



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:17 PM UTC

PDB ID : 6MSJ / pdb_00006msj
EMDB ID : EMD-9221
Title : Cryo-EM structures and dynamics of substrate-engaged human 26S proteasome
Authors : Mao, Y.D.
Deposited on : 2018-10-16
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 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

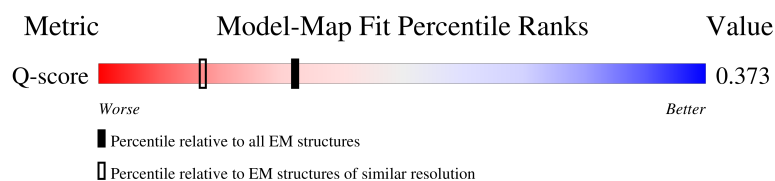
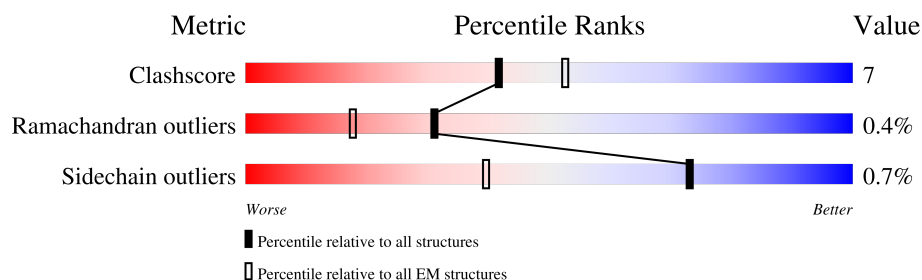
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	U	953	
2	V	533	
3	W	456	
4	X	422	

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Mol	Chain	Length	Quality of chain
5	Y	389	
6	Z	324	
7	a	376	
8	b	377	
9	c	309	
10	d	349	
11	e	70	
12	f	892	
13	A	433	
14	B	440	
15	C	398	
16	D	418	
17	E	403	
18	F	439	
19	v	36	
20	G	245	
21	H	233	
21	h	233	
22	I	260	
22	i	260	
23	J	247	
23	j	247	
24	K	240	
24	k	240	
25	L	268	

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Mol	Chain	Length	Quality of chain
25	l	268	
26	M	254	
26	m	254	
27	N	238	
27	n	238	
28	O	276	
28	o	276	
29	P	204	
29	p	204	
30	Q	201	
30	q	201	
31	R	262	
31	r	262	
32	S	240	
32	s	240	
33	T	263	
33	t	263	
34	g	240	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 105316 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	480	Total	C	N	O	S	0	0
			3852	2444	684	710	14		

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

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

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 11 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	e	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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

- Molecule 13 is a protein called 26S proteasome regulatory subunit 7.

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

- Molecule 14 is a protein called Rpt2, NP_002793.2 (26SHA chain B).

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

- Molecule 15 is a protein called 26S proteasome regulatory subunit 8.

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

- Molecule 16 is a protein called 26S proteasome regulatory subunit 6B.

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

- Molecule 17 is a protein called 26S proteasome regulatory subunit 10B.

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

- Molecule 18 is a protein called 26S proteasome regulatory subunit 6A.

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

- Molecule 19 is a protein called substrate.

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

- Molecule 20 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G	239	Total	C	N	O	S	0	0
			1836	1168	305	350	13		

- Molecule 21 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	230	Total	C	N	O	S	0	0
			1723	1097	289	332	5		
21	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 22 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	I	248	Total	C	N	O	S	0	0
			1908	1204	326	369	9		
22	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 23 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	J	239	Total	C	N	O	S	0	0
			1739	1077	317	340	5		
23	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 24 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	K	228	Total	C	N	O	S	0	0
			1729	1086	284	349	10		
24	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 25 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		
25	l	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 26 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	m	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 27 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		
27	n	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 28 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
28	o	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 29 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		
29	p	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 30 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
30	q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 31 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
31	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 32 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
32	s	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

- Molecule 33 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
33	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

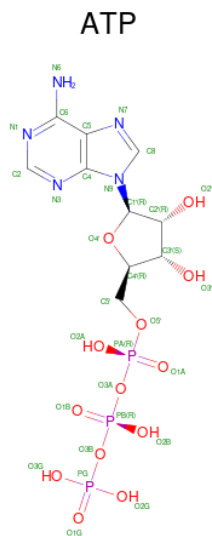
- Molecule 34 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

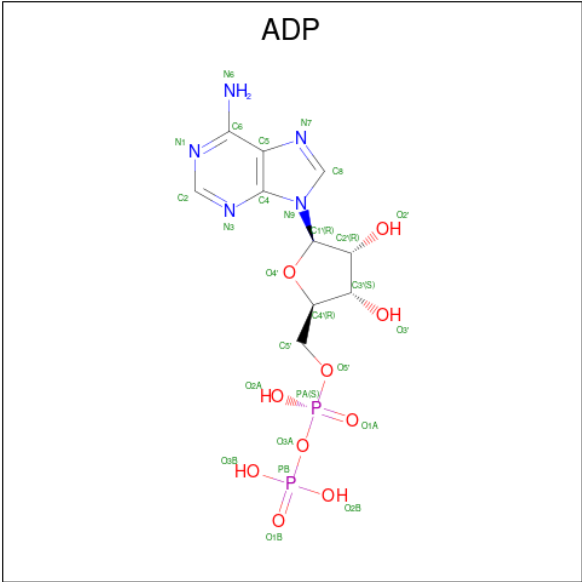


Mol	Chain	Residues	Atoms					AltConf
36	A	1	Total 31	C 10	N 5	O 13	P 3	0
36	B	1	Total 31	C 10	N 5	O 13	P 3	0
36	C	1	Total 31	C 10	N 5	O 13	P 3	0
36	D	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



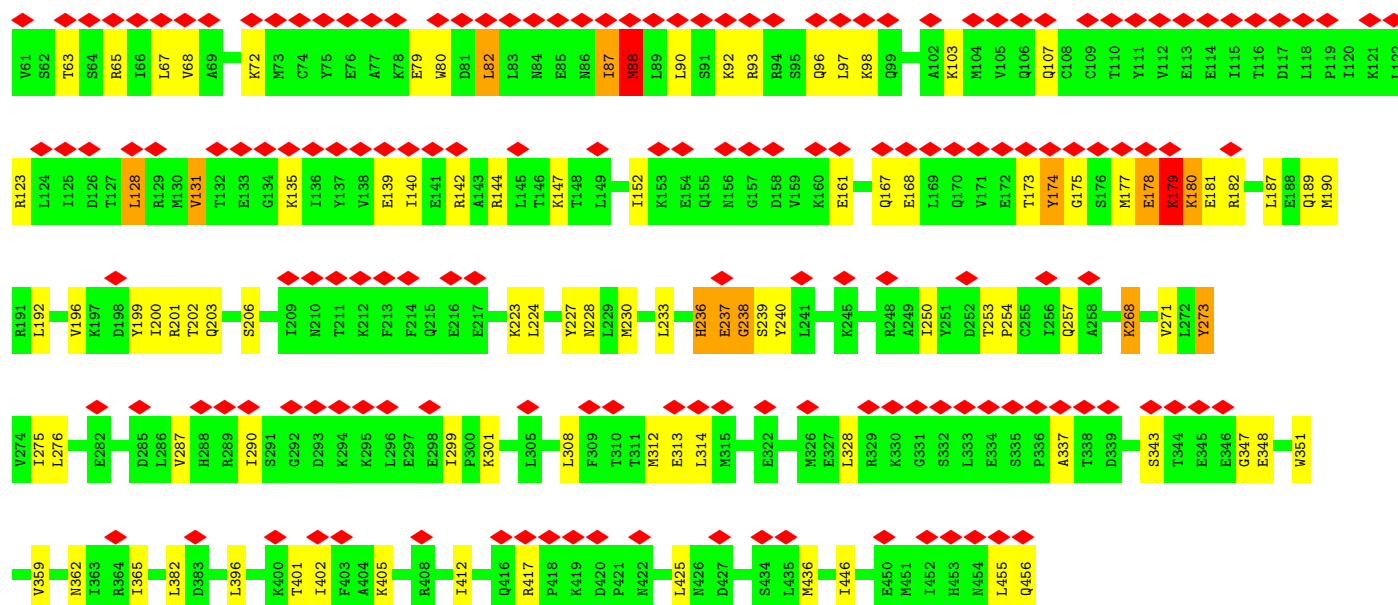
Mol	Chain	Residues	Atoms					AltConf
38	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

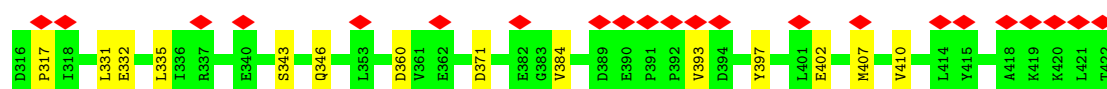
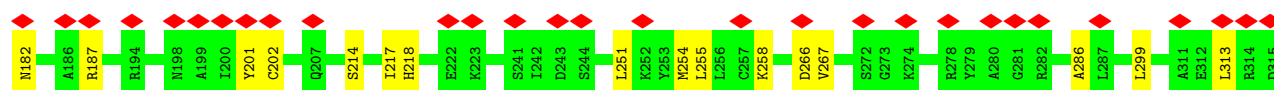
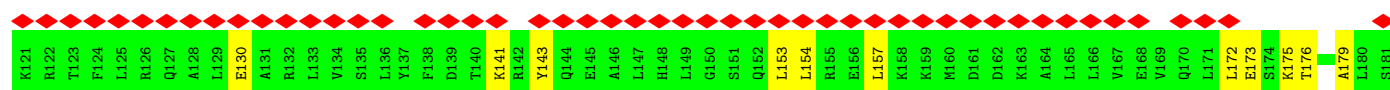
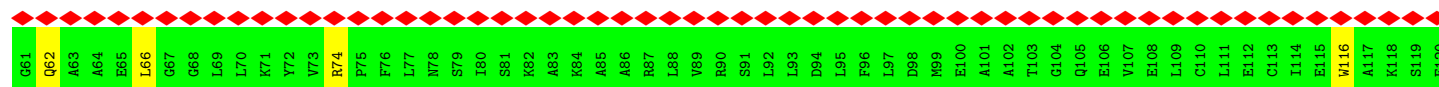
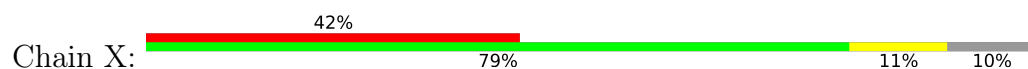
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

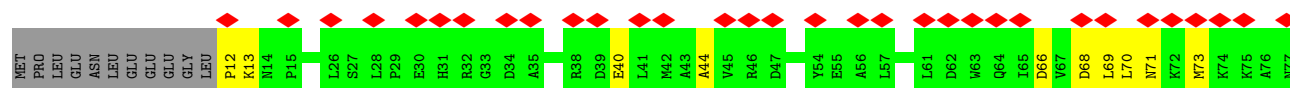
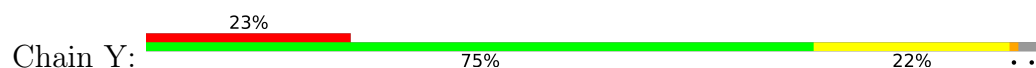


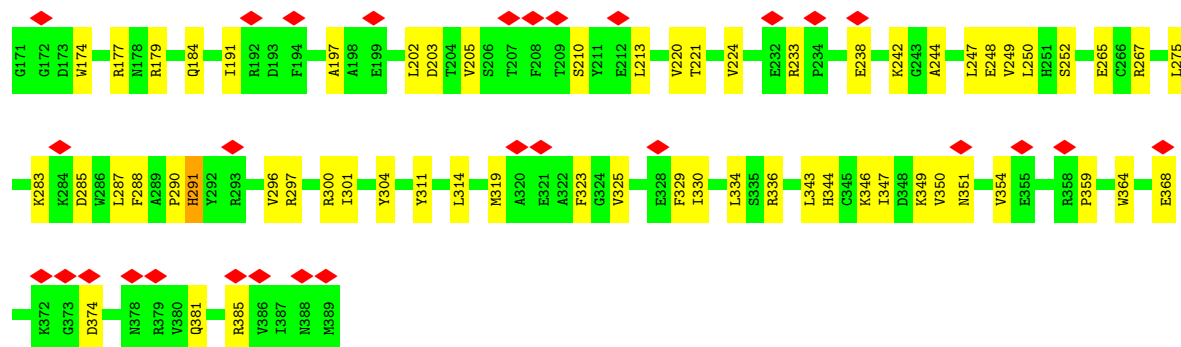


• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

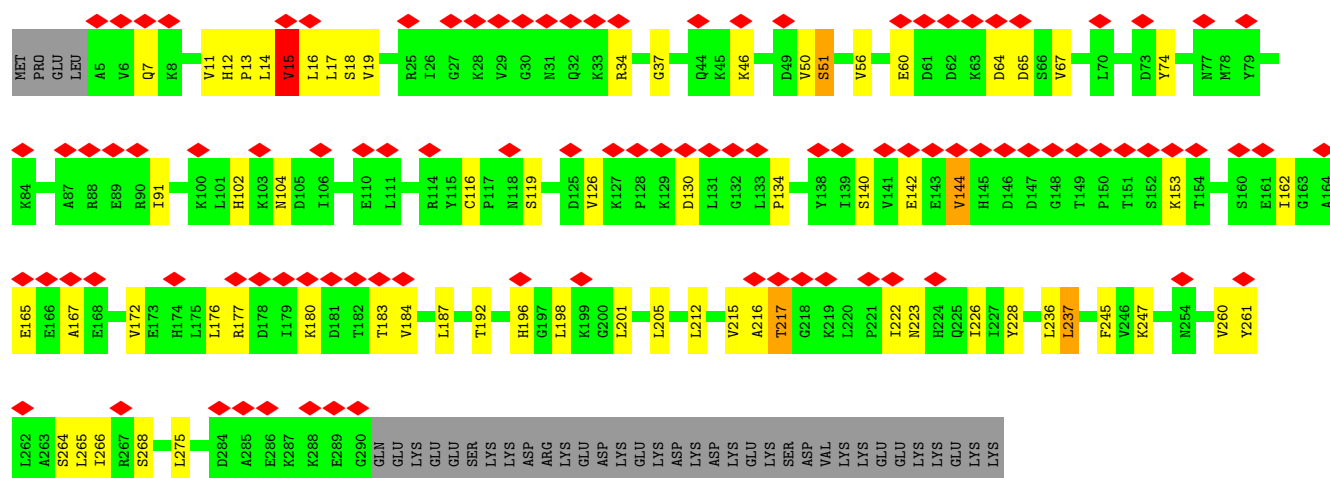


• Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

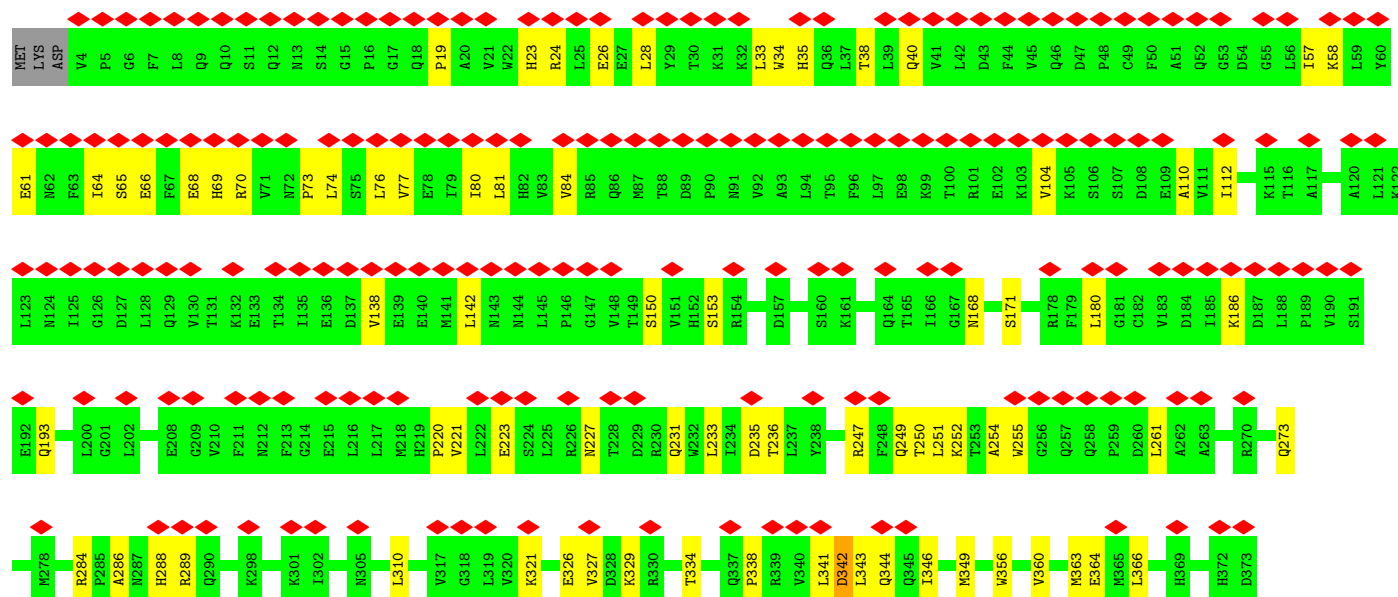
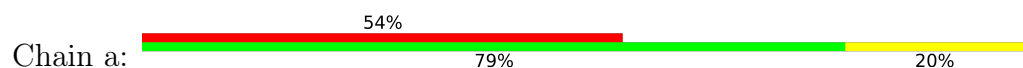


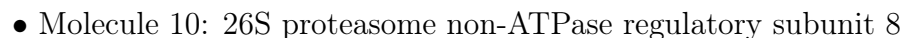


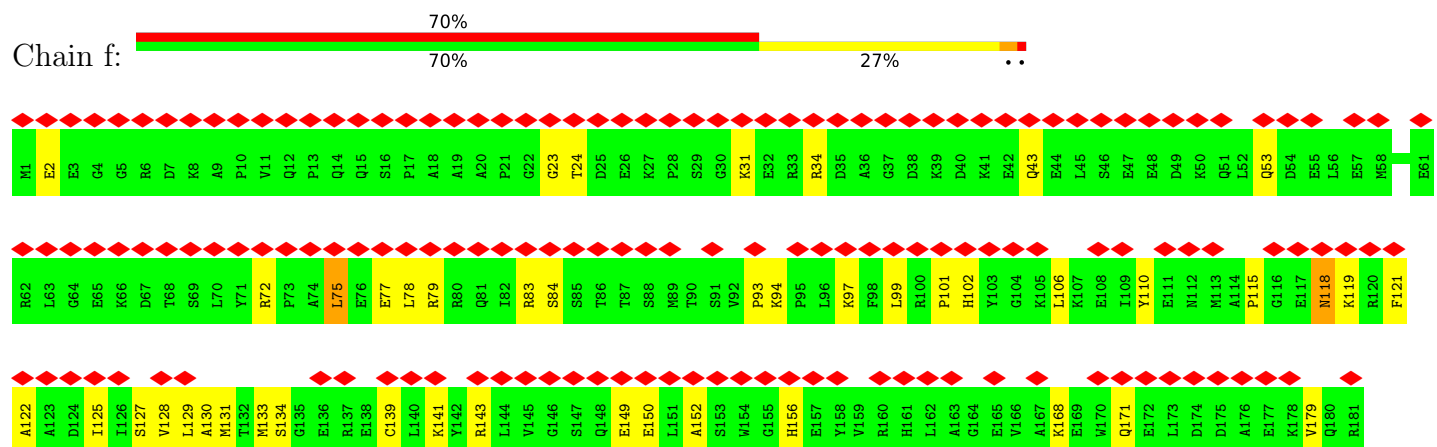
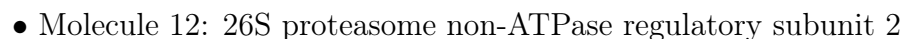
• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

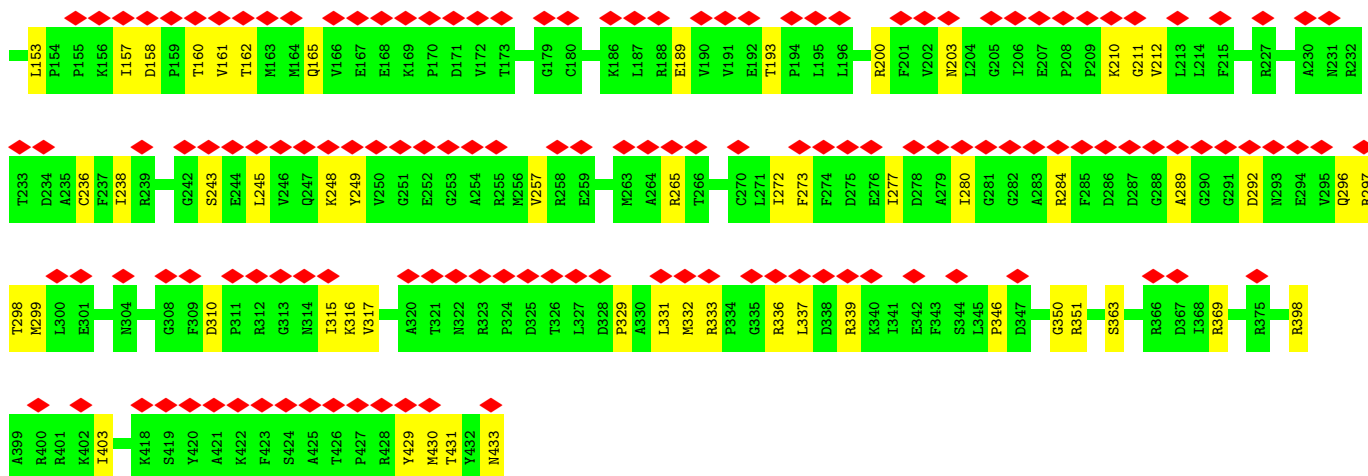


• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13



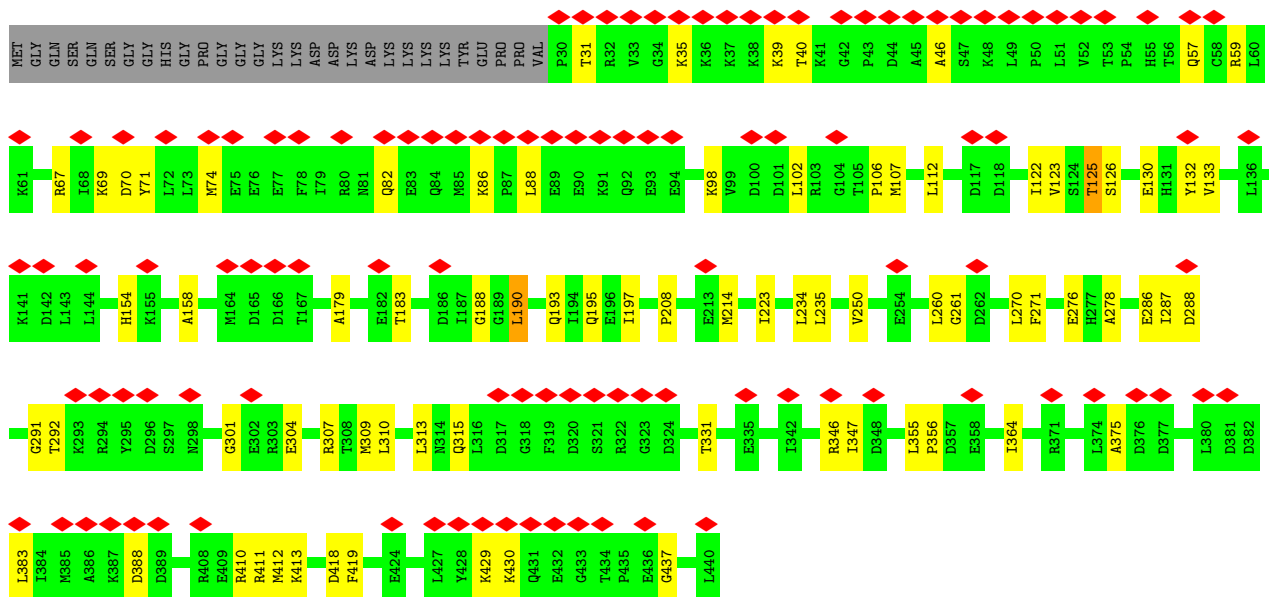






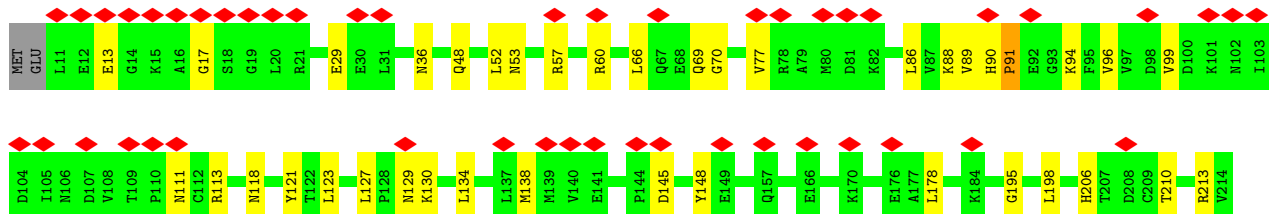
- Molecule 14: Rpt2, NP_002793.2 (26SHA chain B)

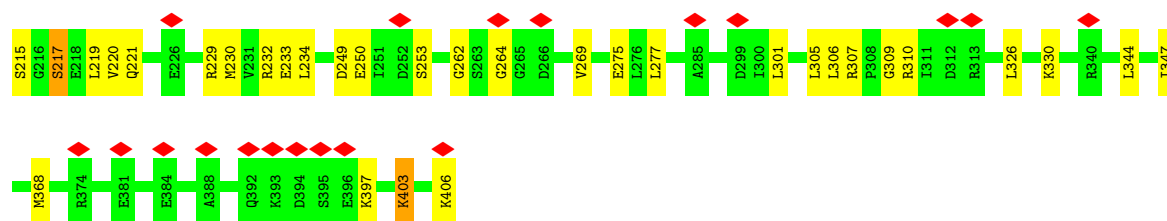
Chain B: 25% 76% 17% 7%



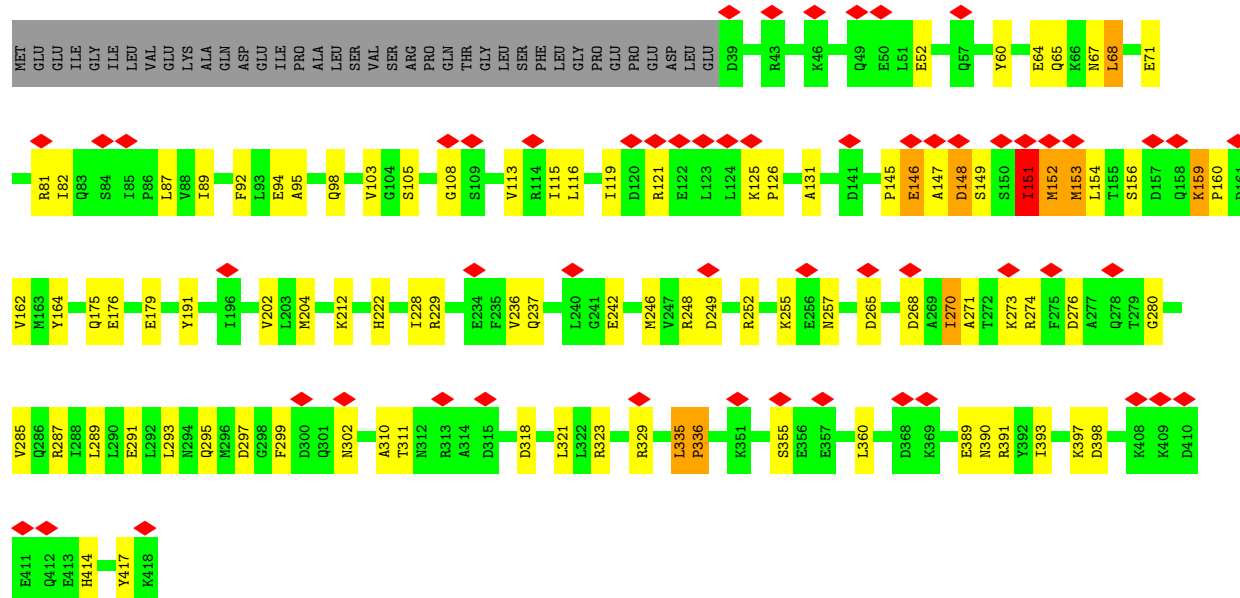
- Molecule 15: 26S proteasome regulatory subunit 8

Chain C: 17% 82% 17%

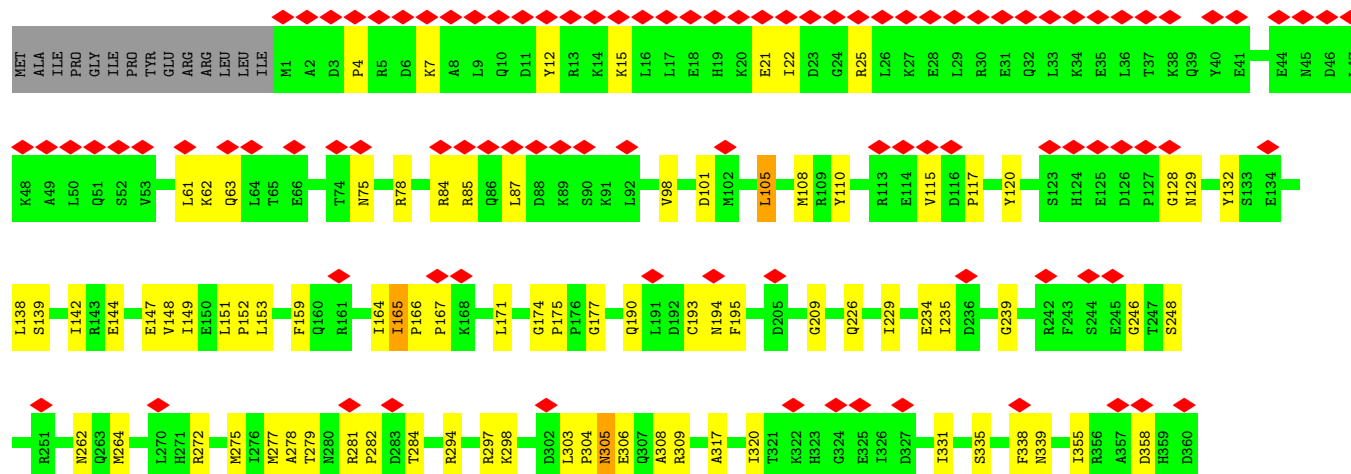
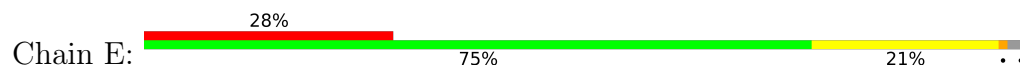


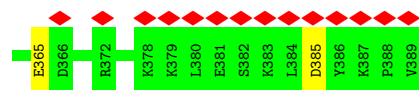


• Molecule 16: 26S proteasome regulatory subunit 6B



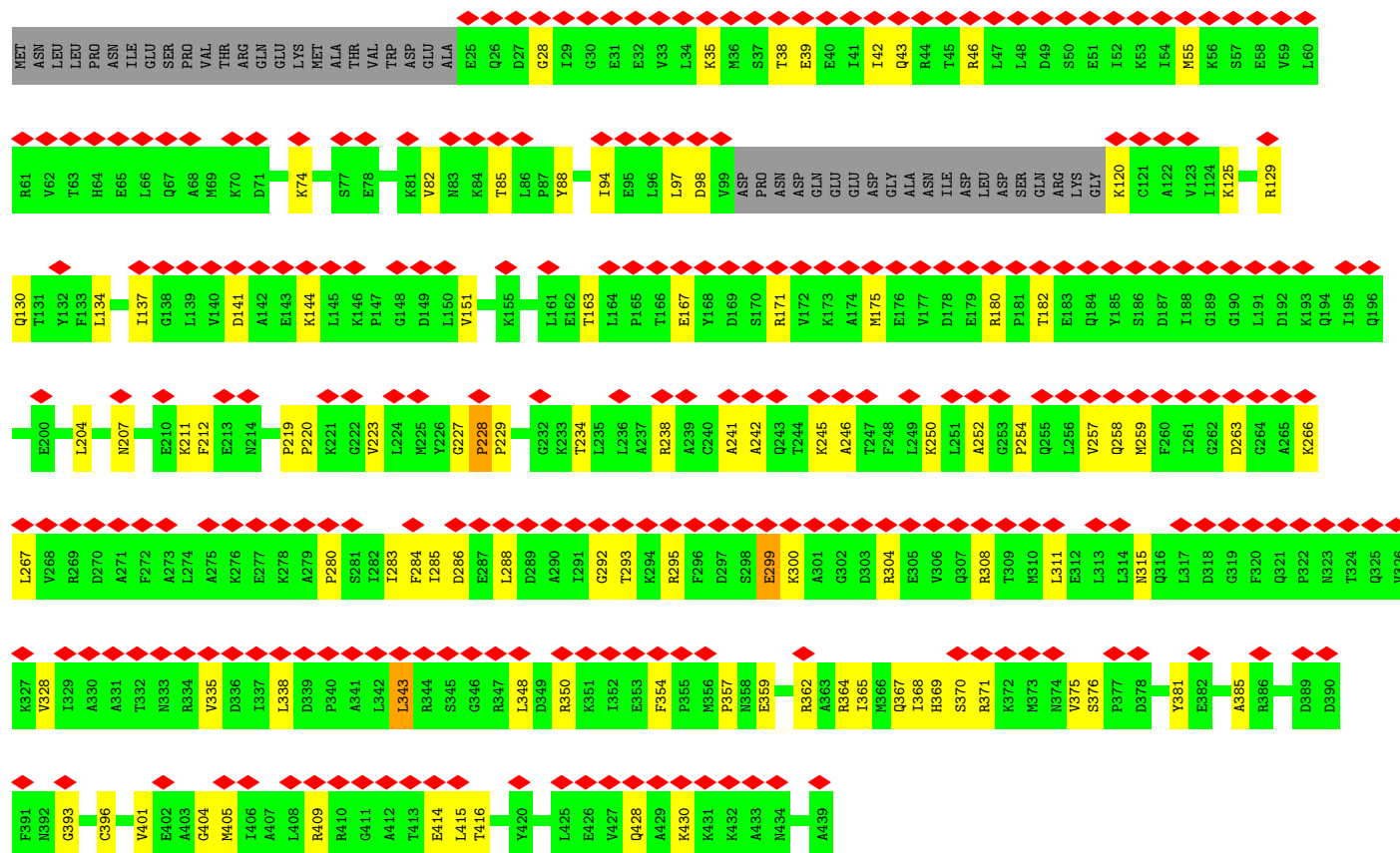
• Molecule 17: 26S proteasome regulatory subunit 10B





