Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 04:03 PM EST

PDB ID	:	7S78
EMDB ID	:	EMD-24881
Title	:	Structure of a cell-entry defective human adenovirus provides insights into precursor proteins and capsid maturation
Authors	:	Reddy, V.S.; Yu, X.
Deposited on	:	2021-09-15
Resolution	:	3.72 Å(reported)
Based on initial model	:	3IYN

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:

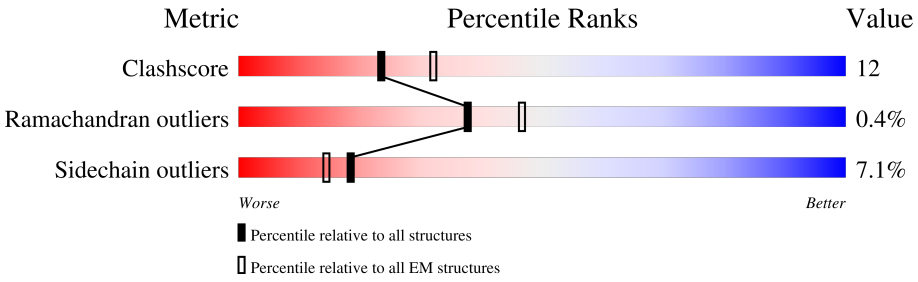
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.72 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 <=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	67% 28%
1	B	952	68% 26%
1	C	952	67% 28%
1	D	952	69% 26%
1	E	952	65% 29%
1	F	952	66% 28%
1	G	952	70% 25%
1	H	952	69% 27%

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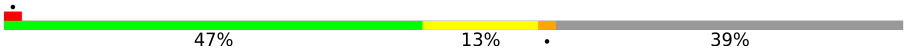
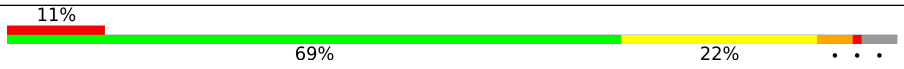
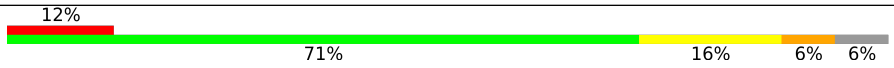
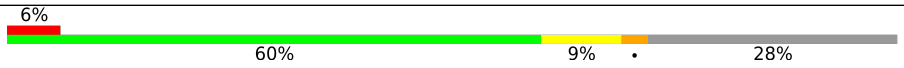
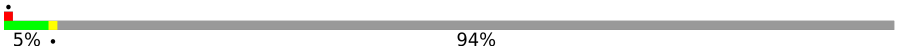
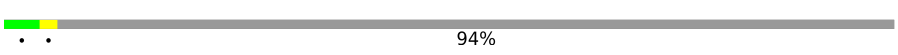
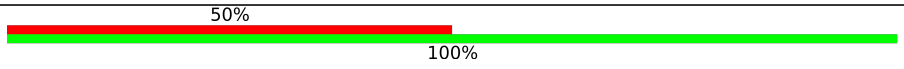
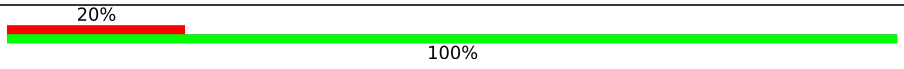
Mol	Chain	Length	Quality of chain
1	I	952	
1	J	952	
1	K	952	
1	L	952	
2	N	571	
3	M	585	
4	P	140	
4	Q	140	
4	R	140	
4	S	140	
5	U	227	
5	V	227	
6	0	250	
6	1	250	
6	2	250	
6	3	250	
6	4	250	
6	W	250	
6	X	250	
6	Y	250	
6	Z	250	
7	5	16	
8	6	10	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 104715 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	929	Total	C	N	O	S	0	0
			7427	4718	1258	1415	36		
1	B	929	Total	C	N	O	S	0	0
			7429	4719	1258	1416	36		
1	C	933	Total	C	N	O	S	0	0
			7456	4736	1262	1422	36		
1	D	929	Total	C	N	O	S	0	0
			7427	4718	1258	1415	36		
1	E	926	Total	C	N	O	S	0	0
			7408	4708	1255	1409	36		
1	F	929	Total	C	N	O	S	0	0
			7430	4721	1258	1415	36		
1	G	931	Total	C	N	O	S	0	0
			7441	4726	1260	1419	36		
1	H	933	Total	C	N	O	S	0	0
			7455	4736	1262	1420	37		
1	I	927	Total	C	N	O	S	0	0
			7417	4713	1256	1412	36		
1	J	928	Total	C	N	O	S	0	0
			7419	4713	1256	1414	36		
1	K	931	Total	C	N	O	S	0	0
			7442	4728	1260	1418	36		
1	L	929	Total	C	N	O	S	0	0
			7427	4718	1258	1415	36		

- Molecule 2 is a protein called Penton protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	466	Total	C	N	O	S	0	0
			3734	2365	646	711	12		

- Molecule 3 is a protein called Pre-hexon-linking protein IIIa.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	359	Total	C	N	O	S	0	0
			2813	1752	517	535	9		

- Molecule 4 is a protein called Hexon-interlacing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	134	Total	C	N	O	S	0	0
			972	600	171	199	2		
4	Q	131	Total	C	N	O	S	0	0
			952	587	168	195	2		
4	R	101	Total	C	N	O	S	0	0
			751	470	128	151	2		
4	S	97	Total	C	N	O	S	0	0
			727	448	128	149	2		

- Molecule 5 is a protein called Pre-hexon-linking protein VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	165	Total	C	N	O	S	0	0
			1268	797	223	243	5		
5	V	184	Total	C	N	O	S	0	0
			1414	890	248	272	4		

- Molecule 6 is a protein called Pre-protein VI.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	W	35	Total	C	N	O	S	0	0
			262	165	48	47	2		
6	X	78	Total	C	N	O	S	0	0
			577	361	107	106	3		
6	Y	61	Total	C	N	O	S	0	0
			485	305	90	87	3		
6	Z	25	Total	C	N	O	S	0	0
			179	109	35	34	1		
6	0	16	Total	C	N	O	S	0	0
			114	68	23	22	1		
6	1	57	Total	C	N	O	S	0	0
			449	279	84	83	3		
6	2	19	Total	C	N	O	S	0	0
			133	81	26	25	1		
6	3	60	Total	C	N	O	S	0	0
			471	293	87	88	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	4	15	Total	C	N	O	S	0	0
			106	64	21	20	1		

- Molecule 7 is a protein called Unknown-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	5	16	Total	C	N	O	0	0
			80	48	16	16		

- Molecule 8 is a protein called Unknown-2.

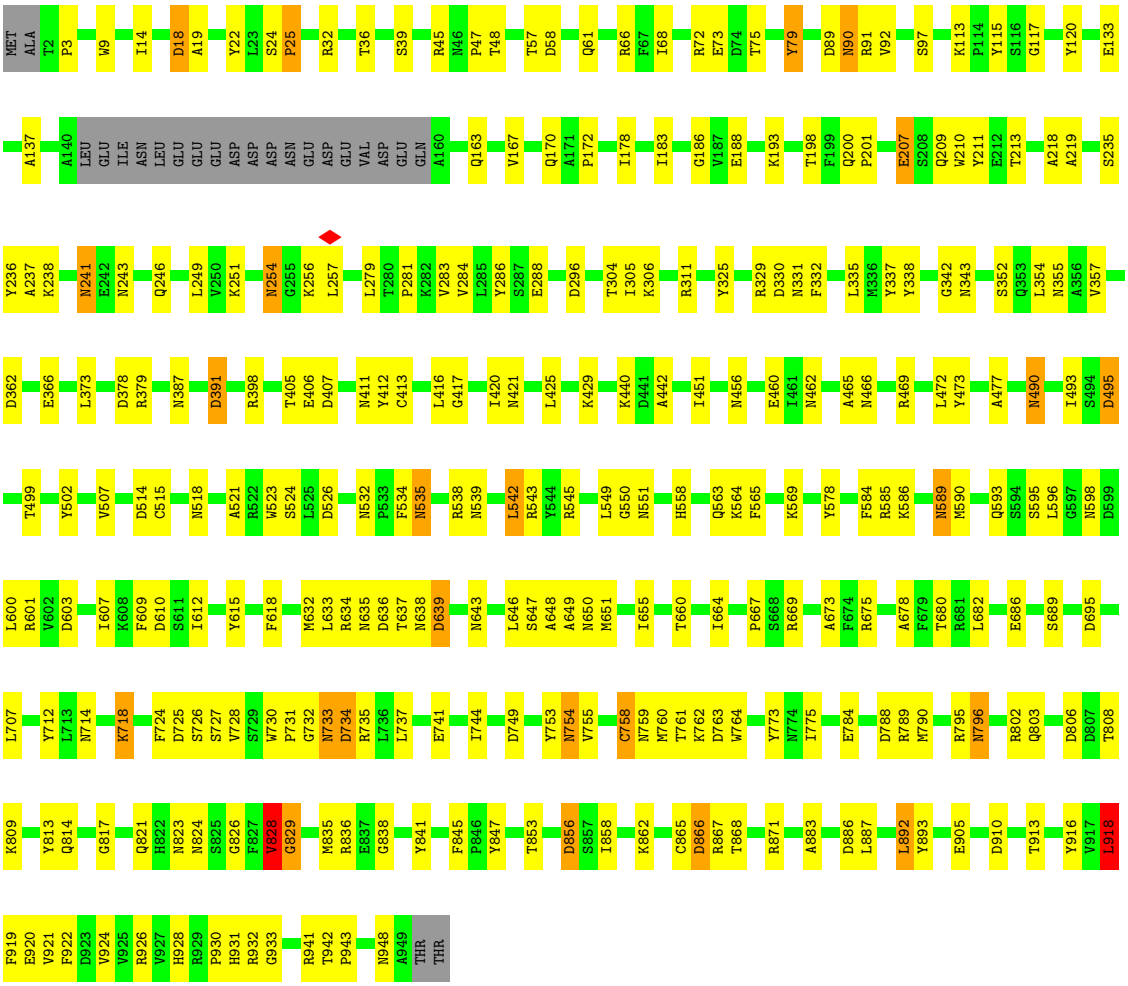
Mol	Chain	Residues	Atoms				AltConf	Trace
8	6	10	Total	C	N	O	0	0
			50	30	10	10		

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.

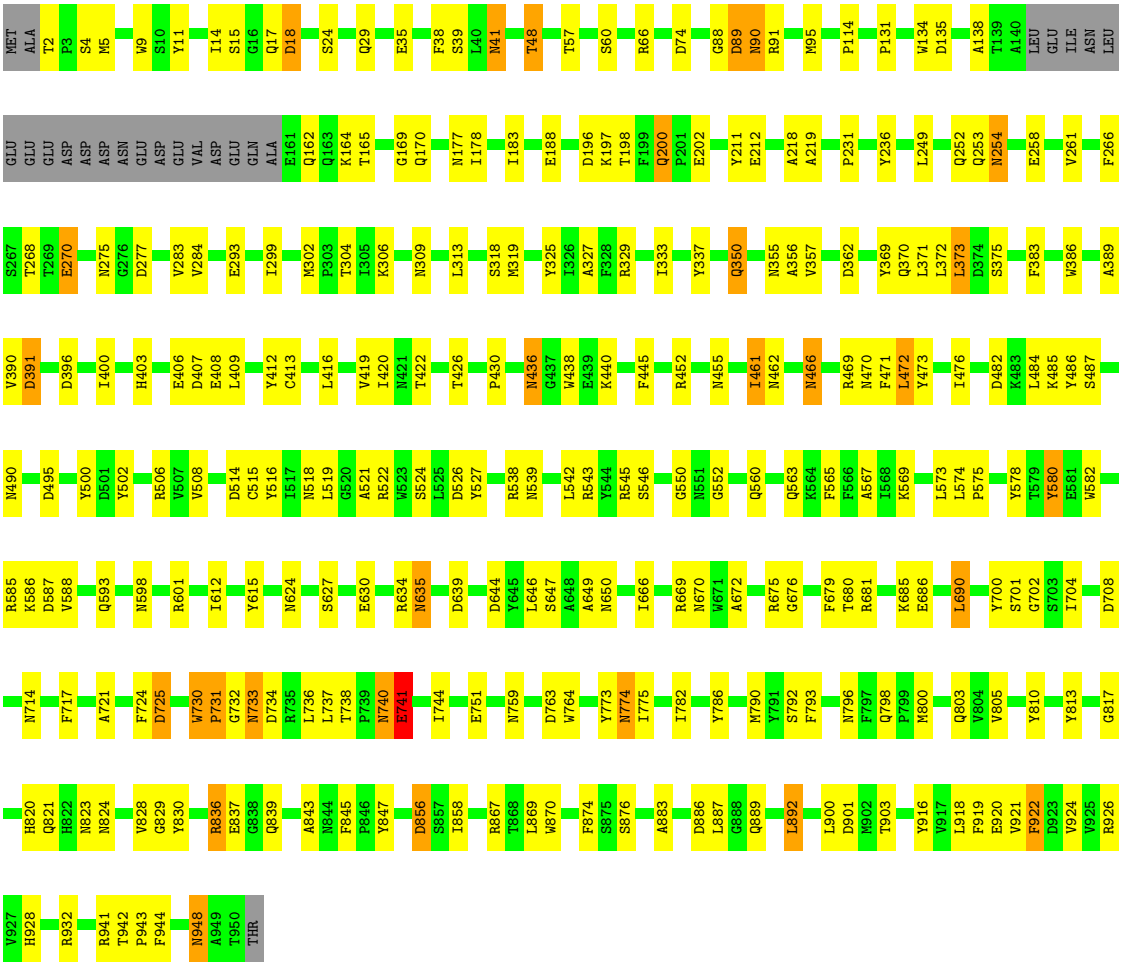
• Molecule 1: Hexon protein

Chain A:



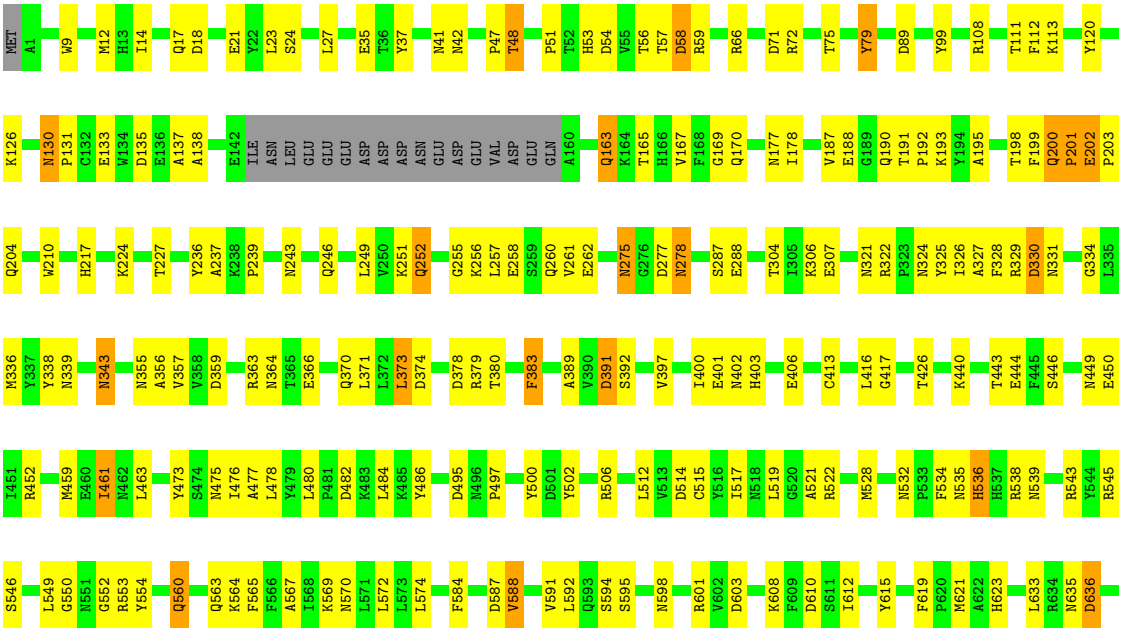
• Molecule 1: Hexon protein

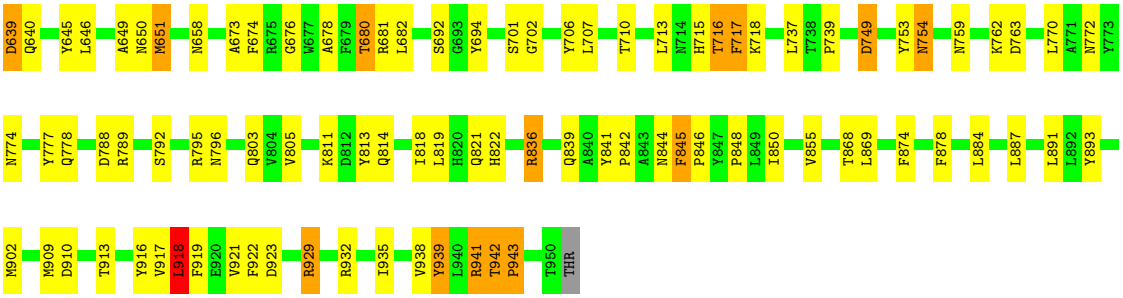
Chain B:



• Molecule 1: Hexon protein

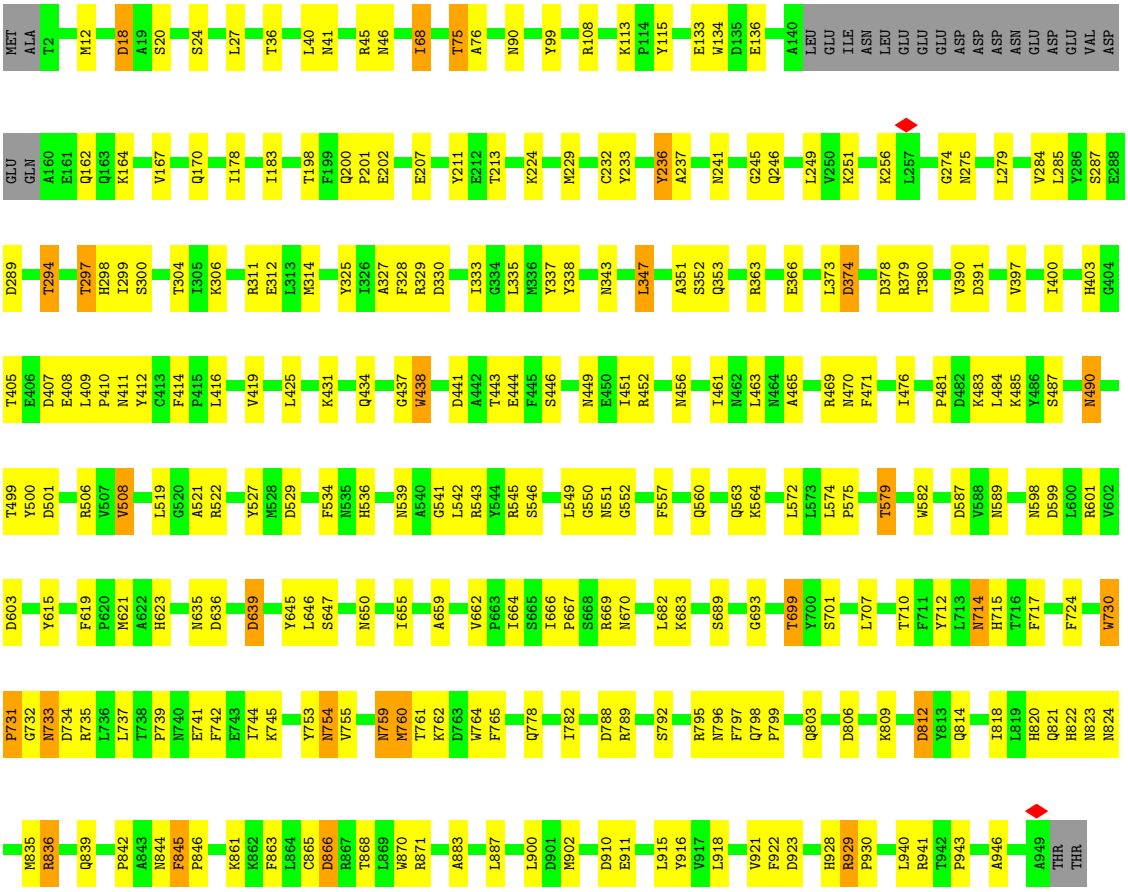
Chain C:





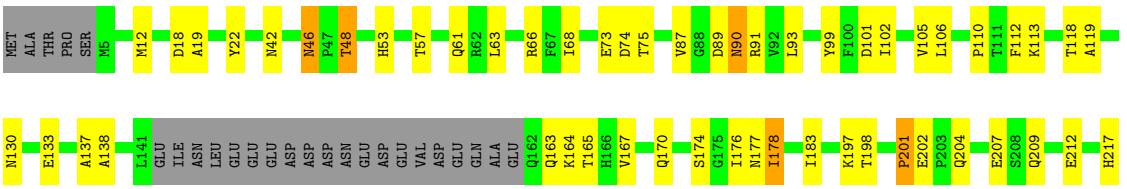
• Molecule 1: Hexon protein

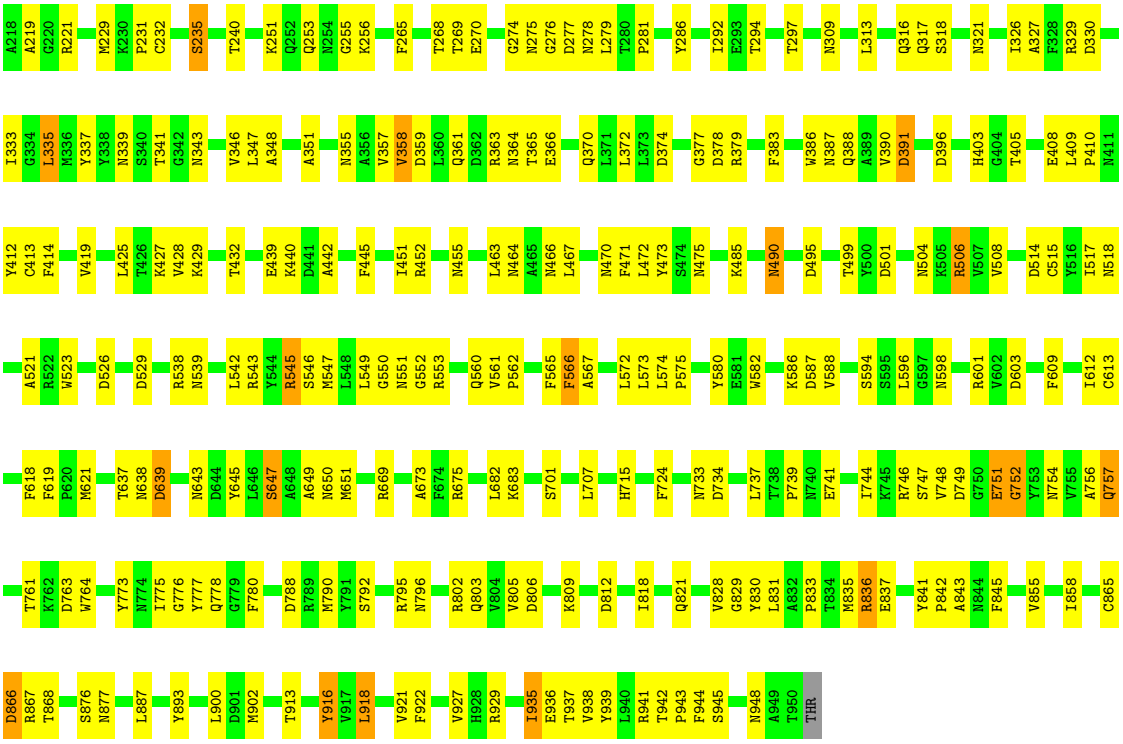
Chain D:



• Molecule 1: Hexon protein

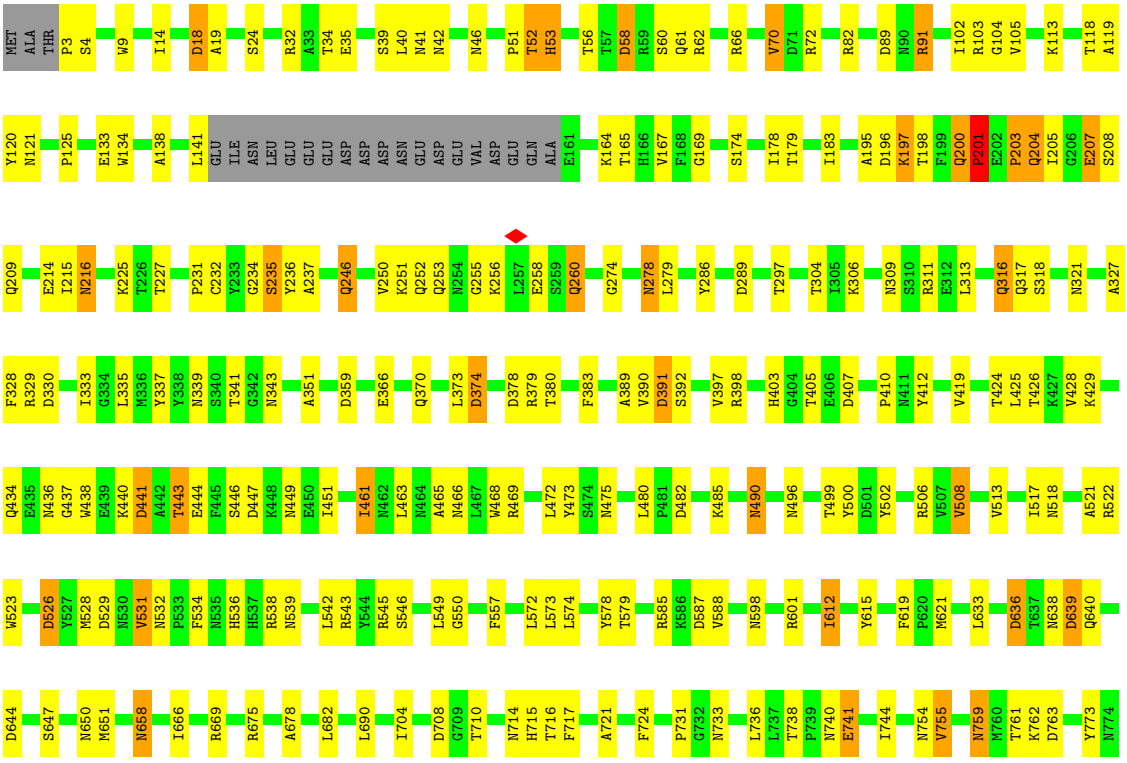
Chain E:

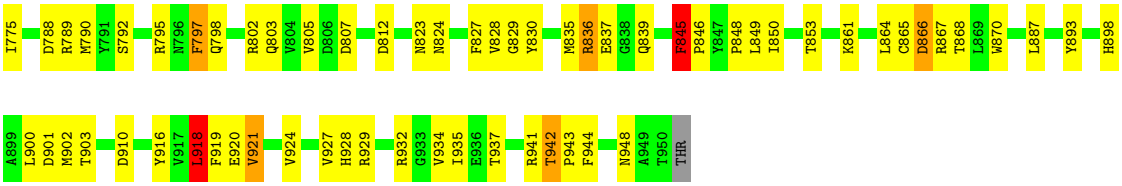




• Molecule 1: Hexon protein

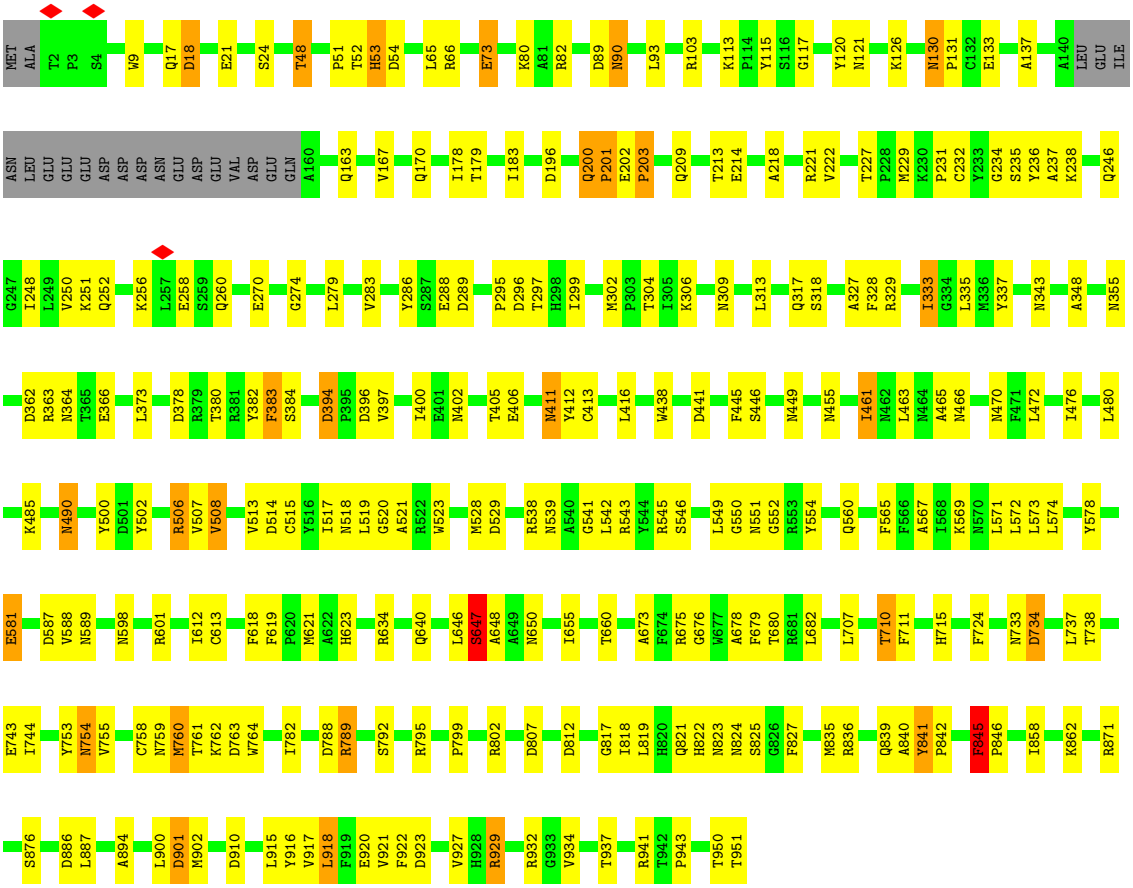
Chain F:





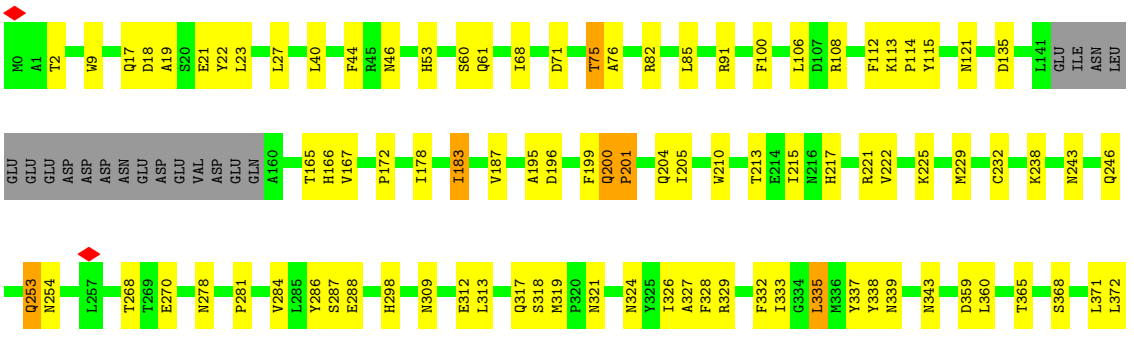
• Molecule 1: Hexon protein

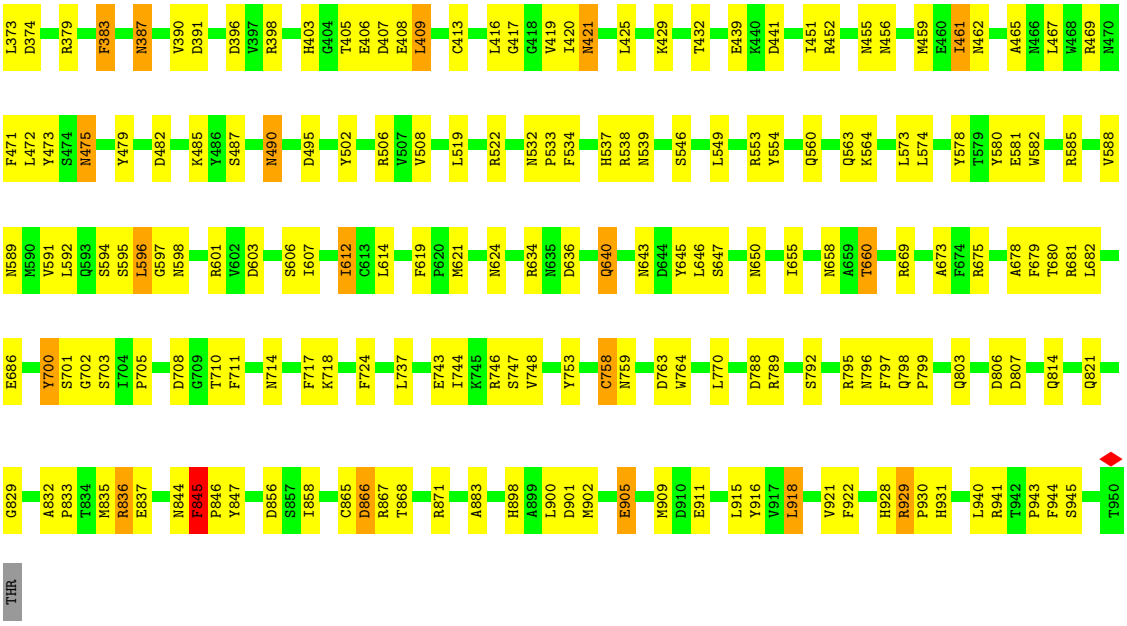
Chain G:



• Molecule 1: Hexon protein

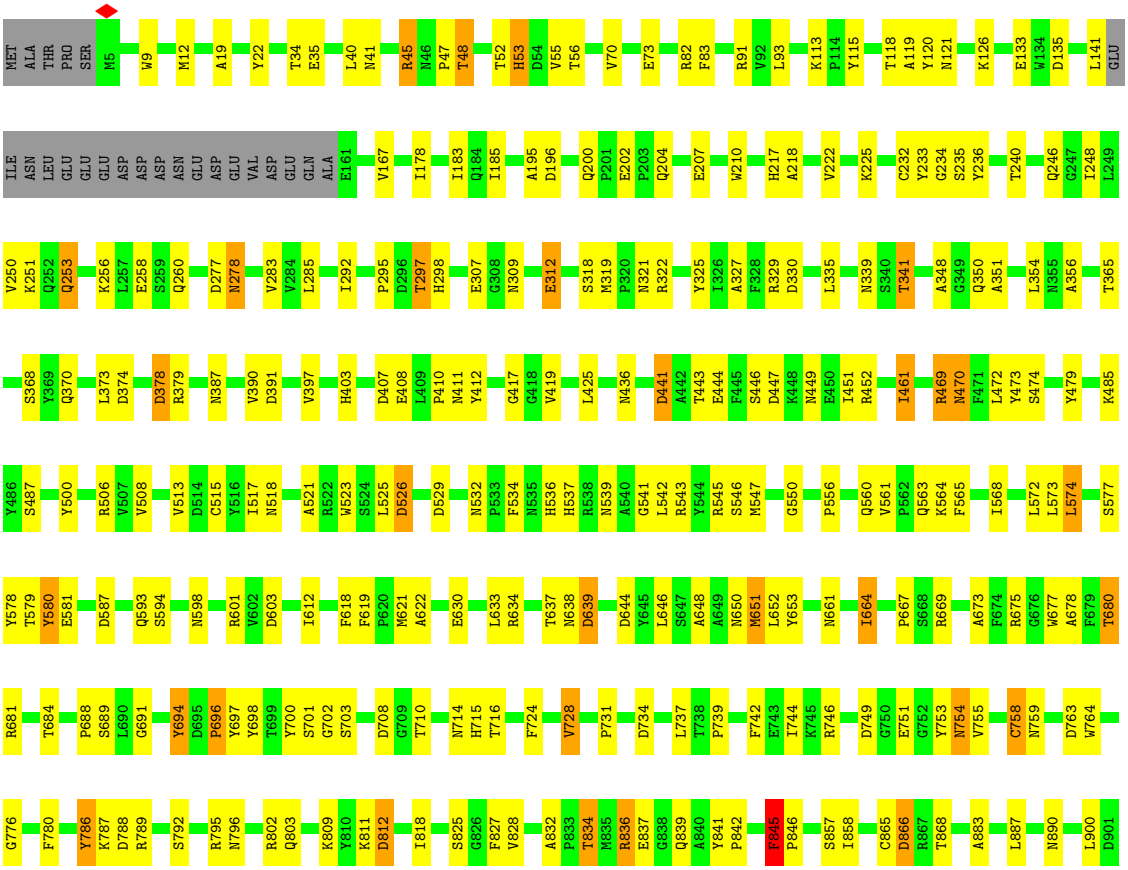
Chain H:





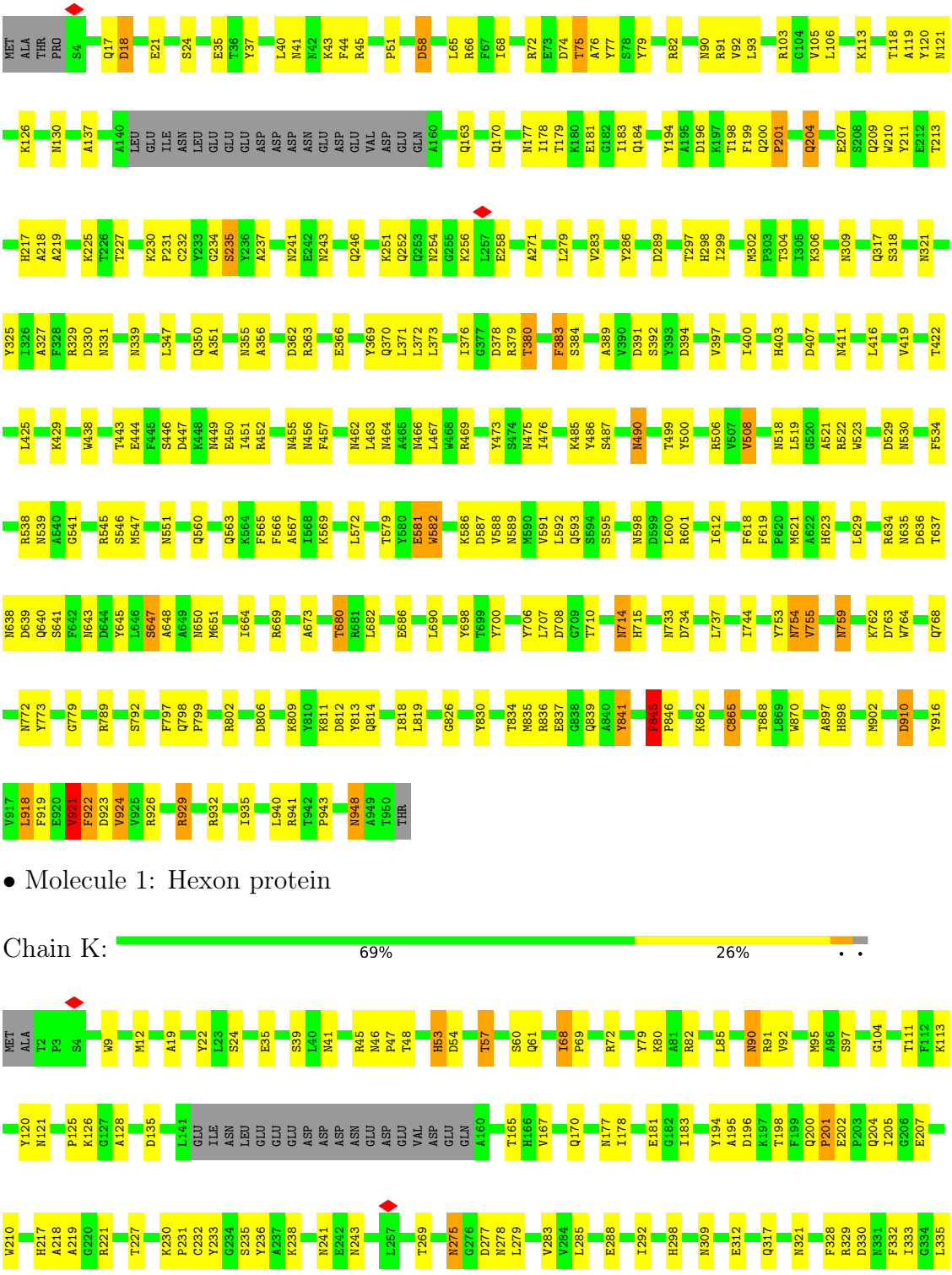
- Molecule 1: Hexon protein

Chain I:



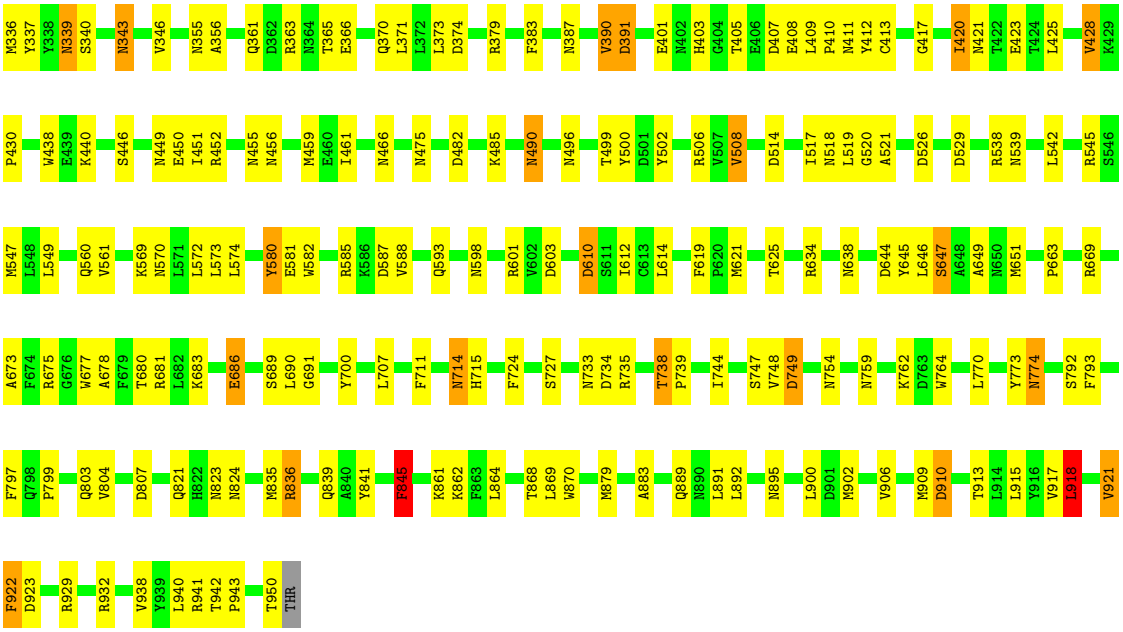
• Molecule 1: Hexon protein

Chain J:



