1%)	68	79
6	G	205/210 (98%)	205 (100%)	0	100	100
6	g	202/210 (96%)	200 (99%)	2 (1%)	68	79
7	H	188/191 (98%)	188 (100%)	0	100	100
7	h	188/191 (98%)	188 (100%)	0	100	100
8	I	207/221 (94%)	205 (99%)	2 (1%)	68	79
8	i	206/221 (93%)	206 (100%)	0	100	100
9	J	201/211 (95%)	201 (100%)	0	100	100
9	j	196/211 (93%)	196 (100%)	0	100	100
10	K	193/203 (95%)	193 (100%)	0	100	100
10	k	195/203 (96%)	195 (100%)	0	100	100
11	L	202/230 (88%)	202 (100%)	0	100	100
11	l	201/230 (87%)	201 (100%)	0	100	100
12	M	196/212 (92%)	196 (100%)	0	100	100
12	m	198/212 (93%)	198 (100%)	0	100	100
13	N	157/181 (87%)	157 (100%)	0	100	100
13	n	156/181 (86%)	156 (100%)	0	100	100
14	O	179/228 (78%)	179 (100%)	0	100	100
14	o	181/228 (79%)	181 (100%)	0	100	100
15	P	172/174 (99%)	172 (100%)	0	100	100
15	p	173/174 (99%)	173 (100%)	0	100	100
16	Q	168/171 (98%)	168 (100%)	0	100	100
16	q	168/171 (98%)	168 (100%)	0	100	100
17	R	156/202 (77%)	156 (100%)	0	100	100
17	r	156/202 (77%)	156 (100%)	0	100	100
18	S	175/199 (88%)	175 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	s	178/199 (89%)	178 (100%)	0	100	100
19	T	178/215 (83%)	178 (100%)	0	100	100
19	t	179/215 (83%)	179 (100%)	0	100	100
20	U	649/816 (80%)	649 (100%)	0	100	100
21	V	391/460 (85%)	390 (100%)	1 (0%)	86	87
22	W	410/416 (99%)	407 (99%)	3 (1%)	76	82
23	X	327/362 (90%)	327 (100%)	0	100	100
24	Y	334/344 (97%)	331 (99%)	3 (1%)	70	80
25	Z	257/295 (87%)	257 (100%)	0	100	100
26	a	333/336 (99%)	331 (99%)	2 (1%)	78	83
27	b	167/312 (54%)	167 (100%)	0	100	100
28	d	231/294 (79%)	231 (100%)	0	100	100
29	f	745/763 (98%)	745 (100%)	0	100	100
30	x	64/439 (15%)	64 (100%)	0	100	100
31	c	252/268 (94%)	252 (100%)	0	100	100
32	F	357/379 (94%)	356 (100%)	1 (0%)	86	87
33	u	68/68 (100%)	68 (100%)	0	100	100
34	e	44/63 (70%)	44 (100%)	0	100	100
All	All	11432/13133 (87%)	11410 (100%)	22 (0%)	85	89

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	ASP
1	A	403	ILE
2	B	125	THR
3	C	109	THR
3	C	210	THR
5	E	383	LYS
5	E	384	LEU
5	E	387	LYS
8	I	7[A]	SER
8	I	7[B]	SER
21	V	106	ARG
22	W	117	ASP
22	W	118	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	W	120	ILE
24	Y	46	ARG
24	Y	47	ASP
24	Y	48	ASN
26	a	122	LYS
26	a	124	ASN
6	g	222	VAL
6	g	224	ASN
32	F	416	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	231	ASN
1	A	247	GLN
2	B	242	GLN
3	C	32	GLN
3	C	64	GLN
3	C	67	GLN
3	C	118	ASN
4	D	98	GLN
4	D	237	GLN
4	D	376	ASN
4	D	414	HIS
5	E	55	GLN
5	E	155	ASN
5	E	220	ASN
5	E	280	ASN
6	G	68	HIS
6	G	75	ASN
6	G	128	ASN
7	H	88	HIS
8	I	102	GLN
9	J	54	GLN
9	J	92	GLN
9	J	154	HIS
10	K	97	GLN
10	K	99	HIS
10	K	204	GLN
11	L	16	GLN
14	O	66	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	O	165	ASN
15	P	7	ASN
16	Q	168	GLN
17	R	70	ASN
17	R	89	GLN
18	S	79	ASN
18	S	151	ASN
19	T	3	ASN
19	T	69	GLN
19	T	147	GLN
19	T	213	HIS
20	U	207	ASN
20	U	340	GLN
20	U	632	GLN
20	U	718	ASN
20	U	888	GLN
21	V	257	ASN
21	V	266	GLN
21	V	311	ASN
21	V	365	GLN
21	V	376	ASN
21	V	387	GLN
21	V	401	ASN
21	V	427	GLN
22	W	86	ASN
22	W	210	ASN
22	W	218	ASN
22	W	235	GLN
22	W	395	ASN
22	W	426	ASN
23	X	144	GLN
23	X	292	GLN
23	X	296	ASN
23	X	380	GLN
24	Y	31	HIS
24	Y	94	ASN
26	a	144	ASN
26	a	257	GLN
26	a	288	HIS
26	a	369	HIS
27	b	105	HIS
27	b	161	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	f	198	HIS
29	f	199	ASN
29	f	202	HIS
29	f	224	ASN
29	f	238	ASN
29	f	382	ASN
29	f	387	GLN
29	f	457	ASN
29	f	565	ASN
6	g	128	ASN
6	g	224	ASN
7	h	109	GLN
7	h	166	ASN
7	h	169	ASN
8	i	40	ASN
8	i	142	HIS
8	i	177	GLN
9	j	85	ASN
9	j	122	ASN
9	j	154	HIS
9	j	175	ASN
9	j	215	GLN
10	k	73	HIS
10	k	99	HIS
10	k	221	GLN
10	k	227	HIS
11	l	90	GLN
12	m	32	ASN
13	n	77	HIS
13	n	110	GLN
14	o	165	ASN
14	o	193	ASN
15	p	81	GLN
16	q	71	ASN
16	q	82	ASN
16	q	101	ASN
17	r	162	GLN
17	r	196	HIS
19	t	3	ASN
19	t	81	HIS
19	t	89	HIS
19	t	147	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	x	44	GLN
30	x	65	ASN
31	c	197	ASN
31	c	214	GLN
31	c	274	ASN
32	F	83	ASN
32	F	208	HIS
32	F	243	GLN
33	u	41	GLN
34	e	47	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
37	ADP	C	501	36	28,29,29	1.38	4 (14%)	43,45,45	1.93	8 (18%)
35	ATP	A	501	36	32,33,33	1.40	5 (15%)	48,52,52	1.80	9 (18%)
35	ATP	E	501	36	32,33,33	0.52	0	48,52,52	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	ADP	F	501	36	28,29,29	1.37	4 (14%)	43,45,45	1.91	8 (18%)
35	ATP	D	501	36	32,33,33	0.41	0	48,52,52	0.32	0
35	ATP	B	501	36	32,33,33	1.42	6 (18%)	48,52,52	1.71	10 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	ADP	C	501	36	-	2/16/32/32	0/3/3/3
35	ATP	A	501	36	-	1/22/38/38	0/3/3/3
35	ATP	E	501	36	-	8/22/38/38	0/3/3/3
37	ADP	F	501	36	-	5/16/32/32	0/3/3/3
35	ATP	D	501	36	-	4/22/38/38	0/3/3/3
35	ATP	B	501	36	-	1/22/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	B	501	ATP	C5-C4	4.65	1.47	1.39
37	C	501	ADP	C5-C4	4.63	1.47	1.39
35	A	501	ATP	C5-C4	4.60	1.47	1.39
37	F	501	ADP	C5-C4	4.55	1.47	1.39
35	A	501	ATP	C5-N7	-2.79	1.34	1.39
37	C	501	ADP	C5-N7	-2.61	1.34	1.39
37	F	501	ADP	C5-N7	-2.61	1.34	1.39
35	B	501	ATP	C5-C6	2.58	1.48	1.41
37	C	501	ADP	C5-C6	2.55	1.48	1.41
35	B	501	ATP	C5-N7	-2.52	1.34	1.39
37	F	501	ADP	C5-C6	2.48	1.47	1.41
35	A	501	ATP	C5-C6	2.41	1.47	1.41
35	B	501	ATP	C4-N9	-2.17	1.33	1.37
35	A	501	ATP	PB-O3B	2.15	1.61	1.59
37	C	501	ADP	C8-N7	2.12	1.35	1.31
35	B	501	ATP	PA-O3A	2.10	1.61	1.59
35	B	501	ATP	C8-N7	2.10	1.35	1.31
37	F	501	ADP	C8-N7	2.05	1.35	1.31
35	A	501	ATP	PA-O3A	2.01	1.61	1.59

