



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 02:34 PM EST

PDB ID : 7TAU
EMDB ID : EMD-25786
Title : Refined capsid structure of human adenovirus D26 at 3.4 Å resolution
Authors : Reddy, V.S.; Yu, X.; Barry, M.A.
Deposited on : 2021-12-21
Resolution : 3.38 Å (reported)
Based on initial model : 5TX1

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

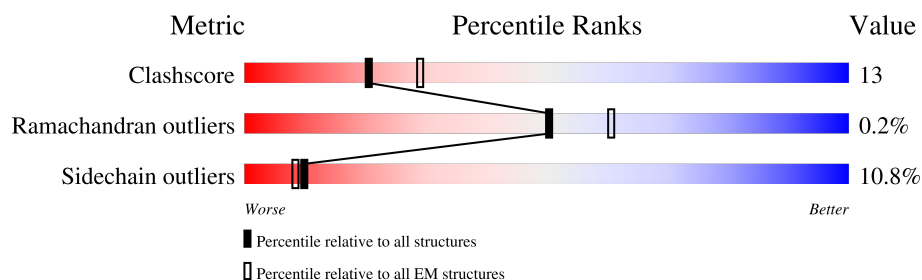
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.38 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	952	<div> <div>29%</div> <div>66%</div> <div>29%</div> <div>.</div> </div>
1	B	952	<div> <div>23%</div> <div>61%</div> <div>32%</div> <div>6%</div> </div>
1	C	952	<div> <div>22%</div> <div>65%</div> <div>30%</div> <div>.</div> </div>
1	D	952	<div> <div>30%</div> <div>66%</div> <div>29%</div> <div>.</div> </div>
1	E	952	<div> <div>28%</div> <div>66%</div> <div>30%</div> <div>.</div> </div>
1	F	952	<div> <div>26%</div> <div>64%</div> <div>32%</div> <div>.</div> </div>
1	G	952	<div> <div>31%</div> <div>65%</div> <div>29%</div> <div>5%</div> </div>
1	H	952	<div> <div>28%</div> <div>62%</div> <div>32%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	952	
1	J	952	
1	K	952	
1	L	952	
2	N	519	
3	O	374	
4	M	560	
5	P	134	
5	Q	134	
5	R	134	
5	S	134	
6	U	227	
6	V	227	
7	1	234	
7	2	234	
7	3	234	
7	4	234	
7	5	234	
7	6	234	
7	7	234	
7	8	234	
7	9	234	
8	X	15	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 105672 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 Hexon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	951	Total	C	N	O	S	0	0
			7551	4796	1276	1444	35		
1	B	949	Total	C	N	O	S	0	0
			7536	4787	1274	1441	34		
1	C	946	Total	C	N	O	S	0	0
			7519	4777	1271	1437	34		
1	D	947	Total	C	N	O	S	0	0
			7526	4780	1272	1440	34		
1	E	947	Total	C	N	O	S	0	0
			7526	4780	1272	1440	34		
1	F	949	Total	C	N	O	S	0	0
			7539	4789	1274	1441	35		
1	G	947	Total	C	N	O	S	0	0
			7526	4780	1272	1440	34		
1	H	947	Total	C	N	O	S	0	0
			7526	4780	1272	1440	34		
1	I	949	Total	C	N	O	S	0	0
			7536	4787	1274	1441	34		
1	J	951	Total	C	N	O	S	0	0
			7551	4795	1276	1446	34		
1	K	950	Total	C	N	O	S	0	0
			7546	4792	1275	1445	34		
1	L	947	Total	C	N	O	S	0	0
			7524	4780	1272	1438	34		

- Molecule 2 is a protein called Penton protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	471	Total	C	N	O	S	0	0
			3786	2404	640	728	14		

- Molecule 3 is a protein called Fiber.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	17	Total	C	N	O	0	0
			147	96	24	27		

- Molecule 4 is a protein called Pre-hexon-linking protein IIIa.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	362	Total	C	N	O	S	0	0
			2829	1771	508	541	9		

- Molecule 5 is a protein called PIX.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	122	Total	C	N	O	S	0	0
			889	547	157	181	4		
5	Q	114	Total	C	N	O	S	0	0
			821	508	143	166	4		
5	R	133	Total	C	N	O	S	0	0
			957	587	168	198	4		
5	S	122	Total	C	N	O	S	0	0
			887	545	157	182	3		

- Molecule 6 is a protein called PVIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	190	Total	C	N	O	S	0	0
			1462	919	252	285	6		
6	V	188	Total	C	N	O	S	0	0
			1449	911	250	282	6		

- Molecule 7 is a protein called Pre-protein VI.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1	30	Total	C	N	O	S	0	0
			236	147	43	45	1		
7	2	26	Total	C	N	O	S	0	0
			203	128	38	36	1		
7	3	27	Total	C	N	O	S	0	0
			211	132	40	38	1		
7	4	29	Total	C	N	O	S	0	0
			227	142	42	42	1		
7	5	28	Total	C	N	O	S	0	0
			219	138	41	39	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	27	Total	C	N	O	S	0	0
			211	132	40	38	1		
7	7	27	Total	C	N	O	S	0	0
			211	132	40	38	1		
7	8	29	Total	C	N	O	S	0	0
			227	142	42	42	1		
7	9	28	Total	C	N	O	S	0	0
			219	138	41	39	1		

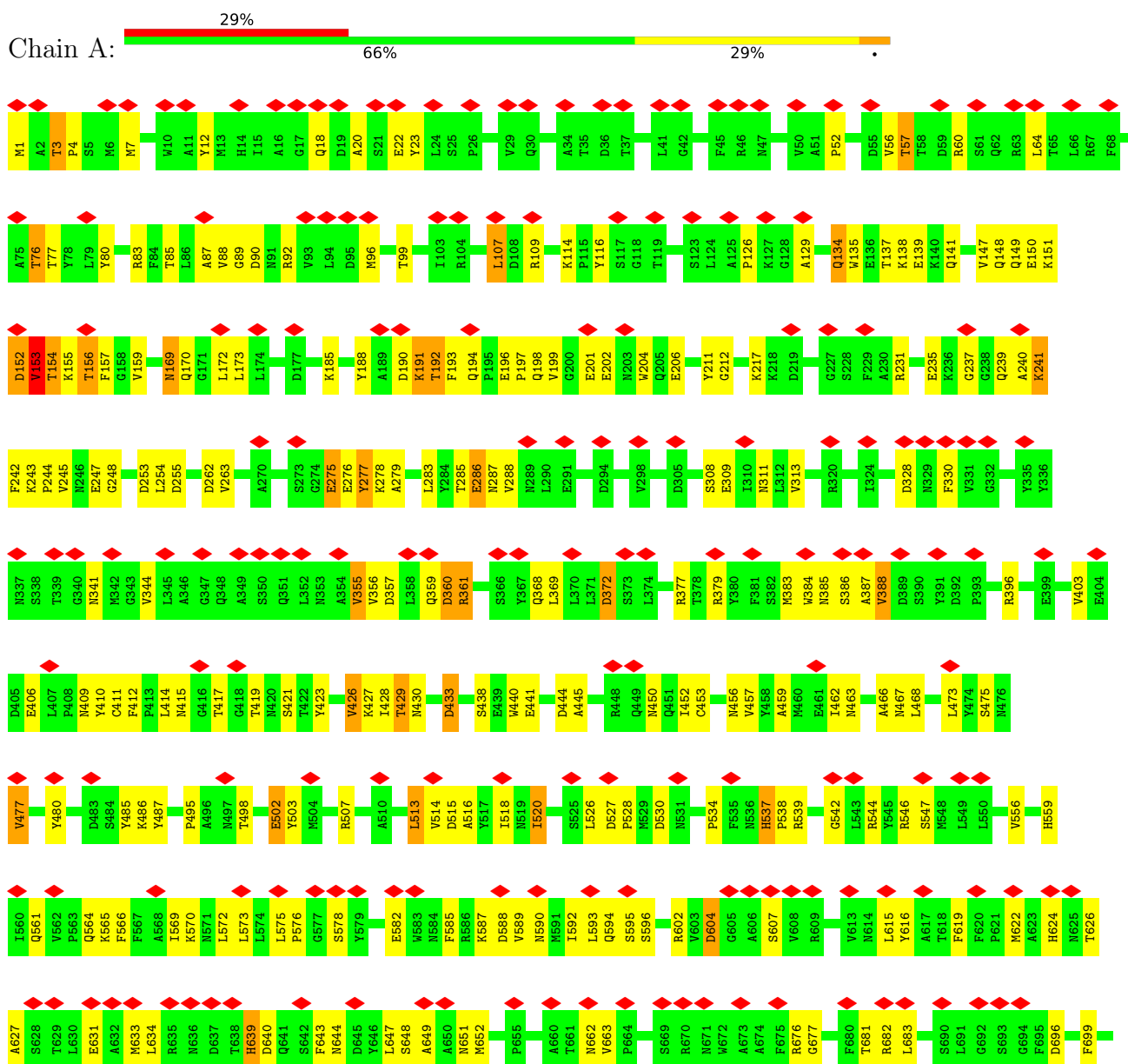
- Molecule 8 is a protein called Unknown fragment.

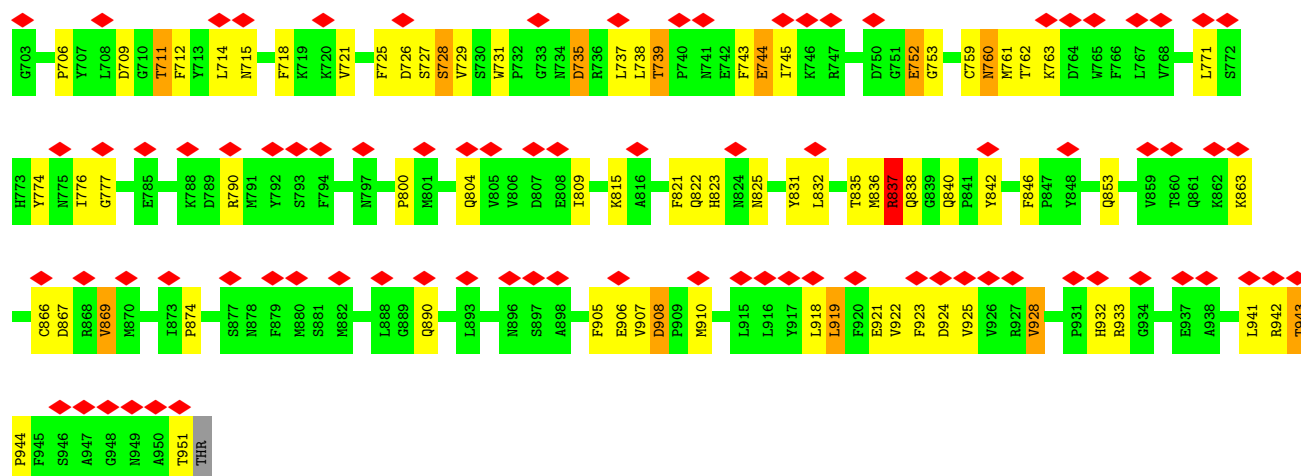
Mol	Chain	Residues	Atoms				AltConf	Trace
8	X	15	Total	C	N	O	0	0
			75	45	15	15		

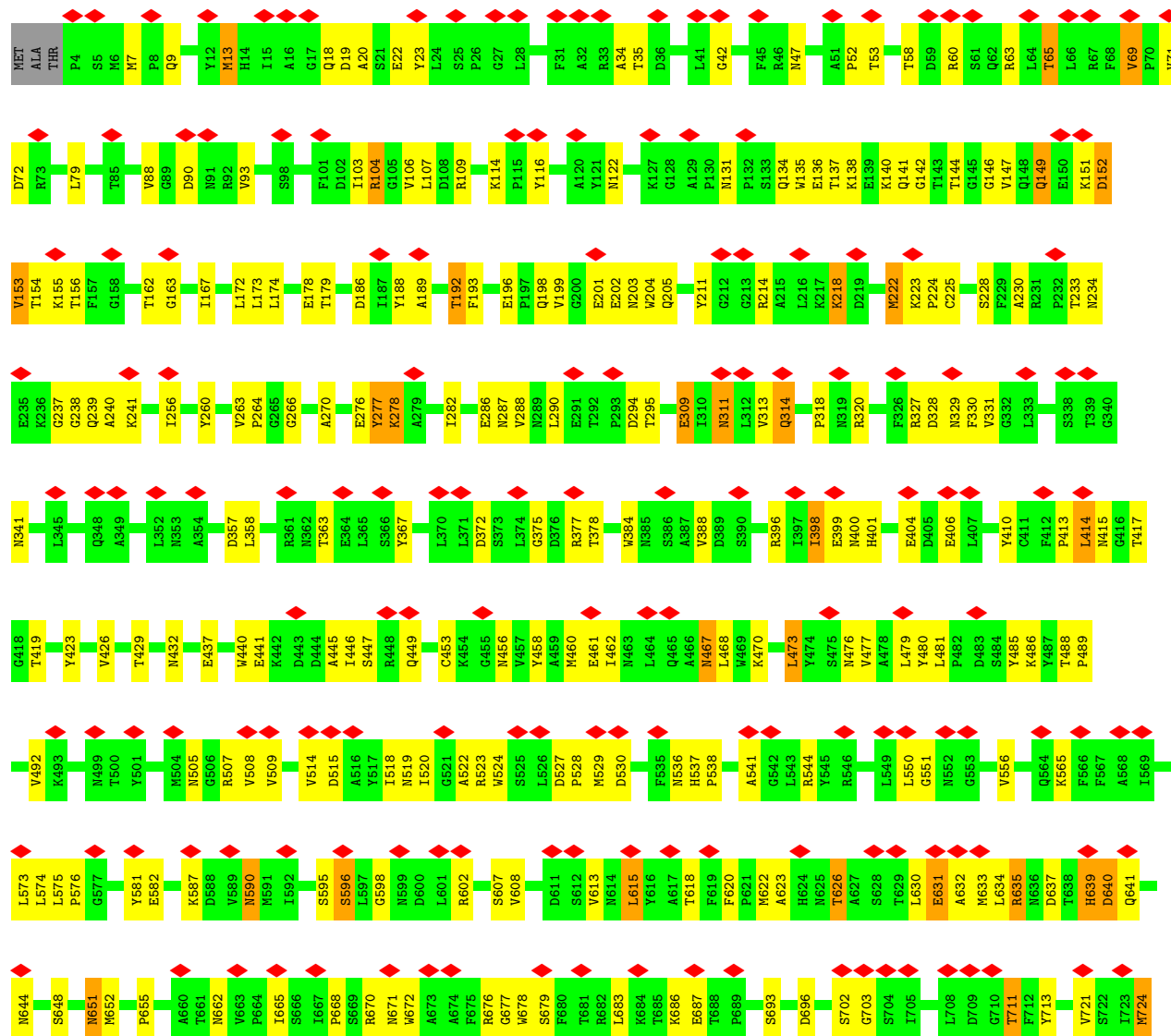
3 Residue-property plots [i](#)

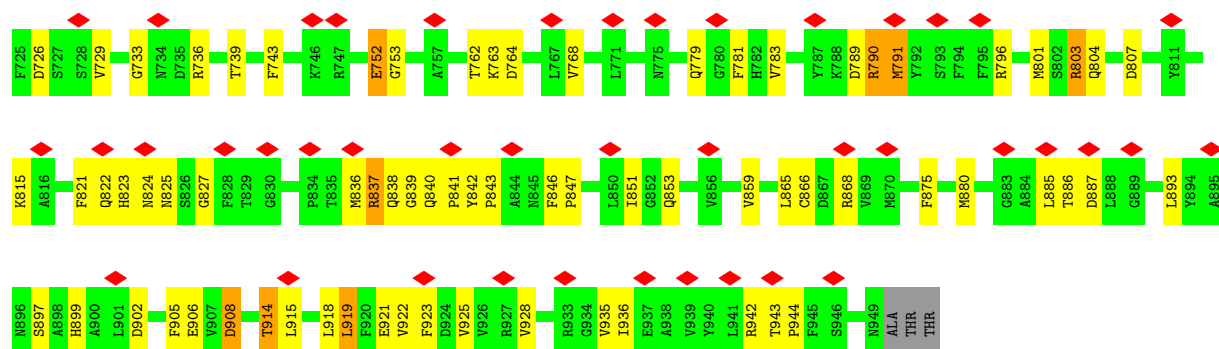
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Hexon protein

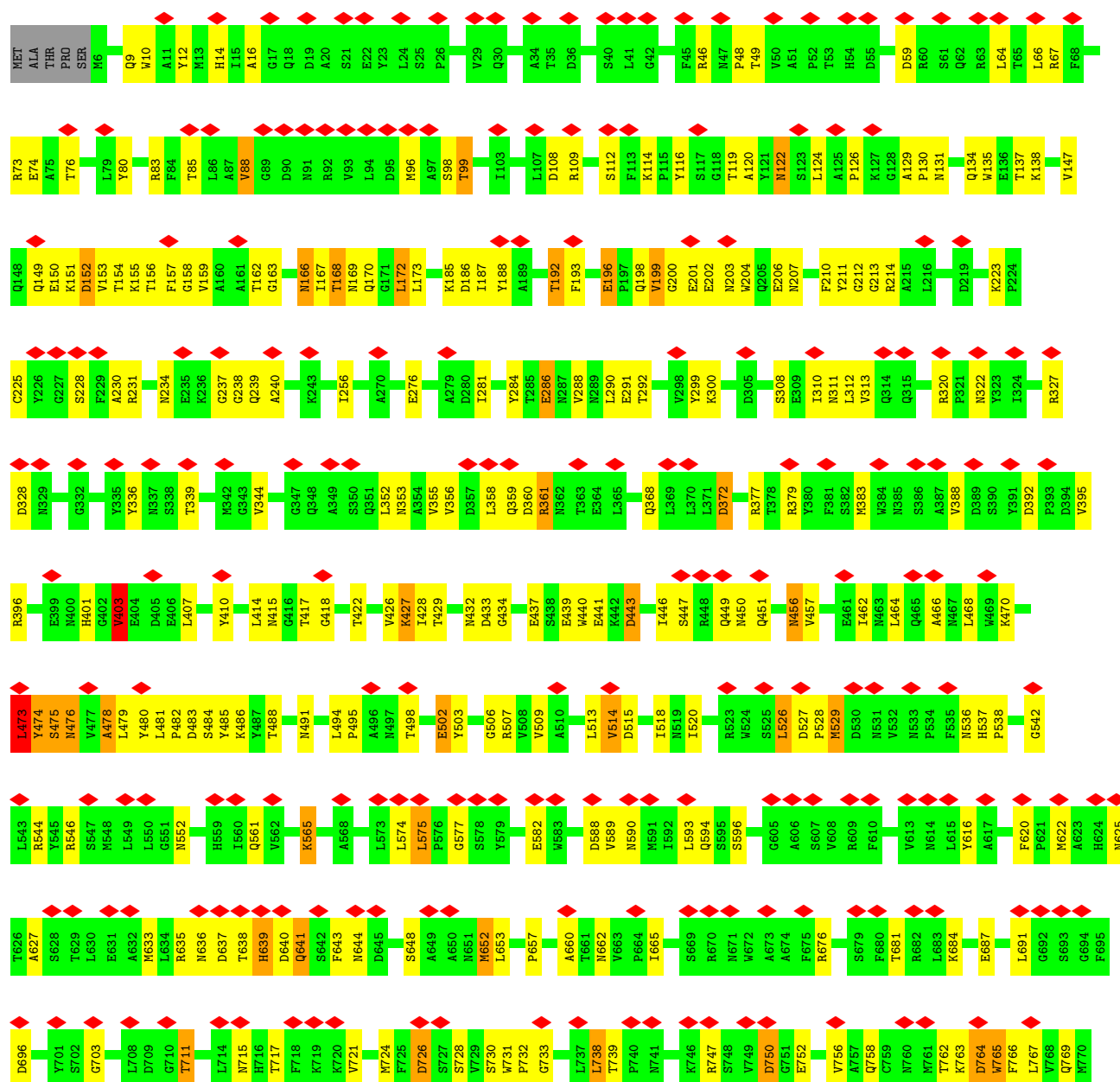


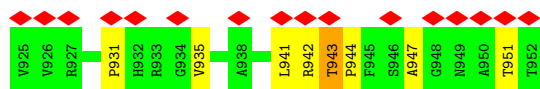
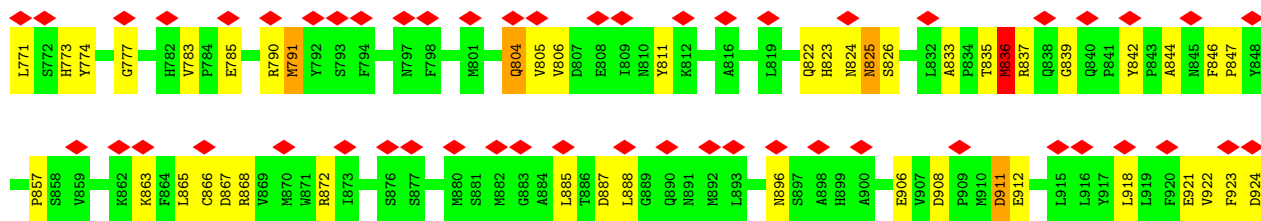




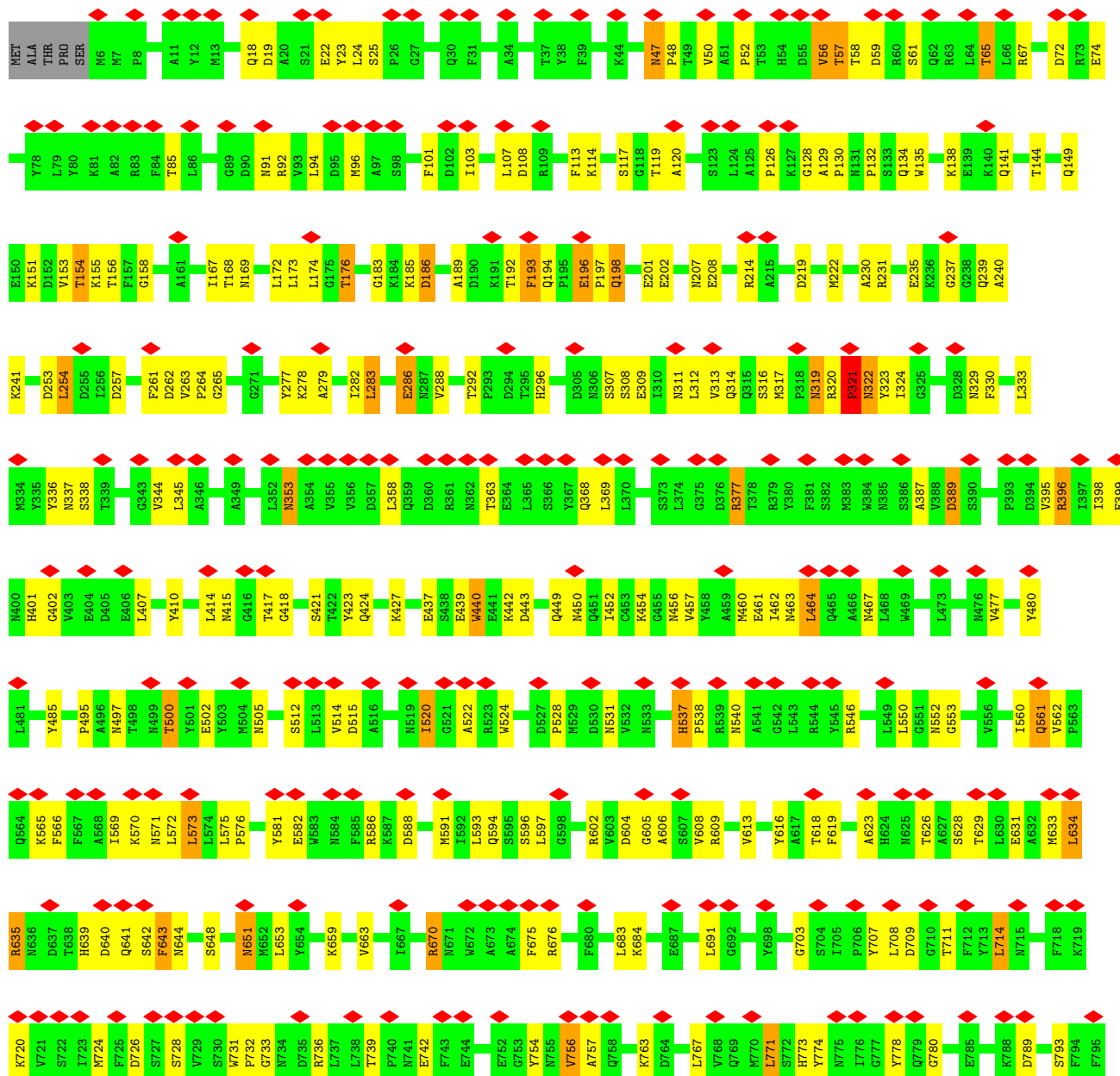


• Molecule 1: Hexon protein



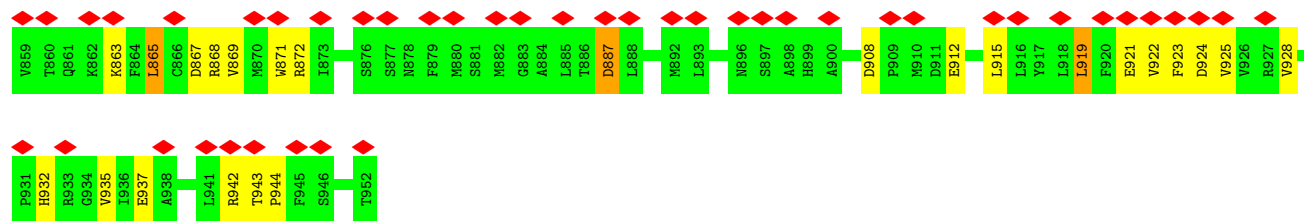


• Molecule 1: Hexon protein

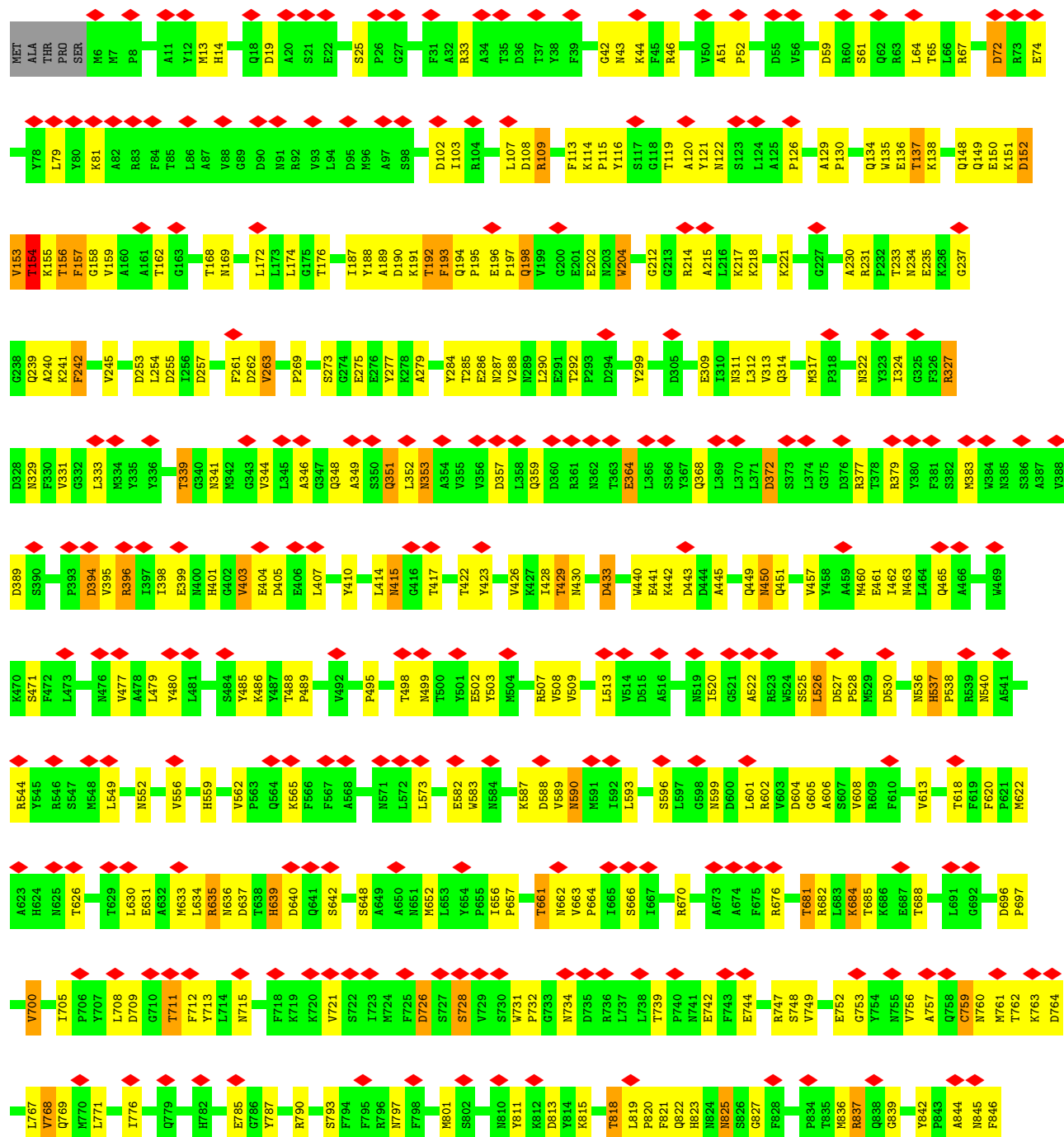


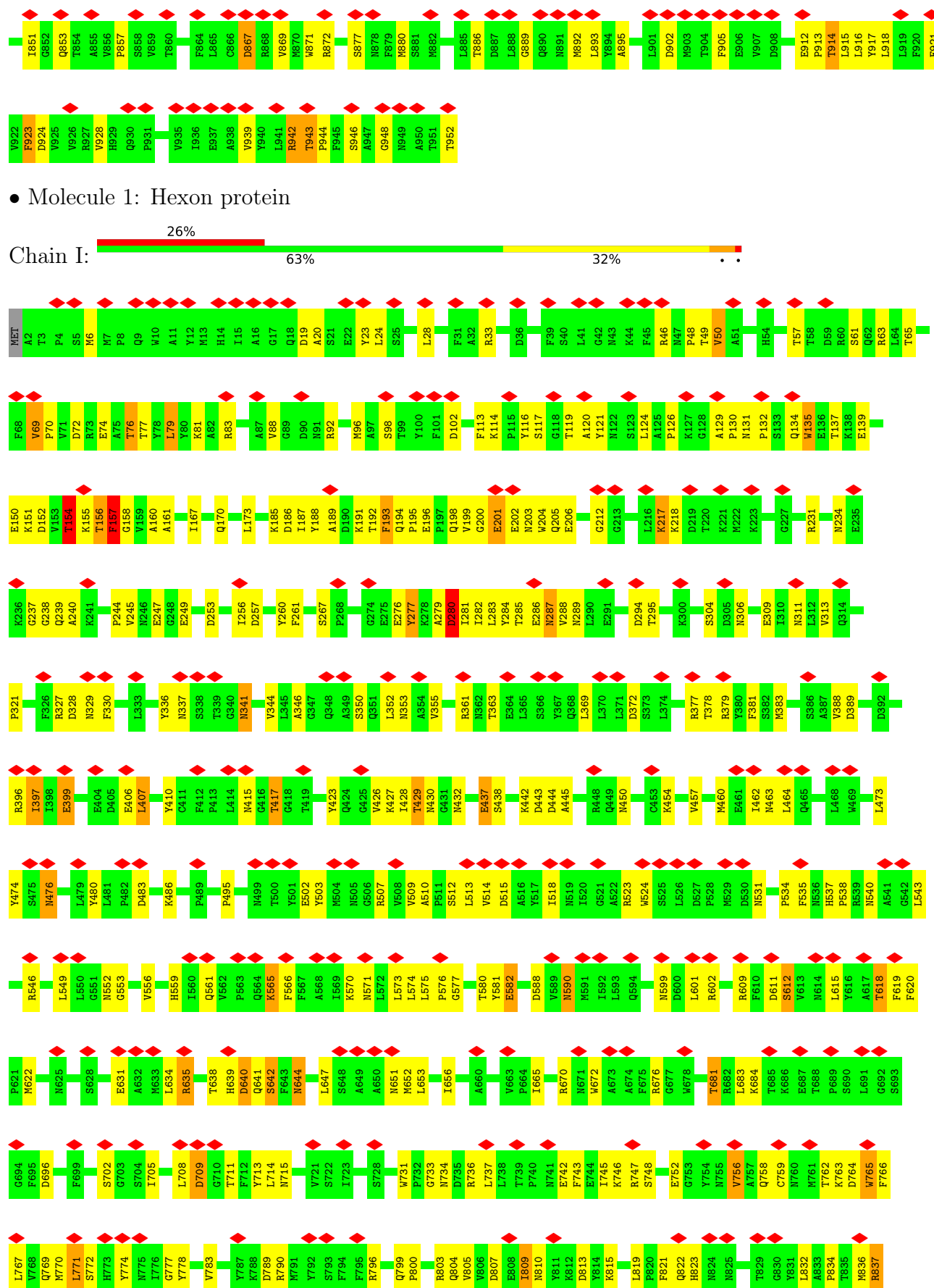


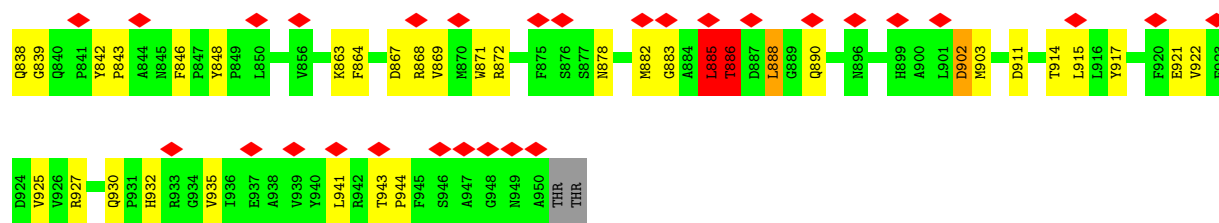




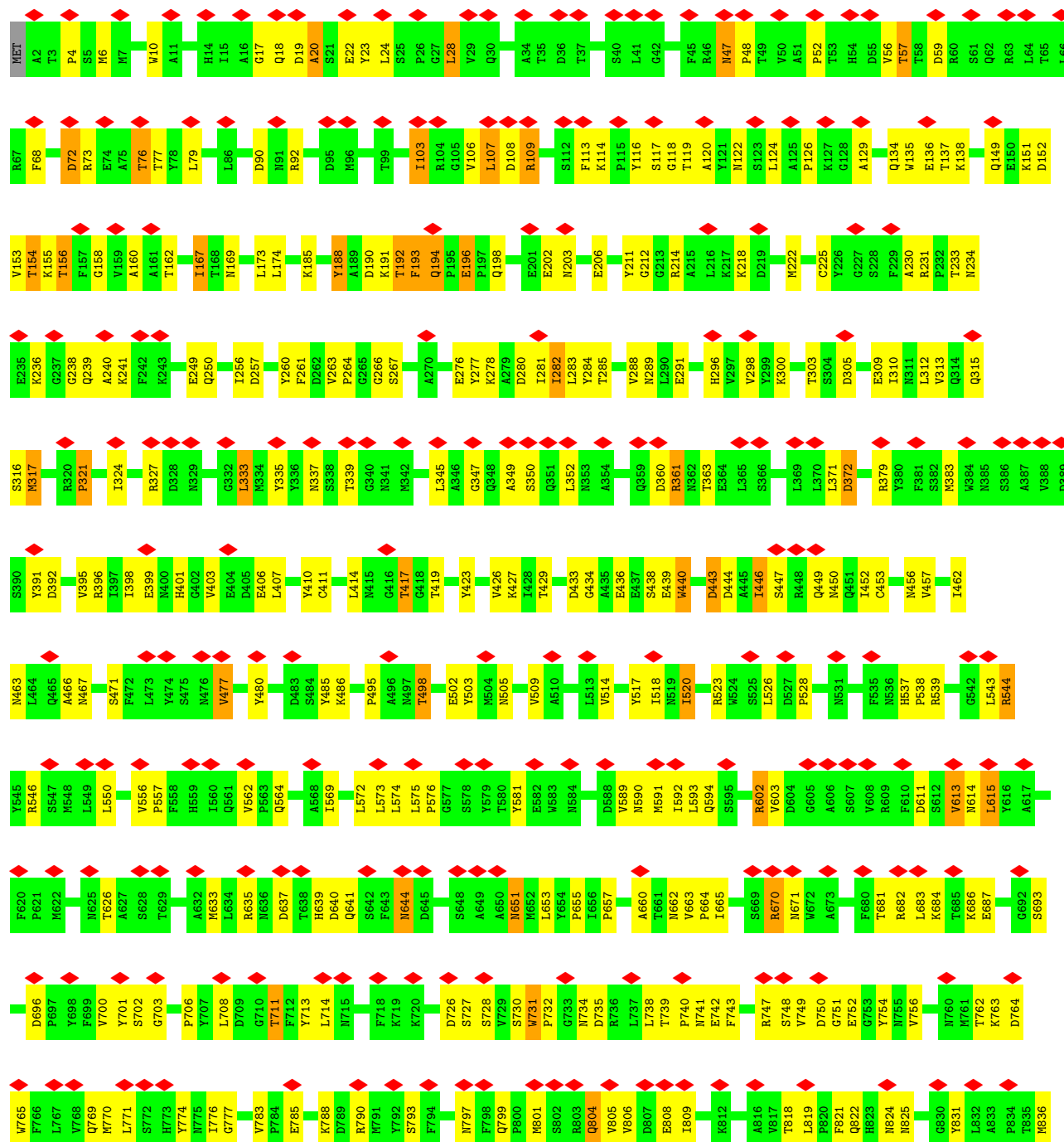
• Molecule 1: Hexon protein

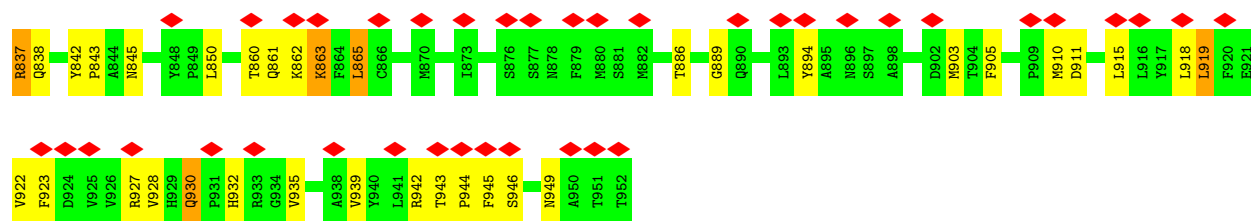




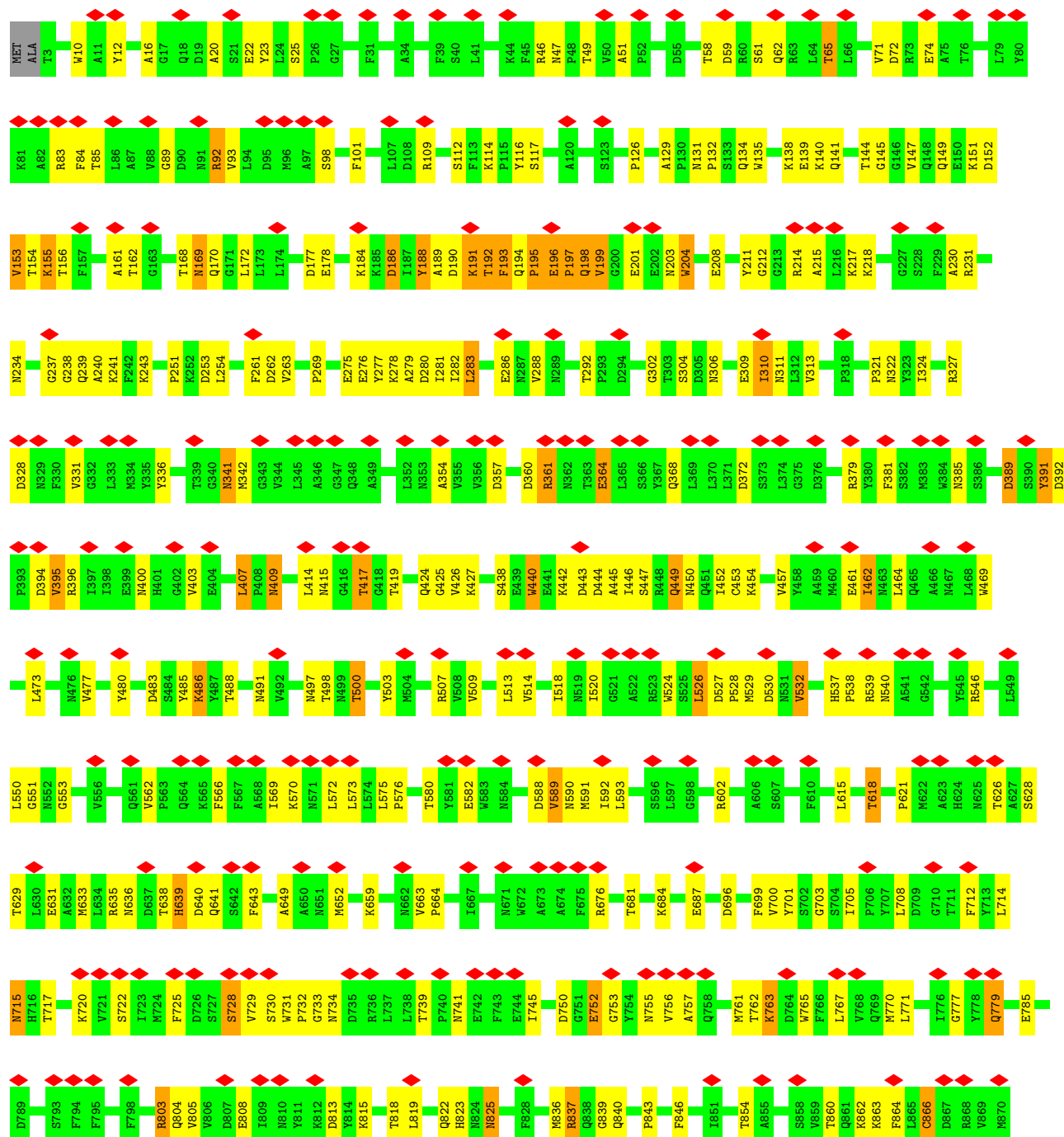


• Molecule 1: Hexon protein



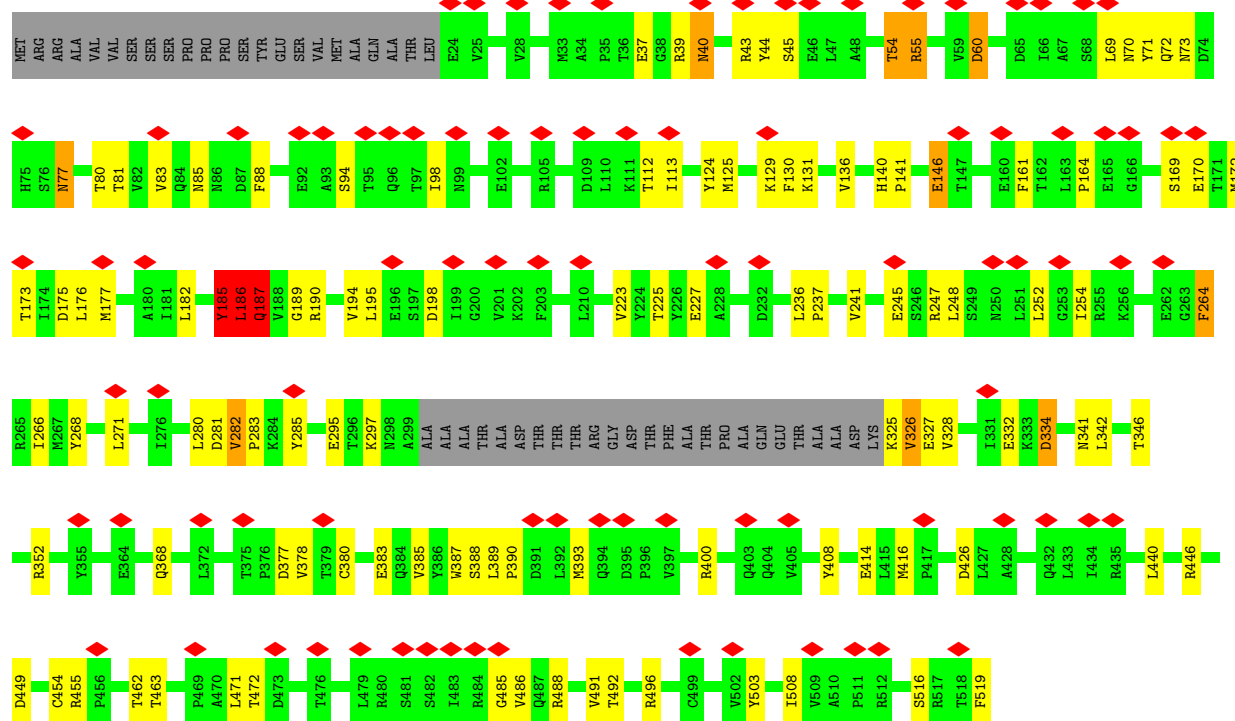


• Molecule 1: Hexon protein

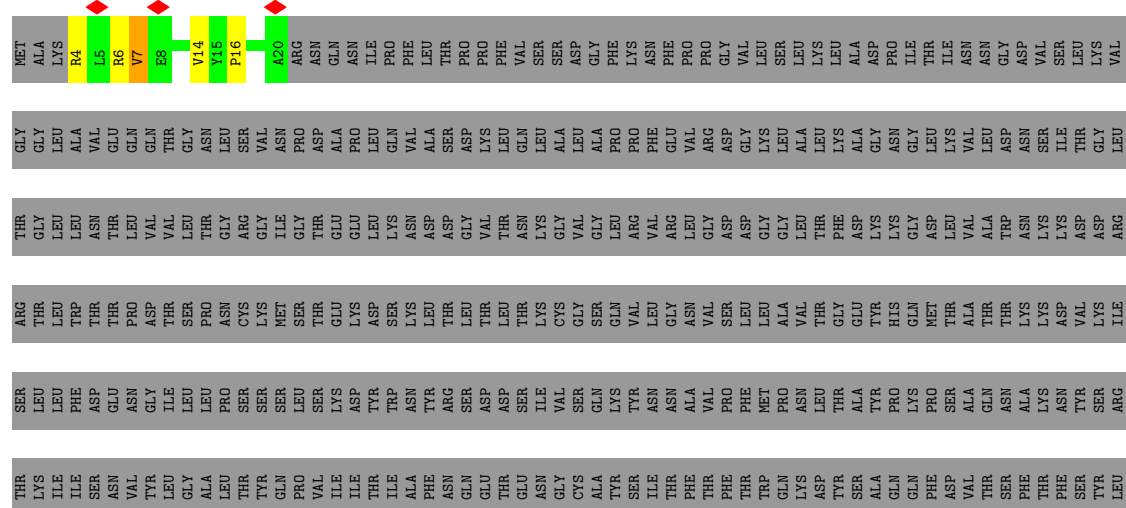


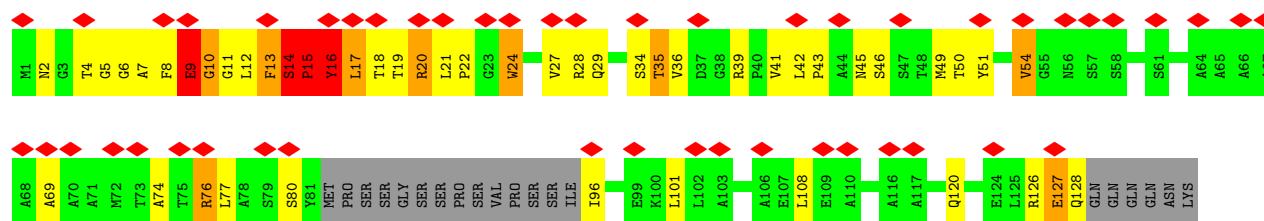


• Molecule 2: Penton protein

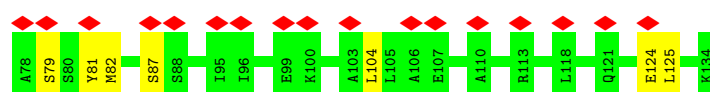
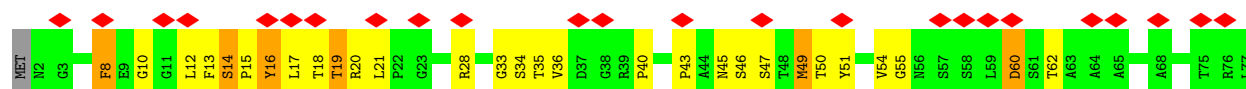


