



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2024 – 04:35 AM EDT

PDB ID : 6CGV  
Title : Revised crystal structure of human adenovirus  
Authors : Natchiar, S.K.; Venkataraman, S.; Nemerow, G.R.; Reddy, V.S.  
Deposited on : 2018-02-21  
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

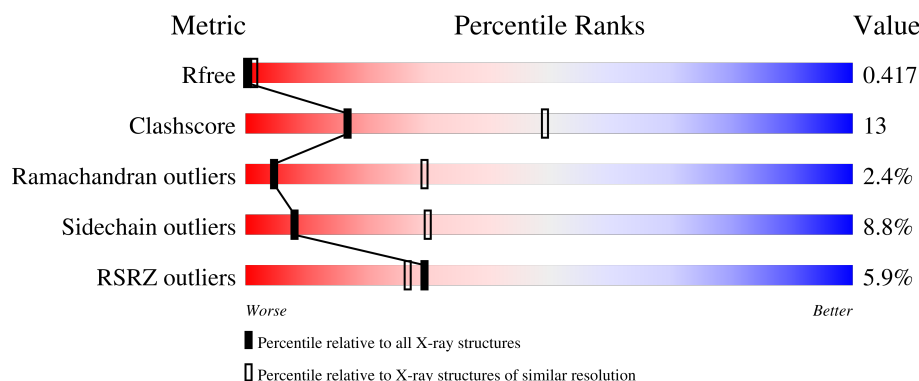
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1025 (3.98-3.62)
Clashscore	180529	1005 (3.96-3.64)
Ramachandran outliers	177936	1044 (3.98-3.62)
Sidechain outliers	177891	1039 (3.98-3.62)
RSRZ outliers	164620	1025 (3.98-3.62)

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

Mol	Chain	Length	Quality of chain
1	A	949	 6% 67% 27% . .
1	B	949	 5% 68% 23% . .
1	C	949	 8% 67% 27% . .
1	D	949	 5% 69% 24% . .
1	E	949	 4% 71% 22% . .

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Mol	Chain	Length	Quality of chain
1	F	949	
1	G	949	
1	H	949	
1	I	949	
1	J	949	
1	K	949	
1	L	949	
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	W	24	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 99723 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
1	A	917	Total	C	N	O	S	0	0	0
			7345	4668	1243	1400	34			
1	B	911	Total	C	N	O	S	0	0	0
			7295	4636	1235	1390	34			
1	C	921	Total	C	N	O	S	0	0	0
			7374	4686	1247	1405	36			
1	D	917	Total	C	N	O	S	0	0	0
			7345	4668	1243	1400	34			
1	E	910	Total	C	N	O	S	0	0	0
			7302	4645	1235	1388	34			
1	F	914	Total	C	N	O	S	0	0	0
			7325	4658	1239	1393	35			
1	G	909	Total	C	N	O	S	0	0	0
			7291	4636	1234	1387	34			
1	H	913	Total	C	N	O	S	0	0	0
			7317	4653	1238	1392	34			
1	I	917	Total	C	N	O	S	0	0	0
			7345	4669	1243	1398	35			
1	J	915	Total	C	N	O	S	0	0	0
			7329	4658	1240	1397	34			
1	K	904	Total	C	N	O	S	0	0	0
			7247	4606	1227	1380	34			
1	L	918	Total	C	N	O	S	0	0	0
			7353	4673	1244	1401	35			

- Molecule 2 is a protein called Penton protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	447	Total	C	N	O	S	0	0	0
			3577	2264	621	680	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	0
			2343	1447	430	460	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	95	Total	C	N	O	S	0	0	0
			717	443	126	146	2			
4	Q	133	Total	C	N	O	S	0	0	0
			965	594	170	199	2			
4	R	98	Total	C	N	O	S	0	0	0
			734	450	132	150	2			
4	S	96	Total	C	N	O	S	0	0	0
			728	450	129	147	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	U	171	Total	C	N	O	S	0	0	0
			1329	839	235	250	5			
5	V	174	Total	C	N	O	S	0	0	0
			1346	848	238	255	5			

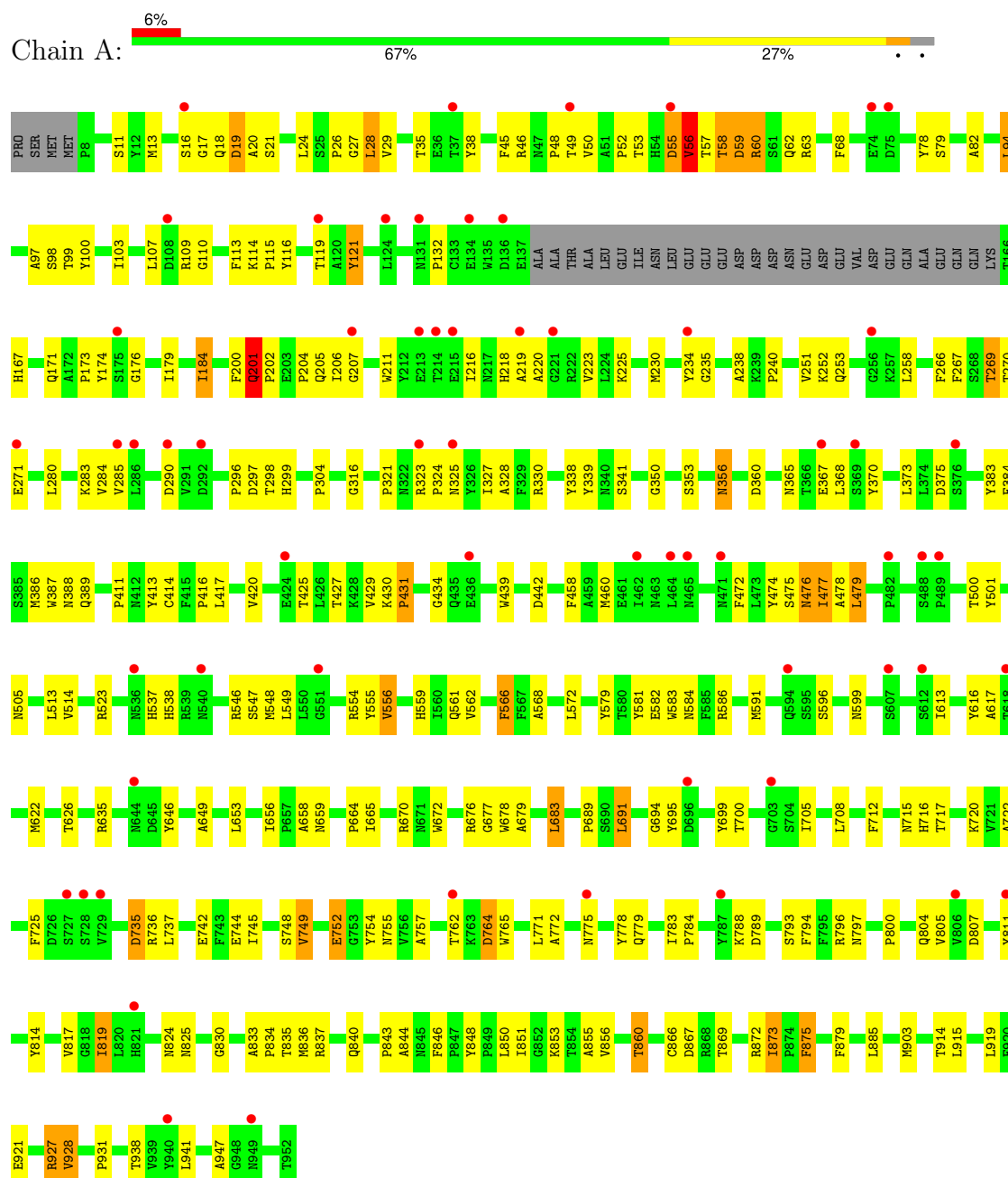
- Molecule 6 is a protein called Pre-protein VI.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	W	24	Total	C	N	O	0	0	0
			116	68	24	24			

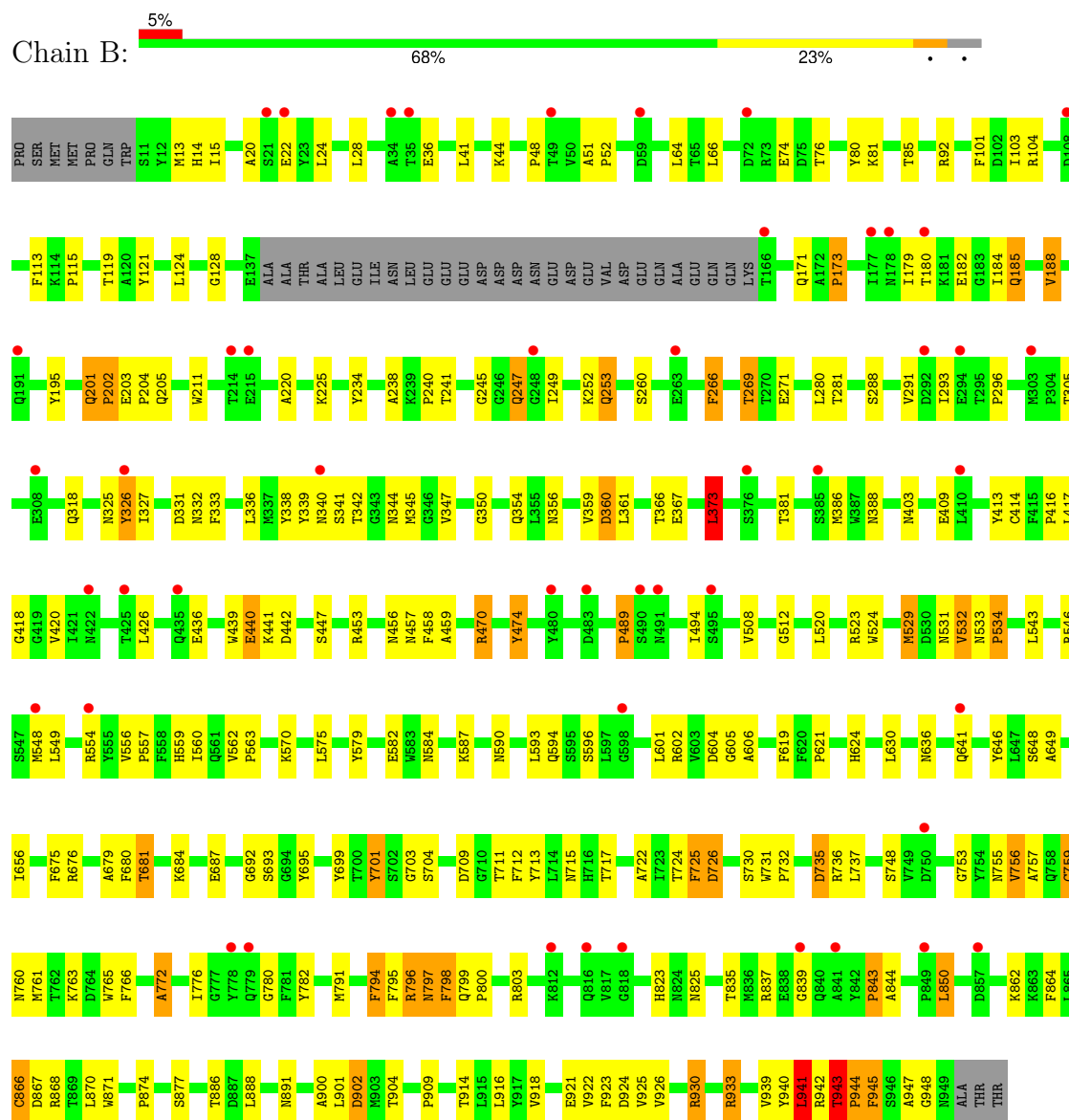
### 3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