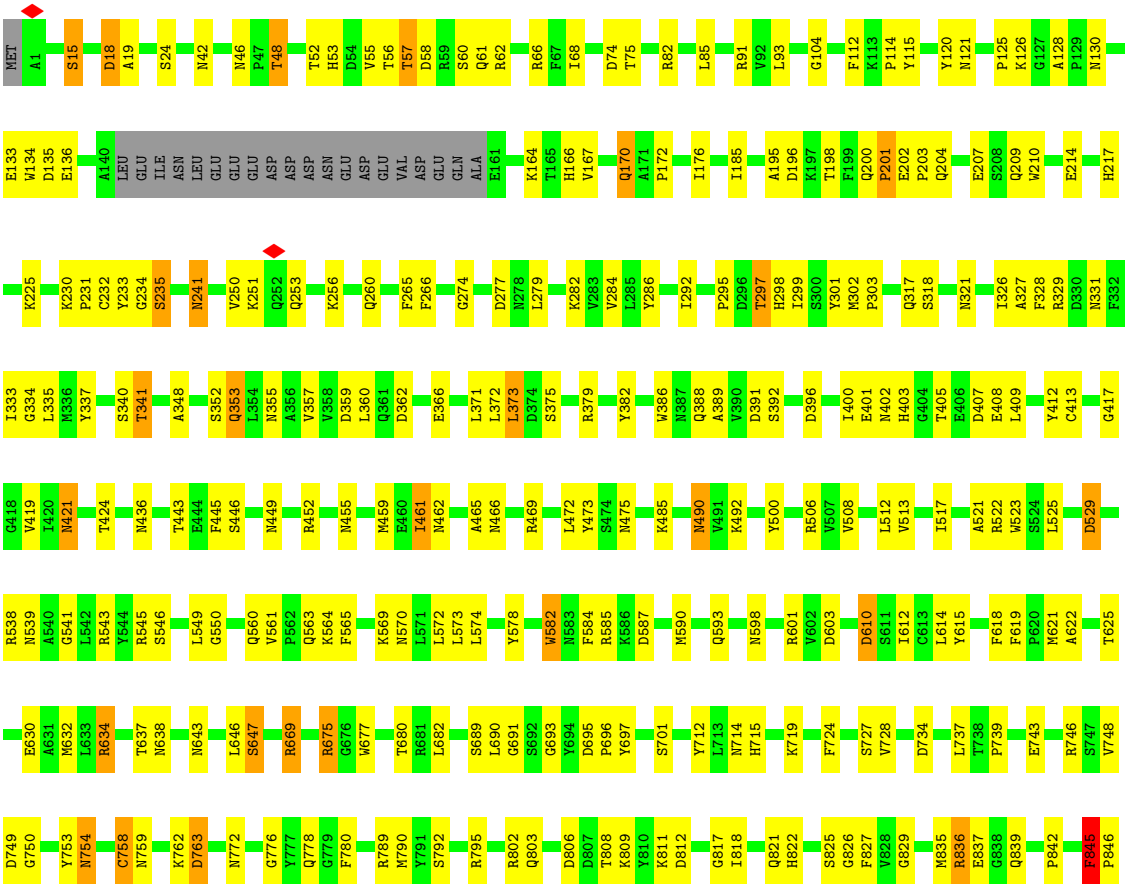
• Molecule 1: Hexon protein

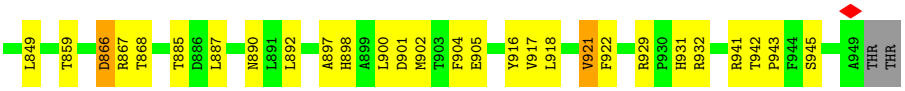
Chain K:



• Molecule 1: Hexon protein

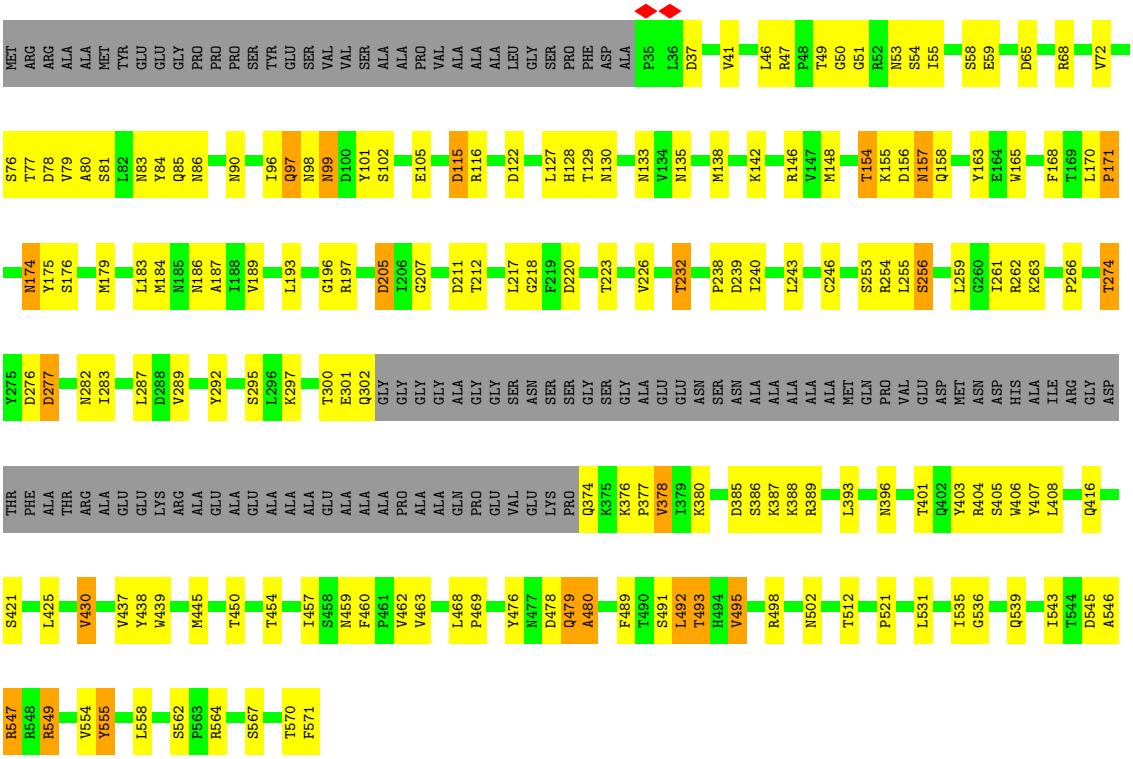
Chain L:





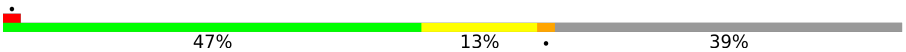
• Molecule 2: Penton protein

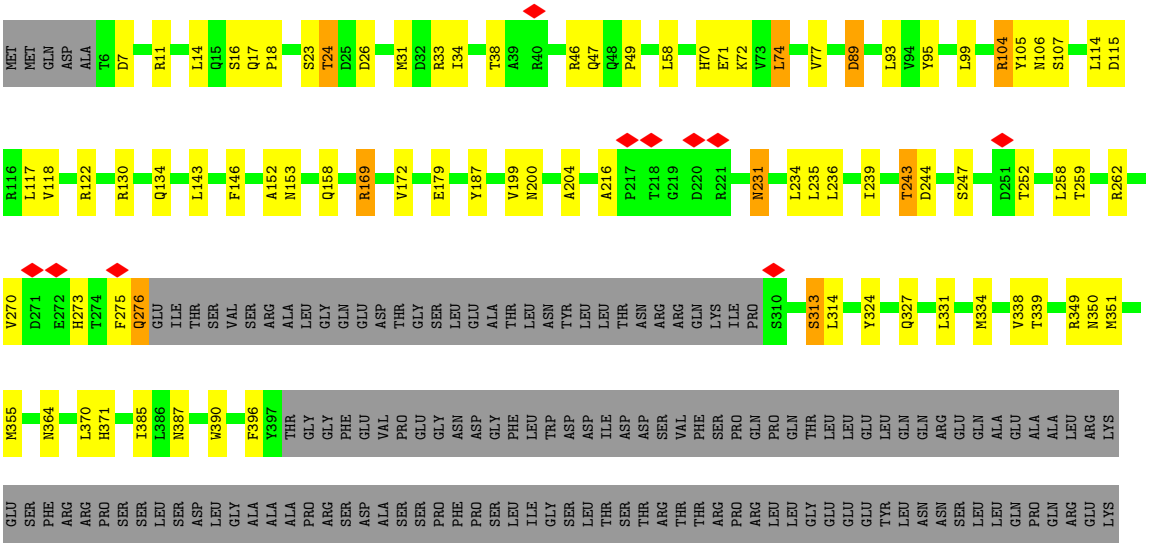
Chain N:



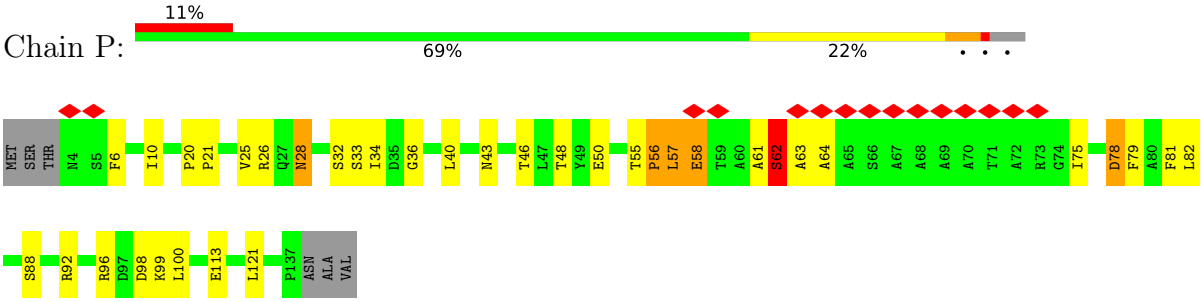
• Molecule 3: Pre-hexon-linking protein IIIa

Chain M:

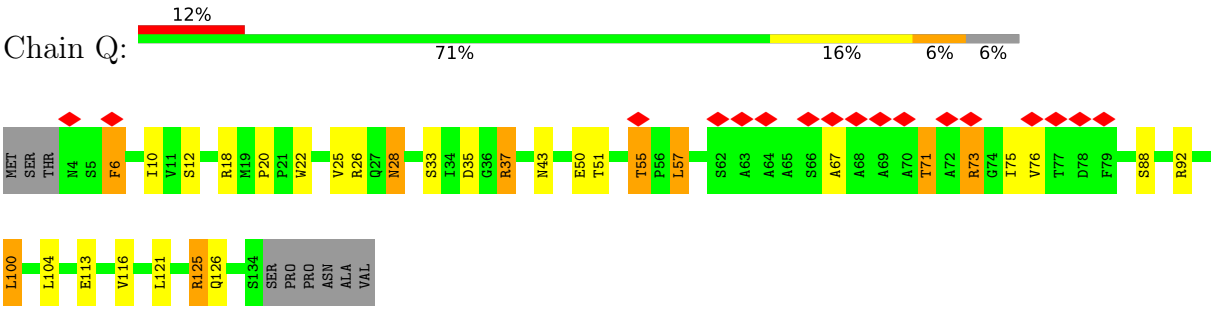




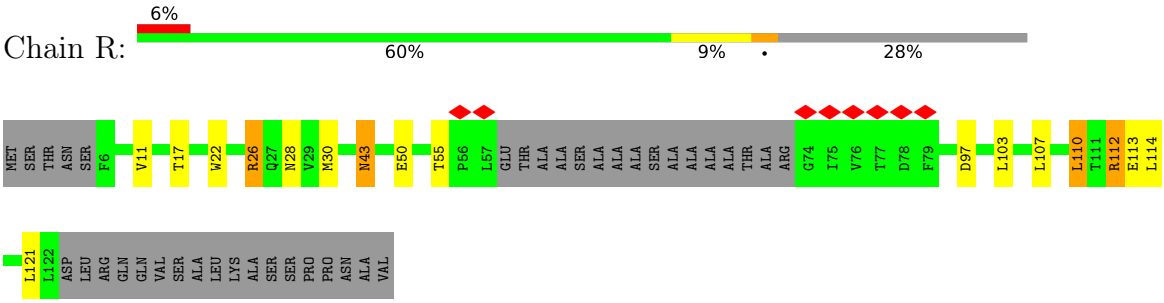
• Molecule 4: Hexon-interlacing protein



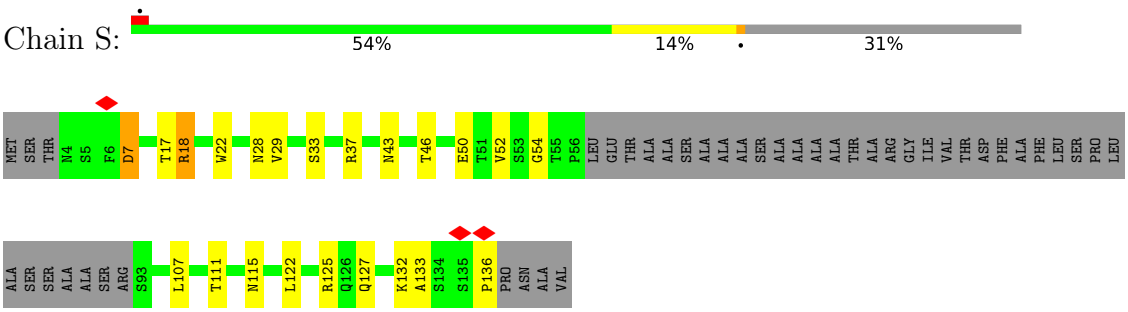
• Molecule 4: Hexon-interlacing protein



• Molecule 4: Hexon-interlacing protein

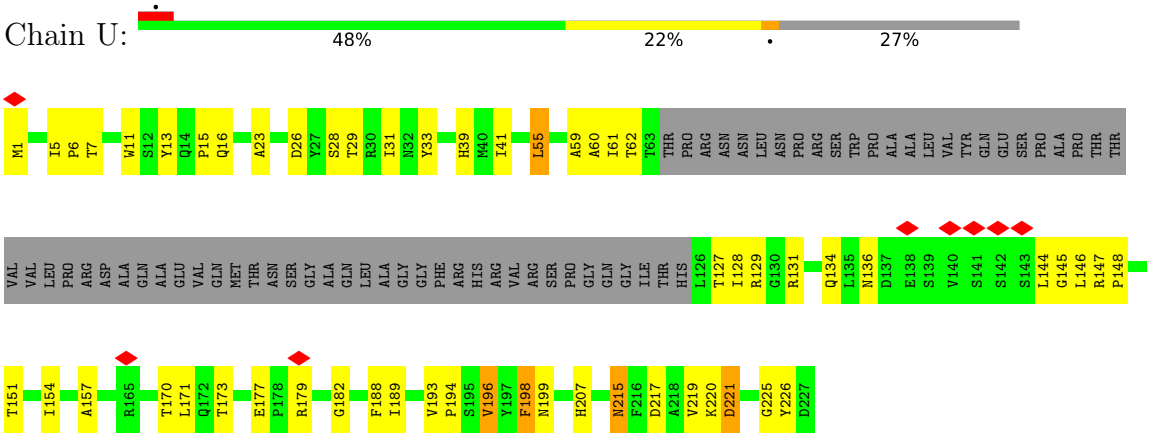


• Molecule 4: Hexon-interlacing protein



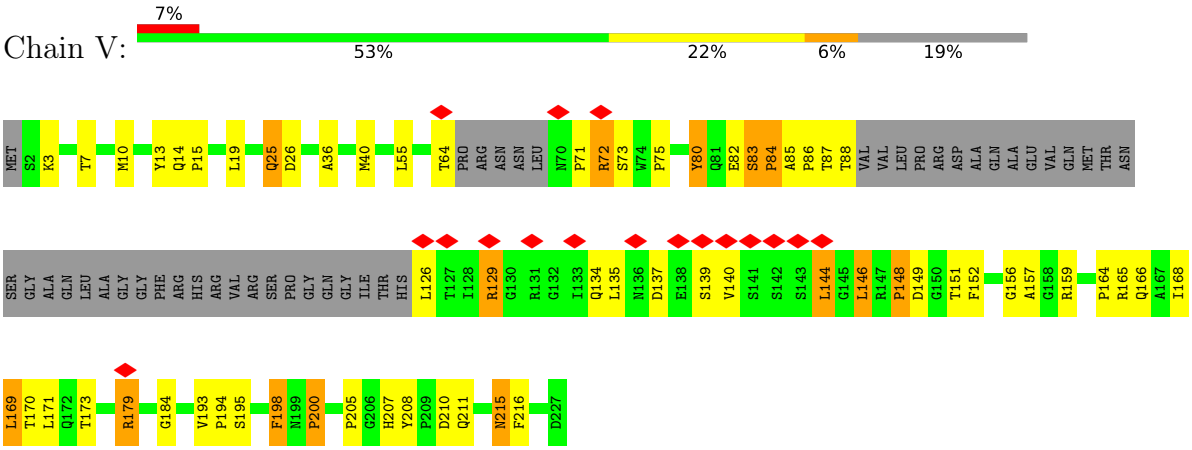
• Molecule 5: Pre-hexon-linking protein VIII

Chain U:



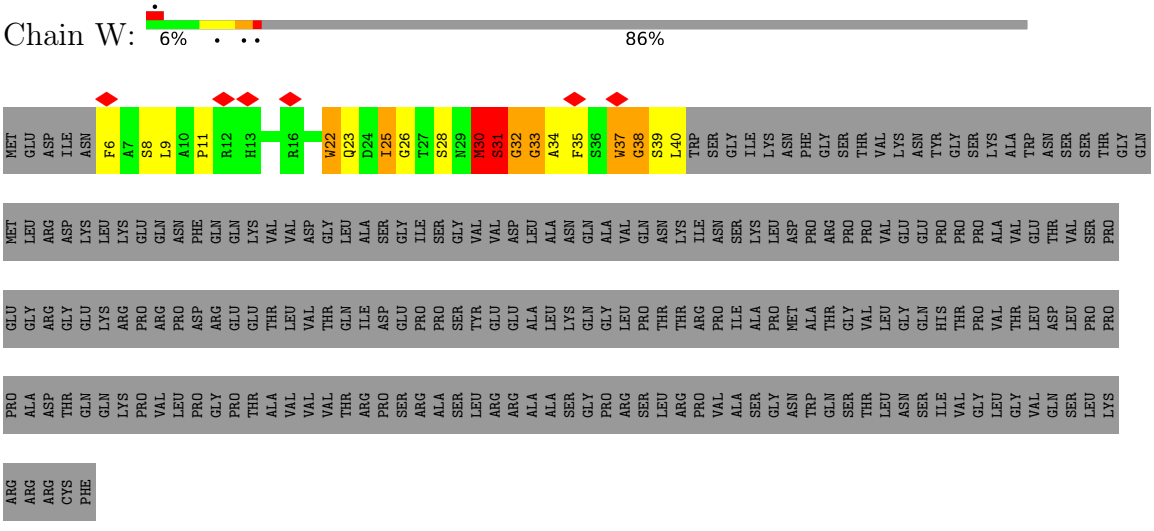
• Molecule 5: Pre-hexon-linking protein VIII

Chain V:



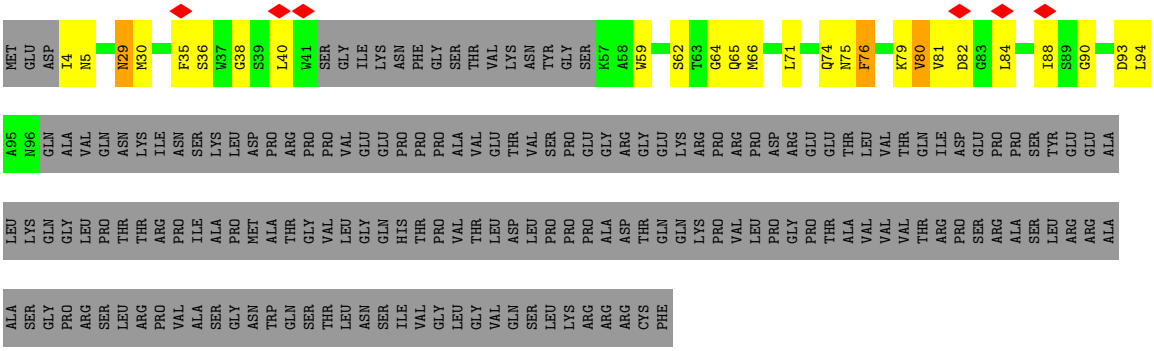
• Molecule 6: Pre-protein VI

Chain W:



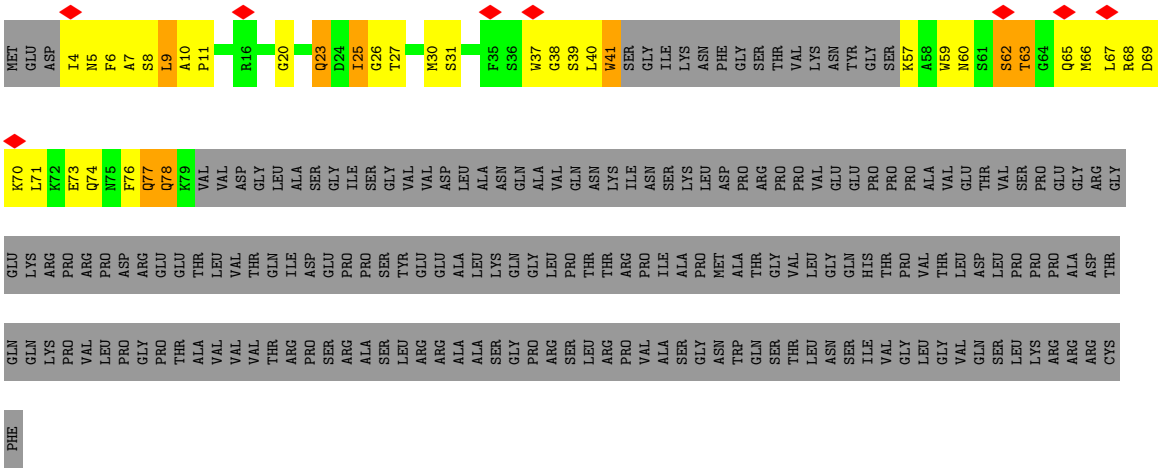
• Molecule 6: Pre-protein VI

Chain X:



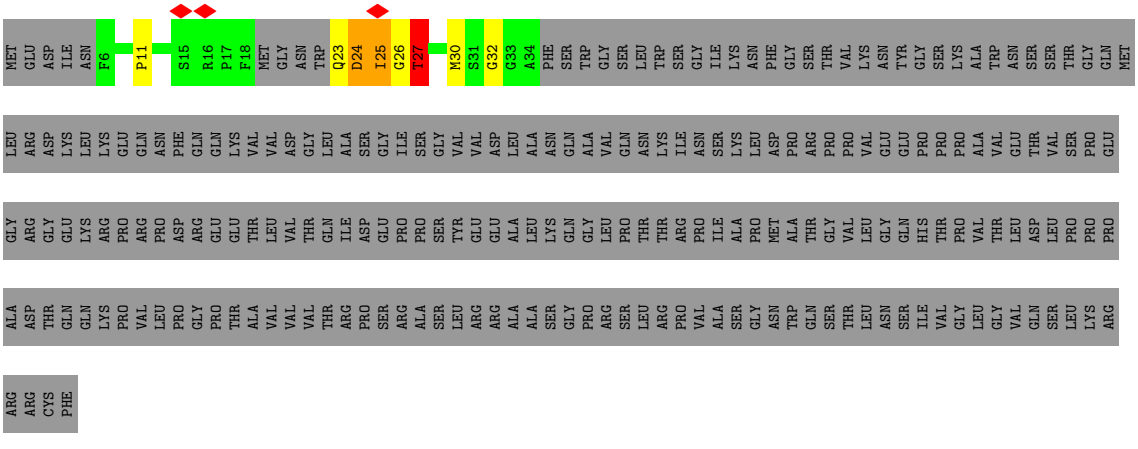
• Molecule 6: Pre-protein VI

Chain Y:



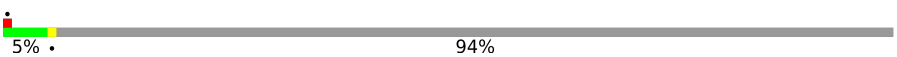
• Molecule 6: Pre-protein VI

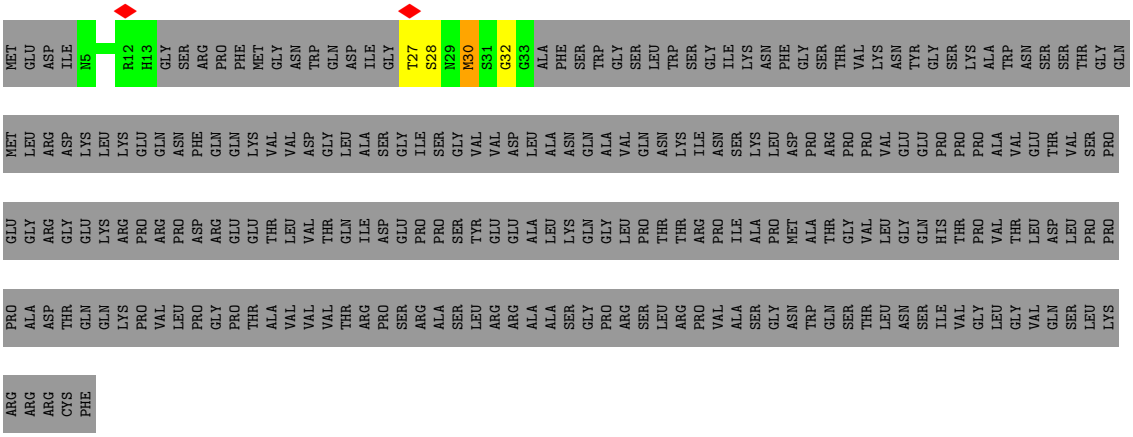
Chain Z:



• Molecule 6: Pre-protein VI

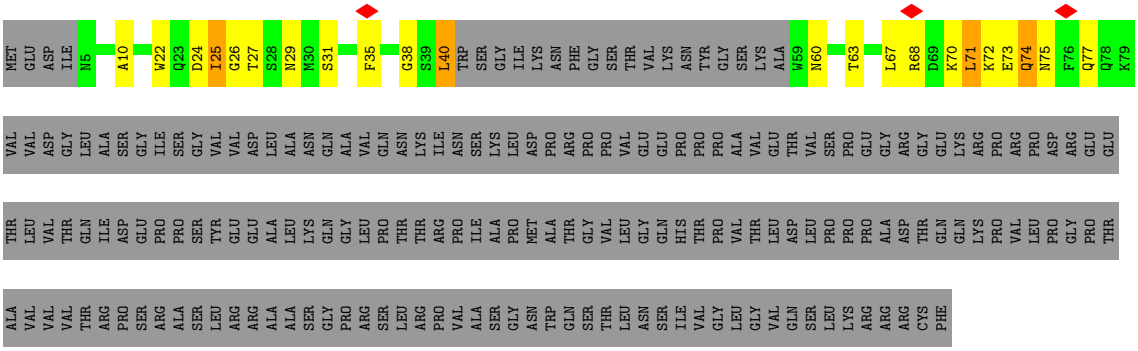
Chain 0:





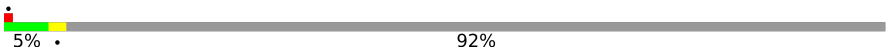
• Molecule 6: Pre-protein VI

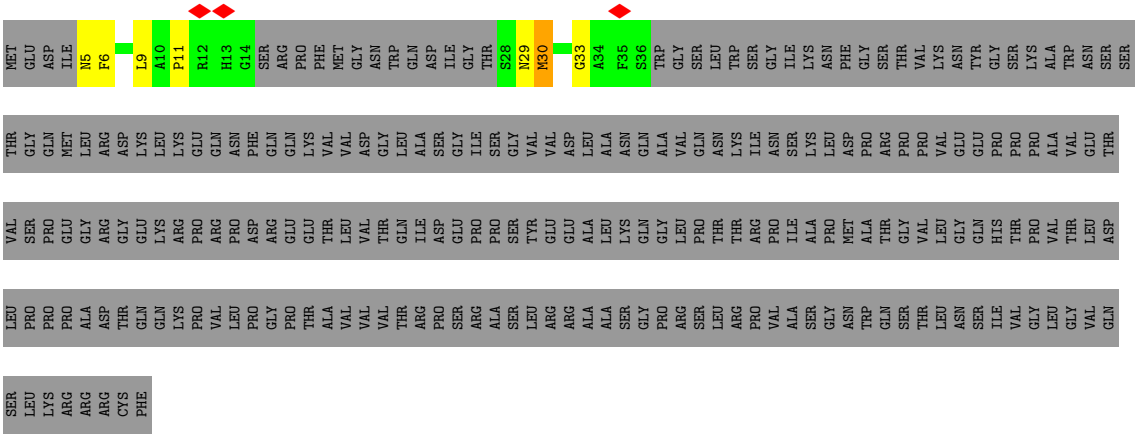
Chain 1:



• Molecule 6: Pre-protein VI

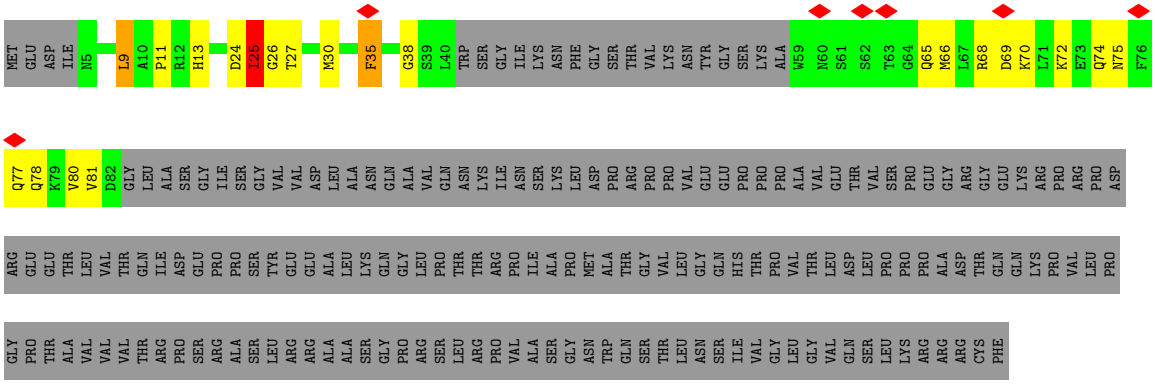
Chain 2:



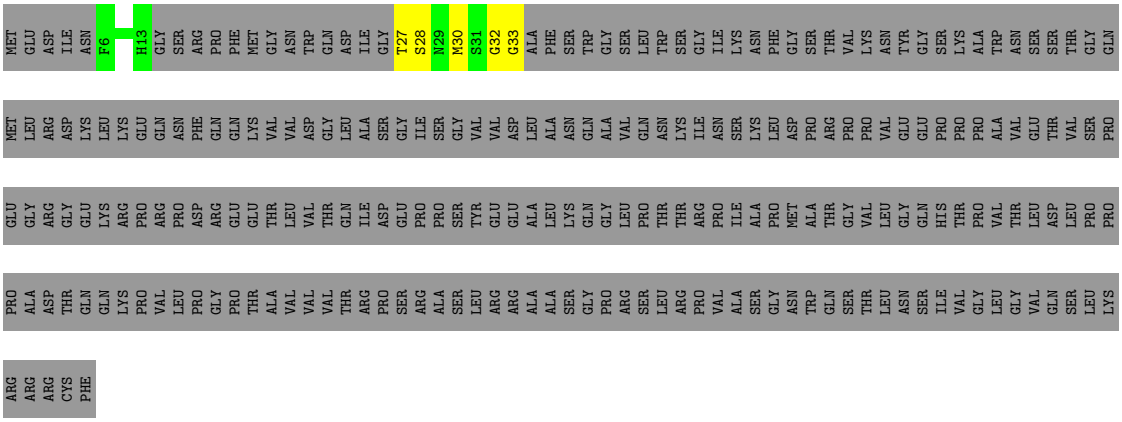


• Molecule 6: Pre-protein VI

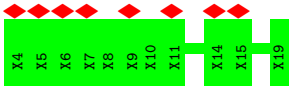
Chain 3:



• Molecule 6: Pre-protein VI



• Molecule 7: Unknown-1



• Molecule 8: Unknown-2

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	11277	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	12	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	36.862	Depositor
Minimum map value	-27.573	Depositor
Average map value	-0.024	Depositor
Map value standard deviation	3.164	Depositor
Recommended contour level	3.15	Depositor
Map size (Å)	1089.9199, 1089.9199, 1089.9199	wwPDB
Map dimensions	832, 832, 832	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.65	1/7626 (0.0%)	0.62	8/10371 (0.1%)
1	B	0.61	1/7628 (0.0%)	0.60	8/10374 (0.1%)
1	C	0.59	0/7655	0.60	8/10411 (0.1%)
1	D	0.67	2/7626 (0.0%)	0.62	9/10371 (0.1%)
1	E	0.63	0/7606	0.58	2/10343 (0.0%)
1	F	0.65	1/7629 (0.0%)	0.61	7/10374 (0.1%)
1	G	0.58	1/7640 (0.0%)	0.56	3/10391 (0.0%)
1	H	0.57	2/7654 (0.0%)	0.57	5/10409 (0.0%)
1	I	0.57	2/7615 (0.0%)	0.55	3/10355 (0.0%)
1	J	0.65	2/7617 (0.0%)	0.61	7/10357 (0.1%)
1	K	0.58	0/7641	0.58	5/10392 (0.0%)
1	L	0.62	2/7626 (0.0%)	0.60	6/10371 (0.1%)
2	N	0.83	0/3827	0.80	4/5215 (0.1%)
3	M	0.44	0/2869	0.51	1/3908 (0.0%)
4	P	0.61	2/986 (0.2%)	0.66	1/1347 (0.1%)
4	Q	0.40	0/964	0.50	0/1315
4	R	0.59	0/762	0.55	0/1039
4	S	0.31	0/736	0.44	0/1002
5	U	0.78	0/1300	0.66	0/1764
5	V	0.75	0/1452	0.77	6/1977 (0.3%)
6	0	0.65	0/115	0.82	0/152
6	1	1.05	0/460	1.23	5/615 (0.8%)
6	2	0.68	0/135	0.94	1/178 (0.6%)
6	3	0.55	0/482	0.95	2/646 (0.3%)
6	4	0.81	0/107	0.96	1/141 (0.7%)
6	W	1.08	1/271 (0.4%)	1.40	8/365 (2.2%)
6	X	0.72	0/590	0.92	3/794 (0.4%)
6	Y	1.01	0/498	1.27	4/667 (0.6%)
6	Z	1.09	0/182	1.20	1/242 (0.4%)
All	All	0.63	17/107299 (0.0%)	0.62	108/145886 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	SER	CA-C	-5.97	1.37	1.52
1	F	201	PRO	CA-C	-5.85	1.41	1.52
1	I	694	TYR	CB-CG	-5.59	1.43	1.51
1	I	696	PRO	CA-C	-5.49	1.41	1.52
6	W	30	MET	CA-C	-5.36	1.39	1.52
1	J	582	TRP	CB-CG	-5.36	1.40	1.50
1	B	731	PRO	CA-C	-5.31	1.42	1.52
1	L	677	TRP	CB-CG	-5.27	1.40	1.50
1	L	15	SER	CA-CB	-5.26	1.45	1.52
1	H	594	SER	CA-C	-5.25	1.39	1.52
4	P	56	PRO	CA-C	-5.24	1.42	1.52
1	D	731	PRO	CA-C	-5.21	1.42	1.52
1	D	667	PRO	CA-C	-5.21	1.42	1.52
1	H	594	SER	CA-CB	-5.16	1.45	1.52
4	P	32	SER	CA-CB	-5.14	1.45	1.52
1	G	647	SER	CA-CB	-5.05	1.45	1.52
1	J	921	VAL	CA-CB	-5.03	1.44	1.54

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	3	26	GLY	N-CA-C	14.88	150.30	113.10
6	1	26	GLY	N-CA-C	12.63	144.68	113.10
6	Y	26	GLY	N-CA-C	12.62	144.65	113.10
6	W	26	GLY	N-CA-C	9.94	137.94	113.10
1	A	45	ARG	N-CA-C	9.08	135.50	111.00
1	K	649	ALA	N-CA-C	-8.99	86.73	111.00
1	C	255	GLY	N-CA-C	-8.65	91.48	113.10
1	D	201	PRO	N-CA-C	-8.64	89.64	112.10
1	K	201	PRO	N-CA-C	-8.45	90.13	112.10
6	W	32	GLY	N-CA-C	-8.39	92.14	113.10
1	C	845	PHE	N-CA-C	8.21	133.16	111.00
1	E	201	PRO	N-CA-C	-7.92	91.50	112.10
1	J	201	PRO	N-CA-C	-7.83	91.75	112.10
1	J	347	LEU	N-CA-C	-7.52	90.71	111.00
5	V	146	LEU	N-CA-C	7.49	131.23	111.00
1	H	201	PRO	N-CA-C	-7.37	92.95	112.10
1	D	845	PHE	N-CA-C	7.32	130.77	111.00
1	C	942	THR	N-CA-C	7.25	130.57	111.00
1	C	201	PRO	N-CA-C	-7.18	93.42	112.10
1	D	200	GLN	N-CA-C	6.89	129.62	111.00
1	K	845	PHE	N-CA-C	6.87	129.54	111.00
4	P	56	PRO	N-CA-C	-6.85	94.28	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	845	PHE	N-CA-C	6.80	129.37	111.00
2	N	98	ASN	N-CA-C	-6.76	92.74	111.00
1	C	918	LEU	CA-CB-CG	6.68	130.67	115.30
1	E	649	ALA	N-CA-C	-6.56	93.28	111.00
1	G	201	PRO	N-CA-C	-6.52	95.14	112.10
1	J	581	GLU	CB-CA-C	-6.43	97.55	110.40
1	D	730	TRP	N-CA-C	6.40	128.29	111.00
1	L	201	PRO	N-CA-C	-6.40	95.45	112.10
1	B	200	GLN	N-CA-C	6.38	128.22	111.00
1	F	845	PHE	N-CA-C	6.30	128.00	111.00
1	C	200	GLN	N-CA-C	6.26	127.91	111.00
1	B	738	THR	N-CA-C	-6.20	94.26	111.00
1	J	921	VAL	CB-CA-C	-6.15	99.71	111.40
1	A	200	GLN	N-CA-C	6.13	127.54	111.00
1	G	845	PHE	N-CA-C	6.12	127.53	111.00
6	1	77	GLN	N-CA-C	6.09	127.44	111.00
5	V	149	ASP	N-CA-C	-6.07	94.61	111.00
1	D	666	ILE	N-CA-C	-6.07	94.62	111.00
6	W	31	SER	N-CA-CB	-6.07	101.40	110.50
1	C	943	PRO	N-CA-C	-6.02	96.45	112.10
6	W	37	TRP	N-CA-C	6.00	127.21	111.00
1	F	200	GLN	N-CA-C	5.99	127.18	111.00
5	V	200	PRO	N-CA-C	5.99	127.68	112.10
1	A	845	PHE	N-CA-C	5.97	127.12	111.00
1	H	592	LEU	N-CA-C	-5.93	95.00	111.00
1	F	105	VAL	CB-CA-C	-5.92	100.16	111.40
1	J	918	LEU	CA-CB-CG	5.88	128.83	115.30
1	I	845	PHE	N-CA-C	5.86	126.81	111.00
1	L	917	VAL	CB-CA-C	-5.79	100.39	111.40
1	F	531	VAL	CB-CA-C	-5.78	100.42	111.40
6	Y	9	LEU	CA-CB-CG	5.78	128.58	115.30
6	Y	38	GLY	N-CA-C	5.77	127.53	113.10
6	2	29	ASN	N-CA-C	-5.72	95.56	111.00
6	4	28	SER	N-CA-C	-5.71	95.60	111.00
1	A	732	GLY	N-CA-C	5.69	127.32	113.10
3	M	313	SER	N-CA-C	5.69	126.35	111.00
5	V	84	PRO	N-CA-C	5.67	126.84	112.10
6	X	90	GLY	N-CA-C	5.65	127.24	113.10
6	Y	40	LEU	N-CA-C	-5.64	95.77	111.00
1	I	918	LEU	CB-CA-C	-5.63	99.50	110.20
1	F	918	LEU	CA-CB-CG	5.63	128.25	115.30
5	V	198	PHE	N-CA-C	5.62	126.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	W	38	GLY	N-CA-C	5.59	127.07	113.10
1	I	691	GLY	N-CA-C	5.59	127.06	113.10
1	D	662	VAL	CB-CA-C	-5.58	100.80	111.40
1	G	200	GLN	N-CA-C	5.56	126.00	111.00
6	W	31	SER	N-CA-C	5.55	125.99	111.00
1	L	680	THR	CB-CA-C	-5.54	96.64	111.60
2	N	378	VAL	CB-CA-C	-5.54	100.87	111.40
1	B	736	LEU	CB-CG-CD1	-5.53	101.61	111.00
6	Z	27	THR	N-CA-C	5.52	125.91	111.00
1	A	918	LEU	CA-CB-CG	5.50	127.95	115.30
1	L	921	VAL	CB-CA-C	-5.50	100.95	111.40
1	H	845	PHE	C-N-CD	5.47	139.88	128.40
1	F	845	PHE	C-N-CD	5.44	139.83	128.40
1	H	200	GLN	N-CA-C	5.40	125.58	111.00
1	A	829	GLY	N-CA-C	5.39	126.57	113.10
1	L	845	PHE	C-N-CD	5.38	139.71	128.40
1	K	918	LEU	CA-CB-CG	5.37	127.64	115.30
2	N	50	GLY	N-CA-C	-5.36	99.70	113.10
6	X	94	LEU	N-CA-C	5.31	125.34	111.00
1	H	701	SER	CB-CA-C	-5.31	100.01	110.10
6	W	30	MET	CB-CA-C	-5.30	99.79	110.40
6	1	38	GLY	N-CA-C	5.26	126.26	113.10
2	N	555	TYR	CA-CB-CG	5.26	123.39	113.40
1	B	730	TRP	N-CA-C	5.23	125.13	111.00
1	K	921	VAL	CB-CA-C	-5.22	101.48	111.40
1	L	693	GLY	N-CA-C	-5.22	100.05	113.10
1	B	649	ALA	N-CA-C	-5.20	96.97	111.00
1	F	921	VAL	CB-CA-C	-5.20	101.53	111.40
1	B	270	GLU	N-CA-C	-5.17	97.04	111.00
6	1	27	THR	CB-CA-C	-5.17	97.65	111.60
6	3	25	ILE	CG1-CB-CG2	-5.14	100.10	111.40
1	J	680	THR	CB-CA-C	-5.13	97.74	111.60
1	D	300	SER	CB-CA-C	-5.11	100.39	110.10
1	A	649	ALA	N-CA-C	-5.11	97.20	111.00
1	D	670	ASN	N-CA-C	-5.08	97.29	111.00
6	X	76	PHE	N-CA-CB	-5.07	101.48	110.60
1	B	730	TRP	C-N-CD	5.05	139.01	128.40
1	D	294	THR	C-N-CD	5.05	139.00	128.40
5	V	83	SER	CB-CA-C	5.04	119.68	110.10
1	B	741	GLU	CB-CA-C	-5.03	100.34	110.40
6	1	10	ALA	N-CA-C	5.03	124.57	111.00
6	W	33	GLY	N-CA-C	-5.02	100.55	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	39	SER	CB-CA-C	-5.02	100.57	110.10
1	C	917	VAL	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

There are no planarity outliers.

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	7427	0	7124	208	0
1	B	7429	0	7126	204	0
1	C	7456	0	7156	210	0
1	D	7427	0	7124	199	0
1	E	7408	0	7112	210	0
1	F	7430	0	7131	210	0
1	G	7441	0	7138	190	0
1	H	7455	0	7159	197	0
1	I	7417	0	7118	212	0
1	J	7419	0	7116	202	0
1	K	7442	0	7142	199	0
1	L	7427	0	7127	219	0
2	N	3734	0	3656	102	0
3	M	2813	0	2767	53	0
4	P	972	0	978	31	0
4	Q	952	0	959	27	0
4	R	751	0	757	14	0
4	S	727	0	732	11	0
5	U	1268	0	1227	42	0
5	V	1414	0	1360	39	0
6	0	114	0	104	2	0
6	1	449	0	419	15	0
6	2	133	0	119	3	0
6	3	471	0	441	13	0
6	4	106	0	98	3	0
6	W	262	0	238	20	0
6	X	577	0	526	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Y	485	0	458	25	0
6	Z	179	0	166	10	0
7	5	80	0	19	0	0
8	6	50	0	12	0	0
All	All	104715	0	100609	2514	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 12.