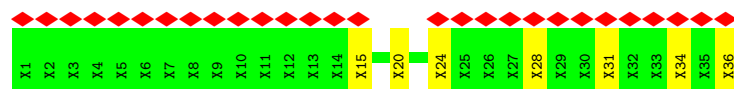
• Molecule 18: 26S proteasome regulatory subunit 6A

Chain F: 61% 67% 23% 10%



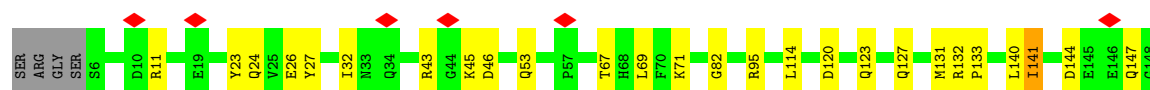
• Molecule 19: substrate

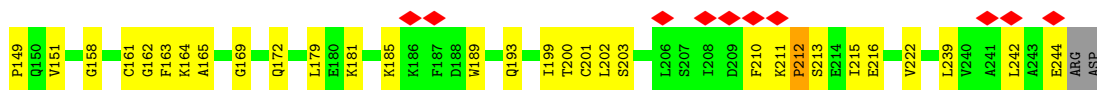
Chain v: 78% 81% 19%



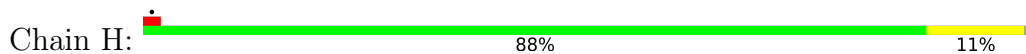
• Molecule 20: Proteasome subunit alpha type-6

Chain G: 7% 75% 22% 2%

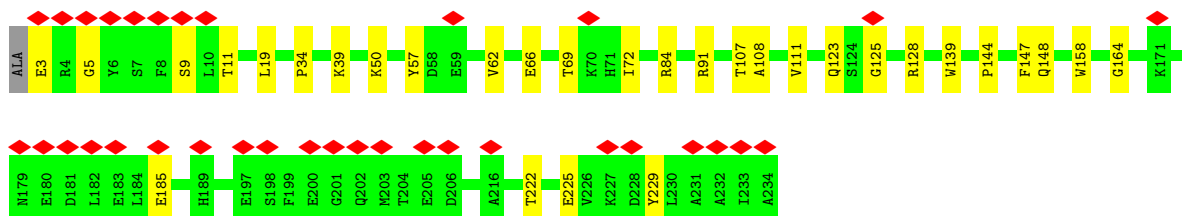
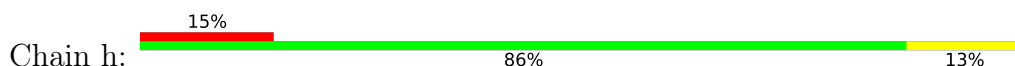




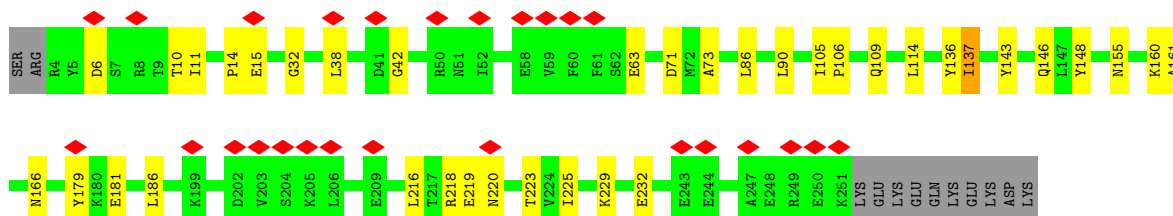
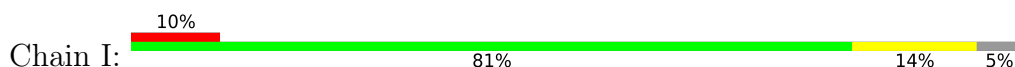
- Molecule 21: Proteasome subunit alpha type-2



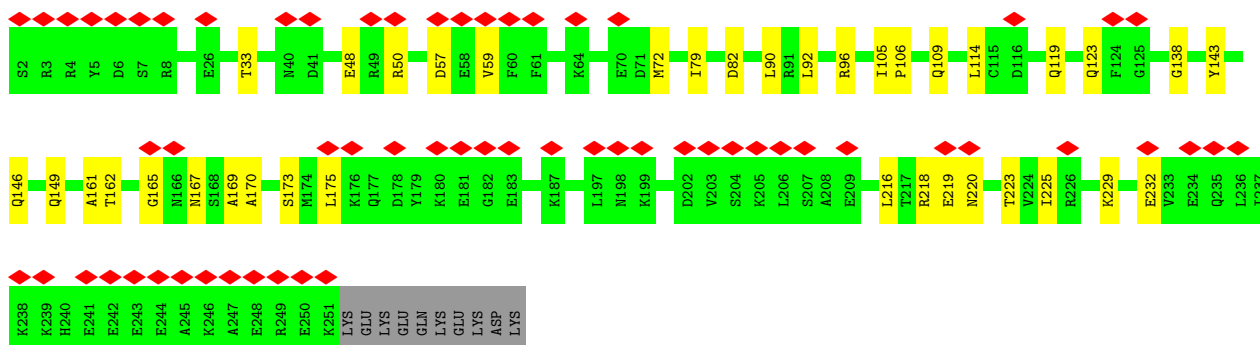
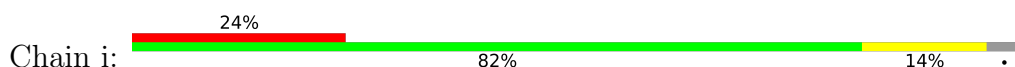
- Molecule 21: Proteasome subunit alpha type-2



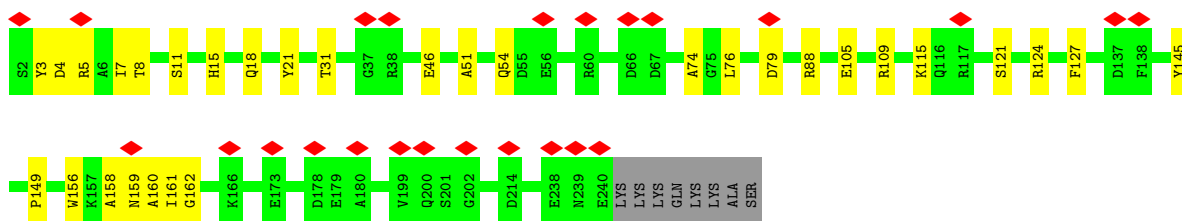
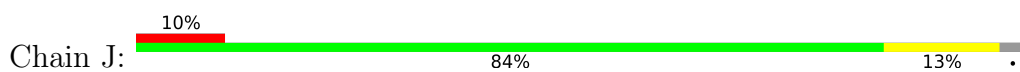
- Molecule 22: Proteasome subunit alpha type-4



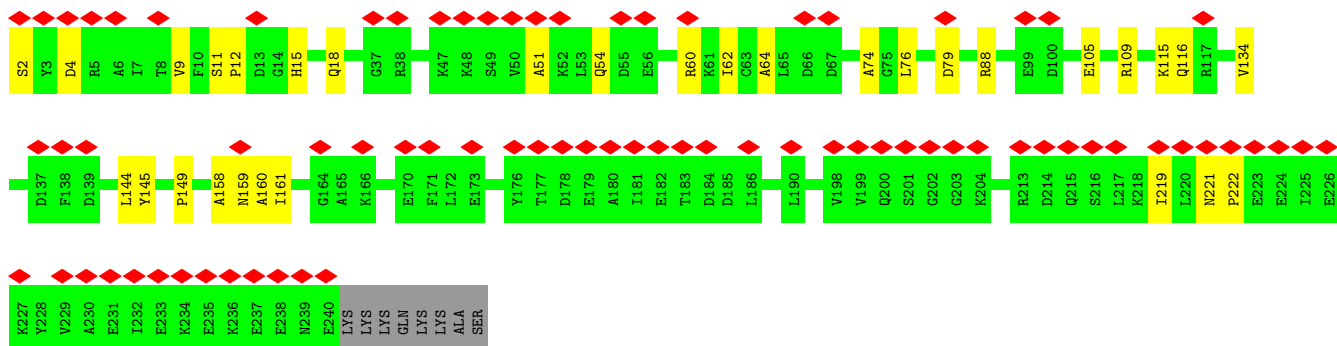
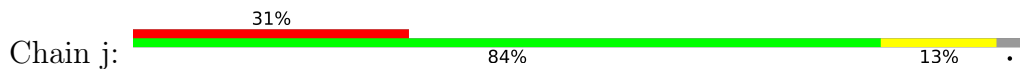
- Molecule 22: Proteasome subunit alpha type-4



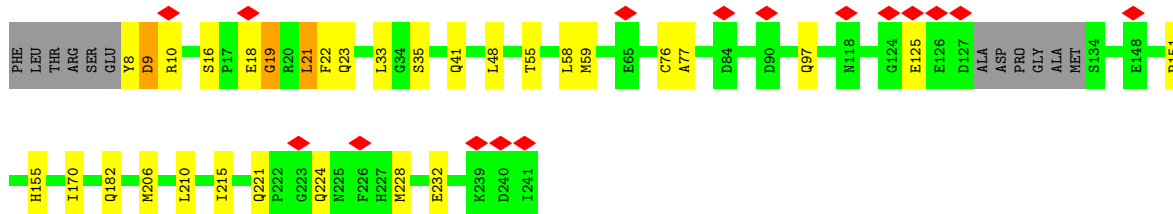
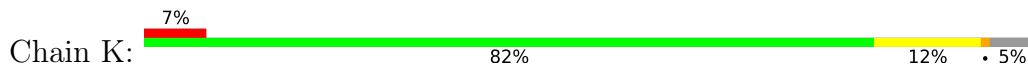
- Molecule 23: Proteasome subunit alpha type-7



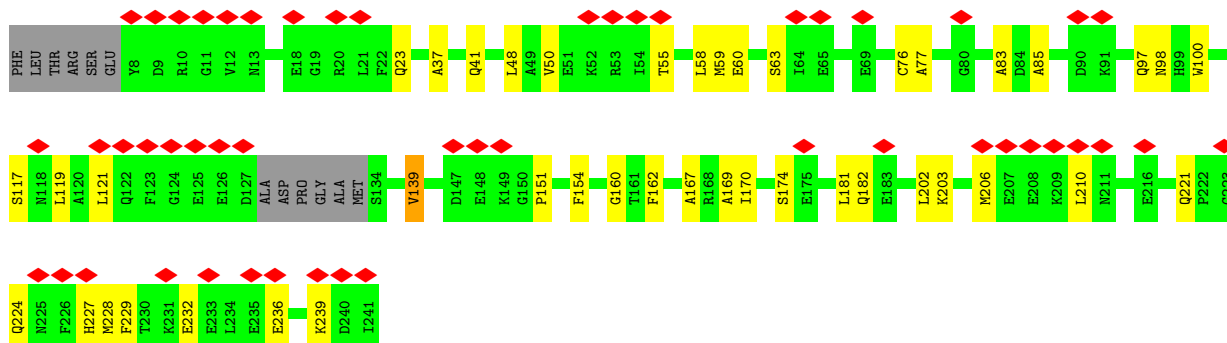
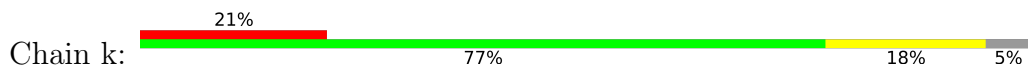
• Molecule 23: Proteasome subunit alpha type-7



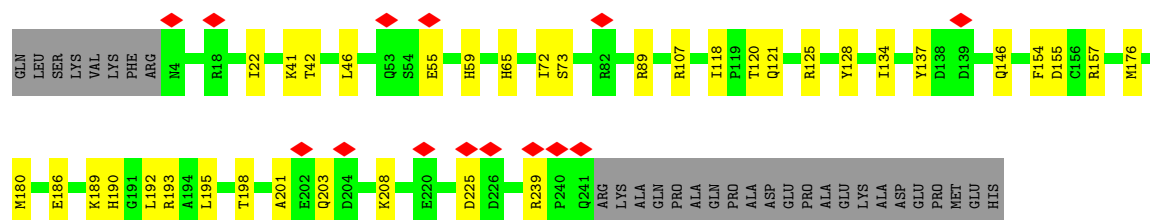
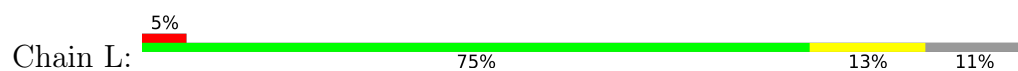
• Molecule 24: Proteasome subunit alpha type-5



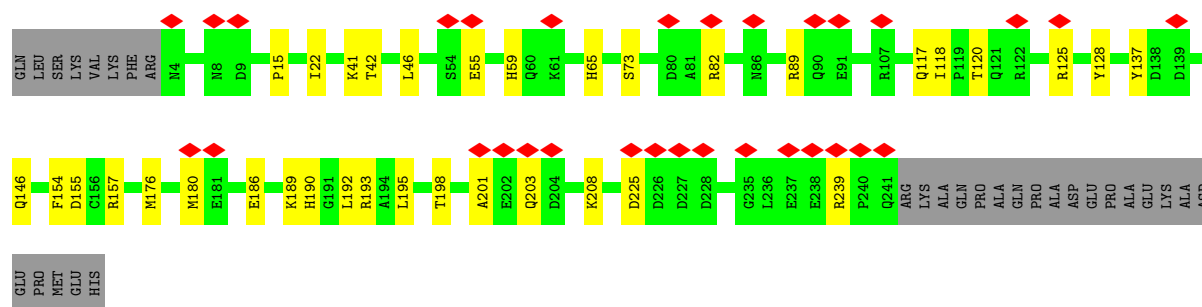
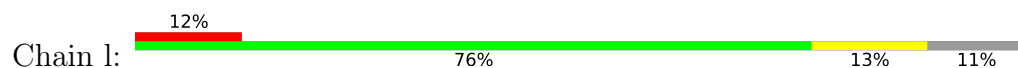
• Molecule 24: Proteasome subunit alpha type-5



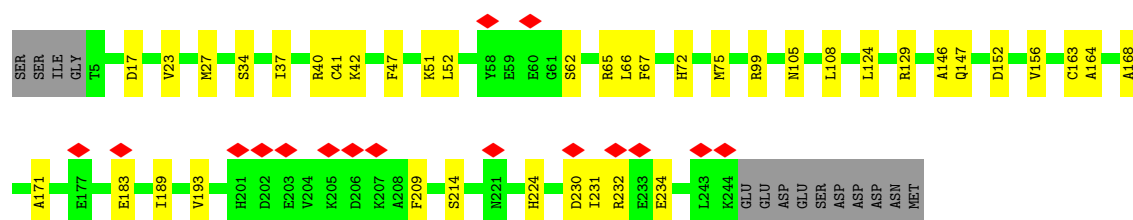
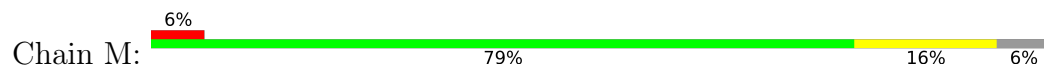
- Molecule 25: Proteasome subunit alpha type-1



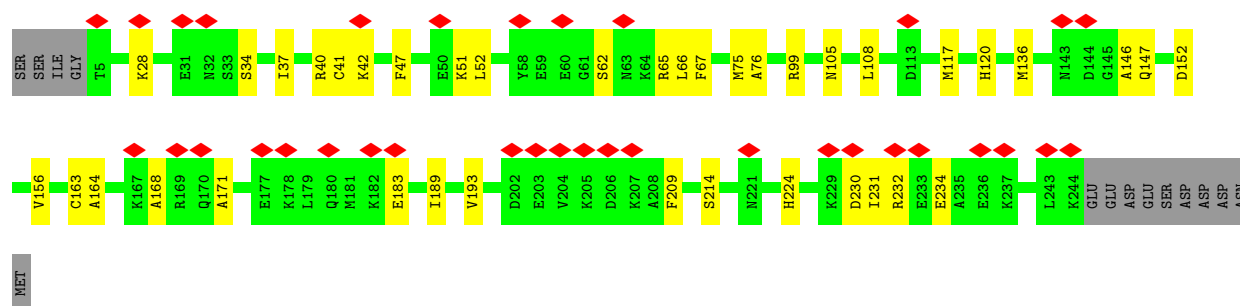
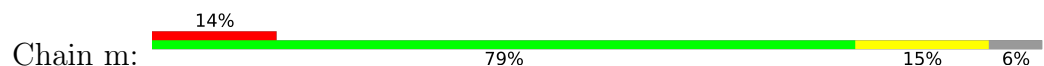
- Molecule 25: Proteasome subunit alpha type-1



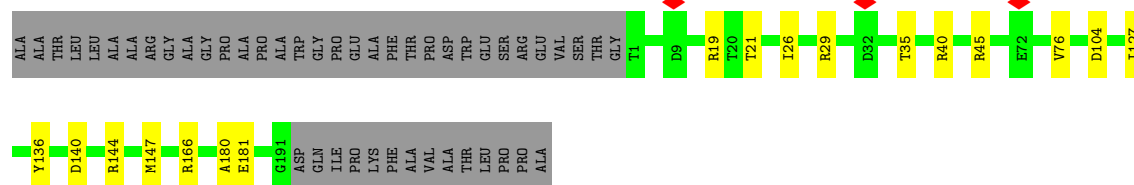
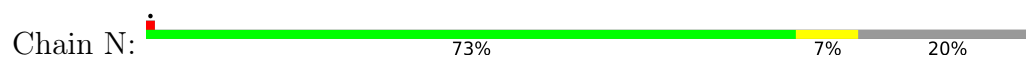
- Molecule 26: Proteasome subunit alpha type-3



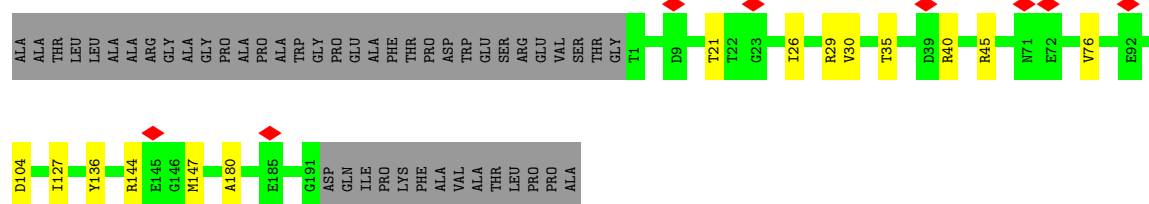
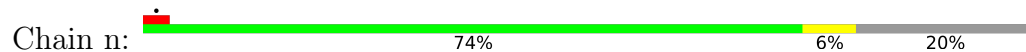
- Molecule 26: Proteasome subunit alpha type-3



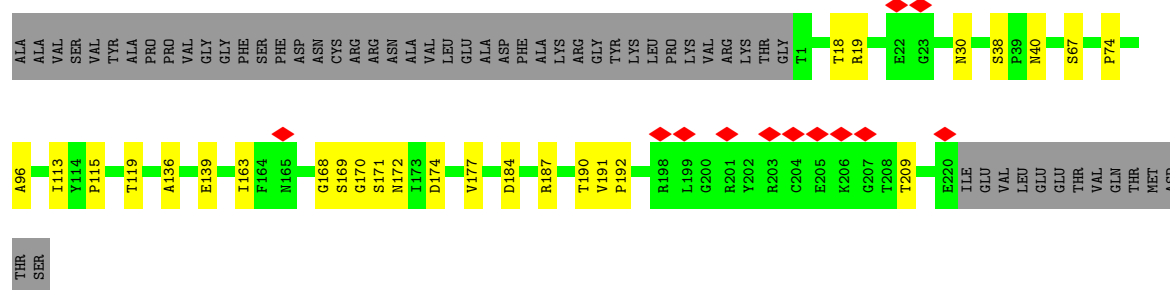
- Molecule 27: Proteasome subunit beta type-6



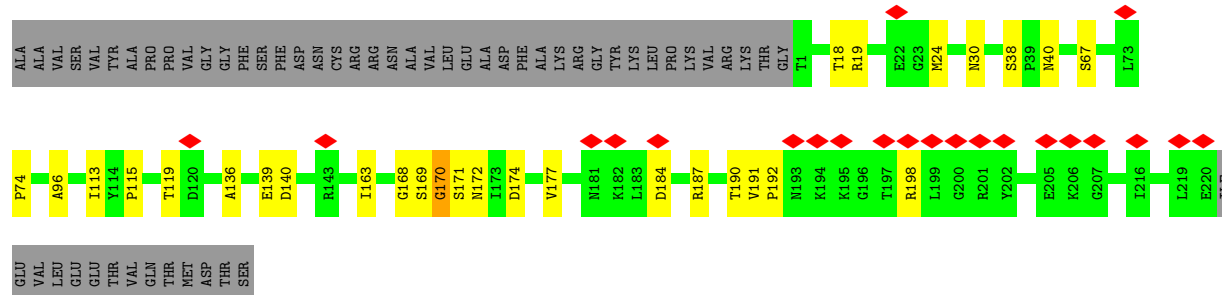
- Molecule 27: Proteasome subunit beta type-6



- Molecule 28: Proteasome subunit beta type-7

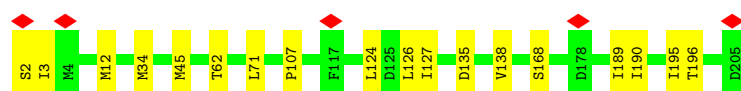


- Molecule 28: Proteasome subunit beta type-7



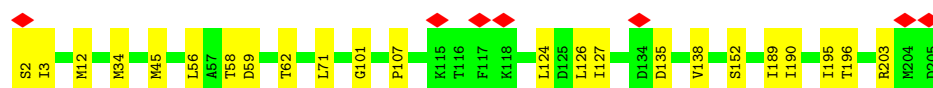
- Molecule 29: Proteasome subunit beta type-3

Chain P:  91% 9%



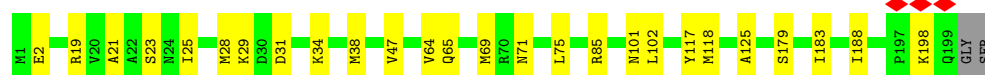
- Molecule 29: Proteasome subunit beta type-3

Chain p:  89% 11%



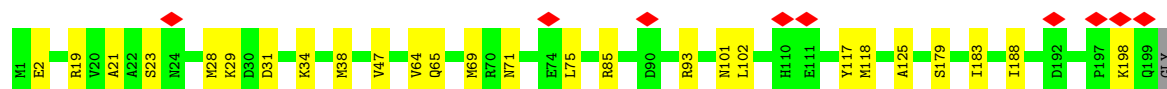
- Molecule 30: Proteasome subunit beta type-2

Chain Q:  86% 13%



- Molecule 30: Proteasome subunit beta type-2

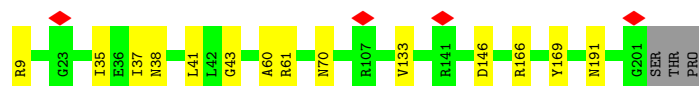
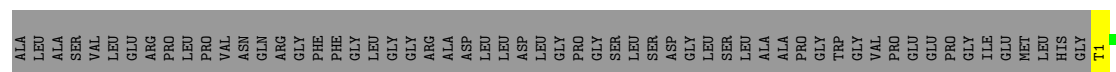
Chain q:  86% 13%



SER

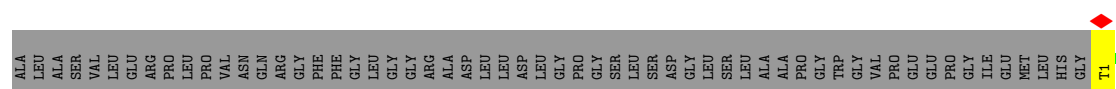
- Molecule 31: Proteasome subunit beta type-5

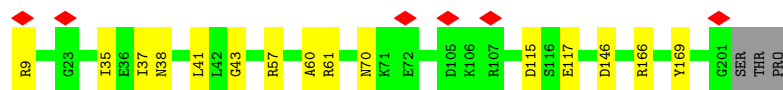
Chain R:  71% 6% 23%



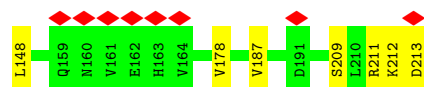
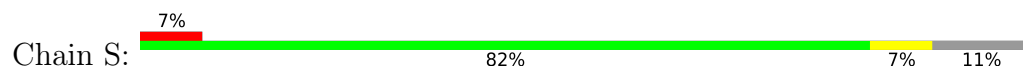
- Molecule 31: Proteasome subunit beta type-5

Chain r:  71% 6% 23%

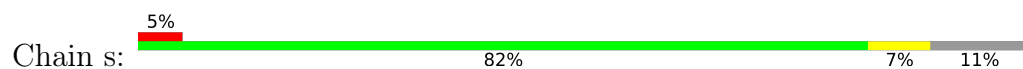




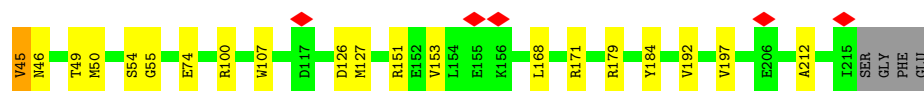
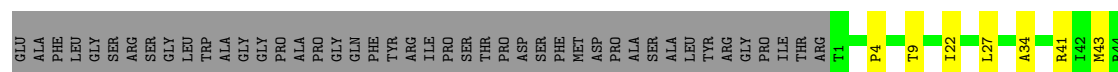
- Molecule 32: Proteasome subunit beta type-1



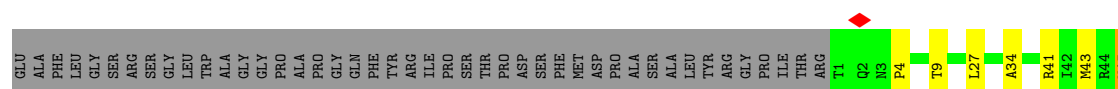
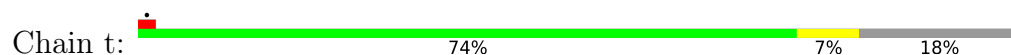
- Molecule 32: Proteasome subunit beta type-1



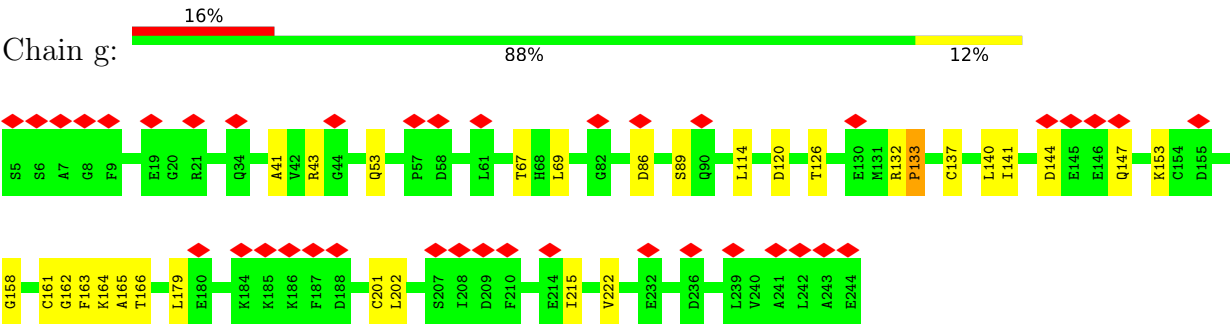
- Molecule 33: Proteasome subunit beta type-4



- Molecule 33: Proteasome subunit beta type-4



- Molecule 34: Proteasome subunit alpha type-6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	288915	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.018	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size ($\text{\AA}$)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.685, 0.685, 0.685	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ADP, MG, 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	U	0.27	0/6945	0.65	7/9382 (0.1%)
2	V	0.28	0/3929	0.70	2/5309 (0.0%)
3	W	0.30	0/3751	0.72	4/5042 (0.1%)
4	X	0.26	0/3053	0.55	0/4115
5	Y	0.30	0/3173	0.69	0/4273
6	Z	0.29	0/2324	0.73	4/3150 (0.1%)
7	a	0.27	0/3053	0.68	0/4133
8	b	0.25	0/1478	0.64	0/2001
9	c	0.29	0/2302	0.70	0/3110
10	d	0.27	0/2162	0.63	0/2919
11	e	0.28	0/338	0.72	1/450 (0.2%)
12	f	0.33	1/6980 (0.0%)	0.82	11/9433 (0.1%)
13	A	0.30	0/3283	0.66	0/4433
14	B	0.32	0/3254	0.63	0/4388
15	C	0.37	0/3146	0.73	5/4226 (0.1%)
16	D	0.36	0/3090	0.75	3/4168 (0.1%)
17	E	0.32	0/3145	0.67	4/4233 (0.1%)
18	F	0.28	0/3137	0.65	2/4223 (0.0%)
20	G	0.39	0/1870	0.70	0/2536
21	H	0.39	0/1759	0.58	0/2389
21	h	0.29	0/1743	0.48	0/2372
22	I	0.37	0/1938	0.68	2/2621 (0.1%)
22	i	0.27	0/1942	0.58	0/2628
23	J	0.37	0/1763	0.58	0/2398
23	j	0.28	0/1728	0.52	0/2358
24	K	0.37	0/1755	0.67	4/2375 (0.2%)
24	k	0.28	0/1747	0.51	0/2364
25	L	0.36	0/1885	0.58	0/2552
25	l	0.36	0/1885	0.58	0/2552
26	M	0.33	0/1891	0.58	0/2552
26	m	0.33	0/1891	0.58	0/2552
27	N	0.33	0/1454	0.51	0/1967

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	n	0.33	0/1454	0.51	0/1967
28	O	0.31	0/1670	0.47	0/2265
28	o	0.31	0/1670	0.47	0/2265
29	P	0.31	0/1614	0.43	0/2177
29	p	0.31	0/1614	0.43	0/2177
30	Q	0.34	0/1603	0.53	0/2174
30	q	0.34	0/1603	0.53	0/2174
31	R	0.32	0/1579	0.41	0/2134
31	r	0.32	0/1579	0.41	0/2134
32	S	0.31	0/1671	0.47	0/2253
32	s	0.31	0/1671	0.47	0/2253
33	T	0.33	0/1700	0.47	0/2305
33	t	0.33	0/1700	0.48	0/2305
34	g	0.30	0/1859	0.59	1/2523 (0.0%)
All	All	0.31	1/106781 (0.0%)	0.63	50/144310 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	U	0	7
2	V	0	2
3	W	0	2
4	X	0	1
5	Y	0	4
6	Z	0	4
7	a	0	1
9	c	0	4
10	d	0	4
11	e	0	1
12	f	0	14
13	A	0	2
14	B	0	2
15	C	0	3
16	D	0	5
17	E	0	5
18	F	0	3
20	G	0	3
22	I	0	1
24	K	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
24	k	0	1
28	O	0	1
28	o	0	1
33	T	0	1
33	t	0	1
34	g	0	1
All	All	0	77

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	f	860	LYS	CA-CB	-5.33	1.45	1.53

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	21	LEU	CA-C-N	9.42	138.65	121.70
24	K	21	LEU	C-N-CA	9.42	138.65	121.70
22	I	15	GLU	CA-C-N	8.78	137.50	121.70
22	I	15	GLU	C-N-CA	8.78	137.50	121.70
6	Z	15	VAL	N-CA-C	8.00	118.06	110.30
24	K	19	GLY	CA-C-N	6.73	133.82	121.70
24	K	19	GLY	C-N-CA	6.73	133.82	121.70
16	D	397	LYS	N-CA-C	-6.68	105.70	114.31
6	Z	217	THR	N-CA-C	-6.63	104.13	111.36
3	W	44	ILE	CA-C-N	6.54	130.63	120.82
3	W	44	ILE	C-N-CA	6.54	130.63	120.82
15	C	397	LYS	CA-C-N	6.53	134.01	121.54
15	C	397	LYS	C-N-CA	6.53	134.01	121.54
3	W	196	VAL	N-CA-C	-6.52	106.16	112.29
1	U	873	PRO	CA-C-N	6.24	133.46	121.54
1	U	873	PRO	C-N-CA	6.24	133.46	121.54
34	g	133	PRO	CA-C-O	-6.02	116.74	121.38
18	F	299	GLU	CA-C-N	6.00	132.99	121.54
18	F	299	GLU	C-N-CA	6.00	132.99	121.54
15	C	217	SER	N-CA-C	-5.89	105.45	114.16
12	f	875	ALA	CA-C-N	5.75	132.52	121.54
12	f	875	ALA	C-N-CA	5.75	132.52	121.54
3	W	88	MET	N-CA-C	5.70	122.94	110.80
1	U	213	PHE	N-CA-C	5.50	116.97	110.97
6	Z	64	ASP	CA-C-N	5.48	132.01	121.54
6	Z	64	ASP	C-N-CA	5.48	132.01	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	27	PRO	N-CA-C	5.44	117.34	110.70
17	E	305	ASN	CA-C-N	5.43	131.91	121.54
17	E	305	ASN	C-N-CA	5.43	131.91	121.54
12	f	852	VAL	CA-C-N	5.43	131.74	121.97
12	f	852	VAL	C-N-CA	5.43	131.74	121.97
12	f	868	HIS	CA-C-N	5.37	131.80	121.54
12	f	868	HIS	C-N-CA	5.37	131.80	121.54
2	V	28	PRO	N-CA-C	5.30	117.17	110.70
12	f	822	VAL	CA-C-N	5.29	131.64	121.54
12	f	822	VAL	C-N-CA	5.29	131.64	121.54
1	U	223	LEU	CA-C-N	5.27	131.61	121.54
1	U	223	LEU	C-N-CA	5.27	131.61	121.54
17	E	115	VAL	CA-C-N	5.26	134.63	121.80
17	E	115	VAL	C-N-CA	5.26	134.63	121.80
11	e	56	LEU	CA-CB-CG	5.22	134.58	116.30
12	f	847	GLY	N-CA-C	5.17	118.49	112.50
15	C	250	GLU	CA-C-N	-5.08	116.87	121.65
15	C	250	GLU	C-N-CA	-5.08	116.87	121.65
16	D	98	GLN	CA-C-N	5.05	131.20	121.54
16	D	98	GLN	C-N-CA	5.05	131.20	121.54
1	U	397	THR	CA-C-N	5.05	131.19	121.54
1	U	397	THR	C-N-CA	5.05	131.19	121.54
12	f	828	ARG	CA-C-N	5.03	127.91	120.82
12	f	828	ARG	C-N-CA	5.03	127.91	120.82

There are no chirality outliers.