• Molecule 3: Fiber

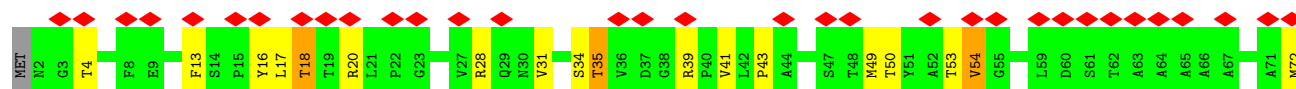




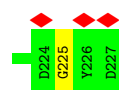
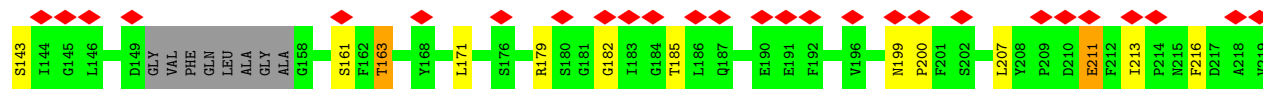
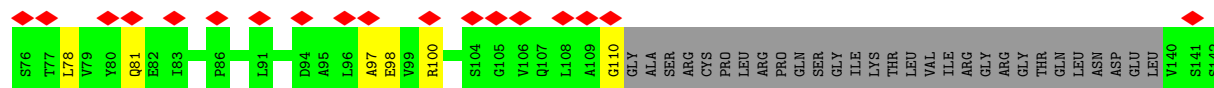
• Molecule 5: PIX



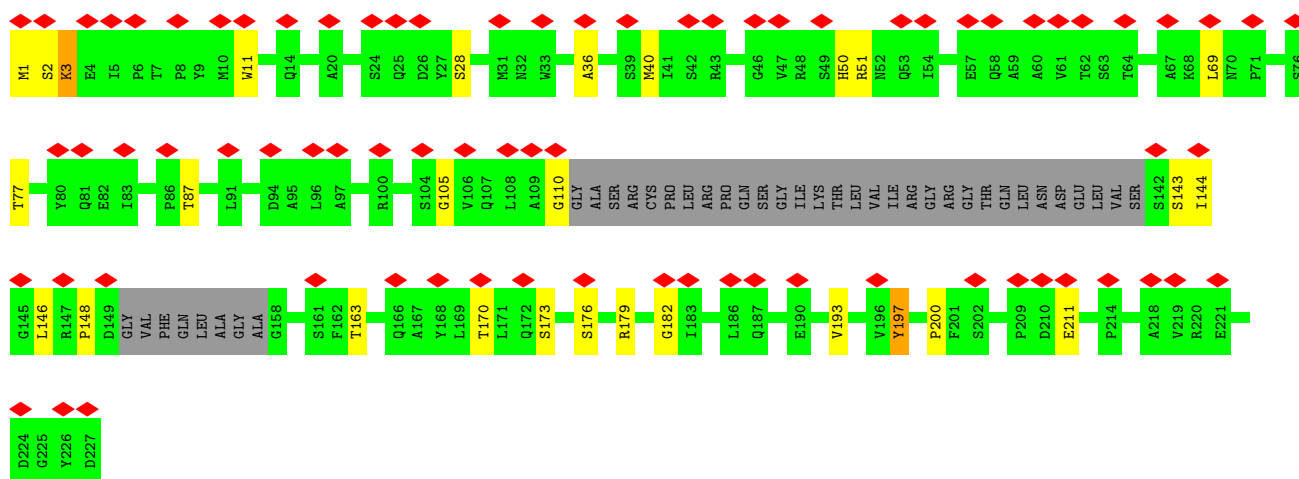
• Molecule 5: PIX



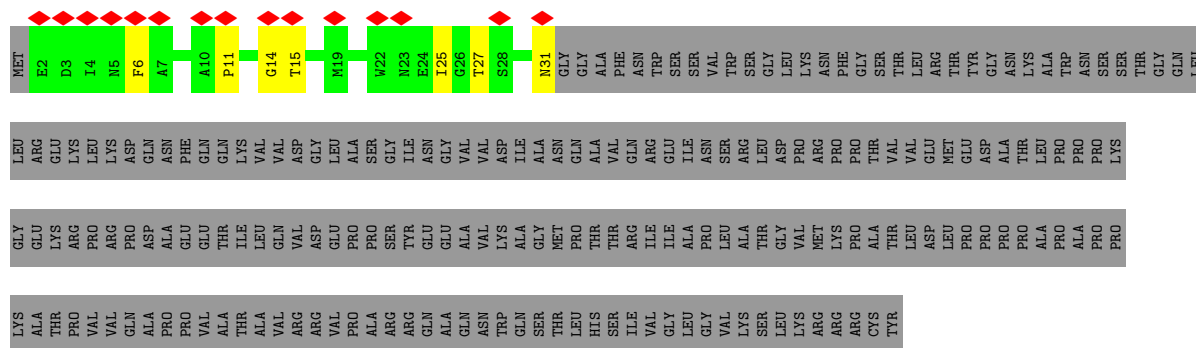
• Molecule 6: PVIII



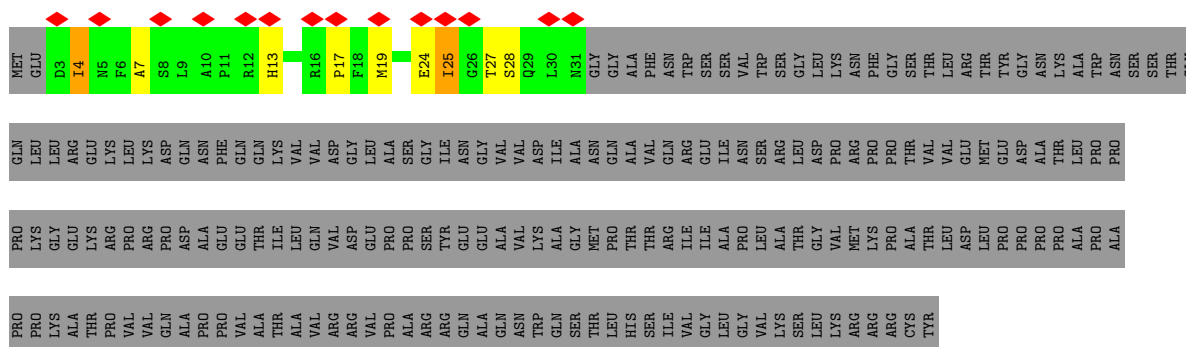
• Molecule 6: PVIII



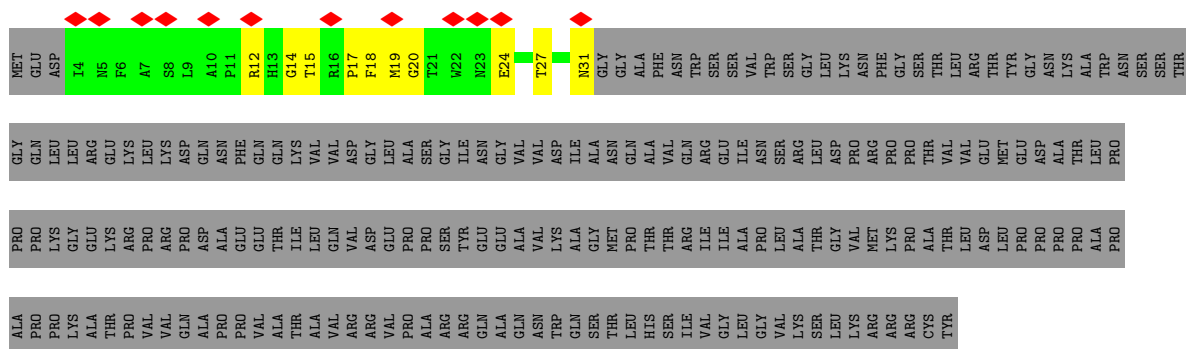
• Molecule 7: Pre-protein VI



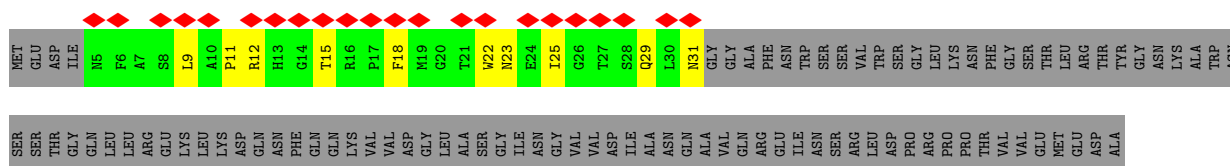
- Molecule 7: Pre-protein VI

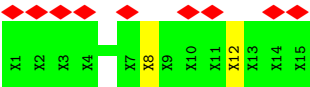
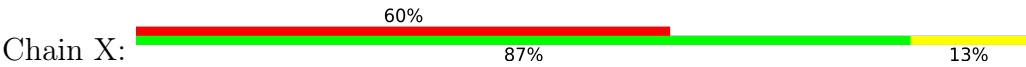


- Molecule 7: Pre-protein VI



- Molecule 7: Pre-protein VI





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	30834	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	54.450	Depositor
Minimum map value	-32.776	Depositor
Average map value	-0.056	Depositor
Map value standard deviation	3.692	Depositor
Recommended contour level	1.8	Depositor
Map size (\AA)	1089.9199, 1089.9199, 1089.9199	wwPDB
Map dimensions	832, 832, 832	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.31, 1.31, 1.31	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.46	0/7758	0.52	3/10554 (0.0%)
1	B	0.52	2/7743 (0.0%)	0.56	5/10534 (0.0%)
1	C	0.46	4/7726 (0.1%)	0.51	3/10509 (0.0%)
1	D	0.59	5/7732 (0.1%)	0.57	4/10517 (0.0%)
1	E	0.51	1/7732 (0.0%)	0.54	3/10517 (0.0%)
1	F	0.57	1/7746 (0.0%)	0.57	4/10537 (0.0%)
1	G	0.51	4/7732 (0.1%)	0.53	3/10517 (0.0%)
1	H	0.59	1/7732 (0.0%)	0.58	4/10517 (0.0%)
1	I	0.67	4/7743 (0.1%)	0.62	8/10534 (0.1%)
1	J	0.53	1/7758 (0.0%)	0.55	1/10554 (0.0%)
1	K	0.63	7/7753 (0.1%)	0.58	5/10547 (0.0%)
1	L	0.58	5/7731 (0.1%)	0.58	6/10516 (0.1%)
2	N	0.62	3/3879 (0.1%)	0.60	2/5280 (0.0%)
3	O	0.61	0/152	0.70	1/207 (0.5%)
4	M	0.63	0/2884	0.61	2/3926 (0.1%)
5	P	1.28	11/898 (1.2%)	1.26	14/1216 (1.2%)
5	Q	1.08	9/830 (1.1%)	1.04	11/1127 (1.0%)
5	R	0.29	0/970	0.45	0/1318
5	S	0.42	0/896	0.61	1/1214 (0.1%)
6	U	0.99	4/1499 (0.3%)	0.75	0/2041
6	V	0.34	0/1486	0.44	0/2023
7	1	0.25	0/242	0.51	0/328
7	2	0.89	0/209	1.38	5/283 (1.8%)
7	3	0.26	0/217	0.44	0/294
7	4	0.78	0/233	0.86	1/316 (0.3%)
7	5	0.25	0/225	0.47	0/305
7	6	0.64	0/217	0.73	0/294
7	7	0.27	0/217	0.44	0/294
7	8	0.61	0/233	0.89	2/316 (0.6%)
7	9	0.26	0/225	0.42	0/305
All	All	0.58	62/108398 (0.1%)	0.58	88/147440 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	3
1	K	0	1
1	L	0	1
2	N	0	3
4	M	0	1
All	All	0	9

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	15	PRO	CA-C	-9.18	1.34	1.52
5	P	17	LEU	CA-C	-7.49	1.33	1.52
5	Q	17	LEU	CA-C	-7.48	1.33	1.52
5	Q	15	PRO	CA-C	-7.08	1.38	1.52
6	U	12	SER	CA-CB	-7.03	1.42	1.52
5	P	16	TYR	N-CA	-6.97	1.32	1.46
1	K	193	PHE	CB-CG	-6.94	1.39	1.51
1	K	628	SER	CA-CB	-6.85	1.42	1.52
5	Q	13	PHE	CA-C	-6.62	1.35	1.52
1	I	642	SER	CA-CB	-6.60	1.43	1.52
5	P	36	VAL	N-CA	-6.34	1.33	1.46
5	Q	15	PRO	CA-CB	-6.29	1.41	1.53
1	L	135	TRP	CB-CG	-6.21	1.39	1.50
5	P	34	SER	CA-C	-6.18	1.36	1.52
1	G	702	SER	CA-CB	-6.11	1.43	1.52
1	L	596	SER	CA-CB	-6.10	1.43	1.52
2	N	185	TYR	CA-C	-6.07	1.37	1.52
1	H	154	THR	N-CA	-6.01	1.34	1.46
1	D	826	SER	CA-CB	-5.97	1.44	1.52
1	D	765	TRP	CB-CG	-5.84	1.39	1.50
1	C	595	SER	CA-CB	-5.82	1.44	1.52
1	K	197	PRO	CA-C	-5.79	1.41	1.52
1	K	61	SER	CA-CB	-5.76	1.44	1.52
6	U	24	SER	CA-CB	-5.72	1.44	1.52
1	C	702	SER	CA-CB	-5.63	1.44	1.52
1	G	192	THR	CA-C	-5.63	1.38	1.52
5	Q	24	TRP	CB-CG	-5.62	1.40	1.50
5	P	14	SER	CA-C	-5.59	1.38	1.52
1	B	826	SER	CA-CB	-5.56	1.44	1.52
2	N	187	GLN	C-O	5.55	1.33	1.23
5	Q	9	GLU	CA-C	-5.54	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	944	PRO	CA-CB	-5.51	1.42	1.53
1	K	631	GLU	CA-C	-5.43	1.38	1.52
2	N	185	TYR	C-O	-5.42	1.13	1.23
1	I	154	THR	N-CA	-5.42	1.35	1.46
1	I	765	TRP	CB-CG	-5.41	1.40	1.50
5	P	22	PRO	CA-CB	-5.39	1.42	1.53
1	B	240	ALA	N-CA	-5.36	1.35	1.46
5	Q	13	PHE	CA-CB	-5.35	1.42	1.53
1	G	459	ALA	CA-CB	-5.34	1.41	1.52
5	P	14	SER	C-N	-5.33	1.24	1.34
1	K	193	PHE	CA-CB	-5.33	1.42	1.53
1	C	596	SER	CA-CB	-5.32	1.45	1.52
5	P	15	PRO	N-CA	-5.31	1.38	1.47
1	K	16	ALA	CA-CB	-5.31	1.41	1.52
1	J	316	SER	CA-CB	-5.27	1.45	1.52
5	P	22	PRO	CA-C	-5.25	1.42	1.52
1	L	135	TRP	CE3-CZ3	-5.25	1.29	1.38
5	P	42	LEU	CA-C	-5.24	1.39	1.52
1	L	154	THR	N-CA	-5.24	1.35	1.46
1	E	316	SER	CA-CB	-5.18	1.45	1.52
1	D	473	LEU	C-O	-5.17	1.13	1.23
1	D	769	GLN	CA-CB	-5.14	1.42	1.53
1	I	157	PHE	CA-C	-5.12	1.39	1.52
6	U	20	ALA	CA-CB	-5.11	1.41	1.52
5	Q	14	SER	C-N	-5.10	1.24	1.34
1	F	763	LYS	CA-C	-5.09	1.39	1.52
5	Q	13	PHE	N-CA	-5.07	1.36	1.46
6	U	42	SER	CA-CB	-5.04	1.45	1.52
1	G	193	PHE	N-CA	-5.02	1.36	1.46
1	C	595	SER	CA-C	-5.01	1.40	1.52
1	D	478	ALA	CA-C	-5.00	1.40	1.52

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	44	ALA	N-CA-C	-17.22	64.52	111.00
7	2	26	GLY	N-CA-C	15.26	151.25	113.10
1	G	193	PHE	N-CA-C	-11.83	79.06	111.00
5	Q	11	GLY	N-CA-C	-10.93	85.77	113.10
5	P	11	GLY	N-CA-C	-9.76	88.70	113.10
5	P	16	TYR	N-CA-C	-9.74	84.71	111.00
1	H	157	PHE	N-CA-C	-9.00	86.69	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	48	THR	N-CA-C	-8.72	87.45	111.00
5	Q	15	PRO	N-CA-C	8.26	133.59	112.10
4	M	395	TYR	O-C-N	-8.11	109.73	122.70
1	I	280	ASP	N-CA-C	7.76	131.94	111.00
4	M	395	TYR	CA-C-O	7.59	136.04	120.10
1	F	203	ASN	CB-CA-C	-7.47	95.45	110.40
1	G	194	GLN	N-CA-C	-7.36	91.12	111.00
7	8	28	SER	N-CA-C	7.32	130.76	111.00
1	A	241	LYS	N-CA-C	-7.22	91.50	111.00
1	B	455	GLY	N-CA-C	7.08	130.81	113.10
1	C	703	GLY	N-CA-C	-6.99	95.62	113.10
1	B	436	GLU	N-CA-C	-6.93	92.28	111.00
1	B	696	ASP	N-CA-C	-6.93	92.30	111.00
1	D	823	HIS	N-CA-C	6.92	129.68	111.00
5	P	34	SER	CB-CA-C	-6.85	97.08	110.10
1	I	615	LEU	CA-CB-CG	6.83	131.01	115.30
1	B	692	GLY	N-CA-C	-6.73	96.27	113.10
1	I	46	ARG	CB-CA-C	-6.70	96.99	110.40
1	I	156	THR	N-CA-C	6.48	128.48	111.00
5	P	17	LEU	CB-CA-C	-6.40	98.04	110.20
5	Q	19	THR	N-CA-C	-6.38	93.77	111.00
1	H	152	ASP	N-CA-C	6.38	128.23	111.00
5	Q	20	ARG	N-CA-C	-6.35	93.86	111.00
7	4	25	ILE	CB-CA-C	-6.31	98.98	111.60
5	P	42	LEU	C-N-CD	6.10	141.21	128.40
1	J	321	PRO	CB-CA-C	-6.09	96.77	112.00
1	H	844	ALA	CB-CA-C	-6.04	101.04	110.10
1	K	915	LEU	CB-CA-C	-6.03	98.75	110.20
1	C	823	HIS	N-CA-C	5.95	127.07	111.00
5	Q	9	GLU	CB-CA-C	-5.93	98.54	110.40
1	F	714	LEU	CA-CB-CG	5.89	128.85	115.30
7	2	27	THR	CB-CA-C	-5.89	95.70	111.60
2	N	44	TYR	N-CA-C	-5.88	95.12	111.00
1	D	478	ALA	C-N-CA	-5.84	107.10	121.70
5	P	17	LEU	N-CA-C	-5.80	95.34	111.00
5	P	46	SER	N-CA-C	5.79	126.62	111.00
5	Q	15	PRO	CB-CA-C	-5.76	97.60	112.00
1	E	321	PRO	CB-CA-C	-5.76	97.61	112.00
2	N	389	LEU	N-CA-C	-5.74	95.50	111.00
1	I	281	ILE	N-CA-C	-5.71	95.59	111.00
1	L	869	VAL	CB-CA-C	-5.70	100.56	111.40
1	L	595	SER	O-C-N	-5.67	113.62	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	837	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	E	316	SER	N-CA-CB	-5.65	102.02	110.50
1	G	192	THR	N-CA-C	-5.65	95.75	111.00
1	K	920	PHE	N-CA-C	-5.64	95.77	111.00
1	L	837	ARG	CB-CA-C	-5.63	99.13	110.40
1	D	403	VAL	CB-CA-C	-5.59	100.78	111.40
7	2	27	THR	N-CA-C	5.58	126.08	111.00
1	I	886	THR	N-CA-C	-5.57	95.97	111.00
1	B	429	THR	N-CA-C	5.53	125.93	111.00
1	K	915	LEU	CA-CB-CG	5.50	127.94	115.30
1	K	192	THR	N-CA-C	-5.48	96.22	111.00
1	C	595	SER	CB-CA-C	-5.47	99.70	110.10
5	Q	17	LEU	CB-CA-C	-5.47	99.81	110.20
3	O	16	PRO	N-CA-C	-5.45	97.92	112.10
5	P	15	PRO	N-CA-C	5.44	126.24	112.10
5	P	14	SER	C-N-CA	-5.40	99.32	122.00
1	L	945	PHE	N-CA-C	-5.38	96.48	111.00
7	8	27	THR	N-CA-C	5.36	125.47	111.00
7	2	9	LEU	C-N-CA	5.36	135.09	121.70
5	P	12	LEU	N-CA-C	5.35	125.44	111.00
5	Q	24	TRP	CA-CB-CG	5.33	123.84	113.70
1	E	286	GLU	CB-CA-C	-5.32	99.75	110.40
5	Q	16	TYR	N-CA-C	-5.28	96.76	111.00
1	A	739	THR	N-CA-C	-5.27	96.78	111.00
1	D	836	MET	CB-CG-SD	-5.25	96.66	112.40
5	Q	9	GLU	N-CA-C	5.24	125.14	111.00
1	I	642	SER	CB-CA-C	-5.21	100.21	110.10
1	F	715	ASN	CB-CA-C	-5.17	100.05	110.40
5	P	18	THR	C-N-CA	-5.17	108.77	121.70
1	L	700	VAL	CB-CA-C	-5.17	101.58	111.40
5	P	20	ARG	N-CA-C	-5.15	97.10	111.00
5	S	74	ALA	N-CA-CB	5.13	117.28	110.10
5	Q	16	TYR	CA-CB-CG	5.11	123.10	113.40
1	L	151	LYS	CB-CA-C	-5.07	100.26	110.40
7	2	25	ILE	CB-CA-C	5.06	121.72	111.60
1	H	153	VAL	N-CA-C	-5.06	97.35	111.00
1	I	612	SER	CB-CA-C	-5.05	100.51	110.10
1	F	202	GLU	N-CA-C	-5.02	97.44	111.00
1	K	12	TYR	CA-CB-CG	5.01	122.92	113.40

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	474	TYR	Mainchain
1	D	475	SER	Mainchain
1	D	476	ASN	Mainchain
1	K	186	ASP	Mainchain
1	L	595	SER	Mainchain
4	M	395	TYR	Mainchain
2	N	185	TYR	Mainchain
2	N	186	LEU	Mainchain
2	N	187	GLN	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7551	0	7226	240	0
1	B	7536	0	7207	265	0
1	C	7519	0	7191	231	0
1	D	7526	0	7197	243	0
1	E	7526	0	7197	227	0
1	F	7539	0	7214	270	0
1	G	7526	0	7197	235	0
1	H	7526	0	7197	263	0
1	I	7536	0	7207	250	0
1	J	7551	0	7221	240	0
1	K	7546	0	7216	242	0
1	L	7524	0	7196	248	0
2	N	3786	0	3699	56	0
3	O	147	0	132	2	0
4	M	2829	0	2795	27	0
5	P	889	0	889	44	0
5	Q	821	0	822	55	0
5	R	957	0	950	44	0
5	S	887	0	882	17	0
6	U	1462	0	1416	32	0
6	V	1449	0	1402	14	0
7	1	236	0	219	7	0
7	2	203	0	192	5	0
7	3	211	0	198	7	0
7	4	227	0	213	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	5	219	0	209	9	0
7	6	211	0	198	8	0
7	7	211	0	198	1	0
7	8	227	0	213	4	0
7	9	219	0	209	8	0
8	X	75	0	17	1	0
All	All	105672	0	101319	2791	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 13.