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	501	ADP	C5-C4-N3	-6.50	117.76	126.72
35	A	501	ATP	C5-C4-N3	-6.40	117.90	126.72
37	F	501	ADP	C5-C4-N3	-6.32	118.01	126.72
35	B	501	ATP	C5-C4-N3	-5.49	119.16	126.72
35	A	501	ATP	N3-C4-N9	5.35	136.26	127.17
37	C	501	ADP	N3-C4-N9	5.32	136.21	127.17
37	F	501	ADP	N3-C4-N9	5.14	135.92	127.17
35	B	501	ATP	N3-C4-N9	4.34	134.55	127.17
37	C	501	ADP	C2-N3-C4	3.94	121.44	111.83
37	F	501	ADP	C2-N3-C4	3.87	121.27	111.83
35	A	501	ATP	C2-N3-C4	3.74	120.96	111.83
35	B	501	ATP	C2-N3-C4	3.61	120.66	111.83
35	B	501	ATP	N3-C2-N1	-3.56	123.19	128.58
37	C	501	ADP	N3-C2-N1	-3.26	123.65	128.58
37	F	501	ADP	N3-C2-N1	-3.25	123.66	128.58
37	F	501	ADP	C4-C5-N7	-3.22	106.91	110.58
37	C	501	ADP	C4-C5-N7	-3.17	106.96	110.58
35	B	501	ATP	C4-C5-N7	-3.12	107.02	110.58
35	A	501	ATP	N3-C2-N1	-3.02	124.01	128.58
35	A	501	ATP	C4-C5-N7	-2.81	107.36	110.58
37	F	501	ADP	C3'-C2'-C1'	2.69	106.55	101.46
37	C	501	ADP	C3'-C2'-C1'	2.59	106.35	101.46
35	B	501	ATP	C3'-C2'-C1'	2.57	106.33	101.46
37	C	501	ADP	C5-N7-C8	2.44	107.28	103.45
37	F	501	ADP	C5-N7-C8	2.43	107.27	103.45
35	B	501	ATP	C2-N1-C6	2.42	122.70	118.73
35	A	501	ATP	C3'-C2'-C1'	2.39	105.99	101.46
37	F	501	ADP	C4-N9-C8	2.35	108.20	105.74
35	B	501	ATP	C4-N9-C8	2.32	108.17	105.74
37	C	501	ADP	C4-N9-C8	2.29	108.14	105.74
35	A	501	ATP	C5-N7-C8	2.23	106.95	103.45
35	B	501	ATP	C5-N7-C8	2.21	106.92	103.45
35	A	501	ATP	C4-N9-C8	2.12	107.97	105.74
35	B	501	ATP	C6-C5-N7	2.04	136.02	132.09
35	A	501	ATP	N6-C6-N1	2.03	122.90	118.38

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	501	ATP	C5'-O5'-PA-O3A
35	D	501	ATP	PB-O3B-PG-O2G
35	D	501	ATP	C5'-O5'-PA-O2A

Continued on next page...

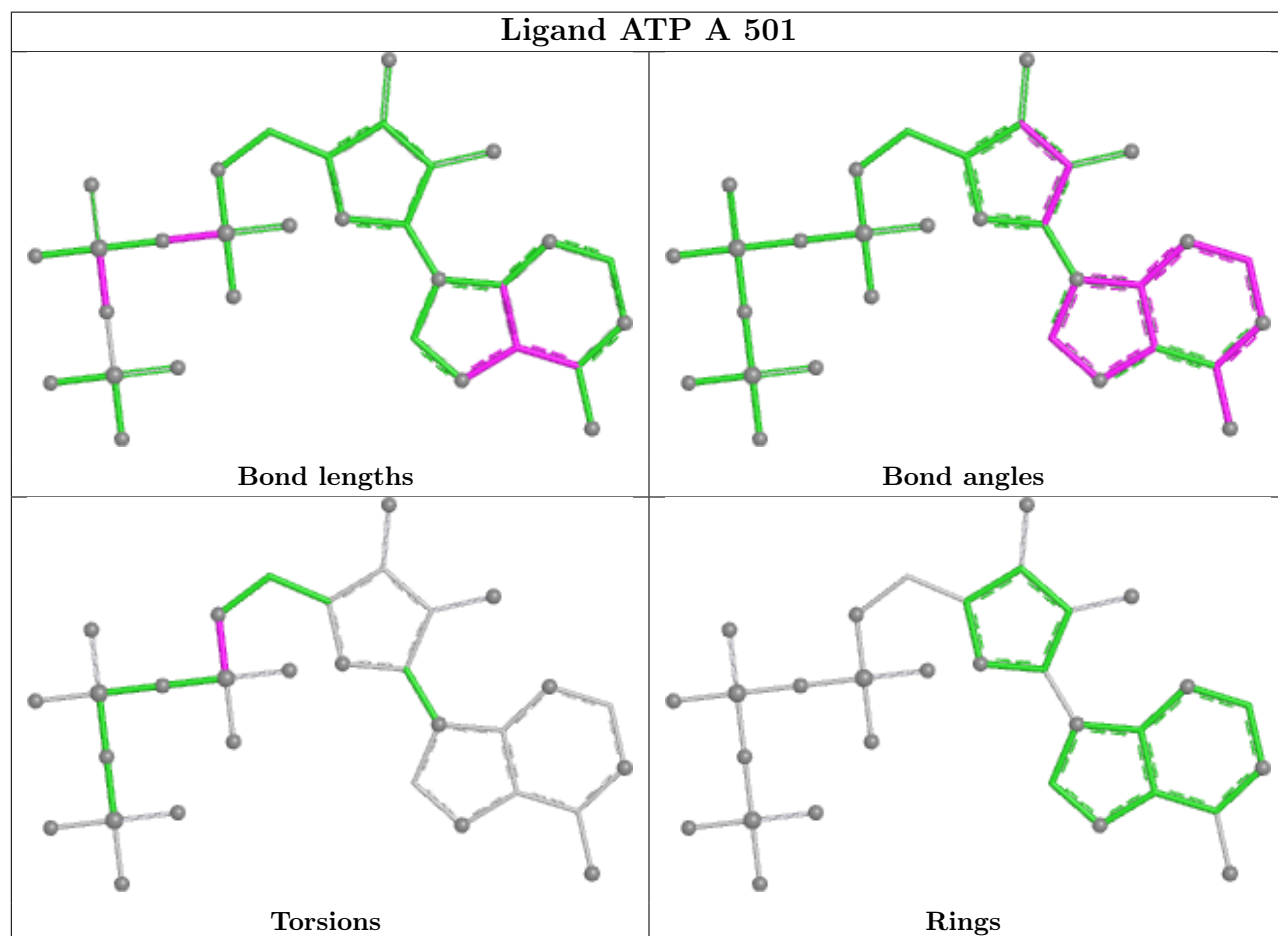
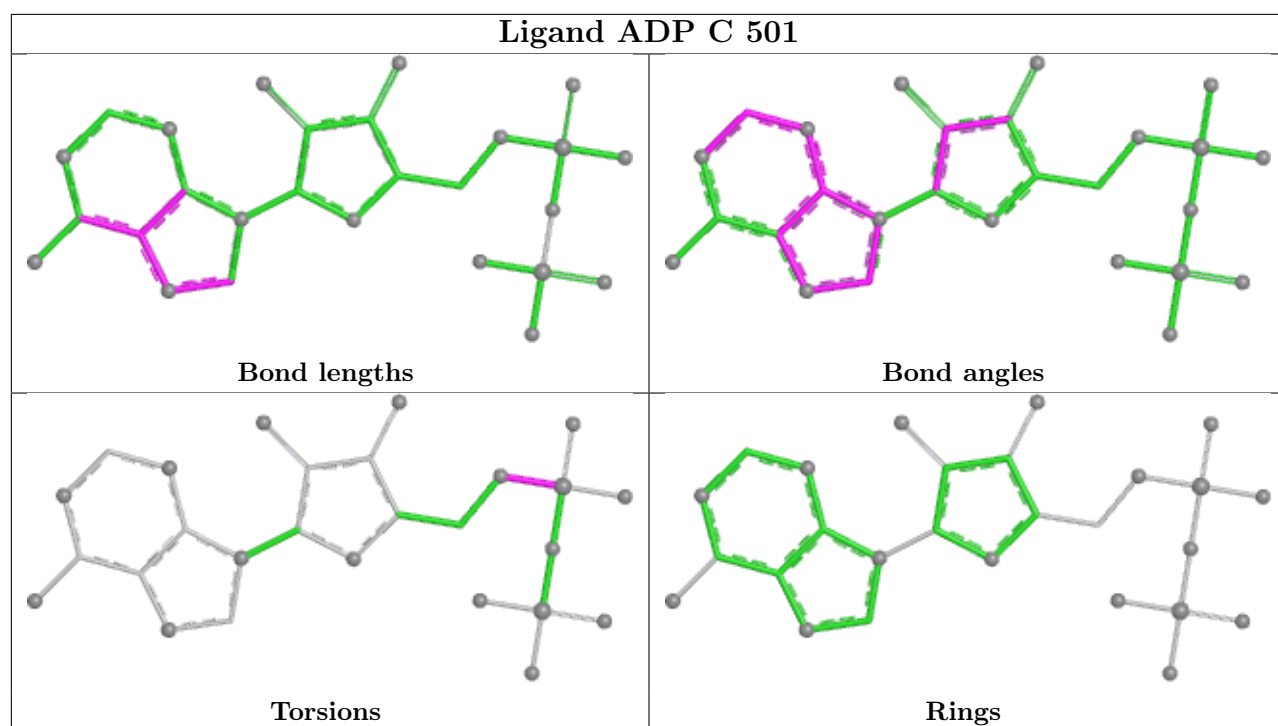
Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	E	501	ATP	C5'-O5'-PA-O1A
37	C	501	ADP	C5'-O5'-PA-O2A
37	C	501	ADP	C5'-O5'-PA-O3A
37	F	501	ADP	PA-O3A-PB-O2B
37	F	501	ADP	C5'-O5'-PA-O1A
37	F	501	ADP	C3'-C4'-C5'-O5'
35	E	501	ATP	C3'-C4'-C5'-O5'
37	F	501	ADP	O4'-C4'-C5'-O5'
35	E	501	ATP	O4'-C4'-C5'-O5'
35	D	501	ATP	C5'-O5'-PA-O3A
35	E	501	ATP	C5'-O5'-PA-O2A
35	E	501	ATP	C5'-O5'-PA-O3A
35	D	501	ATP	PB-O3B-PG-O1G
37	F	501	ADP	PA-O3A-PB-O3B
35	E	501	ATP	PG-O3B-PB-O2B
35	E	501	ATP	C2'-C1'-N9-C8
35	B	501	ATP	PB-O3A-PA-O2A
35	E	501	ATP	PG-O3B-PB-O1B