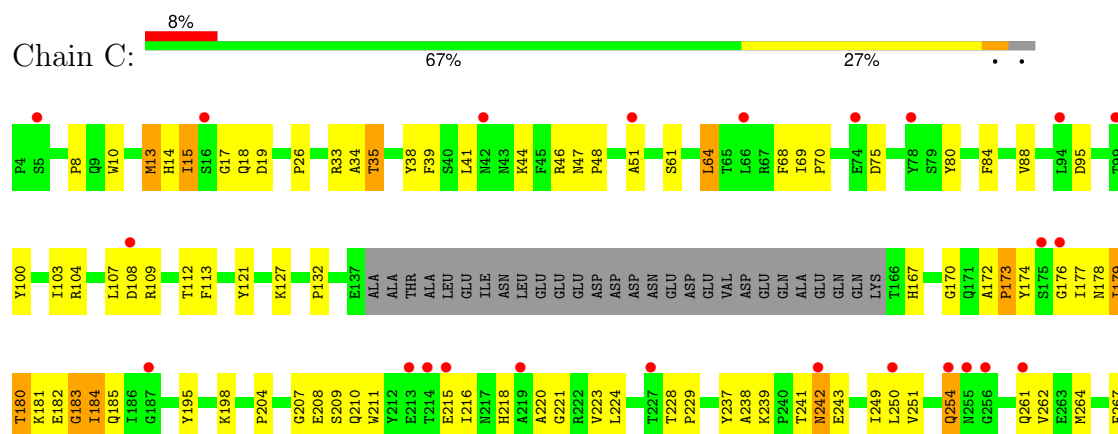
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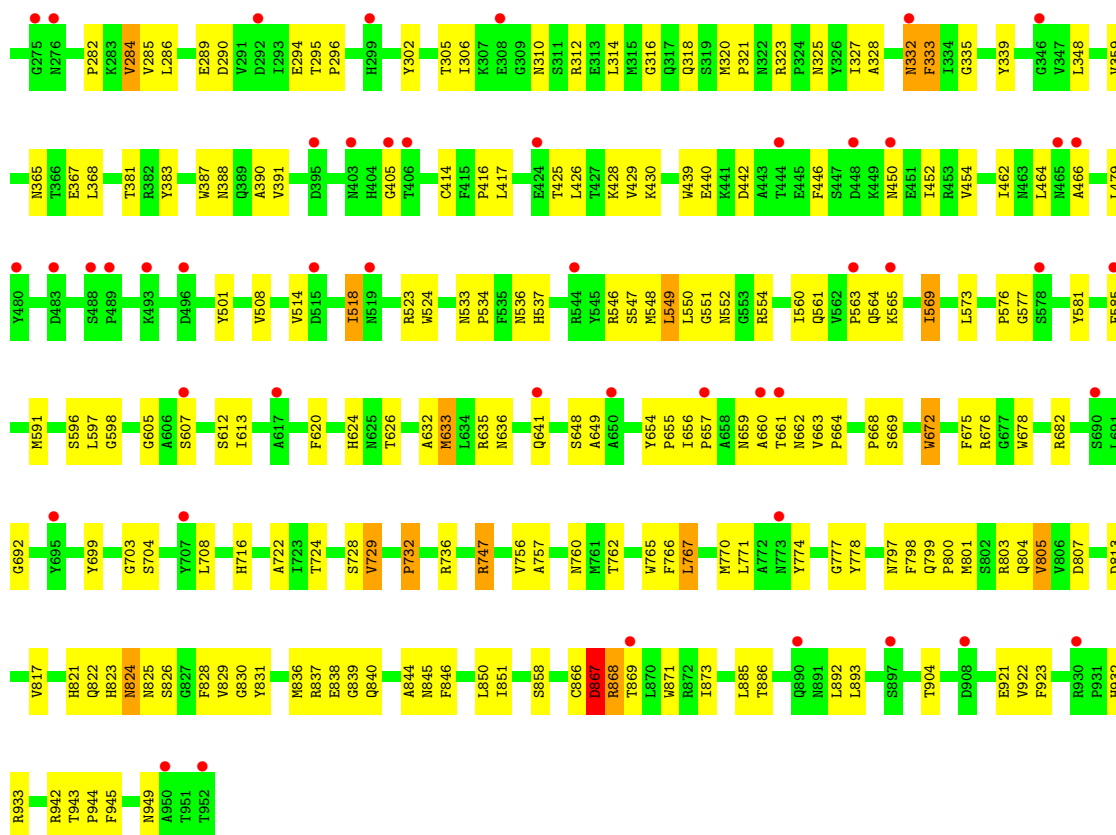


