



Full wwPDB EM Validation Report ⓘ

Jun 30, 2025 – 08:47 AM EDT

PDB ID : 9CGC / pdb_00009cgc
EMDB ID : EMD-45579
Title : Yeast 26S proteasome non-substrate-engaged (S1 state)
Authors : Arkinson, C.; Gee, C.L.; Martin, A.
Deposited on : 2024-06-28
Resolution : 3.61 Å(reported)
Based on initial model : 6j2q

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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

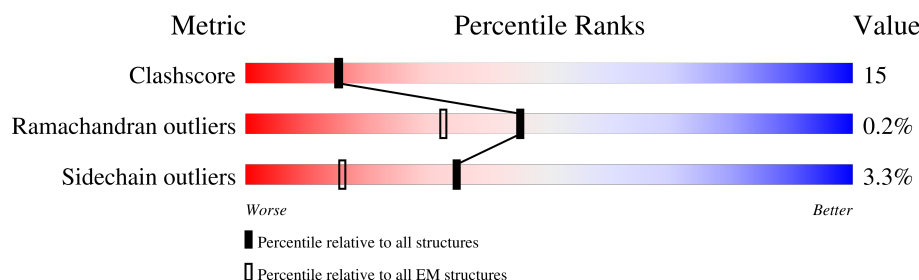
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.61 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1	215	<div> <div>18%</div> <div>57%</div> <div>37%</div> <div>5%</div> </div>
1	b	215	<div> <div>60%</div> <div>69%</div> <div>26%</div> <div>5%</div> </div>
2	2	261	<div> <div>18%</div> <div>56%</div> <div>28%</div> <div>15%</div> </div>
2	i	261	<div> <div>59%</div> <div>56%</div> <div>29%</div> <div>15%</div> </div>
3	3	205	<div> <div>25%</div> <div>61%</div> <div>37%</div> <div>.</div> </div>
3	h	205	<div> <div>77%</div> <div>58%</div> <div>41%</div> <div>.</div> </div>
4	4	198	<div> <div>23%</div> <div>64%</div> <div>35%</div> <div>.</div> </div>
4	g	198	<div> <div>73%</div> <div>61%</div> <div>38%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
5	5	287	
5	f	287	
6	6	241	
6	e	241	
7	7	266	
7	a	266	
8	A	252	
9	B	250	
10	C	258	
11	D	254	
12	E	260	
13	F	234	
14	G	288	
15	I	437	
16	K	428	
17	L	437	
18	O	393	
19	P	445	
20	R	429	
21	S	523	
22	V	306	
23	W	268	
24	Y	89	
25	J	405	
26	H	467	

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Mol	Chain	Length	Quality of chain
27	M	434	
28	Q	434	
29	U	338	
30	N	945	
31	T	274	
32	o	993	

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 92952 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 Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	205	Total	C	N	O	S	0	0
			1576	996	261	312	7		
1	b	205	Total	C	N	O	S	0	0
			1576	996	261	312	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	222	Total	C	N	O	S	0	0
			1684	1061	293	323	7		
2	i	222	Total	C	N	O	S	0	0
			1684	1061	293	323	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		
3	h	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	198	Total	C	N	O	S	0	0
			1585	1005	269	305	6		
4	g	198	Total	C	N	O	S	0	0
			1585	1005	269	305	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
5	f	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
6	e	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	233	Total	C	N	O	S	0	0
			1824	1154	312	351	7		
7	a	233	Total	C	N	O	S	0	0
			1824	1154	312	351	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	243	Total	C	N	O	S	0	0
			1921	1221	322	370	8		

- Molecule 9 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		

- Molecule 10 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

- Molecule 11 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	241	Total	C	N	O	S	0	0
			1890	1181	331	374	4		

- Molecule 12 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		

- Molecule 14 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	243	Total	C	N	O	S	0	0
			1888	1201	328	355	4		

- Molecule 15 is a protein called 26S proteasome regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	392	Total	C	N	O	S	0	0
			3078	1937	516	608	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	383	Total	C	N	O	S	0	0
			3035	1908	532	585	10		

- Molecule 17 is a protein called 26S proteasome subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	359	Total	C	N	O	S	0	0
			2820	1783	490	535	12		

- Molecule 18 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	386	Total	C	N	O	S	0	0
			3169	2040	517	604	8		

- Molecule 19 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	436	Total	C	N	O	S	0	0
			3575	2279	597	690	9		

- Molecule 20 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	397	Total	C	N	O	S	0	0
			3195	2043	524	618	10		

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	461	Total	C	N	O	S	0	0
			3770	2412	629	714	15		

- Molecule 22 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	288	Total	C	N	O	S	0	0
			2267	1421	388	444	14		

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	190	Total	C	N	O	S	0	0
			1484	933	262	287	2		

- Molecule 24 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Y	33	Total	C	N	O	0	0
			281	176	38	67		

- Molecule 25 is a protein called 26S proteasome regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	J	370	Total	C	N	O	S	0	0
			2913	1836	524	536	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	H	385	Total	C	N	O	S	0	0
			3016	1896	540	563	17		

- Molecule 27 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	M	363	Total	C	N	O	S	0	0
			2827	1771	493	550	13		

- Molecule 28 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Q	411	Total	C	N	O	S	0	0
			3347	2137	552	643	15		

- Molecule 29 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	292	Total	C	N	O	S	0	0
			2333	1476	401	449	7		

- Molecule 30 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	N	869	Total	C	N	O	S	0	0
			6725	4275	1130	1292	28		

- Molecule 31 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	T	257	Total	C	N	O	S	0	0
			2106	1357	335	410	4		

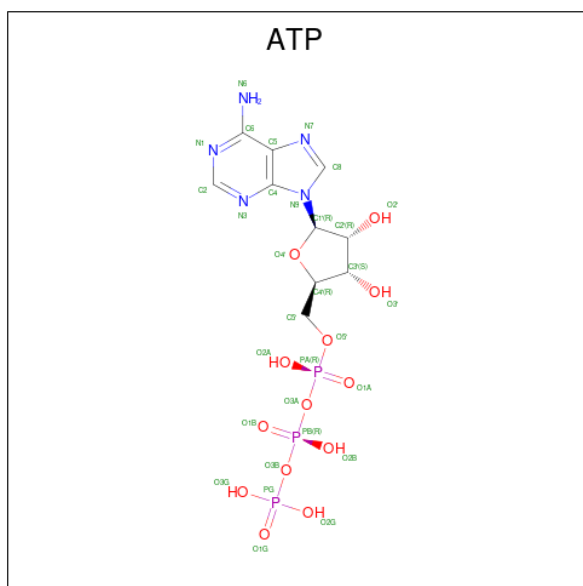
- Molecule 32 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	o	819	Total	C	N	O	S	0	0
			6347	4039	1040	1239	29		

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
33	I	1	Total	Mg	0
			1	1	
33	K	1	Total	Mg	0
			1	1	
33	L	1	Total	Mg	0
			1	1	
33	H	1	Total	Mg	0
			1	1	
33	M	1	Total	Mg	0
			1	1	

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

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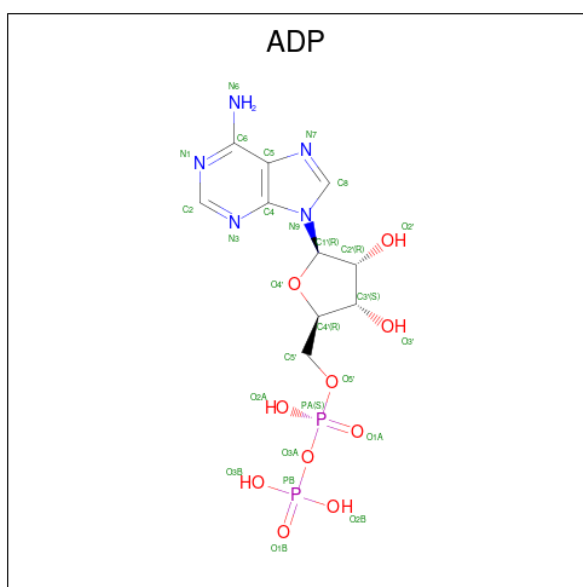
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Mol	Chain	Residues	Atoms					AltConf
34	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	M	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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

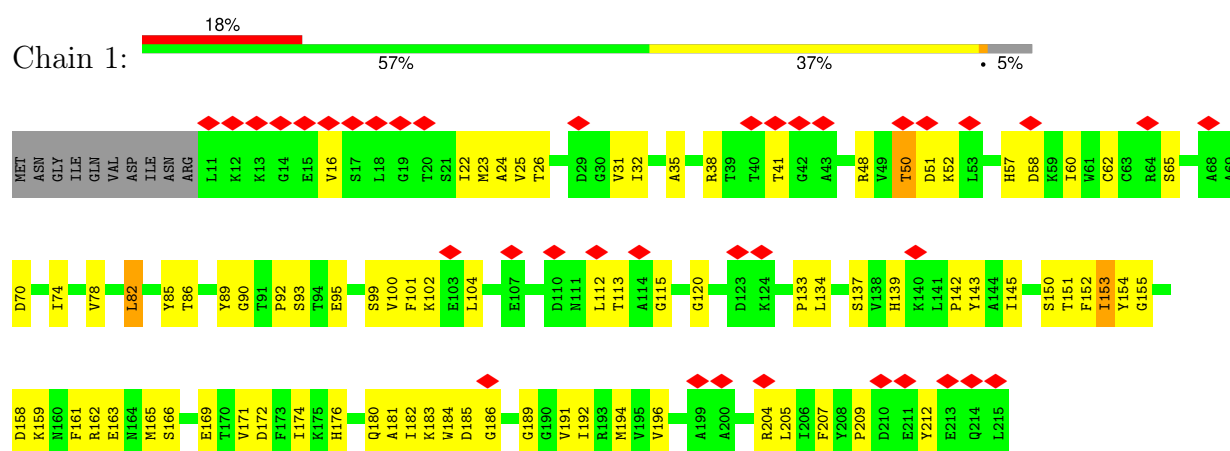


Mol	Chain	Residues	Atoms					AltConf
36	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

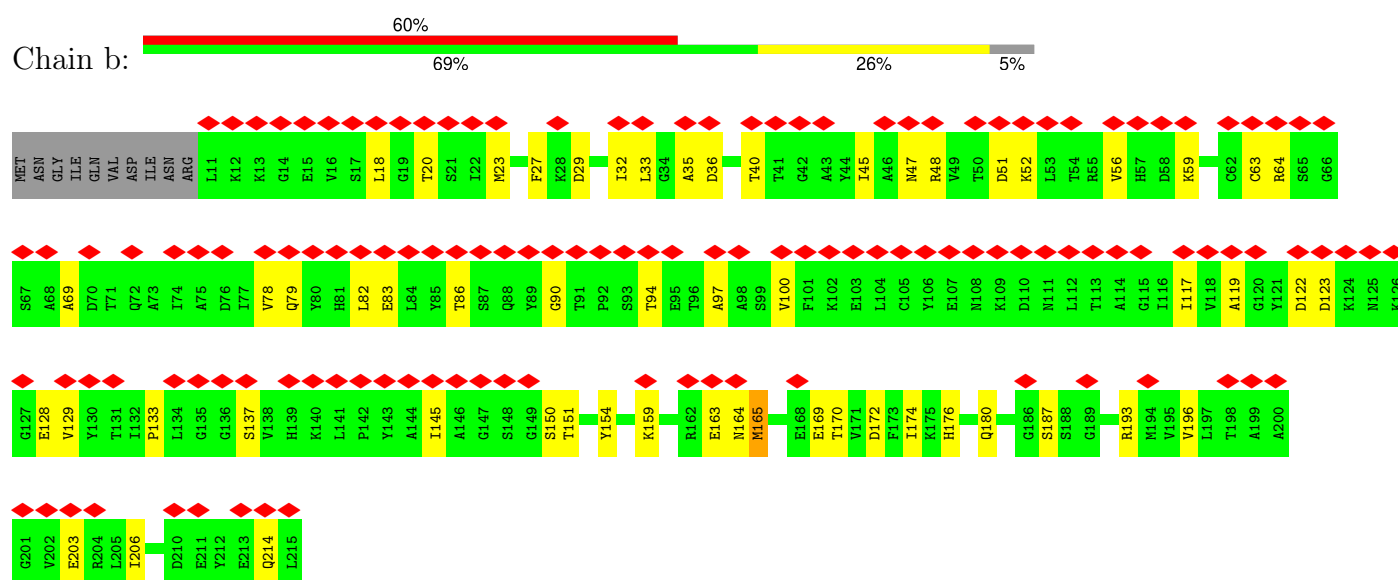
3 Residue-property plots

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: Proteasome subunit beta type-1



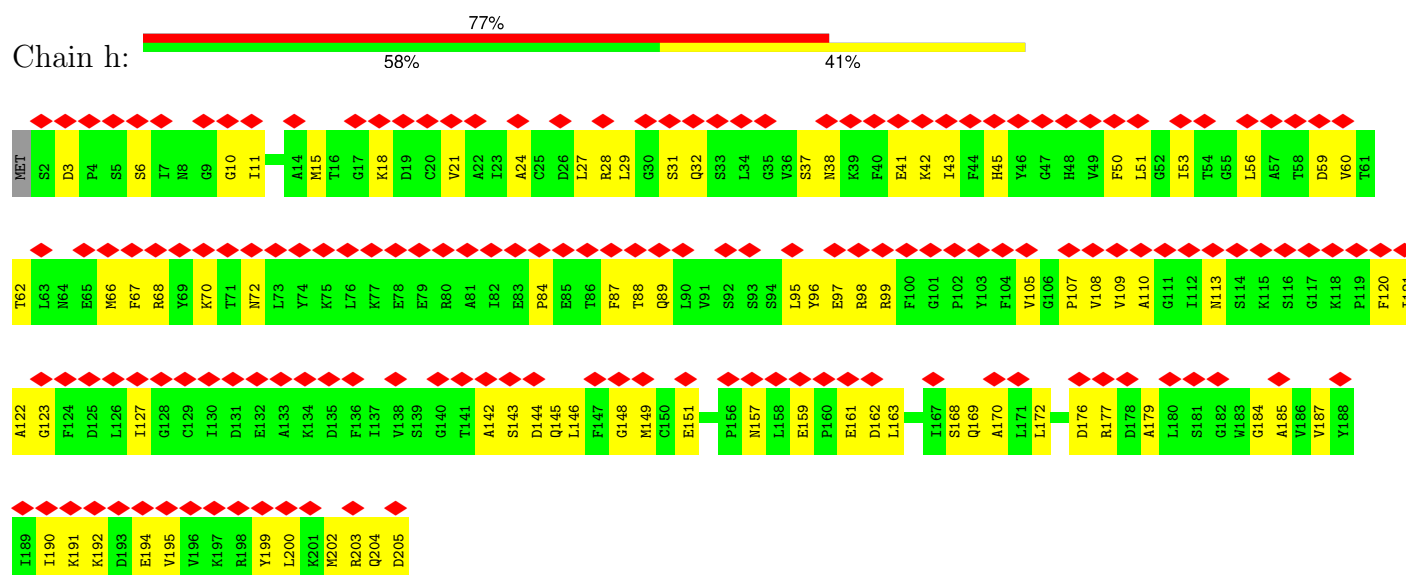
• Molecule 1: Proteasome subunit beta type-1



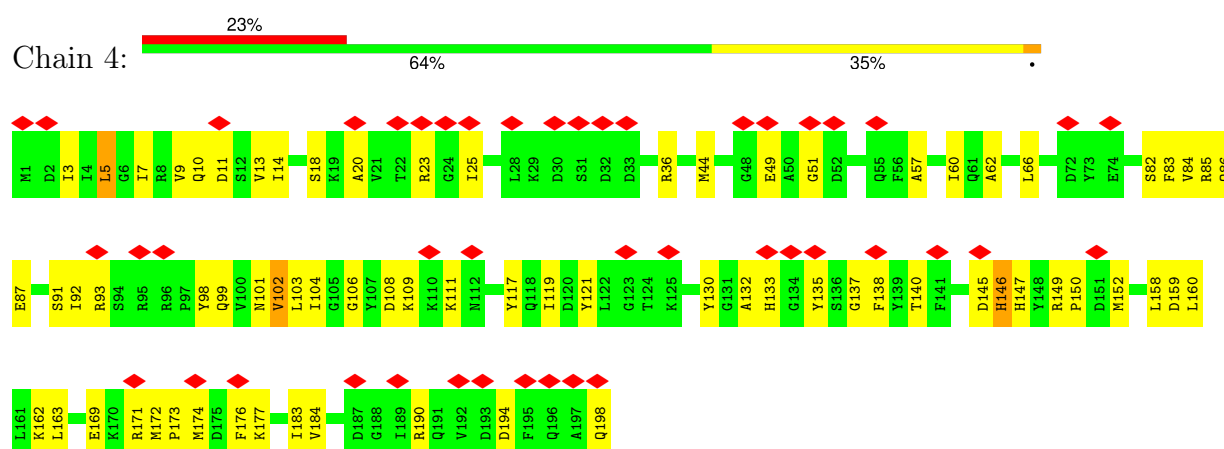
• Molecule 2: Proteasome subunit beta type-2



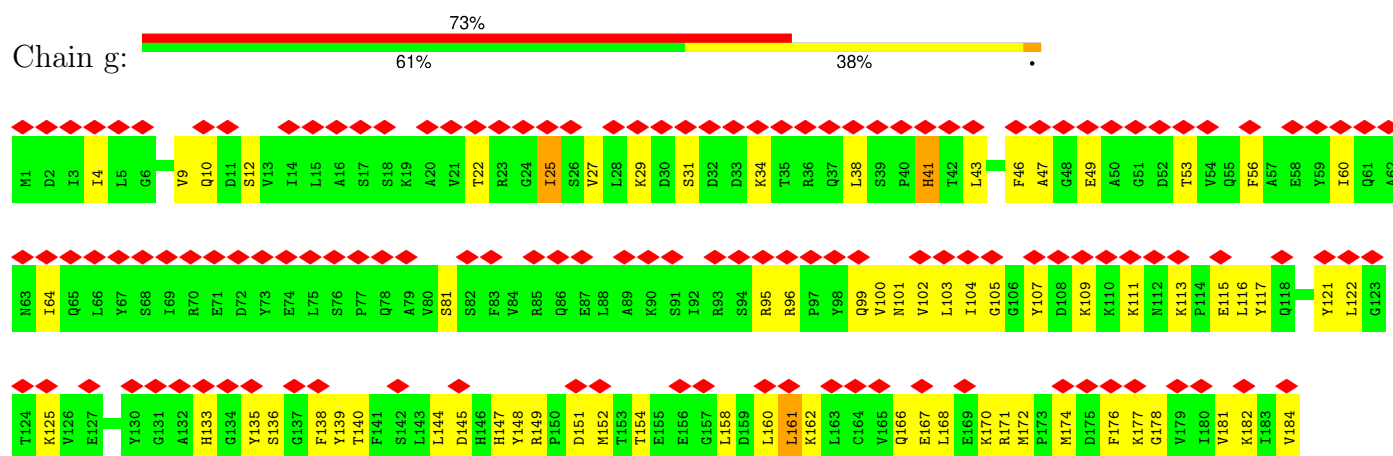
- Molecule 3: Proteasome subunit beta type-3

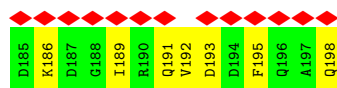


- Molecule 4: Proteasome subunit beta type-4

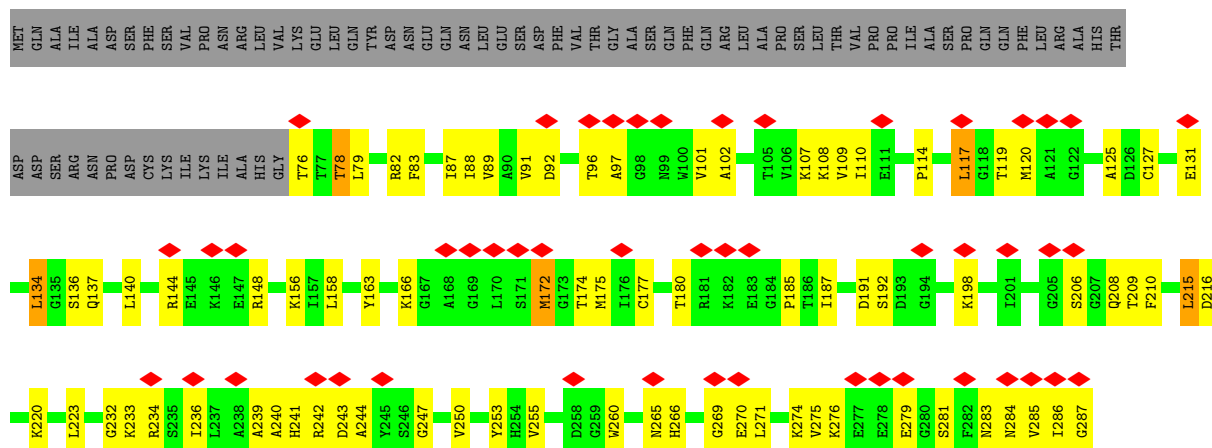
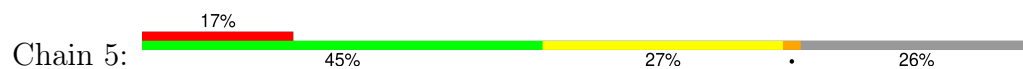


- Molecule 4: Proteasome subunit beta type-4





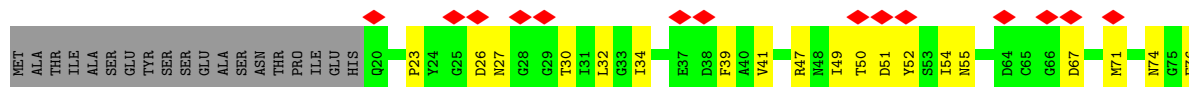
• Molecule 5: Proteasome subunit beta type-5

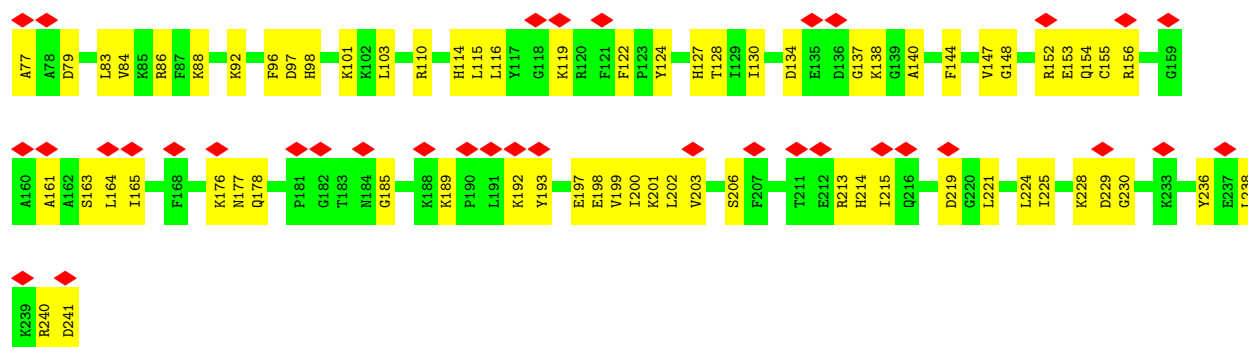


• Molecule 5: Proteasome subunit beta type-5

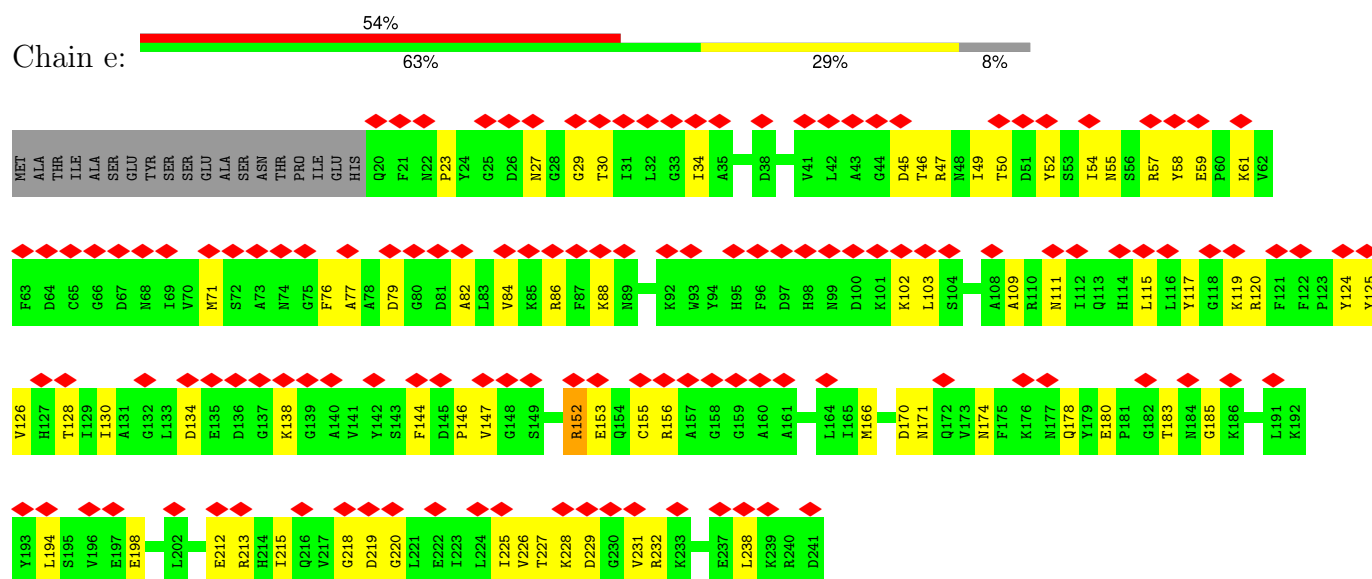


• Molecule 6: Proteasome subunit beta type-6

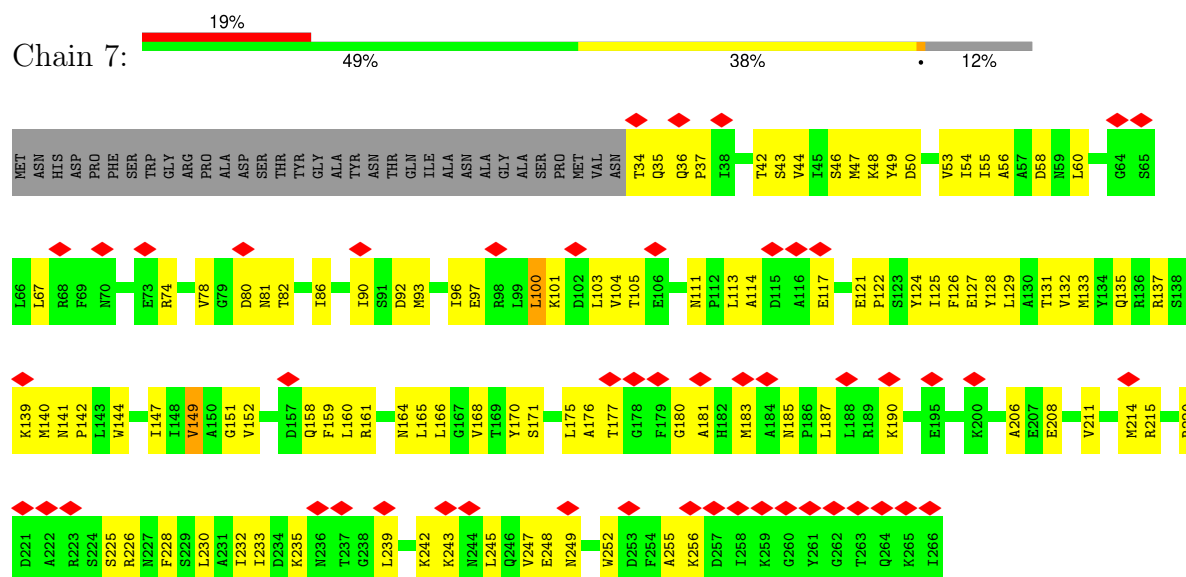




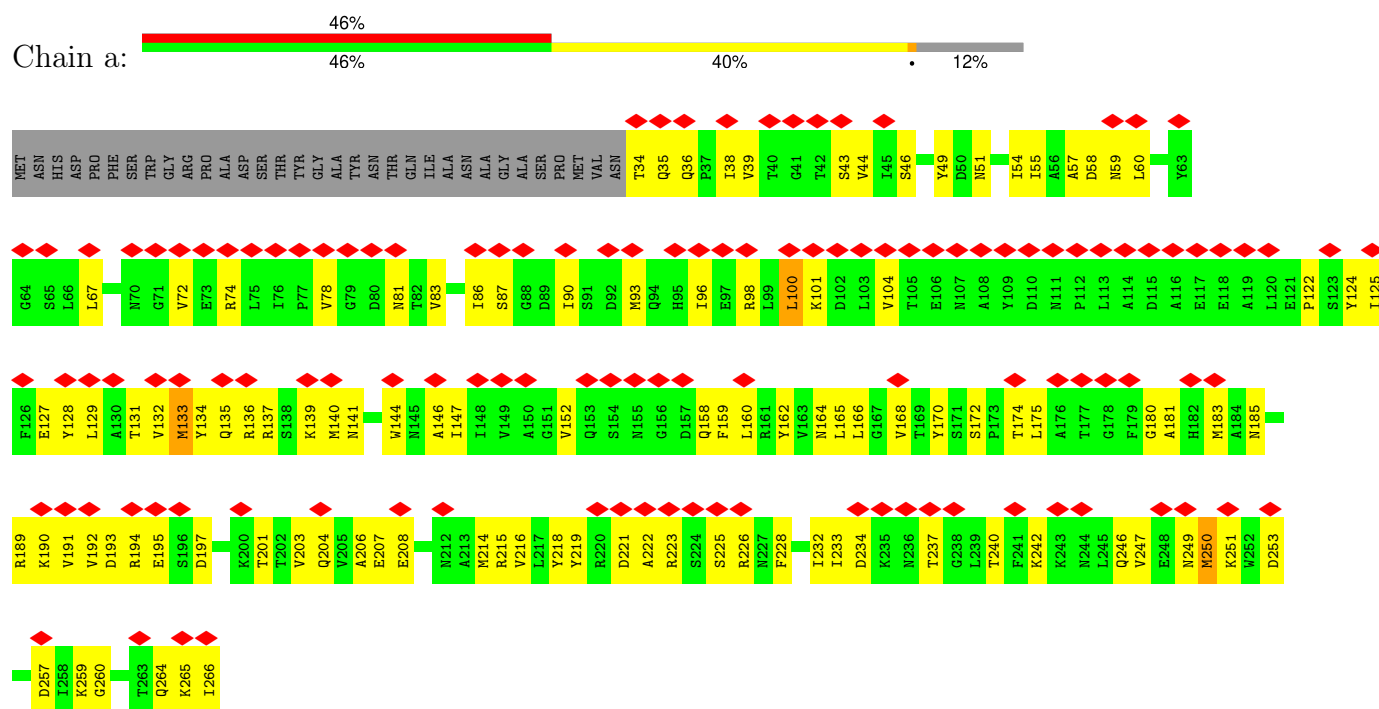
• Molecule 6: Proteasome subunit beta type-6



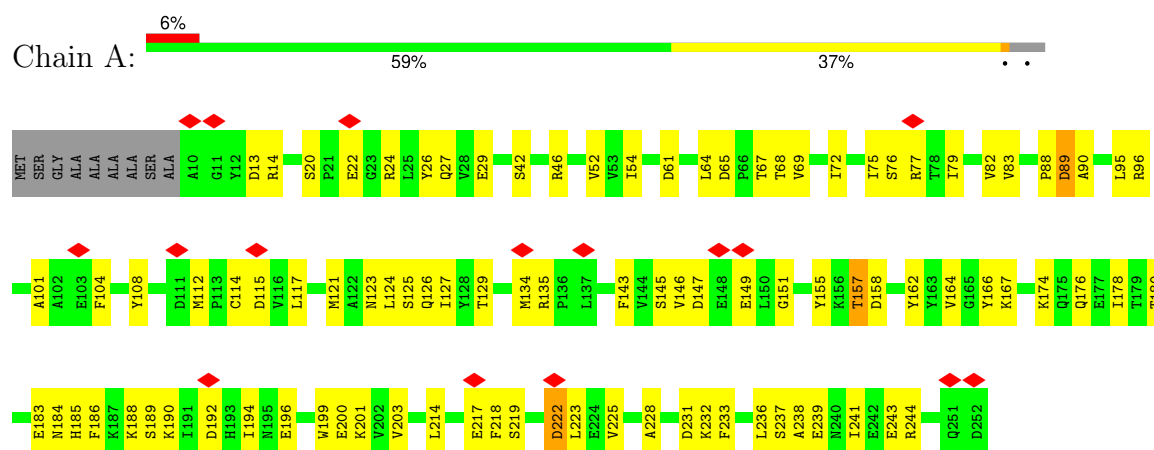
• Molecule 7: Proteasome subunit beta type-7



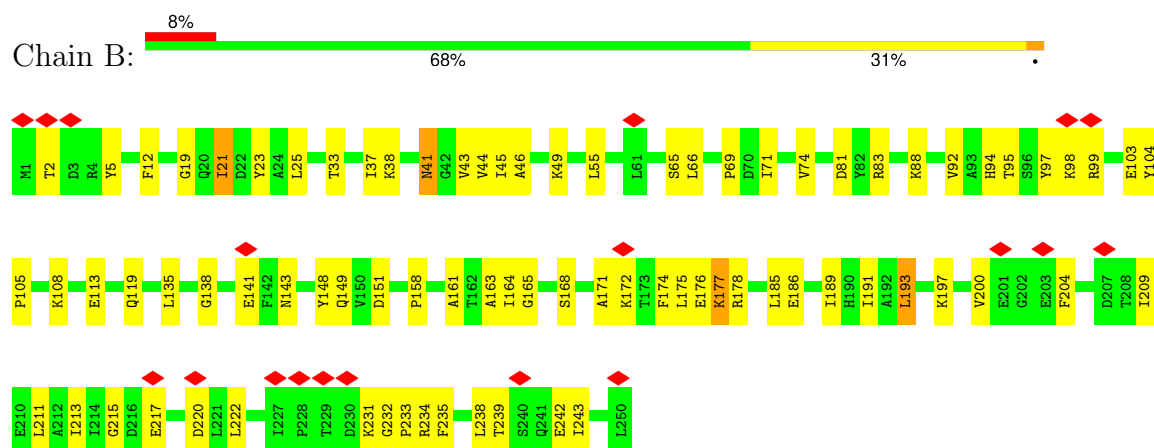
• Molecule 7: Proteasome subunit beta type-7



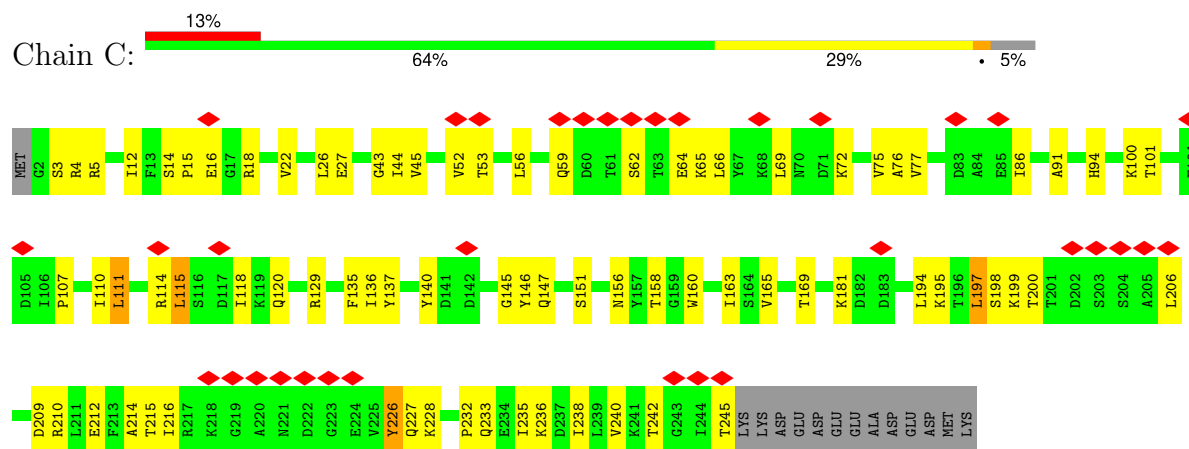
• Molecule 8: Proteasome subunit alpha type-1



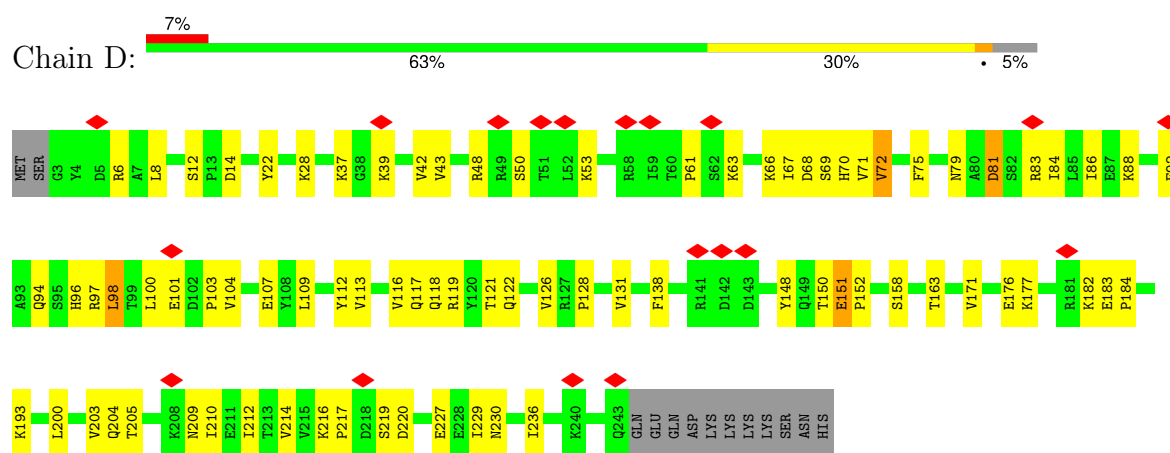
• Molecule 9: Proteasome subunit alpha type-2



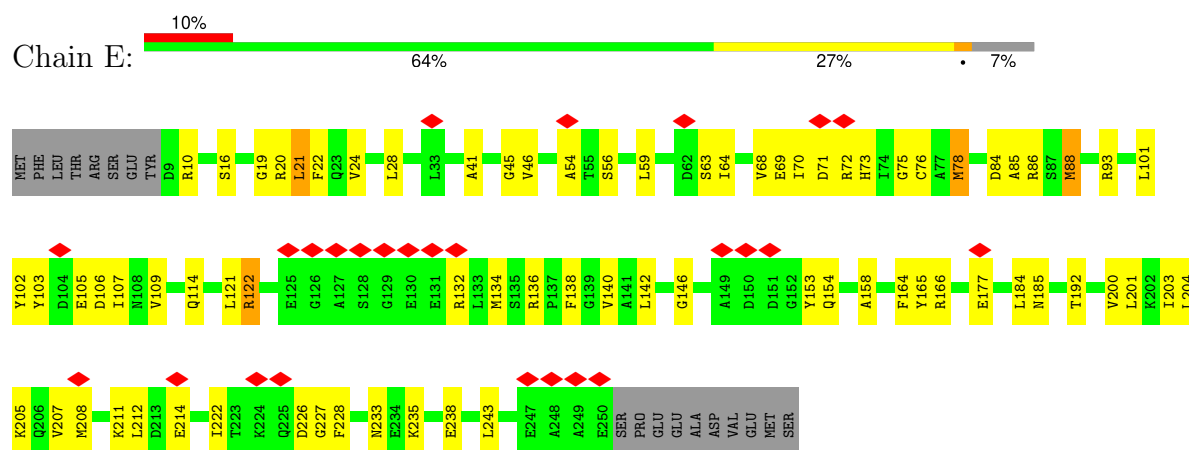
- Molecule 10: Proteasome subunit alpha type-3



- Molecule 11: Proteasome subunit alpha type-4

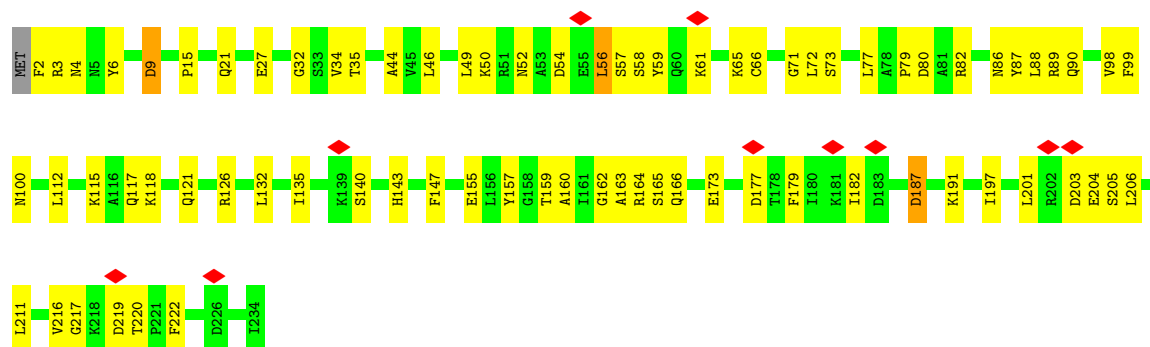


- Molecule 12: Proteasome subunit alpha type-5



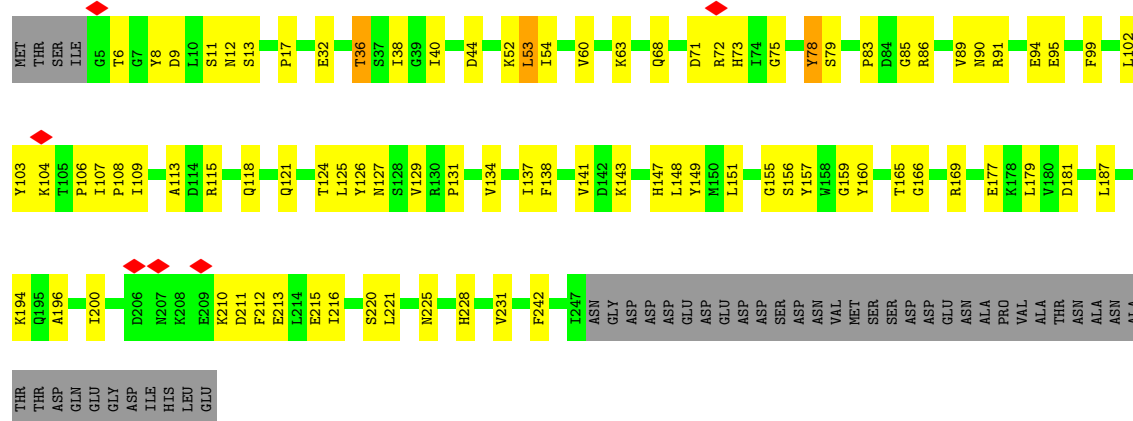
- Molecule 13: Proteasome subunit alpha type-6





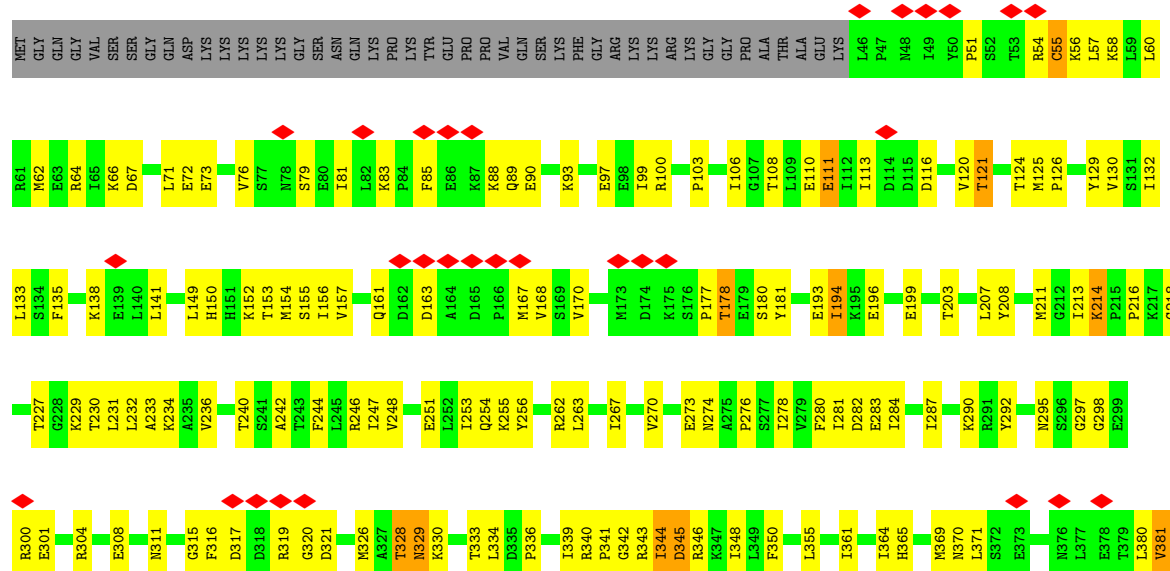
- Molecule 14: Probable proteasome subunit alpha type-7

Chain G: 55% 29% 16%



- Molecule 15: 26S proteasome regulatory subunit 4 homolog

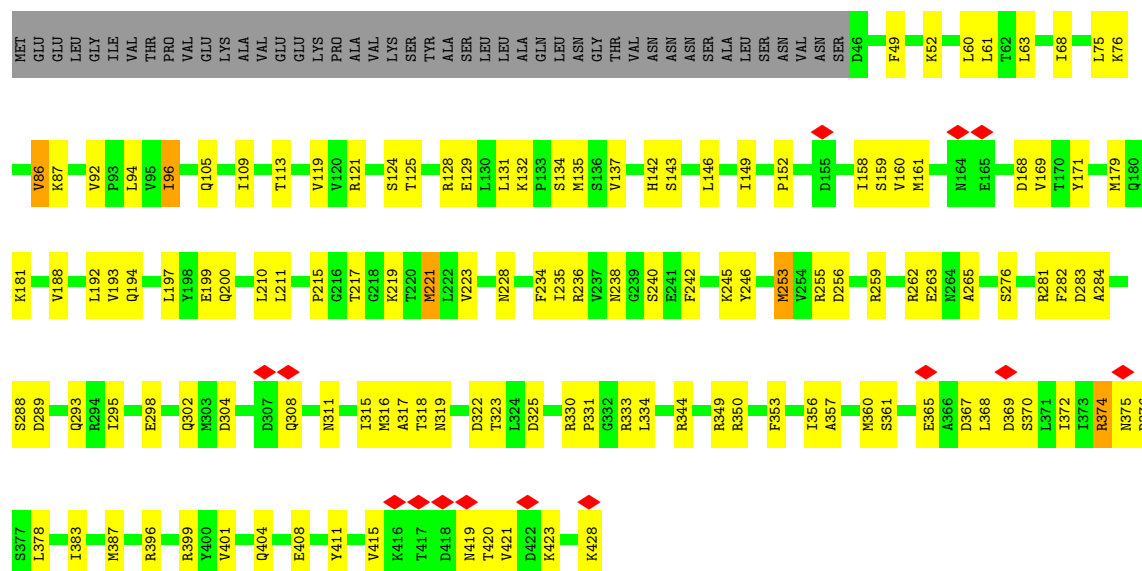
Chain I: 9% 53% 34% 10%





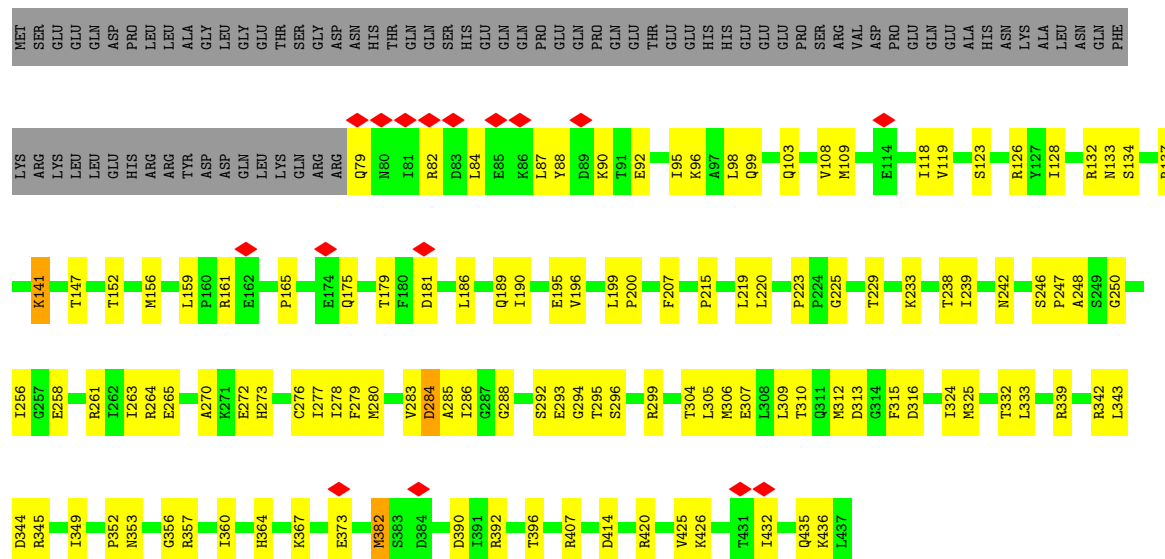
- Molecule 16: 26S proteasome regulatory subunit 6B homolog