All (2791) 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)
5:Q:15:PRO:HB2	5:Q:17:LEU:H	1.22	1.01
1:A:154:THR:HG23	1:A:155:LYS:HG2	1.47	0.96
1:K:196:GLU:HG2	1:L:823:HIS:HB3	1.47	0.94
1:K:194:GLN:HB2	1:K:197:PRO:HD2	1.52	0.91
1:I:762:THR:HG22	1:I:763:LYS:N	1.84	0.90
1:E:337:ASN:HD21	1:E:363:THR:H	1.18	0.89
1:A:135:TRP:CZ2	1:A:153:VAL:HB	2.09	0.87
1:G:449:GLN:HB3	1:H:153:VAL:HG13	1.54	0.86
1:G:194:GLN:HB3	1:G:197:PRO:HD2	1.55	0.85
1:J:134:GLN:HB2	1:J:154:THR:HG23	1.56	0.85
1:D:837:ARG:HD2	1:E:457:VAL:HG23	1.59	0.85
1:A:152:ASP:O	1:C:445:ALA:HB2	1.77	0.84
1:A:721:VAL:HG12	1:A:743:PHE:HB2	1.58	0.84
1:L:822:GLN:HB2	1:L:846:PHE:HB2	1.59	0.84
5:P:35:THR:HG21	5:P:40:PRO:HA	1.59	0.84
1:E:824:ASN:HA	1:E:844:ALA:HB1	1.58	0.84
1:C:897:SER:HG	1:C:899:HIS:HE2	1.24	0.83
1:A:262:ASP:HA	1:A:279:ALA:HB3	1.59	0.83
1:F:170:GLN:HB2	1:F:185:LYS:HD2	1.61	0.83
1:H:822:GLN:HB2	1:H:846:PHE:HB2	1.62	0.82
1:A:151:LYS:HB3	1:A:154:THR:HG21	1.60	0.82
1:I:267:SER:HB2	1:I:276:GLU:HA	1.60	0.82
1:C:138:LYS:HG2	1:C:149:GLN:HB3	1.61	0.81
1:L:155:LYS:HG3	1:L:261:PHE:HZ	1.43	0.81
1:A:403:VAL:HG11	1:A:466:ALA:HA	1.63	0.81
1:D:135:TRP:HE1	1:D:156:THR:HG1	1.27	0.81
1:K:138:LYS:HG2	1:K:149:GLN:HB2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:GLN:HB2	1:A:846:PHE:HB2	1.62	0.80
1:J:126:PRO:HG2	1:J:129:ALA:HB2	1.61	0.80
1:F:822:GLN:HB2	1:F:846:PHE:HB2	1.63	0.80
1:E:19:ASP:HA	1:E:48:PRO:HD2	1.62	0.80
1:I:244:PRO:HG3	1:I:253:ASP:HB3	1.62	0.79
1:D:126:PRO:HG2	1:D:129:ALA:HB2	1.65	0.79
1:F:203:ASN:HB2	1:F:204:TRP:HD1	1.47	0.79
5:Q:16:TYR:HB3	5:Q:18:THR:HG22	1.65	0.79
1:K:193:PHE:CZ	1:K:212:GLY:HA3	2.18	0.78
1:B:239:GLN:HE21	1:B:240:ALA:H	1.32	0.78
1:E:240:ALA:HB3	1:E:288:VAL:HB	1.64	0.78
1:I:762:THR:CG2	1:I:763:LYS:N	2.45	0.78
1:B:445:ALA:HB3	1:B:449:GLN:NE2	1.99	0.78
1:F:20:ALA:HB3	7:4:25:ILE:HG22	1.65	0.77
1:D:822:GLN:HB2	1:D:846:PHE:HB2	1.65	0.77
1:A:126:PRO:HG2	1:A:129:ALA:HB2	1.66	0.77
1:K:822:GLN:HB2	1:K:846:PHE:HB2	1.65	0.77
1:D:377:ARG:HB3	1:D:388:VAL:HG11	1.66	0.77
1:K:189:ALA:HA	1:K:241:LYS:HE3	1.65	0.77
1:L:267:SER:HB3	1:L:276:GLU:HA	1.65	0.77
1:C:822:GLN:HB2	1:C:846:PHE:HB2	1.67	0.76
1:H:67:ARG:HH12	1:I:752:GLU:HB2	1.50	0.76
1:L:908:ASP:OD1	1:L:908:ASP:N	2.19	0.76
1:I:126:PRO:HG2	1:I:129:ALA:HB2	1.68	0.75
1:L:399:GLU:HB3	1:L:523:ARG:HA	1.69	0.75
1:B:887:ASP:OD1	1:B:887:ASP:N	2.20	0.75
1:J:249:GLU:HG3	1:J:250:GLN:HG2	1.67	0.75
1:I:377:ARG:HB3	1:I:388:VAL:HG21	1.68	0.75
1:K:140:LYS:HB3	1:K:147:VAL:HG13	1.68	0.75
1:B:444:ASP:HA	1:C:151:LYS:O	1.87	0.75
1:F:698:TYR:HD1	5:R:33:GLY:HA3	1.50	0.75
1:H:344:VAL:HG22	1:H:582:GLU:HG2	1.68	0.75
1:K:438:SER:HB2	1:L:278:LYS:HD2	1.68	0.74
1:K:922:VAL:HB	1:K:944:PRO:HD2	1.70	0.74
1:H:525:SER:OG	1:H:801:MET:SD	2.46	0.74
5:Q:15:PRO:HB2	5:Q:17:LEU:N	1.99	0.74
1:J:135:TRP:HE1	1:J:156:THR:HG1	1.36	0.74
1:F:377:ARG:HB3	1:F:388:VAL:HG21	1.70	0.74
1:A:244:PRO:HD2	1:A:253:ASP:O	1.87	0.74
5:S:41:VAL:H	5:S:43:PRO:HG3	1.53	0.73
1:H:162:THR:HB	1:H:212:GLY:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:167:ILE:HD12	1:I:280:ASP:HB3	1.68	0.73
1:B:72:ASP:OD2	1:B:83:ARG:NH1	2.21	0.73
1:L:126:PRO:HG2	1:L:129:ALA:HB2	1.71	0.73
1:A:188:TYR:HA	1:A:192:THR:HB	1.69	0.73
1:I:114:LYS:HE2	1:I:294:ASP:HB2	1.70	0.73
1:K:361:ARG:NH1	1:K:924:ASP:OD2	2.22	0.73
1:D:552:ASN:O	1:E:804:GLN:NE2	2.21	0.73
1:G:681:THR:HG22	1:G:715:ASN:HB3	1.71	0.72
1:G:715:ASN:ND2	1:G:869:VAL:O	2.22	0.72
1:G:822:GLN:HB2	1:G:846:PHE:HB2	1.70	0.72
1:L:135:TRP:CZ3	1:L:309:GLU:HB3	2.24	0.72
1:E:427:LYS:HB3	1:E:439:GLU:HB2	1.71	0.72
1:F:74:GLU:HB3	1:F:81:LYS:HB3	1.70	0.72
1:D:410:TYR:HE1	1:E:414:LEU:HD21	1.54	0.72
1:J:160:ALA:HB3	1:J:281:ILE:HD11	1.72	0.72
1:C:188:TYR:O	1:C:241:LYS:NZ	2.22	0.72
1:B:633:MET:O	1:B:639:HIS:NE2	2.23	0.72
1:D:726:ASP:OD1	1:D:726:ASP:N	2.20	0.72
1:C:122:ASN:ND2	1:C:225:CYS:SG	2.61	0.71
1:F:602:ARG:HB2	5:R:35:THR:HB	1.72	0.71
1:C:7:MET:O	1:C:9:GLN:N	2.23	0.71
1:C:633:MET:O	1:C:639:HIS:NE2	2.23	0.71
1:L:389:ASP:OD1	1:L:546:ARG:NH2	2.21	0.71
1:A:153:VAL:HG13	1:C:449:GLN:HB3	1.73	0.71
1:B:822:GLN:HB2	1:B:846:PHE:HB2	1.72	0.71
1:C:135:TRP:N	1:C:154:THR:OG1	2.23	0.71
1:D:589:VAL:HG23	1:D:593:LEU:HD12	1.73	0.71
1:H:726:ASP:N	1:H:726:ASP:OD1	2.20	0.71
1:F:114:LYS:NZ	1:F:116:TYR:O	2.24	0.71
1:H:114:LYS:NZ	1:H:116:TYR:O	2.21	0.71
1:F:203:ASN:HB2	1:F:204:TRP:CD1	2.25	0.71
1:D:457:VAL:O	1:F:837:ARG:NH1	2.23	0.71
1:I:715:ASN:ND2	1:I:869:VAL:O	2.23	0.71
1:A:172:LEU:HD11	1:A:212:GLY:HA3	1.71	0.70
1:F:657:PRO:HB3	5:Q:13:PHE:HZ	1.55	0.70
1:G:486:LYS:HG2	1:G:509:VAL:HG22	1.72	0.70
1:G:648:SER:OG	1:G:676:ARG:NH1	2.24	0.70
1:K:551:GLY:HA3	1:L:804:GLN:HE21	1.55	0.70
1:E:553:GLY:H	1:F:804:GLN:HG3	1.54	0.70
5:R:34:SER:HA	5:R:43:PRO:HD2	1.74	0.70
1:E:922:VAL:HB	1:E:944:PRO:HD2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:924:ASP:HB3	1:G:942:ARG:HG3	1.73	0.70
1:L:943:THR:HB	1:L:944:PRO:HD3	1.72	0.70
1:B:88:VAL:HG22	1:B:576:PRO:HA	1.73	0.70
1:L:168:THR:HG23	1:L:170:GLN:H	1.57	0.70
1:H:329:ASN:OD1	1:H:377:ARG:NH2	2.23	0.70
1:B:20:ALA:H	1:B:47:ASN:HB3	1.57	0.70
1:E:155:LYS:HD3	1:E:283:LEU:HD13	1.72	0.70
1:C:188:TYR:HA	1:C:192:THR:HB	1.73	0.70
1:D:154:THR:HG23	1:D:155:LYS:HD2	1.74	0.70
1:J:315:GLN:NE2	1:L:203:ASN:OD1	2.24	0.70
1:A:134:GLN:HB2	1:A:155:LYS:HD3	1.73	0.70
1:H:151:LYS:HB3	1:H:154:THR:HG21	1.74	0.70
1:J:450:ASN:ND2	1:K:154:THR:O	2.24	0.70
1:B:246:ASN:ND2	1:B:249:GLU:O	2.25	0.69
1:I:709:ASP:HB3	1:I:711:THR:HG22	1.73	0.69
1:L:151:LYS:O	1:L:154:THR:HB	1.92	0.69
5:Q:12:LEU:HG	5:Q:15:PRO:HD3	1.75	0.69
1:D:198:GLN:OE1	1:F:456:ASN:ND2	2.24	0.69
1:J:463:ASN:O	1:J:467:ASN:ND2	2.25	0.69
1:B:126:PRO:HG2	1:B:129:ALA:HB2	1.74	0.69
1:B:693:SER:HB2	2:N:69:LEU:O	1.91	0.69
1:H:633:MET:O	1:H:639:HIS:NE2	2.25	0.69
1:K:172:LEU:HD13	1:K:193:PHE:HZ	1.57	0.69
5:Q:96:ILE:N	5:S:94:SER:HG	1.89	0.69
1:H:192:THR:HB	1:H:214:ARG:HD2	1.74	0.69
1:J:401:HIS:NE2	1:L:548:MET:SD	2.63	0.69
1:D:124:LEU:HB2	1:E:825:ASN:HD21	1.58	0.69
1:F:230:ALA:O	1:F:239:GLN:NE2	2.26	0.69
1:J:653:LEU:HD22	1:J:915:LEU:HD23	1.74	0.69
1:J:603:VAL:HA	5:P:40:PRO:HB3	1.73	0.69
1:F:198:GLN:C	1:F:200:GLY:H	1.97	0.69
1:I:389:ASP:OD1	1:I:540:ASN:ND2	2.24	0.69
1:I:822:GLN:HB2	1:I:846:PHE:HB2	1.75	0.69
1:J:135:TRP:NE1	1:J:156:THR:OG1	2.25	0.69
1:K:172:LEU:CD1	1:K:193:PHE:HZ	2.05	0.69
1:D:169:ASN:OD1	1:F:432:ASN:ND2	2.25	0.68
1:D:486:LYS:O	1:D:507:ARG:NH2	2.26	0.68
1:G:726:ASP:O	1:G:728:SER:N	2.26	0.68
1:J:456:ASN:HB3	1:L:837:ARG:HH12	1.57	0.68
1:L:14:HIS:O	1:L:46:ARG:NH1	2.27	0.68
1:B:449:GLN:HG3	1:B:450:ASN:OD1	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:GLN:HE21	1:C:240:ALA:H	1.40	0.68
1:J:17:GLY:H	1:J:48:PRO:HG3	1.58	0.68
1:G:196:GLU:HG3	1:G:197:PRO:HD3	1.75	0.68
1:J:19:ASP:HB2	7:9:14:GLY:HA3	1.75	0.68
1:B:415:ASN:HD21	1:B:418:GLY:HA2	1.59	0.68
1:K:109:ARG:HD3	1:K:324:ILE:HB	1.75	0.68
1:B:686:LYS:HE2	1:B:701:TYR:HB2	1.75	0.68
1:D:681:THR:HG23	1:D:715:ASN:HB3	1.73	0.68
1:J:230:ALA:O	1:J:239:GLN:NE2	2.26	0.68
1:H:214:ARG:HH22	1:H:241:LYS:HE2	1.58	0.68
1:I:543:LEU:HD23	1:I:546:ARG:HH21	1.57	0.68
1:L:240:ALA:HB3	1:L:288:VAL:HB	1.74	0.68
1:C:536:ASN:HB3	1:C:596:SER:O	1.93	0.68
1:F:135:TRP:N	1:F:154:THR:OG1	2.20	0.68
1:C:20:ALA:H	1:C:47:ASN:HB3	1.58	0.68
1:D:747:ARG:HE	1:D:750:ASP:HB2	1.59	0.68
1:I:415:ASN:ND2	1:I:417:THR:O	2.27	0.68
2:N:170:GLU:HB3	2:N:378:VAL:HG12	1.76	0.68
1:J:173:LEU:HB2	1:J:185:LYS:HZ2	1.59	0.67
1:A:589:VAL:HG23	1:A:593:LEU:HD12	1.76	0.67
1:K:194:GLN:CB	1:K:197:PRO:HD2	2.23	0.67
1:B:196:GLU:HG3	1:B:197:PRO:HD3	1.75	0.67
1:A:415:ASN:ND2	1:A:417:THR:O	2.21	0.67
1:C:676:ARG:NH1	1:C:921:GLU:OE1	2.27	0.67
1:D:198:GLN:NE2	1:D:199:VAL:O	2.26	0.67
1:H:152:ASP:C	1:H:154:THR:H	1.96	0.67
5:Q:45:ASN:HB2	5:Q:49:MET:HG2	1.76	0.67
1:A:409:ASN:ND2	1:C:467:ASN:OD1	2.27	0.67
1:H:769:GLN:NE2	1:H:872:ARG:H	1.92	0.67
2:N:334:ASP:OD1	2:N:334:ASP:N	2.25	0.67
1:E:837:ARG:NH1	1:F:457:VAL:O	2.28	0.67
1:F:196:GLU:OE1	1:F:196:GLU:N	2.24	0.67
1:J:633:MET:O	1:J:639:HIS:NE2	2.27	0.67
1:K:327:ARG:NH1	1:K:591:MET:O	2.28	0.67
1:G:414:LEU:HD21	1:I:410:TYR:HE1	1.58	0.67
1:J:414:LEU:HD21	1:L:410:TYR:HE1	1.60	0.67
1:B:46:ARG:NH1	1:C:644:ASN:OD1	2.28	0.67
1:B:202:GLU:HA	1:C:313:VAL:HG11	1.75	0.67
1:G:460:MET:HG3	1:I:460:MET:HE1	1.76	0.67
1:A:56:VAL:HG13	1:A:57:THR:HG22	1.77	0.67
1:K:937:GLU:HB2	6:U:36:ALA:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:282:VAL:HG13	2:N:283:PRO:HD3	1.76	0.67
1:H:697:PRO:O	5:Q:34:SER:N	2.27	0.67
1:H:771:LEU:HD22	1:H:880:MET:HG2	1.76	0.67
1:K:47:ASN:HD21	7:8:25:ILE:HG22	1.59	0.67
1:L:47:ASN:ND2	7:9:24:GLU:O	2.28	0.67
1:H:135:TRP:CZ3	1:H:137:THR:HB	2.30	0.66
1:K:25:SER:H	1:L:639:HIS:CE1	2.12	0.66
1:K:440:TRP:CZ2	1:L:276:GLU:HB3	2.31	0.66
1:G:199:VAL:HG11	1:G:206:GLU:HG3	1.76	0.66
1:I:399:GLU:HB3	1:I:523:ARG:HA	1.77	0.66
1:C:908:ASP:OD1	1:C:908:ASP:N	2.15	0.66
1:F:922:VAL:HB	1:F:944:PRO:HD2	1.78	0.66
1:I:287:ASN:OD1	1:I:287:ASN:N	2.27	0.66
1:K:240:ALA:HB3	1:K:288:VAL:HB	1.77	0.66
1:A:444:ASP:HA	1:B:152:ASP:HA	1.78	0.66
1:B:134:GLN:HA	1:B:154:THR:O	1.95	0.66
1:H:135:TRP:CH2	1:H:309:GLU:HB2	2.31	0.66
1:I:117:SER:HA	1:I:321:PRO:HG3	1.78	0.66
1:B:836:MET:O	1:B:837:ARG:NE	2.28	0.66
1:J:837:ARG:NE	1:J:837:ARG:O	2.28	0.66
2:N:280:LEU:HD13	2:N:328:VAL:HG13	1.76	0.66
6:V:179:ARG:NH2	6:V:182:GLY:O	2.28	0.66
1:H:233:THR:O	1:I:815:LYS:NZ	2.24	0.66
1:I:681:THR:HG22	1:I:715:ASN:HB3	1.78	0.66
1:J:124:LEU:HB2	1:K:825:ASN:HD21	1.60	0.66
2:N:164:PRO:HD2	2:N:176:LEU:HD21	1.78	0.66
1:B:211:TYR:H	1:B:281:ILE:HG22	1.61	0.66
1:D:159:VAL:HG21	1:E:841:PRO:HD2	1.76	0.66
1:E:107:LEU:HD13	1:E:608:VAL:HG12	1.76	0.66
1:K:126:PRO:HG2	1:K:129:ALA:HB2	1.78	0.66
1:G:474:TYR:HA	1:G:478:ALA:HB3	1.78	0.66
1:K:280:ASP:OD1	1:K:280:ASP:N	2.29	0.66
1:L:134:GLN:HA	1:L:155:LYS:H	1.61	0.66
6:U:179:ARG:NH2	6:U:182:GLY:O	2.29	0.66
1:B:194:GLN:O	1:B:198:GLN:NE2	2.29	0.65
1:E:684:LYS:HA	1:E:914:THR:HG22	1.77	0.65
1:J:333:LEU:HD22	1:J:562:VAL:HG21	1.76	0.65
1:K:46:ARG:HG2	1:L:642:SER:HB2	1.78	0.65
1:A:426:VAL:HA	1:A:440:TRP:HA	1.78	0.65
1:A:542:GLY:O	1:A:546:ARG:NH1	2.29	0.65
1:A:815:LYS:NZ	1:C:233:THR:O	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:TRP:HD1	1:C:441:GLU:HG2	1.60	0.65
1:D:676:ARG:NH2	1:D:921:GLU:OE1	2.27	0.65
1:J:222:MET:HE1	1:J:312:LEU:HD22	1.79	0.65
1:K:409:ASN:ND2	1:K:462:ILE:O	2.28	0.65
1:K:681:THR:HG23	1:K:715:ASN:HB3	1.77	0.65
1:F:241:LYS:HD3	1:F:256:ILE:HD11	1.77	0.65
1:G:154:THR:HG23	1:G:155:LYS:HG2	1.77	0.65
1:K:114:LYS:NZ	1:K:116:TYR:O	2.28	0.65
1:K:681:THR:HG21	1:K:712:PHE:HB3	1.78	0.65
1:D:198:GLN:NE2	1:D:200:GLY:O	2.30	0.65
1:E:189:ALA:O	1:E:241:LYS:NZ	2.28	0.65
1:G:427:LYS:HB2	1:G:441:GLU:HG2	1.77	0.65
1:K:168:THR:HG23	1:K:170:GLN:H	1.61	0.65
5:Q:35:THR:HA	5:Q:43:PRO:HD2	1.77	0.65
1:J:240:ALA:HB3	1:J:288:VAL:HB	1.78	0.65
1:L:289:ASN:OD1	1:L:289:ASN:N	2.29	0.65
4:M:246:VAL:HB	4:M:249:ASN:HB2	1.76	0.65
1:B:344:VAL:HG13	1:B:582:GLU:HB3	1.79	0.65
1:D:122:ASN:ND2	1:D:225:CYS:SG	2.70	0.65
1:D:503:TYR:OH	1:D:507:ARG:NH1	2.30	0.65
1:H:255:ASP:OD2	1:H:287:ASN:ND2	2.30	0.65
1:K:162:THR:HB	1:K:193:PHE:HE1	1.61	0.65
1:L:33:ARG:HE	7:9:22:TRP:HB3	1.61	0.65
1:H:711:THR:OG1	1:H:711:THR:O	2.14	0.65
1:L:188:TYR:O	1:L:241:LYS:NZ	2.29	0.65
5:R:49:MET:SD	5:R:50:THR:N	2.69	0.65
1:I:217:LYS:NZ	1:I:287:ASN:OD1	2.29	0.65
1:I:762:THR:HG22	1:I:764:ASP:H	1.61	0.65
1:K:135:TRP:NE1	1:K:156:THR:OG1	2.29	0.65
1:G:443:ASP:N	1:G:443:ASP:OD1	2.30	0.65
1:J:114:LYS:NZ	1:J:116:TYR:O	2.29	0.65
1:K:837:ARG:NE	1:K:837:ARG:O	2.30	0.65
2:N:247:ARG:NH2	2:N:380:CYS:O	2.29	0.65
1:F:657:PRO:HD3	5:Q:13:PHE:HE2	1.61	0.65
1:G:323:TYR:H	1:G:596:SER:HB3	1.62	0.65
1:J:526:LEU:HG	1:J:528:PRO:HD2	1.79	0.65
1:L:155:LYS:HZ3	1:L:285:THR:HG23	1.61	0.64
1:L:744:GLU:O	1:L:762:THR:OG1	2.14	0.64
5:Q:34:SER:OG	5:Q:35:THR:N	2.30	0.64
1:A:633:MET:O	1:A:639:HIS:NE2	2.30	0.64
1:D:14:HIS:O	1:D:46:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:LYS:HZ3	1:E:283:LEU:HD22	1.62	0.64
1:F:837:ARG:NE	1:F:837:ARG:O	2.28	0.64
1:G:201:GLU:OE1	1:G:201:GLU:N	2.29	0.64
1:G:845:ASN:HB3	1:I:239:GLN:HE22	1.62	0.64
1:K:161:ALA:HB2	1:L:840:GLN:HE21	1.63	0.64
1:A:648:SER:OG	1:A:676:ARG:NH2	2.30	0.64
1:H:552:ASN:O	1:I:804:GLN:NE2	2.29	0.64
1:I:922:VAL:HB	1:I:944:PRO:HD2	1.80	0.64
1:J:403:VAL:HG11	1:J:466:ALA:HA	1.78	0.64
1:A:907:VAL:HG23	1:A:908:ASP:H	1.62	0.64
1:C:140:LYS:HA	1:C:147:VAL:HG22	1.78	0.64
1:F:320:ARG:NH1	1:F:479:LEU:O	2.31	0.64
1:F:681:THR:CG2	1:F:715:ASN:ND2	2.60	0.64
1:I:762:THR:CG2	1:I:763:LYS:H	2.11	0.64
5:P:42:LEU:HB2	5:P:43:PRO:HD3	1.79	0.64
1:G:230:ALA:O	1:G:239:GLN:NE2	2.29	0.64
1:G:403:VAL:HG11	1:G:466:ALA:HA	1.79	0.64
1:H:415:ASN:OD1	1:H:415:ASN:N	2.31	0.64
5:S:35:THR:OG1	5:S:39:ARG:N	2.28	0.64
1:B:443:ASP:OD1	1:B:443:ASP:N	2.31	0.64
1:C:375:GLY:O	1:C:790:ARG:NH1	2.30	0.64
1:D:152:ASP:O	1:D:154:THR:N	2.31	0.64
1:E:103:ILE:HG13	1:E:613:VAL:HG22	1.79	0.64
1:E:512:SER:HA	1:E:515:ASP:HB2	1.79	0.64
1:I:114:LYS:NZ	1:I:116:TYR:O	2.30	0.64
1:J:154:THR:HG22	1:J:155:LYS:HG2	1.80	0.64
1:K:198:GLN:HG2	1:L:839:GLY:N	2.11	0.64
5:R:54:VAL:HG12	5:R:55:GLY:H	1.63	0.64
1:I:731:TRP:O	1:I:733:GLY:N	2.31	0.64
1:C:426:VAL:HG12	1:C:440:TRP:HB3	1.79	0.64
1:F:196:GLU:HG2	1:F:197:PRO:HD3	1.79	0.64
1:G:19:ASP:OD1	1:G:47:ASN:ND2	2.31	0.64
1:G:126:PRO:HG2	1:G:129:ALA:HB2	1.79	0.64
1:H:759:CYS:SG	1:H:760:ASN:N	2.70	0.64
1:A:468:LEU:HD21	1:B:464:LEU:HD22	1.79	0.64
1:D:747:ARG:NH2	1:D:752:GLU:OE2	2.29	0.64
1:E:138:LYS:HD3	1:E:149:GLN:HB2	1.80	0.64
1:L:211:TYR:H	1:L:281:ILE:HG22	1.63	0.64
1:A:328:ASP:OD2	1:A:368:GLN:NE2	2.26	0.64
1:F:328:ASP:OD2	1:F:368:GLN:NE2	2.31	0.64
1:C:224:PRO:HD3	1:C:314:GLN:HG2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:ASP:OD2	1:D:377:ARG:NH2	2.31	0.63
1:F:789:ASP:OD1	1:F:796:ARG:NH1	2.31	0.63
1:H:14:HIS:O	1:H:46:ARG:NH1	2.31	0.63
1:I:756:VAL:HG13	1:I:763:LYS:HG2	1.80	0.63
1:K:98:SER:HB2	1:K:618:THR:HG23	1.81	0.63
6:U:69:LEU:HB2	6:U:211:GLU:HG3	1.79	0.63
1:B:139:GLU:HG3	1:B:152:ASP:HB2	1.79	0.63
1:B:379:ARG:NH2	1:C:789:ASP:OD2	2.31	0.63
1:C:295:THR:HG22	1:C:318:PRO:HA	1.80	0.63
1:E:186:ASP:OD1	1:E:186:ASP:N	2.31	0.63
1:E:389:ASP:O	1:E:868:ARG:NH2	2.30	0.63
1:F:682:ARG:NH2	1:F:914:THR:OG1	2.30	0.63
1:L:422:THR:HB	1:L:450:ASN:H	1.63	0.63
1:L:538:PRO:O	1:L:544:ARG:NE	2.32	0.63
1:I:24:LEU:HD13	1:I:28:LEU:HD12	1.81	0.63
1:J:651:ASN:HB3	1:J:919:LEU:HB3	1.81	0.63
1:L:167:ILE:HD13	1:L:282:ILE:HG23	1.81	0.63
1:A:526:LEU:HG	1:A:528:PRO:HD2	1.80	0.63
1:D:750:ASP:OD1	1:D:750:ASP:N	2.32	0.63
1:J:337:ASN:HD21	1:J:363:THR:H	1.45	0.63
1:B:449:GLN:HE21	1:B:450:ASN:H	1.47	0.63
1:L:79:LEU:O	1:L:587:LYS:NZ	2.30	0.63
1:B:533:ASN:ND2	1:B:536:ASN:OD1	2.32	0.63
1:E:633:MET:O	1:E:639:HIS:NE2	2.31	0.63
1:F:137:THR:OG1	1:F:138:LYS:N	2.32	0.63
1:D:228:SER:HB2	1:D:290:LEU:HD11	1.80	0.62
1:H:344:VAL:HB	1:H:353:ASN:HB2	1.81	0.62
1:I:943:THR:HB	1:I:944:PRO:HD3	1.81	0.62
1:A:546:ARG:NH2	1:A:594:GLN:OE1	2.30	0.62
1:B:135:TRP:CH2	1:B:309:GLU:HB2	2.34	0.62
1:B:162:THR:HG21	1:B:172:LEU:HD13	1.81	0.62
1:B:747:ARG:NH2	1:B:752:GLU:OE1	2.32	0.62
1:E:345:LEU:HD13	1:E:581:TYR:HD1	1.63	0.62
1:G:6:MET:SD	1:G:6:MET:N	2.72	0.62
1:A:89:GLY:HA3	1:A:92:ARG:HE	1.64	0.62
1:F:657:PRO:HB3	5:Q:13:PHE:CZ	2.34	0.62
1:H:52:PRO:HD3	7:7:11:PRO:HA	1.79	0.62
1:H:914:THR:OG1	1:H:915:LEU:N	2.30	0.62
1:K:89:GLY:HA3	1:K:92:ARG:HD3	1.80	0.62
1:A:590:ASN:ND2	1:A:699:PHE:O	2.32	0.62
1:B:13:MET:HB3	1:C:925:VAL:HG21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:594:GLN:HB2	1:E:703:GLY:HA2	1.80	0.62
1:F:152:ASP:O	1:F:154:THR:N	2.33	0.62
1:L:486:LYS:HG2	1:L:509:VAL:HG22	1.82	0.62
1:A:202:GLU:HA	1:B:313:VAL:HG11	1.81	0.62
1:I:537:HIS:CG	1:I:538:PRO:HD2	2.34	0.62
1:J:233:THR:O	1:K:815:LYS:NZ	2.29	0.62
6:U:143:SER:OG	7:1:6:PHE:N	2.32	0.62
1:A:198:GLN:HG2	1:B:838:GLN:HB2	1.82	0.62
1:B:539:ARG:NH1	1:C:404:GLU:OE2	2.32	0.62
1:E:25:SER:H	1:F:639:HIS:CE1	2.18	0.62
1:G:364:GLU:OE1	1:G:565:LYS:NZ	2.32	0.62
1:I:135:TRP:CZ2	1:I:309:GLU:HB3	2.34	0.62
1:L:262:ASP:OD1	1:L:279:ALA:N	2.27	0.62
1:D:308:SER:OG	1:D:311:ASN:ND2	2.32	0.62
1:F:701:TYR:CZ	1:F:703:GLY:HA3	2.35	0.62
1:I:902:ASP:OD1	1:I:902:ASP:N	2.32	0.62
1:D:300:LYS:HB3	1:D:491:ASN:HD21	1.64	0.62
1:G:360:ASP:OD1	1:G:361:ARG:N	2.33	0.62
1:J:202:GLU:HA	1:K:313:VAL:HG11	1.81	0.62
1:J:711:THR:O	1:J:711:THR:OG1	2.18	0.62
1:B:474:TYR:HA	1:B:478:ALA:HB3	1.82	0.62
1:E:594:GLN:NE2	1:E:703:GLY:O	2.33	0.62
1:F:813:ASP:OD1	1:F:813:ASP:N	2.29	0.62
1:B:741:ASN:OD1	1:B:741:ASN:N	2.23	0.62
1:D:415:ASN:ND2	1:D:417:THR:O	2.33	0.62
1:F:240:ALA:HB3	1:F:288:VAL:HB	1.82	0.62
1:J:886:THR:HG23	1:J:889:GLY:H	1.65	0.62
1:C:902:ASP:OD1	1:C:902:ASP:N	2.33	0.61
1:D:636:ASN:OD1	1:D:637:ASP:N	2.29	0.61
1:K:231:ARG:NH1	1:L:813:ASP:OD2	2.33	0.61
1:G:503:TYR:OH	1:G:507:ARG:NH1	2.33	0.61
1:I:88:VAL:HG12	1:I:619:PHE:HE2	1.65	0.61
1:K:360:ASP:OD1	1:K:942:ARG:NH1	2.33	0.61
1:K:450:ASN:HB2	1:L:156:THR:HA	1.82	0.61
1:D:653:LEU:HD13	1:D:691:LEU:HD11	1.83	0.61
1:J:327:ARG:NH2	1:J:703:GLY:O	2.34	0.61
1:F:192:THR:HB	1:F:214:ARG:HD2	1.80	0.61
1:H:837:ARG:NH1	1:I:457:VAL:O	2.34	0.61
5:Q:35:THR:OG1	5:Q:36:VAL:O	2.19	0.61
1:D:327:ARG:NH1	1:D:703:GLY:O	2.30	0.61
1:F:756:VAL:HB	1:F:763:LYS:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:635:ARG:NH1	1:G:932:HIS:O	2.34	0.61
1:H:379:ARG:NH2	1:I:789:ASP:OD2	2.33	0.61
1:K:417:THR:HB	1:K:457:VAL:HG12	1.83	0.61
1:B:648:SER:OG	1:B:676:ARG:NH2	2.33	0.61
1:D:482:PRO:HD3	1:D:529:MET:HB3	1.82	0.61
1:G:726:ASP:N	1:G:726:ASP:OD1	2.33	0.61
1:H:25:SER:H	1:I:639:HIS:CE1	2.18	0.61
1:H:445:ALA:HB3	1:H:449:GLN:HG3	1.81	0.61
1:L:280:ASP:OD1	1:L:280:ASP:N	2.16	0.61
1:A:463:ASN:O	1:A:467:ASN:ND2	2.33	0.61
1:B:470:LYS:NZ	1:B:515:ASP:OD1	2.32	0.61
1:D:135:TRP:N	1:D:154:THR:OG1	2.34	0.61
1:E:47:ASN:N	1:E:47:ASN:OD1	2.33	0.61
1:F:234:ASN:HD21	1:F:238:GLY:HA3	1.65	0.61
1:F:575:LEU:HB3	1:F:576:PRO:HD2	1.83	0.61
1:F:640:ASP:N	1:F:640:ASP:OD1	2.34	0.61
1:G:461:GLU:HG2	1:I:126:PRO:HB3	1.83	0.61
1:H:346:ALA:HB2	1:H:353:ASN:HA	1.82	0.61
1:H:648:SER:OG	1:H:676:ARG:NH2	2.33	0.61
5:R:12:LEU:HD21	5:R:17:LEU:HD11	1.82	0.61
1:A:90:ASP:OD2	1:A:933:ARG:NH1	2.34	0.61
1:H:311:ASN:OD1	1:H:314:GLN:NE2	2.33	0.61
1:H:656:ILE:HD11	1:H:916:LEU:HB2	1.82	0.61
1:H:749:VAL:HG22	5:R:51:TYR:HE2	1.66	0.61
1:B:449:GLN:NE2	1:B:450:ASN:H	1.98	0.61
1:D:239:GLN:OE1	1:E:823:HIS:NE2	2.31	0.61
1:D:514:VAL:HA	1:D:518:ILE:HG21	1.82	0.61
1:F:698:TYR:CD1	5:R:33:GLY:HA3	2.33	0.61
1:A:922:VAL:HB	1:A:944:PRO:HD2	1.83	0.60
1:C:135:TRP:CH2	1:C:309:GLU:HB3	2.36	0.60
1:F:173:LEU:HA	1:F:185:LYS:HA	1.83	0.60
1:H:262:ASP:OD1	1:H:263:VAL:N	2.34	0.60
1:I:566:PHE:O	1:I:570:LYS:HB2	2.01	0.60
2:N:408:TYR:O	2:N:496:ARG:NH2	2.34	0.60
1:G:162:THR:H	1:G:211:TYR:HD1	1.48	0.60
1:H:952:THR:OXT	1:J:734:ASN:ND2	2.34	0.60
1:A:774:TYR:HB2	1:A:776:ILE:HG12	1.83	0.60
1:B:540:ASN:O	1:B:543:LEU:N	2.31	0.60
1:E:117:SER:HA	1:E:321:PRO:HG3	1.82	0.60
1:F:760:ASN:HD22	5:P:54:VAL:HB	1.66	0.60
1:G:813:ASP:OD2	1:I:231:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:449:GLN:HG2	1:H:450:ASN:H	1.65	0.60
1:K:589:VAL:HG23	1:K:593:LEU:HD12	1.83	0.60
1:C:240:ALA:HB3	1:C:288:VAL:HB	1.82	0.60
1:H:916:LEU:HD13	1:H:918:LEU:H	1.66	0.60
1:L:135:TRP:CH2	1:L:309:GLU:HB3	2.36	0.60
1:E:644:ASN:HB3	1:E:925:VAL:HG12	1.84	0.60
1:F:445:ALA:HB1	1:F:448:ARG:HB2	1.83	0.60
1:G:887:ASP:OD1	1:G:887:ASP:N	2.33	0.60
1:I:234:ASN:HD21	1:I:238:GLY:HA3	1.65	0.60
1:L:669:SER:HA	1:L:899:HIS:O	2.02	0.60
1:C:47:ASN:N	1:C:47:ASN:OD1	2.34	0.60
1:H:351:GLN:O	1:L:92:ARG:NH2	2.30	0.60
1:J:486:LYS:HB3	1:J:509:VAL:HG22	1.84	0.60
1:A:80:TYR:HB2	1:A:587:LYS:HE3	1.83	0.60
1:B:917:TYR:CZ	1:B:919:LEU:HD21	2.37	0.60
1:C:131:ASN:ND2	1:C:223:LYS:O	2.30	0.60
1:D:403:VAL:HG11	1:D:466:ALA:HA	1.84	0.60
1:E:415:ASN:HD21	1:E:418:GLY:HA2	1.67	0.60
1:G:441:GLU:OE1	1:G:442:LYS:N	2.32	0.60
1:H:331:VAL:HG13	1:H:364:GLU:HG2	1.82	0.60
1:H:886:THR:HG23	1:H:889:GLY:H	1.66	0.60
1:L:150:GLU:C	1:L:152:ASP:H	2.05	0.60
1:C:587:LYS:NZ	1:C:608:VAL:O	2.35	0.60
1:F:399:GLU:HB3	1:F:523:ARG:HG3	1.84	0.60
1:F:515:ASP:OD1	1:F:516:ALA:N	2.30	0.60
1:F:640:ASP:OD2	1:F:927:ARG:NH1	2.35	0.60
1:K:715:ASN:ND2	1:K:866:CYS:O	2.31	0.60
1:L:20:ALA:HB3	7:9:24:GLU:HB3	1.84	0.60
1:G:837:ARG:NH2	1:H:457:VAL:O	2.31	0.60
1:K:327:ARG:NH2	1:K:703:GLY:O	2.35	0.60
1:L:72:ASP:OD2	1:L:83:ARG:NH1	2.35	0.60
1:D:633:MET:O	1:D:639:HIS:ND1	2.34	0.60
1:E:588:ASP:OD2	1:E:602:ARG:NH2	2.35	0.60
1:J:122:ASN:ND2	1:J:225:CYS:SG	2.75	0.60
1:J:664:PRO:HG2	5:P:15:PRO:O	2.02	0.60
5:P:10:GLY:O	5:P:12:LEU:N	2.35	0.60
1:A:313:VAL:HG22	1:C:204:TRP:HE3	1.66	0.59
1:E:231:ARG:NH1	1:F:813:ASP:OD2	2.35	0.59
1:F:427:LYS:HB3	1:F:439:GLU:HB3	1.83	0.59
1:F:486:LYS:HG2	1:F:509:VAL:HG12	1.84	0.59
1:I:575:LEU:HD21	1:I:634:LEU:HD23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:162:THR:HB	1:K:193:PHE:CE1	2.36	0.59
1:B:575:LEU:HB3	1:B:576:PRO:HD2	1.85	0.59
1:C:22:GLU:OE1	7:1:15:THR:OG1	2.21	0.59
1:E:277:TYR:CZ	1:E:279:ALA:HB2	2.37	0.59
1:F:341:ASN:OD1	1:F:341:ASN:N	2.35	0.59
1:G:496:ALA:HB3	5:R:87:SER:HA	1.82	0.59
1:H:589:VAL:HG23	1:H:593:LEU:HD12	1.83	0.59
1:C:519:ASN:OD1	1:C:803:ARG:NH1	2.35	0.59
1:F:214:ARG:NH2	1:F:286:GLU:OE2	2.34	0.59
1:J:731:TRP:CD1	1:J:732:PRO:HD3	2.37	0.59
2:N:94:SER:O	2:N:485:GLY:HA3	2.02	0.59
1:A:544:ARG:HA	1:A:547:SER:HB3	1.83	0.59
1:C:648:SER:OG	1:C:676:ARG:NH2	2.35	0.59
1:E:196:GLU:HB2	1:F:831:TYR:HD1	1.67	0.59
1:G:433:ASP:OD1	1:G:434:GLY:N	2.35	0.59
1:H:202:GLU:HA	1:I:313:VAL:HG11	1.85	0.59
1:L:95:ASP:OD1	1:L:96:MET:N	2.36	0.59
1:A:196:GLU:N	1:A:196:GLU:OE2	2.35	0.59
1:B:90:ASP:OD1	1:B:933:ARG:NH2	2.36	0.59
1:F:137:THR:HG23	1:F:152:ASP:HB2	1.85	0.59
1:F:523:ARG:NH2	1:F:799:GLN:OE1	2.34	0.59
1:G:88:VAL:HG23	1:G:92:ARG:HB2	1.83	0.59
1:G:731:TRP:CD1	1:G:732:PRO:HD3	2.37	0.59
1:G:758:GLN:HG3	1:I:549:LEU:HD21	1.85	0.59
5:S:35:THR:HG1	5:S:39:ARG:H	1.50	0.59
1:A:387:ALA:O	1:A:546:ARG:NH1	2.35	0.59
1:D:839:GLY:HA2	1:F:198:GLN:HG2	1.83	0.59
1:E:396:ARG:NH1	1:E:867:ASP:OD2	2.35	0.59
1:F:539:ARG:HA	1:F:544:ARG:HH21	1.67	0.59
1:K:239:GLN:OE1	1:L:823:HIS:NE2	2.32	0.59
1:L:247:GLU:OE1	1:L:248:GLY:N	2.35	0.59
1:C:18:GLN:HA	7:1:15:THR:HG23	1.84	0.59
1:C:19:ASP:OD1	1:C:20:ALA:N	2.35	0.59
1:E:132:PRO:HB3	1:E:158:GLY:HA2	1.84	0.59
1:H:286:GLU:OE2	1:I:842:TYR:OH	2.21	0.59
1:J:590:ASN:ND2	1:J:701:TYR:O	2.36	0.59
1:L:113:PHE:HD1	1:L:324:ILE:HG13	1.67	0.59
1:L:306:ASN:O	1:L:311:ASN:ND2	2.32	0.59
2:N:247:ARG:NH2	2:N:383:GLU:OE2	2.36	0.59
1:C:486:LYS:HG2	1:C:509:VAL:HG12	1.85	0.59
1:D:426:VAL:HG12	1:D:440:TRP:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:ARG:NH2	1:E:241:LYS:HE2	2.17	0.59
1:E:337:ASN:HD21	1:E:363:THR:N	1.97	0.59
1:G:261:PHE:HB2	1:G:281:ILE:HG23	1.84	0.59
1:H:333:LEU:HD23	1:H:562:VAL:HG11	1.85	0.59
1:H:676:ARG:NH2	1:H:921:GLU:OE1	2.35	0.59
1:J:337:ASN:ND2	1:J:363:THR:H	2.00	0.59
1:A:309:GLU:O	1:C:205:GLN:NE2	2.34	0.59
1:E:214:ARG:HH22	1:E:241:LYS:HE2	1.67	0.59
1:E:424:GLN:HA	1:E:449:GLN:HG2	1.83	0.59
1:E:573:LEU:HB3	1:E:641:GLN:HE21	1.67	0.59
1:C:230:ALA:O	1:C:239:GLN:NE2	2.35	0.59
1:E:495:PRO:HG3	1:E:502:GLU:HG3	1.83	0.59
1:H:134:GLN:HG3	1:H:155:LYS:NZ	2.18	0.59
1:J:738:LEU:HB3	1:J:754:TYR:HE2	1.67	0.59
5:P:35:THR:OG1	5:P:36:VAL:N	2.35	0.59
1:F:47:ASN:HB3	7:4:25:ILE:HB	1.84	0.58
1:K:590:ASN:ND2	1:K:699:PHE:O	2.36	0.58
1:L:214:ARG:NH2	1:L:286:GLU:OE2	2.36	0.58
5:P:29:GLN:N	5:R:8:PHE:O	2.29	0.58
1:C:541:ALA:HA	1:C:544:ARG:HD3	1.84	0.58
1:D:449:GLN:HB3	1:E:153:VAL:HG13	1.84	0.58
1:E:670:ARG:NH1	1:E:944:PRO:O	2.36	0.58
1:G:589:VAL:HG23	1:G:593:LEU:HD22	1.86	0.58
2:N:325:LYS:O	3:O:6:ARG:NH2	2.35	0.58
1:D:804:GLN:HE21	1:F:551:GLY:HA3	1.68	0.58
1:E:173:LEU:HB2	1:E:185:LYS:HZ3	1.69	0.58
1:G:922:VAL:HB	1:G:944:PRO:HD2	1.85	0.58
1:L:731:TRP:O	1:L:733:GLY:N	2.35	0.58
1:A:410:TYR:HE1	1:B:414:LEU:HD21	1.69	0.58
1:A:760:ASN:O	1:A:760:ASN:ND2	2.35	0.58
1:C:93:VAL:HG21	1:C:630:LEU:HD12	1.85	0.58
1:D:202:GLU:HB3	1:E:313:VAL:HG11	1.84	0.58
1:D:842:TYR:OH	1:F:286:GLU:OE2	2.22	0.58
1:E:344:VAL:HG22	1:E:582:GLU:HG2	1.84	0.58
1:E:893:LEU:O	1:E:899:HIS:NE2	2.34	0.58
1:G:124:LEU:HB2	1:H:825:ASN:HD21	1.69	0.58
1:G:737:LEU:O	1:I:63:ARG:NH1	2.35	0.58
1:K:239:GLN:HE21	1:K:240:ALA:H	1.49	0.58
1:K:483:ASP:OD1	1:K:507:ARG:NH1	2.37	0.58
1:L:300:LYS:NZ	1:L:305:ASP:OD1	2.34	0.58
5:P:17:LEU:HA	5:R:14:SER:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:GLN:OE1	1:B:451:GLN:N	2.37	0.58
1:G:257:ASP:N	1:G:257:ASP:OD1	2.36	0.58
1:I:486:LYS:HG2	1:I:509:VAL:HG12	1.86	0.58
1:B:19:ASP:HA	1:B:48:PRO:HD2	1.86	0.58
1:D:360:ASP:O	1:D:361:ARG:HG3	2.04	0.58
1:E:239:GLN:HE21	1:E:240:ALA:H	1.52	0.58
1:G:114:LYS:NZ	1:G:116:TYR:O	2.30	0.58
1:K:22:GLU:O	6:V:176:SER:OG	2.22	0.58
1:K:253:ASP:OD1	1:K:254:LEU:N	2.31	0.58
1:A:262:ASP:OD2	1:A:279:ALA:N	2.36	0.58
1:B:695:PHE:H	2:N:72:GLN:HE22	1.52	0.58
1:F:681:THR:HG22	1:F:715:ASN:ND2	2.19	0.58
1:G:633:MET:O	1:G:639:HIS:NE2	2.37	0.58
1:H:825:ASN:O	1:H:825:ASN:ND2	2.37	0.58
1:A:379:ARG:NH1	1:B:789:ASP:OD2	2.33	0.58
1:E:96:MET:HG2	1:E:569:ILE:HG22	1.85	0.58
1:H:433:ASP:OD1	1:H:433:ASP:N	2.37	0.58
1:J:152:ASP:HA	1:L:444:ASP:HA	1.85	0.58
1:J:557:PRO:HD2	1:K:860:THR:HG21	1.85	0.58
1:K:151:LYS:HB3	1:K:154:THR:HG21	1.85	0.58
1:B:436:GLU:O	1:B:437:GLU:HB2	2.03	0.58
1:D:887:ASP:OD1	1:D:887:ASP:N	2.37	0.58
1:K:151:LYS:O	1:K:154:THR:OG1	2.21	0.58
4:M:141:LEU:HD22	4:M:170:VAL:HG21	1.86	0.58
1:C:214:ARG:NH2	1:C:286:GLU:OE2	2.37	0.57
1:D:447:SER:HB2	1:E:264:PRO:HB3	1.85	0.57
1:F:731:TRP:O	1:F:733:GLY:N	2.36	0.57
1:H:480:TYR:OH	1:H:538:PRO:HD3	2.03	0.57
1:L:480:TYR:OH	1:L:538:PRO:HD3	2.04	0.57
1:A:433:ASP:OD2	1:B:169:ASN:N	2.35	0.57
1:B:107:LEU:HG	1:B:608:VAL:HG12	1.86	0.57
1:F:483:ASP:OD1	1:F:507:ARG:NH1	2.37	0.57
1:F:603:VAL:HA	5:R:40:PRO:HB3	1.86	0.57
1:H:681:THR:OG1	1:H:682:ARG:N	2.37	0.57
1:H:769:GLN:HE21	1:H:872:ARG:H	1.50	0.57
1:J:804:GLN:HE22	1:L:551:GLY:HA3	1.70	0.57
2:N:130:PHE:HB3	2:N:248:LEU:HD12	1.85	0.57
6:V:3:LYS:H	6:V:3:LYS:HD2	1.69	0.57
1:E:329:ASN:OD1	1:E:377:ARG:NH2	2.37	0.57
1:H:33:ARG:NH1	7:5:20:GLY:O	2.37	0.57
1:I:651:ASN:ND2	1:I:917:TYR:OH	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:569:ILE:HA	1:K:572:LEU:HD22	1.86	0.57
1:L:135:TRP:CZ3	1:L:156:THR:HB	2.39	0.57
1:L:298:VAL:HB	1:L:317:MET:HG2	1.86	0.57
1:A:604:ASP:OD1	1:A:604:ASP:N	2.37	0.57
1:A:831:TYR:HB3	1:A:838:GLN:NE2	2.20	0.57
1:D:239:GLN:HE21	1:D:240:ALA:H	1.50	0.57
1:D:622:MET:HG3	1:D:627:ALA:HB2	1.85	0.57
1:D:731:TRP:CG	1:D:732:PRO:HD3	2.39	0.57
1:E:653:LEU:HD23	1:E:915:LEU:HG	1.85	0.57
1:H:670:ARG:NH1	1:H:944:PRO:O	2.36	0.57
1:I:244:PRO:HD3	1:I:253:ASP:C	2.25	0.57
1:J:360:ASP:OD1	1:J:361:ARG:N	2.36	0.57
1:K:771:LEU:HD13	1:K:777:GLY:HA3	1.86	0.57
1:B:161:ALA:HB3	1:B:198:GLN:HB3	1.84	0.57
1:B:384:TRP:NE1	1:C:781:PHE:O	2.28	0.57
1:C:637:ASP:OD1	1:C:637:ASP:N	2.37	0.57
1:D:137:THR:HG22	1:D:152:ASP:HB2	1.87	0.57
1:G:377:ARG:HB3	1:G:388:VAL:HG11	1.85	0.57
1:H:155:LYS:HG3	1:H:261:PHE:CZ	2.39	0.57
1:H:405:ASP:OD2	1:H:463:ASN:ND2	2.38	0.57
1:I:132:PRO:HB3	1:I:158:GLY:HA2	1.86	0.57
1:L:405:ASP:OD2	1:L:463:ASN:ND2	2.35	0.57
1:G:319:ASN:H	1:G:319:ASN:HD22	1.53	0.57
1:H:253:ASP:OD1	1:H:254:LEU:N	2.36	0.57
2:N:414:GLU:OE2	2:N:472:THR:OG1	2.23	0.57
7:6:12:ARG:NH2	7:6:15:THR:O	2.37	0.57
1:A:433:ASP:N	1:A:433:ASP:OD1	2.37	0.57
1:C:152:ASP:O	1:C:154:THR:N	2.38	0.57
1:C:914:THR:OG1	1:C:915:LEU:N	2.38	0.57
1:E:333:LEU:HD23	1:E:562:VAL:HG11	1.86	0.57
1:G:135:TRP:NE1	1:G:156:THR:OG1	2.38	0.57
1:I:113:PHE:HE2	1:I:553:GLY:H	1.53	0.57
1:J:4:PRO:HG2	6:U:58:GLN:HE21	1.70	0.57
1:J:327:ARG:NH1	1:J:591:MET:O	2.36	0.57
1:K:389:ASP:OD1	1:K:540:ASN:ND2	2.27	0.57
1:K:590:ASN:HB2	1:K:602:ARG:HG3	1.87	0.57
1:L:364:GLU:HB2	1:L:708:LEU:HB2	1.86	0.57
1:D:138:LYS:HA	1:D:149:GLN:HA	1.85	0.57
1:E:731:TRP:N	1:E:732:PRO:HD2	2.19	0.57
1:H:744:GLU:OE2	1:H:747:ARG:NH1	2.38	0.57
1:I:483:ASP:OD1	1:I:507:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:423:TYR:HE1	1:K:263:VAL:HG22	1.69	0.57
1:K:755:ASN:O	1:K:763:LYS:NZ	2.35	0.57
2:N:70:ASN:HB2	2:N:73:ASN:HB2	1.85	0.57
2:N:385:VAL:HG13	2:N:416:MET:HG2	1.87	0.57
1:D:911:ASP:OD1	1:D:911:ASP:N	2.29	0.57
1:E:726:ASP:N	1:E:726:ASP:OD1	2.37	0.57
1:F:417:THR:HG22	1:F:457:VAL:HG13	1.87	0.57
1:A:445:ALA:N	1:B:152:ASP:O	2.37	0.57
1:A:771:LEU:HD13	1:A:777:GLY:HA3	1.87	0.57
1:B:121:TYR:HA	1:C:824:ASN:OD1	2.05	0.57
1:C:481:LEU:HD23	1:C:529:MET:HE3	1.87	0.57
1:C:644:ASN:HB3	1:C:925:VAL:HG12	1.87	0.57
1:C:726:ASP:OD1	1:C:726:ASP:N	2.32	0.57
1:E:167:ILE:HD13	1:E:282:ILE:HB	1.86	0.57
1:E:173:LEU:HD13	1:E:185:LYS:HZ3	1.70	0.57
1:F:107:LEU:HD11	1:F:593:LEU:HD11	1.85	0.57
1:G:239:GLN:HB3	1:G:241:LYS:HZ1	1.70	0.57
1:H:162:THR:HG23	1:H:193:PHE:CE2	2.40	0.57
1:H:230:ALA:O	1:H:239:GLN:NE2	2.37	0.57
1:H:916:LEU:HD22	1:H:917:TYR:H	1.69	0.57
1:B:728:SER:OG	1:B:729:VAL:N	2.38	0.56
1:D:486:LYS:HG2	1:D:509:VAL:HG22	1.86	0.56
1:E:198:GLN:NE2	1:F:839:GLY:O	2.23	0.56
1:E:561:GLN:NE2	1:F:756:VAL:O	2.37	0.56
1:L:614:ASN:N	1:L:614:ASN:OD1	2.37	0.56
1:B:235:GLU:OE1	1:B:235:GLU:N	2.37	0.56
1:D:639:HIS:HD2	1:F:25:SER:H	1.53	0.56
1:H:352:LEU:HB3	6:V:110:GLY:HA2	1.87	0.56
1:H:423:TYR:O	1:H:449:GLN:NE2	2.38	0.56
1:I:134:GLN:HG2	1:I:155:LYS:HD3	1.87	0.56
1:I:480:TYR:OH	1:I:538:PRO:HD3	2.05	0.56
1:J:590:ASN:OD1	1:J:602:ARG:NE	2.36	0.56
5:Q:74:ALA:HA	5:Q:77:LEU:HB3	1.86	0.56
1:A:135:TRP:CH2	1:A:309:GLU:HB2	2.40	0.56
1:A:450:ASN:HD21	1:B:154:THR:HG23	1.70	0.56
1:D:648:SER:OG	1:D:922:VAL:O	2.21	0.56
1:G:294:ASP:O	1:G:319:ASN:ND2	2.37	0.56
1:G:410:TYR:HE1	1:H:414:LEU:HD21	1.69	0.56
1:K:198:GLN:HG3	1:K:199:VAL:N	2.18	0.56
1:L:602:ARG:HD2	5:Q:80:SER:HB2	1.87	0.56
5:P:16:TYR:HB3	5:P:18:THR:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:56:ASN:N	5:P:56:ASN:OD1	2.36	0.56
1:F:415:ASN:O	1:F:417:THR:N	2.38	0.56
1:F:427:LYS:HB2	1:F:442:LYS:HD2	1.88	0.56
1:J:682:ARG:NH2	1:J:910:MET:SD	2.79	0.56
2:N:326:VAL:HG23	3:O:7:VAL:HG23	1.87	0.56
4:M:116:LEU:O	4:M:120:VAL:HG23	2.06	0.56
6:U:2:SER:OG	6:U:3:LYS:O	2.23	0.56
1:D:339:THR:OG1	1:D:359:GLN:NE2	2.33	0.56
1:D:711:THR:O	1:D:711:THR:OG1	2.22	0.56
1:H:661:THR:OG1	1:H:662:ASN:N	2.36	0.56
1:I:762:THR:HG22	1:I:763:LYS:H	1.69	0.56
1:J:602:ARG:HG2	5:P:35:THR:HG23	1.88	0.56
1:J:635:ARG:NH1	1:J:932:HIS:O	2.39	0.56
5:R:60:ASP:N	5:R:60:ASP:OD1	2.37	0.56
1:C:151:LYS:HG2	1:C:154:THR:HG21	1.87	0.56
1:E:389:ASP:OD1	1:E:540:ASN:ND2	2.31	0.56
1:G:804:GLN:NE2	1:I:552:ASN:O	2.39	0.56
1:J:825:ASN:HD21	1:L:124:LEU:HB2	1.70	0.56
1:L:234:ASN:HD21	1:L:238:GLY:HA3	1.69	0.56
7:5:12:ARG:NH2	7:5:15:THR:O	2.38	0.56
1:C:470:LYS:NZ	1:C:515:ASP:OD1	2.34	0.56
1:C:724:MET:HG2	1:C:729:VAL:HG23	1.88	0.56
1:F:456:ASN:OD1	1:F:457:VAL:N	2.38	0.56
1:G:94:LEU:HD21	1:G:617:ALA:HB1	1.88	0.56
1:J:360:ASP:OD1	1:J:942:ARG:NH2	2.38	0.56
1:B:676:ARG:NH2	1:B:921:GLU:OE1	2.39	0.56
1:G:194:GLN:HB3	1:G:197:PRO:CD	2.31	0.56
1:G:328:ASP:O	1:G:330:PHE:N	2.39	0.56
1:K:485:TYR:HB3	1:K:513:LEU:HD21	1.88	0.56
1:L:93:VAL:HG21	1:L:630:LEU:HD23	1.86	0.56
1:B:486:LYS:HG2	1:B:509:VAL:HG12	1.86	0.56
1:C:538:PRO:O	1:C:544:ARG:NH1	2.39	0.56
1:F:463:ASN:O	1:F:467:ASN:ND2	2.30	0.56
1:J:663:VAL:HG13	1:J:905:PHE:HB2	1.88	0.56
1:L:188:TYR:HA	1:L:192:THR:HG23	1.87	0.56
7:6:23:ASN:C	7:6:25:ILE:H	2.10	0.56
1:B:523:ARG:NH2	1:B:799:GLN:OE1	2.36	0.56
1:G:793:SER:O	1:G:797:ASN:ND2	2.39	0.56
1:K:450:ASN:CB	1:L:156:THR:HA	2.36	0.56
1:K:636:ASN:HB3	1:K:639:HIS:CE1	2.41	0.56
1:L:320:ARG:NH2	1:L:479:LEU:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ASP:O	1:A:154:THR:N	2.37	0.55
1:D:150:GLU:HB3	1:F:443:ASP:HB3	1.86	0.55
1:H:349:ALA:O	1:L:933:ARG:NH2	2.39	0.55
1:H:489:PRO:HD3	1:H:508:VAL:HG12	1.88	0.55
1:J:296:HIS:CE1	1:J:317:MET:HG2	2.42	0.55
1:B:5:SER:HA	6:U:185:THR:HB	1.87	0.55
1:B:424:GLN:NE2	1:C:276:GLU:OE2	2.39	0.55
1:C:399:GLU:OE2	1:C:401:HIS:NE2	2.35	0.55
1:D:151:LYS:O	1:F:444:ASP:HA	2.07	0.55
1:D:163:GLY:N	1:D:199:VAL:HB	2.21	0.55
1:D:842:TYR:HE2	1:F:239:GLN:HG2	1.71	0.55
1:G:152:ASP:N	1:G:152:ASP:OD1	2.34	0.55
1:G:239:GLN:HE21	1:G:240:ALA:H	1.54	0.55
1:H:684:LYS:NZ	1:H:713:TYR:OH	2.40	0.55
1:I:715:ASN:O	1:I:871:TRP:NE1	2.36	0.55
2:N:60:ASP:OD1	2:N:60:ASP:N	2.37	0.55
5:Q:8:PHE:CD1	5:R:28:ARG:HG2	2.41	0.55
1:A:169:ASN:OD1	1:C:432:ASN:ND2	2.39	0.55
1:C:752:GLU:OE1	1:C:753:GLY:N	2.40	0.55
1:B:192:THR:OG1	1:B:214:ARG:NH1	2.39	0.55
1:B:230:ALA:HB3	1:B:239:GLN:HE22	1.71	0.55
1:B:327:ARG:NH1	1:B:703:GLY:O	2.40	0.55
1:C:141:GLN:O	1:C:146:GLY:N	2.33	0.55
1:E:651:ASN:N	1:E:651:ASN:OD1	2.40	0.55
1:H:588:ASP:OD2	1:H:602:ARG:NH2	2.40	0.55
1:I:609:ARG:NH1	1:I:611:ASP:OD1	2.40	0.55
1:L:588:ASP:OD1	1:L:591:MET:N	2.39	0.55
1:C:489:PRO:HG2	1:C:492:VAL:HG21	1.87	0.55
1:H:327:ARG:HH21	1:H:705:ILE:HG12	1.71	0.55
1:J:427:LYS:N	1:J:439:GLU:O	2.39	0.55
1:J:480:TYR:OH	1:J:538:PRO:HD3	2.07	0.55
1:L:648:SER:OG	1:L:676:ARG:NH2	2.39	0.55
1:B:360:ASP:OD1	1:B:361:ARG:N	2.39	0.55
1:D:437:GLU:OE1	1:D:437:GLU:N	2.39	0.55
1:D:538:PRO:O	1:D:544:ARG:NH2	2.39	0.55
1:E:320:ARG:HG2	1:E:505:ASN:OD1	2.07	0.55
1:F:178:GLU:OE1	1:F:179:THR:OG1	2.19	0.55
1:J:73:ARG:NH2	1:J:611:ASP:O	2.38	0.55
1:J:313:VAL:HG21	1:L:202:GLU:HG3	1.89	0.55
1:J:748:SER:OG	1:J:749:VAL:N	2.39	0.55
1:K:327:ARG:HH21	1:K:705:ILE:HG13	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:PHE:O	1:B:536:ASN:ND2	2.39	0.55
1:B:680:PHE:HB3	1:B:918:LEU:HD13	1.88	0.55
1:D:199:VAL:HG11	1:D:211:TYR:CE2	2.42	0.55
1:D:396:ARG:NH1	1:D:867:ASP:OD2	2.40	0.55
1:E:308:SER:OG	1:E:311:ASN:OD1	2.24	0.55
1:E:497:ASN:OD1	1:E:500:THR:OG1	2.21	0.55
1:F:46:ARG:NH2	7:4:28:SER:H	2.05	0.55
1:F:389:ASP:N	1:F:389:ASP:OD1	2.40	0.55
1:F:931:PRO:O	1:F:932:HIS:ND1	2.40	0.55
1:E:609:ARG:HH12	5:P:62:THR:HG21	1.71	0.55
1:G:135:TRP:N	1:G:154:THR:OG1	2.34	0.55
1:G:811:TYR:HD2	1:G:814:TYR:HB2	1.72	0.55
1:B:43:ASN:OD1	1:B:44:LYS:NZ	2.35	0.55
1:B:362:ASN:OD1	1:B:651:ASN:ND2	2.40	0.55
1:D:168:THR:OG1	1:D:185:LYS:NZ	2.39	0.55
1:D:731:TRP:CD2	1:D:732:PRO:HD3	2.41	0.55
1:F:277:TYR:HD1	1:F:277:TYR:H	1.55	0.55
1:G:228:SER:HB2	1:G:290:LEU:HD11	1.88	0.55
1:J:117:SER:HA	1:J:321:PRO:HG3	1.87	0.55
1:J:398:ILE:HD11	1:J:477:VAL:HG21	1.89	0.55
1:J:592:ILE:HG13	1:J:593:LEU:HD22	1.89	0.55
1:K:566:PHE:O	1:K:570:LYS:HB2	2.07	0.55
1:L:361:ARG:NH2	1:L:924:ASP:OD1	2.40	0.55
6:V:146:LEU:HG	6:V:148:PRO:HD3	1.89	0.55
1:A:87:ALA:HA	1:A:578:SER:HA	1.88	0.55
1:A:414:LEU:HD21	1:C:410:TYR:HE2	1.72	0.55
1:A:681:THR:HG21	1:A:712:PHE:HB3	1.89	0.55
1:B:377:ARG:NH1	1:B:386:SER:OG	2.40	0.55
1:F:320:ARG:HH11	1:F:479:LEU:HB3	1.72	0.55
1:H:151:LYS:HB3	1:H:154:THR:CG2	2.37	0.55
1:I:151:LYS:HB3	1:I:154:THR:HG21	1.88	0.55
1:I:306:ASN:O	1:I:311:ASN:ND2	2.39	0.55
1:I:759:CYS:HB3	1:I:800:PRO:HB3	1.87	0.55
1:J:327:ARG:NH1	1:J:593:LEU:O	2.39	0.55
1:K:155:LYS:HD3	1:K:283:LEU:HD13	1.87	0.55
1:L:20:ALA:H	1:L:47:ASN:HB3	1.71	0.55
1:L:161:ALA:H	1:L:198:GLN:HE22	1.53	0.55
1:B:250:GLN:NE2	1:B:251:PRO:O	2.41	0.54
1:D:456:ASN:OD1	1:D:456:ASN:N	2.37	0.54
1:F:140:LYS:HA	1:F:147:VAL:HA	1.88	0.54
1:F:298:VAL:HB	1:F:317:MET:HG2	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:666:SER:HB3	5:Q:16:TYR:CE1	2.43	0.54
1:H:688:THR:O	5:Q:28:ARG:NH2	2.40	0.54
1:K:306:ASN:O	1:K:311:ASN:ND2	2.40	0.54
1:D:199:VAL:HG11	1:D:211:TYR:HE2	1.73	0.54
1:H:403:VAL:HG23	1:H:465:GLN:HB3	1.89	0.54
1:I:462:ILE:HG12	1:I:463:ASN:H	1.70	0.54
1:J:134:GLN:OE1	1:J:155:LYS:NZ	2.31	0.54
1:J:257:ASP:N	1:J:257:ASP:OD1	2.41	0.54
1:J:550:LEU:HB3	1:J:556:VAL:HG11	1.87	0.54
1:K:497:ASN:OD1	1:K:500:THR:OG1	2.25	0.54
1:A:277:TYR:HD1	1:A:277:TYR:H	1.54	0.54
1:C:134:GLN:HA	1:C:155:LYS:H	1.70	0.54
1:G:156:THR:HG22	1:G:157:PHE:HD1	1.71	0.54
1:G:456:ASN:ND2	1:I:839:GLY:H	2.04	0.54
1:J:135:TRP:O	1:J:154:THR:OG1	2.14	0.54
1:J:433:ASP:OD1	1:J:434:GLY:N	2.41	0.54
1:K:196:GLU:CG	1:L:823:HIS:HB3	2.31	0.54
1:B:223:LYS:HE2	1:B:292:THR:HG21	1.90	0.54
1:F:480:TYR:OH	1:F:538:PRO:HD3	2.07	0.54
1:F:682:ARG:NH1	1:F:910:MET:SD	2.81	0.54
1:F:756:VAL:HG11	1:F:766:PHE:HB2	1.88	0.54
1:G:427:LYS:O	1:G:439:GLU:N	2.37	0.54
1:L:161:ALA:H	1:L:198:GLN:NE2	2.05	0.54
5:Q:12:LEU:HG	5:Q:15:PRO:CD	2.38	0.54
1:C:837:ARG:O	1:C:837:ARG:NE	2.34	0.54
1:H:486:LYS:HG2	1:H:509:VAL:HG12	1.89	0.54
1:H:818:THR:HB	1:H:820:PRO:HD2	1.90	0.54
1:L:155:LYS:HG3	1:L:261:PHE:CZ	2.33	0.54
1:A:384:TRP:NE1	1:B:781:PHE:O	2.36	0.54
1:A:823:HIS:NE2	1:C:239:GLN:OE1	2.40	0.54
1:C:172:LEU:HD13	1:C:193:PHE:HZ	1.71	0.54
1:D:480:TYR:OH	1:D:538:PRO:HD3	2.08	0.54
1:H:590:ASN:HD21	1:H:601:LEU:H	1.55	0.54
1:I:257:ASP:OD1	1:I:285:THR:OG1	2.23	0.54
1:J:410:TYR:HE1	1:K:414:LEU:HD21	1.72	0.54
1:K:135:TRP:CH2	1:K:309:GLU:HB2	2.43	0.54
1:K:217:LYS:N	1:K:286:GLU:O	2.34	0.54
5:P:12:LEU:HD22	5:P:15:PRO:HD3	1.89	0.54
1:A:539:ARG:NH2	1:B:404:GLU:OE2	2.34	0.54
1:D:401:HIS:CE1	1:F:544:ARG:HD3	2.42	0.54
1:E:648:SER:O	1:E:648:SER:OG	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:661:THR:HG22	1:F:909:PRO:HG3	1.90	0.54
1:F:908:ASP:N	1:F:908:ASP:OD1	2.36	0.54
1:J:190:ASP:HB3	1:J:236:LYS:HB3	1.90	0.54
1:K:161:ALA:HB1	1:K:198:GLN:HB2	1.89	0.54
1:K:443:ASP:HB3	1:L:151:LYS:H	1.71	0.54
1:L:667:ILE:HG22	1:L:668:PRO:O	2.08	0.54
1:A:244:PRO:HD3	1:A:255:ASP:N	2.23	0.54
1:B:8:PRO:HB3	6:U:18:GLY:HA3	1.89	0.54
1:C:485:TYR:CZ	1:C:528:PRO:HB3	2.43	0.54
1:C:662:ASN:HA	1:C:906:GLU:HA	1.89	0.54
1:E:135:TRP:CH2	1:E:309:GLU:HB2	2.43	0.54
1:F:172:LEU:HD22	1:F:193:PHE:HZ	1.72	0.54
1:G:400:ASN:ND2	1:G:518:ILE:O	2.41	0.54
1:C:607:SER:O	1:C:607:SER:OG	2.20	0.54
1:G:277:TYR:OH	1:G:280:ASP:OD2	2.20	0.54
1:K:445:ALA:HB3	1:K:449:GLN:HE21	1.73	0.54
1:A:835:THR:OG1	1:C:201:GLU:OE2	2.22	0.54
1:A:842:TYR:HE2	1:C:239:GLN:HG2	1.72	0.54
1:B:388:VAL:HG21	1:B:791:MET:HE1	1.90	0.54
1:B:651:ASN:N	1:B:651:ASN:OD1	2.39	0.54
1:D:730:SER:O	1:D:733:GLY:N	2.41	0.54
1:D:825:ASN:HD21	1:F:124:LEU:H	1.56	0.54
1:E:151:LYS:HB3	1:E:154:THR:HG21	1.90	0.54
1:H:113:PHE:HE1	1:H:324:ILE:H	1.55	0.54
1:I:188:TYR:HB2	1:I:256:ILE:HG21	1.88	0.54
1:J:670:ARG:HG3	1:J:671:ASN:N	2.22	0.54
1:J:821:PHE:HD1	1:L:194:GLN:HE22	1.53	0.54
1:K:354:ALA:O	1:K:940:TYR:OH	2.24	0.54
1:K:473:LEU:O	1:K:477:VAL:HG12	2.08	0.54
1:K:649:ALA:HA	1:K:922:VAL:HG22	1.89	0.54
1:K:825:ASN:O	1:K:825:ASN:ND2	2.40	0.54
1:A:88:VAL:HG23	1:A:619:PHE:HE2	1.73	0.53
1:A:417:THR:HG22	1:A:419:THR:H	1.72	0.53
1:E:24:LEU:HD22	1:F:639:HIS:HD1	1.73	0.53
1:E:440:TRP:CZ2	1:F:276:GLU:HG3	2.43	0.53
1:I:341:ASN:OD1	1:I:341:ASN:N	2.41	0.53
1:K:186:ASP:HB3	1:K:191:LYS:O	2.08	0.53
1:K:427:LYS:HD3	1:K:442:LYS:HG2	1.89	0.53
1:B:47:ASN:HD21	7:1:25:ILE:HG12	1.71	0.53
1:H:19:ASP:N	1:H:19:ASP:OD1	2.41	0.53
1:I:789:ASP:O	1:I:796:ARG:NH2	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:655:PRO:HG2	5:P:17:LEU:HD22	1.89	0.53
1:K:58:THR:HG23	1:L:736:ARG:NH2	2.23	0.53
1:K:237:GLY:HA3	1:L:821:PHE:HB3	1.90	0.53
1:K:331:VAL:HG13	1:K:364:GLU:HG2	1.90	0.53
2:N:185:TYR:HE1	2:N:194:VAL:HG23	1.72	0.53
1:A:676:ARG:NH2	1:A:921:GLU:OE1	2.41	0.53
1:E:18:GLN:HB3	1:E:22:GLU:HB2	1.88	0.53
1:G:152:ASP:HA	1:I:444:ASP:HA	1.90	0.53
1:J:793:SER:O	1:J:797:ASN:ND2	2.40	0.53
1:K:241:LYS:NZ	1:K:286:GLU:OE1	2.39	0.53
1:D:676:ARG:HE	1:D:921:GLU:HB3	1.73	0.53
1:D:837:ARG:HD2	1:E:457:VAL:CG2	2.37	0.53
1:E:52:PRO:HD3	7:3:11:PRO:HA	1.89	0.53
1:H:636:ASN:HB2	1:H:639:HIS:NE2	2.23	0.53
1:I:537:HIS:CD2	1:I:538:PRO:HD2	2.43	0.53
1:I:575:LEU:HB3	1:I:576:PRO:HD2	1.90	0.53
1:K:425:GLY:HA3	1:K:444:ASP:HB2	1.89	0.53
1:A:752:GLU:OE1	1:A:753:GLY:N	2.41	0.53
1:B:315:GLN:HE22	1:B:835:THR:HA	1.73	0.53
1:D:922:VAL:HB	1:D:944:PRO:HD2	1.91	0.53
1:G:135:TRP:CH2	1:G:309:GLU:HB2	2.43	0.53
1:G:240:ALA:HB3	1:G:288:VAL:HG23	1.91	0.53
1:G:842:TYR:HE2	1:I:239:GLN:HG2	1.73	0.53
1:I:134:GLN:HA	1:I:154:THR:O	2.07	0.53
1:K:214:ARG:HH12	1:K:241:LYS:HZ1	1.56	0.53
1:K:728:SER:OG	1:K:729:VAL:N	2.41	0.53
1:L:76:THR:HG22	1:L:77:THR:H	1.74	0.53
1:L:813:ASP:N	1:L:813:ASP:OD1	2.39	0.53
5:P:10:GLY:HA2	5:P:13:PHE:HD1	1.74	0.53
1:A:239:GLN:HE21	1:A:240:ALA:H	1.56	0.53
1:A:277:TYR:CZ	1:A:279:ALA:HB2	2.44	0.53
1:E:192:THR:HB	1:E:214:ARG:HD2	1.89	0.53
1:E:449:GLN:HG3	1:E:450:ASN:H	1.73	0.53
1:G:584:ASN:N	1:G:584:ASN:OD1	2.41	0.53
1:I:277:TYR:CZ	1:I:279:ALA:HB2	2.44	0.53
1:L:190:ASP:OD1	1:L:191:LYS:N	2.42	0.53
1:A:457:VAL:O	1:C:837:ARG:NH1	2.42	0.53
1:C:167:ILE:HD13	1:C:282:ILE:HG23	1.89	0.53
1:C:480:TYR:OH	1:C:538:PRO:HD3	2.09	0.53
1:I:396:ARG:NH1	1:I:867:ASP:OD2	2.40	0.53
1:I:445:ALA:HB3	1:I:450:ASN:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:83:ARG:HG3	1:K:582:GLU:HB2	1.90	0.53
1:K:379:ARG:NH2	1:L:789:ASP:OD2	2.40	0.53
1:L:135:TRP:HZ3	1:L:156:THR:HG21	1.74	0.53
5:P:9:GLU:OE2	5:P:10:GLY:N	2.42	0.53
6:V:36:ALA:HB1	6:V:40:MET:HB2	1.91	0.53
1:B:135:TRP:CZ3	1:B:137:THR:HB	2.43	0.53
1:B:436:GLU:HG2	1:C:270:ALA:HB1	1.89	0.53
1:C:172:LEU:HD22	1:C:193:PHE:CE1	2.44	0.53
1:D:441:GLU:HG2	1:D:443:ASP:H	1.72	0.53
1:E:135:TRP:N	1:E:154:THR:OG1	2.38	0.53
1:F:186:ASP:OD1	1:F:187:ILE:N	2.42	0.53
1:H:13:MET:HG3	1:I:941:LEU:HD22	1.90	0.53