All (77) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	A	22	ILE	Peptide
13	A	310	ASP	Peptide
14	B	278	ALA	Peptide
14	B	355	LEU	Peptide
15	C	220	VAL	Peptide
15	C	262	GLY	Peptide
15	C	403	LYS	Peptide
16	D	125	LYS	Peptide
16	D	159	LYS	Peptide
16	D	265	ASP	Peptide
16	D	335	LEU	Peptide
16	D	336	PRO	Peptide
17	E	165	ILE	Peptide

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Mol	Chain	Res	Type	Group
17	E	166	PRO	Peptide
17	E	246	GLY	Peptide
17	E	281	ARG	Peptide
17	E	304	PRO	Peptide
18	F	228	PRO	Peptide
18	F	295	ARG	Peptide
18	F	343	LEU	Peptide
20	G	210	PHE	Peptide
20	G	222	VAL	Peptide
20	G	242	LEU	Peptide
22	I	10	THR	Peptide
24	K	19	GLY	Peptide
24	K	232	GLU	Peptide
24	K	8	TYR	Peptide
28	O	170	GLY	Peptide
33	T	45	VAL	Peptide
1	U	211	PRO	Peptide
1	U	212	ASP	Peptide
1	U	24	LEU	Peptide
1	U	806	CYS	Peptide
1	U	821	LYS	Peptide
1	U	873	PRO	Peptide
1	U	880	ASN	Peptide
2	V	264	TYR	Peptide
2	V	83	GLU	Peptide
3	W	273	TYR	Peptide
3	W	313	GLU	Peptide
4	X	202	CYS	Peptide
5	Y	169	GLU	Peptide
5	Y	174	TRP	Peptide
5	Y	291	HIS	Peptide
5	Y	349	LYS	Peptide
6	Z	144	VAL	Peptide
6	Z	167	ALA	Peptide
6	Z	183	THR	Peptide
6	Z	184	VAL	Peptide
7	a	341	LEU	Peptide
9	c	185	ASN	Peptide
9	c	232	GLN	Peptide
9	c	279	ASP	Peptide
9	c	65	TYR	Peptide
10	d	186	TYR	Peptide

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Mol	Chain	Res	Type	Group
10	d	198	LEU	Peptide
10	d	201	ASN	Peptide
10	d	88	GLN	Peptide
11	e	6	GLN	Peptide
12	f	249	LEU	Peptide
12	f	340	MET	Peptide
12	f	620	PHE	Peptide
12	f	642	ALA	Peptide
12	f	737	ASN	Peptide
12	f	755	ASP	Peptide
12	f	807	ARG	Peptide
12	f	809	ILE	Peptide
12	f	816	TYR	Peptide
12	f	822	VAL	Peptide
12	f	823	ALA	Peptide
12	f	854	GLY	Peptide
12	f	870	THR	Peptide
12	f	875	ALA	Peptide
34	g	222	VAL	Peptide
24	k	232	GLU	Peptide
28	o	170	GLY	Peptide
33	t	45	VAL	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	6828	0	6884	97	0
2	V	3852	0	3893	70	0
3	W	3703	0	3822	99	0
4	X	3009	0	3113	29	0
5	Y	3115	0	3120	52	0
6	Z	2281	0	2312	60	0
7	a	2995	0	3012	52	0
8	b	1458	0	1505	33	0
9	c	2260	0	2276	33	0
10	d	2116	0	2146	35	0
11	e	334	0	294	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	f	6866	0	6866	191	0
13	A	3229	0	3261	75	0
14	B	3207	0	3277	56	0
15	C	3105	0	3219	48	0
16	D	3040	0	3075	68	0
17	E	3097	0	3174	58	0
18	F	3098	0	3187	66	0
19	v	180	0	45	16	0
20	G	1836	0	1813	36	0
21	H	1723	0	1655	21	0
21	h	1708	0	1594	21	0
22	I	1908	0	1864	24	0
22	i	1912	0	1851	21	0
23	J	1739	0	1590	21	0
23	j	1704	0	1517	21	0
24	K	1729	0	1680	22	0
24	k	1722	0	1673	29	0
25	L	1850	0	1822	23	0
25	l	1850	0	1822	22	0
26	M	1856	0	1814	26	0
26	m	1856	0	1814	24	0
27	N	1430	0	1398	11	0
27	n	1430	0	1398	9	0
28	O	1643	0	1644	15	0
28	o	1643	0	1644	19	0
29	P	1585	0	1598	11	0
29	p	1585	0	1598	19	0
30	Q	1570	0	1547	16	0
30	q	1570	0	1547	16	0
31	R	1548	0	1499	10	0
31	r	1548	0	1499	11	0
32	S	1641	0	1618	12	0
32	s	1641	0	1618	9	0
33	T	1667	0	1628	19	0
33	t	1667	0	1628	14	0
34	g	1826	0	1796	18	0
35	c	1	0	0	0	0
36	A	31	0	12	0	0
36	B	31	0	12	1	0
36	C	31	0	12	1	0
36	D	31	0	12	0	0
37	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	B	1	0	0	0	0
37	C	1	0	0	0	0
37	D	1	0	0	0	0
38	E	27	0	12	0	0
All	All	105316	0	104710	1433	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 7.