Chain K: 59% 29% 11%



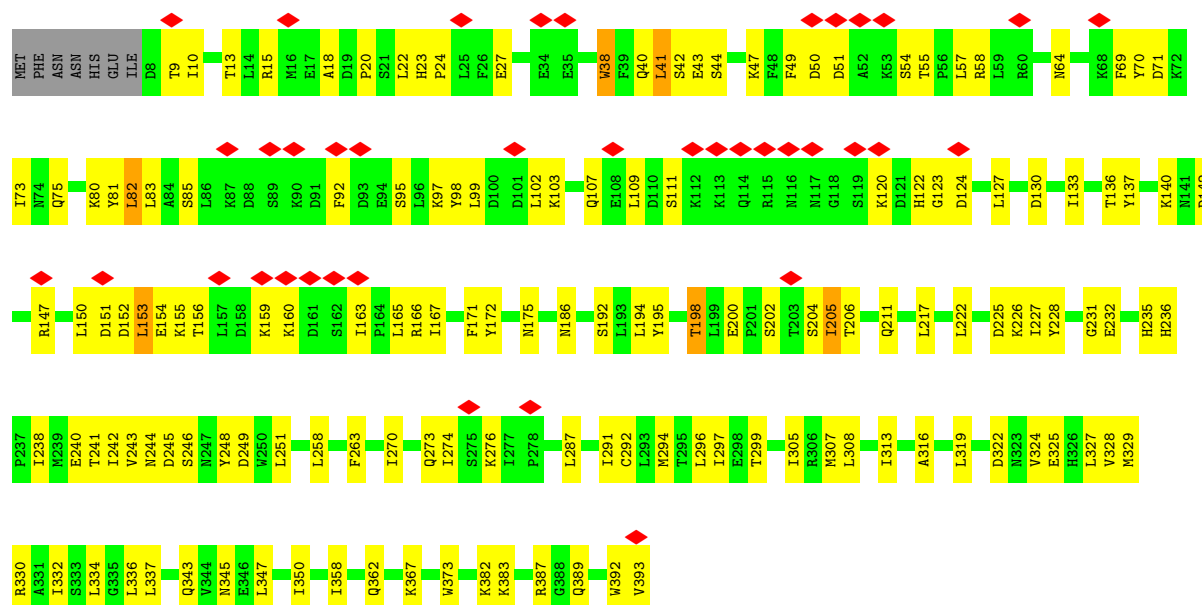
- Molecule 17: 26S proteasome subunit RPT4

Chain L: 55% 27% 18%

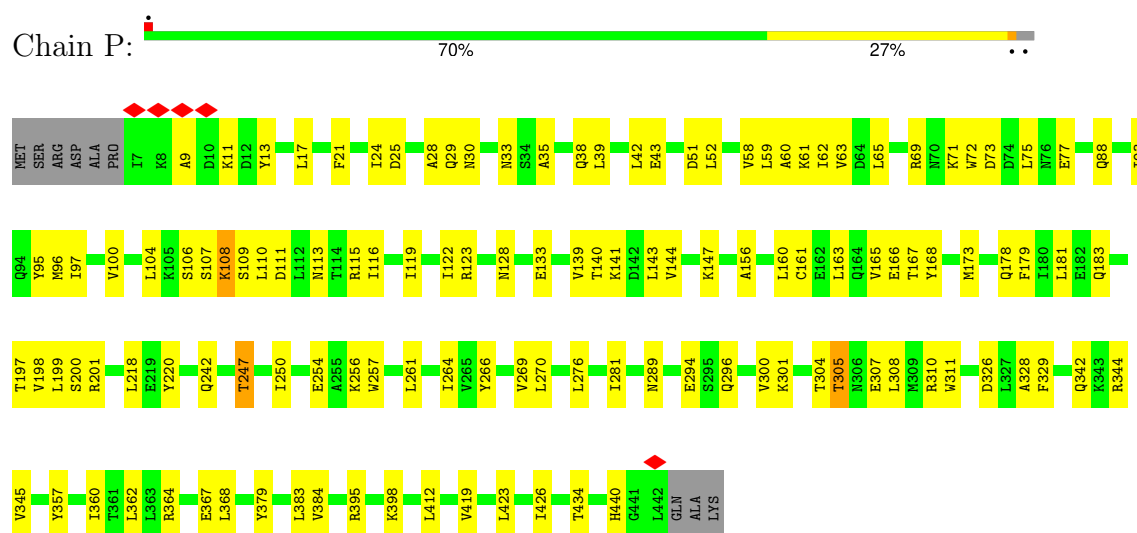


- Molecule 18: 26S proteasome regulatory subunit RPN9

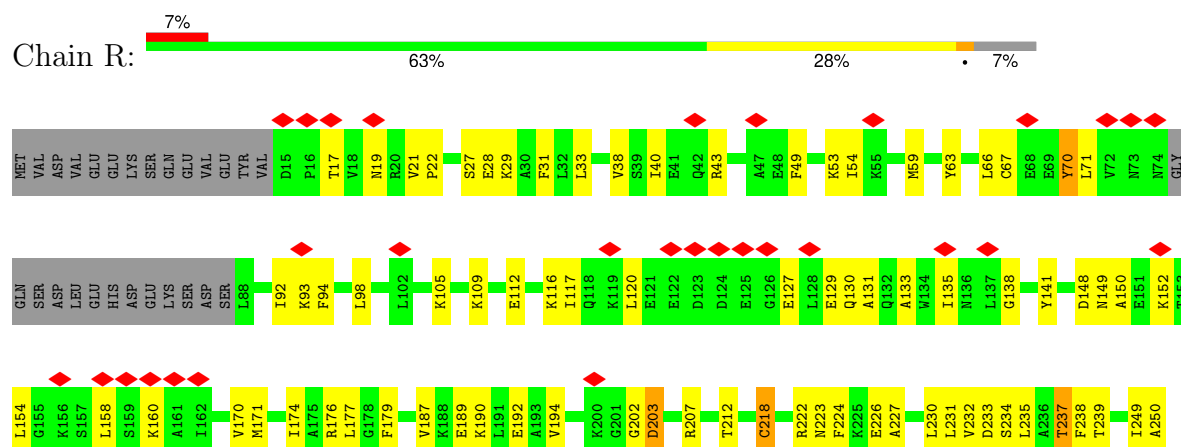
Chain O: 10% 60% 36%

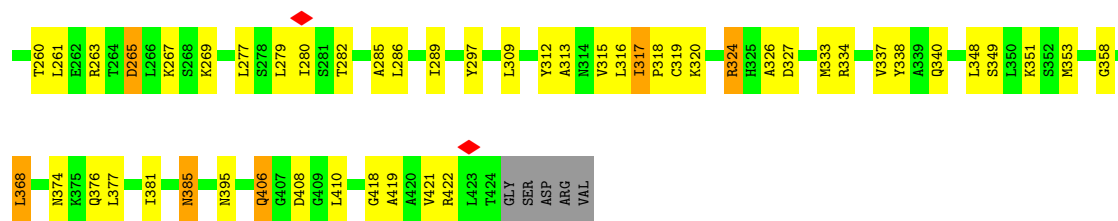


• Molecule 19: 26S proteasome regulatory subunit RPN5



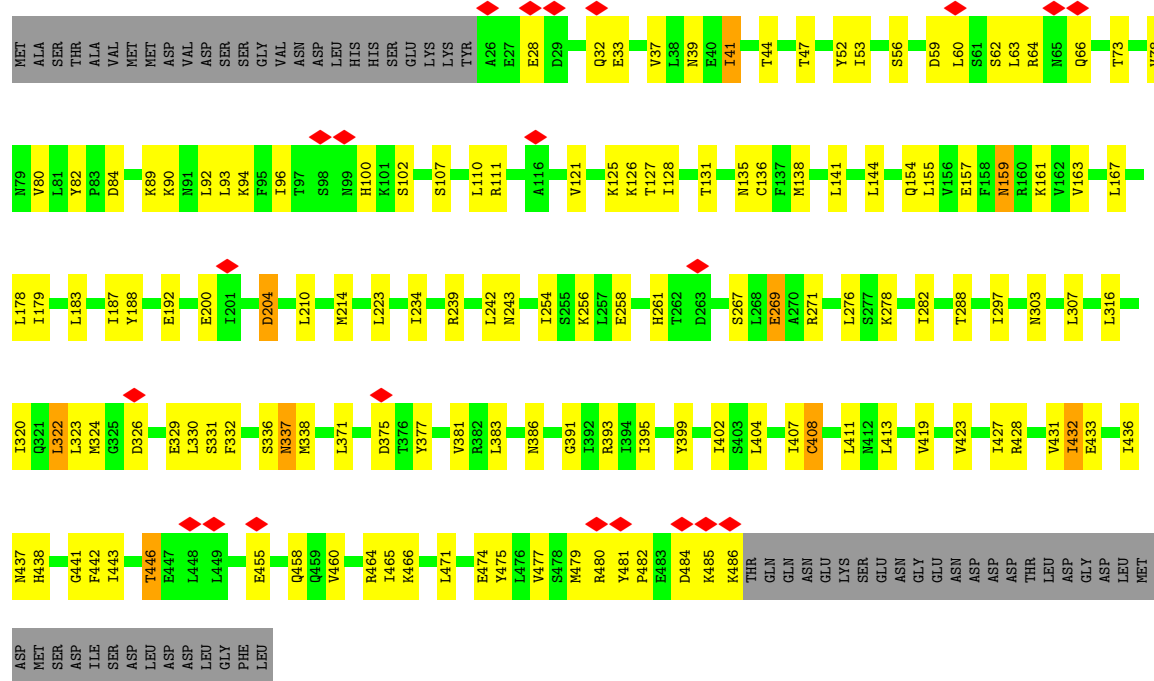
• Molecule 20: 26S proteasome regulatory subunit RPN7





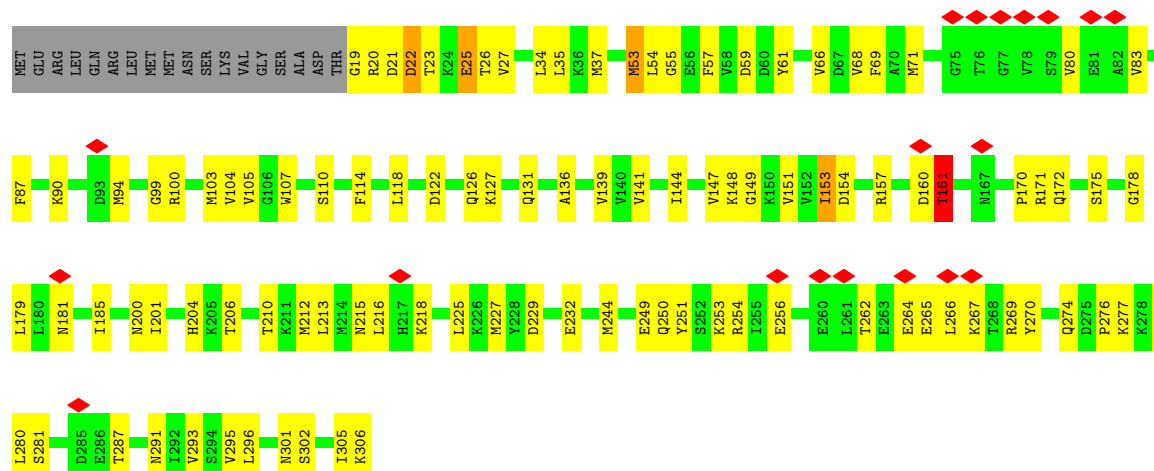
• Molecule 21: 26S proteasome regulatory subunit RPN3

Chain S: 61% 25% 12%

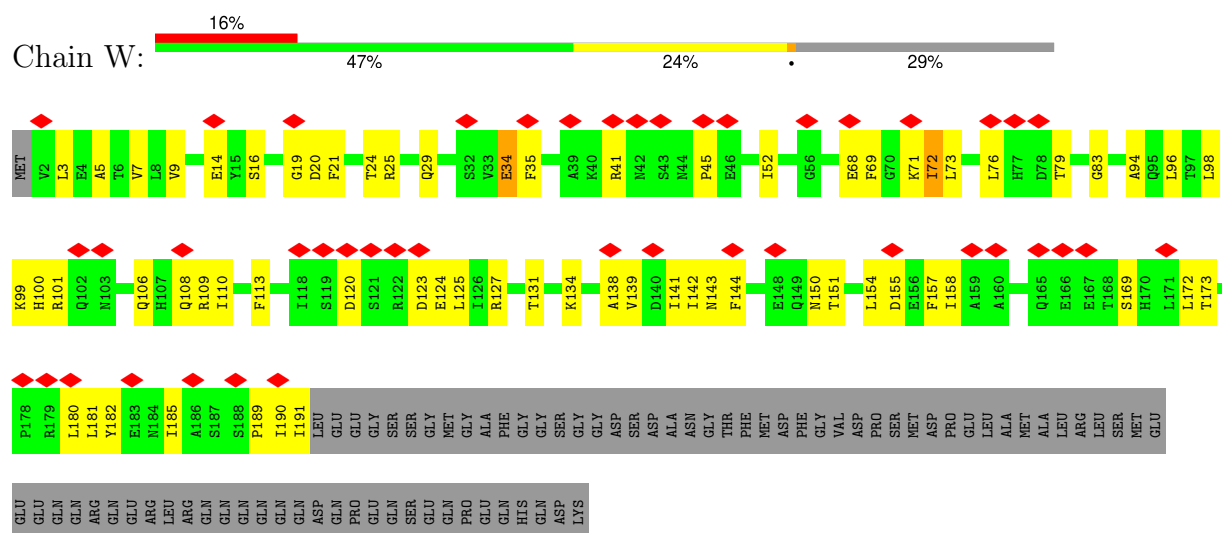


• Molecule 22: Ubiquitin carboxyl-terminal hydrolase RPN11

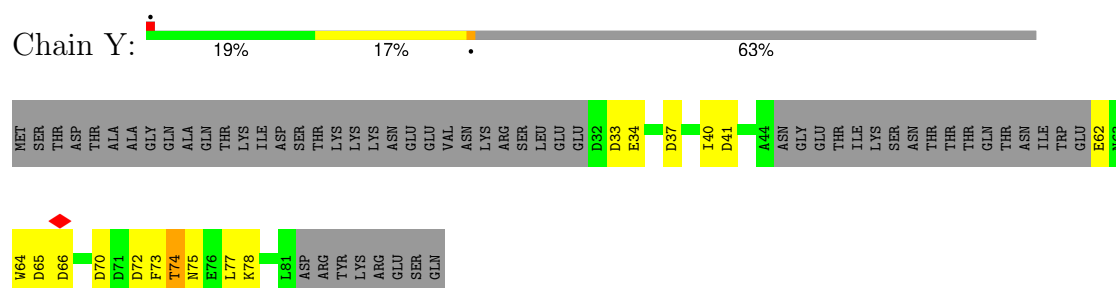
Chain V: 6% 60% 32% 6%



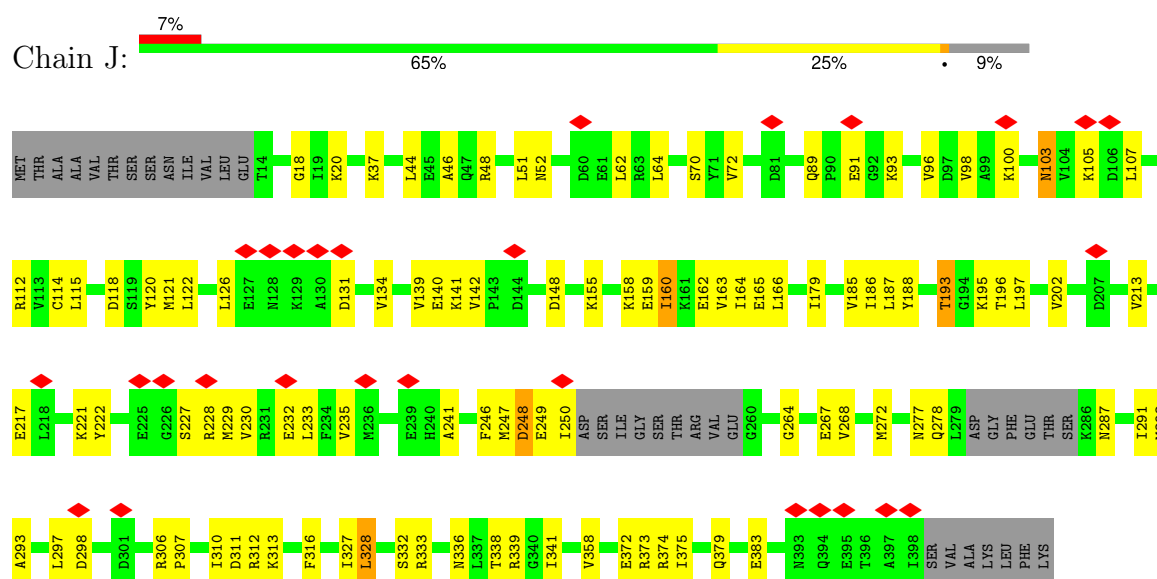
- Molecule 23: 26S proteasome regulatory subunit RPN10



- Molecule 24: 26S proteasome complex subunit SEM1

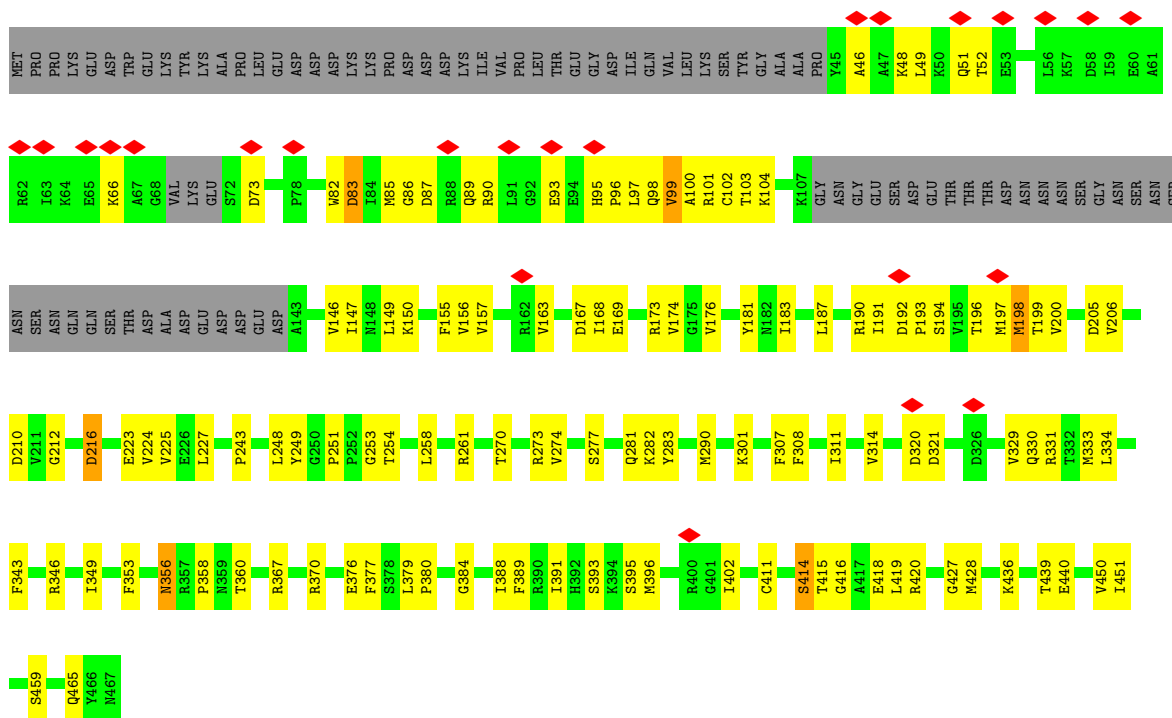


- Molecule 25: 26S proteasome regulatory subunit 8 homolog

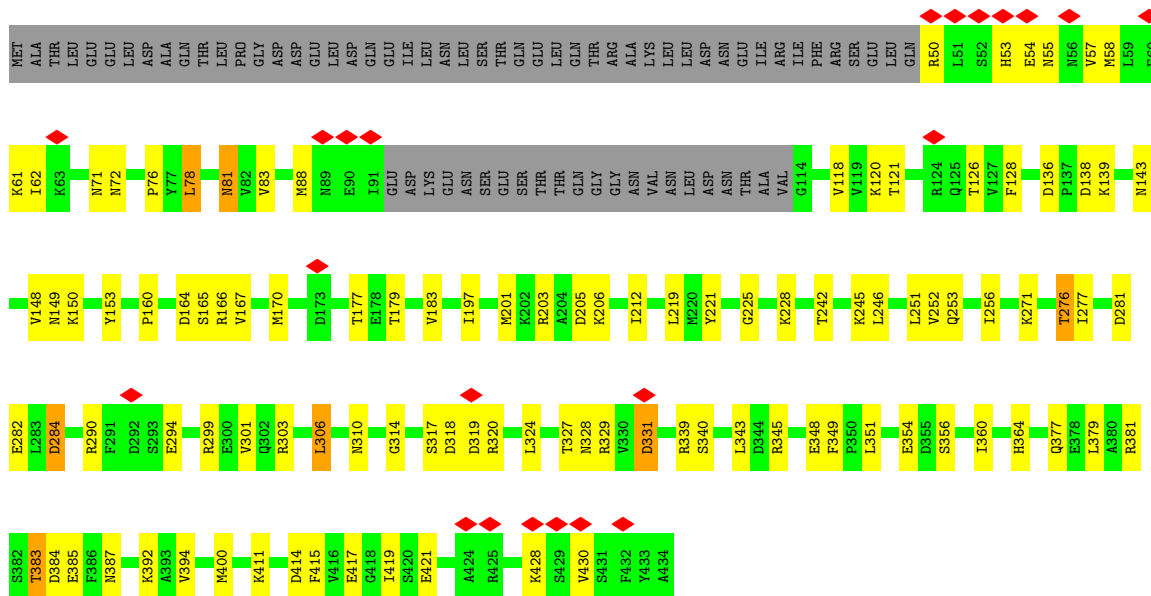


- Molecule 26: 26S proteasome regulatory subunit 7 homolog

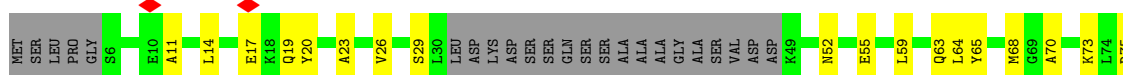


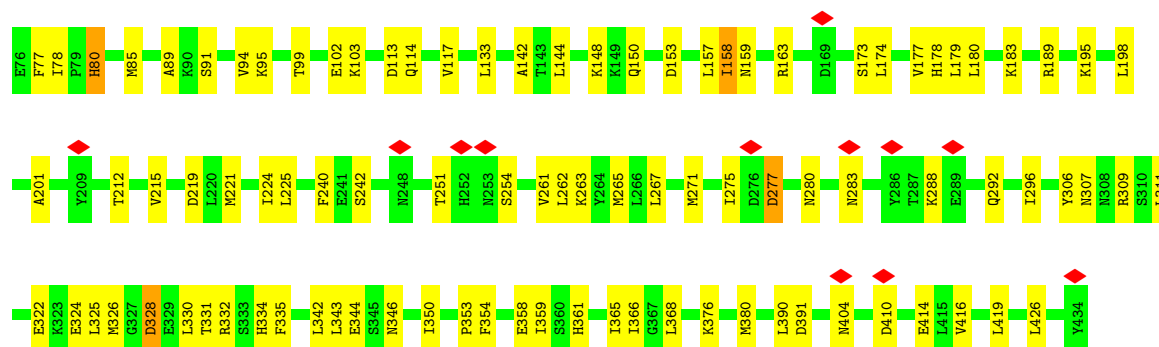


- Molecule 27: 26S proteasome regulatory subunit 6A

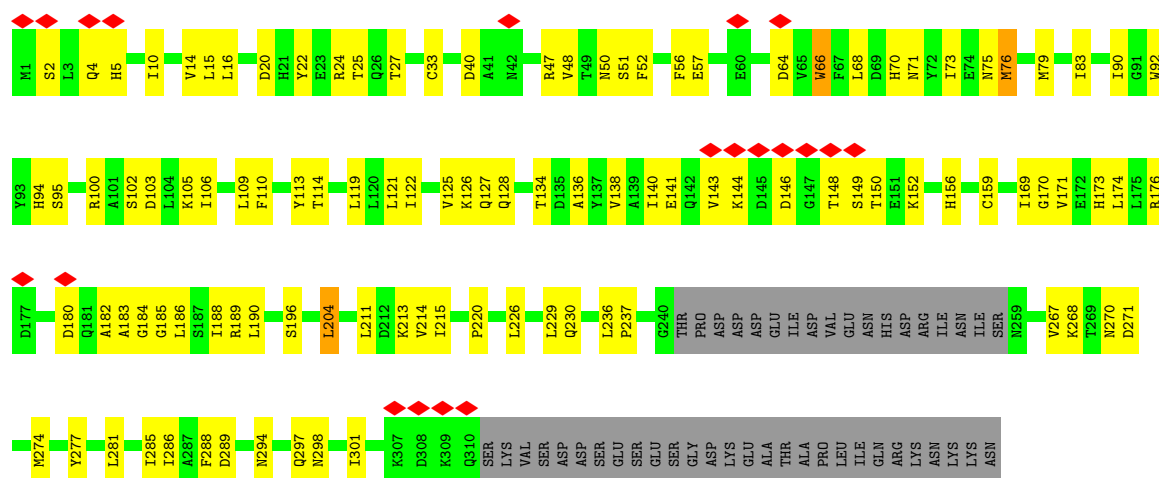


- Molecule 28: 26S proteasome regulatory subunit RPN6

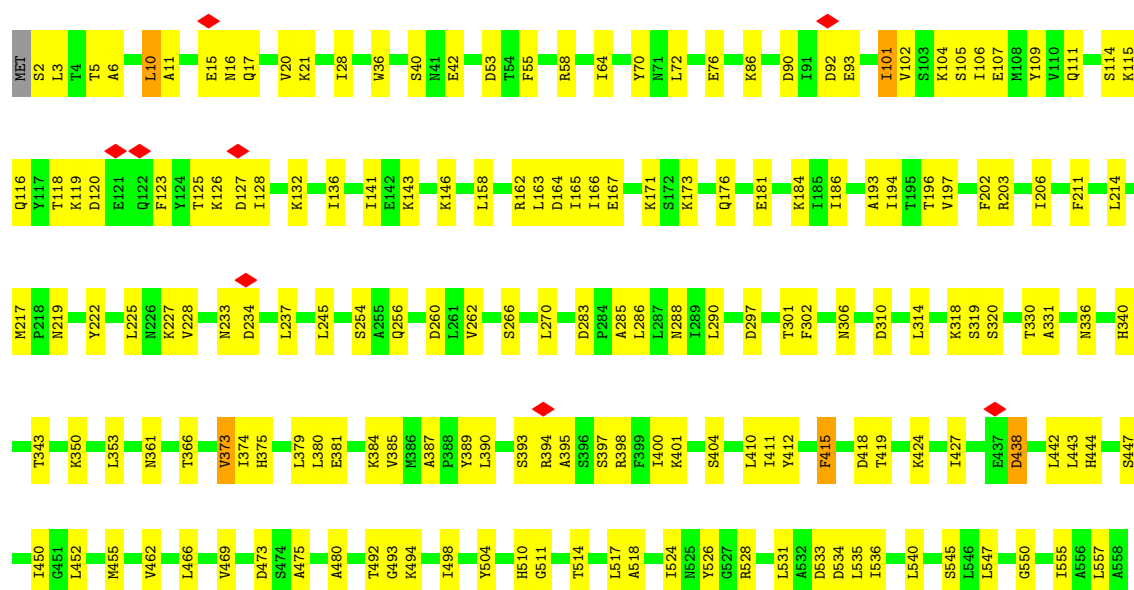


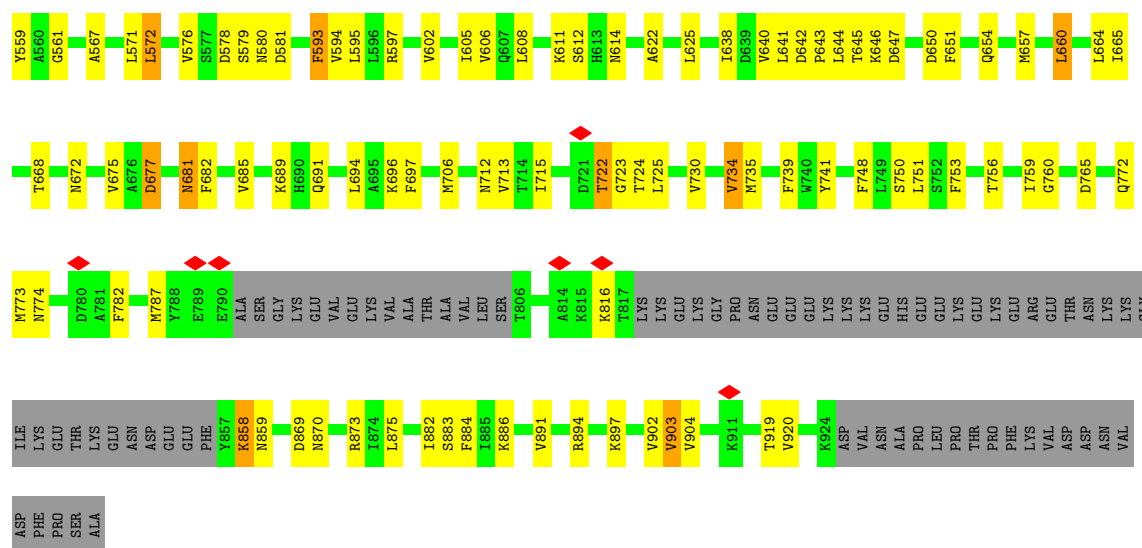


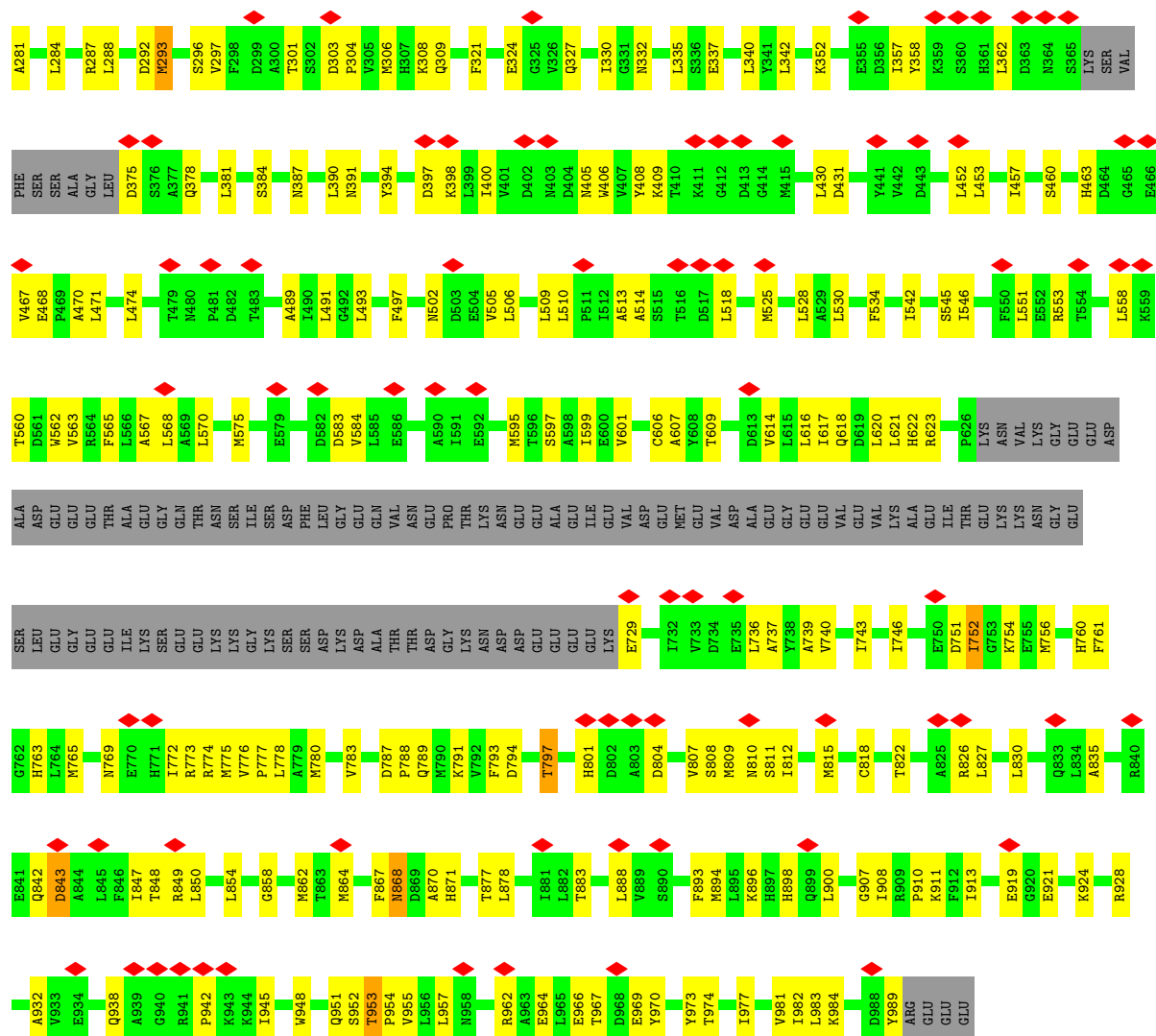
• Molecule 29: 26S proteasome regulatory subunit RPN8



• Molecule 30: 26S proteasome regulatory subunit RPN2







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110527	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.926	Depositor
Minimum map value	-0.797	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.33	Depositor
Map size (Å)	379.1, 379.1, 379.1	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.115, 1.115, 1.115	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.11	0/1605	0.30	0/2171
1	b	0.11	0/1605	0.28	0/2171
2	2	0.11	0/1715	0.31	0/2326
2	i	0.09	0/1715	0.27	0/2326
3	3	0.11	0/1611	0.29	0/2174
3	h	0.11	0/1611	0.28	0/2174
4	4	0.11	0/1613	0.34	0/2173
4	g	0.11	0/1613	0.32	0/2173
5	5	0.10	0/1681	0.30	0/2274
5	f	0.09	0/1681	0.29	0/2274
6	6	0.10	0/1795	0.29	0/2420
6	e	0.09	0/1795	0.24	0/2420
7	7	0.12	0/1855	0.36	0/2514
7	a	0.12	0/1855	0.36	0/2514
8	A	0.13	0/1959	0.33	0/2652
9	B	0.13	0/1952	0.37	1/2642 (0.0%)
10	C	0.11	0/1934	0.31	0/2618
11	D	0.12	0/1919	0.31	0/2598
12	E	0.11	0/1886	0.29	0/2541
13	F	0.16	0/1823	0.34	0/2463
14	G	0.14	0/1928	0.37	0/2603
15	I	0.14	0/3120	0.42	1/4204 (0.0%)
16	K	0.14	0/3078	0.35	0/4154
17	L	0.14	0/2862	0.35	0/3851
18	O	0.11	0/3230	0.33	0/4357
19	P	0.11	0/3629	0.31	0/4894
20	R	0.12	0/3249	0.33	0/4385
21	S	0.11	0/3839	0.31	0/5186
22	V	0.15	0/2302	0.39	0/3105
23	W	0.11	0/1507	0.29	0/2045
24	Y	0.15	0/287	0.40	0/391
25	J	0.13	0/2950	0.35	0/3960

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	H	0.14	0/3063	0.37	0/4120
27	M	0.13	0/2863	0.36	0/3855
28	Q	0.12	0/3402	0.31	0/4577
29	U	0.14	0/2364	0.37	0/3190
30	N	0.12	0/6835	0.32	1/9243 (0.0%)
31	T	0.12	0/2147	0.32	0/2900
32	o	0.12	0/6462	0.32	0/8771
All	All	0.12	0/94340	0.33	3/127409 (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
16	K	0	1
32	o	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	I	381	VAL	N-CA-C	-6.17	107.27	113.20
30	N	86	LYS	CB-CA-C	-5.48	109.78	117.23
9	B	2	THR	CB-CA-C	-5.32	109.46	115.79

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	K	92	VAL	Peptide
32	o	953	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1576	0	1552	62	0
1	b	1576	0	1552	51	0
2	2	1684	0	1685	62	0
2	i	1684	0	1685	54	0
3	3	1581	0	1571	62	0
3	h	1581	0	1571	62	0
4	4	1585	0	1590	58	0
4	g	1585	0	1590	61	0
5	5	1644	0	1592	66	0
5	f	1644	0	1592	55	0
6	6	1757	0	1708	66	0
6	e	1757	0	1708	55	0
7	7	1824	0	1829	79	0
7	a	1824	0	1829	81	0
8	A	1921	0	1910	73	0
9	B	1915	0	1929	59	0
10	C	1904	0	1901	57	0
11	D	1890	0	1900	59	0
12	E	1861	0	1836	60	0
13	F	1795	0	1797	61	0
14	G	1888	0	1880	71	0
15	I	3078	0	3147	131	0
16	K	3035	0	3099	102	0
17	L	2820	0	2895	99	0
18	O	3169	0	3196	105	0
19	P	3575	0	3662	99	0
20	R	3195	0	3214	94	0
21	S	3770	0	3819	101	0
22	V	2267	0	2266	77	0
23	W	1484	0	1494	47	0
24	Y	281	0	224	15	0
25	J	2913	0	3050	89	0
26	H	3016	0	3086	111	0
27	M	2827	0	2887	89	0
28	Q	3347	0	3380	75	0
29	U	2333	0	2396	83	0
30	N	6725	0	6796	189	0
31	T	2106	0	2099	50	0
32	o	6347	0	6319	192	0
33	H	1	0	0	0	0
33	I	1	0	0	0	0
33	K	1	0	0	0	0
33	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	M	1	0	0	0	0
34	H	31	0	12	3	0
34	J	31	0	12	3	0
34	K	31	0	12	6	0
34	L	31	0	12	0	0
34	M	31	0	12	4	0
35	V	1	0	0	0	0
36	J	27	0	12	4	0
All	All	92952	0	93308	2720	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 15.