1:I:653:LEU:HB3	1:I:915:LEU:HD12	1.90	0.53
1:I:813:ASP:OD1	1:I:813:ASP:N	2.41	0.53
1:J:202:GLU:HG3	1:J:206:GLU:HB2	1.89	0.53
1:L:552:ASN:O	1:L:552:ASN:ND2	2.41	0.53
2:N:40:ASN:O	2:N:40:ASN:ND2	2.41	0.53
1:D:414:LEU:HD21	1:F:410:TYR:HE1	1.74	0.53
1:F:711:THR:O	1:F:711:THR:OG1	2.20	0.53
1:G:715:ASN:HB2	1:G:871:TRP:NE1	2.24	0.53
1:K:51:ALA:HB1	1:L:882:MET:HG3	1.91	0.53
1:K:190:ASP:O	1:K:192:THR:HG22	2.09	0.53
4:M:178:VAL:HG21	6:U:207:LEU:HD21	1.91	0.53
1:B:8:PRO:HG2	1:B:11:ALA:HB3	1.90	0.53
1:G:817:VAL:HG12	1:I:237:GLY:HA2	1.90	0.53
1:B:162:THR:HA	1:B:193:PHE:CE2	2.45	0.52
1:B:461:GLU:OE1	1:B:461:GLU:N	2.43	0.52
1:D:639:HIS:HB3	1:F:24:LEU:HD22	1.90	0.52
1:E:65:THR:HB	1:E:618:THR:HG22	1.90	0.52
1:E:194:GLN:O	1:E:197:PRO:HD2	2.09	0.52
1:F:135:TRP:CH2	1:F:309:GLU:HB3	2.44	0.52
1:F:202:GLU:O	1:F:203:ASN:C	2.46	0.52
1:G:825:ASN:HD21	1:I:124:LEU:HG	1.74	0.52
1:G:842:TYR:OH	1:I:286:GLU:OE2	2.27	0.52
1:I:531:ASN:HB2	1:I:714:LEU:HD11	1.91	0.52
1:J:153:VAL:HG12	1:J:156:THR:HG23	1.92	0.52
1:L:150:GLU:C	1:L:152:ASP:N	2.63	0.52
1:L:156:THR:HG23	1:L:157:PHE:N	2.24	0.52
4:M:228:PRO:HB2	6:U:4:GLU:HB3	1.91	0.52
5:Q:14:SER:O	5:R:15:PRO:HB2	2.09	0.52
1:C:234:ASN:HD21	1:C:238:GLY:HA3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:836:MET:HA	1:E:410:TYR:OH	2.08	0.52
1:F:126:PRO:HG2	1:F:129:ALA:HB2	1.91	0.52
1:F:161:ALA:O	1:F:199:VAL:HG23	2.09	0.52
1:L:922:VAL:HB	1:L:944:PRO:HD2	1.90	0.52
2:N:186:LEU:O	2:N:187:GLN:C	2.46	0.52
4:M:227:THR:HG22	4:M:229:ASN:H	1.75	0.52
1:B:194:GLN:O	1:B:197:PRO:HD2	2.09	0.52
1:C:590:ASN:HB2	1:C:602:ARG:HE	1.73	0.52
1:F:139:GLU:OE1	1:F:140:LYS:N	2.40	0.52
1:B:427:LYS:HD2	1:B:441:GLU:HG3	1.91	0.52
1:D:433:ASP:OD1	1:D:434:GLY:N	2.33	0.52
1:H:288:VAL:HG23	1:H:290:LEU:HB2	1.92	0.52
1:J:19:ASP:O	1:J:22:GLU:N	2.36	0.52
1:J:406:GLU:HG2	1:L:479:LEU:HD11	1.91	0.52
4:M:373:ALA:HA	6:U:100:ARG:HB2	1.92	0.52
1:C:256:ILE:HD13	1:C:286:GLU:HB3	1.91	0.52
1:C:693:SER:OG	1:K:750:ASP:OD2	2.27	0.52
1:F:134:GLN:OE1	1:F:155:LYS:NZ	2.32	0.52
1:G:758:GLN:HE21	1:I:549:LEU:HD21	1.74	0.52
1:H:389:ASP:OD1	1:H:540:ASN:ND2	2.34	0.52
1:H:498:THR:HG23	1:H:503:TYR:CE2	2.44	0.52
1:L:445:ALA:HB3	1:L:450:ASN:HB2	1.90	0.52
1:A:572:LEU:HD13	1:A:928:VAL:HG21	1.92	0.52
1:A:867:ASP:N	1:A:867:ASP:OD1	2.41	0.52
1:B:548:MET:HE3	1:C:523:ARG:HG3	1.92	0.52
1:B:552:ASN:HB3	1:C:522:ALA:HB2	1.91	0.52
1:D:119:THR:OG1	1:D:120:ALA:N	2.42	0.52
1:D:756:VAL:HG23	1:F:561:GLN:HE22	1.75	0.52
1:E:575:LEU:HB3	1:E:576:PRO:HD2	1.90	0.52
1:G:198:GLN:OE1	1:H:839:GLY:N	2.29	0.52
1:H:748:SER:HA	5:R:54:VAL:HG13	1.92	0.52
1:I:212:GLY:HA2	1:I:282:ILE:O	2.10	0.52
1:I:523:ARG:NH2	1:I:799:GLN:OE1	2.33	0.52
1:J:423:TYR:HB3	1:K:261:PHE:HB3	1.92	0.52
1:J:845:ASN:HB3	1:L:239:GLN:HE22	1.75	0.52
5:S:35:THR:HA	5:S:43:PRO:HG2	1.90	0.52
1:A:139:GLU:HB2	1:A:150:GLU:HB2	1.90	0.52
1:D:388:VAL:HG21	1:D:791:MET:HE1	1.92	0.52
1:F:670:ARG:NH2	1:F:944:PRO:O	2.43	0.52
1:F:760:ASN:HB2	5:P:54:VAL:HG21	1.91	0.52
1:J:564:GLN:HE21	1:J:569:ILE:HB	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:662:ASN:ND2	5:Q:22:PRO:HG3	2.25	0.52
1:L:282:ILE:HD12	1:L:284:TYR:HE1	1.75	0.52
1:A:706:PRO:HA	1:A:711:THR:HG23	1.91	0.52
1:C:575:LEU:HB3	1:C:576:PRO:HD2	1.92	0.52
1:C:640:ASP:OD1	1:C:640:ASP:N	2.35	0.52
1:D:715:ASN:ND2	1:D:866:CYS:O	2.43	0.52
1:E:399:GLU:OE2	1:E:401:HIS:NE2	2.43	0.52
1:F:188:TYR:HA	1:F:192:THR:HA	1.91	0.52
1:F:241:LYS:HG2	1:F:286:GLU:HG3	1.92	0.52
1:G:319:ASN:OD1	1:G:501:TYR:OH	2.23	0.52
1:H:339:THR:HB	1:J:740:PRO:HG2	1.90	0.52
1:I:240:ALA:HB3	1:I:288:VAL:HB	1.92	0.52
1:I:765:TRP:O	1:I:766:PHE:C	2.43	0.52
1:K:539:ARG:NH2	1:L:404:GLU:OE2	2.34	0.52
5:P:40:PRO:O	5:P:41:VAL:C	2.48	0.52
1:A:662:ASN:HA	1:A:906:GLU:HA	1.92	0.52
1:B:214:ARG:NH2	1:B:286:GLU:OE2	2.43	0.52
1:G:821:PHE:HB3	1:I:237:GLY:HA3	1.91	0.52
1:I:588:ASP:OD2	1:I:602:ARG:NH2	2.43	0.52
1:J:523:ARG:NH2	1:J:799:GLN:OE1	2.43	0.52
1:J:735:ASP:OD1	1:L:63:ARG:NH1	2.43	0.52
1:L:417:THR:HG23	1:L:458:TYR:H	1.74	0.52
1:L:812:LYS:H	1:L:812:LYS:HD2	1.74	0.52
4:M:257:THR:HA	4:M:260:ARG:HH11	1.74	0.52
1:A:60:ARG:HD2	1:A:624:HIS:CE1	2.45	0.52
1:A:139:GLU:OE1	1:A:141:GLN:HB2	2.10	0.52
1:C:596:SER:C	1:C:598:GLY:N	2.62	0.52
1:D:59:ASP:N	1:D:59:ASP:OD1	2.43	0.52
1:E:720:LYS:HG2	1:E:906:GLU:HB3	1.92	0.52
1:F:167:ILE:HD13	1:F:282:ILE:HG23	1.92	0.52
1:L:608:VAL:HG21	5:Q:69:ALA:HB1	1.91	0.52
1:L:608:VAL:HG22	1:L:609:ARG:HG3	1.92	0.52
1:C:417:THR:HG21	1:C:453:CYS:HB2	1.91	0.51
1:F:111:PRO:HD2	1:F:604:ASP:HB3	1.93	0.51
1:G:231:ARG:O	1:G:240:ALA:HB2	2.10	0.51
1:G:651:ASN:HB3	1:G:919:LEU:HD12	1.92	0.51
1:H:241:LYS:HB2	1:H:254:LEU:HD22	1.92	0.51
1:K:172:LEU:CD1	1:K:193:PHE:CZ	2.92	0.51
1:L:94:LEU:HG	1:L:95:ASP:N	2.25	0.51
5:Q:5:GLY:C	5:Q:7:ALA:N	2.63	0.51
5:Q:10:GLY:C	5:Q:12:LEU:N	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:ASP:OD1	1:A:640:ASP:N	2.43	0.51
1:D:468:LEU:HD21	1:E:464:LEU:HD22	1.92	0.51
1:G:515:ASP:OD1	1:G:516:ALA:N	2.38	0.51
1:H:13:MET:HB3	1:I:925:VAL:HG21	1.93	0.51
1:H:214:ARG:NH2	1:H:286:GLU:OE2	2.43	0.51
1:K:196:GLU:HG2	1:L:823:HIS:CB	2.29	0.51
1:K:731:TRP:N	1:K:732:PRO:HD2	2.25	0.51
1:C:320:ARG:NH2	1:C:479:LEU:O	2.43	0.51
1:D:738:LEU:HD23	1:D:738:LEU:H	1.75	0.51
1:F:96:MET:HG2	1:F:574:LEU:HD22	1.91	0.51
1:F:757:ALA:O	1:F:759:CYS:N	2.42	0.51
1:G:428:ILE:HD12	1:H:169:ASN:HB3	1.91	0.51
1:J:188:TYR:HA	1:J:192:THR:HG23	1.92	0.51
1:L:47:ASN:OD1	7:9:27:THR:OG1	2.27	0.51
5:Q:5:GLY:HA3	5:Q:8:PHE:O	2.09	0.51
1:B:217:LYS:NZ	1:B:257:ASP:OD2	2.39	0.51
1:B:277:TYR:CE2	1:B:279:ALA:HB2	2.45	0.51
1:C:135:TRP:NE1	1:C:156:THR:OG1	2.41	0.51
1:C:922:VAL:HG23	1:C:944:PRO:HG2	1.93	0.51
1:D:135:TRP:NE1	1:D:156:THR:OG1	2.36	0.51
1:D:443:ASP:N	1:D:443:ASP:OD1	2.43	0.51
1:D:924:ASP:HB3	1:D:942:ARG:HG3	1.93	0.51
1:E:731:TRP:O	1:E:733:GLY:N	2.44	0.51
1:F:720:LYS:HG3	1:F:744:GLU:HG3	1.92	0.51
1:G:240:ALA:HB3	1:G:288:VAL:CG2	2.39	0.51
1:H:590:ASN:HB2	1:H:602:ARG:HE	1.76	0.51
1:J:495:PRO:HG3	1:J:502:GLU:HG3	1.93	0.51
1:K:731:TRP:O	1:K:733:GLY:N	2.44	0.51
1:L:319:ASN:ND2	1:L:505:ASN:OD1	2.42	0.51
1:L:536:ASN:HB3	1:L:596:SER:O	2.10	0.51
1:L:720:LYS:HG2	1:L:906:GLU:HB3	1.92	0.51
7:5:17:PRO:HB2	7:5:19:MET:HG2	1.92	0.51
1:B:151:LYS:HE2	1:B:218:LYS:HD3	1.91	0.51
1:B:339:THR:OG1	1:B:359:GLN:OE1	2.21	0.51
1:B:644:ASN:HB3	1:B:925:VAL:HG12	1.91	0.51
1:B:842:TYR:CG	1:B:843:PRO:HD2	2.45	0.51
1:D:494:LEU:HD11	1:D:506:GLY:HA3	1.91	0.51
1:D:657:PRO:HG2	1:D:660:ALA:HB2	1.93	0.51
1:E:239:GLN:HG2	1:F:842:TYR:HE2	1.74	0.51
1:E:336:TYR:CZ	1:E:565:LYS:HG3	2.46	0.51
1:H:107:LEU:HD23	1:H:108:ASP:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:785:GLU:OE1	1:K:785:GLU:N	2.43	0.51
1:L:199:VAL:HG22	1:L:206:GLU:HG2	1.93	0.51
1:A:263:VAL:HG22	1:C:423:TYR:HE1	1.75	0.51
1:B:438:SER:HB2	1:C:278:LYS:HB3	1.91	0.51
1:B:446:ILE:N	1:B:449:GLN:HB2	2.26	0.51
1:D:495:PRO:HG3	1:D:502:GLU:HB3	1.92	0.51
1:D:640:ASP:OD1	1:D:640:ASP:N	2.41	0.51
1:F:315:GLN:N	1:F:315:GLN:OE1	2.44	0.51
1:H:158:GLY:O	1:H:159:VAL:C	2.49	0.51
1:I:705:ILE:O	1:I:709:ASP:HB2	2.10	0.51
1:J:345:LEU:HD23	1:J:569:ILE:HD12	1.93	0.51
1:L:114:LYS:HE2	1:L:116:TYR:O	2.11	0.51
1:L:759:CYS:SG	1:L:760:ASN:N	2.82	0.51
1:A:190:ASP:OD1	1:A:191:LYS:N	2.41	0.51
1:C:486:LYS:HB2	1:C:507:ARG:HH11	1.76	0.51
1:C:897:SER:OG	1:C:899:HIS:NE2	2.25	0.51
1:D:552:ASN:HD22	1:E:522:ALA:HB2	1.74	0.51
1:D:639:HIS:CD2	1:F:25:SER:H	2.28	0.51
1:E:50:VAL:HG22	7:3:12:ARG:HB2	1.91	0.51
1:H:756:VAL:HG13	1:H:763:LYS:HG2	1.93	0.51
1:J:107:LEU:HD23	1:J:556:VAL:HB	1.93	0.51
2:N:454:CYS:SG	2:N:455:ARG:N	2.84	0.51
5:R:45:ASN:O	5:R:46:SER:OG	2.28	0.51
1:A:514:VAL:HA	1:A:518:ILE:HG21	1.93	0.51
1:A:590:ASN:HB2	1:A:602:ARG:HG3	1.91	0.51
1:A:663:VAL:HG13	1:A:905:PHE:HB2	1.93	0.51
1:C:489:PRO:HD3	1:C:508:VAL:HG12	1.92	0.51
1:D:83:ARG:HG3	1:D:582:GLU:HB3	1.93	0.51
1:D:234:ASN:HD21	1:D:238:GLY:HA3	1.75	0.51
1:D:358:LEU:HD21	1:D:947:ALA:HB2	1.93	0.51
1:D:474:TYR:O	1:D:475:SER:C	2.46	0.51
1:J:240:ALA:O	1:J:241:LYS:HD3	2.11	0.51
1:J:443:ASP:OD1	1:J:443:ASP:N	2.43	0.51
1:A:696:ASP:OD1	1:A:696:ASP:N	2.43	0.51
1:D:478:ALA:C	1:D:480:TYR:N	2.56	0.51
1:E:812:LYS:H	1:E:812:LYS:HD2	1.75	0.51
1:F:194:GLN:O	1:F:197:PRO:HD2	2.11	0.51
1:G:789:ASP:OD2	1:I:379:ARG:NH2	2.30	0.51
1:K:302:GLY:O	1:K:491:ASN:ND2	2.44	0.51
1:L:358:LEU:HD23	1:L:361:ARG:HH12	1.76	0.51
1:A:7:MET:HG3	1:A:12:TYR:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:ARG:NH2	1:E:789:ASP:OD2	2.34	0.51
1:E:676:ARG:NH2	1:E:921:GLU:OE1	2.44	0.51
1:G:539:ARG:NH2	1:H:404:GLU:OE2	2.44	0.51
1:J:922:VAL:HG12	1:J:944:PRO:HG2	1.93	0.51
2:N:237:PRO:HA	2:N:268:TYR:CG	2.46	0.51
1:A:330:PHE:CZ	1:A:385:ASN:HB2	2.46	0.50
1:B:119:THR:OG1	1:B:120:ALA:N	2.44	0.50
1:B:480:TYR:OH	1:B:538:PRO:HD3	2.11	0.50
1:C:103:ILE:H	1:C:103:ILE:HD12	1.75	0.50
1:C:651:ASN:HB3	1:C:919:LEU:HB3	1.93	0.50
1:C:711:THR:O	1:C:711:THR:OG1	2.29	0.50
1:H:426:VAL:HG12	1:H:440:TRP:HB3	1.93	0.50
1:I:188:TYR:HA	1:I:192:THR:HG23	1.93	0.50
1:J:134:GLN:HA	1:J:154:THR:O	2.11	0.50
2:N:185:TYR:O	2:N:186:LEU:C	2.45	0.50
1:A:99:THR:HB	1:A:615:LEU:HD11	1.94	0.50
1:A:308:SER:OG	1:A:311:ASN:OD1	2.29	0.50
1:D:392:ASP:HB3	1:D:395:VAL:HG12	1.92	0.50
1:G:103:ILE:HG23	1:G:613:VAL:HG22	1.94	0.50
1:H:135:TRP:HE1	1:H:156:THR:HG23	1.76	0.50
1:J:446:ILE:HG23	1:J:447:SER:H	1.75	0.50
1:J:923:PHE:O	1:J:942:ARG:HA	2.11	0.50
1:L:102:ASP:OD1	1:L:559:HIS:NE2	2.44	0.50
1:A:427:LYS:HD2	1:A:441:GLU:HB3	1.92	0.50
1:D:286:GLU:OE2	1:E:842:TYR:OH	2.30	0.50
1:D:415:ASN:HD21	1:D:418:GLY:HA2	1.77	0.50
1:F:785:GLU:OE1	1:F:785:GLU:N	2.42	0.50
1:H:269:PRO:HD2	1:H:273:SER:HB3	1.94	0.50
1:I:83:ARG:HA	1:I:582:GLU:HB2	1.92	0.50
1:K:914:THR:OG1	1:K:915:LEU:N	2.44	0.50
1:L:94:LEU:HB2	1:L:619:PHE:CE2	2.46	0.50
1:L:187:ILE:HG12	1:L:189:ALA:H	1.76	0.50
1:A:804:GLN:HE22	1:C:551:GLY:HA3	1.76	0.50
1:E:531:ASN:HB2	1:E:714:LEU:HD11	1.93	0.50
1:F:931:PRO:HD2	1:F:935:VAL:HG13	1.93	0.50
1:G:240:ALA:O	1:G:288:VAL:HG23	2.11	0.50
1:H:155:LYS:HG3	1:H:261:PHE:HZ	1.76	0.50
1:H:589:VAL:HG21	1:H:606:ALA:HB1	1.92	0.50
1:H:685:THR:O	5:Q:28:ARG:NH1	2.44	0.50
1:K:813:ASP:OD1	1:K:813:ASP:N	2.44	0.50
1:L:698:TYR:O	1:L:700:VAL:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:11:TRP:HZ2	6:V:69:LEU:HD12	1.77	0.50
1:A:385:ASN:OD1	1:A:546:ARG:HD2	2.12	0.50
1:A:456:ASN:HD21	1:C:838:GLN:HA	1.76	0.50
1:A:575:LEU:HD21	1:A:634:LEU:HD23	1.92	0.50
1:B:237:GLY:HA3	1:C:821:PHE:HB3	1.92	0.50
1:B:417:THR:HA	1:B:457:VAL:HG12	1.94	0.50
1:C:671:ASN:OD1	1:C:672:TRP:N	2.44	0.50
1:D:173:LEU:HB2	1:D:185:LYS:HD3	1.92	0.50
1:H:721:VAL:HG22	1:H:905:PHE:HD1	1.76	0.50
1:I:476:ASN:HB2	1:I:537:HIS:HE1	1.77	0.50
6:U:2:SER:HB3	6:U:199:ASN:HA	1.92	0.50
1:B:20:ALA:HA	1:B:23:TYR:CE2	2.47	0.50
1:B:102:ASP:OD2	1:C:763:LYS:NZ	2.45	0.50
1:C:367:TYR:HD2	1:C:565:LYS:HZ3	1.58	0.50
1:D:200:GLY:HA3	1:D:206:GLU:CD	2.32	0.50
1:F:662:ASN:ND2	5:P:22:PRO:HG2	2.26	0.50
1:G:196:GLU:HG2	1:H:823:HIS:HB3	1.93	0.50
1:H:527:ASP:HA	1:H:530:ASP:HB2	1.92	0.50
1:I:684:LYS:NZ	1:I:713:TYR:OH	2.34	0.50
1:J:203:ASN:N	1:J:203:ASN:OD1	2.44	0.50
1:K:230:ALA:O	1:K:239:GLN:NE2	2.44	0.50
5:Q:41:VAL:HG22	5:Q:43:PRO:HG3	1.92	0.50
1:B:103:ILE:HG12	1:B:613:VAL:HG22	1.94	0.50
1:B:426:VAL:HG12	1:B:440:TRP:HB3	1.93	0.50
1:B:604:ASP:OD1	1:B:604:ASP:N	2.35	0.50
1:D:137:THR:CG2	1:D:152:ASP:HB2	2.41	0.50
1:F:289:ASN:N	1:F:289:ASN:OD1	2.44	0.50
1:I:429:THR:HG22	1:I:430:ASN:H	1.76	0.50
1:I:771:LEU:HD21	1:I:778:TYR:CZ	2.47	0.50
1:L:83:ARG:HA	1:L:582:GLU:HB2	1.92	0.50
5:P:10:GLY:HA2	5:P:13:PHE:CD1	2.46	0.50
1:B:246:ASN:ND2	1:B:247:GLU:O	2.45	0.50
1:C:447:SER:O	1:C:449:GLN:HG2	2.12	0.50
1:E:67:ARG:HG3	1:E:616:TYR:CZ	2.46	0.50
1:F:371:LEU:HB3	1:F:377:ARG:HD3	1.94	0.50
1:G:719:LYS:NZ	1:G:908:ASP:OD1	2.29	0.50
1:I:510:ALA:HA	1:I:832:LEU:O	2.12	0.50
1:J:198:GLN:HE22	1:K:840:GLN:HB3	1.75	0.50
1:K:193:PHE:O	1:K:194:GLN:C	2.46	0.50
1:K:392:ASP:OD2	1:K:395:VAL:N	2.44	0.50
1:L:711:THR:O	1:L:711:THR:OG1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ASN:HA	1:C:825:ASN:HD22	1.76	0.50
1:B:479:LEU:HD11	1:C:406:GLU:HG2	1.93	0.50
1:E:91:ASN:OD1	1:E:628:SER:OG	2.30	0.50
1:H:485:TYR:CE2	1:H:528:PRO:HB3	2.46	0.50
1:J:234:ASN:HD21	1:J:238:GLY:HA3	1.76	0.50
1:K:424:GLN:NE2	1:L:276:GLU:OE2	2.44	0.50
1:K:513:LEU:HD13	1:K:819:LEU:HD22	1.94	0.50
1:K:696:ASP:OD1	1:K:696:ASP:N	2.45	0.50
1:L:656:ILE:HD13	1:L:682:ARG:HH12	1.75	0.50
5:P:34:SER:OG	5:P:35:THR:HG22	2.11	0.50
7:6:23:ASN:C	7:6:25:ILE:N	2.64	0.50
1:A:752:GLU:O	1:C:104:ARG:NH1	2.45	0.49
1:B:121:TYR:CE2	1:C:847:PRO:HG2	2.47	0.49
1:B:328:ASP:OD2	1:B:377:ARG:NH2	2.45	0.49
1:C:203:ASN:OD1	1:C:203:ASN:N	2.38	0.49
1:H:620:PHE:CD2	1:H:622:MET:HG2	2.47	0.49
1:I:304:SER:OG	1:I:306:ASN:OD1	2.30	0.49
1:I:442:LYS:HG2	1:I:443:ASP:H	1.76	0.49
1:K:203:ASN:OD1	1:K:203:ASN:N	2.45	0.49
1:L:132:PRO:HB3	1:L:157:PHE:O	2.12	0.49
1:L:165:ILE:HD11	1:L:173:LEU:HD22	1.94	0.49
1:B:96:MET:HG2	1:B:569:ILE:HG22	1.93	0.49
1:B:422:THR:HG23	1:B:449:GLN:O	2.12	0.49
1:D:96:MET:O	1:D:99:THR:OG1	2.31	0.49
1:D:320:ARG:NH1	1:D:479:LEU:O	2.41	0.49
1:F:203:ASN:ND2	1:F:203:ASN:H	2.11	0.49
1:G:278:LYS:HA	1:I:438:SER:HB3	1.95	0.49
1:G:730:SER:OG	1:G:732:PRO:HD2	2.12	0.49
1:I:187:ILE:HG22	1:I:189:ALA:H	1.76	0.49
2:N:77:ASN:HD21	2:N:488:ARG:HE	1.58	0.49
2:N:189:GLY:HA3	2:N:194:VAL:HG22	1.94	0.49
2:N:245:GLU:N	2:N:245:GLU:OE1	2.45	0.49
1:A:80:TYR:O	1:A:585:PHE:N	2.44	0.49
1:A:139:GLU:HG2	1:A:152:ASP:CG	2.33	0.49
1:A:263:VAL:HG22	1:C:423:TYR:CE1	2.47	0.49
1:B:943:THR:HG23	1:B:944:PRO:HD3	1.94	0.49
1:C:20:ALA:HA	1:C:23:TYR:CE2	2.47	0.49
1:C:189:ALA:O	1:C:241:LYS:NZ	2.36	0.49
1:E:480:TYR:OH	1:E:538:PRO:HD3	2.11	0.49
1:F:396:ARG:HD3	1:F:534:PRO:HB3	1.94	0.49
1:H:119:THR:OG1	1:H:120:ALA:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:150:GLU:HB2	1:L:152:ASP:OD1	2.12	0.49
1:B:214:ARG:HH22	1:B:241:LYS:HE2	1.77	0.49
1:C:419:THR:HB	1:C:453:CYS:HA	1.95	0.49
1:D:193:PHE:CD2	1:D:213:GLY:HA2	2.48	0.49
1:D:526:LEU:HD13	1:D:528:PRO:HD2	1.93	0.49
1:D:824:ASN:OD1	1:F:121:TYR:HA	2.11	0.49
1:F:153:VAL:O	1:F:156:THR:OG1	2.20	0.49
1:F:664:PRO:O	5:R:17:LEU:HB2	2.12	0.49
1:G:150:GLU:HB3	1:I:443:ASP:HB2	1.94	0.49
1:H:72:ASP:OD1	1:H:72:ASP:N	2.45	0.49
1:A:159:VAL:HG21	1:B:841:PRO:HD2	1.94	0.49
1:B:204:TRP:CZ2	1:B:415:ASN:HA	2.47	0.49
1:E:771:LEU:HD21	1:E:778:TYR:CE2	2.47	0.49
1:F:764:ASP:OD1	1:F:765:TRP:N	2.45	0.49
1:H:664:PRO:HB3	5:R:19:THR:HG23	1.95	0.49
1:I:33:ARG:HD3	7:6:22:TRP:NE1	2.26	0.49
1:I:590:ASN:O	1:I:590:ASN:ND2	2.46	0.49
1:J:804:GLN:OE1	1:L:556:VAL:HG12	2.13	0.49
1:K:684:LYS:HB3	1:K:687:GLU:HG2	1.95	0.49
1:L:676:ARG:NH2	1:L:921:GLU:OE1	2.44	0.49
1:B:224:PRO:HG2	1:B:316:SER:HB3	1.94	0.49
1:C:71:VAL:HG12	1:E:72:ASP:HB3	1.94	0.49
1:E:202:GLU:HB3	1:F:313:VAL:HG11	1.93	0.49
1:G:500:THR:HG23	1:G:503:TYR:H	1.77	0.49
1:I:33:ARG:HD3	7:6:22:TRP:HE1	1.77	0.49
1:I:98:SER:HB2	1:I:618:THR:HG23	1.94	0.49
1:J:211:TYR:HE2	1:L:454:LYS:HE2	1.78	0.49
1:J:665:ILE:HG12	1:J:903:MET:HB2	1.95	0.49
1:K:112:SER:O	1:K:322:ASN:ND2	2.46	0.49
1:C:65:THR:HB	1:C:618:THR:HG22	1.95	0.49
1:C:633:MET:HE3	6:U:171:LEU:HD13	1.95	0.49
1:F:168:THR:OG1	1:F:169:ASN:N	2.44	0.49
1:H:441:GLU:HG2	1:H:442:LYS:HB2	1.95	0.49
1:I:155:LYS:HG3	1:I:261:PHE:CZ	2.48	0.49
1:J:198:GLN:NE2	1:K:840:GLN:HB3	2.28	0.49
1:K:141:GLN:O	1:K:145:GLY:HA3	2.13	0.49
5:R:18:THR:O	5:R:20:ARG:N	2.42	0.49
1:A:243:LYS:HA	1:A:254:LEU:HA	1.95	0.49
1:B:527:ASP:OD1	1:B:863:LYS:NZ	2.45	0.49
1:C:69:VAL:HG21	1:E:74:GLU:HB3	1.93	0.49
1:C:134:GLN:HE21	1:C:218:LYS:H	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:PRO:HG3	1:F:204:TRP:CZ2	2.47	0.49
1:D:771:LEU:HD13	1:D:777:GLY:HA3	1.94	0.49
1:E:387:ALA:HB3	1:E:546:ARG:HG3	1.94	0.49
1:F:491:ASN:N	1:F:491:ASN:OD1	2.46	0.49
1:H:46:ARG:NE	1:I:644:ASN:OD1	2.41	0.49
1:H:396:ARG:NH1	1:H:867:ASP:OD2	2.46	0.49
1:I:513:LEU:HD13	1:I:819:LEU:HD22	1.95	0.49
1:J:538:PRO:O	1:J:544:ARG:NE	2.45	0.49
1:K:426:VAL:HG12	1:K:440:TRP:HB3	1.93	0.49
1:B:135:TRP:HE1	1:B:156:THR:HG1	1.60	0.49
1:D:456:ASN:HD22	1:F:838:GLN:HA	1.77	0.49
1:G:19:ASP:OD1	1:G:20:ALA:N	2.45	0.49
1:H:700:VAL:HG13	5:Q:34:SER:HB2	1.94	0.49
1:J:4:PRO:HG2	6:U:58:GLN:NE2	2.28	0.49
1:J:573:LEU:HB3	1:J:641:GLN:HE21	1.78	0.49
1:K:588:ASP:OD2	1:K:602:ARG:NH2	2.37	0.49
1:L:219:ASP:OD2	1:L:287:ASN:ND2	2.45	0.49
1:L:392:ASP:HB3	1:L:395:VAL:HG22	1.95	0.49
4:M:221:THR:OG1	4:M:222:VAL:N	2.45	0.49
1:A:194:GLN:NE2	1:A:237:GLY:O	2.44	0.49
1:A:644:ASN:HD21	7:2:29:GLN:HE21	1.61	0.49
1:B:333:LEU:HA	1:B:586:ARG:HB3	1.94	0.49
1:G:256:ILE:HG13	1:G:286:GLU:HB3	1.94	0.49
1:H:760:ASN:HB3	5:R:54:VAL:HG11	1.95	0.49
1:I:888:LEU:HD12	1:I:888:LEU:HA	1.66	0.49
1:J:842:TYR:CG	1:J:843:PRO:HD2	2.47	0.49
1:K:25:SER:HG	1:L:639:HIS:CE1	2.28	0.49
1:K:275:GLU:HG3	1:K:276:GLU:HG3	1.94	0.49
1:L:199:VAL:HG21	1:L:211:TYR:HE1	1.78	0.49
1:L:417:THR:HG21	1:L:453:CYS:SG	2.53	0.49
1:B:173:LEU:HD11	1:B:183:GLY:HA3	1.94	0.48
1:D:620:PHE:CD2	1:D:622:MET:HB3	2.47	0.48
1:E:119:THR:OG1	1:E:120:ALA:N	2.46	0.48
1:E:222:MET:HG2	1:E:307:SER:HA	1.95	0.48
1:E:691:LEU:HD12	1:E:707:TYR:HE2	1.77	0.48
1:F:119:THR:OG1	1:F:120:ALA:N	2.46	0.48
1:G:239:GLN:HG2	1:H:842:TYR:HE2	1.78	0.48
1:G:378:THR:O	1:G:378:THR:OG1	2.31	0.48
1:G:527:ASP:HA	1:G:530:ASP:HB2	1.95	0.48
1:H:549:LEU:HG	1:I:758:GLN:HG3	1.94	0.48
1:K:109:ARG:NH2	1:K:550:LEU:HB2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:419:THR:HB	1:K:453:CYS:HB2	1.95	0.48
1:K:715:ASN:O	1:K:871:TRP:NE1	2.44	0.48
1:L:96:MET:N	1:L:572:LEU:O	2.46	0.48
1:L:513:LEU:HD13	1:L:819:LEU:HD22	1.95	0.48
1:L:794:PHE:HA	1:L:869:VAL:HG11	1.95	0.48
5:P:72:MET:HG2	5:P:76:ARG:HE	1.77	0.48
1:A:515:ASP:OD1	1:A:516:ALA:N	2.40	0.48
1:B:476:ASN:O	1:B:478:ALA:N	2.46	0.48
1:D:327:ARG:HD3	1:D:594:GLN:HB2	1.95	0.48
1:E:19:ASP:HB3	7:3:14:GLY:HA3	1.94	0.48
1:G:106:VAL:HG21	1:G:609:ARG:HH21	1.77	0.48
1:G:133:SER:OG	1:G:134:GLN:N	2.45	0.48
1:G:847:PRO:HG2	1:I:121:TYR:CE1	2.48	0.48
1:H:42:GLY:HA2	7:5:24:GLU:HG2	1.95	0.48
1:J:657:PRO:HG2	1:J:660:ALA:HB2	1.95	0.48
1:K:192:THR:OG1	1:K:193:PHE:N	2.43	0.48
5:S:16:TYR:O	5:S:18:THR:N	2.39	0.48
1:B:162:THR:H	1:B:211:TYR:HD1	1.60	0.48
1:B:385:ASN:HD21	1:B:546:ARG:HG3	1.78	0.48
1:B:663:VAL:HG13	1:B:905:PHE:HB2	1.95	0.48
1:C:842:TYR:CG	1:C:843:PRO:HD2	2.48	0.48
1:D:214:ARG:HD3	1:D:284:TYR:HB2	1.94	0.48
1:D:353:ASN:OD1	1:D:355:VAL:HG12	2.13	0.48
1:D:941:LEU:HD22	1:F:13:MET:HG3	1.95	0.48
1:E:94:LEU:HB2	1:E:619:PHE:CE2	2.48	0.48
1:E:807:ASP:OD2	1:E:810:ASN:ND2	2.37	0.48
1:F:172:LEU:HD13	1:F:193:PHE:HE2	1.77	0.48
1:F:539:ARG:HA	1:F:544:ARG:NH2	2.29	0.48
1:G:135:TRP:HE1	1:G:156:THR:HG1	1.60	0.48
1:H:204:TRP:HH2	1:I:130:PRO:HG3	1.78	0.48
1:H:731:TRP:N	1:H:732:PRO:HD2	2.28	0.48
4:M:388:TRP:CZ2	4:M:391:PRO:HD3	2.47	0.48
1:A:152:ASP:C	1:A:154:THR:H	2.15	0.48
1:A:173:LEU:HA	1:A:185:LYS:HA	1.94	0.48
1:A:217:LYS:HG2	1:A:285:THR:HG22	1.95	0.48
1:A:837:ARG:HH11	1:B:457:VAL:HG23	1.78	0.48
1:C:696:ASP:N	1:C:696:ASP:OD1	2.46	0.48
1:D:427:LYS:HG2	1:D:441:GLU:HB2	1.95	0.48
1:G:233:THR:O	1:H:815:LYS:NZ	2.32	0.48
1:H:107:LEU:HD22	1:H:109:ARG:HD2	1.95	0.48
1:I:514:VAL:HA	1:I:518:ILE:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:635:ARG:HG3	1:I:930:GLN:O	2.14	0.48
1:J:20:ALA:HA	1:J:23:TYR:CE2	2.49	0.48
1:J:198:GLN:HG3	1:K:839:GLY:HA2	1.96	0.48
1:K:243:LYS:HG2	1:K:251:PRO:HB2	1.95	0.48
1:L:396:ARG:HD3	1:L:534:PRO:HB3	1.95	0.48
2:N:113:ILE:HG13	2:N:471:LEU:HG	1.94	0.48
1:B:203:ASN:HD21	1:B:415:ASN:HB3	1.78	0.48
1:D:377:ARG:NH2	1:D:388:VAL:HG12	2.28	0.48
1:E:663:VAL:HG13	1:E:905:PHE:HB2	1.95	0.48
1:F:719:LYS:HE3	1:F:908:ASP:HB3	1.95	0.48
1:G:608:VAL:HG12	1:G:609:ARG:HD3	1.95	0.48
1:H:631:GLU:OE1	1:H:635:ARG:NH1	2.46	0.48
1:I:191:LYS:O	1:I:193:PHE:N	2.43	0.48
1:J:449:GLN:HB3	1:K:153:VAL:HG13	1.95	0.48
1:K:188:TYR:HD1	1:K:188:TYR:H	1.59	0.48
1:K:193:PHE:CE2	1:K:212:GLY:HA3	2.48	0.48
1:L:510:ALA:HA	1:L:832:LEU:O	2.13	0.48
4:M:388:TRP:CH2	4:M:391:PRO:HD3	2.48	0.48
1:A:372:ASP:OD2	1:A:790:ARG:HB3	2.13	0.48
1:B:219:ASP:OD2	1:B:287:ASN:ND2	2.45	0.48
1:B:890:GLN:HG3	4:M:50:ALA:HB2	1.95	0.48
1:C:441:GLU:HB2	1:C:446:ILE:HG23	1.95	0.48
1:G:476:ASN:O	1:G:478:ALA:N	2.47	0.48
1:G:676:ARG:NH2	7:6:31:ASN:H	2.11	0.48
1:K:400:ASN:HD22	1:K:469:TRP:HZ2	1.62	0.48
2:N:426:ASP:OD1	2:N:426:ASP:N	2.47	0.48
1:A:278:LYS:HD2	1:C:437:GLU:O	2.14	0.48
1:B:3:THR:OG1	1:B:4:PRO:HD2	2.14	0.48
1:C:791:MET:SD	1:C:868:ARG:NH1	2.86	0.48
1:D:196:GLU:HG3	1:E:823:HIS:HB3	1.96	0.48
1:E:130:PRO:HG3	1:E:312:LEU:HG	1.96	0.48
1:F:172:LEU:HD13	1:F:193:PHE:CE2	2.49	0.48
1:F:684:LYS:NZ	1:F:713:TYR:OH	2.47	0.48
1:G:219:ASP:HB2	1:G:287:ASN:HD21	1.78	0.48
1:H:154:THR:O	1:H:156:THR:N	2.47	0.48
1:J:498:THR:O	1:J:498:THR:OG1	2.26	0.48
1:L:135:TRP:HE1	1:L:137:THR:HG23	1.79	0.48
1:L:296:HIS:CE1	1:L:317:MET:HG3	2.49	0.48
1:A:64:LEU:HB2	1:B:736:ARG:O	2.14	0.48
1:B:112:SER:OG	1:B:322:ASN:ND2	2.47	0.48
1:C:88:VAL:HB	1:C:576:PRO:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:PRO:HG3	1:F:204:TRP:HZ2	1.79	0.48
1:H:257:ASP:OD1	1:H:285:THR:OG1	2.29	0.48
1:H:538:PRO:O	1:H:544:ARG:NH2	2.43	0.48
1:H:640:ASP:OD1	1:H:640:ASP:N	2.41	0.48
1:I:76:THR:HG22	1:I:77:THR:H	1.79	0.48
1:I:476:ASN:HB2	1:I:537:HIS:CE1	2.48	0.48
1:J:637:ASP:N	1:J:637:ASP:OD1	2.46	0.48
1:J:774:TYR:HB2	1:J:776:ILE:HG12	1.95	0.48
1:K:328:ASP:OD2	1:K:368:GLN:NE2	2.46	0.48
1:L:725:PHE:HD2	1:L:731:TRP:HB2	1.78	0.48
4:M:215:PRO:HG2	4:M:221:THR:HG21	1.95	0.48
5:Q:14:SER:HB3	5:R:15:PRO:HB3	1.94	0.48
1:A:682:ARG:NH2	1:A:910:MET:HG3	2.28	0.48
1:F:680:PHE:HB3	1:F:918:LEU:HD12	1.96	0.48
1:G:246:ASN:ND2	1:G:250:GLN:O	2.40	0.48
1:J:808:GLU:OE1	1:J:808:GLU:N	2.46	0.48
1:K:443:ASP:HB3	1:L:150:GLU:HB3	1.95	0.48
1:K:526:LEU:HD13	1:K:528:PRO:HD2	1.95	0.48
1:L:722:SER:OG	1:L:904:THR:OG1	2.30	0.48
1:B:445:ALA:C	1:B:449:GLN:HB2	2.34	0.48
1:C:152:ASP:O	1:C:154:THR:HG22	2.13	0.48
1:D:804:GLN:NE2	1:F:556:VAL:HG12	2.28	0.48
1:G:140:LYS:HA	1:G:147:VAL:HA	1.95	0.48
1:I:336:TYR:CZ	1:I:565:LYS:HG2	2.49	0.48
1:D:12:TYR:OH	6:U:161:SER:OG	2.23	0.47
1:D:152:ASP:C	1:D:154:THR:N	2.68	0.47
1:D:313:VAL:HG11	1:F:202:GLU:HA	1.95	0.47
1:E:201:GLU:H	1:E:201:GLU:HG2	1.50	0.47
1:E:253:ASP:OD1	1:E:254:LEU:N	2.37	0.47
1:F:657:PRO:HD2	5:R:12:LEU:HD22	1.94	0.47
1:G:52:PRO:HD3	7:6:11:PRO:HA	1.96	0.47
1:G:309:GLU:OE2	1:I:205:GLN:NE2	2.41	0.47
1:G:456:ASN:HD21	1:I:839:GLY:H	1.61	0.47
1:I:151:LYS:HB3	1:I:154:THR:CB	2.44	0.47
1:I:193:PHE:HE2	1:I:284:TYR:CG	2.32	0.47
1:J:72:ASP:N	1:J:72:ASP:OD1	2.46	0.47
1:J:137:THR:OG1	1:J:138:LYS:N	2.46	0.47
1:K:58:THR:OG1	1:K:59:ASP:N	2.47	0.47
1:K:169:ASN:OD1	1:K:169:ASN:N	2.47	0.47
1:K:336:TYR:HE1	1:K:566:PHE:HB2	1.78	0.47
1:L:308:SER:O	1:L:310:ILE:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:13:PHE:CD2	5:P:14:SER:N	2.82	0.47
5:P:39:ARG:HH21	5:P:41:VAL:HG21	1.79	0.47
1:A:355:VAL:HB	1:A:569:ILE:HD11	1.95	0.47
1:A:651:ASN:HB3	1:A:919:LEU:HD12	1.95	0.47
1:A:831:TYR:H	1:A:838:GLN:HE21	1.62	0.47
1:B:403:VAL:HG11	1:B:466:ALA:HA	1.96	0.47
1:B:426:VAL:HA	1:B:440:TRP:HA	1.95	0.47
1:D:200:GLY:HA3	1:D:206:GLU:OE1	2.14	0.47
1:D:207:ASN:OD1	1:D:207:ASN:N	2.47	0.47
1:D:288:VAL:HG13	1:D:290:LEU:H	1.80	0.47
1:E:449:GLN:HG3	1:E:450:ASN:N	2.30	0.47
1:F:134:GLN:HG2	1:F:155:LYS:HG2	1.96	0.47
1:H:187:ILE:O	1:H:191:LYS:N	2.45	0.47
1:I:20:ALA:HA	1:I:23:TYR:CE2	2.49	0.47
1:J:264:PRO:HD3	1:L:423:TYR:HA	1.95	0.47
1:K:629:THR:O	1:K:633:MET:HG2	2.13	0.47
1:K:767:LEU:O	1:K:771:LEU:HB2	2.14	0.47
1:K:952:THR:H	6:U:33:TRP:HZ2	1.60	0.47
2:N:280:LEU:HD11	2:N:285:TYR:HB2	1.96	0.47
2:N:281:ASP:OD1	2:N:281:ASP:N	2.47	0.47
1:B:230:ALA:HB3	1:B:239:GLN:NE2	2.27	0.47
1:B:678:TRP:HE1	1:B:901:LEU:HD21	1.79	0.47
1:C:152:ASP:C	1:C:154:THR:N	2.67	0.47
1:D:427:LYS:HG3	1:D:439:GLU:HB2	1.95	0.47
1:D:833:ALA:C	1:D:835:THR:H	2.17	0.47
1:F:20:ALA:HA	1:F:23:TYR:CE2	2.49	0.47
1:G:548:MET:HE1	1:H:399:GLU:HG3	1.96	0.47
1:H:813:ASP:OD1	1:H:813:ASP:N	2.46	0.47
1:J:122:ASN:HA	1:K:825:ASN:HA	1.95	0.47
1:J:278:LYS:HZ1	1:L:428:ILE:HG22	1.79	0.47
1:J:426:VAL:HG12	1:J:440:TRP:HD1	1.79	0.47
1:J:764:ASP:OD1	1:J:765:TRP:N	2.46	0.47
4:M:86:ARG:HB2	4:M:89:GLU:HG3	1.96	0.47
5:S:72:MET:O	5:S:74:ALA:N	2.47	0.47
6:U:2:SER:HB2	6:U:200:PRO:HD3	1.96	0.47
6:U:26:ASP:OD2	6:U:29:THR:OG1	2.31	0.47
1:E:322:ASN:ND2	1:E:597:LEU:H	2.13	0.47
1:E:872:ARG:NH2	7:3:30:LEU:O	2.45	0.47
1:F:513:LEU:HD13	1:F:819:LEU:HD22	1.97	0.47
1:H:102:ASP:OD1	1:H:559:HIS:NE2	2.48	0.47
1:H:217:LYS:HD2	1:H:287:ASN:HD21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:676:ARG:HD3	1:H:923:PHE:CE2	2.50	0.47
1:I:267:SER:HB3	1:I:277:TYR:CD1	2.50	0.47
1:I:495:PRO:HG2	1:I:502:GLU:HG3	1.96	0.47
1:I:842:TYR:CG	1:I:843:PRO:HD2	2.49	0.47
1:J:589:VAL:HG23	1:J:593:LEU:HD23	1.96	0.47
1:J:693:SER:OG	5:P:25:ALA:N	2.37	0.47
1:J:804:GLN:OE1	1:J:860:THR:HB	2.14	0.47
1:K:452:ILE:HG23	1:L:158:GLY:O	2.13	0.47
1:L:429:THR:HG22	1:L:430:ASN:H	1.79	0.47
1:L:684:LYS:HE2	1:L:713:TYR:OH	2.14	0.47
5:P:39:ARG:HB3	5:P:41:VAL:HG23	1.96	0.47
1:A:622:MET:HG3	1:A:627:ALA:HB2	1.97	0.47
1:B:49:THR:HG21	7:1:27:THR:HG21	1.96	0.47
1:E:172:LEU:HD11	1:E:282:ILE:HG21	1.95	0.47
1:G:548:MET:SD	1:H:401:HIS:NE2	2.88	0.47
1:G:561:GLN:HE22	1:H:756:VAL:HA	1.80	0.47
5:S:34:SER:OG	5:S:35:THR:N	2.47	0.47
1:D:344:VAL:HG22	1:D:582:GLU:HG2	1.97	0.47
1:D:478:ALA:C	1:D:480:TYR:H	2.17	0.47
1:D:696:ASP:OD1	1:D:696:ASP:N	2.45	0.47
1:H:526:LEU:HD13	1:H:528:PRO:HD2	1.95	0.47
1:H:715:ASN:HB2	1:H:871:TRP:NE1	2.29	0.47
1:J:590:ASN:OD1	1:J:602:ARG:HB2	2.14	0.47
1:L:112:SER:O	1:L:112:SER:OG	2.30	0.47
1:B:907:VAL:HG23	1:B:908:ASP:H	1.79	0.47
1:C:58:THR:HB	1:C:623:ALA:HA	1.97	0.47
1:D:112:SER:O	1:D:322:ASN:ND2	2.47	0.47
1:D:639:HIS:CD2	1:F:25:SER:HG	2.30	0.47
1:D:924:ASP:N	1:D:924:ASP:OD1	2.47	0.47
1:F:228:SER:HB2	1:F:290:LEU:HD11	1.97	0.47
1:F:681:THR:CG2	1:F:715:ASN:HD21	2.27	0.47
1:F:886:THR:HG23	1:F:889:GLY:H	1.79	0.47
1:G:88:VAL:HG22	1:G:576:PRO:HA	1.97	0.47
1:G:137:THR:OG1	1:G:138:LYS:N	2.46	0.47
1:G:234:ASN:HD21	1:G:238:GLY:HA3	1.80	0.47
1:G:341:ASN:O	1:G:341:ASN:ND2	2.44	0.47
1:G:457:VAL:O	1:I:837:ARG:NH1	2.48	0.47
1:G:485:TYR:CZ	1:G:528:PRO:HB3	2.50	0.47
1:H:193:PHE:HE1	1:H:198:GLN:HB3	1.79	0.47
1:H:198:GLN:NE2	1:I:838:GLN:HB2	2.30	0.47
1:H:240:ALA:O	1:H:288:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:656:ILE:HG12	1:H:663:VAL:HG21	1.97	0.47
1:I:244:PRO:HD3	1:I:253:ASP:O	2.15	0.47
1:I:767:LEU:O	1:I:771:LEU:HB2	2.14	0.47
1:I:872:ARG:NH1	7:5:31:ASN:O	2.48	0.47
1:J:188:TYR:O	1:J:192:THR:OG1	2.29	0.47
1:J:639:HIS:CD2	1:L:28:LEU:HD12	2.50	0.47
1:K:214:ARG:HH22	1:K:241:LYS:HZ3	1.62	0.47
1:K:514:VAL:HA	1:K:518:ILE:HG21	1.96	0.47
2:N:341:ASN:ND2	2:N:341:ASN:O	2.48	0.47
5:Q:127:GLU:HG2	5:Q:128:GLN:HG3	1.96	0.47
1:A:923:PHE:O	1:A:942:ARG:HA	2.15	0.47
1:C:266:GLY:HA3	1:C:277:TYR:CE1	2.50	0.47
1:E:113:PHE:HE1	1:E:324:ILE:H	1.61	0.47
1:F:442:LYS:HG2	1:F:443:ASP:H	1.79	0.47
1:G:383:MET:HA	1:H:757:ALA:HA	1.96	0.47
1:G:771:LEU:HD21	1:G:778:TYR:CE2	2.50	0.47
1:H:237:GLY:HA3	1:I:821:PHE:HB3	1.95	0.47
1:J:52:PRO:HB2	1:J:56:VAL:HG21	1.97	0.47
1:J:419:THR:HB	1:J:453:CYS:HB2	1.97	0.47
1:K:138:LYS:HA	1:K:149:GLN:HA	1.96	0.47
1:K:204:TRP:CD1	1:K:415:ASN:HB3	2.50	0.47
1:L:287:ASN:OD1	1:L:287:ASN:N	2.47	0.47
1:L:597:LEU:HD12	1:L:597:LEU:HA	1.70	0.47
1:L:811:TYR:CD1	1:L:857:PRO:HD2	2.50	0.47
1:A:237:GLY:HA3	1:B:821:PHE:HB2	1.97	0.47
1:A:530:ASP:OD2	1:A:863:LYS:NZ	2.42	0.47
1:B:638:THR:HG23	1:B:639:HIS:ND1	2.30	0.47
1:D:152:ASP:O	1:D:154:THR:HG22	2.15	0.47
1:E:756:VAL:HG13	1:E:763:LYS:HG2	1.95	0.47
1:F:657:PRO:HG2	1:F:660:ALA:HB2	1.96	0.47
1:G:636:ASN:OD1	1:G:637:ASP:N	2.47	0.47
1:G:640:ASP:HB2	1:G:928:VAL:O	2.14	0.47
1:H:148:GLN:HG3	1:H:150:GLU:OE1	2.15	0.47
1:I:328:ASP:O	1:I:329:ASN:C	2.52	0.47
5:R:12:LEU:HD11	5:R:17:LEU:HD21	1.96	0.47
1:A:3:THR:HG23	1:A:4:PRO:HD3	1.97	0.47
1:D:372:ASP:OD2	1:D:790:ARG:HB3	2.15	0.47
1:G:216:LEU:HB3	1:G:220:THR:HG21	1.96	0.47
1:H:189:ALA:O	1:H:241:LYS:NZ	2.39	0.47
1:J:59:ASP:OD1	1:J:59:ASP:N	2.47	0.47
1:J:438:SER:HB3	1:K:278:LYS:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:42:GLU:HG3	4:M:45:ARG:NH1	2.30	0.47
1:A:96:MET:HE2	1:A:569:ILE:HG22	1.97	0.46
1:B:64:LEU:HD21	1:B:621:PRO:HG3	1.97	0.46
1:C:263:VAL:O	1:C:277:TYR:OH	2.23	0.46
1:D:152:ASP:C	1:D:154:THR:H	2.19	0.46
1:D:299:TYR:OH	1:F:202:GLU:HG2	2.15	0.46
1:D:451:GLN:HB2	1:E:156:THR:O	2.15	0.46
1:D:825:ASN:OD1	1:F:124:LEU:HB2	2.15	0.46
1:E:675:PHE:HE1	1:E:920:PHE:HB3	1.79	0.46
1:F:154:THR:HG23	1:F:155:LYS:HG3	1.96	0.46
1:G:640:ASP:OD1	1:G:640:ASP:N	2.44	0.46
1:I:74:GLU:HB3	1:I:81:LYS:HB3	1.97	0.46
1:I:204:TRP:CD2	1:I:415:ASN:HB3	2.50	0.46
1:I:329:ASN:O	1:I:330:PHE:C	2.51	0.46
1:J:278:LYS:HZ3	1:L:438:SER:HB3	1.80	0.46
1:J:824:ASN:HD22	1:J:825:ASN:HB2	1.80	0.46
1:K:191:LYS:HA	1:K:191:LYS:HD2	1.54	0.46
1:K:503:TYR:OH	1:K:507:ARG:NH1	2.47	0.46
1:L:34:ALA:HA	7:9:19:MET:HG2	1.97	0.46
1:A:842:TYR:OH	1:C:286:GLU:OE2	2.33	0.46
1:G:367:TYR:CD2	1:G:565:LYS:HE2	2.50	0.46
1:G:429:THR:HG22	1:G:439:GLU:HB2	1.97	0.46
1:H:195:PRO:HG2	1:I:823:HIS:CD2	2.50	0.46
1:I:79:LEU:HD21	1:I:341:ASN:HD22	1.80	0.46
1:I:590:ASN:HB3	1:I:602:ARG:HH21	1.81	0.46
1:I:676:ARG:NH2	1:I:921:GLU:OE1	2.47	0.46
1:J:113:PHE:CG	1:J:113:PHE:O	2.69	0.46
5:S:49:MET:SD	5:S:50:THR:N	2.89	0.46
1:A:564:GLN:HE22	1:A:569:ILE:HD12	1.80	0.46
1:A:759:CYS:HB3	1:A:800:PRO:HB3	1.98	0.46
1:B:415:ASN:OD1	1:B:418:GLY:N	2.37	0.46
1:C:204:TRP:HE1	1:C:415:ASN:HB2	1.80	0.46
1:C:631:GLU:C	1:C:633:MET:H	2.19	0.46
1:D:724:MET:HG3	1:D:728:SER:O	2.16	0.46
1:E:773:HIS:CE1	1:E:872:ARG:HH11	2.34	0.46
1:F:731:TRP:N	1:F:732:PRO:HD2	2.31	0.46
1:G:575:LEU:HB3	1:G:576:PRO:HD2	1.97	0.46
1:J:392:ASP:HB3	1:J:395:VAL:HG12	1.97	0.46
1:J:670:ARG:NH2	1:J:946:SER:H	2.13	0.46
1:L:575:LEU:HB3	1:L:576:PRO:HD2	1.96	0.46
1:A:255:ASP:O	1:A:286:GLU:HB3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:THR:HB	1:D:193:PHE:CD1	2.50	0.46
1:D:239:GLN:HG2	1:E:842:TYR:HE2	1.80	0.46
1:E:754:TYR:O	1:E:763:LYS:N	2.46	0.46
1:F:759:CYS:SG	1:F:760:ASN:N	2.88	0.46
1:G:28:LEU:HD12	1:H:639:HIS:ND1	2.31	0.46
1:G:237:GLY:HA3	1:H:821:PHE:HB3	1.97	0.46
1:H:64:LEU:HD13	1:I:736:ARG:HD2	1.96	0.46
1:H:913:PRO:HB2	5:P:8:PHE:HB2	1.98	0.46
1:I:161:ALA:HB3	1:I:198:GLN:NE2	2.29	0.46
1:J:266:GLY:HA3	1:J:276:GLU:HA	1.96	0.46
1:J:831:TYR:HD1	1:L:196:GLU:HB2	1.80	0.46
1:K:292:THR:O	1:K:292:THR:OG1	2.34	0.46
1:L:423:TYR:N	1:L:450:ASN:O	2.31	0.46
5:Q:4:THR:HB	5:Q:13:PHE:CE1	2.50	0.46
5:Q:101:LEU:HD22	5:S:96:ILE:HG13	1.97	0.46
1:A:423:TYR:HE1	1:B:263:VAL:HG22	1.80	0.46
1:A:495:PRO:HG3	1:A:502:GLU:HB3	1.96	0.46
1:B:403:VAL:HG22	1:B:465:GLN:HB3	1.98	0.46
1:B:449:GLN:HE21	1:B:449:GLN:HA	1.80	0.46
1:D:237:GLY:HA3	1:E:821:PHE:HB3	1.98	0.46
1:D:256:ILE:HA	1:D:286:GLU:HB3	1.97	0.46
1:D:401:HIS:NE2	1:F:544:ARG:HD3	2.30	0.46
1:D:414:LEU:HD21	1:F:410:TYR:CE1	2.50	0.46
1:F:198:GLN:C	1:F:200:GLY:N	2.64	0.46
1:F:932:HIS:C	1:F:934:GLY:H	2.18	0.46
1:G:449:GLN:HG2	1:H:153:VAL:HG22	1.97	0.46
1:H:44:LYS:HE3	1:I:573:LEU:HB2	1.97	0.46
1:H:573:LEU:HD23	1:H:634:LEU:HD21	1.98	0.46
1:I:155:LYS:HG3	1:I:261:PHE:HZ	1.79	0.46
1:J:18:GLN:O	1:J:22:GLU:HB2	2.15	0.46
1:J:241:LYS:HD2	1:J:256:ILE:HD11	1.97	0.46
1:J:747:ARG:NH2	1:J:752:GLU:OE2	2.41	0.46
2:N:131:LYS:NZ	2:N:245:GLU:OE2	2.33	0.46
4:M:254:HIS:O	4:M:257:THR:OG1	2.26	0.46
1:A:737:LEU:O	1:C:63:ARG:NH1	2.48	0.46
1:C:827:GLY:HA2	1:C:839:GLY:C	2.36	0.46
1:D:223:LYS:HD3	1:D:292:THR:HG23	1.97	0.46
1:E:767:LEU:O	1:E:771:LEU:HB2	2.15	0.46
1:F:392:ASP:HB3	1:F:395:VAL:HG22	1.98	0.46
1:H:115:PRO:HD2	1:H:116:TYR:HD1	1.81	0.46
1:J:6:MET:HE1	6:U:51:ARG:HH22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:162:THR:H	1:J:211:TYR:HD1	1.64	0.46
1:J:762:THR:OG1	1:J:763:LYS:N	2.48	0.46
1:K:310:ILE:HD12	1:K:311:ASN:H	1.80	0.46
1:L:150:GLU:O	1:L:152:ASP:N	2.43	0.46
1:A:275:GLU:OE1	1:A:276:GLU:N	2.47	0.46
1:A:438:SER:HB3	1:B:278:LYS:HD2	1.97	0.46
1:A:475:SER:OG	1:B:406:GLU:OE1	2.21	0.46
1:B:651:ASN:ND2	1:B:917:TYR:OH	2.49	0.46
1:B:767:LEU:O	1:B:771:LEU:HB2	2.15	0.46
1:C:19:ASP:HB2	7:1:14:GLY:HA3	1.96	0.46
1:D:138:LYS:HG2	1:D:147:VAL:HG12	1.97	0.46
1:F:364:GLU:HB2	1:F:708:LEU:HB2	1.96	0.46
1:G:239:GLN:HG2	1:H:842:TYR:CE2	2.51	0.46
1:G:771:LEU:HD12	1:G:775:ASN:HA	1.98	0.46
1:H:61:SER:HA	1:I:734:ASN:HB2	1.97	0.46
1:H:604:ASP:OD1	1:H:605:GLY:N	2.39	0.46
1:I:512:SER:HA	1:I:515:ASP:HB2	1.98	0.46
1:J:135:TRP:CZ3	1:J:137:THR:HB	2.50	0.46
1:J:261:PHE:O	1:J:280:ASP:N	2.45	0.46
1:K:49:THR:HG22	1:L:884:ALA:H	1.81	0.46
1:K:269:PRO:HG3	1:K:277:TYR:HB3	1.98	0.46
1:L:109:ARG:HH21	1:L:556:VAL:HG11	1.81	0.46
1:A:573:LEU:HD23	1:A:634:LEU:HD21	1.98	0.46
1:A:728:SER:OG	1:A:729:VAL:N	2.49	0.46
1:B:162:THR:HG23	1:B:193:PHE:CD1	2.50	0.46
1:B:198:GLN:HB2	1:C:838:GLN:O	2.16	0.46
1:B:573:LEU:HD23	1:B:573:LEU:HA	1.79	0.46
1:B:595:SER:HB2	1:B:601:LEU:HD21	1.97	0.46
1:C:163:GLY:HA2	1:C:211:TYR:HA	1.97	0.46
1:C:476:ASN:O	1:C:537:HIS:NE2	2.29	0.46
1:F:369:LEU:HD12	1:F:647:LEU:HD13	1.97	0.46
1:G:151:LYS:HD3	1:G:154:THR:HG21	1.97	0.46
1:G:775:ASN:N	1:G:775:ASN:OD1	2.48	0.46
1:I:361:ARG:HG2	1:I:363:THR:HG23	1.97	0.46
1:J:350:SER:O	1:J:352:LEU:N	2.48	0.46
1:J:399:GLU:HB3	1:J:523:ARG:HB3	1.96	0.46
1:K:527:ASP:HA	1:K:530:ASP:HB2	1.98	0.46
1:K:808:GLU:OE1	1:K:808:GLU:N	2.49	0.46
1:L:650:ALA:HB2	1:L:942:ARG:HE	1.80	0.46
4:M:40:ASN:OD1	4:M:40:ASN:N	2.49	0.46
1:D:422:THR:HA	1:D:450:ASN:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:575:LEU:HB3	1:D:635:ARG:NH2	2.31	0.46
1:D:785:GLU:H	1:D:785:GLU:HG2	1.61	0.46
1:E:239:GLN:HG2	1:F:842:TYR:CE2	2.51	0.46
1:F:360:ASP:OD1	1:F:942:ARG:NH1	2.37	0.46
1:F:771:LEU:HD13	1:F:879:PHE:HB2	1.98	0.46
1:G:441:GLU:OE1	1:G:443:ASP:N	2.29	0.46
1:G:836:MET:HA	1:H:410:TYR:OH	2.16	0.46
1:H:51:ALA:HB2	1:I:883:GLY:HA3	1.98	0.46
1:K:750:ASP:N	1:K:750:ASP:OD1	2.49	0.46
1:K:888:LEU:HD12	1:K:888:LEU:HA	1.79	0.46
1:L:377:ARG:HH12	1:L:386:SER:HB2	1.81	0.46
5:Q:14:SER:C	5:R:15:PRO:CB	2.85	0.46
7:3:21:THR:O	7:3:23:ASN:N	2.48	0.46
1:A:76:THR:HG22	1:A:77:THR:H	1.80	0.46
1:A:575:LEU:HD11	1:A:634:LEU:HB3	1.98	0.46
1:B:372:ASP:O	1:B:790:ARG:NH1	2.49	0.46
1:B:486:LYS:O	1:B:507:ARG:NH1	2.49	0.46
1:C:537:HIS:CG	1:C:538:PRO:HD2	2.51	0.46
1:C:807:ASP:HB3	1:C:859:VAL:HB	1.97	0.46
1:E:296:HIS:CE1	1:E:317:MET:HG2	2.51	0.46
1:H:728:SER:O	1:H:728:SER:OG	2.33	0.46
1:I:151:LYS:HB3	1:I:154:THR:CG2	2.46	0.46
1:I:734:ASN:OD1	1:I:736:ARG:NH1	2.46	0.46
1:I:772:SER:OG	1:I:872:ARG:HG2	2.16	0.46
1:J:726:ASP:O	1:J:727:SER:OG	2.34	0.46
2:N:124:TYR:CD2	2:N:125:MET:HG3	2.51	0.46
1:A:52:PRO:HD3	7:2:11:PRO:HA	1.96	0.45
1:B:423:TYR:CE1	1:C:263:VAL:HG22	2.51	0.45
1:D:66:LEU:HD23	1:D:66:LEU:HA	1.82	0.45
1:D:151:LYS:HD3	1:D:151:LYS:HA	1.83	0.45
1:E:19:ASP:O	1:E:23:TYR:HE1	1.99	0.45
1:E:336:TYR:CE2	1:E:565:LYS:HG3	2.51	0.45
1:F:69:VAL:HG23	1:F:70:PRO:HD2	1.97	0.45
1:G:407:LEU:HD11	1:I:474:TYR:HB3	1.98	0.45
1:G:473:LEU:HD12	1:G:473:LEU:HA	1.84	0.45
1:H:135:TRP:CZ2	1:H:309:GLU:HB2	2.51	0.45
1:I:350:SER:O	1:I:352:LEU:N	2.47	0.45
1:J:315:GLN:HE22	1:J:836:MET:H	1.64	0.45
1:K:444:ASP:OD1	1:K:444:ASP:N	2.49	0.45
1:A:410:TYR:OH	1:C:836:MET:HA	2.16	0.45
1:A:735:ASP:N	1:A:735:ASP:OD1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:TYR:HA	1:C:264:PRO:HD3	1.97	0.45
1:E:58:THR:OG1	1:E:59:ASP:N	2.49	0.45
1:E:421:SER:OG	1:E:452:ILE:O	2.34	0.45
1:G:210:PHE:HD1	1:G:280:ASP:HA	1.81	0.45
1:G:801:MET:HE2	1:G:801:MET:HB2	1.91	0.45
1:H:191:LYS:C	1:H:193:PHE:H	2.19	0.45
1:I:696:ASP:OD1	1:I:696:ASP:N	2.46	0.45
1:J:68:PHE:HB2	1:J:615:LEU:HD23	1.98	0.45
1:J:327:ARG:NH2	1:J:702:SER:O	2.49	0.45
1:J:514:VAL:HA	1:J:518:ILE:HG21	1.98	0.45
1:K:208:GLU:HB2	1:K:211:TYR:CZ	2.51	0.45
1:L:519:ASN:OD1	1:L:803:ARG:NH1	2.50	0.45
1:L:693:SER:OG	1:L:694:GLY:N	2.48	0.45
1:B:233:THR:OG1	1:B:240:ALA:HA	2.15	0.45
1:B:328:ASP:O	1:B:331:VAL:HG22	2.16	0.45
1:B:392:ASP:HB3	1:B:395:VAL:HG12	1.98	0.45
1:B:825:ASN:O	1:B:829:THR:HG22	2.16	0.45
1:C:514:VAL:HA	1:C:518:ILE:HG21	1.97	0.45
1:C:678:TRP:HD1	1:C:918:LEU:HD11	1.81	0.45
1:D:167:ILE:HG22	1:D:172:LEU:HA	1.98	0.45
1:D:764:ASP:OD1	1:D:764:ASP:N	2.35	0.45
1:E:126:PRO:HG2	1:E:129:ALA:HB2	1.97	0.45
1:E:135:TRP:HE1	1:E:156:THR:HG22	1.81	0.45
1:F:911:ASP:N	1:F:911:ASP:OD1	2.50	0.45
1:G:449:GLN:CB	1:H:153:VAL:HG13	2.37	0.45
1:G:644:ASN:HB3	1:G:925:VAL:HG12	1.97	0.45
1:I:20:ALA:O	1:I:24:LEU:HG	2.16	0.45
1:I:50:VAL:HG13	7:5:12:ARG:HB2	1.98	0.45
1:I:809:ILE:HD12	1:I:810:ASN:H	1.82	0.45
1:K:731:TRP:HE1	1:K:888:LEU:HD23	1.81	0.45
1:L:884:ALA:HB1	7:8:29:GLN:NE2	2.31	0.45
4:M:145:LEU:HD23	4:M:145:LEU:HA	1.76	0.45
1:A:412:PHE:CE2	1:A:459:ALA:HB2	2.50	0.45
1:A:417:THR:HG21	1:A:453:CYS:HB2	1.99	0.45
1:A:607:SER:O	1:A:607:SER:OG	2.28	0.45
1:B:124:LEU:HB2	1:C:825:ASN:HD21	1.82	0.45
1:C:620:PHE:HD2	1:C:622:MET:HB2	1.82	0.45
1:D:336:TYR:CZ	1:D:565:LYS:HG2	2.51	0.45
1:E:320:ARG:CZ	1:E:597:LEU:HD11	2.47	0.45
1:F:531:ASN:HB2	1:F:714:LEU:HD11	1.98	0.45
1:F:827:GLY:HA2	1:F:839:GLY:C	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:GLN:HA	7:6:15:THR:HG23	1.99	0.45
1:G:20:ALA:HA	1:G:23:TYR:CE2	2.51	0.45
1:G:249:GLU:HG3	1:G:250:GLN:HG2	1.99	0.45
1:H:198:GLN:HE22	1:I:838:GLN:HB2	1.80	0.45
1:H:536:ASN:HB3	1:H:596:SER:O	2.16	0.45
1:K:950:ALA:HA	6:U:48:ARG:HH12	1.82	0.45
1:L:172:LEU:HD12	1:L:282:ILE:HD11	1.98	0.45
5:P:42:LEU:HB2	5:P:43:PRO:CD	2.47	0.45
1:A:738:LEU:HD23	1:A:738:LEU:HA	1.75	0.45
1:B:94:LEU:HB2	1:B:619:PHE:CE2	2.51	0.45
1:D:172:LEU:HD11	1:D:212:GLY:HA3	1.99	0.45
1:E:59:ASP:N	1:E:59:ASP:OD1	2.48	0.45
1:E:586:ARG:NH1	1:E:591:MET:HG2	2.32	0.45
1:G:698:TYR:HA	5:R:81:TYR:HB2	1.98	0.45
1:H:189:ALA:HB1	1:H:234:ASN:ND2	2.31	0.45
1:H:239:GLN:HE21	1:H:240:ALA:H	1.63	0.45
1:H:451:GLN:HE21	1:I:157:PHE:HE1	1.63	0.45
1:I:503:TYR:CZ	1:I:507:ARG:HD2	2.51	0.45
5:P:17:LEU:HD23	5:R:14:SER:HA	1.97	0.45
1:A:240:ALA:HB3	1:A:288:VAL:HG23	1.98	0.45
1:A:357:ASP:HB3	1:A:566:PHE:HE1	1.81	0.45
1:B:261:PHE:O	1:B:280:ASP:HA	2.15	0.45
1:E:25:SER:H	1:F:639:HIS:HE1	1.60	0.45
1:E:155:LYS:HD2	1:E:261:PHE:CZ	2.52	0.45
1:E:192:THR:HG22	1:E:193:PHE:CD1	2.52	0.45
1:E:684:LYS:HB2	1:E:684:LYS:HE3	1.71	0.45
1:F:172:LEU:HD22	1:F:193:PHE:CZ	2.50	0.45
1:G:139:GLU:HB3	1:G:152:ASP:OD2	2.17	0.45
1:G:202:GLU:HB2	1:G:205:GLN:HB2	1.98	0.45
1:G:204:TRP:CE3	1:H:313:VAL:HG22	2.51	0.45
1:G:595:SER:HB3	1:G:702:SER:OG	2.17	0.45
1:H:636:ASN:HB2	1:H:639:HIS:HE2	1.81	0.45
1:J:134:GLN:CD	1:J:155:LYS:HZ3	2.16	0.45
1:K:25:SER:H	1:L:639:HIS:HE1	1.59	0.45
1:K:342:MET:HE3	1:K:357:ASP:HB2	1.99	0.45
6:V:143:SER:HB2	6:V:170:THR:O	2.17	0.45
1:A:239:GLN:HG2	1:B:842:TYR:HE2	1.82	0.45
1:A:421:SER:OG	1:A:452:ILE:O	2.35	0.45
1:A:438:SER:HB3	1:B:278:LYS:HB3	1.98	0.45
1:A:649:ALA:HA	1:A:922:VAL:HG22	1.99	0.45
1:B:424:GLN:HA	1:B:449:GLN:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:MET:HA	1:E:757:ALA:HA	1.99	0.45
1:F:26:PRO:HA	1:F:29:VAL:HG12	1.99	0.45
1:F:152:ASP:C	1:F:154:THR:N	2.69	0.45
1:F:739:THR:O	1:F:741:ASN:N	2.41	0.45
1:G:193:PHE:CG	1:G:194:GLN:N	2.85	0.45
1:G:410:TYR:OH	1:I:836:MET:HA	2.16	0.45
1:G:676:ARG:NH2	1:G:921:GLU:OE1	2.50	0.45
1:H:426:VAL:O	1:I:260:TYR:HB2	2.17	0.45
1:H:657:PRO:HG3	5:Q:12:LEU:HD22	1.99	0.45
2:N:195:LEU:HD12	2:N:195:LEU:HA	1.80	0.45
4:M:322:TYR:OH	4:M:348:ASN:O	2.24	0.45
1:C:162:THR:HB	1:C:193:PHE:CD1	2.52	0.45
1:C:631:GLU:OE2	1:C:632:ALA:N	2.50	0.45
1:D:684:LYS:HB3	1:D:687:GLU:HG2	1.99	0.45
1:E:237:GLY:HA3	1:F:821:PHE:HB3	1.98	0.45
1:F:947:ALA:HA	1:H:728:SER:HA	1.98	0.45
1:G:315:GLN:NE2	1:I:203:ASN:OD1	2.50	0.45
1:H:138:LYS:HD3	1:H:149:GLN:HB2	1.99	0.45
1:I:186:ASP:OD1	1:I:187:ILE:N	2.49	0.45
1:J:263:VAL:HG22	1:L:423:TYR:CE1	2.52	0.45
1:J:300:LYS:NZ	1:J:305:ASP:OD1	2.46	0.45
1:K:10:TRP:CZ2	1:L:674:ALA:HB2	2.52	0.45
1:K:730:SER:OG	1:K:741:ASN:OD1	2.21	0.45
1:L:52:PRO:HD3	7:8:11:PRO:HA	1.99	0.45
1:L:387:ALA:HB3	1:L:546:ARG:HE	1.81	0.45
2:N:173:THR:O	2:N:177:MET:HG3	2.17	0.45
1:A:715:ASN:ND2	1:A:869:VAL:HG13	2.32	0.45
1:B:290:LEU:HD12	1:B:290:LEU:HA	1.81	0.45
1:B:524:TRP:CH2	1:B:863:LYS:HG2	2.52	0.45
1:D:515:ASP:H	1:D:518:ILE:HG12	1.82	0.45
1:D:811:TYR:CD1	1:D:857:PRO:HD2	2.52	0.45
1:E:56:VAL:HG13	1:E:57:THR:HG22	1.99	0.45
1:E:813:ASP:OD1	1:E:813:ASP:N	2.47	0.45
1:G:456:ASN:HD22	1:G:456:ASN:HA	1.63	0.45
1:H:214:ARG:NH2	1:H:241:LYS:HE2	2.30	0.45
1:H:589:VAL:HG21	1:H:606:ALA:CB	2.47	0.45
1:I:651:ASN:OD1	1:I:651:ASN:N	2.50	0.45
1:I:759:CYS:HB2	1:I:864:PHE:HB3	1.99	0.45
1:J:76:THR:HG22	1:J:77:THR:H	1.82	0.45
1:K:190:ASP:CG	1:K:191:LYS:H	2.19	0.45
5:P:15:PRO:HG3	5:R:14:SER:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:81:TYR:CD2	5:R:82:MET:HG3	2.52	0.45
5:S:4:THR:HB	5:S:13:PHE:HE1	1.82	0.45
1:A:595:SER:OG	1:A:596:SER:N	2.49	0.45
1:A:721:VAL:CG1	1:A:743:PHE:HB2	2.40	0.45
1:C:141:GLN:HG3	1:C:142:GLY:H	1.82	0.45
1:C:153:VAL:O	1:C:156:THR:OG1	2.24	0.45
1:C:400:ASN:ND2	1:C:518:ILE:O	2.42	0.45
1:D:73:ARG:NH1	1:D:80:TYR:OH	2.50	0.45
1:E:485:TYR:CZ	1:E:528:PRO:HB3	2.52	0.45
1:F:113:PHE:HE1	1:F:324:ILE:H	1.65	0.45
1:F:239:GLN:HE21	1:F:240:ALA:H	1.63	0.45