All (2514) 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)
1:C:251:LYS:HG2	1:C:258:GLU:HB2	1.48	0.96
4:P:58:GLU:HA	4:P:61:ALA:HB3	1.52	0.92
2:N:51:GLY:HA2	2:N:116:ARG:NH2	1.87	0.90
1:B:635:ASN:HD22	3:M:18:PRO:HB3	1.37	0.87
1:H:432:THR:HB	1:H:439:GLU:HB2	1.57	0.86
6:W:32:GLY:C	6:W:34:ALA:H	1.71	0.86
1:C:921:VAL:HB	1:C:943:PRO:HD2	1.58	0.85
1:E:795:ARG:HH22	6:Y:41:TRP:HA	1.41	0.85
3:M:89:ASP:OD1	3:M:89:ASP:N	2.10	0.84
1:D:574:LEU:H	1:D:929:ARG:HH12	1.25	0.84
1:E:105:VAL:HB	4:P:56:PRO:HG3	1.60	0.81
1:H:574:LEU:H	1:H:929:ARG:HH12	1.28	0.80
1:E:499:THR:HG22	1:E:501:ASP:H	1.46	0.80
1:D:659:ALA:HA	4:R:11:VAL:HG21	1.65	0.79
1:D:485:LYS:HG2	1:D:508:VAL:HB	1.65	0.79
3:M:216:ALA:HA	3:M:252:THR:HA	1.65	0.79
6:W:32:GLY:C	6:W:34:ALA:N	2.36	0.79
1:E:235:SER:HB3	1:E:292:ILE:HD11	1.65	0.78
1:F:18:ASP:OD1	1:F:18:ASP:N	2.14	0.78
1:C:678:ALA:HB3	1:C:918:LEU:HG	1.66	0.78
1:G:647:SER:HB3	1:G:675:ARG:HH22	1.48	0.78
1:J:58:ASP:HB2	5:V:148:PRO:HG2	1.66	0.78
2:N:51:GLY:HA2	2:N:116:ARG:HH21	1.48	0.77
1:B:686:GLU:HG2	1:B:700:TYR:CZ	2.20	0.77
1:J:921:VAL:HG12	1:J:943:PRO:HG2	1.64	0.77
1:H:573:LEU:HA	1:H:929:ARG:HH22	1.48	0.77
1:L:251:LYS:HB3	1:L:256:LYS:HA	1.66	0.77
1:G:573:LEU:HA	1:G:929:ARG:HH12	1.47	0.76
1:B:803:GLN:HE22	1:C:550:GLY:HA3	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ALA:HB1	1:C:200:GLN:HB3	1.66	0.76
1:J:18:ASP:N	1:J:18:ASP:OD1	2.17	0.76
4:P:79:PHE:HA	4:P:82:LEU:HB2	1.66	0.75
1:B:138:ALA:HB3	1:B:162:GLN:HB3	1.67	0.75
1:L:714:ASN:ND2	1:L:868:THR:O	2.20	0.75
1:C:788:ASP:OD2	1:C:795:ARG:NH1	2.20	0.75
1:G:113:LYS:NZ	1:G:115:TYR:O	2.21	0.74
2:N:292:TYR:HD1	2:N:378:VAL:HA	1.51	0.74
1:L:763:ASP:OD1	1:L:763:ASP:N	2.17	0.74
1:E:821:GLN:HB2	1:E:845:PHE:HB2	1.68	0.74
2:N:493:THR:HB	2:N:495:VAL:HG23	1.68	0.74
1:L:697:TYR:O	4:P:26:ARG:NH2	2.20	0.74
1:L:921:VAL:HB	1:L:943:PRO:HD2	1.69	0.74
1:I:572:LEU:O	1:I:929:ARG:NH1	2.20	0.74
1:L:754:ASN:OD1	1:L:754:ASN:N	2.20	0.74
1:J:714:ASN:ND2	1:J:868:THR:O	2.21	0.74
6:W:31:SER:HB2	6:W:33:GLY:H	1.52	0.73
1:C:72:ARG:NE	1:C:79:TYR:OH	2.22	0.73
1:F:379:ARG:HE	1:F:390:VAL:HB	1.53	0.73
1:J:485:LYS:HG2	1:J:508:VAL:HB	1.70	0.73
1:B:502:TYR:OH	1:B:506:ARG:NH1	2.22	0.73
1:E:795:ARG:HH22	6:Y:41:TRP:CA	2.01	0.72
1:H:178:ILE:HG12	1:H:217:HIS:HD2	1.52	0.72
1:A:18:ASP:HA	1:A:47:PRO:HD2	1.71	0.72
1:F:921:VAL:HB	1:F:943:PRO:HD2	1.70	0.72
1:H:195:ALA:HB1	1:H:200:GLN:HB3	1.70	0.71
1:E:803:GLN:HE22	1:F:550:GLY:HA3	1.53	0.71
1:D:714:ASN:ND2	1:D:868:THR:O	2.22	0.71
1:J:330:ASP:OD1	1:J:331:ASN:ND2	2.24	0.71
1:K:485:LYS:HG2	1:K:508:VAL:HB	1.72	0.71
1:D:754:ASN:ND2	4:P:50:GLU:OE1	2.23	0.71
5:V:129:ARG:HA	5:V:134:GLN:HA	1.72	0.71
1:D:113:LYS:NZ	1:D:115:TYR:O	2.23	0.71
1:I:545:ARG:NH2	1:I:593:GLN:OE1	2.24	0.71
2:N:156:ASP:O	2:N:157:ASN:ND2	2.24	0.71
1:D:550:GLY:HA3	1:F:803:GLN:HE22	1.55	0.70
1:L:573:LEU:HA	1:L:929:ARG:HH12	1.56	0.70
1:C:400:ILE:HD11	1:C:476:ILE:HG12	1.73	0.70
1:J:411:ASN:ND2	1:K:466:ASN:OD1	2.25	0.70
1:B:138:ALA:HB2	1:B:164:LYS:HB2	1.74	0.70
1:E:638:ASN:ND2	1:F:24:SER:OG	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:58:ASP:OD1	1:J:58:ASP:N	2.24	0.70
1:D:456:ASN:O	1:E:836:ARG:NH1	2.25	0.69
1:H:379:ARG:HE	1:H:390:VAL:HB	1.56	0.69
1:K:379:ARG:HE	1:K:390:VAL:HB	1.56	0.69
1:C:502:TYR:OH	1:C:506:ARG:NH1	2.25	0.69
1:L:905:GLU:OE2	4:Q:22:TRP:NE1	2.23	0.69
1:A:391:ASP:OD1	1:A:391:ASP:N	2.23	0.69
2:N:171:PRO:HB2	2:N:174:ASN:HD21	1.58	0.69
1:C:754:ASN:N	1:C:754:ASN:OD1	2.25	0.69
1:I:35:GLU:OE2	1:I:41:ASN:ND2	2.26	0.69
4:P:28:ASN:ND2	4:P:43:ASN:OD1	2.25	0.69
5:V:71:PRO:O	5:V:75:PRO:HD2	1.92	0.69
1:I:680:THR:OG1	1:I:681:ARG:N	2.26	0.69
2:N:68:ARG:NH1	2:N:562:SER:OG	2.26	0.69
1:D:134:TRP:NE1	1:D:136:GLU:OE1	2.25	0.69
1:I:446:SER:O	1:I:449:ASN:ND2	2.24	0.69
1:K:572:LEU:O	1:K:929:ARG:NH1	2.22	0.69
2:N:295:SER:HB3	2:N:377:PRO:HD2	1.74	0.69
1:I:694:TYR:CE2	1:I:696:PRO:HA	2.28	0.69
1:B:252:GLN:HB3	1:B:258:GLU:HG3	1.73	0.69
1:H:407:ASP:OD2	1:H:462:ASN:ND2	2.26	0.69
1:C:921:VAL:HG12	1:C:943:PRO:HB2	1.75	0.68
1:I:235:SER:HB2	1:I:292:ILE:HD11	1.74	0.68
1:D:45:ARG:HH11	6:Z:27:THR:HG22	1.56	0.68
2:N:277:ASP:OD1	2:N:277:ASP:N	2.26	0.68
1:D:46:ASN:O	6:Z:27:THR:HG21	1.93	0.68
1:E:866:ASP:OD1	1:E:866:ASP:N	2.23	0.68
1:K:803:GLN:HE21	1:L:550:GLY:HA3	1.59	0.68
1:L:669:ARG:HH22	1:L:945:SER:H	1.42	0.68
1:A:550:GLY:HA3	1:C:803:GLN:HE22	1.58	0.68
1:I:178:ILE:HG12	1:I:183:ILE:HG22	1.75	0.68
1:K:921:VAL:HG12	1:K:943:PRO:HG2	1.75	0.68
1:G:231:PRO:HG3	1:G:318:SER:HB2	1.74	0.68
1:L:866:ASP:N	1:L:866:ASP:OD1	2.27	0.68
1:D:803:GLN:HE22	1:E:550:GLY:HA3	1.58	0.68
1:H:866:ASP:OD1	1:H:866:ASP:N	2.25	0.68
1:L:795:ARG:NH1	6:3:74:GLN:O	2.27	0.68
1:D:823:ASN:HD22	1:D:846:PRO:HD3	1.59	0.68
1:K:361:GLN:NE2	1:K:690:LEU:O	2.24	0.68
1:F:304:THR:HG22	1:F:306:LYS:H	1.59	0.68
1:A:113:LYS:NZ	1:A:115:TYR:O	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:ASN:HB2	1:B:60:SER:HA	1.76	0.67
1:C:188:GLU:HB2	1:C:193:LYS:HE3	1.76	0.67
1:G:550:GLY:HA3	1:I:803:GLN:HE22	1.58	0.67
1:K:574:LEU:HG	1:K:929:ARG:HH11	1.58	0.67
1:F:389:ALA:O	1:F:545:ARG:NH1	2.27	0.67
1:C:391:ASP:HB3	1:C:539:ASN:HD21	1.59	0.67
1:D:251:LYS:HA	1:D:256:LYS:HA	1.76	0.67
1:G:170:GLN:O	1:I:839:GLN:NE2	2.28	0.67
1:G:647:SER:HB3	1:G:675:ARG:NH2	2.08	0.67
1:G:894:ALA:HB3	1:H:2:THR:HG21	1.76	0.67
1:B:790:MET:SD	1:B:867:ARG:NH2	2.67	0.67
1:D:587:ASP:OD1	1:D:601:ARG:NH2	2.27	0.67
1:G:405:THR:HG21	1:G:465:ALA:HA	1.77	0.67
1:J:759:ASN:OD1	1:J:759:ASN:N	2.28	0.67
1:L:529:ASP:OD2	1:L:715:HIS:NE2	2.25	0.67
1:L:789:ARG:HH11	6:3:75:ASN:HD21	1.40	0.67
1:H:634:ARG:NH1	1:H:931:HIS:O	2.28	0.67
1:J:813:TYR:O	1:J:814:GLN:NE2	2.28	0.67
1:L:407:ASP:OD2	1:L:462:ASN:ND2	2.25	0.66
1:B:737:LEU:HB2	1:B:763:ASP:OD2	1.94	0.66
1:F:317:GLN:HE22	1:F:835:MET:HB2	1.60	0.66
1:G:201:PRO:HG2	1:G:286:TYR:CD1	2.29	0.66
1:H:405:THR:HG21	1:H:465:ALA:HA	1.75	0.66
1:A:311:ARG:NH1	1:B:211:TYR:OH	2.27	0.66
1:E:587:ASP:OD2	1:E:601:ARG:NH2	2.29	0.66
1:E:683:LYS:HA	1:E:913:THR:HG22	1.77	0.66
1:H:485:LYS:HG2	1:H:508:VAL:HB	1.76	0.66
1:B:403:HIS:HD1	1:C:325:TYR:HH	1.41	0.66
1:C:89:ASP:OD1	1:C:932:ARG:NH1	2.28	0.66
1:L:104:GLY:HA2	1:L:610:ASP:HB2	1.77	0.66
1:L:362:ASP:HB2	1:L:941:ARG:HH12	1.60	0.66
6:2:6:PHE:HB3	6:2:9:LEU:HD13	1.78	0.66
1:C:572:LEU:HB3	1:C:640:GLN:HE22	1.60	0.66
1:C:304:THR:HG22	1:C:306:LYS:H	1.61	0.66
1:A:643:ASN:HB3	1:A:924:VAL:HG12	1.78	0.66
1:E:419:VAL:HG21	1:E:452:ARG:HB2	1.77	0.66
1:L:921:VAL:HG12	1:L:943:PRO:HB2	1.78	0.66
4:S:7:ASP:OD1	4:S:7:ASP:N	2.25	0.66
1:B:721:ALA:HB3	1:B:903:THR:HB	1.77	0.66
1:I:754:ASN:OD1	1:I:754:ASN:N	2.28	0.66
1:E:372:LEU:HD12	1:E:645:TYR:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:429:LYS:N	1:H:439:GLU:O	2.29	0.66
1:H:686:GLU:HG2	1:H:700:TYR:CZ	2.30	0.65
1:D:170:GLN:O	1:F:839:GLN:NE2	2.29	0.65
1:K:446:SER:O	1:K:449:ASN:ND2	2.29	0.65
1:E:231:PRO:HG3	1:E:318:SER:HB2	1.77	0.65
1:F:89:ASP:OD1	1:F:932:ARG:NH1	2.29	0.65
1:J:120:TYR:HE1	1:L:846:PRO:HB2	1.61	0.65
1:K:950:THR:HA	5:U:1:MET:HB3	1.77	0.65
3:M:72:LYS:NZ	3:M:115:ASP:OD1	2.25	0.65
1:B:686:GLU:HG2	1:B:700:TYR:CE2	2.32	0.65
1:D:379:ARG:HE	1:D:390:VAL:HB	1.61	0.65
1:I:195:ALA:HB1	1:I:200:GLN:HB3	1.79	0.65
1:L:250:VAL:O	1:L:260:GLN:NE2	2.29	0.65
6:3:24:ASP:O	6:3:25:ILE:HG13	1.97	0.65
1:C:788:ASP:O	1:C:795:ARG:NH1	2.29	0.65
1:E:572:LEU:O	1:E:929:ARG:NH1	2.28	0.65
1:I:419:VAL:HG21	1:I:452:ARG:HB2	1.79	0.65
1:J:218:ALA:HB3	1:J:283:VAL:HG22	1.78	0.65
1:J:329:ARG:HE	1:J:593:GLN:HB2	1.61	0.65
1:L:331:ASN:OD1	1:L:379:ARG:NH2	2.29	0.65
2:N:205:ASP:OD1	2:N:205:ASP:N	2.30	0.65
1:D:304:THR:HG22	1:D:306:LYS:H	1.62	0.65
1:F:391:ASP:HB3	1:F:539:ASN:HD21	1.62	0.65
1:J:304:THR:HG22	1:J:306:LYS:H	1.61	0.65
1:L:405:THR:HG21	1:L:465:ALA:HA	1.77	0.65
1:A:646:LEU:HG	1:A:648:ALA:HB2	1.79	0.65
1:D:839:GLN:NE2	1:E:170:GLN:O	2.29	0.65
1:A:237:ALA:HB3	1:A:246:GLN:NE2	2.12	0.65
1:H:429:LYS:HG3	1:H:441:ASP:HB2	1.78	0.65
1:D:759:ASN:N	1:D:759:ASN:OD1	2.28	0.64
1:D:916:TYR:CZ	1:D:918:LEU:HD21	2.32	0.64
1:K:681:ARG:NH2	1:K:909:MET:SD	2.70	0.64
4:P:58:GLU:HA	4:P:61:ALA:CB	2.27	0.64
1:B:823:ASN:OD1	1:B:824:ASN:ND2	2.30	0.64
1:E:66:ARG:NH2	1:E:613:CYS:SG	2.70	0.64
1:A:758:CYS:SG	1:A:759:ASN:N	2.69	0.64
1:B:164:LYS:HE2	1:C:446:SER:HA	1.79	0.64
1:A:411:ASN:ND2	1:B:466:ASN:OD1	2.31	0.64
1:A:803:GLN:HE22	1:B:550:GLY:HA3	1.63	0.64
1:B:18:ASP:N	1:B:18:ASP:OD1	2.31	0.64
1:B:304:THR:HG22	1:B:306:LYS:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:485:LYS:HG2	1:E:508:VAL:HB	1.78	0.64
1:A:440:LYS:HE2	1:A:442:ALA:HB2	1.78	0.64
1:A:754:ASN:OD1	1:A:754:ASN:N	2.28	0.64
1:H:221:ARG:NH1	1:H:288:GLU:OE2	2.31	0.64
1:J:589:ASN:OD1	1:J:601:ARG:NE	2.30	0.64
1:J:940:LEU:HD23	1:K:12:MET:HG3	1.80	0.64
1:I:487:SER:OG	1:I:506:ARG:NH1	2.30	0.64
2:N:254:ARG:C	2:N:256:SER:H	2.01	0.64
3:M:327:GLN:HA	5:U:147:ARG:HH21	1.60	0.64
1:E:378:ASP:OD1	1:E:379:ARG:N	2.32	0.63
1:B:635:ASN:OD1	1:B:635:ASN:N	2.30	0.63
1:J:121:ASN:ND2	1:J:232:CYS:SG	2.68	0.63
1:E:752:GLY:HA2	1:F:103:ARG:HH21	1.62	0.63
1:G:178:ILE:HG12	1:G:183:ILE:HG22	1.81	0.63
1:G:825:SER:OG	1:G:840:ALA:HA	1.97	0.63
1:I:485:LYS:HG2	1:I:508:VAL:HB	1.80	0.63
1:J:137:ALA:HB2	1:J:163:GLN:HG2	1.80	0.63
1:H:196:ASP:H	1:H:200:GLN:HB2	1.63	0.63
1:A:32:ARG:HD2	6:W:22:TRP:HA	1.80	0.63
1:C:35:GLU:OE2	1:C:41:ASN:ND2	2.31	0.63
1:J:839:GLN:NE2	1:K:170:GLN:O	2.32	0.63
1:C:322:ARG:NH1	1:C:478:LEU:O	2.32	0.63
1:D:683:LYS:NZ	1:D:712:TYR:OH	2.31	0.63
1:J:929:ARG:HD2	1:J:935:ILE:HG12	1.80	0.63
1:B:218:ALA:HB3	1:B:283:VAL:HG22	1.81	0.63
1:E:348:ALA:HB2	1:E:355:ASN:HA	1.80	0.63
1:K:121:ASN:ND2	1:K:232:CYS:SG	2.71	0.63
1:K:339:ASN:HD21	1:K:365:THR:H	1.46	0.63
1:A:254:ASN:OD1	1:A:254:ASN:N	2.30	0.63
1:C:482:ASP:OD2	1:C:506:ARG:NH1	2.32	0.63
1:E:639:ASP:N	1:E:639:ASP:OD1	2.32	0.63
1:J:196:ASP:H	1:J:200:GLN:HB2	1.64	0.63
1:F:500:TYR:HB2	1:F:598:ASN:HD22	1.64	0.62
1:F:789:ARG:N	1:F:792:SER:OG	2.31	0.62
1:I:916:TYR:CZ	1:I:918:LEU:HD21	2.33	0.62
1:K:401:GLU:OE2	6:3:68:ARG:NH2	2.32	0.62
1:L:485:LYS:HG2	1:L:508:VAL:HB	1.81	0.62
1:A:634:ARG:NH1	1:A:931:HIS:O	2.31	0.62
1:D:366:GLU:HG3	1:D:707:LEU:HD22	1.81	0.62
1:D:446:SER:O	1:D:449:ASN:ND2	2.32	0.62
1:I:809:LYS:NZ	4:R:55:THR:OG1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:ASP:N	1:C:58:ASP:OD1	2.31	0.62
1:D:739:PRO:HG2	1:L:341:THR:HB	1.80	0.62
1:L:130:ASN:ND2	1:L:230:LYS:O	2.32	0.62
2:N:133:ASN:ND2	2:N:430:VAL:O	2.32	0.62
1:K:407:ASP:O	1:L:126:LYS:NZ	2.32	0.62
1:A:514:ASP:OD1	1:A:515:CYS:N	2.28	0.62
1:C:587:ASP:OD2	1:C:601:ARG:NH2	2.30	0.62
1:H:598:ASN:ND2	1:H:603:ASP:OD2	2.32	0.62
1:I:234:GLY:HA3	1:I:297:THR:HG21	1.80	0.62
1:C:339:ASN:ND2	1:C:359:ASP:OD1	2.30	0.62
1:D:522:ARG:NH2	1:D:798:GLN:OE1	2.32	0.62
1:K:680:THR:HG21	1:K:711:PHE:HB3	1.81	0.62
1:A:589:ASN:OD1	1:A:601:ARG:NE	2.33	0.62
1:C:502:TYR:CZ	1:C:506:ARG:HD2	2.34	0.62
1:D:487:SER:OG	1:D:506:ARG:NH1	2.32	0.62
2:N:211:ASP:OD1	2:N:212:THR:N	2.33	0.62
6:W:30:MET:O	6:W:32:GLY:N	2.32	0.62
1:A:172:PRO:HG3	1:C:839:GLN:HB3	1.80	0.62
1:B:792:SER:O	1:B:796:ASN:ND2	2.32	0.62
1:J:635:ASN:ND2	5:V:171:LEU:O	2.33	0.62
1:L:758:CYS:SG	1:L:759:ASN:N	2.72	0.62
1:E:790:MET:SD	1:E:867:ARG:NH2	2.73	0.62
1:H:18:ASP:OD1	1:H:19:ALA:N	2.33	0.62
1:L:391:ASP:HB3	1:L:539:ASN:HD21	1.63	0.62
1:F:736:LEU:HD22	1:F:763:ASP:HB3	1.81	0.61
1:G:446:SER:O	1:G:449:ASN:ND2	2.32	0.61
1:G:572:LEU:O	1:G:929:ARG:NH2	2.33	0.61
1:J:587:ASP:OD1	1:J:601:ARG:NH1	2.33	0.61
1:K:759:ASN:ND2	1:K:861:LYS:O	2.33	0.61
1:L:401:GLU:HG3	1:L:522:ARG:HG3	1.82	0.61
6:Y:39:SER:HB3	6:Y:41:TRP:O	1.99	0.61
1:A:183:ILE:HG21	1:A:219:ALA:HB2	1.80	0.61
1:E:921:VAL:HB	1:E:943:PRO:HD2	1.83	0.61
1:J:339:ASN:ND2	1:J:363:ARG:O	2.33	0.61
1:L:573:LEU:HD12	1:L:929:ARG:HH12	1.65	0.61
1:D:619:PHE:HD2	1:D:621:MET:HG3	1.65	0.61
1:K:733:ASN:ND2	1:L:58:ASP:O	2.34	0.61
4:Q:33:SER:OG	4:Q:37:ARG:N	2.33	0.61
1:E:339:ASN:HD21	1:E:365:THR:HG23	1.64	0.61
1:F:250:VAL:O	1:F:260:GLN:NE2	2.33	0.61
1:H:647:SER:OG	1:H:675:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:678:ALA:HB3	1:K:918:LEU:HG	1.81	0.61
4:R:28:ASN:ND2	4:R:43:ASN:OD1	2.27	0.61
1:D:822:HIS:O	1:D:822:HIS:ND1	2.34	0.61
1:F:102:ILE:HA	1:F:612:ILE:HG22	1.81	0.61
1:L:630:GLU:OE2	1:L:634:ARG:NH1	2.33	0.61
1:D:470:ASN:O	1:D:471:PHE:C	2.37	0.61
1:E:390:VAL:HG21	1:E:790:MET:HE1	1.82	0.61
1:I:55:VAL:HG12	1:I:56:THR:HG23	1.83	0.61
1:J:17:GLN:HB3	1:J:21:GLU:HB2	1.83	0.61
1:A:796:ASN:ND2	1:A:866:ASP:O	2.30	0.61
1:E:165:THR:N	1:F:444:GLU:O	2.34	0.61
1:I:754:ASN:ND2	4:R:50:GLU:OE1	2.34	0.61
1:D:821:GLN:HG2	1:D:845:PHE:HB2	1.83	0.61
1:F:759:ASN:N	1:F:759:ASN:OD1	2.31	0.61
1:L:598:ASN:ND2	1:L:603:ASP:OD2	2.34	0.61
1:D:411:ASN:HD22	1:D:463:LEU:H	1.48	0.60
1:F:836:ARG:NE	1:F:836:ARG:O	2.32	0.60
1:I:202:GLU:OE1	1:I:204:GLN:NE2	2.32	0.60
1:I:250:VAL:O	1:I:260:GLN:NE2	2.33	0.60
1:J:210:TRP:HB3	1:L:835:MET:HE1	1.83	0.60
1:K:407:ASP:N	1:K:407:ASP:OD1	2.34	0.60
1:J:455:ASN:ND2	1:L:207:GLU:O	2.34	0.60
1:K:227:THR:O	1:K:309:ASN:ND2	2.32	0.60
1:H:940:LEU:HD23	1:I:12:MET:HG3	1.83	0.60
1:K:104:GLY:HA2	1:K:610:ASP:HB2	1.83	0.60
1:A:733:ASN:O	1:A:734:ASP:C	2.37	0.60
1:E:18:ASP:OD1	1:E:19:ALA:N	2.31	0.60
1:F:717:PHE:HB3	1:F:744:ILE:HD13	1.83	0.60
1:K:647:SER:HB2	1:K:675:ARG:NH2	2.16	0.60
4:Q:28:ASN:ND2	4:Q:43:ASN:OD1	2.30	0.60
1:B:39:SER:N	1:C:778:GLN:OE1	2.32	0.60
1:H:456:ASN:O	1:I:836:ARG:NH2	2.33	0.60
1:H:814:GLN:NE2	1:I:240:THR:O	2.34	0.60
1:K:231:PRO:O	1:K:235:SER:OG	2.20	0.60
1:L:419:VAL:HG21	1:L:452:ARG:HB2	1.81	0.60
1:F:201:PRO:HG2	1:F:286:TYR:CE2	2.36	0.60
1:K:183:ILE:HG21	1:K:219:ALA:HB2	1.83	0.60
3:M:153:ASN:HA	3:M:158:GLN:HE22	1.65	0.60
1:A:589:ASN:HD22	1:A:600:LEU:HB2	1.66	0.60
1:B:390:VAL:HG11	1:B:790:MET:HE1	1.84	0.60
1:C:598:ASN:ND2	1:C:603:ASP:OD2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:LYS:NZ	1:E:321:ASN:O	2.29	0.60
1:G:137:ALA:HB2	1:G:163:GLN:HG2	1.83	0.60
1:H:883:ALA:H	1:I:48:THR:HG1	1.49	0.60
1:J:806:ASP:OD1	1:J:809:LYS:N	2.28	0.60
1:E:391:ASP:N	1:E:391:ASP:OD1	2.34	0.60
1:F:225:LYS:O	1:F:309:ASN:ND2	2.35	0.60
1:H:758:CYS:SG	1:H:759:ASN:N	2.75	0.60
1:G:250:VAL:HB	1:G:260:GLN:HE21	1.67	0.60
1:J:400:ILE:HD11	1:J:476:ILE:HG12	1.83	0.60
1:G:538:ARG:HA	1:G:543:ARG:HH21	1.67	0.60
1:G:754:ASN:OD1	1:G:754:ASN:N	2.32	0.60
1:I:73:GLU:OE2	1:J:66:ARG:NH2	2.30	0.60
1:I:866:ASP:N	1:I:866:ASP:OD1	2.35	0.60
1:K:569:LYS:NZ	1:K:570:ASN:OD1	2.34	0.60
2:N:51:GLY:N	2:N:54:SER:OG	2.35	0.60
2:N:295:SER:CB	2:N:377:PRO:HD2	2.32	0.60
2:N:130:ASN:ND2	2:N:130:ASN:O	2.35	0.59
5:V:165:ARG:O	5:V:169:LEU:HB2	2.02	0.59
1:B:403:HIS:ND1	1:C:325:TYR:OH	2.32	0.59
1:C:329:ARG:NH1	1:C:702:GLY:O	2.27	0.59
1:D:68:ILE:HD13	1:D:68:ILE:H	1.65	0.59
1:D:689:SER:OG	4:R:26:ARG:NH1	2.35	0.59
1:J:183:ILE:HG21	1:J:219:ALA:HB2	1.83	0.59
1:J:317:GLN:HE22	1:J:834:THR:HB	1.67	0.59
1:J:755:VAL:HG13	1:J:762:LYS:HG2	1.84	0.59
1:K:518:ASN:HB3	1:K:521:ALA:HB3	1.84	0.59
1:L:251:LYS:HG3	1:L:253:GLN:H	1.68	0.59
1:K:61:GLN:OE1	1:K:91:ARG:NH1	2.35	0.59
1:K:420:ILE:HD12	1:K:421:ASN:H	1.67	0.59
1:L:66:ARG:HE	1:L:68:ILE:HD11	1.67	0.59
1:H:743:GLU:OE1	1:H:746:ARG:NH1	2.35	0.59
1:L:790:MET:SD	1:L:867:ARG:NH2	2.75	0.59
5:V:139:SER:HB3	5:V:164:PRO:CD	2.32	0.59
1:B:921:VAL:HB	1:B:943:PRO:HD2	1.85	0.59
1:I:946:ALA:HA	1:L:728:VAL:HG22	1.84	0.59
1:L:806:ASP:OD1	1:L:808:THR:N	2.35	0.59
3:M:234:LEU:HD22	5:U:198:PHE:HD2	1.66	0.59
4:P:58:GLU:O	4:P:62:SER:N	2.35	0.59
1:E:440:LYS:HE2	1:E:442:ALA:HB2	1.84	0.59
1:G:400:ILE:HD11	1:G:476:ILE:HG12	1.84	0.59
1:H:588:VAL:HG12	1:H:607:ILE:HG22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:803:GLN:HE21	1:I:550:GLY:HA3	1.66	0.59
1:I:684:THR:O	4:Q:26:ARG:NH2	2.36	0.59
6:W:39:SER:HB3	6:X:82:ASP:HB2	1.85	0.59
1:A:79:TYR:HE1	1:A:584:PHE:HB2	1.68	0.59
1:A:718:LYS:HB3	1:A:905:GLU:HG3	1.85	0.59
1:C:553:ARG:NH2	1:C:554:TYR:OH	2.35	0.59
1:G:348:ALA:HB2	1:G:355:ASN:HA	1.84	0.59
1:I:921:VAL:HB	1:I:943:PRO:HD2	1.83	0.59
1:A:535:ASN:ND2	1:A:535:ASN:O	2.34	0.59
1:C:343:ASN:N	1:C:343:ASN:OD1	2.33	0.59
1:H:836:ARG:NH1	1:H:836:ARG:O	2.36	0.59
1:A:493:ILE:HD11	1:A:502:TYR:CD1	2.37	0.59
1:B:403:HIS:HE1	1:C:543:ARG:HB3	1.68	0.59
1:F:207:GLU:OE1	1:F:208:SER:N	2.36	0.59
1:G:529:ASP:OD1	1:G:715:HIS:NE2	2.36	0.59
1:A:538:ARG:HA	1:A:543:ARG:HH11	1.66	0.59
1:B:362:ASP:OD1	1:B:941:ARG:NH2	2.31	0.59
1:B:407:ASP:OD2	1:B:462:ASN:ND2	2.36	0.59
1:D:400:ILE:HD11	1:D:476:ILE:HG12	1.85	0.59
1:H:298:HIS:ND1	1:H:321:ASN:OD1	2.27	0.59
1:C:792:SER:O	1:C:796:ASN:ND2	2.36	0.58
1:J:105:VAL:HG11	4:Q:57:LEU:HA	1.85	0.58
2:N:135:ASN:HD21	2:N:138:MET:HB2	1.67	0.58
3:M:70:HIS:CE1	3:M:99:LEU:HD21	2.38	0.58
1:B:135:ASP:HA	1:B:165:THR:HA	1.85	0.58
1:C:278:ASN:N	1:C:278:ASN:OD1	2.35	0.58
1:F:678:ALA:HB3	1:F:918:LEU:HG	1.84	0.58
1:H:368:SER:HG	1:H:646:LEU:H	1.49	0.58
1:L:112:PHE:HD1	1:L:326:ILE:HB	1.68	0.58
1:C:749:ASP:OD1	1:C:749:ASP:N	2.36	0.58
1:E:313:LEU:O	1:E:316:GLN:NE2	2.36	0.58
1:I:927:VAL:HG22	1:I:937:THR:HG22	1.85	0.58
1:F:178:ILE:HG12	1:F:183:ILE:HG22	1.85	0.58
2:N:122:ASP:OD1	2:N:564:ARG:NH1	2.36	0.58
3:M:47:GLN:HB2	6:W:8:SER:HB3	1.86	0.58
4:Q:20:PRO:HG2	4:Q:25:VAL:HG11	1.85	0.58
4:R:110:LEU:HA	4:R:114:LEU:HD23	1.85	0.58
1:A:639:ASP:OD2	1:A:926:ARG:NH1	2.36	0.58
1:B:355:ASN:ND2	1:B:357:VAL:O	2.35	0.58
1:E:792:SER:O	1:E:796:ASN:ND2	2.36	0.58
1:G:130:ASN:OD1	1:G:130:ASN:N	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:436:ASN:N	1:I:436:ASN:OD1	2.35	0.58
1:J:130:ASN:ND2	1:J:230:LYS:O	2.37	0.58
1:J:487:SER:OG	1:J:506:ARG:NH1	2.37	0.58
1:B:647:SER:HB3	1:B:675:ARG:HH21	1.68	0.58
1:G:518:ASN:HB3	1:G:521:ALA:HB3	1.84	0.58
1:G:841:TYR:CZ	1:H:221:ARG:HB3	2.39	0.58
1:J:170:GLN:O	1:L:839:GLN:NE2	2.36	0.58
1:D:24:SER:OG	1:F:638:ASN:ND2	2.36	0.58
1:J:113:LYS:NZ	1:J:321:ASN:O	2.36	0.58
1:J:231:PRO:O	1:J:235:SER:OG	2.20	0.58
1:J:425:LEU:HD12	1:J:451:ILE:HD12	1.85	0.58
1:D:378:ASP:OD1	1:D:379:ARG:N	2.37	0.58
1:L:475:ASN:OD1	1:L:538:ARG:NE	2.37	0.58
1:C:24:SER:OG	3:M:16:SER:O	2.20	0.58
1:B:231:PRO:HG3	1:B:318:SER:HB2	1.85	0.58
1:B:730:TRP:O	1:B:731:PRO:C	2.38	0.58
1:C:789:ARG:HD3	6:X:76:PHE:HZ	1.68	0.58
1:G:648:ALA:HA	1:G:921:VAL:HG22	1.85	0.58
1:H:268:THR:HG22	1:H:270:GLU:H	1.68	0.58
1:K:53:HIS:ND1	1:K:54:ASP:OD2	2.36	0.58
2:N:146:ARG:HB2	2:N:165:TRP:CD2	2.38	0.58
4:S:33:SER:OG	4:S:37:ARG:N	2.31	0.58
1:G:218:ALA:HB3	1:G:283:VAL:HG22	1.85	0.57
1:L:574:LEU:H	1:L:929:ARG:NH1	2.01	0.57
4:S:111:THR:O	4:S:115:ASN:ND2	2.36	0.57
1:A:137:ALA:HA	1:A:163:GLN:HA	1.84	0.57
1:A:325:TYR:N	1:A:595:SER:OG	2.36	0.57
1:B:485:LYS:HG2	1:B:508:VAL:HB	1.85	0.57
4:R:110:LEU:O	4:R:114:LEU:HB2	2.05	0.57
1:D:391:ASP:HB3	1:D:539:ASN:HD21	1.69	0.57
1:J:910:ASP:OD1	1:J:910:ASP:N	2.35	0.57
5:U:221:ASP:N	5:U:221:ASP:OD1	2.37	0.57
1:A:632:MET:HG3	5:U:170:THR:HG22	1.87	0.57
1:B:889:GLN:HA	1:B:892:LEU:HD23	1.87	0.57
1:D:403:HIS:NE2	1:E:547:MET:SD	2.77	0.57
1:F:797:PHE:O	1:F:798:GLN:NE2	2.37	0.57
1:G:274:GLY:HA3	1:G:279:LEU:HB2	1.86	0.57
1:I:560:GLN:OE1	1:I:560:GLN:N	2.38	0.57
3:M:270:VAL:HA	3:M:273:HIS:CE1	2.40	0.57
1:A:871:ARG:NH2	6:X:30:MET:SD	2.77	0.57
1:C:251:LYS:HG3	1:C:252:GLN:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:LYS:NZ	1:C:570:ASN:OD1	2.35	0.57
1:H:534:PHE:HE2	1:H:867:ARG:HH21	1.53	0.57
1:I:694:TYR:HE2	1:I:696:PRO:HA	1.70	0.57
1:K:910:ASP:OD1	1:K:910:ASP:N	2.30	0.57
1:K:170:GLN:HG3	1:L:452:ARG:HB3	1.86	0.57
6:3:65:GLN:HG2	6:3:68:ARG:HB2	1.86	0.57
1:C:674:PHE:HA	1:C:943:PRO:HG2	1.87	0.57
1:D:639:ASP:OD1	1:D:639:ASP:N	2.36	0.57
1:E:268:THR:HG22	1:E:270:GLU:H	1.69	0.57
1:I:350:GLN:OE1	1:I:577:SER:OG	2.22	0.57
1:D:669:ARG:HB3	1:D:669:ARG:HH11	1.69	0.57
1:E:317:GLN:HE22	1:E:835:MET:H	1.52	0.57
1:E:529:ASP:OD1	1:E:715:HIS:NE2	2.37	0.57
1:E:650:ASN:HB3	1:E:916:TYR:HE1	1.69	0.57
1:I:669:ARG:NH2	1:I:945:SER:H	2.03	0.57
1:J:325:TYR:N	1:J:595:SER:OG	2.36	0.57
1:K:135:ASP:OD1	1:K:165:THR:OG1	2.22	0.57
1:K:675:ARG:HD3	1:K:922:PHE:HE1	1.70	0.57
1:L:274:GLY:HA2	1:L:277:ASP:HB3	1.87	0.57
1:D:229:MET:HE1	1:D:314:MET:HA	1.85	0.57
1:F:252:GLN:O	1:F:256:LYS:HB3	2.05	0.57
1:G:520:GLY:HA3	1:H:114:PRO:HG2	1.87	0.57
1:J:103:ARG:NH1	1:L:750:GLY:O	2.36	0.57
1:J:639:ASP:OD2	1:J:926:ARG:NH2	2.37	0.57
1:L:210:TRP:CZ3	1:L:417:GLY:HA3	2.40	0.57
1:L:446:SER:O	1:L:449:ASN:ND2	2.37	0.57
1:H:553:ARG:NH1	1:H:554:TYR:OH	2.38	0.57
1:H:846:PRO:HB2	1:I:120:TYR:HE1	1.69	0.57
2:N:283:ILE:HD12	2:N:403:TYR:HB3	1.86	0.57
4:P:61:ALA:O	4:P:64:ALA:HB2	2.05	0.57
1:K:940:LEU:HD13	5:U:31:ILE:HG12	1.87	0.56
1:L:334:GLY:N	1:L:366:GLU:OE2	2.35	0.56
1:D:589:ASN:ND2	1:D:599:ASP:OD1	2.38	0.56
1:I:574:LEU:HG	1:I:929:ARG:HH11	1.70	0.56
1:A:79:TYR:CE1	1:A:584:PHE:HB2	2.40	0.56
1:A:330:ASP:OD1	1:A:331:ASN:ND2	2.35	0.56
1:A:589:ASN:HD21	1:A:601:ARG:HG3	1.70	0.56
1:A:686:GLU:OE1	1:A:712:TYR:OH	2.23	0.56
1:C:475:ASN:OD1	1:C:538:ARG:NE	2.38	0.56
1:D:921:VAL:HG12	1:D:943:PRO:HG2	1.86	0.56
1:E:110:PRO:HD3	1:E:553:ARG:HH21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:669:ARG:HH12	1:E:944:PHE:HA	1.70	0.56
1:F:523:TRP:CD1	1:F:802:ARG:HD3	2.41	0.56
1:G:910:ASP:OD1	1:G:910:ASP:N	2.31	0.56
1:I:905:GLU:OE1	4:R:22:TRP:NE1	2.30	0.56
1:J:389:ALA:HB3	1:J:545:ARG:HE	1.69	0.56
2:N:282:ASN:HA	2:N:404:ARG:HG2	1.88	0.56
1:E:183:ILE:HG21	1:E:219:ALA:HB2	1.86	0.56
5:U:59:ALA:HB2	5:U:193:VAL:HG21	1.87	0.56
1:G:24:SER:HB3	1:I:638:ASN:HD21	1.69	0.56
1:G:675:ARG:NH2	1:G:920:GLU:OE1	2.39	0.56
1:H:792:SER:O	1:H:796:ASN:ND2	2.38	0.56
1:K:82:ARG:NH1	1:K:581:GLU:OE2	2.39	0.56
4:P:20:PRO:HB2	4:P:25:VAL:HG21	1.86	0.56
1:B:422:THR:HG22	1:B:452:ARG:HB2	1.88	0.56
1:D:735:ARG:HB3	1:E:63:LEU:HG	1.88	0.56
1:J:547:MET:SD	1:L:403:HIS:NE2	2.79	0.56
1:K:403:HIS:HE1	1:L:543:ARG:HB3	1.70	0.56
4:Q:67:ALA:O	4:Q:71:THR:OG1	2.21	0.56
5:V:164:PRO:O	5:V:168:ILE:HB	2.06	0.56
1:C:363:ARG:NE	1:C:923:ASP:OD2	2.39	0.56
1:D:946:ALA:HA	1:I:728:VAL:HG12	1.87	0.56
1:H:327:ALA:HB2	1:H:546:SER:HA	1.86	0.56
1:I:526:ASP:OD1	1:I:526:ASP:N	2.38	0.56
1:I:639:ASP:OD1	1:I:639:ASP:N	2.38	0.56
1:J:35:GLU:OE2	1:J:41:ASN:ND2	2.39	0.56
1:K:456:ASN:O	1:L:836:ARG:NH2	2.37	0.56
5:V:80:TYR:HE1	5:V:195:SER:HB2	1.70	0.56
1:D:294:THR:HB	1:D:297:THR:HG23	1.86	0.56
1:E:364:ASN:HB2	1:E:650:ASN:ND2	2.21	0.56
1:E:387:ASN:HB3	1:E:545:ARG:HD2	1.86	0.56
1:I:573:LEU:HA	1:I:929:ARG:NH2	2.20	0.56
1:I:936:GLU:HB3	5:V:157:ALA:HA	1.87	0.56
1:K:735:ARG:NH2	1:L:57:THR:O	2.36	0.56
1:B:948:ASN:OD1	1:B:948:ASN:N	2.39	0.56
1:G:406:GLU:OE1	1:H:475:ASN:ND2	2.39	0.56
1:J:126:LYS:NZ	1:L:407:ASP:O	2.29	0.56
1:K:346:VAL:HA	1:K:355:ASN:HD21	1.70	0.56
1:A:730:TRP:O	1:A:731:PRO:C	2.33	0.56
1:E:176:ILE:O	1:E:217:HIS:ND1	2.32	0.56
1:H:807:ASP:N	1:H:807:ASP:OD1	2.37	0.56
1:I:19:ALA:HA	1:I:22:TYR:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:113:LYS:NZ	1:I:321:ASN:O	2.34	0.56
1:I:356:ALA:HA	5:V:156:GLY:H	1.71	0.56
1:L:421:ASN:OD1	1:L:421:ASN:N	2.38	0.56
1:A:405:THR:HG21	1:A:465:ALA:HA	1.88	0.55
1:A:813:TYR:O	1:A:814:GLN:NE2	2.39	0.55
1:A:883:ALA:H	1:B:48:THR:HG1	1.54	0.55
1:B:732:GLY:O	1:B:734:ASP:N	2.38	0.55
1:C:645:TYR:CZ	6:W:30:MET:HA	2.41	0.55
1:E:209:GLN:OE1	1:E:209:GLN:N	2.39	0.55
5:U:148:PRO:HD3	5:U:154:ILE:HD12	1.88	0.55
1:A:133:GLU:HG2	1:A:167:VAL:HG13	1.89	0.55
1:A:532:ASN:ND2	1:A:535:ASN:OD1	2.39	0.55
1:A:856:ASP:N	1:A:856:ASP:OD1	2.38	0.55
1:F:790:MET:SD	1:F:867:ARG:NH2	2.79	0.55
1:G:394:ASP:OD2	1:G:397:VAL:N	2.37	0.55
1:H:714:ASN:ND2	1:H:868:THR:O	2.39	0.55
1:I:379:ARG:HE	1:I:390:VAL:HB	1.72	0.55
1:I:523:TRP:CD1	1:I:802:ARG:HD3	2.41	0.55
1:K:35:GLU:OE2	1:K:41:ASN:ND2	2.39	0.55
6:X:80:VAL:C	6:X:82:ASP:H	2.10	0.55
1:C:137:ALA:HA	1:C:163:GLN:HB3	1.88	0.55
1:C:532:ASN:OD1	1:C:535:ASN:N	2.37	0.55
1:C:772:ASN:HA	6:W:35:PHE:CE2	2.41	0.55
1:D:408:GLU:OE1	1:D:408:GLU:N	2.37	0.55
1:F:251:LYS:HG2	1:F:258:GLU:HB3	1.88	0.55
1:F:339:ASN:ND2	1:F:359:ASP:OD1	2.36	0.55
1:H:455:ASN:HD22	1:I:837:GLU:HA	1.71	0.55
1:I:354:LEU:HD23	1:J:91:ARG:HH21	1.69	0.55
5:V:3:LYS:HB3	5:V:200:PRO:HD2	1.88	0.55
1:A:407:ASP:OD2	1:A:462:ASN:ND2	2.33	0.55
1:B:337:TYR:CZ	1:B:585:ARG:HG3	2.42	0.55
1:C:18:ASP:OD1	1:C:18:ASP:N	2.31	0.55
1:D:574:LEU:H	1:D:929:ARG:NH1	2.00	0.55
1:F:587:ASP:OD2	1:F:601:ARG:NH2	2.40	0.55
5:U:179:ARG:HH22	5:U:182:GLY:N	2.04	0.55
1:A:545:ARG:NH2	1:A:593:GLN:OE1	2.39	0.55
1:B:134:TRP:HB2	1:B:309:ASN:HB3	1.89	0.55
1:F:644:ASP:O	1:F:647:SER:OG	2.20	0.55
1:J:350:GLN:O	1:J:351:ALA:C	2.44	0.55
1:J:391:ASP:OD1	1:J:545:ARG:NH2	2.38	0.55
1:J:635:ASN:OD1	1:J:636:ASP:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:733:ASN:HB3	1:L:60:SER:HA	1.87	0.55
1:B:408:GLU:OE1	1:B:408:GLU:N	2.35	0.55
1:C:261:VAL:HG13	1:C:287:SER:O	2.06	0.55
1:C:893:TYR:OH	1:E:948:ASN:ND2	2.39	0.55
1:E:598:ASN:ND2	1:E:603:ASP:OD2	2.39	0.55
1:H:372:LEU:HD12	1:H:645:TYR:HB2	1.88	0.55
1:J:924:VAL:HG11	1:K:12:MET:HB3	1.88	0.55
1:K:207:GLU:O	1:L:455:ASN:ND2	2.39	0.55
1:D:425:LEU:HD12	1:D:451:ILE:HD12	1.88	0.55
1:D:529:ASP:OD2	1:D:715:HIS:NE2	2.40	0.55
1:D:820:HIS:HA	1:E:204:GLN:HE22	1.72	0.55
1:E:573:LEU:HA	1:E:929:ARG:HH22	1.72	0.55
1:I:758:CYS:SG	1:I:759:ASN:N	2.79	0.55
1:K:210:TRP:CZ3	1:K:417:GLY:HA3	2.41	0.55
1:K:587:ASP:OD2	1:K:601:ARG:NH2	2.40	0.55
1:B:803:GLN:OE1	1:C:552:GLY:N	2.39	0.55
1:C:334:GLY:N	1:C:366:GLU:OE2	2.35	0.55
1:C:813:TYR:O	1:C:814:GLN:NE2	2.37	0.55
1:C:929:ARG:HG2	1:C:935:ILE:HG12	1.87	0.55
1:D:814:GLN:NE2	1:E:240:THR:O	2.39	0.55
1:E:102:ILE:HD13	1:E:609:PHE:HE2	1.72	0.55
1:E:805:VAL:HG13	1:E:855:VAL:HG21	1.89	0.55
1:F:740:ASN:HB3	1:F:741:GLU:HG3	1.89	0.55
1:J:444:GLU:HA	1:L:164:LYS:HG2	1.89	0.55
1:L:675:ARG:HH22	6:4:30:MET:HB3	1.72	0.55
1:A:207:GLU:HB2	1:B:455:ASN:HD21	1.71	0.55
1:D:764:TRP:HZ2	1:D:870:TRP:HB3	1.72	0.55
1:E:42:ASN:OD1	1:E:42:ASN:N	2.36	0.55
1:E:929:ARG:HH21	1:E:935:ILE:HD11	1.72	0.55
1:H:682:LEU:HD22	1:H:705:PRO:HB2	1.87	0.55
2:N:207:GLY:HA2	2:N:243:LEU:HB2	1.89	0.55
3:M:14:LEU:HD21	3:M:74:LEU:HB3	1.88	0.55
1:C:680:THR:OG1	1:C:681:ARG:N	2.40	0.55
1:E:514:ASP:OD1	1:E:515:CYS:N	2.32	0.55
1:G:733:ASN:HB3	1:H:60:SER:HA	1.89	0.55
1:G:812:ASP:OD2	1:H:238:LYS:NZ	2.37	0.55
1:G:927:VAL:HG22	1:G:937:THR:HG22	1.89	0.55
1:J:452:ARG:HB3	1:L:170:GLN:HB3	1.90	0.55
1:A:733:ASN:OD1	1:A:733:ASN:N	2.39	0.54
1:D:416:LEU:HD21	1:E:412:TYR:HE1	1.72	0.54
1:E:174:SER:OG	1:E:207:GLU:OE2	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:496:ASN:OD1	1:F:499:THR:N	2.41	0.54
1:G:130:ASN:HD22	1:I:842:PRO:HD3	1.73	0.54
1:L:646:LEU:O	1:L:647:SER:C	2.45	0.54
2:N:536:GLY:H	2:N:539:GLN:HE21	1.55	0.54
1:F:195:ALA:HB1	1:F:200:GLN:HB3	1.89	0.54
1:F:274:GLY:HA3	1:F:279:LEU:HD21	1.89	0.54
1:G:758:CYS:HB3	1:G:799:PRO:HB3	1.90	0.54
1:I:845:PHE:O	1:I:846:PRO:C	2.38	0.54
1:J:227:THR:OG1	1:J:289:ASP:OD1	2.25	0.54
1:J:394:ASP:OD1	1:J:397:VAL:N	2.36	0.54
1:K:500:TYR:HB2	1:K:598:ASN:HD22	1.71	0.54
1:K:764:TRP:HZ2	1:K:870:TRP:HB3	1.72	0.54
1:L:386:TRP:HB2	1:L:388:GLN:HG3	1.89	0.54
1:B:88:GLY:HA3	1:B:91:ARG:NH1	2.22	0.54
1:B:391:ASP:HB3	1:B:539:ASN:HD21	1.73	0.54
1:D:866:ASP:N	1:D:866:ASP:OD1	2.39	0.54
1:I:556:PRO:HG3	4:S:54:GLY:HA3	1.89	0.54
1:I:573:LEU:HA	1:I:929:ARG:HH22	1.71	0.54
2:N:468:LEU:HD12	2:N:469:PRO:HD2	1.89	0.54
1:B:74:ASP:OD1	1:B:586:LYS:NZ	2.39	0.54
1:B:469:ARG:NH2	1:B:828:VAL:HG21	2.22	0.54
1:G:650:ASN:HB3	1:G:916:TYR:HE1	1.71	0.54
1:H:61:GLN:OE1	1:H:91:ARG:NH1	2.41	0.54
1:A:598:ASN:ND2	1:A:603:ASP:OD2	2.41	0.54
1:A:806:ASP:OD1	1:A:809:LYS:N	2.32	0.54
1:B:14:ILE:HG22	1:B:15:SER:H	1.72	0.54
1:C:111:THR:O	1:C:324:ASN:ND2	2.39	0.54
1:D:689:SER:HG	4:R:26:ARG:NH1	2.05	0.54
1:E:573:LEU:HA	1:E:929:ARG:NH2	2.23	0.54
1:H:718:LYS:HB2	1:H:905:GLU:HB3	1.89	0.54
1:I:218:ALA:HB3	1:I:283:VAL:HG22	1.90	0.54
1:A:391:ASP:HB3	1:A:539:ASN:HD21	1.72	0.54
1:A:919:PHE:O	1:A:921:VAL:HG13	2.07	0.54
1:B:942:THR:HG21	1:C:9:TRP:HH2	1.72	0.54
1:C:330:ASP:OD2	1:C:370:GLN:NE2	2.36	0.54
1:D:444:GLU:HB3	1:F:164:LYS:HA	1.89	0.54
1:G:196:ASP:H	1:G:200:GLN:HB2	1.72	0.54
1:H:636:ASP:HA	1:H:928:HIS:HE1	1.72	0.54
1:J:789:ARG:NH2	6:3:35:PHE:O	2.40	0.54
1:A:893:TYR:OH	5:U:226:TYR:HA	2.08	0.54
1:E:425:LEU:HD12	1:E:451:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:500:TYR:HB2	1:G:598:ASN:HD22	1.72	0.54
1:I:650:ASN:HB3	1:I:916:TYR:HE1	1.73	0.54
1:K:178:ILE:HG22	1:K:183:ILE:HG22	1.89	0.54
1:K:391:ASP:HB3	1:K:539:ASN:HD21	1.72	0.54
1:K:500:TYR:HB2	1:K:598:ASN:ND2	2.23	0.54
2:N:115:ASP:N	2:N:115:ASP:OD1	2.37	0.54
2:N:254:ARG:C	2:N:256:SER:N	2.60	0.54
1:C:639:ASP:N	1:C:639:ASP:OD1	2.40	0.54
1:D:635:ASN:OD1	1:D:636:ASP:N	2.41	0.54
1:E:201:PRO:HG2	1:E:286:TYR:CG	2.42	0.54
1:E:346:VAL:HG13	1:E:355:ASN:HB3	1.90	0.54
1:E:795:ARG:NH2	6:Y:41:TRP:HA	2.17	0.54
1:J:231:PRO:HG2	1:J:318:SER:HB2	1.88	0.54
1:K:167:VAL:N	1:L:449:ASN:OD1	2.40	0.54
2:N:83:ASN:HB2	2:N:86:ASN:HB2	1.89	0.54
1:B:680:THR:HG22	1:B:681:ARG:H	1.72	0.54
1:F:830:TYR:N	1:F:837:GLU:OE2	2.35	0.54
1:H:113:LYS:NZ	1:H:321:ASN:O	2.30	0.54
1:J:201:PRO:HG2	1:J:286:TYR:CD1	2.42	0.54
1:L:391:ASP:OD1	1:L:545:ARG:NH1	2.41	0.54
5:V:126:LEU:N	5:V:137:ASP:OD1	2.41	0.54
1:C:929:ARG:HB2	1:C:929:ARG:HH11	1.73	0.53
1:I:469:ARG:HH12	1:I:828:VAL:HG11	1.72	0.53
3:M:143:LEU:HD22	3:M:172:VAL:HG21	1.89	0.53
1:A:362:ASP:OD2	1:A:948:ASN:ND2	2.41	0.53
1:A:673:ALA:HB2	1:B:9:TRP:CZ2	2.43	0.53
1:D:615:TYR:CZ	1:F:762:LYS:HE3	2.43	0.53
1:G:485:LYS:HG2	1:G:508:VAL:HB	1.91	0.53
1:G:523:TRP:CD1	1:G:802:ARG:HD3	2.43	0.53
1:K:340:SER:OG	1:K:343:ASN:O	2.25	0.53
1:K:529:ASP:OD1	1:K:862:LYS:NZ	2.40	0.53
1:L:825:SER:O	1:L:827:PHE:CD2	2.61	0.53
2:N:218:GLY:HA3	2:N:226:VAL:HG13	1.90	0.53
5:V:7:THR:OG1	5:V:25:GLN:OE1	2.24	0.53
1:B:565:PHE:HD1	1:B:567:ALA:H	1.57	0.53
1:E:429:LYS:O	1:E:439:GLU:N	2.34	0.53
1:I:651:MET:SD	4:Q:18:ARG:NH1	2.81	0.53
1:I:916:TYR:CE2	1:I:918:LEU:HD21	2.44	0.53
1:J:669:ARG:N	1:J:898:HIS:O	2.37	0.53
1:K:895:ASN:HB3	5:U:194:PRO:HD3	1.89	0.53
1:L:231:PRO:O	1:L:235:SER:OG	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:341:THR:OG1	1:E:361:GLN:NE2	2.32	0.53
1:E:429:LYS:N	1:E:439:GLU:O	2.29	0.53
1:G:252:GLN:CD	1:G:258:GLU:HG2	2.29	0.53
1:H:487:SER:OG	1:H:506:ARG:NH1	2.38	0.53
1:I:737:LEU:N	1:I:763:ASP:OD2	2.29	0.53
1:J:812:ASP:OD2	1:K:238:LYS:NZ	2.34	0.53
2:N:193:LEU:O	2:N:197:ARG:NH1	2.42	0.53
1:C:277:ASP:OD1	1:C:278:ASN:N	2.42	0.53
1:F:485:LYS:HG2	1:F:508:VAL:HB	1.91	0.53
1:I:734:ASP:HA	1:I:739:PRO:HB3	1.91	0.53
1:L:125:PRO:HG2	1:L:128:ALA:HB2	1.89	0.53
5:V:36:ALA:HB1	5:V:40:MET:HB3	1.89	0.53
1:B:371:LEU:O	1:B:372:LEU:C	2.45	0.53
1:D:669:ARG:HB3	1:D:669:ARG:NH1	2.24	0.53
1:D:730:TRP:O	1:D:731:PRO:C	2.39	0.53
1:G:413:CYS:HA	1:H:461:ILE:HB	1.90	0.53
1:G:922:PHE:O	1:G:941:ARG:HA	2.08	0.53
1:A:218:ALA:HB3	1:A:283:VAL:HG22	1.90	0.53
1:A:237:ALA:HB3	1:A:246:GLN:CD	2.29	0.53
1:B:744:ILE:HG12	1:B:764:TRP:CD2	2.44	0.53
1:C:130:ASN:N	1:C:130:ASN:OD1	2.41	0.53
1:E:452:ARG:NH2	1:E:455:ASN:O	2.40	0.53
1:F:446:SER:O	1:F:449:ASN:ND2	2.42	0.53
1:K:312:GLU:OE2	1:L:209:GLN:NE2	2.42	0.53
1:A:493:ILE:HD11	1:A:502:TYR:HD1	1.74	0.53
1:D:598:ASN:ND2	1:D:603:ASP:OD2	2.42	0.53
1:J:572:LEU:O	1:J:929:ARG:NH2	2.41	0.53
1:L:235:SER:HB3	1:L:292:ILE:HD11	1.90	0.53
1:B:29:GLN:NE2	6:X:5:ASN:OD1	2.42	0.53
1:F:482:ASP:OD2	1:F:506:ARG:NH2	2.42	0.53
1:G:724:PHE:CE1	1:G:900:LEU:HD13	2.44	0.53
1:H:829:GLY:HA2	1:H:837:GLU:HG2	1.91	0.53
1:I:598:ASN:ND2	1:I:603:ASP:OD2	2.41	0.53
4:Q:28:ASN:N	4:Q:28:ASN:OD1	2.42	0.53
1:A:170:GLN:O	1:C:839:GLN:NE2	2.42	0.53
1:A:675:ARG:NH1	1:A:920:GLU:OE1	2.40	0.53
1:A:789:ARG:NH2	6:X:35:PHE:O	2.37	0.53
1:G:304:THR:HG22	1:G:306:LYS:H	1.72	0.53
1:H:225:LYS:O	1:H:309:ASN:ND2	2.42	0.53
1:H:522:ARG:NH2	1:H:798:GLN:OE1	2.42	0.53
1:I:500:TYR:HB2	1:I:598:ASN:HD22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:195:ALA:HB1	1:L:200:GLN:HB3	1.91	0.53
4:P:43:ASN:ND2	4:P:43:ASN:O	2.41	0.53
1:C:588:VAL:HG12	1:C:592:LEU:HD12	1.90	0.52
1:C:836:ARG:NE	1:C:836:ARG:O	2.40	0.52
1:D:598:ASN:O	1:D:701:SER:OG	2.27	0.52
1:F:531:VAL:O	1:F:532:ASN:C	2.48	0.52
6:W:28:SER:HB3	6:X:84:LEU:HD22	1.91	0.52
1:D:871:ARG:HH12	6:0:30:MET:HG2	1.74	0.52
1:I:441:ASP:N	1:I:441:ASP:OD1	2.43	0.52
1:J:518:ASN:HB3	1:J:521:ALA:HB3	1.91	0.52
1:J:737:LEU:HD13	1:J:753:TYR:CD1	2.44	0.52
1:K:724:PHE:HE1	1:K:900:LEU:HD13	1.74	0.52
5:V:126:LEU:N	5:V:137:ASP:H	2.07	0.52
1:B:396:ASP:OD1	6:X:65:GLN:HB2	2.08	0.52
1:D:410:PRO:HB2	1:D:412:TYR:CE1	2.44	0.52
1:E:279:LEU:HB3	1:F:438:TRP:HB2	1.92	0.52
1:I:410:PRO:HB2	1:I:412:TYR:CE2	2.45	0.52
1:I:587:ASP:OD2	1:I:601:ARG:NH1	2.42	0.52
2:N:386:SER:C	2:N:388:LYS:H	2.12	0.52
2:N:547:ARG:HD3	2:N:549:ARG:HD3	1.90	0.52
1:A:329:ARG:HG2	1:A:593:GLN:HB2	1.92	0.52
1:A:639:ASP:OD1	1:A:639:ASP:N	2.42	0.52
1:B:253:GLN:HG3	1:B:254:ASN:H	1.74	0.52
1:B:325:TYR:HE2	1:B:543:ARG:HG2	1.73	0.52
1:D:115:TYR:HE2	1:F:850:ILE:HD13	1.73	0.52
1:F:636:ASP:OD1	1:F:636:ASP:N	2.42	0.52
1:F:714:ASN:HB3	1:F:870:TRP:NE1	2.24	0.52
1:G:103:ARG:NH2	1:I:751:GLU:O	2.41	0.52
1:G:565:PHE:HD1	1:G:567:ALA:H	1.55	0.52
1:L:355:ASN:ND2	1:L:357:VAL:O	2.42	0.52
4:P:33:SER:O	4:P:36:GLY:N	2.43	0.52
4:S:50:GLU:HG2	4:S:52:VAL:HG23	1.90	0.52
1:C:789:ARG:HD3	6:X:76:PHE:CZ	2.44	0.52
1:D:759:ASN:ND2	1:D:861:LYS:O	2.36	0.52
1:F:513:VAL:HG13	1:F:517:ILE:HG21	1.91	0.52
1:J:422:THR:OG1	1:J:450:GLU:OE1	2.21	0.52
1:L:301:TYR:CZ	1:L:303:PRO:HG3	2.45	0.52
1:L:897:ALA:O	1:L:898:HIS:ND1	2.42	0.52
3:M:104:ARG:HG3	3:M:105:TYR:HD1	1.74	0.52
1:A:730:TRP:O	1:A:730:TRP:CG	2.62	0.52
1:G:744:ILE:HG12	1:G:764:TRP:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:176:ILE:O	1:L:217:HIS:ND1	2.43	0.52
1:A:178:ILE:HG12	1:A:183:ILE:HG22	1.92	0.52
1:B:725:ASP:N	1:B:725:ASP:OD1	2.42	0.52
1:B:886:ASP:OD1	1:B:886:ASP:N	2.43	0.52
1:D:211:TYR:HE1	1:F:311:ARG:HH21	1.55	0.52
1:F:526:ASP:C	1:F:528:MET:N	2.60	0.52
1:G:113:LYS:HE2	1:G:296:ASP:HB2	1.92	0.52
1:G:825:SER:O	1:G:827:PHE:CD2	2.62	0.52
2:N:76:SER:O	2:N:77:THR:C	2.44	0.52
4:Q:125:ARG:HG3	4:Q:126:GLN:N	2.23	0.52
1:A:355:ASN:OD1	1:A:357:VAL:N	2.37	0.52
1:G:734:ASP:N	1:G:734:ASP:OD1	2.43	0.52
1:K:686:GLU:HG3	1:K:700:TYR:CE2	2.44	0.52
1:K:744:ILE:HG12	1:K:764:TRP:CD2	2.44	0.52
1:L:121:ASN:ND2	1:L:232:CYS:SG	2.79	0.52
1:L:359:ASP:OD1	1:L:360:LEU:N	2.42	0.52
3:M:243:THR:O	3:M:262:ARG:NH2	2.40	0.52
1:D:655:ILE:HD11	1:D:915:LEU:HB2	1.92	0.52
1:D:789:ARG:N	1:D:792:SER:OG	2.43	0.52
1:G:363:ARG:NE	1:G:923:ASP:OD2	2.40	0.52
1:G:724:PHE:HE1	1:G:900:LEU:HD13	1.75	0.52
1:H:921:VAL:HG12	1:H:943:PRO:HG2	1.92	0.52
1:K:19:ALA:HA	1:K:22:TYR:CE2	2.45	0.52
1:L:669:ARG:N	1:L:898:HIS:O	2.40	0.52
2:N:238:PRO:HB2	2:N:259:LEU:O	2.10	0.52
1:A:675:ARG:HH22	6:X:30:MET:HB3	1.75	0.52
1:B:545:ARG:NH2	1:B:593:GLN:OE1	2.42	0.52
1:D:928:HIS:NE2	1:D:930:PRO:HG3	2.25	0.52
1:E:229:MET:HG3	1:E:309:ASN:ND2	2.24	0.52
1:H:199:PHE:HA	1:H:221:ARG:NH2	2.25	0.52
1:H:409:LEU:HD11	1:I:473:TYR:HB3	1.92	0.52
1:J:327:ALA:HB2	1:J:546:SER:HA	1.92	0.52
5:U:11:TRP:HA	5:U:23:ALA:HB2	1.92	0.52
1:A:66:ARG:NH2	1:E:73:GLU:OE1	2.41	0.51
1:D:18:ASP:OD1	1:D:18:ASP:N	2.43	0.51
1:F:58:ASP:N	1:F:58:ASP:OD1	2.43	0.51
1:J:298:HIS:ND1	1:J:321:ASN:OD1	2.29	0.51
1:J:648:ALA:HA	1:J:921:VAL:HG22	1.92	0.51
1:K:921:VAL:HB	1:K:943:PRO:HD2	1.91	0.51
1:L:133:GLU:HG2	1:L:167:VAL:HG13	1.91	0.51
1:L:241:ASN:OD1	1:L:241:ASN:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:298:HIS:ND1	1:L:321:ASN:OD1	2.34	0.51
1:L:829:GLY:HA2	1:L:837:GLU:HG2	1.92	0.51
2:N:99:ASN:H	2:N:99:ASN:HD22	1.57	0.51
3:M:106:ASN:OD1	3:M:107:SER:N	2.43	0.51
6:X:40:LEU:H	6:X:40:LEU:HD23	1.74	0.51
1:B:406:GLU:OE2	1:C:538:ARG:NH2	2.43	0.51
1:C:131:PRO:HB3	1:C:169:GLY:HA2	1.93	0.51
1:D:699:THR:O	1:D:699:THR:OG1	2.23	0.51
1:E:201:PRO:HG2	1:E:286:TYR:CD1	2.45	0.51
1:E:734:ASP:HA	1:E:739:PRO:HB3	1.92	0.51
1:K:95:MET:HE1	1:K:580:TYR:HE2	1.76	0.51
1:A:120:TYR:HE1	1:C:846:PRO:HB2	1.75	0.51
1:D:689:SER:HG	4:R:26:ARG:HH11	1.57	0.51
1:H:806:ASP:HB2	1:H:858:ILE:HG23	1.93	0.51
1:I:341:THR:HB	1:L:739:PRO:HG2	1.93	0.51
1:J:246:GLN:HE21	1:L:822:HIS:CE1	2.28	0.51
1:K:298:HIS:ND1	1:K:321:ASN:OD1	2.32	0.51
1:L:234:GLY:HA3	1:L:297:THR:HG21	1.91	0.51
2:N:128:HIS:HD2	2:N:521:PRO:HB3	1.76	0.51
4:P:61:ALA:O	4:P:62:SER:C	2.47	0.51
5:U:215:ASN:N	5:U:215:ASN:OD1	2.44	0.51
1:B:400:ILE:HG12	1:B:524:SER:HA	1.93	0.51
1:B:856:ASP:OD1	1:B:856:ASP:N	2.42	0.51
1:C:355:ASN:ND2	1:C:357:VAL:O	2.43	0.51
1:D:108:ARG:HH12	1:D:549:LEU:HB3	1.75	0.51
1:D:241:ASN:HD21	1:D:245:GLY:HA3	1.75	0.51
1:E:475:ASN:OD1	1:E:538:ARG:NE	2.44	0.51
1:G:113:LYS:NZ	1:G:117:GLY:O	2.40	0.51
1:K:230:LYS:HB2	1:K:292:ILE:HD11	1.93	0.51
1:K:332:PHE:HB3	1:K:335:LEU:HD12	1.92	0.51
1:K:574:LEU:HG	1:K:929:ARG:NH1	2.25	0.51
2:N:171:PRO:HD2	2:N:183:LEU:HD21	1.91	0.51
4:P:40:LEU:HD12	4:P:46:THR:HG21	1.93	0.51
1:D:572:LEU:O	1:D:929:ARG:NH2	2.44	0.51
1:F:52:THR:OG1	1:F:53:HIS:N	2.43	0.51
1:F:196:ASP:O	1:F:197:LYS:C	2.49	0.51
1:F:829:GLY:HA2	1:F:837:GLU:HG2	1.91	0.51
1:G:48:THR:HB	1:I:883:ALA:H	1.75	0.51
1:G:574:LEU:H	1:G:929:ARG:NH1	2.09	0.51