- Molecule 1: Hexon protein

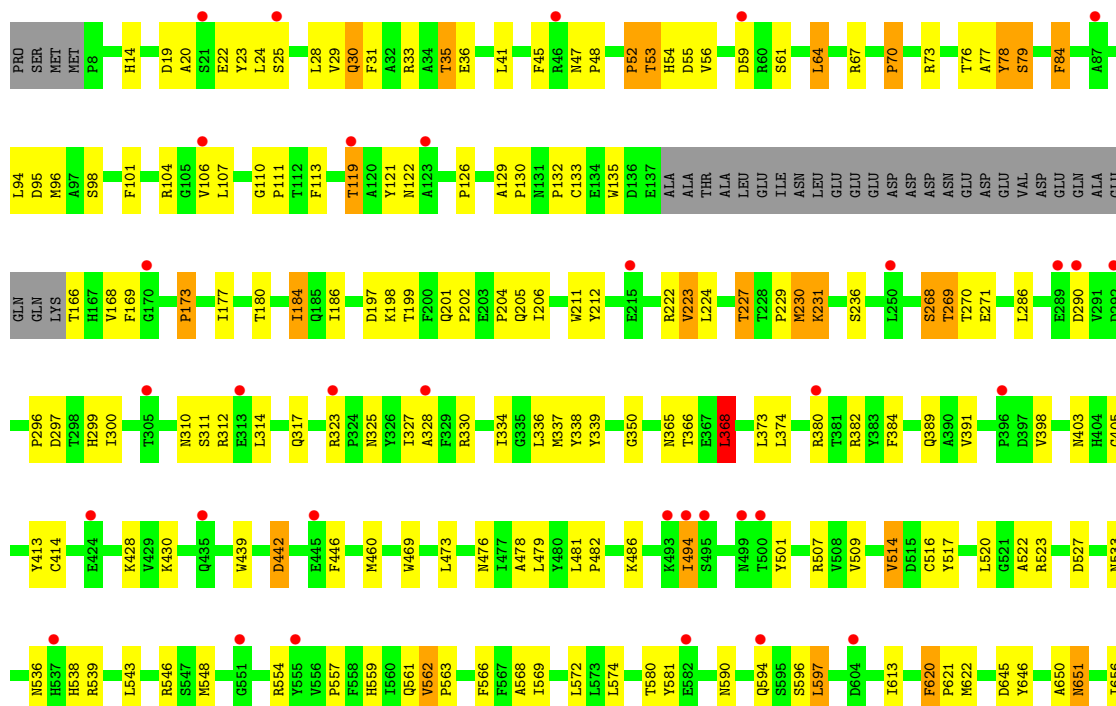


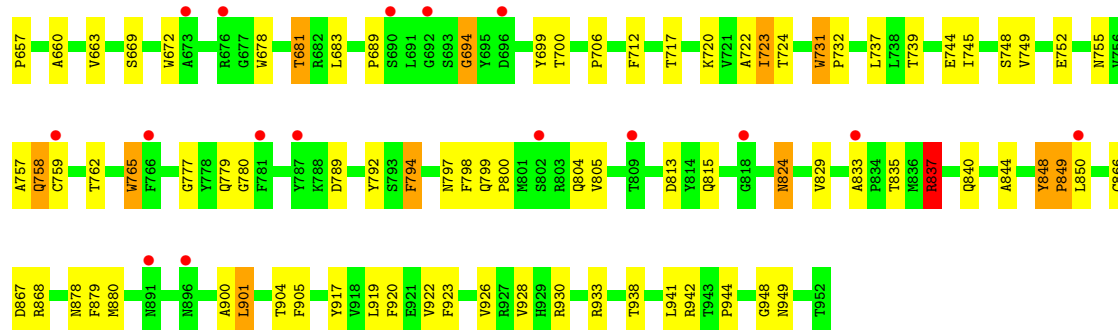
- Molecule 1: Hexon protein



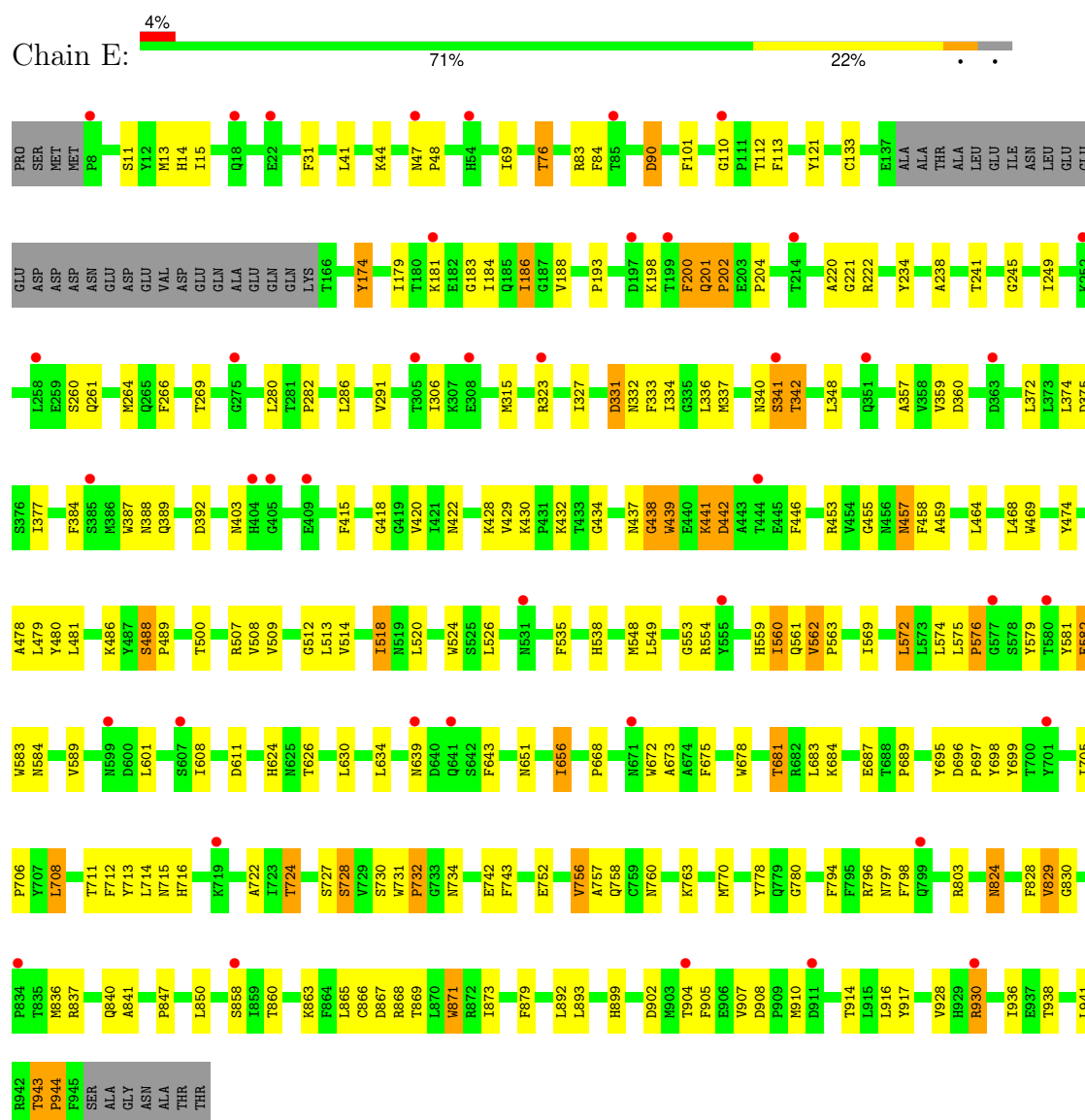


### • Molecule 1: Hexon protein



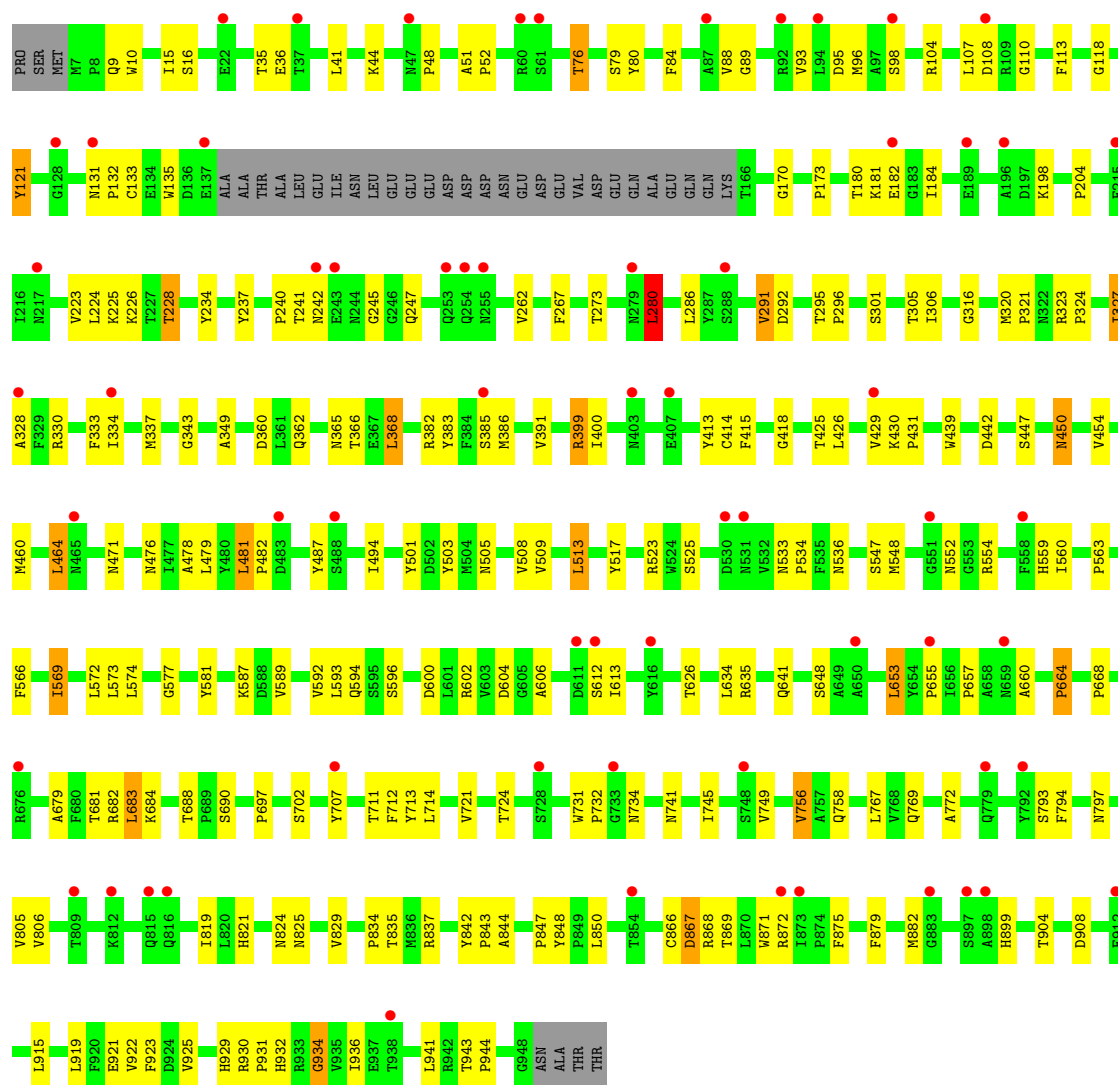


• Molecule 1: Hexon protein

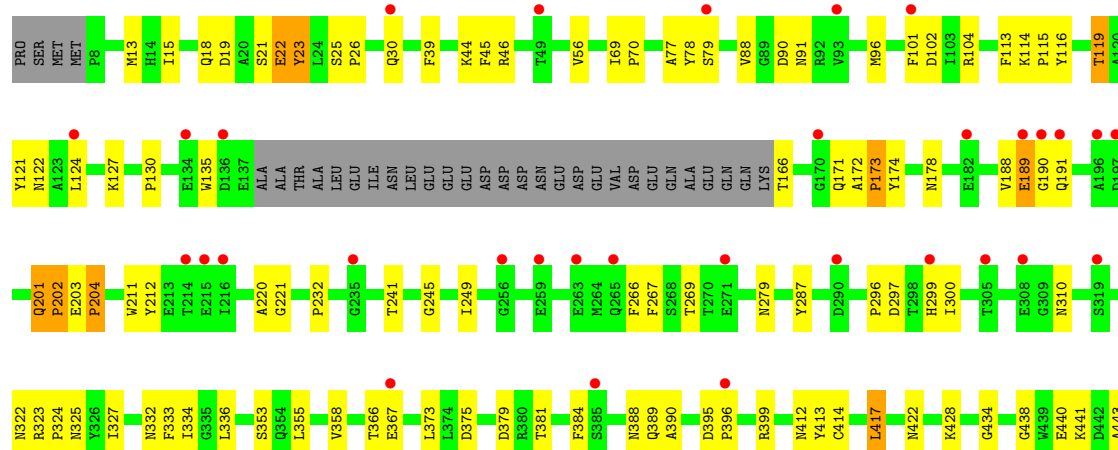


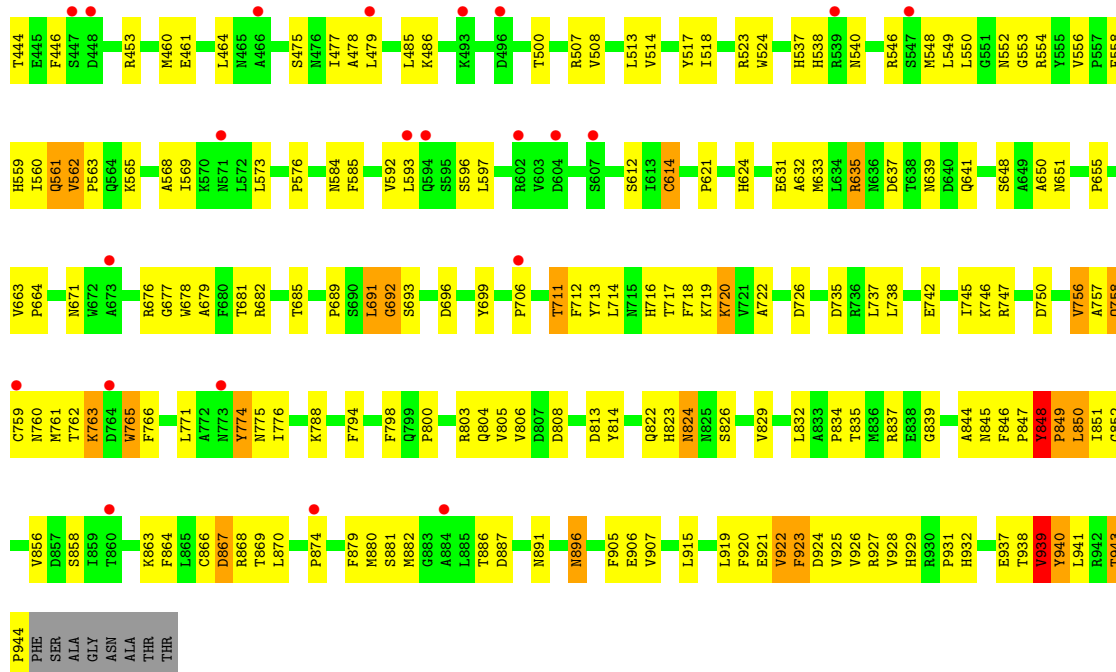
• Molecule 1: Hexon protein



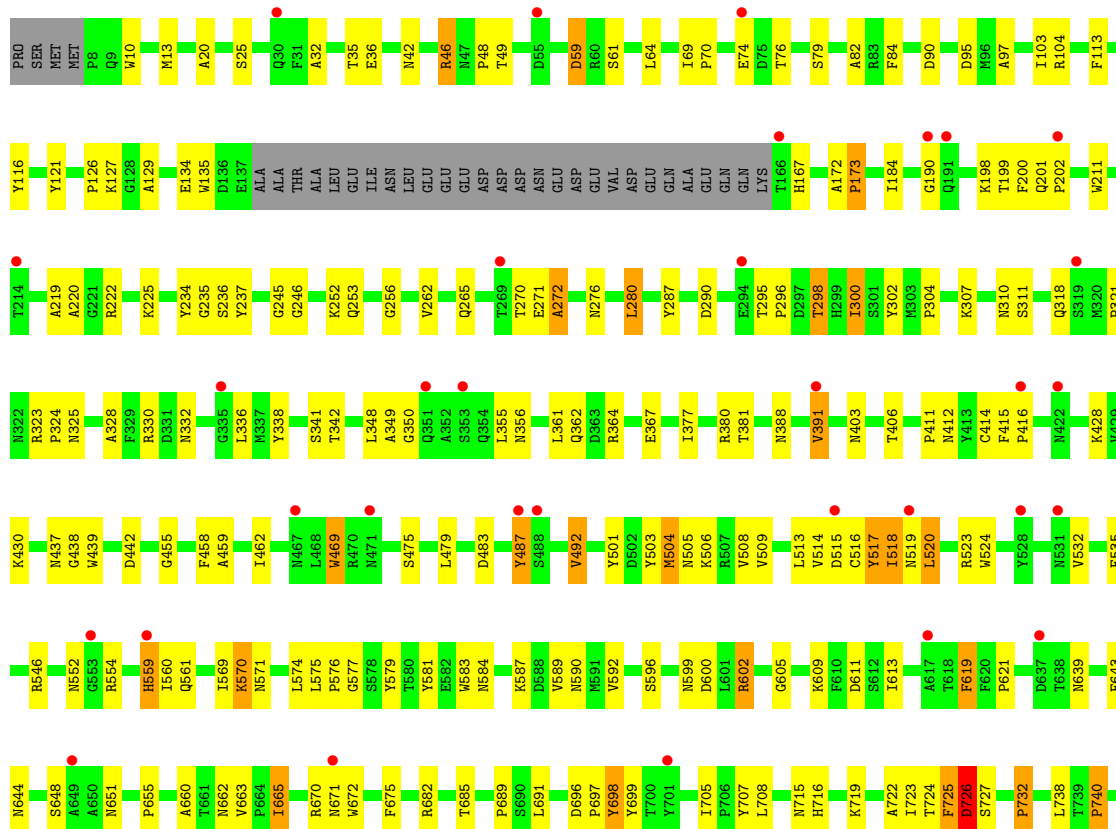


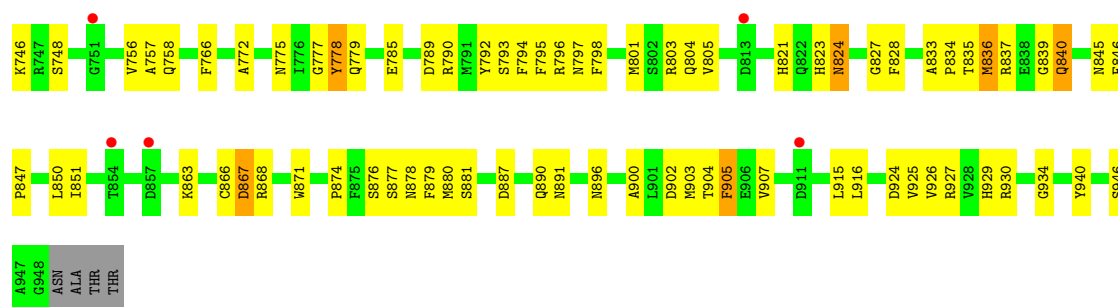
• Molecule 1: Hexon protein



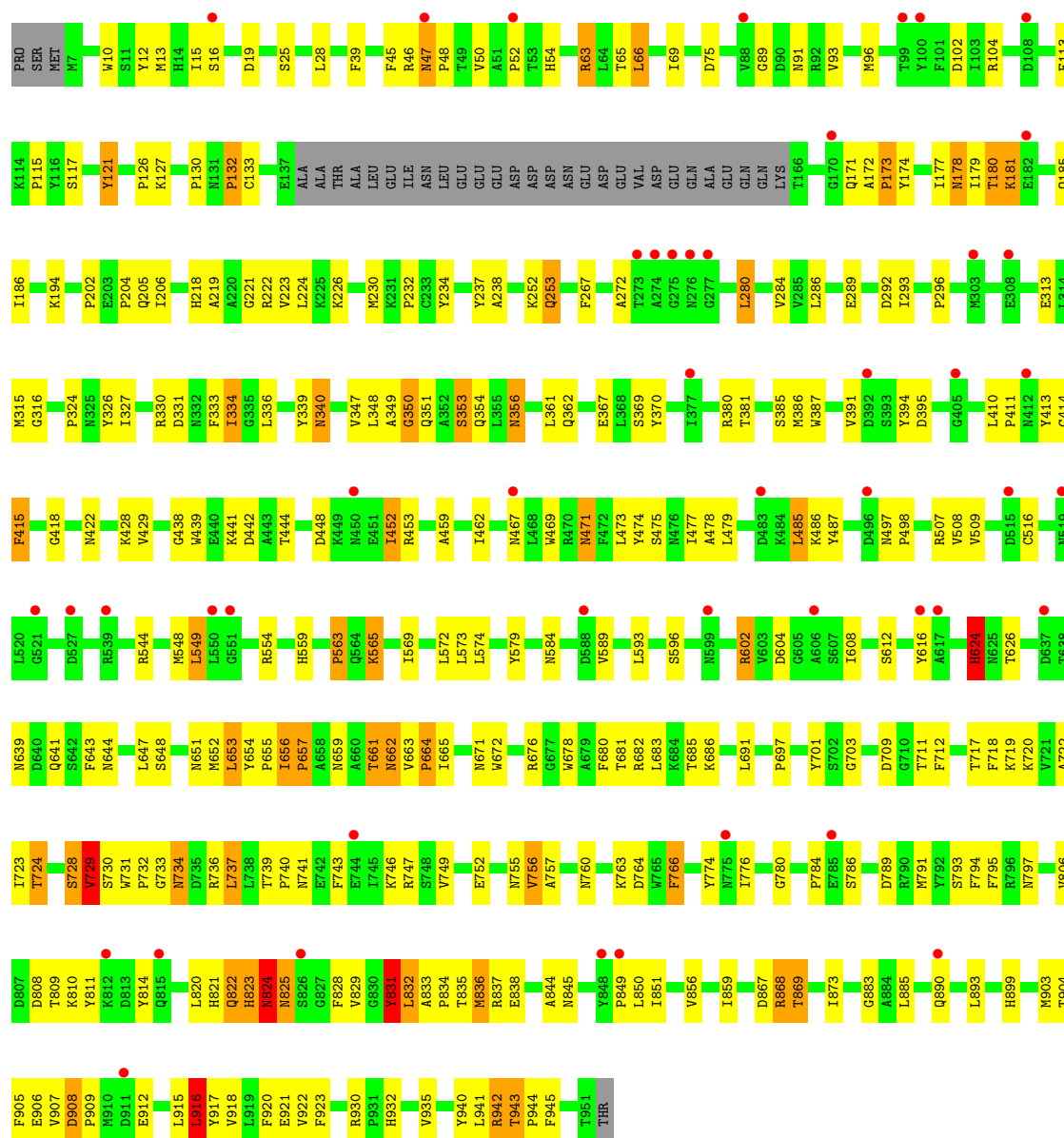


• Molecule 1: Hexon protein