1:F:337:ASN:ND2	1:F:361:ARG:O	2.50	0.45
1:F:346:ALA:O	1:F:580:THR:HG22	2.16	0.45
1:H:134:GLN:HA	1:H:154:THR:O	2.16	0.45
1:I:640:ASP:OD1	1:I:640:ASP:N	2.46	0.45
1:J:240:ALA:O	1:J:288:VAL:HG12	2.17	0.45
1:J:456:ASN:HB2	1:L:837:ARG:HH22	1.82	0.45
1:K:755:ASN:H	1:K:763:LYS:NZ	2.16	0.45
1:L:489:PRO:HD3	1:L:508:VAL:HG12	1.99	0.45
5:P:12:LEU:HA	5:P:12:LEU:HD23	1.64	0.45
7:2:30:LEU:O	7:2:31:ASN:C	2.52	0.45
1:A:170:GLN:HG2	1:A:185:LYS:HG3	1.98	0.44
1:A:204:TRP:CZ2	1:A:415:ASN:HA	2.52	0.44
1:A:890:GLN:OE1	1:C:53:THR:OG1	2.35	0.44
1:B:323:TYR:H	1:B:596:SER:HB3	1.82	0.44
1:B:922:VAL:HB	1:B:944:PRO:HD2	1.98	0.44
1:F:152:ASP:O	1:F:154:THR:HG22	2.17	0.44
1:F:188:TYR:HB2	1:F:192:THR:HG23	1.98	0.44
1:G:480:TYR:OH	1:G:538:PRO:HD3	2.17	0.44
1:G:657:PRO:HG2	1:G:660:ALA:HB2	1.99	0.44
1:H:924:ASP:OD1	1:H:924:ASP:N	2.49	0.44
1:J:277:TYR:OH	1:J:280:ASP:OD2	2.27	0.44
1:J:298:VAL:HG21	1:J:317:MET:HB3	1.98	0.44
1:J:546:ARG:NH2	1:J:594:GLN:OE1	2.48	0.44
1:C:733:GLY:O	1:C:736:ARG:HG2	2.17	0.44
1:F:681:THR:HG21	1:F:715:ASN:HD21	1.81	0.44
1:G:280:ASP:OD1	1:G:280:ASP:N	2.49	0.44
1:J:152:ASP:O	1:L:445:ALA:N	2.50	0.44
1:J:155:LYS:HG3	1:J:261:PHE:CZ	2.52	0.44
1:J:452:ILE:HG21	1:K:281:ILE:HD11	1.99	0.44
1:K:445:ALA:HB2	1:L:152:ASP:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:747:ARG:HE	1:L:750:ASP:HB3	1.82	0.44
1:B:240:ALA:O	1:B:241:LYS:HG3	2.17	0.44
1:C:574:LEU:HD23	1:C:574:LEU:HA	1.77	0.44
1:G:525:SER:HB2	1:G:863:LYS:HZ1	1.82	0.44
1:J:20:ALA:O	1:J:24:LEU:HG	2.18	0.44
1:K:10:TRP:HZ2	1:L:674:ALA:HB2	1.83	0.44
1:K:177:ASP:HB2	1:K:184:LYS:HE3	1.99	0.44
1:K:763:LYS:HZ3	1:K:763:LYS:HB2	1.81	0.44
1:L:94:LEU:O	1:L:95:ASP:HB2	2.17	0.44
1:A:198:GLN:HG3	1:A:199:VAL:O	2.17	0.44
1:B:667:ILE:HD12	1:B:901:LEU:HD23	2.00	0.44
1:C:172:LEU:HD22	1:C:193:PHE:HE1	1.83	0.44
1:C:178:GLU:HG2	1:C:179:THR:N	2.33	0.44
1:C:922:VAL:HG23	1:C:944:PRO:HD2	1.97	0.44
1:D:842:TYR:CE2	1:F:239:GLN:HG2	2.51	0.44
1:E:423:TYR:HA	1:F:264:PRO:HD3	2.00	0.44
1:E:609:ARG:HH22	5:P:62:THR:HG21	1.82	0.44
1:F:512:SER:HA	1:F:515:ASP:HB2	1.99	0.44
1:F:657:PRO:HD3	5:Q:13:PHE:CE2	2.47	0.44
1:F:725:PHE:O	1:F:901:LEU:HA	2.17	0.44
1:G:328:ASP:O	1:G:329:ASN:C	2.55	0.44
1:H:162:THR:HA	1:H:193:PHE:CZ	2.52	0.44
1:I:88:VAL:HG23	1:I:577:GLY:H	1.83	0.44
1:I:277:TYR:CE1	1:I:279:ALA:HB2	2.53	0.44
1:I:746:LYS:HE3	1:I:746:LYS:HB3	1.72	0.44
1:J:383:MET:HA	1:K:757:ALA:HA	1.98	0.44
1:J:575:LEU:HB3	1:J:576:PRO:HD2	2.00	0.44
1:K:391:TYR:H	1:K:391:TYR:HD1	1.65	0.44
1:L:202:GLU:HB3	1:L:206:GLU:HB2	1.99	0.44
5:P:8:PHE:O	5:Q:29:GLN:HB2	2.17	0.44
1:A:313:VAL:HG11	1:C:202:GLU:HB2	1.99	0.44
1:A:932:HIS:CG	1:A:933:ARG:H	2.35	0.44
1:B:517:TYR:HA	1:B:520:ILE:HG23	1.99	0.44
1:D:747:ARG:NE	1:D:750:ASP:HB2	2.31	0.44
1:E:173:LEU:HB2	1:E:185:LYS:NZ	2.33	0.44
1:E:537:HIS:CG	1:E:538:PRO:HD2	2.52	0.44
1:E:933:ARG:NH2	1:J:349:ALA:O	2.50	0.44
1:F:520:ILE:H	1:F:520:ILE:HG13	1.46	0.44
1:G:172:LEU:HD11	1:G:212:GLY:HA3	2.00	0.44
1:G:328:ASP:C	1:G:330:PHE:N	2.68	0.44
1:H:103:ILE:HG23	1:H:613:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:189:ALA:HB1	1:H:234:ASN:HD21	1.83	0.44
1:I:135:TRP:CH2	1:I:309:GLU:HB3	2.51	0.44
1:J:28:LEU:HD12	1:K:639:HIS:CD2	2.52	0.44
1:J:167:ILE:HD11	1:J:260:TYR:HD1	1.81	0.44
1:J:730:SER:OG	1:J:741:ASN:O	2.32	0.44
1:K:155:LYS:HD3	1:K:283:LEU:HD22	1.99	0.44
1:K:190:ASP:C	1:K:192:THR:H	2.21	0.44
1:K:514:VAL:HG23	1:K:518:ILE:HG12	2.00	0.44
1:K:590:ASN:HD21	1:K:701:TYR:H	1.66	0.44
1:A:204:TRP:CE3	1:B:313:VAL:HG13	2.53	0.44
1:A:360:ASP:OD1	1:A:360:ASP:N	2.48	0.44
1:A:924:ASP:N	1:A:924:ASP:OD1	2.47	0.44
1:C:635:ARG:HE	1:C:635:ARG:HB3	1.46	0.44
1:D:74:GLU:OE1	1:D:74:GLU:N	2.51	0.44
1:D:481:LEU:HD23	1:D:529:MET:HG2	1.98	0.44
1:F:152:ASP:C	1:F:154:THR:H	2.21	0.44
1:F:286:GLU:OE1	1:F:286:GLU:N	2.51	0.44
1:H:134:GLN:HG3	1:H:155:LYS:HZ3	1.83	0.44
1:H:242:PHE:HD1	1:H:242:PHE:HA	1.72	0.44
1:I:119:THR:OG1	1:I:120:ALA:N	2.51	0.44
1:I:524:TRP:CH2	1:I:863:LYS:HE3	2.53	0.44
1:I:665:ILE:HG12	1:I:903:MET:HB2	1.98	0.44
1:K:385:ASN:OD1	1:K:546:ARG:HG2	2.18	0.44
1:K:676:ARG:NH1	1:K:922:VAL:O	2.50	0.44
1:L:236:LYS:HE2	1:L:236:LYS:HB3	1.82	0.44
2:N:254:ILE:HG22	2:N:264:PHE:CZ	2.52	0.44
4:M:144:PHE:HZ	4:M:203:PHE:CE1	2.36	0.44
1:B:638:THR:HG21	4:M:16:SER:O	2.17	0.44
1:C:137:THR:HG23	1:C:152:ASP:HB2	1.99	0.44
1:H:43:ASN:OD1	1:I:571:ASN:ND2	2.51	0.44
1:H:573:LEU:HD12	1:H:573:LEU:HA	1.84	0.44
1:H:948:GLY:O	6:V:105:GLY:HA2	2.18	0.44
1:I:635:ARG:NH2	1:I:932:HIS:O	2.51	0.44
1:J:644:ASN:OD1	1:L:46:ARG:NE	2.43	0.44
1:K:101:PHE:HB2	1:K:562:VAL:HG23	1.99	0.44
1:K:341:ASN:O	1:K:341:ASN:ND2	2.47	0.44
1:L:309:GLU:HA	1:L:312:LEU:HB2	1.98	0.44
1:L:644:ASN:HB3	1:L:925:VAL:HG12	1.99	0.44
5:Q:45:ASN:O	5:Q:46:SER:OG	2.28	0.44
1:A:135:TRP:CH2	1:A:153:VAL:HB	2.48	0.44
1:B:262:ASP:OD2	1:B:279:ALA:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:912:GLU:OE1	1:B:912:GLU:N	2.51	0.44
1:C:721:VAL:HG23	1:C:743:PHE:HB2	2.00	0.44
1:D:64:LEU:HB2	1:E:736:ARG:O	2.17	0.44
1:D:116:TYR:HB2	1:E:402:GLY:HA3	1.98	0.44
1:D:137:THR:OG1	1:D:138:LYS:N	2.51	0.44
1:D:644:ASN:OD1	1:F:46:ARG:NE	2.51	0.44
1:F:19:ASP:OD1	1:F:47:ASN:ND2	2.51	0.44
1:F:280:ASP:OD1	1:F:280:ASP:N	2.51	0.44
1:F:720:LYS:HB3	1:F:742:GLU:HG3	2.00	0.44
1:G:332:GLY:O	1:G:586:ARG:NH1	2.46	0.44
1:H:445:ALA:HB2	1:I:152:ASP:HB3	2.00	0.44
1:H:503:TYR:CE2	1:H:507:ARG:HD2	2.52	0.44
1:H:620:PHE:HD2	1:H:622:MET:HG2	1.82	0.44
1:J:347:GLY:O	1:J:350:SER:N	2.35	0.44
1:J:517:TYR:HA	1:J:520:ILE:HG23	1.99	0.44
1:K:730:SER:HB2	1:K:732:PRO:HD2	2.00	0.44
1:K:752:GLU:H	1:K:752:GLU:HG3	1.54	0.44
1:L:239:GLN:O	1:L:241:LYS:HG3	2.17	0.44
1:L:400:ASN:HB3	1:L:469:TRP:HZ2	1.82	0.44
1:L:442:LYS:HG2	1:L:443:ASP:H	1.82	0.44
5:Q:13:PHE:CD1	5:Q:13:PHE:N	2.86	0.44
6:U:19:LEU:HD11	6:U:74:TRP:HE1	1.82	0.44
1:A:135:TRP:CZ2	1:A:309:GLU:HB2	2.51	0.44
1:A:244:PRO:HD3	1:A:254:LEU:C	2.38	0.44
1:A:473:LEU:HD12	1:A:473:LEU:HA	1.84	0.44
1:A:485:TYR:CZ	1:A:528:PRO:HB3	2.53	0.44
1:B:193:PHE:O	1:B:198:GLN:NE2	2.46	0.44
1:B:444:ASP:HB3	1:B:449:GLN:OE1	2.17	0.44
1:B:726:ASP:N	1:B:900:ALA:O	2.31	0.44
1:C:687:GLU:OE2	1:C:713:TYR:OH	2.27	0.44
1:D:98:SER:HB3	1:E:780:GLY:H	1.83	0.44
1:D:526:LEU:HA	1:D:526:LEU:HD22	1.81	0.44
1:D:847:PRO:HG2	1:F:121:TYR:CE2	2.53	0.44
1:E:263:VAL:O	1:E:265:GLY:N	2.50	0.44
1:E:344:VAL:HB	1:E:353:ASN:HB2	2.00	0.44
1:F:344:VAL:HG22	1:F:582:GLU:HG2	2.00	0.44
1:K:446:ILE:HG13	1:K:447:SER:H	1.83	0.44
1:K:573:LEU:HD12	1:K:573:LEU:HA	1.84	0.44
1:K:917:TYR:CG	1:K:917:TYR:O	2.68	0.44
1:L:277:TYR:CE2	1:L:279:ALA:HB2	2.52	0.44
5:P:15:PRO:HG3	5:R:14:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:8:PHE:HE1	5:R:28:ARG:HH11	1.65	0.44
5:S:72:MET:O	5:S:73:THR:C	2.57	0.44
1:A:718:PHE:HB3	1:A:745:ILE:HG13	2.00	0.43
1:B:336:TYR:HE2	1:B:565:LYS:HD2	1.82	0.43
1:B:656:ILE:HD11	1:B:916:LEU:HB2	1.99	0.43
1:C:655:PRO:HA	1:C:915:LEU:HB3	2.00	0.43
1:E:230:ALA:O	1:E:239:GLN:NE2	2.51	0.43
1:E:323:TYR:H	1:E:596:SER:HB3	1.83	0.43
1:E:456:ASN:H	1:E:456:ASN:HD22	1.66	0.43
1:F:47:ASN:HA	1:F:48:PRO:HD2	1.84	0.43
1:F:398:ILE:HG22	1:F:524:TRP:O	2.18	0.43
1:H:445:ALA:O	1:H:449:GLN:HB2	2.18	0.43
1:K:65:THR:HG23	1:L:738:LEU:HD13	1.99	0.43
1:A:473:LEU:O	1:A:477:VAL:HG12	2.17	0.43
1:A:825:ASN:HA	1:C:122:ASN:HA	2.00	0.43
1:B:204:TRP:CE3	1:C:313:VAL:HG22	2.53	0.43
1:B:526:LEU:HB3	1:B:528:PRO:HD2	2.00	0.43
1:C:398:ILE:HD12	1:C:473:LEU:HD11	1.99	0.43
1:C:524:TRP:CD2	1:C:803:ARG:HG2	2.53	0.43
1:C:686:LYS:HE3	1:C:686:LYS:HB2	1.90	0.43
1:D:756:VAL:HB	1:D:763:LYS:HG3	2.00	0.43
1:E:192:THR:HG22	1:E:193:PHE:CE1	2.53	0.43
1:E:604:ASP:OD1	1:E:605:GLY:N	2.44	0.43
1:G:66:LEU:HA	1:G:66:LEU:HD23	1.80	0.43
1:G:357:ASP:HB3	1:G:566:PHE:HE1	1.83	0.43
1:G:414:LEU:HD23	1:G:414:LEU:HA	1.83	0.43
1:G:440:TRP:HE1	1:H:277:TYR:HA	1.83	0.43
1:H:113:PHE:CE2	1:H:115:PRO:HG3	2.52	0.43
1:H:479:LEU:HD11	1:I:406:GLU:HG2	2.00	0.43
1:I:151:LYS:HB3	1:I:154:THR:HB	2.00	0.43
1:J:17:GLY:H	1:J:48:PRO:CG	2.29	0.43
1:J:278:LYS:NZ	1:L:438:SER:HB3	2.33	0.43
1:J:417:THR:HA	1:J:457:VAL:HG13	2.00	0.43
1:J:573:LEU:HB3	1:J:641:GLN:NE2	2.34	0.43
1:J:640:ASP:OD1	1:J:640:ASP:N	2.47	0.43
1:J:687:GLU:OE2	1:J:713:TYR:OH	2.32	0.43
1:K:190:ASP:C	1:K:192:THR:N	2.71	0.43
1:K:277:TYR:CZ	1:K:279:ALA:HB2	2.53	0.43
1:K:886:THR:HG23	1:K:889:GLY:H	1.83	0.43
1:L:531:ASN:HB2	1:L:714:LEU:HD11	2.00	0.43
5:Q:76:ARG:HB3	5:Q:76:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:28:ARG:HD3	5:S:31:VAL:HG11	2.00	0.43
1:A:411:CYS:SG	1:C:460:MET:HG3	2.58	0.43
1:A:718:PHE:CD1	1:A:907:VAL:HG12	2.53	0.43
1:A:744:GLU:O	1:A:762:THR:OG1	2.29	0.43
1:B:109:ARG:NH1	1:B:324:ILE:O	2.51	0.43
1:C:327:ARG:HD2	1:C:331:VAL:HG23	1.98	0.43
1:C:677:GLY:H	1:C:875:PHE:HB2	1.83	0.43
1:D:825:ASN:HD21	1:F:124:LEU:HG	1.83	0.43
1:G:130:PRO:HG3	1:G:312:LEU:HG	1.99	0.43
1:I:69:VAL:HG22	1:I:70:PRO:HD2	1.99	0.43
1:I:369:LEU:HD12	1:I:647:LEU:HD13	2.00	0.43
1:J:706:PRO:HB3	1:J:711:THR:O	2.18	0.43
1:J:894:TYR:HD1	1:L:4:PRO:HD2	1.82	0.43
1:K:58:THR:HG23	1:L:736:ARG:HH22	1.82	0.43
1:K:134:GLN:HE21	1:K:154:THR:HB	1.84	0.43
1:L:189:ALA:C	1:L:241:LYS:HZ2	2.19	0.43
4:M:203:PHE:HB2	4:M:206:LEU:HD13	1.99	0.43
5:Q:9:GLU:OE2	5:Q:10:GLY:N	2.51	0.43
6:V:69:LEU:HD23	6:V:69:LEU:H	1.83	0.43
1:A:151:LYS:O	1:C:445:ALA:N	2.51	0.43
1:A:194:GLN:O	1:A:197:PRO:HD2	2.18	0.43
1:A:231:ARG:O	1:A:240:ALA:HB2	2.18	0.43
1:A:368:GLN:NE2	1:A:709:ASP:OD1	2.51	0.43
1:B:3:THR:HG23	1:B:5:SER:H	1.83	0.43
1:B:67:ARG:HB2	1:B:616:TYR:CE2	2.54	0.43
1:B:138:LYS:HG2	1:B:149:GLN:HB3	2.00	0.43
1:D:162:THR:HG22	1:D:212:GLY:O	2.19	0.43
1:D:230:ALA:O	1:E:845:ASN:HB3	2.18	0.43
1:D:428:ILE:HD11	1:E:169:ASN:HB3	2.00	0.43
1:E:198:GLN:HB2	1:F:838:GLN:O	2.19	0.43
1:G:169:ASN:HB3	1:I:428:ILE:HD13	1.99	0.43
1:G:524:TRP:CD2	1:G:803:ARG:HG2	2.54	0.43
1:H:109:ARG:H	1:H:109:ARG:HG2	1.64	0.43
1:H:372:ASP:OD2	1:H:790:ARG:HB3	2.18	0.43
1:H:785:GLU:HG3	1:H:787:TYR:CE1	2.54	0.43
1:I:193:PHE:HZ	1:I:284:TYR:CZ	2.36	0.43
1:K:480:TYR:OH	1:K:538:PRO:HD3	2.19	0.43
1:K:524:TRP:CD2	1:K:803:ARG:HG2	2.54	0.43
1:L:228:SER:HA	1:L:292:THR:HG22	2.00	0.43
5:Q:51:TYR:O	5:Q:54:VAL:HG13	2.18	0.43
1:D:738:LEU:HA	1:F:63:ARG:NH1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:836:MET:HB3	1:D:836:MET:HE3	1.70	0.43
1:E:437:GLU:O	1:F:278:LYS:HD2	2.17	0.43
1:F:732:PRO:HB3	1:F:743:PHE:CE1	2.54	0.43
1:G:520:ILE:H	1:G:520:ILE:HG13	1.46	0.43
1:G:759:CYS:SG	1:G:761:MET:HB3	2.59	0.43
1:I:746:LYS:HG2	1:I:864:PHE:HE1	1.83	0.43
1:L:90:ASP:OD1	1:L:91:ASN:N	2.52	0.43
5:Q:49:MET:HG3	5:Q:50:THR:H	1.82	0.43
1:A:414:LEU:HD21	1:C:410:TYR:CE2	2.52	0.43
1:A:725:PHE:HE1	1:A:731:TRP:HB2	1.83	0.43
1:A:842:TYR:CE2	1:C:239:GLN:HG2	2.52	0.43
1:C:34:ALA:HB1	7:2:10:ALA:HB2	2.00	0.43
1:D:170:GLN:CD	1:D:185:LYS:HG3	2.38	0.43
1:D:536:ASN:HB3	1:D:596:SER:O	2.18	0.43
1:D:620:PHE:HE1	1:E:880:MET:HE1	1.83	0.43
1:I:462:ILE:HG12	1:I:463:ASN:N	2.34	0.43
1:J:193:PHE:HZ	1:J:284:TYR:CZ	2.37	0.43
1:J:819:LEU:HA	1:J:822:GLN:CD	2.38	0.43
4:M:234:LEU:HD11	4:M:252:LEU:HD22	2.01	0.43
5:Q:42:LEU:N	5:Q:43:PRO:HD3	2.34	0.43
7:4:4:ILE:HG13	7:4:7:ALA:HB2	1.99	0.43
1:A:80:TYR:HD2	1:A:585:PHE:HB2	1.82	0.43
1:A:241:LYS:HE2	1:A:286:GLU:HG2	2.01	0.43
1:A:738:LEU:HG	1:C:65:THR:HG23	1.99	0.43
1:B:172:LEU:HD21	1:B:212:GLY:HA3	2.00	0.43
1:B:379:ARG:H	1:B:379:ARG:HG2	1.60	0.43
1:C:922:VAL:HG22	1:C:923:PHE:N	2.34	0.43
1:F:308:SER:OG	1:F:311:ASN:ND2	2.44	0.43
1:G:320:ARG:CZ	1:G:597:LEU:HD11	2.49	0.43
1:H:764:ASP:O	1:H:768:VAL:HG12	2.19	0.43
1:I:771:LEU:HD13	1:I:777:GLY:HA3	2.01	0.43
1:K:239:GLN:NE2	1:K:240:ALA:H	2.15	0.43
1:K:537:HIS:ND1	1:K:538:PRO:HD2	2.33	0.43
1:L:47:ASN:OD1	1:L:47:ASN:N	2.50	0.43
6:U:81:GLN:NE2	6:U:179:ARG:O	2.52	0.43
1:B:423:TYR:HE1	1:C:263:VAL:HG22	1.84	0.43
1:C:679:SER:HB2	1:C:919:LEU:HG	2.01	0.43
1:D:158:GLY:O	1:F:452:ILE:HA	2.19	0.43
1:F:46:ARG:HH12	7:4:27:THR:HG23	1.83	0.43
1:G:838:GLN:HB3	1:I:200:GLY:HA3	2.00	0.43
1:I:684:LYS:HG2	1:I:914:THR:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:748:SER:HA	5:S:54:VAL:HG23	2.00	0.43
1:I:803:ARG:HH21	1:I:805:VAL:HG11	1.84	0.43
1:J:440:TRP:NE1	1:K:276:GLU:O	2.50	0.43
1:J:763:LYS:HE3	1:J:763:LYS:HB2	1.83	0.43
1:L:824:ASN:OD1	1:L:825:ASN:N	2.52	0.43
2:N:198:ASP:HA	2:N:236:LEU:HD11	2.01	0.43
1:B:320:ARG:NH2	1:B:479:LEU:O	2.52	0.43
1:B:736:ARG:HA	1:B:736:ARG:HD3	1.84	0.43
1:C:114:LYS:NZ	1:C:116:TYR:O	2.33	0.43
1:C:152:ASP:C	1:C:154:THR:H	2.22	0.43
1:C:413:PRO:HD3	1:C:458:TYR:O	2.19	0.43
1:D:230:ALA:HB3	1:D:239:GLN:NE2	2.34	0.43
1:D:923:PHE:O	1:D:942:ARG:HA	2.19	0.43
1:E:631:GLU:OE2	1:E:635:ARG:NH1	2.45	0.43
1:E:846:PHE:HB3	1:E:847:PRO:HD3	2.00	0.43
1:G:76:THR:HG22	1:G:77:THR:H	1.83	0.43
1:G:396:ARG:NH2	1:G:865:LEU:HD11	2.34	0.43
1:G:867:ASP:N	1:G:867:ASP:OD1	2.52	0.43
1:H:231:ARG:O	1:H:240:ALA:HB2	2.19	0.43
1:H:513:LEU:HD13	1:H:819:LEU:HD22	2.00	0.43
1:I:327:ARG:HH21	1:I:705:ILE:HG12	1.84	0.43
1:J:372:ASP:OD2	1:J:790:ARG:HB3	2.19	0.43
1:J:738:LEU:HB3	1:J:754:TYR:CE2	2.52	0.43
4:M:257:THR:O	4:M:261:GLU:HG2	2.17	0.43
6:V:197:TYR:OH	6:V:200:PRO:O	2.32	0.43
1:A:537:HIS:ND1	1:A:538:PRO:HD2	2.34	0.43
1:A:726:ASP:O	1:A:727:SER:OG	2.35	0.43
1:B:387:ALA:HB3	1:B:546:ARG:HH11	1.83	0.43
1:D:407:LEU:HD11	1:F:474:TYR:HB3	2.00	0.43
1:E:842:TYR:CD1	1:E:843:PRO:HD2	2.54	0.43
1:F:6:MET:HE3	1:F:10:TRP:HE1	1.82	0.43
1:F:794:PHE:HA	1:F:869:VAL:HG11	2.01	0.43
1:F:808:GLU:OE1	1:F:808:GLU:N	2.34	0.43
1:G:198:GLN:HB2	1:H:839:GLY:N	2.34	0.43
1:G:336:TYR:OH	1:G:565:LYS:HG2	2.19	0.43
1:H:192:THR:HG22	1:H:284:TYR:CG	2.54	0.43
1:I:737:LEU:HD11	1:I:743:PHE:CE2	2.53	0.43
1:J:732:PRO:HG3	1:J:743:PHE:CZ	2.54	0.43
1:K:161:ALA:N	1:K:212:GLY:O	2.47	0.43
1:K:836:MET:HA	1:L:410:TYR:OH	2.18	0.43
4:M:207:ARG:HA	4:M:210:TRP:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:16:TYR:HB3	5:P:18:THR:CG2	2.49	0.43
6:V:87:THR:HG23	6:V:173:SER:HB3	2.00	0.43
1:A:836:MET:HG2	1:A:837:ARG:H	1.84	0.42
1:B:533:ASN:OD1	1:B:533:ASN:N	2.53	0.42
1:C:676:ARG:O	1:C:921:GLU:HB2	2.19	0.42
1:D:204:TRP:CZ2	1:D:415:ASN:HA	2.54	0.42
1:D:372:ASP:HB2	1:D:377:ARG:HD3	2.01	0.42
1:F:500:THR:HG23	1:F:503:TYR:H	1.84	0.42
1:F:790:ARG:H	1:F:793:SER:HB3	1.84	0.42
1:G:261:PHE:HB3	1:I:423:TYR:HB3	2.01	0.42
1:G:385:ASN:OD1	1:G:546:ARG:HD2	2.19	0.42
1:G:943:THR:HB	1:G:944:PRO:HD3	2.01	0.42
1:H:126:PRO:HG2	1:H:129:ALA:HB2	2.01	0.42
1:H:460:MET:HE2	1:H:460:MET:HB2	1.86	0.42
1:I:19:ASP:HB2	7:5:14:GLY:HA3	2.01	0.42
1:J:109:ARG:NH1	1:J:324:ILE:O	2.52	0.42
1:K:117:SER:HA	1:K:321:PRO:HB3	2.01	0.42
1:L:923:PHE:O	1:L:942:ARG:HA	2.18	0.42
2:N:189:GLY:CA	2:N:194:VAL:HG22	2.49	0.42
6:U:24:SER:O	6:U:25:GLN:C	2.56	0.42
1:A:114:LYS:HE2	1:A:116:TYR:CE1	2.54	0.42
1:A:206:GLU:O	1:A:211:TYR:OH	2.37	0.42
1:A:520:ILE:H	1:A:520:ILE:HG12	1.53	0.42
1:B:162:THR:HG23	1:B:193:PHE:CG	2.54	0.42
1:C:668:PRO:HG3	1:K:664:PRO:HG3	2.00	0.42
1:D:473:LEU:HD12	1:D:473:LEU:HA	1.78	0.42
1:E:101:PHE:CZ	1:E:581:TYR:HE2	2.37	0.42
1:E:114:LYS:HE2	1:E:319:ASN:O	2.20	0.42
1:E:198:GLN:HB2	1:F:838:GLN:HB2	2.01	0.42
1:E:450:ASN:HD22	1:F:155:LYS:HB2	1.85	0.42
1:E:456:ASN:H	1:E:456:ASN:ND2	2.17	0.42
1:E:629:THR:O	1:E:633:MET:HG2	2.19	0.42
1:F:661:THR:HA	1:F:907:VAL:O	2.18	0.42
1:G:31:PHE:O	1:G:35:THR:HG22	2.19	0.42
1:G:111:PRO:HG3	1:G:554:ARG:HH12	1.84	0.42
1:H:666:SER:CB	5:Q:16:TYR:HE1	2.32	0.42
1:L:135:TRP:CD1	1:L:135:TRP:C	2.93	0.42
1:L:685:THR:HG21	1:L:913:PRO:HG2	2.00	0.42
2:N:146:GLU:H	2:N:146:GLU:HG3	1.52	0.42
1:A:137:THR:OG1	1:A:138:LYS:N	2.52	0.42
1:A:138:LYS:HA	1:A:149:GLN:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:LYS:O	1:A:507:ARG:NH1	2.52	0.42
1:B:520:ILE:H	1:B:520:ILE:HG12	1.46	0.42
1:E:58:THR:HB	1:E:623:ALA:HA	2.01	0.42
1:H:760:ASN:CG	5:R:54:VAL:HG21	2.39	0.42
1:I:353:ASN:OD1	1:I:355:VAL:HG12	2.19	0.42
1:K:589:VAL:O	1:K:593:LEU:HB2	2.19	0.42
1:L:310:ILE:HD12	1:L:310:ILE:HA	1.88	0.42
1:L:337:ASN:ND2	1:L:357:ASP:OD1	2.52	0.42
1:L:422:THR:HA	1:L:451:GLN:HA	2.00	0.42
1:L:642:SER:HA	1:L:926:VAL:O	2.19	0.42
1:B:334:MET:O	1:B:583:TRP:NE1	2.49	0.42
1:B:389:ASP:OD2	1:B:594:GLN:NE2	2.40	0.42
1:B:745:ILE:HG23	1:B:765:TRP:CD1	2.55	0.42
1:C:228:SER:HB2	1:C:290:LEU:HD11	2.01	0.42
1:C:377:ARG:NH2	1:C:388:VAL:HG22	2.34	0.42
1:D:187:ILE:O	1:D:192:THR:N	2.52	0.42
1:E:924:ASP:HB3	1:E:942:ARG:HG3	2.01	0.42
1:F:396:ARG:NH2	1:F:865:LEU:HD11	2.34	0.42
1:G:552:ASN:HB3	1:H:522:ALA:HB2	2.00	0.42
1:G:734:ASN:HB3	1:I:61:SER:HA	2.01	0.42
1:H:537:HIS:ND1	1:H:538:PRO:HD2	2.34	0.42
1:I:745:ILE:HG23	1:I:765:TRP:CD1	2.54	0.42
1:I:885:LEU:HB3	1:I:886:THR:H	1.60	0.42
1:J:135:TRP:CH2	1:J:309:GLU:HB2	2.54	0.42
1:J:136:GLU:OE2	1:J:151:LYS:HE2	2.19	0.42
1:J:214:ARG:HH22	1:J:241:LYS:CE	2.32	0.42
1:K:58:THR:HG22	1:K:621:PRO:O	2.19	0.42
1:L:574:LEU:HD12	1:L:574:LEU:HA	1.85	0.42
1:L:715:ASN:HD21	1:L:869:VAL:HG23	1.84	0.42
8:X:8:UNK:O	8:X:12:UNK:N	2.52	0.42
1:A:480:TYR:OH	1:A:538:PRO:HD3	2.19	0.42
1:A:559:HIS:HE1	1:B:753:GLY:HA2	1.85	0.42
1:A:809:ILE:HG21	5:P:78:ALA:HB1	2.01	0.42
1:B:385:ASN:OD1	1:B:546:ARG:HD2	2.19	0.42
1:B:920:PHE:O	1:B:922:VAL:HG13	2.20	0.42
1:C:286:GLU:OE1	1:C:286:GLU:N	2.52	0.42
1:D:239:GLN:HG2	1:E:842:TYR:CE2	2.55	0.42
1:E:128:GLY:HA2	1:E:314:GLN:O	2.18	0.42
1:E:524:TRP:CD1	1:E:803:ARG:HD3	2.54	0.42
1:F:912:GLU:HG3	1:F:913:PRO:HD2	2.01	0.42
1:G:597:LEU:HD12	1:G:597:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:620:PHE:O	1:G:622:MET:N	2.49	0.42
1:H:394:ASP:OD1	1:H:394:ASP:N	2.29	0.42
1:H:811:TYR:CD1	1:H:857:PRO:HD2	2.54	0.42
1:J:310:ILE:H	1:J:310:ILE:HG13	1.58	0.42
1:K:194:GLN:O	1:K:195:PRO:C	2.56	0.42
1:L:193:PHE:HZ	1:L:284:TYR:CG	2.38	0.42
7:9:5:ASN:OD1	7:9:5:ASN:N	2.52	0.42
1:A:487:TYR:OH	1:A:832:LEU:O	2.26	0.42
1:B:20:ALA:HA	1:B:23:TYR:CD2	2.54	0.42
1:B:140:LYS:HA	1:B:146:GLY:O	2.20	0.42
1:B:341:ASN:OD1	1:B:341:ASN:N	2.52	0.42
1:C:42:GLY:HA2	7:2:25:ILE:HG23	2.01	0.42
1:C:358:LEU:HD22	1:C:942:ARG:NH1	2.34	0.42
1:C:575:LEU:HD22	1:C:631:GLU:HB3	2.01	0.42
1:C:893:LEU:HD13	6:U:225:GLY:HA3	2.01	0.42
1:D:388:VAL:O	1:D:542:GLY:HA3	2.19	0.42
1:D:476:ASN:OD1	1:D:476:ASN:N	2.52	0.42
1:E:520:ILE:H	1:E:520:ILE:HG12	1.53	0.42
1:E:937:GLU:HA	6:U:110:GLY:HA3	2.01	0.42
1:F:327:ARG:HB3	1:F:331:VAL:HG22	2.02	0.42
1:F:745:ILE:HG23	1:F:765:TRP:CD1	2.55	0.42
1:G:440:TRP:HH2	1:H:275:GLU:H	1.67	0.42
1:G:446:ILE:HG12	1:G:447:SER:H	1.85	0.42
1:G:546:ARG:NH2	1:G:594:GLN:OE1	2.48	0.42
1:H:423:TYR:HB3	1:I:261:PHE:HB3	2.01	0.42
1:H:485:TYR:HE2	1:H:528:PRO:HB3	1.85	0.42
1:H:744:GLU:O	1:H:762:THR:OG1	2.36	0.42
1:I:167:ILE:HD13	1:I:282:ILE:HB	2.00	0.42
1:I:474:TYR:OH	1:I:834:PRO:HG3	2.19	0.42
1:J:751:GLY:O	1:L:104:ARG:NH2	2.53	0.42
1:K:47:ASN:ND2	7:8:25:ILE:HG22	2.31	0.42
1:K:262:ASP:HA	1:K:280:ASP:HA	2.02	0.42
1:K:745:ILE:HG23	1:K:765:TRP:CD1	2.55	0.42
1:L:155:LYS:NZ	1:L:215:ALA:HB3	2.34	0.42
1:L:738:LEU:HD12	1:L:738:LEU:HA	1.75	0.42
2:N:80:THR:OG1	2:N:81:THR:N	2.53	0.42
5:P:8:PHE:HD1	5:Q:28:ARG:HD3	1.84	0.42
5:S:98:GLU:H	5:S:98:GLU:CD	2.23	0.42
1:A:18:GLN:HB3	1:A:22:GLU:HG3	2.01	0.42
1:A:423:TYR:CE1	1:B:263:VAL:HG22	2.54	0.42
1:B:313:VAL:HG12	1:B:313:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:GLU:HB3	1:B:708:LEU:HB2	2.00	0.42
1:D:198:GLN:HB3	1:E:838:GLN:HB2	2.02	0.42
1:D:446:ILE:HG13	1:E:141:GLN:HB3	2.02	0.42
1:D:765:TRP:O	1:D:766:PHE:C	2.53	0.42
1:E:135:TRP:CH2	1:E:153:VAL:HB	2.55	0.42
1:E:460:MET:HB2	1:E:460:MET:HE2	1.85	0.42
1:G:683:LEU:O	1:G:915:LEU:N	2.45	0.42
1:G:738:LEU:HD12	1:G:738:LEU:HA	1.85	0.42
1:G:842:TYR:CE2	1:I:239:GLN:HG2	2.53	0.42
1:H:107:LEU:HB3	1:H:556:VAL:HG13	2.01	0.42
1:H:715:ASN:HB2	1:H:871:TRP:HE1	1.85	0.42
1:I:151:LYS:O	1:I:154:THR:HB	2.19	0.42
1:I:534:PRO:HG2	1:I:535:PHE:CD1	2.55	0.42
1:J:162:THR:HG22	1:J:212:GLY:N	2.35	0.42
1:J:714:LEU:HD12	1:J:714:LEU:HA	1.85	0.42
1:K:360:ASP:OD1	1:K:361:ARG:N	2.53	0.42
1:L:372:ASP:OD2	1:L:790:ARG:HB3	2.20	0.42
1:L:495:PRO:HG2	1:L:503:TYR:HB2	2.00	0.42
2:N:169:SER:O	2:N:172:MET:N	2.41	0.42
2:N:225:THR:HG22	2:N:227:GLU:H	1.84	0.42
5:P:45:ASN:O	5:P:46:SER:CB	2.67	0.42
5:P:49:MET:HB3	5:P:50:THR:H	1.73	0.42
5:Q:2:ASN:HA	5:Q:6:GLY:HA3	2.02	0.42
6:V:2:SER:HB3	6:V:200:PRO:HD2	2.02	0.42
6:V:211:GLU:H	6:V:211:GLU:HG2	1.67	0.42
1:A:357:ASP:HB3	1:A:566:PHE:CE1	2.55	0.42
1:B:495:PRO:HG3	1:B:502:GLU:HB3	2.02	0.42
1:B:514:VAL:HA	1:B:518:ILE:HG21	2.02	0.42
1:B:575:LEU:O	1:B:577:GLY:N	2.52	0.42
1:D:312:LEU:HB3	1:F:204:TRP:CH2	2.55	0.42
1:F:108:ASP:HA	1:F:554:ARG:O	2.20	0.42
1:F:353:ASN:OD1	1:F:354:ALA:N	2.53	0.42
1:G:191:LYS:HB2	1:G:191:LYS:HE2	1.57	0.42
1:G:514:VAL:HA	1:G:518:ILE:HG21	2.01	0.42
1:H:234:ASN:OD1	1:H:234:ASN:N	2.53	0.42
1:I:160:ALA:HB1	1:I:212:GLY:C	2.40	0.42
1:J:683:LEU:O	1:J:915:LEU:N	2.46	0.42
1:K:197:PRO:HG3	1:L:831:TYR:CE1	2.55	0.42
1:K:234:ASN:HD21	1:K:238:GLY:HA3	1.85	0.42
5:P:35:THR:O	5:P:36:VAL:C	2.53	0.42
5:Q:8:PHE:HD1	5:R:28:ARG:HG2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:NH1	1:A:582:GLU:OE1	2.53	0.42
1:A:152:ASP:C	1:A:154:THR:N	2.73	0.42
1:A:159:VAL:HG11	1:B:840:GLN:HB2	2.02	0.42
1:A:244:PRO:HD2	1:A:253:ASP:C	2.39	0.42
1:A:838:GLN:HB2	1:C:198:GLN:HG2	2.00	0.42
1:B:233:THR:O	1:C:815:LYS:HE3	2.19	0.42
1:B:530:ASP:OD1	1:B:531:ASN:N	2.53	0.42
1:C:222:MET:HE3	1:C:311:ASN:HB3	2.02	0.42
1:C:328:ASP:O	1:C:329:ASN:C	2.56	0.42
1:D:662:ASN:HB3	1:D:906:GLU:HG2	2.02	0.42
1:E:19:ASP:N	1:E:19:ASP:OD1	2.47	0.42
1:F:334:MET:HG3	1:F:336:TYR:CE2	2.55	0.42
1:F:524:TRP:CD2	1:F:803:ARG:HG2	2.54	0.42
1:G:313:VAL:HB	1:I:203:ASN:HB2	2.00	0.42
1:G:572:LEU:HD11	1:G:928:VAL:HG11	2.02	0.42
1:H:240:ALA:O	1:H:241:LYS:HD3	2.19	0.42
1:H:827:GLY:HA2	1:H:839:GLY:C	2.40	0.42
1:I:256:ILE:HD13	1:I:286:GLU:HB3	2.02	0.42
1:I:337:ASN:ND2	1:I:361:ARG:HB3	2.34	0.42
1:I:747:ARG:HG3	1:I:748:SER:O	2.20	0.42
1:I:764:ASP:OD1	1:I:764:ASP:N	2.52	0.42
1:J:635:ARG:HG3	1:J:930:GLN:O	2.20	0.42
1:K:172:LEU:HD11	1:K:193:PHE:CZ	2.54	0.42
1:L:599:ASN:O	1:L:702:SER:HB3	2.20	0.42
1:L:783:VAL:HG12	1:L:795:PHE:CZ	2.54	0.42
1:L:837:ARG:H	1:L:837:ARG:HG3	1.29	0.42
2:N:241:VAL:HG22	2:N:266:ILE:HB	2.01	0.42
1:A:360:ASP:O	1:A:361:ARG:HG3	2.20	0.42
1:B:320:ARG:N	1:B:505:ASN:OD1	2.43	0.42
1:B:600:ASP:OD1	1:B:602:ARG:N	2.53	0.42
1:B:668:PRO:HB2	2:N:88:PHE:CE1	2.55	0.42
1:B:808:GLU:HG3	1:B:814:TYR:CE2	2.54	0.42
1:D:652:MET:N	1:D:652:MET:SD	2.93	0.42
1:D:888:LEU:HA	1:D:888:LEU:HD23	1.87	0.42
1:E:176:THR:HA	1:E:183:GLY:HA2	2.01	0.42
1:E:240:ALA:O	1:E:288:VAL:HG12	2.20	0.42
1:E:442:LYS:HD3	1:E:442:LYS:HA	1.90	0.42
1:F:594:GLN:HG3	1:F:703:GLY:O	2.20	0.42
1:F:726:ASP:H	1:F:729:VAL:HG13	1.84	0.42
1:F:759:CYS:HG	1:F:761:MET:H	1.68	0.42
1:G:202:GLU:HB3	1:H:313:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:649:ALA:HA	1:G:922:VAL:HG22	2.02	0.42
1:I:231:ARG:O	1:I:240:ALA:HB2	2.20	0.42
1:K:486:LYS:HB3	1:K:509:VAL:HG22	2.02	0.42
5:S:74:ALA:O	5:S:75:THR:C	2.57	0.42
6:U:97:ALA:HB2	6:U:163:THR:HG21	2.02	0.42
1:A:677:GLY:HA3	1:A:874:PRO:HA	2.02	0.41
1:B:505:ASN:O	1:B:505:ASN:ND2	2.50	0.41
1:B:706:PRO:HB3	1:B:711:THR:O	2.19	0.41
1:C:172:LEU:HD23	1:C:174:LEU:HD23	2.01	0.41
1:C:199:VAL:O	1:C:201:GLU:N	2.51	0.41
1:C:530:ASP:OD1	1:C:865:LEU:HD21	2.20	0.41
1:C:573:LEU:HD23	1:C:634:LEU:HD21	2.02	0.41
1:C:763:LYS:HE3	1:C:763:LYS:HB2	1.93	0.41
1:D:231:ARG:O	1:D:240:ALA:HB2	2.20	0.41
1:D:483:ASP:O	1:D:484:SER:C	2.57	0.41
1:E:155:LYS:HZ3	1:E:283:LEU:HB3	1.84	0.41
1:E:358:LEU:HD21	1:E:947:ALA:HB2	2.01	0.41
1:E:641:GLN:HB3	1:E:643:PHE:CZ	2.55	0.41
1:G:166:ASN:O	1:G:173:LEU:HB3	2.20	0.41
1:G:288:VAL:HG13	1:G:290:LEU:H	1.84	0.41
1:H:121:TYR:O	1:H:122:ASN:C	2.58	0.41
1:H:130:PRO:HG3	1:H:312:LEU:HG	2.02	0.41
1:H:403:VAL:CG2	1:H:465:GLN:HB3	2.50	0.41
1:I:170:GLN:HB3	1:I:185:LYS:HE2	2.01	0.41
1:I:437:GLU:OE1	1:I:438:SER:N	2.53	0.41
1:J:401:HIS:CE1	1:L:544:ARG:HD2	2.55	0.41
1:L:904:THR:OG1	1:L:904:THR:O	2.38	0.41
2:N:129:LYS:HA	2:N:161:PHE:O	2.20	0.41
5:R:16:TYR:HD1	5:R:16:TYR:HA	1.65	0.41
1:A:202:GLU:HA	1:B:313:VAL:CG1	2.48	0.41
1:B:222:MET:HE2	1:B:307:SER:HB2	2.02	0.41
1:B:336:TYR:CE2	1:B:565:LYS:HB2	2.55	0.41
1:B:429:THR:HB	1:B:430:ASN:H	1.39	0.41
1:C:623:ALA:HB3	1:C:626:THR:HG23	2.02	0.41
1:C:865:LEU:HA	1:C:865:LEU:HD23	1.83	0.41
1:D:134:GLN:HA	1:D:155:LYS:H	1.84	0.41
1:D:641:GLN:HE21	1:D:641:GLN:H	1.67	0.41
1:E:642:SER:HA	1:E:926:VAL:O	2.20	0.41
1:E:845:ASN:N	1:E:845:ASN:OD1	2.53	0.41
1:F:705:ILE:H	1:F:705:ILE:HG12	1.61	0.41
1:G:94:LEU:HD23	1:G:619:PHE:CE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:731:TRP:CG	1:G:732:PRO:HD3	2.55	0.41
1:H:136:GLU:HG3	1:H:137:THR:N	2.35	0.41
1:H:155:LYS:HZ1	1:H:215:ALA:HB3	1.85	0.41
1:H:194:GLN:O	1:H:197:PRO:HD2	2.19	0.41
1:H:352:LEU:HD23	1:H:352:LEU:HA	1.96	0.41
1:H:943:THR:HG23	1:H:944:PRO:HD3	2.02	0.41
1:I:328:ASP:HB2	1:I:546:ARG:NH1	2.35	0.41
1:I:427:LYS:HB2	1:I:442:LYS:HD2	2.02	0.41
1:I:878:ASN:HD21	1:I:882:MET:CE	2.33	0.41
1:J:103:ILE:HA	1:J:613:VAL:HA	2.02	0.41
1:K:304:SER:OG	1:K:306:ASN:OD1	2.37	0.41
1:L:135:TRP:HZ3	1:L:156:THR:CG2	2.33	0.41
5:Q:13:PHE:CG	5:Q:14:SER:N	2.88	0.41
1:A:503:TYR:CZ	1:A:507:ARG:HD2	2.55	0.41
1:A:941:LEU:HB3	1:C:13:MET:HG2	2.03	0.41
1:B:86:LEU:HD23	1:B:581:TYR:HB2	2.02	0.41
1:B:164:GLY:HA2	1:B:174:LEU:HA	2.01	0.41
1:B:566:PHE:HD2	1:B:569:ILE:HG13	1.85	0.41
1:C:260:TYR:CD2	1:C:282:ILE:HG22	2.55	0.41
1:C:328:ASP:O	1:C:330:PHE:N	2.52	0.41
1:D:88:VAL:HG13	1:D:577:GLY:H	1.86	0.41
1:D:114:LYS:HE3	1:D:116:TYR:O	2.21	0.41
1:D:475:SER:O	1:D:476:ASN:C	2.58	0.41
1:F:481:LEU:O	1:F:486:LYS:NZ	2.53	0.41
1:G:230:ALA:HB1	1:G:288:VAL:HG22	2.02	0.41
1:G:410:TYR:CE1	1:H:414:LEU:HD21	2.52	0.41
1:H:262:ASP:OD2	1:H:279:ALA:N	2.54	0.41
1:H:429:THR:HG22	1:H:430:ASN:H	1.84	0.41
1:H:495:PRO:HG3	1:H:502:GLU:HB2	2.00	0.41
1:H:836:MET:HE3	1:H:837:ARG:HH21	1.85	0.41
1:I:150:GLU:HB2	1:I:152:ASP:OD1	2.19	0.41
1:I:202:GLU:HB2	1:I:206:GLU:HB2	2.01	0.41
1:I:346:ALA:O	1:I:580:THR:HG22	2.19	0.41
1:J:739:THR:O	1:J:739:THR:OG1	2.33	0.41
1:L:327:ARG:HB3	1:L:331:VAL:HG22	2.03	0.41
1:L:419:THR:HG22	1:L:451:GLN:HB2	2.01	0.41
2:N:271:LEU:O	2:N:352:ARG:HD3	2.20	0.41
4:M:361:ILE:O	4:M:365:MET:HG2	2.20	0.41
1:B:236:LYS:HD2	1:B:236:LYS:HA	1.97	0.41
1:B:293:PRO:O	1:B:295:THR:OG1	2.36	0.41
1:B:771:LEU:HD12	1:B:771:LEU:HA	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:LEU:HD22	1:E:193:PHE:HE2	1.85	0.41
1:E:463:ASN:O	1:E:467:ASN:ND2	2.43	0.41
1:E:524:TRP:CG	1:E:803:ARG:HD3	2.55	0.41
1:F:589:VAL:HG23	1:F:593:LEU:HD12	2.02	0.41
1:G:294:ASP:N	1:G:294:ASP:OD1	2.52	0.41
1:I:48:PRO:HG2	7:5:14:GLY:HA2	2.01	0.41
1:I:428:ILE:HD11	1:I:432:ASN:HA	2.03	0.41
1:J:684:LYS:HD2	1:J:686:LYS:HE2	2.01	0.41
1:J:801:MET:HG2	1:J:863:LYS:O	2.20	0.41
1:K:717:THR:HB	1:K:908:ASP:HB2	2.02	0.41
1:L:151:LYS:HE2	1:L:218:LYS:HD2	2.02	0.41
5:Q:16:TYR:CG	5:R:18:THR:OG1	2.62	0.41
5:R:13:PHE:CG	5:R:14:SER:N	2.88	0.41
6:U:211:GLU:H	6:U:211:GLU:HG2	1.61	0.41
1:A:278:LYS:HD2	1:C:437:GLU:HG3	2.03	0.41
1:A:377:ARG:NH1	1:A:386:SER:OG	2.52	0.41
1:A:396:ARG:NH1	1:A:534:PRO:HG3	2.35	0.41
1:A:415:ASN:HD22	1:B:157:PHE:HZ	1.68	0.41
1:B:24:LEU:HG	1:C:639:HIS:HB3	2.01	0.41
1:C:60:ARG:NH2	6:U:98:GLU:OE2	2.54	0.41
1:E:135:TRP:HE1	1:E:156:THR:CG2	2.33	0.41
1:E:369:LEU:HD23	7:3:30:LEU:HD13	2.01	0.41
1:F:536:ASN:HB3	1:F:596:SER:O	2.20	0.41
1:F:803:ARG:NH1	1:F:861:GLN:OE1	2.53	0.41
1:F:859:VAL:HG23	5:P:58:SER:HA	2.01	0.41
1:F:894:TYR:OH	1:J:949:ASN:OD1	2.37	0.41
1:I:88:VAL:HG12	1:I:619:PHE:CE2	2.49	0.41
1:I:346:ALA:HB2	1:I:353:ASN:HA	2.03	0.41
1:J:543:LEU:O	1:J:546:ARG:N	2.53	0.41
1:K:198:GLN:HG2	1:L:839:GLY:H	1.83	0.41
6:U:41:ILE:HD13	6:U:41:ILE:HG21	1.85	0.41
6:U:213:ILE:HB	6:U:216:PHE:HB2	2.02	0.41
1:A:107:LEU:HA	1:A:607:SER:HB2	2.01	0.41
1:A:588:ASP:O	1:A:592:ILE:HG12	2.20	0.41
1:B:135:TRP:HE1	1:B:156:THR:HG21	1.86	0.41
1:B:942:ARG:O	1:B:946:SER:HA	2.21	0.41
1:C:724:MET:HB3	1:C:729:VAL:HA	2.03	0.41
1:D:166:ASN:HA	1:D:210:PHE:CD2	2.56	0.41
1:D:276:GLU:HB2	1:F:440:TRP:CE3	2.54	0.41
1:D:470:LYS:HE2	1:F:124:LEU:HD11	2.02	0.41
1:F:204:TRP:HD1	1:F:204:TRP:H	1.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:698:TYR:CZ	5:R:47:SER:HB2	2.56	0.41
1:G:559:HIS:CE1	1:H:753:GLY:HA2	2.55	0.41
1:H:752:GLU:CD	1:H:752:GLU:H	2.24	0.41
1:I:151:LYS:C	1:I:154:THR:HB	2.40	0.41
1:I:766:PHE:O	1:I:767:LEU:C	2.58	0.41
1:K:923:PHE:O	1:K:942:ARG:HA	2.21	0.41
1:L:334:MET:HB2	1:L:336:TYR:CE2	2.55	0.41
1:L:634:LEU:HD12	1:L:634:LEU:HA	1.82	0.41
5:P:16:TYR:C	5:P:18:THR:N	2.73	0.41
5:R:54:VAL:HG12	5:R:55:GLY:N	2.31	0.41
1:A:1:MET:HG3	1:B:931:PRO:HG2	2.02	0.41
1:A:718:PHE:HB2	1:A:745:ILE:HG21	2.03	0.41
1:A:763:LYS:HE3	1:A:763:LYS:HB2	1.87	0.41
1:C:328:ASP:C	1:C:330:PHE:N	2.72	0.41
1:D:122:ASN:OD1	1:D:122:ASN:N	2.54	0.41
1:D:173:LEU:HA	1:D:185:LYS:HA	2.02	0.41
1:D:824:ASN:HA	1:D:844:ALA:CB	2.51	0.41
1:D:896:ASN:ND2	1:F:3:THR:O	2.49	0.41
1:D:931:PRO:HD2	1:D:935:VAL:HG23	2.03	0.41
1:E:724:MET:HG3	1:E:728:SER:O	2.20	0.41
1:F:721:VAL:HG13	1:F:743:PHE:HB2	2.03	0.41
1:G:211:TYR:HE2	1:I:454:LYS:HE2	1.85	0.41
1:G:822:GLN:HE21	1:G:822:GLN:C	2.23	0.41
1:H:322:ASN:HA	1:H:596:SER:OG	2.21	0.41
1:H:422:THR:HA	1:H:450:ASN:O	2.21	0.41
1:H:715:ASN:ND2	1:H:869:VAL:O	2.54	0.41
1:I:631:GLU:O	1:I:635:ARG:HB2	2.21	0.41
1:J:119:THR:OG1	1:J:120:ALA:N	2.53	0.41
1:J:444:ASP:HA	1:K:152:ASP:HA	2.02	0.41
1:J:471:SER:HA	1:K:407:LEU:HD11	2.02	0.41
1:J:485:TYR:CZ	1:J:528:PRO:HB3	2.55	0.41
1:K:243:LYS:HG3	1:K:253:ASP:O	2.21	0.41
1:K:529:MET:HG2	1:K:532:VAL:HG11	2.02	0.41
1:K:714:LEU:HD23	1:K:714:LEU:HA	1.91	0.41
1:K:863:LYS:HG2	1:K:864:PHE:H	1.86	0.41
5:R:10:GLY:O	5:R:12:LEU:N	2.53	0.41
6:U:36:ALA:HB1	6:U:40:MET:HB2	2.02	0.41
7:4:17:PRO:HB2	7:4:19:MET:HG3	2.02	0.41
1:B:567:PHE:HA	1:B:570:LYS:HE2	2.03	0.41
1:B:685:THR:HG21	1:B:913:PRO:HB2	2.02	0.41
1:B:835:THR:HG22	1:B:836:MET:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:527:ASP:N	1:C:528:PRO:HD2	2.36	0.41
1:D:478:ALA:O	1:D:479:LEU:C	2.53	0.41
1:D:717:THR:HB	1:D:908:ASP:HB2	2.03	0.41
1:D:773:HIS:CE1	1:D:872:ARG:HD3	2.55	0.41
1:D:943:THR:OG1	1:D:944:PRO:HD3	2.21	0.41
1:E:134:GLN:HA	1:E:155:LYS:H	1.86	0.41
1:E:254:LEU:HD22	1:E:254:LEU:HA	1.83	0.41
1:E:443:ASP:HB2	1:F:150:GLU:HB3	2.02	0.41
1:G:733:GLY:C	1:G:735:ASP:H	2.24	0.41
1:H:74:GLU:HG2	1:H:81:LYS:HB3	2.02	0.41
1:H:785:GLU:OE1	1:H:785:GLU:N	2.54	0.41
1:H:790:ARG:H	1:H:793:SER:HB3	1.86	0.41
1:I:88:VAL:HG23	1:I:577:GLY:N	2.36	0.41
1:I:102:ASP:OD2	1:I:559:HIS:NE2	2.45	0.41
1:J:212:GLY:HA2	1:J:282:ILE:O	2.20	0.41
1:K:132:PRO:HB2	1:K:215:ALA:HA	2.03	0.41
1:L:261:PHE:O	1:L:280:ASP:HA	2.21	0.41
5:Q:36:VAL:O	5:Q:39:ARG:N	2.53	0.41
1:A:88:VAL:HG13	1:A:576:PRO:HA	2.01	0.41
1:A:498:THR:HG23	1:A:503:TYR:CE2	2.56	0.41
1:A:513:LEU:HD13	1:A:513:LEU:HA	1.88	0.41
1:A:821:PHE:HB3	1:C:237:GLY:HA3	2.03	0.41
1:A:823:HIS:HB3	1:C:196:GLU:CD	2.41	0.41
1:B:134:GLN:HE22	1:B:217:LYS:HG3	1.85	0.41
1:B:396:ARG:NH1	1:B:867:ASP:OD2	2.54	0.41
1:B:771:LEU:HD21	1:B:778:TYR:CE2	2.56	0.41
1:B:811:TYR:CD1	1:B:857:PRO:HD2	2.56	0.41
1:B:924:ASP:HB3	1:B:942:ARG:HG2	2.02	0.41
1:C:488:THR:HG22	1:C:507:ARG:HG2	2.03	0.41
1:C:615:LEU:HD23	1:C:615:LEU:HA	1.84	0.41
1:D:16:ALA:HA	1:D:48:PRO:HB3	2.03	0.41
1:D:410:TYR:OH	1:F:836:MET:HA	2.21	0.41
1:D:432:ASN:O	1:E:168:THR:OG1	2.31	0.41
1:D:485:TYR:CZ	1:D:528:PRO:HB3	2.56	0.41
1:D:546:ARG:NH2	1:D:594:GLN:OE1	2.53	0.41
1:E:330:PHE:CZ	1:E:560:ILE:HB	2.55	0.41
1:E:872:ARG:NH2	7:3:30:LEU:HG	2.36	0.41
1:F:46:ARG:HH22	7:4:28:SER:H	1.66	0.41
1:F:185:LYS:HE3	1:F:185:LYS:HB2	1.85	0.41
1:F:190:ASP:OD1	1:F:191:LYS:N	2.54	0.41
1:F:214:ARG:HH12	1:F:241:LYS:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:319:ASN:OD1	1:F:505:ASN:ND2	2.46	0.41
1:F:760:ASN:CB	5:P:54:VAL:HG21	2.50	0.41
1:G:201:GLU:HA	1:H:836:MET:HE2	2.03	0.41
1:G:313:VAL:HG12	1:I:204:TRP:CE2	2.54	0.41
1:G:417:THR:HG21	1:G:453:CYS:SG	2.61	0.41
1:G:839:GLY:HA2	1:I:198:GLN:HG3	2.03	0.41
1:H:168:THR:OG1	1:H:169:ASN:N	2.54	0.41
1:H:368:GLN:HG2	1:H:709:ASP:O	2.21	0.41
1:H:681:THR:HG21	1:H:712:PHE:CD1	2.56	0.41
1:H:892:MET:HA	1:H:895:ALA:HB3	2.02	0.41
1:I:599:ASN:O	1:I:702:SER:OG	2.34	0.41
1:I:771:LEU:HD21	1:I:778:TYR:CE2	2.56	0.41
1:I:771:LEU:HD12	1:I:771:LEU:HA	1.87	0.41
1:J:79:LEU:HD22	1:J:335:TYR:HE2	1.86	0.41
1:J:158:GLY:HA3	1:J:283:LEU:HD11	2.01	0.41
1:J:396:ARG:NH2	1:J:865:LEU:HD11	2.36	0.41
1:J:539:ARG:HB2	1:J:539:ARG:HH11	1.86	0.41
1:J:633:MET:C	1:J:639:HIS:HE2	2.21	0.41
1:J:825:ASN:HA	1:L:122:ASN:HA	2.01	0.41
1:L:240:ALA:O	1:L:288:VAL:HG12	2.20	0.41
1:L:282:ILE:HD12	1:L:284:TYR:CE1	2.55	0.41
1:L:290:LEU:HD12	1:L:290:LEU:HA	1.87	0.41
1:L:350:SER:O	1:L:352:LEU:N	2.53	0.41
2:N:140:HIS:ND1	2:N:141:PRO:HD2	2.36	0.41
2:N:182:LEU:HD21	2:N:446:ARG:HD2	2.02	0.41
2:N:462:THR:OG1	2:N:463:THR:N	2.52	0.41
4:M:98:LEU:HD23	4:M:98:LEU:HA	1.88	0.41
1:A:156:THR:O	1:A:157:PHE:C	2.59	0.41
1:A:640:ASP:HB2	1:A:928:VAL:O	2.20	0.41
1:B:288:VAL:HG23	1:B:290:LEU:HB2	2.03	0.41
1:C:109:ARG:NH2	1:C:550:LEU:HB2	2.35	0.41
1:C:789:ASP:N	1:C:789:ASP:OD1	2.54	0.41
1:D:203:ASN:HD21	1:D:415:ASN:HB3	1.86	0.41
1:E:85:THR:O	1:E:85:THR:OG1	2.37	0.41
1:E:108:ASP:HB3	1:E:606:ALA:HB3	2.04	0.41
1:E:323:TYR:OH	1:F:401:HIS:HB3	2.21	0.41
1:E:477:VAL:HG11	1:E:514:VAL:HG21	2.03	0.41
1:E:566:PHE:O	1:E:570:LYS:N	2.53	0.41
1:F:135:TRP:CZ3	1:F:137:THR:HB	2.56	0.41
1:F:163:GLY:HA2	1:F:210:PHE:O	2.21	0.41
1:F:757:ALA:C	1:F:759:CYS:N	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:471:SER:HA	1:I:407:LEU:HD11	2.02	0.41
1:H:526:LEU:HD22	1:H:526:LEU:HA	1.91	0.41
1:I:309:GLU:H	1:I:309:GLU:HG3	1.70	0.41
1:J:198:GLN:CG	1:K:839:GLY:HA2	2.51	0.41
1:J:231:ARG:O	1:J:240:ALA:HB2	2.21	0.41
1:J:696:ASP:OD1	1:J:696:ASP:N	2.50	0.41
1:J:771:LEU:HG	1:J:777:GLY:HA3	2.02	0.41
1:K:20:ALA:HA	1:K:23:TYR:CE2	2.56	0.41
1:K:62:GLN:HE21	1:K:62:GLN:HB2	1.61	0.41
1:K:943:THR:HB	1:K:944:PRO:HD3	2.03	0.41
2:N:189:GLY:O	2:N:190:ARG:C	2.58	0.41
5:Q:8:PHE:CE1	5:R:28:ARG:HG2	2.56	0.41
1:A:20:ALA:HA	1:A:23:TYR:CE2	2.56	0.40
1:A:99:THR:HA	1:A:616:TYR:O	2.21	0.40
1:A:429:THR:HG22	1:A:430:ASN:H	1.87	0.40
1:A:556:VAL:HG12	1:B:804:GLN:NE2	2.36	0.40
1:B:461:GLU:OE2	1:C:414:LEU:HA	2.21	0.40
1:B:630:LEU:O	1:B:634:LEU:HB2	2.21	0.40
1:B:637:ASP:OD1	1:B:929:HIS:ND1	2.29	0.40
1:C:764:ASP:O	1:C:768:VAL:HG12	2.21	0.40
1:D:201:GLU:H	1:D:201:GLU:CD	2.24	0.40
1:E:61:SER:HA	1:F:734:ASN:HB2	2.02	0.40
1:E:155:LYS:HD2	1:E:261:PHE:CE1	2.56	0.40
1:E:842:TYR:CG	1:E:843:PRO:HD2	2.55	0.40
1:E:875:PHE:O	1:E:888:LEU:HB2	2.21	0.40
1:F:901:LEU:HD13	1:F:903:MET:HG3	2.02	0.40
1:G:167:ILE:HD11	1:G:260:TYR:CD1	2.56	0.40
1:G:588:ASP:O	1:G:592:ILE:HG12	2.20	0.40
1:G:807:ASP:OD2	1:G:810:ASN:ND2	2.54	0.40
1:H:162:THR:HA	1:H:193:PHE:CE1	2.56	0.40
1:I:201:GLU:CD	1:I:202:GLU:H	2.24	0.40
1:I:676:ARG:HH12	7:5:31:ASN:H	1.69	0.40
1:J:196:GLU:CD	1:K:823:HIS:HB3	2.41	0.40
1:J:785:GLU:HB2	1:J:788:LYS:HB2	2.03	0.40
1:K:575:LEU:HB3	1:K:576:PRO:HD2	2.03	0.40
1:K:779:GLN:HE22	1:L:39:PHE:HA	1.86	0.40
1:L:31:PHE:HD2	7:9:6:PHE:HD1	1.68	0.40
1:L:518:ILE:H	1:L:518:ILE:HG13	1.74	0.40
2:N:377:ASP:N	2:N:377:ASP:OD1	2.54	0.40
5:R:10:GLY:O	5:R:13:PHE:N	2.53	0.40
6:U:75:PRO:HD2	6:U:78:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:4:4:ILE:H	7:4:4:ILE:HG12	1.70	0.40
1:A:201:GLU:H	1:A:201:GLU:CD	2.21	0.40
1:A:283:LEU:HD23	1:A:283:LEU:HA	1.92	0.40
1:A:388:VAL:O	1:A:542:GLY:HA3	2.21	0.40
1:A:922:VAL:HA	1:A:944:PRO:HG2	2.04	0.40
1:B:222:MET:HE2	1:B:222:MET:HB3	1.91	0.40
1:B:392:ASP:O	1:B:395:VAL:HG12	2.22	0.40
1:C:277:TYR:CD1	1:C:277:TYR:N	2.89	0.40
1:D:203:ASN:H	1:E:313:VAL:CG1	2.35	0.40
1:E:208:GLU:OE1	1:E:208:GLU:N	2.54	0.40
1:E:240:ALA:O	1:E:241:LYS:HD3	2.21	0.40
1:E:588:ASP:OD1	1:E:591:MET:N	2.41	0.40
1:E:597:LEU:HD12	1:E:597:LEU:HA	1.93	0.40
1:E:924:ASP:OD1	1:E:924:ASP:N	2.53	0.40
1:F:89:GLY:O	1:F:576:PRO:HB3	2.21	0.40
1:F:227:GLY:HA3	1:F:295:THR:HG21	2.03	0.40
1:F:560:ILE:H	1:F:560:ILE:HG13	1.77	0.40
1:G:415:ASN:OD1	1:G:417:THR:N	2.53	0.40
1:G:696:ASP:OD1	1:G:696:ASP:N	2.44	0.40
1:G:823:HIS:CD2	1:I:195:PRO:HG2	2.57	0.40
1:H:499:ASN:O	1:H:599:ASN:HB2	2.21	0.40
1:H:590:ASN:HD22	1:H:602:ARG:HG3	1.87	0.40
1:H:696:ASP:OD1	1:H:696:ASP:N	2.48	0.40
1:I:96:MET:HE2	1:I:574:LEU:HD22	2.03	0.40
1:I:397:ILE:HG21	1:I:523:ARG:HG2	2.03	0.40
1:I:620:PHE:O	1:I:622:MET:N	2.52	0.40
1:J:114:LYS:NZ	1:J:118:GLY:O	2.48	0.40
1:J:174:LEU:HD13	1:J:191:LYS:HE2	2.03	0.40
1:K:498:THR:HG23	1:K:503:TYR:CE2	2.56	0.40
1:K:593:LEU:HD23	1:K:593:LEU:HA	1.74	0.40
2:N:54:THR:HG22	2:N:55:ARG:H	1.86	0.40
5:Q:9:GLU:HG3	5:R:21:LEU:HD12	2.03	0.40
5:Q:20:ARG:O	5:Q:21:LEU:C	2.59	0.40
1:A:918:LEU:HD23	1:A:919:LEU:N	2.37	0.40
1:A:943:THR:OG1	1:A:944:PRO:HD3	2.21	0.40
1:B:753:GLY:O	1:B:763:LYS:NZ	2.53	0.40
1:B:851:ILE:H	1:B:851:ILE:HD13	1.86	0.40
1:C:52:PRO:HG3	7:1:11:PRO:HG3	2.04	0.40
1:E:634:LEU:HD12	1:E:634:LEU:HA	1.86	0.40
1:F:359:GLN:NE2	1:F:692:GLY:HA2	2.35	0.40
1:G:202:GLU:OE2	1:H:299:TYR:OH	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:771:LEU:HD12	1:G:771:LEU:HA	1.89	0.40
1:G:771:LEU:HD13	1:G:777:GLY:HA3	2.04	0.40
1:H:442:LYS:HG2	1:H:443:ASP:H	1.85	0.40
1:H:630:LEU:O	1:H:634:LEU:HB2	2.21	0.40
1:H:634:LEU:HD12	1:H:634:LEU:HA	1.88	0.40
1:H:682:ARG:NH2	1:H:914:THR:HG21	2.36	0.40
1:H:942:ARG:O	1:H:946:SER:HA	2.21	0.40
1:J:57:THR:HG21	1:K:877:SER:OG	2.21	0.40
1:J:574:LEU:HA	1:J:574:LEU:HD23	1.87	0.40
1:J:763:LYS:HD3	1:L:100:TYR:OH	2.22	0.40
1:J:911:ASP:OD1	1:J:911:ASP:N	2.47	0.40
1:K:109:ARG:NH1	1:K:553:GLY:O	2.55	0.40
1:K:722:SER:O	1:K:903:MET:HA	2.20	0.40
1:L:74:GLU:HG3	1:L:81:LYS:HE3	2.03	0.40
1:L:589:VAL:HB	1:L:606:ALA:HA	2.02	0.40
1:L:946:SER:O	1:L:947:ALA:C	2.58	0.40
2:N:112:THR:HB	2:N:387:TRP:CZ2	2.55	0.40
2:N:332:GLU:H	2:N:332:GLU:HG3	1.77	0.40
1:A:313:VAL:HG22	1:C:204:TRP:CE3	2.51	0.40
1:A:566:PHE:O	1:A:570:LYS:HB2	2.21	0.40
1:A:589:VAL:O	1:A:593:LEU:HB2	2.21	0.40
1:A:647:LEU:HD11	1:A:919:LEU:HD21	2.04	0.40
1:C:192:THR:HG21	1:C:214:ARG:HH11	1.85	0.40
1:D:67:ARG:HB2	1:D:616:TYR:CE1	2.56	0.40
1:E:651:ASN:HB3	1:E:917:TYR:HE1	1.87	0.40
1:F:663:VAL:HG13	5:R:17:LEU:HD12	2.04	0.40
1:I:199:VAL:HB	1:I:206:GLU:HG2	2.02	0.40
1:J:47:ASN:OD1	1:J:47:ASN:N	2.53	0.40
1:J:138:LYS:HG2	1:J:149:GLN:HG3	2.02	0.40
1:J:194:GLN:HB2	1:J:196:GLU:OE1	2.21	0.40
1:J:411:CYS:HB3	1:L:462:ILE:HB	2.02	0.40
1:K:725:PHE:CD1	1:K:731:TRP:HB2	2.56	0.40
1:K:752:GLU:OE1	1:K:753:GLY:N	2.55	0.40
2:N:39:ARG:NH1	2:N:516:SER:OG	2.54	0.40
5:S:102:LEU:HD12	5:S:102:LEU:HA	1.91	0.40
1:A:426:VAL:HG23	1:B:260:TYR:HB2	2.03	0.40
1:B:76:THR:HG22	1:B:77:THR:H	1.85	0.40
1:B:159:VAL:HG21	1:C:841:PRO:HD2	2.04	0.40
1:B:193:PHE:HZ	1:B:199:VAL:HG23	1.86	0.40
1:C:721:VAL:HG12	1:C:905:PHE:HD2	1.86	0.40
1:D:574:LEU:HD12	1:D:574:LEU:HA	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:620:PHE:HD2	1:D:622:MET:HB3	1.87	0.40
1:F:94:LEU:HD23	1:F:574:LEU:HD21	2.03	0.40
1:F:423:TYR:OH	1:F:454:LYS:HG3	2.22	0.40
1:F:427:LYS:HD2	1:F:442:LYS:HE3	2.02	0.40
1:G:46:ARG:HB2	1:G:46:ARG:HH11	1.85	0.40
1:G:127:LYS:HE2	1:G:127:LYS:HB2	1.92	0.40
1:G:358:LEU:HD22	1:G:942:ARG:NH1	2.36	0.40
1:I:283:LEU:HD23	1:I:283:LEU:HA	1.83	0.40
1:J:503:TYR:C	1:J:505:ASN:H	2.25	0.40
1:J:942:ARG:HD2	1:J:945:PHE:O	2.21	0.40
1:K:71:VAL:HG21	1:K:85:THR:HG23	2.04	0.40
1:L:154:THR:HG23	1:L:155:LYS:HG2	2.03	0.40
1:L:192:THR:HG21	1:L:214:ARG:HH11	1.87	0.40
1:L:309:GLU:C	1:L:312:LEU:H	2.22	0.40
1:L:750:ASP:OD1	1:L:750:ASP:N	2.55	0.40
5:Q:41:VAL:H	5:Q:43:PRO:HD3	1.86	0.40
5:R:34:SER:OG	5:R:35:THR:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	949/952 (100%)	825 (87%)	121 (13%)	3 (0%)	41	73
1	B	947/952 (100%)	843 (89%)	101 (11%)	3 (0%)	41	73
1	C	944/952 (99%)	803 (85%)	139 (15%)	2 (0%)	47	78
1	D	945/952 (99%)	821 (87%)	122 (13%)	2 (0%)	47	78
1	E	945/952 (99%)	841 (89%)	104 (11%)	0	100	100
1	F	947/952 (100%)	815 (86%)	129 (14%)	3 (0%)	41	73
1	G	945/952 (99%)	817 (86%)	123 (13%)	5 (0%)	29	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	945/952 (99%)	817 (86%)	127 (13%)	1 (0%)	51	82
1	I	947/952 (100%)	818 (86%)	128 (14%)	1 (0%)	51	82
1	J	949/952 (100%)	830 (88%)	118 (12%)	1 (0%)	51	82
1	K	948/952 (100%)	833 (88%)	115 (12%)	0	100	100
1	L	945/952 (99%)	821 (87%)	120 (13%)	4 (0%)	34	68
2	N	467/519 (90%)	434 (93%)	32 (7%)	1 (0%)	47	78
3	O	15/374 (4%)	13 (87%)	2 (13%)	0	100	100
4	M	358/560 (64%)	344 (96%)	14 (4%)	0	100	100
5	P	118/134 (88%)	96 (81%)	19 (16%)	3 (2%)	5	29
5	Q	110/134 (82%)	84 (76%)	24 (22%)	2 (2%)	8	35
5	R	131/134 (98%)	109 (83%)	22 (17%)	0	100	100
5	S	118/134 (88%)	98 (83%)	18 (15%)	2 (2%)	9	36
6	U	184/227 (81%)	172 (94%)	12 (6%)	0	100	100
6	V	182/227 (80%)	167 (92%)	15 (8%)	0	100	100
7	1	28/234 (12%)	20 (71%)	8 (29%)	0	100	100
7	2	24/234 (10%)	16 (67%)	8 (33%)	0	100	100
7	3	25/234 (11%)	20 (80%)	5 (20%)	0	100	100
7	4	27/234 (12%)	18 (67%)	9 (33%)	0	100	100
7	5	26/234 (11%)	21 (81%)	5 (19%)	0	100	100
7	6	25/234 (11%)	21 (84%)	4 (16%)	0	100	100
7	7	25/234 (11%)	20 (80%)	5 (20%)	0	100	100
7	8	27/234 (12%)	24 (89%)	3 (11%)	0	100	100
7	9	26/234 (11%)	20 (77%)	6 (23%)	0	100	100
All	All	13272/15973 (83%)	11581 (87%)	1658 (12%)	33 (0%)	50	78