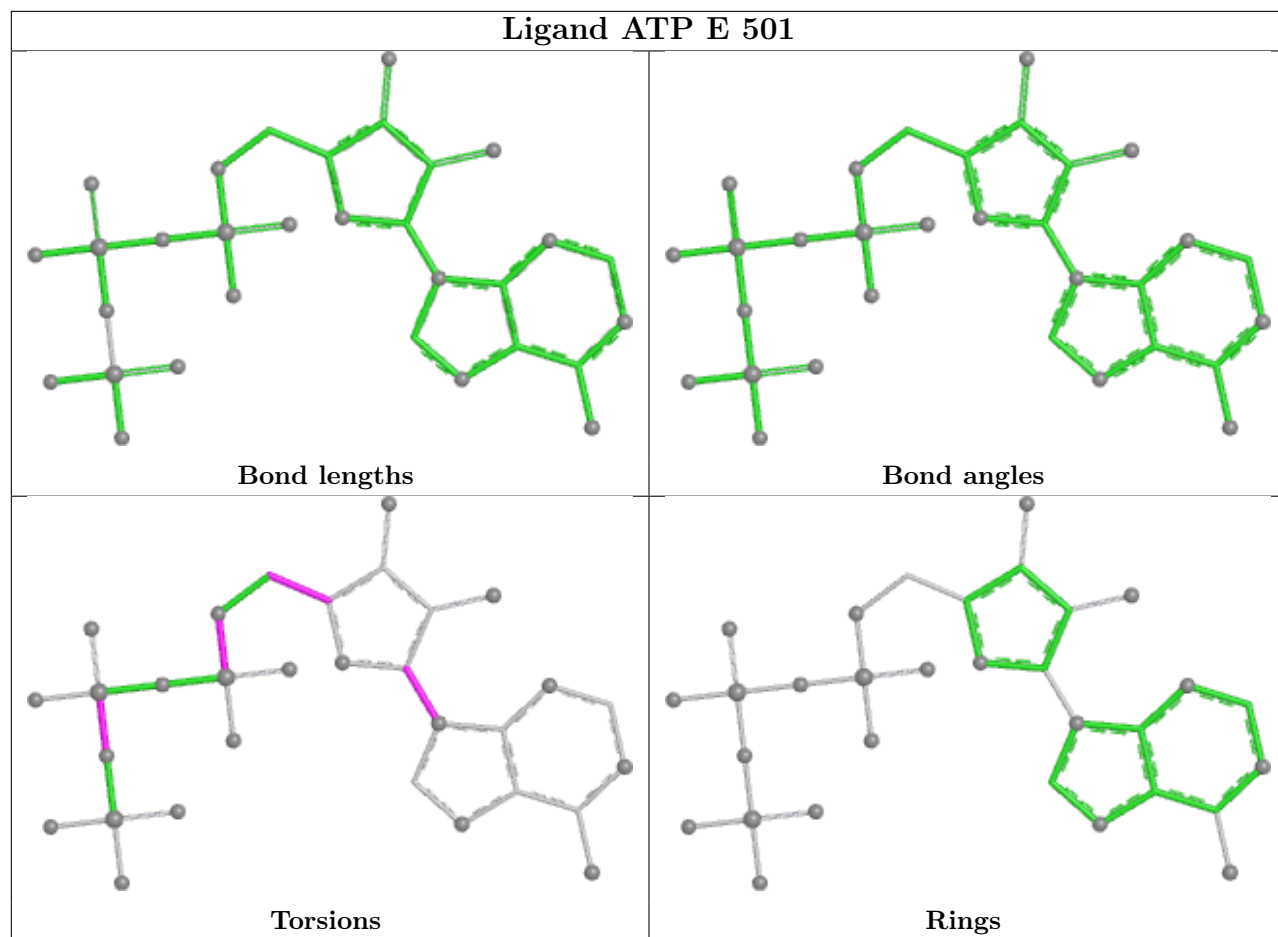
There are no ring outliers.

No monomer is involved in short contacts.