All (2720) 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)
16:K:61:LEU:HD21	25:J:37:LYS:HB3	1.49	0.94
28:Q:419:LEU:HD23	29:U:285:ILE:HD12	1.48	0.93
29:U:126:LYS:HB2	29:U:128:GLN:HE22	1.36	0.90
15:I:67:ASP:HB3	32:o:614:VAL:HG11	1.58	0.85
12:E:166:ARG:HG2	13:F:58:SER:HB3	1.59	0.82
19:P:97:ILE:HD11	19:P:122:ILE:HG23	1.61	0.81
25:J:230:VAL:HG11	25:J:268:VAL:HG13	1.62	0.81
13:F:179:PHE:HA	13:F:182:ILE:HD12	1.62	0.80
3:h:187:VAL:HG23	3:h:200:LEU:HD21	1.64	0.79
32:o:470:ALA:O	32:o:474:LEU:HB2	1.82	0.79
32:o:737:ALA:HA	32:o:775:MET:HE1	1.64	0.79
6:6:47:ARG:HB2	6:6:219:ASP:HB2	1.65	0.79
16:K:282:PHE:HE2	16:K:293:GLN:HB2	1.48	0.78
28:Q:277:ASP:N	28:Q:277:ASP:OD1	2.16	0.78
21:S:465:ILE:HD11	29:U:277:TYR:HA	1.66	0.78
22:V:216:LEU:HD13	29:U:171:VAL:HG11	1.66	0.77
21:S:482:PRO:HB3	29:U:298:ASN:HB2	1.67	0.77
4:g:174:MET:HE3	4:g:174:MET:H	1.49	0.76
19:P:59:LEU:HD13	19:P:62:ILE:HD11	1.68	0.76
32:o:894:MET:HB3	32:o:900:LEU:HD11	1.67	0.76
18:O:242:ILE:HG21	18:O:248:TYR:HB2	1.66	0.76
30:N:657:MET:HE1	30:N:685:VAL:HG21	1.67	0.75
11:D:122:GLN:NE2	12:E:134:MET:SD	2.60	0.75
4:4:162:LYS:NZ	4:4:194:ASP:O	2.20	0.75
16:K:245:LYS:NZ	17:L:258:GLU:OE2	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:212:MET:SD	29:U:15:LEU:HD21	2.27	0.74
30:N:254:SER:HB3	30:N:286:LEU:HD21	1.67	0.74
16:K:378:LEU:HD21	16:K:415:VAL:HG21	1.69	0.74
13:F:173:GLU:OE2	27:M:381:ARG:NH1	2.20	0.74
14:G:107:ILE:HD12	14:G:108:PRO:HD2	1.67	0.74
17:L:87:LEU:HA	17:L:90:LYS:HD2	1.69	0.74
21:S:431:VAL:HG13	21:S:432:ILE:HG12	1.69	0.74
7:a:226:ARG:HG3	7:a:247:VAL:HG23	1.69	0.74
4:4:62:ALA:HB2	11:D:98:LEU:HD11	1.70	0.74
25:J:52:ASN:HD21	30:N:612:SER:HA	1.51	0.74
10:C:206:LEU:HA	10:C:210:ARG:HH12	1.51	0.74
32:o:597:SER:HB2	32:o:623:ARG:HH22	1.53	0.74
10:C:107:PRO:HG2	10:C:110:ILE:HG12	1.68	0.73
17:L:88:TYR:OH	27:M:61:LYS:HB2	1.88	0.73
3:3:15:MET:HB2	3:3:22:ALA:HB3	1.70	0.73
2:2:196:LEU:HB3	6:e:215:ILE:HB	1.68	0.73
20:R:218:CYS:SG	20:R:223:ASN:ND2	2.62	0.73
4:4:103:LEU:HD13	4:4:133:HIS:HE1	1.52	0.73
31:T:90:PHE:HB3	31:T:132:HIS:HD2	1.54	0.73
22:V:178:GLY:HA2	22:V:200:ASN:HD21	1.54	0.73
22:V:19:GLY:HA2	30:N:361:ASN:HD21	1.52	0.73
29:U:144:LYS:HD3	29:U:148:THR:HB	1.70	0.72
18:O:160:LYS:HB2	18:O:163:ILE:HG22	1.71	0.72
18:O:200:GLU:HG2	18:O:202:SER:H	1.55	0.72
21:S:258:GLU:OE1	21:S:258:GLU:N	2.21	0.72
32:o:384:SER:HB3	32:o:406:TRP:HZ2	1.54	0.72
13:F:49:LEU:HB2	13:F:197:ILE:HD11	1.70	0.72
21:S:155:LEU:O	21:S:159:ASN:ND2	2.23	0.72
5:f:80:ALA:HB3	5:f:175:MET:HE2	1.71	0.72
27:M:242:THR:HB	27:M:276:THR:HG22	1.71	0.72
30:N:518:ALA:HB1	30:N:550:GLY:HA3	1.71	0.72
15:I:100:ARG:NH2	26:H:73:ASP:O	2.22	0.72
8:A:184:ASN:OD1	8:A:185:HIS:N	2.23	0.72
30:N:557:LEU:HD21	30:N:734:VAL:HG21	1.71	0.71
5:5:242:ARG:HH22	5:5:284:ASN:HD21	1.38	0.71
26:H:48:LYS:O	26:H:52:THR:OG1	2.09	0.71
22:V:179:LEU:HB3	30:N:694:LEU:HD21	1.73	0.71
25:J:195:LYS:NZ	36:J:502:ADP:O1B	2.23	0.71
32:o:474:LEU:HD13	32:o:493:LEU:HG	1.72	0.71
15:I:66:LYS:NZ	26:H:52:THR:O	2.23	0.71
26:H:258:LEU:HD22	34:H:501:ATP:H2'	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Q:65:TYR:HA	28:Q:68:MET:HE2	1.72	0.71
16:K:135:MET:HE2	16:K:135:MET:HA	1.73	0.71
7:a:164:ASN:HD21	7:a:168:VAL:HB	1.55	0.71
26:H:331:ARG:HD3	27:M:252:VAL:HG21	1.74	0.70
32:o:268:ALA:HA	32:o:271:ILE:HD12	1.73	0.70
20:R:261:LEU:HB3	20:R:265:ASP:HB2	1.71	0.70
11:D:204:GLN:O	11:D:205:THR:OG1	2.10	0.70
4:4:172:MET:HA	4:4:172:MET:HE3	1.71	0.70
9:B:189:ILE:HD12	9:B:213:ILE:HD11	1.74	0.70
15:I:253:ILE:HD11	15:I:287:ILE:HA	1.74	0.70
28:Q:309:ARG:O	28:Q:346:ASN:ND2	2.24	0.70
10:C:69:LEU:HD11	10:C:75:VAL:HB	1.74	0.70
15:I:120:VAL:HG21	15:I:149:LEU:HD21	1.71	0.70
32:o:777:PRO:HB3	32:o:811:SER:HA	1.74	0.70
13:F:82:ARG:HH21	13:F:86:ASN:HD21	1.38	0.70
19:P:59:LEU:HD12	19:P:96:MET:HG3	1.74	0.69
7:a:83:VAL:HG12	7:a:233:ILE:HD11	1.73	0.69
2:i:235:PRO:O	2:i:238:THR:OG1	2.10	0.69
9:B:103:GLU:OE1	9:B:103:GLU:N	2.25	0.69
21:S:90:LYS:HG2	21:S:94:LYS:HE3	1.74	0.69
11:D:148:TYR:HE1	11:D:158:SER:HB2	1.57	0.69
18:O:50:ASP:OD1	18:O:80:LYS:NZ	2.25	0.69
3:3:164:PHE:HB2	3:3:189:ILE:HD11	1.75	0.69
3:3:96:TYR:HA	3:3:99:ARG:HH12	1.57	0.69
5:5:82:ARG:HD2	5:5:185:PRO:HB2	1.75	0.69
16:K:105:GLN:NE2	22:V:267:LYS:O	2.26	0.69
17:L:284:ASP:OD2	27:M:290:ARG:NH1	2.26	0.69
21:S:93:LEU:HD23	21:S:96:ILE:HD11	1.75	0.69
2:2:197:GLY:H	6:e:52:TYR:HE1	1.41	0.69
13:F:72:LEU:HD11	13:F:88:LEU:HD23	1.74	0.69
19:P:119:ILE:HG21	19:P:143:LEU:HB2	1.75	0.69
19:P:160:LEU:HG	19:P:183:GLN:HG3	1.73	0.69
6:6:185:GLY:HA3	2:i:240:ALA:HB2	1.75	0.68
27:M:294:GLU:OE1	27:M:294:GLU:N	2.25	0.68
30:N:194:ILE:HA	30:N:203:ARG:HH12	1.56	0.68
1:1:158:ASP:HB3	1:b:180:GLN:HE22	1.58	0.68
13:F:100:ASN:O	13:F:100:ASN:ND2	2.27	0.68
11:D:48:ARG:HB2	11:D:209:ASN:HB2	1.74	0.68
2:2:243:LYS:HB3	3:3:199:TYR:HD2	1.58	0.68
4:4:3:ILE:HD13	4:4:176:PHE:HB3	1.76	0.68
1:b:165:MET:SD	1:b:170:THR:OG1	2.50	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:95:LEU:HD22	14:G:118:GLN:HG3	1.75	0.68
12:E:85:ALA:HB2	12:E:140:VAL:HG21	1.76	0.68
29:U:148:THR:HG22	29:U:149:SER:H	1.59	0.68
1:b:196:VAL:HB	1:b:203:GLU:HB2	1.76	0.68
26:H:147:ILE:HD12	26:H:157:VAL:HB	1.76	0.68
32:o:452:LEU:HD11	32:o:474:LEU:HD23	1.75	0.68
7:a:137:ARG:NH1	6:e:23:PRO:O	2.26	0.68
30:N:301:THR:HG22	30:N:920:VAL:HG23	1.76	0.68
16:K:94:LEU:HB2	17:L:128:ILE:HB	1.76	0.68
19:P:165:VAL:HA	19:P:168:TYR:HD2	1.59	0.67
5:f:220:LYS:HB2	5:f:223:LEU:HG	1.75	0.67
16:K:219:LYS:NZ	34:K:501:ATP:O1G	2.27	0.67
17:L:179:THR:HG23	17:L:181:ASP:H	1.58	0.67
6:e:171:ASN:OD1	6:e:178:GLN:NE2	2.26	0.67
2:2:39:ASN:ND2	2:2:208:GLU:OE2	2.28	0.67
32:o:812:ILE:HD11	32:o:847:ILE:HG23	1.76	0.67
11:D:163:THR:HG21	11:D:171:VAL:HB	1.76	0.67
1:1:32:ILE:HD12	1:1:196:VAL:HG22	1.76	0.67
19:P:384:VAL:HG11	28:Q:353:PRO:HB3	1.75	0.67
2:i:105:VAL:HG21	2:i:138:HIS:HB2	1.76	0.67
30:N:578:ASP:OD1	30:N:579:SER:N	2.28	0.67
19:P:119:ILE:HD12	19:P:139:VAL:HG13	1.76	0.67
4:4:172:MET:HE3	4:4:173:PRO:HD2	1.77	0.67
15:I:231:LEU:HD22	34:J:501:ATP:H2'	1.77	0.67
19:P:266:TYR:OH	19:P:296:GLN:NE2	2.27	0.67
19:P:357:TYR:HD2	19:P:360:ILE:HB	1.60	0.67
22:V:215:ASN:HA	22:V:218:LYS:HD3	1.77	0.67
25:J:185:VAL:HG13	25:J:312:ARG:HB2	1.77	0.67
2:2:105:VAL:HG11	2:2:138:HIS:HB2	1.77	0.66
16:K:420:THR:OG1	16:K:421:VAL:N	2.28	0.66
22:V:26:THR:HG22	22:V:200:ASN:HB2	1.77	0.66
31:T:60:ARG:O	31:T:64:VAL:HG23	1.95	0.66
32:o:843:ASP:OD1	32:o:843:ASP:N	2.28	0.66
7:7:126:PHE:HB2	7:7:149:VAL:HG11	1.76	0.66
7:a:43:SER:OG	7:a:180:GLY:N	2.27	0.66
7:a:34:THR:N	7:a:140:MET:O	2.28	0.66
1:1:60:ILE:HD13	1:1:120:GLY:HA3	1.76	0.66
4:4:152:MET:HE1	4:4:160:LEU:HD12	1.77	0.66
10:C:4:ARG:HG2	11:D:6:ARG:HH22	1.61	0.66
17:L:88:TYR:HE1	27:M:58:MET:HE2	1.60	0.66
4:g:158:LEU:O	4:g:162:LYS:HG2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:164:MET:HA	2:2:167:LEU:HG	1.78	0.66
20:R:138:GLY:HA3	20:R:154:LEU:HD21	1.77	0.66
7:a:38:ILE:HG22	7:a:39:VAL:HG23	1.78	0.66
6:e:49:ILE:HG22	6:e:54:ILE:HA	1.76	0.66
6:e:120:ARG:HD2	5:f:170:LEU:HD21	1.77	0.66
8:A:243:GLU:OE1	8:A:244:ARG:NH1	2.29	0.66
16:K:194:GLN:OE1	25:J:373:ARG:NH2	2.29	0.66
18:O:163:ILE:HD12	18:O:167:ILE:HB	1.77	0.66
22:V:59:ASP:OD1	22:V:61:TYR:N	2.28	0.66
32:o:463:HIS:ND1	32:o:468:GLU:OE2	2.29	0.66
6:6:49:ILE:HG22	6:6:54:ILE:HA	1.76	0.66
30:N:2:SER:OG	30:N:3:LEU:N	2.29	0.66
32:o:736:LEU:HD13	32:o:772:ILE:HD11	1.78	0.66
20:R:238:PHE:O	25:J:339:ARG:NH1	2.29	0.65
7:7:60:LEU:HD11	7:7:67:LEU:HB3	1.78	0.65
13:F:6:TYR:OH	14:G:9:ASP:OD2	2.09	0.65
22:V:148:LYS:HG2	29:U:169:ILE:HD12	1.79	0.65
10:C:91:ALA:HB2	10:C:115:LEU:HD21	1.77	0.65
7:a:166:LEU:HB3	6:e:76:PHE:HZ	1.62	0.65
8:A:135:ARG:HB3	14:G:13:SER:HB2	1.77	0.65
22:V:100:ARG:NH2	29:U:20:ASP:OD2	2.29	0.65
4:4:169:GLU:O	4:g:177:LYS:NZ	2.29	0.65
22:V:126:GLN:NE2	22:V:136:ALA:O	2.30	0.65
22:V:225:LEU:O	22:V:301:ASN:ND2	2.28	0.65
23:W:98:LEU:HD13	23:W:108:GLN:HB3	1.78	0.65
29:U:14:VAL:HG21	29:U:48:VAL:HG12	1.78	0.65
30:N:283:ASP:HB3	30:N:286:LEU:HD12	1.78	0.65
3:3:23:ILE:HG23	3:3:188:TYR:HB2	1.77	0.65
3:3:201:LYS:HG2	5:f:273:TRP:HZ2	1.61	0.65
16:K:256:ASP:OD1	16:K:259:ARG:NH2	2.29	0.65
18:O:171:PHE:O	18:O:175:ASN:ND2	2.30	0.65
26:H:206:VAL:HG21	26:H:261:ARG:HB3	1.79	0.65
7:7:161:ARG:HE	7:7:171:SER:HB2	1.61	0.65
17:L:339:ARG:HH21	17:L:342:ARG:HG3	1.61	0.65
20:R:319:CYS:SG	20:R:320:LYS:N	2.69	0.65
10:C:137:TYR:HE1	10:C:151:SER:HB3	1.63	0.64
11:D:83:ARG:HA	11:D:86:ILE:HD12	1.78	0.64
20:R:408:ASP:OD1	21:S:464:ARG:NE	2.30	0.64
32:o:514:ALA:HB2	32:o:545:SER:HB3	1.79	0.64
4:4:102:VAL:HG12	4:4:119:ILE:HB	1.78	0.64
10:C:53:THR:HG21	10:C:210:ARG:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:48:ARG:NH2	2:i:153:TYR:OH	2.30	0.64
32:o:161:ILE:HD11	32:o:203:LEU:HD23	1.80	0.64
20:R:406:GLN:HB3	28:Q:416:VAL:HG11	1.79	0.64
1:b:52:LYS:HA	1:b:64:ARG:HH21	1.62	0.64
30:N:691:GLN:HB2	30:N:696:LYS:HE2	1.80	0.64
15:I:51:PRO:HD2	15:I:58:LYS:HB2	1.79	0.64
32:o:788:PRO:HG3	32:o:822:THR:HG21	1.80	0.64
4:4:171:ARG:HE	4:g:27:VAL:HB	1.62	0.64
6:6:116:LEU:HD13	6:6:148:GLY:HA2	1.79	0.64
11:D:69:SER:OG	11:D:219:SER:OG	2.15	0.64
7:a:86:ILE:HD12	7:a:147:ILE:HG12	1.78	0.64
26:H:330:GLN:O	26:H:334:LEU:HG	1.98	0.64
28:Q:306:TYR:HA	28:Q:342:LEU:HD21	1.79	0.64
32:o:108:ASP:N	32:o:108:ASP:OD1	2.31	0.64
8:A:46:ARG:NH2	8:A:192:ASP:OD1	2.31	0.64
18:O:319:LEU:HD12	18:O:327:LEU:HD12	1.80	0.64
22:V:21:ASP:O	22:V:172:GLN:NE2	2.31	0.64
22:V:53:MET:HG3	22:V:68:VAL:HG12	1.80	0.64
28:Q:325:LEU:HD13	28:Q:335:PHE:HE2	1.63	0.64
30:N:125:THR:HB	30:N:128:ILE:HG12	1.80	0.64
1:1:48:ARG:NH2	2:2:153:TYR:OH	2.31	0.63
9:B:239:THR:OG1	9:B:242:GLU:OE1	2.16	0.63
28:Q:366:ILE:HG23	28:Q:368:LEU:H	1.62	0.63
9:B:5:TYR:OH	14:G:127:ASN:ND2	2.30	0.63
10:C:160:TRP:CD2	10:C:163:ILE:HD13	2.33	0.63
2:2:42:VAL:HB	2:2:206:VAL:HG13	1.79	0.63
8:A:238:ALA:HA	8:A:241:ILE:HD12	1.79	0.63
11:D:203:VAL:HG11	11:D:210:ILE:HD11	1.79	0.63
15:I:124:THR:OG1	15:I:125:MET:SD	2.55	0.63
16:K:68:ILE:HD11	30:N:608:LEU:HG	1.80	0.63
20:R:170:VAL:O	20:R:174:ILE:HD12	1.97	0.63
13:F:9:ASP:OD1	13:F:9:ASP:N	2.30	0.63
16:K:255:ARG:HG2	16:K:302:GLN:HE21	1.62	0.63
19:P:266:TYR:HB3	19:P:329:PHE:HE2	1.63	0.63
22:V:280:LEU:HD23	29:U:286:ILE:HD11	1.80	0.63
6:6:215:ILE:HB	2:i:196:LEU:HB3	1.81	0.63
16:K:215:PRO:HB3	16:K:319:ASN:HD22	1.62	0.63
4:g:182:LYS:HG2	4:g:191:GLN:HG3	1.80	0.63
17:L:285:ALA:HB1	27:M:303:ARG:HD3	1.81	0.63
3:3:67:PHE:O	3:3:71:THR:HG23	1.99	0.63
15:I:138:LYS:HA	15:I:141:LEU:HD12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:K:236:ARG:HH11	17:L:315:PHE:HB3	1.64	0.63
1:1:162:ARG:HH22	1:1:169:GLU:HB3	1.64	0.62
4:4:36:ARG:HB2	4:4:44:MET:HB3	1.81	0.62
8:A:147:ASP:O	8:A:151:GLY:N	2.31	0.62
27:M:201:MET:HE1	27:M:277:ILE:HD11	1.80	0.62
30:N:677:ASP:OD1	30:N:677:ASP:N	2.26	0.62
12:E:10:ARG:HH21	13:F:3:ARG:HD3	1.65	0.62
19:P:39:LEU:HD13	19:P:62:ILE:HG22	1.81	0.62
29:U:2:SER:HB2	29:U:4:GLN:HG2	1.80	0.62
29:U:134:THR:OG1	29:U:159:CYS:SG	2.55	0.62
30:N:163:LEU:HA	30:N:166:ILE:HD12	1.80	0.62
30:N:306:ASN:O	30:N:712:ASN:ND2	2.32	0.62
4:4:108:ASP:OD2	4:4:111:LYS:NZ	2.31	0.62
10:C:158:THR:OG1	10:C:160:TRP:NE1	2.32	0.62
19:P:133:GLU:HB3	19:P:168:TYR:HD1	1.63	0.62
20:R:54:ILE:HD13	20:R:63:TYR:HD1	1.64	0.62
26:H:248:LEU:HD22	26:H:377:PHE:HE2	1.63	0.62
5:5:131:GLU:OE2	5:5:174:THR:OG1	2.16	0.62
15:I:89:GLN:HG2	15:I:90:GLU:H	1.64	0.62
16:K:200:GLN:NE2	25:J:375:ILE:O	2.26	0.62
27:M:71:ASN:OD1	27:M:72:ASN:ND2	2.32	0.62
3:h:18:LYS:NZ	3:h:157:ASN:O	2.28	0.62
30:N:211:PHE:HB2	30:N:228:VAL:HG11	1.82	0.62
30:N:645:THR:HG23	30:N:646:LYS:HE2	1.80	0.62
16:K:330:ARG:NH1	25:J:140:GLU:O	2.33	0.62
20:R:63:TYR:OH	20:R:93:LYS:O	2.18	0.62
29:U:64:ASP:OD2	29:U:105:LYS:NZ	2.32	0.62
5:f:179:TYR:O	5:f:181:ARG:NH2	2.33	0.62
2:2:56:ALA:O	6:e:213:ARG:NH2	2.33	0.62
2:2:58:LYS:NZ	6:e:212:GLU:O	2.31	0.62
7:7:35:GLN:NE2	7:7:142:PRO:O	2.32	0.62
10:C:62:SER:OG	10:C:64:GLU:OE2	2.13	0.62
16:K:360:MET:HE1	16:K:387:MET:HB3	1.82	0.62
18:O:18:ALA:HB2	18:O:57:LEU:HD21	1.82	0.62
19:P:133:GLU:HB3	19:P:168:TYR:CD1	2.35	0.62
6:6:23:PRO:O	7:7:137:ARG:NH1	2.33	0.62
11:D:107:GLU:HA	11:D:148:TYR:HE2	1.65	0.62
2:i:64:HIS:HB3	2:i:85:THR:HG21	1.80	0.62
3:3:118:LYS:NZ	3:3:119:PRO:O	2.33	0.62
22:V:293:VAL:HG21	29:U:189:ARG:HE	1.65	0.62
31:T:200:LEU:HD12	31:T:201:PRO:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:48:ARG:HH12	2:2:55:VAL:HG21	1.65	0.61
9:B:33:THR:HA	9:B:165:GLY:HA3	1.81	0.61
12:E:41:ALA:HA	12:E:46:VAL:HG22	1.81	0.61
14:G:79:SER:OG	14:G:165:THR:OG1	2.09	0.61
19:P:218:LEU:HD21	19:P:247:THR:HG21	1.82	0.61
3:h:143:SER:HA	3:h:146:LEU:HD12	1.81	0.61
25:J:195:LYS:HG2	25:J:316:PHE:HD2	1.65	0.61
26:H:104:LYS:NZ	27:M:160:PRO:O	2.33	0.61
27:M:331:ASP:OD1	27:M:331:ASP:N	2.32	0.61
20:R:368:LEU:HD22	20:R:381:ILE:HD11	1.82	0.61
28:Q:198:LEU:HD13	28:Q:225:LEU:HD12	1.81	0.61
28:Q:288:LYS:HA	28:Q:292:GLN:HB2	1.82	0.61
14:G:137:ILE:HD11	14:G:165:THR:HG23	1.82	0.61
16:K:96:ILE:O	16:K:113:THR:OG1	2.18	0.61
16:K:331:PRO:O	25:J:141:LYS:NZ	2.30	0.61
17:L:292:SER:OG	17:L:293:GLU:OE1	2.17	0.61
21:S:322:LEU:HB3	21:S:383:LEU:HD21	1.82	0.61
7:a:232:ILE:HB	7:a:240:THR:HB	1.81	0.61
10:C:233:GLN:HA	10:C:236:LYS:HE2	1.81	0.61
17:L:223:PRO:HB3	17:L:432:ILE:HG21	1.82	0.61
32:o:68:LEU:HD11	32:o:114:SER:HB2	1.82	0.61
18:O:130:ASP:HA	18:O:133:ILE:HD12	1.81	0.61
22:V:53:MET:HE1	22:V:139:VAL:HG21	1.82	0.61
23:W:142:ILE:HG23	23:W:172:LEU:HD23	1.83	0.61
21:S:210:LEU:HG	21:S:214:MET:HE2	1.82	0.61
6:e:229:ASP:OD1	6:e:232:ARG:NH2	2.33	0.61
2:i:115:HIS:HA	2:i:118:LYS:HE3	1.83	0.61
30:N:447:SER:HB2	30:N:466:LEU:HD11	1.82	0.61
31:T:79:GLU:OE2	31:T:112:ASN:ND2	2.33	0.61
5:5:276:LYS:NZ	5:5:287:GLY:O	2.28	0.61
7:7:181:ALA:O	7:7:185:ASN:ND2	2.32	0.61
15:I:255:LYS:NZ	25:J:217:GLU:HB3	2.16	0.61
7:a:87:SER:HB3	7:a:146:ALA:HB3	1.83	0.61
2:2:48:ARG:HH22	6:e:215:ILE:HG22	1.66	0.61
22:V:212:MET:HG2	29:U:127:GLN:HE21	1.64	0.61
26:H:216:ASP:N	26:H:216:ASP:OD1	2.33	0.61
30:N:222:TYR:HA	30:N:225:LEU:HD12	1.81	0.61
8:A:200:GLU:OE1	8:A:201:LYS:NZ	2.34	0.61
16:K:236:ARG:NH1	17:L:315:PHE:O	2.34	0.61
7:a:132:VAL:O	7:a:136:ARG:HG2	2.01	0.61
32:o:55:ARG:HB2	32:o:67:SER:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:87:ILE:HB	5:5:255:VAL:HB	1.83	0.61
11:D:122:GLN:OE1	12:E:136:ARG:NH1	2.34	0.61
16:K:193:VAL:HG12	16:K:194:GLN:HG3	1.83	0.61
4:g:47:ALA:N	4:g:101:ASN:O	2.32	0.61
25:J:372:GLU:OE1	25:J:374:ARG:NH2	2.34	0.61
2:2:192:ILE:HB	2:2:199:GLY:HA2	1.81	0.60
7:7:54:ILE:HG12	7:7:232:ILE:HG13	1.82	0.60
13:F:219:ASP:N	13:F:219:ASP:OD1	2.34	0.60
17:L:196:VAL:HG13	17:L:215:PRO:HG2	1.83	0.60
20:R:54:ILE:HA	20:R:59:MET:HG2	1.81	0.60
15:I:369:MET:HB3	15:I:371:LEU:HG	1.83	0.60
21:S:204:ASP:N	21:S:204:ASP:OD1	2.31	0.60
6:e:71:MET:HE1	6:e:84:VAL:HG22	1.83	0.60
6:6:77:ALA:HB3	7:7:168:VAL:HG12	1.82	0.60
11:D:70:HIS:NE2	11:D:104:VAL:O	2.30	0.60
13:F:35:THR:OG1	13:F:73:SER:OG	2.17	0.60
6:e:153:GLU:HG3	6:e:156:ARG:HG3	1.84	0.60
26:H:253:GLY:O	26:H:415:THR:OG1	2.15	0.60
27:M:299:ARG:O	27:M:303:ARG:NH2	2.34	0.60
32:o:280:ASP:O	32:o:284:LEU:HD12	2.00	0.60
5:5:79:LEU:HD13	5:5:215:LEU:HD21	1.83	0.60
6:6:41:VAL:HG12	6:6:225:ILE:HG13	1.82	0.60
15:I:130:VAL:HG13	15:I:155:SER:HA	1.83	0.60
7:a:214:MET:HE1	7:a:247:VAL:HA	1.82	0.60
26:H:89:GLN:O	26:H:95:HIS:NE2	2.34	0.60
3:3:125:ASP:OD1	3:3:129:CYS:N	2.33	0.60
15:I:256:TYR:HE1	16:K:281:ARG:HH22	1.49	0.60
20:R:334:ARG:NH1	24:Y:70:ASP:OD2	2.35	0.60
15:I:60:LEU:O	15:I:64:ARG:HG2	2.01	0.60
22:V:151:VAL:H	29:U:173:HIS:HD2	1.50	0.60
7:a:125:ILE:O	7:a:129:LEU:HG	2.01	0.60
4:g:176:PHE:HD1	4:g:178:GLY:H	1.50	0.60
27:M:88:MET:O	27:M:88:MET:HE3	2.02	0.60
30:N:606:VAL:HG21	30:N:625:LEU:HD21	1.83	0.60
32:o:525:MET:HA	32:o:528:LEU:HD12	1.83	0.60
11:D:37:LYS:HB3	11:D:42:VAL:HG23	1.83	0.60
11:D:151:GLU:HG3	11:D:152:PRO:HD2	1.84	0.60
13:F:32:GLY:O	13:F:163:ALA:N	2.33	0.60
23:W:155:ASP:N	23:W:155:ASP:OD1	2.33	0.60
7:a:60:LEU:HD11	7:a:67:LEU:HB3	1.82	0.60
5:f:82:ARG:NH1	5:f:185:PRO:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:o:518:LEU:O	32:o:553:ARG:NH1	2.28	0.60
5:5:156:LYS:HE2	11:D:101:GLU:HB2	1.83	0.60
16:K:378:LEU:HD13	16:K:383:ILE:HG22	1.82	0.60
18:O:186:ASN:OD1	18:O:226:LYS:N	2.35	0.60
21:S:84:ASP:OD1	21:S:89:LYS:NZ	2.34	0.60
21:S:482:PRO:HA	21:S:485:LYS:HB2	1.84	0.60
7:a:46:SER:HB2	7:a:55:ILE:HG13	1.82	0.60
1:1:58:ASP:N	1:1:58:ASP:OD1	2.34	0.60
20:R:21:VAL:O	20:R:176:ARG:NH1	2.34	0.60
20:R:358:GLY:HA2	24:Y:78:LYS:HE2	1.83	0.60
32:o:135:LEU:HD11	32:o:160:GLU:HB3	1.84	0.60
8:A:126:GLN:HE21	9:B:81:ASP:HA	1.67	0.59
17:L:284:ASP:OD1	17:L:284:ASP:N	2.34	0.59
18:O:107:GLN:O	18:O:111:SER:HB3	2.02	0.59
20:R:313:ALA:HA	20:R:317:ILE:HD11	1.84	0.59
7:a:60:LEU:HD22	7:a:225:SER:HB3	1.82	0.59
7:7:180:GLY:HA2	7:7:183:MET:HB2	1.84	0.59
8:A:72:ILE:HG12	8:A:82:VAL:HG22	1.82	0.59
15:I:246:ARG:HH12	25:J:278:GLN:HB3	1.68	0.59
15:I:329:ASN:OD1	15:I:329:ASN:N	2.35	0.59
17:L:270:ALA:HB2	17:L:278:ILE:HD11	1.83	0.59
22:V:55:GLY:HA2	22:V:66:VAL:HG23	1.84	0.59
3:3:28:ARG:NH2	3:3:205:ASP:OXT	2.36	0.59
6:6:165:ILE:HD12	6:6:206:SER:HB3	1.85	0.59
11:D:182:LYS:HG3	11:D:183:GLU:HG2	1.84	0.59
15:I:113:ILE:HD12	15:I:113:ILE:O	2.02	0.59
15:I:240:THR:HG22	15:I:242:ALA:H	1.67	0.59
18:O:58:ARG:HB3	18:O:85:SER:HA	1.82	0.59
26:H:193:PRO:O	26:H:196:THR:OG1	2.16	0.59
2:2:48:ARG:NH2	2:2:196:LEU:O	2.36	0.59
7:7:113:LEU:HB3	7:7:117:GLU:HB3	1.84	0.59
15:I:55:CYS:HG	32:o:248:TYR:HH	1.51	0.59
15:I:282:ASP:OD1	15:I:283:GLU:N	2.35	0.59
17:L:84:LEU:HB3	27:M:58:MET:HE3	1.83	0.59
18:O:130:ASP:HB2	18:O:153:LEU:HD21	1.83	0.59
6:e:34:ILE:HD13	6:e:155:CYS:HB3	1.85	0.59
32:o:774:ARG:O	32:o:810:ASN:ND2	2.35	0.59
2:2:47:THR:HB	2:2:59:ASN:HA	1.85	0.59
9:B:215:GLY:O	9:B:234:ARG:NH1	2.35	0.59
17:L:79:GLN:OE1	17:L:82:ARG:NH1	2.36	0.59
4:g:46:PHE:HD2	4:g:53:THR:HB	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:56:ALA:HB2	7:7:230:LEU:HD13	1.84	0.59
8:A:176:GLN:O	8:A:180:THR:HG23	2.02	0.59
26:H:270:THR:HG21	26:H:301:LYS:HD3	1.83	0.59
32:o:868:ASN:OD1	32:o:868:ASN:N	2.35	0.59
8:A:68:THR:HG21	14:G:159:GLY:HA3	1.84	0.59
12:E:201:LEU:HB3	12:E:243:LEU:HD22	1.83	0.59
14:G:71:ASP:OD1	14:G:72:ARG:N	2.35	0.59
15:I:103:PRO:HG3	25:J:120:TYR:HB2	1.85	0.59
17:L:84:LEU:HD22	27:M:58:MET:HE1	1.85	0.59
5:f:166:LYS:O	4:g:96:ARG:NH2	2.36	0.59
28:Q:75:ARG:HH21	28:Q:113:ASP:HA	1.67	0.59
30:N:398:ARG:HD2	30:N:438:ASP:HA	1.85	0.59
14:G:177:GLU:HG3	17:L:420:ARG:HH12	1.67	0.59
15:I:129:TYR:HB3	26:H:97:LEU:HB2	1.83	0.59
15:I:380:LEU:HD22	15:I:381:VAL:HG23	1.84	0.59
16:K:142:HIS:ND1	16:K:142:HIS:O	2.36	0.59
7:a:54:ILE:HG12	7:a:232:ILE:HG12	1.83	0.59
6:e:71:MET:HB3	6:e:130:ILE:HG22	1.84	0.59
4:4:3:ILE:HB	4:4:18:SER:HB3	1.85	0.59
13:F:46:LEU:HG	13:F:135:ILE:HD13	1.85	0.59
14:G:52:LYS:HZ3	14:G:213:GLU:HG3	1.67	0.59
15:I:196:GLU:O	15:I:208:TYR:OH	2.18	0.59
19:P:161:CYS:HA	19:P:183:GLN:HE21	1.67	0.59
31:T:7:LEU:HB3	31:T:30:ILE:HG12	1.85	0.59
15:I:135:PHE:HD1	26:H:82:TRP:HB2	1.68	0.58
16:K:255:ARG:NH1	16:K:298:GLU:OE2	2.34	0.58
20:R:312:TYR:HE1	20:R:326:ALA:HB1	1.68	0.58
24:Y:73:PHE:O	24:Y:75:ASN:N	2.35	0.58
5:5:241:HIS:CE1	3:h:204:GLN:HB3	2.38	0.58
7:7:60:LEU:HD21	7:7:67:LEU:HD13	1.84	0.58
15:I:73:GLU:O	26:H:66:LYS:NZ	2.36	0.58
16:K:121:ARG:HH22	25:J:64:LEU:HD13	1.68	0.58
17:L:186:LEU:HD12	17:L:189:GLN:HB2	1.84	0.58
18:O:330:ARG:NH1	19:P:307:GLU:OE2	2.35	0.58
6:e:46:THR:HB	6:e:59:GLU:H	1.68	0.58
30:N:498:ILE:HG23	30:N:535:LEU:HD21	1.84	0.58
32:o:924:LYS:HG2	32:o:953:THR:HG21	1.84	0.58
10:C:233:GLN:CD	10:C:233:GLN:H	2.11	0.58
20:R:27:SER:OG	20:R:320:LYS:NZ	2.36	0.58
1:b:40:THR:HG22	1:b:45:ILE:HG12	1.85	0.58
8:A:54:ILE:HD11	8:A:223:LEU:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:250:MET:HA	7:a:250:MET:HE3	1.85	0.58
28:Q:158:ILE:HG12	28:Q:177:VAL:HG23	1.84	0.58
29:U:119:LEU:HD11	29:U:136:ALA:HB1	1.85	0.58
3:3:101:GLY:O	4:4:93:ARG:NH1	2.36	0.58
20:R:285:ALA:HB1	20:R:315:VAL:HG22	1.85	0.58
23:W:68:GLU:HB2	23:W:71:LYS:HZ2	1.68	0.58
25:J:264:GLY:HA2	25:J:267:GLU:HB3	1.85	0.58
26:H:174:VAL:HG11	26:H:183:ILE:HG12	1.86	0.58
4:4:83:PHE:O	4:4:87:GLU:HG2	2.03	0.58
6:6:26:ASP:OD2	6:6:27:ASN:N	2.37	0.58
15:I:236:VAL:O	15:I:240:THR:OG1	2.22	0.58
21:S:261:HIS:ND1	21:S:269:GLU:OE2	2.35	0.58
7:a:139:LYS:NZ	7:a:141:ASN:O	2.36	0.58
7:a:140:MET:H	7:a:140:MET:HE2	1.69	0.58
3:h:113:ASN:O	3:h:192:LYS:NZ	2.37	0.58
26:H:356:ASN:N	26:H:356:ASN:OD1	2.36	0.58
28:Q:359:ILE:HD11	28:Q:390:LEU:HD11	1.84	0.58
32:o:617:ILE:HD12	32:o:743:ILE:HG13	1.84	0.58
9:B:222:LEU:HD13	9:B:232:GLY:HA2	1.85	0.58
16:K:124:SER:HA	16:K:128:ARG:HH22	1.69	0.58
21:S:256:LYS:NZ	30:N:40:SER:OG	2.30	0.58
30:N:452:LEU:HD11	30:N:751:LEU:HD11	1.84	0.58
32:o:938:GLN:HB2	32:o:942:PRO:HG3	1.85	0.58
9:B:119:GLN:HG3	10:C:86:ILE:HD11	1.85	0.58
10:C:59:GLN:NE2	10:C:209:ASP:O	2.35	0.58
19:P:25:ASP:O	19:P:29:GLN:NE2	2.36	0.58
6:6:97:ASP:OD1	6:6:98:HIS:ND1	2.37	0.58
15:I:311:ASN:O	15:I:315:GLY:N	2.37	0.58
20:R:222:ARG:NH1	24:Y:62:GLU:O	2.35	0.58
2:i:63:LEU:HD13	2:i:205:CYS:HB2	1.85	0.58
2:2:86:GLN:NE2	9:B:98:LYS:O	2.37	0.58
6:6:47:ARG:NH1	6:6:215:ILE:O	2.37	0.58
7:7:50:ASP:O	7:7:158:GLN:NE2	2.37	0.58
17:L:246:SER:HB3	17:L:280:MET:HA	1.84	0.58
18:O:92:PHE:HB2	18:O:140:LYS:HE2	1.86	0.58
19:P:122:ILE:HG21	19:P:139:VAL:HG21	1.86	0.58
23:W:3:LEU:HB3	23:W:106:GLN:HG2	1.85	0.58
4:g:38:LEU:HD11	4:g:60:ILE:HG13	1.85	0.58
3:h:84:PRO:HA	3:h:87:PHE:HB3	1.86	0.58
29:U:186:LEU:HD21	31:T:267:ALA:HB1	1.85	0.58
30:N:127:ASP:O	30:N:128:ILE:HD13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:N:380:LEU:HG	30:N:381:GLU:HG2	1.86	0.58
32:o:808:SER:O	32:o:812:ILE:HG23	2.04	0.58
4:4:101:ASN:HB3	4:4:133:HIS:CD2	2.39	0.57
15:I:130:VAL:HG11	15:I:156:ILE:HG13	1.86	0.57
16:K:282:PHE:HE1	16:K:284:ALA:HB2	1.69	0.57
17:L:277:ILE:HG22	17:L:277:ILE:O	2.03	0.57
18:O:172:TYR:HB3	18:O:195:TYR:HB2	1.86	0.57
18:O:186:ASN:HD21	18:O:225:ASP:H	1.51	0.57
25:J:18:GLY:O	25:J:20:LYS:N	2.36	0.57
32:o:157:LEU:HD11	32:o:207:ILE:HD11	1.86	0.57
32:o:804:ASP:O	32:o:807:VAL:N	2.35	0.57
8:A:218:PHE:HB3	8:A:223:LEU:HD22	1.86	0.57
11:D:158:SER:HB3	12:E:63:SER:HB2	1.86	0.57
13:F:54:ASP:O	13:F:57:SER:OG	2.21	0.57
15:I:229:LYS:NZ	34:J:501:ATP:O2B	2.36	0.57
22:V:301:ASN:O	22:V:305:ILE:HB	2.03	0.57
28:Q:426:LEU:HD11	29:U:289:ASP:HB2	1.86	0.57
30:N:772:GLN:NE2	30:N:869:ASP:OD1	2.37	0.57
9:B:88:LYS:O	9:B:92:VAL:HG12	2.04	0.57
26:H:51:GLN:N	26:H:51:GLN:OE1	2.33	0.57
27:M:120:LYS:HG2	27:M:126:THR:HG22	1.86	0.57
27:M:197:ILE:HG13	27:M:324:LEU:HD21	1.86	0.57
30:N:314:LEU:HD21	30:N:336:ASN:HB2	1.87	0.57
2:2:137:SER:O	2:2:138:HIS:ND1	2.36	0.57
2:2:188:ILE:HD13	2:2:202:VAL:HG13	1.86	0.57
4:4:9:VAL:HG23	4:4:11:ASP:H	1.69	0.57
4:4:25:ILE:HD11	5:5:209:THR:HG21	1.86	0.57
5:5:244:ALA:HB1	3:h:179:ALA:HB1	1.87	0.57
11:D:117:GLN:NE2	11:D:151:GLU:O	2.36	0.57
14:G:78:TYR:HD2	14:G:85:GLY:HA3	1.69	0.57
20:R:38:VAL:O	20:R:43:ARG:NH2	2.37	0.57
22:V:178:GLY:O	22:V:181:ASN:ND2	2.37	0.57
7:a:131:THR:O	7:a:135:GLN:HG2	2.05	0.57
9:B:148:TYR:HE1	9:B:158:PRO:HB3	1.70	0.57
5:f:280:GLY:O	5:f:283:ASN:ND2	2.29	0.57
25:J:89:GLN:OE1	25:J:89:GLN:N	2.29	0.57
25:J:195:LYS:HE2	25:J:293:ALA:HB1	1.87	0.57
25:J:306:ARG:NE	25:J:307:PRO:O	2.34	0.57
29:U:70:HIS:ND1	29:U:113:TYR:OH	2.31	0.57
1:1:57:HIS:ND1	1:1:58:ASP:OD1	2.37	0.57
13:F:135:ILE:HD11	13:F:222:PHE:HE1	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:K:262:ARG:NH2	16:K:302:GLN:OE1	2.38	0.57
30:N:120:ASP:OD2	30:N:125:THR:OG1	2.21	0.57
3:3:28:ARG:HB2	3:3:183:TRP:HB2	1.86	0.57
19:P:43:GLU:OE2	19:P:88:GLN:NE2	2.35	0.57
20:R:277:LEU:HA	20:R:280:ILE:HD12	1.86	0.57
22:V:71:MET:HE2	22:V:71:MET:HA	1.85	0.57
22:V:153:ILE:HG22	22:V:201:ILE:HG13	1.86	0.57
7:a:183:MET:HE2	7:a:183:MET:HA	1.86	0.57
32:o:135:LEU:HD12	32:o:135:LEU:H	1.68	0.57
4:4:49:GLU:OE2	4:4:51:GLY:N	2.35	0.57
4:4:92:ILE:HD12	4:4:93:ARG:HG3	1.85	0.57
11:D:216:LYS:HB2	11:D:220:ASP:HB3	1.87	0.57
20:R:263:ARG:NH2	20:R:297:TYR:O	2.37	0.57
18:O:246:SER:HA	18:O:249:ASP:HB2	1.87	0.57
23:W:41:ARG:HD3	23:W:45:PRO:HA	1.86	0.57
5:f:152:ALA:O	5:f:156:LYS:HG2	2.04	0.57
25:J:103:ASN:N	25:J:103:ASN:OD1	2.38	0.57
26:H:311:ILE:HG21	26:H:353:PHE:HD1	1.68	0.57
30:N:536:ILE:HD12	30:N:555:ILE:HG12	1.86	0.57
32:o:42:ASP:OD2	32:o:43:ALA:N	2.38	0.57
6:6:116:LEU:HD23	6:6:124:TYR:HD2	1.70	0.57
10:C:195:LYS:HG2	10:C:199:LYS:HZ2	1.69	0.57
15:I:62:MET:O	15:I:66:LYS:HG3	2.04	0.57
19:P:395:ARG:NH2	28:Q:358:GLU:OE1	2.38	0.57
30:N:245:LEU:HD21	30:N:254:SER:HA	1.87	0.57
2:2:235:PRO:O	2:2:238:THR:OG1	2.22	0.56
5:5:134:LEU:HG	5:5:158:LEU:HD13	1.86	0.56
5:5:266:HIS:HB3	5:5:271:LEU:HD11	1.87	0.56
12:E:154:GLN:HG2	12:E:166:ARG:HH12	1.69	0.56
17:L:286:ILE:O	17:L:286:ILE:HG13	2.05	0.56
21:S:455:GLU:OE2	31:T:258:ASN:ND2	2.38	0.56
6:e:125:TYR:HA	6:e:146:PRO:HB3	1.86	0.56
30:N:605:ILE:HD12	30:N:605:ILE:H	1.69	0.56
30:N:759:ILE:HG23	30:N:902:VAL:HG13	1.86	0.56
5:5:241:HIS:ND1	3:h:204:GLN:O	2.38	0.56
10:C:16:GLU:OE2	10:C:18:ARG:HG2	2.04	0.56
23:W:125:LEU:HB3	23:W:157:PHE:CE1	2.40	0.56
6:e:76:PHE:HB3	6:e:79:ASP:HB2	1.86	0.56
26:H:411:CYS:SG	26:H:414:SER:OG	2.63	0.56
27:M:379:LEU:HD21	27:M:415:PHE:HB3	1.85	0.56
5:5:234:ARG:HH12	5:5:279:GLU:HG3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:9:ALA:HB2	19:P:51:ASP:HB2	1.87	0.56
19:P:69:ARG:HB2	19:P:71:LYS:HG2	1.87	0.56
20:R:33:LEU:HD22	20:R:71:LEU:HD21	1.86	0.56
6:e:47:ARG:HB2	6:e:219:ASP:HB2	1.87	0.56
31:T:67:LEU:HA	31:T:70:ILE:HG22	1.87	0.56
32:o:52:LEU:HD22	32:o:67:SER:HA	1.88	0.56
7:7:103:LEU:HD21	7:7:125:ILE:HG22	1.87	0.56
15:I:319:ARG:CZ	15:I:320:GLY:H	2.18	0.56
18:O:307:MET:N	18:O:307:MET:SD	2.79	0.56
21:S:52:TYR:O	21:S:56:SER:OG	2.22	0.56
27:M:384:ASP:OD1	27:M:384:ASP:N	2.36	0.56
30:N:127:ASP:N	30:N:127:ASP:OD1	2.38	0.56
1:1:204:ARG:HG2	7:a:259:LYS:HE3	1.87	0.56
3:3:104:PHE:HD1	3:3:126:LEU:HD11	1.71	0.56
3:3:205:ASP:HB2	5:f:247:GLY:HA3	1.88	0.56
4:4:147:HIS:HB3	4:4:160:LEU:HD21	1.88	0.56
7:7:187:LEU:O	7:7:190:LYS:NZ	2.34	0.56
11:D:121:THR:HG22	11:D:128:PRO:HB3	1.88	0.56
13:F:118:LYS:HA	13:F:118:LYS:HE3	1.87	0.56
16:K:356:ILE:HD11	34:K:501:ATP:H2	1.70	0.56
5:f:134:LEU:HD22	5:f:158:LEU:HB2	1.88	0.56
29:U:182:ALA:O	29:U:184:GLY:N	2.38	0.56
2:2:240:ALA:HB2	6:e:185:GLY:HA3	1.87	0.56
6:6:86:ARG:HE	6:6:115:LEU:HD22	1.71	0.56
19:P:59:LEU:HB3	19:P:96:MET:HB2	1.87	0.56
23:W:101:ARG:HH12	23:W:108:GLN:HE21	1.52	0.56
2:i:47:THR:HG21	2:i:217:ARG:HH22	1.70	0.56
27:M:167:VAL:HA	27:M:170:MET:SD	2.45	0.56
30:N:638:ILE:HG23	30:N:660:LEU:HD21	1.87	0.56
5:5:76:THR:O	5:5:206:SER:N	2.36	0.56
8:A:64:LEU:HD22	14:G:160:TYR:HE2	1.70	0.56
15:I:421:GLU:O	15:I:425:LYS:HG2	2.05	0.56
1:b:79:GLN:O	1:b:83:GLU:HG2	2.06	0.56
27:M:225:GLY:N	34:M:501:ATP:O1B	2.34	0.56
32:o:778:LEU:HD11	32:o:888:LEU:HD23	1.88	0.56
5:5:236:ILE:HD13	5:5:250:VAL:HG13	1.88	0.56
5:5:283:ASN:ND2	4:g:148:TYR:O	2.39	0.56
8:A:96:ARG:O	8:A:96:ARG:HD3	2.06	0.56
8:A:135:ARG:NH1	14:G:124:THR:O	2.39	0.56
13:F:82:ARG:HH21	13:F:86:ASN:ND2	2.04	0.56
17:L:407:ARG:NH2	17:L:414:ASP:OD2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:107:TRP:NE1	22:V:126:GLN:OE1	2.32	0.56
31:T:79:GLU:O	31:T:83:ASN:ND2	2.39	0.56
31:T:171:ILE:HD13	31:T:174:PHE:CE2	2.40	0.56
32:o:256:LEU:HD21	32:o:260:GLU:HB2	1.87	0.56
6:6:163:SER:HB2	3:h:145:GLN:HG2	1.88	0.56
8:A:157:THR:OG1	8:A:158:ASP:N	2.38	0.56
7:a:180:GLY:HA2	7:a:183:MET:HB2	1.87	0.56
25:J:310:ILE:O	25:J:313:LYS:NZ	2.39	0.56
27:M:356:SER:O	27:M:360:ILE:HG12	2.05	0.56
1:1:23:MET:HE1	1:1:143:TYR:HB2	1.87	0.56
13:F:80:ASP:OD1	13:F:126:ARG:NH2	2.34	0.56
13:F:187:ASP:N	13:F:187:ASP:OD1	2.39	0.56
32:o:304:PRO:O	32:o:308:LYS:HG3	2.07	0.56
2:2:75:ALA:N	2:2:126:TYR:O	2.39	0.55
10:C:15:PRO:HA	11:D:22:TYR:CZ	2.41	0.55
16:K:357:ALA:HB2	16:K:387:MET:HE1	1.87	0.55
18:O:228:TYR:HA	18:O:294:MET:HE1	1.88	0.55
19:P:183:GLN:HB3	19:P:199:LEU:HD23	1.87	0.55
22:V:35:LEU:HD12	29:U:16:LEU:HD12	1.88	0.55
3:h:41:GLU:OE1	3:h:43:ILE:N	2.36	0.55
3:h:177:ARG:HA	3:h:177:ARG:HH11	1.71	0.55
28:Q:242:SER:HB2	28:Q:261:VAL:HG21	1.88	0.55
31:T:59:LYS:NZ	31:T:98:GLU:O	2.40	0.55
5:5:175:MET:HA	5:5:175:MET:HE3	1.89	0.55
6:6:176:LYS:HD2	3:h:203:ARG:NH2	2.21	0.55
20:R:222:ARG:NH1	24:Y:62:GLU:OE1	2.39	0.55
5:f:112:ILE:HG23	5:f:135:GLY:HA2	1.88	0.55
32:o:951:GLN:HB3	32:o:955:VAL:HG11	1.88	0.55
7:7:90:ILE:HA	7:7:93:MET:HG2	1.87	0.55
7:7:97:GLU:O	7:7:101:LYS:HG2	2.05	0.55
7:7:105:THR:HA	14:G:72:ARG:HH21	1.70	0.55
7:7:256:LYS:HB3	1:b:206:ILE:HG21	1.89	0.55
9:B:174:PHE:HA	9:B:177:LYS:HE2	1.86	0.55
22:V:291:ASN:O	22:V:295:VAL:HG23	2.06	0.55
29:U:70:HIS:HD1	29:U:113:TYR:HH	1.46	0.55
1:1:23:MET:HG3	1:1:174:ILE:HD11	1.88	0.55
2:2:153:TYR:HB2	2:2:167:LEU:HD13	1.88	0.55
15:I:263:LEU:O	15:I:267:ILE:HG12	2.06	0.55
18:O:325:GLU:O	18:O:329:MET:HG2	2.05	0.55
23:W:100:HIS:CE1	29:U:57:GLU:HG3	2.41	0.55
16:K:349:ARG:HH12	16:K:375:ASN:HA	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:172:LEU:HD22	3:h:202:MET:HB3	1.88	0.55
30:N:657:MET:HG2	30:N:682:PHE:HE1	1.72	0.55
1:1:23:MET:HE2	1:1:145:ILE:HG23	1.88	0.55
5:5:96:THR:HG22	5:5:101:VAL:HG22	1.89	0.55
7:7:58:ASP:HA	7:7:228:PHE:HA	1.89	0.55
7:7:111:ASN:HB3	7:7:114:ALA:HB2	1.87	0.55
10:C:44:ILE:HB	10:C:216:ILE:HD12	1.88	0.55
10:C:76:ALA:HB3	10:C:136:ILE:HB	1.89	0.55
14:G:109:ILE:HG21	14:G:147:HIS:HB2	1.89	0.55
15:I:254:GLN:NE2	25:J:228:ARG:O	2.32	0.55
15:I:308:GLU:OE1	26:H:277:SER:OG	2.24	0.55
21:S:60:LEU:HD11	21:S:144:LEU:HD13	1.89	0.55
21:S:125:LYS:HB2	21:S:127:THR:HG22	1.89	0.55
5:f:83:PHE:HE1	5:f:88:ILE:HG12	1.72	0.55
32:o:301:THR:HG21	32:o:306:MET:HB2	1.89	0.55
1:1:50:THR:OG1	1:1:51:ASP:N	2.40	0.55
12:E:146:GLY:HA2	12:E:222:ILE:HG12	1.88	0.55
18:O:343:GLN:HE22	19:P:364:ARG:HG2	1.71	0.55
19:P:52:LEU:H	19:P:52:LEU:HD23	1.72	0.55
21:S:157:GLU:O	21:S:161:LYS:HB2	2.07	0.55
21:S:254:ILE:HD13	21:S:276:LEU:HD11	1.87	0.55
5:f:145:GLU:HB3	5:f:147:GLU:HG2	1.88	0.55
2:i:188:ILE:HG21	2:i:202:VAL:HG13	1.89	0.55
1:1:70:ASP:HB3	1:1:112:LEU:HD13	1.88	0.55
6:6:27:ASN:HD22	6:6:77:ALA:HB2	1.71	0.55
12:E:22:PHE:O	12:E:24:VAL:N	2.39	0.55
19:P:24:ILE:HD11	19:P:35:ALA:HA	1.88	0.55
19:P:72:TRP:HA	19:P:75:LEU:HB3	1.89	0.55
7:a:101:LYS:HA	7:a:104:VAL:HG12	1.87	0.55
32:o:867:PHE:HD2	32:o:871:HIS:HA	1.70	0.55
12:E:72:ARG:HE	12:E:227:GLY:HA3	1.72	0.55
30:N:375:HIS:CD2	30:N:385:VAL:HG11	2.42	0.55
30:N:602:VAL:O	30:N:606:VAL:HG22	2.07	0.55
1:1:192:ILE:HB	1:1:207:PHE:HB2	1.88	0.55
1:1:194:MET:HA	1:1:194:MET:HE3	1.89	0.55
3:3:144:ASP:OD1	3:3:144:ASP:N	2.36	0.55
12:E:114:GLN:HE21	12:E:114:GLN:C	2.15	0.55
7:a:81:ASN:ND2	7:a:152:VAL:O	2.40	0.55
25:J:131:ASP:OD1	25:J:134:VAL:HG23	2.07	0.55
27:M:299:ARG:HG3	27:M:303:ARG:HH21	1.70	0.55
28:Q:14:LEU:HD23	28:Q:19:GLN:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:90:SER:OG	9:B:99:ARG:NH1	2.40	0.54
6:6:119:LYS:NZ	6:6:122:PHE:O	2.38	0.54
7:7:36:GLN:NE2	7:7:37:PRO:O	2.37	0.54
10:C:44:ILE:HD11	10:C:146:TYR:HB3	1.88	0.54
21:S:391:GLY:O	21:S:395:ILE:HG12	2.07	0.54
7:a:204:GLN:H	7:a:204:GLN:CD	2.14	0.54
5:f:156:LYS:HD3	5:f:196:ARG:HH12	1.72	0.54
4:g:104:ILE:HB	4:g:117:TYR:HB2	1.87	0.54
15:I:168:VAL:HG21	15:I:270:VAL:HG21	1.89	0.54
17:L:109:MET:HE1	17:L:126:ARG:HE	1.72	0.54
17:L:132:ARG:NH2	17:L:134:SER:OG	2.41	0.54
6:e:147:VAL:HG22	5:f:125:ALA:HB3	1.89	0.54
30:N:722:THR:OG1	30:N:723:GLY:N	2.40	0.54
6:6:101:LYS:NZ	12:E:105:GLU:OE2	2.40	0.54
16:K:119:VAL:N	25:J:70:SER:O	2.36	0.54
19:P:104:LEU:O	19:P:115:ARG:NH2	2.41	0.54
21:S:62:SER:O	21:S:66:GLN:NE2	2.40	0.54
25:J:118:ASP:OD1	25:J:118:ASP:N	2.40	0.54
30:N:387:ALA:HA	30:N:390:LEU:HD12	1.89	0.54
32:o:575:MET:HA	32:o:607:ALA:HA	1.89	0.54
8:A:194:ILE:HG22	8:A:196:GLU:H	1.72	0.54
12:E:122:ARG:NH2	12:E:132:ARG:O	2.41	0.54
7:a:191:VAL:HG12	7:a:192:VAL:HG23	1.90	0.54
28:Q:159:ASN:HB3	28:Q:163:ARG:HH21	1.72	0.54
3:3:188:TYR:HE1	3:3:197:LYS:HG3	1.72	0.54
5:5:250:VAL:HB	5:5:266:HIS:HB2	1.88	0.54
6:6:201:LYS:HB2	2:i:229:GLN:HG2	1.90	0.54
7:7:131:THR:O	7:7:135:GLN:HG2	2.07	0.54
17:L:313:ASP:OD1	17:L:342:ARG:NE	2.41	0.54
5:f:165:TYR:HB3	5:f:170:LEU:HD12	1.89	0.54
4:g:10:GLN:NE2	4:g:151:ASP:O	2.41	0.54
3:h:53:ILE:HG22	3:h:60:VAL:HG22	1.89	0.54
30:N:665:ILE:HD13	30:N:715:ILE:HG13	1.90	0.54
9:B:46:ALA:HB2	9:B:211:LEU:HD13	1.89	0.54
11:D:48:ARG:HE	11:D:209:ASN:HA	1.72	0.54
14:G:126:TYR:HB2	14:G:129:VAL:HG12	1.89	0.54
17:L:295:THR:OG1	17:L:296:SER:N	2.41	0.54
19:P:60:ALA:HB2	19:P:95:TYR:HE2	1.72	0.54
19:P:254:GLU:HA	19:P:257:TRP:NE1	2.23	0.54
29:U:141:GLU:HA	29:U:152:LYS:HA	1.88	0.54
31:T:104:LYS:HE2	31:T:171:ILE:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:230:THR:N	34:J:501:ATP:O1B	2.37	0.54
16:K:87:LYS:HE3	16:K:125:THR:HG21	1.90	0.54
18:O:152:ASP:HA	18:O:155:LYS:HD2	1.89	0.54
21:S:136:CYS:HB3	21:S:179:ILE:HG21	1.90	0.54
7:a:58:ASP:HA	7:a:228:PHE:HA	1.88	0.54
3:h:199:TYR:HB2	2:i:243:LYS:H	1.72	0.54
28:Q:20:TYR:HB2	28:Q:64:LEU:HD13	1.90	0.54
28:Q:275:ILE:HG21	28:Q:307:ASN:HB2	1.90	0.54
30:N:17:GLN:O	30:N:21:LYS:HG2	2.07	0.54
32:o:797:THR:HG22	32:o:801:HIS:HE1	1.72	0.54
5:5:82:ARG:NH1	5:5:185:PRO:O	2.41	0.54
9:B:69:PRO:HB3	9:B:233:PRO:HB3	1.90	0.54
9:B:213:ILE:HD12	9:B:238:LEU:HD21	1.88	0.54
15:I:177:PRO:O	15:I:178:THR:OG1	2.20	0.54
18:O:82:LEU:HD23	18:O:83:LEU:HD23	1.90	0.54
18:O:231:GLY:O	18:O:235:HIS:ND1	2.41	0.54
20:R:203:ASP:N	20:R:203:ASP:OD1	2.37	0.54
20:R:312:TYR:HA	20:R:316:LEU:HD13	1.88	0.54
23:W:180:LEU:HD12	23:W:182:TYR:CE2	2.42	0.54
8:A:104:PHE:CD1	8:A:112:MET:HB3	2.43	0.54
9:B:178:ARG:HB3	9:B:191:ILE:HD12	1.89	0.54
16:K:131:LEU:HD23	16:K:149:ILE:HD12	1.88	0.54
19:P:294:GLU:OE1	19:P:294:GLU:N	2.41	0.54
20:R:117:ILE:HG12	20:R:133:ALA:HB1	1.90	0.54
4:4:149:ARG:HH12	5:f:281:SER:HA	1.73	0.54
7:7:42:THR:H	7:7:74:ARG:HH22	1.54	0.54
7:7:139:LYS:HE3	7:7:141:ASN:HB3	1.89	0.54
16:K:322:ASP:OD2	16:K:323:THR:N	2.40	0.54
20:R:149:ASN:HA	20:R:152:LYS:HD2	1.90	0.54
20:R:289:ILE:HG12	20:R:315:VAL:HG21	1.89	0.54
1:b:78:VAL:HG22	1:b:100:VAL:HG12	1.90	0.54
4:g:56:PHE:O	4:g:60:ILE:HG23	2.06	0.54
28:Q:17:GLU:HB2	28:Q:19:GLN:HG2	1.88	0.54
32:o:471:LEU:HB2	32:o:497:PHE:HZ	1.73	0.54
5:5:140:LEU:HB3	5:5:144:ARG:HH22	1.74	0.53
6:6:134:ASP:OD1	6:6:138:LYS:N	2.31	0.53
7:7:248:GLU:OE1	7:7:248:GLU:N	2.41	0.53
8:A:200:GLU:HG2	8:A:244:ARG:HH21	1.72	0.53
15:I:167:MET:HE1	25:J:229:MET:H	1.72	0.53
17:L:225:GLY:HA3	27:M:339:ARG:HD3	1.91	0.53
17:L:435:GLN:NE2	17:L:436:LYS:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:U:66:TRP:CE2	29:U:106:ILE:HG12	2.42	0.53
30:N:101:ILE:O	30:N:105:SER:OG	2.24	0.53
32:o:280:ASP:OD1	32:o:280:ASP:N	2.40	0.53
10:C:5:ARG:NH2	14:G:11:SER:OG	2.40	0.53
15:I:72:GLU:HG2	32:o:760:HIS:CE1	2.44	0.53
15:I:194:ILE:HG21	15:I:232:LEU:HD21	1.90	0.53
16:K:242:PHE:HB3	16:K:295:ILE:HD13	1.89	0.53
20:R:22:PRO:HG3	20:R:177:LEU:HD23	1.90	0.53
20:R:189:GLU:HG3	20:R:190:LYS:HE2	1.90	0.53
21:S:466:LYS:NZ	31:T:265:ASP:OD2	2.28	0.53
26:H:98:GLN:O	26:H:176:VAL:N	2.41	0.53
7:7:129:LEU:HA	7:7:132:VAL:HG12	1.91	0.53
15:I:79:SER:O	15:I:83:LYS:HG2	2.09	0.53
15:I:124:THR:HG21	25:J:91:GLU:HB3	1.90	0.53
20:R:237:THR:O	20:R:237:THR:OG1	2.25	0.53
6:e:50:THR:OG1	6:e:55:ASN:OD1	2.23	0.53
6:e:156:ARG:HG2	6:e:166:MET:HE1	1.89	0.53
4:4:66:LEU:HB2	11:D:94:GLN:HG3	1.91	0.53
7:7:92:ASP:O	7:7:96:ILE:HG12	2.09	0.53
20:R:17:THR:HG22	20:R:19:ASN:H	1.74	0.53
21:S:28:GLU:O	21:S:32:GLN:HG2	2.08	0.53
30:N:373:VAL:HG23	30:N:410:LEU:HD21	1.90	0.53
32:o:809:MET:HE1	32:o:843:ASP:HB2	1.90	0.53
5:5:89:VAL:HG22	5:5:253:TYR:HB2	1.91	0.53
6:6:71:MET:HB2	6:6:130:ILE:HG22	1.90	0.53
10:C:232:PRO:HA	10:C:235:ILE:HB	1.90	0.53
12:E:16:SER:OG	12:E:20:ARG:O	2.23	0.53
17:L:294:GLY:O	17:L:299:ARG:NH2	2.40	0.53
17:L:373:GLU:H	17:L:373:GLU:CD	2.16	0.53
3:h:11:ILE:HG21	3:h:142:ALA:HB3	1.91	0.53
25:J:103:ASN:HB3	25:J:105:LYS:HE2	1.91	0.53
27:M:364:HIS:NE2	34:M:501:ATP:O2'	2.42	0.53
32:o:567:ALA:HB2	32:o:599:ILE:HD12	1.90	0.53
2:2:101:ARG:NH2	8:A:115:ASP:OD2	2.41	0.53
2:2:212:ASP:OD1	2:2:213:ALA:N	2.41	0.53
4:4:82:SER:HA	4:4:85:ARG:HG2	1.90	0.53
6:6:76:PHE:HB3	6:6:79:ASP:HB2	1.90	0.53
8:A:164:VAL:HG13	8:A:166:TYR:HE1	1.74	0.53
18:O:42:SER:HB3	18:O:73:ILE:HD13	1.91	0.53
2:2:66:ILE:HB	2:2:70:ILE:HG23	1.91	0.53
10:C:114:ARG:O	10:C:118:ILE:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:370:ASN:ND2	15:I:409:MET:O	2.41	0.53
16:K:350:ARG:NH2	16:K:368:LEU:HB2	2.24	0.53
17:L:339:ARG:NH2	17:L:342:ARG:HG3	2.22	0.53
20:R:28:GLU:HA	20:R:320:LYS:HD2	1.90	0.53
23:W:143:ASN:HB3	23:W:173:THR:HA	1.90	0.53
4:g:107:TYR:HE2	4:g:186:LYS:HG3	1.74	0.53
4:g:181:VAL:HB	4:g:192:VAL:HB	1.91	0.53
26:H:384:GLY:O	26:H:388:ILE:HG12	2.07	0.53
3:3:15:MET:HA	3:3:15:MET:HE3	1.89	0.53
8:A:46:ARG:NH2	8:A:192:ASP:O	2.37	0.53
14:G:54:ILE:O	14:G:210:LYS:NZ	2.30	0.53
21:S:44:THR:HG21	21:S:53:ILE:HD11	1.91	0.53
26:H:393:SER:O	26:H:393:SER:OG	2.24	0.53
32:o:335:LEU:HD11	32:o:910:PRO:HG2	1.90	0.53
5:5:269:GLY:HA3	3:h:203:ARG:HH11	1.74	0.53
8:A:89:ASP:HA	14:G:121:GLN:HE22	1.74	0.53
19:P:106:SER:HA	19:P:108:LYS:HE2	1.90	0.53
19:P:242:GLN:N	19:P:264:ILE:HD11	2.24	0.53
6:e:46:THR:OG1	6:e:219:ASP:O	2.27	0.53
3:h:110:ALA:HA	3:h:121:ILE:HG22	1.91	0.53
2:i:220:LEU:HG	2:i:222:PRO:HD3	1.91	0.53
8:A:183:GLU:HG2	9:B:55:LEU:HG	1.91	0.53
10:C:145:GLY:O	10:C:147:GLN:NE2	2.42	0.53
10:C:238:ILE:H	10:C:238:ILE:HD12	1.72	0.53
12:E:204:LEU:HA	12:E:207:VAL:HG12	1.91	0.53
5:f:95:ALA:HB2	5:f:106:VAL:HG21	1.90	0.53
27:M:55:ASN:HA	27:M:58:MET:HG3	1.90	0.53
32:o:597:SER:O	32:o:601:VAL:HG22	2.09	0.53
7:7:176:ALA:HB3	7:7:181:ALA:HA	1.91	0.52
12:E:71:ASP:OD2	12:E:73:HIS:ND1	2.28	0.52
13:F:98:VAL:HG12	13:F:99:PHE:HD2	1.74	0.52
14:G:91:ARG:O	14:G:91:ARG:HD3	2.08	0.52
15:I:55:CYS:SG	32:o:248:TYR:OH	2.65	0.52
18:O:232:GLU:HA	18:O:235:HIS:HE1	1.74	0.52
19:P:301:LYS:O	19:P:305:THR:OG1	2.28	0.52
21:S:438:HIS:O	21:S:438:HIS:ND1	2.35	0.52
30:N:227:LYS:HE2	30:N:722:THR:HA	1.91	0.52
7:7:103:LEU:HD22	7:7:128:TYR:HD2	1.73	0.52
14:G:60:VAL:HG13	14:G:63:LYS:HB2	1.92	0.52
15:I:116:ASP:OD2	26:H:89:GLN:NE2	2.31	0.52
18:O:165:LEU:O	18:O:167:ILE:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:13:TYR:O	19:P:17:LEU:N	2.33	0.52
3:h:84:PRO:HB2	3:h:120:PHE:HE2	1.74	0.52
30:N:76:GLU:OE2	30:N:76:GLU:N	2.39	0.52
30:N:109:TYR:OH	30:N:162:ARG:NH1	2.32	0.52
30:N:389:TYR:HB3	30:N:404:SER:HB2	1.92	0.52
5:5:119:THR:OG1	5:5:175:MET:N	2.40	0.52
12:E:214:GLU:HG3	12:E:233:ASN:HB3	1.91	0.52
17:L:264:ARG:NE	17:L:307:GLU:OE2	2.39	0.52
22:V:87:PHE:CZ	29:U:79:MET:HB3	2.44	0.52
7:a:152:VAL:HG22	7:a:158:GLN:HG3	1.91	0.52
30:N:533:ASP:OD1	30:N:559:TYR:OH	2.27	0.52
3:3:84:PRO:HB2	3:3:120:PHE:HD2	1.74	0.52
9:B:185:LEU:HD21	9:B:213:ILE:HG21	1.92	0.52
10:C:72:LYS:HD2	10:C:140:TYR:HB3	1.91	0.52
13:F:77:LEU:HG	13:F:79:PRO:HD2	1.90	0.52
15:I:99:ILE:O	26:H:90:ARG:NH1	2.40	0.52
16:K:361:SER:O	16:K:401:VAL:HG23	2.09	0.52
20:R:226:GLU:O	20:R:230:LEU:HG	2.08	0.52
21:S:484:ASP:HB2	25:J:46:ALA:HB2	1.89	0.52
30:N:181:GLU:HA	30:N:184:LYS:HD2	1.90	0.52
32:o:546:ILE:HG21	32:o:570:LEU:HB2	1.90	0.52
6:6:192:LYS:NZ	6:6:193:TYR:O	2.42	0.52
16:K:316:MET:HE3	16:K:334:LEU:HD11	1.90	0.52
17:L:247:PRO:HG2	17:L:250:GLY:HA3	1.92	0.52
6:6:137:GLY:O	6:6:228:LYS:NZ	2.43	0.52
15:I:234:LYS:NZ	25:J:277:ASN:OD1	2.36	0.52
17:L:108:VAL:HG22	17:L:119:VAL:HG12	1.92	0.52
23:W:101:ARG:NH1	23:W:106:GLN:O	2.42	0.52
30:N:572:LEU:O	30:N:576:VAL:HG23	2.09	0.52
5:5:136:SER:OG	5:5:137:GLN:OE1	2.27	0.52
7:7:80:ASP:OD2	7:7:81:ASN:N	2.43	0.52
7:7:86:ILE:HD11	7:7:93:MET:HA	1.92	0.52
15:I:150:HIS:CE1	15:I:152:LYS:H	2.28	0.52
17:L:261:ARG:O	17:L:265:GLU:HG2	2.10	0.52
22:V:94:MET:HE3	29:U:76:MET:HE2	1.92	0.52
7:a:133:MET:HG3	7:a:165:LEU:HA	1.91	0.52
4:g:193:ASP:OD1	4:g:193:ASP:N	2.43	0.52
28:Q:153:ASP:N	28:Q:153:ASP:OD1	2.39	0.52
30:N:773:MET:HG2	30:N:884:PHE:HA	1.90	0.52
8:A:200:GLU:HG2	8:A:244:ARG:NH2	2.25	0.52
16:K:368:LEU:HD12	16:K:368:LEU:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:e:117:TYR:OH	5:f:126:ASP:OD1	2.18	0.52
6:e:152:ARG:HD3	6:e:153:GLU:N	2.25	0.52
3:h:27:LEU:HG	3:h:185:ALA:HA	1.91	0.52
28:Q:261:VAL:O	28:Q:265:MET:HG2	2.10	0.52
28:Q:283:ASN:O	28:Q:288:LYS:NZ	2.42	0.52
30:N:11:ALA:HB1	31:T:80:ASN:HB3	1.92	0.52
32:o:776:VAL:O	32:o:780:MET:HG2	2.09	0.52
32:o:862:MET:SD	32:o:908:ILE:HD11	2.50	0.52
2:2:87:LEU:HD12	9:B:99:ARG:HH22	1.75	0.52
3:3:25:CYS:HB2	3:3:43:ILE:HD11	1.92	0.52
14:G:102:LEU:HD23	14:G:103:TYR:CD2	2.44	0.52
17:L:219:LEU:HB2	17:L:343:LEU:HD12	1.92	0.52
20:R:19:ASN:HB3	20:R:21:VAL:HG22	1.90	0.52
21:S:458:GLN:NE2	29:U:270:ASN:OD1	2.43	0.52
21:S:482:PRO:O	21:S:486:LYS:N	2.43	0.52
6:e:220:GLY:HA2	6:e:238:LEU:H	1.75	0.52
25:J:98:VAL:HA	25:J:122:LEU:HB2	1.92	0.52
25:J:197:LEU:HD22	36:J:502:ADP:H2'	1.92	0.52
26:H:395:SER:OG	26:H:396:MET:N	2.42	0.52
30:N:735:MET:HG3	30:N:748:PHE:CD2	2.45	0.52
31:T:32:ILE:HG22	31:T:36:LYS:HE3	1.92	0.52
8:A:123:ASN:O	8:A:127:ILE:HG12	2.09	0.52
10:C:215:THR:O	10:C:227:GLN:NE2	2.43	0.52
13:F:157:TYR:HE1	14:G:60:VAL:HA	1.74	0.52
15:I:83:LYS:HB3	15:I:88:LYS:HG3	1.91	0.52
1:b:117:ILE:HD11	1:b:129:VAL:HG13	1.91	0.52
25:J:112:ARG:HH21	25:J:126:LEU:HD23	1.74	0.52
28:Q:11:ALA:HA	28:Q:14:LEU:HD12	1.92	0.52
30:N:55:PHE:HB3	30:N:58:ARG:HG2	1.92	0.52
31:T:4:LEU:O	31:T:8:THR:HG23	2.10	0.52
31:T:76:ASP:OD1	31:T:76:ASP:N	2.41	0.52
5:5:96:THR:HA	5:5:101:VAL:HA	1.92	0.51
15:I:218:GLY:HA3	15:I:344:ILE:HG22	1.92	0.51
20:R:131:ALA:O	20:R:135:ILE:HG12	2.10	0.51
21:S:271:ARG:NE	24:Y:37:ASP:OD2	2.35	0.51
22:V:160:ASP:O	22:V:161:THR:HG23	2.10	0.51
32:o:95:THR:O	32:o:99:LEU:HD22	2.10	0.51
10:C:136:ILE:HD11	10:C:165:VAL:HG22	1.93	0.51
14:G:99:PHE:CG	14:G:107:ILE:HD13	2.46	0.51
21:S:239:ARG:NH1	21:S:243:ASN:OD1	2.44	0.51
23:W:20:ASP:OD1	23:W:21:PHE:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:153:TYR:HB2	2:i:167:LEU:HD13	1.91	0.51
2:i:177:LYS:HE3	2:i:206:VAL:HG11	1.93	0.51
32:o:381:LEU:HD21	32:o:898:HIS:CD2	2.45	0.51
2:2:51:GLN:OE1	2:2:51:GLN:N	2.41	0.51
6:6:161:ALA:HB2	6:6:214:HIS:HD2	1.74	0.51
18:O:232:GLU:HA	18:O:235:HIS:CE1	2.46	0.51
21:S:393:ARG:HA	21:S:432:ILE:HD11	1.93	0.51
5:f:138:CYS:HB2	5:f:149:ILE:HG21	1.92	0.51
27:M:284:ASP:OD1	27:M:284:ASP:N	2.35	0.51
3:3:31:SER:N	3:3:34:LEU:O	2.43	0.51
4:4:160:LEU:HD23	4:4:163:LEU:HD12	1.92	0.51
7:7:160:LEU:HG	7:7:175:LEU:HD23	1.92	0.51
12:E:205:LYS:HA	12:E:208:MET:HG2	1.92	0.51
15:I:242:ALA:HB2	15:I:276:PRO:HG2	1.91	0.51
7:7:122:PRO:HB2	7:7:159:PHE:HD2	1.76	0.51
8:A:219:SER:N	8:A:222:ASP:OD2	2.38	0.51
19:P:310:ARG:NH1	19:P:367:GLU:O	2.37	0.51
1:b:214:GLN:OE1	1:b:214:GLN:N	2.43	0.51
4:g:95:ARG:HH11	4:g:96:ARG:HB2	1.75	0.51
26:H:282:LYS:HG2	26:H:283:TYR:CD2	2.46	0.51
26:H:343:PHE:HD2	27:M:245:LYS:HD3	1.76	0.51
28:Q:52:ASN:HA	28:Q:55:GLU:HG2	1.92	0.51
3:3:203:ARG:O	3:3:203:ARG:NH1	2.43	0.51
15:I:316:PHE:HD2	26:H:273:ARG:HD2	1.76	0.51
17:L:293:GLU:OE1	17:L:293:GLU:N	2.43	0.51
20:R:218:CYS:HG	20:R:223:ASN:ND2	2.07	0.51
24:Y:77:LEU:HD23	24:Y:77:LEU:H	1.75	0.51
1:b:48:ARG:NE	2:i:168:GLU:OE2	2.43	0.51
2:i:30:THR:HG21	2:i:75:ALA:HA	1.93	0.51
28:Q:410:ASP:O	28:Q:414:GLU:HG2	2.10	0.51
32:o:737:ALA:CA	32:o:775:MET:HE1	2.38	0.51
32:o:761:PHE:HB3	32:o:776:VAL:HG13	1.92	0.51
4:4:5:LEU:HD21	4:4:140:THR:HG21	1.92	0.51
15:I:339:ILE:HA	15:I:344:ILE:HD11	1.92	0.51
18:O:22:LEU:HD13	18:O:57:LEU:HD11	1.93	0.51
20:R:54:ILE:HG12	20:R:59:MET:HB2	1.93	0.51
21:S:433:GLU:OE1	21:S:446:THR:OG1	2.26	0.51
7:a:260:GLY:HA2	7:a:264:GLN:HE21	1.76	0.51
25:J:160:ILE:HD11	25:J:187:LEU:HD21	1.92	0.51
26:H:98:GLN:HB3	26:H:149:LEU:HD21	1.92	0.51
30:N:330:THR:HG23	30:N:366:THR:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:125:ALA:HB1	2:2:127:LEU:HD21	1.93	0.51
6:6:140:ALA:HA	6:6:152:ARG:HH12	1.76	0.51
7:7:122:PRO:HG3	7:7:151:GLY:HA3	1.92	0.51
11:D:67:ILE:HG21	11:D:109:LEU:HD11	1.92	0.51
17:L:95:ILE:O	17:L:99:GLN:HG2	2.11	0.51
17:L:165:PRO:HD3	27:M:83:VAL:HG13	1.92	0.51
17:L:258:GLU:OE1	17:L:258:GLU:HA	2.11	0.51
30:N:427:ILE:HD13	30:N:443:LEU:HD13	1.93	0.51
31:T:39:LEU:HB3	31:T:58:THR:HG21	1.93	0.51
32:o:812:ILE:HD12	32:o:848:THR:HA	1.92	0.51
1:1:159:LYS:HG3	1:b:180:GLN:HE21	1.75	0.51
7:7:34:THR:N	7:7:140:MET:O	2.44	0.51
11:D:116:VAL:HA	11:D:119:ARG:NH1	2.26	0.51
15:I:380:LEU:HD21	15:I:416:PHE:CD2	2.45	0.51
20:R:348:LEU:HD12	20:R:349:SER:H	1.76	0.51
25:J:96:VAL:HG11	25:J:115:LEU:HD22	1.92	0.51
30:N:104:LYS:HA	30:N:107:GLU:HG2	1.93	0.51
32:o:309:GLN:HG3	32:o:982:ILE:HG13	1.92	0.51
15:I:56:LYS:HE2	32:o:226:GLU:HB3	1.93	0.51
23:W:141:ILE:HD13	23:W:154:LEU:HD22	1.93	0.51
4:g:184:VAL:HG22	4:g:189:ILE:HG12	1.93	0.51
25:J:188:TYR:CE1	25:J:297:LEU:HD11	2.45	0.51
25:J:213:VAL:HG11	25:J:233:LEU:HD22	1.93	0.51
2:2:54:ILE:HD11	3:3:147:PHE:HD2	1.77	0.50
15:I:290:LYS:HB3	15:I:292:TYR:CE1	2.46	0.50
17:L:279:PHE:HD1	17:L:324:ILE:HB	1.75	0.50
22:V:127:LYS:O	22:V:131:GLN:HG2	2.11	0.50
28:Q:344:GLU:HG2	28:Q:376:LYS:HE3	1.92	0.50
32:o:279:THR:OG1	32:o:280:ASP:OD1	2.29	0.50
32:o:387:ASN:ND2	32:o:397:ASP:OD2	2.36	0.50
32:o:751:ASP:OD1	32:o:751:ASP:N	2.40	0.50
1:1:78:VAL:HG22	1:1:100:VAL:HG23	1.93	0.50
8:A:125:SER:O	8:A:129:THR:HG23	2.11	0.50
15:I:244:PHE:HD1	15:I:278:ILE:HB	1.76	0.50
16:K:109:ILE:HG12	16:K:119:VAL:HG22	1.92	0.50
20:R:171:MET:HA	20:R:174:ILE:CD1	2.41	0.50
20:R:224:PHE:O	20:R:260:THR:HG21	2.11	0.50
21:S:404:LEU:N	21:S:441:GLY:O	2.45	0.50
26:H:102:CYS:SG	26:H:103:THR:N	2.84	0.50
32:o:74:SER:O	32:o:78:SER:N	2.43	0.50
4:4:44:MET:HE2	4:4:44:MET:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:189:SER:O	8:A:190:LYS:HG3	2.10	0.50
8:A:228:ALA:HB2	8:A:233:PHE:HD1	1.76	0.50
11:D:148:TYR:CE1	11:D:158:SER:HB2	2.43	0.50
12:E:86:ARG:HG2	12:E:86:ARG:HH11	1.77	0.50
12:E:122:ARG:O	12:E:122:ARG:NE	2.43	0.50
13:F:177:ASP:OD1	13:F:177:ASP:N	2.39	0.50
20:R:66:LEU:HD22	20:R:92:ILE:HG21	1.94	0.50
21:S:183:LEU:O	21:S:187:ILE:HG12	2.10	0.50
22:V:296:LEU:HD23	29:U:190:LEU:HD22	1.93	0.50
4:g:49:GLU:O	4:g:53:THR:HG23	2.11	0.50
26:H:93:GLU:O	26:H:96:PRO:HD2	2.11	0.50
6:6:240:ARG:HD3	2:i:193:TRP:HB3	1.94	0.50
9:B:217:GLU:HB2	9:B:231:LYS:HE2	1.93	0.50
12:E:184:LEU:HA	13:F:56:LEU:HD11	1.93	0.50
15:I:273:GLU:HG3	15:I:274:ASN:HD22	1.77	0.50
16:K:171:TYR:O	16:K:181:LYS:NZ	2.37	0.50
20:R:148:ASP:OD1	20:R:148:ASP:N	2.45	0.50
21:S:307:LEU:HD21	21:S:337:ASN:HB2	1.94	0.50
2:i:206:VAL:HB	2:i:214:GLU:HB2	1.93	0.50
27:M:246:LEU:HD11	27:M:251:LEU:HG	1.93	0.50
29:U:15:LEU:C	29:U:15:LEU:HD23	2.35	0.50
1:1:163:GLU:N	1:1:163:GLU:OE2	2.43	0.50
3:3:99:ARG:NH2	3:3:127:ILE:HG23	2.25	0.50
6:6:32:LEU:HD23	6:6:203:VAL:HG13	1.92	0.50
7:7:152:VAL:HG11	7:7:235:LYS:HB3	1.92	0.50
15:I:76:VAL:HB	26:H:66:LYS:HZ1	1.74	0.50
15:I:262:ARG:NH2	26:H:281:GLN:OE1	2.44	0.50
18:O:75:GLN:HB3	18:O:122:HIS:CD2	2.45	0.50
3:h:108:VAL:HA	3:h:123:GLY:HA2	1.94	0.50
25:J:112:ARG:HE	25:J:126:LEU:HD23	1.77	0.50
27:M:203:ARG:HE	27:M:206:LYS:HD2	1.76	0.50
32:o:609:THR:HG21	32:o:878:LEU:HD21	1.92	0.50
1:1:176:HIS:HA	1:b:159:LYS:HZ3	1.77	0.50
1:1:194:MET:HB2	1:1:205:LEU:HB3	1.94	0.50
3:3:66:MET:O	3:3:70:LYS:HG2	2.11	0.50
8:A:101:ALA:HA	8:A:112:MET:SD	2.51	0.50
11:D:43:VAL:HG22	11:D:214:VAL:HG22	1.94	0.50
21:S:59:ASP:O	21:S:63:LEU:HG	2.11	0.50
7:a:204:GLN:O	7:a:208:GLU:HG2	2.11	0.50
7:a:215:ARG:NH1	7:a:249:ASN:OD1	2.44	0.50
1:b:163:GLU:HG3	1:b:164:ASN:OD1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:H:501:ATP:H5'2	34:H:501:ATP:C8	2.47	0.50
28:Q:85:MET:SD	28:Q:89:ALA:HB3	2.51	0.50
30:N:256:GLN:HE22	30:N:903:VAL:HA	1.75	0.50
4:4:104:ILE:HG23	4:4:117:TYR:HB2	1.93	0.50
5:5:208:GLN:OE1	5:5:208:GLN:N	2.41	0.50
32:o:973:TYR:HE1	32:o:984:LYS:HB3	1.77	0.50
4:4:13:VAL:HG13	4:4:184:VAL:HB	1.94	0.50
5:5:210:PHE:HB3	5:5:239:ALA:HA	1.94	0.50
8:A:143:PHE:N	8:A:155:TYR:O	2.42	0.50
16:K:221:MET:HE1	34:K:501:ATP:H2'	1.93	0.50
19:P:173:MET:HE2	19:P:173:MET:HA	1.94	0.50
20:R:202:GLY:HA2	20:R:207:ARG:HH21	1.77	0.50
20:R:317:ILE:HG13	20:R:318:PRO:HD3	1.94	0.50
22:V:90:LYS:O	22:V:94:MET:HG2	2.12	0.50
22:V:154:ASP:OD1	22:V:154:ASP:N	2.44	0.50
22:V:265:GLU:O	22:V:269:ARG:N	2.45	0.50
23:W:19:GLY:HA2	23:W:24:THR:HA	1.94	0.50
25:J:217:GLU:OE1	25:J:217:GLU:N	2.45	0.50
26:H:173:ARG:HD2	26:H:190:ARG:HB2	1.94	0.50
28:Q:328:ASP:O	28:Q:331:THR:N	2.40	0.50
30:N:654:GLN:HE22	30:N:694:LEU:HD12	1.77	0.50
32:o:117:ASP:O	32:o:121:ILE:HG12	2.12	0.50
5:5:109:VAL:HG11	5:5:253:TYR:CE2	2.47	0.50
14:G:147:HIS:HB3	14:G:149:TYR:CE1	2.47	0.50
15:I:110:GLU:OE1	15:I:111:GLU:HB2	2.12	0.50
18:O:49:PHE:O	18:O:58:ARG:NH2	2.41	0.50
18:O:389:GLN:HA	18:O:392:TRP:CD1	2.47	0.50
20:R:179:PHE:CZ	20:R:187:VAL:HG11	2.47	0.50
23:W:125:LEU:HD22	23:W:157:PHE:HZ	1.77	0.50
28:Q:198:LEU:HD12	28:Q:221:MET:HG3	1.93	0.50
30:N:657:MET:HE2	30:N:681:ASN:HD21	1.77	0.50
32:o:774:ARG:HB2	32:o:810:ASN:ND2	2.27	0.50
1:1:85:TYR:HE2	1:1:92:PRO:HA	1.77	0.49
5:5:220:LYS:HB3	5:5:223:LEU:HG	1.93	0.49
13:F:4:ASN:OD1	13:F:6:TYR:N	2.32	0.49
13:F:6:TYR:CE2	13:F:15:PRO:HD3	2.46	0.49
16:K:210:LEU:HB2	16:K:334:LEU:HD23	1.94	0.49
17:L:88:TYR:CE1	27:M:62:ILE:HG13	2.46	0.49
30:N:119:LYS:HG3	30:N:120:ASP:H	1.77	0.49
30:N:297:ASP:O	30:N:301:THR:HG23	2.12	0.49
30:N:594:VAL:HG12	30:N:595:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:117:LEU:HB2	5:5:177:CYS:HB2	1.92	0.49
17:L:79:GLN:HA	17:L:82:ARG:HH11	1.76	0.49
20:R:33:LEU:HA	20:R:43:ARG:HG3	1.94	0.49
23:W:123:ASP:N	23:W:123:ASP:OD1	2.43	0.49
7:a:59:ASN:O	7:a:72:VAL:N	2.44	0.49
3:h:68:ARG:NH1	3:h:72:ASN:OD1	2.45	0.49
3:h:162:ASP:HA	2:i:236:ARG:CZ	2.42	0.49
29:U:75:ASN:O	29:U:79:MET:HG2	2.12	0.49
31:T:258:ASN:O	31:T:260:ILE:N	2.44	0.49
32:o:826:ARG:HH22	32:o:830:LEU:HD11	1.77	0.49
5:5:114:PRO:HA	5:5:260:TRP:NE1	2.27	0.49
9:B:217:GLU:HB3	9:B:231:LYS:HB2	1.94	0.49
21:S:329:GLU:OE2	21:S:331:SER:OG	2.30	0.49
5:f:82:ARG:HE	5:f:221:TRP:HZ3	1.58	0.49
25:J:52:ASN:ND2	30:N:611:LYS:O	2.45	0.49
30:N:111:GLN:O	30:N:115:LYS:HG2	2.12	0.49
30:N:158:LEU:HD21	30:N:206:ILE:HD12	1.93	0.49
1:1:155:GLY:O	1:b:180:GLN:NE2	2.46	0.49
15:I:126:PRO:HG2	26:H:98:GLN:HE22	1.77	0.49
17:L:229:THR:HG21	27:M:314:GLY:HA2	1.93	0.49
18:O:10:ILE:HG21	18:O:64:ASN:HB3	1.95	0.49
21:S:141:LEU:HA	21:S:144:LEU:HD12	1.93	0.49
7:a:194:ARG:NE	7:a:195:GLU:OE1	2.45	0.49
4:g:111:LYS:HD2	4:g:113:LYS:HB2	1.95	0.49
30:N:438:ASP:OD1	30:N:438:ASP:N	2.44	0.49
30:N:750:SER:HA	30:N:753:PHE:HD2	1.76	0.49
9:B:38:LYS:HG3	9:B:43:VAL:HG22	1.94	0.49
11:D:66:LYS:HA	11:D:72:VAL:HG23	1.93	0.49
14:G:52:LYS:NZ	14:G:215:GLU:HB2	2.27	0.49
16:K:137:VAL:HB	16:K:146:LEU:HD21	1.95	0.49
18:O:299:THR:HG21	18:O:316:ALA:HB1	1.95	0.49
22:V:37:MET:HB3	22:V:141:VAL:HG11	1.94	0.49
23:W:3:LEU:HG	23:W:106:GLN:HE21	1.77	0.49
7:a:204:GLN:HA	7:a:207:GLU:OE1	2.12	0.49
7:a:218:TYR:CD2	7:a:247:VAL:HG21	2.48	0.49
1:b:69:ALA:HB3	2:i:145:HIS:CD2	2.47	0.49
5:f:82:ARG:HG2	5:f:200:ASP:HB3	1.93	0.49
2:i:137:SER:HB3	2:i:209:ILE:HD11	1.94	0.49
28:Q:65:TYR:CE2	28:Q:73:LYS:HB3	2.47	0.49
1:1:85:TYR:HA	1:1:89:TYR:HD1	1.77	0.49
1:1:85:TYR:CD1	14:G:103:TYR:HE1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:174:MET:HE2	4:4:174:MET:HA	1.93	0.49
5:5:78:THR:HG22	5:5:91:VAL:HG13	1.95	0.49
5:5:232:GLY:O	5:5:236:ILE:HG22	2.11	0.49
8:A:185:HIS:O	8:A:188:LYS:HG3	2.13	0.49
11:D:39:LYS:HD3	11:D:184:PRO:HG2	1.94	0.49
13:F:203:ASP:OD1	13:F:204:GLU:N	2.45	0.49
21:S:399:TYR:HB3	21:S:402:ILE:HB	1.94	0.49
7:a:221:ASP:OD1	7:a:223:ARG:NH2	2.45	0.49
26:H:192:ASP:OD1	26:H:194:SER:N	2.39	0.49
28:Q:114:GLN:HB3	28:Q:144:LEU:HD13	1.95	0.49
29:U:40:ASP:OD2	29:U:47:ARG:NH1	2.45	0.49
32:o:928:ARG:HG3	32:o:966:GLU:HB2	1.94	0.49
5:5:83:PHE:HE1	5:5:88:ILE:HG12	1.78	0.49
5:5:97:ALA:HB2	5:5:102:ALA:HB2	1.94	0.49
12:E:205:LYS:NZ	12:E:212:LEU:H	2.11	0.49
15:I:216:PRO:HG3	15:I:346:ARG:HD2	1.94	0.49
17:L:309:LEU:HG	17:L:342:ARG:CZ	2.43	0.49
3:h:168:SER:O	3:h:172:LEU:HG	2.12	0.49
26:H:251:PRO:O	26:H:254:THR:OG1	2.22	0.49
26:H:416:GLY:HA2	26:H:419:LEU:HD23	1.94	0.49
30:N:894:ARG:HH21	30:N:897:LYS:HZ3	1.59	0.49
32:o:405:ASN:HA	32:o:408:TYR:HD2	1.77	0.49
5:5:108:LYS:HB3	5:5:120:MET:HB2	1.94	0.49
6:6:83:LEU:HD21	6:6:124:TYR:CD2	2.47	0.49
11:D:79:ASN:O	11:D:83:ARG:NH1	2.45	0.49
12:E:142:LEU:HB2	12:E:158:ALA:HB3	1.95	0.49
19:P:357:TYR:CD2	19:P:360:ILE:HB	2.44	0.49
23:W:113:PHE:CE1	23:W:142:ILE:HD12	2.47	0.49
27:M:317:SER:C	27:M:319:ASP:H	2.20	0.49
28:Q:89:ALA:O	28:Q:91:SER:N	2.44	0.49
28:Q:326:MET:HB3	28:Q:332:ARG:HD3	1.95	0.49
30:N:750:SER:HA	30:N:753:PHE:CD2	2.48	0.49
32:o:391:ASN:ND2	32:o:397:ASP:OD1	2.45	0.49
32:o:924:LYS:HA	32:o:953:THR:HB	1.95	0.49
3:3:41:GLU:OE2	3:3:41:GLU:N	2.35	0.49
9:B:220:ASP:N	9:B:220:ASP:OD1	2.46	0.49
14:G:151:LEU:HD13	14:G:157:TYR:HB3	1.94	0.49
16:K:179:MET:HA	16:K:179:MET:HE3	1.94	0.49
19:P:72:TRP:H	19:P:72:TRP:CD1	2.31	0.49
21:S:80:VAL:O	21:S:111:ARG:NH2	2.46	0.49
21:S:411:LEU:HB3	21:S:413:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:94:MET:HE3	29:U:76:MET:CE	2.43	0.49
1:b:56:VAL:HG12	1:b:79:GLN:HB2	1.93	0.49
2:i:32:ILE:HD11	2:i:156:LEU:HB3	1.95	0.49
26:H:46:ALA:HA	26:H:49:LEU:HB2	1.95	0.49
32:o:616:LEU:O	32:o:620:LEU:HD23	2.13	0.49
1:1:23:MET:SD	1:1:25:VAL:HG23	2.52	0.49
3:3:65:GLU:OE1	10:C:100:LYS:HD3	2.13	0.49
8:A:24:ARG:HH21	8:A:26:TYR:HE1	1.61	0.49
9:B:204:PHE:CE1	9:B:209:ILE:HD11	2.48	0.49
12:E:204:LEU:O	12:E:208:MET:N	2.46	0.49
19:P:344:ARG:HA	19:P:344:ARG:HD3	1.57	0.49
20:R:312:TYR:CE1	20:R:326:ALA:HB1	2.48	0.49
21:S:41:ILE:HG22	21:S:56:SER:HB3	1.95	0.49
21:S:481:TYR:HB2	21:S:482:PRO:HD3	1.95	0.49
23:W:109:ARG:HD2	23:W:138:ALA:HB3	1.95	0.49
2:i:124:GLY:HA2	2:i:144:ALA:HB1	1.95	0.49
26:H:197:MET:SD	26:H:197:MET:N	2.85	0.49
26:H:314:VAL:HG23	26:H:314:VAL:O	2.13	0.49
26:H:402:ILE:HG13	26:H:440:GLU:HB2	1.95	0.49
27:M:149:ASN:OD1	27:M:150:LYS:N	2.46	0.49
28:Q:322:GLU:OE1	28:Q:322:GLU:N	2.41	0.49
2:2:115:HIS:C	2:2:115:HIS:HD1	2.19	0.48
9:B:211:LEU:HD23	9:B:243:ILE:HD13	1.94	0.48
13:F:117:GLN:HB3	13:F:118:LYS:HD2	1.95	0.48
15:I:316:PHE:CD2	26:H:273:ARG:HD2	2.47	0.48
16:K:370:SER:OG	16:K:404:GLN:NE2	2.36	0.48
19:P:254:GLU:HA	19:P:257:TRP:CD1	2.48	0.48
20:R:40:ILE:HG12	20:R:43:ARG:HH12	1.77	0.48
20:R:154:LEU:HD13	20:R:170:VAL:HG13	1.95	0.48
20:R:154:LEU:HD12	20:R:174:ILE:HG13	1.95	0.48
20:R:190:LYS:O	20:R:194:VAL:HG23	2.12	0.48
21:S:188:TYR:CZ	21:S:192:GLU:HG3	2.47	0.48
22:V:34:LEU:HD23	29:U:174:LEU:HD21	1.95	0.48
5:f:94:ARG:H	5:f:108:LYS:NZ	2.10	0.48
5:f:243:ASP:HB3	5:f:246:SER:HB3	1.95	0.48
26:H:101:ARG:NH1	27:M:165:SER:OG	2.41	0.48
32:o:309:GLN:OE1	32:o:973:TYR:HB2	2.13	0.48
1:1:182:ILE:HG23	1:1:189:GLY:HA2	1.95	0.48
3:3:13:VAL:HA	3:3:138:VAL:HG12	1.95	0.48
3:3:160:PRO:HA	3:3:163:LEU:HD23	1.96	0.48
7:7:82:THR:HG21	7:7:125:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:K:350:ARG:HH22	16:K:368:LEU:HB2	1.76	0.48
19:P:141:LYS:O	19:P:144:VAL:HG12	2.14	0.48
19:P:198:VAL:HA	19:P:201:ARG:HH22	1.77	0.48
21:S:336:SER:OG	21:S:337:ASN:N	2.40	0.48
23:W:110:ILE:HB	23:W:139:VAL:HG12	1.95	0.48
7:a:168:VAL:HG22	6:e:77:ALA:HB3	1.95	0.48
3:h:15:MET:HE2	3:h:15:MET:HA	1.95	0.48
25:J:248:ASP:OD1	25:J:248:ASP:N	2.32	0.48
25:J:328:LEU:O	25:J:332:SER:HB3	2.12	0.48
29:U:100:ARG:N	29:U:103:ASP:OD2	2.41	0.48
30:N:650:ASP:OD1	30:N:651:PHE:N	2.44	0.48
31:T:258:ASN:C	31:T:259:ILE:HD12	2.37	0.48
32:o:617:ILE:HD11	32:o:746:ILE:HB	1.94	0.48
4:4:86:GLN:OE1	10:C:101:THR:HA	2.13	0.48
6:6:47:ARG:NH2	6:6:241:ASP:O	2.47	0.48
6:6:67:ASP:OD2	6:6:103:LEU:N	2.38	0.48
7:7:255:ALA:O	1:b:193:ARG:NH2	2.46	0.48
11:D:50:SER:HB2	11:D:209:ASN:HD21	1.78	0.48
11:D:212:ILE:HD12	11:D:229:ILE:HD12	1.94	0.48
12:E:75:GLY:HA3	12:E:228:PHE:CE2	2.48	0.48
12:E:185:ASN:OD1	12:E:185:ASN:N	2.45	0.48
21:S:479:MET:O	21:S:482:PRO:HD2	2.13	0.48
22:V:147:VAL:HA	29:U:169:ILE:HD11	1.94	0.48
5:f:254:HIS:O	5:f:261:ILE:N	2.45	0.48
27:M:205:ASP:N	27:M:205:ASP:OD1	2.45	0.48
28:Q:189:ARG:HD3	28:Q:189:ARG:HA	1.61	0.48
30:N:10:LEU:HD11	30:N:42:GLU:OE2	2.13	0.48
32:o:765:MET:HE1	32:o:773:ARG:HG2	1.95	0.48
8:A:158:ASP:OD1	8:A:162:TYR:N	2.45	0.48
9:B:45:ILE:HB	9:B:74:VAL:HG21	1.95	0.48
16:K:52:LYS:HE3	30:N:196:THR:HG23	1.94	0.48
18:O:358:ILE:HG23	18:O:362:GLN:HB2	1.96	0.48
20:R:348:LEU:HD12	20:R:349:SER:N	2.29	0.48
21:S:78:VAL:HG21	21:S:92:LEU:HD22	1.94	0.48
27:M:164:ASP:HB3	27:M:167:VAL:HG23	1.95	0.48
27:M:339:ARG:NH1	27:M:340:SER:O	2.46	0.48
28:Q:212:THR:HA	28:Q:215:VAL:HG12	1.95	0.48
29:U:68:LEU:HD21	29:U:73:ILE:HD11	1.94	0.48
32:o:254:PRO:HG2	32:o:255:LEU:HD12	1.95	0.48
1:1:145:ILE:HB	1:1:150:SER:HB2	1.95	0.48
2:2:123:ILE:HG22	2:2:125:ALA:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:234:PHE:O	2:2:236:ARG:NH1	2.46	0.48
15:I:290:LYS:NZ	15:I:292:TYR:OH	2.46	0.48
15:I:386:ASP:C	15:I:387:LEU:HD22	2.39	0.48
18:O:240:GLU:HA	18:O:243:VAL:HB	1.95	0.48
19:P:250:ILE:HG23	19:P:256:LYS:HB3	1.96	0.48
22:V:262:THR:OG1	22:V:264:GLU:OE1	2.19	0.48
32:o:155:ARG:O	32:o:159:LEU:HG	2.13	0.48
32:o:303:ASP:HB3	32:o:306:MET:HG3	1.95	0.48
32:o:502:ASN:HB3	32:o:505:VAL:HB	1.95	0.48
1:1:16:VAL:HG21	2:2:143:HIS:ND1	2.28	0.48
6:6:74:ASN:O	6:6:127:HIS:N	2.37	0.48
11:D:68:ASP:OD2	11:D:97:ARG:NH2	2.45	0.48
11:D:227:GLU:HA	11:D:230:ASN:HD21	1.77	0.48
13:F:86:ASN:O	13:F:90:GLN:HG2	2.13	0.48
15:I:256:TYR:HE1	16:K:281:ARG:NH2	2.11	0.48
4:g:122:LEU:H	4:g:122:LEU:HD12	1.78	0.48
3:h:28:ARG:NH2	3:h:205:ASP:OXT	2.46	0.48
2:i:88:ILE:HD12	2:i:111:MET:SD	2.54	0.48
2:i:140:PHE:HB3	2:i:150:VAL:HG22	1.95	0.48
25:J:193:THR:N	36:J:502:ADP:O1A	2.45	0.48
30:N:625:LEU:HD12	30:N:641:LEU:HG	1.95	0.48
32:o:117:ASP:OD2	32:o:138:ARG:NH1	2.46	0.48
1:1:137:SER:OG	1:1:139:HIS:NE2	2.44	0.48
2:2:152:TYR:OH	7:a:257:ASP:HB2	2.14	0.48
7:7:37:PRO:HD3	7:7:144:TRP:CD1	2.49	0.48
11:D:97:ARG:HH12	11:D:103:PRO:HG3	1.78	0.48
11:D:118:GLN:NE2	12:E:84:ASP:HA	2.28	0.48
15:I:167:MET:HE3	25:J:228:ARG:HB2	1.96	0.48
16:K:169:VAL:O	16:K:228:ASN:ND2	2.31	0.48
16:K:399:ARG:HG2	19:P:128:ASN:O	2.13	0.48
21:S:267:SER:OG	21:S:271:ARG:NH1	2.47	0.48
23:W:127:ARG:O	23:W:131:THR:OG1	2.31	0.48
7:a:49:TYR:CE1	7:a:54:ILE:HG13	2.49	0.48
29:U:52:PHE:CD1	29:U:76:MET:HG3	2.49	0.48
32:o:138:ARG:CZ	32:o:146:PHE:HB3	2.44	0.48
32:o:453:LEU:HD11	32:o:491:LEU:HD23	1.96	0.48
32:o:740:VAL:HA	32:o:743:ILE:HG22	1.94	0.48
32:o:815:MET:HB3	32:o:827:LEU:HD21	1.95	0.48
1:1:180:GLN:O	1:1:184:TRP:HB2	2.13	0.48
13:F:46:LEU:HD13	13:F:73:SER:HB2	1.95	0.48
14:G:194:LYS:HB3	14:G:242:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:44:SER:HA	18:O:47:LYS:HB2	1.95	0.48
21:S:126:LYS:HD3	21:S:126:LYS:HA	1.70	0.48
7:a:36:GLN:HE21	7:a:38:ILE:HD11	1.79	0.48
1:b:18:LEU:O	1:b:20:THR:HG23	2.13	0.48
3:h:31:SER:O	3:h:32:GLN:NE2	2.47	0.48
2:i:186:ASP:HA	2:i:189:GLN:HE21	1.78	0.48
26:H:155:PHE:CE1	27:M:78:LEU:HD13	2.48	0.48
27:M:364:HIS:CD2	27:M:392:LYS:HB2	2.49	0.48
29:U:126:LYS:HB2	29:U:128:GLN:NE2	2.18	0.48
30:N:473:ASP:OD1	30:N:504:TYR:OH	2.26	0.48
32:o:224:LEU:HA	32:o:227:ILE:HG22	1.96	0.48
32:o:324:GLU:OE1	32:o:324:GLU:N	2.45	0.48
1:l:65:SER:OG	1:l:115:GLY:O	2.22	0.48
2:2:101:ARG:NH1	8:A:149:GLU:OE1	2.47	0.48
3:3:30:GLY:HA2	3:3:35:GLY:HA2	1.96	0.48
15:I:125:MET:SD	15:I:125:MET:N	2.86	0.48
19:P:104:LEU:HD22	19:P:115:ARG:HH21	1.79	0.48
19:P:123:ARG:NH1	19:P:140:THR:OG1	2.39	0.48
21:S:480:ARG:NH2	25:J:44:LEU:HD23	2.29	0.48
23:W:101:ARG:NH1	23:W:108:GLN:HE21	2.10	0.48
5:f:119:THR:OG1	5:f:175:MET:N	2.46	0.48
4:g:34:LYS:HZ1	4:g:47:ALA:HA	1.78	0.48
30:N:90:ASP:OD1	30:N:93:GLU:N	2.36	0.48
30:N:735:MET:HE2	30:N:735:MET:HA	1.96	0.48
31:T:90:PHE:HB3	31:T:132:HIS:CD2	2.41	0.48
32:o:400:ILE:HD12	32:o:406:TRP:HE1	1.79	0.48
6:6:164:LEU:HD22	3:h:148:GLY:H	1.79	0.48
11:D:79:ASN:ND2	15:I:437:LEU:O	2.47	0.48
11:D:81:ASP:N	11:D:81:ASP:OD1	2.47	0.48
5:f:93:SER:HB2	5:f:106:VAL:H	1.78	0.48
27:M:118:VAL:HG22	27:M:128:PHE:HD1	1.78	0.48
30:N:697:PHE:HE1	30:N:739:PHE:HE2	1.61	0.48
1:l:153:ILE:HD11	1:l:181:ALA:HB2	1.95	0.47
14:G:141:VAL:HG11	14:G:221:LEU:HG	1.95	0.47
15:I:111:GLU:HG2	15:I:113:ILE:HG23	1.95	0.47
16:K:223:VAL:HG13	16:K:234:PHE:HZ	1.79	0.47
30:N:411:ILE:HG22	30:N:412:TYR:HD1	1.78	0.47
32:o:139:LEU:O	32:o:141:SER:N	2.47	0.47
32:o:597:SER:HB2	32:o:623:ARG:NH2	2.23	0.47
2:2:59:ASN:N	2:2:59:ASN:OD1	2.47	0.47
2:2:171:TRP:O	7:a:251:LYS:NZ	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:130:TYR:OH	4:4:145:ASP:OD1	2.32	0.47
23:W:14:GLU:OE2	23:W:83:GLY:N	2.45	0.47
23:W:16:SER:O	23:W:25:ARG:HB2	2.14	0.47
4:g:41:HIS:HD2	4:g:109:LYS:HD3	1.79	0.47
25:J:186:ILE:HD13	25:J:292:MET:HB3	1.96	0.47
29:U:211:LEU:O	29:U:215:ILE:HG23	2.14	0.47
30:N:760:GLY:H	30:N:870:ASN:HD21	1.61	0.47
1:1:180:GLN:HA	1:1:183:LYS:HG2	1.95	0.47
8:A:178:ILE:HD11	8:A:214:LEU:HD21	1.96	0.47
12:E:114:GLN:O	12:E:114:GLN:NE2	2.39	0.47
14:G:8:TYR:CD2	14:G:17:PRO:HD3	2.49	0.47
15:I:246:ARG:HH22	25:J:278:GLN:HB2	1.78	0.47
18:O:42:SER:O	18:O:81:TYR:OH	2.31	0.47
19:P:379:TYR:O	19:P:383:LEU:HG	2.14	0.47
19:P:395:ARG:HG3	28:Q:354:PHE:HE1	1.80	0.47
21:S:82:TYR:OH	21:S:135:ASN:OD1	2.28	0.47
22:V:170:PRO:C	22:V:171:ARG:HG2	2.38	0.47
1:b:32:ILE:HG12	1:b:196:VAL:HA	1.96	0.47
26:H:163:VAL:HG21	26:H:168:ILE:HD11	1.97	0.47
30:N:450:ILE:HD11	30:N:462:VAL:HG22	1.97	0.47
3:3:172:LEU:HD22	3:3:202:MET:SD	2.53	0.47
4:4:36:ARG:HG3	4:4:57:ALA:HB1	1.95	0.47
7:7:126:PHE:O	7:7:129:LEU:HD12	2.14	0.47
12:E:69:GLU:N	12:E:69:GLU:OE2	2.48	0.47
13:F:140:SER:OG	13:F:143:HIS:NE2	2.41	0.47
18:O:358:ILE:HD12	29:U:226:LEU:HB3	1.96	0.47
22:V:232:GLU:OE1	22:V:232:GLU:N	2.43	0.47
6:e:76:PHE:HD2	6:e:79:ASP:H	1.63	0.47
3:h:89:GLN:OE1	3:h:89:GLN:N	2.45	0.47
2:i:192:ILE:HG12	2:i:199:GLY:HA2	1.96	0.47
26:H:224:VAL:HG12	26:H:225:VAL:HG23	1.95	0.47
26:H:428:MET:HE2	26:H:428:MET:HB2	1.74	0.47
30:N:302:PHE:CE2	30:N:712:ASN:HB3	2.48	0.47
32:o:752:ILE:O	32:o:756:MET:HG2	2.14	0.47
4:4:60:ILE:HG12	4:4:84:VAL:HG12	1.97	0.47
5:5:92:ASP:OD1	5:5:92:ASP:N	2.42	0.47
6:6:55:ASN:HB3	7:7:170:TYR:CE2	2.50	0.47
9:B:163:ALA:O	9:B:168:SER:OG	2.32	0.47
14:G:78:TYR:H	14:G:78:TYR:HD1	1.63	0.47
16:K:293:GLN:NE2	25:J:221:LYS:O	2.48	0.47
17:L:325:MET:SD	17:L:343:LEU:HD21	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:212:THR:OG1	20:R:234:SER:OG	2.32	0.47
22:V:225:LEU:HD12	29:U:196:SER:HB3	1.96	0.47
30:N:20:VAL:HG23	31:T:35:ILE:HD11	1.95	0.47