1:I:339:ASN:OD1	1:I:365:THR:N	2.33	0.51
1:I:697:TYR:O	4:Q:26:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:825:SER:O	1:L:827:PHE:N	2.44	0.51
2:N:72:VAL:HG23	2:N:558:LEU:HD13	1.93	0.51
1:B:212:GLU:OE1	1:B:212:GLU:N	2.41	0.51
1:B:704:ILE:N	1:B:708:ASP:OD2	2.43	0.51
1:D:441:ASP:OD1	1:D:443:THR:OG1	2.21	0.51
1:J:768:GLN:O	1:J:772:ASN:ND2	2.35	0.51
1:D:499:THR:HG22	1:D:501:ASP:H	1.76	0.51
1:E:942:THR:HB	1:E:943:PRO:HD3	1.92	0.51
1:F:754:ASN:OD1	1:F:754:ASN:N	2.38	0.51
1:H:337:TYR:CZ	1:H:585:ARG:HG2	2.46	0.51
1:H:650:ASN:HB3	1:H:916:TYR:HE1	1.74	0.51
1:I:574:LEU:HD13	1:I:630:GLU:HG3	1.93	0.51
1:J:378:ASP:OD1	1:J:380:THR:N	2.43	0.51
1:K:355:ASN:OD1	1:K:356:ALA:N	2.43	0.51
1:L:582:TRP:HB3	1:L:584:PHE:HE1	1.75	0.51
5:V:169:LEU:O	5:V:173:THR:OG1	2.29	0.51
1:A:304:THR:HG22	1:A:306:LYS:H	1.75	0.51
1:D:224:LYS:HG2	1:D:287:SER:HB2	1.93	0.51
1:D:824:ASN:ND2	1:D:824:ASN:O	2.43	0.51
1:G:950:THR:O	1:G:951:THR:OG1	2.27	0.51
1:H:650:ASN:OD1	1:H:916:TYR:OH	2.20	0.51
1:I:298:HIS:ND1	1:I:321:ASN:OD1	2.35	0.51
1:I:563:GLN:OE1	1:I:564:LYS:N	2.44	0.51
1:I:919:PHE:O	1:I:921:VAL:HG13	2.10	0.51
1:K:330:ASP:OD1	1:K:379:ARG:NH2	2.44	0.51
1:C:330:ASP:OD1	1:C:331:ASN:ND2	2.43	0.51
1:F:715:HIS:CD2	1:F:716:THR:HG23	2.46	0.51
1:H:871:ARG:HH11	6:1:31:SER:HB3	1.75	0.51
1:K:452:ARG:NE	1:K:455:ASN:O	2.39	0.51
1:L:19:ALA:N	1:L:46:ASN:OD1	2.43	0.51
1:L:746:ARG:HB3	1:L:749:ASP:HB2	1.93	0.51
1:L:942:THR:HB	1:L:943:PRO:HD3	1.92	0.51
5:V:215:ASN:OD1	5:V:215:ASN:N	2.43	0.51
1:B:2:THR:HG22	1:B:4:SER:H	1.75	0.51
1:C:789:ARG:N	1:C:792:SER:OG	2.44	0.51
1:E:795:ARG:HH22	6:Y:41:TRP:C	2.13	0.51
1:G:18:ASP:OD1	1:G:18:ASP:N	2.41	0.51
1:K:195:ALA:HB1	1:K:200:GLN:HB3	1.93	0.51
2:N:133:ASN:H	2:N:175:TYR:HE1	1.59	0.51
1:B:89:ASP:OD1	1:B:89:ASP:N	2.43	0.50
1:B:482:ASP:OD1	1:B:506:ARG:NH1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133:GLU:HG2	1:G:167:VAL:HG13	1.93	0.50
1:I:45:ARG:HH11	1:I:45:ARG:HG3	1.76	0.50
1:K:496:ASN:OD1	1:K:499:THR:N	2.44	0.50
3:M:200:ASN:HB2	5:U:199:ASN:ND2	2.27	0.50
5:V:19:LEU:HD11	5:V:88:THR:HG21	1.93	0.50
1:C:187:VAL:HG12	1:C:192:PRO:HA	1.92	0.50
1:C:307:GLU:OE1	1:C:307:GLU:N	2.39	0.50
1:C:402:ASN:ND2	1:C:517:ILE:O	2.35	0.50
1:E:756:ALA:O	1:E:757:GLN:C	2.48	0.50
1:F:398:ARG:NH2	1:F:866:ASP:OD2	2.37	0.50
1:F:425:LEU:HD12	1:F:451:ILE:HD12	1.93	0.50
1:G:822:HIS:HE1	1:H:246:GLN:NE2	2.09	0.50
1:H:821:GLN:HB2	1:H:845:PHE:HB2	1.91	0.50
1:K:413:CYS:SG	1:K:459:MET:HB2	2.51	0.50
2:N:297:LYS:O	2:N:300:THR:HB	2.11	0.50
1:A:758:CYS:HG	1:A:760:MET:H	1.57	0.50
1:C:921:VAL:CB	1:C:943:PRO:HD2	2.38	0.50
1:D:363:ARG:NE	1:D:923:ASP:OD2	2.44	0.50
1:D:434:GLN:HG3	1:D:437:GLY:N	2.25	0.50
1:E:900:LEU:HD11	1:E:902:MET:HG2	1.92	0.50
1:J:37:TYR:HB2	1:K:879:MET:HE3	1.93	0.50
1:J:650:ASN:HB3	1:J:916:TYR:HE1	1.77	0.50
2:N:396:ASN:OD1	2:N:396:ASN:N	2.39	0.50
3:M:313:SER:O	3:M:314:LEU:HB2	2.10	0.50
6:W:32:GLY:O	6:W:34:ALA:N	2.43	0.50
1:A:753:TYR:O	1:A:762:LYS:HG3	2.12	0.50
1:B:325:TYR:CE2	1:B:543:ARG:HG2	2.47	0.50
1:E:297:THR:OG1	1:E:318:SER:OG	2.28	0.50
1:F:113:LYS:NZ	1:F:321:ASN:O	2.27	0.50
1:F:227:THR:OG1	1:F:289:ASP:OD1	2.25	0.50
1:H:135:ASP:OD2	1:H:225:LYS:NZ	2.29	0.50
1:I:708:ASP:HB3	1:I:710:THR:HG23	1.94	0.50
1:I:812:ASP:N	1:I:812:ASP:OD1	2.44	0.50
1:J:389:ALA:O	1:J:545:ARG:NH2	2.44	0.50
1:A:113:LYS:HE2	1:A:296:ASP:HB2	1.93	0.50
1:A:646:LEU:HG	1:A:648:ALA:CB	2.41	0.50
1:D:133:GLU:HG2	1:D:167:VAL:HG22	1.94	0.50
1:G:203:PRO:HD3	1:G:221:ARG:HD2	1.92	0.50
1:I:307:GLU:OE1	1:I:307:GLU:N	2.44	0.50
1:I:391:ASP:OD1	1:I:539:ASN:ND2	2.42	0.50
1:J:529:ASP:OD1	1:J:715:HIS:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:724:PHE:CE1	1:K:900:LEU:HD13	2.47	0.50
1:A:744:ILE:HG12	1:A:764:TRP:CD2	2.47	0.50
1:A:789:ARG:NH2	6:X:36:SER:O	2.40	0.50
1:B:17:GLN:NE2	5:U:177:GLU:O	2.39	0.50
1:B:165:THR:N	1:C:444:GLU:O	2.25	0.50
1:C:18:ASP:HA	1:C:47:PRO:HD2	1.94	0.50
1:C:426:THR:HG21	1:C:440:LYS:HE3	1.92	0.50
1:E:673:ALA:HB2	1:F:9:TRP:CZ2	2.47	0.50
1:F:35:GLU:OE1	1:F:41:ASN:ND2	2.44	0.50
1:F:447:ASP:OD1	1:F:447:ASP:N	2.43	0.50
1:G:121:ASN:ND2	1:G:232:CYS:SG	2.82	0.50
1:H:425:LEU:HD12	1:H:451:ILE:HD13	1.93	0.50
1:H:588:VAL:HG11	1:H:606:SER:HA	1.93	0.50
1:I:937:THR:HG1	1:I:939:TYR:HE1	1.60	0.50
1:J:72:ARG:HD3	1:J:79:TYR:OH	2.10	0.50
1:K:892:LEU:HD13	5:U:189:ILE:HD11	1.93	0.50
1:L:371:LEU:O	1:L:372:LEU:C	2.49	0.50
3:M:236:LEU:HD22	3:M:258:LEU:HD21	1.94	0.50
4:P:28:ASN:OD1	4:P:28:ASN:N	2.44	0.50
1:B:669:ARG:HH22	2:N:101:TYR:HE1	1.60	0.50
1:B:773:TYR:HH	1:B:792:SER:HG	1.59	0.50
1:C:224:LYS:HG3	1:C:288:GLU:O	2.11	0.50
1:E:936:GLU:HG2	5:U:157:ALA:HA	1.94	0.50
1:G:921:VAL:HA	1:G:943:PRO:HG2	1.93	0.50
1:H:680:THR:HG21	1:H:711:PHE:HB3	1.93	0.50
1:H:844:ASN:HB3	1:I:246:GLN:HE21	1.77	0.50
1:I:677:TRP:NE1	1:I:902:MET:SD	2.84	0.50
1:J:355:ASN:OD1	1:J:356:ALA:N	2.44	0.50
1:J:714:ASN:OD1	1:J:714:ASN:N	2.43	0.50
1:J:754:ASN:N	1:J:754:ASN:OD1	2.44	0.50
1:K:196:ASP:H	1:K:200:GLN:HB2	1.77	0.50
5:U:179:ARG:NH2	5:U:182:GLY:O	2.44	0.50
1:C:113:LYS:NZ	1:C:321:ASN:O	2.31	0.50
1:C:910:ASP:OD1	1:C:910:ASP:N	2.30	0.50
1:E:327:ALA:HB2	1:E:546:SER:HA	1.94	0.50
1:E:518:ASN:HB3	1:E:521:ALA:HB3	1.94	0.50
1:E:865:CYS:SG	1:E:868:THR:HG21	2.52	0.50
1:G:380:THR:HG21	6:1:72:LYS:HG2	1.94	0.50
1:J:207:GLU:HB3	1:K:455:ASN:HD21	1.77	0.50
1:K:669:ARG:HD3	5:U:28:SER:HB3	1.93	0.50
1:A:90:ASN:OD1	1:A:90:ASN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:732:GLY:O	1:D:734:ASP:N	2.45	0.50
1:F:51:PRO:HD3	6:Z:11:PRO:HA	1.94	0.50
1:G:839:GLN:HG2	1:H:172:PRO:HG3	1.93	0.50
1:J:447:ASP:N	1:J:447:ASP:OD1	2.43	0.50
1:K:39:SER:O	1:L:778:GLN:NE2	2.45	0.50
1:K:644:ASP:OD1	1:K:645:TYR:N	2.43	0.50
4:Q:71:THR:HG22	4:Q:75:ILE:HG23	1.94	0.50
1:B:268:THR:C	1:B:270:GLU:H	2.14	0.49
1:B:514:ASP:OD1	1:B:515:CYS:N	2.40	0.49
1:D:338:TYR:OH	1:D:564:LYS:N	2.31	0.49
1:E:90:ASN:N	1:E:90:ASN:OD1	2.45	0.49
1:G:238:LYS:NZ	1:I:812:ASP:OD2	2.35	0.49
1:I:532:ASN:HD21	1:I:703:SER:HB3	1.76	0.49
1:J:830:TYR:N	1:J:837:GLU:OE1	2.35	0.49
1:K:401:GLU:HG2	1:K:403:HIS:CD2	2.46	0.49
2:N:189:VAL:O	2:N:193:LEU:HG	2.12	0.49
5:U:13:TYR:CE2	5:U:15:PRO:HA	2.46	0.49
1:A:456:ASN:O	1:B:836:ARG:NH1	2.45	0.49
1:E:413:CYS:HA	1:F:461:ILE:HB	1.94	0.49
1:H:329:ARG:HB2	1:H:333:ILE:H	1.77	0.49
1:H:475:ASN:OD1	1:H:538:ARG:NE	2.44	0.49
1:J:92:VAL:HG21	1:J:629:LEU:HD23	1.94	0.49
1:J:650:ASN:ND2	1:J:650:ASN:H	2.10	0.49
1:K:412:TYR:OH	1:L:835:MET:HA	2.12	0.49
1:K:839:GLN:NE2	1:L:170:GLN:O	2.45	0.49
1:C:572:LEU:HB3	1:C:640:GLN:NE2	2.26	0.49
1:H:655:ILE:HD11	1:H:915:LEU:HB2	1.94	0.49
1:I:121:ASN:ND2	1:I:232:CYS:SG	2.68	0.49
1:I:469:ARG:HG2	1:I:515:CYS:HB3	1.95	0.49
1:J:225:LYS:O	1:J:309:ASN:ND2	2.45	0.49
6:4:32:GLY:O	6:4:33:GLY:C	2.50	0.49
1:B:41:ASN:N	1:B:41:ASN:OD1	2.46	0.49
1:B:724:PHE:CE1	1:B:900:LEU:HD13	2.48	0.49
1:D:732:GLY:O	1:D:733:ASN:C	2.49	0.49
1:E:733:ASN:HB3	1:F:60:SER:HA	1.95	0.49
1:G:455:ASN:HD21	1:I:207:GLU:HB3	1.78	0.49
1:H:700:TYR:CZ	1:H:702:GLY:HA3	2.47	0.49
1:I:500:TYR:HB2	1:I:598:ASN:ND2	2.27	0.49
1:J:929:ARG:NH1	1:J:929:ARG:HB2	2.27	0.49
1:B:500:TYR:HB2	1:B:598:ASN:HD22	1.77	0.49
1:C:251:LYS:HB3	1:C:256:LYS:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:THR:HG21	1:D:465:ALA:HA	1.93	0.49
1:D:551:ASN:HB3	1:F:521:ALA:HB2	1.94	0.49
1:D:803:GLN:OE1	1:E:552:GLY:N	2.45	0.49
1:E:99:TYR:HE2	1:E:560:GLN:HE21	1.59	0.49
1:G:237:ALA:HB3	1:G:246:GLN:HG2	1.94	0.49
1:H:339:ASN:HD21	1:H:365:THR:HG23	1.78	0.49
1:H:482:ASP:OD2	1:H:502:TYR:OH	2.31	0.49
1:K:677:TRP:NE1	1:K:902:MET:SD	2.85	0.49
2:N:51:GLY:HA2	2:N:116:ARG:HH22	1.75	0.49
1:A:636:ASP:HA	1:A:928:HIS:HE1	1.78	0.49
1:B:407:ASP:O	1:C:126:LYS:NZ	2.34	0.49
1:B:430:PRO:HA	1:B:438:TRP:CD1	2.47	0.49
1:C:210:TRP:CZ3	1:C:417:GLY:HA3	2.48	0.49
1:C:473:TYR:O	1:C:477:ALA:HB3	2.12	0.49
1:G:789:ARG:O	1:G:792:SER:OG	2.31	0.49
1:H:112:PHE:CD1	1:H:326:ILE:HB	2.48	0.49
1:I:710:THR:O	1:I:710:THR:OG1	2.31	0.49
1:J:764:TRP:HZ2	1:J:870:TRP:HB3	1.78	0.49
1:J:789:ARG:O	1:J:792:SER:OG	2.30	0.49
1:A:495:ASP:OD1	1:A:495:ASP:N	2.46	0.49
1:A:796:ASN:OD1	1:A:796:ASN:N	2.46	0.49
1:C:819:LEU:HD21	4:P:78:ASP:HB3	1.94	0.49
1:D:731:PRO:HG3	1:D:742:PHE:CE1	2.48	0.49
1:D:754:ASN:OD1	1:D:754:ASN:N	2.45	0.49
1:G:552:GLY:N	1:I:803:GLN:OE1	2.44	0.49
1:G:678:ALA:HB3	1:G:918:LEU:HG	1.95	0.49
1:H:407:ASP:O	1:I:126:LYS:NZ	2.40	0.49
1:H:669:ARG:HH22	1:H:945:SER:H	1.59	0.49
1:K:337:TYR:CZ	1:K:585:ARG:HG2	2.48	0.49
1:L:587:ASP:OD2	1:L:601:ARG:NH2	2.46	0.49
3:M:14:LEU:HD23	3:M:74:LEU:HD22	1.93	0.49
5:V:179:ARG:H	5:V:179:ARG:NE	2.09	0.49
1:A:115:TYR:CG	1:C:519:LEU:HG	2.48	0.49
1:A:251:LYS:HB2	1:A:256:LYS:HG2	1.95	0.49
1:B:197:LYS:HB3	1:B:261:VAL:HG11	1.94	0.49
1:B:400:ILE:HD12	1:B:476:ILE:HD13	1.95	0.49
1:B:587:ASP:OD2	1:B:601:ARG:NH2	2.40	0.49
1:E:574:LEU:HG	1:E:929:ARG:HH11	1.76	0.49
1:F:573:LEU:HD11	1:F:578:TYR:CZ	2.48	0.49
1:G:539:ASN:OD1	1:G:542:LEU:N	2.38	0.49
1:H:928:HIS:HD2	1:H:930:PRO:HD3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:678:ALA:O	1:I:918:LEU:N	2.41	0.49
1:K:714:ASN:ND2	1:K:868:THR:O	2.42	0.49
1:F:66:ARG:HG3	1:F:615:TYR:CZ	2.48	0.49
1:J:686:GLU:HG2	1:J:700:TYR:CZ	2.47	0.49
1:K:57:THR:HG21	1:K:61:GLN:HG3	1.93	0.49
1:L:299:ILE:HG21	1:L:302:MET:HB2	1.94	0.49
1:L:329:ARG:HD3	1:L:593:GLN:HB2	1.93	0.49
2:N:212:THR:HG22	2:N:238:PRO:HA	1.95	0.49
1:A:865:CYS:SG	1:A:868:THR:HG21	2.52	0.49
1:G:73:GLU:HB2	1:G:80:LYS:HE2	1.95	0.49
1:G:327:ALA:HB2	1:G:546:SER:HA	1.95	0.49
1:H:407:ASP:OD1	1:H:407:ASP:N	2.42	0.49
1:I:594:SER:OG	1:I:701:SER:OG	2.28	0.49
1:J:178:ILE:HG12	1:J:183:ILE:HG22	1.94	0.49
1:K:428:VAL:HG12	1:K:440:LYS:HA	1.95	0.49
1:C:805:VAL:HG13	1:C:855:VAL:HG21	1.95	0.48
1:D:90:ASN:HD22	1:D:623:HIS:HB3	1.77	0.48
1:D:940:LEU:HD23	1:E:12:MET:HG3	1.94	0.48
1:G:845:PHE:O	1:G:846:PRO:C	2.41	0.48
1:H:403:HIS:ND1	1:I:325:TYR:OH	2.35	0.48
1:H:747:SER:OG	1:H:748:VAL:N	2.46	0.48
1:L:754:ASN:ND2	4:Q:50:GLU:OE1	2.46	0.48
1:L:803:GLN:NE2	1:L:859:THR:OG1	2.38	0.48
1:A:420:ILE:HG13	1:A:421:ASN:OD1	2.14	0.48
1:B:178:ILE:HD13	1:B:284:VAL:HG23	1.95	0.48
1:F:337:TYR:HA	1:F:585:ARG:HH21	1.78	0.48
1:I:327:ALA:HB2	1:I:546:SER:HA	1.95	0.48
1:I:667:PRO:O	1:I:669:ARG:N	2.46	0.48
1:K:727:SER:HB2	5:U:16:GLN:HE21	1.78	0.48
1:L:201:PRO:HG3	1:L:286:TYR:CG	2.49	0.48
4:P:99:LYS:HD3	4:P:100:LEU:HG	1.93	0.48
5:U:217:ASP:HB3	5:U:220:LYS:O	2.12	0.48
1:C:108:ARG:NH1	1:C:550:GLY:O	2.34	0.48
1:C:397:VAL:HG11	1:C:536:HIS:CD2	2.48	0.48
1:C:486:TYR:O	1:C:506:ARG:NE	2.44	0.48
1:F:61:GLN:HE22	1:F:91:ARG:HB3	1.78	0.48
1:H:210:TRP:CE3	1:H:417:GLY:HA3	2.47	0.48
1:J:75:THR:HG22	1:J:76:ALA:H	1.79	0.48
1:L:436:ASN:N	1:L:436:ASN:OD1	2.46	0.48
1:L:513:VAL:HG13	1:L:517:ILE:HG21	1.94	0.48
1:B:200:GLN:O	1:B:202:GLU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:ASP:O	1:C:591:VAL:HG22	2.13	0.48
1:D:36:THR:HG21	6:Z:11:PRO:HG3	1.95	0.48
1:D:329:ARG:HB2	1:D:333:ILE:H	1.78	0.48
1:G:755:VAL:HG12	1:G:762:LYS:HE2	1.95	0.48
1:H:19:ALA:HA	1:H:22:TYR:CE2	2.49	0.48
1:I:118:THR:OG1	1:I:119:ALA:N	2.46	0.48
1:K:714:ASN:OD1	1:K:714:ASN:N	2.45	0.48
1:A:585:ARG:HD2	1:A:590:MET:HG2	1.94	0.48
1:D:207:GLU:OE2	1:D:213:THR:OG1	2.31	0.48
1:D:541:GLY:O	1:D:545:ARG:HG3	2.13	0.48
1:E:357:VAL:HG13	1:E:565:PHE:CE2	2.48	0.48
1:E:377:GLY:HA2	6:Y:37:TRP:HZ3	1.79	0.48
1:G:929:ARG:HB3	1:G:934:VAL:O	2.14	0.48
1:H:23:LEU:HD22	1:H:27:LEU:HD23	1.94	0.48
1:H:686:GLU:HG2	1:H:700:TYR:CE1	2.48	0.48
1:J:198:THR:HB	1:J:241:ASN:CG	2.34	0.48
1:J:330:ASP:HB2	1:J:545:ARG:NH2	2.29	0.48
2:N:261:ILE:HG23	2:N:406:TRP:CZ2	2.48	0.48
1:A:72:ARG:HE	1:A:79:TYR:HD2	1.61	0.48
1:B:666:ILE:HB	1:B:900:LEU:HB3	1.95	0.48
1:D:883:ALA:H	1:E:48:THR:HG1	1.61	0.48
1:E:330:ASP:OD2	1:E:379:ARG:NH2	2.46	0.48
1:J:329:ARG:NH2	1:J:592:LEU:O	2.47	0.48
1:J:444:GLU:HB3	1:L:164:LYS:HA	1.95	0.48
1:K:410:PRO:HB2	1:K:412:TYR:CE1	2.49	0.48
1:A:113:LYS:NZ	1:A:117:GLY:O	2.44	0.48
1:A:835:MET:HE2	1:B:416:LEU:HD23	1.95	0.48
1:D:717:PHE:HB3	1:D:744:ILE:HD13	1.96	0.48
1:F:216:ASN:OD1	1:F:216:ASN:N	2.46	0.48
1:F:754:ASN:HA	1:F:761:THR:HA	1.95	0.48
1:H:379:ARG:HD2	1:H:379:ARG:HA	1.71	0.48
1:J:43:LYS:HG2	1:L:570:ASN:O	2.14	0.48
2:N:193:LEU:HB3	2:N:197:ARG:HH22	1.79	0.48
1:A:186:GLY:O	1:A:193:LYS:N	2.39	0.48
1:B:88:GLY:HA3	1:B:91:ARG:HH11	1.79	0.48
1:B:924:VAL:HG21	1:C:12:MET:HB3	1.96	0.48
1:C:378:ASP:OD1	1:C:378:ASP:N	2.47	0.48
1:D:351:ALA:HB1	1:G:932:ARG:HH12	1.79	0.48
1:D:412:TYR:OH	1:E:835:MET:HA	2.14	0.48
1:E:358:VAL:HG23	1:E:939:TYR:CZ	2.49	0.48
1:F:373:LEU:HD13	1:F:379:ARG:HH12	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:SER:HB2	1:I:842:PRO:HB3	1.95	0.48
1:G:329:ARG:HD3	1:G:333:ILE:HG22	1.95	0.48
1:H:200:GLN:O	1:H:201:PRO:C	2.46	0.48
1:I:796:ASN:O	1:I:865:CYS:HA	2.14	0.48
1:K:520:GLY:HA3	1:L:114:PRO:HG2	1.96	0.48
1:L:809:LYS:NZ	4:Q:55:THR:OG1	2.32	0.48
1:A:538:ARG:NH2	1:C:406:GLU:OE2	2.37	0.48
1:B:839:GLN:NE2	1:C:170:GLN:O	2.47	0.48
1:C:574:LEU:HB2	1:C:929:ARG:HD2	1.95	0.48
1:C:821:GLN:NE2	1:C:845:PHE:CG	2.81	0.48
1:E:255:GLY:O	1:E:256:LYS:HG2	2.13	0.48
1:F:313:LEU:O	1:F:316:GLN:HG2	2.14	0.48
1:F:429:LYS:HZ1	1:F:443:THR:HG1	1.54	0.48
1:G:9:TRP:CZ2	1:I:673:ALA:HB2	2.49	0.48
1:H:201:PRO:HG3	1:H:286:TYR:CD1	2.49	0.48
1:L:563:GLN:OE1	1:L:565:PHE:N	2.40	0.48
5:V:144:LEU:HD13	5:V:144:LEU:HA	1.72	0.48
1:F:572:LEU:O	1:F:929:ARG:NH2	2.47	0.48
1:F:639:ASP:OD1	1:F:639:ASP:N	2.46	0.48
1:F:807:ASP:N	1:F:807:ASP:OD1	2.46	0.48
1:H:490:ASN:OD1	1:H:490:ASN:N	2.47	0.48
1:J:118:THR:OG1	1:J:119:ALA:N	2.46	0.48
1:J:407:ASP:OD2	1:J:462:ASN:ND2	2.31	0.48
1:L:601:ARG:HH12	1:L:696:PRO:HA	1.78	0.48
3:M:23:SER:OG	3:M:24:THR:N	2.46	0.48
1:A:406:GLU:OE2	1:B:538:ARG:NH2	2.47	0.47
1:B:329:ARG:HB2	1:B:333:ILE:H	1.79	0.47
1:B:786:TYR:HD1	6:X:93:ASP:CB	2.27	0.47
1:D:46:ASN:H	6:Z:27:THR:CG2	2.27	0.47
1:G:378:ASP:OD1	1:G:380:THR:N	2.47	0.47
1:G:560:GLN:OE1	1:G:560:GLN:N	2.47	0.47
1:G:679:PHE:HB3	1:G:917:VAL:HG22	1.95	0.47
1:G:823:ASN:O	1:G:824:ASN:C	2.51	0.47
1:I:225:LYS:O	1:I:309:ASN:ND2	2.46	0.47
1:J:560:GLN:OE1	1:J:560:GLN:N	2.47	0.47
1:K:425:LEU:HD12	1:K:451:ILE:HD13	1.96	0.47
1:K:738:THR:HG22	1:K:739:PRO:HD2	1.94	0.47
2:N:476:TYR:HD1	2:N:512:THR:O	1.97	0.47
6:X:76:PHE:N	6:X:76:PHE:CD1	2.82	0.47
1:B:676:GLY:O	1:B:920:GLU:HB2	2.13	0.47
1:C:565:PHE:HD1	1:C:567:ALA:H	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:TYR:OH	1:D:693:GLY:O	2.21	0.47
1:F:200:GLN:HB3	1:F:201:PRO:HD3	1.94	0.47
1:F:675:ARG:HH21	1:F:920:GLU:HB3	1.78	0.47
1:G:807:ASP:OD1	1:G:807:ASP:N	2.46	0.47
1:H:204:GLN:H	1:H:204:GLN:HG2	1.38	0.47
1:H:865:CYS:SG	1:H:868:THR:HG21	2.54	0.47
1:J:234:GLY:HA3	1:J:297:THR:HG21	1.96	0.47
1:J:446:SER:HG	1:L:166:HIS:CE1	2.29	0.47
1:K:482:ASP:OD2	1:K:502:TYR:OH	2.29	0.47
2:N:127:LEU:HD11	2:N:554:VAL:HG13	1.97	0.47
3:M:200:ASN:HB2	5:U:199:ASN:HD21	1.79	0.47
1:A:236:TYR:CZ	1:C:848:PRO:HD3	2.49	0.47
1:A:817:GLY:O	1:A:821:GLN:HG3	2.13	0.47
1:E:133:GLU:HB3	1:E:167:VAL:HG13	1.96	0.47
1:E:619:PHE:O	1:E:621:MET:N	2.46	0.47
1:E:777:TYR:O	1:E:778:GLN:NE2	2.35	0.47
1:F:475:ASN:OD1	1:F:538:ARG:NE	2.31	0.47
1:I:675:ARG:HH21	1:I:920:GLU:HB3	1.79	0.47
1:K:411:ASN:ND2	1:L:466:ASN:OD1	2.39	0.47
1:A:762:LYS:HE2	1:B:615:TYR:CE2	2.50	0.47
1:B:369:TYR:O	1:B:370:GLN:C	2.49	0.47
1:B:487:SER:N	1:B:506:ARG:HE	2.11	0.47
1:C:594:SER:OG	1:C:701:SER:O	2.28	0.47
1:F:41:ASN:HB2	6:Y:25:ILE:HA	1.95	0.47
1:F:121:ASN:ND2	1:F:232:CYS:SG	2.87	0.47
1:F:921:VAL:HG21	1:F:941:ARG:HD3	1.96	0.47
1:H:737:LEU:HB2	1:H:763:ASP:OD1	2.14	0.47
1:J:845:PHE:O	1:J:846:PRO:C	2.44	0.47
1:L:746:ARG:HD3	1:L:749:ASP:CB	2.44	0.47
1:A:337:TYR:CZ	1:A:585:ARG:HG2	2.50	0.47
1:B:724:PHE:HE1	1:B:900:LEU:HD13	1.80	0.47
1:C:178:ILE:HG13	1:C:217:HIS:HB3	1.96	0.47
1:D:490:ASN:N	1:D:490:ASN:OD1	2.47	0.47
1:D:645:TYR:HD1	6:0:28:SER:O	1.97	0.47
1:J:673:ALA:HB2	1:K:9:TRP:CZ2	2.49	0.47
1:K:545:ARG:NH2	1:K:593:GLN:OE1	2.47	0.47
1:K:836:ARG:NE	1:K:836:ARG:O	2.48	0.47
1:L:297:THR:OG1	1:L:318:SER:OG	2.25	0.47
1:L:789:ARG:N	1:L:792:SER:OG	2.46	0.47
3:M:234:LEU:HD22	5:U:198:PHE:CD2	2.47	0.47
6:Z:25:ILE:HG12	6:Z:26:GLY:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:LEU:HD21	1:B:412:TYR:HE1	1.80	0.47
1:A:524:SER:O	1:A:862:LYS:NZ	2.36	0.47
1:B:327:ALA:HB2	1:B:546:SER:HA	1.96	0.47
1:C:163:GLN:O	1:C:163:GLN:NE2	2.48	0.47
1:F:522:ARG:NH2	1:F:798:GLN:OE1	2.47	0.47
1:I:351:ALA:HA	1:J:932:ARG:HH22	1.80	0.47
1:I:543:ARG:O	1:I:547:MET:HG3	2.15	0.47
1:J:24:SER:HB3	1:L:638:ASN:HD21	1.80	0.47
1:J:733:ASN:HB3	1:K:60:SER:HA	1.96	0.47
2:N:135:ASN:OD1	2:N:138:MET:N	2.37	0.47
2:N:385:ASP:OD2	2:N:502:ASN:HB2	2.15	0.47
6:3:9:LEU:HD23	6:3:9:LEU:H	1.79	0.47
1:A:241:ASN:ND2	1:A:243:ASN:H	2.13	0.47
1:A:678:ALA:O	1:A:918:LEU:N	2.41	0.47
1:C:636:ASP:OD1	1:C:636:ASP:N	2.46	0.47
1:D:842:PRO:HG3	1:E:130:ASN:ND2	2.29	0.47
1:E:574:LEU:HB3	1:E:575:PRO:HD2	1.96	0.47
1:F:658:ASN:N	1:F:658:ASN:OD1	2.48	0.47
1:G:90:ASN:OD1	1:G:90:ASN:N	2.47	0.47
1:G:120:TYR:CD2	1:G:236:TYR:HB2	2.49	0.47
1:G:251:LYS:HE2	1:G:256:LYS:HD2	1.97	0.47
1:G:411:ASN:OD1	1:G:411:ASN:N	2.47	0.47
1:H:165:THR:N	1:I:444:GLU:O	2.46	0.47
1:I:278:ASN:N	1:I:278:ASN:OD1	2.47	0.47
1:I:513:VAL:HG13	1:I:517:ILE:HG21	1.97	0.47
1:I:539:ASN:HB3	1:I:542:LEU:HB3	1.95	0.47
1:I:541:GLY:O	1:I:545:ARG:HD3	2.15	0.47
1:J:330:ASP:OD2	1:J:379:ARG:NH2	2.45	0.47
1:L:712:TYR:HA	1:L:866:ASP:HB3	1.97	0.47
2:N:51:GLY:CA	2:N:116:ARG:HH21	2.23	0.47
2:N:148:MET:HG2	2:N:163:TYR:CE1	2.50	0.47
2:N:262:ARG:HG2	2:N:263:LYS:H	1.80	0.47
4:Q:73:ARG:NH2	4:Q:76:VAL:HG21	2.30	0.47
5:V:10:MET:HG2	5:V:26:ASP:HB2	1.97	0.47
5:V:166:GLN:O	5:V:170:THR:OG1	2.22	0.47
6:W:39:SER:HB3	6:X:82:ASP:CB	2.44	0.47
1:A:643:ASN:ND2	6:X:29:ASN:OD1	2.48	0.47
1:D:449:ASN:OD1	1:F:167:VAL:N	2.46	0.47
1:F:234:GLY:HA3	1:F:297:THR:HG21	1.97	0.47
1:H:619:PHE:O	1:H:621:MET:N	2.45	0.47
1:I:387:ASN:OD1	1:I:545:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:650:ASN:ND2	1:I:650:ASN:H	2.12	0.47
1:I:714:ASN:ND2	1:I:868:THR:O	2.48	0.47
1:J:254:ASN:O	1:J:254:ASN:ND2	2.48	0.47
1:K:90:ASN:N	1:K:90:ASN:OD1	2.47	0.47
1:K:519:LEU:HD13	1:L:115:TYR:CD2	2.50	0.47
1:K:749:ASP:OD1	1:K:749:ASP:N	2.48	0.47
1:L:695:ASP:O	1:L:697:TYR:N	2.48	0.47
2:N:535:ILE:HG22	2:N:536:GLY:H	1.79	0.47
1:B:372:LEU:O	1:B:375:SER:N	2.48	0.47
1:D:274:GLY:HA2	1:D:279:LEU:HD11	1.96	0.47
1:D:823:ASN:OD1	1:D:824:ASN:N	2.48	0.47
1:E:643:ASN:N	1:E:643:ASN:OD1	2.48	0.47
1:F:865:CYS:SG	1:F:868:THR:HG21	2.55	0.47
1:I:942:THR:HB	1:I:943:PRO:HD3	1.97	0.47
1:J:299:ILE:HG21	1:J:302:MET:HB2	1.97	0.47
1:J:541:GLY:O	1:J:545:ARG:HG3	2.15	0.47
1:K:950:THR:HB	5:U:33:TYR:OH	2.14	0.47
2:N:196:GLY:O	2:N:197:ARG:C	2.51	0.47
6:3:66:MET:HG2	6:3:70:LYS:HE3	1.97	0.47
1:A:3:PRO:HG3	3:M:355:MET:HE1	1.96	0.47
1:A:578:TYR:CZ	1:A:933:GLY:HA2	2.50	0.47
1:A:638:ASN:ND2	1:B:24:SER:OG	2.48	0.47
1:B:700:TYR:CZ	1:B:702:GLY:HA3	2.50	0.47
1:B:876:SER:HB2	1:C:56:THR:HG21	1.97	0.47
1:C:658:ASN:N	1:C:909:MET:O	2.39	0.47
1:D:500:TYR:HB2	1:D:598:ASN:ND2	2.30	0.47
1:E:61:GLN:HE22	1:E:91:ARG:HG2	1.79	0.47
1:F:19:ALA:HB3	6:Y:25:ILE:HB	1.97	0.47
1:I:210:TRP:CZ3	1:I:417:GLY:HA3	2.50	0.47
1:I:325:TYR:CE2	1:I:543:ARG:HG2	2.50	0.47
1:J:714:ASN:HB3	1:J:870:TRP:NE1	2.30	0.47
1:J:819:LEU:HD12	1:J:819:LEU:H	1.79	0.47
1:K:619:PHE:O	1:K:621:MET:N	2.48	0.47
1:L:82:ARG:NH2	1:L:353:GLN:OE1	2.48	0.47
1:L:265:PHE:HD1	1:L:284:VAL:HG22	1.80	0.47
1:L:389:ALA:HB3	1:L:545:ARG:HD2	1.97	0.47
2:N:535:ILE:H	2:N:535:ILE:HG12	1.41	0.47
1:A:598:ASN:OD1	1:A:598:ASN:N	2.45	0.46
1:C:328:PHE:CE2	1:C:549:LEU:HD11	2.51	0.46
1:D:797:PHE:CZ	1:D:799:PRO:HG3	2.50	0.46
1:E:812:ASP:OD1	1:E:812:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:207:GLU:OE1	1:F:209:GLN:N	2.48	0.46
1:F:391:ASP:OD1	1:F:391:ASP:N	2.48	0.46
1:G:299:ILE:HG21	1:G:302:MET:HB2	1.96	0.46
1:G:737:LEU:HD13	1:G:753:TYR:CE1	2.50	0.46
1:H:312:GLU:OE1	1:H:312:GLU:N	2.31	0.46
1:H:669:ARG:N	1:H:898:HIS:O	2.46	0.46
1:I:661:ASN:O	4:Q:12:SER:HB3	2.15	0.46
2:N:97:GLN:H	2:N:97:GLN:HG2	1.61	0.46
3:M:204:ALA:HB2	3:M:231:ASN:HD21	1.80	0.46
6:1:25:ILE:H	6:1:25:ILE:HG12	1.35	0.46
1:B:792:SER:OG	1:B:793:PHE:N	2.48	0.46
1:C:54:ASP:N	1:C:54:ASP:OD1	2.48	0.46
1:E:277:ASP:O	1:E:279:LEU:N	2.48	0.46
1:E:927:VAL:HG22	1:E:937:THR:HG22	1.98	0.46
1:F:327:ALA:HB2	1:F:546:SER:HA	1.97	0.46
1:G:51:PRO:HD3	6:2:11:PRO:HA	1.98	0.46
1:G:89:ASP:OD2	1:G:932:ARG:NH2	2.45	0.46
1:G:131:PRO:HB2	1:G:222:VAL:HA	1.97	0.46
1:G:466:ASN:O	1:G:470:ASN:ND2	2.42	0.46
1:H:329:ARG:HG3	1:H:333:ILE:O	2.16	0.46
1:J:818:ILE:H	1:J:818:ILE:HD12	1.80	0.46
1:K:423:GLU:O	1:K:450:GLU:HA	2.14	0.46
1:K:475:ASN:OD1	1:K:538:ARG:NE	2.48	0.46
1:K:681:ARG:HH21	1:K:913:THR:HG21	1.79	0.46
1:K:797:PHE:CE2	1:K:799:PRO:HG3	2.51	0.46
3:M:199:VAL:HG11	3:M:235:LEU:HD23	1.97	0.46
1:D:419:VAL:HG21	1:D:452:ARG:HB2	1.97	0.46
1:D:778:GLN:OE1	1:F:39:SER:N	2.48	0.46
1:E:724:PHE:CE1	1:E:900:LEU:HD13	2.50	0.46
1:E:843:ALA:HB3	1:F:120:TYR:HD2	1.80	0.46
1:F:472:LEU:HA	1:F:472:LEU:HD23	1.73	0.46
1:H:744:ILE:HG12	1:H:764:TRP:CE2	2.50	0.46
1:J:529:ASP:OD2	1:J:862:LYS:NZ	2.39	0.46
1:K:113:LYS:NZ	1:K:321:ASN:O	2.35	0.46
1:L:902:MET:HE3	1:L:904:PHE:HE1	1.80	0.46
2:N:86:ASN:HB3	2:N:90:ASN:O	2.16	0.46
2:N:478:ASP:C	2:N:480:ALA:H	2.17	0.46
1:C:120:TYR:CD2	1:C:236:TYR:HB2	2.50	0.46
1:C:484:LEU:HD22	4:P:75:ILE:HD11	1.96	0.46
1:D:237:ALA:HB3	1:D:246:GLN:CD	2.36	0.46
1:E:265:PHE:HB3	1:E:281:PRO:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:427:LYS:HD2	1:E:445:PHE:CD2	2.51	0.46
1:E:472:LEU:O	1:E:473:TYR:C	2.53	0.46
1:F:70:VAL:HG12	1:F:82:ARG:HG2	1.97	0.46
1:F:397:VAL:HG11	1:F:536:HIS:CD2	2.50	0.46
1:H:359:ASP:OD1	1:H:360:LEU:N	2.49	0.46
1:H:596:LEU:HD12	1:H:596:LEU:HA	1.56	0.46
1:J:198:THR:HB	1:J:241:ASN:OD1	2.15	0.46
1:J:918:LEU:O	1:J:919:PHE:C	2.49	0.46
1:L:134:TRP:CH2	1:L:166:HIS:HB2	2.49	0.46
2:N:301:GLU:O	2:N:302:GLN:C	2.54	0.46
3:M:152:ALA:O	3:M:158:GLN:NE2	2.49	0.46
5:U:55:LEU:HD12	5:U:55:LEU:HA	1.43	0.46
1:B:830:TYR:N	1:B:837:GLU:OE2	2.35	0.46
1:C:275:ASN:N	1:C:275:ASN:OD1	2.46	0.46
1:E:235:SER:HB3	1:E:292:ILE:CD1	2.41	0.46
1:G:416:LEU:HD23	1:G:416:LEU:H	1.80	0.46
1:G:655:ILE:HD11	1:G:915:LEU:HB2	1.97	0.46
1:J:929:ARG:HB2	1:J:929:ARG:HH11	1.81	0.46
1:K:120:TYR:CD2	1:K:236:TYR:HB2	2.50	0.46
1:K:646:LEU:HD21	1:K:918:LEU:HD22	1.98	0.46
1:L:669:ARG:NH2	1:L:945:SER:H	2.11	0.46
1:B:470:ASN:O	1:B:471:PHE:C	2.51	0.46
1:D:714:ASN:N	1:D:714:ASN:OD1	2.49	0.46
1:F:251:LYS:HD2	1:F:251:LYS:HA	1.67	0.46
1:F:795:ARG:HE	1:F:795:ARG:HB2	1.50	0.46
1:G:17:GLN:HB3	1:G:21:GLU:HB2	1.98	0.46
1:H:108:ARG:NH2	1:H:549:LEU:HB2	2.30	0.46
1:H:335:LEU:HD23	1:H:591:VAL:HG11	1.96	0.46
1:H:737:LEU:HD13	1:H:753:TYR:CD1	2.51	0.46
1:I:945:SER:O	1:L:727:SER:OG	2.31	0.46
1:J:77:TYR:O	1:J:586:LYS:N	2.48	0.46
1:K:343:ASN:N	1:K:343:ASN:OD1	2.48	0.46
1:K:598:ASN:ND2	1:K:603:ASP:OD2	2.48	0.46
1:L:201:PRO:HG3	1:L:286:TYR:CD1	2.51	0.46
1:B:744:ILE:HG23	1:B:764:TRP:CD1	2.51	0.46
1:B:932:ARG:HH12	3:M:93:LEU:HA	1.80	0.46
1:D:714:ASN:HB3	1:D:870:TRP:NE1	2.30	0.46
1:E:87:VAL:HB	1:E:575:PRO:HA	1.96	0.46
1:H:413:CYS:SG	1:H:459:MET:HB2	2.55	0.46
1:I:133:GLU:HG2	1:I:167:VAL:HG13	1.98	0.46
1:J:90:ASN:HD22	1:J:623:HIS:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:456:ASN:O	1:K:836:ARG:NH1	2.48	0.46
1:J:744:ILE:HG12	1:J:764:TRP:CE2	2.51	0.46
1:L:887:LEU:HD12	1:L:887:LEU:HA	1.74	0.46
4:P:61:ALA:O	4:P:63:ALA:N	2.49	0.46
1:A:89:ASP:OD1	1:A:932:ARG:NH1	2.48	0.46
1:B:350:GLN:HE21	1:B:350:GLN:HB3	1.47	0.46
1:C:236:TYR:CG	1:C:237:ALA:N	2.83	0.46
1:D:921:VAL:HB	1:D:943:PRO:HD2	1.98	0.46
1:F:138:ALA:HB3	1:F:164:LYS:HD2	1.97	0.46
1:F:572:LEU:HB3	1:F:640:GLN:HE22	1.81	0.46
1:G:402:ASN:ND2	1:G:515:CYS:O	2.42	0.46
1:G:921:VAL:HB	1:G:943:PRO:HD2	1.97	0.46
1:I:574:LEU:HD12	1:I:634:ARG:HE	1.80	0.46
1:J:473:TYR:CD2	1:L:409:LEU:HD21	2.50	0.46
1:K:549:LEU:HD23	1:K:549:LEU:HA	1.75	0.46
1:K:754:ASN:O	1:K:762:LYS:HE2	2.16	0.46
1:K:821:GLN:HB2	1:K:845:PHE:HB2	1.98	0.46
1:L:340:SER:OG	1:L:690:LEU:O	2.22	0.46
4:R:112:ARG:HD3	4:R:112:ARG:HA	1.71	0.46
1:B:773:TYR:OH	1:B:792:SER:OG	2.29	0.46
1:B:942:THR:HB	1:B:943:PRO:HD3	1.97	0.46
1:D:484:LEU:HD11	1:D:527:TYR:CD1	2.51	0.46
1:D:835:MET:HA	1:F:412:TYR:OH	2.16	0.46
1:E:594:SER:OG	1:E:701:SER:OG	2.26	0.46
1:E:747:SER:O	1:E:749:ASP:N	2.48	0.46
1:F:518:ASN:ND2	1:F:523:TRP:HD1	2.14	0.46
1:H:82:ARG:HG3	1:H:581:GLU:HG2	1.98	0.46
1:H:196:ASP:H	1:H:200:GLN:CB	2.27	0.46
1:I:479:TYR:OH	1:I:537:HIS:ND1	2.27	0.46
1:J:551:ASN:HB3	1:L:521:ALA:HB2	1.98	0.46
1:K:573:LEU:HA	1:K:929:ARG:NH2	2.30	0.46
1:A:534:PHE:HZ	1:A:867:ARG:HG3	1.81	0.46
1:B:573:LEU:HD11	1:B:578:TYR:CE2	2.51	0.46
1:B:836:ARG:O	1:B:836:ARG:NE	2.49	0.46
1:C:922:PHE:O	1:C:941:ARG:HA	2.16	0.46
1:D:330:ASP:HB2	1:D:545:ARG:HH21	1.81	0.46
1:E:830:TYR:N	1:E:837:GLU:OE2	2.40	0.46
1:F:201:PRO:CD	1:F:286:TYR:HE2	2.29	0.46
1:J:500:TYR:HB2	1:J:598:ASN:HD22	1.81	0.46
1:L:500:TYR:HB2	1:L:598:ASN:ND2	2.31	0.46
3:M:14:LEU:HD11	3:M:71:GLU:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ALA:HA	1:A:22:TYR:CE2	2.51	0.45
1:B:372:LEU:O	1:B:373:LEU:C	2.54	0.45
1:B:805:VAL:HG21	1:B:847:TYR:HD2	1.81	0.45
1:C:364:ASN:HB2	1:C:650:ASN:ND2	2.32	0.45
1:C:739:PRO:HG2	1:E:341:THR:HB	1.98	0.45
1:C:874:PHE:CE1	1:C:887:LEU:HB3	2.51	0.45
1:D:730:TRP:O	1:D:730:TRP:CG	2.67	0.45
1:E:68:ILE:HD13	1:E:68:ILE:HA	1.84	0.45
1:E:941:ARG:O	1:E:945:SER:HA	2.16	0.45
1:F:3:PRO:HB2	1:F:4:SER:H	1.56	0.45
1:F:724:PHE:HE2	1:F:893:TYR:HE2	1.64	0.45
1:G:221:ARG:HH12	1:G:288:GLU:CD	2.20	0.45
1:H:178:ILE:HG22	1:H:183:ILE:HA	1.97	0.45
1:H:329:ARG:HB2	1:H:333:ILE:N	2.32	0.45
1:I:529:ASP:OD1	1:I:715:HIS:NE2	2.27	0.45
1:I:724:PHE:CE1	1:I:900:LEU:HD13	2.51	0.45
1:J:271:ALA:HB3	1:J:279:LEU:HD13	1.98	0.45
1:K:430:PRO:HA	1:K:438:TRP:CD1	2.51	0.45
1:K:490:ASN:N	1:K:490:ASN:OD1	2.48	0.45
1:K:646:LEU:HD11	1:K:918:LEU:HD21	1.97	0.45
1:L:327:ALA:HB2	1:L:546:SER:HA	1.98	0.45
1:L:572:LEU:O	1:L:929:ARG:NH2	2.49	0.45
1:A:490:ASN:N	1:A:490:ASN:OD1	2.49	0.45
1:A:728:VAL:HG21	5:U:226:TYR:CE2	2.51	0.45
1:A:932:ARG:HH22	1:E:351:ALA:HA	1.80	0.45
1:B:212:GLU:H	1:B:212:GLU:CD	2.16	0.45
1:B:764:TRP:HZ2	1:B:870:TRP:HB3	1.81	0.45
1:C:188:GLU:HB3	1:C:191:THR:HB	1.98	0.45
1:E:596:LEU:HA	1:E:596:LEU:HD12	1.76	0.45
1:E:876:SER:HB2	1:F:56:THR:HG21	1.99	0.45
1:F:619:PHE:O	1:F:621:MET:N	2.47	0.45
1:H:744:ILE:HG12	1:H:764:TRP:CD2	2.52	0.45
1:K:181:GLU:HB2	1:K:194:TYR:CD1	2.52	0.45
1:L:563:GLN:OE1	1:L:564:LYS:N	2.50	0.45
2:N:189:VAL:HG11	2:N:498:ARG:HD2	1.97	0.45
3:M:334:MET:SD	5:U:151:THR:OG1	2.70	0.45
1:C:200:GLN:O	1:C:201:PRO:C	2.53	0.45
1:F:436:ASN:N	1:F:436:ASN:OD1	2.49	0.45
1:F:572:LEU:HB3	1:F:640:GLN:NE2	2.32	0.45
1:H:210:TRP:CZ3	1:H:417:GLY:HA3	2.52	0.45
1:I:858:ILE:HD12	1:I:858:ILE:HA	1.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:339:ASN:ND2	1:K:363:ARG:O	2.50	0.45
1:L:348:ALA:HB2	1:L:355:ASN:HA	1.97	0.45
1:L:746:ARG:HD3	1:L:749:ASP:HB2	1.98	0.45
2:N:80:ALA:O	2:N:81:SER:C	2.53	0.45
5:V:72:ARG:HG3	5:V:73:SER:N	2.31	0.45
1:A:24:SER:O	1:A:25:PRO:C	2.54	0.45
1:A:462:ASN:O	1:A:466:ASN:ND2	2.33	0.45
1:A:473:TYR:O	1:A:477:ALA:HB3	2.16	0.45
1:B:817:GLY:O	1:B:821:GLN:HG3	2.17	0.45
1:C:239:PRO:HA	1:C:246:GLN:HA	1.98	0.45
1:D:391:ASP:OD1	1:D:545:ARG:NH2	2.34	0.45
1:E:829:GLY:HA2	1:E:837:GLU:HG2	1.98	0.45
1:G:201:PRO:HG2	1:G:286:TYR:CE1	2.51	0.45
1:H:121:ASN:ND2	1:H:232:CYS:SG	2.83	0.45
1:H:409:LEU:HD13	1:I:470:ASN:HA	1.99	0.45
1:H:678:ALA:HB3	1:H:918:LEU:HG	1.99	0.45
1:I:126:LYS:HG2	1:I:233:TYR:CD2	2.51	0.45
1:K:68:ILE:HG22	1:K:69:PRO:HD2	1.98	0.45
1:K:638:ASN:HD21	1:L:24:SER:HB3	1.81	0.45
4:Q:6:PHE:HD1	4:Q:6:PHE:HA	1.69	0.45
1:A:210:TRP:CZ3	1:A:417:GLY:HA3	2.51	0.45
1:A:235:SER:HB2	1:C:842:PRO:HA	1.97	0.45
1:A:660:THR:O	1:A:660:THR:OG1	2.33	0.45
1:A:733:ASN:O	1:A:735:ARG:HG2	2.17	0.45
1:D:397:VAL:HG11	1:D:536:HIS:CE1	2.51	0.45
1:D:823:ASN:ND2	1:D:846:PRO:HD3	2.30	0.45
1:E:565:PHE:O	1:E:567:ALA:N	2.50	0.45
1:F:133:GLU:HG2	1:F:167:VAL:HG13	1.99	0.45
1:F:253:GLN:H	1:F:253:GLN:CD	2.20	0.45
1:G:120:TYR:HE2	1:G:295:PRO:HG2	1.81	0.45
1:I:204:GLN:H	1:I:204:GLN:HG2	1.56	0.45
1:I:251:LYS:HE3	1:I:253:GLN:HB2	1.99	0.45
1:J:640:GLN:NE2	1:J:929:ARG:HH22	2.14	0.45
1:J:789:ARG:NH1	6:3:38:GLY:HA2	2.31	0.45
1:J:865:CYS:SG	1:J:868:THR:HG21	2.57	0.45
1:K:526:ASP:N	1:K:526:ASP:OD1	2.50	0.45
2:N:459:ASN:O	2:N:460:PHE:C	2.55	0.45
5:V:19:LEU:HD21	5:V:88:THR:OG1	2.17	0.45
1:D:552:GLY:N	1:F:803:GLN:OE1	2.40	0.45
1:D:560:GLN:OE1	1:D:560:GLN:N	2.50	0.45
1:D:574:LEU:HB3	1:D:575:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:ASP:OD1	1:E:278:ASN:N	2.45	0.45
1:E:922:PHE:CE2	1:F:14:ILE:HG23	2.52	0.45
1:E:936:GLU:OE1	5:U:144:LEU:HB2	2.16	0.45
1:F:118:THR:OG1	1:F:119:ALA:N	2.50	0.45
1:F:721:ALA:HB3	1:F:903:THR:HB	1.98	0.45
1:F:942:THR:OG1	1:F:943:PRO:HD3	2.17	0.45
1:J:200:GLN:O	1:J:201:PRO:C	2.47	0.45
3:M:77:VAL:HG21	3:M:95:TYR:HA	1.99	0.45
4:Q:88:SER:HB2	4:Q:92:ARG:HH11	1.80	0.45
6:Y:23:GLN:HE21	6:Y:23:GLN:HB2	1.48	0.45
1:A:823:ASN:O	1:A:824:ASN:C	2.52	0.45
1:C:79:TYR:HB3	1:C:584:PHE:HB2	1.99	0.45
1:D:330:ASP:HB2	1:D:545:ARG:NH2	2.31	0.45
1:E:773:TYR:OH	1:E:792:SER:OG	2.31	0.45
1:E:776:GLY:HA2	1:E:780:PHE:CE1	2.52	0.45
1:F:203:PRO:O	1:F:205:ILE:N	2.49	0.45
1:F:927:VAL:HG22	1:F:937:THR:HG22	1.98	0.45
1:G:202:GLU:O	1:G:203:PRO:C	2.55	0.45
1:H:703:SER:O	1:H:705:PRO:HD3	2.17	0.45
1:J:523:TRP:CD1	1:J:802:ARG:HD3	2.52	0.45
1:J:948:ASN:OD1	1:J:948:ASN:N	2.49	0.45
1:L:112:PHE:CD1	1:L:326:ILE:HB	2.51	0.45
2:N:416:GLN:O	2:N:421:SER:OG	2.32	0.45
6:Y:77:GLN:HB2	6:Y:78:GLN:H	1.46	0.45
1:A:246:GLN:OE1	1:C:822:HIS:HE1	2.00	0.45
1:A:352:SER:O	1:A:354:LEU:N	2.44	0.45
1:A:469:ARG:NH1	1:A:828:VAL:HG21	2.32	0.45
1:A:615:TYR:CE2	1:C:762:LYS:HE2	2.51	0.45
1:C:676:GLY:HA2	1:C:874:PHE:HB2	1.99	0.45
1:D:922:PHE:O	1:D:941:ARG:HA	2.17	0.45
1:E:523:TRP:CD1	1:E:802:ARG:HD3	2.52	0.45
1:G:362:ASP:OD2	1:G:941:ARG:NH2	2.44	0.45
1:G:383:PHE:HD1	1:G:384:SER:N	2.14	0.45
3:M:385:ILE:HD12	3:M:385:ILE:HA	1.84	0.45
4:S:133:ALA:O	4:S:136:PRO:HD2	2.17	0.45
6:W:39:SER:O	6:W:40:LEU:C	2.55	0.45
1:A:892:LEU:HD13	5:U:225:GLY:HA3	1.97	0.45
1:D:745:LYS:NZ	4:P:48:THR:O	2.46	0.45
1:E:549:LEU:HD23	1:E:549:LEU:HA	1.82	0.45
1:E:836:ARG:O	1:E:836:ARG:NE	2.44	0.45
1:I:120:TYR:HE2	1:I:295:PRO:HG2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:641:SER:OG	1:K:45:ARG:HB2	2.17	0.45
1:L:719:LYS:HE2	1:L:743:GLU:HG2	1.99	0.45
4:R:113:GLU:OE1	4:R:113:GLU:N	2.50	0.45
6:Y:25:ILE:H	6:Y:25:ILE:HG12	1.32	0.45
6:1:40:LEU:HD22	6:1:40:LEU:HA	1.74	0.45
1:A:563:GLN:OE1	1:A:564:LYS:N	2.50	0.45
1:A:789:ARG:NH1	6:X:38:GLY:HA2	2.32	0.45
1:B:413:CYS:HA	1:C:461:ILE:HB	1.99	0.45
1:B:883:ALA:H	1:C:48:THR:HG1	1.58	0.45
1:C:371:LEU:HD13	6:W:30:MET:HE3	1.99	0.45
1:C:392:SER:O	1:C:539:ASN:HA	2.17	0.45
1:F:120:TYR:CD2	1:F:236:TYR:HB2	2.51	0.45
1:F:260:GLN:H	1:F:260:GLN:HG2	1.57	0.45
1:F:574:LEU:HD23	1:F:574:LEU:HA	1.80	0.45
1:G:461:ILE:HG13	1:G:463:LEU:HD12	1.98	0.45
1:I:619:PHE:O	1:I:621:MET:N	2.44	0.45
1:I:646:LEU:HG	1:I:648:ALA:HB2	1.98	0.45
1:I:788:ASP:OD2	1:I:795:ARG:HB2	2.16	0.45
1:I:887:LEU:HD12	1:I:887:LEU:HA	1.80	0.45
1:J:45:ARG:HD3	1:L:643:ASN:OD1	2.17	0.45
1:K:839:GLN:HB3	1:L:172:PRO:HD3	1.98	0.45
1:K:868:THR:OG1	1:K:869:LEU:N	2.50	0.45
1:L:120:TYR:HE2	1:L:295:PRO:HG2	1.82	0.45
2:N:133:ASN:HB3	2:N:175:TYR:HD1	1.82	0.45
1:A:237:ALA:O	1:A:238:LYS:C	2.56	0.44
1:A:607:ILE:HD11	1:A:609:PHE:CE1	2.52	0.44
1:A:724:PHE:CE2	1:A:893:TYR:HE1	2.35	0.44
1:A:828:VAL:HG13	1:A:829:GLY:N	2.31	0.44
1:B:670:ASN:OD1	1:B:672:ALA:N	2.50	0.44
1:C:336:MET:HB2	1:C:338:TYR:CE2	2.52	0.44
1:D:409:LEU:HD23	1:E:833:PRO:HB3	1.99	0.44
1:D:820:HIS:HA	1:E:204:GLN:NE2	2.32	0.44
1:D:836:ARG:O	1:D:836:ARG:NE	2.40	0.44
1:G:52:THR:OG1	1:G:53:HIS:N	2.49	0.44
1:G:229:MET:N	1:G:309:ASN:OD1	2.44	0.44
1:H:254:ASN:N	1:H:254:ASN:OD1	2.50	0.44
1:J:170:GLN:HG3	1:K:452:ARG:HB3	1.99	0.44
1:J:366:GLU:HG3	1:J:707:LEU:HD22	1.99	0.44
1:J:744:ILE:HG12	1:J:764:TRP:CD2	2.52	0.44
1:K:328:PHE:CE1	1:K:549:LEU:HD11	2.52	0.44
1:K:681:ARG:HD2	1:K:906:VAL:HG11	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:297:THR:OG1	1:L:298:HIS:N	2.48	0.44
1:L:402:ASN:OD1	1:L:403:HIS:N	2.50	0.44
2:N:478:ASP:C	2:N:480:ALA:N	2.65	0.44
1:A:886:ASP:OD1	1:A:887:LEU:N	2.50	0.44
1:B:266:PHE:HE2	1:C:449:ASN:HD22	1.65	0.44
1:E:647:SER:HB2	1:E:675:ARG:HH12	1.81	0.44
1:F:201:PRO:CD	1:F:286:TYR:CE2	3.01	0.44
1:F:278:ASN:N	1:F:278:ASN:OD1	2.50	0.44
1:G:126:LYS:NZ	1:I:407:ASP:O	2.34	0.44
1:G:237:ALA:CB	1:G:246:GLN:HG2	2.47	0.44
1:G:886:ASP:OD1	1:G:886:ASP:N	2.49	0.44
1:H:253:GLN:OE1	1:H:254:ASN:N	2.47	0.44
1:I:746:ARG:HE	1:I:749:ASP:HB2	1.82	0.44
1:J:416:LEU:HD23	1:J:416:LEU:H	1.81	0.44
1:J:419:VAL:HG21	1:J:452:ARG:HB2	1.99	0.44
1:L:196:ASP:OD1	1:L:198:THR:N	2.50	0.44
2:N:439:TRP:CZ3	2:N:543:ILE:HD11	2.52	0.44
1:A:9:TRP:CZ2	1:C:673:ALA:HB2	2.52	0.44
1:A:806:ASP:OD1	1:A:808:THR:OG1	2.31	0.44
1:B:821:GLN:HB3	1:B:845:PHE:HB2	2.00	0.44
1:E:130:ASN:OD1	1:E:232:CYS:HA	2.17	0.44
1:H:167:VAL:N	1:I:449:ASN:OD1	2.47	0.44
1:H:413:CYS:HA	1:I:461:ILE:HB	1.99	0.44
1:H:724:PHE:CE1	1:H:900:LEU:HD13	2.53	0.44
1:H:941:ARG:HG3	1:H:944:PHE:O	2.18	0.44
1:I:776:GLY:HA2	1:I:780:PHE:CE1	2.52	0.44
1:J:619:PHE:O	1:J:621:MET:N	2.46	0.44
1:K:673:ALA:HB3	1:K:942:THR:HG21	1.99	0.44
1:K:714:ASN:HB3	1:K:870:TRP:NE1	2.32	0.44
6:W:25:ILE:H	6:W:25:ILE:HG12	1.09	0.44
1:A:784:GLU:CD	1:A:784:GLU:H	2.17	0.44
1:D:329:ARG:HG3	1:D:333:ILE:O	2.18	0.44
1:D:481:PRO:HB2	1:D:483:LYS:HG2	1.99	0.44
1:F:434:GLN:HG3	1:F:437:GLY:H	1.81	0.44
1:G:743:GLU:O	1:G:761:THR:OG1	2.21	0.44
1:G:817:GLY:O	1:G:821:GLN:HG3	2.17	0.44
1:H:844:ASN:N	1:H:844:ASN:OD1	2.49	0.44
1:I:563:GLN:OE1	1:I:565:PHE:N	2.37	0.44
1:I:563:GLN:NE2	1:I:568:ILE:HD11	2.33	0.44
1:J:237:ALA:HB3	1:J:246:GLN:OE1	2.18	0.44
1:J:490:ASN:OD1	1:J:490:ASN:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:221:ARG:NH2	1:K:288:GLU:OE2	2.50	0.44
1:K:883:ALA:H	1:L:48:THR:HG1	1.62	0.44
1:L:204:GLN:H	1:L:204:GLN:HG2	1.45	0.44
1:L:389:ALA:HB3	1:L:545:ARG:CD	2.47	0.44
1:L:845:PHE:O	1:L:846:PRO:C	2.46	0.44
2:N:491:SER:O	2:N:492:LEU:HB2	2.15	0.44
4:P:55:THR:C	4:P:57:LEU:HB2	2.38	0.44
6:Y:10:ALA:O	6:Y:11:PRO:C	2.54	0.44
1:A:866:ASP:N	1:A:866:ASP:OD1	2.47	0.44
1:B:196:ASP:O	1:B:197:LYS:C	2.56	0.44
1:B:598:ASN:N	1:B:598:ASN:OD1	2.49	0.44
1:D:20:SER:HB3	6:Z:23:GLN:HG3	1.99	0.44
1:E:485:LYS:HB3	1:E:506:ARG:HG2	2.00	0.44
1:G:466:ASN:ND2	1:I:411:ASN:OD1	2.44	0.44
1:G:646:LEU:HD12	1:G:646:LEU:HA	1.85	0.44
1:H:85:LEU:HD13	1:H:614:LEU:HD21	1.98	0.44
1:H:485:LYS:O	1:H:506:ARG:NH2	2.51	0.44
1:H:681:ARG:HG3	1:H:717:PHE:CZ	2.53	0.44
1:I:688:PRO:HB3	1:I:698:TYR:CZ	2.53	0.44
1:J:841:TYR:CE1	1:K:221:ARG:HB2	2.53	0.44
5:U:6:PRO:HG2	5:U:196:VAL:HG23	1.99	0.44
1:A:14:ILE:HA	1:A:14:ILE:HD13	1.77	0.44
1:A:407:ASP:N	1:A:407:ASP:OD1	2.51	0.44
1:B:516:TYR:HA	1:B:519:LEU:HD21	2.00	0.44
1:B:773:TYR:O	1:B:775:ILE:HG13	2.18	0.44
1:C:497:PRO:HA	1:C:502:TYR:CG	2.52	0.44
1:F:19:ALA:N	1:F:46:ASN:OD1	2.30	0.44
1:F:426:THR:HG23	1:F:447:ASP:HA	1.98	0.44
1:F:440:LYS:HG2	1:F:441:ASP:H	1.83	0.44
1:G:916:TYR:CZ	1:G:918:LEU:HD22	2.52	0.44
1:H:373:LEU:HB3	1:H:379:ARG:NH1	2.32	0.44
1:H:928:HIS:CD2	1:H:930:PRO:HD3	2.53	0.44
1:J:403:HIS:NE2	1:K:547:MET:SD	2.90	0.44
1:K:200:GLN:O	1:K:201:PRO:C	2.50	0.44
1:L:352:SER:O	1:L:353:GLN:NE2	2.50	0.44
2:N:96:ILE:HD12	2:N:96:ILE:HG23	1.71	0.44
5:V:139:SER:HB3	5:V:164:PRO:HD2	1.98	0.44
1:C:355:ASN:OD1	1:C:356:ALA:N	2.50	0.44
1:C:921:VAL:CG1	1:C:943:PRO:HB2	2.44	0.44
1:E:19:ALA:HA	1:E:22:TYR:CE2	2.52	0.44
1:E:744:ILE:HG12	1:E:764:TRP:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:650:ASN:ND2	1:F:650:ASN:H	2.13	0.44
1:G:299:ILE:HG21	1:G:302:MET:HE2	2.00	0.44
1:G:573:LEU:HD12	1:G:929:ARG:HH12	1.82	0.44
1:I:425:LEU:HD12	1:I:451:ILE:HD13	1.99	0.44
1:K:634:ARG:HH22	1:K:932:ARG:HA	1.81	0.44
1:L:523:TRP:CD1	1:L:802:ARG:HD3	2.53	0.44
1:L:634:ARG:NH2	1:L:932:ARG:HA	2.33	0.44
3:M:275:PHE:O	3:M:276:GLN:C	2.56	0.44
4:P:55:THR:O	4:P:56:PRO:C	2.53	0.44
4:S:122:LEU:HD23	4:S:122:LEU:HA	1.87	0.44
5:V:13:TYR:CE2	5:V:15:PRO:HA	2.53	0.44
1:A:460:GLU:HB2	1:C:416:LEU:HD23	1.99	0.44
1:A:569:LYS:HB3	1:A:569:LYS:HE2	1.69	0.44
1:B:66:ARG:HG3	1:B:615:TYR:CZ	2.53	0.44
1:C:563:GLN:OE1	1:C:565:PHE:N	2.38	0.44
1:C:770:LEU:HB3	1:C:878:PHE:O	2.18	0.44
1:D:45:ARG:NH1	6:Z:27:THR:HG22	2.27	0.44
1:D:99:TYR:OH	1:F:762:LYS:NZ	2.43	0.44
1:G:737:LEU:HB2	1:G:763:ASP:OD2	2.17	0.44
1:G:789:ARG:HH21	6:1:75:ASN:HB3	1.83	0.44
1:H:640:GLN:HE21	1:H:640:GLN:H	1.66	0.44
1:I:397:VAL:HG11	1:I:536:HIS:NE2	2.32	0.44
1:I:716:THR:HB	1:I:907:ASP:HB2	1.99	0.44
1:I:737:LEU:HD13	1:I:753:TYR:CE2	2.52	0.44
1:J:638:ASN:ND2	1:K:24:SER:OG	2.39	0.44
1:K:46:ASN:HB2	6:3:27:THR:OG1	2.18	0.44
1:K:529:ASP:HB3	1:K:715:HIS:NE2	2.33	0.44
1:L:922:PHE:O	1:L:941:ARG:HA	2.17	0.44
4:P:78:ASP:OD1	4:P:79:PHE:N	2.45	0.44