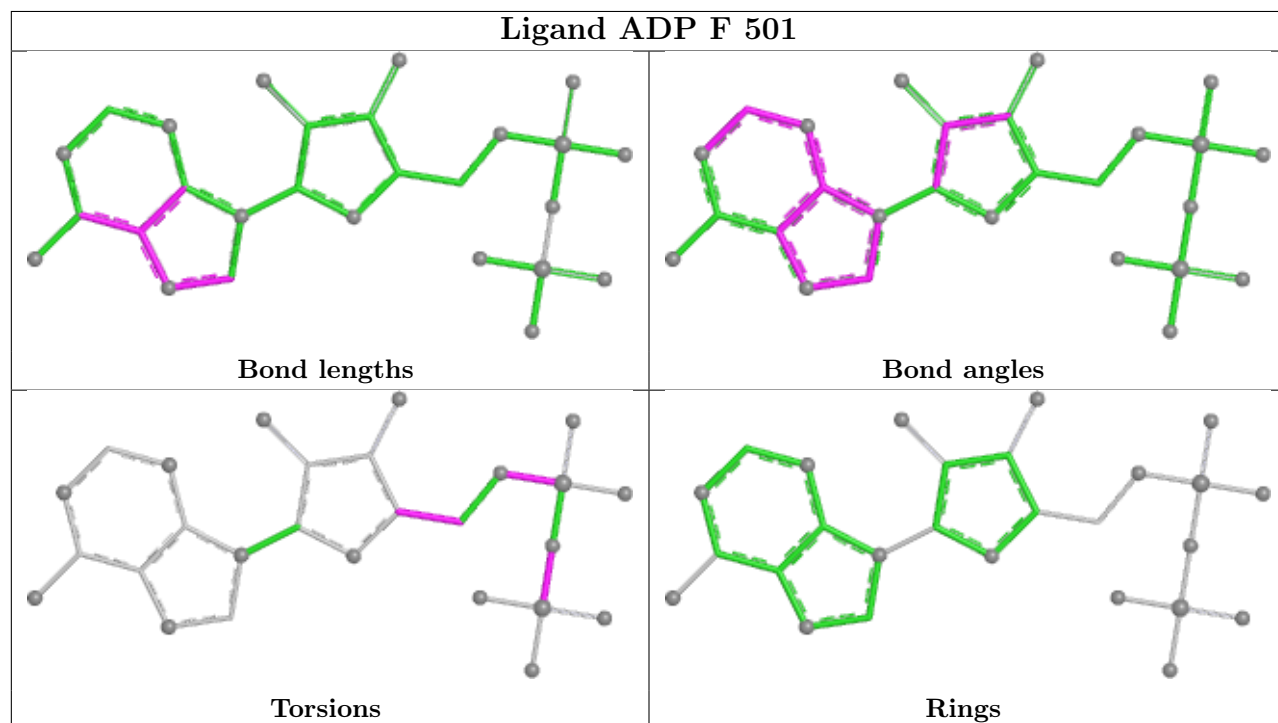
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