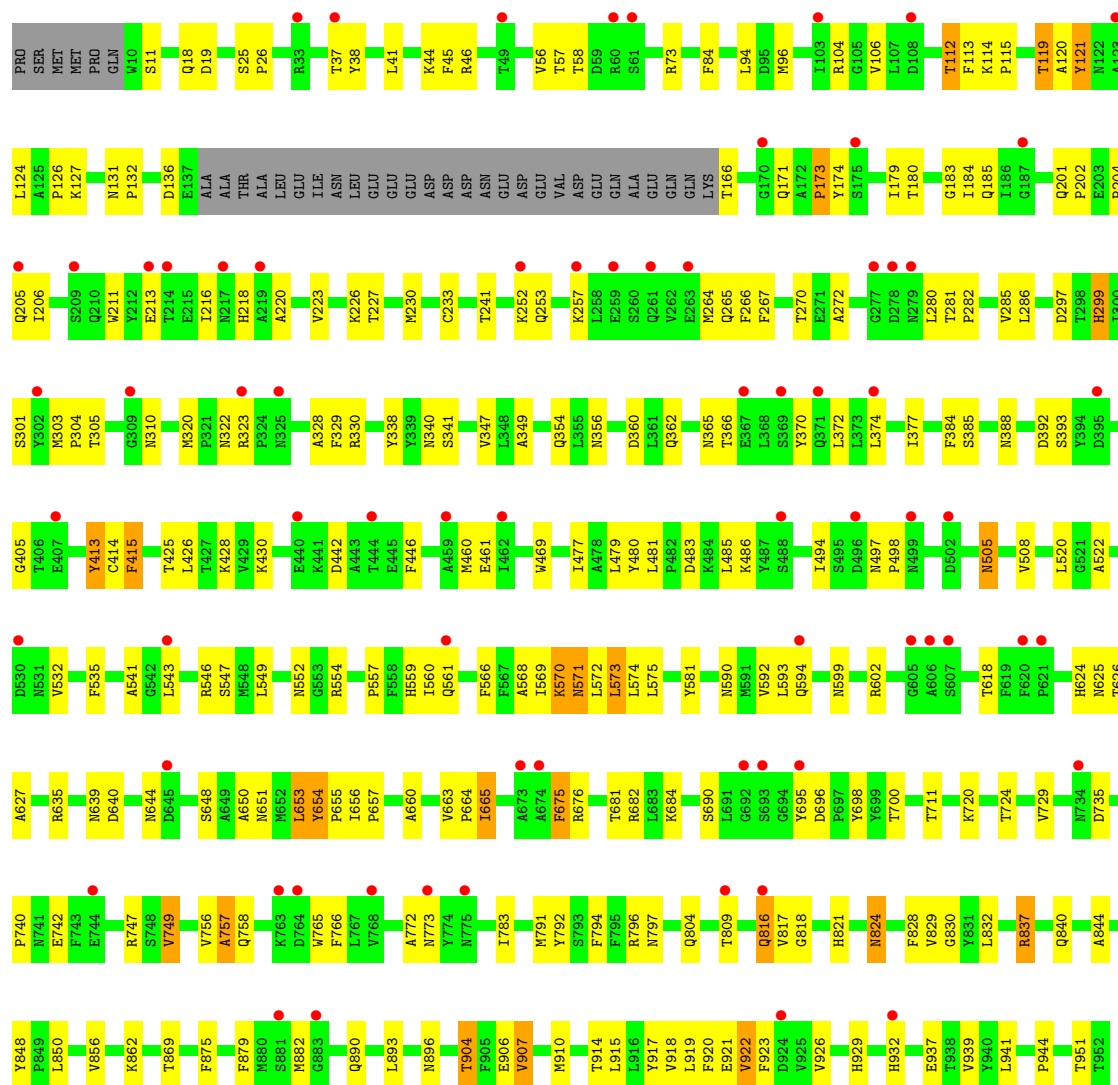




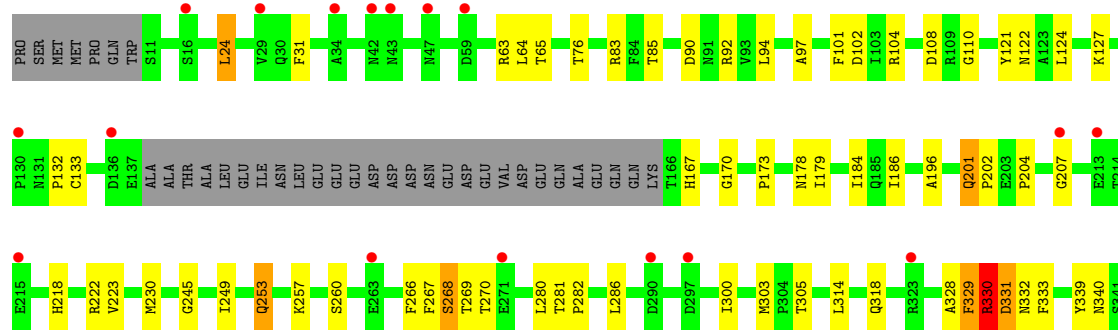
● Molecule 1: Hexon protein

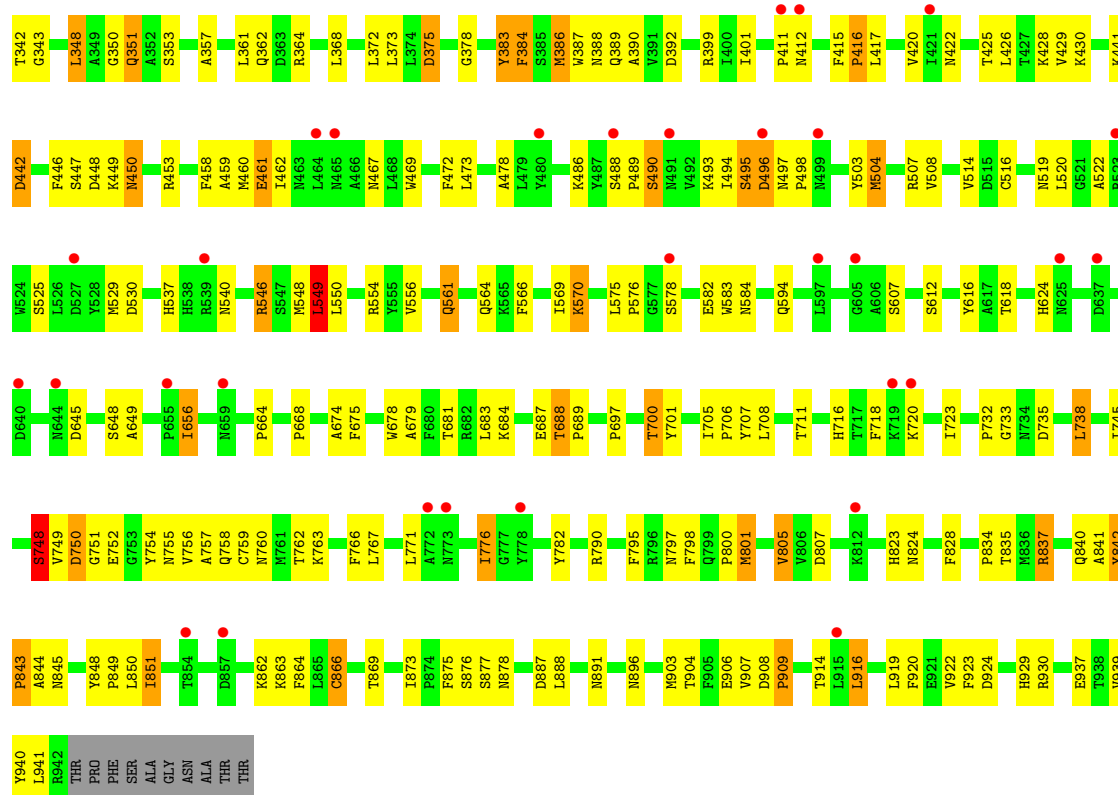


● Molecule 1: Hexon protein

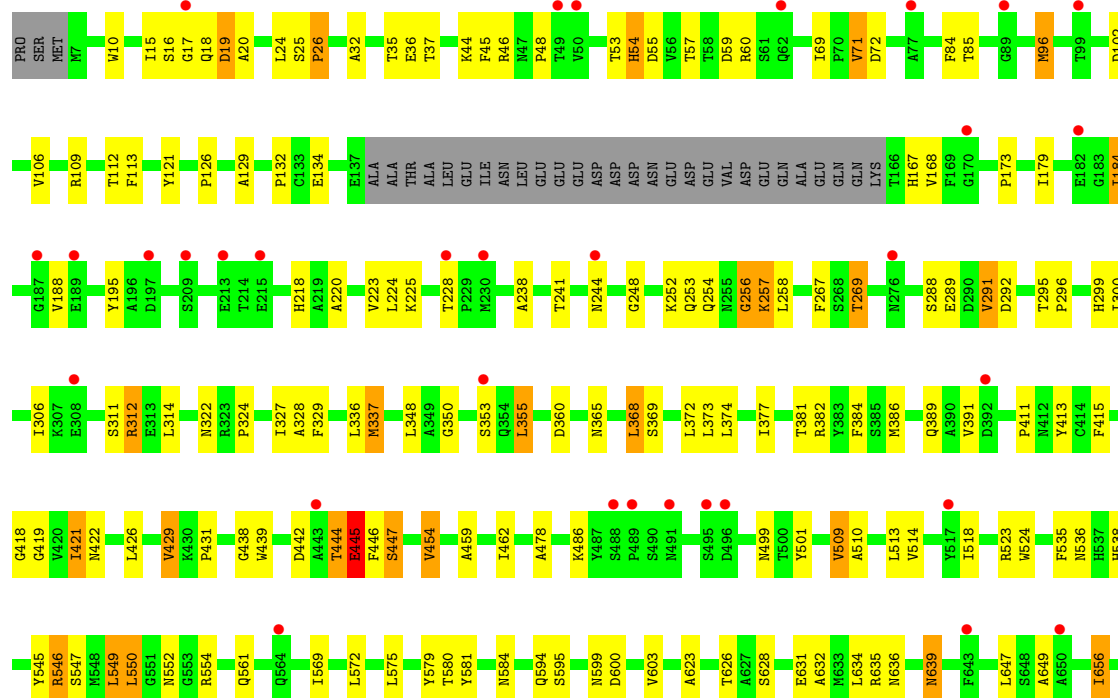


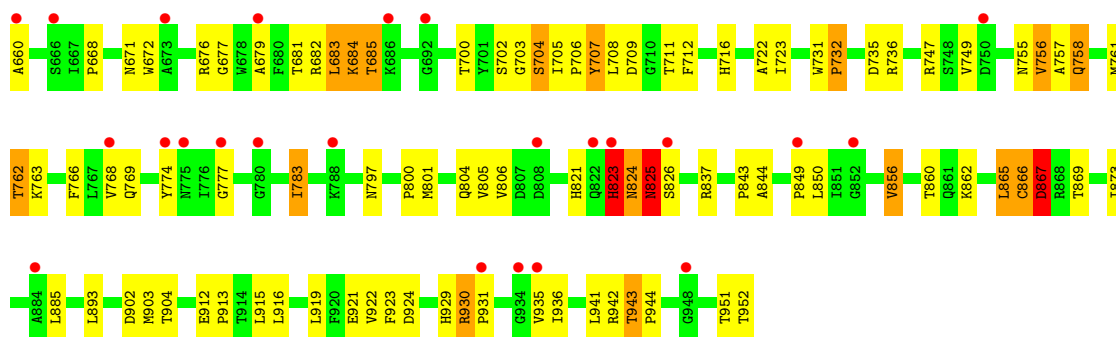
• Molecule 1: Hexon protein



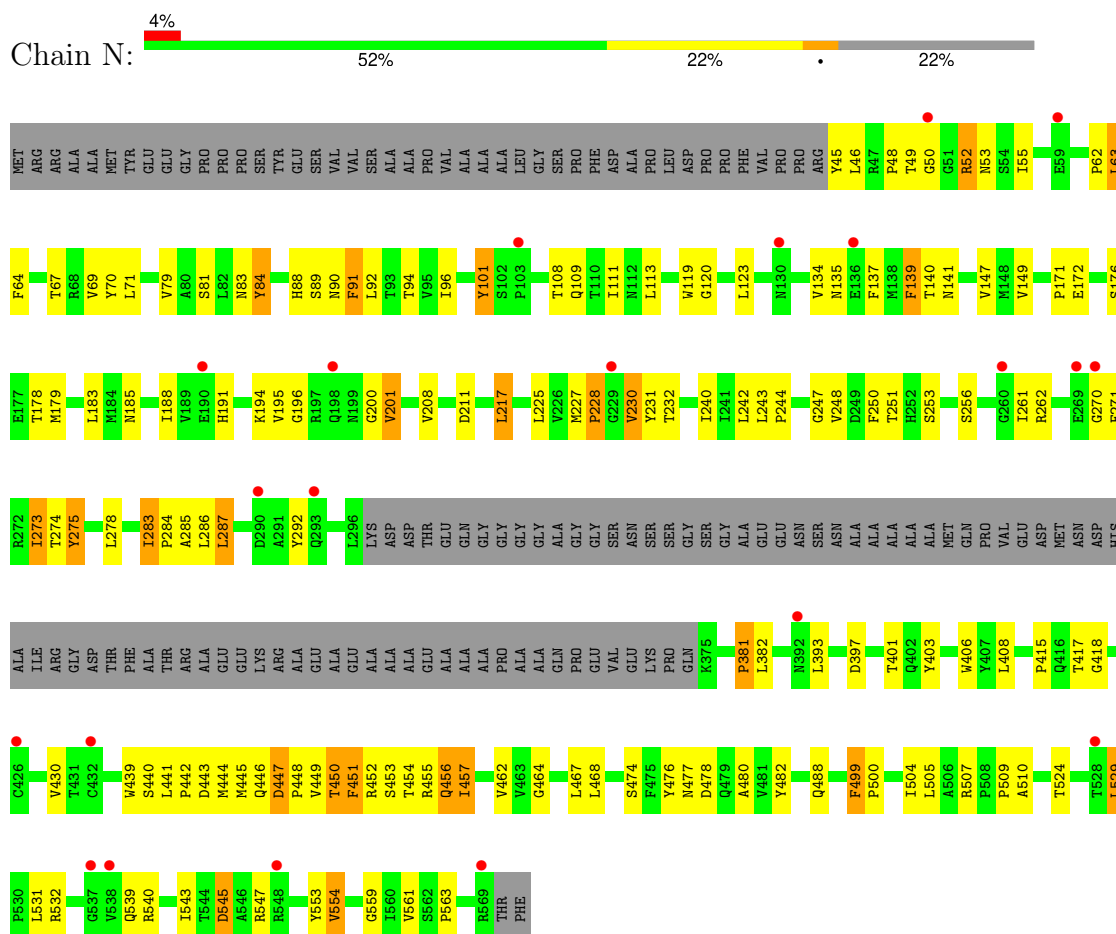


• Molecule 1: Hexon protein

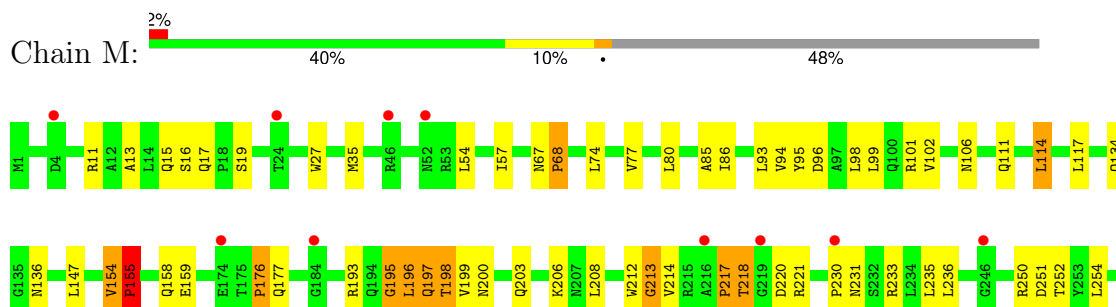


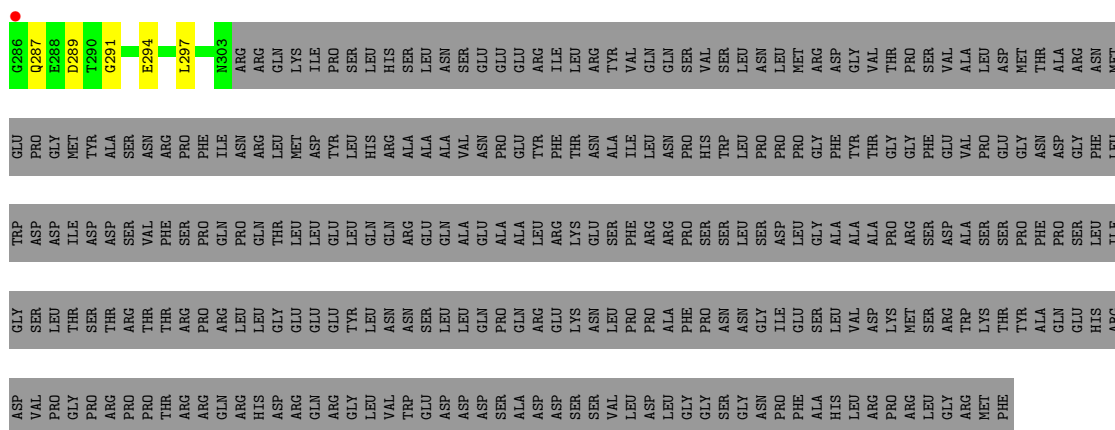


• Molecule 2: Penton protein

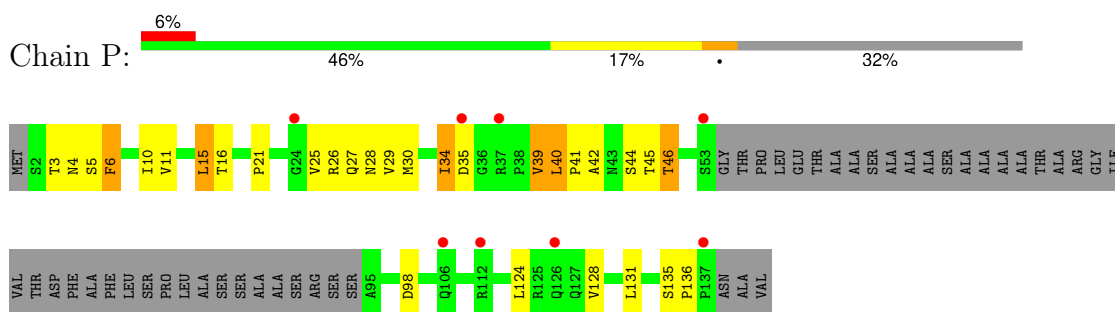


• Molecule 3: Pre-hexon-linking protein IIIa