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	ASP
1	C	153	VAL
1	D	153	VAL
1	F	153	VAL
1	F	203	ASN
1	G	193	PHE

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Mol	Chain	Res	Type
1	I	885	LEU
1	L	152	ASP
5	P	15	PRO
5	P	46	SER
5	Q	9	GLU
5	S	78	ALA
1	G	329	ASN
1	L	95	ASP
1	L	309	GLU
5	Q	10	GLY
1	A	248	GLY
1	G	727	SER
1	L	94	LEU
1	D	152	ASP
1	F	152	ASP
5	S	73	THR
1	C	152	ASP
1	H	845	ASN
1	J	20	ALA
5	P	40	PRO
1	B	429	THR
1	B	456	ASN
1	G	196	GLU
2	N	390	PRO
1	A	153	VAL
1	B	477	VAL
1	G	477	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	817/818 (100%)	741 (91%)	76 (9%)	9	31
1	B	815/818 (100%)	721 (88%)	94 (12%)	5	22
1	C	814/818 (100%)	724 (89%)	90 (11%)	6	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	814/818 (100%)	728 (89%)	86 (11%)	6	25
1	E	814/818 (100%)	730 (90%)	84 (10%)	7	27
1	F	816/818 (100%)	733 (90%)	83 (10%)	7	28
1	G	814/818 (100%)	718 (88%)	96 (12%)	5	20
1	H	814/818 (100%)	712 (88%)	102 (12%)	4	18
1	I	815/818 (100%)	723 (89%)	92 (11%)	6	22
1	J	817/818 (100%)	725 (89%)	92 (11%)	6	22
1	K	817/818 (100%)	721 (88%)	96 (12%)	5	20
1	L	814/818 (100%)	720 (88%)	94 (12%)	5	22
2	N	426/462 (92%)	387 (91%)	39 (9%)	9	32
3	O	15/324 (5%)	12 (80%)	3 (20%)	1	4
4	M	304/472 (64%)	291 (96%)	13 (4%)	29	60
5	P	91/102 (89%)	77 (85%)	14 (15%)	2	12
5	Q	83/102 (81%)	70 (84%)	13 (16%)	2	11
5	R	101/102 (99%)	89 (88%)	12 (12%)	5	20
5	S	91/102 (89%)	83 (91%)	8 (9%)	10	34
6	U	162/190 (85%)	154 (95%)	8 (5%)	25	57
6	V	160/190 (84%)	150 (94%)	10 (6%)	18	49
7	1	25/195 (13%)	24 (96%)	1 (4%)	31	61
7	2	21/195 (11%)	12 (57%)	9 (43%)	0	0
7	3	22/195 (11%)	22 (100%)	0	100	100
7	4	24/195 (12%)	21 (88%)	3 (12%)	4	18
7	5	23/195 (12%)	21 (91%)	2 (9%)	10	35
7	6	22/195 (11%)	19 (86%)	3 (14%)	3	16
7	7	22/195 (11%)	17 (77%)	5 (23%)	1	3
7	8	24/195 (12%)	22 (92%)	2 (8%)	11	37
7	9	23/195 (12%)	21 (91%)	2 (9%)	10	35
All	All	11420/13617 (84%)	10188 (89%)	1232 (11%)	10	25