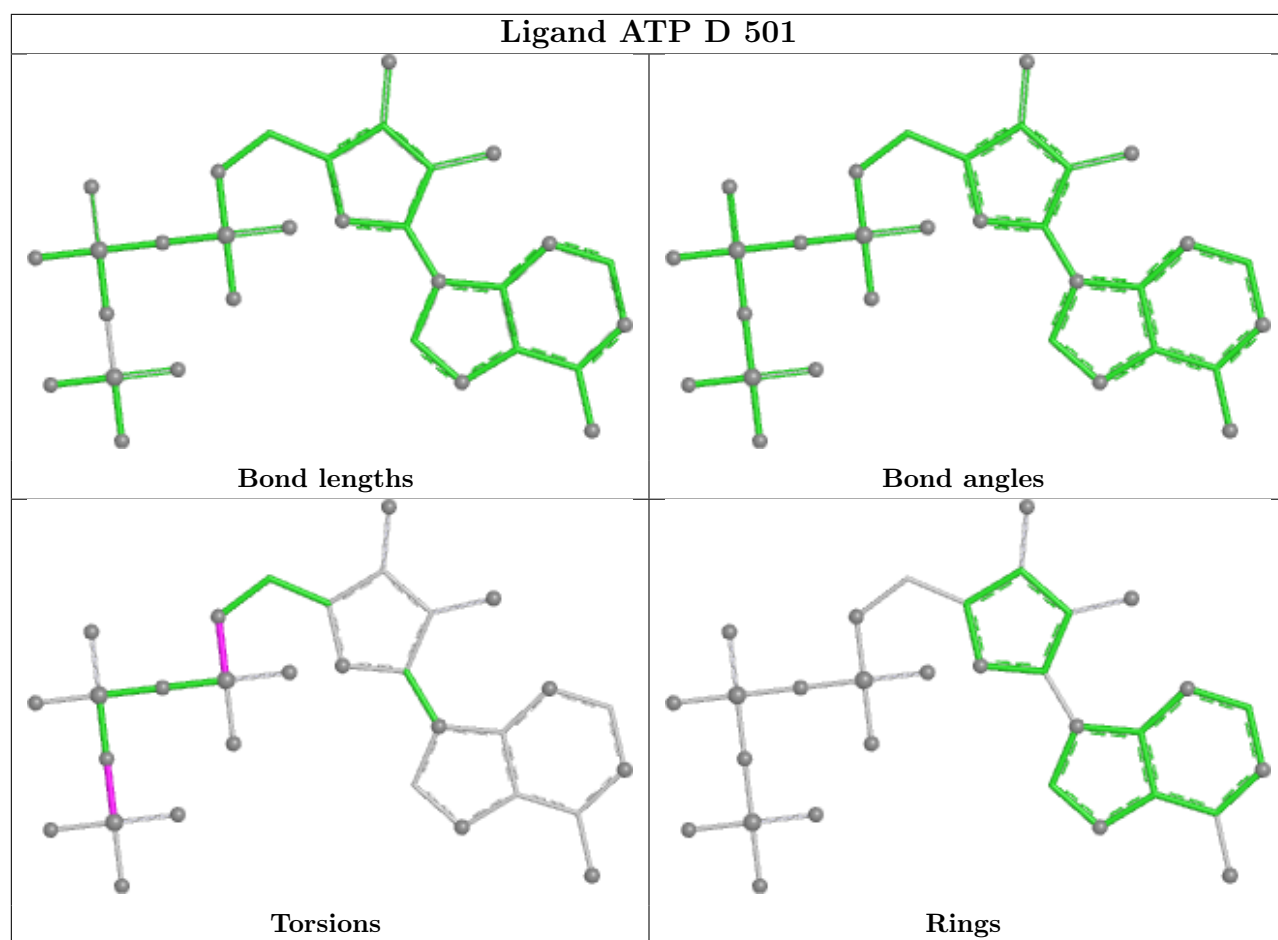


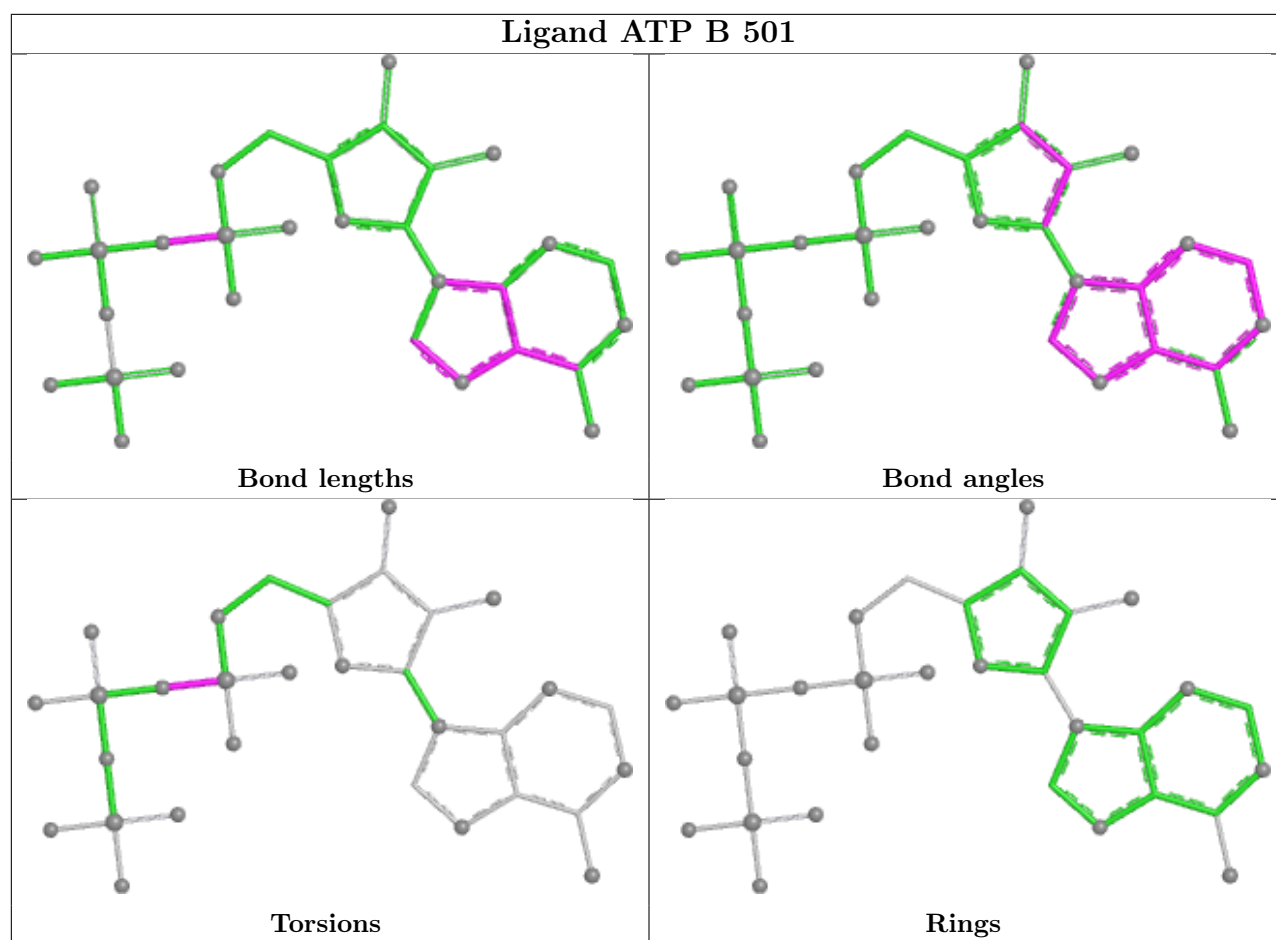
Ligand ATP E 501



Ligand ADP F 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

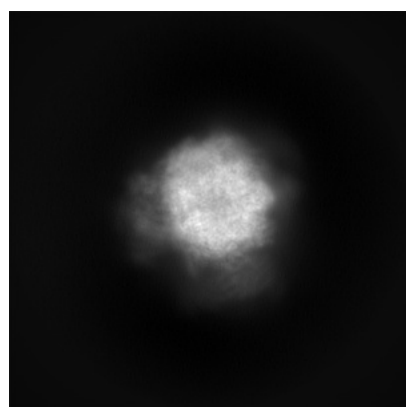
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32273. These allow visual inspection of the internal detail of the map and identification of artifacts.

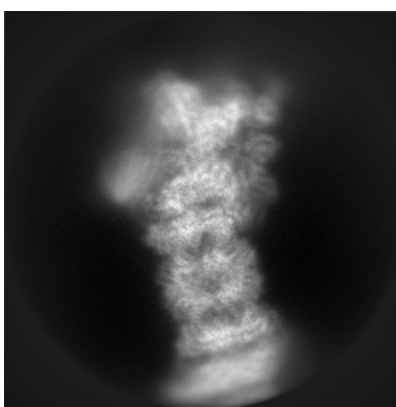
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

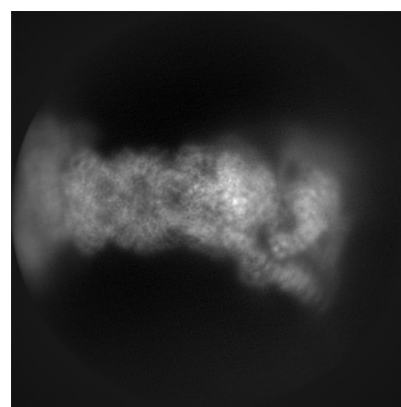
6.1.1 Primary map



X



Y

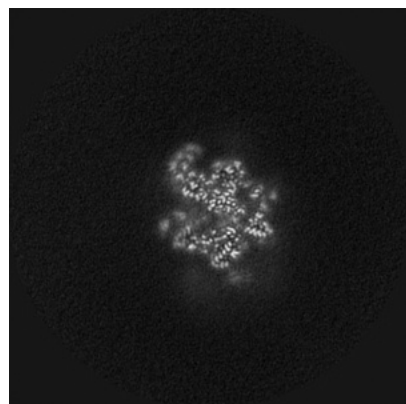


Z

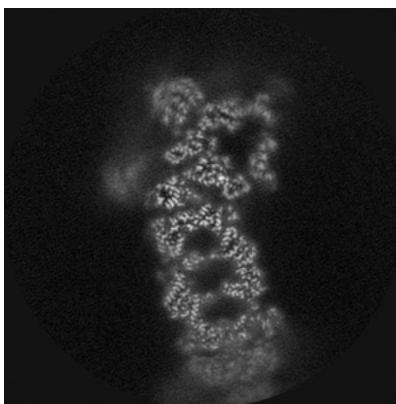
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

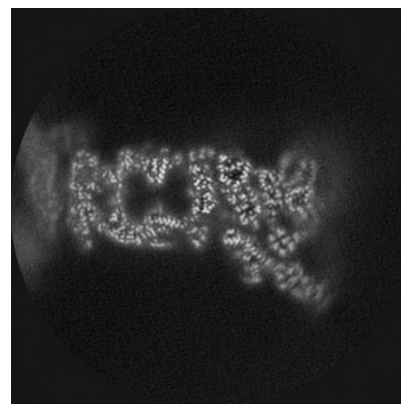
6.2.1 Primary map



X Index: 320



Y Index: 320

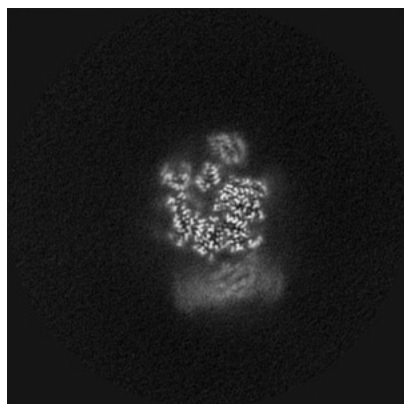


Z Index: 320

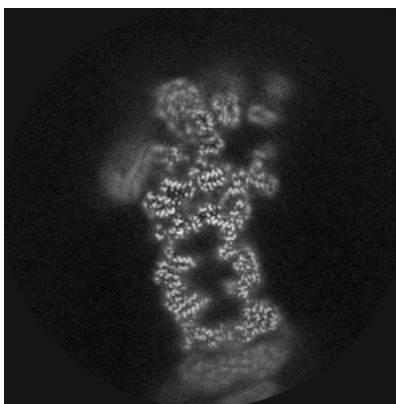
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

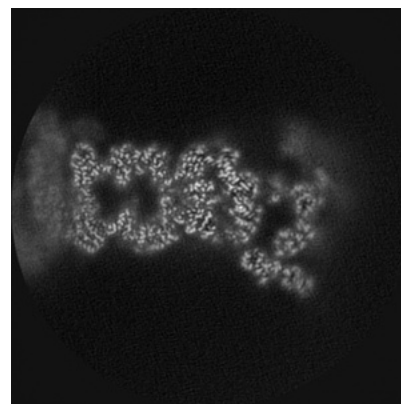
6.3.1 Primary map



X Index: 349



Y Index: 335

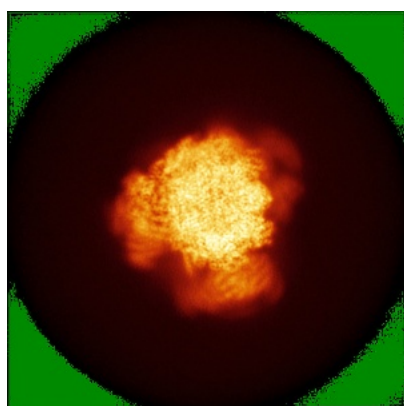


Z Index: 348

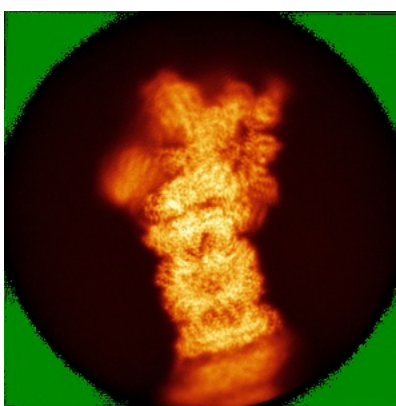
The images above show the largest variance slices of the map in three orthogonal directions.