30:N:262:VAL:HG23	30:N:290:LEU:HD23	1.96	0.47
30:N:593:PHE:CZ	30:N:734:VAL:HG23	2.49	0.47
31:T:258:ASN:HB3	31:T:259:ILE:HD12	1.97	0.47
3:3:105:VAL:HG23	3:3:107:PRO:HD3	1.96	0.47
7:7:230:LEU:O	7:7:242:LYS:NZ	2.48	0.47
8:A:52:VAL:HG21	8:A:203:VAL:HG22	1.95	0.47
12:E:177:GLU:N	12:E:177:GLU:OE1	2.47	0.47
15:I:193:GLU:HB3	15:I:346:ARG:HH12	1.79	0.47
15:I:326:MET:HE3	15:I:344:ILE:HG21	1.96	0.47
16:K:152:PRO:HG2	16:K:263:GLU:OE2	2.14	0.47
21:S:408:CYS:HB2	21:S:419:VAL:HG21	1.96	0.47
21:S:428:ARG:HD3	31:T:192:ASN:HA	1.97	0.47
23:W:172:LEU:HD13	23:W:189:PRO:HG3	1.97	0.47
1:b:51:ASP:O	1:b:64:ARG:NH2	2.48	0.47
3:h:169:GLN:NE2	2:i:239:THR:OG1	2.45	0.47
27:M:78:LEU:HB3	27:M:148:VAL:HG13	1.95	0.47
30:N:102:VAL:O	30:N:106:ILE:HG13	2.14	0.47
32:o:321:PHE:O	32:o:330:ILE:HD12	2.13	0.47
1:1:23:MET:SD	1:1:24:ALA:N	2.87	0.47
1:1:172:ASP:OD2	1:1:176:HIS:HD2	1.98	0.47
2:2:154:LEU:HD12	2:2:154:LEU:HA	1.80	0.47
2:2:163:ALA:HB1	2:2:187:ALA:HB1	1.95	0.47
3:3:9:GLY:HA2	3:3:141:THR:HG21	1.95	0.47
6:6:178:GLN:HE22	6:6:189:LYS:HD2	1.80	0.47
6:6:213:ARG:HE	3:h:151:GLU:HG3	1.79	0.47
7:7:252:TRP:HH2	1:b:48:ARG:HB2	1.79	0.47
10:C:43:GLY:HA2	10:C:146:TYR:CZ	2.49	0.47
15:I:211:MET:O	26:H:396:MET:HA	2.14	0.47
17:L:316:ASP:OD1	17:L:316:ASP:N	2.47	0.47
18:O:38:TRP:HA	18:O:41:LEU:HB3	1.96	0.47
21:S:107:SER:HB3	21:S:110:LEU:HB2	1.97	0.47
23:W:190:ILE:HG22	23:W:191:ILE:HG23	1.97	0.47
5:f:105:THR:O	5:f:105:THR:OG1	2.29	0.47
3:h:21:VAL:HG23	3:h:190:ILE:HB	1.95	0.47
25:J:162:GLU:HA	25:J:166:LEU:HB2	1.97	0.47
28:Q:173:SER:O	28:Q:177:VAL:HG12	2.15	0.47
28:Q:311:LEU:HD13	28:Q:343:LEU:HD13	1.96	0.47
29:U:94:HIS:NE2	29:U:122:ILE:HG22	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:103:LEU:HD13	4:4:133:HIS:CE1	2.41	0.47
18:O:270:ILE:O	18:O:274:ILE:HB	2.14	0.47
19:P:73:ASP:N	19:P:73:ASP:OD1	2.44	0.47
20:R:227:ALA:O	20:R:231:LEU:HD23	2.15	0.47
21:S:200:GLU:O	31:T:92:ASN:ND2	2.48	0.47
22:V:23:THR:HA	22:V:171:ARG:CZ	2.45	0.47
26:H:46:ALA:HA	26:H:49:LEU:HD13	1.97	0.47
28:Q:322:GLU:O	28:Q:326:MET:HG3	2.15	0.47
32:o:60:ASP:OD2	32:o:62:SER:OG	2.33	0.47
1:1:16:VAL:HG13	1:1:41:THR:HG22	1.96	0.47
6:6:114:HIS:NE2	12:E:102:TYR:HA	2.29	0.47
8:A:22:GLU:HB2	8:A:24:ARG:HG3	1.96	0.47
9:B:95:THR:HA	9:B:99:ARG:HG3	1.97	0.47
10:C:156:ASN:ND2	15:I:434:GLY:O	2.47	0.47
20:R:419:ALA:HA	20:R:422:ARG:HD3	1.96	0.47
21:S:163:VAL:HG21	21:S:187:ILE:HD11	1.96	0.47
24:Y:40:ILE:HD12	24:Y:41:ASP:H	1.80	0.47
7:a:58:ASP:OD1	7:a:74:ARG:NH2	2.48	0.47
7:a:140:MET:HE2	7:a:140:MET:N	2.28	0.47
1:b:23:MET:HB3	1:b:145:ILE:HG22	1.96	0.47
3:h:96:TYR:CZ	3:h:99:ARG:HD2	2.50	0.47
3:h:184:GLY:N	3:h:202:MET:HE2	2.30	0.47
26:H:281:GLN:HE21	26:H:290:MET:HE3	1.80	0.47
28:Q:95:LYS:O	28:Q:99:THR:HG22	2.15	0.47
6:6:176:LYS:HA	6:6:176:LYS:HD3	1.64	0.47
13:F:117:GLN:HE22	14:G:83:PRO:HB2	1.80	0.47
14:G:75:GLY:HA3	14:G:228:HIS:CE1	2.50	0.47
15:I:284:ILE:HG22	15:I:328:THR:HB	1.96	0.47
16:K:188:VAL:O	16:K:192:LEU:HG	2.15	0.47
16:K:200:GLN:HE21	25:J:336:ASN:HD22	1.62	0.47
18:O:204:SER:C	18:O:205:ILE:HG13	2.40	0.47
20:R:222:ARG:HH12	20:R:324:ARG:HH12	1.63	0.47
20:R:333:MET:HA	20:R:333:MET:HE2	1.96	0.47
6:e:86:ARG:NH1	6:e:115:LEU:O	2.48	0.47
26:H:100:ALA:HB2	26:H:149:LEU:HD23	1.97	0.47
27:M:384:ASP:HB2	27:M:385:GLU:OE2	2.15	0.47
1:1:26:THR:HG22	1:1:31:VAL:HB	1.96	0.46
5:5:274:LYS:HG3	5:5:275:VAL:N	2.30	0.46
14:G:102:LEU:HD23	14:G:103:TYR:HD2	1.80	0.46
15:I:180:SER:OG	15:I:181:TYR:N	2.48	0.46
16:K:276:SER:HB3	17:L:306:MET:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:358:ILE:HG21	29:U:226:LEU:HD12	1.96	0.46
22:V:27:VAL:HB	22:V:201:ILE:HD13	1.97	0.46
22:V:206:THR:O	22:V:210:THR:HG22	2.15	0.46
22:V:262:THR:OG1	22:V:265:GLU:OE1	2.33	0.46
6:e:47:ARG:HH21	6:e:218:GLY:HA3	1.80	0.46
25:J:227:SER:HB2	25:J:232:GLU:HG3	1.97	0.46
27:M:329:ARG:NH2	27:M:331:ASP:OD2	2.48	0.46
29:U:25:THR:OG1	29:U:27:THR:HG23	2.15	0.46
29:U:90:ILE:HG13	29:U:90:ILE:O	2.15	0.46
32:o:601:VAL:HG11	32:o:623:ARG:HD2	1.97	0.46
5:5:283:ASN:HD21	4:g:149:ARG:HD3	1.80	0.46
6:6:197:GLU:HA	6:6:200:ILE:HG12	1.96	0.46
14:G:12:ASN:ND2	14:G:131:PRO:HD3	2.30	0.46
15:I:199:GLU:O	15:I:203:THR:HG22	2.15	0.46
18:O:345:ASN:OD1	18:O:345:ASN:N	2.49	0.46
20:R:22:PRO:HD2	20:R:176:ARG:HD2	1.95	0.46
20:R:385:ASN:N	20:R:385:ASN:OD1	2.49	0.46
21:S:460:VAL:O	21:S:464:ARG:HG2	2.15	0.46
1:b:35:ALA:O	1:b:193:ARG:N	2.41	0.46
26:H:212:GLY:O	34:H:501:ATP:N6	2.47	0.46
26:H:376:GLU:O	26:H:376:GLU:HG2	2.16	0.46
32:o:826:ARG:HH12	32:o:830:LEU:HG	1.80	0.46
32:o:877:THR:HA	32:o:907:GLY:HA3	1.96	0.46
3:3:177:ARG:HA	3:3:177:ARG:HD3	1.69	0.46
4:4:135:TYR:HA	4:4:138:PHE:HE1	1.80	0.46
6:6:34:ILE:HG12	6:6:155:CYS:HB3	1.98	0.46
16:K:378:LEU:HD11	16:K:411:TYR:HE1	1.80	0.46
19:P:165:VAL:HA	19:P:168:TYR:CD2	2.44	0.46
21:S:256:LYS:HD3	30:N:72:LEU:HD21	1.98	0.46
23:W:73:LEU:HA	23:W:76:LEU:HD12	1.97	0.46
1:b:145:ILE:HD12	1:b:150:SER:HB3	1.97	0.46
2:i:84:VAL:O	2:i:88:ILE:HG12	2.15	0.46
25:J:338:THR:O	25:J:341:ILE:HG12	2.14	0.46
26:H:436:LYS:HZ3	32:o:952:SER:HB2	1.80	0.46
32:o:528:LEU:HD21	32:o:565:PHE:HB3	1.98	0.46
7:7:127:GLU:O	7:7:131:THR:OG1	2.25	0.46
8:A:77:ARG:NH2	8:A:231:ASP:O	2.37	0.46
13:F:98:VAL:HG12	13:F:99:PHE:CD2	2.51	0.46
14:G:38:ILE:HD12	14:G:40:ILE:HD11	1.98	0.46
17:L:352:PRO:HB2	17:L:357:ARG:HG2	1.97	0.46
19:P:77:GLU:OE1	19:P:77:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:54:ILE:HD13	20:R:63:TYR:CD1	2.48	0.46
20:R:138:GLY:HA3	20:R:154:LEU:CD2	2.43	0.46
22:V:244:MET:HE1	22:V:287:THR:HG21	1.97	0.46
7:a:160:LEU:HG	7:a:175:LEU:HD12	1.98	0.46
6:e:119:LYS:HD2	6:e:124:TYR:CE2	2.50	0.46
4:g:81:SER:HB3	4:g:104:ILE:HG21	1.97	0.46
27:M:271:LYS:HG3	27:M:318:ASP:OD2	2.15	0.46
32:o:138:ARG:HE	32:o:144:SER:HA	1.80	0.46
32:o:378:GLN:HB3	32:o:842:GLN:NE2	2.31	0.46
32:o:394:TYR:OH	32:o:858:GLY:O	2.27	0.46
7:7:243:LYS:HB3	7:7:243:LYS:HE3	1.72	0.46
17:L:242:ASN:HD22	17:L:273:HIS:HB3	1.80	0.46
17:L:305:LEU:O	17:L:309:LEU:HB2	2.15	0.46
21:S:37:VAL:HG21	21:S:63:LEU:HD11	1.98	0.46
22:V:251:TYR:HD1	22:V:276:PRO:O	1.99	0.46
7:a:124:TYR:O	7:a:127:GLU:HG2	2.16	0.46
3:h:168:SER:HB2	2:i:239:THR:HG21	1.98	0.46
27:M:57:VAL:HG12	27:M:61:LYS:HE3	1.97	0.46
27:M:383:THR:HG23	27:M:419:ILE:HD12	1.97	0.46
30:N:393:SER:OG	30:N:394:ARG:N	2.47	0.46
32:o:811:SER:O	32:o:815:MET:HG2	2.16	0.46
2:2:155:SER:HB3	2:2:164:MET:HB2	1.96	0.46
11:D:158:SER:N	12:E:63:SER:OG	2.32	0.46
16:K:188:VAL:HG21	16:K:315:ILE:HD11	1.97	0.46
16:K:200:GLN:NE2	25:J:375:ILE:HG23	2.31	0.46
18:O:120:LYS:C	18:O:122:HIS:H	2.24	0.46
18:O:192:SER:HB2	18:O:217:LEU:HD13	1.97	0.46
18:O:387:ARG:NE	31:T:261:GLU:OE2	2.32	0.46
20:R:267:LYS:HA	20:R:267:LYS:HD2	1.76	0.46
22:V:213:LEU:HD11	29:U:16:LEU:HD11	1.96	0.46
7:a:172:SER:OG	7:a:174:THR:O	2.33	0.46
4:g:43:LEU:HB2	4:g:189:ILE:HD13	1.98	0.46
26:H:249:TYR:HB2	26:H:358:PRO:HG3	1.97	0.46
30:N:713:VAL:HG21	30:N:753:PHE:HB3	1.97	0.46
1:i:159:LYS:CG	1:b:180:GLN:HE21	2.29	0.46
7:7:220:ARG:NE	2:i:168:GLU:OE2	2.49	0.46
8:A:134:MET:HA	8:A:134:MET:HE3	1.96	0.46
10:C:198:SER:HB3	10:C:206:LEU:HD22	1.98	0.46
13:F:52:ASN:HB2	13:F:57:SER:OG	2.16	0.46
14:G:86:ARG:HG2	14:G:86:ARG:HH11	1.81	0.46
20:R:158:LEU:O	20:R:158:LEU:HD12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:171:MET:HA	20:R:174:ILE:HD12	1.97	0.46
1:b:78:VAL:HG13	1:b:100:VAL:HB	1.98	0.46
1:b:82:LEU:HD21	1:b:97:ALA:HA	1.97	0.46
4:g:101:ASN:HD22	4:g:133:HIS:HB3	1.80	0.46
25:J:105:LYS:H	25:J:105:LYS:HD3	1.81	0.46
25:J:379:GLN:O	25:J:383:GLU:HG2	2.16	0.46
32:o:888:LEU:N	32:o:894:MET:HE3	2.31	0.46
4:4:158:LEU:O	4:4:162:LYS:HG2	2.16	0.46
6:6:50:THR:OG1	6:6:55:ASN:ND2	2.28	0.46
9:B:66:LEU:HD12	9:B:235:PHE:CD2	2.51	0.46
9:B:108:LYS:HA	9:B:148:TYR:HE2	1.80	0.46
15:I:100:ARG:O	15:I:150:HIS:HD2	1.99	0.46
15:I:340:ARG:HH12	15:I:343:ARG:CZ	2.29	0.46
18:O:123:GLY:O	18:O:127:LEU:HG	2.16	0.46
19:P:107:SER:O	19:P:109:SER:N	2.48	0.46
19:P:310:ARG:HH22	19:P:368:LEU:HA	1.80	0.46
22:V:99:GLY:HA3	29:U:24:ARG:HD3	1.97	0.46
1:b:27:PHE:HB2	1:b:165:MET:O	2.15	0.46
6:e:194:LEU:HB3	6:e:198:GLU:HB2	1.97	0.46
6:e:226:VAL:HG22	6:e:231:VAL:HG22	1.97	0.46
4:g:158:LEU:O	4:g:161:LEU:HG	2.15	0.46
2:i:43:ILE:HG12	2:i:207:MET:HE1	1.96	0.46
2:i:74:GLY:HA2	2:i:127:LEU:HD23	1.97	0.46
25:J:196:THR:HG22	36:J:502:ADP:O2A	2.16	0.46
26:H:83:ASP:OD1	26:H:83:ASP:N	2.47	0.46
27:M:299:ARG:HG3	27:M:303:ARG:NH2	2.30	0.46
29:U:185:GLY:O	29:U:188:ILE:HG22	2.16	0.46
32:o:970:TYR:HD2	32:o:983:LEU:HD13	1.80	0.46
10:C:22:VAL:HG21	15:I:435:LEU:HD11	1.97	0.46
10:C:197:LEU:HA	10:C:200:THR:HG22	1.98	0.46
16:K:87:LYS:O	22:V:147:VAL:HG21	2.15	0.46
18:O:222:LEU:HD23	18:O:222:LEU:HA	1.77	0.46
20:R:120:LEU:HD13	20:R:129:GLU:HG3	1.97	0.46
21:S:138:MET:HA	21:S:138:MET:HE3	1.98	0.46
7:a:135:GLN:O	7:a:139:LYS:HG2	2.14	0.46
5:f:152:ALA:HA	5:f:188:TYR:HE2	1.81	0.46
3:h:50:PHE:HE2	3:h:195:VAL:HG21	1.81	0.46
3:h:109:VAL:N	3:h:122:ALA:O	2.43	0.46
28:Q:178:HIS:HB3	28:Q:201:ALA:HB2	1.97	0.46
29:U:10:ILE:HD13	29:U:121:LEU:HD21	1.97	0.46
30:N:285:ALA:HA	30:N:288:ASN:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:T:255:GLN:OE1	31:T:256:LYS:N	2.48	0.46
2:2:109:LEU:HD22	2:2:140:PHE:CD2	2.51	0.46
3:3:80:ARG:NH2	3:3:81:ALA:O	2.40	0.46
5:5:241:HIS:HE1	3:h:204:GLN:HB3	1.77	0.46
7:7:226:ARG:HD3	7:7:247:VAL:HB	1.97	0.46
15:I:400:GLY:HA3	25:J:179:ILE:HG21	1.97	0.46
16:K:52:LYS:HD3	16:K:52:LYS:HA	1.66	0.46
18:O:324:VAL:O	18:O:328:VAL:HG23	2.16	0.46
19:P:412:LEU:HD12	29:U:268:LYS:HG3	1.97	0.46
19:P:440:HIS:ND1	29:U:220:PRO:HG3	2.30	0.46
21:S:336:SER:O	21:S:338:MET:N	2.49	0.46
22:V:250:GLN:HA	22:V:253:LYS:NZ	2.30	0.46
1:b:94:THR:HG21	1:b:128:GLU:HG2	1.98	0.46
6:e:128:THR:HB	6:e:144:PHE:HB2	1.98	0.46
25:J:241:ALA:HB1	25:J:287:ASN:HD21	1.81	0.46
25:J:298:ASP:OD1	25:J:298:ASP:N	2.49	0.46
26:H:181:TYR:H	26:H:181:TYR:HD2	1.64	0.46
32:o:278:LEU:H	32:o:278:LEU:HD12	1.80	0.46
3:3:28:ARG:HH21	3:3:183:TRP:CD1	2.34	0.45
4:4:183:ILE:HG12	4:4:190:ARG:HE	1.82	0.45
8:A:135:ARG:HH12	14:G:125:LEU:HD12	1.80	0.45
15:I:133:LEU:HD12	15:I:157:VAL:HG12	1.98	0.45
16:K:245:LYS:HG3	16:K:246:TYR:N	2.30	0.45
16:K:325:ASP:OD1	25:J:222:TYR:OH	2.32	0.45
19:P:166:GLU:OE1	19:P:166:GLU:N	2.26	0.45
20:R:189:GLU:O	20:R:192:GLU:HG3	2.16	0.45
20:R:279:LEU:O	20:R:282:THR:OG1	2.28	0.45
25:J:341:ILE:HD12	25:J:379:GLN:HB2	1.97	0.45
28:Q:158:ILE:HD11	28:Q:180:LEU:HB3	1.97	0.45
30:N:173:LYS:HA	30:N:176:GLN:HE21	1.80	0.45
30:N:493:GLY:HA2	30:N:524:ILE:HG23	1.98	0.45
30:N:765:ASP:OD1	30:N:765:ASP:N	2.48	0.45
3:3:172:LEU:HD11	3:3:200:LEU:HD13	1.98	0.45
15:I:72:GLU:OE1	32:o:763:HIS:ND1	2.48	0.45
15:I:234:LYS:NZ	25:J:277:ASN:O	2.37	0.45
16:K:288:SER:HA	17:L:256:ILE:HD13	1.96	0.45
18:O:71:ASP:OD1	18:O:109:LEU:HD22	2.17	0.45
18:O:336:LEU:HB2	18:O:337:LEU:HD12	1.98	0.45
21:S:100:HIS:CE1	21:S:102:SER:HB2	2.51	0.45
21:S:188:TYR:HE2	21:S:239:ARG:HD3	1.81	0.45
21:S:323:LEU:HD23	21:S:323:LEU:HA	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:7:VAL:HG11	23:W:94:ALA:HB1	1.98	0.45
7:a:39:VAL:HG12	7:a:90:ILE:HD12	1.97	0.45
7:a:78:VAL:HG11	7:a:100:LEU:HD12	1.99	0.45
5:f:188:TYR:HE1	5:f:198:LYS:HD3	1.80	0.45
25:J:333:ARG:HE	25:J:333:ARG:HB2	1.57	0.45
29:U:33:CYS:O	29:U:95:SER:N	2.50	0.45
31:T:63:GLU:OE2	31:T:89:TYR:OH	2.33	0.45
32:o:358:TYR:CE1	32:o:849:ARG:HG2	2.50	0.45
4:4:10:GLN:NE2	4:4:152:MET:O	2.50	0.45
8:A:115:ASP:HB3	8:A:155:TYR:CZ	2.51	0.45
8:A:237:SER:OG	8:A:239:GLU:OE2	2.34	0.45
9:B:69:PRO:HD2	9:B:104:TYR:CE2	2.51	0.45
9:B:172:LYS:HE2	9:B:172:LYS:HB2	1.82	0.45
12:E:235:LYS:HA	12:E:238:GLU:HG3	1.98	0.45
14:G:52:LYS:HZ2	14:G:215:GLU:HB2	1.80	0.45
16:K:199:GLU:OE2	16:K:308:GLN:NE2	2.47	0.45
19:P:93:ILE:HD13	19:P:93:ILE:HA	1.87	0.45
6:e:225:ILE:O	6:e:232:ARG:NH1	2.49	0.45
5:f:83:PHE:CE1	5:f:88:ILE:HG12	2.51	0.45
5:f:166:LYS:HE3	4:g:96:ARG:NH1	2.32	0.45
5:f:240:ALA:HB1	5:f:247:GLY:HA2	1.97	0.45
3:h:144:ASP:N	3:h:144:ASP:OD1	2.49	0.45
26:H:147:ILE:HG21	26:H:176:VAL:HG21	1.98	0.45
30:N:331:ALA:HB2	30:N:697:PHE:HD2	1.81	0.45
31:T:28:PRO:HA	31:T:31:LYS:HD3	1.99	0.45
32:o:287:ARG:NH2	32:o:870:ALA:O	2.34	0.45
32:o:964:GLU:HA	32:o:977:ILE:HD12	1.97	0.45
3:3:29:LEU:HD13	3:3:40:PHE:HD1	1.82	0.45
5:5:96:THR:HA	5:5:102:ALA:H	1.81	0.45
13:F:217:GLY:N	13:F:220:THR:O	2.50	0.45
14:G:8:TYR:HD2	14:G:17:PRO:HD3	1.80	0.45
15:I:256:TYR:HB3	26:H:282:LYS:HD3	1.98	0.45
15:I:295:ASN:ND2	15:I:298:GLY:O	2.49	0.45
16:K:353:PHE:HD1	16:K:387:MET:HE3	1.81	0.45
19:P:107:SER:HB3	19:P:110:LEU:HD13	1.98	0.45
20:R:59:MET:O	20:R:63:TYR:N	2.44	0.45
22:V:306:LYS:HA	29:U:236:LEU:HD11	1.98	0.45
23:W:181:LEU:O	23:W:185:ILE:HG13	2.16	0.45
23:W:185:ILE:HG23	23:W:189:PRO:HG2	1.97	0.45
26:H:248:LEU:HD22	26:H:377:PHE:CE2	2.48	0.45
27:M:83:VAL:HG23	27:M:120:LYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:N:53:ASP:OD2	30:N:53:ASP:N	2.35	0.45
30:N:397:SER:O	30:N:400:ILE:HG22	2.17	0.45
30:N:526:TYR:HE1	30:N:730:VAL:HG11	1.80	0.45
30:N:578:ASP:OD1	30:N:580:ASN:N	2.48	0.45
32:o:292:ASP:OD1	32:o:292:ASP:N	2.47	0.45
1:1:82:LEU:O	1:1:86:THR:HG22	2.16	0.45
1:1:153:ILE:H	1:1:153:ILE:HD12	1.81	0.45
2:2:211:LYS:HE2	2:2:211:LYS:HB2	1.82	0.45
7:7:44:VAL:H	7:7:177:THR:HB	1.81	0.45
9:B:135:LEU:HG	9:B:164:ILE:HD11	1.99	0.45
13:F:87:TYR:HE2	13:F:115:LYS:HD3	1.82	0.45
15:I:71:LEU:HG	32:o:621:LEU:HD12	1.99	0.45
15:I:153:THR:O	26:H:96:PRO:HG3	2.17	0.45
16:K:240:SER:OG	17:L:307:GLU:OE1	2.34	0.45
16:K:283:ASP:OD2	17:L:296:SER:OG	2.34	0.45
19:P:276:LEU:HD23	19:P:276:LEU:HA	1.82	0.45
21:S:41:ILE:O	21:S:44:THR:HG22	2.16	0.45
21:S:154:GLN:HA	21:S:157:GLU:HB2	1.97	0.45
7:a:128:TYR:CD2	7:a:129:LEU:HD23	2.51	0.45
7:a:265:LYS:C	7:a:265:LYS:HD3	2.41	0.45
4:g:172:MET:SD	4:g:174:MET:HE1	2.57	0.45
26:H:167:ASP:C	26:H:168:ILE:HD13	2.42	0.45
28:Q:263:LYS:NZ	28:Q:324:GLU:HB3	2.31	0.45
30:N:285:ALA:HA	30:N:288:ASN:ND2	2.31	0.45
6:6:110:ARG:NH1	12:E:101:LEU:O	2.48	0.45
8:A:14:ARG:O	8:A:27:GLN:NE2	2.40	0.45
15:I:214:LYS:HE3	26:H:420:ARG:HD3	1.99	0.45
16:K:96:ILE:HD11	17:L:118:ILE:HD13	1.99	0.45
16:K:420:THR:O	16:K:423:LYS:NZ	2.49	0.45
18:O:75:GLN:NE2	18:O:124:ASP:OD1	2.50	0.45
18:O:82:LEU:HD13	18:O:102:LEU:HD11	1.99	0.45
18:O:258:LEU:HD22	18:O:291:ILE:HD11	1.98	0.45
23:W:35:PHE:CD2	23:W:182:TYR:HB2	2.52	0.45
5:f:181:ARG:NH1	5:f:257:GLU:HG3	2.32	0.45
3:h:99:ARG:NH2	3:h:127:ILE:HG13	2.31	0.45
2:i:69:LYS:NZ	2:i:103:PRO:O	2.43	0.45
25:J:100:LYS:HB2	25:J:100:LYS:HE3	1.75	0.45
28:Q:78:ILE:HD12	28:Q:117:VAL:HG11	1.97	0.45
29:U:271:ASP:O	29:U:274:MET:HE3	2.16	0.45
30:N:114:SER:O	30:N:118:THR:OG1	2.26	0.45
32:o:509:LEU:O	32:o:513:ALA:N	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:o:740:VAL:HB	32:o:775:MET:SD	2.57	0.45
5:5:279:GLU:OE1	5:5:281:SER:OG	2.25	0.45
7:7:127:GLU:CD	13:F:100:ASN:HB2	2.42	0.45
10:C:14:SER:OG	10:C:18:ARG:O	2.34	0.45
15:I:106:ILE:HB	25:J:93:LYS:HG3	1.97	0.45
16:K:376:ASP:OD1	16:K:376:ASP:N	2.49	0.45
17:L:390:ASP:OD2	17:L:426:LYS:NZ	2.47	0.45
18:O:358:ILE:HD11	29:U:230:GLN:HB2	1.99	0.45
2:i:37:PHE:HE1	2:i:42:VAL:HG23	1.82	0.45
29:U:56:PHE:CD1	29:U:56:PHE:C	2.95	0.45
30:N:381:GLU:HB3	30:N:384:LYS:HE3	1.98	0.45
31:T:68:ALA:O	31:T:72:THR:OG1	2.30	0.45
32:o:269:TYR:OH	32:o:296:SER:OG	2.34	0.45
5:5:107:LYS:HE2	5:5:107:LYS:HB2	1.86	0.45
6:6:161:ALA:HB2	6:6:214:HIS:CD2	2.51	0.45
9:B:97:TYR:CD1	9:B:105:PRO:HB3	2.52	0.45
9:B:193:LEU:HD21	9:B:243:ILE:HD11	1.98	0.45
15:I:355:LEU:HD12	15:I:355:LEU:HA	1.81	0.45
18:O:24:PRO:HA	18:O:27:GLU:HG2	1.98	0.45
18:O:51:ASP:O	18:O:58:ARG:NH2	2.49	0.45
18:O:136:THR:O	18:O:140:LYS:N	2.49	0.45
21:S:37:VAL:O	21:S:41:ILE:HG23	2.17	0.45
21:S:278:LYS:O	21:S:282:ILE:HG13	2.17	0.45
24:Y:37:ASP:N	24:Y:37:ASP:OD1	2.48	0.45
1:b:56:VAL:HB	1:b:82:LEU:HD12	1.99	0.45
6:e:227:THR:HG22	6:e:228:LYS:N	2.32	0.45
5:f:108:LYS:H	5:f:108:LYS:HG2	1.62	0.45
27:M:81:ASN:OD1	27:M:81:ASN:N	2.48	0.45
27:M:121:THR:HG21	27:M:153:TYR:HE1	1.81	0.45
27:M:377:GLN:O	27:M:381:ARG:HG3	2.16	0.45
27:M:411:LYS:N	27:M:414:ASP:OD2	2.42	0.45
30:N:132:LYS:O	30:N:136:ILE:HG12	2.17	0.45
30:N:782:PHE:HB3	30:N:875:LEU:HD13	1.98	0.45
32:o:337:GLU:HA	32:o:340:LEU:HG	1.99	0.45
32:o:558:LEU:HD22	32:o:595:MET:HE1	1.99	0.45
32:o:977:ILE:HG23	32:o:981:VAL:HG21	1.98	0.45
6:6:50:THR:HG1	6:6:55:ASN:HD21	1.55	0.45
6:6:221:LEU:N	6:6:236:TYR:O	2.48	0.45
10:C:120:GLN:HG2	11:D:84:ILE:HD11	1.97	0.45
12:E:68:VAL:HB	12:E:93:ARG:HH21	1.82	0.45
18:O:9:THR:O	18:O:13:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:24:ILE:HG12	19:P:39:LEU:HG	1.98	0.45
23:W:120:ASP:HB2	23:W:125:LEU:HD11	1.98	0.45
28:Q:262:LEU:HD23	28:Q:296:ILE:HG13	1.99	0.45
30:N:194:ILE:HA	30:N:203:ARG:NH1	2.29	0.45
30:N:418:ASP:OD1	30:N:419:THR:N	2.50	0.45
32:o:119:LEU:HB3	32:o:137:TYR:CE2	2.52	0.45
2:2:116:LEU:HD23	2:2:116:LEU:HA	1.82	0.45
4:4:106:GLY:HA2	4:4:184:VAL:HG11	1.99	0.45
7:7:127:GLU:OE1	13:F:100:ASN:HB2	2.16	0.45
11:D:177:LYS:HB3	11:D:177:LYS:HE2	1.80	0.45
17:L:161:ARG:NE	17:L:272:GLU:OE2	2.50	0.45
17:L:382:MET:HE2	17:L:382:MET:HB2	1.83	0.45
20:R:232:VAL:HG11	20:R:269:LYS:HD2	1.97	0.45
5:f:82:ARG:HH21	5:f:221:TRP:HH2	1.65	0.45
5:f:89:VAL:HB	5:f:253:TYR:HB2	1.99	0.45
4:g:166:GLN:O	4:g:170:LYS:HG2	2.17	0.45
3:h:51:LEU:HD21	3:h:107:PRO:HB3	1.99	0.45
28:Q:150:GLN:HB3	28:Q:153:ASP:OD1	2.16	0.45
30:N:581:ASP:OD2	30:N:614:ASN:ND2	2.34	0.45
1:1:142:PRO:HB2	1:1:161:PHE:CZ	2.51	0.44
2:2:178:GLU:HA	2:2:181:ILE:HG22	1.99	0.44
6:6:229:ASP:OD1	6:6:230:GLY:N	2.50	0.44
8:A:22:GLU:OE1	8:A:22:GLU:N	2.49	0.44
9:B:49:LYS:HE3	9:B:49:LYS:HB2	1.83	0.44
13:F:206:LEU:HD13	13:F:211:LEU:HD22	1.98	0.44
15:I:54:ARG:HH12	32:o:155:ARG:HH21	1.64	0.44
17:L:98:LEU:HD21	27:M:72:ASN:HD22	1.82	0.44
18:O:40:GLN:HA	18:O:43:GLU:CD	2.42	0.44
18:O:156:THR:HA	18:O:159:LYS:HG2	1.98	0.44
18:O:211:GLN:NE2	18:O:241:THR:O	2.51	0.44
22:V:59:ASP:OD1	22:V:59:ASP:C	2.60	0.44
5:f:153:ALA:O	5:f:157:ILE:HG12	2.16	0.44
27:M:54:GLU:O	27:M:58:MET:HG3	2.17	0.44
31:T:256:LYS:HD3	31:T:262:LYS:HE2	2.00	0.44
32:o:528:LEU:HD11	32:o:565:PHE:HB3	1.99	0.44
32:o:913:ILE:HD11	32:o:957:LEU:HD21	2.00	0.44
2:2:32:ILE:HG22	2:2:45:ALA:HB2	1.98	0.44
4:4:146:HIS:O	4:4:149:ARG:NH2	2.50	0.44
5:5:216:ASP:N	5:5:216:ASP:OD1	2.49	0.44
6:6:198:GLU:O	6:6:202:LEU:HG	2.18	0.44
7:7:48:LYS:HA	7:7:53:VAL:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:24:ARG:NH2	8:A:29:GLU:OE1	2.50	0.44
9:B:141:GLU:H	9:B:141:GLU:CD	2.26	0.44
13:F:52:ASN:ND2	13:F:59:TYR:OH	2.50	0.44
15:I:161:GLN:HG2	15:I:163:ASP:HB2	1.99	0.44
15:I:281:ILE:O	15:I:326:MET:HA	2.17	0.44
18:O:292:CYS:HB3	18:O:327:LEU:HD11	1.99	0.44
21:S:371:LEU:HD23	21:S:371:LEU:HA	1.86	0.44
23:W:29:GLN:HG3	23:W:144:PHE:HZ	1.81	0.44
7:a:226:ARG:NH1	7:a:246:GLN:HE21	2.15	0.44
7:a:234:ASP:OD2	7:a:237:THR:N	2.37	0.44
27:M:415:PHE:O	27:M:419:ILE:HG12	2.17	0.44
28:Q:63:GLN:HB2	28:Q:103:LYS:HZ3	1.81	0.44
30:N:394:ARG:HG3	30:N:394:ARG:O	2.18	0.44
32:o:787:ASP:OD1	32:o:787:ASP:N	2.49	0.44
6:6:30:THR:HA	6:6:74:ASN:HD21	1.81	0.44
6:6:39:PHE:HE2	6:6:199:VAL:HG21	1.82	0.44
7:7:164:ASN:HD21	7:7:166:LEU:HB2	1.82	0.44
12:E:86:ARG:HG2	12:E:86:ARG:NH1	2.32	0.44
14:G:90:ASN:O	14:G:94:GLU:HG2	2.17	0.44
14:G:95:GLU:HB3	14:G:115:ARG:HH11	1.82	0.44
15:I:93:LYS:O	15:I:97:GLU:HG2	2.18	0.44
16:K:132:LYS:O	16:K:135:MET:HB2	2.17	0.44
19:P:113:ASN:O	19:P:116:ILE:HG22	2.17	0.44
21:S:159:ASN:N	21:S:159:ASN:HD22	2.15	0.44
21:S:278:LYS:HG2	21:S:316:LEU:HD11	1.99	0.44
6:e:134:ASP:OD1	6:e:138:LYS:N	2.49	0.44
27:M:139:LYS:HD3	27:M:139:LYS:HA	1.74	0.44
30:N:10:LEU:HD12	30:N:10:LEU:HA	1.69	0.44
30:N:528:ARG:HB3	30:N:531:LEU:HB2	1.99	0.44
1:1:102:LYS:HD3	14:G:104:LYS:NZ	2.33	0.44
1:1:151:THR:HA	1:1:154:TYR:CE1	2.52	0.44
1:1:159:LYS:HZ1	1:b:176:HIS:HB3	1.82	0.44
13:F:191:LYS:HE2	13:F:191:LYS:HB2	1.86	0.44
14:G:95:GLU:HB3	14:G:115:ARG:NH1	2.33	0.44
15:I:255:LYS:HZ3	25:J:217:GLU:HB3	1.83	0.44
16:K:129:GLU:H	16:K:129:GLU:HG2	1.57	0.44
16:K:160:VAL:HG22	16:K:235:ILE:HG12	1.99	0.44
17:L:165:PRO:HB2	27:M:143:ASN:OD1	2.18	0.44
18:O:328:VAL:O	18:O:332:ILE:HG12	2.17	0.44
18:O:392:TRP:HZ3	29:U:190:LEU:HB3	1.83	0.44
1:b:172:ASP:O	1:b:176:HIS:ND1	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:e:109:ALA:HA	6:e:144:PHE:HZ	1.81	0.44
25:J:197:LEU:HD12	25:J:197:LEU:HA	1.86	0.44
28:Q:376:LYS:O	28:Q:380:MET:HG2	2.16	0.44
29:U:50:ASN:OD1	29:U:51:SER:N	2.50	0.44
30:N:511:GLY:O	30:N:514:THR:OG1	2.35	0.44
30:N:664:LEU:HB2	30:N:706:MET:HE1	1.99	0.44
1:1:151:THR:HA	1:1:154:TYR:HE1	1.82	0.44
2:2:236:ARG:NH2	3:3:162:ASP:HA	2.33	0.44
3:3:44:PHE:CE2	3:3:64:ASN:HB2	2.52	0.44
5:5:250:VAL:N	5:5:266:HIS:O	2.48	0.44
6:6:49:ILE:HG21	2:i:196:LEU:HD21	2.00	0.44
6:6:176:LYS:HD2	3:h:203:ARG:HH22	1.80	0.44
12:E:54:ALA:HA	12:E:59:LEU:HD23	1.99	0.44
13:F:162:GLY:N	13:F:165:SER:OG	2.50	0.44
14:G:148:LEU:C	14:G:149:TYR:HD1	2.26	0.44
16:K:134:SER:O	16:K:134:SER:OG	2.30	0.44
16:K:221:MET:O	16:K:221:MET:HG3	2.16	0.44
17:L:396:THR:HA	27:M:212:ILE:HD11	1.99	0.44
19:P:311:TRP:CE3	19:P:345:VAL:HG11	2.53	0.44
22:V:25:GLU:CD	22:V:157:ARG:HH22	2.25	0.44
7:a:122:PRO:HB2	7:a:159:PHE:HD2	1.82	0.44
7:a:134:TYR:HE2	6:e:82:ALA:HB2	1.83	0.44
6:e:102:LYS:NZ	6:e:103:LEU:O	2.44	0.44
6:e:227:THR:HG22	6:e:228:LYS:H	1.83	0.44
2:i:129:VAL:HB	2:i:140:PHE:CE1	2.52	0.44
2:i:195:ASP:HB3	2:i:198:SER:HB3	1.99	0.44
26:H:95:HIS:HB2	26:H:96:PRO:HD3	1.98	0.44
26:H:360:THR:O	26:H:360:THR:OG1	2.30	0.44
30:N:186:ILE:HG21	30:N:214:LEU:HD21	1.99	0.44
30:N:475:ALA:HB2	30:N:510:HIS:CD2	2.52	0.44
30:N:492:THR:HG21	30:N:494:LYS:HE2	1.99	0.44
30:N:858:LYS:HD2	30:N:859:ASN:H	1.82	0.44
32:o:293:MET:O	32:o:297:VAL:HG23	2.18	0.44
32:o:357:ILE:HG13	32:o:390:LEU:HD11	2.00	0.44
15:I:150:HIS:CD2	26:H:90:ARG:HH22	2.35	0.44
15:I:194:ILE:HG12	15:I:348:ILE:HD13	1.98	0.44
16:K:304:ASP:OD2	16:K:333:ARG:NH2	2.42	0.44
17:L:141:LYS:HE2	17:L:141:LYS:HB2	1.77	0.44
19:P:63:VAL:HG23	19:P:75:LEU:HD11	2.00	0.44
19:P:362:LEU:HD23	19:P:398:LYS:C	2.43	0.44
20:R:149:ASN:OD1	20:R:150:ALA:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:118:LEU:HD22	22:V:122:ASP:HB3	1.99	0.44
25:J:249:GLU:HG3	25:J:250:ILE:H	1.82	0.44
26:H:86:GLY:O	26:H:90:ARG:HB2	2.18	0.44
27:M:320:ARG:HE	27:M:320:ARG:HB2	1.66	0.44
30:N:374:ILE:HG22	30:N:375:HIS:ND1	2.32	0.44
2:2:87:LEU:HD22	2:2:115:HIS:HD2	1.83	0.44
3:3:109:VAL:O	3:3:121:ILE:HD12	2.18	0.44
3:3:121:ILE:HG13	3:3:137:ILE:HD13	1.99	0.44
4:4:149:ARG:HD3	4:4:149:ARG:HA	1.74	0.44
7:7:228:PHE:N	7:7:245:LEU:O	2.40	0.44
15:I:233:ALA:HA	15:I:236:VAL:HG12	1.99	0.44
18:O:15:ARG:HH21	18:O:23:HIS:CD2	2.36	0.44
18:O:151:ASP:HA	18:O:154:GLU:HG3	1.99	0.44
18:O:373:TRP:CE3	29:U:204:LEU:HD11	2.53	0.44
19:P:326:ASP:O	19:P:328:ALA:N	2.48	0.44
23:W:5:ALA:H	23:W:106:GLN:HB3	1.82	0.44
23:W:9:VAL:HA	23:W:52:ILE:HG23	2.00	0.44
4:g:168:LEU:O	4:g:172:MET:HB2	2.17	0.44
3:h:159:GLU:OE1	3:h:161:GLU:HB3	2.18	0.44
2:i:48:ARG:NH2	2:i:196:LEU:O	2.51	0.44
25:J:327:ILE:HG22	25:J:358:VAL:HG11	1.98	0.44
26:H:82:TRP:CD1	26:H:82:TRP:H	2.34	0.44
26:H:395:SER:O	26:H:396:MET:HB2	2.18	0.44
28:Q:77:PHE:O	28:Q:80:HIS:ND1	2.46	0.44
30:N:193:ALA:HB2	30:N:206:ILE:HD13	1.99	0.44
30:N:301:THR:HG22	30:N:920:VAL:H	1.83	0.44
30:N:536:ILE:O	30:N:540:LEU:HB2	2.17	0.44
30:N:559:TYR:CD2	30:N:567:ALA:HB2	2.53	0.44
31:T:112:ASN:O	31:T:116:GLN:HG2	2.18	0.44
32:o:279:THR:HB	32:o:974:THR:HG23	2.00	0.44
32:o:945:ILE:HD11	32:o:962:ARG:HB2	1.99	0.44
11:D:66:LYS:NZ	11:D:69:SER:HA	2.33	0.44
19:P:423:LEU:O	19:P:426:ILE:HG22	2.17	0.44
20:R:31:PHE:HB3	20:R:320:LYS:HG2	2.00	0.44
21:S:159:ASN:OD1	21:S:187:ILE:HA	2.18	0.44
7:a:49:TYR:HE1	7:a:54:ILE:HG13	1.83	0.44
4:g:29:LYS:HE2	4:g:31:SER:HB2	1.99	0.44
4:g:167:GLU:HG3	4:g:168:LEU:N	2.32	0.44
26:H:320:ASP:OD1	26:H:321:ASP:N	2.51	0.44
26:H:439:THR:OG1	26:H:440:GLU:N	2.51	0.44
27:M:76:PRO:HG2	27:M:150:LYS:NZ	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:N:202:PHE:O	30:N:206:ILE:HG22	2.18	0.44
30:N:443:LEU:HD12	30:N:469:VAL:HG21	2.00	0.44
30:N:646:LYS:HD3	30:N:646:LYS:HA	1.69	0.44
31:T:59:LYS:NZ	31:T:96:LEU:O	2.49	0.44
32:o:620:LEU:HD12	32:o:739:ALA:HA	1.99	0.44
2:2:233:LYS:HA	2:2:233:LYS:HD2	1.90	0.44
7:7:214:MET:HE2	7:7:214:MET:HA	2.00	0.44
16:K:396:ARG:NH2	17:L:195:GLU:OE1	2.51	0.44
20:R:59:MET:SD	20:R:59:MET:N	2.91	0.44
21:S:437:ASN:HB3	21:S:442:PHE:CE1	2.52	0.44
7:a:44:VAL:HG23	7:a:87:SER:HB2	1.99	0.44
4:g:4:ILE:HG22	4:g:103:LEU:HD12	1.99	0.44
3:h:45:HIS:CE1	2:i:247:VAL:HG11	2.53	0.44
26:H:223:GLU:HG2	26:H:227:LEU:HD12	2.00	0.44
26:H:389:PHE:O	26:H:393:SER:HB3	2.18	0.44
28:Q:195:LYS:HD2	28:Q:225:LEU:HD13	1.98	0.44
29:U:71:ASN:OD1	29:U:71:ASN:N	2.51	0.44
29:U:211:LEU:O	29:U:214:VAL:HG12	2.17	0.44
32:o:278:LEU:HA	32:o:281:ALA:HB3	1.99	0.44
6:6:177:ASN:ND2	3:h:176:ASP:OD2	2.25	0.43
7:7:49:TYR:CE1	7:7:54:ILE:HG13	2.52	0.43
14:G:73:HIS:CE1	14:G:106:PRO:HB3	2.53	0.43
15:I:304:ARG:HH21	26:H:329:VAL:HG21	1.83	0.43
17:L:147:THR:OG1	17:L:156:MET:HB2	2.18	0.43
17:L:248:ALA:HB1	17:L:285:ALA:HB3	2.00	0.43
19:P:107:SER:HB3	19:P:110:LEU:HB2	1.99	0.43
19:P:384:VAL:CG1	28:Q:353:PRO:HB3	2.46	0.43
7:a:190:LYS:HA	7:a:190:LYS:HD2	1.73	0.43
4:g:115:GLU:HG2	4:g:117:TYR:CZ	2.53	0.43
30:N:143:LYS:HA	30:N:146:LYS:HD2	2.00	0.43
32:o:497:PHE:CG	32:o:505:VAL:HG21	2.53	0.43
1:1:166:SER:OG	1:1:169:GLU:HG3	2.17	0.43
4:4:103:LEU:HD12	4:4:103:LEU:HA	1.86	0.43
5:5:286:ILE:HD12	5:5:286:ILE:HA	1.91	0.43
6:6:153:GLU:OE1	6:6:156:ARG:NE	2.49	0.43
8:A:65:ASP:OD2	8:A:67:THR:OG1	2.35	0.43
8:A:76:SER:OG	8:A:77:ARG:N	2.51	0.43
9:B:37:ILE:HG22	9:B:161:ALA:HB1	1.99	0.43
10:C:4:ARG:HH12	12:E:10:ARG:HA	1.82	0.43
10:C:181:LYS:HA	10:C:181:LYS:HD3	1.89	0.43
11:D:113:VAL:HG12	11:D:150:THR:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:155:GLU:O	14:G:60:VAL:HG12	2.18	0.43
14:G:83:PRO:O	14:G:86:ARG:HB3	2.18	0.43
17:L:220:LEU:HD22	17:L:349:ILE:HD11	1.99	0.43
18:O:38:TRP:HB3	18:O:69:PHE:CE2	2.52	0.43
18:O:248:TYR:HB3	18:O:251:LEU:HD21	2.00	0.43
18:O:287:LEU:HD12	18:O:287:LEU:HA	1.87	0.43
19:P:33:ASN:OD1	19:P:33:ASN:N	2.50	0.43
19:P:141:LYS:HD2	19:P:179:PHE:HE1	1.83	0.43
21:S:33:GLU:O	21:S:37:VAL:HG23	2.18	0.43
22:V:229:ASP:C	22:V:229:ASP:OD2	2.61	0.43
23:W:34:GLU:HG3	23:W:69:PHE:CZ	2.53	0.43
4:g:135:TYR:HD1	4:g:138:PHE:HE2	1.65	0.43
32:o:457:ILE:HA	32:o:460:SER:HB3	1.98	0.43
32:o:809:MET:HB3	32:o:847:ILE:HD13	2.00	0.43
32:o:967:THR:HG22	32:o:969:GLU:H	1.82	0.43
4:4:44:MET:HE1	4:4:104:ILE:HB	2.00	0.43
5:5:120:MET:SD	5:5:127:CYS:HB2	2.58	0.43
5:5:198:LYS:HA	5:5:198:LYS:HD2	1.82	0.43
7:7:60:LEU:HD22	7:7:225:SER:HB3	2.00	0.43
7:7:208:GLU:HA	7:7:211:VAL:HG12	2.01	0.43
8:A:61:ASP:CG	17:L:420:ARG:HH21	2.23	0.43
8:A:126:GLN:NE2	9:B:81:ASP:HA	2.31	0.43
9:B:94:HIS:O	9:B:99:ARG:HG2	2.17	0.43
13:F:163:ALA:O	13:F:164:ARG:HG2	2.18	0.43
14:G:36:THR:HA	14:G:166:GLY:HA3	2.00	0.43
15:I:150:HIS:O	15:I:154:MET:HG2	2.17	0.43
19:P:300:VAL:O	19:P:304:THR:OG1	2.24	0.43
6:e:180:GLU:O	6:e:183:THR:OG1	2.31	0.43
3:h:24:ALA:HB2	3:h:187:VAL:HG22	1.99	0.43
3:h:95:LEU:HD11	3:h:107:PRO:HG2	2.00	0.43
2:i:47:THR:HB	2:i:59:ASN:HA	2.00	0.43
28:Q:224:ILE:HD12	28:Q:330:LEU:HD22	2.01	0.43
28:Q:275:ILE:H	28:Q:275:ILE:HG13	1.53	0.43
28:Q:390:LEU:HD12	28:Q:391:ASP:H	1.84	0.43
29:U:294:ASN:O	29:U:297:GLN:HG3	2.18	0.43
31:T:202:LEU:HB3	31:T:231:SER:HB2	2.01	0.43
32:o:154:ILE:O	32:o:157:LEU:HG	2.18	0.43
32:o:375:ASP:HB3	32:o:842:GLN:HE22	1.83	0.43
4:4:20:ALA:HB2	4:4:177:LYS:HG2	2.00	0.43
9:B:186:GLU:HA	9:B:189:ILE:HG22	2.00	0.43
11:D:50:SER:O	11:D:50:SER:OG	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:147:ARG:CZ	18:O:150:LEU:HD11	2.49	0.43
22:V:175:SER:OG	30:N:741:TYR:HA	2.18	0.43
24:Y:72:ASP:OD1	24:Y:74:THR:OG1	2.36	0.43
7:a:98:ARG:HG3	7:a:101:LYS:HE2	1.99	0.43
1:b:133:PRO:HD2	1:b:137:SER:O	2.18	0.43
6:e:111:ASN:O	6:e:115:LEU:HG	2.18	0.43
4:g:168:LEU:HB3	4:g:176:PHE:CE2	2.54	0.43
3:h:10:GLY:HA3	3:h:42:LYS:HE2	2.00	0.43
2:i:96:SER:OG	2:i:101:ARG:O	2.31	0.43
27:M:50:ARG:O	27:M:53:HIS:ND1	2.49	0.43
27:M:203:ARG:NE	27:M:206:LYS:HD2	2.34	0.43
28:Q:251:THR:H	28:Q:254:SER:HB3	1.84	0.43
30:N:319:SER:OG	30:N:320:SER:N	2.51	0.43
3:3:18:LYS:NZ	3:3:157:ASN:HB3	2.33	0.43
3:3:65:GLU:CD	10:C:100:LYS:HA	2.43	0.43
3:3:165:GLU:O	3:3:169:GLN:HG2	2.18	0.43
7:7:125:ILE:O	7:7:129:LEU:HG	2.18	0.43
8:A:232:LYS:HA	8:A:232:LYS:HD2	1.81	0.43
9:B:19:GLY:O	9:B:23:TYR:HD1	2.01	0.43
9:B:176:GLU:HG3	10:C:56:LEU:HD23	2.01	0.43
11:D:75:PHE:CE2	11:D:79:ASN:HA	2.53	0.43
11:D:200:LEU:HA	11:D:203:VAL:HG12	1.99	0.43
11:D:203:VAL:O	11:D:204:GLN:HG3	2.17	0.43
18:O:211:GLN:HG2	18:O:241:THR:HB	1.99	0.43
18:O:236:HIS:HB3	18:O:238:ILE:HG22	2.01	0.43
18:O:296:LEU:HD22	18:O:327:LEU:HD22	2.00	0.43
20:R:67:CYS:HB3	20:R:94:PHE:HB2	2.00	0.43
20:R:410:LEU:HD22	29:U:281:LEU:HD21	2.00	0.43
21:S:336:SER:OG	21:S:337:ASN:OD1	2.36	0.43
21:S:423:VAL:O	21:S:427:ILE:HG23	2.18	0.43
21:S:474:GLU:O	21:S:477:VAL:HG12	2.18	0.43
1:b:122:ASP:OD1	1:b:123:ASP:N	2.51	0.43
1:b:151:THR:HA	1:b:154:TYR:HE2	1.83	0.43
1:b:151:THR:HA	1:b:154:TYR:CE2	2.54	0.43
6:e:45:ASP:O	6:e:61:LYS:NZ	2.50	0.43
5:f:107:LYS:HA	5:f:107:LYS:HD2	1.80	0.43
4:g:149:ARG:HB2	4:g:152:MET:HG3	2.00	0.43
4:g:178:GLY:HA3	4:g:195:PHE:CE1	2.53	0.43
30:N:739:PHE:O	30:N:739:PHE:CG	2.71	0.43
31:T:255:GLN:CD	31:T:256:LYS:H	2.27	0.43
32:o:506:LEU:HD12	32:o:534:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:o:583:ASP:OD1	32:o:584:VAL:N	2.51	0.43
32:o:854:LEU:HD12	32:o:854:LEU:O	2.18	0.43
1:l:155:GLY:HA2	1:b:180:GLN:CD	2.42	0.43
4:4:99:GLN:HA	4:4:121:TYR:HB2	2.00	0.43
6:6:224:LEU:HD12	6:6:224:LEU:HA	1.81	0.43
7:7:86:ILE:HG22	7:7:147:ILE:HG23	2.00	0.43
7:7:121:GLU:HB2	7:7:124:TYR:CE2	2.54	0.43
9:B:66:LEU:HD12	9:B:235:PHE:HD2	1.84	0.43
9:B:66:LEU:HD11	9:B:69:PRO:HA	2.00	0.43
17:L:159:LEU:HD11	27:M:128:PHE:CD1	2.54	0.43
17:L:283:VAL:HG21	17:L:325:MET:HE3	1.99	0.43
18:O:150:LEU:HA	18:O:153:LEU:HB2	2.01	0.43
22:V:270:TYR:N	22:V:270:TYR:CD1	2.87	0.43
1:b:20:THR:HG21	1:b:52:LYS:HD2	2.01	0.43
1:b:23:MET:SD	1:b:174:ILE:HG12	2.59	0.43
6:e:29:GLY:HA3	6:e:61:LYS:HE2	2.00	0.43
5:f:82:ARG:HH22	5:f:185:PRO:HD2	1.83	0.43
5:f:113:ASN:C	5:f:115:PHE:H	2.26	0.43
5:f:156:LYS:HZ2	5:f:196:ARG:HH22	1.65	0.43
4:g:81:SER:HB2	4:g:125:LYS:HD2	2.00	0.43
4:g:100:VAL:HG12	4:g:102:VAL:HG13	1.99	0.43
25:J:121:MET:HE2	25:J:121:MET:HB2	1.86	0.43
26:H:168:ILE:HG13	26:H:183:ILE:HG21	2.01	0.43
26:H:331:ARG:CZ	27:M:301:VAL:HG21	2.48	0.43
27:M:354:GLU:OE1	27:M:354:GLU:C	2.61	0.43
28:Q:23:ALA:HA	28:Q:26:VAL:HB	2.00	0.43
30:N:126:LYS:HA	30:N:126:LYS:HD3	1.80	0.43
32:o:509:LEU:HD23	32:o:530:LEU:HG	2.01	0.43
2:2:48:ARG:O	2:2:62:LYS:NZ	2.51	0.43
3:3:46:TYR:OH	3:3:64:ASN:O	2.33	0.43
3:3:201:LYS:HE3	5:f:273:TRP:HE1	1.84	0.43
6:6:55:ASN:HB3	7:7:170:TYR:CZ	2.54	0.43
7:7:42:THR:OG1	7:7:43:SER:N	2.52	0.43
8:A:88:PRO:HD3	14:G:156:SER:HB2	2.00	0.43
18:O:308:LEU:HD23	18:O:308:LEU:HA	1.80	0.43
19:P:257:TRP:CH2	19:P:289:ASN:HB3	2.54	0.43
6:e:86:ARG:NE	6:e:115:LEU:HD22	2.34	0.43
5:f:76:THR:O	5:f:206:SER:N	2.52	0.43
3:h:66:MET:O	3:h:70:LYS:HE3	2.19	0.43
26:H:85:MET:C	26:H:85:MET:HE2	2.43	0.43
26:H:198:MET:HB2	26:H:273:ARG:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:H:367:ARG:HH21	26:H:370:ARG:CZ	2.31	0.43
32:o:52:LEU:HD23	32:o:55:ARG:HH11	1.83	0.43
32:o:769:ASN:HB2	32:o:772:ILE:HD12	2.01	0.43
32:o:789:GLN:OE1	32:o:791:LYS:N	2.43	0.43
4:4:152:MET:H	4:4:152:MET:HG2	1.58	0.43
7:7:144:TRP:HA	7:7:165:LEU:HD22	1.99	0.43
10:C:43:GLY:HA2	10:C:146:TYR:CE1	2.54	0.43
12:E:70:ILE:HD11	12:E:76:CYS:HB3	2.01	0.43
15:I:81:ILE:HA	15:I:85:PHE:CZ	2.54	0.43
15:I:232:LEU:HD13	15:I:350:PHE:HZ	1.84	0.43
15:I:345:ASP:OD1	15:I:345:ASP:N	2.42	0.43
17:L:186:LEU:HD11	17:L:349:ILE:HG23	2.00	0.43
17:L:288:GLY:HA3	27:M:299:ARG:NH1	2.34	0.43
20:R:235:LEU:HD21	20:R:250:ALA:HA	2.00	0.43
21:S:136:CYS:HA	21:S:167:LEU:HD11	2.01	0.43
3:h:66:MET:HE2	3:h:66:MET:HA	2.01	0.43
27:M:228:LYS:HG2	27:M:349:PHE:CD2	2.54	0.43
30:N:101:ILE:HD13	30:N:101:ILE:HA	1.84	0.43
30:N:353:LEU:HD23	30:N:353:LEU:HA	1.82	0.43
30:N:647:ASP:C	30:N:647:ASP:OD1	2.61	0.43
32:o:756:MET:N	32:o:756:MET:HE2	2.33	0.43
32:o:797:THR:HG22	32:o:801:HIS:CE1	2.53	0.43
1:1:86:THR:HA	1:1:90:GLY:O	2.19	0.43
7:7:215:ARG:NH2	7:7:249:ASN:HB3	2.33	0.43
8:A:13:ASP:C	8:A:13:ASP:OD2	2.61	0.43
15:I:300:ARG:O	15:I:304:ARG:HG2	2.18	0.43
16:K:356:ILE:HD11	34:K:501:ATP:C2	2.54	0.43
17:L:156:MET:HE3	17:L:156:MET:HB3	1.92	0.43
17:L:233:LYS:HB2	17:L:233:LYS:HE3	1.79	0.43
18:O:54:SER:OG	18:O:57:LEU:HB2	2.18	0.43
18:O:228:TYR:CE2	18:O:334:LEU:HD13	2.54	0.43
18:O:244:ASN:OD1	18:O:244:ASN:N	2.52	0.43
18:O:387:ARG:O	18:O:387:ARG:NH1	2.52	0.43
19:P:342:GLN:O	19:P:345:VAL:HG12	2.18	0.43
20:R:309:LEU:HD23	20:R:309:LEU:HA	1.85	0.43
4:g:95:ARG:HD2	4:g:95:ARG:C	2.43	0.43
26:H:83:ASP:HB2	26:H:85:MET:HG3	2.00	0.43
26:H:346:ARG:HG2	26:H:349:ILE:HB	2.01	0.43
27:M:290:ARG:NH1	27:M:306:LEU:HD11	2.33	0.43
29:U:138:VAL:HG12	29:U:140:ILE:HG23	2.01	0.43
30:N:104:LYS:O	30:N:107:GLU:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:N:447:SER:HA	30:N:450:ILE:HG22	2.00	0.43
30:N:534:ASP:O	30:N:535:LEU:HB2	2.18	0.43
31:T:108:LEU:HD23	31:T:108:LEU:HA	1.87	0.43
2:2:82:GLU:H	2:2:82:GLU:CD	2.27	0.43
2:2:120:GLN:O	2:2:122:HIS:ND1	2.52	0.43
2:2:166:VAL:O	2:2:169:SER:OG	2.37	0.43
3:3:104:PHE:HA	3:3:126:LEU:HG	2.00	0.43
5:5:172:MET:H	5:5:192:SER:HB3	1.83	0.43
7:7:53:VAL:O	7:7:233:ILE:HG12	2.19	0.43
7:7:137:ARG:HD3	7:7:166:LEU:HA	2.00	0.43
11:D:53:LYS:HD3	11:D:53:LYS:HA	1.74	0.43
11:D:193:LYS:HG3	11:D:236:ILE:HD11	2.00	0.43
14:G:118:GLN:OE1	14:G:118:GLN:HA	2.19	0.43
14:G:221:LEU:HA	14:G:225:ASN:HA	1.99	0.43
16:K:378:LEU:HD23	16:K:378:LEU:HA	1.79	0.43
19:P:281:ILE:HD11	19:P:300:VAL:HG22	2.00	0.43
20:R:98:LEU:HD23	20:R:98:LEU:HA	1.86	0.43
20:R:238:PHE:CE1	20:R:249:ILE:HG13	2.54	0.43
23:W:124:GLU:OE1	23:W:127:ARG:NH1	2.51	0.43
7:a:60:LEU:HD21	7:a:67:LEU:HD13	2.01	0.43
3:h:67:PHE:CD1	3:h:70:LYS:HD2	2.54	0.43
2:i:195:ASP:OD1	2:i:197:GLY:N	2.50	0.43
30:N:442:LEU:HD12	30:N:442:LEU:HA	1.88	0.43
30:N:517:LEU:HD23	30:N:517:LEU:HA	1.89	0.43
30:N:561:GLY:O	30:N:597:ARG:HD2	2.18	0.43
32:o:89:LEU:HA	32:o:92:LEU:HD12	2.00	0.43
3:3:88:THR:HB	3:3:109:VAL:HG21	2.00	0.42
5:5:206:SER:OG	5:5:243:ASP:OD2	2.28	0.42
16:K:238:ASN:OD1	17:L:310:THR:HG21	2.19	0.42
18:O:103:LYS:NZ	18:O:107:GLN:OE1	2.52	0.42
19:P:38:GLN:O	19:P:42:LEU:HD12	2.19	0.42
19:P:281:ILE:HD12	19:P:281:ILE:HA	1.92	0.42
21:S:64:ARG:HD3	21:S:144:LEU:HD22	2.01	0.42
21:S:178:LEU:HD12	21:S:178:LEU:H	1.84	0.42
1:b:33:LEU:HD23	1:b:63:CYS:SG	2.59	0.42
6:e:27:ASN:OD1	6:e:77:ALA:N	2.52	0.42
5:f:139:ARG:HA	5:f:142:GLU:OE1	2.19	0.42
5:f:229:LEU:HD11	5:f:263:HIS:CE1	2.54	0.42
4:g:9:VAL:HG21	4:g:154:THR:HA	2.01	0.42
25:J:230:VAL:HG22	25:J:233:LEU:HD23	2.01	0.42
26:H:87:ASP:HA	26:H:90:ARG:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:N:424:LYS:HE2	30:N:424:LYS:HB3	1.79	0.42
30:N:873:ARG:NH1	30:N:875:LEU:HD11	2.34	0.42
31:T:271:GLU:HA	31:T:271:GLU:OE2	2.18	0.42
32:o:167:ASP:O	32:o:171:LYS:HB2	2.19	0.42
32:o:769:ASN:O	32:o:773:ARG:HG3	2.19	0.42
32:o:867:PHE:CD2	32:o:871:HIS:HA	2.52	0.42
32:o:953:THR:OG1	32:o:954:PRO:HD3	2.19	0.42
1:1:171:VAL:O	1:1:174:ILE:HG22	2.19	0.42
12:E:102:TYR:C	12:E:103:TYR:HD2	2.27	0.42
13:F:159:THR:OG1	13:F:160:ALA:N	2.51	0.42
17:L:242:ASN:ND2	17:L:273:HIS:HB3	2.33	0.42
17:L:356:GLY:O	17:L:360:ILE:HG12	2.19	0.42
18:O:97:LYS:HD3	18:O:97:LYS:HA	1.90	0.42
19:P:140:THR:HG21	19:P:163:LEU:HD13	2.01	0.42
20:R:418:GLY:HA2	20:R:421:VAL:HG22	2.00	0.42
3:h:15:MET:HG3	3:h:163:LEU:HD22	2.01	0.42
25:J:164:ILE:HD13	25:J:164:ILE:HA	1.90	0.42
25:J:247:MET:HE1	25:J:268:VAL:HB	2.00	0.42
27:M:219:LEU:N	27:M:345:ARG:O	2.49	0.42
30:N:379:LEU:HD21	30:N:415:PHE:HD2	1.84	0.42
30:N:536:ILE:HG21	30:N:555:ILE:HD11	2.01	0.42
30:N:858:LYS:HD2	30:N:859:ASN:N	2.33	0.42
2:2:149:ASP:N	2:2:149:ASP:OD1	2.50	0.42
3:3:175:ALA:O	3:3:181:SER:OG	2.37	0.42
4:4:91:SER:HB3	4:4:98:TYR:HD1	1.85	0.42
8:A:83:VAL:HG11	8:A:90:ALA:HB1	2.02	0.42
9:B:171:ALA:O	9:B:175:LEU:HD23	2.20	0.42
14:G:121:GLN:HA	14:G:124:THR:HG22	2.00	0.42
15:I:317:ASP:OD1	15:I:317:ASP:N	2.53	0.42
16:K:161:MET:HE2	16:K:161:MET:HB3	1.80	0.42
34:K:501:ATP:O3G	17:L:342:ARG:NH2	2.44	0.42
20:R:112:GLU:O	20:R:116:LYS:HG2	2.18	0.42
21:S:375:ASP:N	21:S:375:ASP:OD1	2.53	0.42
7:a:226:ARG:HG3	7:a:247:VAL:H	1.84	0.42
3:h:50:PHE:CE2	3:h:195:VAL:HG21	2.54	0.42
2:i:202:VAL:HG12	2:i:204:VAL:HG23	2.02	0.42
26:H:349:ILE:HG22	26:H:349:ILE:O	2.20	0.42
30:N:234:ASP:OD1	30:N:237:LEU:N	2.43	0.42
30:N:331:ALA:HB2	30:N:697:PHE:CD2	2.54	0.42
30:N:444:HIS:CE1	30:N:480:ALA:HB2	2.55	0.42
32:o:793:PHE:O	32:o:797:THR:OG1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:o:794:ASP:OD1	32:o:794:ASP:N	2.41	0.42
1:1:99:SER:HB2	14:G:104:LYS:HG2	2.01	0.42
4:4:159:ASP:O	4:4:163:LEU:HG	2.19	0.42
6:6:153:GLU:HG2	6:6:154:GLN:N	2.34	0.42
7:7:42:THR:N	7:7:74:ARG:HH22	2.16	0.42
8:A:75:ILE:HD13	8:A:75:ILE:HA	1.82	0.42
11:D:92:GLU:HG3	11:D:112:TYR:CG	2.55	0.42
16:K:76:LYS:HE3	25:J:51:LEU:HD22	2.02	0.42
17:L:280:MET:HE2	17:L:280:MET:HB3	1.94	0.42
18:O:330:ARG:HG2	19:P:307:GLU:OE2	2.19	0.42
18:O:382:LYS:HB3	18:O:382:LYS:HE2	1.62	0.42
19:P:181:LEU:HD21	19:P:220:TYR:HB2	2.01	0.42
21:S:326:ASP:OD2	21:S:326:ASP:C	2.62	0.42
22:V:144:ILE:HD13	22:V:144:ILE:HA	1.84	0.42
23:W:172:LEU:HB2	23:W:189:PRO:HG3	2.02	0.42
7:a:35:GLN:HB3	7:a:144:TRP:HE1	1.85	0.42
1:b:27:PHE:HE2	1:b:29:ASP:HB3	1.84	0.42
3:h:56:LEU:O	3:h:60:VAL:HG23	2.19	0.42
25:J:306:ARG:HD2	25:J:307:PRO:HD2	2.01	0.42
26:H:99:VAL:HG23	26:H:187:LEU:HD12	2.01	0.42
26:H:210:ASP:O	26:H:391:ILE:HG21	2.19	0.42
26:H:274:VAL:HB	26:H:308:PHE:HD1	1.84	0.42
27:M:360:ILE:HD12	34:M:501:ATP:N1	2.33	0.42
28:Q:26:VAL:O	28:Q:29:SER:OG	2.34	0.42
28:Q:179:LEU:O	28:Q:183:LYS:HG3	2.19	0.42
28:Q:271:MET:HE1	28:Q:334:HIS:HB3	2.02	0.42
30:N:217:MET:HE2	30:N:219:ASN:O	2.18	0.42
30:N:318:LYS:HB3	30:N:318:LYS:HE2	1.76	0.42
31:T:32:ILE:H	31:T:32:ILE:HG13	1.66	0.42
1:1:113:THR:HG22	1:1:134:LEU:HD22	2.00	0.42
5:5:172:MET:N	5:5:192:SER:HB3	2.34	0.42
6:6:199:VAL:O	6:6:203:VAL:HG23	2.20	0.42
8:A:225:VAL:HG13	8:A:236:LEU:HB2	2.02	0.42
11:D:28:LYS:HE3	11:D:28:LYS:HB2	1.78	0.42
18:O:20:PRO:HA	18:O:23:HIS:CG	2.55	0.42
19:P:197:THR:O	19:P:200:SER:OG	2.31	0.42
21:S:436:ILE:HD13	21:S:443:ILE:HG12	2.00	0.42
7:a:93:MET:HA	7:a:96:ILE:HG12	2.01	0.42
7:a:170:TYR:CZ	6:e:55:ASN:HB3	2.54	0.42
1:b:165:MET:HG2	1:b:169:GLU:HB3	2.02	0.42
6:e:46:THR:HB	6:e:58:TYR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:H:146:VAL:HG22	26:H:156:VAL:HG22	2.01	0.42
26:H:465:GLN:NE2	26:H:465:GLN:HA	2.35	0.42
27:M:281:ASP:OD1	27:M:282:GLU:N	2.53	0.42
28:Q:70:ALA:HB3	28:Q:73:LYS:HB2	2.02	0.42
32:o:729:GLU:N	32:o:729:GLU:OE1	2.52	0.42
1:1:50:THR:HG23	1:1:52:LYS:HZ1	1.85	0.42
2:2:124:GLY:HA2	2:2:144:ALA:HB1	2.02	0.42
10:C:94:HIS:CG	10:C:114:ARG:HG2	2.55	0.42
15:I:130:VAL:HG22	15:I:154:MET:O	2.19	0.42
16:K:265:ALA:HB1	16:K:311:ASN:OD1	2.20	0.42
16:K:369:ASP:HA	16:K:372:ILE:HG12	2.01	0.42
17:L:263:ILE:HD12	17:L:304:THR:HG23	2.00	0.42
18:O:273:GLN:HA	18:O:276:LYS:HD3	2.00	0.42
7:a:193:ASP:CG	6:e:57:ARG:HH22	2.28	0.42
32:o:117:ASP:OD1	32:o:138:ARG:NH2	2.53	0.42
32:o:568:LEU:HD21	32:o:883:THR:HA	2.02	0.42
32:o:893:PHE:HA	32:o:896:LYS:HE2	2.02	0.42
32:o:911:LYS:HE2	32:o:911:LYS:HB3	1.68	0.42
32:o:919:GLU:HB2	32:o:921:GLU:OE1	2.19	0.42
2:2:48:ARG:HD3	2:2:199:GLY:C	2.44	0.42
6:6:84:VAL:HG12	6:6:88:LYS:HD2	2.02	0.42
8:A:123:ASN:OD1	9:B:83:ARG:NH2	2.52	0.42
12:E:88:MET:HE3	12:E:138:PHE:CD1	2.55	0.42
13:F:61:LYS:HB2	13:F:61:LYS:HE2	1.84	0.42
14:G:53:LEU:HD12	14:G:53:LEU:HA	1.80	0.42
19:P:9:ALA:C	19:P:11:LYS:H	2.28	0.42
19:P:58:VAL:O	19:P:62:ILE:HG23	2.20	0.42
22:V:254:ARG:HH22	22:V:277:LYS:HD3	1.84	0.42
4:g:139:TYR:CE2	4:g:171:ARG:HB2	2.54	0.42
4:g:166:GLN:NE2	4:g:198:GLN:OE1	2.53	0.42
25:J:155:LYS:O	25:J:158:LYS:HB3	2.19	0.42
26:H:150:LYS:HD3	26:H:150:LYS:HA	1.87	0.42
26:H:379:LEU:HA	26:H:380:PRO:HD3	1.95	0.42
27:M:76:PRO:HG2	27:M:150:LYS:HZ1	1.84	0.42
28:Q:361:HIS:O	28:Q:365:ILE:HG12	2.19	0.42
29:U:301:ILE:HD13	29:U:301:ILE:HA	1.90	0.42
32:o:948:TRP:CD1	32:o:948:TRP:H	2.37	0.42
1:1:38:ARG:NH1	1:1:186:GLY:O	2.39	0.42
3:3:135:ASP:OD1	3:3:136:PHE:N	2.50	0.42
5:5:242:ARG:HH21	4:g:145:ASP:CG	2.27	0.42
7:7:46:SER:HB3	7:7:55:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:217:GLU:OE2	8:A:218:PHE:N	2.53	0.42
12:E:19:GLY:HA3	13:F:27:GLU:OE1	2.20	0.42
15:I:213:ILE:HD13	26:H:427:GLY:HA3	2.01	0.42
15:I:246:ARG:HG2	15:I:247:ILE:N	2.34	0.42
16:K:322:ASP:OD2	16:K:323:THR:HG23	2.20	0.42
16:K:333:ARG:NH1	25:J:139:VAL:O	2.37	0.42
19:P:30:ASN:OD1	19:P:30:ASN:N	2.52	0.42
22:V:25:GLU:HA	22:V:61:TYR:O	2.20	0.42
23:W:134:LYS:HD3	23:W:134:LYS:HA	1.76	0.42
23:W:143:ASN:HD21	23:W:150:ASN:HB2	1.84	0.42
1:b:40:THR:HG21	1:b:187:SER:HA	2.02	0.42
5:f:201:ILE:HD11	5:f:219:TYR:CD1	2.54	0.42
25:J:246:PHE:HA	25:J:291:ILE:O	2.19	0.42
26:H:191:ILE:HD12	26:H:191:ILE:HA	1.79	0.42
27:M:290:ARG:HD3	27:M:306:LEU:HD21	2.01	0.42
27:M:327:THR:OG1	27:M:328:ASN:N	2.53	0.42
27:M:400:MET:HE3	27:M:400:MET:O	2.18	0.42
28:Q:267:LEU:HD22	28:Q:331:THR:HG22	2.02	0.42
29:U:110:PHE:O	29:U:114:THR:OG1	2.32	0.42
30:N:17:GLN:O	30:N:20:VAL:HG12	2.20	0.42
31:T:25:LYS:HA	31:T:25:LYS:HD3	1.67	0.42
31:T:139:ASP:HB3	31:T:142:LEU:HD12	2.01	0.42
32:o:327:GLN:HA	32:o:330:ILE:HG12	2.01	0.42
32:o:595:MET:O	32:o:599:ILE:HG12	2.20	0.42
3:3:29:LEU:HD13	3:3:40:PHE:CD1	2.55	0.42
4:4:158:LEU:HD13	4:4:198:GLN:HE22	1.85	0.42
8:A:96:ARG:HH11	8:A:124:LEU:HD22	1.85	0.42
10:C:27:GLU:OE2	15:I:431:ASN:ND2	2.52	0.42
10:C:69:LEU:HD22	10:C:111:LEU:HD11	2.02	0.42
11:D:176:GLU:OE2	12:E:56:SER:OG	2.32	0.42
14:G:38:ILE:HD11	14:G:196:ALA:HA	2.02	0.42
15:I:193:GLU:HB3	15:I:346:ARG:NH1	2.35	0.42
26:H:281:GLN:NE2	26:H:290:MET:HE3	2.35	0.42
26:H:307:PHE:O	26:H:307:PHE:CG	2.72	0.42
28:Q:263:LYS:HZ3	28:Q:324:GLU:HB3	1.85	0.42
29:U:102:SER:O	29:U:106:ILE:HG13	2.20	0.42
30:N:194:ILE:HD13	30:N:203:ARG:NH1	2.35	0.42
32:o:201:LEU:HA	32:o:204:CYS:SG	2.59	0.42
32:o:754:LYS:HD2	32:o:783:VAL:O	2.19	0.42
3:3:203:ARG:H	3:3:203:ARG:HD3	1.85	0.42
7:7:53:VAL:HG11	7:7:160:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:167:LYS:HB3	8:A:186:PHE:HE2	1.84	0.42
11:D:84:ILE:O	11:D:88:LYS:HG3	2.20	0.42
13:F:82:ARG:HD2	13:F:82:ARG:HA	1.96	0.42
13:F:155:GLU:HG2	14:G:60:VAL:HG11	2.00	0.42
15:I:89:GLN:CG	15:I:90:GLU:N	2.83	0.42
16:K:119:VAL:HG21	25:J:114:CYS:SG	2.59	0.42
17:L:333:LEU:HD23	17:L:333:LEU:HA	1.87	0.42
17:L:367:LYS:HA	17:L:367:LYS:HD3	1.92	0.42
19:P:28:ALA:O	19:P:69:ARG:NH2	2.46	0.42
19:P:198:VAL:HA	19:P:201:ARG:NH2	2.34	0.42
20:R:127:GLU:O	20:R:130:GLN:HG2	2.19	0.42
20:R:358:GLY:C	24:Y:78:LYS:HG2	2.45	0.42
22:V:90:LYS:HG2	22:V:94:MET:HE2	2.02	0.42
7:a:181:ALA:O	7:a:185:ASN:ND2	2.52	0.42
4:g:136:SER:O	4:g:140:THR:HG23	2.19	0.42
4:g:147:HIS:HB2	4:g:160:LEU:HD13	2.02	0.42
3:h:59:ASP:HA	3:h:62:THR:HG22	2.01	0.42
27:M:351:LEU:HD22	27:M:387:ASN:HB3	2.02	0.42
28:Q:142:ALA:HB2	28:Q:157:LEU:HD22	2.02	0.42
29:U:22:TYR:CD1	29:U:125:VAL:HG11	2.55	0.42
30:N:171:LYS:HE2	30:N:171:LYS:HB2	1.85	0.42
32:o:265:LEU:HB3	32:o:288:LEU:HD11	2.02	0.42
32:o:525:MET:HE2	32:o:562:TRP:CZ3	2.55	0.42
32:o:864:MET:HE2	32:o:864:MET:HA	2.02	0.42
32:o:969:GLU:OE2	32:o:989:TYR:HB3	2.19	0.42
3:3:39:LYS:HZ1	5:f:284:ASN:HB3	1.85	0.41
8:A:145:SER:OG	8:A:146:VAL:N	2.53	0.41
9:B:44:VAL:HG23	9:B:211:LEU:HD11	2.02	0.41
9:B:197:LYS:HD3	9:B:204:PHE:CE2	2.55	0.41
14:G:32:GLU:HB2	14:G:169:ARG:HH21	1.85	0.41
16:K:211:LEU:O	16:K:317:ALA:HA	2.20	0.41
17:L:92:GLU:O	17:L:96:LYS:HG3	2.20	0.41
20:R:105:LYS:HE2	20:R:109:LYS:HE2	2.02	0.41
22:V:54:LEU:HD21	22:V:69:PHE:HE1	1.85	0.41
23:W:96:LEU:HD23	23:W:96:LEU:HA	1.90	0.41
3:h:97:GLU:OE1	3:h:98:ARG:NH1	2.53	0.41
29:U:170:GLY:O	29:U:174:LEU:HD23	2.20	0.41
30:N:640:VAL:O	30:N:643:PRO:HD2	2.20	0.41
30:N:672:ASN:HB3	30:N:675:VAL:HG23	2.02	0.41
32:o:235:GLN:OE1	32:o:235:GLN:N	2.52	0.41
1:1:22:ILE:HG22	1:1:35:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:75:ILE:HB	8:A:79:ILE:HG22	2.02	0.41
10:C:66:LEU:HD13	10:C:214:ALA:HB2	2.01	0.41
10:C:135:PHE:H	10:C:151:SER:HG	1.65	0.41
11:D:96:HIS:NE2	11:D:100:LEU:HD12	2.35	0.41
16:K:344:ARG:O	16:K:349:ARG:NH2	2.44	0.41
18:O:226:LYS:C	18:O:227:ILE:HD12	2.45	0.41
21:S:82:TYR:HB3	21:S:89:LYS:HB2	2.03	0.41
23:W:99:LYS:HG2	23:W:100:HIS:CD2	2.54	0.41
7:a:189:ARG:NH2	6:e:54:ILE:O	2.43	0.41
7:a:203:VAL:O	7:a:206:ALA:HB3	2.20	0.41
1:b:33:LEU:HD11	1:b:119:ALA:HB3	2.01	0.41
6:e:84:VAL:HG12	6:e:88:LYS:NZ	2.35	0.41
5:f:273:TRP:O	5:f:276:LYS:HG2	2.19	0.41
2:i:51:GLN:OE1	2:i:51:GLN:N	2.53	0.41
26:H:205:ASP:OD1	32:o:362:LEU:HD13	2.21	0.41
29:U:79:MET:O	29:U:83:ILE:HG12	2.21	0.41
30:N:340:HIS:HB2	30:N:374:ILE:HG12	2.00	0.41
30:N:504:TYR:HD2	30:N:517:LEU:HD11	1.85	0.41
5:5:125:ALA:HB3	6:6:147:VAL:HG22	2.01	0.41
6:6:128:THR:HG22	6:6:144:PHE:HB2	2.01	0.41
7:7:47:MET:HE1	7:7:206:ALA:HA	2.03	0.41
12:E:21:LEU:H	12:E:21:LEU:HD12	1.84	0.41
16:K:86:VAL:HG23	25:J:62:LEU:HB2	2.02	0.41
18:O:186:ASN:ND2	18:O:225:ASP:H	2.17	0.41
18:O:248:TYR:O	18:O:251:LEU:HG	2.20	0.41
19:P:24:ILE:HD12	19:P:24:ILE:HA	1.81	0.41
19:P:96:MET:O	19:P:100:VAL:HG23	2.21	0.41
21:S:330:LEU:H	24:Y:64:TRP:HZ3	1.67	0.41
23:W:158:ILE:HG13	23:W:169:SER:OG	2.20	0.41
7:a:197:ASP:O	7:a:201:THR:HG22	2.21	0.41
3:h:29:LEU:HB3	3:h:37:SER:HB3	2.03	0.41
2:i:133:ASP:OD1	2:i:136:GLY:N	2.53	0.41
27:M:428:LYS:HD2	27:M:428:LYS:HA	1.71	0.41
29:U:92:TRP:CH2	29:U:106:ILE:HB	2.55	0.41
30:N:15:GLU:HG2	30:N:16:ASN:H	1.85	0.41
30:N:256:GLN:OE1	30:N:904:VAL:N	2.47	0.41
3:3:183:TRP:HZ2	5:f:242:ARG:HA	1.85	0.41
4:4:23:ARG:NH2	5:5:191:ASP:OD2	2.51	0.41
5:5:187:ILE:H	5:5:198:LYS:NZ	2.18	0.41
5:5:270:GLU:H	5:5:270:GLU:HG3	1.73	0.41
9:B:41:ASN:ND2	9:B:41:ASN:H	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:44:ALA:HB3	13:F:216:VAL:HG12	2.03	0.41
16:K:158:ILE:HD11	16:K:253:MET:HE1	2.02	0.41
17:L:247:PRO:HB3	27:M:310:ASN:ND2	2.36	0.41
17:L:312:MET:HE3	17:L:342:ARG:HD3	2.01	0.41
18:O:194:LEU:O	18:O:198:THR:OG1	2.26	0.41
19:P:72:TRP:NE1	19:P:110:LEU:HD11	2.35	0.41
19:P:111:ASP:O	19:P:115:ARG:HG3	2.19	0.41
20:R:29:LYS:HG3	20:R:49:PHE:CD2	2.56	0.41
7:a:265:LYS:HD3	7:a:266:ILE:N	2.35	0.41
6:e:170:ASP:HA	6:e:174:ASN:HB2	2.02	0.41
4:g:140:THR:O	4:g:144:LEU:HG	2.20	0.41
2:i:163:ALA:HB1	2:i:187:ALA:HB1	2.02	0.41
32:o:575:MET:HB3	32:o:606:CYS:SG	2.61	0.41
3:3:110:ALA:HB2	3:3:121:ILE:HD13	2.02	0.41
4:4:132:ALA:HB3	4:4:137:GLY:HA2	2.02	0.41
7:7:152:VAL:HG23	7:7:233:ILE:HD12	2.03	0.41
9:B:12:PHE:HE1	10:C:129:ARG:HH11	1.69	0.41
9:B:143:ASN:OD1	9:B:143:ASN:N	2.54	0.41
11:D:138:PHE:CE1	11:D:217:PRO:HG3	2.55	0.41
12:E:21:LEU:HD11	13:F:77:LEU:HD21	2.02	0.41
12:E:106:ASP:OD1	12:E:107:ILE:N	2.53	0.41
13:F:50:LYS:HD2	13:F:59:TYR:HB3	2.01	0.41
13:F:121:GLN:OE1	13:F:121:GLN:HA	2.21	0.41
14:G:44:ASP:OD2	14:G:220:SER:HB2	2.20	0.41
17:L:353:ASN:OD1	17:L:353:ASN:N	2.50	0.41
18:O:137:TYR:HA	18:O:140:LYS:HB2	2.02	0.41
18:O:329:MET:HE3	19:P:308:LEU:HD22	2.01	0.41
20:R:351:LYS:HE2	20:R:351:LYS:HB2	1.89	0.41
22:V:20:ARG:C	22:V:172:GLN:HE21	2.28	0.41
23:W:72:ILE:O	23:W:76:LEU:HG	2.20	0.41
3:h:191:LYS:HB2	3:h:194:GLU:O	2.21	0.41
2:i:128:ILE:HA	2:i:141:SER:HA	2.02	0.41
25:J:230:VAL:HG13	25:J:272:MET:HE1	2.02	0.41
26:H:450:VAL:HG12	26:H:451:ILE:HD13	2.02	0.41
28:Q:148:LYS:HE2	28:Q:148:LYS:HB2	1.81	0.41
29:U:102:SER:HA	29:U:105:LYS:HG3	2.02	0.41
29:U:143:VAL:HA	29:U:150:THR:HA	2.03	0.41
30:N:116:GLN:O	30:N:120:ASP:N	2.54	0.41
32:o:44:LYS:NZ	32:o:48:ASP:OD1	2.40	0.41
32:o:835:ALA:HB2	32:o:848:THR:HG21	2.02	0.41
32:o:932:ALA:HB1	32:o:962:ARG:HE	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:107:SER:HB2	8:A:108:TYR:HD2	1.86	0.41
2:2:217:ARG:HD2	2:2:217:ARG:HA	1.87	0.41
4:4:101:ASN:HB3	4:4:133:HIS:HD2	1.85	0.41
6:6:30:THR:HB	6:6:161:ALA:HB3	2.02	0.41
11:D:12:SER:OG	11:D:14:ASP:OD1	2.24	0.41
12:E:10:ARG:NH2	13:F:3:ARG:HD3	2.35	0.41
12:E:109:VAL:HB	12:E:154:GLN:OE1	2.21	0.41
12:E:122:ARG:HD2	12:E:122:ARG:HA	1.79	0.41
12:E:211:LYS:HD3	12:E:211:LYS:HA	1.88	0.41
13:F:71:GLY:HA3	13:F:222:PHE:CE1	2.56	0.41
15:I:207:LEU:H	15:I:207:LEU:HD12	1.86	0.41
15:I:336:PRO:O	26:H:459:SER:OG	2.30	0.41
16:K:330:ARG:NH1	25:J:140:GLU:OE1	2.52	0.41
17:L:103:GLN:O	27:M:128:PHE:N	2.53	0.41
17:L:345:ARG:H	17:L:345:ARG:HG2	1.66	0.41
18:O:383:LYS:HE2	18:O:383:LYS:HB3	1.79	0.41
19:P:198:VAL:HA	19:P:201:ARG:HH12	1.85	0.41
22:V:256:GLU:HA	22:V:256:GLU:OE1	2.21	0.41
24:Y:33:ASP:OD2	24:Y:34:GLU:N	2.53	0.41
7:a:214:MET:SD	7:a:214:MET:C	3.03	0.41
7:a:242:LYS:HB2	7:a:242:LYS:HE2	1.72	0.41
2:i:32:ILE:HD12	2:i:128:ILE:HG22	2.01	0.41
25:J:186:ILE:HG13	25:J:310:ILE:HG21	2.02	0.41
27:M:221:TYR:CD1	27:M:221:TYR:C	2.97	0.41
27:M:385:GLU:OE2	27:M:385:GLU:N	2.54	0.41
30:N:28:ILE:HG22	30:N:64:ILE:HD11	2.02	0.41
32:o:542:ILE:O	32:o:546:ILE:HG12	2.20	0.41
32:o:774:ARG:HB2	32:o:810:ASN:HD22	1.85	0.41
5:5:240:ALA:HB1	5:5:247:GLY:HA2	2.03	0.41
7:7:230:LEU:HB3	7:7:242:LYS:HE2	2.01	0.41
8:A:135:ARG:HH11	14:G:125:LEU:HA	1.85	0.41
10:C:209:ASP:OD1	10:C:209:ASP:N	2.51	0.41
14:G:113:ALA:HA	14:G:138:PHE:HZ	1.86	0.41
14:G:179:LEU:HD11	14:G:187:LEU:HD22	2.03	0.41
15:I:229:LYS:HG2	15:I:350:PHE:CD2	2.56	0.41
15:I:330:LYS:HE3	15:I:330:LYS:HB3	1.88	0.41
16:K:350:ARG:O	16:K:350:ARG:HD3	2.21	0.41
20:R:141:TYR:HB3	20:R:150:ALA:HB2	2.01	0.41
21:S:475:TYR:HE2	29:U:288:PHE:HB2	1.86	0.41
22:V:254:ARG:HD2	22:V:254:ARG:C	2.46	0.41
4:g:99:GLN:HA	4:g:121:TYR:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:J:159:GLU:O	25:J:163:VAL:HG23	2.21	0.41
31:T:185:ILE:O	31:T:189:ILE:HG13	2.21	0.41
32:o:332:ASN:ND2	32:o:335:LEU:HD22	2.35	0.41
32:o:406:TRP:HA	32:o:409:LYS:HD3	2.03	0.41
8:A:115:ASP:OD1	8:A:115:ASP:N	2.51	0.41
9:B:200:VAL:HG11	9:B:204:PHE:CD1	2.56	0.41
10:C:65:LYS:HE2	10:C:77:VAL:O	2.21	0.41
10:C:240:VAL:HG12	10:C:245:THR:HG23	2.03	0.41
12:E:59:LEU:HD12	12:E:59:LEU:HA	1.88	0.41
12:E:134:MET:HB2	12:E:134:MET:HE2	1.76	0.41
13:F:66:CYS:HB2	13:F:89:ARG:HG3	2.02	0.41
15:I:334:LEU:HD23	15:I:334:LEU:HA	1.85	0.41
15:I:341:PRO:HG2	26:H:418:GLU:HG3	2.01	0.41
15:I:342:GLY:HA2	26:H:420:ARG:HH22	1.85	0.41
17:L:207:PHE:HE2	17:L:215:PRO:HD2	1.86	0.41
18:O:95:SER:O	18:O:99:LEU:HG	2.21	0.41
18:O:137:TYR:HB3	18:O:142:ASP:HB2	2.03	0.41
18:O:392:TRP:CE3	18:O:392:TRP:HA	2.55	0.41
21:S:377:TYR:O	21:S:381:VAL:HG23	2.21	0.41
22:V:227:MET:CE	22:V:301:ASN:HD22	2.34	0.41
1:b:36:ASP:C	1:b:52:LYS:HZ1	2.29	0.41
1:b:86:THR:HA	1:b:90:GLY:O	2.20	0.41
4:g:168:LEU:HB3	4:g:176:PHE:HE2	1.85	0.41
27:M:221:TYR:HE1	27:M:348:GLU:HG2	1.85	0.41
28:Q:63:GLN:HB2	28:Q:103:LYS:NZ	2.36	0.41
32:o:618:GLN:O	32:o:622:HIS:ND1	2.53	0.41
1:1:158:ASP:HB3	1:b:180:GLN:NE2	2.31	0.41
2:2:189:GLN:HA	2:2:192:ILE:HG12	2.03	0.41
3:3:39:LYS:NZ	5:f:284:ASN:HB3	2.35	0.41
3:3:202:MET:HB3	3:3:203:ARG:NH1	2.35	0.41
5:5:163:TYR:O	5:5:166:LYS:HG2	2.21	0.41
6:6:92:LYS:HB3	6:6:92:LYS:HE2	1.93	0.41
6:6:96:PHE:HE1	13:F:65:LYS:HE2	1.86	0.41
7:7:103:LEU:HD22	7:7:128:TYR:CD2	2.55	0.41
9:B:21:ILE:O	9:B:25:LEU:HD23	2.21	0.41
10:C:26:LEU:HD23	10:C:26:LEU:HA	1.94	0.41
10:C:226:TYR:HB2	10:C:228:LYS:NZ	2.35	0.41
12:E:45:GLY:HA2	12:E:153:TYR:CD1	2.56	0.41
12:E:205:LYS:HZ1	12:E:212:LEU:H	1.68	0.41
13:F:201:LEU:HD13	13:F:205:SER:HA	2.03	0.41
14:G:86:ARG:O	14:G:89:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:248:VAL:N	15:I:251:GLU:OE2	2.37	0.41
17:L:199:LEU:HB3	17:L:200:PRO:HD3	2.02	0.41
18:O:343:GLN:NE2	19:P:364:ARG:HG2	2.35	0.41
18:O:367:LYS:HE2	18:O:367:LYS:HB3	1.91	0.41
19:P:147:LYS:HB3	19:P:156:ALA:HB2	2.02	0.41
20:R:70:TYR:HB3	20:R:71:LEU:H	1.71	0.41
20:R:374:ASN:HB2	20:R:376:GLN:HG3	2.02	0.41
21:S:223:LEU:HD11	30:N:70:TYR:CE1	2.56	0.41
21:S:278:LYS:HG2	21:S:316:LEU:CD1	2.51	0.41
22:V:149:GLY:O	29:U:176:ARG:NH1	2.52	0.41
23:W:108:GLN:CD	23:W:108:GLN:H	2.29	0.41
7:a:44:VAL:HG13	7:a:57:ALA:HB2	2.02	0.41
4:g:105:GLY:HA2	4:g:116:LEU:HA	2.03	0.41
2:i:217:ARG:HE	2:i:218:ASN:ND2	2.18	0.41
26:H:169:GLU:N	26:H:169:GLU:OE1	2.54	0.41
28:Q:174:LEU:HA	28:Q:177:VAL:CG1	2.51	0.41
29:U:213:LYS:HA	29:U:213:LYS:HD3	1.81	0.41
30:N:141:ILE:HD12	30:N:165:ILE:HG21	2.03	0.41
30:N:163:LEU:O	30:N:167:GLU:HG3	2.21	0.41
30:N:389:TYR:CB	30:N:404:SER:HB2	2.50	0.41
30:N:642:ASP:OD1	30:N:642:ASP:C	2.63	0.41
31:T:103:SER:HB2	31:T:141:LEU:HD12	2.02	0.41
31:T:112:ASN:O	31:T:115:SER:OG	2.38	0.41
32:o:76:LYS:HG3	32:o:149:TRP:CZ3	2.55	0.41
32:o:223:LEU:HA	32:o:226:GLU:HG3	2.01	0.41
32:o:273:LEU:HD23	32:o:273:LEU:HA	1.83	0.41
2:2:38:ASN:OD1	2:2:39:ASN:N	2.50	0.41
4:4:109:LYS:HA	4:4:109:LYS:HD3	1.79	0.41
4:4:150:PRO:HD3	5:f:283:ASN:OD1	2.21	0.41
10:C:4:ARG:NH1	12:E:10:ARG:HA	2.37	0.41
10:C:66:LEU:HD11	10:C:212:GLU:HB3	2.02	0.41
14:G:36:THR:HA	14:G:165:THR:O	2.19	0.41
14:G:211:ASP:OD1	14:G:212:PHE:N	2.51	0.41
14:G:216:ILE:HG13	14:G:231:VAL:HB	2.03	0.41
15:I:280:PHE:O	15:I:280:PHE:CG	2.74	0.41
18:O:242:ILE:HG23	18:O:245:ASP:HB3	2.03	0.41
19:P:61:LYS:NZ	19:P:65:LEU:HG	2.36	0.41
21:S:242:LEU:HD23	21:S:242:LEU:HA	1.86	0.41
22:V:110:SER:HA	22:V:141:VAL:HG23	2.03	0.41
1:b:47:ASN:OD1	1:b:48:ARG:N	2.54	0.41
3:h:3:ASP:OD2	3:h:6:SER:OG	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:H:223:GLU:HA	26:H:227:LEU:HD12	2.03	0.41
27:M:166:ARG:HH11	27:M:253:GLN:NE2	2.19	0.41
30:N:17:GLN:HE22	31:T:32:ILE:HD11	1.86	0.41
30:N:622:ALA:HB2	30:N:644:LEU:HD13	2.01	0.41
31:T:93:ASN:HB3	31:T:96:LEU:HB3	2.03	0.41
32:o:224:LEU:HD13	32:o:233:LEU:HB2	2.03	0.41
32:o:560:THR:O	32:o:563:VAL:HG22	2.21	0.41
32:o:948:TRP:CD1	32:o:948:TRP:N	2.89	0.41
1:1:74:ILE:HG23	1:1:101:PHE:HE1	1.86	0.40
2:2:233:LYS:HE3	3:3:162:ASP:HB3	2.03	0.40
3:3:25:CYS:SG	3:3:42:LYS:HB2	2.61	0.40
3:3:107:PRO:HG2	3:3:124:PHE:HD2	1.86	0.40
3:3:194:GLU:HG3	3:3:195:VAL:H	1.86	0.40
5:5:233:LYS:HE2	5:5:233:LYS:HB2	1.72	0.40
6:6:50:THR:O	6:6:52:TYR:N	2.54	0.40
6:6:221:LEU:HB2	6:6:238:LEU:HD11	2.03	0.40
8:A:88:PRO:HB3	14:G:155:GLY:C	2.46	0.40
10:C:160:TRP:CG	10:C:163:ILE:HD13	2.56	0.40
12:E:200:VAL:O	12:E:203:ILE:HG22	2.22	0.40
14:G:137:ILE:HG22	14:G:148:LEU:HD11	2.02	0.40
15:I:108:THR:OG1	15:I:121:THR:O	2.39	0.40
16:K:367:ASP:OD2	16:K:370:SER:N	2.53	0.40
16:K:374:ARG:HD2	16:K:411:TYR:HE2	1.86	0.40
17:L:133:ASN:HA	17:L:137:ARG:HH21	1.85	0.40
18:O:297:ILE:HD11	18:O:336:LEU:HB3	2.03	0.40
19:P:270:LEU:HD23	19:P:270:LEU:HA	1.78	0.40
19:P:395:ARG:HG3	28:Q:354:PHE:CE1	2.56	0.40
21:S:121:VAL:HG12	21:S:128:ILE:HG22	2.03	0.40
21:S:223:LEU:HD23	21:S:223:LEU:HA	1.85	0.40
22:V:22:ASP:O	22:V:171:ARG:NH2	2.54	0.40
22:V:293:VAL:HG21	29:U:189:ARG:NE	2.35	0.40
1:b:59:LYS:HA	1:b:59:LYS:HD2	1.69	0.40
6:e:30:THR:H	6:e:45:ASP:CG	2.29	0.40
5:f:134:LEU:HD12	5:f:134:LEU:HA	1.95	0.40
4:g:38:LEU:HD12	4:g:64:ILE:HG13	2.03	0.40
25:J:48:ARG:NH2	30:N:608:LEU:O	2.54	0.40
25:J:160:ILE:CG2	25:J:202:VAL:HG21	2.51	0.40
26:H:308:PHE:O	26:H:353:PHE:HA	2.21	0.40
28:Q:174:LEU:HA	28:Q:177:VAL:HG12	2.03	0.40
30:N:90:ASP:OD1	30:N:92:ASP:N	2.54	0.40
30:N:395:ALA:HB3	30:N:401:LYS:HE3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:N:498:ILE:HG12	30:N:524:ILE:HG21	2.02	0.40
30:N:774:ASN:N	30:N:883:SER:O	2.51	0.40
31:T:38:ASN:O	31:T:51:TYR:OH	2.37	0.40
31:T:157:TYR:HA	31:T:160:ALA:HB3	2.03	0.40
32:o:115:LEU:HD12	32:o:115:LEU:HA	1.89	0.40
32:o:474:LEU:HD23	32:o:474:LEU:HA	1.90	0.40
1:1:204:ARG:HD2	1:1:204:ARG:HA	1.95	0.40
4:4:173:PRO:HG3	4:g:22:THR:HG21	2.03	0.40
5:5:110:ILE:N	5:5:110:ILE:HD12	2.36	0.40
5:5:148:ARG:NH2	5:5:180:THR:HA	2.35	0.40
5:5:265:ASN:OD1	5:5:265:ASN:C	2.64	0.40
5:5:285:VAL:HA	3:h:38:ASN:ND2	2.36	0.40
7:7:78:VAL:HG11	7:7:100:LEU:HG	2.02	0.40
7:7:97:GLU:HG2	7:7:101:LYS:HE2	2.03	0.40
10:C:194:LEU:HD12	10:C:242:THR:HG21	2.02	0.40
15:I:57:LEU:HD21	32:o:252:CYS:HA	2.02	0.40
34:K:501:ATP:O3B	17:L:339:ARG:NH1	2.52	0.40
17:L:98:LEU:HD12	17:L:98:LEU:HA	1.89	0.40
18:O:296:LEU:HD13	18:O:313:ILE:HG23	2.03	0.40
21:S:223:LEU:HD11	30:N:70:TYR:HE1	1.86	0.40
22:V:57:PHE:CE1	22:V:105:VAL:HG13	2.56	0.40
22:V:80:VAL:HG11	22:V:107:TRP:HZ3	1.86	0.40
7:a:222:ALA:HB3	7:a:223:ARG:NH1	2.36	0.40
3:h:149:MET:HE1	3:h:170:ALA:HA	2.03	0.40
2:i:81:THR:HB	2:i:127:LEU:HD21	2.03	0.40
27:M:228:LYS:HB2	34:M:501:ATP:O2B	2.21	0.40
28:Q:133:LEU:HD12	28:Q:133:LEU:HA	1.86	0.40
29:U:236:LEU:HD12	29:U:237:PRO:HD2	2.02	0.40
30:N:545:SER:HB2	30:N:580:ASN:HD22	1.87	0.40
30:N:555:ILE:HG21	30:N:571:LEU:HG	2.03	0.40
31:T:69:SER:HB2	31:T:74:ASN:HB3	2.03	0.40
31:T:164:LEU:HD11	31:T:181:LEU:HB3	2.02	0.40
32:o:93:ARG:NH1	32:o:125:THR:O	2.54	0.40
32:o:352:LYS:HB2	32:o:390:LEU:HD13	2.02	0.40
1:1:152:PHE:HE2	1:1:185:ASP:HB2	1.86	0.40
1:1:209:PRO:HA	1:1:212:TYR:CE2	2.55	0.40
4:4:135:TYR:HD2	4:g:25:ILE:HD12	1.87	0.40
7:7:42:THR:HG22	7:7:74:ARG:NH1	2.36	0.40
7:7:80:ASP:O	7:7:239:LEU:HB2	2.21	0.40
8:A:112:MET:HE2	8:A:117:LEU:HB2	2.03	0.40
8:A:121:MET:HE3	8:A:121:MET:HB3	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:65:SER:OG	9:B:66:LEU:N	2.54	0.40
9:B:71:ILE:HG12	9:B:138:GLY:HA3	2.02	0.40
9:B:149:GLN:NE2	9:B:151:ASP:OD1	2.54	0.40
13:F:132:LEU:HB2	13:F:147:PHE:HB3	2.03	0.40
15:I:297:GLY:HA3	15:I:301:GLU:HB2	2.04	0.40
16:K:365:GLU:OE1	16:K:365:GLU:N	2.54	0.40
17:L:344:ASP:O	17:L:345:ARG:C	2.64	0.40
20:R:130:GLN:HG3	20:R:160:LYS:HE3	2.03	0.40
21:S:316:LEU:HD23	21:S:320:ILE:HG12	2.03	0.40
22:V:274:GLN:HB3	22:V:279:HIS:CD2	2.56	0.40
7:a:51:ASN:HB3	7:a:234:ASP:OD1	2.21	0.40
7:a:122:PRO:HB2	7:a:159:PHE:CD2	2.56	0.40
4:g:9:VAL:HG23	4:g:12:SER:H	1.86	0.40
4:g:95:ARG:NH1	4:g:96:ARG:HB2	2.36	0.40
4:g:113:LYS:HB3	4:g:113:LYS:HE3	1.91	0.40
2:i:79:ALA:O	2:i:82:GLU:HG3	2.22	0.40
26:H:224:VAL:HG22	26:H:243:PRO:HG2	2.03	0.40
30:N:193:ALA:HA	30:N:197:VAL:HG23	2.03	0.40
30:N:302:PHE:HE2	30:N:712:ASN:HB3	1.85	0.40
30:N:350:LYS:HD3	30:N:350:LYS:HA	1.91	0.40
30:N:547:LEU:HD23	30:N:547:LEU:HA	1.88	0.40
32:o:452:LEU:HD21	32:o:489:ALA:HB2	2.02	0.40
1:1:93:SER:OG	1:1:95:GLU:OE2	2.26	0.40
1:1:133:PRO:HD2	1:1:137:SER:O	2.20	0.40
4:4:7:ILE:HG23	4:4:14:ILE:HB	2.04	0.40
5:5:156:LYS:NZ	11:D:98:LEU:O	2.54	0.40
7:7:100:LEU:O	7:7:104:VAL:HG23	2.21	0.40
8:A:174:LYS:HD3	8:A:214:LEU:HD22	2.04	0.40
8:A:199:TRP:HZ3	8:A:236:LEU:HD11	1.85	0.40
11:D:61:PRO:O	11:D:63:LYS:NZ	2.43	0.40
12:E:78:MET:HB2	12:E:78:MET:HE2	1.86	0.40
12:E:164:PHE:C	12:E:165:TYR:HD1	2.29	0.40
13:F:66:CYS:HA	13:F:89:ARG:HE	1.86	0.40
15:I:361:ILE:HA	15:I:364:ILE:HG22	2.04	0.40
15:I:380:LEU:HD21	15:I:416:PHE:HD2	1.86	0.40
17:L:238:THR:CG2	17:L:239:ILE:N	2.84	0.40
17:L:364:HIS:CE1	17:L:392:ARG:HB2	2.56	0.40
20:R:53:LYS:HE2	20:R:53:LYS:HB2	1.94	0.40
21:S:402:ILE:HG21	21:S:407:ILE:HD11	2.04	0.40
21:S:411:LEU:HD23	21:S:411:LEU:HA	1.88	0.40
24:Y:65:ASP:CG	24:Y:66:ASP:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:66:ASP:OD1	24:Y:66:ASP:N	2.54	0.40
7:a:219:TYR:CZ	7:a:250:MET:HE2	2.57	0.40
5:f:188:TYR:CE1	5:f:198:LYS:HD3	2.56	0.40
26:H:98:GLN:N	26:H:176:VAL:O	2.54	0.40
27:M:167:VAL:O	27:M:170:MET:HG2	2.21	0.40
30:N:42:GLU:OE1	30:N:42:GLU:N	2.52	0.40
30:N:233:ASN:HD21	30:N:266:SER:HB3	1.87	0.40
30:N:270:LEU:HD23	30:N:270:LEU:HA	1.80	0.40
30:N:816:LYS:HB2	30:N:816:LYS:HE3	1.90	0.40
31:T:100:ASP:OD1	31:T:101:LYS:HG3	2.21	0.40
32:o:232:LYS:HD3	32:o:235:GLN:NE2	2.36	0.40
1:1:134:LEU:HD23	1:1:134:LEU:HA	1.91	0.40
2:2:54:ILE:HD11	3:3:147:PHE:CD2	2.55	0.40
14:G:157:TYR:CD1	14:G:157:TYR:C	2.99	0.40
16:K:334:LEU:H	16:K:334:LEU:HD12	1.86	0.40
17:L:88:TYR:OH	27:M:58:MET:O	2.38	0.40
18:O:337:LEU:HD22	18:O:350:ILE:HD12	2.02	0.40
20:R:338:TYR:HB3	20:R:377:LEU:HD21	2.03	0.40
21:S:47:THR:HG21	21:S:52:TYR:CE1	2.57	0.40
21:S:482:PRO:HB2	29:U:294:ASN:OD1	2.21	0.40
23:W:185:ILE:O	23:W:189:PRO:HD2	2.22	0.40
4:g:162:LYS:HD2	4:g:198:GLN:CD	2.46	0.40
3:h:161:GLU:O	2:i:236:ARG:NH2	2.54	0.40
25:J:186:ILE:HG12	25:J:310:ILE:HG12	2.04	0.40
26:H:333:MET:SD	26:H:334:LEU:HD23	2.61	0.40
28:Q:350:ILE:O	28:Q:353:PRO:HD2	2.22	0.40
30:N:6:ALA:O	30:N:10:LEU:HB2	2.21	0.40
30:N:310:ASP:HA	30:N:787:MET:HE1	2.02	0.40
30:N:882:ILE:HD13	30:N:882:ILE:HA	1.88	0.40
30:N:886:LYS:H	30:N:886:LYS:HG2	1.57	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	1	203/215 (94%)	195 (96%)	8 (4%)	0	100	100
1	b	203/215 (94%)	197 (97%)	6 (3%)	0	100	100
2	2	220/261 (84%)	217 (99%)	3 (1%)	0	100	100
2	i	220/261 (84%)	217 (99%)	3 (1%)	0	100	100
3	3	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
3	h	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
4	4	196/198 (99%)	191 (97%)	5 (3%)	0	100	100
4	g	196/198 (99%)	192 (98%)	4 (2%)	0	100	100
5	5	210/287 (73%)	207 (99%)	3 (1%)	0	100	100
5	f	210/287 (73%)	206 (98%)	4 (2%)	0	100	100
6	6	220/241 (91%)	214 (97%)	5 (2%)	1 (0%)	25	59
6	e	220/241 (91%)	217 (99%)	3 (1%)	0	100	100
7	7	231/266 (87%)	223 (96%)	8 (4%)	0	100	100
7	a	231/266 (87%)	224 (97%)	7 (3%)	0	100	100
8	A	241/252 (96%)	236 (98%)	5 (2%)	0	100	100
9	B	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
10	C	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	30	62
11	D	239/254 (94%)	231 (97%)	8 (3%)	0	100	100
12	E	240/260 (92%)	232 (97%)	8 (3%)	0	100	100
13	F	231/234 (99%)	223 (96%)	8 (4%)	0	100	100
14	G	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
15	I	390/437 (89%)	345 (88%)	43 (11%)	2 (0%)	25	59
16	K	381/428 (89%)	336 (88%)	43 (11%)	2 (0%)	25	59
17	L	357/437 (82%)	320 (90%)	36 (10%)	1 (0%)	37	67
18	O	384/393 (98%)	356 (93%)	25 (6%)	3 (1%)	16	50
19	P	434/445 (98%)	415 (96%)	18 (4%)	1 (0%)	44	73
20	R	393/429 (92%)	373 (95%)	19 (5%)	1 (0%)	37	67
21	S	459/523 (88%)	430 (94%)	28 (6%)	1 (0%)	44	73
22	V	286/306 (94%)	265 (93%)	20 (7%)	1 (0%)	37	67
23	W	188/268 (70%)	172 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	Y	29/89 (33%)	26 (90%)	2 (7%)	1 (3%)	3	24
25	J	364/405 (90%)	345 (95%)	19 (5%)	0	100	100
26	H	379/467 (81%)	333 (88%)	46 (12%)	0	100	100
27	M	359/434 (83%)	330 (92%)	28 (8%)	1 (0%)	37	67
28	Q	407/434 (94%)	385 (95%)	22 (5%)	0	100	100
29	U	288/338 (85%)	270 (94%)	17 (6%)	1 (0%)	37	67
30	N	863/945 (91%)	816 (95%)	47 (5%)	0	100	100
31	T	253/274 (92%)	237 (94%)	15 (6%)	1 (0%)	30	62
32	o	811/993 (82%)	756 (93%)	55 (7%)	0	100	100
All	All	11671/13187 (88%)	11029 (94%)	624 (5%)	18 (0%)	45	73