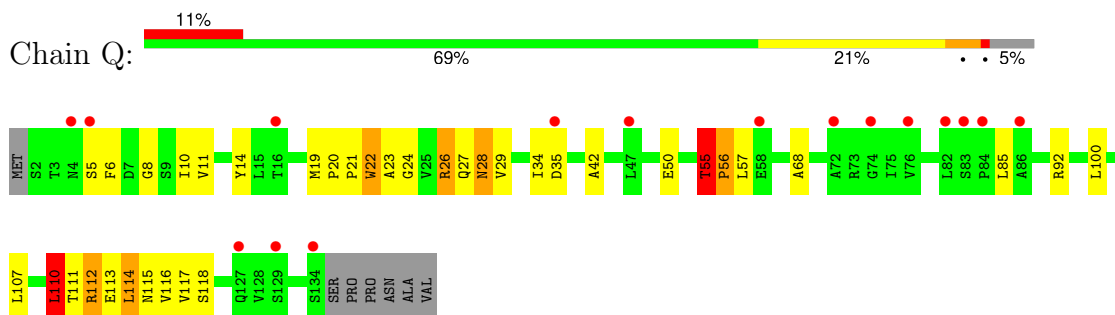




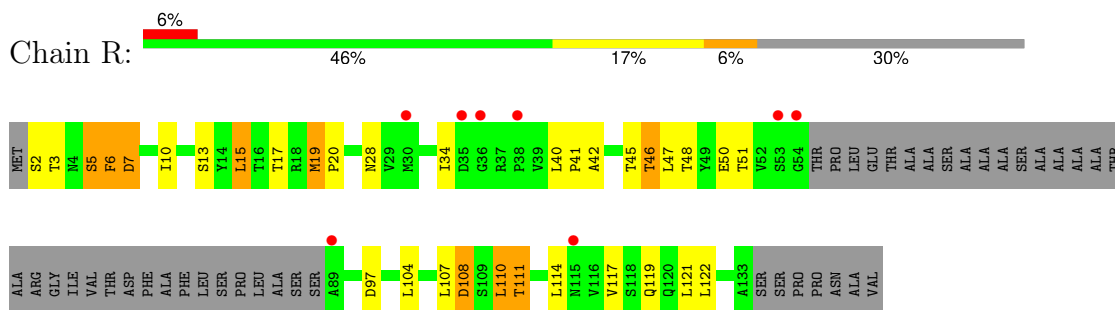
- Molecule 4: Hexon-interlacing protein



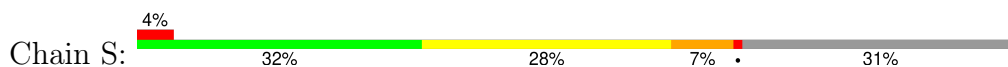
- Molecule 4: Hexon-interlacing protein

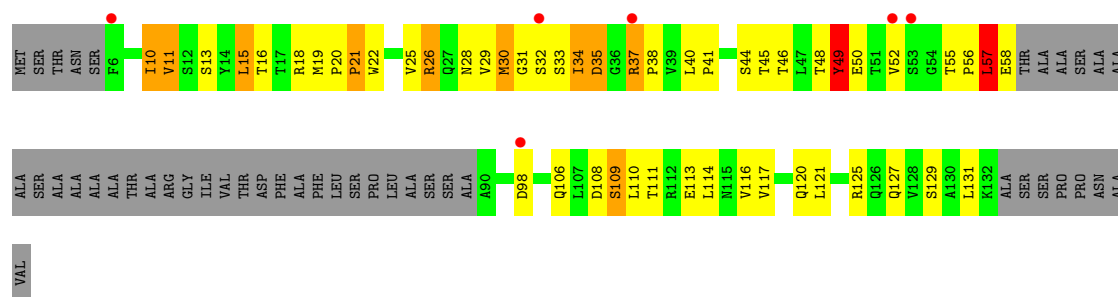


- Molecule 4: Hexon-interlacing protein

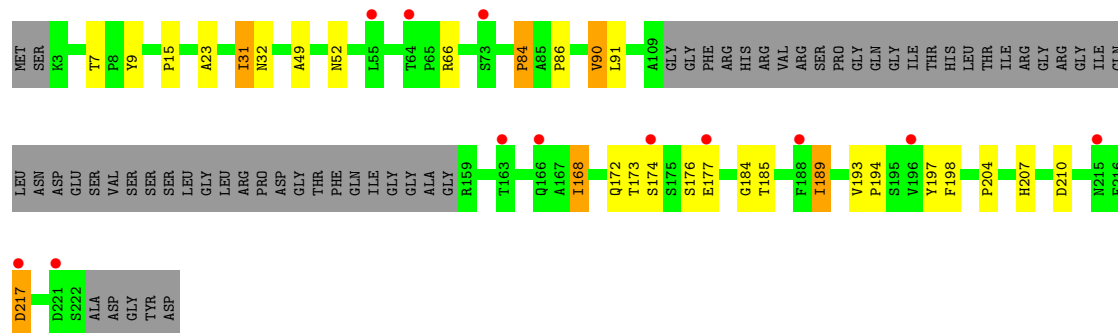


- Molecule 4: Hexon-interlacing protein

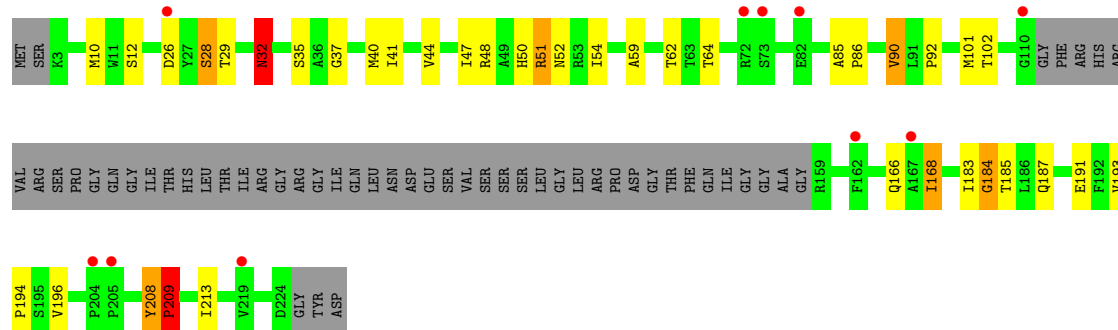




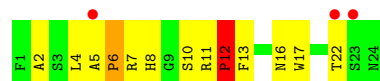
• Molecule 5: Pre-hexon-linking protein VIII



• Molecule 5: Pre-hexon-linking protein VIII



• Molecule 6: Pre-protein VI



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	854.25Å 855.32Å 865.91Å 60.38° 60.43° 61.98°	Depositor
Resolution (Å)	129.00 – 3.80 129.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (129.00-3.80) 52.6 (129.00-3.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.36	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 3.78Å)	Xtriage
Refinement program	REFMAC 5.8	Depositor
R, $R_{free}$	0.422 , 0.427 0.413 , 0.417	Depositor DCC
$R_{free}$ test set	277724 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 0.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.25$ , $\langle L^2 \rangle = 0.10$	Xtriage