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

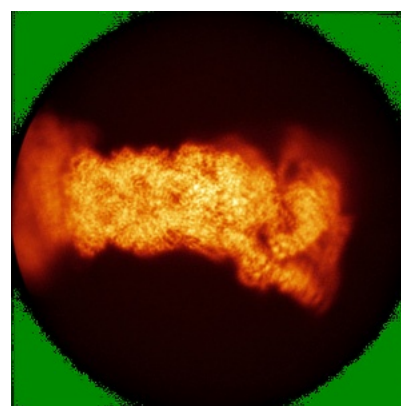
6.4.1 Primary map



X



Y

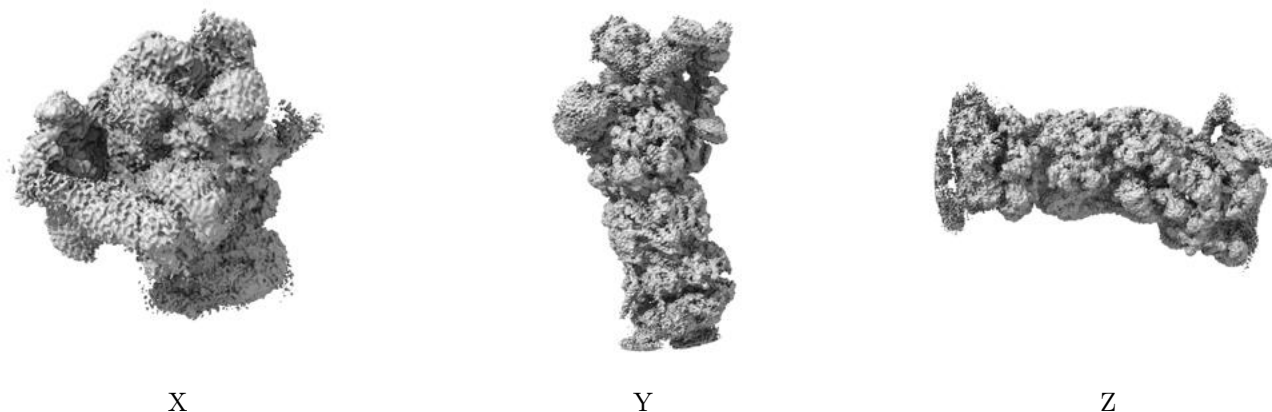


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

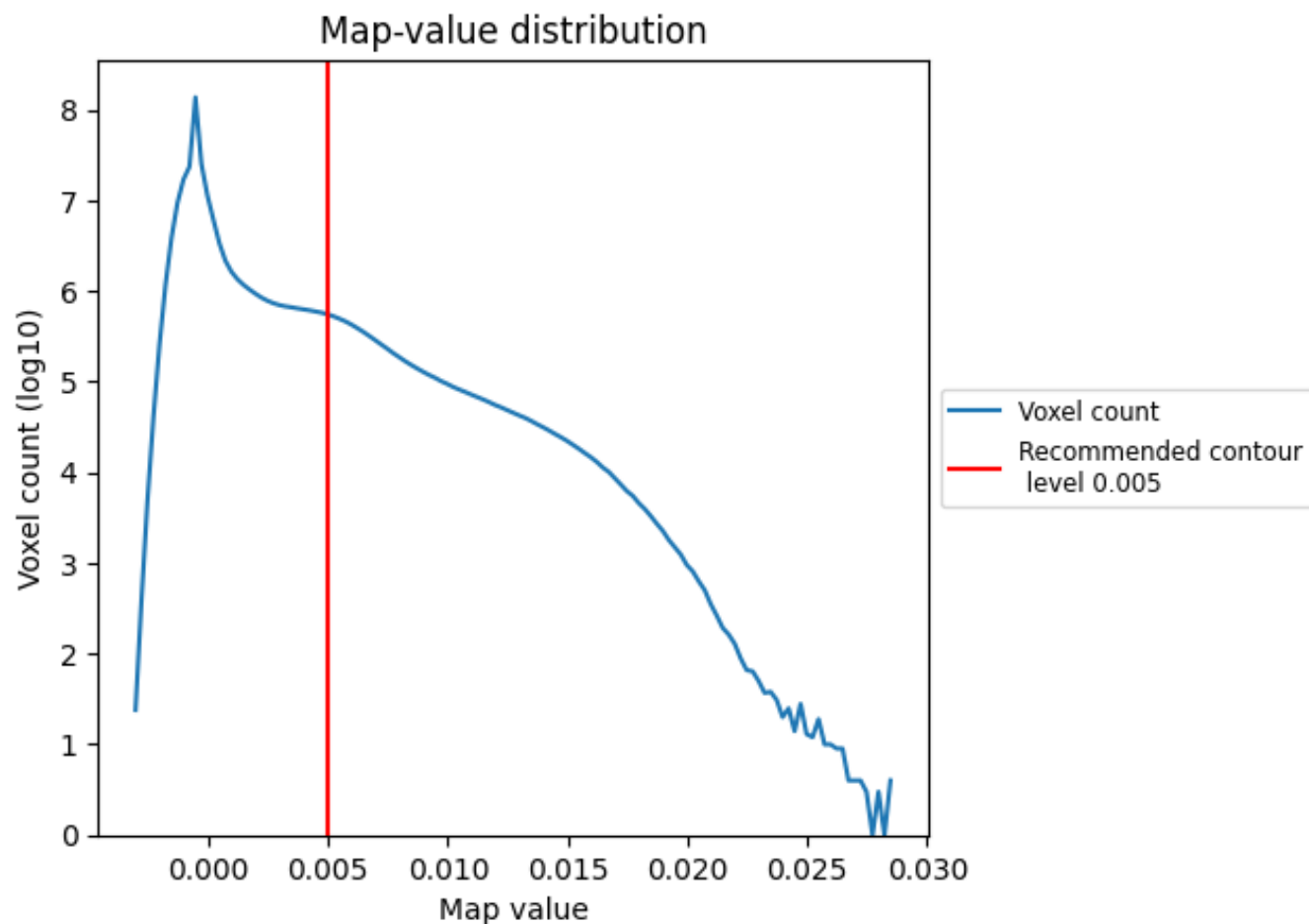
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