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	K	143	SER
18	O	205	ILE
22	V	161	THR
15	I	178	THR
17	L	175	GLN
18	O	166	ARG
24	Y	74	THR
6	6	51	ASP
19	P	108	LYS
16	K	419	ASN
18	O	305	ILE
15	I	386	ASP
20	R	70	TYR
29	U	183	ALA
27	M	430	VAL
31	T	259	ILE
10	C	52	VAL
21	S	432	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	169/178 (95%)	162 (96%)	7 (4%)	26	54
1	b	169/178 (95%)	168 (99%)	1 (1%)	84	91
2	2	181/214 (85%)	177 (98%)	4 (2%)	47	69
2	i	181/214 (85%)	178 (98%)	3 (2%)	56	75
3	3	172/173 (99%)	167 (97%)	5 (3%)	37	63
3	h	172/173 (99%)	170 (99%)	2 (1%)	67	82
4	4	175/175 (100%)	172 (98%)	3 (2%)	56	75
4	g	175/175 (100%)	172 (98%)	3 (2%)	56	75
5	5	169/235 (72%)	164 (97%)	5 (3%)	36	62
5	f	169/235 (72%)	164 (97%)	5 (3%)	36	62
6	6	185/201 (92%)	185 (100%)	0	100	100
6	e	185/201 (92%)	183 (99%)	2 (1%)	70	83
7	7	199/224 (89%)	196 (98%)	3 (2%)	60	77
7	a	199/224 (89%)	193 (97%)	6 (3%)	36	62
8	A	207/210 (99%)	200 (97%)	7 (3%)	32	59
9	B	209/209 (100%)	204 (98%)	5 (2%)	44	67
10	C	203/216 (94%)	195 (96%)	8 (4%)	27	56
11	D	213/226 (94%)	205 (96%)	8 (4%)	28	57
12	E	198/215 (92%)	189 (96%)	9 (4%)	23	52
13	F	192/193 (100%)	184 (96%)	8 (4%)	25	54
14	G	200/239 (84%)	191 (96%)	9 (4%)	23	52
15	I	349/385 (91%)	333 (95%)	16 (5%)	23	51
16	K	336/374 (90%)	319 (95%)	17 (5%)	20	48
17	L	305/377 (81%)	296 (97%)	9 (3%)	36	62
18	O	361/368 (98%)	348 (96%)	13 (4%)	30	58
19	P	408/415 (98%)	399 (98%)	9 (2%)	47	69
20	R	349/379 (92%)	332 (95%)	17 (5%)	21	49
21	S	433/489 (88%)	414 (96%)	19 (4%)	24	53
22	V	252/268 (94%)	237 (94%)	15 (6%)	16	44
23	W	165/230 (72%)	161 (98%)	4 (2%)	44	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	Y	31/82 (38%)	31 (100%)	0	100	100
25	J	322/352 (92%)	310 (96%)	12 (4%)	29	57
26	H	326/399 (82%)	318 (98%)	8 (2%)	42	66
27	M	311/375 (83%)	294 (94%)	17 (6%)	18	47
28	Q	374/391 (96%)	363 (97%)	11 (3%)	37	63
29	U	265/308 (86%)	255 (96%)	10 (4%)	28	57
30	N	729/797 (92%)	701 (96%)	28 (4%)	28	57
31	T	240/256 (94%)	237 (99%)	3 (1%)	65	80
32	o	697/850 (82%)	677 (97%)	20 (3%)	37	63
All	All	10175/11403 (89%)	9844 (97%)	331 (3%)	35	60