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<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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Property	Value	Source
Estimated twinning fraction	0.226 for h-l,h,h-k 0.226 for k,k-l,-h+k 0.220 for h-k,h-l,h 0.220 for l,-h+l,-k+l 0.226 for -k+l,l,-h+l 0.226 for k-l,-h+k,k 0.220 for l,h,k 0.220 for k,l,h 0.226 for -l,k-l,h-l 0.226 for -h+l,-h+k,-h 0.220 for -k,h-k,-k+l 0.220 for -h+k,-h,-h+l 0.226 for h-k,-k+l,-k 0.226 for h-l,-l,k-l 0.226 for h,h-k,h-l 0.226 for -h+k,k,k-l 0.226 for -h,-l,-k 0.236 for -k,-h,-l 0.226 for k-l,h-l,-l 0.226 for -k+l,-k,h-k 0.226 for -h+l,-k+l,l 0.226 for -l,-k,-h 0.226 for -h,-h+l,-h+k	Xtriage
$F_o, F_c$ correlation	0.14	EDS
Total number of atoms	99723	wwPDB-VP
Average B, all atoms ( $\text{\AA}^2$ )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.24% of the height of the origin peak. No significant pseudotranslation is detected.*

## 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	0.53	0/7543	0.77	12/10258 (0.1%)
1	B	0.49	0/7490	0.72	11/10185 (0.1%)
1	C	0.50	0/7573	0.72	8/10298 (0.1%)
1	D	0.48	1/7543 (0.0%)	0.71	11/10258 (0.1%)
1	E	0.46	0/7500	0.66	1/10200 (0.0%)
1	F	0.46	1/7523 (0.0%)	0.65	2/10231 (0.0%)
1	G	0.54	3/7488 (0.0%)	0.78	10/10184 (0.1%)
1	H	0.49	0/7515	0.74	7/10220 (0.1%)
1	I	0.52	1/7543 (0.0%)	0.77	11/10259 (0.1%)
1	J	0.46	0/7526	0.68	4/10235 (0.0%)
1	K	0.50	0/7440	0.73	5/10116 (0.0%)
1	L	0.50	0/7551	0.73	13/10269 (0.1%)
2	N	0.60	1/3663 (0.0%)	0.87	9/4989 (0.2%)
3	M	0.46	0/2380	0.70	2/3240 (0.1%)
4	P	0.78	4/726 (0.6%)	0.96	4/989 (0.4%)
4	Q	0.78	2/977 (0.2%)	1.00	4/1333 (0.3%)
4	R	0.67	2/741 (0.3%)	0.97	3/1006 (0.3%)
4	S	1.08	4/736 (0.5%)	1.26	4/1000 (0.4%)
5	U	0.43	0/1367	0.63	0/1868
5	V	0.53	0/1384	0.72	2/1891 (0.1%)
6	W	0.80	0/115	1.29	2/157 (1.3%)
All	All	0.51	19/102324 (0.0%)	0.74	125/139186 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
3	M	0	1
All	All	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	56	PRO	CA-C	9.69	1.72	1.52
4	Q	55	THR	C-N	9.24	1.51	1.34
4	S	56	PRO	C-N	8.73	1.54	1.34
4	P	6	PHE	N-CA	8.02	1.62	1.46
4	S	57	LEU	N-CA	7.83	1.62	1.46
4	Q	55	THR	CA-C	7.07	1.71	1.52
1	I	794	PHE	CB-CG	-6.69	1.40	1.51
1	G	22	GLU	CB-CG	6.58	1.64	1.52
1	G	21	SER	C-N	6.51	1.49	1.34
4	R	6	PHE	N-CA	6.13	1.58	1.46
2	N	292	TYR	CB-CG	6.13	1.60	1.51
1	G	562	VAL	C-N	5.90	1.45	1.34
4	P	5	SER	CA-C	5.87	1.68	1.52
1	D	54	HIS	CB-CG	5.82	1.60	1.50
4	S	22	TRP	CB-CG	5.56	1.60	1.50
1	F	712	PHE	N-CA	5.51	1.57	1.46
4	P	4	ASN	N-CA	5.41	1.57	1.46
4	R	5	SER	C-N	5.21	1.46	1.34
4	P	5	SER	C-N	5.04	1.45	1.34