5:V:87:THR:O	5:V:88:THR:C	2.56	0.44
1:A:378:ASP:OD1	1:A:379:ARG:N	2.50	0.44
1:B:495:ASP:OD1	1:B:495:ASP:N	2.49	0.44
1:B:774:ASN:N	1:B:774:ASN:OD1	2.51	0.44
1:C:257:LEU:HD23	1:C:257:LEU:HA	1.83	0.44
1:C:715:HIS:HD2	1:C:716:THR:HG23	1.83	0.44
1:E:409:LEU:HD21	1:F:473:TYR:CG	2.53	0.44
1:E:724:PHE:HE1	1:E:900:LEU:HD13	1.82	0.44
1:F:797:PHE:HD1	1:F:798:GLN:N	2.15	0.44
1:H:222:VAL:O	1:H:287:SER:HA	2.18	0.44
1:H:789:ARG:NH2	6:1:35:PHE:O	2.51	0.44
1:H:856:ASP:OD1	1:H:856:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:734:ASP:O	1:L:62:ARG:HG2	2.18	0.44
5:V:80:TYR:CE1	5:V:195:SER:HB2	2.51	0.44
1:A:325:TYR:HD2	1:A:543:ARG:HA	1.83	0.43
1:A:325:TYR:HE2	1:A:543:ARG:HG3	1.82	0.43
1:A:558:HIS:O	1:A:558:HIS:ND1	2.51	0.43
1:A:678:ALA:HB3	1:A:918:LEU:HB2	1.99	0.43
1:B:730:TRP:C	1:B:732:GLY:N	2.60	0.43
1:D:327:ALA:HB2	1:D:546:SER:HA	1.99	0.43
1:D:542:LEU:HA	1:D:545:ARG:NH1	2.32	0.43
1:D:619:PHE:O	1:D:621:MET:N	2.49	0.43
1:D:844:ASN:OD1	1:D:844:ASN:N	2.50	0.43
1:G:795:ARG:HH21	6:1:73:GLU:C	2.22	0.43
1:H:178:ILE:HD12	1:H:284:VAL:HG23	1.99	0.43
1:J:690:LEU:HD12	1:J:706:TYR:HE2	1.82	0.43
1:L:55:VAL:HG12	1:L:56:THR:HG23	1.99	0.43
1:L:512:LEU:HD23	1:L:818:ILE:HG12	1.99	0.43
1:L:724:PHE:CE1	1:L:900:LEU:HD13	2.53	0.43
5:V:146:LEU:HD12	5:V:152:PHE:CE2	2.53	0.43
6:X:80:VAL:C	6:X:82:ASP:N	2.71	0.43
1:A:178:ILE:HD13	1:A:284:VAL:HG12	2.01	0.43
1:A:425:LEU:HD12	1:A:451:ILE:HB	2.01	0.43
1:B:183:ILE:HG21	1:B:219:ALA:HB2	2.00	0.43
1:B:231:PRO:CG	1:B:318:SER:HB2	2.48	0.43
1:B:574:LEU:HB3	1:B:575:PRO:HD2	2.00	0.43
1:E:379:ARG:HD2	1:E:379:ARG:HA	1.72	0.43
1:F:231:PRO:HG3	1:F:318:SER:HB2	1.99	0.43
1:G:328:PHE:CD2	1:G:549:LEU:HD11	2.53	0.43
1:G:490:ASN:OD1	1:G:490:ASN:N	2.51	0.43
1:J:45:ARG:HH12	6:4:27:THR:HG23	1.83	0.43
1:J:177:ASN:H	1:J:184:GLN:HB3	1.83	0.43
1:J:475:ASN:OD1	1:J:538:ARG:NE	2.51	0.43
1:K:80:LYS:HE2	1:K:581:GLU:OE1	2.18	0.43
1:K:646:LEU:O	1:K:647:SER:C	2.52	0.43
1:L:57:THR:OG1	1:L:58:ASP:N	2.52	0.43
1:L:392:SER:O	1:L:539:ASN:HA	2.18	0.43
1:L:818:ILE:H	1:L:818:ILE:HD12	1.83	0.43
2:N:142:LYS:O	2:N:253:SER:OG	2.20	0.43
6:Y:8:SER:O	6:Y:10:ALA:N	2.51	0.43
1:A:325:TYR:HH	1:C:403:HIS:CE1	2.36	0.43
1:A:921:VAL:HB	1:A:943:PRO:HD2	1.99	0.43
1:B:254:ASN:OD1	1:B:254:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:THR:HG21	1:B:440:LYS:HE3	1.99	0.43
1:B:518:ASN:HB3	1:B:521:ALA:HB3	1.99	0.43
1:D:414:PHE:HB2	1:F:125:PRO:HG3	2.01	0.43
1:E:788:ASP:OD2	1:E:795:ARG:HB2	2.17	0.43
1:F:666:ILE:HD11	1:F:919:PHE:CZ	2.52	0.43
1:G:227:THR:O	1:G:309:ASN:ND2	2.41	0.43
1:H:166:HIS:CE1	1:I:446:SER:HB2	2.53	0.43
1:H:332:PHE:CE2	1:H:387:ASN:HB2	2.53	0.43
1:H:643:ASN:OD1	1:I:45:ARG:HD3	2.18	0.43
1:J:181:GLU:HB2	1:J:194:TYR:CD2	2.54	0.43
1:L:541:GLY:O	1:L:545:ARG:HD3	2.18	0.43
1:L:634:ARG:HG3	1:L:929:ARG:O	2.18	0.43
1:L:825:SER:C	1:L:827:PHE:H	2.22	0.43
3:M:31:MET:SD	3:M:34:ILE:HD11	2.59	0.43
6:1:74:GLN:HE21	6:1:74:GLN:HB2	1.70	0.43
1:A:288:GLU:OE2	1:C:841:TYR:OH	2.25	0.43
1:A:523:TRP:CD1	1:A:802:ARG:HD3	2.53	0.43
1:B:759:ASN:OD1	1:B:759:ASN:N	2.43	0.43
1:B:782:ILE:HD11	1:C:383:PHE:HB2	2.00	0.43
1:C:71:ASP:OD1	1:C:72:ARG:N	2.52	0.43
1:C:327:ALA:HB2	1:C:546:SER:HA	2.00	0.43
1:D:910:ASP:N	1:D:910:ASP:OD1	2.52	0.43
1:E:164:LYS:HD3	1:F:444:GLU:HA	2.00	0.43
1:E:197:LYS:O	1:E:221:ARG:NH2	2.51	0.43
1:G:317:GLN:OE1	1:G:835:MET:HB3	2.18	0.43
1:H:419:VAL:HG21	1:H:452:ARG:HB2	1.99	0.43
1:H:660:THR:O	1:H:660:THR:OG1	2.26	0.43
1:I:248:ILE:HG22	1:I:250:VAL:H	1.84	0.43
1:I:724:PHE:HE1	1:I:900:LEU:HD13	1.82	0.43
1:K:366:GLU:HG3	1:K:707:LEU:HD22	2.01	0.43
2:N:148:MET:HG2	2:N:163:TYR:HE1	1.83	0.43
1:A:257:LEU:HD12	1:A:257:LEU:H	1.82	0.43
1:A:332:PHE:HB3	1:A:335:LEU:HD12	2.00	0.43
1:A:650:ASN:HB3	1:A:916:TYR:HE1	1.83	0.43
1:A:655:ILE:HB	1:A:913:THR:O	2.18	0.43
1:A:689:SER:OG	1:A:695:ASP:OD2	2.27	0.43
1:B:90:ASN:N	1:B:90:ASN:OD1	2.52	0.43
1:B:170:GLN:HG3	1:C:452:ARG:HB3	1.99	0.43
1:C:23:LEU:HD22	1:C:27:LEU:HD23	2.00	0.43
1:C:373:LEU:HB3	1:C:379:ARG:HD3	2.01	0.43
1:C:389:ALA:O	1:C:545:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:LEU:HD23	1:C:528:MET:SD	2.58	0.43
1:C:495:ASP:OD1	1:C:495:ASP:N	2.51	0.43
1:D:902:MET:HE2	1:D:902:MET:HB2	1.86	0.43
1:D:923:ASP:HA	1:D:941:ARG:HB3	1.99	0.43
1:E:403:HIS:HE1	1:F:543:ARG:HB3	1.84	0.43
1:F:773:TYR:O	1:F:775:ILE:HG13	2.19	0.43
1:G:472:LEU:HD23	1:G:472:LEU:HA	1.78	0.43
1:H:408:GLU:HG3	1:I:474:SER:HB2	2.00	0.43
1:H:479:TYR:OH	1:H:537:HIS:ND1	2.41	0.43
1:H:563:GLN:NE2	1:H:580:TYR:OH	2.33	0.43
1:H:737:LEU:HD13	1:H:753:TYR:CE1	2.54	0.43
1:I:818:ILE:HD12	1:I:818:ILE:H	1.83	0.43
1:I:825:SER:O	1:I:827:PHE:N	2.51	0.43
1:J:565:PHE:O	1:J:567:ALA:N	2.52	0.43
1:K:363:ARG:NE	1:K:923:ASP:OD2	2.41	0.43
2:N:274:THR:H	2:N:277:ASP:CG	2.20	0.43
6:Y:76:PHE:HD1	6:Y:77:GLN:H	1.64	0.43
1:A:73:GLU:O	1:A:79:TYR:HB2	2.19	0.43
1:A:788:ASP:OD2	1:A:795:ARG:NE	2.51	0.43
1:C:401:GLU:HG2	1:C:522:ARG:HG3	2.01	0.43
1:C:500:TYR:HB2	1:C:598:ASN:ND2	2.34	0.43
1:D:298:HIS:O	1:D:299:ILE:C	2.53	0.43
1:D:373:LEU:HD23	1:D:373:LEU:HA	1.74	0.43
1:E:737:LEU:HB2	1:E:763:ASP:OD2	2.18	0.43
1:E:830:TYR:CZ	1:E:831:LEU:HD13	2.53	0.43
1:F:828:VAL:HG12	1:F:829:GLY:N	2.32	0.43
1:G:541:GLY:O	1:G:545:ARG:HG3	2.18	0.43
1:H:421:ASN:N	1:H:421:ASN:OD1	2.50	0.43
1:I:83:PHE:N	1:I:580:TYR:O	2.44	0.43
1:J:371:LEU:HB3	1:J:645:TYR:HE2	1.84	0.43
1:J:392:SER:N	1:J:539:ASN:OD1	2.40	0.43
1:J:425:LEU:O	1:J:449:ASN:ND2	2.39	0.43
1:J:601:ARG:NH2	1:J:698:TYR:O	2.52	0.43
1:K:835:MET:HE1	1:L:210:TRP:N	2.33	0.43
4:Q:73:ARG:NH1	4:Q:73:ARG:HB3	2.34	0.43
1:B:409:LEU:HD23	1:B:409:LEU:HA	1.90	0.43
1:B:647:SER:HB3	1:B:675:ARG:NH2	2.32	0.43
1:C:681:ARG:O	1:C:713:LEU:HB2	2.18	0.43
1:C:918:LEU:O	1:C:919:PHE:C	2.54	0.43
1:D:431:LYS:HE2	1:D:434:GLN:HB3	2.01	0.43
1:F:480:LEU:HD23	1:F:528:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:241:ASN:OD1	1:K:243:ASN:N	2.51	0.43
1:K:792:SER:OG	1:K:793:PHE:N	2.52	0.43
1:L:372:LEU:O	1:L:373:LEU:C	2.55	0.43
1:L:492:LYS:HA	1:L:492:LYS:HD2	1.82	0.43
2:N:76:SER:C	2:N:78:ASP:N	2.68	0.43
2:N:220:ASP:OD2	2:N:223:THR:N	2.44	0.43
4:R:103:LEU:HD23	4:R:103:LEU:HA	1.82	0.43
6:W:31:SER:HB2	6:W:33:GLY:N	2.28	0.43
1:A:342:GLY:HA2	1:K:749:ASP:HB3	2.00	0.43
1:A:788:ASP:OD2	1:A:795:ARG:HB2	2.19	0.43
1:B:131:PRO:HB3	1:B:169:GLY:HA2	2.00	0.43
1:B:396:ASP:OD2	6:X:62:SER:HB3	2.17	0.43
1:B:526:ASP:N	1:B:526:ASP:OD1	2.51	0.43
1:B:565:PHE:O	1:B:569:LYS:HB3	2.19	0.43
1:B:639:ASP:OD2	1:B:926:ARG:NH1	2.52	0.43
1:C:619:PHE:O	1:C:621:MET:N	2.49	0.43
1:D:760:MET:HG2	1:D:765:PHE:HB2	2.01	0.43
1:G:373:LEU:HD23	1:G:373:LEU:HA	1.81	0.43
1:G:789:ARG:HH21	6:1:75:ASN:CB	2.32	0.43
1:H:85:LEU:N	1:H:578:TYR:O	2.52	0.43
1:H:318:SER:OG	1:H:319:MET:N	2.51	0.43
1:H:332:PHE:CZ	1:H:387:ASN:HB2	2.54	0.43
1:I:55:VAL:O	1:I:622:ALA:N	2.46	0.43
1:I:373:LEU:HD13	1:I:379:ARG:HH12	1.83	0.43
1:I:694:TYR:OH	4:Q:33:SER:O	2.37	0.43
1:K:409:LEU:HD21	1:L:473:TYR:CG	2.54	0.43
1:L:93:LEU:HB2	1:L:618:PHE:CE2	2.54	0.43
1:L:859:THR:O	4:Q:51:THR:HA	2.19	0.43
3:M:17:GLN:HB2	3:M:18:PRO:HD3	2.00	0.43
4:P:96:ARG:HD3	4:P:96:ARG:HA	1.84	0.43
4:S:18:ARG:H	4:S:18:ARG:HG2	1.67	0.43
5:U:127:THR:HG22	5:U:136:ASN:OD1	2.19	0.43
1:A:79:TYR:HB3	1:A:586:LYS:HE3	2.01	0.43
1:A:635:ASN:OD1	5:U:171:LEU:O	2.37	0.43
1:A:737:LEU:HB2	1:A:763:ASP:OD2	2.19	0.43
1:A:826:GLY:HA2	1:A:838:GLY:C	2.39	0.43
1:B:95:MET:HE1	1:B:580:TYR:HE2	1.84	0.43
1:B:196:ASP:H	1:B:200:GLN:HB2	1.84	0.43
1:B:436:ASN:OD1	1:B:436:ASN:N	2.51	0.43
1:B:635:ASN:ND2	3:M:18:PRO:HB3	2.19	0.43
1:C:891:LEU:HD11	3:M:324:TYR:HD1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:634:ARG:NH2	1:G:932:ARG:HA	2.34	0.43
1:G:871:ARG:NH1	6:2:30:MET:SD	2.92	0.43
1:H:229:MET:N	1:H:309:ASN:OD1	2.51	0.43
1:H:373:LEU:HD23	1:H:373:LEU:HA	1.76	0.43
1:H:679:PHE:O	1:H:680:THR:OG1	2.33	0.43
1:I:196:ASP:N	1:I:196:ASP:OD1	2.51	0.43
1:J:797:PHE:CE2	1:J:799:PRO:HG3	2.53	0.43
1:K:269:THR:OG1	1:L:424:THR:O	2.34	0.43
1:L:66:ARG:HB2	1:L:615:TYR:CE2	2.54	0.43
1:L:472:LEU:HA	1:L:472:LEU:HD23	1.77	0.43
1:L:490:ASN:N	1:L:490:ASN:OD1	2.50	0.43
1:L:634:ARG:NH2	1:L:931:HIS:O	2.52	0.43
4:P:33:SER:O	4:P:34:ILE:C	2.55	0.43
6:Y:62:SER:O	6:Y:65:GLN:HB3	2.18	0.43
1:A:730:TRP:N	1:A:731:PRO:HD2	2.34	0.43
1:A:921:VAL:HG12	1:A:943:PRO:HB2	2.01	0.43
1:D:275:ASN:OD1	1:D:275:ASN:N	2.52	0.43
1:E:19:ALA:HB2	1:E:46:ASN:HB3	2.00	0.43
1:E:383:PHE:HB3	1:E:388:GLN:HB3	2.00	0.43
1:E:410:PRO:HB2	1:E:412:TYR:CE2	2.53	0.43
1:E:490:ASN:OD1	1:E:490:ASN:N	2.49	0.43
1:F:490:ASN:OD1	1:F:490:ASN:N	2.50	0.43
1:F:900:LEU:HD11	1:F:902:MET:HG2	2.00	0.43
1:G:53:HIS:ND1	1:G:54:ASP:OD1	2.52	0.43
1:H:589:ASN:HB2	1:H:601:ARG:HE	1.84	0.43
1:H:708:ASP:HB3	1:H:710:THR:HG23	2.01	0.43
1:J:177:ASN:HA	1:J:217:HIS:CD2	2.54	0.43
1:J:811:LYS:HG2	1:J:812:ASP:OD1	2.18	0.43
1:K:683:LYS:HA	1:K:913:THR:HG22	2.00	0.43
1:L:317:GLN:HE22	1:L:835:MET:H	1.65	0.43
2:N:53:ASN:OD1	2:N:53:ASN:N	2.50	0.43
6:W:32:GLY:HA2	6:W:35:PHE:CD2	2.54	0.43
1:A:472:LEU:HD23	1:A:472:LEU:HA	1.85	0.42
1:D:232:CYS:O	1:D:233:TYR:C	2.53	0.42
1:D:444:GLU:O	1:F:165:THR:N	2.52	0.42
1:F:398:ARG:HH12	1:F:529:ASP:HA	1.84	0.42
1:G:221:ARG:NH2	1:G:288:GLU:OE2	2.46	0.42
1:G:412:TYR:OH	1:H:835:MET:HA	2.19	0.42
1:G:673:ALA:HB2	1:H:9:TRP:CZ2	2.53	0.42
1:H:534:PHE:CZ	1:H:710:THR:HB	2.54	0.42
1:J:389:ALA:HB1	1:J:541:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:111:THR:HG21	1:K:603:ASP:OD2	2.19	0.42
1:K:332:PHE:CZ	1:K:387:ASN:HB2	2.53	0.42
1:L:560:GLN:OE1	1:L:560:GLN:N	2.52	0.42
1:L:598:ASN:O	1:L:701:SER:OG	2.29	0.42
1:L:737:LEU:HD13	1:L:753:TYR:CE2	2.54	0.42
2:N:81:SER:HA	2:N:84:TYR:CE2	2.54	0.42
2:N:438:TYR:HB3	2:N:462:VAL:HG13	2.00	0.42
3:M:169:ARG:HB2	3:M:169:ARG:HH11	1.83	0.42
6:Y:73:GLU:HB3	6:Y:74:GLN:H	1.70	0.42
1:B:740:ASN:HB2	1:B:741:GLU:HG3	2.00	0.42
1:C:66:ARG:HG3	1:C:615:TYR:CZ	2.54	0.42
1:D:521:ALA:HB2	1:E:551:ASN:HB3	2.01	0.42
1:D:664:ILE:CG1	1:D:902:MET:HB3	2.49	0.42
1:D:788:ASP:OD2	1:D:795:ARG:HB2	2.18	0.42
1:D:887:LEU:HD23	1:D:887:LEU:HA	1.72	0.42
1:E:746:ARG:HB2	1:E:761:THR:HG22	2.00	0.42
1:H:178:ILE:HD11	1:H:281:PRO:O	2.19	0.42
1:I:865:CYS:SG	1:I:868:THR:OG1	2.64	0.42
1:J:589:ASN:HD21	1:J:600:LEU:H	1.67	0.42
1:J:744:ILE:HG23	1:J:764:TRP:CD1	2.54	0.42
1:K:329:ARG:HG3	1:K:333:ILE:O	2.19	0.42
1:K:774:ASN:OD1	1:K:774:ASN:N	2.52	0.42
1:L:905:GLU:HG3	4:Q:22:TRP:HZ2	1.84	0.42
6:W:37:TRP:HB2	6:W:38:GLY:H	1.70	0.42
6:X:74:GLN:HE21	6:X:74:GLN:HB2	1.59	0.42
1:A:201:PRO:HG2	1:A:286:TYR:CD1	2.54	0.42
1:A:332:PHE:CZ	1:A:387:ASN:HB2	2.54	0.42
1:A:646:LEU:O	1:A:647:SER:C	2.57	0.42
1:B:786:TYR:CD1	6:X:93:ASP:CB	3.01	0.42
1:C:138:ALA:H	1:C:163:GLN:HA	1.83	0.42
1:E:118:THR:OG1	1:E:119:ALA:N	2.52	0.42
1:E:921:VAL:HG12	1:E:943:PRO:HB2	2.00	0.42
1:G:234:GLY:HA3	1:G:297:THR:HG21	2.00	0.42
1:G:519:LEU:HD23	1:G:519:LEU:HA	1.86	0.42
1:H:472:LEU:O	1:H:473:TYR:C	2.57	0.42
1:H:710:THR:O	1:H:710:THR:OG1	2.35	0.42
1:J:643:ASN:OD1	1:K:45:ARG:HD2	2.19	0.42
1:K:770:LEU:HD23	1:K:770:LEU:HA	1.92	0.42
1:L:85:LEU:N	1:L:578:TYR:O	2.53	0.42
2:N:183:LEU:O	2:N:186:ASN:HB3	2.18	0.42
2:N:217:LEU:HD23	2:N:232:THR:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:393:LEU:HA	2:N:401:THR:HA	2.00	0.42
4:Q:113:GLU:O	4:Q:116:VAL:HG22	2.19	0.42
1:A:413:CYS:HA	1:B:461:ILE:HB	2.02	0.42
1:B:646:LEU:HA	1:B:646:LEU:HD12	1.53	0.42
1:B:918:LEU:O	1:B:919:PHE:C	2.55	0.42
1:C:17:GLN:HB3	1:C:21:GLU:HB2	2.02	0.42
1:C:649:ALA:O	1:C:651:MET:HG2	2.19	0.42
1:D:519:LEU:HA	1:D:519:LEU:HD23	1.77	0.42
1:D:646:LEU:O	1:D:647:SER:C	2.57	0.42
1:E:138:ALA:HB3	1:E:164:LYS:HG3	2.00	0.42
1:E:167:VAL:N	1:F:449:ASN:OD1	2.46	0.42
1:E:363:ARG:NH1	1:E:566:PHE:HE1	2.17	0.42
1:E:414:PHE:CE1	1:F:827:PHE:HD1	2.37	0.42
1:E:751:GLU:H	1:E:751:GLU:HG3	1.69	0.42
1:F:330:ASP:OD2	1:F:370:GLN:NE2	2.33	0.42
1:G:65:LEU:HD12	1:G:618:PHE:CE2	2.54	0.42
1:G:120:TYR:HE1	1:I:846:PRO:HB2	1.83	0.42
1:G:514:ASP:O	1:G:517:ILE:HG22	2.19	0.42
1:I:653:TYR:CD1	1:I:664:ILE:HD11	2.54	0.42
1:I:678:ALA:HB3	1:I:918:LEU:HB2	2.02	0.42
1:K:514:ASP:O	1:K:517:ILE:HG22	2.19	0.42
1:L:337:TYR:CE2	1:L:585:ARG:HG2	2.54	0.42
1:L:619:PHE:O	1:L:621:MET:N	2.48	0.42
2:N:154:THR:OG1	2:N:158:GLN:O	2.25	0.42
3:M:11:ARG:HD3	3:M:122:ARG:NH1	2.34	0.42
5:U:59:ALA:O	5:U:60:ALA:C	2.56	0.42
5:V:137:ASP:OD1	5:V:137:ASP:N	2.52	0.42
6:Y:5:ASN:C	6:Y:7:ALA:H	2.22	0.42
1:A:366:GLU:HG3	1:A:707:LEU:HD22	2.01	0.42
1:A:412:TYR:HE2	1:B:836:ARG:H	1.67	0.42
1:A:589:ASN:ND2	1:A:600:LEU:HB2	2.34	0.42
1:A:942:THR:HB	1:A:943:PRO:HD3	2.00	0.42
1:B:650:ASN:HD22	1:B:650:ASN:N	2.18	0.42
1:D:409:LEU:HB2	1:E:470:ASN:OD1	2.19	0.42
1:D:737:LEU:HD13	1:D:753:TYR:CD1	2.55	0.42
1:D:812:ASP:N	1:D:812:ASP:OD1	2.52	0.42
1:E:514:ASP:O	1:E:517:ILE:HG22	2.19	0.42
1:F:542:LEU:HA	1:F:542:LEU:HD12	1.74	0.42
1:G:782:ILE:HD11	1:H:383:PHE:HB2	2.00	0.42
1:H:75:THR:HG22	1:H:76:ALA:H	1.85	0.42
1:J:329:ARG:HH21	1:J:593:GLN:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:669:ARG:O	1:J:898:HIS:N	2.47	0.42
3:M:33:ARG:HG3	3:M:38:THR:HG21	2.01	0.42
4:Q:100:LEU:HD22	4:Q:100:LEU:HA	1.84	0.42
5:U:131:ARG:HH21	5:U:171:LEU:HD21	1.84	0.42
6:Y:5:ASN:O	6:Y:6:PHE:HB2	2.20	0.42
1:A:97:SER:HB3	1:C:777:TYR:O	2.20	0.42
1:B:389:ALA:O	1:B:545:ARG:NH1	2.53	0.42
1:C:324:ASN:HA	1:C:595:SER:OG	2.20	0.42
1:C:822:HIS:H	1:C:844:ASN:HD21	1.68	0.42
1:C:884:LEU:HD13	1:C:922:PHE:HE2	1.85	0.42
1:E:333:ILE:HD11	1:E:370:GLN:HE21	1.85	0.42
1:F:253:GLN:O	1:F:255:GLY:N	2.53	0.42
1:F:405:THR:OG1	1:F:407:ASP:OD1	2.38	0.42
1:F:724:PHE:CE2	1:F:893:TYR:HE2	2.38	0.42
1:H:371:LEU:HD12	1:H:646:LEU:HD13	2.01	0.42
1:I:298:HIS:NE2	1:I:319:MET:SD	2.92	0.42
1:I:318:SER:OG	1:I:319:MET:N	2.52	0.42
1:J:572:LEU:HA	1:J:572:LEU:HD12	1.78	0.42
1:K:573:LEU:HA	1:K:929:ARG:HH22	1.84	0.42
1:L:382:TYR:HD1	1:L:389:ALA:HA	1.84	0.42
2:N:243:LEU:HD23	2:N:243:LEU:HA	1.92	0.42
2:N:406:TRP:CH2	2:N:425:LEU:HD12	2.54	0.42
5:V:55:LEU:HD21	5:V:194:PRO:HB2	2.01	0.42
5:V:84:PRO:C	5:V:86:PRO:HD3	2.39	0.42
1:B:484:LEU:HD11	1:B:527:TYR:CD1	2.55	0.42
1:C:366:GLU:HG3	1:C:707:LEU:HD22	2.02	0.42
1:C:373:LEU:HD23	1:C:373:LEU:HA	1.83	0.42
1:D:285:LEU:HD23	1:D:285:LEU:HA	1.88	0.42
1:E:93:LEU:HB2	1:E:618:PHE:CE1	2.54	0.42
1:E:110:PRO:HD2	1:E:603:ASP:O	2.19	0.42
1:E:724:PHE:CE2	1:E:893:TYR:HE2	2.37	0.42
1:E:776:GLY:HA2	1:E:780:PHE:HE1	1.83	0.42
1:F:46:ASN:ND2	6:Y:25:ILE:O	2.53	0.42
1:F:788:ASP:OD2	1:F:795:ARG:HB2	2.19	0.42
1:G:480:LEU:HD23	1:G:528:MET:SD	2.59	0.42
1:G:573:LEU:HD12	1:G:929:ARG:NH1	2.34	0.42
1:H:770:LEU:HD23	1:H:770:LEU:HA	1.90	0.42
1:J:209:GLN:CD	1:J:211:TYR:HB3	2.40	0.42
1:J:835:MET:HA	1:L:412:TYR:OH	2.19	0.42
1:K:339:ASN:OD1	1:K:339:ASN:N	2.53	0.42
1:K:542:LEU:HA	1:K:545:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:823:ASN:OD1	1:K:824:ASN:N	2.53	0.42
1:L:301:TYR:CE2	1:L:303:PRO:HG3	2.55	0.42
1:L:337:TYR:CZ	1:L:585:ARG:HG2	2.55	0.42
1:L:817:GLY:O	1:L:821:GLN:HG3	2.19	0.42
1:A:305:ILE:H	1:A:305:ILE:HG13	1.63	0.42
1:A:338:TYR:CZ	1:A:564:LYS:HB2	2.54	0.42
1:A:773:TYR:O	1:A:775:ILE:HG13	2.20	0.42
1:B:178:ILE:HG12	1:B:183:ILE:HG22	2.01	0.42
1:D:12:MET:HB3	1:F:924:VAL:HG11	2.02	0.42
1:D:41:ASN:HA	6:Z:24:ASP:O	2.20	0.42
1:D:438:TRP:HH2	1:F:179:THR:HA	1.84	0.42
1:D:534:PHE:CE1	1:D:710:THR:HB	2.55	0.42
1:E:251:LYS:HG3	1:E:256:LYS:HA	2.01	0.42
1:E:470:ASN:O	1:E:471:PHE:C	2.55	0.42
1:F:32:ARG:HG3	6:Y:20:GLY:O	2.20	0.42
1:F:203:PRO:O	1:F:204:GLN:C	2.57	0.42
1:G:887:LEU:HA	1:G:887:LEU:HD23	1.78	0.42
1:I:251:LYS:HB2	1:I:258:GLU:H	1.84	0.42
1:I:368:SER:OG	1:I:644:ASP:OD1	2.28	0.42
1:I:525:LEU:HD23	1:I:525:LEU:HA	1.86	0.42
1:I:731:PRO:HG3	1:I:742:PHE:CE1	2.55	0.42
1:I:786:TYR:CE1	1:I:787:LYS:HG3	2.55	0.42
1:I:918:LEU:O	1:I:919:PHE:C	2.57	0.42
1:J:457:PHE:HE1	1:K:459:MET:HE1	1.84	0.42
1:J:463:LEU:O	1:J:464:ASN:C	2.56	0.42
1:J:690:LEU:HD23	1:J:690:LEU:HA	1.79	0.42
2:N:217:LEU:HD12	2:N:217:LEU:HA	1.66	0.42
2:N:255:LEU:HA	2:N:255:LEU:HD23	1.74	0.42
1:A:61:GLN:HE21	1:A:91:ARG:HE	1.67	0.42
1:A:667:PRO:HG3	1:K:663:PRO:HG3	2.02	0.42
1:B:391:ASP:OD1	1:B:391:ASP:N	2.39	0.42
1:B:486:TYR:C	1:B:506:ARG:HE	2.23	0.42
1:B:717:PHE:HB3	1:B:744:ILE:HD12	2.02	0.42
1:D:724:PHE:CE1	1:D:900:LEU:HD13	2.55	0.42
1:D:733:ASN:O	1:D:734:ASP:C	2.58	0.42
1:D:818:ILE:H	1:D:818:ILE:HD12	1.85	0.42
1:E:724:PHE:HE2	1:E:893:TYR:HE2	1.67	0.42
1:F:333:ILE:HG12	1:F:366:GLU:OE1	2.20	0.42
1:F:370:GLN:HG3	1:F:708:ASP:HA	2.02	0.42
1:G:571:LEU:HD11	1:G:927:VAL:HG11	2.02	0.42
1:G:835:MET:HA	1:I:412:TYR:OH	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:915:LEU:HG	1:G:917:VAL:HG23	2.02	0.42
1:H:100:PHE:HD2	1:H:612:ILE:HD11	1.85	0.42
1:H:681:ARG:NH2	1:H:909:MET:SD	2.93	0.42
1:H:797:PHE:CD1	1:H:799:PRO:HD3	2.55	0.42
1:I:335:LEU:HD23	1:I:561:VAL:HG21	2.02	0.42
1:K:85:LEU:HD13	1:K:614:LEU:HD21	2.02	0.42
1:K:218:ALA:HB3	1:K:283:VAL:HG22	2.01	0.42
1:K:413:CYS:HA	1:L:461:ILE:HB	2.01	0.42
1:L:126:LYS:HE2	1:L:233:TYR:CE2	2.55	0.42
3:M:387:ASN:HA	5:U:145:GLY:O	2.20	0.42
4:P:88:SER:O	4:P:92:ARG:HG2	2.19	0.42
6:Y:68:ARG:O	6:Y:69:ASP:C	2.57	0.42
1:A:725:ASP:O	1:A:726:SER:OG	2.34	0.42
1:B:874:PHE:CE2	1:B:887:LEU:HB3	2.55	0.42
1:C:450:GLU:OE1	1:C:450:GLU:N	2.52	0.42
1:E:164:LYS:HA	1:F:444:GLU:HB3	2.01	0.42
1:E:177:ASN:OD1	1:E:178:ILE:N	2.50	0.42
1:F:633:LEU:HA	1:F:633:LEU:HD23	1.86	0.42
1:F:836:ARG:H	1:F:836:ARG:HG3	1.66	0.42
1:F:887:LEU:HD23	1:F:887:LEU:HA	1.90	0.42
1:G:519:LEU:HD22	1:H:115:TYR:CG	2.55	0.42
1:G:710:THR:O	1:G:710:THR:OG1	2.29	0.42
1:I:737:LEU:HB2	1:I:763:ASP:OD1	2.19	0.42
1:J:251:LYS:HA	1:J:256:LYS:HA	2.02	0.42
1:K:72:ARG:HD2	1:K:79:TYR:OH	2.20	0.42
3:M:114:LEU:O	3:M:118:VAL:HG13	2.20	0.42
4:P:58:GLU:HA	4:P:61:ALA:H	1.85	0.42
4:Q:35:ASP:OD2	4:Q:37:ARG:NH2	2.48	0.42
5:U:61:ILE:HG13	5:U:62:THR:H	1.84	0.42
5:V:210:ASP:HB3	5:V:216:PHE:CE2	2.55	0.42
6:Y:63:THR:H	6:Y:63:THR:HG22	1.55	0.42
1:A:237:ALA:O	1:A:246:GLN:HG2	2.20	0.41
1:D:557:PHE:HD1	1:D:557:PHE:H	1.68	0.41
1:E:93:LEU:HB2	1:E:618:PHE:HE1	1.84	0.41
1:E:773:TYR:O	1:E:775:ILE:HG13	2.20	0.41
1:F:237:ALA:HB3	1:F:246:GLN:HG2	2.01	0.41
1:F:316:GLN:HG2	1:F:316:GLN:H	1.58	0.41
1:G:382:TYR:CE2	6:1:68:ARG:HD3	2.55	0.41
1:G:513:VAL:HG13	1:G:517:ILE:HG21	2.02	0.41
1:G:523:TRP:CZ3	1:G:862:LYS:HG2	2.54	0.41
1:G:587:ASP:OD2	1:G:601:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:40:LEU:HD12	1:H:40:LEU:HA	1.85	0.41
1:H:472:LEU:HD12	1:H:472:LEU:HA	1.77	0.41
1:I:82:ARG:HG3	1:I:581:GLU:HB2	2.02	0.41
1:I:378:ASP:OD1	1:I:378:ASP:N	2.43	0.41
1:I:950:THR:HA	1:L:890:ASN:HD21	1.85	0.41
1:K:126:LYS:HG2	1:K:233:TYR:CD2	2.55	0.41
1:L:333:ILE:HG12	1:L:366:GLU:OE1	2.19	0.41
1:L:695:ASP:O	1:L:696:PRO:C	2.55	0.41
2:N:276:ASP:OD1	2:N:276:ASP:N	2.53	0.41
3:M:26:ASP:OD1	3:M:26:ASP:N	2.43	0.41
1:A:551:ASN:CG	1:C:521:ALA:HB2	2.41	0.41
1:A:675:ARG:NH2	6:X:30:MET:HB3	2.34	0.41
1:A:803:GLN:OE1	1:B:552:GLY:N	2.50	0.41
1:B:630:GLU:O	1:B:634:ARG:HG3	2.20	0.41
1:B:690:LEU:HD23	1:B:690:LEU:HA	1.84	0.41
1:C:574:LEU:HD23	1:C:574:LEU:HA	1.78	0.41
1:C:635:ASN:OD1	1:C:636:ASP:N	2.54	0.41
1:C:737:LEU:HD13	1:C:753:TYR:CE1	2.55	0.41
1:D:328:PHE:CD1	1:D:549:LEU:HD11	2.55	0.41
1:D:782:ILE:HD11	1:E:383:PHE:HB2	2.01	0.41
1:E:74:ASP:OD1	1:E:586:LYS:NZ	2.38	0.41
1:E:265:PHE:HB2	1:F:428:VAL:O	2.20	0.41
1:E:463:LEU:O	1:E:464:ASN:C	2.53	0.41
1:E:539:ASN:HB3	1:E:542:LEU:HB3	2.03	0.41
1:E:744:ILE:HG23	1:E:764:TRP:CD1	2.55	0.41
1:E:806:ASP:OD1	1:E:809:LYS:N	2.37	0.41
1:F:174:SER:HB2	1:F:215:ILE:HD13	2.02	0.41
1:F:373:LEU:HD23	1:F:373:LEU:HA	1.83	0.41
1:F:468:TRP:O	1:F:469:ARG:C	2.58	0.41
1:F:690:LEU:HD12	1:F:690:LEU:HA	1.84	0.41
1:G:549:LEU:HD23	1:G:549:LEU:HA	1.86	0.41
1:G:660:THR:O	1:G:660:THR:OG1	2.33	0.41
1:G:680:THR:HG21	1:G:711:PHE:HB3	2.01	0.41
1:G:762:LYS:HE3	1:G:762:LYS:HB2	1.87	0.41
1:H:519:LEU:HD13	1:I:115:TYR:CD2	2.55	0.41
1:H:922:PHE:O	1:H:941:ARG:HA	2.20	0.41
1:H:930:PRO:O	1:H:931:HIS:ND1	2.49	0.41
1:I:135:ASP:OD1	1:I:225:LYS:HD2	2.20	0.41
1:I:348:ALA:O	1:I:579:THR:HG22	2.20	0.41
1:J:43:LYS:O	1:J:44:PHE:CG	2.73	0.41
1:K:747:SER:OG	1:K:748:VAL:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:196:ASP:HB3	1:L:200:GLN:HB2	2.02	0.41
2:N:479:GLN:O	2:N:480:ALA:C	2.58	0.41
1:A:563:GLN:OE1	1:A:565:PHE:N	2.40	0.41
1:B:197:LYS:O	1:B:198:THR:C	2.56	0.41
1:B:764:TRP:CZ2	1:B:870:TRP:HB3	2.54	0.41
1:C:112:PHE:HE1	1:C:326:ILE:H	1.67	0.41
1:C:413:CYS:SG	1:C:459:MET:HB2	2.60	0.41
1:C:713:LEU:HD23	1:C:713:LEU:HA	1.84	0.41
1:D:845:PHE:O	1:D:846:PRO:C	2.56	0.41
1:E:877:ASN:ND2	1:F:56:THR:OG1	2.52	0.41
1:G:900:LEU:HD21	1:G:902:MET:HE1	2.02	0.41
1:H:199:PHE:CD2	1:H:243:ASN:HB3	2.55	0.41
1:H:788:ASP:OD2	1:H:795:ARG:NE	2.53	0.41
1:I:397:VAL:HG11	1:I:536:HIS:HE2	1.84	0.41
1:I:408:GLU:H	1:I:408:GLU:HG2	1.60	0.41
1:J:737:LEU:HB2	1:J:763:ASP:OD2	2.20	0.41
1:K:210:TRP:CE3	1:K:417:GLY:HA3	2.56	0.41
1:K:917:VAL:O	1:K:918:LEU:C	2.53	0.41
1:L:135:ASP:OD1	1:L:225:LYS:HD2	2.20	0.41
1:L:202:GLU:HG3	1:L:203:PRO:HD2	2.02	0.41
1:L:335:LEU:HD23	1:L:561:VAL:HG21	2.02	0.41
2:N:129:THR:HG22	2:N:554:VAL:HA	2.02	0.41
2:N:385:ASP:OD2	2:N:389:ARG:HB2	2.20	0.41
3:M:130:ARG:O	3:M:134:GLN:HB2	2.20	0.41
4:P:56:PRO:O	4:P:57:LEU:C	2.56	0.41
4:S:28:ASN:OD1	4:S:43:ASN:ND2	2.53	0.41
1:A:650:ASN:OD1	1:A:918:LEU:HD13	2.21	0.41
1:A:675:ARG:HD2	1:A:922:PHE:CE1	2.55	0.41
1:A:928:HIS:HD2	1:A:930:PRO:HD3	1.85	0.41
1:B:14:ILE:O	1:B:15:SER:C	2.58	0.41
1:B:318:SER:OG	1:B:319:MET:N	2.53	0.41
1:B:420:ILE:O	1:B:422:THR:N	2.53	0.41
1:C:177:ASN:HA	1:C:217:HIS:CD2	2.55	0.41
1:C:463:LEU:HD23	1:C:463:LEU:HA	1.85	0.41
1:C:563:GLN:OE1	1:C:564:LYS:N	2.53	0.41
1:D:136:GLU:OE1	1:D:311:ARG:HB2	2.21	0.41
1:D:162:GLN:HE22	1:D:164:LYS:HG3	1.85	0.41
1:E:818:ILE:HD12	1:E:818:ILE:H	1.86	0.41
1:F:196:ASP:H	1:F:200:GLN:HB2	1.86	0.41
1:F:378:ASP:OD1	1:F:380:THR:N	2.54	0.41
1:F:534:PHE:CE2	1:F:710:THR:HB	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:731:PRO:O	1:F:733:ASN:N	2.54	0.41
1:F:845:PHE:O	1:F:846:PRO:C	2.50	0.41
1:G:634:ARG:HH22	1:G:932:ARG:HA	1.84	0.41
1:G:841:TYR:O	1:G:842:PRO:C	2.54	0.41
1:G:900:LEU:HD12	1:G:901:ASP:N	2.35	0.41
1:H:589:ASN:CB	1:H:601:ARG:HE	2.33	0.41
1:I:52:THR:OG1	1:I:53:HIS:N	2.53	0.41
1:I:329:ARG:NH1	1:I:702:GLY:O	2.36	0.41
1:J:372:LEU:HD12	1:J:645:TYR:HB2	2.02	0.41
1:J:635:ASN:OD1	1:J:637:THR:HG22	2.21	0.41
1:A:58:ASP:N	1:A:58:ASP:OD1	2.53	0.41
1:C:51:PRO:HD3	6:W:11:PRO:HA	2.01	0.41
1:C:133:GLU:HG2	1:C:167:VAL:HG13	2.02	0.41
1:C:325:TYR:CD2	1:C:543:ARG:HA	2.56	0.41
1:D:347:LEU:HA	1:D:579:THR:O	2.21	0.41
1:D:451:ILE:HA	1:F:169:GLY:O	2.20	0.41
1:E:275:ASN:O	1:E:275:ASN:ND2	2.54	0.41
1:E:432:THR:OG1	1:E:439:GLU:HB2	2.20	0.41
1:F:329:ARG:NH1	1:F:704:ILE:HG13	2.36	0.41
1:F:578:TYR:HE2	1:F:935:ILE:HG13	1.86	0.41
1:F:669:ARG:O	1:F:898:HIS:N	2.39	0.41
1:G:589:ASN:HD21	1:G:601:ARG:HB2	1.85	0.41
1:H:112:PHE:CE2	1:H:114:PRO:HD3	2.55	0.41
1:H:335:LEU:HD23	1:H:335:LEU:HA	1.77	0.41
1:J:204:GLN:H	1:J:204:GLN:HG2	1.39	0.41
1:J:362:ASP:HB2	1:J:941:ARG:HH22	1.85	0.41
1:J:429:LYS:HE2	1:J:429:LYS:HB3	1.86	0.41
1:J:522:ARG:NH2	1:J:798:GLN:OE1	2.54	0.41
1:K:329:ARG:HB2	1:K:333:ILE:H	1.85	0.41
1:K:689:SER:O	1:K:691:GLY:N	2.52	0.41
1:L:400:ILE:HD13	1:L:525:LEU:HG	2.03	0.41
1:L:825:SER:O	1:L:827:PHE:HD2	2.02	0.41
2:N:154:THR:HB	2:N:156:ASP:OD1	2.21	0.41
3:M:259:THR:HA	3:M:262:ARG:NH1	2.36	0.41
1:A:379:ARG:HD2	1:A:379:ARG:HA	1.70	0.41
1:B:355:ASN:OD1	1:B:356:ALA:N	2.53	0.41
1:C:99:TYR:CD2	1:C:560:GLN:HB3	2.55	0.41
1:C:202:GLU:O	1:C:203:PRO:C	2.57	0.41
1:D:407:ASP:OD1	1:D:407:ASP:N	2.54	0.41
1:D:792:SER:O	1:D:796:ASN:ND2	2.54	0.41
1:E:212:GLU:H	1:E:212:GLU:HG2	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:328:PHE:CE1	1:F:549:LEU:HD11	2.55	0.41
1:F:374:ASP:OD1	1:F:789:ARG:HB3	2.20	0.41
1:F:864:LEU:HD23	1:F:864:LEU:HA	1.83	0.41
1:G:754:ASN:HD22	1:G:759:ASN:HA	1.85	0.41
1:H:532:ASN:HA	1:H:533:PRO:HD3	1.94	0.41
1:H:624:ASN:OD1	1:H:624:ASN:N	2.53	0.41
1:H:673:ALA:HB2	1:I:9:TRP:CZ2	2.56	0.41
1:I:40:LEU:HA	1:I:40:LEU:HD23	1.88	0.41
1:J:93:LEU:HB2	1:J:618:PHE:CE2	2.55	0.41
1:K:125:PRO:HG2	1:K:128:ALA:HB2	2.01	0.41
1:K:275:ASN:O	1:K:279:LEU:N	2.54	0.41
1:K:889:GLN:NE2	1:L:52:THR:HG22	2.35	0.41
2:N:407:TYR:O	2:N:408:LEU:C	2.56	0.41
5:V:80:TYR:CE2	5:V:82:GLU:HA	2.56	0.41
6:Y:63:THR:HA	6:Y:66:MET:HG2	2.02	0.41
6:1:22:TRP:HE3	6:1:22:TRP:H	1.68	0.41
1:A:281:PRO:HD3	1:B:438:TRP:CE3	2.55	0.41
1:B:810:TYR:HD2	1:B:813:TYR:N	2.18	0.41
1:B:829:GLY:HA2	1:B:837:GLU:HG2	2.03	0.41
1:C:737:LEU:HB2	1:C:763:ASP:OD2	2.20	0.41
1:D:45:ARG:HD2	6:Z:27:THR:HG22	2.03	0.41
1:D:572:LEU:HA	1:D:572:LEU:HD12	1.88	0.41
1:E:842:PRO:HB3	1:F:235:SER:HB2	2.03	0.41
1:F:482:ASP:OD2	1:F:502:TYR:OH	2.39	0.41
1:G:209:GLN:NE2	1:I:312:GLU:O	2.51	0.41
1:G:574:LEU:HD23	1:G:574:LEU:HA	1.86	0.41
1:I:744:ILE:HG12	1:I:764:TRP:CD2	2.56	0.41
1:J:369:TYR:HE1	1:J:569:LYS:HE3	1.85	0.41
1:J:779:GLY:N	1:K:97:SER:OG	2.53	0.41
1:J:921:VAL:HB	1:J:922:PHE:H	1.65	0.41
1:K:285:LEU:HD23	1:K:285:LEU:HA	1.83	0.41
1:L:55:VAL:O	1:L:622:ALA:N	2.43	0.41
1:L:372:LEU:O	1:L:375:SER:N	2.54	0.41
1:L:372:LEU:HD23	1:L:569:LYS:NZ	2.36	0.41
2:N:58:SER:OG	2:N:59:GLU:OE1	2.20	0.41
2:N:105:GLU:OE1	2:N:105:GLU:N	2.52	0.41
4:S:46:THR:O	4:S:46:THR:OG1	2.31	0.41
1:A:910:ASP:OD1	1:A:910:ASP:N	2.39	0.41
1:A:921:VAL:HA	1:A:943:PRO:HG2	2.02	0.41
1:B:275:ASN:ND2	1:B:277:ASP:HB3	2.36	0.41
1:C:112:PHE:HD1	1:C:326:ILE:HB	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ASP:HA	1:C:165:THR:HA	2.02	0.41
1:C:364:ASN:ND2	1:C:706:TYR:O	2.54	0.41
1:C:534:PHE:CZ	1:C:710:THR:HB	2.56	0.41
1:C:759:ASN:OD1	1:C:759:ASN:N	2.51	0.41
1:D:40:LEU:HD23	1:D:40:LEU:HA	1.82	0.41
1:D:90:ASN:OD1	1:D:90:ASN:N	2.52	0.41
1:D:236:TYR:CE2	1:F:848:PRO:HD3	2.56	0.41
1:D:374:ASP:OD1	1:D:789:ARG:HB3	2.21	0.41
1:D:745:LYS:NZ	4:P:48:THR:OG1	2.50	0.41
1:F:398:ARG:NH1	1:F:529:ASP:HA	2.35	0.41
1:F:463:LEU:HD23	1:F:463:LEU:HA	1.85	0.41
1:G:66:ARG:NH2	1:G:613:CYS:SG	2.93	0.41
1:G:366:GLU:HG3	1:G:707:LEU:HD22	2.02	0.41
1:G:538:ARG:HD3	6:1:67:LEU:HD11	2.03	0.41
1:H:112:PHE:HD1	1:H:326:ILE:HB	1.84	0.41
1:H:113:LYS:HE2	1:H:115:TYR:O	2.21	0.41
1:H:391:ASP:HB3	1:H:539:ASN:HD21	1.85	0.41
1:J:634:ARG:HD3	1:J:929:ARG:O	2.20	0.41
1:K:373:LEU:HD23	1:K:373:LEU:HA	1.82	0.41
1:K:915:LEU:HG	1:K:917:VAL:HG22	2.03	0.41
3:M:146:PHE:HB2	3:M:187:TYR:CG	2.56	0.41
1:A:91:ARG:HD3	1:A:618:PHE:CD2	2.56	0.41
1:B:35:GLU:OE2	1:B:41:ASN:ND2	2.54	0.41
1:B:95:MET:HE3	1:B:95:MET:HB3	1.88	0.41
1:B:472:LEU:O	1:B:473:TYR:C	2.57	0.41
1:B:843:ALA:HB3	1:C:120:TYR:HD2	1.86	0.41
1:C:199:PHE:CD2	1:C:243:ASN:HB3	2.56	0.41
1:C:633:LEU:HD23	1:C:633:LEU:HA	1.88	0.41
1:C:713:LEU:HA	1:C:715:HIS:CE1	2.56	0.41
1:C:770:LEU:HD23	1:C:770:LEU:HA	1.89	0.41
1:D:806:ASP:OD1	1:D:809:LYS:N	2.37	0.41
1:E:112:PHE:CD1	1:E:326:ILE:HB	2.56	0.41
1:E:137:ALA:HA	1:E:163:GLN:HA	2.02	0.41
1:E:412:TYR:OH	1:F:835:MET:HA	2.21	0.41
1:E:539:ASN:O	1:E:543:ARG:HG3	2.21	0.41
1:E:650:ASN:OD1	1:E:918:LEU:HD23	2.21	0.41
1:E:737:LEU:HA	1:F:62:ARG:HH21	1.85	0.41
1:E:939:TYR:N	1:E:939:TYR:CD1	2.89	0.41
1:F:392:SER:O	1:F:539:ASN:HA	2.21	0.41
1:F:724:PHE:CE1	1:F:900:LEU:HD13	2.56	0.41
1:F:866:ASP:OD1	1:F:866:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:910:ASP:OD1	1:F:910:ASP:N	2.52	0.41
1:G:82:ARG:HA	1:G:581:GLU:HA	2.03	0.41
1:G:93:LEU:HB2	1:G:618:PHE:CE1	2.55	0.41
1:G:213:THR:C	1:G:214:GLU:HG3	2.41	0.41
1:G:565:PHE:O	1:G:569:LYS:HB3	2.20	0.41
1:H:328:PHE:HD1	1:H:549:LEU:HD11	1.86	0.41
1:H:371:LEU:HB3	1:H:645:TYR:HE2	1.85	0.41
1:H:373:LEU:HD13	1:H:379:ARG:HH12	1.85	0.41
1:H:595:SER:C	1:H:597:GLY:N	2.73	0.41
1:I:93:LEU:HB2	1:I:618:PHE:CE2	2.56	0.41
1:I:222:VAL:HG11	1:I:285:LEU:HD13	2.03	0.41
1:I:534:PHE:CZ	1:I:710:THR:HB	2.56	0.41
1:I:789:ARG:N	1:I:792:SER:OG	2.53	0.41
1:J:199:PHE:CD2	1:J:243:ASN:HB3	2.55	0.41
1:J:251:LYS:HD2	1:J:256:LYS:HD2	2.03	0.41
1:J:373:LEU:HD23	1:J:373:LEU:HA	1.81	0.41
1:J:446:SER:O	1:J:449:ASN:ND2	2.52	0.41
1:K:336:MET:HG3	1:K:561:VAL:HG11	2.03	0.41
1:L:210:TRP:CE3	1:L:417:GLY:HA3	2.56	0.41
1:L:373:LEU:HD23	1:L:373:LEU:HA	1.84	0.41
1:L:753:TYR:O	1:L:762:LYS:HB2	2.21	0.41
2:N:168:PHE:HD2	2:N:187:ALA:HB1	1.86	0.41
2:N:170:LEU:HD22	2:N:183:LEU:HG	2.02	0.41
3:M:349:ARG:O	3:M:351:MET:N	2.51	0.41
4:Q:10:ILE:HG12	4:R:26:ARG:HA	2.03	0.41
5:U:128:ILE:H	5:U:128:ILE:HD12	1.86	0.41
5:V:205:PRO:HA	5:V:208:TYR:CE2	2.56	0.41
1:A:335:LEU:HD23	1:A:335:LEU:HA	1.87	0.41
1:A:456:ASN:OD1	1:A:456:ASN:N	2.54	0.41
1:A:542:LEU:HD23	1:A:542:LEU:HA	1.84	0.41
1:A:633:LEU:HD23	1:A:633:LEU:HA	1.87	0.41
1:B:500:TYR:HB2	1:B:598:ASN:ND2	2.36	0.41
1:B:820:HIS:HA	1:C:204:GLN:HE22	1.86	0.41
1:C:59:ARG:HD2	1:C:623:HIS:CE1	2.56	0.41
1:C:329:ARG:NH2	1:C:592:LEU:O	2.54	0.41
1:C:646:LEU:HD12	1:C:646:LEU:HA	1.84	0.41
1:D:380:THR:HG21	6:Y:71:LEU:HA	2.02	0.41
1:E:574:LEU:HD23	1:E:574:LEU:HA	1.84	0.41
1:F:104:GLY:HA3	1:F:557:PHE:CZ	2.56	0.41
1:G:502:TYR:OH	1:G:506:ARG:NE	2.54	0.41
1:G:554:TYR:HB2	1:I:857:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:338:TYR:CZ	1:H:564:LYS:HB2	2.56	0.41
1:I:447:ASP:N	1:I:447:ASP:OD1	2.54	0.41
1:I:573:LEU:HD11	1:I:578:TYR:CE2	2.56	0.41
1:I:776:GLY:HA2	1:I:780:PHE:HE1	1.86	0.41
1:I:832:ALA:O	1:I:834:THR:N	2.49	0.41
1:J:51:PRO:HD3	6:3:11:PRO:HA	2.03	0.41
1:J:252:GLN:HG3	1:J:258:GLU:CD	2.41	0.41
1:J:407:ASP:O	1:K:126:LYS:NZ	2.42	0.41
1:J:664:ILE:HD11	1:J:902:MET:HG3	2.02	0.41
1:K:277:ASP:OD1	1:K:277:ASP:N	2.53	0.41
1:L:328:PHE:CD2	1:L:549:LEU:HD11	2.56	0.41
1:L:413:CYS:SG	1:L:459:MET:HB2	2.61	0.41
1:L:691:GLY:HA3	4:P:21:PRO:O	2.21	0.41
1:L:772:ASN:N	1:L:772:ASN:OD1	2.53	0.41
2:N:179:MET:HE3	2:N:179:MET:HB3	1.79	0.41
2:N:183:LEU:O	2:N:184:MET:C	2.57	0.41
3:M:235:LEU:O	3:M:239:ILE:HG13	2.21	0.41
3:M:244:ASP:O	3:M:247:SER:OG	2.30	0.41
4:Q:104:LEU:HD23	4:Q:104:LEU:HA	1.91	0.41
5:U:13:TYR:HB2	5:U:188:PHE:CE2	2.56	0.41
5:V:13:TYR:OH	5:V:184:GLY:O	2.25	0.41
5:V:211:GLN:H	5:V:211:GLN:HG2	1.60	0.41
1:A:680:THR:HG23	1:A:714:ASN:ND2	2.36	0.40
1:A:835:MET:HE3	1:A:835:MET:HB3	1.71	0.40
1:C:512:LEU:HD23	1:C:818:ILE:HG12	2.03	0.40
1:C:514:ASP:OD1	1:C:515:CYS:N	2.45	0.40
1:C:692:SER:OG	1:C:694:TYR:O	2.34	0.40
1:D:456:ASN:OD1	1:E:836:ARG:HD2	2.21	0.40
1:D:560:GLN:NE2	1:F:755:VAL:HG12	2.36	0.40
1:E:61:GLN:NE2	1:E:91:ARG:HG2	2.36	0.40
1:E:818:ILE:HA	1:E:821:GLN:HG2	2.03	0.40
1:F:201:PRO:CG	1:F:286:TYR:CE2	3.02	0.40
1:G:90:ASN:HD22	1:G:623:HIS:HB3	1.86	0.40
1:G:640:GLN:HG2	1:H:44:PHE:HE1	1.86	0.40
1:G:676:GLY:N	1:G:920:GLU:HB2	2.35	0.40
1:H:832:ALA:HA	1:H:833:PRO:HD3	1.93	0.40
1:I:178:ILE:HG13	1:I:217:HIS:HD2	1.86	0.40
1:I:251:LYS:HB3	1:I:256:LYS:C	2.42	0.40
1:I:373:LEU:HD23	1:I:373:LEU:HA	1.80	0.40
1:I:633:LEU:HD23	1:I:633:LEU:HA	1.86	0.40
1:J:65:LEU:HD23	1:J:65:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:534:PHE:CE1	1:J:710:THR:HB	2.56	0.40
1:K:942:THR:O	5:U:29:THR:HG22	2.21	0.40
1:L:776:GLY:HA2	1:L:780:PHE:CE1	2.57	0.40
2:N:102:SER:HB2	2:N:105:GLU:OE1	2.20	0.40
3:M:179:GLU:OE2	5:U:207:HIS:NE2	2.38	0.40
6:X:62:SER:O	6:X:64:GLY:N	2.48	0.40
6:1:24:ASP:N	6:1:24:ASP:OD1	2.52	0.40
6:3:77:GLN:O	6:3:78:GLN:C	2.59	0.40
1:A:421:ASN:OD1	1:A:421:ASN:N	2.54	0.40
1:A:518:ASN:HB3	1:A:521:ALA:HB3	2.03	0.40
1:B:680:THR:HG23	1:B:714:ASN:OD1	2.21	0.40
1:C:251:LYS:HB2	1:C:258:GLU:O	2.20	0.40
1:C:681:ARG:HH21	1:C:913:THR:HG21	1.85	0.40
1:C:774:ASN:OD1	1:C:774:ASN:N	2.55	0.40
1:E:294:THR:HB	1:E:297:THR:HG23	2.02	0.40
1:E:335:LEU:HA	1:E:335:LEU:HD23	1.87	0.40
1:E:757:GLN:HE21	1:E:757:GLN:HB2	1.73	0.40
1:F:759:ASN:ND2	1:F:861:LYS:O	2.43	0.40
1:G:758:CYS:SG	1:G:760:MET:HB3	2.61	0.40
1:G:876:SER:OG	1:G:886:ASP:OD2	2.30	0.40
1:H:871:ARG:NH1	6:1:31:SER:HB3	2.37	0.40
1:I:650:ASN:HB3	1:I:916:TYR:CE1	2.55	0.40
1:J:588:VAL:HA	1:J:591:VAL:HG22	2.03	0.40
1:K:864:LEU:HA	1:K:864:LEU:HD23	1.43	0.40
1:L:587:ASP:OD1	1:L:590:MET:N	2.54	0.40
1:L:789:ARG:HH22	6:3:80:VAL:HG11	1.86	0.40
1:B:371:LEU:HD23	1:B:371:LEU:HA	1.83	0.40
1:B:624:ASN:N	1:B:624:ASN:OD1	2.53	0.40
1:B:646:LEU:O	1:B:647:SER:C	2.57	0.40
1:B:922:PHE:CE2	1:C:14:ILE:HG23	2.56	0.40
1:C:357:VAL:HA	1:C:939:TYR:OH	2.22	0.40
1:D:325:TYR:HD2	1:D:543:ARG:HA	1.86	0.40
1:G:573:LEU:HD11	1:G:578:TYR:CZ	2.56	0.40
1:G:818:ILE:H	1:G:818:ILE:HD12	1.86	0.40
1:H:17:GLN:HB3	1:H:21:GLU:HB2	2.03	0.40
1:H:788:ASP:OD2	1:H:795:ARG:HB2	2.21	0.40
1:J:40:LEU:HD23	1:J:40:LEU:HA	1.89	0.40
1:K:177:ASN:HA	1:K:217:HIS:CD2	2.57	0.40
1:K:807:ASP:N	1:K:807:ASP:OD1	2.54	0.40
1:L:18:ASP:OD1	1:L:18:ASP:N	2.54	0.40
1:L:136:GLU:HB3	1:L:166:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:266:PHE:O	1:L:282:LYS:N	2.46	0.40
1:L:811:LYS:HE3	1:L:811:LYS:HB2	1.76	0.40
1:L:825:SER:C	1:L:827:PHE:N	2.75	0.40
2:N:226:VAL:O	2:N:287:LEU:HB3	2.21	0.40
3:M:99:LEU:HA	3:M:99:LEU:HD12	1.83	0.40
4:S:107:LEU:HD23	4:S:107:LEU:HA	1.89	0.40
5:V:210:ASP:HB3	5:V:216:PHE:CD2	2.56	0.40
1:A:36:THR:HG21	6:W:11:PRO:HG2	2.03	0.40
1:A:790:MET:SD	1:A:867:ARG:NH1	2.95	0.40
1:A:853:THR:OG1	1:B:293:GLU:OE2	2.33	0.40
1:B:114:PRO:HA	1:B:325:TYR:CD1	2.57	0.40
1:B:177:ASN:OD1	1:B:178:ILE:N	2.53	0.40
1:B:299:ILE:HG13	1:B:302:MET:HE1	2.02	0.40
1:B:522:ARG:NH2	1:B:798:GLN:OE1	2.52	0.40
1:B:685:LYS:HB3	1:B:685:LYS:HE2	1.87	0.40
1:B:941:ARG:HD2	1:B:944:PHE:O	2.21	0.40
1:D:75:THR:HG22	1:D:76:ALA:H	1.87	0.40
1:D:178:ILE:HD13	1:D:284:VAL:HG23	2.03	0.40
1:D:755:VAL:HG13	1:D:762:LYS:HG2	2.04	0.40
1:E:274:GLY:O	1:E:276:GLY:N	2.55	0.40
1:E:887:LEU:HD12	1:E:887:LEU:HA	1.89	0.40
1:F:134:TRP:HB2	1:F:309:ASN:HB3	2.03	0.40
1:F:405:THR:HG21	1:F:465:ALA:HA	2.03	0.40
1:F:823:ASN:O	1:F:824:ASN:C	2.58	0.40
1:H:213:THR:O	1:H:215:ILE:HG13	2.21	0.40
1:H:398:ARG:CZ	1:H:533:PRO:HG3	2.51	0.40
1:J:82:ARG:HD2	1:J:581:GLU:OE2	2.22	0.40
1:J:897:ALA:O	1:J:898:HIS:ND1	2.54	0.40
1:K:371:LEU:HD12	1:K:646:LEU:HD13	2.03	0.40
1:K:938:VAL:HG13	5:U:33:TYR:HB3	2.03	0.40
1:L:85:LEU:HD13	1:L:614:LEU:HD21	2.01	0.40
4:P:58:GLU:O	4:P:62:SER:HB3	2.22	0.40
1:A:209:GLN:HB3	1:A:211:TYR:CE1	2.56	0.40
1:B:679:PHE:HA	1:B:916:TYR:O	2.21	0.40
1:C:177:ASN:OD1	1:C:178:ILE:N	2.52	0.40
1:D:178:ILE:HG12	1:D:183:ILE:HG22	2.03	0.40
1:D:249:LEU:HD23	1:D:249:LEU:HA	1.79	0.40
1:E:269:THR:OG1	1:F:424:THR:O	2.36	0.40
1:E:329:ARG:HG3	1:E:333:ILE:O	2.22	0.40
1:E:366:GLU:HG3	1:E:707:LEU:HD22	2.03	0.40
1:F:351:ALA:HB3	1:F:934:VAL:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:941:ARG:HD2	1:F:944:PHE:O	2.21	0.40
1:G:196:ASP:H	1:G:200:GLN:CB	2.35	0.40
1:G:248:ILE:HG21	1:G:289:ASP:HB2	2.03	0.40
1:G:551:ASN:CG	1:I:521:ALA:HB2	2.42	0.40
1:G:619:PHE:O	1:G:621:MET:N	2.55	0.40
1:H:324:ASN:HA	1:H:595:SER:OG	2.21	0.40
1:H:471:PHE:O	1:H:475:ASN:HB2	2.22	0.40
1:I:178:ILE:HG13	1:I:217:HIS:CD2	2.55	0.40
1:I:312:GLU:H	1:I:312:GLU:HG3	1.60	0.40
1:I:518:ASN:OD1	1:I:802:ARG:NH1	2.48	0.40
1:I:936:GLU:HA	5:V:156:GLY:O	2.22	0.40
1:J:68:ILE:HD13	1:J:68:ILE:HA	1.81	0.40
1:J:370:GLN:HE21	1:J:708:ASP:HA	1.87	0.40
1:J:383:PHE:HD1	1:J:384:SER:N	2.20	0.40
1:J:572:LEU:HB3	1:J:640:GLN:HE22	1.86	0.40
1:K:317:GLN:HE22	1:K:835:MET:HB3	1.87	0.40
1:L:573:LEU:HA	1:L:929:ARG:NH1	2.31	0.40
2:N:386:SER:C	2:N:388:LYS:N	2.74	0.40
2:N:445:MET:HB2	2:N:463:VAL:HG11	2.03	0.40
2:N:545:ASP:CG	2:N:546:ALA:H	2.24	0.40
3:M:115:ASP:O	3:M:118:VAL:HG22	2.21	0.40
3:M:259:THR:HG22	3:M:262:ARG:HH12	1.86	0.40
6:X:64:GLY:C	6:X:66:MET:N	2.72	0.40
6:Y:30:MET:HB3	6:Y:31:SER:H	1.26	0.40
6:1:71:LEU:O	6:1:73:GLU:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	925/952 (97%)	858 (93%)	65 (7%)	2 (0%)	47 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	925/952 (97%)	855 (92%)	69 (8%)	1 (0%)	51 83
1	C	929/952 (98%)	859 (92%)	69 (7%)	1 (0%)	51 83
1	D	925/952 (97%)	855 (92%)	69 (8%)	1 (0%)	51 83
1	E	922/952 (97%)	854 (93%)	63 (7%)	5 (0%)	29 65
1	F	925/952 (97%)	854 (92%)	66 (7%)	5 (0%)	29 65
1	G	927/952 (97%)	850 (92%)	76 (8%)	1 (0%)	51 83
1	H	929/952 (98%)	857 (92%)	71 (8%)	1 (0%)	51 83
1	I	923/952 (97%)	842 (91%)	78 (8%)	3 (0%)	41 74
1	J	924/952 (97%)	853 (92%)	66 (7%)	5 (0%)	29 65
1	K	927/952 (97%)	850 (92%)	75 (8%)	2 (0%)	47 78
1	L	925/952 (97%)	855 (92%)	67 (7%)	3 (0%)	41 74
2	N	462/571 (81%)	427 (92%)	31 (7%)	4 (1%)	17 53
3	M	355/585 (61%)	328 (92%)	26 (7%)	1 (0%)	41 74
4	P	132/140 (94%)	117 (89%)	14 (11%)	1 (1%)	19 56
4	Q	129/140 (92%)	112 (87%)	17 (13%)	0	100 100
4	R	97/140 (69%)	82 (84%)	15 (16%)	0	100 100
4	S	93/140 (66%)	87 (94%)	6 (6%)	0	100 100
5	U	161/227 (71%)	140 (87%)	21 (13%)	0	100 100
5	V	178/227 (78%)	148 (83%)	26 (15%)	4 (2%)	6 38
6	0	12/250 (5%)	11 (92%)	0	1 (8%)	1 11
6	1	53/250 (21%)	45 (85%)	8 (15%)	0	100 100
6	2	15/250 (6%)	10 (67%)	4 (27%)	1 (7%)	1 17
6	3	56/250 (22%)	52 (93%)	3 (5%)	1 (2%)	8 41
6	4	11/250 (4%)	6 (54%)	5 (46%)	0	100 100
6	W	33/250 (13%)	28 (85%)	4 (12%)	1 (3%)	4 32
6	X	74/250 (30%)	56 (76%)	15 (20%)	3 (4%)	3 26
6	Y	57/250 (23%)	46 (81%)	8 (14%)	3 (5%)	2 21
6	Z	21/250 (8%)	17 (81%)	1 (5%)	3 (14%)	0 3
All	All	13045/15844 (82%)	11954 (92%)	1038 (8%)	53 (0%)	38 69