All (331) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	50	THR
1	1	62	CYS
1	1	82	LEU
1	1	104	LEU
1	1	153	ILE
1	1	165	MET
1	1	191	VAL
2	2	59	ASN
2	2	112	LEU
2	2	149	ASP
2	2	249	ILE
3	3	16	THR
3	3	23	ILE
3	3	25	CYS
3	3	64	ASN
3	3	82	ILE
4	4	5	LEU
4	4	102	VAL
4	4	146	HIS
5	5	78	THR
5	5	117	LEU
5	5	134	LEU
5	5	172	MET
5	5	215	LEU
7	7	100	LEU

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Mol	Chain	Res	Type
7	7	133	MET
7	7	149	VAL
8	A	20	SER
8	A	42	SER
8	A	69	VAL
8	A	89	ASP
8	A	114	CYS
8	A	157	THR
8	A	222	ASP
9	B	21	ILE
9	B	41	ASN
9	B	113	GLU
9	B	177	LYS
9	B	193	LEU
10	C	3	SER
10	C	12	ILE
10	C	45	VAL
10	C	111	LEU
10	C	115	LEU
10	C	169	THR
10	C	197	LEU
10	C	226	TYR
11	D	8	LEU
11	D	71	VAL
11	D	72	VAL
11	D	81	ASP
11	D	98	LEU
11	D	126	VAL
11	D	131	VAL
11	D	151	GLU
12	E	21	LEU
12	E	28	LEU
12	E	64	ILE
12	E	78	MET
12	E	88	MET
12	E	121	LEU
12	E	122	ARG
12	E	192	THR
12	E	226	ASP
13	F	2	PHE
13	F	9	ASP
13	F	21	GLN