All (1232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR

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Mol	Chain	Res	Type
1	A	57	THR
1	A	76	THR
1	A	85	THR
1	A	107	LEU
1	A	109	ARG
1	A	134	GLN
1	A	147	VAL
1	A	148	GLN
1	A	153	VAL
1	A	154	THR
1	A	156	THR
1	A	169	ASN
1	A	191	LYS
1	A	192	THR
1	A	193	PHE
1	A	235	GLU
1	A	242	PHE
1	A	245	VAL
1	A	247	GLU
1	A	275	GLU
1	A	277	TYR
1	A	286	GLU
1	A	287	ASN
1	A	341	ASN
1	A	344	VAL
1	A	355	VAL
1	A	356	VAL
1	A	359	GLN
1	A	360	ASP
1	A	361	ARG
1	A	369	LEU
1	A	372	ASP
1	A	383	MET
1	A	388	VAL
1	A	406	GLU
1	A	426	VAL
1	A	428	ILE
1	A	429	THR
1	A	433	ASP
1	A	462	ILE
1	A	477	VAL
1	A	502	GLU

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Mol	Chain	Res	Type
1	A	513	LEU
1	A	520	ILE
1	A	527	ASP
1	A	537	HIS
1	A	561	GLN
1	A	565	LYS
1	A	604	ASP
1	A	626	THR
1	A	631	GLU
1	A	639	HIS
1	A	643	PHE
1	A	652	MET
1	A	683	LEU
1	A	711	THR
1	A	714	LEU
1	A	728	SER
1	A	735	ASP
1	A	739	THR
1	A	744	GLU
1	A	752	GLU
1	A	760	ASN
1	A	761	MET
1	A	837	ARG
1	A	840	GLN
1	A	853	GLN
1	A	866	CYS
1	A	869	VAL
1	A	908	ASP
1	A	919	LEU
1	A	925	VAL
1	A	928	VAL
1	A	943	THR
1	A	951	THR
1	B	3	THR
1	B	9	GLN
1	B	49	THR
1	B	58	THR
1	B	66	LEU
1	B	69	VAL
1	B	76	THR
1	B	78	TYR
1	B	79	LEU

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Mol	Chain	Res	Type
1	B	86	LEU
1	B	88	VAL
1	B	109	ARG
1	B	119	THR
1	B	131	ASN
1	B	141	GLN
1	B	149	GLN
1	B	150	GLU
1	B	154	THR
1	B	156	THR
1	B	157	PHE
1	B	166	ASN
1	B	186	ASP
1	B	188	TYR
1	B	193	PHE
1	B	196	GLU
1	B	203	ASN
1	B	206	GLU
1	B	214	ARG
1	B	231	ARG
1	B	239	GLN
1	B	241	LYS
1	B	262	ASP
1	B	278	LYS
1	B	292	THR
1	B	295	THR
1	B	311	ASN
1	B	335	TYR
1	B	339	THR
1	B	341	ASN
1	B	344	VAL
1	B	345	LEU
1	B	348	GLN
1	B	361	ARG
1	B	364	GLU
1	B	372	ASP
1	B	379	ARG
1	B	396	ARG
1	B	433	ASP
1	B	443	ASP
1	B	446	ILE
1	B	449	GLN

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Mol	Chain	Res	Type
1	B	450	ASN
1	B	456	ASN
1	B	457	VAL
1	B	462	ILE
1	B	464	LEU
1	B	500	THR
1	B	505	ASN
1	B	514	VAL
1	B	520	ILE
1	B	529	MET
1	B	537	HIS
1	B	544	ARG
1	B	548	MET
1	B	561	GLN
1	B	573	LEU
1	B	581	TYR
1	B	626	THR
1	B	651	ASN
1	B	652	MET
1	B	661	THR
1	B	695	PHE
1	B	696	ASP
1	B	734	ASN
1	B	741	ASN
1	B	771	LEU
1	B	774	TYR
1	B	785	GLU
1	B	790	ARG
1	B	813	ASP
1	B	818	THR
1	B	821	PHE
1	B	835	THR
1	B	837	ARG
1	B	840	GLN
1	B	851	ILE
1	B	863	LYS
1	B	868	ARG
1	B	887	ASP
1	B	893	LEU
1	B	907	VAL
1	B	908	ASP
1	B	927	ARG

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Mol	Chain	Res	Type
1	B	943	THR
1	C	13	MET
1	C	35	THR
1	C	65	THR
1	C	69	VAL
1	C	72	ASP
1	C	79	LEU
1	C	90	ASP
1	C	104	ARG
1	C	106	VAL
1	C	107	LEU
1	C	136	GLU
1	C	144	THR
1	C	149	GLN
1	C	173	LEU
1	C	186	ASP
1	C	192	THR
1	C	218	LYS
1	C	222	MET
1	C	277	TYR
1	C	278	LYS
1	C	287	ASN
1	C	294	ASP
1	C	309	GLU
1	C	311	ASN
1	C	314	GLN
1	C	341	ASN
1	C	357	ASP
1	C	363	THR
1	C	372	ASP
1	C	378	THR
1	C	384	TRP
1	C	396	ARG
1	C	398	ILE
1	C	414	LEU
1	C	429	THR
1	C	456	ASN
1	C	461	GLU
1	C	462	ILE
1	C	467	ASN
1	C	468	LEU
1	C	473	LEU

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Mol	Chain	Res	Type
1	C	477	VAL
1	C	505	ASN
1	C	520	ILE
1	C	556	VAL
1	C	581	TYR
1	C	582	GLU
1	C	590	ASN
1	C	613	VAL
1	C	615	LEU
1	C	626	THR
1	C	631	GLU
1	C	635	ARG
1	C	639	HIS
1	C	640	ASP
1	C	641	GLN
1	C	651	ASN
1	C	652	MET
1	C	665	ILE
1	C	670	ARG
1	C	683	LEU
1	C	711	THR
1	C	724	MET
1	C	739	THR
1	C	752	GLU
1	C	762	THR
1	C	779	GLN
1	C	783	VAL
1	C	790	ARG
1	C	791	MET
1	C	796	ARG
1	C	801	MET
1	C	803	ARG
1	C	804	GLN
1	C	837	ARG
1	C	840	GLN
1	C	851	ILE
1	C	853	GLN
1	C	866	CYS
1	C	880	MET
1	C	885	LEU
1	C	886	THR
1	C	887	ASP

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Mol	Chain	Res	Type
1	C	908	ASP
1	C	914	THR
1	C	919	LEU
1	C	928	VAL
1	C	935	VAL
1	C	936	ILE
1	C	943	THR
1	D	9	GLN
1	D	10	TRP
1	D	49	THR
1	D	76	THR
1	D	85	THR
1	D	88	VAL
1	D	99	THR
1	D	108	ASP
1	D	109	ARG
1	D	122	ASN
1	D	131	ASN
1	D	157	PHE
1	D	166	ASN
1	D	168	THR
1	D	172	LEU
1	D	186	ASP
1	D	188	TYR
1	D	192	THR
1	D	196	GLU
1	D	199	VAL
1	D	281	ILE
1	D	286	GLU
1	D	291	GLU
1	D	310	ILE
1	D	352	LEU
1	D	356	VAL
1	D	361	ARG
1	D	368	GLN
1	D	372	ASP
1	D	403	VAL
1	D	427	LYS
1	D	429	THR
1	D	443	ASP
1	D	456	ASN
1	D	462	ILE

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Mol	Chain	Res	Type
1	D	464	LEU
1	D	473	LEU
1	D	488	THR
1	D	498	THR
1	D	502	GLU
1	D	513	LEU
1	D	514	VAL
1	D	520	ILE
1	D	526	LEU
1	D	527	ASP
1	D	529	MET
1	D	537	HIS
1	D	561	GLN
1	D	565	LYS
1	D	575	LEU
1	D	588	ASP
1	D	590	ASN
1	D	625	ASN
1	D	638	THR
1	D	639	HIS
1	D	641	GLN
1	D	643	PHE
1	D	652	MET
1	D	665	ILE
1	D	711	THR
1	D	721	VAL
1	D	726	ASP
1	D	738	LEU
1	D	739	THR
1	D	750	ASP
1	D	758	GLN
1	D	762	THR
1	D	764	ASP
1	D	767	LEU
1	D	774	TYR
1	D	783	VAL
1	D	791	MET
1	D	804	GLN
1	D	805	VAL
1	D	806	VAL
1	D	825	ASN
1	D	836	MET

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Mol	Chain	Res	Type
1	D	863	LYS
1	D	865	LEU
1	D	868	ARG
1	D	885	LEU
1	D	911	ASP
1	D	912	GLU
1	D	918	LEU
1	D	943	THR
1	D	951	THR
1	E	47	ASN
1	E	56	VAL
1	E	57	THR
1	E	65	THR
1	E	92	ARG
1	E	144	THR
1	E	154	THR
1	E	174	LEU
1	E	176	THR
1	E	186	ASP
1	E	193	PHE
1	E	196	GLU
1	E	198	GLN
1	E	207	ASN
1	E	219	ASP
1	E	235	GLU
1	E	254	LEU
1	E	257	ASP
1	E	262	ASP
1	E	278	LYS
1	E	283	LEU
1	E	286	GLU
1	E	292	THR
1	E	319	ASN
1	E	321	PRO
1	E	322	ASN
1	E	338	SER
1	E	353	ASN
1	E	368	GLN
1	E	377	ARG
1	E	389	ASP
1	E	395	VAL
1	E	396	ARG

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Mol	Chain	Res	Type
1	E	398	ILE
1	E	407	LEU
1	E	417	THR
1	E	440	TRP
1	E	454	LYS
1	E	461	GLU
1	E	462	ILE
1	E	464	LEU
1	E	500	THR
1	E	520	ILE
1	E	537	HIS
1	E	550	LEU
1	E	552	ASN
1	E	561	GLN
1	E	571	ASN
1	E	572	LEU
1	E	573	LEU
1	E	593	LEU
1	E	626	THR
1	E	634	LEU
1	E	635	ARG
1	E	640	ASP
1	E	643	PHE
1	E	651	ASN
1	E	659	LYS
1	E	670	ARG
1	E	683	LEU
1	E	708	LEU
1	E	709	ASP
1	E	711	THR
1	E	714	LEU
1	E	739	THR
1	E	742	GLU
1	E	756	VAL
1	E	771	LEU
1	E	774	TYR
1	E	793	SER
1	E	804	GLN
1	E	807	ASP
1	E	809	ILE
1	E	811	TYR
1	E	825	ASN

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Mol	Chain	Res	Type
1	E	837	ARG
1	E	851	ILE
1	E	854	THR
1	E	877	SER
1	E	885	LEU
1	E	902	ASP
1	E	919	LEU
1	E	927	ARG
1	E	930	GLN
1	F	1	MET
1	F	35	THR
1	F	47	ASN
1	F	50	VAL
1	F	65	THR
1	F	69	VAL
1	F	71	VAL
1	F	72	ASP
1	F	76	THR
1	F	86	LEU
1	F	88	VAL
1	F	90	ASP
1	F	92	ARG
1	F	137	THR
1	F	156	THR
1	F	172	LEU
1	F	185	LYS
1	F	188	TYR
1	F	193	PHE
1	F	203	ASN
1	F	204	TRP
1	F	218	LYS
1	F	233	THR
1	F	249	GLU
1	F	277	TYR
1	F	280	ASP
1	F	289	ASN
1	F	341	ASN
1	F	344	VAL
1	F	363	THR
1	F	372	ASP
1	F	389	ASP
1	F	407	LEU

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Mol	Chain	Res	Type
1	F	409	ASN
1	F	428	ILE
1	F	437	GLU
1	F	461	GLU
1	F	473	LEU
1	F	476	ASN
1	F	491	ASN
1	F	502	GLU
1	F	507	ARG
1	F	520	ILE
1	F	565	LYS
1	F	570	LYS
1	F	581	TYR
1	F	582	GLU
1	F	615	LEU
1	F	626	THR
1	F	635	ARG
1	F	640	ASP
1	F	652	MET
1	F	656	ILE
1	F	672	TRP
1	F	683	LEU
1	F	686	LYS
1	F	695	PHE
1	F	705	ILE
1	F	711	THR
1	F	721	VAL
1	F	725	PHE
1	F	729	VAL
1	F	734	ASN
1	F	739	THR
1	F	754	TYR
1	F	762	THR
1	F	769	GLN
1	F	771	LEU
1	F	774	TYR
1	F	783	VAL
1	F	803	ARG
1	F	804	GLN
1	F	806	VAL
1	F	813	ASP
1	F	837	ARG

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Mol	Chain	Res	Type
1	F	877	SER
1	F	885	LEU
1	F	890	GLN
1	F	902	ASP
1	F	915	LEU
1	F	925	VAL
1	F	935	VAL
1	F	943	THR
1	G	6	MET
1	G	9	GLN
1	G	10	TRP
1	G	13	MET
1	G	28	LEU
1	G	46	ARG
1	G	54	HIS
1	G	58	THR
1	G	63	ARG
1	G	72	ASP
1	G	76	THR
1	G	78	TYR
1	G	85	THR
1	G	88	VAL
1	G	93	VAL
1	G	152	ASP
1	G	154	THR
1	G	167	ILE
1	G	191	LYS
1	G	192	THR
1	G	193	PHE
1	G	196	GLU
1	G	199	VAL
1	G	222	MET
1	G	225	CYS
1	G	257	ASP
1	G	282	ILE
1	G	286	GLU
1	G	291	GLU
1	G	310	ILE
1	G	319	ASN
1	G	320	ARG
1	G	327	ARG
1	G	341	ASN

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Mol	Chain	Res	Type
1	G	344	VAL
1	G	355	VAL
1	G	361	ARG
1	G	372	ASP
1	G	376	ASP
1	G	378	THR
1	G	379	ARG
1	G	388	VAL
1	G	407	LEU
1	G	409	ASN
1	G	438	SER
1	G	441	GLU
1	G	443	ASP
1	G	461	GLU
1	G	508	VAL
1	G	514	VAL
1	G	520	ILE
1	G	529	MET
1	G	561	GLN
1	G	565	LYS
1	G	580	THR
1	G	583	TRP
1	G	584	ASN
1	G	607	SER
1	G	609	ARG
1	G	631	GLU
1	G	638	THR
1	G	651	ASN
1	G	652	MET
1	G	653	LEU
1	G	665	ILE
1	G	676	ARG
1	G	681	THR
1	G	688	THR
1	G	700	VAL
1	G	708	LEU
1	G	720	LYS
1	G	721	VAL
1	G	726	ASP
1	G	728	SER
1	G	738	LEU
1	G	756	VAL

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Mol	Chain	Res	Type
1	G	758	GLN
1	G	769	GLN
1	G	775	ASN
1	G	783	VAL
1	G	801	MET
1	G	803	ARG
1	G	822	GLN
1	G	836	MET
1	G	837	ARG
1	G	840	GLN
1	G	850	LEU
1	G	865	LEU
1	G	868	ARG
1	G	872	ARG
1	G	887	ASP
1	G	912	GLU
1	G	919	LEU
1	G	923	PHE
1	G	935	VAL
1	G	937	GLU
1	H	59	ASP
1	H	65	THR
1	H	72	ASP
1	H	79	LEU
1	H	109	ARG
1	H	137	THR
1	H	154	THR
1	H	156	THR
1	H	157	PHE
1	H	172	LEU
1	H	174	LEU
1	H	176	THR
1	H	188	TYR
1	H	190	ASP
1	H	192	THR
1	H	193	PHE
1	H	196	GLU
1	H	198	GLN
1	H	204	TRP
1	H	218	LYS
1	H	221	LYS
1	H	235	GLU

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Mol	Chain	Res	Type
1	H	242	PHE
1	H	245	VAL
1	H	263	VAL
1	H	292	THR
1	H	317	MET
1	H	327	ARG
1	H	339	THR
1	H	341	ASN
1	H	348	GLN
1	H	351	GLN
1	H	353	ASN
1	H	357	ASP
1	H	359	GLN
1	H	364	GLU
1	H	372	ASP
1	H	383	MET
1	H	394	ASP
1	H	395	VAL
1	H	396	ARG
1	H	398	ILE
1	H	403	VAL
1	H	407	LEU
1	H	415	ASN
1	H	417	THR
1	H	428	ILE
1	H	429	THR
1	H	433	ASP
1	H	450	ASN
1	H	461	GLU
1	H	462	ILE
1	H	477	VAL
1	H	488	THR
1	H	520	ILE
1	H	526	LEU
1	H	537	HIS
1	H	565	LYS
1	H	583	TRP
1	H	587	LYS
1	H	590	ASN
1	H	608	VAL
1	H	618	THR
1	H	626	THR