All (1433) 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)
13:A:118:PHE:HZ	19:v:28:UNK:CB	1.50	1.24
3:W:179:LYS:O	3:W:180:LYS:CG	1.88	1.21
6:Z:12:HIS:CD2	6:Z:51:SER:HB3	1.75	1.21
13:A:118:PHE:CZ	19:v:28:UNK:CB	2.24	1.19
3:W:179:LYS:O	3:W:180:LYS:HG3	0.99	1.15
12:f:659:LEU:HD11	12:f:667:GLY:HA2	1.28	1.15
12:f:659:LEU:CD1	12:f:667:GLY:HA2	1.78	1.14
14:B:301:GLY:HA3	19:v:20:UNK:CB	1.78	1.13
12:f:664:GLU:HG3	12:f:665:GLU:H	1.14	1.10
12:f:659:LEU:HD11	12:f:671:ALA:HB3	1.27	1.07
12:f:662:MET:HE2	13:A:65:ILE:HG23	1.41	1.02
3:W:173:THR:HB	3:W:182:ARG:HH11	1.22	1.02
12:f:662:MET:CE	13:A:65:ILE:HG23	1.88	1.02
12:f:664:GLU:HG3	12:f:665:GLU:N	1.68	1.00
6:Z:12:HIS:HD2	6:Z:51:SER:HB3	0.86	0.99
16:D:148:ASP:OD1	17:E:62:LYS:HB2	1.63	0.98
3:W:174:TYR:C	3:W:174:TYR:CD2	2.40	0.98
14:B:260:LEU:HD22	19:v:24:UNK:CB	1.94	0.97
6:Z:12:HIS:HD2	6:Z:51:SER:CB	1.78	0.94
12:f:659:LEU:HD11	12:f:671:ALA:CB	1.98	0.92
12:f:659:LEU:HD13	12:f:667:GLY:CA	2.00	0.92
12:f:659:LEU:CD1	12:f:667:GLY:CA	2.50	0.90
29:p:56:LEU:HG	29:p:58:THR:HG22	1.54	0.89
16:D:148:ASP:OD2	17:E:61:LEU:HB3	1.73	0.88
12:f:653:ALA:O	12:f:657:ILE:HG13	1.73	0.86
3:W:236:HIS:O	3:W:236:HIS:ND1	2.08	0.85
6:Z:216:ALA:HB2	7:a:346:ILE:HG21	1.57	0.85
16:D:147:ALA:O	17:E:62:LYS:HD2	1.78	0.84
3:W:173:THR:HB	3:W:182:ARG:NH1	1.93	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:144:ARG:CG	19:v:31:UNK:CB	2.55	0.84
12:f:664:GLU:CG	12:f:665:GLU:N	2.41	0.83
12:f:659:LEU:CD1	12:f:671:ALA:HB3	2.08	0.83
13:A:144:ARG:HG2	19:v:31:UNK:CB	2.07	0.83
12:f:659:LEU:HD13	12:f:667:GLY:HA3	1.61	0.83
13:A:118:PHE:CE1	19:v:28:UNK:CB	2.65	0.79
3:W:174:TYR:C	3:W:174:TYR:HD2	1.91	0.78
3:W:179:LYS:C	3:W:180:LYS:HG3	2.05	0.78
12:f:661:ALA:O	12:f:662:MET:SD	2.43	0.77
6:Z:11:VAL:HB	6:Z:162:ILE:HD13	1.66	0.77
17:E:62:LYS:HG2	17:E:63:GLN:N	2.00	0.77
29:p:58:THR:HG23	29:p:59:ASP:N	2.00	0.77
13:A:118:PHE:HE1	19:v:28:UNK:N	1.83	0.77
17:E:62:LYS:HG2	17:E:63:GLN:H	1.50	0.75
6:Z:15:VAL:O	6:Z:19:VAL:HG23	1.88	0.74
20:G:200:THR:HA	20:G:203:SER:HB2	1.70	0.73
17:E:305:ASN:HB3	17:E:308:ALA:H	1.52	0.73
14:B:260:LEU:CD2	19:v:24:UNK:CB	2.66	0.73
1:U:47:VAL:HG12	1:U:48:LEU:N	2.04	0.73
12:f:662:MET:C	14:B:82:GLN:HE22	1.96	0.73
6:Z:16:LEU:HG	6:Z:17:LEU:N	2.04	0.73
16:D:148:ASP:OD1	17:E:62:LYS:CB	2.36	0.73
3:W:173:THR:HA	3:W:182:ARG:HE	1.53	0.72
3:W:178:GLU:HG2	3:W:182:ARG:HD3	1.71	0.72
12:f:664:GLU:O	12:f:666:ILE:N	2.21	0.72
8:b:177:PRO:O	8:b:178:SER:HB2	1.89	0.71
12:f:662:MET:HE1	13:A:65:ILE:HG23	1.71	0.71
3:W:174:TYR:CD2	3:W:175:GLY:N	2.58	0.71
3:W:299:ILE:HG22	3:W:301:LYS:H	1.55	0.71
3:W:237:GLU:OE2	3:W:237:GLU:HA	1.91	0.71
16:D:212:LYS:NZ	16:D:311:THR:O	2.25	0.70
1:U:47:VAL:O	1:U:50:GLU:N	2.24	0.70
12:f:673:ARG:HH22	12:f:709:THR:HA	1.57	0.70
2:V:280:ALA:HB1	2:V:284:GLU:HB3	1.74	0.69
15:C:307:ARG:HD2	15:C:309:GLY:H	1.56	0.69
18:F:359:GLU:HB3	18:F:385:ALA:HB1	1.74	0.69
3:W:93:ARG:NH1	3:W:139:GLU:O	2.25	0.69
13:A:122:VAL:HB	18:F:88:TYR:HB2	1.75	0.69
3:W:173:THR:CB	3:W:182:ARG:HH11	2.04	0.68
12:f:653:ALA:O	12:f:657:ILE:CG1	2.41	0.68
12:f:704:LEU:HA	12:f:707:LEU:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:79:VAL:HG13	2:V:81:GLN:H	1.58	0.68
23:j:74:ALA:HB2	23:j:161:ILE:HD13	1.76	0.67
16:D:147:ALA:O	17:E:62:LYS:CD	2.42	0.67
12:f:53:GLN:HA	13:A:32:LEU:HG	1.75	0.67
15:C:269:VAL:HG11	16:D:287:ARG:HH22	1.60	0.67
6:Z:16:LEU:HG	6:Z:17:LEU:H	1.59	0.67
16:D:153:MET:HE1	16:D:257:ASN:ND2	2.10	0.66
10:d:61:TRP:HB3	10:d:65:ARG:HH11	1.61	0.65
1:U:26:LYS:HE2	10:d:36:LEU:HB2	1.77	0.65
3:W:53:GLN:HG3	3:W:103:LYS:HE3	1.78	0.65
16:D:237:GLN:HA	17:E:209:GLY:HA3	1.77	0.65
22:I:143:TYR:HB2	22:I:146:GLN:HE21	1.61	0.65
1:U:694:ILE:HG23	1:U:695:MET:HG3	1.78	0.65
6:Z:212:LEU:HA	6:Z:215:VAL:HG12	1.79	0.65
3:W:425:LEU:HB2	6:Z:247:LYS:HD3	1.78	0.65
8:b:161:ASN:HB2	8:b:165:GLY:HA3	1.78	0.65
16:D:145:PRO:O	16:D:146:GLU:C	2.39	0.65
2:V:265:ASP:O	2:V:269:LYS:NZ	2.30	0.64
26:M:214:SER:OG	26:M:224:HIS:NE2	2.30	0.64
6:Z:12:HIS:O	6:Z:15:VAL:HG12	1.97	0.64
12:f:828:ARG:CZ	12:f:843:SER:OG	2.45	0.64
26:m:214:SER:OG	26:m:224:HIS:NE2	2.30	0.64
3:W:273:TYR:HB2	3:W:276:LEU:HB2	1.79	0.64
15:C:113:ARG:NH2	15:C:129:ASN:O	2.30	0.64
16:D:160:PRO:HB2	16:D:162:VAL:HG12	1.80	0.64
1:U:885:MET:H	1:U:888:GLN:HE21	1.47	0.63
12:f:659:LEU:HD13	12:f:659:LEU:C	2.23	0.63
14:B:304:GLU:HG3	14:B:307:ARG:HH11	1.62	0.63
22:I:218:ARG:NH1	22:I:223:THR:OG1	2.31	0.63
8:b:177:PRO:O	8:b:178:SER:CB	2.45	0.63
13:A:210:LYS:HG2	13:A:316:LYS:HE3	1.79	0.63
3:W:343:SER:HB3	3:W:347:GLY:H	1.63	0.63
3:W:12:ARG:HD2	3:W:24:VAL:HG22	1.80	0.63
12:f:2:GLU:OE1	13:A:23:ARG:NH1	2.32	0.63
12:f:127:SER:HA	12:f:131:MET:HB2	1.80	0.62
12:f:585:GLU:HG3	12:f:588:ARG:HE	1.64	0.62
5:Y:163:LYS:HG3	5:Y:167:LEU:HD12	1.81	0.62
12:f:659:LEU:CD1	12:f:671:ALA:CB	2.74	0.62
12:f:665:GLU:HG2	12:f:669:GLU:HG3	1.81	0.62
18:F:357:PRO:O	18:F:362:ARG:NH1	2.33	0.62
12:f:594:LEU:O	12:f:635:LYS:NZ	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:828:ARG:NE	12:f:843:SER:OG	2.33	0.62
16:D:156:SER:H	16:D:159:LYS:HE3	1.65	0.62
3:W:179:LYS:O	3:W:180:LYS:CB	2.47	0.62
14:B:412:MET:HE1	15:C:178:LEU:HA	1.81	0.62
1:U:366:HIS:HE1	1:U:395:ARG:HD2	1.65	0.62
12:f:77:GLU:OE1	12:f:79:ARG:NH1	2.33	0.61
15:C:215:SER:HA	15:C:249:ASP:HB2	1.81	0.61
1:U:607:VAL:HG12	16:D:67:ASN:HD22	1.65	0.61
12:f:302:GLY:HA2	12:f:317:LEU:HD11	1.83	0.61
16:D:237:GLN:NE2	16:D:246:MET:SD	2.72	0.61
24:K:221:GLN:HB2	24:K:224:GLN:HB3	1.82	0.61
2:V:33:GLN:NE2	2:V:83:GLU:O	2.33	0.61
10:d:188:LYS:HD2	10:d:221:ASN:HD21	1.65	0.61
12:f:828:ARG:HD2	12:f:843:SER:OG	2.00	0.61
13:A:162:THR:HA	13:A:165:GLN:HB3	1.81	0.61
21:h:50:LYS:NZ	21:h:62:VAL:O	2.33	0.61
29:p:58:THR:CG2	29:p:59:ASP:N	2.63	0.61
16:D:355:SER:HB3	16:D:393:ILE:HD11	1.81	0.61
23:j:60:ARG:HH22	23:j:219:ILE:HD11	1.65	0.61
1:U:108:TYR:OH	1:U:159:ARG:NH1	2.34	0.61
1:U:559:ARG:HB3	1:U:562:GLU:HB2	1.82	0.61
3:W:401:THR:HG23	3:W:402:ILE:HD12	1.83	0.61
12:f:99:LEU:HG	12:f:101:PRO:HD2	1.82	0.61
17:E:21:GLU:OE2	17:E:25:ARG:NH2	2.34	0.61
2:V:494:MET:HB3	6:Z:275:LEU:HD23	1.81	0.61
6:Z:16:LEU:CG	6:Z:17:LEU:H	2.13	0.61
12:f:586:PRO:HA	12:f:589:SER:HB2	1.83	0.61
12:f:836:GLU:H	12:f:840:LEU:HD21	1.65	0.61
14:B:122:ILE:HD11	14:B:130:GLU:HB3	1.83	0.60
26:M:51:LYS:NZ	26:M:62:SER:O	2.34	0.60
12:f:125:ILE:HD13	12:f:129:LEU:HB2	1.81	0.60
13:A:144:ARG:HG3	19:v:31:UNK:CB	2.31	0.60
18:F:35:LYS:HB2	18:F:38:THR:HB	1.82	0.60
26:m:51:LYS:NZ	26:m:62:SER:O	2.34	0.60
33:t:27:LEU:HD22	33:t:184:TYR:HB2	1.83	0.60
2:V:345:ARG:HH12	2:V:353:LEU:HD11	1.66	0.60
26:M:231:ILE:HG22	26:M:232:ARG:HG3	1.83	0.60
12:f:634:LYS:HD2	12:f:637:LYS:HD2	1.83	0.60
22:I:219:GLU:OE2	22:I:220:ASN:ND2	2.34	0.60
22:i:106:PRO:HD2	22:i:109:GLN:HE21	1.66	0.60
1:U:205:TYR:HB3	1:U:215:ASN:HD22	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:411:ARG:NH1	14:B:413:LYS:O	2.34	0.60
32:s:27:THR:HB	32:s:40:SER:H	1.67	0.60
6:Z:37:GLY:HA2	6:Z:56:VAL:HG12	1.83	0.60
33:T:27:LEU:HD22	33:T:184:TYR:HB2	1.83	0.60
29:p:56:LEU:CG	29:p:58:THR:HG22	2.28	0.60
10:d:19:CYS:SG	10:d:65:ARG:NH1	2.75	0.60
12:f:662:MET:O	14:B:82:GLN:NE2	2.35	0.60
12:f:672:LEU:HD21	12:f:690:VAL:HG22	1.82	0.60
13:A:24:ALA:O	14:B:410:ARG:NH2	2.30	0.60
14:B:46:ALA:HB3	14:B:179:ALA:H	1.67	0.60
3:W:80:TRP:HE1	20:G:244:GLU:HB2	1.66	0.60
13:A:38:GLN:NE2	13:A:40:THR:OG1	2.35	0.60
26:m:231:ILE:HG22	26:m:232:ARG:HG3	1.83	0.60
1:U:10:SER:HB2	10:d:73:ARG:HG3	1.84	0.59
6:Z:12:HIS:CE1	6:Z:165:GLU:OE1	2.55	0.59
6:Z:13:PRO:HA	6:Z:16:LEU:HD21	1.84	0.59
12:f:125:ILE:HD11	12:f:128:VAL:HB	1.83	0.59
20:G:123:GLN:NE2	21:H:82:ASP:OD1	2.35	0.59
23:j:116:GLN:HE22	24:k:83:ALA:HB1	1.67	0.59
13:A:339:ARG:NH2	18:F:405:MET:SD	2.75	0.59
6:Z:177:ARG:H	6:Z:180:LYS:HZ1	1.50	0.59
27:N:29:ARG:NH1	28:O:139:GLU:OE1	2.34	0.59
32:S:27:THR:HB	32:S:40:SER:H	1.67	0.59
22:i:219:GLU:OE2	22:i:220:ASN:ND2	2.35	0.59
2:V:349:ARG:HA	2:V:353:LEU:HD23	1.85	0.59
12:f:221:ILE:HA	12:f:224:ASN:HB2	1.85	0.59
33:T:192:VAL:HG12	33:T:197:VAL:HG22	1.84	0.59
13:A:165:GLN:NE2	13:A:236:CYS:SG	2.76	0.59
2:V:476:PHE:HB3	6:Z:260:VAL:HG21	1.84	0.59
27:n:40:ARG:NH1	27:n:180:ALA:O	2.36	0.59
20:G:165:ALA:HB1	20:G:179:LEU:HD13	1.85	0.58
13:A:257:VAL:HG21	13:A:298:THR:HG23	1.83	0.58
23:J:4:ASP:O	23:J:18:GLN:NE2	2.36	0.58
27:N:40:ARG:NH1	27:N:180:ALA:O	2.36	0.58
12:f:721:VAL:HG11	14:B:208:PRO:HD2	1.85	0.58
7:a:363:MET:HG2	7:a:366:LEU:HD12	1.85	0.58
12:f:150:GLU:O	12:f:156:HIS:ND1	2.36	0.58
12:f:469:TYR:O	12:f:472:HIS:ND1	2.30	0.58
18:F:151:VAL:HG12	18:F:163:THR:HG23	1.86	0.58
23:j:4:ASP:O	23:j:18:GLN:NE2	2.34	0.58
12:f:552:ASP:HB3	12:f:556:ARG:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:429:LYS:HG2	14:B:430:LYS:HG3	1.84	0.58
2:V:200:ARG:NH1	2:V:242:HIS:O	2.37	0.58
12:f:717:ALA:HB1	12:f:760:PHE:HB2	1.84	0.58
10:d:203:PRO:HG2	10:d:206:MET:H	1.69	0.58
12:f:680:ARG:HB2	12:f:716:ASP:HA	1.84	0.58
16:D:248:ARG:HG2	16:D:295:GLN:HE22	1.69	0.58
3:W:131:VAL:O	3:W:144:ARG:NH1	2.36	0.58
14:B:429:LYS:HE2	14:B:430:LYS:HE2	1.86	0.58
24:K:9:ASP:HB3	24:K:22:PHE:HB3	1.86	0.58
1:U:796:LYS:HA	1:U:924:LEU:HD11	1.86	0.58
5:Y:160:ASN:HA	5:Y:163:LYS:HB2	1.86	0.58
22:i:143:TYR:HB2	22:i:146:GLN:HE21	1.67	0.58
33:t:192:VAL:HG12	33:t:197:VAL:HG22	1.84	0.58
5:Y:191:ILE:HD13	11:e:40:GLU:HG2	1.84	0.57
5:Y:288:PHE:HA	5:Y:291:HIS:HD2	1.69	0.57
7:a:286:ALA:HA	7:a:289:ARG:HB3	1.85	0.57
12:f:556:ARG:HD3	12:f:786:GLN:HB2	1.85	0.57
13:A:118:PHE:CE1	19:v:28:UNK:N	2.70	0.57
14:B:375:ALA:HB2	14:B:413:LYS:HB3	1.85	0.57
20:G:127:GLN:NE2	21:H:128:ARG:O	2.37	0.57
1:U:642:GLU:O	15:C:53:ASN:ND2	2.36	0.57
8:b:157:VAL:HG21	8:b:170:LEU:HB2	1.87	0.57
18:F:246:ALA:HB1	18:F:280:PRO:HB2	1.85	0.57
23:J:51:ALA:H	23:J:54:GLN:HE22	1.51	0.57
27:N:127:ILE:HD11	27:N:136:TYR:HD1	1.70	0.57
12:f:828:ARG:CD	12:f:843:SER:OG	2.52	0.57
34:g:120:ASP:OD1	21:h:84:ARG:NH1	2.38	0.57
23:j:115:LYS:HD3	23:j:149:PRO:HA	1.85	0.57
4:X:182:ASN:ND2	5:Y:248:GLU:OE2	2.36	0.57
6:Z:13:PRO:HA	6:Z:16:LEU:CD2	2.35	0.57
6:Z:261:TYR:HA	6:Z:265:LEU:HD13	1.86	0.57
1:U:216:VAL:HA	1:U:220:LEU:HD13	1.86	0.57
2:V:280:ALA:HB3	2:V:285:TRP:HB2	1.86	0.57
15:C:264:GLY:O	16:D:280:GLY:N	2.36	0.57
26:M:52:LEU:HA	26:M:209:PHE:HA	1.87	0.57
25:l:42:THR:O	25:l:137:TYR:OH	2.23	0.57
27:n:127:ILE:HD11	27:n:136:TYR:HD1	1.70	0.57
7:a:24:ARG:NH1	7:a:40:GLN:OE1	2.38	0.57
12:f:198:HIS:O	12:f:202:HIS:N	2.36	0.57
12:f:378:ASN:OD1	12:f:382:ASN:ND2	2.37	0.57
6:Z:12:HIS:HB2	6:Z:51:SER:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:70:GLY:HA3	16:D:113:VAL:HG12	1.86	0.57
30:Q:198:LYS:H	30:q:198:LYS:H	1.53	0.57
3:W:201:ARG:NH1	16:D:389:GLU:O	2.37	0.57
7:a:73:PRO:HB3	7:a:104:VAL:HG21	1.87	0.57
9:c:128:ASN:HD21	19:v:36:UNK:HA	1.69	0.57
20:G:67:THR:HG23	20:G:216:GLU:HG2	1.87	0.57
20:G:201:CYS:SG	20:G:202:LEU:N	2.77	0.57
3:W:238:GLY:O	3:W:240:TYR:N	2.38	0.57
12:f:441:LYS:HB2	12:f:477:MET:HE1	1.86	0.57
15:C:88:LYS:HB2	15:C:94:LYS:HG2	1.87	0.57
23:J:74:ALA:HB2	23:J:161:ILE:HD13	1.85	0.57
9:c:134:GLU:OE1	9:c:161:ARG:NH1	2.38	0.56
18:F:180:ARG:HH21	18:F:241:ALA:HB3	1.69	0.56
2:V:68:ASP:O	2:V:72:LEU:N	2.37	0.56
12:f:378:ASN:HD21	12:f:392:THR:HG22	1.70	0.56
15:C:217:SER:OG	16:D:248:ARG:NH2	2.39	0.56
25:L:42:THR:O	25:L:137:TYR:OH	2.23	0.56
21:h:39:LYS:HE2	21:h:144:PRO:HG2	1.86	0.56
3:W:199:TYR:CE2	3:W:236:HIS:HD2	2.23	0.56
12:f:691:PRO:HA	12:f:694:LEU:HB2	1.87	0.56
15:C:52:LEU:HB3	16:D:68:LEU:HD12	1.87	0.56
17:E:171:LEU:HB3	17:E:298:LYS:HG2	1.86	0.56
30:Q:38:MET:O	30:Q:65:GLN:NE2	2.38	0.56
3:W:174:TYR:HB2	17:E:139:SER:HB2	1.87	0.56
5:Y:381:GLN:HB3	5:Y:385:ARG:HH12	1.71	0.56
7:a:65:SER:HA	7:a:68:GLU:HB2	1.87	0.56
12:f:209:MET:HG3	12:f:211:ILE:H	1.68	0.56
25:l:65:HIS:O	25:l:89:ARG:NH2	2.38	0.56
27:n:21:THR:HG22	27:n:26:ILE:HG13	1.88	0.56
1:U:505:ASP:HB3	1:U:508:THR:HG22	1.88	0.56
2:V:412:LEU:O	5:Y:346:LYS:NZ	2.39	0.56
12:f:571:GLU:HG3	12:f:573:ILE:H	1.71	0.56
23:J:115:LYS:HD3	23:J:149:PRO:HA	1.88	0.56
25:L:186:GLU:HA	25:L:189:LYS:HG2	1.86	0.56
25:l:186:GLU:HA	25:l:189:LYS:HG2	1.86	0.56
6:Z:198:LEU:HG	6:Z:201:LEU:HD12	1.88	0.56
15:C:138:MET:SD	15:C:138:MET:N	2.77	0.56
21:H:148:GLN:OE1	21:H:158:TRP:NE1	2.39	0.56
2:V:228:ARG:O	2:V:232:HIS:ND1	2.37	0.56
10:d:41:THR:HG22	10:d:44:THR:H	1.71	0.56
17:E:275:MET:HB3	17:E:277:MET:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:94:ILE:HD11	18:F:125:LYS:HB2	1.87	0.56
18:F:401:VAL:HG12	18:F:405:MET:HE2	1.87	0.56
20:G:71:LYS:O	20:G:95:ARG:NH2	2.39	0.56
24:K:97:GLN:HG3	31:R:61:ARG:HG2	1.88	0.56
24:k:41:GLN:NE2	24:k:151:PRO:O	2.39	0.56
26:m:52:LEU:HA	26:m:209:PHE:HA	1.87	0.56
1:U:660:CYS:SG	1:U:665:ASN:ND2	2.78	0.56
2:V:37:MET:SD	2:V:92:ARG:NH1	2.78	0.56
3:W:40:LEU:HG	3:W:41:GLN:HG3	1.88	0.56
3:W:348:GLU:HA	3:W:351:TRP:HD1	1.71	0.56
12:f:252:ALA:O	12:f:257:ARG:NH1	2.39	0.56
14:B:125:THR:OG1	14:B:126:SER:N	2.36	0.56
30:q:38:MET:O	30:q:65:GLN:NE2	2.38	0.56
3:W:179:LYS:HZ3	3:W:179:LYS:HB3	1.70	0.56
24:K:21:LEU:HB3	24:K:23:GLN:H	1.71	0.56
29:p:62:THR:OG1	30:q:85:ARG:NH2	2.39	0.56
5:Y:336:ARG:NH1	11:e:55:GLN:OE1	2.39	0.55
6:Z:34:ARG:NH1	6:Z:60:GLU:OE1	2.39	0.55
16:D:175:GLN:NE2	16:D:179:GLU:OE2	2.38	0.55
22:i:79:ILE:HG22	22:i:82:ASP:H	1.71	0.55
6:Z:16:LEU:CG	6:Z:17:LEU:N	2.68	0.55
12:f:110:TYR:OH	12:f:118:ASN:ND2	2.39	0.55
18:F:39:GLU:HA	18:F:42:ILE:HB	1.89	0.55
1:U:47:VAL:O	1:U:49:TYR:N	2.39	0.55
1:U:70:HIS:HB2	2:V:236:ARG:HH12	1.71	0.55
2:V:55:THR:OG1	15:C:36:ASN:ND2	2.39	0.55
9:c:174:PRO:O	9:c:176:GLN:NE2	2.39	0.55
18:F:171:ARG:NH2	18:F:258:GLN:OE1	2.40	0.55
18:F:304:ARG:O	18:F:308:ARG:NH1	2.39	0.55
12:f:497:VAL:HA	12:f:500:LEU:HB2	1.89	0.55
22:I:106:PRO:HD2	22:I:109:GLN:HE21	1.70	0.55
13:A:211:GLY:HA3	13:A:337:LEU:HA	1.87	0.55
3:W:35:ALA:HA	3:W:48:LEU:HD13	1.88	0.55
6:Z:216:ALA:CB	7:a:346:ILE:HG21	2.33	0.55
15:C:195:GLY:HA2	15:C:198:LEU:HD13	1.88	0.55
15:C:368:MET:HG2	16:D:329:ARG:HH22	1.71	0.55
15:C:406:LYS:NZ	22:I:63:GLU:OE2	2.38	0.55
16:D:119:ILE:O	16:D:121:ARG:NH1	2.39	0.55
25:L:65:HIS:O	25:L:89:ARG:NH2	2.38	0.55
9:c:173:GLU:HG3	9:c:175:ARG:HD2	1.88	0.55
29:p:58:THR:HG23	29:p:59:ASP:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:p:189:ILE:HG23	29:p:196:THR:HB	1.88	0.55
7:a:180:LEU:HD21	7:a:221:VAL:HG11	1.89	0.55
12:f:447:ALA:HA	12:f:450:ILE:HD12	1.89	0.55
13:A:114:ASN:HB3	13:A:120:LYS:HG2	1.88	0.55
7:a:227:ASN:O	7:a:231:GLN:NE2	2.39	0.55
12:f:171:GLN:HG3	12:f:179:VAL:HG22	1.88	0.55
24:K:48:LEU:HD21	24:K:77:ALA:HB2	1.87	0.55
21:h:66:GLU:OE2	21:h:91:ARG:NH2	2.40	0.55
2:V:290:TYR:OH	2:V:294:ARG:NH2	2.40	0.55
12:f:283:THR:O	12:f:287:ASP:N	2.40	0.55
12:f:664:GLU:O	12:f:667:GLY:N	2.39	0.55
29:P:189:ILE:HG23	29:P:196:THR:HB	1.88	0.55
5:Y:297:ARG:NH1	11:e:51:ASP:OD2	2.41	0.54
15:C:217:SER:OG	16:D:291:GLU:OE1	2.24	0.54
22:i:92:LEU:HD22	22:i:96:ARG:HH21	1.72	0.54
23:j:109:ARG:NH2	31:r:70:ASN:OD1	2.40	0.54
9:c:49:VAL:HG23	9:c:50:PRO:HD3	1.89	0.54
12:f:591:ALA:HA	12:f:594:LEU:HD23	1.88	0.54
12:f:812:GLY:HA3	12:f:853:VAL:HA	1.87	0.54
13:A:212:VAL:HG22	13:A:339:ARG:HB3	1.89	0.54
18:F:430:LYS:NZ	24:K:18:GLU:OE2	2.40	0.54
24:k:76:CYS:SG	24:k:77:ALA:N	2.80	0.54
1:U:804:SER:HA	1:U:892:LEU:HA	1.88	0.54
2:V:480:ILE:HD11	6:Z:260:VAL:HA	1.90	0.54
3:W:1:MET:HB3	3:W:43:VAL:HB	1.90	0.54
3:W:254:PRO:HA	3:W:257:GLN:HB2	1.89	0.54
7:a:35:HIS:NE2	8:b:14:GLU:O	2.40	0.54
5:Y:325:VAL:O	11:e:66:LYS:NZ	2.37	0.54
12:f:811:LEU:HD11	12:f:862:ILE:HB	1.90	0.54
32:S:148:LEU:HD23	32:S:178:VAL:HG12	1.89	0.54
6:Z:172:VAL:HG22	9:c:217:LEU:HD21	1.89	0.54
20:G:169:GLY:O	20:G:172:GLN:NE2	2.41	0.54
2:V:137:GLU:HA	2:V:140:ASP:HB2	1.90	0.54
3:W:396:LEU:HD13	3:W:402:ILE:HD13	1.90	0.54
14:B:190:LEU:HD13	14:B:193:GLN:HB2	1.90	0.54
24:K:210:LEU:HD11	24:K:215:ILE:HG12	1.90	0.54
1:U:18:GLN:HE21	10:d:27:LYS:HD2	1.71	0.54
10:d:131:VAL:HA	10:d:134:LYS:HB3	1.90	0.54
12:f:790:GLN:HG2	12:f:794:ALA:HB3	1.89	0.54
22:I:229:LYS:N	22:I:232:GLU:OE2	2.41	0.54
24:K:41:GLN:NE2	24:K:151:PRO:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:N:21:THR:HG22	27:N:26:ILE:HG13	1.88	0.54
3:W:362:ASN:HD22	3:W:365:ILE:HD11	1.73	0.54
4:X:57:LEU:HD23	4:X:62:GLN:HE21	1.73	0.54
15:C:307:ARG:HE	15:C:310:ARG:HG3	1.73	0.54
16:D:274:ARG:NH2	16:D:276:ASP:O	2.40	0.54
18:F:250:LYS:HA	18:F:284:PHE:HB3	1.89	0.54
22:i:90:LEU:HD12	22:i:114:LEU:HD22	1.89	0.54
22:i:229:LYS:N	22:i:232:GLU:OE2	2.41	0.54
32:s:148:LEU:HD23	32:s:178:VAL:HG12	1.89	0.54
2:V:167:LEU:HD12	2:V:169:LEU:H	1.72	0.54
12:f:291:GLN:HE21	12:f:879:ARG:HH21	1.55	0.54
20:G:212:PRO:HG3	20:G:239:LEU:HD23	1.90	0.54
32:S:123:SER:HB3	32:S:136:LYS:HG3	1.90	0.54
13:A:38:GLN:HG2	14:B:57:GLN:HB3	1.90	0.53
32:S:187:VAL:HG21	28:o:24:MET:HE3	1.89	0.53
1:U:803:LYS:HB3	1:U:877:LEU:HD23	1.89	0.53
1:U:862:LYS:HD2	1:U:863:GLU:HB3	1.90	0.53
7:a:186:LYS:O	7:a:193:GLN:NE2	2.42	0.53
12:f:373:ALA:HB2	12:f:744:MET:HA	1.89	0.53
12:f:664:GLU:C	12:f:666:ILE:N	2.66	0.53
17:E:101:ASP:HB3	17:E:105:LEU:H	1.73	0.53
18:F:227:GLY:HA3	18:F:354:PHE:HB2	1.90	0.53
21:H:7:SER:O	21:H:21:GLN:NE2	2.41	0.53
5:Y:314:LEU:O	5:Y:354:VAL:N	2.42	0.53
12:f:240:VAL:O	12:f:257:ARG:NH2	2.37	0.53
12:f:875:ALA:O	12:f:876:HIS:ND1	2.41	0.53
18:F:97:LEU:O	18:F:120:LYS:N	2.41	0.53
25:l:41:LYS:NZ	25:l:180:MET:O	2.38	0.53
22:I:90:LEU:HD12	22:I:114:LEU:HD22	1.90	0.53
4:X:201:TYR:HD1	21:H:177:ARG:HA	1.73	0.53
15:C:198:LEU:HD11	36:C:407:ATP:H2'	1.89	0.53
22:i:161:ALA:HB1	22:i:175:LEU:HD13	1.90	0.53
26:m:34:SER:OG	26:m:65:ARG:NH2	2.42	0.53
1:U:189:GLN:NE2	1:U:595:ASN:OD1	2.41	0.53
3:W:72:LYS:HD3	3:W:123:ARG:HA	1.91	0.53
5:Y:314:LEU:HD21	5:Y:319:MET:HE3	1.90	0.53
6:Z:215:VAL:HG22	6:Z:222:ILE:HG22	1.90	0.53
8:b:24:THR:HG22	8:b:26:LEU:H	1.74	0.53
12:f:202:HIS:ND1	12:f:242:GLU:OE2	2.42	0.53
16:D:87:LEU:HD13	16:D:131:ALA:HB1	1.89	0.53
30:Q:19:ARG:HH11	30:Q:179:SER:HB3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:q:19:ARG:HH11	30:q:179:SER:HB3	1.73	0.53
1:U:21:GLU:O	1:U:25:HIS:N	2.42	0.53
8:b:124:LEU:HD13	8:b:156:PHE:HB2	1.90	0.53
12:f:288:VAL:HA	12:f:291:GLN:HG2	1.89	0.53
12:f:758:ASN:HB2	12:f:809:ILE:HG21	1.91	0.53
13:A:272:ILE:HB	13:A:317:VAL:HG22	1.89	0.53
2:V:72:LEU:O	2:V:76:LYS:N	2.39	0.53
2:V:166:TYR:OH	2:V:216:ARG:NH1	2.42	0.53
4:X:74:ARG:HH22	4:X:116:TRP:HB2	1.73	0.53
12:f:378:ASN:O	12:f:382:ASN:ND2	2.42	0.53
13:A:116:LYS:O	13:A:249:TYR:OH	2.24	0.53
3:W:65:ARG:HG3	3:W:67:LEU:H	1.74	0.53
4:X:332:GLU:HA	4:X:335:LEU:HB2	1.90	0.53
5:Y:13:LYS:HE3	5:Y:146:ARG:HD2	1.91	0.53
7:a:273:GLN:HB3	7:a:310:LEU:HD11	1.91	0.53
12:f:816:TYR:HB3	12:f:821:LEU:HD13	1.90	0.53
23:J:109:ARG:NH2	31:R:70:ASN:OD1	2.42	0.53
24:k:48:LEU:HD21	24:k:77:ALA:HB2	1.90	0.53
7:a:33:LEU:HA	8:b:18:ASN:HB2	1.91	0.53
10:d:45:LYS:NZ	10:d:86:LYS:O	2.41	0.53
17:E:355:ILE:HG21	18:F:212:PHE:HE1	1.74	0.53
12:f:119:LYS:HA	12:f:122:ALA:HB3	1.91	0.52
12:f:673:ARG:NH1	12:f:708:ASP:OD2	2.42	0.52
1:U:885:MET:HB3	1:U:888:GLN:HG2	1.91	0.52
3:W:82:LEU:HB3	3:W:90:LEU:HD11	1.92	0.52
3:W:98:LYS:HD3	3:W:140:ILE:HG12	1.90	0.52
3:W:128:LEU:HA	3:W:147:LYS:HZ3	1.74	0.52
21:H:108:ALA:HA	21:H:147:PHE:HE2	1.74	0.52
22:I:38:LEU:HG	22:I:160:LYS:HB3	1.91	0.52
26:m:163:CYS:SG	26:m:164:ALA:N	2.83	0.52
6:Z:16:LEU:N	6:Z:16:LEU:HD23	2.23	0.52
15:C:69:GLN:HB3	15:C:118:ASN:HD21	1.74	0.52
17:E:144:GLU:O	17:E:297:ARG:NH2	2.42	0.52
25:L:46:LEU:HD13	25:L:73:SER:HB2	1.92	0.52
3:W:175:GLY:O	3:W:178:GLU:HG3	2.09	0.52
6:Z:12:HIS:HB2	6:Z:50:VAL:O	2.09	0.52
7:a:284:ARG:HH21	7:a:288:HIS:HB2	1.75	0.52
10:d:183:GLU:OE2	10:d:215:TRP:NE1	2.37	0.52
17:E:101:ASP:HB2	17:E:108:MET:HE3	1.90	0.52
29:p:58:THR:CG2	29:p:59:ASP:H	2.22	0.52
1:U:811:PHE:HZ	1:U:888:GLN:HB3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:88:GLY:O	2:V:118:GLN:NE2	2.41	0.52
5:Y:66:ASP:HA	5:Y:69:LEU:HD13	1.90	0.52
5:Y:311:TYR:HD2	5:Y:314:LEU:HD12	1.75	0.52
6:Z:216:ALA:HB2	7:a:346:ILE:CG2	2.34	0.52
14:B:383:LEU:HD11	14:B:419:PHE:HB3	1.92	0.52
16:D:151:ILE:HG12	16:D:151:ILE:O	2.08	0.52
16:D:271:ALA:HA	16:D:289:LEU:HD21	1.90	0.52
17:E:226:GLN:HE21	17:E:272:ARG:HB2	1.74	0.52
18:F:82:VAL:O	18:F:85:THR:OG1	2.27	0.52
18:F:204:LEU:HD23	18:F:207:ASN:HD22	1.74	0.52
23:J:7:ILE:HD12	23:J:8:THR:HG23	1.91	0.52
26:M:34:SER:OG	26:M:65:ARG:NH2	2.42	0.52
26:M:163:CYS:SG	26:M:164:ALA:N	2.83	0.52
34:g:165:ALA:HB1	34:g:179:LEU:HD13	1.90	0.52
22:i:123:GLN:NE2	23:j:79:ASP:OD1	2.43	0.52
24:k:117:SER:HB3	25:l:82:ARG:HH22	1.75	0.52
33:t:27:LEU:HD11	33:t:34:ALA:HB1	1.92	0.52
3:W:312:MET:HG2	3:W:314:LEU:HA	1.91	0.52
5:Y:117:LYS:HD3	5:Y:151:TYR:HD2	1.73	0.52
12:f:872:VAL:HG21	12:f:881:GLU:H	1.75	0.52
15:C:232:ARG:NH1	15:C:275:GLU:OE2	2.42	0.52
20:G:199:ILE:O	20:G:203:SER:N	2.41	0.52
29:p:135:ASP:OD1	29:p:135:ASP:N	2.41	0.52
3:W:60:MET:HG3	3:W:107:GLN:HG3	1.92	0.52
10:d:44:THR:OG1	10:d:47:GLN:NE2	2.43	0.52
20:G:158:GLY:O	21:H:84:ARG:NH2	2.42	0.52
24:k:121:LEU:HD11	24:k:160:GLY:HA3	1.92	0.52
10:d:78:LEU:HD13	10:d:98:LEU:HD21	1.90	0.52
10:d:203:PRO:HB2	10:d:205:LYS:H	1.74	0.52
32:s:123:SER:HB3	32:s:136:LYS:HG3	1.90	0.52
1:U:168:LEU:HD13	1:U:204:ILE:HD11	1.91	0.52
2:V:401:ASN:HA	2:V:404:LYS:HB2	1.92	0.52
15:C:145:ASP:OD1	15:C:145:ASP:N	2.41	0.52
17:E:317:ALA:HA	17:E:320:ILE:HD12	1.91	0.52
32:S:125:ASP:OD1	32:S:129:SER:N	2.42	0.52
34:g:144:ASP:HB3	34:g:147:GLN:HB2	1.92	0.52
21:H:65:VAL:HG11	21:H:211:GLY:HA3	1.92	0.52
25:L:189:LYS:O	25:L:193:ARG:NH1	2.43	0.52
33:T:45:VAL:HB	33:T:49:THR:HG23	1.92	0.52
33:t:45:VAL:HB	33:t:49:THR:HG23	1.92	0.52
16:D:249:ASP:OD1	16:D:252:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:K:228:MET:N	24:K:228:MET:SD	2.83	0.51
1:U:772:TRP:HD1	1:U:775:LEU:HG	1.74	0.51
2:V:80:LYS:O	2:V:87:SER:N	2.43	0.51
2:V:100:MET:H	2:V:103:SER:HB2	1.75	0.51
2:V:416:ARG:NH1	5:Y:351:ASN:OD1	2.42	0.51
3:W:174:TYR:HD2	3:W:174:TYR:O	1.91	0.51
12:f:465:LEU:O	12:f:481:SER:OG	2.27	0.51
12:f:682:GLY:HA3	12:f:687:ARG:HH11	1.73	0.51
12:f:829:MET:H	12:f:845:ARG:HB3	1.75	0.51
18:F:175:MET:HE1	18:F:267:LEU:HD21	1.91	0.51
25:L:157:ARG:HD2	25:L:176:MET:HE3	1.92	0.51
30:Q:21:ALA:HB3	30:Q:29:LYS:HB3	1.92	0.51
1:U:94:SER:HB3	1:U:97:VAL:HG12	1.92	0.51
12:f:809:ILE:HG23	12:f:810:ILE:HG12	1.92	0.51
24:K:16:SER:OG	24:K:18:GLU:OE1	2.27	0.51
32:S:4:PRO:HB2	33:T:100:ARG:HH21	1.74	0.51
32:S:211:ARG:NH2	32:S:213:ASP:OD2	2.42	0.51
28:o:177:VAL:HB	28:o:184:ASP:HB2	1.93	0.51
5:Y:364:TRP:NE1	5:Y:368:GLU:OE2	2.44	0.51
7:a:74:LEU:HD23	7:a:110:ALA:HB2	1.93	0.51
12:f:149:GLU:HG3	12:f:152:ALA:HB2	1.91	0.51
12:f:664:GLU:O	12:f:665:GLU:C	2.51	0.51
15:C:277:LEU:O	15:C:310:ARG:NH1	2.37	0.51
18:F:234:THR:O	18:F:238:ARG:N	2.36	0.51
18:F:368:ILE:HG23	18:F:371:ARG:HH12	1.74	0.51
25:L:41:LYS:NZ	25:L:180:MET:O	2.38	0.51
8:b:131:LEU:HD22	8:b:136:VAL:HB	1.93	0.51
9:c:100:LYS:HG2	9:c:105:PRO:HB3	1.91	0.51
15:C:113:ARG:NH2	16:D:94:GLU:OE1	2.39	0.51
17:E:385:ASP:HB3	26:M:17:ASP:HB3	1.93	0.51
26:M:47:PHE:HB2	26:M:214:SER:HB3	1.93	0.51
32:s:125:ASP:OD1	32:s:129:SER:N	2.42	0.51
3:W:41:GLN:NE2	17:E:365:GLU:OE2	2.44	0.51
3:W:167:GLN:HG3	3:W:168:GLU:HG3	1.93	0.51
3:W:223:LYS:HD2	3:W:227:TYR:HE2	1.75	0.51
24:K:9:ASP:OD1	24:K:9:ASP:N	2.39	0.51
26:M:40:ARG:NH1	26:M:146:ALA:O	2.44	0.51
25:l:46:LEU:HD13	25:l:73:SER:HB2	1.92	0.51
25:l:189:LYS:O	25:l:193:ARG:NH1	2.43	0.51
3:W:92:LYS:HD3	3:W:96:GLN:HG2	1.91	0.51
8:b:54:LEU:HD13	8:b:84:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:179:ALA:O	10:d:183:GLU:N	2.44	0.51
12:f:240:VAL:HG13	12:f:257:ARG:HE	1.75	0.51
26:M:168:ALA:HB1	26:M:171:ALA:HB3	1.93	0.51
23:j:105:GLU:HA	23:j:145:TYR:HE2	1.75	0.51
25:l:157:ARG:HD2	25:l:176:MET:HE3	1.92	0.51
2:V:90:GLU:HG2	2:V:134:PHE:HB3	1.93	0.51
9:c:224:SER:HB2	9:c:227:GLU:HB3	1.93	0.51
12:f:712:LYS:HD3	12:f:715:HIS:HB2	1.93	0.51
13:A:346:PRO:O	13:A:351:ARG:NH1	2.44	0.51
31:R:166:ARG:NH2	29:p:34:MET:O	2.43	0.51
26:m:40:ARG:NH1	26:m:146:ALA:O	2.44	0.51
1:U:107:HIS:HA	1:U:110:LYS:HE3	1.93	0.51
3:W:88:MET:SD	20:G:203:SER:HA	2.51	0.51
3:W:446:ILE:HG22	6:Z:226:ILE:HD12	1.93	0.51
4:X:172:LEU:HD12	4:X:175:LYS:HD3	1.92	0.51
7:a:19:PRO:HA	7:a:23:HIS:HD2	1.75	0.51
12:f:606:VAL:HG11	14:B:70:ASP:HB3	1.92	0.51
12:f:873:LEU:HG	12:f:875:ALA:H	1.74	0.51
3:W:201:ARG:HH11	16:D:390:ASN:HB2	1.75	0.50
14:B:197:ILE:HG21	14:B:235:LEU:HD11	1.93	0.50
24:k:97:GLN:HG3	31:r:61:ARG:HG2	1.92	0.50
33:t:43:MET:HE3	33:t:45:VAL:HG22	1.93	0.50
6:Z:228:TYR:HB2	7:a:338:PRO:HB2	1.93	0.50
7:a:247:ARG:HH21	7:a:250:THR:HG23	1.76	0.50
33:T:27:LEU:HD11	33:T:34:ALA:HB1	1.92	0.50
34:g:53:GLN:HA	34:g:215:ILE:HA	1.93	0.50
22:i:109:GLN:OE1	30:q:71:ASN:ND2	2.44	0.50
13:A:329:PRO:O	13:A:333:ARG:N	2.45	0.50
14:B:106:PRO:O	14:B:154:HIS:NE2	2.44	0.50
21:h:185:GLU:O	21:h:229:TYR:OH	2.30	0.50
2:V:85:ALA:O	2:V:89:LYS:NZ	2.38	0.50
12:f:692:LEU:HD22	14:B:40:THR:HB	1.92	0.50
13:A:369:ARG:NH2	24:K:206:MET:O	2.39	0.50
33:T:43:MET:HE3	33:T:45:VAL:HG22	1.93	0.50
30:q:21:ALA:HB3	30:q:29:LYS:HB3	1.92	0.50
2:V:452:ASN:HB3	2:V:457:TYR:HB2	1.93	0.50
5:Y:40:GLU:O	5:Y:44:ALA:N	2.45	0.50
20:G:114:LEU:HD22	20:G:140:LEU:HD21	1.92	0.50
2:V:337:LEU:HD22	2:V:367:VAL:HG11	1.94	0.50
2:V:467:TYR:HH	4:X:397:TYR:HH	1.51	0.50
4:X:299:LEU:HD11	4:X:331:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:28:LEU:HG	7:a:33:LEU:HD11	1.94	0.50
8:b:110:ILE:HG22	8:b:139:ASP:HB2	1.93	0.50
12:f:482:ILE:HD11	12:f:517:VAL:HG23	1.94	0.50
15:C:60:ARG:NH2	16:D:71:GLU:OE1	2.45	0.50
17:E:303:LEU:HD23	17:E:338:PHE:HB3	1.92	0.50
22:i:216:LEU:HD12	22:i:225:ILE:HG12	1.93	0.50
2:V:264:TYR:HB2	10:d:121:ARG:HH21	1.77	0.50
14:B:437:GLY:O	22:I:155:ASN:ND2	2.43	0.50
15:C:66:LEU:HD23	16:D:82:ILE:HD13	1.94	0.50
22:I:109:GLN:OE1	30:Q:71:ASN:ND2	2.39	0.50
3:W:152:ILE:HG13	3:W:161:GLU:HB3	1.94	0.49
34:g:137:CYS:SG	34:g:153:LYS:NZ	2.80	0.49
1:U:376:MET:HA	1:U:739:ALA:HA	1.94	0.49
3:W:206:SER:OG	3:W:230:MET:SD	2.68	0.49
8:b:20:ASP:OD1	8:b:25:ARG:NE	2.42	0.49
12:f:139:CYS:O	12:f:143:ARG:NH1	2.44	0.49
28:O:177:VAL:HB	28:O:184:ASP:HB2	1.93	0.49
22:i:218:ARG:NH1	22:i:223:THR:OG1	2.45	0.49
26:m:168:ALA:HB1	26:m:171:ALA:HB3	1.93	0.49
1:U:82:LEU:O	1:U:129:ARG:NE	2.45	0.49
13:A:331:LEU:HB3	13:A:337:LEU:HD12	1.94	0.49
1:U:12:LEU:O	1:U:20:LYS:NZ	2.43	0.49
1:U:580:ARG:HH22	1:U:768:GLN:HE22	1.60	0.49
2:V:136:GLU:O	2:V:140:ASP:N	2.43	0.49
5:Y:275:LEU:HD21	5:Y:296:VAL:HG13	1.94	0.49
6:Z:11:VAL:HB	6:Z:162:ILE:CD1	2.41	0.49
25:L:121:GLN:HG3	26:M:129:ARG:HG2	1.94	0.49
26:m:47:PHE:HB2	26:m:214:SER:HB3	1.93	0.49
29:p:190:ILE:HG22	29:p:195:ILE:HG23	1.95	0.49
4:X:187:ARG:HH21	4:X:217:ILE:HG22	1.77	0.49
12:f:742:ALA:O	12:f:746:ARG:NE	2.44	0.49
13:A:29:ASP:HA	13:A:32:LEU:HD23	1.94	0.49
20:G:43:ARG:HH21	20:G:164:LYS:HG2	1.77	0.49
2:V:139:MET:HE1	2:V:181:TYR:HB3	1.94	0.49
6:Z:216:ALA:CB	7:a:346:ILE:CG2	2.91	0.49
13:A:248:LYS:NZ	14:B:261:GLY:O	2.45	0.49
13:A:433:ASN:OD1	24:K:35:SER:OG	2.30	0.49
17:E:358:ASP:OD1	18:F:211:LYS:NZ	2.45	0.49
29:P:135:ASP:OD1	29:P:135:ASP:N	2.41	0.49
30:Q:64:VAL:HG13	30:Q:75:LEU:HD12	1.95	0.49
3:W:179:LYS:O	3:W:179:LYS:HE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:253:THR:O	3:W:257:GLN:NE2	2.46	0.49
6:Z:260:VAL:O	6:Z:264:SER:OG	2.28	0.49
7:a:23:HIS:ND1	7:a:26:GLU:OE2	2.41	0.49
8:b:15:TYR:O	8:b:25:ARG:NH1	2.45	0.49
8:b:53:THR:HG22	8:b:59:GLU:H	1.77	0.49
12:f:184:LEU:HG	14:B:59:ARG:HB2	1.95	0.49
12:f:276:GLU:O	12:f:286:LYS:NZ	2.36	0.49
15:C:344:LEU:HA	15:C:347:ILE:HD12	1.94	0.49
18:F:370:SER:HB2	18:F:375:VAL:HG21	1.95	0.49
25:l:189:LYS:HA	25:l:192:LEU:HG	1.94	0.49
5:Y:238:GLU:HA	5:Y:242:LYS:HB2	1.95	0.49
12:f:414:LEU:HD23	12:f:417:ILE:HD12	1.93	0.49
12:f:659:LEU:CD1	12:f:659:LEU:C	2.86	0.49
13:A:158:ASP:OD2	13:A:162:THR:OG1	2.25	0.49
17:E:75:ASN:HD21	18:F:130:GLN:HG2	1.78	0.49
20:G:181:LYS:O	20:G:185:LYS:NZ	2.45	0.49
23:J:3:TYR:HB3	24:K:10:ARG:HH22	1.78	0.49
34:g:114:LEU:HD22	34:g:140:LEU:HD21	1.95	0.49
3:W:142:ARG:CZ	3:W:181:GLU:HG2	2.43	0.49
7:a:247:ARG:HH12	7:a:251:LEU:HD13	1.78	0.49
12:f:94:LYS:HA	12:f:97:LYS:HB2	1.94	0.49
12:f:564:LEU:HD22	12:f:776:LEU:HG	1.94	0.49
14:B:411:ARG:NH2	14:B:418:ASP:OD2	2.43	0.49
23:j:76:LEU:HD12	23:j:79:ASP:H	1.78	0.49
24:k:203:LYS:HB3	24:k:210:LEU:HD22	1.95	0.49
25:l:225:ASP:OD1	25:l:225:ASP:N	2.45	0.49
4:X:286:ALA:HB1	4:X:313:LEU:HD22	1.95	0.48
6:Z:205:LEU:HD11	7:a:356:TRP:CD1	2.48	0.48
25:L:225:ASP:N	25:L:225:ASP:OD1	2.44	0.48
29:P:190:ILE:HG22	29:P:195:ILE:HG23	1.95	0.48
34:g:41:ALA:HB3	34:g:166:THR:HB	1.95	0.48
25:l:15:PRO:O	26:m:28:LYS:NZ	2.33	0.48
3:W:179:LYS:NZ	3:W:180:LYS:NZ	2.62	0.48
12:f:637:LYS:HE2	12:f:673:ARG:HB2	1.95	0.48
12:f:680:ARG:HD2	12:f:762:VAL:HG23	1.95	0.48
13:A:160:THR:HG23	13:A:161:VAL:HG23	1.95	0.48
21:h:108:ALA:HA	21:h:147:PHE:HE2	1.78	0.48
23:j:134:VAL:HG22	23:j:144:LEU:HB2	1.94	0.48
2:V:228:ARG:NH2	2:V:253:LEU:O	2.46	0.48
5:Y:265:GLU:OE1	5:Y:267:ARG:NH2	2.41	0.48
12:f:24:THR:HG23	12:f:31:LYS:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:35:THR:O	13:A:39:SER:OG	2.30	0.48
17:E:62:LYS:CG	17:E:63:GLN:H	2.25	0.48
18:F:98:ASP:OD1	18:F:120:LYS:N	2.46	0.48
23:J:158:ALA:HB3	24:K:58:LEU:HD13	1.96	0.48
29:p:101:GLY:O	30:q:93:ARG:NH1	2.43	0.48
2:V:132:LEU:HD23	2:V:135:LEU:HD12	1.96	0.48
2:V:194:LYS:HD3	2:V:241:ARG:HH22	1.79	0.48
6:Z:67:VAL:HG21	8:b:91:ARG:HD2	1.95	0.48
22:I:38:LEU:HD12	22:I:161:ALA:HB2	1.94	0.48
24:k:182:GLN:NE2	25:l:55:GLU:OE1	2.40	0.48
1:U:11:LEU:HD22	1:U:19:LEU:HD11	1.96	0.48
1:U:885:MET:HG2	1:U:887:ALA:H	1.77	0.48
2:V:81:GLN:HB3	2:V:85:ALA:HB3	1.95	0.48
2:V:163:VAL:HA	2:V:175:MET:HE2	1.95	0.48
3:W:328:LEU:HD13	3:W:337:ALA:HB1	1.95	0.48
6:Z:14:LEU:O	6:Z:18:SER:N	2.42	0.48
25:L:189:LYS:HA	25:L:192:LEU:HG	1.94	0.48
34:g:163:PHE:HB3	21:h:57:TYR:HA	1.94	0.48
1:U:397:THR:OG1	1:U:401:LYS:NZ	2.46	0.48
1:U:889:LEU:HD13	1:U:909:GLY:H	1.77	0.48
4:X:154:LEU:HD23	4:X:157:LEU:HB2	1.95	0.48
8:b:180:ALA:HA	8:b:183:LEU:HD13	1.94	0.48
10:d:179:ALA:HA	10:d:182:ILE:HG22	1.95	0.48
15:C:230:MET:HA	15:C:233:GLU:HB2	1.95	0.48
16:D:176:GLU:OE2	16:D:329:ARG:NH1	2.46	0.48
20:G:45:LYS:HG3	20:G:46:ASP:H	1.79	0.48
23:J:159:ASN:OD1	23:J:160:ALA:N	2.46	0.48
29:P:62:THR:OG1	30:Q:85:ARG:NH2	2.46	0.48
33:T:179:ARG:HH22	28:o:136:ALA:HB2	1.78	0.48
3:W:38:GLY:HA2	3:W:44:ILE:HA	1.96	0.48
5:Y:138:LEU:HB2	5:Y:168:ILE:HG21	1.95	0.48
6:Z:16:LEU:CD2	6:Z:17:LEU:H	2.27	0.48
9:c:59:GLY:HA3	9:c:69:VAL:HA	1.95	0.48
13:A:73:ALA:O	13:A:78:TRP:NE1	2.42	0.48
14:B:234:LEU:HD11	36:B:441:ATP:H2'	1.94	0.48
17:E:84:ARG:O	17:E:85:ARG:NE	2.42	0.48
26:M:72:HIS:HE2	26:M:105:ASN:HB3	1.78	0.48
26:M:152:ASP:OD1	26:M:156:VAL:N	2.46	0.48
2:V:30:PRO:HA	2:V:33:GLN:HB2	1.95	0.48
2:V:203:LEU:HA	2:V:206:VAL:HB	1.96	0.48
2:V:477:HIS:CG	10:d:245:GLN:HE21	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:173:THR:CA	3:W:182:ARG:HE	2.22	0.48
4:X:258:LYS:HD3	4:X:266:ASP:HB2	1.94	0.48
17:E:264:MET:HE3	17:E:294:ARG:HD3	1.96	0.48
28:O:136:ALA:HB2	33:t:179:ARG:HH22	1.78	0.48
34:g:161:CYS:SG	34:g:162:GLY:N	2.87	0.48
21:h:139:TRP:HA	21:h:144:PRO:HA	1.96	0.48
24:k:236:GLU:HA	24:k:239:LYS:HE3	1.95	0.48
3:W:236:HIS:HD1	3:W:236:HIS:C	2.16	0.48
5:Y:304:TYR:HE1	5:Y:323:PHE:HZ	1.62	0.48
13:A:48:VAL:HG13	14:B:69:LYS:HZ3	1.79	0.48
16:D:293:LEU:HD21	16:D:321:LEU:HD22	1.96	0.48
1:U:522:GLY:O	1:U:559:ARG:NH2	2.47	0.48
8:b:25:ARG:NH1	8:b:145:GLU:OE1	2.33	0.48
9:c:284:LEU:O	9:c:286:GLU:N	2.47	0.48
12:f:253:LEU:HD11	12:f:272:LEU:HB3	1.95	0.48
13:A:284:ARG:NH2	18:F:254:PRO:O	2.45	0.48
34:g:43:ARG:HH21	34:g:164:LYS:HG2	1.79	0.48
34:g:67:THR:HG22	34:g:69:LEU:H	1.78	0.48
32:s:4:PRO:HB2	33:t:100:ARG:HH21	1.78	0.48
1:U:47:VAL:O	1:U:48:LEU:C	2.57	0.47
1:U:643:SER:O	15:C:57:ARG:NH2	2.36	0.47
7:a:168:ASN:OD1	7:a:171:SER:OG	2.29	0.47
12:f:23:GLY:HA3	12:f:34:ARG:HH22	1.78	0.47
16:D:116:LEU:O	16:D:121:ARG:NH2	2.40	0.47
17:E:193:CYS:SG	17:E:194:ASN:N	2.86	0.47
21:h:222:THR:OG1	21:h:225:GLU:OE1	2.26	0.47
22:i:48:GLU:OE2	22:i:50:ARG:NH2	2.46	0.47
28:o:198:ARG:NH1	29:p:152:SER:O	2.47	0.47
1:U:167:ILE:HD12	1:U:204:ILE:HG21	1.95	0.47
3:W:425:LEU:HA	6:Z:247:LYS:HZ3	1.79	0.47
5:Y:301:ILE:HG13	5:Y:343:LEU:HD12	1.95	0.47
12:f:202:HIS:CE1	12:f:241:PRO:HB2	2.49	0.47
12:f:640:LYS:HD3	12:f:651:GLY:HA3	1.96	0.47
12:f:852:VAL:HG22	12:f:853:VAL:HG13	1.96	0.47
14:B:39:LYS:HG2	14:B:276:GLU:HB3	1.95	0.47
16:D:92:PHE:HA	16:D:103:VAL:HG12	1.96	0.47
26:M:41:CYS:HB3	26:M:189:ILE:HG13	1.95	0.47
30:q:64:VAL:HG13	30:q:75:LEU:HD12	1.95	0.47
2:V:252:ASN:ND2	2:V:284:GLU:OE2	2.47	0.47
3:W:412:ILE:HG12	7:a:327:VAL:HG23	1.95	0.47
13:A:189:GLU:HG2	18:F:409:ARG:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:G:144:ASP:HB3	20:G:147:GLN:HB2	1.96	0.47
22:i:33:THR:OG1	22:i:167:ASN:ND2	2.47	0.47
26:m:41:CYS:HB3	26:m:189:ILE:HG13	1.95	0.47
27:n:29:ARG:NH1	28:o:139:GLU:OE1	2.46	0.47
28:o:113:ILE:HG12	28:o:119:THR:HG22	1.95	0.47
30:q:102:LEU:HB2	30:q:118:MET:HB3	1.96	0.47
3:W:174:TYR:CG	3:W:175:GLY:N	2.82	0.47
12:f:674:THR:O	12:f:678:LEU:N	2.42	0.47
13:A:125:LEU:HA	13:A:149:ILE:HB	1.96	0.47
18:F:311:LEU:O	18:F:315:ASN:N	2.47	0.47
23:j:158:ALA:HB3	24:k:58:LEU:HD13	1.96	0.47
26:m:152:ASP:OD1	26:m:156:VAL:N	2.46	0.47
6:Z:192:THR:O	6:Z:196:HIS:ND1	2.48	0.47
6:Z:212:LEU:HD22	7:a:349:MET:HE3	1.96	0.47
10:d:125:LYS:HE3	10:d:130:ASN:HB2	1.96	0.47
13:A:200:ARG:HA	13:A:203:ASN:HB2	1.95	0.47
16:D:417:TYR:HA	21:H:79:MET:HA	1.95	0.47
24:K:182:GLN:NE2	25:L:55:GLU:OE1	2.40	0.47
25:l:195:LEU:O	25:l:198:THR:OG1	2.31	0.47