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	733	ASN
1	D	733	ASN
1	F	197	LYS
1	F	203	PRO
2	N	495	VAL
5	V	85	ALA
6	W	31	SER
1	A	734	ASP
1	E	562	PRO
1	E	566	PHE
1	E	754	ASN
1	F	204	GLN
1	J	647	SER
1	L	826	GLY
6	Z	25	ILE
6	Z	27	THR
1	C	717	PHE
1	E	752	GLY
1	F	410	PRO
1	I	845	PHE
1	I	919	PHE
1	J	566	PHE
1	J	845	PHE
1	L	647	SER
2	N	480	ALA
6	Y	9	LEU
6	Y	59	TRP
6	Y	62	SER
1	F	845	PHE
1	G	845	PHE
2	N	266	PRO
4	P	62	SER
5	V	80	TYR
5	V	83	SER
6	X	75	ASN
6	X	88	ILE
1	I	47	PRO
1	L	845	PHE
2	N	380	LYS
3	M	350	ASN
6	X	81	VAL
6	Z	32	GLY
1	H	845	PHE

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Mol	Chain	Res	Type
1	J	826	GLY
1	K	47	PRO
1	K	845	PHE
6	0	32	GLY
1	A	828	VAL
6	3	25	ILE
1	E	748	VAL
1	J	921	VAL
5	V	148	PRO
6	2	33	GLY