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Mol	Chain	Res	Type
1	H	635	ARG
1	H	637	ASP
1	H	639	HIS
1	H	642	SER
1	H	652	MET
1	H	661	THR
1	H	681	THR
1	H	684	LYS
1	H	700	VAL
1	H	708	LEU
1	H	711	THR
1	H	726	ASP
1	H	728	SER
1	H	734	ASN
1	H	739	THR
1	H	742	GLU
1	H	759	CYS
1	H	761	MET
1	H	767	LEU
1	H	768	VAL
1	H	776	ILE
1	H	797	ASN
1	H	818	THR
1	H	825	ASN
1	H	837	ARG
1	H	851	ILE
1	H	853	GLN
1	H	867	ASP
1	H	877	SER
1	H	893	LEU
1	H	902	ASP
1	H	912	GLU
1	H	914	THR
1	H	923	PHE
1	H	928	VAL
1	H	939	VAL
1	H	942	ARG
1	H	943	THR
1	I	6	MET
1	I	49	THR
1	I	50	VAL
1	I	57	THR

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Mol	Chain	Res	Type
1	I	65	THR
1	I	69	VAL
1	I	72	ASP
1	I	76	THR
1	I	79	LEU
1	I	92	ARG
1	I	131	ASN
1	I	135	TRP
1	I	137	THR
1	I	139	GLU
1	I	154	THR
1	I	156	THR
1	I	157	PHE
1	I	173	LEU
1	I	193	PHE
1	I	194	GLN
1	I	196	GLU
1	I	201	GLU
1	I	217	LYS
1	I	218	LYS
1	I	245	VAL
1	I	247	GLU
1	I	249	GLU
1	I	277	TYR
1	I	280	ASP
1	I	287	ASN
1	I	289	ASN
1	I	295	THR
1	I	341	ASN
1	I	344	VAL
1	I	372	ASP
1	I	378	THR
1	I	381	PHE
1	I	383	MET
1	I	397	ILE
1	I	399	GLU
1	I	407	LEU
1	I	417	THR
1	I	426	VAL
1	I	429	THR
1	I	437	GLU
1	I	464	LEU

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Mol	Chain	Res	Type
1	I	473	LEU
1	I	476	ASN
1	I	556	VAL
1	I	561	GLN
1	I	565	LYS
1	I	581	TYR
1	I	582	GLU
1	I	590	ASN
1	I	601	LEU
1	I	612	SER
1	I	618	THR
1	I	635	ARG
1	I	638	THR
1	I	640	ASP
1	I	641	GLN
1	I	642	SER
1	I	644	ASN
1	I	652	MET
1	I	656	ILE
1	I	670	ARG
1	I	672	TRP
1	I	681	THR
1	I	683	LEU
1	I	708	LEU
1	I	709	ASP
1	I	742	GLU
1	I	756	VAL
1	I	769	GLN
1	I	770	MET
1	I	771	LEU
1	I	774	TYR
1	I	783	VAL
1	I	790	ARG
1	I	807	ASP
1	I	809	ILE
1	I	837	ARG
1	I	848	TYR
1	I	868	ARG
1	I	885	LEU
1	I	886	THR
1	I	888	LEU
1	I	890	GLN

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Mol	Chain	Res	Type
1	I	902	ASP
1	I	911	ASP
1	I	927	ARG
1	I	935	VAL
1	J	10	TRP
1	J	28	LEU
1	J	47	ASN
1	J	57	THR
1	J	72	ASP
1	J	76	THR
1	J	90	ASP
1	J	92	ARG
1	J	103	ILE
1	J	106	VAL
1	J	107	LEU
1	J	108	ASP
1	J	109	ARG
1	J	154	THR
1	J	156	THR
1	J	167	ILE
1	J	169	ASN
1	J	188	TYR
1	J	192	THR
1	J	193	PHE
1	J	194	GLN
1	J	196	GLU
1	J	218	LYS
1	J	267	SER
1	J	282	ILE
1	J	285	THR
1	J	289	ASN
1	J	291	GLU
1	J	303	THR
1	J	317	MET
1	J	333	LEU
1	J	339	THR
1	J	361	ARG
1	J	371	LEU
1	J	372	ASP
1	J	379	ARG
1	J	391	TYR
1	J	407	LEU

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Mol	Chain	Res	Type
1	J	417	THR
1	J	429	THR
1	J	436	GLU
1	J	440	TRP
1	J	443	ASP
1	J	446	ILE
1	J	462	ILE
1	J	477	VAL
1	J	498	THR
1	J	520	ILE
1	J	537	HIS
1	J	544	ARG
1	J	572	LEU
1	J	581	TYR
1	J	602	ARG
1	J	613	VAL
1	J	614	ASN
1	J	615	LEU
1	J	626	THR
1	J	644	ASN
1	J	651	ASN
1	J	670	ARG
1	J	681	THR
1	J	700	VAL
1	J	708	LEU
1	J	711	THR
1	J	728	SER
1	J	731	TRP
1	J	742	GLU
1	J	750	ASP
1	J	756	VAL
1	J	769	GLN
1	J	770	MET
1	J	783	VAL
1	J	804	GLN
1	J	805	VAL
1	J	806	VAL
1	J	809	ILE
1	J	818	THR
1	J	837	ARG
1	J	838	GLN
1	J	850	LEU

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Mol	Chain	Res	Type
1	J	861	GLN
1	J	862	LYS
1	J	863	LYS
1	J	865	LEU
1	J	918	LEU
1	J	919	LEU
1	J	927	ARG
1	J	928	VAL
1	J	930	GLN
1	J	935	VAL
1	J	939	VAL
1	J	943	THR
1	K	65	THR
1	K	72	ASP
1	K	74	GLU
1	K	84	PHE
1	K	92	ARG
1	K	93	VAL
1	K	131	ASN
1	K	139	GLU
1	K	144	THR
1	K	153	VAL
1	K	155	LYS
1	K	169	ASN
1	K	178	GLU
1	K	188	TYR
1	K	191	LYS
1	K	195	PRO
1	K	196	GLU
1	K	198	GLN
1	K	199	VAL
1	K	201	GLU
1	K	204	TRP
1	K	218	LYS
1	K	282	ILE
1	K	283	LEU
1	K	310	ILE
1	K	341	ASN
1	K	361	ARG
1	K	364	GLU
1	K	372	ASP
1	K	381	PHE

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Mol	Chain	Res	Type
1	K	389	ASP
1	K	391	TYR
1	K	394	ASP
1	K	395	VAL
1	K	396	ARG
1	K	403	VAL
1	K	407	LEU
1	K	409	ASN
1	K	417	THR
1	K	440	TRP
1	K	449	GLN
1	K	454	LYS
1	K	461	GLU
1	K	462	ILE
1	K	464	LEU
1	K	486	LYS
1	K	488	THR
1	K	500	THR
1	K	520	ILE
1	K	526	LEU
1	K	532	VAL
1	K	580	THR
1	K	589	VAL
1	K	592	ILE
1	K	615	LEU
1	K	618	THR
1	K	626	THR
1	K	635	ARG
1	K	638	THR
1	K	639	HIS
1	K	640	ASP
1	K	641	GLN
1	K	643	PHE
1	K	652	MET
1	K	659	LYS
1	K	663	VAL
1	K	700	VAL
1	K	708	LEU
1	K	715	ASN
1	K	720	LYS
1	K	728	SER
1	K	734	ASN

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Mol	Chain	Res	Type
1	K	739	THR
1	K	752	GLU
1	K	756	VAL
1	K	761	MET
1	K	762	THR
1	K	763	LYS
1	K	770	MET
1	K	779	GLN
1	K	803	ARG
1	K	804	GLN
1	K	805	VAL
1	K	818	THR
1	K	825	ASN
1	K	837	ARG
1	K	843	PRO
1	K	854	THR
1	K	862	LYS
1	K	866	CYS
1	K	877	SER
1	K	914	THR
1	K	927	ARG
1	K	930	GLN
1	K	941	LEU
1	K	949	ASN
1	L	28	LEU
1	L	71	VAL
1	L	86	LEU
1	L	88	VAL
1	L	104	ARG
1	L	134	GLN
1	L	137	THR
1	L	154	THR
1	L	173	LEU
1	L	187	ILE
1	L	196	GLU
1	L	218	LYS
1	L	235	GLU
1	L	242	PHE
1	L	247	GLU
1	L	277	TYR
1	L	280	ASP
1	L	285	THR

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Mol	Chain	Res	Type
1	L	289	ASN
1	L	303	THR
1	L	309	GLU
1	L	313	VAL
1	L	333	LEU
1	L	341	ASN
1	L	345	LEU
1	L	355	VAL
1	L	356	VAL
1	L	357	ASP
1	L	371	LEU
1	L	372	ASP
1	L	388	VAL
1	L	399	GLU
1	L	403	VAL
1	L	407	LEU
1	L	429	THR
1	L	440	TRP
1	L	462	ILE
1	L	464	LEU
1	L	494	LEU
1	L	502	GLU
1	L	505	ASN
1	L	508	VAL
1	L	520	ILE
1	L	529	MET
1	L	537	HIS
1	L	543	LEU
1	L	544	ARG
1	L	546	ARG
1	L	582	GLU
1	L	596	SER
1	L	597	LEU
1	L	601	LEU
1	L	613	VAL
1	L	614	ASN
1	L	631	GLU
1	L	634	LEU
1	L	635	ARG
1	L	652	MET
1	L	656	ILE
1	L	659	LYS

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Mol	Chain	Res	Type
1	L	665	ILE
1	L	672	TRP
1	L	695	PHE
1	L	700	VAL
1	L	711	THR
1	L	714	LEU
1	L	725	PHE
1	L	726	ASP
1	L	729	VAL
1	L	734	ASN
1	L	738	LEU
1	L	756	VAL
1	L	759	CYS
1	L	769	GLN
1	L	774	TYR
1	L	782	HIS
1	L	803	ARG
1	L	806	VAL
1	L	812	LYS
1	L	813	ASP
1	L	829	THR
1	L	837	ARG
1	L	853	GLN
1	L	867	ASP
1	L	868	ARG
1	L	869	VAL
1	L	877	SER
1	L	885	LEU
1	L	890	GLN
1	L	901	LEU
1	L	907	VAL
1	L	908	ASP
1	L	935	VAL
1	L	937	GLU
2	N	37	GLU
2	N	40	ASN
2	N	43	ARG
2	N	45	SER
2	N	54	THR
2	N	55	ARG
2	N	60	ASP
2	N	71	TYR

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Mol	Chain	Res	Type
2	N	77	ASN
2	N	83	VAL
2	N	85	ASN
2	N	98	ILE
2	N	136	VAL
2	N	146	GLU
2	N	175	ASP
2	N	186	LEU
2	N	223	VAL
2	N	252	LEU
2	N	264	PHE
2	N	282	VAL
2	N	295	GLU
2	N	297	LYS
2	N	326	VAL
2	N	327	GLU
2	N	334	ASP
2	N	342	LEU
2	N	346	THR
2	N	368	GLN
2	N	388	SER
2	N	393	MET
2	N	400	ARG
2	N	440	LEU
2	N	449	ASP
2	N	486	VAL
2	N	491	VAL
2	N	492	THR
2	N	503	TYR
2	N	508	ILE
2	N	519	PHE
3	O	4	ARG
3	O	7	VAL
3	O	14	VAL
4	M	15	GLN
4	M	34	MET
4	M	45	ARG
4	M	58	GLU
4	M	92	LEU
4	M	107	THR
4	M	110	GLN
4	M	119	ASP

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Mol	Chain	Res	Type
4	M	157	ASP
4	M	159	TYR
4	M	201	GLN
4	M	203	PHE
4	M	381	ASN
5	P	4	THR
5	P	9	GLU
5	P	13	PHE
5	P	14	SER
5	P	16	TYR
5	P	17	LEU
5	P	22	PRO
5	P	24	TRP
5	P	36	VAL
5	P	50	THR
5	P	54	VAL
5	P	56	ASN
5	P	60	ASP
5	P	109	GLU
5	Q	9	GLU
5	Q	14	SER
5	Q	15	PRO
5	Q	16	TYR
5	Q	24	TRP
5	Q	27	VAL
5	Q	35	THR
5	Q	54	VAL
5	Q	76	ARG
5	Q	108	LEU
5	Q	120	GLN
5	Q	126	ARG
5	Q	127	GLU
5	R	8	PHE
5	R	14	SER
5	R	16	TYR
5	R	19	THR
5	R	36	VAL
5	R	49	MET
5	R	60	ASP
5	R	62	THR
5	R	79	SER
5	R	104	LEU

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Mol	Chain	Res	Type
5	R	124	GLU
5	R	125	LEU
5	S	17	LEU
5	S	18	THR
5	S	20	ARG
5	S	35	THR
5	S	53	THR
5	S	54	VAL
5	S	75	THR
5	S	81	TYR
6	U	2	SER
6	U	3	LYS
6	U	19	LEU
6	U	28	SER
6	U	43	ARG
6	U	51	ARG
6	U	163	THR
6	U	211	GLU
6	V	1	MET
6	V	3	LYS
6	V	28	SER
6	V	50	HIS
6	V	51	ARG
6	V	77	THR
6	V	144	ILE
6	V	163	THR
6	V	193	VAL
6	V	197	TYR
7	1	31	ASN
7	2	6	PHE
7	2	12	ARG
7	2	13	HIS
7	2	15	THR
7	2	22	TRP
7	2	25	ILE
7	2	27	THR
7	2	30	LEU
7	2	31	ASN
7	4	4	ILE
7	4	13	HIS
7	4	24	GLU
7	5	18	PHE

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Mol	Chain	Res	Type
7	5	27	THR
7	6	9	LEU
7	6	18	PHE
7	6	29	GLN
7	7	9	LEU
7	7	13	HIS
7	7	15	THR
7	7	27	THR
7	7	31	ASN
7	8	27	THR
7	8	31	ASN
7	9	18	PHE
7	9	22	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	715	ASN
1	A	741	ASN
1	B	134	GLN
1	B	239	GLN
1	B	315	GLN
1	B	449	GLN
1	B	450	ASN
1	B	456	ASN
1	B	715	ASN
1	C	825	ASN
1	C	878	ASN
1	D	134	GLN
1	D	804	GLN
1	E	319	ASN
1	E	322	ASN
1	E	337	ASN
1	E	599	ASN
1	E	715	ASN
1	E	797	ASN
1	F	203	ASN
1	F	715	ASN
1	G	9	GLN
1	G	456	ASN
1	H	134	GLN
1	H	198	GLN

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Mol	Chain	Res	Type
1	H	769	GLN
1	I	537	HIS
1	I	614	ASN
1	I	641	GLN
1	I	838	GLN
1	J	337	ASN
1	J	519	ASN
1	J	662	ASN
1	J	804	GLN
1	J	822	GLN
1	K	62	GLN
1	L	134	GLN
1	L	840	GLN
2	N	72	GLN
4	M	110	GLN
7	2	29	GLN
7	8	31	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

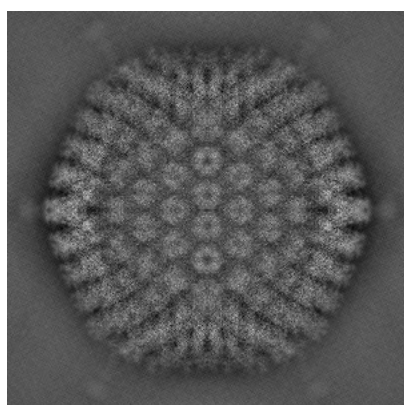
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25786. These allow visual inspection of the internal detail of the map and identification of artifacts.

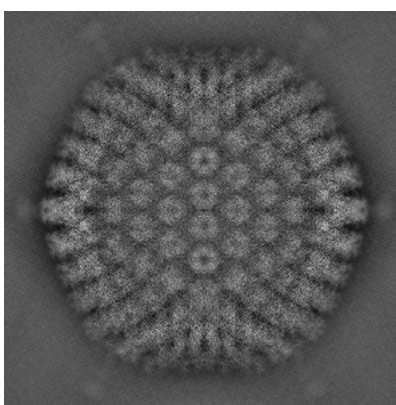
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

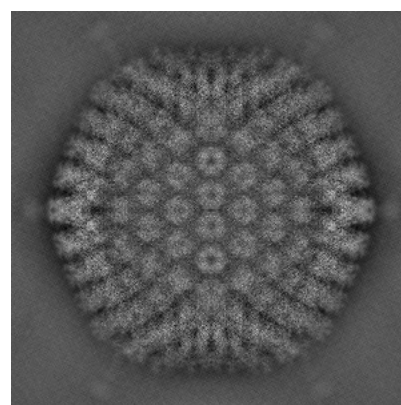
6.1.1 Primary map



X



Y

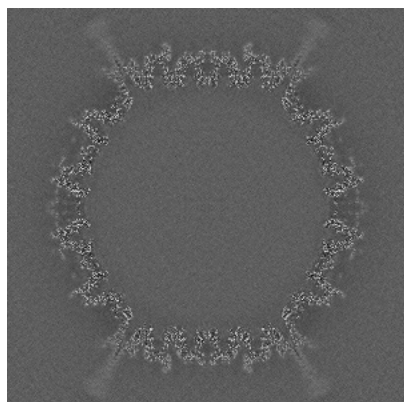


Z

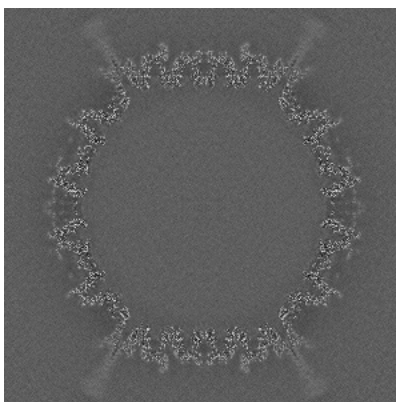
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

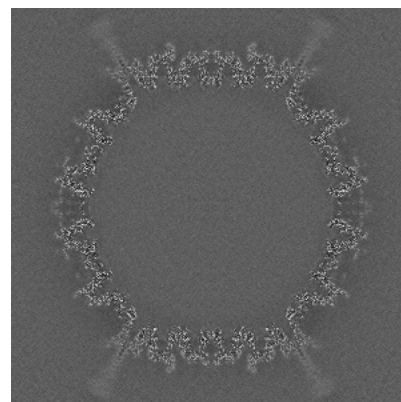
6.2.1 Primary map



X Index: 416



Y Index: 416

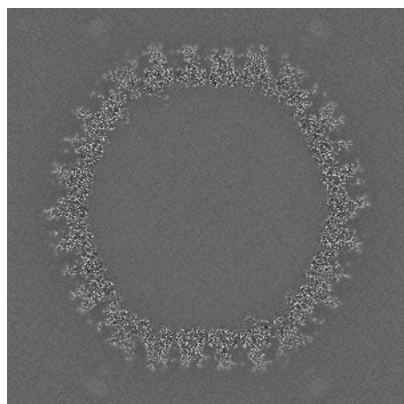


Z Index: 416

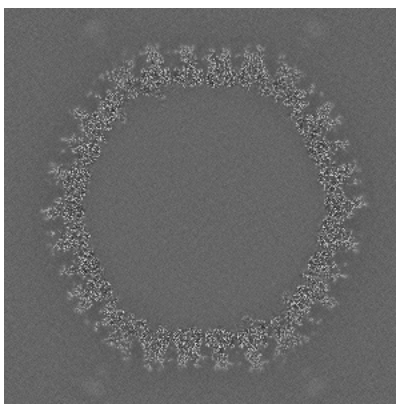
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

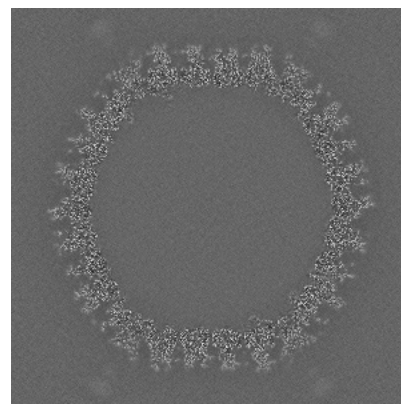
6.3.1 Primary map



X Index: 431



Y Index: 431



Z Index: 431

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

6.4 Orthogonal surface views [i](#)

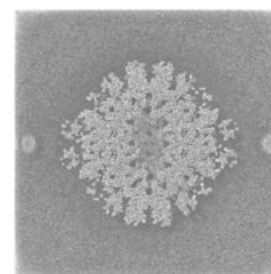
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

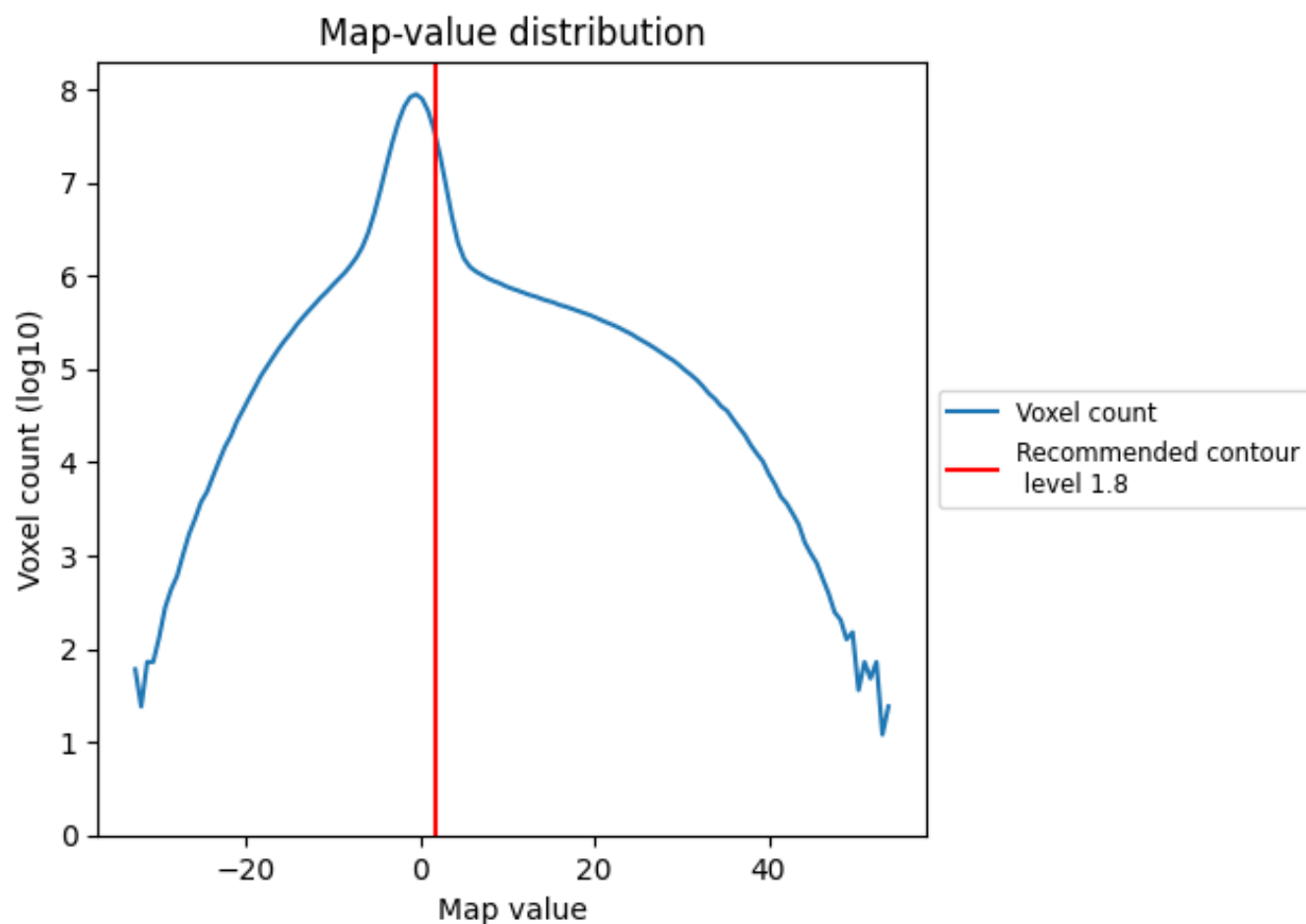
6.5 Mask visualisation

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

7 Map analysis [i](#)

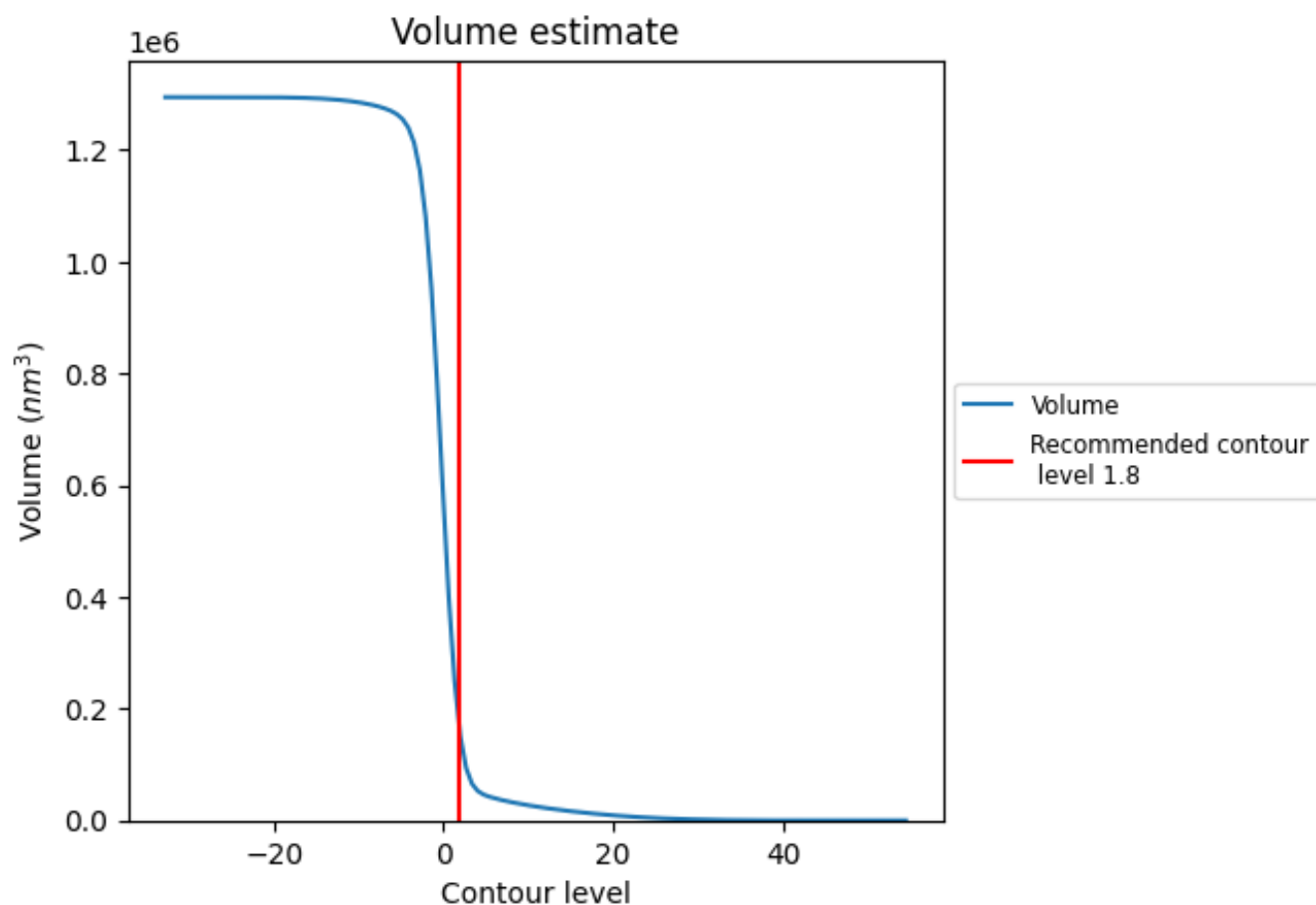
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

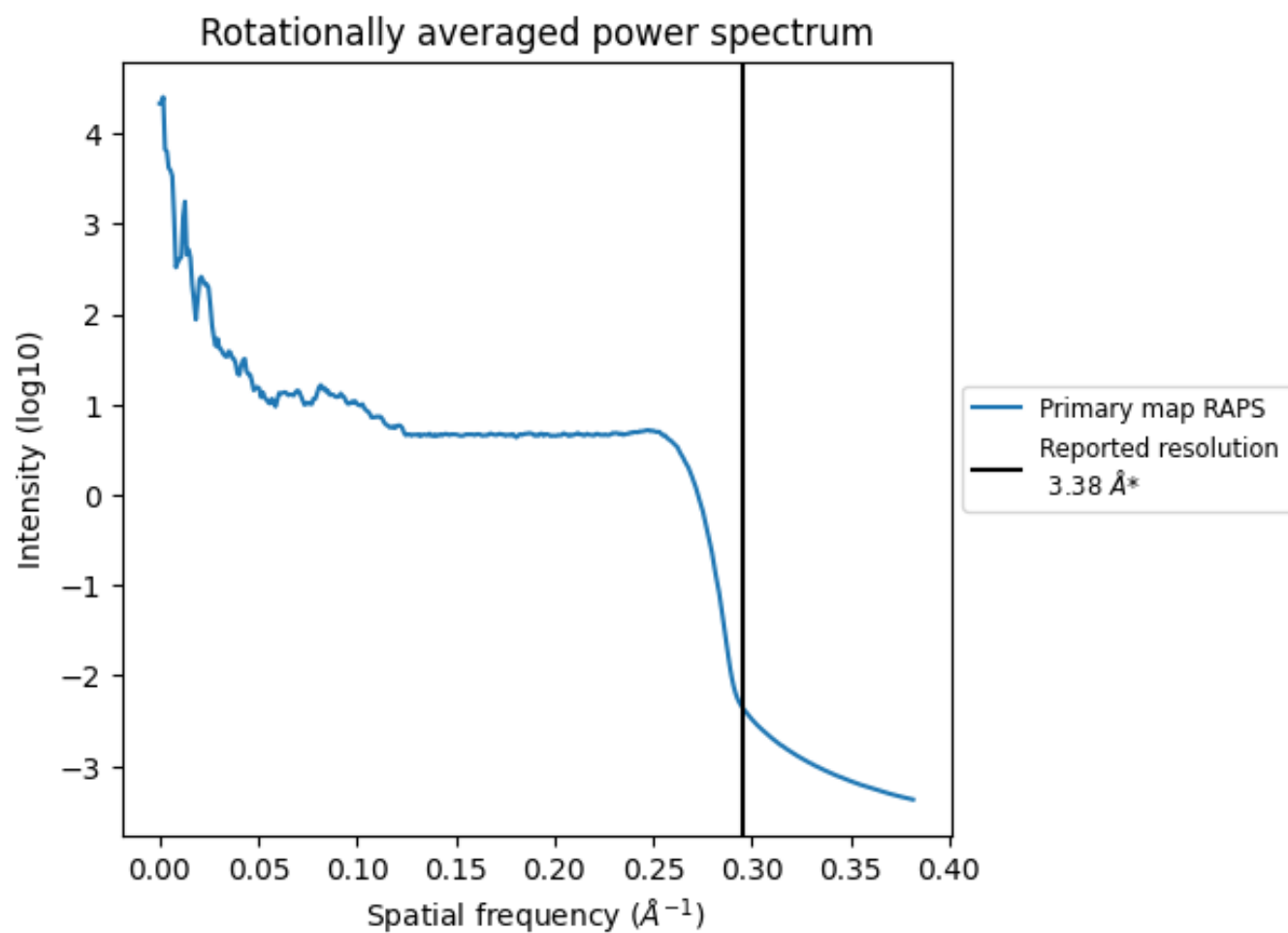
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 176024 nm³; this corresponds to an approximate mass of 159007 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 ⓘ

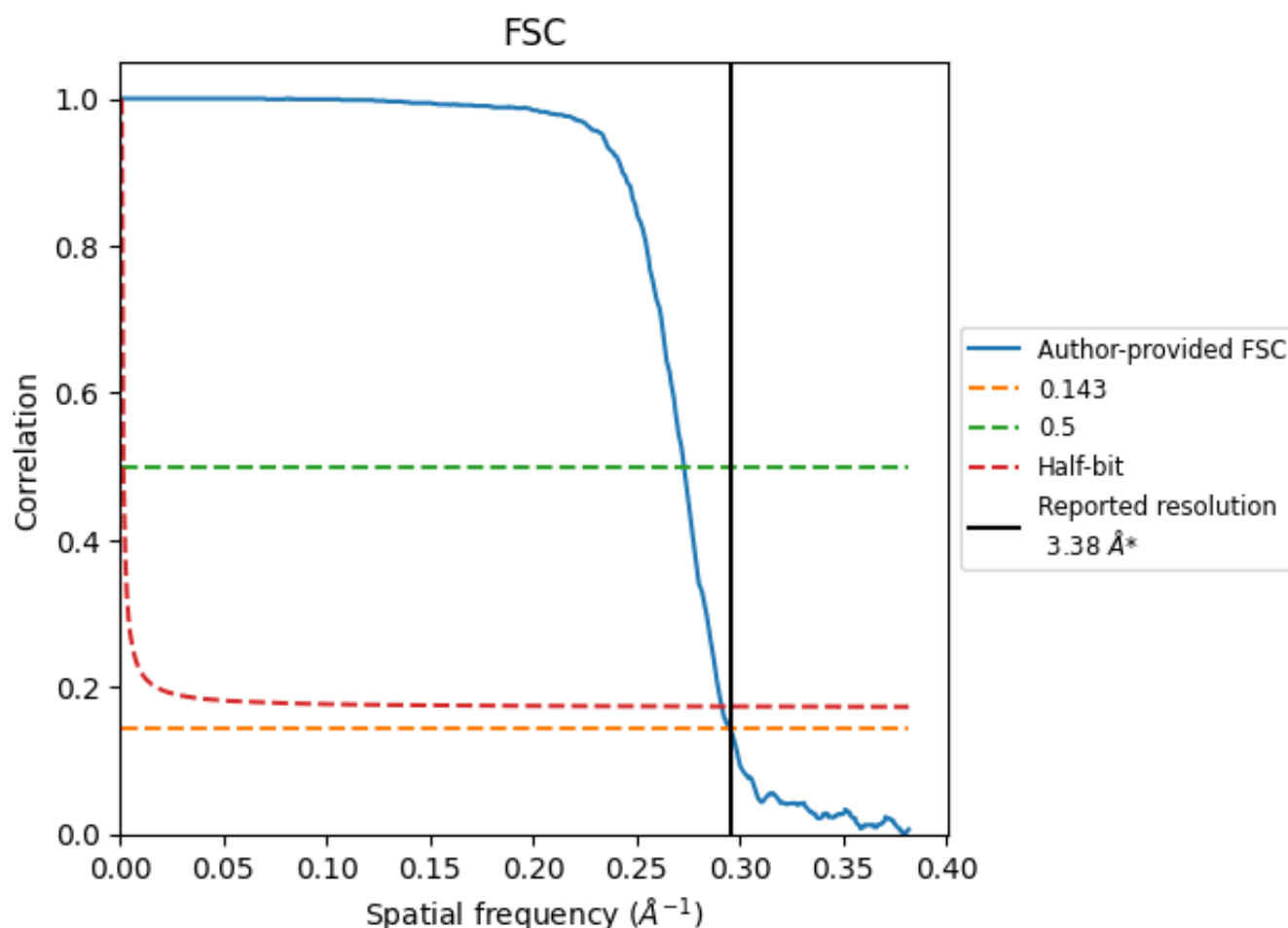


*Reported resolution corresponds to spatial frequency of 0.296 Å⁻¹

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 0.296 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.38	-	-
Author-provided FSC curve	3.39	3.66	3.43
Unmasked-calculated*	-	-	-

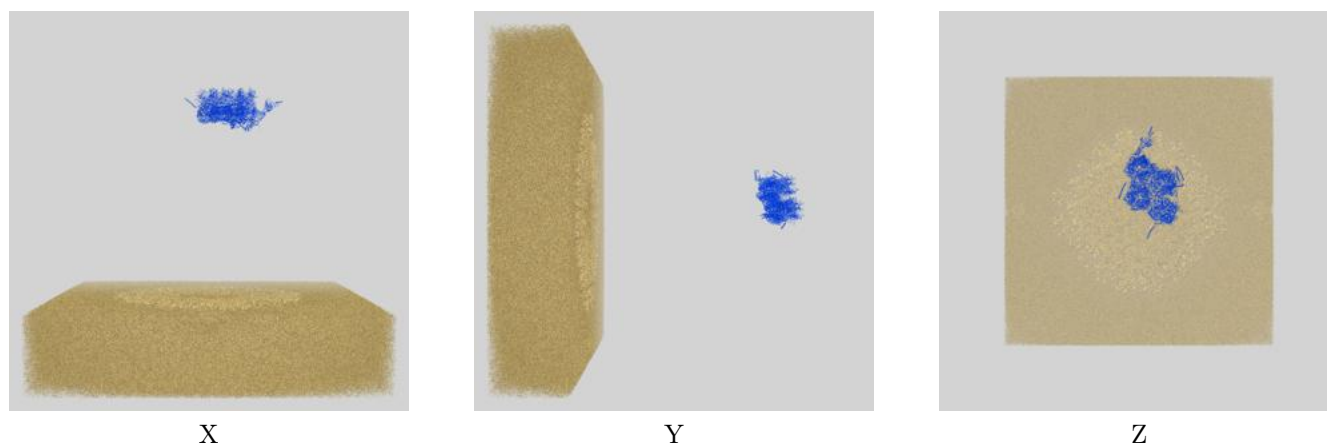
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

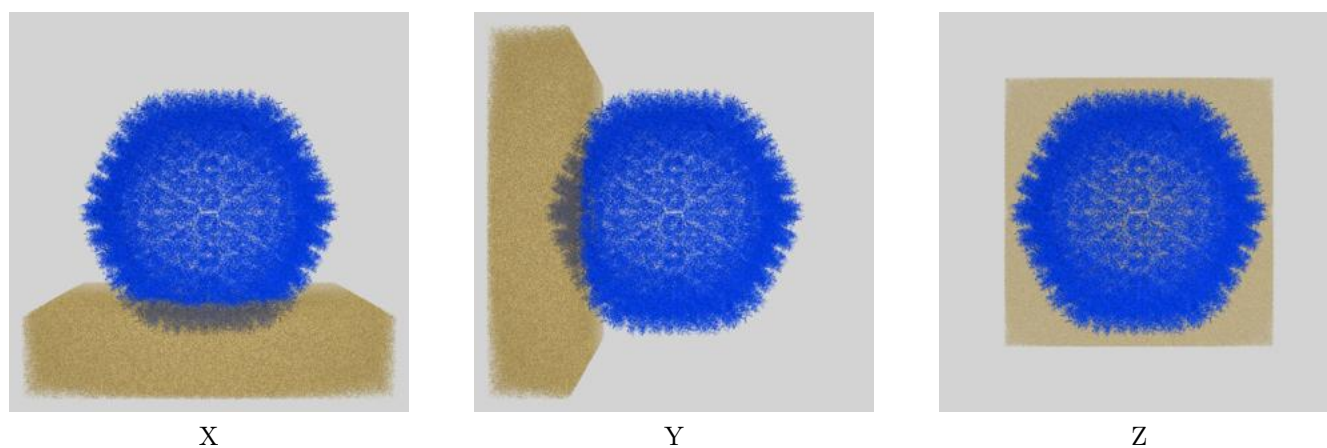
This section contains information regarding the fit between EMDB map EMD-25786 and PDB model 7TAU. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)



9.1.2 Map-model assembly overlay [i](#)



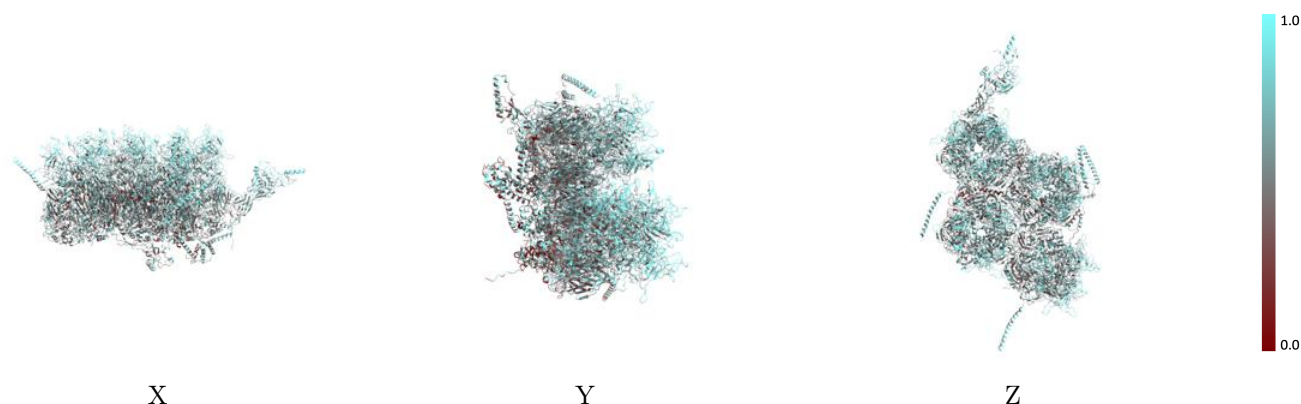
The images above show the 3D surface view of the map at the recommended contour level 1.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



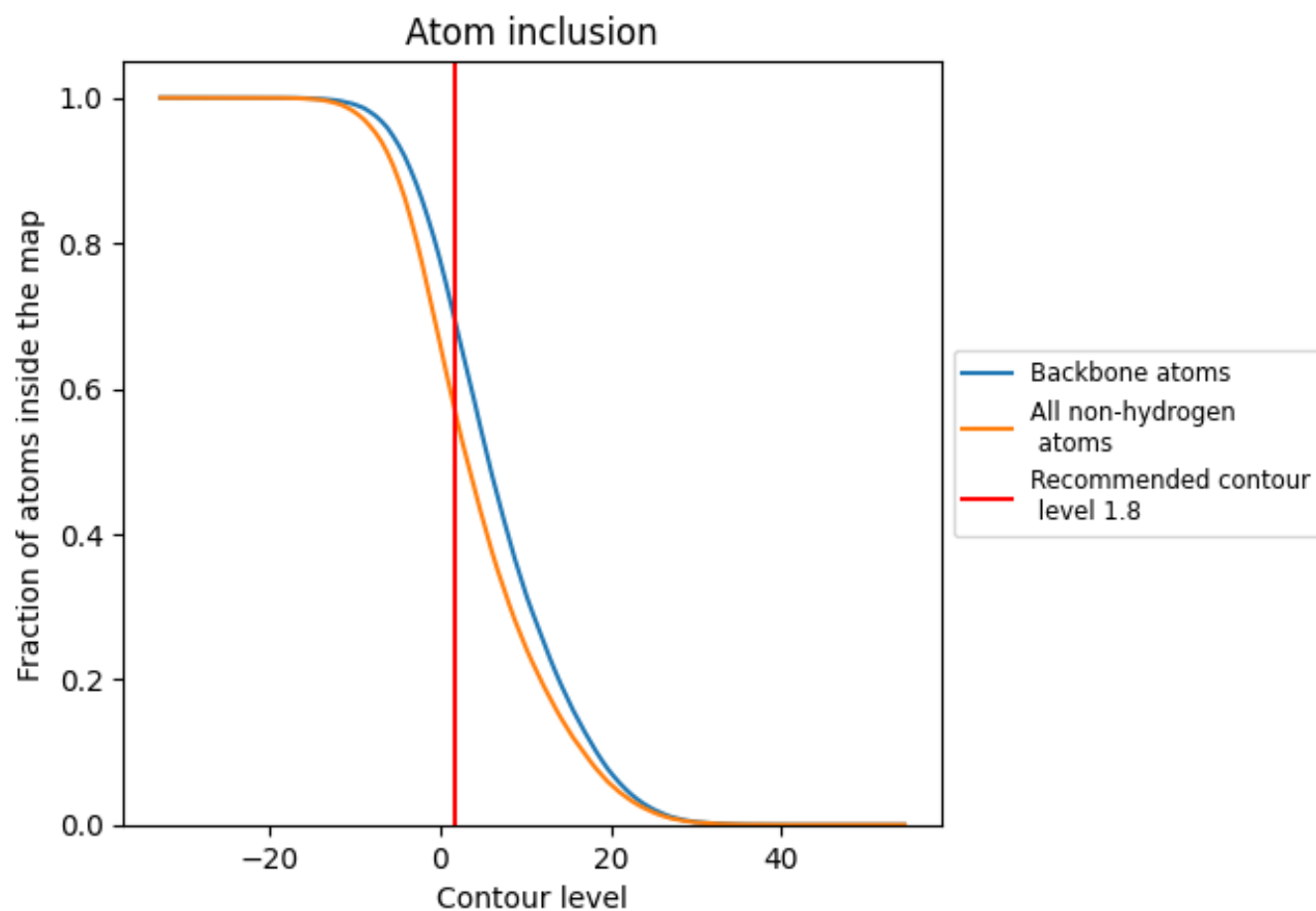
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (1.8).

































































9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 57% 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 (1.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5664	 0.0400
1	 0.4156	 0.0680
2	 0.5404	 0.0510
3	 0.3058	 0.0190
4	 0.4595	 0.0290
5	 0.4439	 0.1130
6	 0.2476	 -0.0080
7	 0.3107	 -0.0030
8	 0.4550	 0.0800
9	 0.2804	 0.0020
A	 0.5802	 0.0330
B	 0.6067	 0.0440
C	 0.6045	 0.0580
D	 0.5586	 0.0200
E	 0.5667	 0.0260
F	 0.5716	 0.0430
G	 0.5536	 0.0240
H	 0.5606	 0.0350
I	 0.5723	 0.0460
J	 0.5644	 0.0340
K	 0.5833	 0.0410
L	 0.5977	 0.0630
M	 0.4192	 0.0430
N	 0.6184	 0.0650
O	 0.6071	 0.0450
P	 0.4948	 0.0330
Q	 0.4981	 0.0410
R	 0.5909	 0.1010
S	 0.5316	 0.0800
U	 0.4884	 0.0120
V	 0.4936	 0.0190
X	 0.3600	 0.0470