1:U:92:ASP:HB3	1:U:140:ARG:HH12	1.79	0.47
1:U:336:GLU:O	1:U:340:GLN:N	2.46	0.47
12:f:705:ASN:OD1	12:f:706:ILE:N	2.48	0.47
18:F:223:VAL:HG22	18:F:350:ARG:HD3	1.96	0.47
28:O:113:ILE:HG12	28:O:119:THR:HG22	1.95	0.47
25:l:146:GLN:HE21	25:l:154:PHE:HD2	1.63	0.47
1:U:261:LEU:HA	1:U:264:VAL:HG12	1.97	0.47
3:W:359:VAL:HG23	3:W:382:LEU:HD22	1.95	0.47
5:Y:184:GLN:HG2	5:Y:197:ALA:HA	1.96	0.47
9:c:139:ARG:HB2	9:c:161:ARG:HE	1.80	0.47
10:d:79:LYS:HG3	10:d:121:ARG:HH12	1.79	0.47
12:f:777:THR:HG22	12:f:803:PHE:HA	1.95	0.47
13:A:41:TYR:HA	13:A:44:GLN:HB3	1.96	0.47
13:A:118:PHE:CE1	19:v:28:UNK:CA	2.98	0.47
13:A:245:LEU:HB3	13:A:298:THR:HG21	1.97	0.47
16:D:105:SER:OG	16:D:108:GLY:O	2.32	0.47
17:E:4:PRO:HG2	17:E:7:LYS:HB3	1.97	0.47
17:E:128:GLY:HA3	17:E:129:ASN:HA	1.68	0.47
23:J:11:SER:OG	23:J:15:HIS:N	2.47	0.47
25:L:107:ARG:HH12	33:T:74:GLU:HG3	1.79	0.47
34:g:201:CYS:SG	34:g:202:LEU:N	2.87	0.47
23:j:116:GLN:NE2	24:k:83:ALA:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:q:183:ILE:HG12	30:q:188:ILE:HG13	1.97	0.47
18:F:263:ASP:HA	18:F:266:LYS:HB2	1.97	0.47
1:U:21:GLU:HA	1:U:24:LEU:HG	1.96	0.47
2:V:99:ARG:HH12	2:V:100:MET:HE3	1.80	0.47
4:X:173:GLU:HA	4:X:176:THR:HG22	1.97	0.47
5:Y:102:ASP:HA	5:Y:105:MET:HG2	1.96	0.47
5:Y:113:ARG:HB3	5:Y:114:ILE:HD12	1.97	0.47
6:Z:142:GLU:OE2	6:Z:153:LYS:NZ	2.40	0.47
12:f:93:PRO:HB2	12:f:97:LYS:HG3	1.97	0.47
12:f:331:LEU:HD21	12:f:810:ILE:HD11	1.96	0.47
16:D:270:ILE:H	16:D:270:ILE:HG13	1.49	0.47
17:E:175:PRO:HB2	17:E:303:LEU:HD11	1.96	0.47
18:F:283:ILE:HD12	18:F:328:VAL:HG22	1.95	0.47
34:g:126:THR:HG22	21:h:128:ARG:HH22	1.80	0.47
7:a:252:LYS:HA	7:a:255:TRP:HD1	1.80	0.47
16:D:414:HIS:CE1	20:G:26:GLU:HB2	2.50	0.47
30:Q:47:VAL:O	30:Q:101:ASN:N	2.42	0.47
24:k:228:MET:SD	24:k:228:MET:N	2.88	0.47
12:f:697:ILE:HG12	12:f:737:ASN:HD21	1.80	0.46
20:G:11:ARG:O	20:G:24:GLN:NE2	2.42	0.46
21:H:107:THR:HG21	21:H:138:GLY:HA3	1.97	0.46
27:N:76:VAL:HG23	27:N:104:ASP:HB2	1.97	0.46
2:V:294:ARG:HE	2:V:331:LEU:HD22	1.81	0.46
2:V:450:SER:OG	10:d:186:TYR:OH	2.33	0.46
8:b:6:THR:HB	8:b:49:VAL:HG22	1.97	0.46
9:c:284:LEU:HB3	9:c:285:GLU:H	1.46	0.46
12:f:487:LEU:HD11	12:f:804:LEU:HD12	1.96	0.46
12:f:659:LEU:HD21	12:f:671:ALA:HB2	1.96	0.46
16:D:398:ASP:OD1	16:D:398:ASP:N	2.47	0.46
30:Q:2:GLU:HG3	30:Q:34:LYS:HE2	1.97	0.46
21:h:148:GLN:OE1	21:h:158:TRP:NE1	2.48	0.46
23:j:64:ALA:O	23:j:88:ARG:NH1	2.48	0.46
25:l:186:GLU:O	25:l:190:HIS:N	2.48	0.46
1:U:325:MET:HA	1:U:328:ILE:HG12	1.97	0.46
1:U:792:ASN:HB3	1:U:914:LEU:HB3	1.97	0.46
2:V:264:TYR:OH	10:d:114:GLU:OE1	2.29	0.46
7:a:70:ARG:HE	8:b:17:ARG:HA	1.79	0.46
8:b:18:ASN:N	8:b:18:ASN:OD1	2.48	0.46
12:f:184:LEU:HD11	14:B:59:ARG:H	1.80	0.46
12:f:705:ASN:HB3	12:f:787:LEU:HD21	1.97	0.46
18:F:134:LEU:HD13	18:F:137:ILE:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:G:211:LYS:O	20:G:213:SER:N	2.48	0.46
23:J:31:THR:H	23:J:46:GLU:HG2	1.80	0.46
30:Q:183:ILE:HG12	30:Q:188:ILE:HG13	1.97	0.46
1:U:351:MET:HE1	1:U:818:GLU:HA	1.97	0.46
1:U:751:ARG:NH1	1:U:909:GLY:O	2.48	0.46
1:U:803:LYS:HD2	1:U:875:PHE:HB2	1.97	0.46
4:X:130:GLU:HG3	4:X:153:LEU:HD11	1.96	0.46
8:b:9:CYS:HB3	8:b:111:ALA:HA	1.98	0.46
12:f:130:ALA:O	12:f:134:SER:N	2.48	0.46
13:A:74:PRO:HA	13:A:75:PRO:HD3	1.78	0.46
16:D:153:MET:HE1	16:D:257:ASN:HD21	1.81	0.46
18:F:428:GLN:HG2	18:F:430:LYS:HG2	1.97	0.46
1:U:469:SER:OG	1:U:470:ASN:N	2.49	0.46
7:a:23:HIS:HA	7:a:26:GLU:HG2	1.98	0.46
7:a:73:PRO:HA	7:a:76:LEU:HB3	1.98	0.46
7:a:81:LEU:HA	7:a:84:VAL:HG12	1.97	0.46
16:D:60:TYR:O	16:D:64:GLU:N	2.42	0.46
18:F:365:ILE:O	18:F:369:HIS:ND1	2.32	0.46
25:L:146:GLN:HE21	25:L:154:PHE:HD2	1.63	0.46
24:k:221:GLN:HB2	24:k:224:GLN:HB3	1.98	0.46
25:l:203:GLN:O	25:l:239:ARG:NH2	2.49	0.46
1:U:265:ILE:HG13	1:U:268:LEU:HD22	1.98	0.46
3:W:98:LYS:HD2	3:W:140:ILE:H	1.81	0.46
12:f:75:LEU:HD12	12:f:78:LEU:HD13	1.97	0.46
13:A:45:ILE:HG21	14:B:57:GLN:HE22	1.80	0.46
13:A:346:PRO:HB3	13:A:350:GLY:HA3	1.97	0.46
14:B:98:LYS:O	14:B:102:LEU:N	2.49	0.46
28:O:96:ALA:H	28:O:115:PRO:HB3	1.81	0.46
30:Q:102:LEU:HB2	30:Q:118:MET:HB3	1.96	0.46
28:o:18:THR:HB	28:o:30:ASN:HA	1.98	0.46
2:V:106:ARG:O	2:V:110:HIS:ND1	2.47	0.46
13:A:103:ASN:HA	13:A:136:GLU:HG2	1.98	0.46
13:A:363:SER:HB2	14:B:214:MET:HG2	1.97	0.46
16:D:270:ILE:HG22	16:D:285:VAL:HG13	1.98	0.46
22:I:73:ALA:HB3	22:I:137:ILE:HD11	1.96	0.46
24:K:155:HIS:CE1	24:K:170:ILE:HG21	2.50	0.46
28:O:38:SER:OG	28:O:40:ASN:OD1	2.30	0.46
3:W:63:THR:HB	3:W:68:VAL:HA	1.98	0.46
3:W:268:LYS:HA	3:W:271:VAL:HG12	1.97	0.46
5:Y:81:LEU:HB3	5:Y:107:LYS:HD3	1.98	0.46
7:a:233:LEU:HA	7:a:236:THR:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:257:ARG:HG2	12:f:272:LEU:HD13	1.97	0.46
12:f:755:ASP:N	12:f:755:ASP:OD1	2.46	0.46
22:I:179:TYR:OH	22:I:181:GLU:OE1	2.26	0.46
30:Q:25:ILE:HD11	31:R:133:VAL:HG11	1.97	0.46
21:h:225:GLU:O	21:h:229:TYR:N	2.47	0.46
28:o:96:ALA:H	28:o:115:PRO:HB3	1.81	0.46
30:q:23:SER:HB2	30:q:28:MET:HE2	1.98	0.46
12:f:258:LYS:HG2	12:f:297:MET:HG3	1.98	0.46
13:A:56:LEU:O	13:A:60:ASN:ND2	2.49	0.46
14:B:313:LEU:O	14:B:346:ARG:NH1	2.49	0.46
15:C:48:GLN:HB3	16:D:65:GLN:HE22	1.79	0.46
25:L:186:GLU:O	25:L:190:HIS:N	2.48	0.46
25:L:195:LEU:O	25:L:198:THR:OG1	2.31	0.46
28:O:209:THR:HG21	29:P:168:SER:HB3	1.97	0.46
34:g:132:ARG:HA	34:g:133:PRO:HD3	1.78	0.46
2:V:276:PHE:HB2	2:V:278:GLU:HG2	1.98	0.46
3:W:203:GLN:HB3	3:W:233:LEU:HD21	1.98	0.46
6:Z:130:ASP:OD1	6:Z:130:ASP:N	2.41	0.46
9:c:92:GLN:HE21	9:c:96:LEU:HD11	1.80	0.46
18:F:212:PHE:HB3	18:F:219:PRO:HD3	1.97	0.46
26:M:99:ARG:NH2	26:M:105:ASN:OD1	2.49	0.46
24:k:167:ALA:HB3	24:k:181:LEU:HD21	1.98	0.46
25:l:155:ASP:HB3	26:m:62:SER:HB2	1.97	0.46
27:n:76:VAL:HG23	27:n:104:ASP:HB2	1.97	0.46
1:U:496:LEU:HA	1:U:499:THR:HG22	1.98	0.45
7:a:360:VAL:HG22	9:c:308:VAL:HG13	1.98	0.45
9:c:192:LEU:HA	9:c:196:LEU:HB2	1.98	0.45
12:f:852:VAL:O	12:f:854:GLY:N	2.43	0.45
14:B:112:LEU:HD23	14:B:123:VAL:HG12	1.98	0.45
14:B:291:GLY:HA2	14:B:309:MET:HE2	1.98	0.45
16:D:154:LEU:HD11	16:D:229:ARG:HG2	1.99	0.45
17:E:235:ILE:HG13	17:E:277:MET:HB3	1.97	0.45
26:m:66:LEU:HD13	26:m:214:SER:HB2	1.98	0.45
1:U:541:HIS:HB2	1:U:544:ILE:HG22	1.98	0.45
1:U:636:VAL:HG23	1:U:637:VAL:HG23	1.98	0.45
2:V:176:MET:HE3	2:V:180:ARG:HE	1.81	0.45
3:W:187:LEU:HA	3:W:190:MET:HE3	1.97	0.45
10:d:139:LEU:HD11	10:d:151:VAL:HG13	1.99	0.45
16:D:273:LYS:HB3	16:D:318:ASP:HA	1.98	0.45
18:F:220:PRO:HG2	18:F:350:ARG:HD2	1.98	0.45
22:I:14:PRO:HB3	23:J:21:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:r:1:THR:N	31:r:169:TYR:O	2.50	0.45
3:W:405:LYS:HD3	4:X:343:SER:HB3	1.98	0.45
4:X:346:GLN:HA	4:X:384:VAL:HA	1.98	0.45
8:b:137:ASN:ND2	8:b:166:THR:OG1	2.50	0.45
24:K:76:CYS:SG	24:K:77:ALA:N	2.90	0.45
25:L:125:ARG:HH21	25:L:128:TYR:HE1	1.64	0.45
25:L:203:GLN:O	25:L:239:ARG:NH2	2.49	0.45
26:M:66:LEU:HD13	26:M:214:SER:HB2	1.98	0.45
26:M:67:PHE:HB2	26:M:75:MET:HB2	1.98	0.45
28:O:18:THR:HB	28:O:30:ASN:HA	1.98	0.45
28:O:174:ASP:OD2	28:O:187:ARG:NH1	2.49	0.45
1:U:756:HIS:HB3	1:U:758:PRO:HD2	1.98	0.45
17:E:139:SER:HA	17:E:142:ILE:HD12	1.98	0.45
23:J:121:SER:HB3	23:J:124:ARG:HD3	1.98	0.45
26:m:99:ARG:NH2	26:m:105:ASN:OD1	2.49	0.45
12:f:407:MET:HE3	12:f:439:TYR:HB2	1.99	0.45
15:C:368:MET:HE1	16:D:191:TYR:HE1	1.81	0.45
16:D:164:TYR:HB2	16:D:222:HIS:CD2	2.51	0.45
21:H:52:GLN:HB3	21:H:57:TYR:HD2	1.81	0.45
23:J:79:ASP:HB3	23:J:127:PHE:HD1	1.80	0.45
29:P:126:LEU:HD12	29:P:127:ILE:HG23	1.99	0.45
31:R:1:THR:N	31:R:169:TYR:O	2.50	0.45
33:T:9:THR:O	33:T:41:ARG:NH2	2.49	0.45
28:o:174:ASP:OD2	28:o:187:ARG:NH1	2.49	0.45
29:p:45:MET:HE3	29:p:71:LEU:HD22	1.98	0.45
1:U:92:ASP:HB2	1:U:140:ARG:HH22	1.82	0.45
1:U:900:TYR:HB3	1:U:914:LEU:HD21	1.97	0.45
2:V:55:THR:HG21	2:V:196:SER:HB3	1.97	0.45
5:Y:285:ASP:HB3	5:Y:288:PHE:HB2	1.97	0.45
6:Z:56:VAL:HG23	6:Z:74:TYR:HD2	1.81	0.45
12:f:261:ARG:HG2	12:f:266:LEU:HD13	1.98	0.45
13:A:333:ARG:HH21	13:A:336:ARG:HH22	1.64	0.45
20:G:67:THR:HG22	20:G:69:LEU:H	1.80	0.45
22:i:57:ASP:HB3	22:i:59:VAL:HG13	1.99	0.45
33:t:46:ASN:OD1	33:t:46:ASN:N	2.50	0.45
10:d:155:LYS:HD3	10:d:171:LEU:HD11	1.99	0.45
12:f:359:GLY:HA3	14:B:31:THR:HB	1.98	0.45
12:f:456:ARG:HE	12:f:492:SER:HG	1.63	0.45
12:f:520:LEU:HD11	12:f:557:TRP:CD1	2.52	0.45
13:A:99:THR:HG22	13:A:115:VAL:HA	1.99	0.45
17:E:62:LYS:CG	17:E:63:GLN:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:N:144:ARG:H	27:N:147:MET:HE3	1.82	0.45
24:k:100:TRP:O	31:r:57:ARG:NH2	2.49	0.45
12:f:72:ARG:HH12	12:f:83:ARG:HA	1.81	0.45
12:f:369:ARG:NH2	12:f:791:VAL:O	2.47	0.45
18:F:204:LEU:HA	18:F:207:ASN:HB2	1.99	0.45
21:H:66:GLU:OE2	21:H:91:ARG:NH2	2.50	0.45
26:M:232:ARG:HB3	26:M:234:GLU:HG2	1.99	0.45
29:P:45:MET:HE3	29:P:71:LEU:HD22	1.98	0.45
24:k:55:THR:OG1	24:k:59:MET:SD	2.71	0.45
27:n:144:ARG:H	27:n:147:MET:HE3	1.82	0.45
1:U:788:VAL:HG23	1:U:882:ALA:HB3	1.98	0.45
1:U:792:ASN:HB3	1:U:914:LEU:H	1.81	0.45
5:Y:210:SER:N	5:Y:213:LEU:O	2.50	0.45
10:d:3:GLU:HB2	10:d:25:ARG:HD3	1.98	0.45
14:B:271:PHE:HD2	14:B:315:GLN:HG3	1.82	0.45
16:D:204:MET:HE3	16:D:310:ALA:HB2	1.98	0.45
24:K:125:GLU:HG2	25:L:125:ARG:HH12	1.82	0.45
1:U:62:LEU:HD12	1:U:84:ALA:HB1	1.99	0.45
3:W:312:MET:HB3	3:W:314:LEU:HD23	1.99	0.45
7:a:138:VAL:O	7:a:142:LEU:N	2.48	0.45
9:c:88:ASP:HB3	9:c:91:PHE:HB3	1.99	0.45
15:C:403:LYS:HB3	21:H:156:PHE:CZ	2.51	0.45
16:D:92:PHE:HZ	16:D:95:ALA:HB2	1.82	0.45
24:K:55:THR:OG1	24:K:59:MET:SD	2.72	0.45
28:O:163:ILE:HA	28:O:168:GLY:HA3	1.99	0.45
26:m:232:ARG:HB3	26:m:234:GLU:HG2	1.99	0.45
1:U:554:LEU:HG	1:U:588:MET:HE1	1.99	0.44
3:W:253:THR:HG22	3:W:257:GLN:HE22	1.82	0.44
7:a:34:TRP:HD1	8:b:18:ASN:HA	1.83	0.44
12:f:43:GLN:HG3	12:f:121:PHE:HB2	1.99	0.44
12:f:612:LEU:HD21	12:f:636:ASP:HA	2.00	0.44
12:f:796:LEU:HA	12:f:799:VAL:HG12	1.97	0.44
17:E:98:VAL:HA	17:E:110:TYR:HA	2.00	0.44
30:Q:23:SER:HB2	30:Q:28:MET:HE2	1.98	0.44
24:k:202:LEU:HB3	24:k:206:MET:HE3	1.98	0.44
29:p:126:LEU:HD12	29:p:127:ILE:HG23	1.99	0.44
30:q:47:VAL:O	30:q:101:ASN:N	2.42	0.44
1:U:47:VAL:C	1:U:49:TYR:N	2.74	0.44
1:U:118:LEU:HD13	1:U:122:GLU:HG3	1.98	0.44
1:U:695:MET:HE3	1:U:695:MET:HB2	1.80	0.44
1:U:699:THR:O	1:U:702:THR:OG1	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:255:LEU:HD22	2:V:291:TYR:HB3	2.00	0.44
8:b:5:SER:HB3	8:b:64:LEU:HD21	1.98	0.44
9:c:196:LEU:HA	9:c:197:ASN:HA	1.72	0.44
14:B:107:MET:HB2	15:C:96:VAL:HB	1.98	0.44
21:H:6:TYR:HE1	22:I:6:ASP:HB3	1.82	0.44
32:S:35:ILE:HB	33:T:151:ARG:HH12	1.81	0.44
28:o:67:SER:HB3	28:o:74:PRO:HG3	1.99	0.44
1:U:643:SER:O	1:U:649:ARG:NH1	2.50	0.44
10:d:8:GLU:O	10:d:13:SER:OG	2.34	0.44
12:f:281:ILE:HA	12:f:282:PHE:HA	1.55	0.44
17:E:148:VAL:HG13	17:E:149:ILE:HG13	1.98	0.44
20:G:11:ARG:NE	20:G:27:TYR:OH	2.50	0.44
20:G:131:MET:HE3	26:M:124:LEU:HD13	1.99	0.44
20:G:163:PHE:HB3	21:H:57:TYR:HA	1.98	0.44
22:I:86:LEU:HD22	22:I:114:LEU:HD11	2.00	0.44
33:T:171:ARG:NH2	28:o:140:ASP:OD2	2.50	0.44
26:m:67:PHE:HB2	26:m:75:MET:HB2	1.98	0.44
28:o:172:ASN:HD22	28:o:191:VAL:HG22	1.82	0.44
30:q:2:GLU:HG3	30:q:34:LYS:HE2	1.98	0.44
5:Y:203:ASP:N	5:Y:203:ASP:OD1	2.42	0.44
5:Y:329:PHE:CG	11:e:66:LYS:HD3	2.52	0.44
13:A:296:GLN:HA	13:A:299:MET:HB3	2.00	0.44
18:F:285:ILE:HG21	18:F:288:LEU:HD13	1.99	0.44
26:M:108:LEU:HD23	26:M:147:GLN:HB2	2.00	0.44
23:j:2:SER:HA	23:j:12:PRO:HD3	1.99	0.44
1:U:625:ILE:HG13	1:U:626:LEU:HG	1.99	0.44
3:W:60:MET:HE2	3:W:107:GLN:HB3	1.99	0.44
3:W:200:ILE:HD12	3:W:203:GLN:HE21	1.83	0.44
12:f:505:MET:HE3	12:f:537:THR:HG22	2.00	0.44
15:C:213:ARG:HD2	16:D:299:PHE:CD2	2.53	0.44
3:W:87:ILE:HD12	3:W:88:MET:SD	2.58	0.44
4:X:255:LEU:HD22	4:X:267:VAL:HG13	1.99	0.44
6:Z:187:LEU:HD13	10:d:250:ALA:HB1	1.99	0.44
12:f:269:ALA:HA	12:f:272:LEU:HB2	1.99	0.44
12:f:452:ASN:ND2	12:f:460:ASP:OD1	2.50	0.44
18:F:182:THR:HA	18:F:242:ALA:HB1	1.98	0.44
18:F:393:GLY:HA2	18:F:396:CYS:HB2	2.00	0.44
20:G:120:ASP:OD1	21:H:84:ARG:NH1	2.51	0.44
23:j:159:ASN:OD1	23:j:160:ALA:N	2.51	0.44
24:k:98:ASN:OD1	31:r:61:ARG:NH2	2.45	0.44
25:l:125:ARG:HH21	25:l:128:TYR:HE1	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:m:230:ASP:OD1	26:m:230:ASP:N	2.49	0.44
2:V:411:SER:HB2	2:V:447:ILE:HG12	1.98	0.44
3:W:201:ARG:NH1	16:D:390:ASN:O	2.51	0.44
5:Y:300:ARG:NH2	11:e:59:GLU:OE1	2.51	0.44
6:Z:12:HIS:CD2	6:Z:51:SER:CB	2.69	0.44
10:d:87:GLU:HA	10:d:89:LEU:HD23	1.99	0.44
12:f:747:GLN:HA	12:f:750:GLN:HB3	2.00	0.44
17:E:117:PRO:HA	17:E:120:TYR:HB3	2.00	0.44
22:I:136:TYR:HB2	22:I:148:TYR:HB2	2.00	0.44
28:O:67:SER:HB3	28:O:74:PRO:HG3	1.99	0.44
33:T:212:ALA:HA	27:n:30:VAL:HG21	1.99	0.44
21:h:72:ILE:HG12	21:h:107:THR:HG22	1.99	0.44
1:U:218:GLN:HE22	1:U:752:THR:HB	1.81	0.44
4:X:371:ASP:OD1	5:Y:233:ARG:NH1	2.50	0.44
9:c:152:LYS:HA	16:D:81:ARG:HH22	1.83	0.44
13:A:297:ARG:NE	18:F:259:MET:SD	2.91	0.44
23:j:51:ALA:H	23:j:54:GLN:HE22	1.65	0.44
1:U:596:ASN:HD21	16:D:52:GLU:HB3	1.82	0.44
7:a:34:TRP:HZ3	7:a:64:ILE:HG23	1.83	0.44
12:f:194:TYR:HB3	12:f:234:THR:HG21	2.00	0.44
12:f:269:ALA:O	12:f:273:ASN:N	2.41	0.44
17:E:177:GLY:O	17:E:339:ASN:ND2	2.51	0.44
22:I:105:ILE:HA	22:I:106:PRO:HD3	1.75	0.44
28:O:172:ASN:HD22	28:O:191:VAL:HG22	1.82	0.44
34:g:158:GLY:O	21:h:84:ARG:NH2	2.51	0.44
23:j:60:ARG:NE	23:j:62:ILE:O	2.51	0.44
1:U:697:GLN:NE2	1:U:744:VAL:O	2.51	0.43
4:X:141:LYS:HE3	4:X:179:ALA:HB1	1.99	0.43
4:X:214:SER:O	4:X:218:HIS:ND1	2.46	0.43
5:Y:220:VAL:HG21	5:Y:249:VAL:HG21	2.00	0.43
7:a:57:ILE:O	7:a:61:GLU:N	2.42	0.43
12:f:412:ALA:HA	12:f:447:ALA:HB2	2.00	0.43
13:A:103:ASN:ND2	18:F:167:GLU:OE1	2.51	0.43
27:N:19:ARG:NH2	33:t:181:ALA:HA	2.33	0.43
1:U:419:ALA:HB1	1:U:449:ILE:HD13	2.00	0.43
1:U:839:ALA:HA	1:U:842:LYS:HE3	2.01	0.43
8:b:95:LEU:O	8:b:99:HIS:ND1	2.49	0.43
12:f:828:ARG:HG2	12:f:845:ARG:C	2.43	0.43
13:A:398:ARG:NH1	14:B:195:GLN:HE22	2.16	0.43
20:G:53:GLN:HA	20:G:215:ILE:HA	1.99	0.43
22:I:32:GLY:O	22:I:166:ASN:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:I:42:GLY:HA3	22:I:186:LEU:HD21	1.99	0.43
21:h:9:SER:HA	21:h:125:GLY:HA2	1.99	0.43
2:V:228:ARG:HA	2:V:228:ARG:HD3	1.88	0.43
5:Y:344:HIS:CE1	5:Y:359:PRO:HD3	2.53	0.43
6:Z:7:GLN:HB2	6:Z:46:LYS:HG2	1.99	0.43
7:a:34:TRP:O	7:a:38:THR:OG1	2.26	0.43
7:a:58:LYS:HA	7:a:61:GLU:HB2	2.00	0.43
7:a:150:SER:HA	7:a:153:SER:HB3	1.98	0.43
15:C:127:LEU:O	15:C:130:LYS:NZ	2.36	0.43
16:D:268:ASP:HA	16:D:271:ALA:HB3	2.00	0.43
17:E:153:LEU:HA	17:E:272:ARG:HH12	1.84	0.43
21:H:181:ASP:OD1	21:H:181:ASP:N	2.52	0.43
32:S:211:ARG:HH22	28:o:170:GLY:HA2	1.82	0.43
33:T:46:ASN:OD1	33:T:46:ASN:N	2.50	0.43
21:h:34:PRO:HA	21:h:164:GLY:HA3	2.00	0.43
30:q:117:TYR:HB3	30:q:125:ALA:HB3	2.01	0.43
33:t:9:THR:O	33:t:41:ARG:NH2	2.49	0.43
3:W:12:ARG:HH11	3:W:27:ARG:HB2	1.83	0.43
4:X:251:LEU:HA	4:X:254:MET:HG2	2.01	0.43
5:Y:177:ARG:NH1	5:Y:205:VAL:O	2.40	0.43
6:Z:16:LEU:HD23	6:Z:16:LEU:H	1.83	0.43
7:a:252:LYS:HD2	7:a:255:TRP:CD1	2.53	0.43
10:d:132:TYR:HE1	10:d:160:ALA:HB2	1.84	0.43
14:B:288:ASP:N	14:B:288:ASP:OD1	2.51	0.43
21:H:118:MET:HE2	21:H:151:PRO:HA	1.98	0.43
24:K:21:LEU:HA	24:K:22:PHE:HB2	2.00	0.43
22:i:149:GLN:OE1	22:i:162:THR:OG1	2.36	0.43
1:U:45:ILE:C	1:U:47:VAL:N	2.75	0.43
1:U:432:SER:HB3	1:U:435:SER:HB3	2.00	0.43
1:U:607:VAL:HG11	16:D:64:GLU:HA	2.00	0.43
3:W:79:GLU:HG3	3:W:97:LEU:HD11	2.00	0.43
12:f:370:MET:HE3	12:f:747:GLN:HE22	1.82	0.43
14:B:106:PRO:HB3	15:C:121:TYR:HB2	1.99	0.43
14:B:188:GLY:HA3	14:B:364:ILE:HG12	2.01	0.43
15:C:86:LEU:HD11	15:C:94:LYS:HD2	2.01	0.43
20:G:32:ILE:HA	20:G:82:GLY:HA2	1.99	0.43
33:T:4:PRO:HG3	33:T:107:TRP:CE2	2.53	0.43
32:s:211:ARG:NH2	32:s:213:ASP:OD2	2.42	0.43
3:W:201:ARG:HH22	16:D:391:ARG:HE	1.65	0.43
4:X:360:ASP:OD1	4:X:360:ASP:N	2.52	0.43
34:g:126:THR:O	21:h:128:ARG:NH1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:o:163:ILE:HA	28:o:168:GLY:HA3	1.99	0.43
29:p:2:SER:OG	29:p:3:ILE:N	2.51	0.43
5:Y:247:LEU:HD12	5:Y:250:LEU:HD11	2.01	0.43
9:c:29:GLU:HG3	9:c:65:TYR:HB2	2.00	0.43
17:E:235:ILE:O	17:E:239:GLY:N	2.50	0.43
17:E:306:GLU:HA	17:E:309:ARG:HD2	1.99	0.43
17:E:355:ILE:HD13	18:F:212:PHE:CE1	2.53	0.43
26:m:108:LEU:HD23	26:m:147:GLN:HB2	2.00	0.43
2:V:342:ILE:HD12	2:V:343:PRO:HD2	2.00	0.43
3:W:123:ARG:O	3:W:123:ARG:NH1	2.52	0.43
6:Z:140:SER:OG	6:Z:153:LYS:NZ	2.38	0.43
9:c:124:GLY:HA3	19:v:34:UNK:CB	2.49	0.43
12:f:168:LYS:HD3	12:f:204:ALA:HB1	2.00	0.43
13:A:284:ARG:HA	13:A:289:ALA:HB2	2.00	0.43
22:i:105:ILE:HD11	22:i:109:GLN:HG3	2.00	0.43
28:o:163:ILE:HG21	28:o:171:SER:HB2	2.01	0.43
33:t:4:PRO:HG3	33:t:107:TRP:CE2	2.53	0.43
1:U:890:LYS:HG3	1:U:891:VAL:HG13	2.00	0.43
2:V:18:PRO:HA	2:V:22:GLY:HA3	2.01	0.43
3:W:236:HIS:ND1	3:W:236:HIS:C	2.74	0.43
4:X:402:GLU:HB2	9:c:249:LEU:HD11	2.01	0.43
12:f:460:ASP:OD1	12:f:460:ASP:N	2.49	0.43
12:f:732:VAL:O	12:f:736:THR:OG1	2.36	0.43
13:A:329:PRO:HA	13:A:332:MET:HB2	2.01	0.43
14:B:286:GLU:HA	14:B:331:THR:HG22	2.01	0.43
16:D:248:ARG:HG2	16:D:295:GLN:NE2	2.33	0.43
18:F:299:GLU:HG3	18:F:300:LYS:H	1.84	0.43
18:F:376:SER:HB3	18:F:414:GLU:HB2	2.00	0.43
25:L:59:HIS:ND1	25:L:208:LYS:O	2.51	0.43
29:P:2:SER:OG	29:P:3:ILE:N	2.52	0.43
34:g:89:SER:OG	26:m:117:MET:SD	2.77	0.43
3:W:8:ARG:HB3	3:W:27:ARG:HD3	1.99	0.43
3:W:189:GLN:HA	3:W:192:LEU:HD12	2.01	0.43
4:X:182:ASN:HA	5:Y:244:ALA:HB1	2.01	0.43
6:Z:223:ASN:HB3	6:Z:226:ILE:HG22	2.00	0.43
6:Z:245:PHE:HD1	10:d:236:THR:HG23	1.84	0.43
12:f:253:LEU:HA	12:f:257:ARG:HD3	2.01	0.43
12:f:465:LEU:HB2	12:f:485:LEU:HD12	2.01	0.43
12:f:801:VAL:HB	12:f:804:LEU:HD11	2.01	0.43
13:A:153:LEU:HD22	14:B:132:TYR:CZ	2.54	0.43
17:E:165:ILE:HG22	17:E:167:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:J:76:LEU:HD12	23:J:79:ASP:H	1.83	0.43
24:k:228:MET:HE2	24:k:228:MET:HB2	1.92	0.43
1:U:82:LEU:HD21	1:U:130:LEU:HB3	2.00	0.42
2:V:168:GLN:HE22	2:V:175:MET:HE1	1.83	0.42
3:W:12:ARG:HA	3:W:12:ARG:HD3	1.86	0.42
8:b:161:ASN:HD21	8:b:168:SER:H	1.67	0.42
12:f:205:CYS:SG	12:f:213:GLN:NE2	2.78	0.42
12:f:294:MET:HE1	12:f:456:ARG:HG2	2.01	0.42
18:F:43:GLN:HA	18:F:46:ARG:HG3	2.01	0.42
2:V:36:GLU:HG3	2:V:76:LYS:HG2	2.01	0.42
9:c:176:GLN:HB3	9:c:177:THR:H	1.58	0.42
9:c:225:TRP:HE3	9:c:226:MET:HE3	1.84	0.42
13:A:114:ASN:OD1	13:A:114:ASN:N	2.52	0.42
17:E:75:ASN:ND2	18:F:129:ARG:O	2.52	0.42
20:G:46:ASP:OD1	20:G:46:ASP:N	2.51	0.42
21:H:79:MET:HE2	21:H:79:MET:HB3	1.93	0.42
21:H:79:MET:HG3	21:H:82:ASP:HB2	2.01	0.42
22:I:11:ILE:HD13	23:J:5:ARG:HA	2.01	0.42
1:U:358:ASP:OD1	1:U:358:ASP:N	2.50	0.42
3:W:227:TYR:HB2	3:W:250:ILE:HD11	2.02	0.42
5:Y:334:LEU:HB2	5:Y:347:ILE:HD12	2.01	0.42
6:Z:16:LEU:HD23	6:Z:17:LEU:H	1.85	0.42
6:Z:102:HIS:HD2	6:Z:104:ASN:HB3	1.83	0.42
9:c:185:ASN:ND2	9:c:186:LYS:O	2.51	0.42
9:c:231:LEU:HB3	9:c:233:ASP:HA	2.01	0.42
13:A:346:PRO:HB2	13:A:351:ARG:HG3	2.00	0.42
15:C:99:VAL:HG12	15:C:123:LEU:HD12	2.01	0.42
16:D:152:MET:O	16:D:228:ILE:HG12	2.19	0.42
24:k:169:ALA:O	24:k:174:SER:OG	2.34	0.42
1:U:100:ILE:HA	1:U:103:LYS:HE3	2.00	0.42
12:f:438:ASP:HA	12:f:477:MET:HE2	2.00	0.42
12:f:478:ARG:HG3	12:f:514:VAL:HG11	2.00	0.42
12:f:773:LYS:HA	12:f:774:GLY:HA3	1.77	0.42
15:C:326:LEU:HG	15:C:330:LYS:HE3	2.01	0.42
17:E:234:GLU:N	17:E:278:ALA:O	2.52	0.42
18:F:404:GLY:HA2	18:F:415:LEU:HD21	2.01	0.42
20:G:43:ARG:NH1	20:G:149:PRO:O	2.51	0.42
30:Q:117:TYR:HB3	30:Q:125:ALA:HB3	2.01	0.42
22:i:72:MET:HG2	22:i:138:GLY:HA3	2.02	0.42
22:i:119:GLN:HE21	22:i:123:GLN:HE22	1.66	0.42
29:p:12:MET:HG3	29:p:138:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:r:35:ILE:N	31:r:43:GLY:O	2.50	0.42
1:U:857:ASP:OD1	1:U:857:ASP:N	2.50	0.42
2:V:232:HIS:O	2:V:236:ARG:N	2.47	0.42
2:V:241:ARG:HH21	15:C:29:GLU:HG2	1.85	0.42
2:V:473:GLN:OE1	10:d:245:GLN:NE2	2.52	0.42
3:W:455:LEU:HA	3:W:456:GLN:HA	1.75	0.42
5:Y:70:LEU:HA	5:Y:73:MET:HB2	2.01	0.42
12:f:403:LYS:HG3	12:f:406:GLY:H	1.84	0.42
12:f:659:LEU:CG	12:f:671:ALA:CB	2.97	0.42
13:A:189:GLU:O	13:A:193:THR:OG1	2.26	0.42
13:A:429:TYR:O	13:A:431:THR:N	2.52	0.42
16:D:237:GLN:HE21	16:D:242:GLU:HG3	1.85	0.42
17:E:331:ILE:O	17:E:335:SER:N	2.44	0.42
18:F:141:ASP:OD2	18:F:144:LYS:NZ	2.41	0.42
31:r:9:ARG:NH2	31:r:146:ASP:OD1	2.42	0.42
1:U:456:ASP:O	1:U:460:TYR:N	2.45	0.42
3:W:190:MET:HB2	3:W:202:THR:HG23	2.01	0.42
7:a:254:ALA:HA	7:a:261:LEU:HD23	2.02	0.42
9:c:284:LEU:HD13	9:c:284:LEU:HA	1.92	0.42
14:B:388:ASP:N	14:B:388:ASP:OD1	2.52	0.42
16:D:255:LYS:HD3	16:D:302:ASN:HB3	2.01	0.42
26:M:37:ILE:HD11	26:M:193:VAL:HG13	2.01	0.42
28:O:163:ILE:HG21	28:O:171:SER:HB2	2.01	0.42
34:g:86:ASP:OD1	26:m:120:HIS:NE2	2.41	0.42
22:i:170:ALA:O	22:i:173:SER:OG	2.36	0.42
8:b:176:GLY:HA3	8:b:177:PRO:HD3	1.89	0.42
12:f:828:ARG:NE	12:f:843:SER:HG	2.18	0.42
13:A:157:ILE:HA	13:A:158:ASP:HA	1.67	0.42
14:B:133:VAL:HB	14:B:158:ALA:HA	2.02	0.42
14:B:223:ILE:HG13	14:B:347:ILE:HG21	2.01	0.42
17:E:152:PRO:HG3	17:E:159:PHE:HE2	1.85	0.42
20:G:23:TYR:HA	20:G:26:GLU:HG2	2.01	0.42
25:L:155:ASP:HB3	26:M:62:SER:HB2	2.02	0.42
26:M:230:ASP:N	26:M:230:ASP:OD1	2.49	0.42
33:T:179:ARG:HB3	27:n:29:ARG:HH21	1.84	0.42
26:m:37:ILE:HD11	26:m:193:VAL:HG13	2.01	0.42
29:p:107:PRO:HG2	29:p:124:LEU:HB2	2.02	0.42
1:U:738:ASP:OD1	1:U:742:HIS:NE2	2.53	0.42
3:W:93:ARG:NH2	3:W:135:LYS:HB2	2.35	0.42
12:f:403:LYS:O	12:f:407:MET:N	2.52	0.42
14:B:301:GLY:CA	19:v:20:UNK:CB	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:E:12:TYR:OH	18:F:28:GLY:O	2.38	0.42
32:S:16:ALA:HB2	32:S:121:VAL:HG23	2.02	0.42
21:h:9:SER:OG	21:h:123:GLN:O	2.27	0.42
24:k:203:LYS:HA	24:k:206:MET:HG2	2.02	0.42
7:a:235:ASP:OD2	7:a:249:GLN:NE2	2.49	0.42
8:b:2:VAL:O	8:b:44:ASN:ND2	2.48	0.42
9:c:161:ARG:HH11	9:c:162:LEU:H	1.68	0.42
12:f:84:SER:HA	12:f:115:PRO:HB3	2.02	0.42
12:f:330:PHE:HA	12:f:333:LEU:HB2	2.02	0.42
14:B:86:LYS:HB3	14:B:88:LEU:HD23	2.00	0.42
17:E:174:GLY:HA2	17:E:175:PRO:HD3	1.90	0.42
18:F:365:ILE:HG23	18:F:369:HIS:CE1	2.55	0.42
31:R:38:ASN:HD22	31:R:41:LEU:HD12	1.85	0.42
21:h:111:VAL:HG21	21:h:147:PHE:HD2	1.84	0.42
25:l:117:GLN:O	25:l:120:THR:OG1	2.31	0.42
28:o:190:THR:HG22	28:o:192:PRO:HD3	2.02	0.42
31:r:38:ASN:HD22	31:r:41:LEU:HD12	1.85	0.42
1:U:268:LEU:HD21	1:U:329:LEU:HD12	2.02	0.42
1:U:428:PRO:HA	1:U:439:GLU:HB2	2.02	0.42
3:W:179:LYS:HB3	3:W:179:LYS:NZ	2.33	0.42
10:d:192:THR:OG1	10:d:196:ARG:NH1	2.53	0.42
12:f:469:TYR:OH	12:f:478:ARG:NH1	2.52	0.42
15:C:13:GLU:O	15:C:17:GLY:N	2.52	0.42
24:k:37:ALA:HB2	24:k:50:VAL:HG23	2.02	0.42
1:U:237:VAL:HG13	1:U:242:LEU:HD21	2.02	0.41
12:f:228:LYS:HB3	12:f:231:LEU:HD13	2.02	0.41
13:A:243:SER:HB2	14:B:310:LEU:HD12	2.01	0.41
16:D:297:ASP:OD2	16:D:323:ARG:NH2	2.52	0.41
17:E:279:THR:HG23	17:E:282:PRO:HD3	2.01	0.41
3:W:12:ARG:NH1	3:W:23:THR:O	2.53	0.41
5:Y:179:ARG:HD3	5:Y:179:ARG:HA	1.80	0.41
12:f:102:HIS:CE1	12:f:106:LEU:HG	2.56	0.41
12:f:418:LEU:HD22	12:f:425:GLY:HA2	2.02	0.41
15:C:305:LEU:HA	15:C:310:ARG:HD2	2.02	0.41
16:D:414:HIS:HE1	20:G:26:GLU:HB2	1.85	0.41
1:U:28:ASN:HB3	1:U:63:VAL:HG12	2.01	0.41
5:Y:68:ASP:HA	5:Y:71:ASN:HB2	2.03	0.41
12:f:94:LYS:HE2	12:f:110:TYR:HB2	2.02	0.41
12:f:171:GLN:HE21	12:f:179:VAL:HG13	1.86	0.41
12:f:399:LEU:HD11	12:f:440:ILE:HG12	2.02	0.41
12:f:658:ALA:HA	12:f:662:MET:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:143:ASP:OD2	13:A:146:LYS:N	2.45	0.41
17:E:22:ILE:HG23	18:F:55:MET:HG3	2.02	0.41
26:M:42:LYS:HD3	26:M:183:GLU:HA	2.02	0.41
1:U:540:GLN:O	9:c:68:ARG:NH1	2.54	0.41
12:f:664:GLU:C	12:f:666:ILE:H	2.28	0.41
17:E:132:TYR:HE2	17:E:190:GLN:HG3	1.85	0.41
33:T:153:VAL:HG21	33:T:168:LEU:HD11	2.01	0.41
25:l:59:HIS:ND1	25:l:208:LYS:O	2.52	0.41
1:U:725:MET:HE1	9:c:182:GLY:H	1.85	0.41
3:W:417:ARG:HD3	3:W:417:ARG:HA	1.89	0.41
7:a:77:VAL:HA	7:a:80:ILE:HG22	2.03	0.41
7:a:220:PRO:HA	7:a:223:GLU:HG2	2.03	0.41
8:b:62:THR:HG21	8:b:71:ILE:HG13	2.02	0.41
12:f:171:GLN:HE21	12:f:179:VAL:HA	1.86	0.41
12:f:241:PRO:O	12:f:245:ASN:N	2.47	0.41
12:f:810:ILE:O	12:f:878:GLU:HB2	2.21	0.41
25:L:120:THR:O	26:M:129:ARG:NH1	2.32	0.41
29:P:34:MET:O	31:r:166:ARG:NH2	2.54	0.41
30:Q:19:ARG:HH21	30:Q:31:ASP:HB2	1.86	0.41
25:l:201:ALA:O	25:l:239:ARG:NH1	2.53	0.41
28:o:19:ARG:HB2	28:o:169:SER:HA	2.03	0.41
33:t:153:VAL:HG21	33:t:168:LEU:HD11	2.01	0.41
6:Z:116:CYS:O	6:Z:119:SER:OG	2.37	0.41
6:Z:265:LEU:O	6:Z:268:SER:OG	2.33	0.41
9:c:149:GLN:HB3	9:c:156:VAL:HG21	2.03	0.41
12:f:634:LYS:HA	12:f:637:LYS:HD2	2.03	0.41
20:G:141:ILE:HG22	20:G:151:VAL:HG22	2.02	0.41
22:I:105:ILE:HD11	22:I:109:GLN:HG3	2.02	0.41
31:R:191:ASN:HD21	29:p:203:ARG:HH12	1.69	0.41
31:r:37:ILE:HG23	31:r:60:ALA:HB2	2.02	0.41
1:U:35:TRP:HB3	1:U:70:HIS:CE1	2.56	0.41
1:U:360:VAL:HG13	1:U:365:CYS:HB3	2.02	0.41
1:U:794:ASP:OD1	1:U:794:ASP:N	2.53	0.41
3:W:179:LYS:HZ3	3:W:180:LYS:NZ	2.17	0.41
7:a:326:GLU:HA	7:a:329:LYS:HA	2.03	0.41
12:f:189:LYS:HG2	12:f:190:GLU:HG2	2.02	0.41
12:f:556:ARG:NH1	12:f:784:ASP:O	2.54	0.41
12:f:609:VAL:HG12	14:B:74:MET:HE1	2.02	0.41
17:E:248:SER:HB2	19:v:15:UNK:HA	2.03	0.41
22:I:71:ASP:OD1	22:I:71:ASP:N	2.54	0.41
29:P:12:MET:HG3	29:P:138:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:i:165:GLY:O	22:i:169:ALA:N	2.53	0.41
32:s:16:ALA:HB2	32:s:121:VAL:HG23	2.02	0.41
2:V:166:TYR:HA	2:V:168:GLN:HE21	1.85	0.41
2:V:467:TYR:OH	4:X:397:TYR:OH	2.31	0.41
3:W:436:MET:HE2	6:Z:237:LEU:HB3	2.03	0.41
4:X:57:LEU:HD13	4:X:66:LEU:HA	2.01	0.41
7:a:342:ASP:O	7:a:344:GLN:N	2.54	0.41
12:f:265:ALA:HB3	12:f:268:LEU:HB2	2.02	0.41
15:C:77:VAL:HA	15:C:111:ASN:H	1.86	0.41
18:F:252:ALA:HA	18:F:286:ASP:HB3	2.02	0.41
20:G:161:CYS:SG	20:G:162:GLY:N	2.94	0.41
27:N:166:ARG:NH1	33:t:34:ALA:O	2.45	0.41
33:T:22:ILE:HD12	33:T:50:MET:HE3	2.03	0.41
23:j:9:VAL:HA	24:k:23:GLN:HE22	1.86	0.41
24:k:60:GLU:OE1	24:k:63:SER:N	2.54	0.41
1:U:802:TYR:HB3	1:U:895:PRO:HD3	2.03	0.41
2:V:38:LYS:HA	2:V:41:ALA:HB3	2.03	0.41
4:X:53:LEU:HD23	4:X:56:LEU:HD12	2.02	0.41
5:Y:221:THR:HA	5:Y:224:VAL:HG12	2.03	0.41
6:Z:198:LEU:HD22	7:a:364:GLU:HB2	2.02	0.41
8:b:52:ILE:HD11	8:b:58:CYS:HB3	2.02	0.41
8:b:174:PRO:HA	8:b:175:PRO:HD2	1.96	0.41
10:d:200:PHE:HB3	10:d:203:PRO:HB3	2.03	0.41
12:f:106:LEU:HB2	12:f:141:LYS:HD2	2.03	0.41
12:f:404:ASP:OD1	12:f:404:ASP:N	2.54	0.41
12:f:524:MET:HA	12:f:776:LEU:HD23	2.03	0.41
12:f:830:LEU:HB2	12:f:859:PRO:C	2.46	0.41
13:A:265:ARG:HA	13:A:315:ILE:HD13	2.02	0.41
13:A:331:LEU:HD23	13:A:336:ARG:HD3	2.02	0.41
15:C:148:TYR:HB2	15:C:206:HIS:CD2	2.56	0.41
15:C:229:ARG:NH1	15:C:233:GLU:OE1	2.52	0.41
17:E:12:TYR:HA	17:E:15:LYS:HB2	2.02	0.41
18:F:245:LYS:H	18:F:245:LYS:HD2	1.86	0.41
18:F:335:VAL:HA	18:F:338:LEU:HD12	2.03	0.41
18:F:343:LEU:HD13	18:F:348:LEU:HB2	2.03	0.41
23:J:51:ALA:H	23:J:54:GLN:NE2	2.16	0.41
23:J:88:ARG:NH1	30:Q:69:MET:O	2.53	0.41
25:L:72:ILE:HG22	25:L:134:ILE:HG12	2.03	0.41
25:L:201:ALA:O	25:L:239:ARG:NH1	2.53	0.41
27:N:35:THR:OG1	27:N:45:ARG:NH2	2.54	0.41
28:O:19:ARG:HB2	28:O:169:SER:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:O:190:THR:HG22	28:O:192:PRO:HD3	2.02	0.41
29:P:107:PRO:HG2	29:P:124:LEU:HB2	2.02	0.41
31:R:37:ILE:HG23	31:R:60:ALA:HB2	2.02	0.41
32:S:211:ARG:NH2	28:o:170:GLY:HA2	2.36	0.41
23:j:11:SER:OG	23:j:15:HIS:N	2.54	0.41
24:k:227:HIS:NE2	24:k:229:PHE:O	2.53	0.41
27:n:35:THR:OG1	27:n:45:ARG:NH2	2.54	0.41
28:o:38:SER:OG	28:o:40:ASN:OD1	2.31	0.41
32:s:55:SER:OG	32:s:56:GLY:N	2.54	0.41
3:W:142:ARG:NE	3:W:181:GLU:HG2	2.36	0.41
4:X:407:MET:HA	4:X:410:VAL:HG22	2.02	0.41
7:a:261:LEU:HD12	7:a:261:LEU:HA	1.87	0.41
12:f:662:MET:HE2	13:A:65:ILE:CG2	2.30	0.41
14:B:67:ARG:NH2	14:B:71:TYR:OH	2.51	0.41
16:D:202:VAL:HA	16:D:329:ARG:HB2	2.02	0.41
21:H:111:VAL:HG21	21:H:147:PHE:HD2	1.86	0.41
23:J:31:THR:HA	23:J:162:GLY:HA3	2.02	0.41
33:T:54:SER:OG	33:T:55:GLY:N	2.54	0.41
26:m:42:LYS:HD3	26:m:183:GLU:HA	2.02	0.41
2:V:345:ARG:HH11	2:V:346:LEU:HB3	1.86	0.40
3:W:224:LEU:O	3:W:228:ASN:ND2	2.54	0.40
5:Y:290:PRO:HB3	11:e:40:GLU:HB3	2.03	0.40
6:Z:176:LEU:HB3	6:Z:180:LYS:HG2	2.03	0.40
7:a:66:GLU:HG2	18:F:42:ILE:HG13	2.01	0.40
8:b:33:VAL:HG11	8:b:75:LEU:HD21	2.03	0.40
8:b:153:LEU:HB3	8:b:170:LEU:HD21	2.03	0.40
9:c:57:MET:HG2	9:c:69:VAL:HG21	2.03	0.40
9:c:244:VAL:HB	9:c:291:LEU:HD21	2.03	0.40
12:f:94:LYS:NZ	12:f:133:MET:SD	2.93	0.40
12:f:729:MET:HA	12:f:732:VAL:HG12	2.02	0.40
13:A:238:ILE:O	13:A:273:PHE:N	2.47	0.40
13:A:284:ARG:NH2	18:F:257:VAL:O	2.54	0.40
14:B:107:MET:O	15:C:96:VAL:N	2.51	0.40
18:F:364:ARG:HA	18:F:367:GLN:HG2	2.03	0.40
23:J:156:TRP:CD1	24:K:59:MET:HA	2.56	0.40
31:R:9:ARG:NH2	31:R:146:ASP:OD1	2.42	0.40
33:T:126:ASP:OD1	33:T:127:MET:N	2.54	0.40
21:h:3:GLU:HG3	21:h:5:GLY:H	1.86	0.40
2:V:479:ARG:HH21	5:Y:374:ASP:CG	2.29	0.40
10:d:45:LYS:HA	10:d:48:LEU:HD12	2.02	0.40
10:d:199:PHE:HD1	10:d:199:PHE:HA	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:830:LEU:H	12:f:859:PRO:HB2	1.87	0.40
13:A:277:ILE:HG22	13:A:280:ILE:HD11	2.04	0.40
13:A:292:ASP:HB3	18:F:259:MET:HG3	2.02	0.40
17:E:195:PHE:HD1	17:E:229:ILE:HB	1.86	0.40
20:G:132:ARG:HA	20:G:133:PRO:HD3	1.81	0.40
22:I:216:LEU:HD12	22:I:225:ILE:HG12	2.02	0.40
21:h:11:THR:HG22	21:h:19:LEU:HD22	2.03	0.40
23:j:221:ASN:HA	23:j:222:PRO:HD3	1.96	0.40
24:k:117:SER:HB2	25:l:82:ARG:HH12	1.85	0.40
32:s:209:SER:OG	32:s:212:LYS:NZ	2.55	0.40
2:V:338:LEU:HD21	2:V:397:ARG:HG3	2.01	0.40
3:W:2:ALA:HB2	3:W:43:VAL:HA	2.04	0.40
4:X:143:TYR:CZ	5:Y:252:SER:HB2	2.57	0.40
5:Y:157:ILE:H	5:Y:157:ILE:HG13	1.72	0.40
12:f:417:ILE:HG22	12:f:418:LEU:HD12	2.02	0.40
12:f:531:ASN:HD22	12:f:534:VAL:HB	1.86	0.40
15:C:230:MET:O	15:C:234:LEU:N	2.55	0.40
15:C:301:LEU:HG	15:C:306:LEU:HD11	2.02	0.40
17:E:164:ILE:HD12	17:E:164:ILE:HA	1.97	0.40
20:G:189:TRP:HA	20:G:193:GLN:HB3	2.02	0.40
23:J:105:GLU:HA	23:J:145:TYR:HE2	1.86	0.40
31:R:35:ILE:N	31:R:43:GLY:O	2.50	0.40
24:k:85:ALA:HB2	24:k:139:VAL:HG21	2.04	0.40
26:m:76:ALA:HB3	26:m:136:MET:HB2	2.03	0.40
1:U:399:TRP:CD1	9:c:176:GLN:HG2	2.56	0.40
1:U:824:GLU:HB3	1:U:826:GLU:HB2	2.03	0.40
2:V:194:LYS:HE2	2:V:241:ARG:HH12	1.87	0.40
7:a:321:LYS:O	7:a:334:THR:OG1	2.39	0.40
12:f:764:LEU:HB3	12:f:771:LEU:HD12	2.04	0.40
18:F:74:LYS:HE2	18:F:74:LYS:HB3	1.95	0.40
18:F:375:VAL:HG22	18:F:415:LEU:HD12	2.03	0.40
26:M:23:VAL:HG12	26:M:27:MET:HE3	2.04	0.40
32:S:209:SER:OG	32:S:212:LYS:NZ	2.55	0.40
23:j:88:ARG:NH1	30:q:69:MET:O	2.54	0.40
30:q:19:ARG:HH21	30:q:31:ASP:HB2	1.86	0.40
33:t:126:ASP:OD1	33:t:127:MET:N	2.54	0.40
1:U:475:HIS:CE1	1:U:507:VAL:HG22	2.57	0.40
2:V:107:ARG:HA	2:V:110:HIS:HD1	1.86	0.40
3:W:287:VAL:HA	3:W:290:ILE:HG12	2.03	0.40
5:Y:12:PRO:HB3	5:Y:113:ARG:HB2	2.04	0.40
5:Y:92:GLU:OE2	5:Y:94:ASN:ND2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:283:LYS:HD3	5:Y:288:PHE:CZ	2.57	0.40
14:B:250:VAL:HG21	14:B:270:LEU:HD21	2.04	0.40
16:D:89:ILE:HB	17:E:78:ARG:HB2	2.03	0.40
17:E:147:GLU:HA	17:E:151:LEU:HD12	2.03	0.40
18:F:288:LEU:O	18:F:292:GLY:N	2.54	0.40
18:F:367:GLN:HB3	18:F:381:TYR:CE1	2.56	0.40
27:N:40:ARG:NH2	27:N:181:GLU:O	2.55	0.40
27:N:140:ASP:OD1	27:N:140:ASP:N	2.53	0.40
24:k:154:PHE:HB3	24:k:162:PHE:HE1	1.86	0.40
31:r:115:ASP:HB3	31:r:117:GLU:H	1.86	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	U	868/953 (91%)	785 (90%)	79 (9%)	4 (0%)	24	55
2	V	478/533 (90%)	420 (88%)	58 (12%)	0	100	100
3	W	454/456 (100%)	411 (90%)	36 (8%)	7 (2%)	8	32
4	X	378/422 (90%)	355 (94%)	22 (6%)	1 (0%)	36	65
5	Y	376/389 (97%)	340 (90%)	35 (9%)	1 (0%)	36	65
6	Z	284/324 (88%)	242 (85%)	39 (14%)	3 (1%)	11	39
7	a	371/376 (99%)	332 (90%)	36 (10%)	3 (1%)	16	45
8	b	189/377 (50%)	164 (87%)	22 (12%)	3 (2%)	7	31
9	c	285/309 (92%)	241 (85%)	41 (14%)	3 (1%)	11	39
10	d	255/349 (73%)	215 (84%)	39 (15%)	1 (0%)	30	60
11	e	36/70 (51%)	25 (69%)	11 (31%)	0	100	100
12	f	887/892 (99%)	715 (81%)	158 (18%)	14 (2%)	7	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	A	411/433 (95%)	361 (88%)	48 (12%)	2 (0%)	24	55
14	B	409/440 (93%)	343 (84%)	65 (16%)	1 (0%)	43	71
15	C	394/398 (99%)	340 (86%)	49 (12%)	5 (1%)	9	35
16	D	378/418 (90%)	323 (85%)	49 (13%)	6 (2%)	7	31
17	E	387/403 (96%)	341 (88%)	46 (12%)	0	100	100
18	F	391/439 (89%)	347 (89%)	42 (11%)	2 (0%)	24	55
20	G	237/245 (97%)	214 (90%)	22 (9%)	1 (0%)	30	60
21	H	228/233 (98%)	222 (97%)	6 (3%)	0	100	100
21	h	230/233 (99%)	223 (97%)	7 (3%)	0	100	100
22	I	246/260 (95%)	228 (93%)	18 (7%)	0	100	100
22	i	248/260 (95%)	223 (90%)	25 (10%)	0	100	100
23	J	237/247 (96%)	214 (90%)	23 (10%)	0	100	100
23	j	237/247 (96%)	217 (92%)	20 (8%)	0	100	100
24	K	224/240 (93%)	202 (90%)	21 (9%)	1 (0%)	30	60
24	k	224/240 (93%)	204 (91%)	20 (9%)	0	100	100
25	L	236/268 (88%)	225 (95%)	11 (5%)	0	100	100
25	l	236/268 (88%)	225 (95%)	11 (5%)	0	100	100
26	M	238/254 (94%)	219 (92%)	19 (8%)	0	100	100
26	m	238/254 (94%)	219 (92%)	19 (8%)	0	100	100
27	N	189/238 (79%)	180 (95%)	9 (5%)	0	100	100
27	n	189/238 (79%)	180 (95%)	9 (5%)	0	100	100
28	O	218/276 (79%)	202 (93%)	16 (7%)	0	100	100
28	o	218/276 (79%)	202 (93%)	16 (7%)	0	100	100
29	P	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
29	p	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
30	Q	197/201 (98%)	186 (94%)	11 (6%)	0	100	100
30	q	197/201 (98%)	186 (94%)	11 (6%)	0	100	100
31	R	199/262 (76%)	190 (96%)	9 (4%)	0	100	100
31	r	199/262 (76%)	190 (96%)	9 (4%)	0	100	100
32	S	211/240 (88%)	201 (95%)	10 (5%)	0	100	100
32	s	211/240 (88%)	201 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	T	213/263 (81%)	204 (96%)	9 (4%)	0	100	100
33	t	213/263 (81%)	204 (96%)	9 (4%)	0	100	100
34	g	238/240 (99%)	221 (93%)	17 (7%)	0	100	100
All	All	13386/14838 (90%)	12070 (90%)	1258 (9%)	58 (0%)	31	60