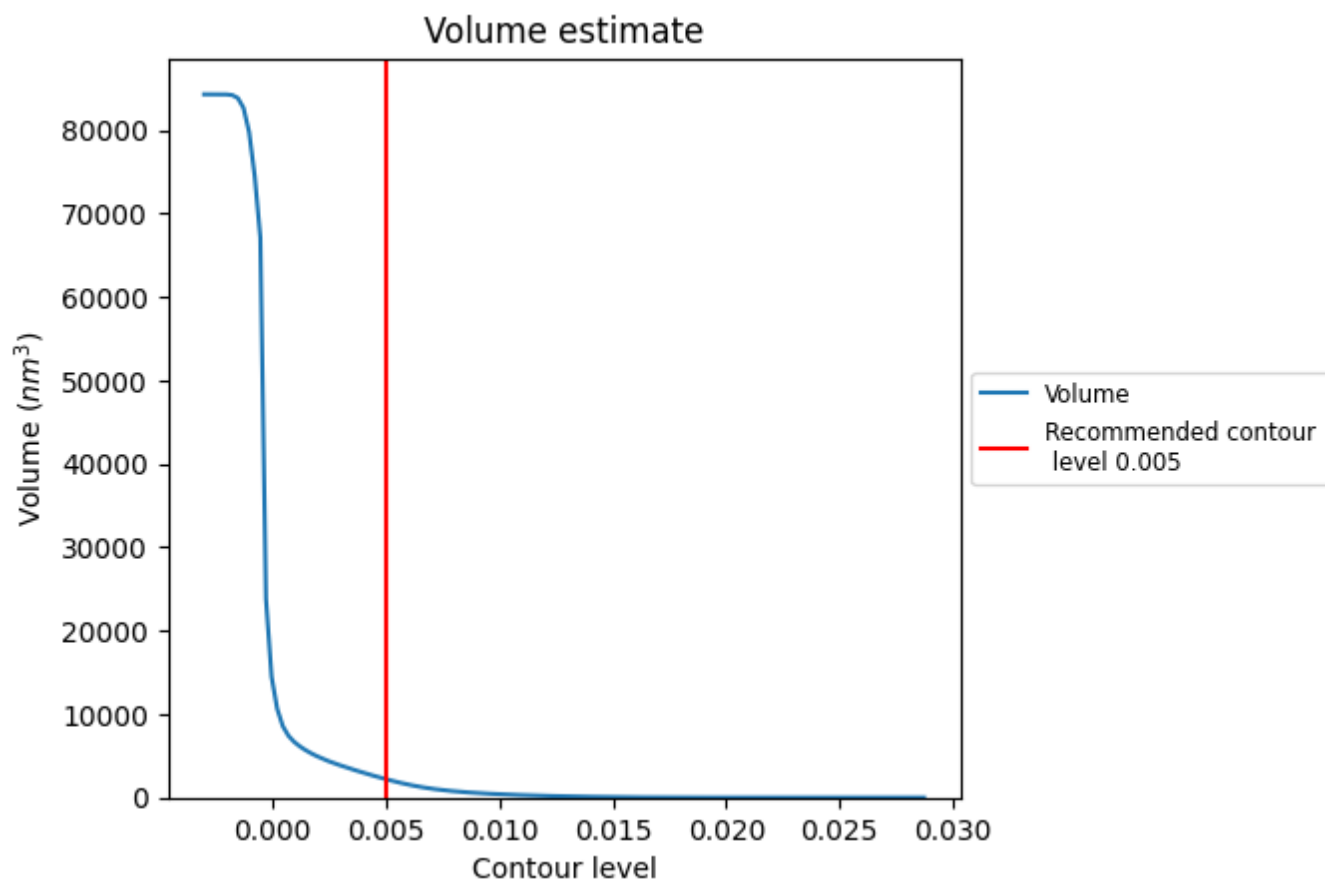
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

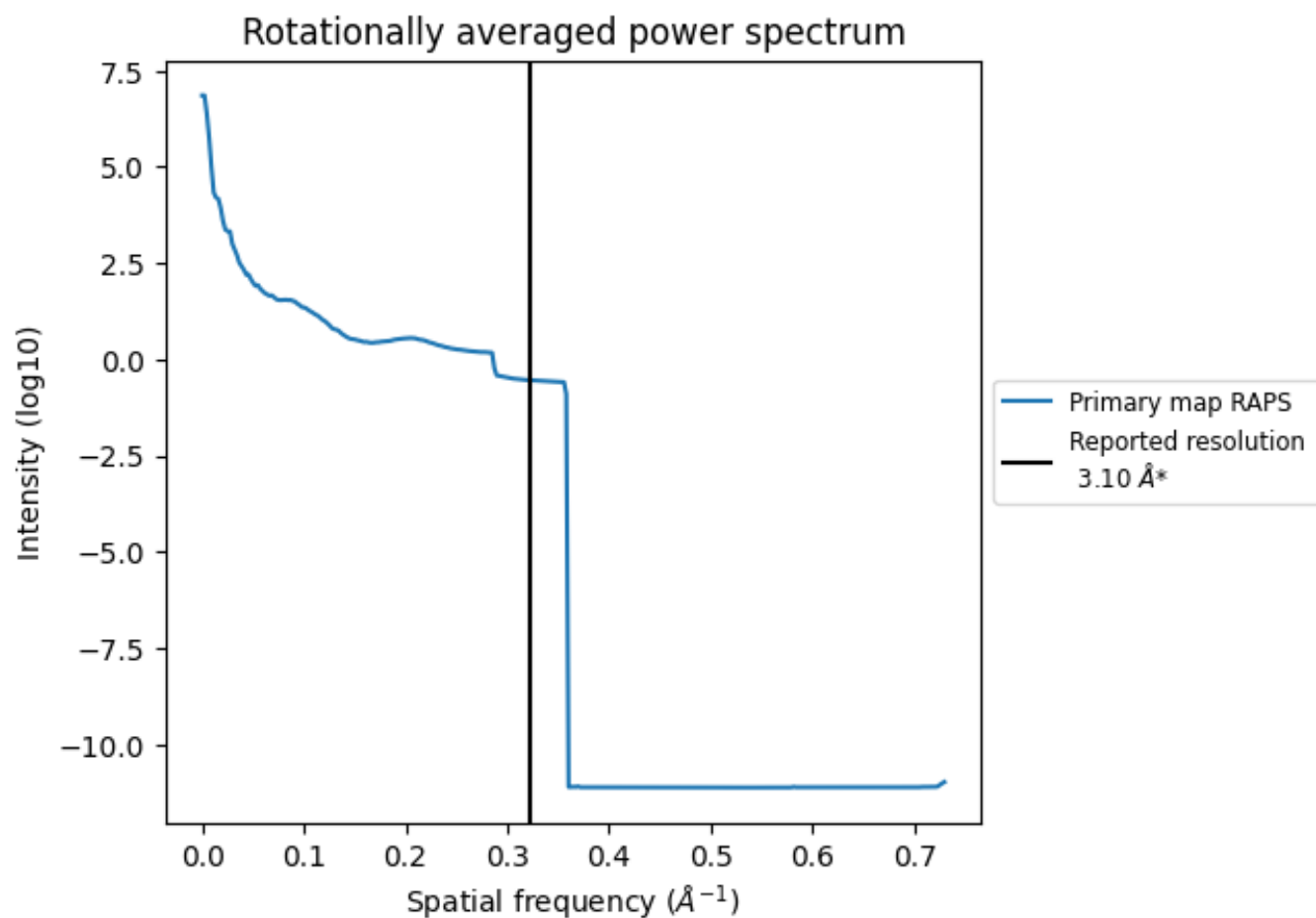
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2193 nm^3 ; this corresponds to an approximate mass of 1981 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 0.323 Å⁻¹

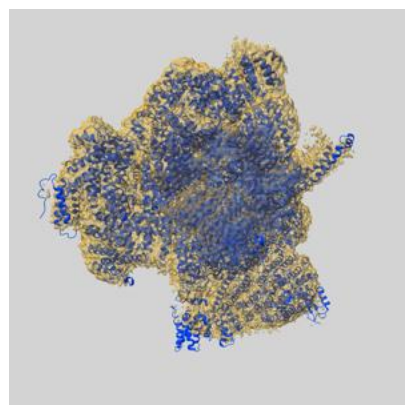
8 Fourier-Shell correlation

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

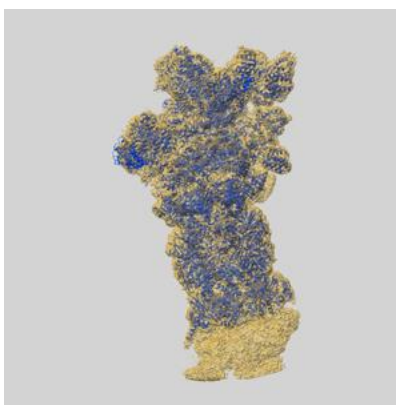
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32273 and PDB model 7W38. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