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Mol	Chain	Res	Type
13	F	34	VAL
13	F	56	LEU
13	F	112	LEU
13	F	166	GLN
13	F	187	ASP
14	G	6	THR
14	G	36	THR
14	G	53	LEU
14	G	68	GLN
14	G	78	TYR
14	G	134	VAL
14	G	143	LYS
14	G	181	ASP
14	G	200	ILE
15	I	55	CYS
15	I	111	GLU
15	I	121	THR
15	I	132	ILE
15	I	170	VAL
15	I	194	ILE
15	I	214	LYS
15	I	227	THR
15	I	321	ASP
15	I	328	THR
15	I	329	ASN
15	I	333	THR
15	I	344	ILE
15	I	345	ASP
15	I	365	HIS
15	I	391	ASP
16	K	49	PHE
16	K	60	LEU
16	K	63	LEU
16	K	75	LEU
16	K	86	VAL
16	K	96	ILE
16	K	159	SER
16	K	168	ASP
16	K	197	LEU
16	K	217	THR
16	K	221	MET
16	K	253	MET

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Mol	Chain	Res	Type
16	K	289	ASP
16	K	318	THR
16	K	374	ARG
16	K	408	GLU
16	K	428	LYS
17	L	123	SER
17	L	141	LYS
17	L	152	THR
17	L	190	ILE
17	L	276	CYS
17	L	284	ASP
17	L	332	THR
17	L	382	MET
17	L	425	VAL
18	O	38	TRP
18	O	41	LEU
18	O	55	THR
18	O	70	TYR
18	O	82	LEU
18	O	98	TYR
18	O	153	LEU
18	O	198	THR
18	O	206	THR
18	O	263	PHE
18	O	322	ASP
18	O	347	LEU
18	O	393	VAL
19	P	21	PHE
19	P	167	THR
19	P	178	GLN
19	P	247	THR
19	P	261	LEU
19	P	269	VAL
19	P	305	THR
19	P	419	VAL
19	P	434	THR
20	R	203	ASP
20	R	218	CYS
20	R	233	ASP
20	R	237	THR
20	R	239	THR
20	R	265	ASP

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Mol	Chain	Res	Type
20	R	286	LEU
20	R	317	ILE
20	R	324	ARG
20	R	327	ASP
20	R	337	VAL
20	R	340	GLN
20	R	353	MET
20	R	368	LEU
20	R	385	ASN
20	R	395	ASN
20	R	406	GLN
21	S	39	ASN
21	S	41	ILE
21	S	73	THR
21	S	131	THR
21	S	159	ASN
21	S	204	ASP
21	S	234	ILE
21	S	269	GLU
21	S	288	THR
21	S	297	ILE
21	S	303	ASN
21	S	322	LEU
21	S	324	MET
21	S	332	PHE
21	S	337	ASN
21	S	386	ASN
21	S	408	CYS
21	S	446	THR
21	S	471	LEU
22	V	22	ASP
22	V	25	GLU
22	V	53	MET
22	V	83	VAL
22	V	103	MET
22	V	104	VAL
22	V	114	PHE
22	V	153	ILE
22	V	161	THR
22	V	185	ILE
22	V	204	HIS
22	V	249	GLU

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Mol	Chain	Res	Type
22	V	266	LEU
22	V	281	SER
22	V	302	SER
23	W	34	GLU
23	W	72	ILE
23	W	79	THR
23	W	151	THR
7	a	100	LEU
7	a	133	MET
7	a	162	TYR
7	a	216	VAL
7	a	250	MET
7	a	253	ASP
1	b	165	MET
6	e	126	VAL
6	e	152	ARG
5	f	108	LYS
5	f	161	LEU
5	f	192	SER
5	f	204	VAL
5	f	245	TYR
4	g	25	ILE
4	g	41	HIS
4	g	161	LEU
3	h	88	THR
3	h	105	VAL
2	i	64	HIS
2	i	95	HIS
2	i	128	ILE
25	J	72	VAL
25	J	103	ASN
25	J	107	LEU
25	J	142	VAL
25	J	148	ASP
25	J	160	ILE
25	J	165	GLU
25	J	193	THR
25	J	235	VAL
25	J	248	ASP
25	J	311	ASP
25	J	328	LEU
26	H	83	ASP

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Mol	Chain	Res	Type
26	H	99	VAL
26	H	198	MET
26	H	199	THR
26	H	200	VAL
26	H	216	ASP
26	H	356	ASN
26	H	414	SER
27	M	78	LEU
27	M	81	ASN
27	M	136	ASP
27	M	138	ASP
27	M	177	THR
27	M	179	THR
27	M	183	VAL
27	M	256	ILE
27	M	276	THR
27	M	284	ASP
27	M	306	LEU
27	M	331	ASP
27	M	343	LEU
27	M	383	THR
27	M	394	VAL
27	M	417	GLU
27	M	421	GLU
28	Q	59	LEU
28	Q	80	HIS
28	Q	94	VAL
28	Q	102	GLU
28	Q	158	ILE
28	Q	219	ASP
28	Q	240	PHE
28	Q	277	ASP
28	Q	280	ASN
28	Q	328	ASP
28	Q	404	ASN
29	U	5	HIS
29	U	66	TRP
29	U	76	MET
29	U	109	LEU
29	U	146	ASP
29	U	156	HIS
29	U	180	ASP

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Mol	Chain	Res	Type
29	U	204	LEU
29	U	229	LEU
29	U	267	VAL
30	N	5	THR
30	N	10	LEU
30	N	36	TRP
30	N	101	ILE
30	N	123	PHE
30	N	164	ASP
30	N	260	ASP
30	N	343	THR
30	N	373	VAL
30	N	415	PHE
30	N	438	ASP
30	N	455	MET
30	N	572	LEU
30	N	593	PHE
30	N	660	LEU
30	N	668	THR
30	N	677	ASP
30	N	681	ASN
30	N	689	LYS
30	N	722	THR
30	N	724	THR
30	N	725	LEU
30	N	734	VAL
30	N	756	THR
30	N	858	LYS
30	N	891	VAL
30	N	903	VAL
30	N	919	THR
31	T	40	LEU
31	T	76	ASP
31	T	119	THR
32	o	68	LEU
32	o	108	ASP
32	o	146	PHE
32	o	225	LEU
32	o	279	THR
32	o	280	ASP
32	o	293	MET
32	o	342	LEU

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Mol	Chain	Res	Type
32	o	398	LYS
32	o	430	LEU
32	o	431	ASP
32	o	467	VAL
32	o	510	LEU
32	o	551	LEU
32	o	752	ILE
32	o	797	THR
32	o	818	CYS
32	o	843	ASP
32	o	850	LEU
32	o	868	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	88	GLN
2	2	201	ASN
2	2	229	GLN
4	4	10	GLN
4	4	65	GLN
4	4	118	GLN
4	4	133	HIS
4	4	198	GLN
5	5	99	ASN
5	5	104	GLN
5	5	254	HIS
5	5	283	ASN
6	6	214	HIS
8	A	15	HIS
8	A	181	ASN
8	A	240	ASN
9	B	20	GLN
9	B	149	GLN
9	B	244	ASN
10	C	96	GLN
11	D	118	GLN
11	D	167	ASN
12	E	114	GLN
12	E	147	HIS
12	E	157	HIS
13	F	60	GLN

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Mol	Chain	Res	Type
13	F	86	ASN
13	F	100	ASN
13	F	166	GLN
13	F	210	ASN
14	G	68	GLN
14	G	183	HIS
16	K	64	GLN
16	K	200	GLN
16	K	319	ASN
16	K	414	GLN
16	K	419	ASN
17	L	273	HIS
17	L	302	GLN
18	O	122	HIS
18	O	175	ASN
18	O	304	ASN
18	O	343	GLN
19	P	178	GLN
19	P	183	GLN
19	P	230	HIS
19	P	246	GLN
20	R	19	ASN
20	R	114	ASN
20	R	132	GLN
20	R	136	ASN
20	R	184	GLN
20	R	406	GLN
21	S	32	GLN
21	S	39	ASN
21	S	70	ASN
21	S	191	HIS
21	S	205	ASN
21	S	227	ASN
21	S	450	ASN
22	V	97	GLN
22	V	111	HIS
22	V	172	GLN
22	V	193	ASN
22	V	200	ASN
22	V	291	ASN
23	W	12	ASN
23	W	80	GLN

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Mol	Chain	Res	Type
23	W	102	GLN
23	W	108	GLN
7	a	35	GLN
7	a	185	ASN
7	a	246	GLN
1	b	180	GLN
4	g	41	HIS
4	g	63	ASN
4	g	166	GLN
3	h	169	GLN
2	i	189	GLN
25	J	52	ASN
25	J	220	GLN
25	J	376	HIS
26	H	467	ASN
27	M	72	ASN
27	M	238	GLN
27	M	253	GLN
28	Q	19	GLN
28	Q	150	GLN
28	Q	418	GLN
28	Q	425	GLN
29	U	127	GLN
29	U	128	GLN
29	U	173	HIS
29	U	181	GLN
29	U	223	HIS
29	U	298	ASN
30	N	176	GLN
30	N	231	ASN
30	N	336	ASN
30	N	361	ASN
30	N	459	ASN
30	N	580	ASN
30	N	613	HIS
31	T	47	GLN
31	T	83	ASN
31	T	112	ASN
31	T	132	HIS
32	o	166	ASN
32	o	347	ASN
32	o	391	ASN

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Mol	Chain	Res	Type
32	o	403	ASN
32	o	801	HIS
32	o	810	ASN
32	o	842	GLN
32	o	874	ASN
32	o	926	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
34	ATP	M	501	33	28,33,33	0.66	0	34,52,52	0.66	1 (2%)
36	ADP	J	502	-	24,29,29	0.89	0	29,45,45	1.28	3 (10%)
34	ATP	J	501	33	28,33,33	0.65	0	34,52,52	0.75	2 (5%)
34	ATP	H	501	33	28,33,33	0.67	0	34,52,52	0.65	1 (2%)
34	ATP	K	501	33	28,33,33	0.68	0	34,52,52	0.68	1 (2%)
34	ATP	L	501	33	28,33,33	0.71	0	34,52,52	0.64	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	ATP	M	501	33	-	3/18/38/38	0/3/3/3
36	ADP	J	502	-	-	2/12/32/32	0/3/3/3
34	ATP	J	501	33	-	4/18/38/38	0/3/3/3
34	ATP	H	501	33	-	4/18/38/38	0/3/3/3
34	ATP	K	501	33	-	1/18/38/38	0/3/3/3
34	ATP	L	501	33	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	J	502	ADP	N3-C2-N1	-3.57	123.82	128.67
34	J	501	ATP	C4'-O4'-C1'	-2.68	107.47	109.92
36	J	502	ADP	C4'-O4'-C1'	2.41	112.13	109.92
36	J	502	ADP	C4-C5-N7	-2.32	106.89	109.34
34	M	501	ATP	C5-C6-N6	2.32	123.84	120.31
34	J	501	ATP	C5-C6-N6	2.31	123.83	120.31
34	H	501	ATP	C5-C6-N6	2.31	123.83	120.31
34	K	501	ATP	C5-C6-N6	2.30	123.82	120.31
34	L	501	ATP	C5-C6-N6	2.28	123.78	120.31

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	L	501	ATP	C5'-O5'-PA-O2A
34	L	501	ATP	C5'-O5'-PA-O3A
34	J	501	ATP	C5'-O5'-PA-O2A
34	J	501	ATP	C5'-O5'-PA-O3A
34	H	501	ATP	O4'-C4'-C5'-O5'
34	H	501	ATP	C3'-C4'-C5'-O5'
36	J	502	ADP	C5'-O5'-PA-O3A
34	L	501	ATP	C4'-C5'-O5'-PA
34	H	501	ATP	C4'-C5'-O5'-PA
34	M	501	ATP	C3'-C4'-C5'-O5'
34	M	501	ATP	O4'-C4'-C5'-O5'

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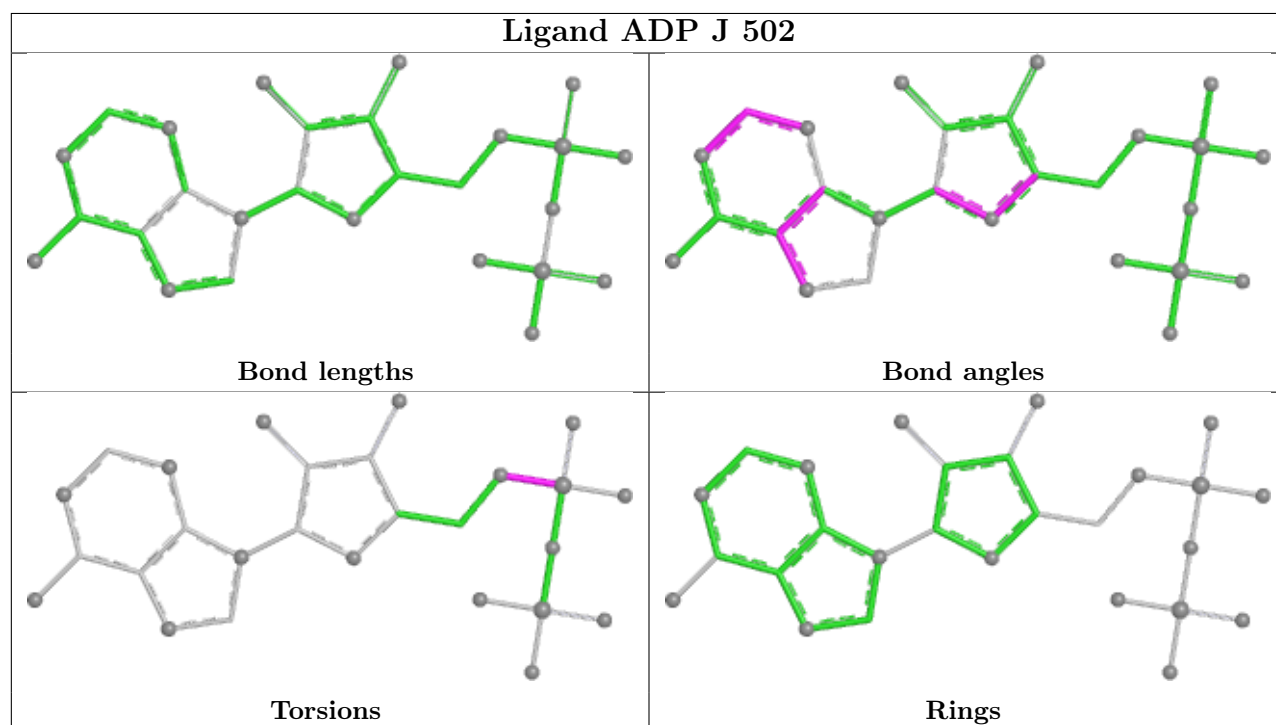
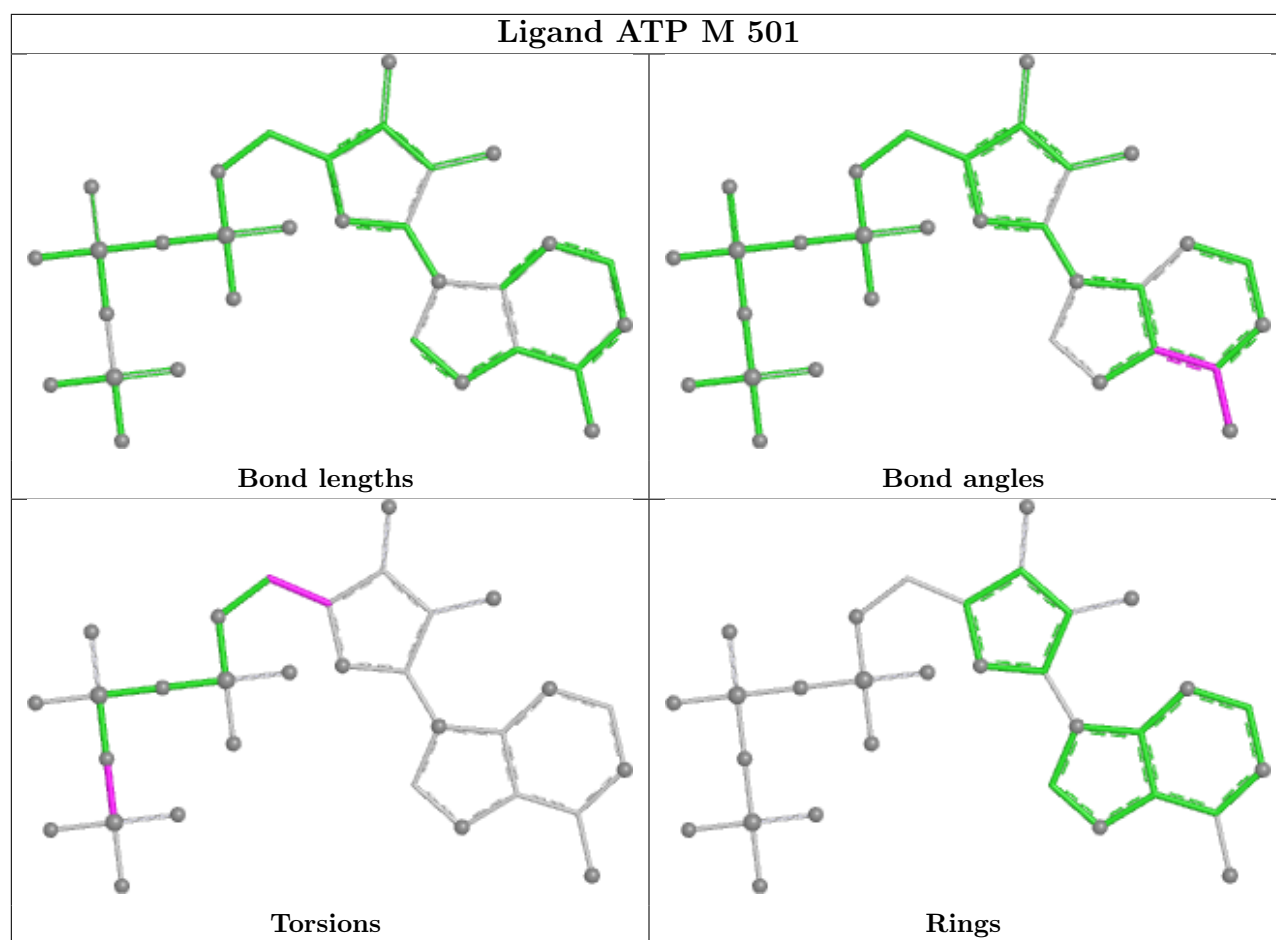
Mol	Chain	Res	Type	Atoms
36	J	502	ADP	C5'-O5'-PA-O1A
34	K	501	ATP	C4'-C5'-O5'-PA
34	J	501	ATP	C4'-C5'-O5'-PA
34	H	501	ATP	PB-O3A-PA-O5'
34	M	501	ATP	PB-O3B-PG-O1G
34	J	501	ATP	O4'-C4'-C5'-O5'

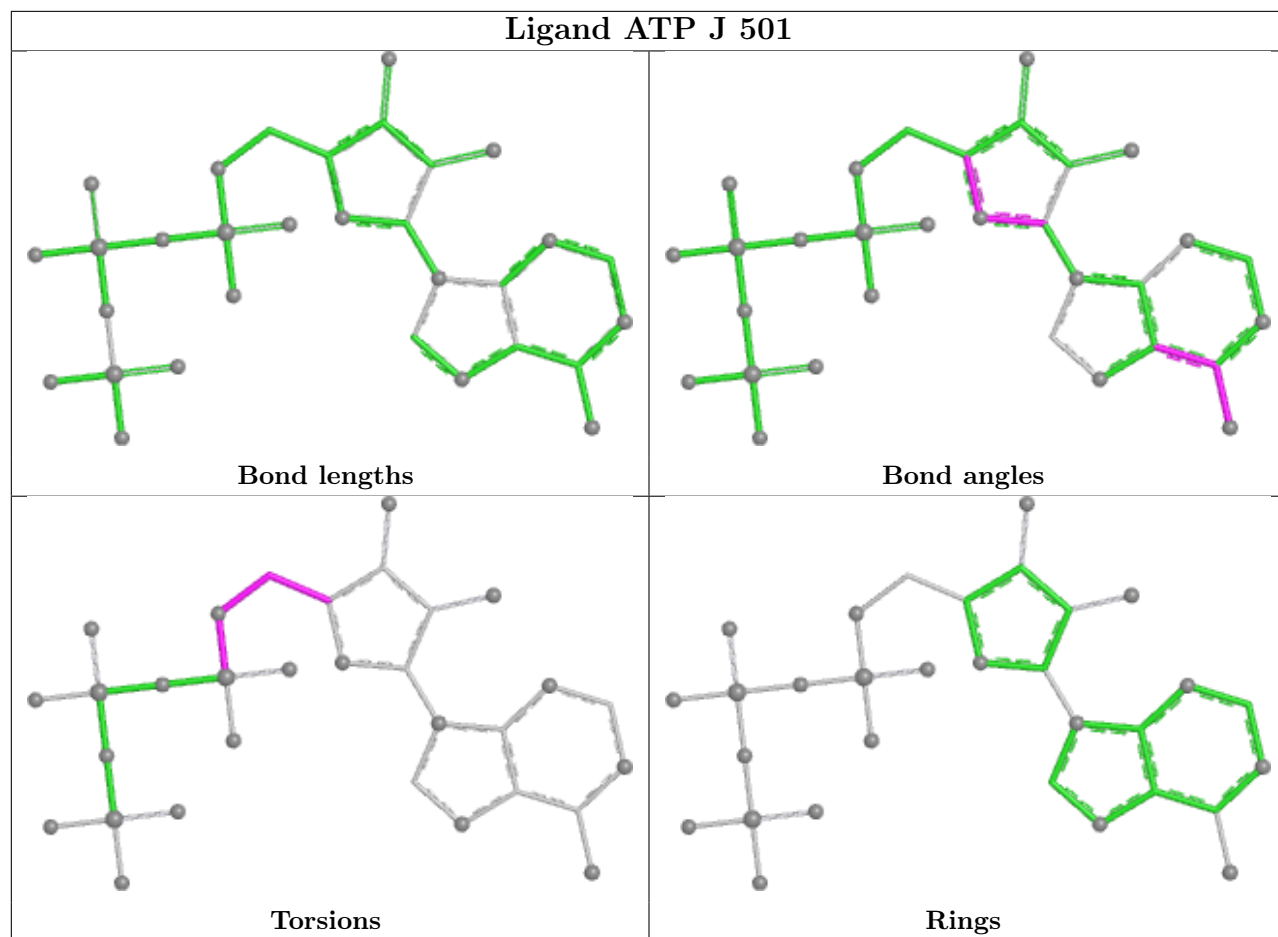
There are no ring outliers.

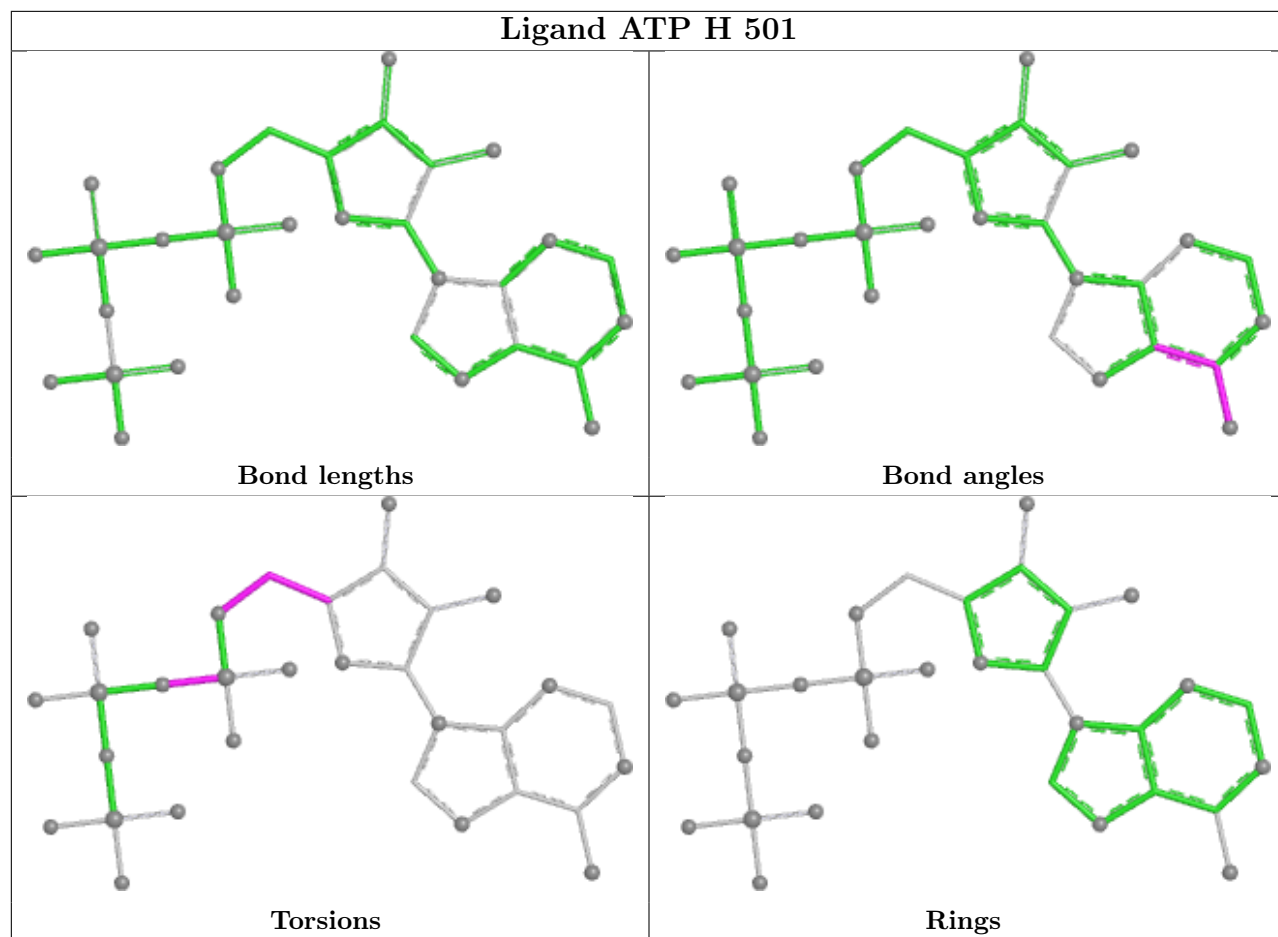
5 monomers are involved in 20 short contacts:

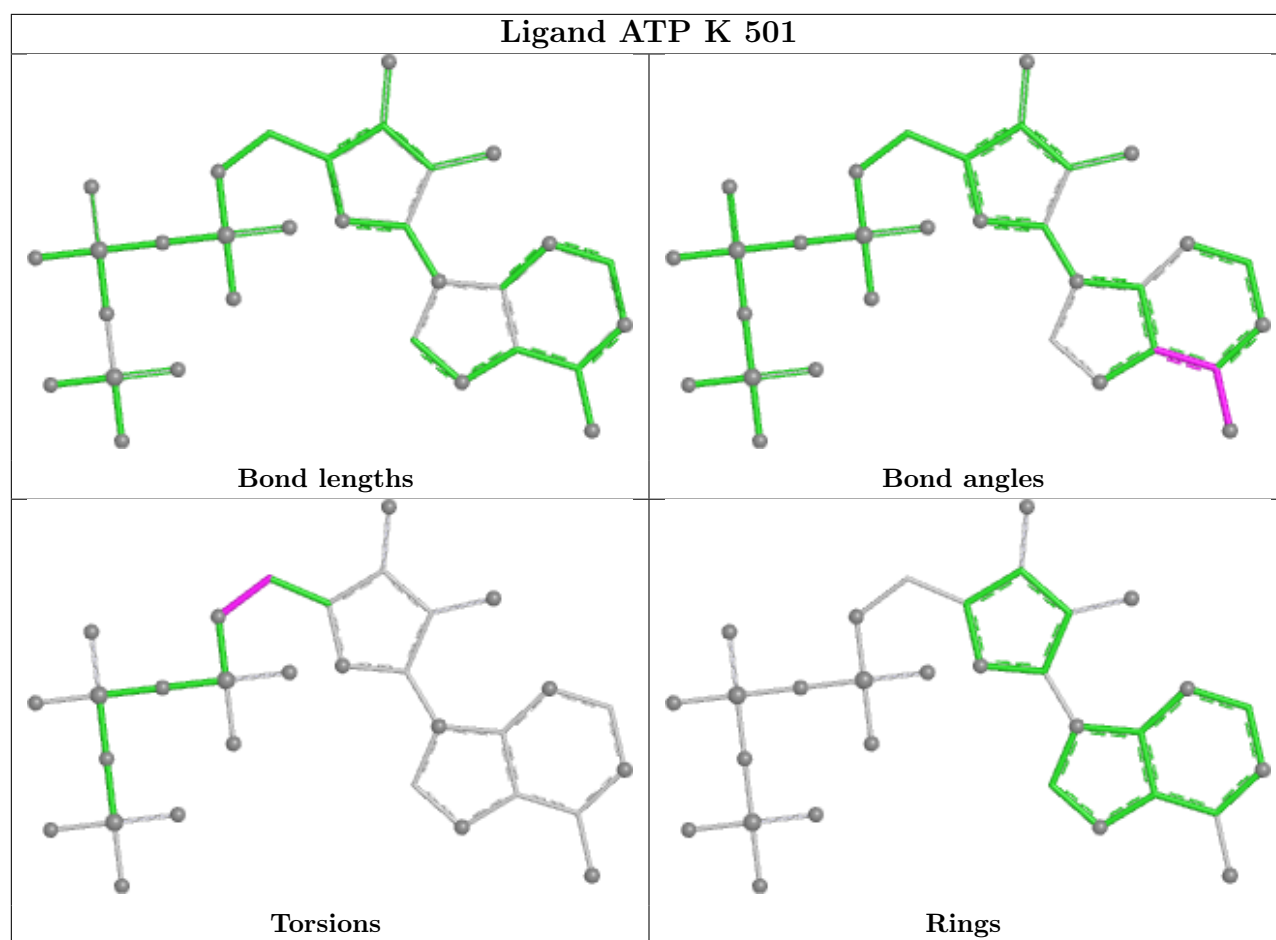
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	M	501	ATP	4	0
36	J	502	ADP	4	0
34	J	501	ATP	3	0
34	H	501	ATP	3	0
34	K	501	ATP	6	0

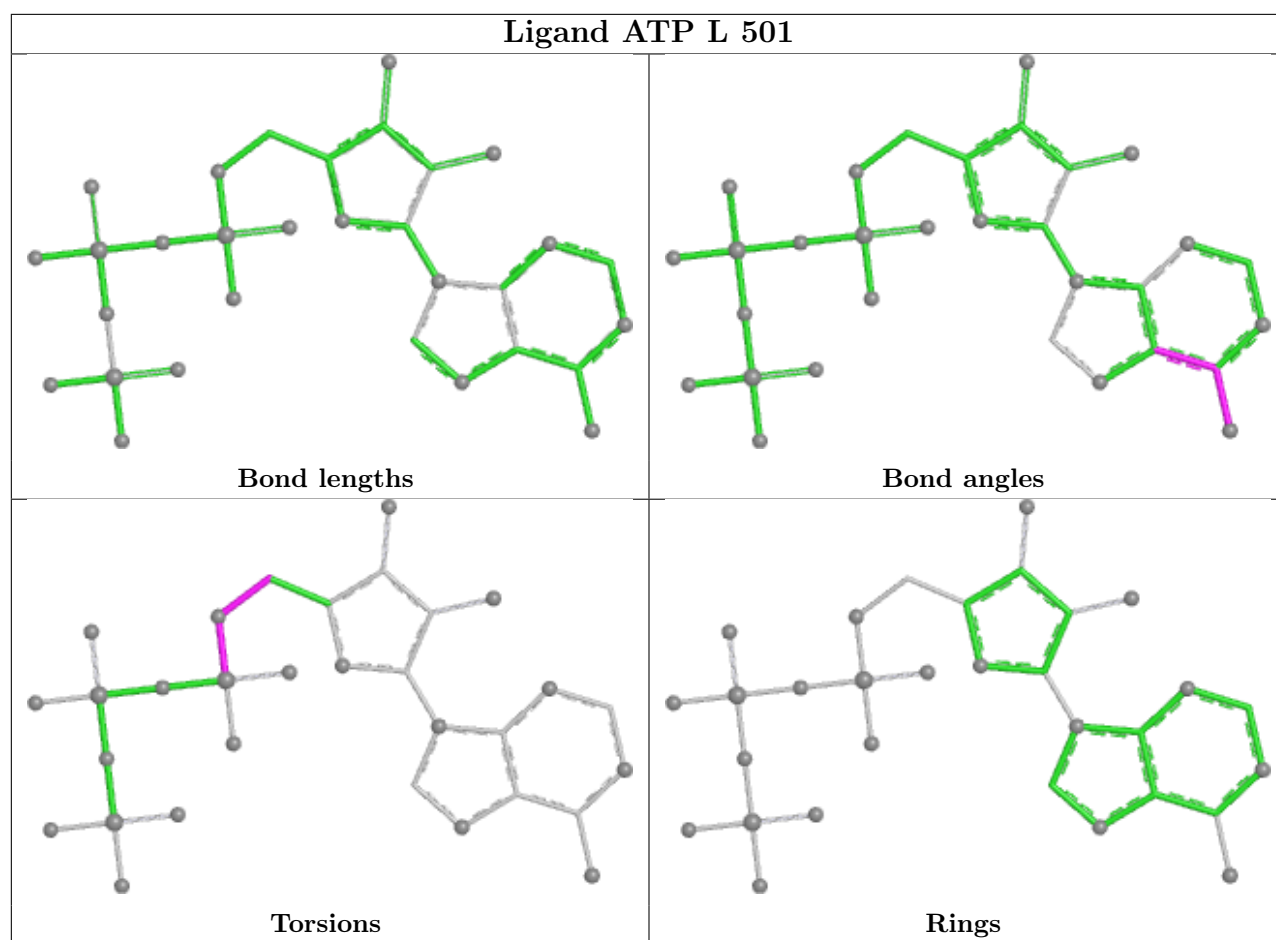
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

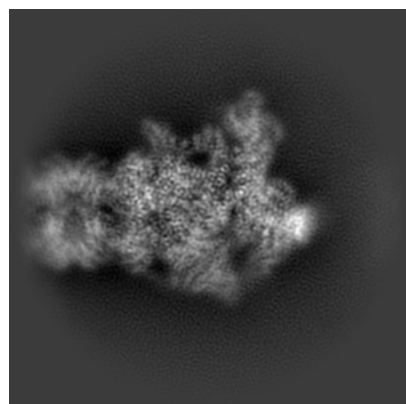
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45579. These allow visual inspection of the internal detail of the map and identification of artifacts.