5.3.2 Protein sidechains (i)

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	806/829 (97%)	746 (93%)	60 (7%)	13 44
1	B	807/829 (97%)	753 (93%)	54 (7%)	16 47
1	C	809/829 (98%)	751 (93%)	58 (7%)	14 45
1	D	806/829 (97%)	765 (95%)	41 (5%)	24 55
1	E	804/829 (97%)	747 (93%)	57 (7%)	14 45
1	F	807/829 (97%)	746 (92%)	61 (8%)	13 43
1	G	808/829 (98%)	762 (94%)	46 (6%)	20 52
1	H	809/829 (98%)	761 (94%)	48 (6%)	19 51
1	I	805/829 (97%)	754 (94%)	51 (6%)	18 49
1	J	804/829 (97%)	758 (94%)	46 (6%)	20 52
1	K	808/829 (98%)	758 (94%)	50 (6%)	18 49
1	L	806/829 (97%)	750 (93%)	56 (7%)	15 46
2	N	423/489 (86%)	376 (89%)	47 (11%)	6 29
3	M	304/500 (61%)	283 (93%)	21 (7%)	15 46
4	P	107/112 (96%)	96 (90%)	11 (10%)	7 31
4	Q	104/112 (93%)	94 (90%)	10 (10%)	8 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	R	86/112 (77%)	77 (90%)	9 (10%)	7 30
4	S	85/112 (76%)	77 (91%)	8 (9%)	8 35
5	U	136/186 (73%)	121 (89%)	15 (11%)	6 29
5	V	152/186 (82%)	136 (90%)	16 (10%)	7 30
6	0	12/210 (6%)	10 (83%)	2 (17%)	2 14
6	1	47/210 (22%)	39 (83%)	8 (17%)	2 13
6	2	13/210 (6%)	11 (85%)	2 (15%)	2 17
6	3	50/210 (24%)	43 (86%)	7 (14%)	3 20
6	4	11/210 (5%)	11 (100%)	0	100 100
6	W	26/210 (12%)	20 (77%)	6 (23%)	1 6
6	X	54/210 (26%)	48 (89%)	6 (11%)	6 29
6	Y	50/210 (24%)	38 (76%)	12 (24%)	0 5
6	Z	18/210 (9%)	16 (89%)	2 (11%)	6 29
All	All	11357/13647 (83%)	10547 (93%)	810 (7%)	18 45

All (810) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	25	PRO
1	A	48	THR
1	A	57	THR
1	A	68	ILE
1	A	75	THR
1	A	79	TYR
1	A	90	ASN
1	A	92	VAL
1	A	188	GLU
1	A	198	THR
1	A	207	GLU
1	A	213	THR
1	A	241	ASN
1	A	249	LEU
1	A	254	ASN
1	A	279	LEU
1	A	343	ASN
1	A	373	LEU

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Mol	Chain	Res	Type
1	A	391	ASP
1	A	398	ARG
1	A	429	LYS
1	A	490	ASN
1	A	495	ASP
1	A	499	THR
1	A	507	VAL
1	A	526	ASP
1	A	535	ASN
1	A	542	LEU
1	A	549	LEU
1	A	589	ASN
1	A	596	LEU
1	A	610	ASP
1	A	612	ILE
1	A	637	THR
1	A	639	ASP
1	A	651	MET
1	A	664	ILE
1	A	669	ARG
1	A	682	LEU
1	A	718	LYS
1	A	727	SER
1	A	733	ASN
1	A	741	GLU
1	A	749	ASP
1	A	754	ASN
1	A	755	VAL
1	A	758	CYS
1	A	761	THR
1	A	796	ASN
1	A	828	VAL
1	A	836	ARG
1	A	841	TYR
1	A	847	TYR
1	A	856	ASP
1	A	858	ILE
1	A	866	ASP
1	A	892	LEU
1	A	918	LEU
1	A	941	ARG
1	B	5	MET

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Mol	Chain	Res	Type
1	B	11	TYR
1	B	18	ASP
1	B	38	PHE
1	B	41	ASN
1	B	48	THR
1	B	57	THR
1	B	89	ASP
1	B	90	ASN
1	B	188	GLU
1	B	236	TYR
1	B	249	LEU
1	B	254	ASN
1	B	313	LEU
1	B	350	GLN
1	B	373	LEU
1	B	383	PHE
1	B	386	TRP
1	B	391	ASP
1	B	419	VAL
1	B	436	ASN
1	B	445	PHE
1	B	461	ILE
1	B	466	ASN
1	B	472	LEU
1	B	490	ASN
1	B	542	LEU
1	B	560	GLN
1	B	563	GLN
1	B	580	TYR
1	B	582	TRP
1	B	588	VAL
1	B	612	ILE
1	B	627	SER
1	B	635	ASN
1	B	644	ASP
1	B	690	LEU
1	B	701	SER
1	B	725	ASP
1	B	733	ASN
1	B	740	ASN
1	B	741	GLU
1	B	751	GLU

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Mol	Chain	Res	Type
1	B	774	ASN
1	B	800	MET
1	B	836	ARG
1	B	856	ASP
1	B	858	ILE
1	B	869	LEU
1	B	892	LEU
1	B	901	ASP
1	B	922	PHE
1	B	928	HIS
1	B	948	ASN
1	C	37	TYR
1	C	42	ASN
1	C	48	THR
1	C	53	HIS
1	C	57	THR
1	C	58	ASP
1	C	75	THR
1	C	79	TYR
1	C	130	ASN
1	C	163	GLN
1	C	190	GLN
1	C	198	THR
1	C	202	GLU
1	C	227	THR
1	C	249	LEU
1	C	252	GLN
1	C	260	GLN
1	C	262	GLU
1	C	275	ASN
1	C	278	ASN
1	C	330	ASP
1	C	343	ASN
1	C	373	LEU
1	C	374	ASP
1	C	380	THR
1	C	383	PHE
1	C	391	ASP
1	C	443	THR
1	C	461	ILE
1	C	536	HIS
1	C	560	GLN

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Mol	Chain	Res	Type
1	C	588	VAL
1	C	608	LYS
1	C	610	ASP
1	C	612	ILE
1	C	636	ASP
1	C	639	ASP
1	C	651	MET
1	C	680	THR
1	C	682	LEU
1	C	716	THR
1	C	717	PHE
1	C	718	LYS
1	C	749	ASP
1	C	754	ASN
1	C	811	LYS
1	C	836	ARG
1	C	850	ILE
1	C	868	THR
1	C	869	LEU
1	C	902	MET
1	C	916	TYR
1	C	918	LEU
1	C	929	ARG
1	C	938	VAL
1	C	939	TYR
1	C	941	ARG
1	C	942	THR
1	D	18	ASP
1	D	27	LEU
1	D	68	ILE
1	D	75	THR
1	D	198	THR
1	D	202	GLU
1	D	236	TYR
1	D	289	ASP
1	D	297	THR
1	D	312	GLU
1	D	335	LEU
1	D	343	ASN
1	D	347	LEU
1	D	352	SER
1	D	353	GLN

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Mol	Chain	Res	Type
1	D	374	ASP
1	D	438	TRP
1	D	461	ILE
1	D	469	ARG
1	D	490	ASN
1	D	508	VAL
1	D	563	GLN
1	D	579	THR
1	D	582	TRP
1	D	639	ASP
1	D	650	ASN
1	D	682	LEU
1	D	699	THR
1	D	714	ASN
1	D	741	GLU
1	D	754	ASN
1	D	759	ASN
1	D	760	MET
1	D	761	THR
1	D	812	ASP
1	D	836	ARG
1	D	863	PHE
1	D	865	CYS
1	D	866	ASP
1	D	911	GLU
1	D	929	ARG
1	E	46	ASN
1	E	48	THR
1	E	53	HIS
1	E	57	THR
1	E	75	THR
1	E	89	ASP
1	E	90	ASN
1	E	101	ASP
1	E	106	LEU
1	E	178	ILE
1	E	198	THR
1	E	202	GLU
1	E	235	SER
1	E	253	GLN
1	E	335	LEU
1	E	337	TYR

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Mol	Chain	Res	Type
1	E	343	ASN
1	E	347	LEU
1	E	358	VAL
1	E	359	ASP
1	E	374	ASP
1	E	386	TRP
1	E	391	ASP
1	E	396	ASP
1	E	405	THR
1	E	408	GLU
1	E	428	VAL
1	E	466	ASN
1	E	467	LEU
1	E	490	ASN
1	E	495	ASP
1	E	504	ASN
1	E	506	ARG
1	E	526	ASP
1	E	545	ARG
1	E	561	VAL
1	E	580	TYR
1	E	582	TRP
1	E	588	VAL
1	E	612	ILE
1	E	637	THR
1	E	639	ASP
1	E	647	SER
1	E	651	MET
1	E	682	LEU
1	E	741	GLU
1	E	751	GLU
1	E	757	GLN
1	E	828	VAL
1	E	836	ARG
1	E	841	TYR
1	E	858	ILE
1	E	866	ASP
1	E	916	TYR
1	E	918	LEU
1	E	935	ILE
1	E	938	VAL
1	F	18	ASP

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Mol	Chain	Res	Type
1	F	34	THR
1	F	40	LEU
1	F	42	ASN
1	F	52	THR
1	F	53	HIS
1	F	58	ASP
1	F	70	VAL
1	F	72	ARG
1	F	91	ARG
1	F	141	LEU
1	F	198	THR
1	F	201	PRO
1	F	207	GLU
1	F	214	GLU
1	F	216	ASN
1	F	235	SER
1	F	246	GLN
1	F	260	GLN
1	F	278	ASN
1	F	316	GLN
1	F	335	LEU
1	F	341	THR
1	F	343	ASN
1	F	374	ASP
1	F	383	PHE
1	F	391	ASP
1	F	403	HIS
1	F	419	VAL
1	F	441	ASP
1	F	443	THR
1	F	461	ILE
1	F	466	ASN
1	F	490	ASN
1	F	508	VAL
1	F	526	ASP
1	F	579	THR
1	F	588	VAL
1	F	612	ILE
1	F	636	ASP
1	F	639	ASP
1	F	651	MET
1	F	658	ASN

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Mol	Chain	Res	Type
1	F	682	LEU
1	F	738	THR
1	F	741	GLU
1	F	755	VAL
1	F	759	ASN
1	F	797	PHE
1	F	805	VAL
1	F	812	ASP
1	F	836	ARG
1	F	849	LEU
1	F	853	THR
1	F	866	ASP
1	F	901	ASP
1	F	916	TYR
1	F	918	LEU
1	F	928	HIS
1	F	942	THR
1	F	948	ASN
1	G	18	ASP
1	G	48	THR
1	G	53	HIS
1	G	73	GLU
1	G	90	ASN
1	G	130	ASN
1	G	179	THR
1	G	203	PRO
1	G	270	GLU
1	G	313	LEU
1	G	333	ILE
1	G	335	LEU
1	G	337	TYR
1	G	343	ASN
1	G	364	ASN
1	G	383	PHE
1	G	394	ASP
1	G	396	ASP
1	G	411	ASN
1	G	438	TRP
1	G	441	ASP
1	G	445	PHE
1	G	461	ILE
1	G	490	ASN

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Mol	Chain	Res	Type
1	G	506	ARG
1	G	507	VAL
1	G	508	VAL
1	G	581	GLU
1	G	588	VAL
1	G	612	ILE
1	G	647	SER
1	G	682	LEU
1	G	710	THR
1	G	734	ASP
1	G	738	THR
1	G	754	ASN
1	G	760	MET
1	G	788	ASP
1	G	789	ARG
1	G	819	LEU
1	G	836	ARG
1	G	841	TYR
1	G	858	ILE
1	G	901	ASP
1	G	918	LEU
1	G	929	ARG
1	H	46	ASN
1	H	53	HIS
1	H	68	ILE
1	H	71	ASP
1	H	75	THR
1	H	106	LEU
1	H	183	ILE
1	H	187	VAL
1	H	205	ILE
1	H	253	GLN
1	H	278	ASN
1	H	313	LEU
1	H	317	GLN
1	H	335	LEU
1	H	343	ASN
1	H	374	ASP
1	H	383	PHE
1	H	387	ASN
1	H	396	ASP
1	H	406	GLU