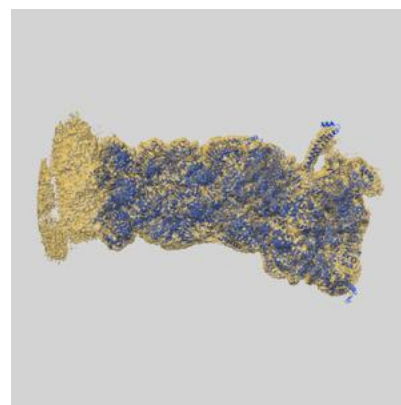
9.1 Map-model overlay [i](#)



X



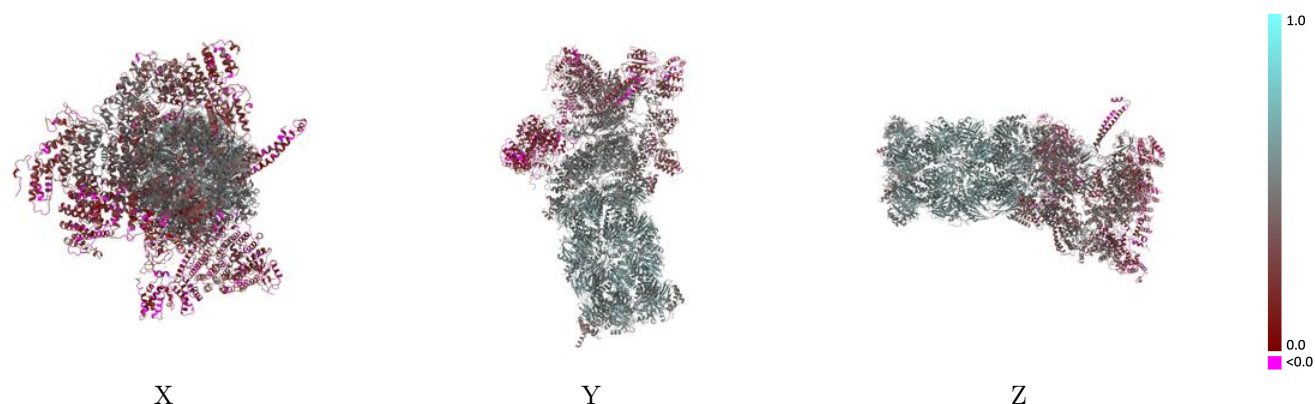
Y



Z

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

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

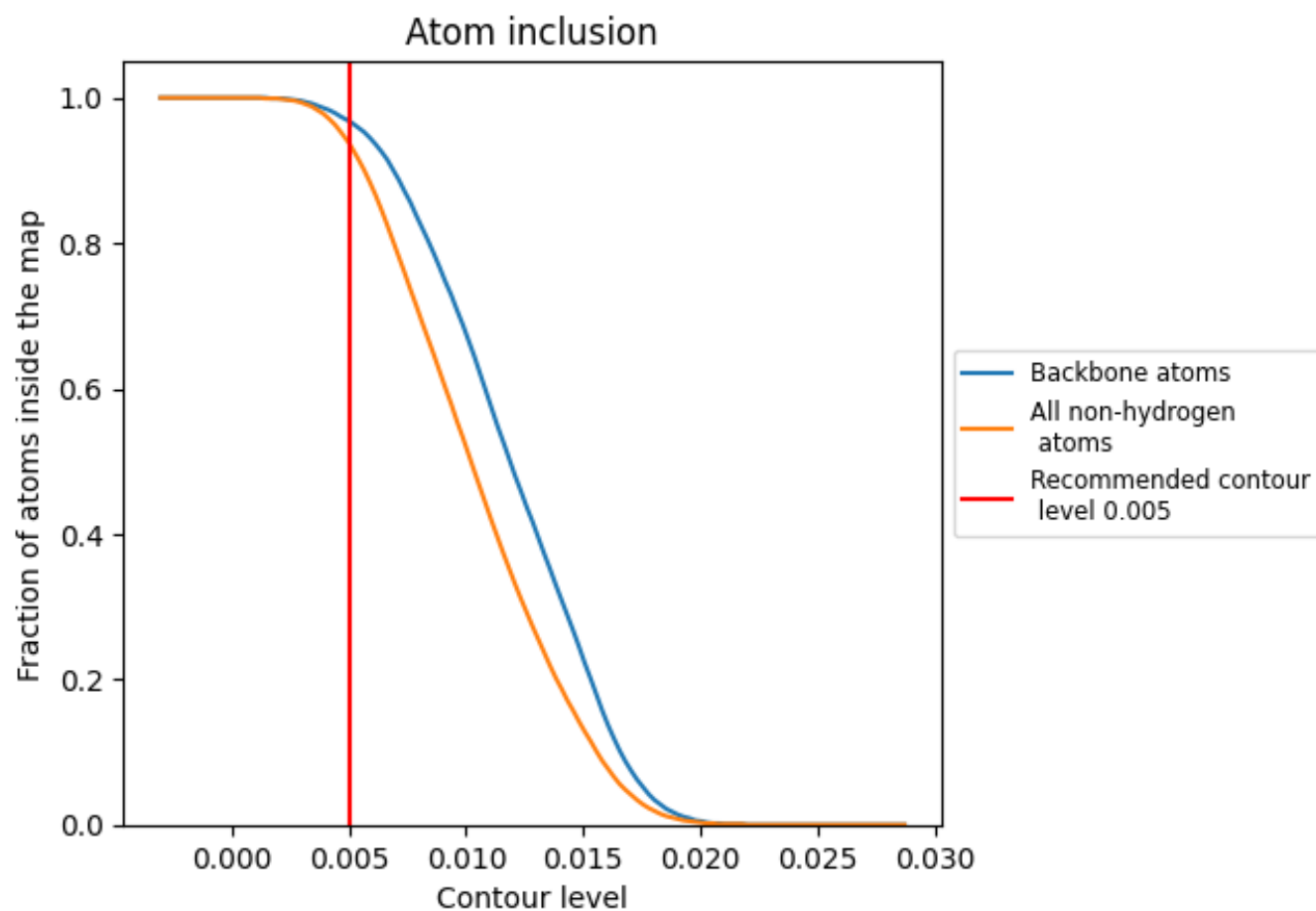


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.9380	 0.4200
A	 0.9340	 0.4190
B	 0.9710	 0.4200
C	 0.9770	 0.4370
D	 0.9810	 0.4350
E	 0.9690	 0.4410
F	 0.9100	 0.4180
G	 0.9860	 0.5260
H	 0.9890	 0.5300
I	 0.9870	 0.5190
J	 0.9790	 0.4880
K	 0.9860	 0.5320
L	 0.9910	 0.5430
M	 0.9880	 0.5290
N	 0.9940	 0.5620
O	 0.9950	 0.5490
P	 0.9970	 0.5570
Q	 0.9960	 0.5510
R	 0.9970	 0.5500
S	 0.9910	 0.5510
T	 0.9900	 0.5610
U	 0.8990	 0.2490
V	 0.8730	 0.2530
W	 0.9070	 0.3040
X	 0.9550	 0.3590
Y	 0.9520	 0.3740
Z	 0.9460	 0.3600
a	 0.9070	 0.2760
b	 0.9150	 0.2090
c	 0.9630	 0.4000
d	 0.6640	 0.1910
e	 0.8930	 0.2990
f	 0.7740	 0.1590
g	 0.9760	 0.5260
h	 0.9900	 0.5320



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.9700	 0.5040
j	 0.9750	 0.4660
k	 0.9790	 0.5160
l	 0.9880	 0.5330
m	 0.9810	 0.5240
n	 0.9950	 0.5690
o	 0.9910	 0.5590
p	 0.9960	 0.5590
q	 0.9970	 0.5540
r	 0.9970	 0.5620
s	 0.9930	 0.5560
t	 0.9910	 0.5630
u	 0.8950	 0.3760
x	 0.1460	 0.1300