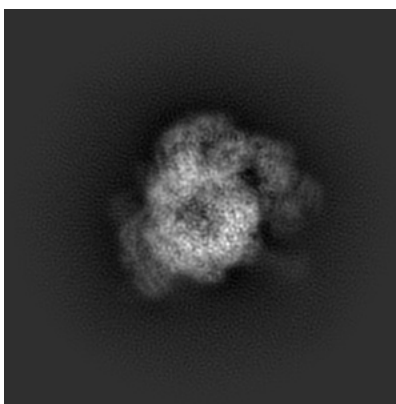
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

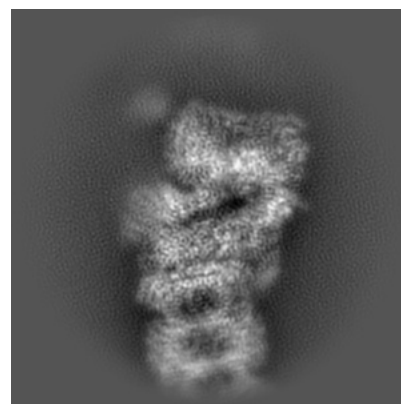
6.1.1 Primary map



X

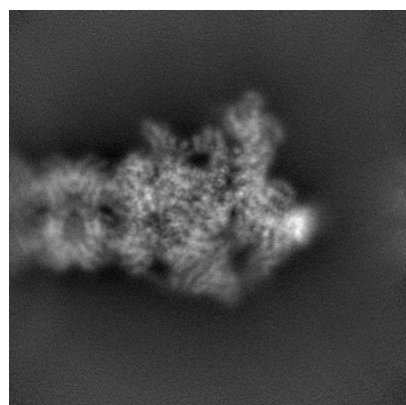


Y

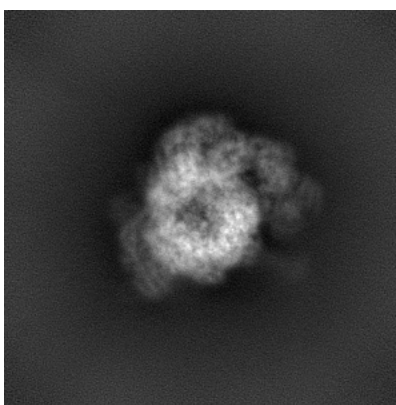


Z

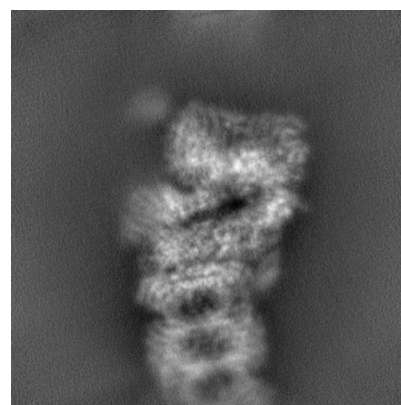
6.1.2 Raw map



X



Y

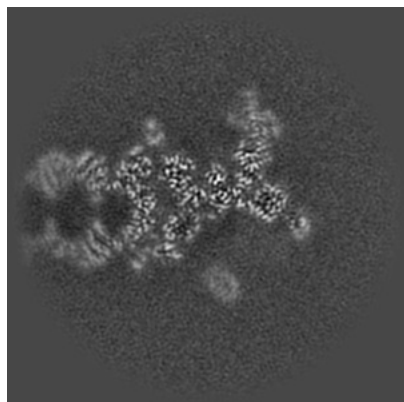


Z

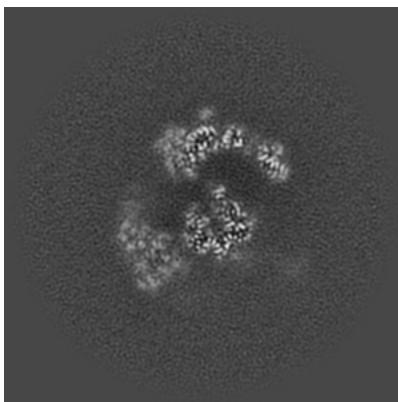
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

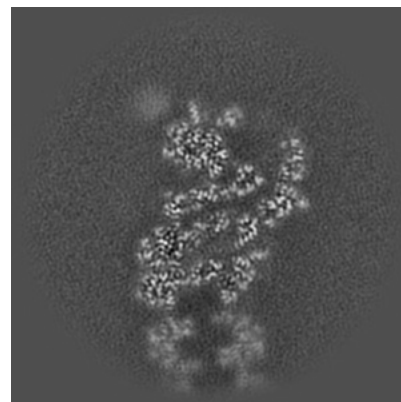
6.2.1 Primary map



X Index: 170

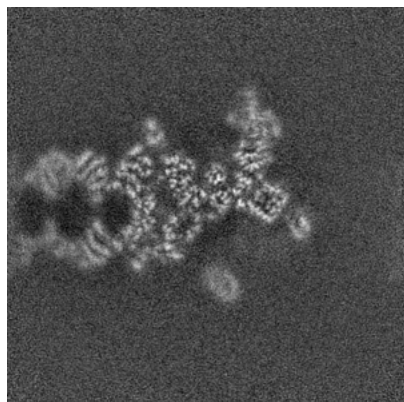


Y Index: 170

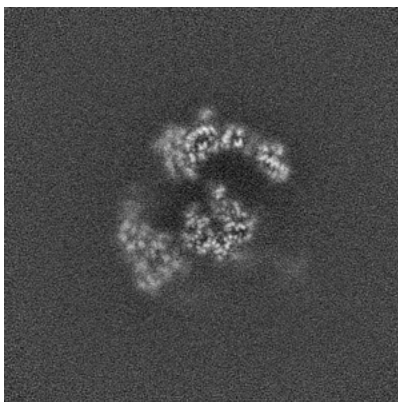


Z Index: 170

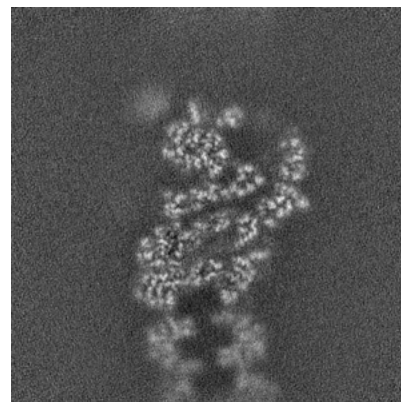
6.2.2 Raw map



X Index: 170



Y Index: 170

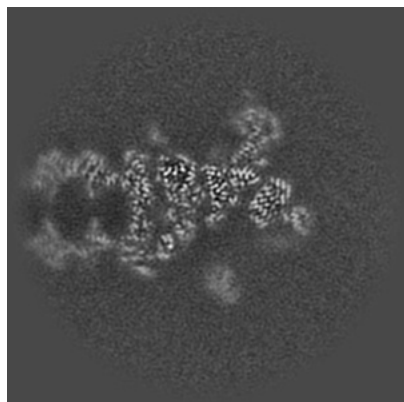


Z Index: 170

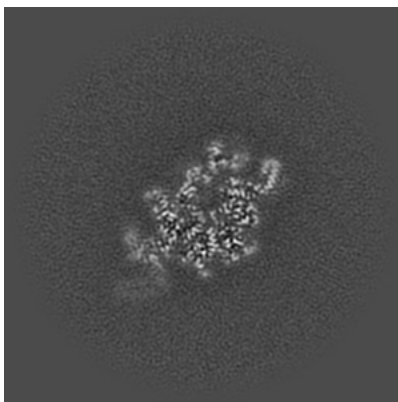
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

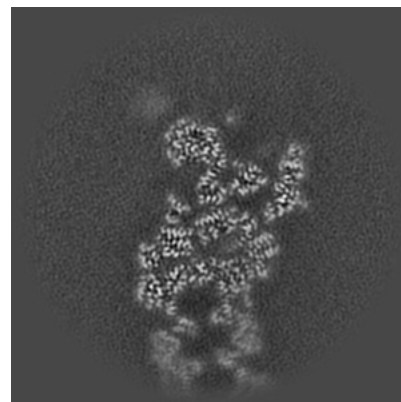
6.3.1 Primary map



X Index: 164

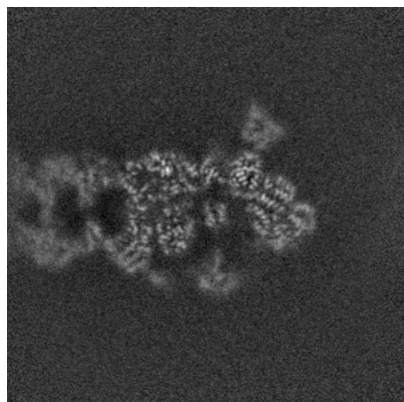


Y Index: 139

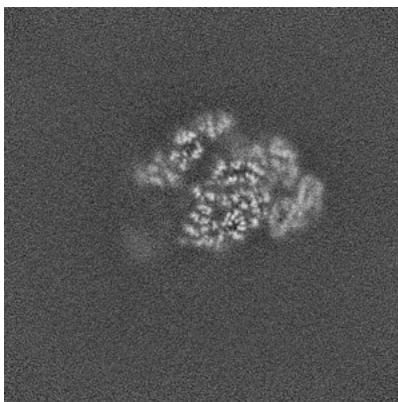


Z Index: 175

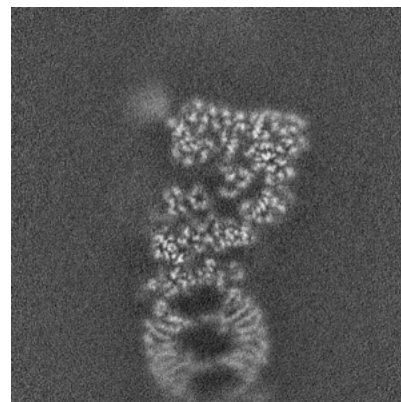
6.3.2 Raw map



X Index: 155



Y Index: 208

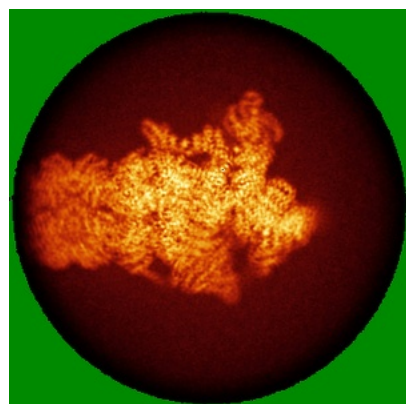


Z Index: 158

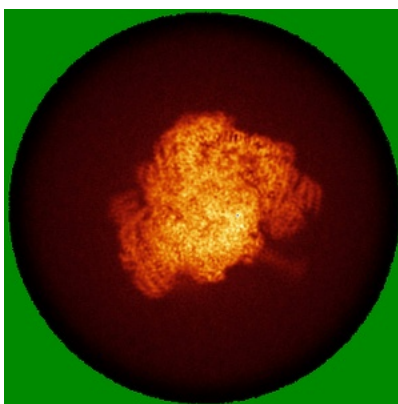
The images above show the largest variance slices of the map in three orthogonal directions.

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

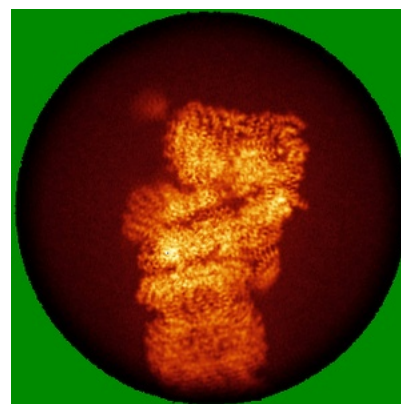
6.4.1 Primary map



X

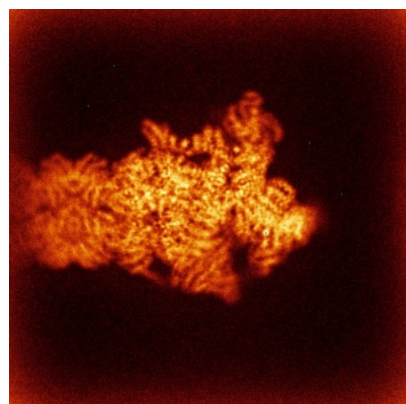


Y

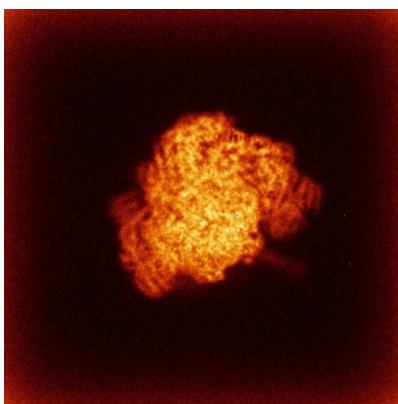


Z

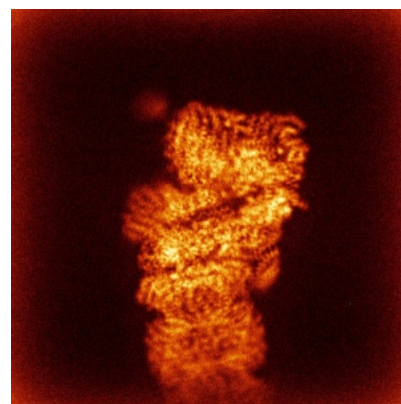
6.4.2 Raw map



X



Y

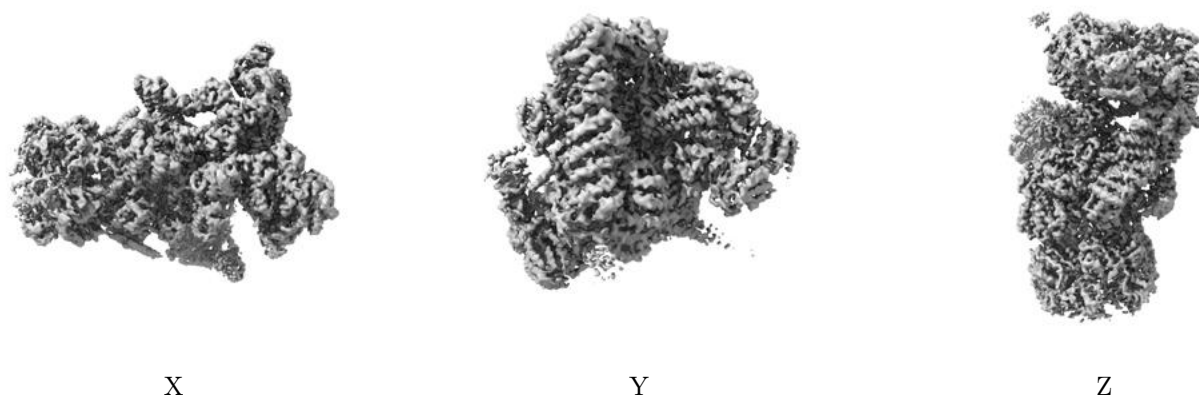


Z

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

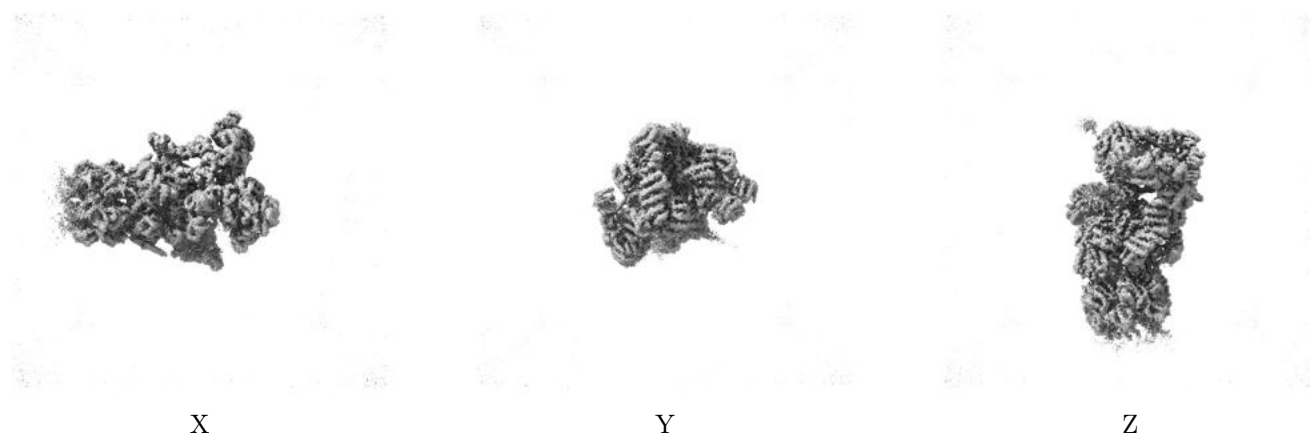
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.33. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

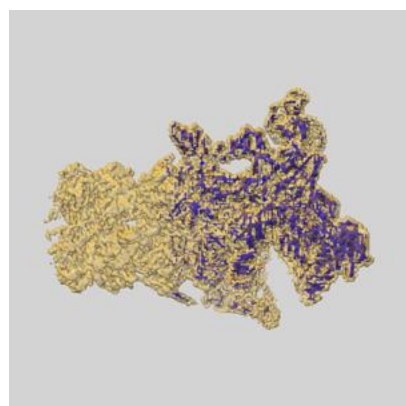
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

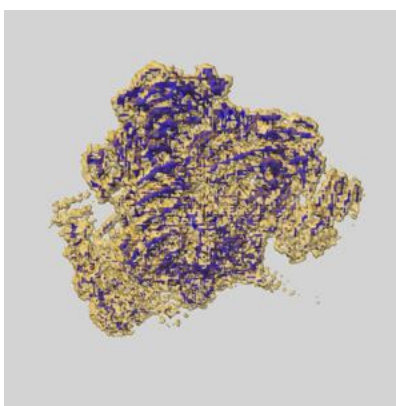
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

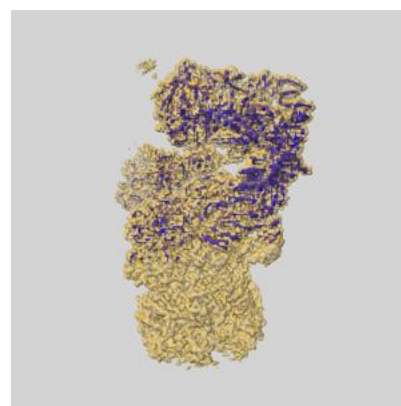
6.6.1 emd_45579_msk_1.map [i](#)



X



Y

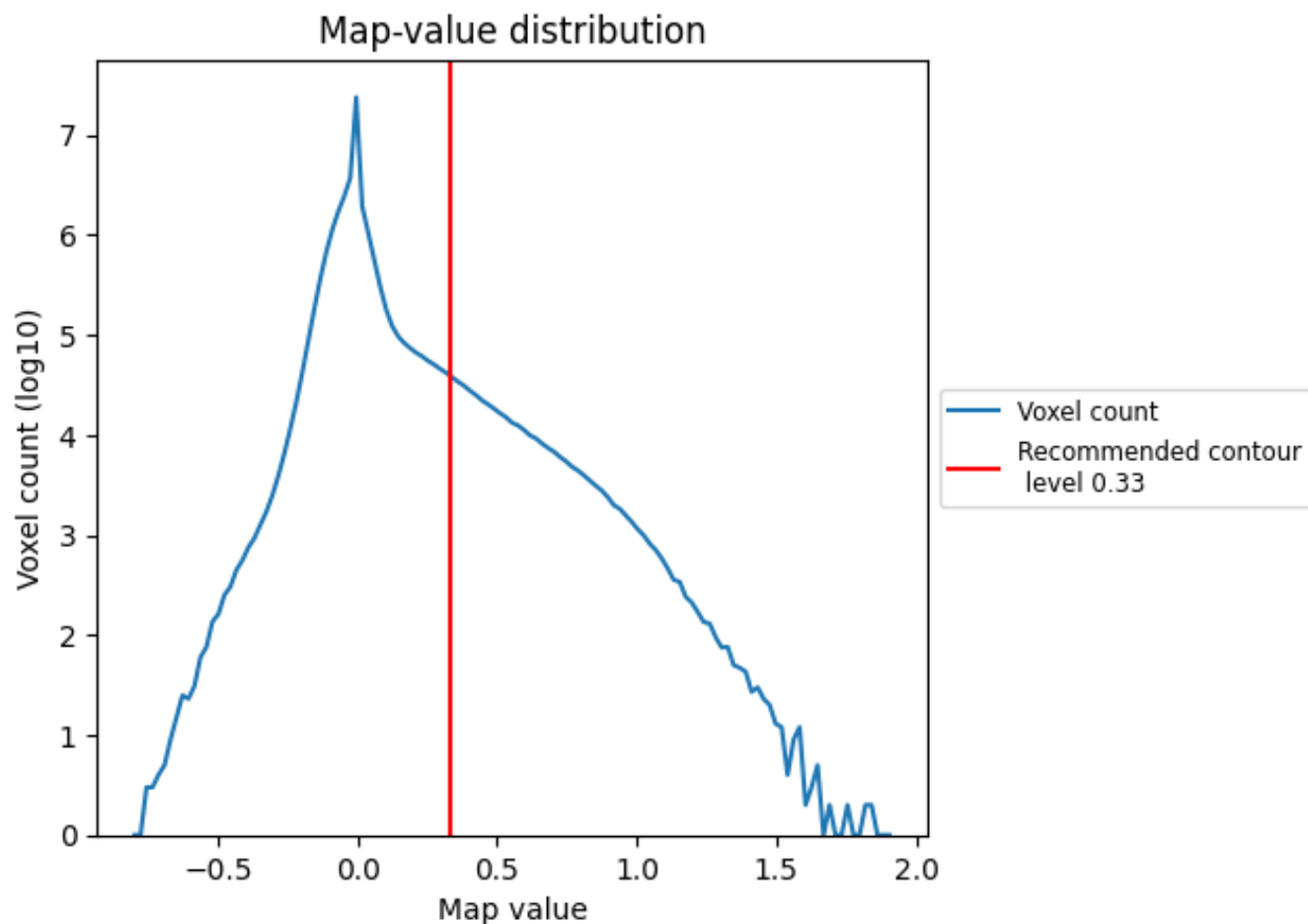


Z

7 Map analysis [i](#)

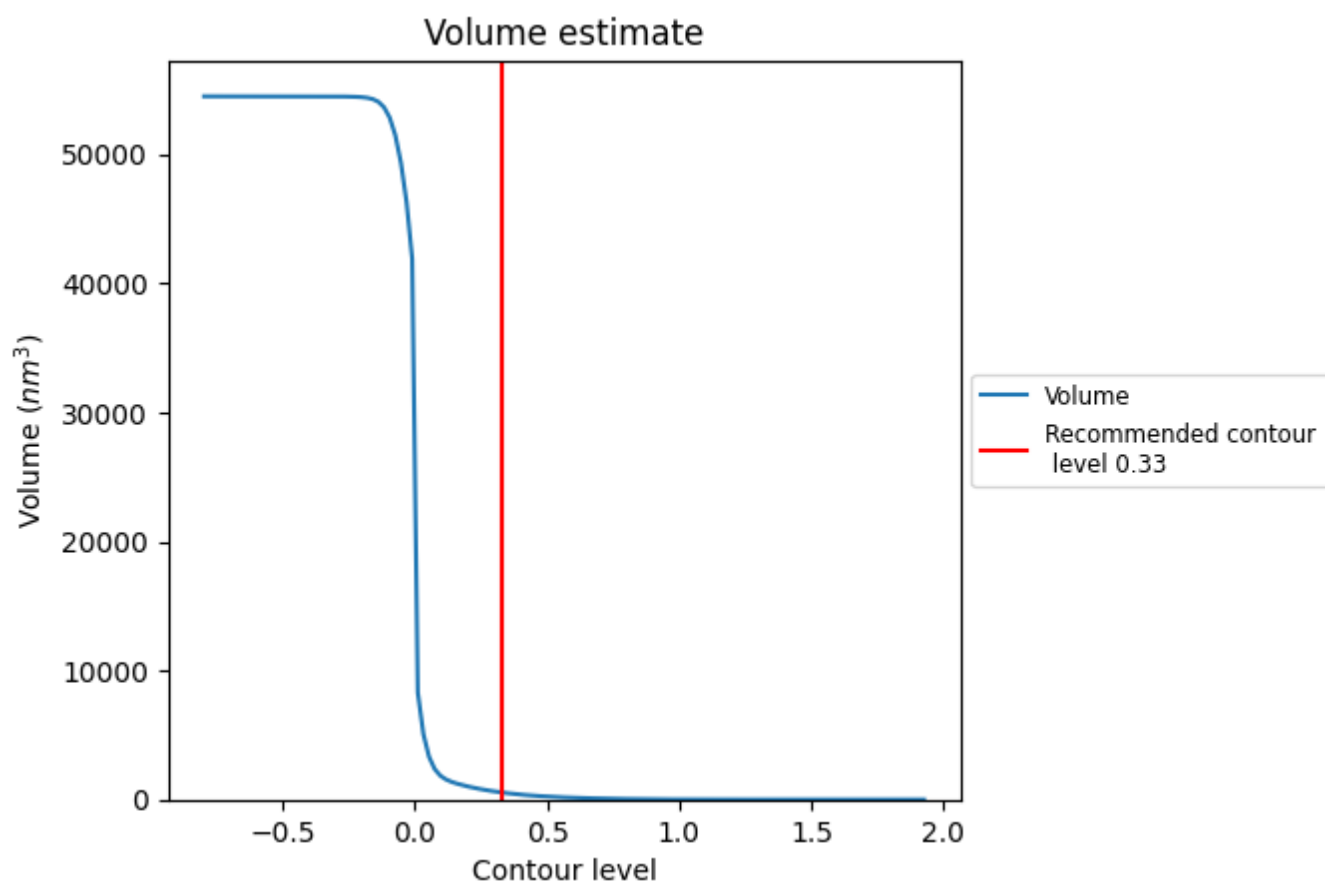
This section contains the results of statistical analysis of the map.

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.

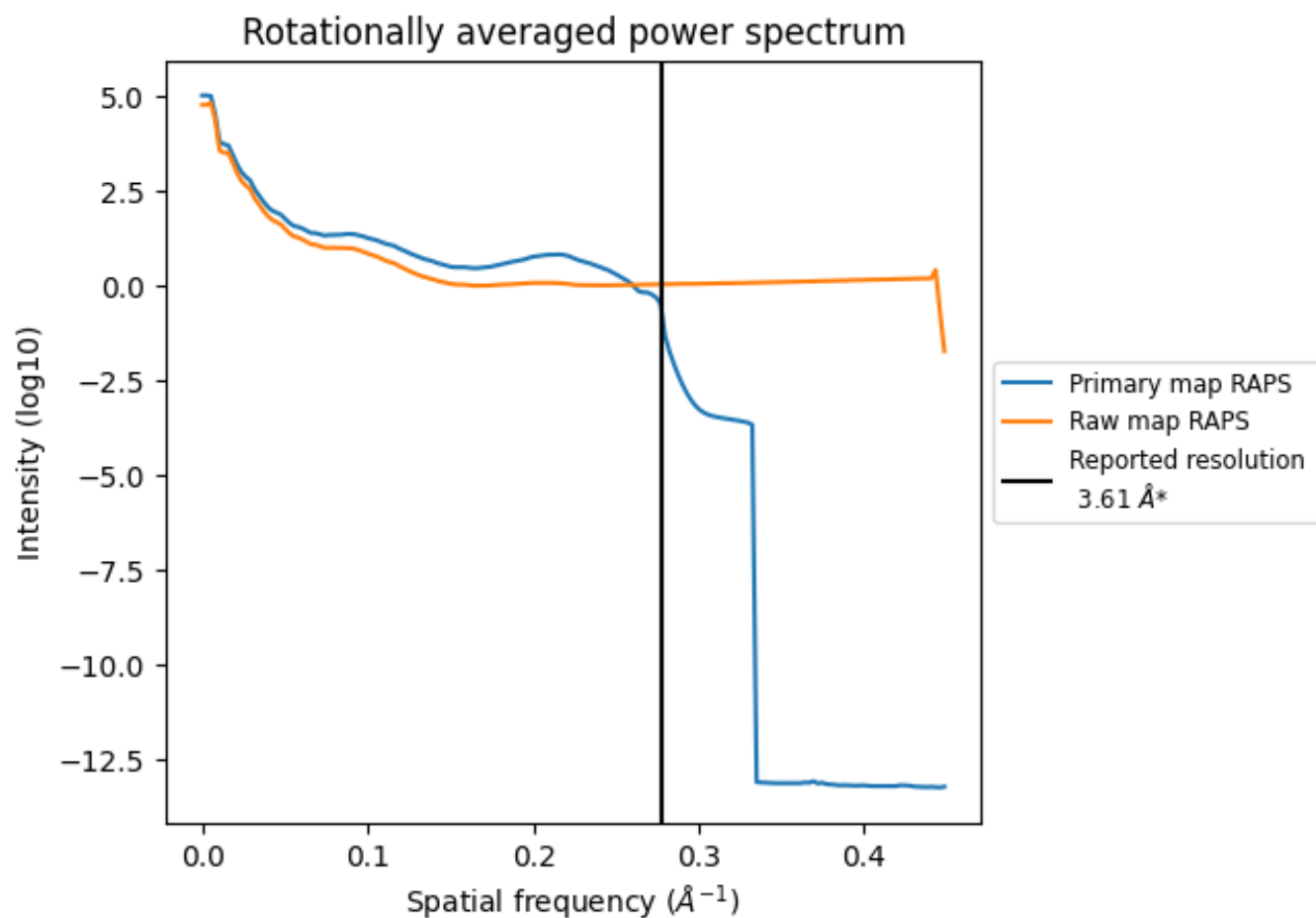
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 547 nm³; this corresponds to an approximate mass of 494 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 ⓘ

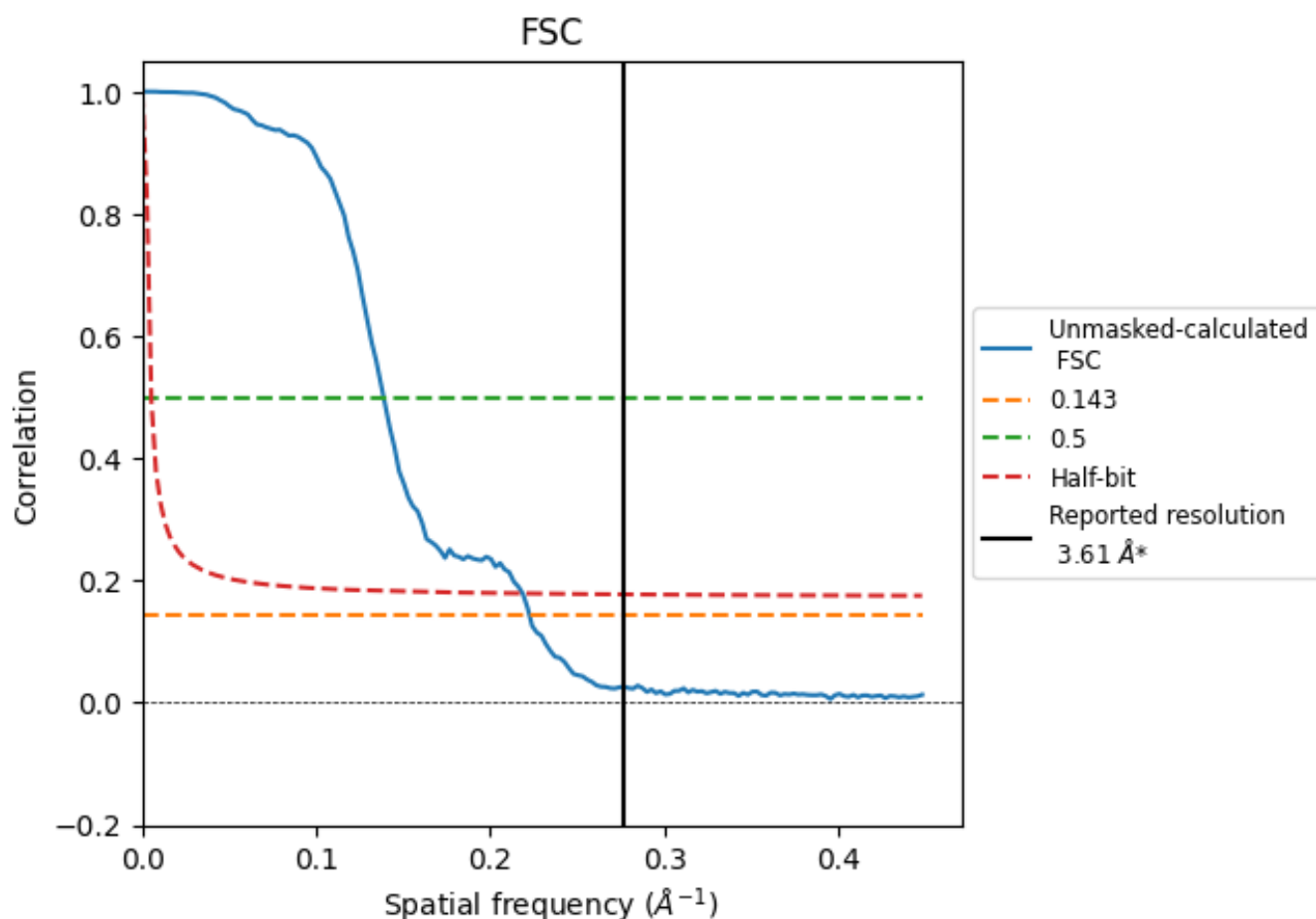


*Reported resolution corresponds to spatial frequency of 0.277 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.277 Å⁻¹

8.2 Resolution estimates [i](#)

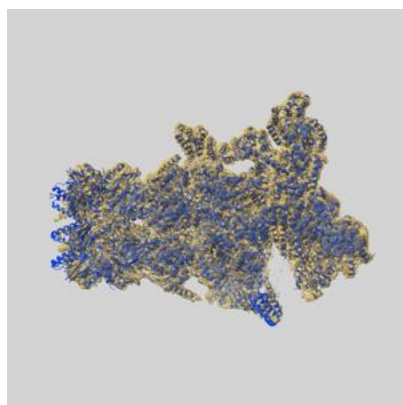
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.61	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.49	7.20	4.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.49 differs from the reported value 3.61 by more than 10 %

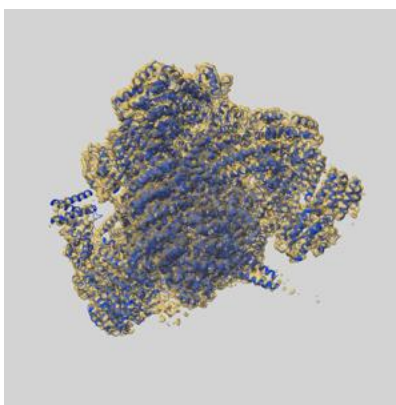
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45579 and PDB model 9CGC. Per-residue inclusion information can be found in section [3](#) on page [12](#).

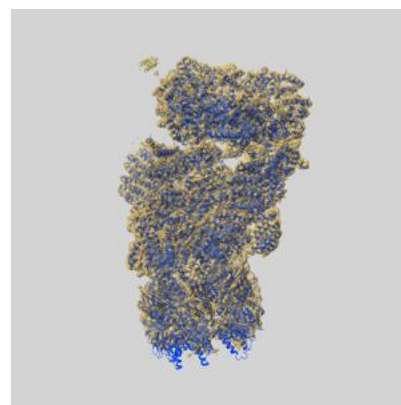
9.1 Map-model overlay [i](#)



X



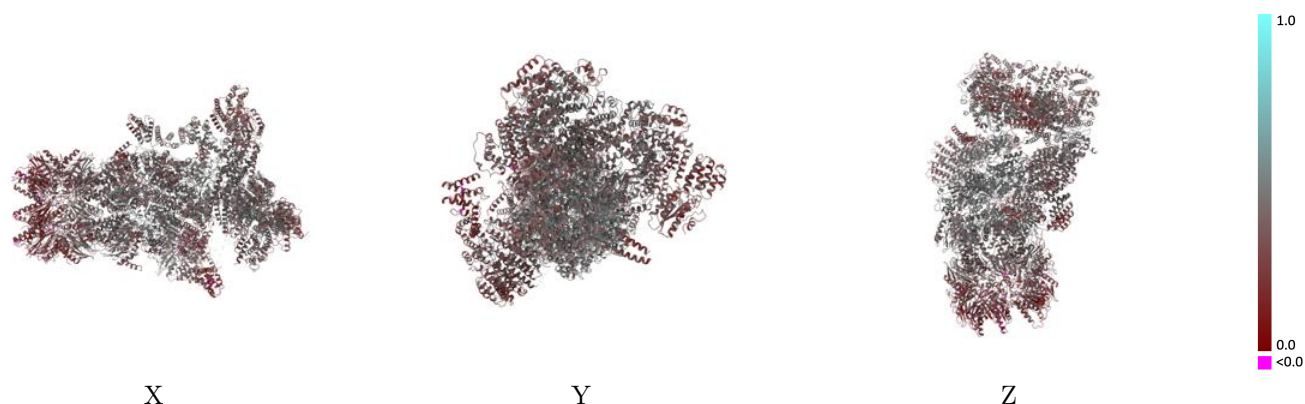
Y



Z

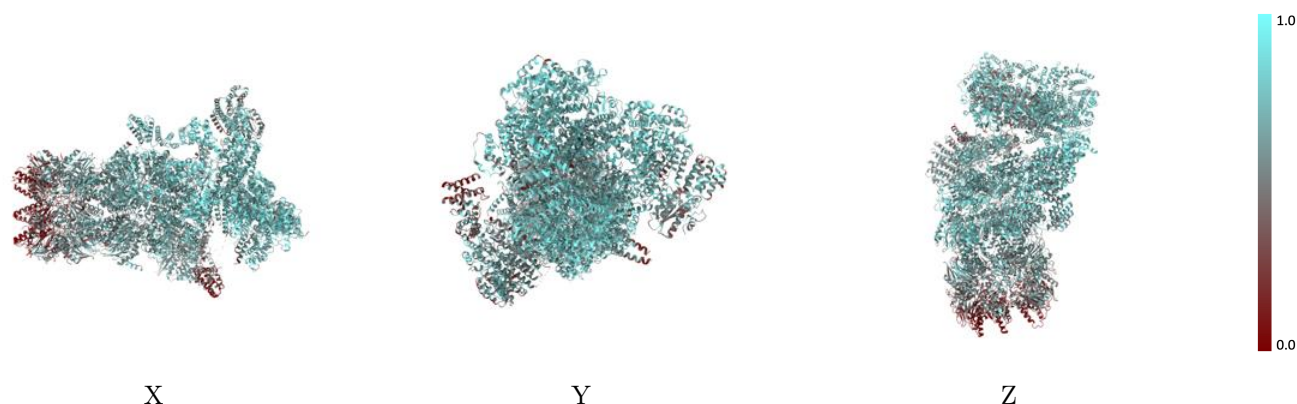
The images above show the 3D surface view of the map at the recommended contour level 0.33 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



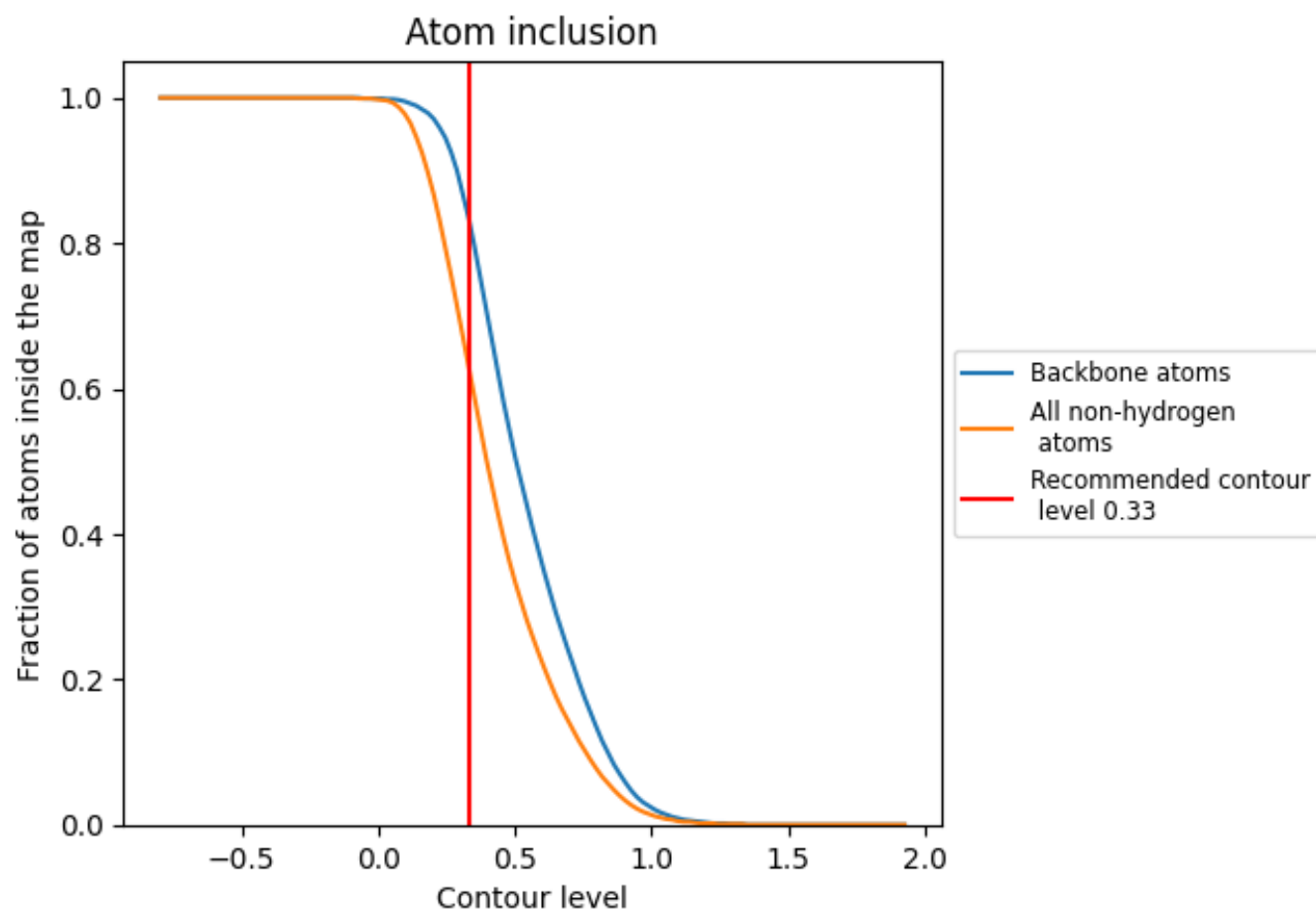
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.33).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 63% 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 (0.33) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6310	 0.3860
1	 0.5810	 0.3460
2	 0.5730	 0.3760
3	 0.5370	 0.3600
4	 0.5320	 0.3400
5	 0.5870	 0.3450
6	 0.5460	 0.3530
7	 0.5670	 0.3600
A	 0.7200	 0.4420
B	 0.6540	 0.4290
C	 0.6240	 0.4010
D	 0.6700	 0.4070
E	 0.6730	 0.4150
F	 0.7210	 0.4440
G	 0.7370	 0.4490
H	 0.7320	 0.4600
I	 0.6590	 0.4290
J	 0.6980	 0.4520
K	 0.7140	 0.4660
L	 0.7360	 0.4620
M	 0.7200	 0.4600
N	 0.7610	 0.4190
O	 0.6520	 0.3500
P	 0.7600	 0.4130
Q	 0.7200	 0.3870
R	 0.7190	 0.3880
S	 0.7450	 0.4140
T	 0.7320	 0.3810
U	 0.7020	 0.4300
V	 0.7380	 0.4550
W	 0.5530	 0.3320
Y	 0.7960	 0.4220
a	 0.3820	 0.2730
b	 0.3350	 0.2400
e	 0.3590	 0.2640



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Chain	Atom inclusion	Q-score
f	 0.3290	 0.2720
g	 0.2470	 0.2470
h	 0.2230	 0.2400
i	 0.2750	 0.2500
o	 0.5520	 0.3300