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	874	ASN
7	a	343	LEU
8	b	178	SER
9	c	285	GLU
12	f	665	GLU
12	f	808	ASN
12	f	853	VAL
13	A	430	MET
16	D	335	LEU
1	U	48	LEU
3	W	88	MET
3	W	178	GLU
3	W	180	LYS
3	W	239	SER
5	Y	350	VAL
12	f	118	ASN
12	f	657	ILE
12	f	876	HIS
16	D	146	GLU
3	W	238	GLY
7	a	69	HIS
7	a	342	ASP
9	c	233	ASP
9	c	284	LEU
12	f	476	THR
12	f	659	LEU
12	f	823	ALA
14	B	356	PRO
16	D	149	SER
18	F	228	PRO
24	K	9	ASP
1	U	820	PRO
1	U	873	PRO

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Mol	Chain	Res	Type
4	X	317	PRO
10	d	199	PHE
15	C	90	HIS
15	C	253	SER
3	W	179	LYS
6	Z	65	ASP
12	f	475	ASN
12	f	662	MET
12	f	809	ILE
15	C	221	GLN
16	D	126	PRO
16	D	336	PRO
12	f	859	PRO
13	A	109	PRO
16	D	151	ILE
6	Z	134	PRO
12	f	755	ASP
15	C	91	PRO
18	F	229	PRO
20	G	212	PRO
15	C	89	VAL
6	Z	144	VAL
8	b	177	PRO
3	W	87	ILE
8	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	U	748/816 (92%)	743 (99%)	5 (1%)	76	80
2	V	414/459 (90%)	413 (100%)	1 (0%)	87	88
3	W	416/416 (100%)	405 (97%)	11 (3%)	40	64
4	X	327/362 (90%)	326 (100%)	1 (0%)	86	86
5	Y	334/344 (97%)	330 (99%)	4 (1%)	63	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Z	257/295 (87%)	249 (97%)	8 (3%)	35	60
7	a	333/336 (99%)	332 (100%)	1 (0%)	86	86
8	b	167/312 (54%)	167 (100%)	0	100	100
9	c	252/267 (94%)	250 (99%)	2 (1%)	73	79
10	d	231/293 (79%)	230 (100%)	1 (0%)	84	84
11	e	38/63 (60%)	38 (100%)	0	100	100
12	f	745/748 (100%)	737 (99%)	8 (1%)	65	76
13	A	348/372 (94%)	347 (100%)	1 (0%)	86	86
14	B	357/385 (93%)	351 (98%)	6 (2%)	53	71
15	C	340/346 (98%)	336 (99%)	4 (1%)	63	75
16	D	333/366 (91%)	324 (97%)	9 (3%)	39	63
17	E	341/353 (97%)	336 (98%)	5 (2%)	57	72
18	F	340/379 (90%)	338 (99%)	2 (1%)	78	81
20	G	196/209 (94%)	195 (100%)	1 (0%)	81	83
21	H	172/190 (90%)	172 (100%)	0	100	100
21	h	164/190 (86%)	163 (99%)	1 (1%)	78	81
22	I	195/220 (89%)	194 (100%)	1 (0%)	81	83
22	i	193/220 (88%)	193 (100%)	0	100	100
23	J	161/210 (77%)	161 (100%)	0	100	100
23	j	152/210 (72%)	152 (100%)	0	100	100
24	K	187/202 (93%)	186 (100%)	1 (0%)	81	83
24	k	186/202 (92%)	183 (98%)	3 (2%)	55	72
25	L	198/229 (86%)	196 (99%)	2 (1%)	68	76
25	l	198/229 (86%)	196 (99%)	2 (1%)	68	76
26	M	192/211 (91%)	192 (100%)	0	100	100
26	m	192/211 (91%)	192 (100%)	0	100	100
27	N	148/180 (82%)	148 (100%)	0	100	100
27	n	148/180 (82%)	148 (100%)	0	100	100
28	O	177/227 (78%)	177 (100%)	0	100	100
28	o	177/227 (78%)	177 (100%)	0	100	100
29	P	172/173 (99%)	172 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	p	172/173 (99%)	172 (100%)	0	100	100
30	Q	164/171 (96%)	164 (100%)	0	100	100
30	q	164/171 (96%)	164 (100%)	0	100	100
31	R	153/201 (76%)	153 (100%)	0	100	100
31	r	153/201 (76%)	153 (100%)	0	100	100
32	S	174/198 (88%)	174 (100%)	0	100	100
32	s	174/198 (88%)	174 (100%)	0	100	100
33	T	175/214 (82%)	175 (100%)	0	100	100
33	t	175/214 (82%)	175 (100%)	0	100	100
34	g	193/205 (94%)	192 (100%)	1 (0%)	81	83
All	All	11226/12578 (89%)	11145 (99%)	81 (1%)	73	80