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Mol	Chain	Res	Type
1	H	409	LEU
1	H	416	LEU
1	H	420	ILE
1	H	421	ASN
1	H	461	ILE
1	H	467	LEU
1	H	469	ARG
1	H	475	ASN
1	H	490	ASN
1	H	495	ASP
1	H	560	GLN
1	H	582	TRP
1	H	596	LEU
1	H	612	ILE
1	H	640	GLN
1	H	658	ASN
1	H	660	THR
1	H	700	TYR
1	H	758	CYS
1	H	836	ARG
1	H	847	TYR
1	H	866	ASP
1	H	901	ASP
1	H	902	MET
1	H	905	GLU
1	H	911	GLU
1	H	918	LEU
1	H	929	ARG
1	I	34	THR
1	I	45	ARG
1	I	48	THR
1	I	53	HIS
1	I	70	VAL
1	I	91	ARG
1	I	141	LEU
1	I	185	ILE
1	I	236	TYR
1	I	253	GLN
1	I	277	ASP
1	I	278	ASN
1	I	297	THR
1	I	312	GLU

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Mol	Chain	Res	Type
1	I	322	ARG
1	I	330	ASP
1	I	341	THR
1	I	370	GLN
1	I	374	ASP
1	I	378	ASP
1	I	403	HIS
1	I	441	ASP
1	I	443	THR
1	I	461	ILE
1	I	469	ARG
1	I	470	ASN
1	I	472	LEU
1	I	526	ASP
1	I	574	LEU
1	I	580	TYR
1	I	612	ILE
1	I	637	THR
1	I	639	ASP
1	I	651	MET
1	I	652	LEU
1	I	664	ILE
1	I	680	THR
1	I	689	SER
1	I	700	TYR
1	I	728	VAL
1	I	754	ASN
1	I	755	VAL
1	I	758	CYS
1	I	786	TYR
1	I	811	LYS
1	I	812	ASP
1	I	834	THR
1	I	836	ARG
1	I	841	TYR
1	I	866	ASP
1	I	890	ASN
1	J	18	ASP
1	J	58	ASP
1	J	74	ASP
1	J	75	THR
1	J	106	LEU

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Mol	Chain	Res	Type
1	J	179	THR
1	J	204	GLN
1	J	213	THR
1	J	235	SER
1	J	376	ILE
1	J	380	THR
1	J	383	PHE
1	J	438	TRP
1	J	443	THR
1	J	466	ASN
1	J	467	LEU
1	J	469	ARG
1	J	486	TYR
1	J	490	ASN
1	J	499	THR
1	J	508	VAL
1	J	519	LEU
1	J	530	ASN
1	J	563	GLN
1	J	579	THR
1	J	582	TRP
1	J	612	ILE
1	J	647	SER
1	J	651	MET
1	J	680	THR
1	J	682	LEU
1	J	714	ASN
1	J	734	ASP
1	J	754	ASN
1	J	755	VAL
1	J	759	ASN
1	J	773	TYR
1	J	836	ARG
1	J	841	TYR
1	J	865	CYS
1	J	910	ASP
1	J	922	PHE
1	J	923	ASP
1	J	924	VAL
1	J	929	ARG
1	J	948	ASN
1	K	48	THR

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Mol	Chain	Res	Type
1	K	53	HIS
1	K	57	THR
1	K	68	ILE
1	K	90	ASN
1	K	92	VAL
1	K	198	THR
1	K	202	GLU
1	K	204	GLN
1	K	205	ILE
1	K	275	ASN
1	K	278	ASN
1	K	339	ASN
1	K	343	ASN
1	K	370	GLN
1	K	374	ASP
1	K	383	PHE
1	K	390	VAL
1	K	391	ASP
1	K	405	THR
1	K	408	GLU
1	K	420	ILE
1	K	428	VAL
1	K	461	ILE
1	K	490	ASN
1	K	506	ARG
1	K	508	VAL
1	K	560	GLN
1	K	580	TYR
1	K	582	TRP
1	K	588	VAL
1	K	610	ASP
1	K	612	ILE
1	K	625	THR
1	K	647	SER
1	K	651	MET
1	K	686	GLU
1	K	714	ASN
1	K	738	THR
1	K	749	ASP
1	K	773	TYR
1	K	774	ASN
1	K	804	VAL

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Mol	Chain	Res	Type
1	K	836	ARG
1	K	841	TYR
1	K	891	LEU
1	K	910	ASP
1	K	918	LEU
1	K	922	PHE
1	K	941	ARG
1	L	15	SER
1	L	18	ASP
1	L	42	ASN
1	L	48	THR
1	L	53	HIS
1	L	57	THR
1	L	61	GLN
1	L	74	ASP
1	L	75	THR
1	L	91	ARG
1	L	170	GLN
1	L	185	ILE
1	L	214	GLU
1	L	235	SER
1	L	241	ASN
1	L	279	LEU
1	L	297	THR
1	L	341	THR
1	L	353	GLN
1	L	373	LEU
1	L	396	ASP
1	L	408	GLU
1	L	421	ASN
1	L	443	THR
1	L	445	PHE
1	L	461	ILE
1	L	469	ARG
1	L	490	ASN
1	L	506	ARG
1	L	529	ASP
1	L	582	TRP
1	L	610	ASP
1	L	612	ILE
1	L	625	THR
1	L	632	MET

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Mol	Chain	Res	Type
1	L	634	ARG
1	L	637	THR
1	L	669	ARG
1	L	675	ARG
1	L	682	LEU
1	L	689	SER
1	L	734	ASP
1	L	748	VAL
1	L	754	ASN
1	L	758	CYS
1	L	763	ASP
1	L	812	ASP
1	L	836	ARG
1	L	842	PRO
1	L	849	LEU
1	L	866	ASP
1	L	885	THR
1	L	892	LEU
1	L	901	ASP
1	L	916	TYR
1	L	918	LEU
2	N	37	ASP
2	N	41	VAL
2	N	46	LEU
2	N	47	ARG
2	N	49	THR
2	N	55	ILE
2	N	65	ASP
2	N	79	VAL
2	N	85	GLN
2	N	97	GLN
2	N	99	ASN
2	N	115	ASP
2	N	154	THR
2	N	155	LYS
2	N	157	ASN
2	N	171	PRO
2	N	174	ASN
2	N	176	SER
2	N	205	ASP
2	N	232	THR
2	N	239	ASP

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Mol	Chain	Res	Type
2	N	240	ILE
2	N	246	CYS
2	N	256	SER
2	N	274	THR
2	N	277	ASP
2	N	289	VAL
2	N	374	GLN
2	N	376	LYS
2	N	387	LYS
2	N	405	SER
2	N	430	VAL
2	N	437	VAL
2	N	450	THR
2	N	454	THR
2	N	457	ILE
2	N	479	GLN
2	N	489	PHE
2	N	492	LEU
2	N	493	THR
2	N	531	LEU
2	N	547	ARG
2	N	549	ARG
2	N	555	TYR
2	N	567	SER
2	N	570	THR
2	N	571	PHE
3	M	7	ASP
3	M	24	THR
3	M	46	ARG
3	M	49	PRO
3	M	58	LEU
3	M	74	LEU
3	M	89	ASP
3	M	104	ARG
3	M	117	LEU
3	M	169	ARG
3	M	231	ASN
3	M	243	THR
3	M	276	GLN
3	M	331	LEU
3	M	338	VAL
3	M	339	THR

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Mol	Chain	Res	Type
3	M	364	ASN
3	M	370	LEU
3	M	371	HIS
3	M	390	TRP
3	M	396	PHE
4	P	6	PHE
4	P	10	ILE
4	P	28	ASN
4	P	57	LEU
4	P	58	GLU
4	P	62	SER
4	P	78	ASP
4	P	81	PHE
4	P	98	ASP
4	P	113	GLU
4	P	121	LEU
4	Q	6	PHE
4	Q	28	ASN
4	Q	37	ARG
4	Q	55	THR
4	Q	57	LEU
4	Q	71	THR
4	Q	73	ARG
4	Q	100	LEU
4	Q	121	LEU
4	Q	125	ARG
4	R	17	THR
4	R	26	ARG
4	R	30	MET
4	R	43	ASN
4	R	97	ASP
4	R	107	LEU
4	R	110	LEU
4	R	112	ARG
4	R	121	LEU
4	S	7	ASP
4	S	17	THR
4	S	18	ARG
4	S	22	TRP
4	S	29	VAL
4	S	125	ARG
4	S	127	GLN

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Mol	Chain	Res	Type
4	S	132	LYS
5	U	5	ILE
5	U	7	THR
5	U	26	ASP
5	U	39	HIS
5	U	41	ILE
5	U	55	LEU
5	U	129	ARG
5	U	134	GLN
5	U	146	LEU
5	U	173	THR
5	U	196	VAL
5	U	198	PHE
5	U	215	ASN
5	U	219	VAL
5	U	221	ASP
5	V	14	GLN
5	V	25	GLN
5	V	64	THR
5	V	72	ARG
5	V	129	ARG
5	V	135	LEU
5	V	140	VAL
5	V	144	LEU
5	V	151	THR
5	V	159	ARG
5	V	169	LEU
5	V	179	ARG
5	V	193	VAL
5	V	198	PHE
5	V	207	HIS
5	V	215	ASN
6	W	6	PHE
6	W	9	LEU
6	W	22	TRP
6	W	23	GLN
6	W	25	ILE
6	W	30	MET
6	X	4	ILE
6	X	29	ASN
6	X	59	TRP
6	X	71	LEU

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Mol	Chain	Res	Type
6	X	79	LYS
6	X	80	VAL
6	Y	4	ILE
6	Y	23	GLN
6	Y	25	ILE
6	Y	27	THR
6	Y	41	TRP
6	Y	57	LYS
6	Y	60	ASN
6	Y	63	THR
6	Y	67	LEU
6	Y	70	LYS
6	Y	77	GLN
6	Y	78	GLN
6	Z	24	ASP
6	Z	30	MET
6	0	27	THR
6	0	30	MET
6	1	25	ILE
6	1	29	ASN
6	1	40	LEU
6	1	60	ASN
6	1	63	THR
6	1	70	LYS
6	1	71	LEU
6	1	74	GLN
6	2	5	ASN
6	2	30	MET
6	3	9	LEU
6	3	13	HIS
6	3	30	MET
6	3	35	PHE
6	3	69	ASP
6	3	72	LYS
6	3	81	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	504	ASN
1	A	822	HIS
1	B	350	GLN

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Mol	Chain	Res	Type
1	C	821	GLN
1	C	822	HIS
1	D	246	GLN
1	D	331	ASN
1	E	264	GLN
1	E	822	HIS
1	F	246	GLN
1	F	317	GLN
1	F	411	ASN
1	F	466	ASN
1	F	560	GLN
1	G	200	GLN
1	G	204	GLN
1	G	252	GLN
1	G	260	GLN
1	G	822	HIS
1	H	217	HIS
1	H	928	HIS
1	J	200	GLN
1	J	204	GLN
1	J	466	ASN
1	J	530	ASN
1	J	583	ASN
1	K	822	HIS
1	L	822	HIS
2	N	99	ASN
2	N	174	ASN
3	M	111	GLN
3	M	273	HIS
3	M	276	GLN
4	Q	127	GLN
6	X	74	GLN
6	Y	13	HIS
6	Y	23	GLN
6	Z	23	GLN
6	1	74	GLN

5.3.3 RNA

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 (i)

There are no chain breaks in this entry.

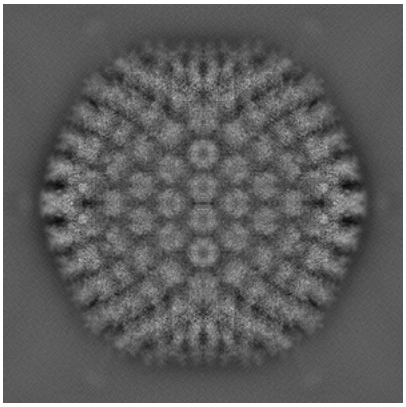
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24881. These allow visual inspection of the internal detail of the map and identification of artifacts.

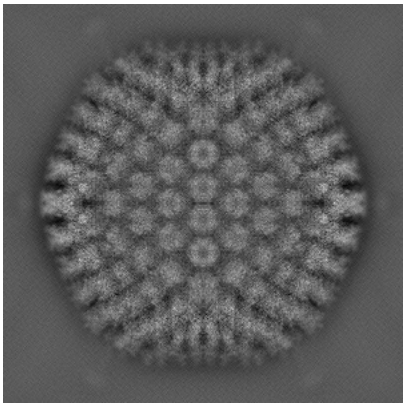
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

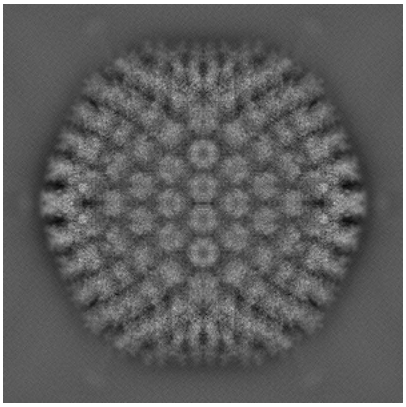
6.1.1 Primary map



X



Y

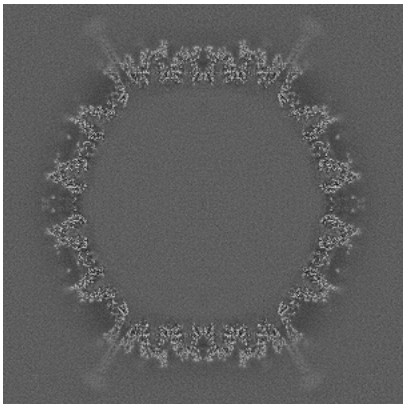


Z

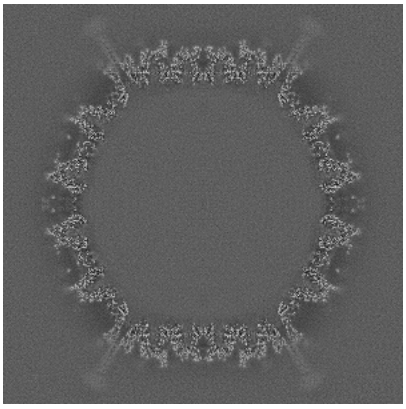
The images above show the map projected in three orthogonal directions.

6.2 Central slices

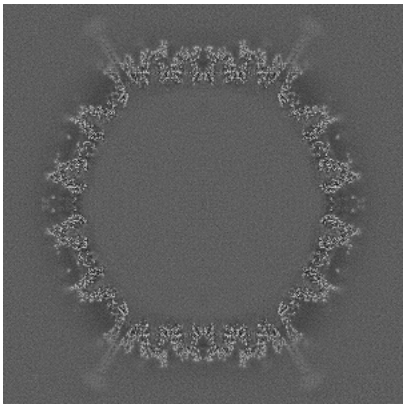
6.2.1 Primary map



X Index: 416



Y Index: 416

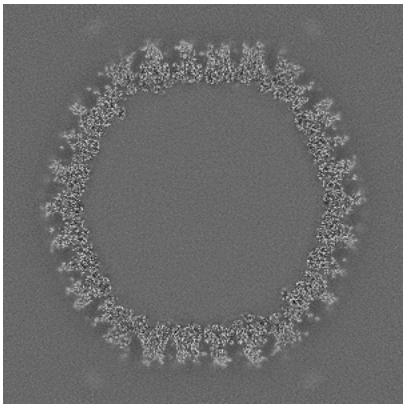


Z Index: 416

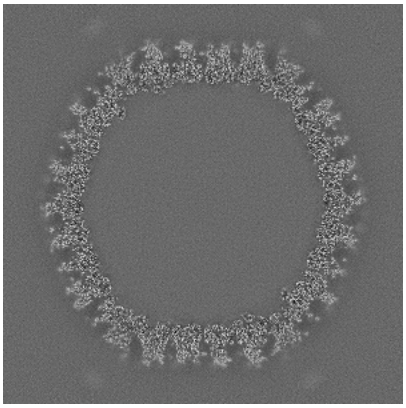
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

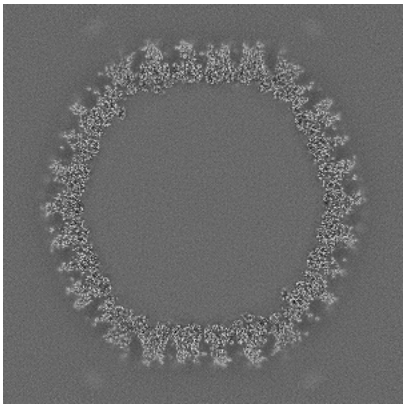
6.3.1 Primary map



X Index: 431



Y Index: 431

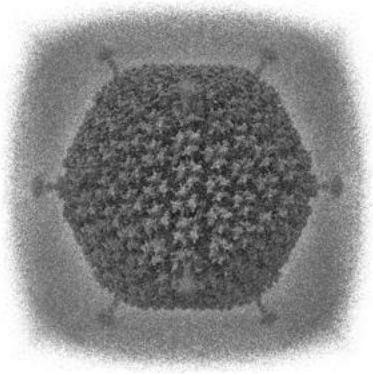


Z Index: 431

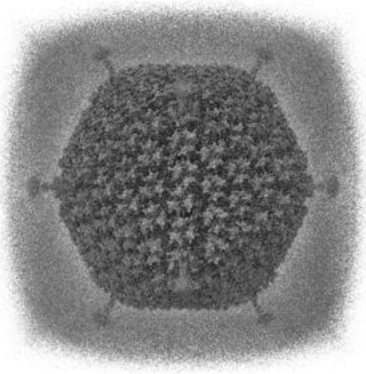
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

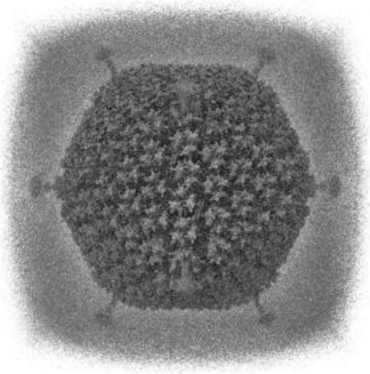
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

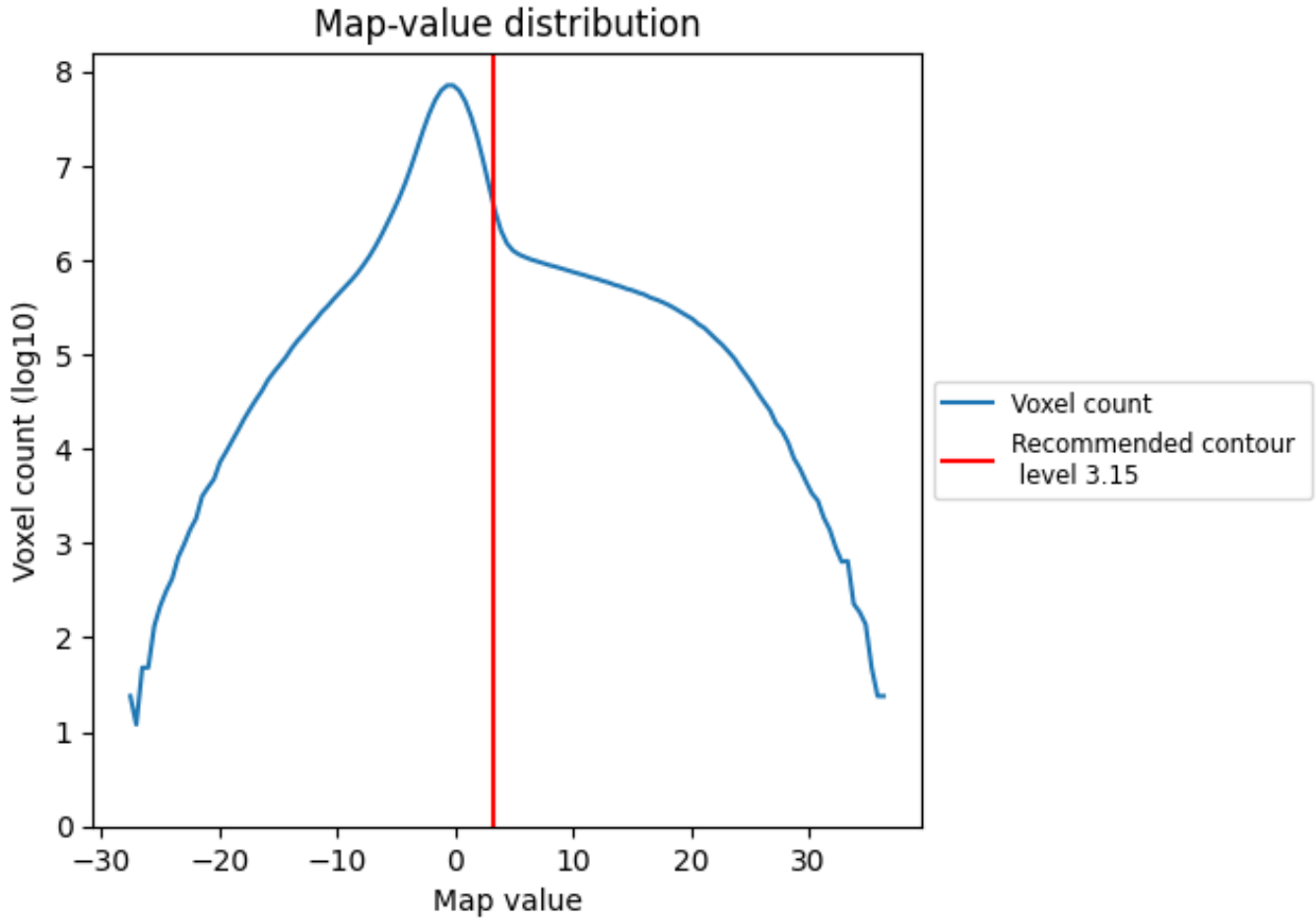
6.5 Mask visualisation (i)

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

7 Map analysis

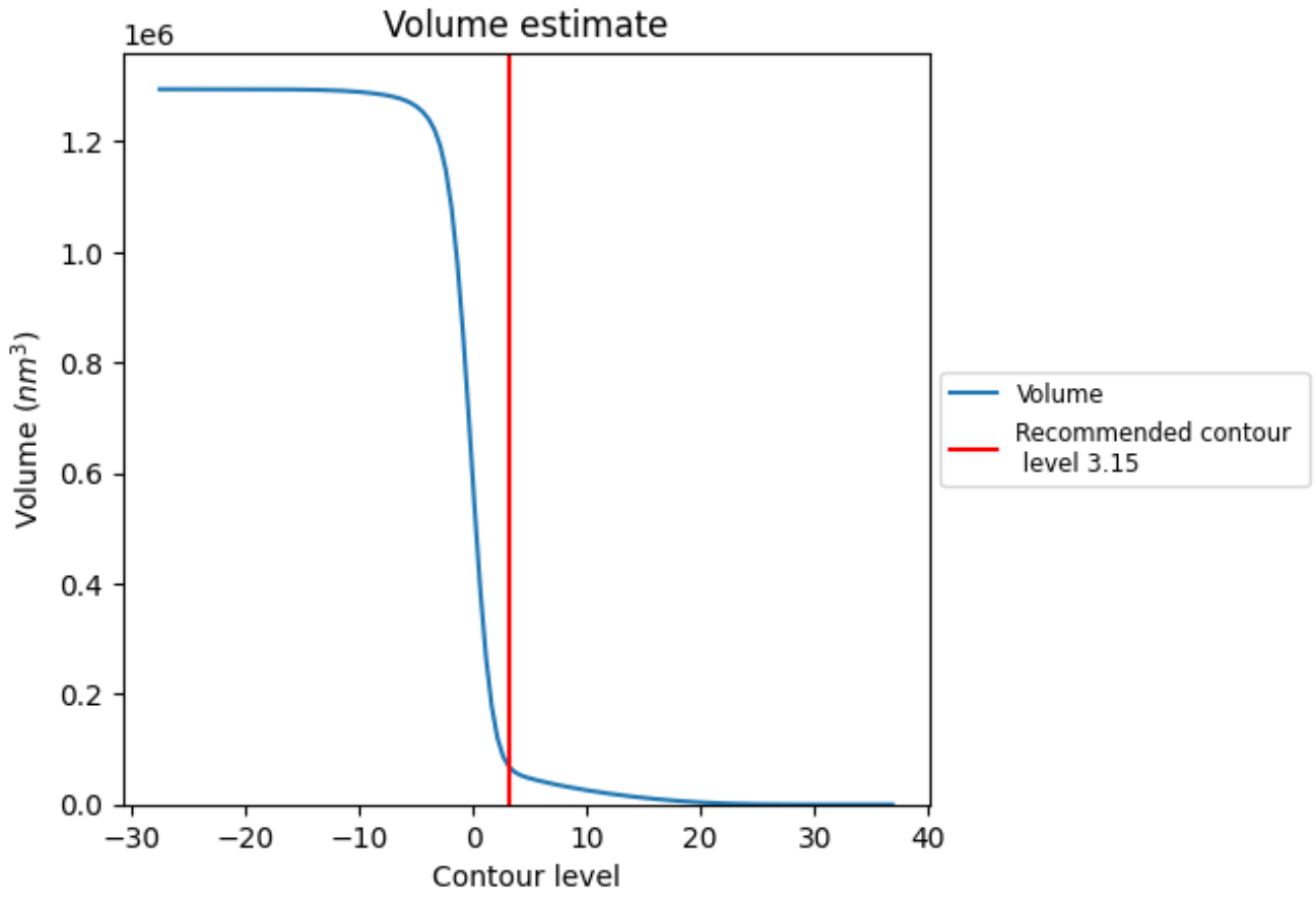
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

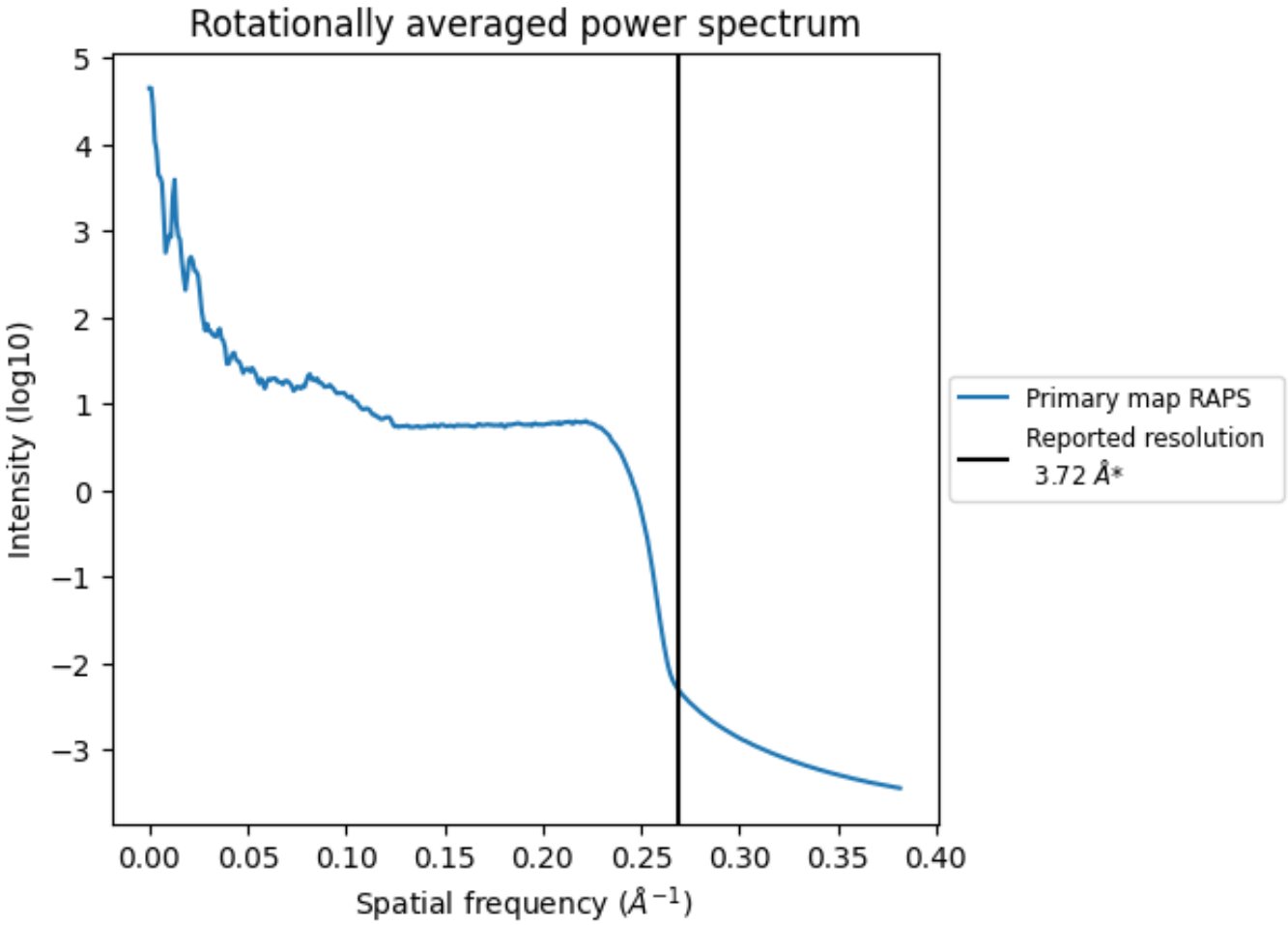
7.2 Volume estimate (i)



The volume at the recommended contour level is 68380 nm^3; this corresponds to an approximate mass of 61769 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 (i)

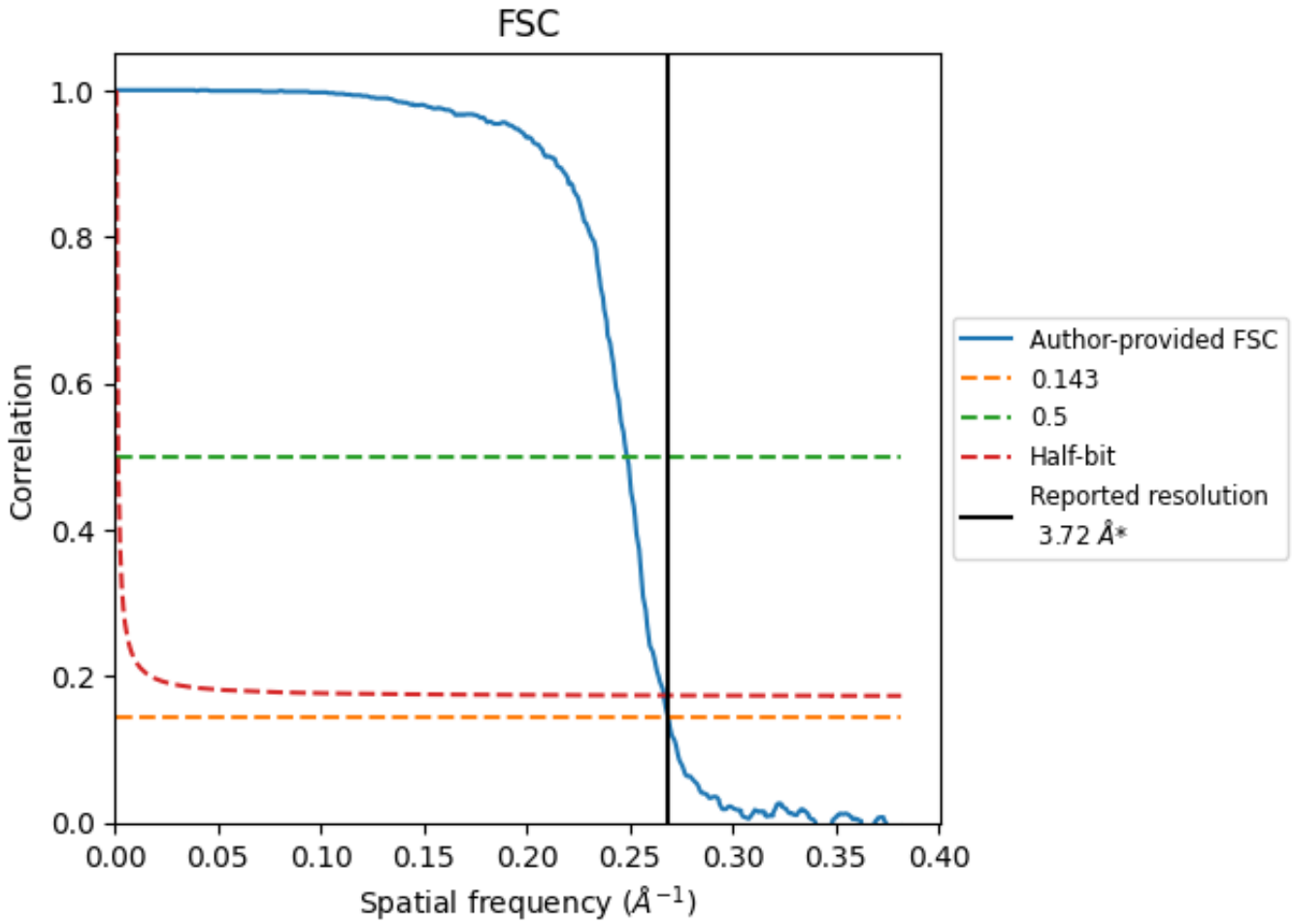


*Reported resolution corresponds to spatial frequency of 0.269 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.269 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.72	-	-
Author-provided FSC curve	3.72	4.02	3.75
Unmasked-calculated*	-	-	-

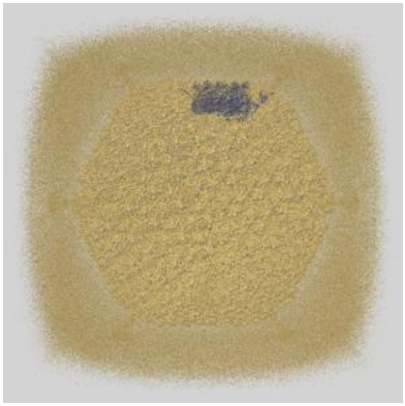
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit

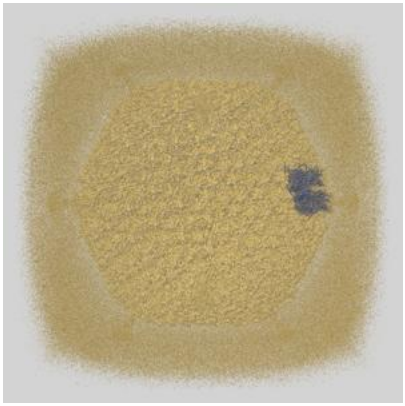
This section contains information regarding the fit between EMDB map EMD-24881 and PDB model 7S78. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

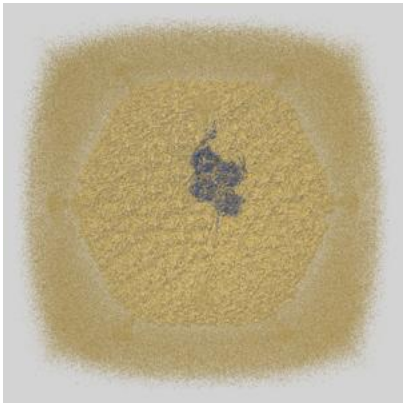
9.1.1 Map-model overlay



X

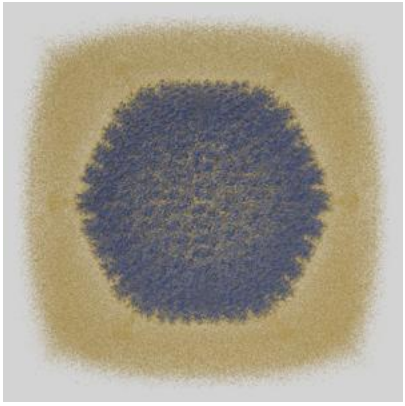


Y

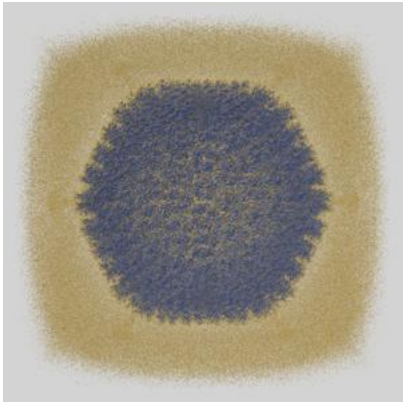


Z

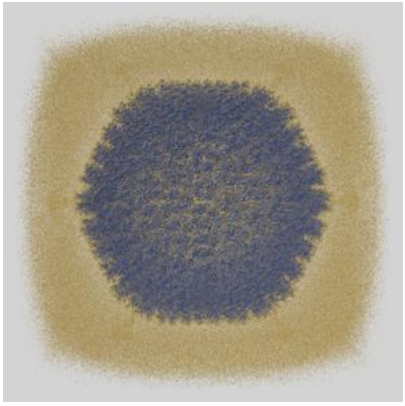
9.1.2 Map-model assembly overlay



X



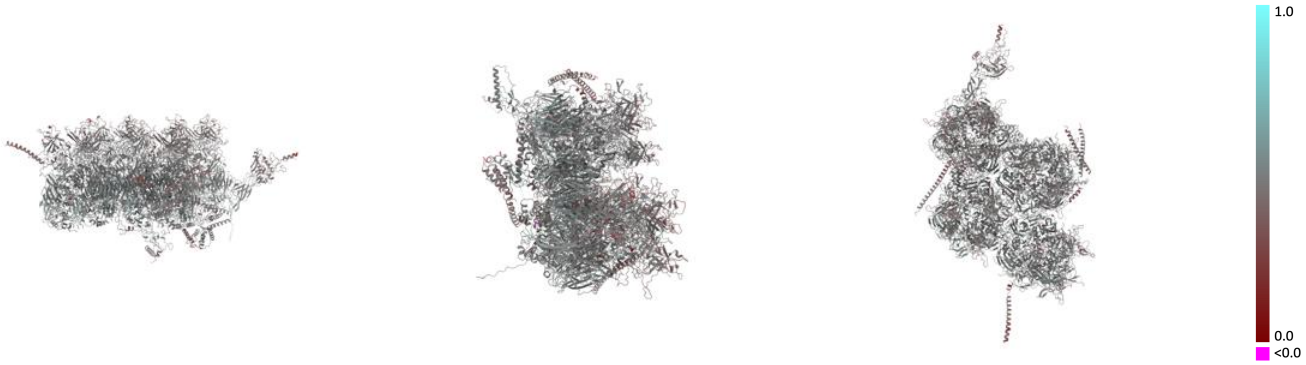
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.15 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.

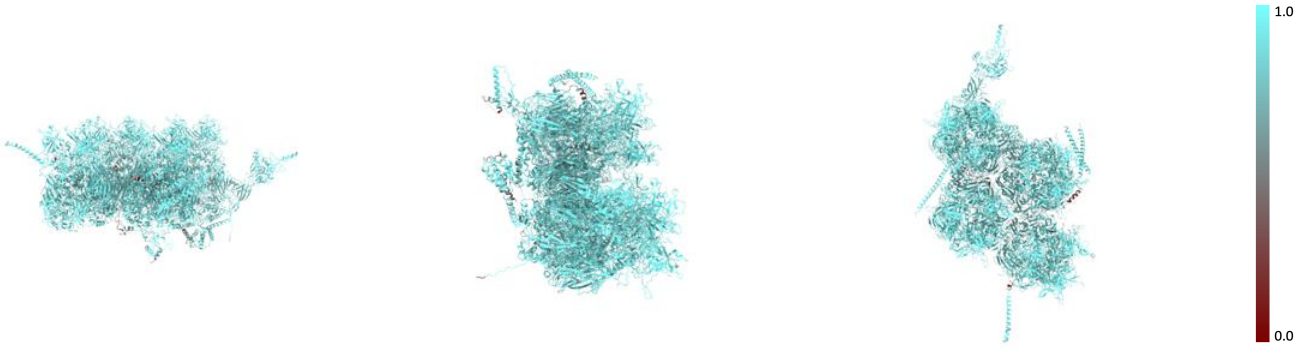
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

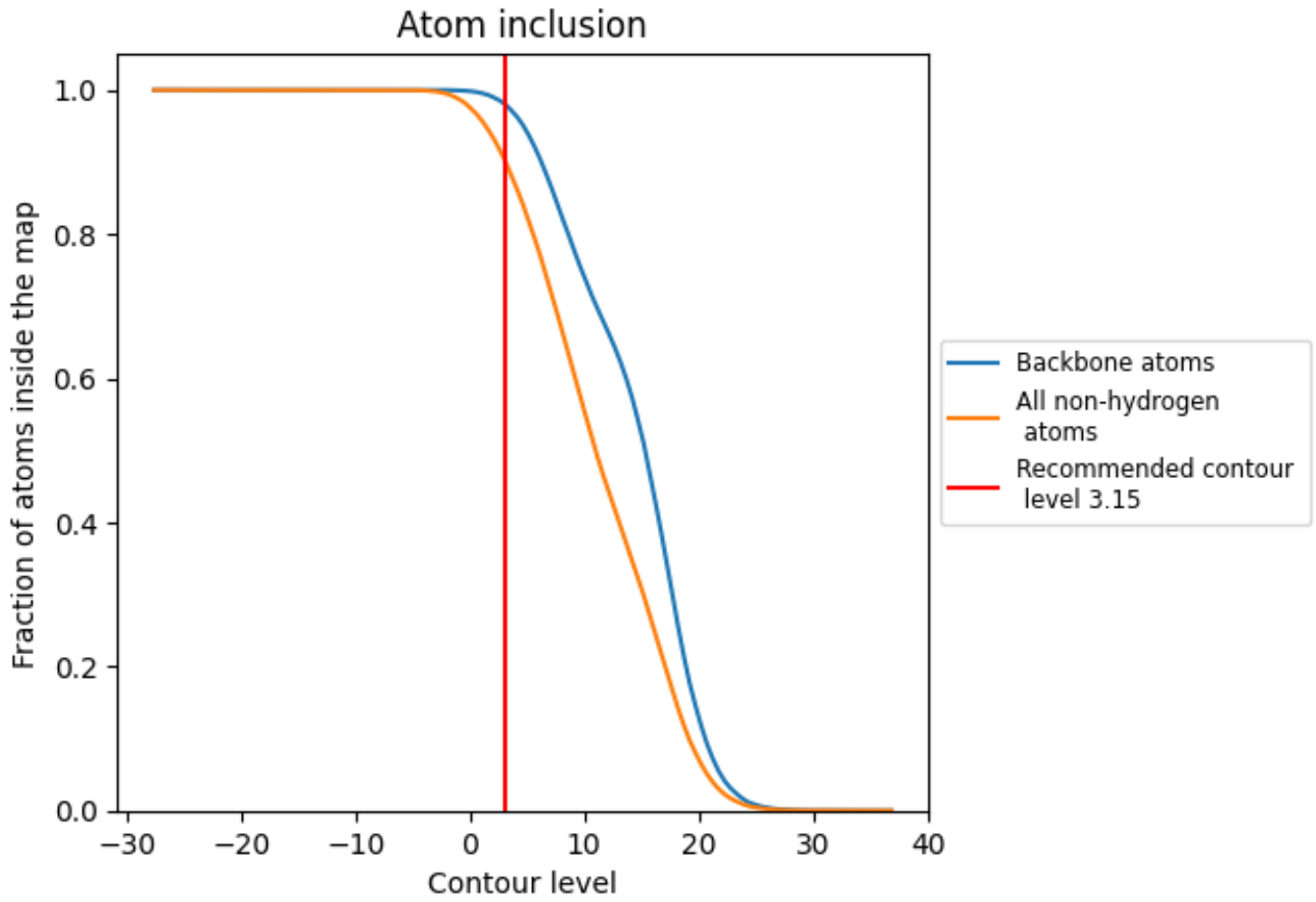
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (3.15).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 90% 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 (3.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8998	0.4710
0	0.7143	0.4920
1	0.7682	0.4890
2	0.6565	0.5190
3	0.7165	0.4610
4	0.6442	0.4730
5	0.5125	0.4670
6	0.6800	0.4480
A	0.9179	0.4710
B	0.9165	0.4650
C	0.9157	0.4680
D	0.9142	0.4770
E	0.9142	0.4770
F	0.9182	0.4790
G	0.9142	0.4810
H	0.9139	0.4810
I	0.9156	0.4790
J	0.9159	0.4770
K	0.9186	0.4740
L	0.9128	0.4770
M	0.8075	0.4370
N	0.8879	0.4510
P	0.7859	0.4080
Q	0.7964	0.4230
R	0.8274	0.4160
S	0.8736	0.4330
U	0.8344	0.4650
V	0.7899	0.4650
W	0.5586	0.4460
X	0.7531	0.4480
Y	0.6800	0.4580
Z	0.6857	0.4860