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	46	GLU
1	U	118	LEU
1	U	603	LEU
1	U	629	THR
1	U	819	VAL
2	V	362	LEU
3	W	82	LEU
3	W	128	LEU
3	W	131	VAL
3	W	174	TYR
3	W	177	MET
3	W	179	LYS
3	W	236	HIS
3	W	237	GLU
3	W	268	LYS
3	W	275	ILE
3	W	308	LEU
4	X	393	VAL
5	Y	81	LEU
5	Y	202	LEU
5	Y	287	LEU
5	Y	330	ILE
6	Z	15	VAL

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Mol	Chain	Res	Type
6	Z	51	SER
6	Z	91	ILE
6	Z	126	VAL
6	Z	217	THR
6	Z	236	LEU
6	Z	237	LEU
6	Z	266	ILE
7	a	112	ILE
9	c	49	VAL
9	c	284	LEU
10	d	178	ILE
12	f	75	LEU
12	f	344	VAL
12	f	615	ILE
12	f	657	ILE
12	f	662	MET
12	f	664	GLU
12	f	672	LEU
12	f	822	VAL
13	A	403	ILE
14	B	35	LYS
14	B	125	THR
14	B	183	THR
14	B	190	LEU
14	B	287	ILE
14	B	292	THR
15	C	91	PRO
15	C	134	LEU
15	C	210	THR
15	C	219	LEU
16	D	68	LEU
16	D	115	ILE
16	D	148	ASP
16	D	151	ILE
16	D	152	MET
16	D	153	MET
16	D	236	VAL
16	D	270	ILE
16	D	360	LEU
17	E	87	LEU
17	E	105	LEU
17	E	138	LEU

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Mol	Chain	Res	Type
17	E	262	ASN
17	E	284	THR
18	F	293	THR
18	F	416	THR
20	G	141	ILE
22	I	137	ILE
24	K	33	LEU
25	L	22	ILE
25	L	118	ILE
34	g	141	ILE
21	h	69	THR
24	k	119	LEU
24	k	139	VAL
24	k	170	ILE
25	l	22	ILE
25	l	118	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (193) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	18	GLN
1	U	79	ASN
1	U	89	ASN
1	U	115	ASN
1	U	145	HIS
1	U	189	GLN
1	U	192	GLN
1	U	207	ASN
1	U	218	GLN
1	U	247	GLN
1	U	366	HIS
1	U	421	GLN
1	U	438	GLN
1	U	491	GLN
1	U	541	HIS
1	U	596	ASN
1	U	632	GLN
1	U	665	ASN
1	U	743	ASN
1	U	768	GLN
1	U	805	ASN
1	U	888	GLN

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Mol	Chain	Res	Type
2	V	62	HIS
2	V	168	GLN
2	V	214	HIS
2	V	473	GLN
3	W	84	ASN
3	W	228	ASN
3	W	257	GLN
3	W	362	ASN
4	X	62	GLN
4	X	198	ASN
4	X	292	GLN
4	X	296	ASN
4	X	329	ASN
5	Y	48	ASN
5	Y	71	ASN
5	Y	77	ASN
5	Y	136	HIS
5	Y	178	ASN
5	Y	291	HIS
6	Z	12	HIS
6	Z	77	ASN
6	Z	96	HIS
6	Z	189	GLN
6	Z	193	ASN
6	Z	229	GLN
7	a	9	GLN
7	a	86	GLN
7	a	143	ASN
7	a	152	HIS
7	a	169	HIS
7	a	227	ASN
7	a	288	HIS
7	a	332	HIS
7	a	370	GLN
8	b	76	HIS
8	b	137	ASN
8	b	161	ASN
9	c	92	GLN
9	c	128	ASN
9	c	130	GLN
9	c	149	GLN
9	c	185	ASN

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Mol	Chain	Res	Type
9	c	254	ASN
9	c	256	ASN
9	c	274	ASN
10	d	116	HIS
10	d	245	GLN
12	f	14	GLN
12	f	43	GLN
12	f	112	ASN
12	f	118	ASN
12	f	213	GLN
12	f	291	GLN
12	f	327	ASN
12	f	378	ASN
12	f	382	ASN
12	f	396	ASN
12	f	457	ASN
12	f	531	ASN
12	f	565	ASN
12	f	737	ASN
12	f	747	GLN
12	f	752	HIS
12	f	757	ASN
12	f	766	GLN
12	f	782	HIS
12	f	786	GLN
12	f	815	HIS
13	A	54	GLN
13	A	60	ASN
13	A	197	HIS
13	A	247	GLN
13	A	305	GLN
13	A	314	ASN
13	A	379	ASN
14	B	57	GLN
14	B	195	GLN
14	B	207	HIS
14	B	241	ASN
14	B	368	HIS
15	C	36	ASN
15	C	53	ASN
15	C	64	GLN
15	C	67	GLN

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Mol	Chain	Res	Type
15	C	90	HIS
15	C	171	HIS
15	C	205	HIS
15	C	221	GLN
15	C	278	ASN
15	C	380	GLN
16	D	65	GLN
16	D	67	ASN
16	D	135	HIS
16	D	173	GLN
16	D	187	HIS
16	D	237	GLN
16	D	257	ASN
16	D	295	GLN
16	D	301	GLN
16	D	304	ASN
16	D	412	GLN
16	D	414	HIS
17	E	39	GLN
17	E	225	HIS
17	E	226	GLN
17	E	262	ASN
17	E	271	HIS
17	E	300	HIS
17	E	339	ASN
17	E	364	GLN
18	F	207	ASN
18	F	208	HIS
18	F	333	ASN
20	G	75	ASN
20	G	123	GLN
20	G	193	GLN
21	H	71	HIS
21	H	102	GLN
21	H	109	GLN
21	H	166	ASN
22	I	123	GLN
22	I	146	GLN
22	I	149	GLN
22	I	166	ASN
22	I	167	ASN
23	J	92	GLN

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Mol	Chain	Res	Type
24	K	41	GLN
24	K	97	GLN
24	K	155	HIS
25	L	20	HIS
28	O	62	ASN
28	O	116	HIS
28	O	172	ASN
29	P	18	ASN
29	P	169	GLN
31	R	10	HIS
31	R	38	ASN
32	S	58	HIS
32	S	79	ASN
32	S	146	GLN
32	S	159	GLN
33	T	69	GLN
34	g	12	HIS
34	g	68	HIS
34	g	127	GLN
21	h	102	GLN
21	h	189	HIS
22	i	119	GLN
22	i	146	GLN
22	i	167	ASN
23	j	92	GLN
23	j	116	GLN
24	k	23	GLN
24	k	41	GLN
24	k	114	GLN
24	k	155	HIS
24	k	214	ASN
25	l	20	HIS
25	l	146	GLN
25	l	152	ASN
26	m	180	GLN
28	o	62	ASN
28	o	116	HIS
28	o	172	ASN
29	p	18	ASN
31	r	10	HIS
31	r	38	ASN
32	s	79	ASN

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Mol	Chain	Res	Type
32	s	146	GLN
32	s	159	GLN
33	t	69	GLN

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	ATP	B	441	37	32,33,33	1.29	5 (15%)	48,52,52	1.81	9 (18%)
38	ADP	E	419	-	28,29,29	1.44	6 (21%)	43,45,45	1.90	8 (18%)
36	ATP	C	407	37	32,33,33	1.25	5 (15%)	48,52,52	1.88	12 (25%)
36	ATP	D	440	37	32,33,33	1.30	5 (15%)	48,52,52	1.76	8 (16%)
36	ATP	A	434	37	32,33,33	1.28	3 (9%)	48,52,52	1.96	11 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ATP	B	441	37	-	3/22/38/38	0/3/3/3
38	ADP	E	419	-	-	0/16/32/32	0/3/3/3
36	ATP	C	407	37	-	0/22/38/38	0/3/3/3
36	ATP	D	440	37	-	1/22/38/38	0/3/3/3
36	ATP	A	434	37	-	0/22/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A	434	ATP	C5-C4	4.50	1.47	1.39
36	D	440	ATP	C5-C4	4.42	1.47	1.39
38	E	419	ADP	C5-C4	4.38	1.46	1.39
36	B	441	ATP	C5-C4	4.23	1.46	1.39
36	C	407	ATP	C5-C4	4.19	1.46	1.39
38	E	419	ADP	C5-N7	-3.15	1.33	1.39
36	D	440	ATP	C5-N7	-2.78	1.34	1.39
36	C	407	ATP	C5-N7	-2.74	1.34	1.39
36	B	441	ATP	C5-N7	-2.69	1.34	1.39
36	A	434	ATP	C5-N7	-2.66	1.34	1.39
36	D	440	ATP	C5-C6	2.45	1.47	1.41
36	A	434	ATP	C5-C6	2.43	1.47	1.41
38	E	419	ADP	C8-N9	-2.36	1.33	1.37
36	B	441	ATP	C5-C6	2.35	1.47	1.41
38	E	419	ADP	C5-C6	2.31	1.47	1.41
36	C	407	ATP	C4-N9	-2.20	1.33	1.37
36	C	407	ATP	C5-C6	2.14	1.46	1.41
36	D	440	ATP	C4-N9	-2.13	1.33	1.37
36	D	440	ATP	C8-N7	2.08	1.35	1.31
38	E	419	ADP	C4-N9	-2.07	1.33	1.37
36	B	441	ATP	C8-N9	-2.06	1.34	1.37
36	B	441	ATP	C4-N9	-2.03	1.33	1.37
38	E	419	ADP	C8-N7	2.01	1.35	1.31
36	C	407	ATP	C8-N9	-2.00	1.34	1.37

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A	434	ATP	C5-C4-N3	-6.67	117.54	126.72
38	E	419	ADP	C5-C4-N3	-6.31	118.02	126.72
36	B	441	ATP	C5-C4-N3	-6.17	118.22	126.72
36	D	440	ATP	C5-C4-N3	-6.02	118.43	126.72
36	C	407	ATP	C5-C4-N3	-5.84	118.67	126.72
36	A	434	ATP	N3-C4-N9	5.65	136.78	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	B	441	ATP	N3-C4-N9	5.08	135.80	127.17
36	C	407	ATP	N3-C4-N9	5.06	135.77	127.17
38	E	419	ADP	N3-C4-N9	4.94	135.57	127.17
36	D	440	ATP	N3-C4-N9	4.74	135.24	127.17
36	A	434	ATP	C2-N3-C4	3.98	121.56	111.83
36	B	441	ATP	C2-N3-C4	3.73	120.95	111.83
36	D	440	ATP	C2-N3-C4	3.72	120.91	111.83
36	C	407	ATP	C2-N3-C4	3.68	120.83	111.83
38	E	419	ADP	C2-N3-C4	3.66	120.76	111.83
38	E	419	ADP	C4-C5-N7	-3.63	106.44	110.58
36	C	407	ATP	N3-C2-N1	-3.52	123.26	128.58
36	D	440	ATP	C4-C5-N7	-3.25	106.86	110.58
36	B	441	ATP	C4-C5-N7	-3.24	106.88	110.58
36	A	434	ATP	N3-C2-N1	-3.19	123.75	128.58
36	C	407	ATP	C4-N9-C8	3.18	109.08	105.74
36	D	440	ATP	N3-C2-N1	-3.14	123.83	128.58
36	B	441	ATP	N3-C2-N1	-3.07	123.94	128.58
36	C	407	ATP	C3'-C2'-C1'	2.89	106.94	101.46
36	C	407	ATP	C4-C5-N7	-2.89	107.28	110.58
36	D	440	ATP	C3'-C2'-C1'	2.88	106.90	101.46
38	E	419	ADP	N3-C2-N1	-2.87	124.24	128.58
36	A	434	ATP	C4-C5-N7	-2.87	107.30	110.58
36	B	441	ATP	C4-N9-C8	2.80	108.68	105.74
36	A	434	ATP	C3'-C2'-C1'	2.74	106.64	101.46
36	B	441	ATP	C3'-C2'-C1'	2.68	106.53	101.46
36	A	434	ATP	C1'-N9-C8	-2.63	121.26	127.09
38	E	419	ADP	C5-N7-C8	2.62	107.56	103.45
36	C	407	ATP	O3A-PB-O1B	-2.60	102.89	110.70
38	E	419	ADP	C3'-C2'-C1'	2.50	106.20	101.46
36	B	441	ATP	C5-N7-C8	2.45	107.30	103.45
36	A	434	ATP	C4-N9-C8	2.39	108.25	105.74
36	C	407	ATP	C5-N7-C8	2.32	107.09	103.45
38	E	419	ADP	C4-N9-C8	2.30	108.15	105.74
36	D	440	ATP	C4-N9-C8	2.29	108.14	105.74
36	D	440	ATP	C5-N7-C8	2.28	107.03	103.45
36	A	434	ATP	O4'-C1'-N9	-2.27	103.73	108.09
36	A	434	ATP	C5-N7-C8	2.27	107.02	103.45
36	C	407	ATP	O2B-PB-O1B	2.17	122.53	112.44
36	C	407	ATP	C2-N1-C6	2.11	122.20	118.73
36	C	407	ATP	N9-C8-N7	-2.08	110.99	113.94
36	A	434	ATP	O3G-PG-O2G	2.04	115.47	107.80
36	B	441	ATP	C2'-C1'-N9	-2.01	108.32	113.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

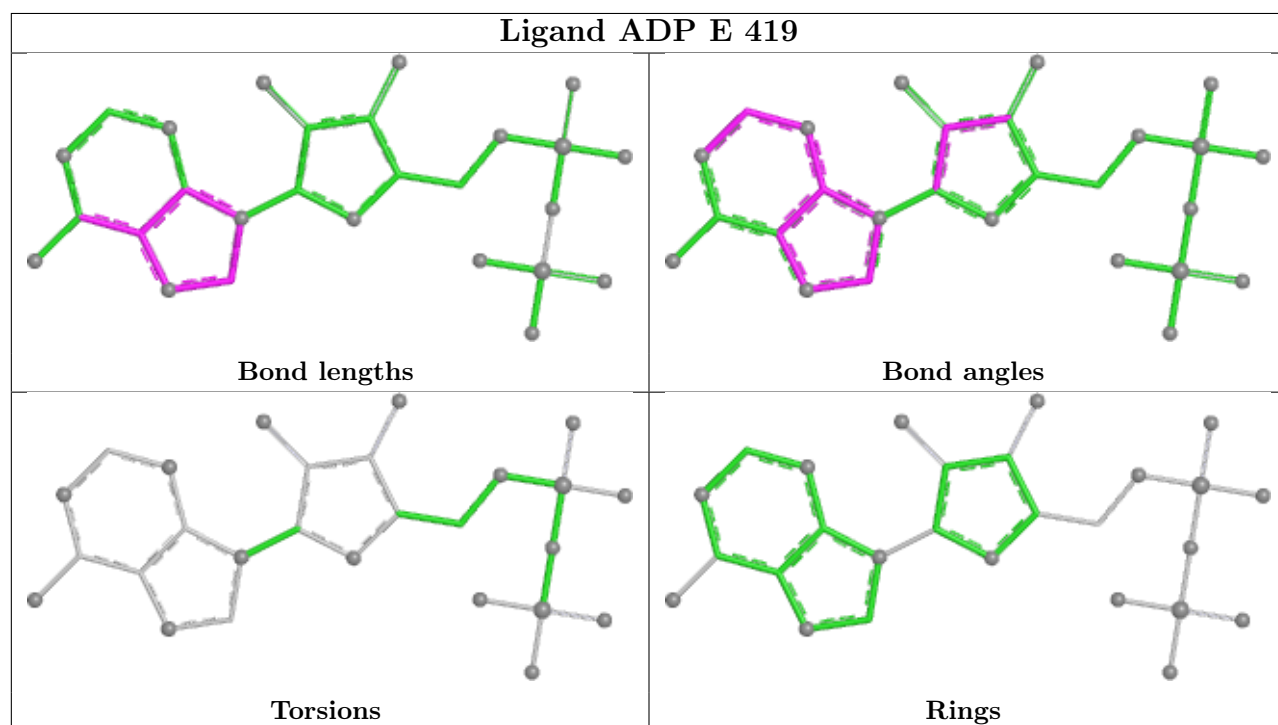
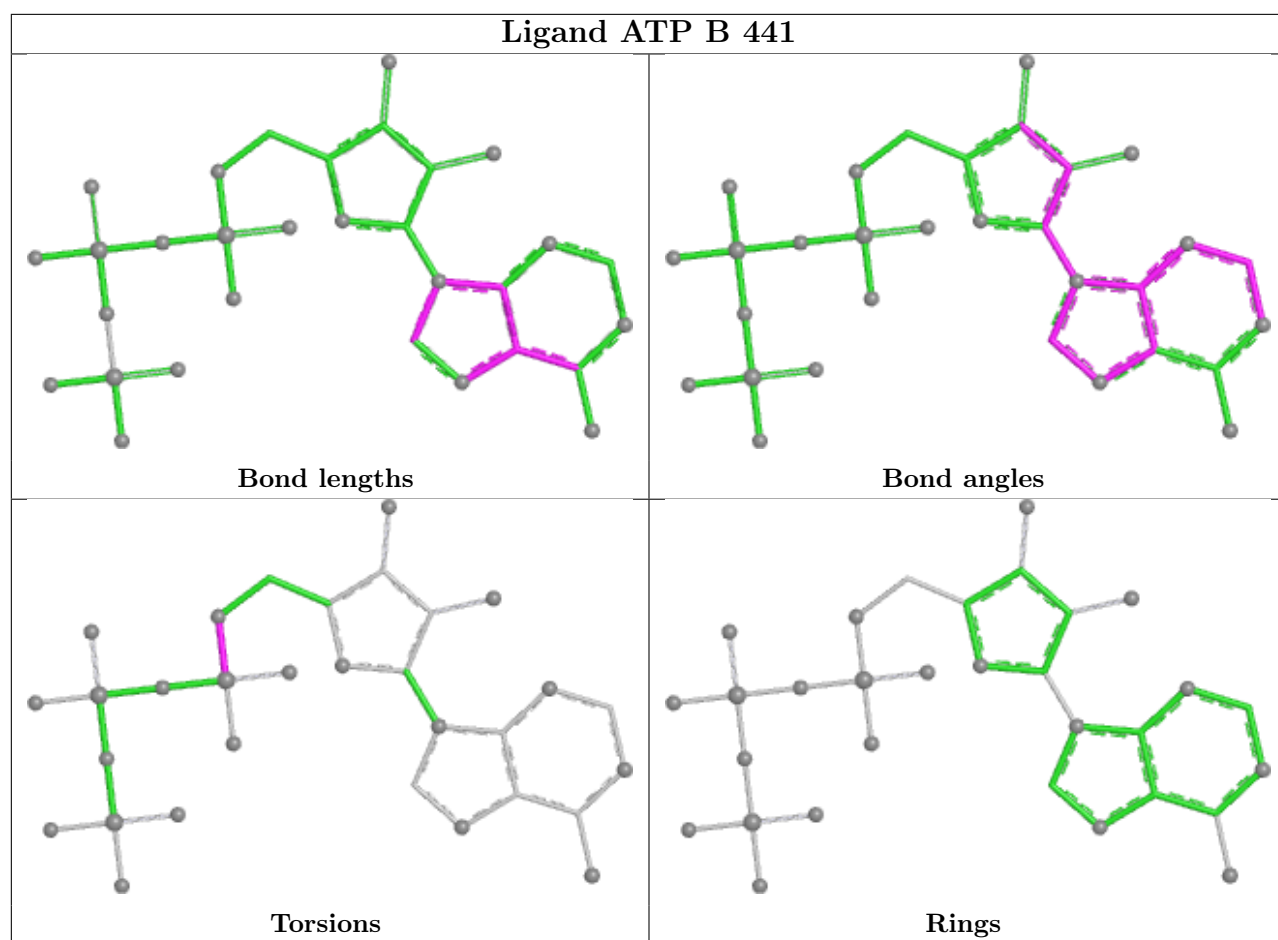
Mol	Chain	Res	Type	Atoms
36	B	441	ATP	C5'-O5'-PA-O1A
36	B	441	ATP	C5'-O5'-PA-O2A
36	B	441	ATP	C5'-O5'-PA-O3A
36	D	440	ATP	PA-O3A-PB-O2B

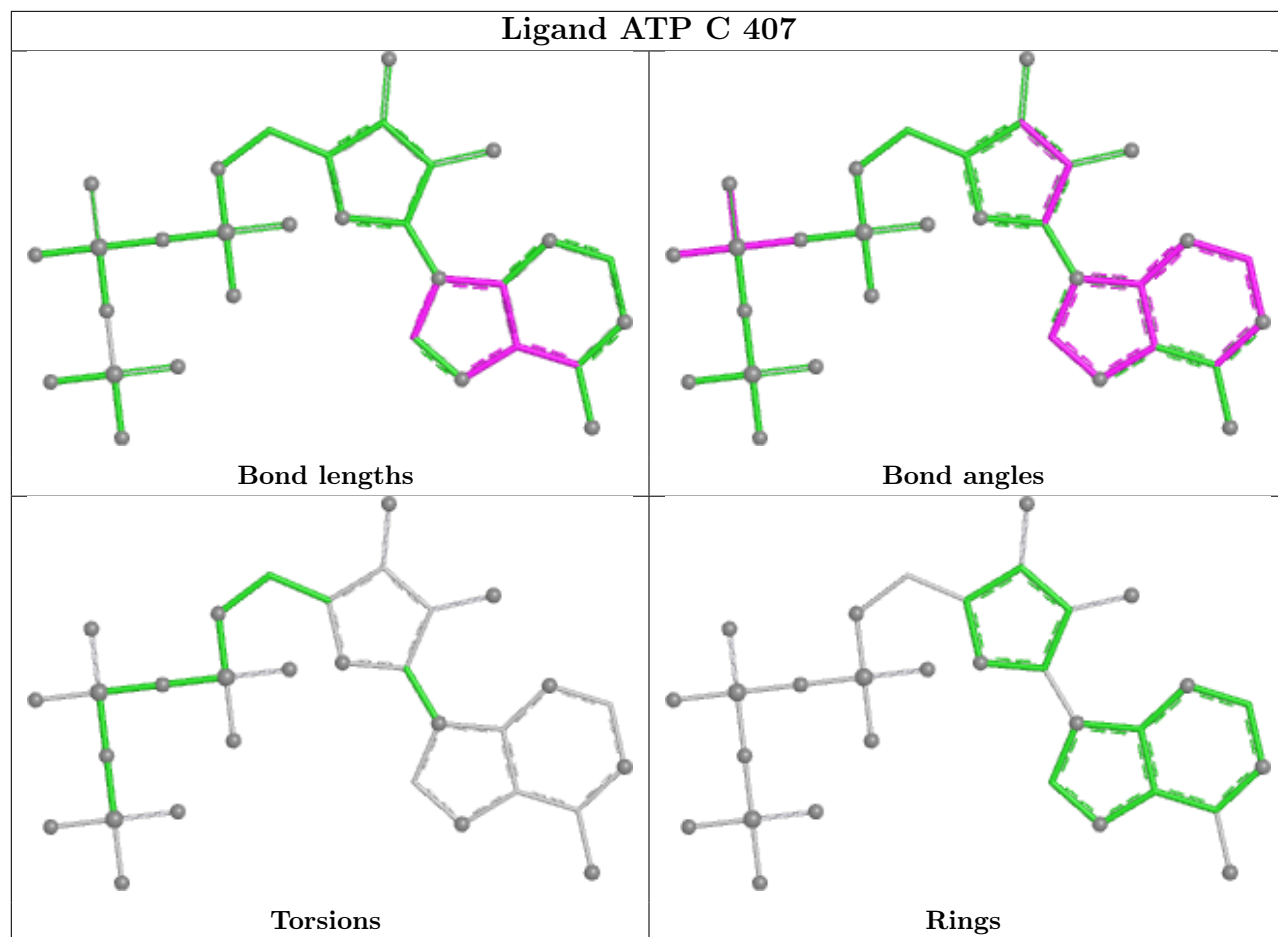
There are no ring outliers.

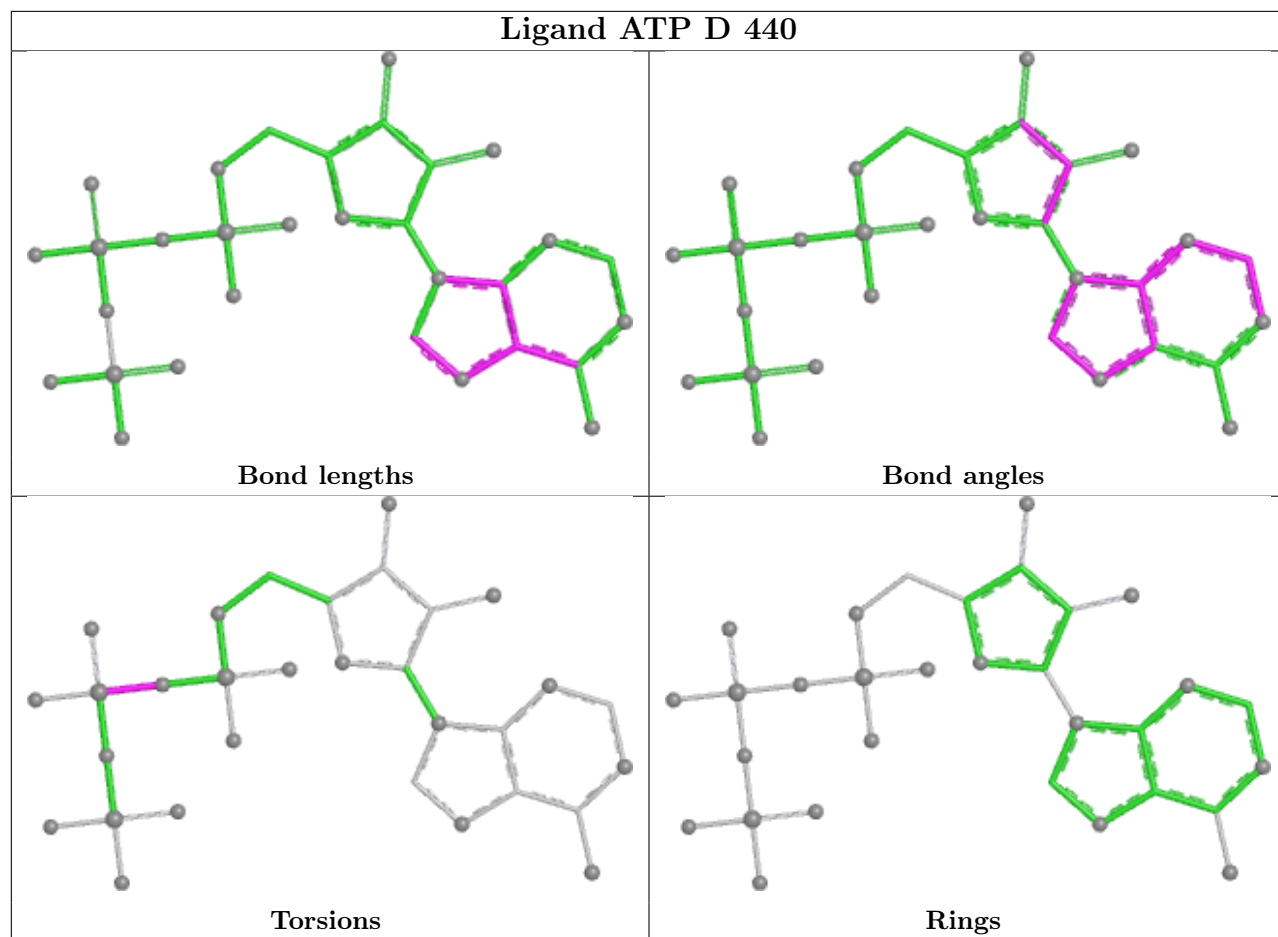
2 monomers are involved in 2 short contacts:

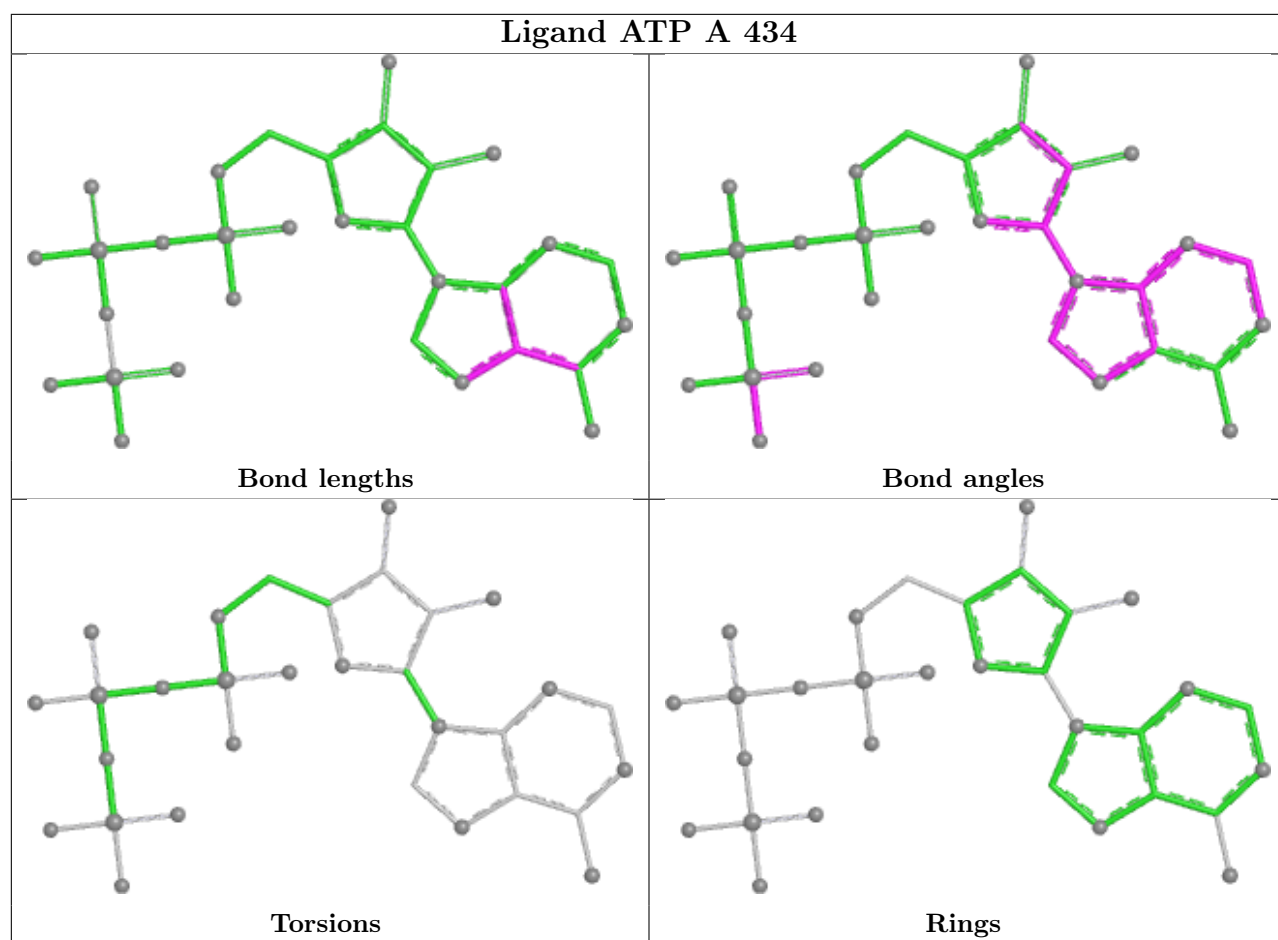
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	B	441	ATP	1	0
36	C	407	ATP	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

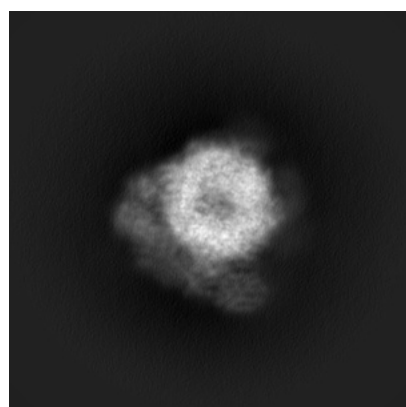
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9221. These allow visual inspection of the internal detail of the map and identification of artifacts.

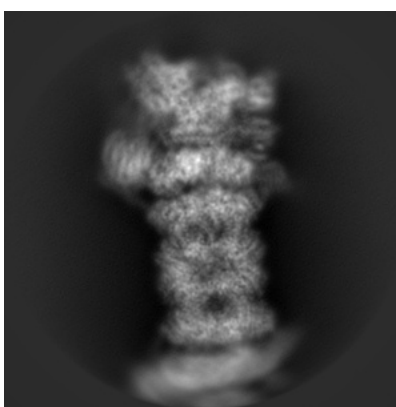
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

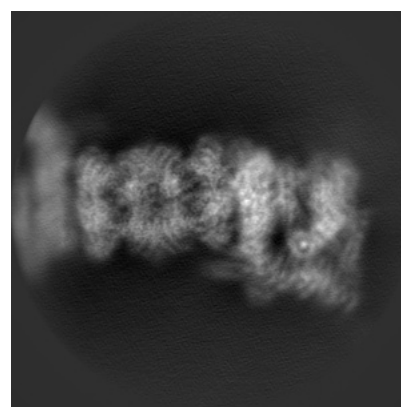
6.1.1 Primary map



X



Y

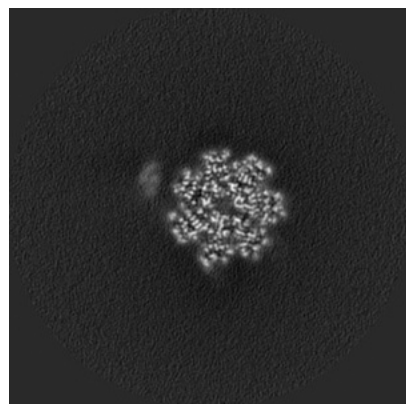


Z

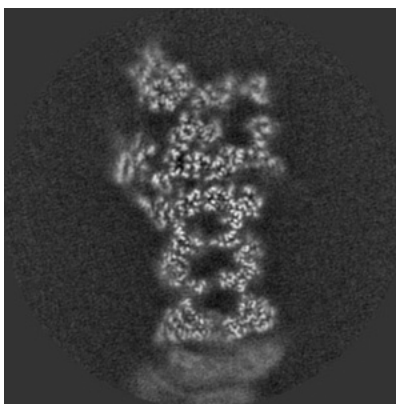
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

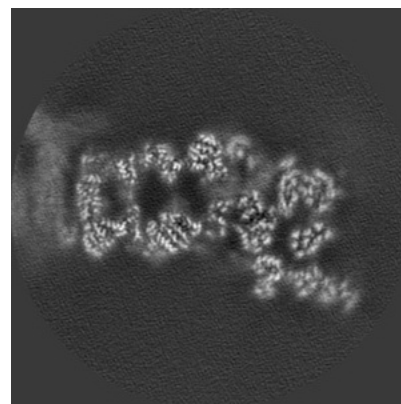
6.2.1 Primary map



X Index: 300



Y Index: 300

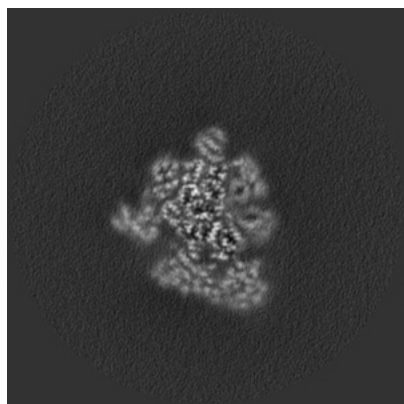


Z Index: 300

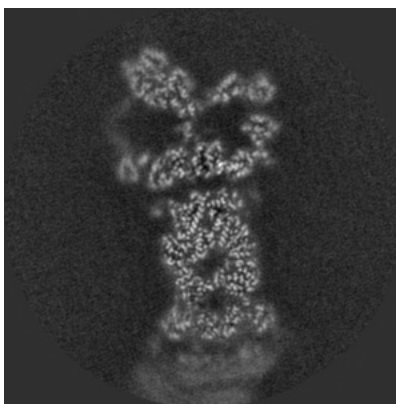
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

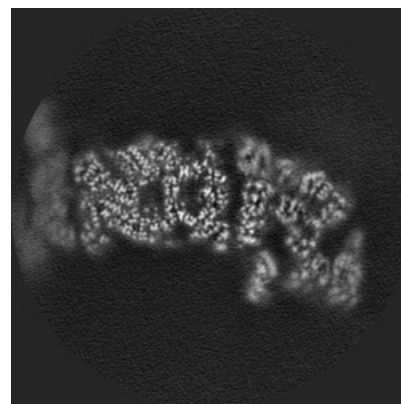
6.3.1 Primary map



X Index: 366



Y Index: 283

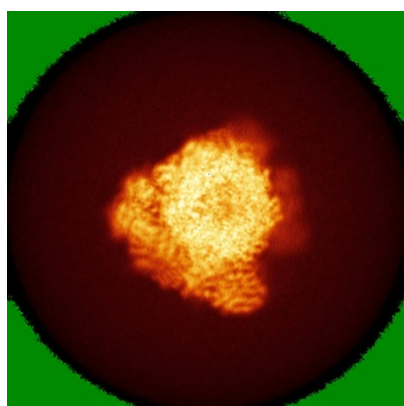


Z Index: 275

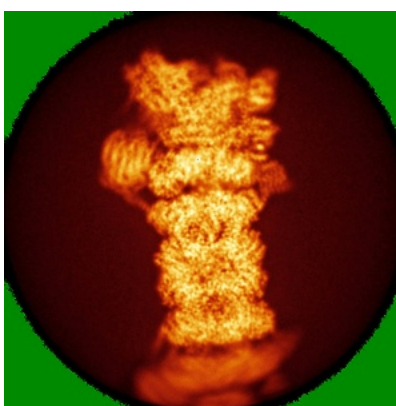
The images above show the largest variance slices of the map in three orthogonal directions.

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

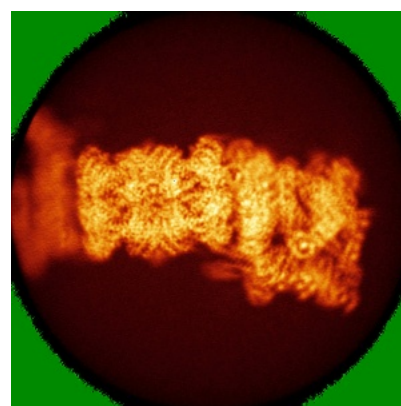
6.4.1 Primary map



X



Y

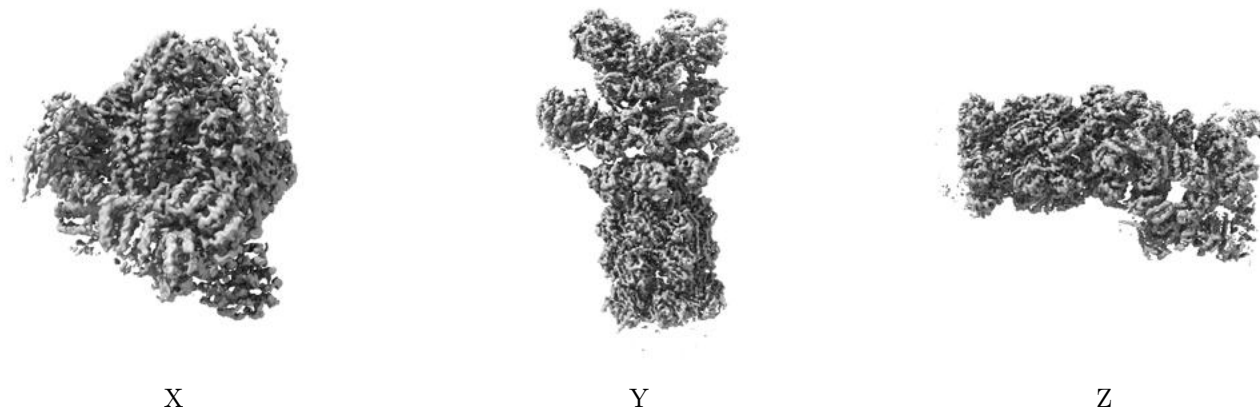


Z

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 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

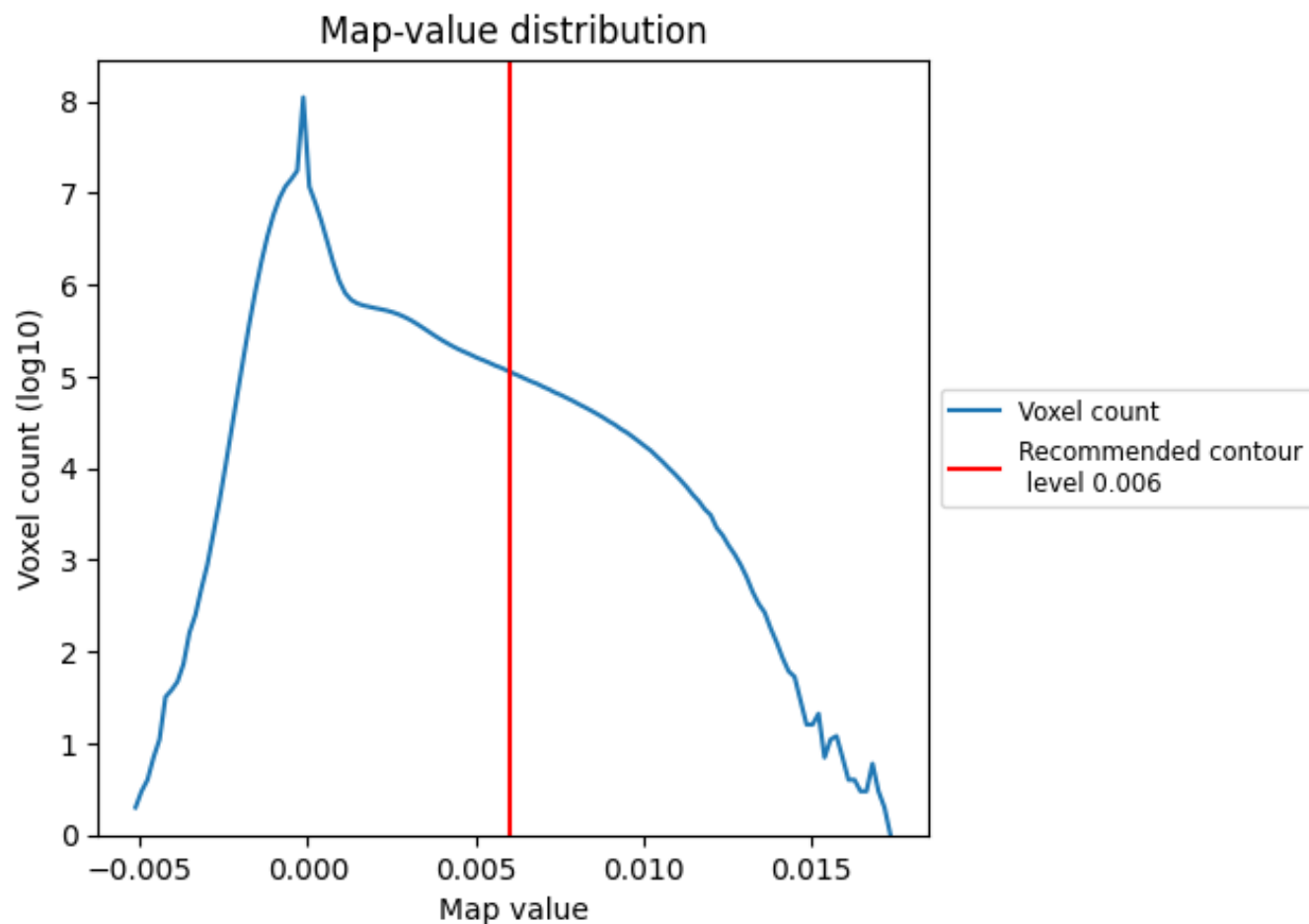
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

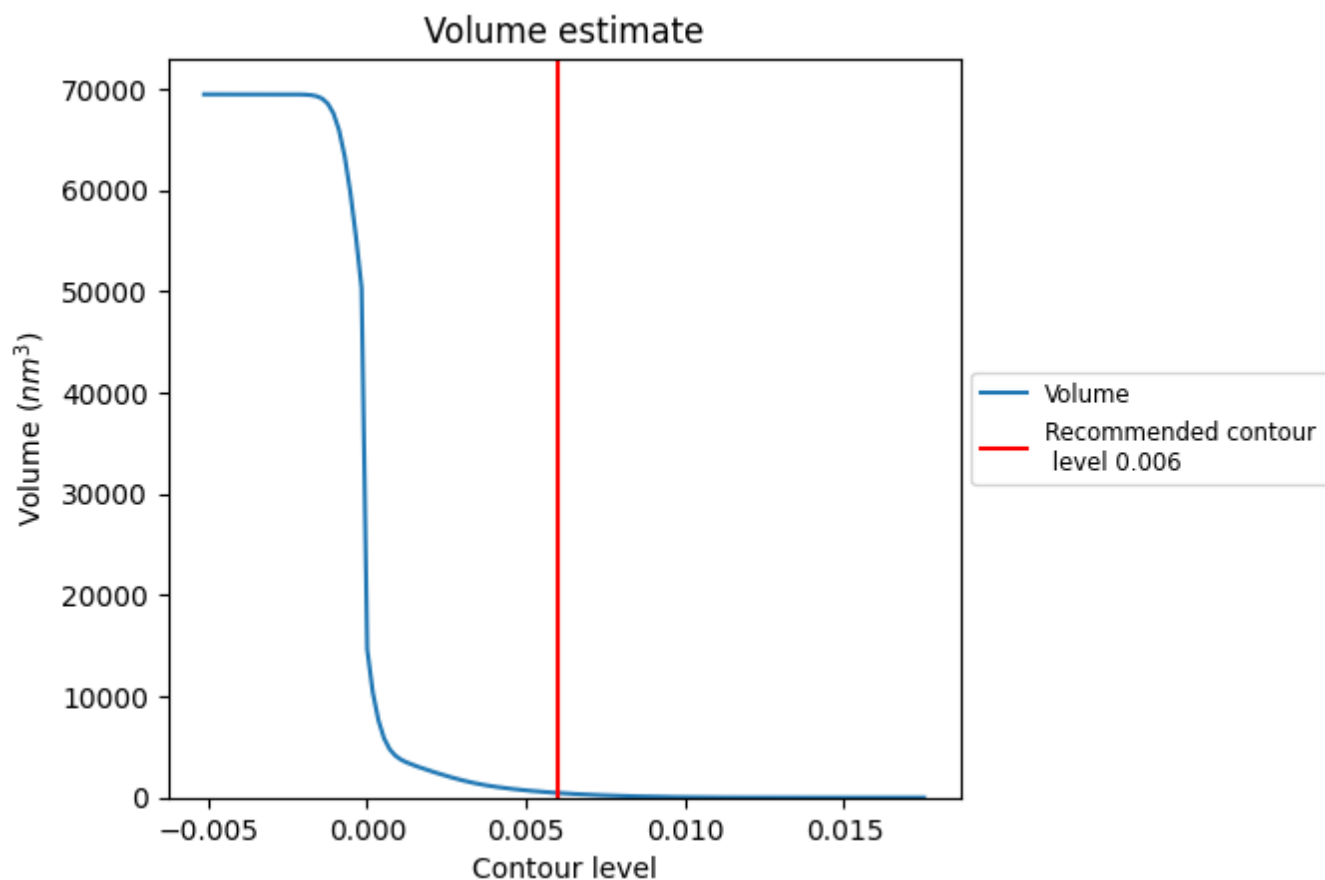
This section contains the results of statistical analysis of the map.

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.

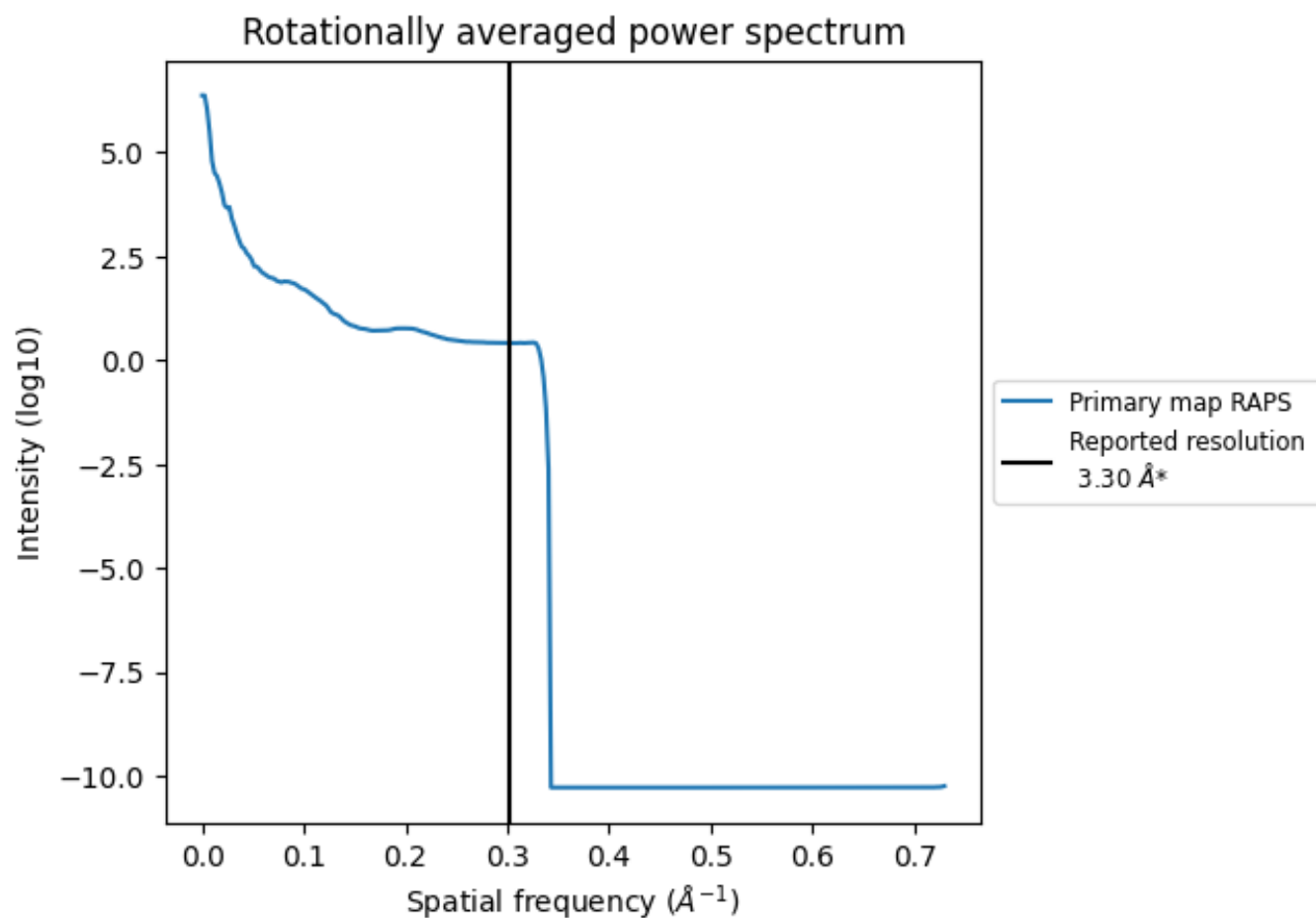
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 456 nm³; this corresponds to an approximate mass of 412 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 0.303 Å⁻¹

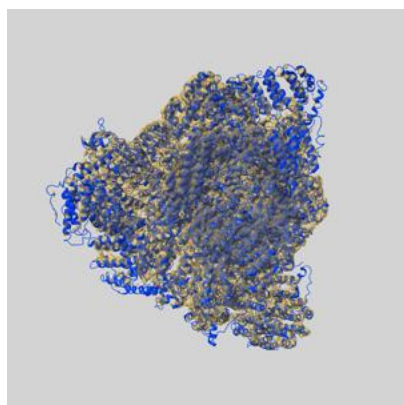
8 Fourier-Shell correlation

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

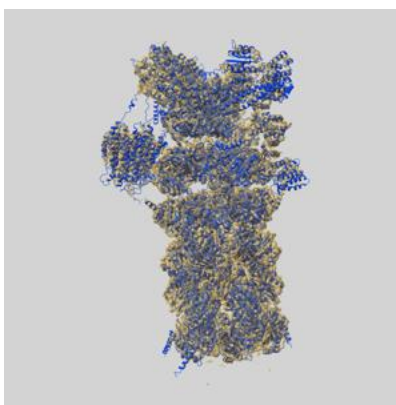
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9221 and PDB model 6MSJ. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

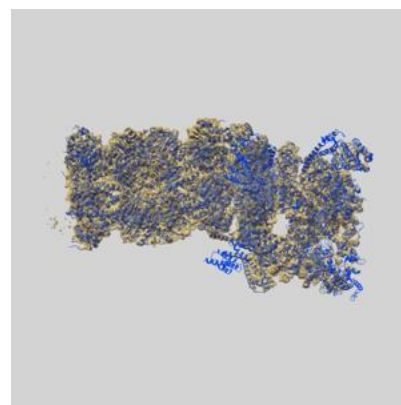
9.1 Map-model overlay [i](#)



X



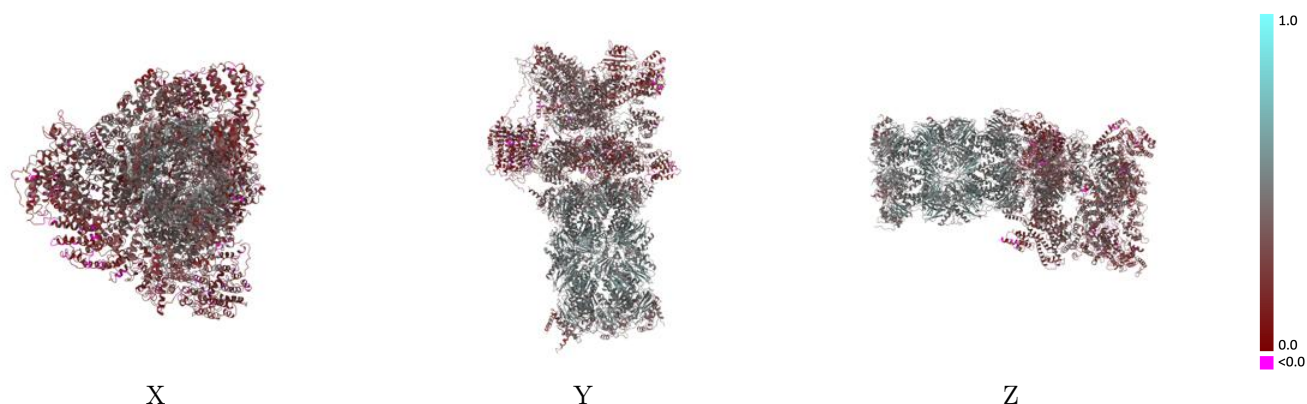
Y



Z

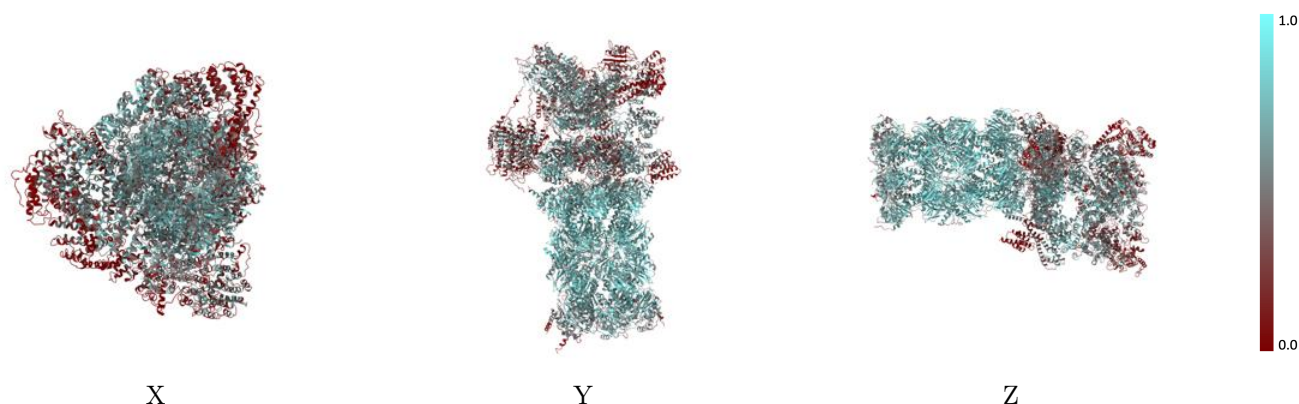
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



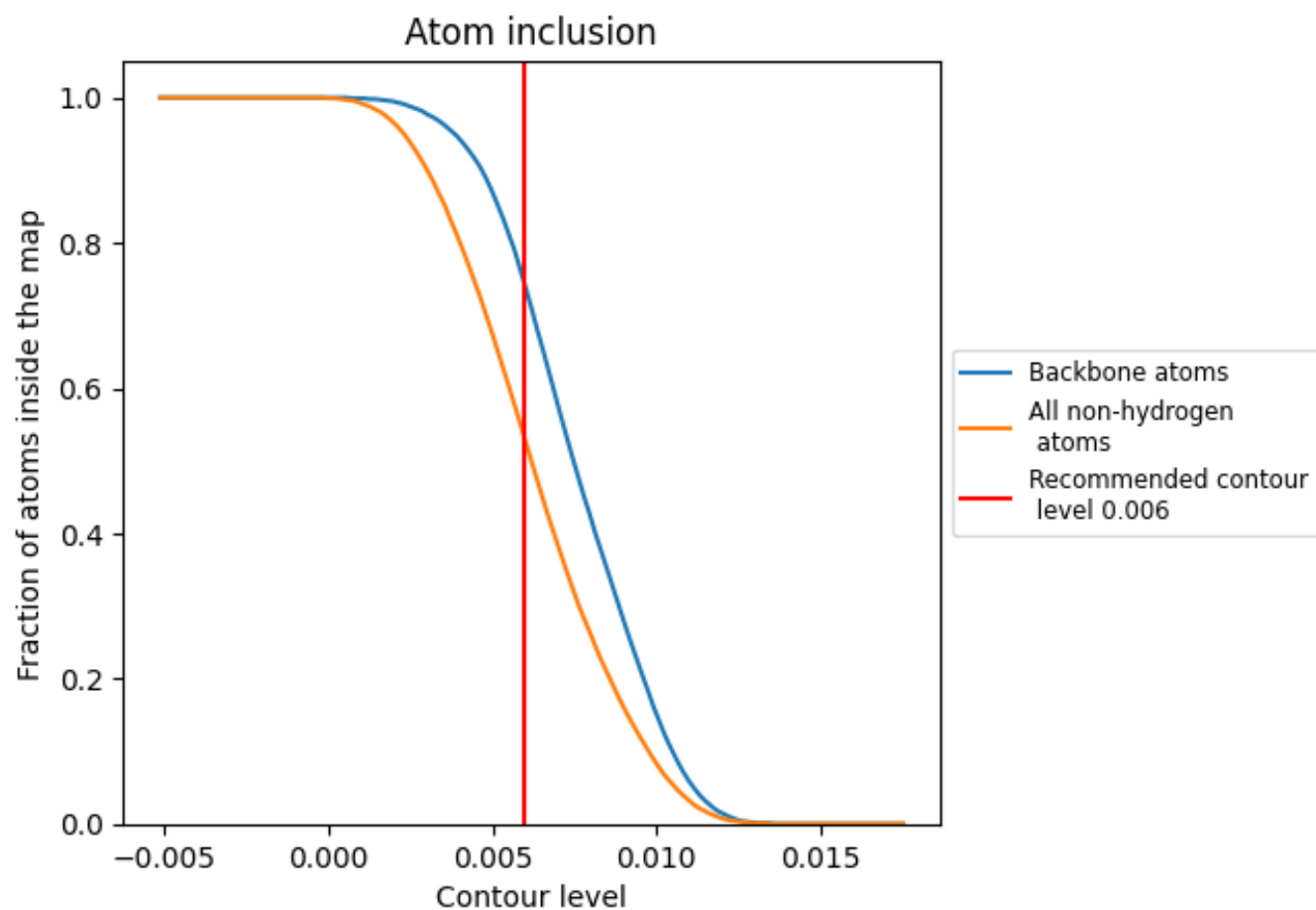
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 53% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5280	 0.3730
A	 0.4000	 0.2830
B	 0.5100	 0.3550
C	 0.5820	 0.3780
D	 0.6020	 0.3820
E	 0.4990	 0.3530
F	 0.2690	 0.2310
G	 0.6960	 0.4450
H	 0.7430	 0.4760
I	 0.6770	 0.4390
J	 0.6700	 0.4350
K	 0.6760	 0.4420
L	 0.7210	 0.4670
M	 0.6960	 0.4400
N	 0.7680	 0.5000
O	 0.7350	 0.4940
P	 0.7460	 0.5090
Q	 0.7390	 0.4910
R	 0.7640	 0.5110
S	 0.6980	 0.5000
T	 0.7530	 0.5010
U	 0.4370	 0.3230
V	 0.3020	 0.2280
W	 0.3970	 0.2770
X	 0.3800	 0.2970
Y	 0.5610	 0.3080
Z	 0.4500	 0.3320
a	 0.3630	 0.2620
b	 0.2100	 0.2630
c	 0.4930	 0.3490
d	 0.1700	 0.2210
e	 0.3270	 0.2450
f	 0.2590	 0.2020
g	 0.5900	 0.4550
h	 0.5920	 0.4570



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Chain	Atom inclusion	Q-score
i	 0.5390	 0.4240
j	 0.5110	 0.4090
k	 0.5500	 0.4340
l	 0.6420	 0.4670
m	 0.6190	 0.4380
n	 0.7430	 0.5100
o	 0.6730	 0.4930
p	 0.7180	 0.5160
q	 0.7180	 0.5030
r	 0.7460	 0.5130
s	 0.7170	 0.5090
t	 0.7520	 0.5110
v	 0.1720	 0.2710