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	23	TYR	CB-CG-CD1	-15.65	111.61	121.00
1	G	23	TYR	CB-CG-CD2	15.43	130.25	121.00
1	D	78	TYR	CB-CG-CD2	-10.26	114.84	121.00
4	R	6	PHE	CB-CG-CD2	9.83	127.68	120.80
1	B	532	VAL	CB-CA-C	-9.69	92.98	111.40
1	J	571	ASN	CB-CA-C	-9.36	91.69	110.40
1	I	831	TYR	CA-CB-CG	-8.62	97.01	113.40
1	L	856	VAL	CB-CA-C	8.54	127.62	111.40
1	D	78	TYR	CB-CG-CD1	8.45	126.07	121.00
4	S	22	TRP	CA-CB-CG	8.15	129.19	113.70
2	N	451	PHE	CB-CG-CD1	-7.95	115.24	120.80
4	Q	22	TRP	CB-CA-C	7.95	126.29	110.40
1	H	504	MET	CB-CA-C	7.89	126.17	110.40
1	G	563	PRO	CB-CA-C	-7.75	92.62	112.00
1	K	496	ASP	N-CA-C	7.63	131.59	111.00
1	G	563	PRO	N-CA-CB	7.48	112.28	103.30
1	C	242	ASN	CB-CA-C	-7.25	95.90	110.40
1	D	794	PHE	CB-CG-CD1	-7.18	115.78	120.80
1	G	21	SER	C-N-CA	-7.16	103.80	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	794	PHE	CB-CA-C	-7.14	96.12	110.40
4	R	6	PHE	CB-CG-CD1	-6.99	115.90	120.80
1	A	689	PRO	CB-CA-C	-6.96	94.59	112.00
1	B	534	PRO	CB-CA-C	-6.95	94.62	112.00
4	Q	55	THR	CA-C-N	6.86	136.32	117.10
1	B	725	PHE	CA-CB-CG	6.83	130.30	113.90
3	M	195	GLY	N-CA-C	-6.80	96.09	113.10
4	P	6	PHE	CB-CG-CD1	6.69	125.49	120.80
6	W	6	PRO	N-CA-CB	6.66	111.29	103.30
1	I	824	ASN	CA-CB-CG	-6.56	98.96	113.40
1	D	52	PRO	CB-CA-C	-6.51	95.72	112.00
1	I	347	VAL	CB-CA-C	-6.47	99.11	111.40
1	D	229	PRO	N-CA-C	-6.43	95.38	112.10
1	L	355	LEU	CA-CB-CG	6.33	129.85	115.30
5	V	185	THR	C-N-CA	-6.28	106.01	121.70
4	P	5	SER	CA-C-N	6.25	130.94	117.20
1	L	758	GLN	CB-CA-C	-6.21	97.99	110.40
1	D	794	PHE	CB-CA-C	-6.20	98.00	110.40
1	E	438	GLY	N-CA-C	-6.19	97.63	113.10
1	K	330	ARG	CB-CA-C	6.16	122.72	110.40
1	K	549	LEU	CA-CB-CG	6.15	129.44	115.30
1	A	664	PRO	CB-CA-C	-6.14	96.65	112.00
1	A	431	PRO	N-CA-C	6.10	127.95	112.10
1	I	823	HIS	CB-CA-C	-6.08	98.23	110.40
2	N	48	PRO	CB-CA-C	-6.02	96.95	112.00
1	F	712	PHE	N-CA-C	6.00	127.21	111.00
1	I	734	ASN	CB-CA-C	5.99	122.39	110.40
1	L	445	GLU	CB-CA-C	5.99	122.39	110.40
2	N	476	TYR	CA-CB-CG	5.99	124.78	113.40
1	C	179	ILE	CB-CA-C	-5.99	99.62	111.60
1	G	848	TYR	CB-CG-CD2	5.97	124.58	121.00
1	L	867	ASP	CB-CA-C	-5.96	98.48	110.40
4	Q	56	PRO	N-CA-CB	5.93	110.41	103.30
4	P	6	PHE	N-CA-C	5.93	127.00	111.00
1	B	188	VAL	CA-C-N	-5.88	104.27	117.20
3	M	117	LEU	CA-CB-CG	5.86	128.78	115.30
1	D	35	THR	CB-CA-C	-5.85	95.80	111.60
1	D	230	MET	CA-CB-CG	5.83	123.21	113.30
1	C	664	PRO	CB-CA-C	-5.79	97.53	112.00
1	F	280	LEU	CA-CB-CG	5.76	128.55	115.30
1	J	654	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	C	13	MET	C-N-CA	5.70	135.95	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	355	LEU	CB-CG-CD1	5.68	120.66	111.00
1	L	756	VAL	CB-CA-C	-5.67	100.62	111.40
1	I	794	PHE	N-CA-CB	-5.67	100.39	110.60
1	C	333	PHE	CB-CG-CD2	-5.66	116.84	120.80
2	N	451	PHE	CB-CG-CD2	5.62	124.73	120.80
1	A	253	GLN	N-CA-C	-5.60	95.89	111.00
1	A	794	PHE	CB-CG-CD1	-5.59	116.89	120.80
1	H	732	PRO	N-CA-CB	5.59	110.01	103.30
1	B	794	PHE	N-CA-C	5.56	126.02	111.00
1	L	54	HIS	CA-CB-CG	-5.56	104.15	113.60
1	A	689	PRO	N-CA-CB	5.55	109.96	103.30
4	Q	110	LEU	CA-CB-CG	5.53	128.02	115.30
1	I	656	ILE	N-CA-C	-5.53	96.07	111.00
2	N	63	LEU	CB-CA-C	5.53	120.70	110.20
1	B	730	SER	C-N-CA	5.51	135.48	121.70
2	N	50	GLY	N-CA-C	-5.51	99.32	113.10
1	B	185	GLN	N-CA-C	-5.50	96.14	111.00
4	S	21	PRO	N-CA-C	5.46	126.30	112.10
1	G	22	GLU	CA-CB-CG	-5.46	101.39	113.40
1	H	867	ASP	CA-CB-CG	-5.46	101.39	113.40
1	A	928	VAL	CB-CA-C	5.45	121.76	111.40
1	A	19	ASP	C-N-CA	5.43	135.29	121.70
1	L	823	HIS	C-N-CA	5.43	135.29	121.70
1	H	271	GLU	CB-CA-C	5.42	121.24	110.40
1	D	368	LEU	CA-CB-CG	5.38	127.68	115.30
1	B	373	LEU	CA-CB-CG	5.38	127.67	115.30
4	R	7	ASP	CA-CB-CG	5.37	125.22	113.40
1	C	173	PRO	CB-CA-C	-5.37	98.58	112.00
1	I	729	VAL	CB-CA-C	5.36	121.59	111.40
1	G	879	PHE	CB-CG-CD2	-5.35	117.05	120.80
1	B	941	LEU	CB-CA-C	-5.35	100.03	110.20
1	J	657	PRO	CB-CA-C	-5.34	98.65	112.00
1	C	867	ASP	C-N-CA	5.32	135.01	121.70
1	D	794	PHE	N-CA-C	5.31	125.33	111.00
6	W	12	PRO	N-CA-CB	5.30	109.66	103.30
1	H	503	TYR	CB-CG-CD2	5.29	124.18	121.00
4	P	4	ASN	CA-C-N	5.27	128.80	117.20
1	B	534	PRO	N-CA-CB	5.26	109.61	103.30
2	N	71	LEU	CA-CB-CG	5.26	127.40	115.30
2	N	48	PRO	N-CA-CB	5.24	109.59	103.30
1	I	348	LEU	CA-CB-CG	5.23	127.33	115.30
1	H	280	LEU	CB-CA-C	5.19	120.06	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	478	ALA	C-N-CA	-5.19	108.74	121.70
1	D	79	SER	CB-CA-C	5.18	119.94	110.10
1	H	272	ALA	N-CA-C	5.15	124.91	111.00
1	I	916	LEU	CA-CB-CG	5.12	127.08	115.30
4	S	109	SER	CA-C-N	-5.12	105.93	117.20
1	L	26	PRO	N-CA-CB	5.11	109.44	103.30
1	J	757	ALA	C-N-CA	5.10	134.44	121.70
1	L	54	HIS	N-CA-C	5.09	124.75	111.00
1	L	254	GLN	CB-CA-C	-5.09	100.22	110.40
1	A	56	VAL	CB-CA-C	-5.08	101.74	111.40
1	I	178	ASN	CB-CA-C	-5.08	100.24	110.40
1	G	922	VAL	CB-CA-C	5.06	121.02	111.40
1	A	867	ASP	CB-CA-C	-5.06	100.28	110.40
1	B	732	PRO	CB-CA-C	-5.06	99.36	112.00
1	K	751	GLY	N-CA-C	-5.06	100.45	113.10
2	N	476	TYR	CB-CG-CD1	5.06	124.03	121.00
1	K	748	SER	C-N-CA	5.05	134.33	121.70
4	S	49	TYR	N-CA-CB	5.03	119.65	110.60
5	V	184	GLY	N-CA-C	-5.02	100.56	113.10
1	C	867	ASP	CA-C-N	-5.01	106.17	117.20
1	L	421	ILE	CB-CA-C	-5.01	101.58	111.60
1	G	558	PHE	CB-CG-CD1	-5.00	117.30	120.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	501	TYR	Sidechain
3	M	106	ASN	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7345	0	7042	232	0
1	B	7295	0	6999	224	0
1	C	7374	0	7074	188	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	7345	0	7045	166	0
1	E	7302	0	7006	150	0
1	F	7325	0	7027	133	0
1	G	7291	0	6997	254	0
1	H	7317	0	7019	237	0
1	I	7345	0	7045	262	0
1	J	7329	0	7028	201	0
1	K	7247	0	6957	211	0
1	L	7353	0	7052	195	0
2	N	3577	0	3508	145	0
3	M	2343	0	2313	52	0
4	P	717	0	724	39	0
4	Q	965	0	971	56	0
4	R	734	0	741	27	0
4	S	728	0	739	59	0
5	U	1329	0	1290	18	0
5	V	1346	0	1302	19	0
6	W	116	0	54	21	0
All	All	99723	0	95933	2464	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (2464) 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:H:698:TYR:CE1	4:Q:24:GLY:HA2	1.10	1.58
1:H:698:TYR:HE1	4:Q:24:GLY:CA	1.19	1.54
4:P:40:LEU:HB2	4:P:41:PRO:CD	1.44	1.46
1:A:18:GLN:HB2	6:W:10:SER:CB	1.30	1.46
6:W:7:ARG:CB	6:W:11:ARG:O	1.65	1.42
1:G:758:GLN:OE1	1:I:549:LEU:CD1	1.69	1.39
1:J:656:ILE:HD11	1:J:910:MET:CG	1.51	1.39
1:G:847:PRO:HG2	1:I:121:TYR:CD1	1.57	1.38
1:I:831:TYR:CG	1:I:831:TYR:O	1.75	1.37
1:L:55:ASP:O	1:L:623:ALA:HB3	1.24	1.32
4:S:37:ARG:HB3	4:S:38:PRO:CD	1.60	1.32
4:P:41:PRO:HG2	4:P:44:SER:CB	1.58	1.31
1:G:332:ASN:O	1:G:565:LYS:NZ	1.65	1.30
1:I:356:ASN:ND2	1:I:940:TYR:CE2	1.99	1.29
1:L:824:ASN:HB3	1:L:844:ALA:CB	1.60	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:698:TYR:CE1	4:Q:24:GLY:CA	2.00	1.29
1:I:728:SER:O	1:I:729:VAL:HG23	1.19	1.28
1:C:182:GLU:O	1:C:264:MET:SD	1.92	1.27
1:I:728:SER:O	1:I:729:VAL:CG2	1.81	1.26
1:J:720:LYS:NZ	4:Q:22:TRP:HZ3	1.35	1.25
1:J:757:ALA:CB	1:L:386:MET:HB3	1.65	1.25
1:G:758:GLN:OE1	1:I:549:LEU:HD11	1.10	1.24
1:C:104:ARG:HD3	1:C:612:SER:OG	1.20	1.24
1:I:831:TYR:O	1:I:831:TYR:CD2	1.91	1.23
1:H:748:SER:HB2	4:R:50:GLU:CD	1.58	1.22
1:G:121:TYR:O	1:H:824:ASN:OD1	1.56	1.21
1:H:748:SER:HB2	4:R:50:GLU:OE1	1.39	1.21
1:A:559:HIS:NE2	1:B:755:ASN:O	1.71	1.21
1:E:13:MET:O	1:E:14:HIS:ND1	1.73	1.21
4:P:40:LEU:CB	4:P:41:PRO:CD	2.18	1.21
2:N:67:THR:O	2:N:563:PRO:HD2	1.34	1.20
1:A:62:GLN:O	1:B:735:ASP:O	1.60	1.19
4:P:41:PRO:CG	4:P:44:SER:HB3	1.73	1.18
1:G:929:HIS:HB2	1:G:937:GLU:HG3	1.24	1.17
1:J:720:LYS:CE	4:Q:22:TRP:CZ3	2.26	1.17
1:I:654:TYR:OH	1:I:665:ILE:HD12	1.43	1.17
1:L:32:ALA:O	1:L:36:GLU:HB3	1.41	1.17
5:V:183:ILE:HG22	5:V:184:GLY:O	1.43	1.16
1:J:757:ALA:HB2	1:L:386:MET:HB3	1.26	1.15
1:J:18:GLN:HG3	1:J:19:ASP:H	1.05	1.15
1:K:755:ASN:ND2	1:K:759:CYS:O	1.79	1.15
6:W:7:ARG:CB	6:W:12:PRO:O	1.94	1.15
4:P:41:PRO:CG	4:P:44:SER:CB	2.23	1.14
1:B:941:LEU:HA	1:B:948:GLY:HA2	1.24	1.13
2:N:287:LEU:O	2:N:381:PRO:HA	1.45	1.13
1:D:868:ARG:HG3	1:D:868:ARG:O	1.43	1.13
1:L:824:ASN:HB3	1:L:844:ALA:HB2	1.30	1.13
2:N:55:ILE:HG21	2:N:67:THR:OG1	1.46	1.12
1:G:759:CYS:SG	1:G:800:PRO:HB3	1.89	1.11
1:J:720:LYS:NZ	4:Q:22:TRP:CZ3	2.17	1.11
1:A:201:GLN:HG2	1:A:202:PRO:HD2	1.32	1.11
1:I:831:TYR:O	1:I:831:TYR:CD1	2.02	1.10
2:N:448:PRO:HB3	2:N:529:LEU:CD2	1.80	1.10
1:I:654:TYR:OH	1:I:665:ILE:CD1	1.98	1.10
1:B:81:LYS:HZ2	2:N:457:ILE:HG21	1.16	1.10
1:G:757:ALA:HA	1:I:386:MET:HB3	1.34	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:824:ASN:HB3	1:L:844:ALA:HB1	1.33	1.10
3:M:196:LEU:O	5:U:197:TYR:CE1	2.03	1.10
1:H:748:SER:CB	4:R:50:GLU:OE2	1.98	1.10
1:I:356:ASN:ND2	1:I:940:TYR:HE2	1.36	1.10
1:A:201:GLN:CG	1:A:202:PRO:HD2	1.81	1.09
1:H:517:TYR:HA	1:H:520:LEU:HD11	1.33	1.09
1:A:793:SER:O	1:A:869:THR:CG2	2.00	1.09
1:G:648:SER:O	1:G:922:VAL:O	1.69	1.09
1:G:850:LEU:CD1	1:G:856:VAL:O	2.00	1.08
1:J:426:LEU:HA	1:K:268:SER:O	1.48	1.08
1:L:824:ASN:CB	1:L:844:ALA:HB2	1.84	1.08
1:A:176:GLY:H	1:A:219:ALA:HB2	0.96	1.07
1:A:269:THR:HA	1:C:426:LEU:HD23	1.29	1.07
1:G:847:PRO:CG	1:I:121:TYR:HD1	1.67	1.07
1:C:747:ARG:HG3	1:C:762:THR:HB	1.29	1.07
1:D:53:THR:O	1:D:56:VAL:HG12	1.55	1.07
2:N:446:GLN:HB2	2:N:532:ARG:NE	1.70	1.07
1:G:121:TYR:O	1:H:824:ASN:CG	1.92	1.06
4:S:48:THR:HG23	4:S:48:THR:O	1.28	1.06
1:A:201:GLN:HG3	1:A:202:PRO:HD3	1.38	1.06
1:C:536:ASN:O	1:C:596:SER:O	1.73	1.06
1:C:318:GLN:HE22	1:C:836:MET:HG3	1.16	1.06
1:J:720:LYS:HD2	4:Q:22:TRP:CZ3	1.90	1.06
1:K:204:PRO:O	1:L:826:SER:O	1.70	1.05
1:G:757:ALA:O	1:G:758:GLN:HG3	1.54	1.05
4:S:37:ARG:HB3	4:S:38:PRO:HD3	1.09	1.05
1:K:489:PRO:HB3	1:K:494:ILE:HG13	1.39	1.04
1:D:135:TRP:NE1	1:D:230:MET:SD	2.29	1.04
1:C:747:ARG:CG	1:C:762:THR:HB	1.88	1.04
1:F:481:LEU:HB3	1:F:482:PRO:HD2	1.37	1.04
1:G:771:LEU:O	1:G:880:MET:O	1.73	1.04
1:A:201:GLN:CG	1:A:202:PRO:CD	2.36	1.04
1:G:758:GLN:CD	1:I:549:LEU:HD11	1.77	1.04
1:H:874:PRO:CB	1:H:879:PHE:O	2.05	1.04
1:I:652:MET:CE	1:I:654:TYR:OH	2.06	1.04
1:I:654:TYR:CZ	1:I:665:ILE:HD12	1.92	1.04
1:J:648:SER:CB	1:J:922:VAL:O	2.06	1.04
1:G:850:LEU:HD13	1:G:856:VAL:O	1.57	1.03
1:H:793:SER:O	1:H:797:ASN:ND2	1.91	1.03
1:D:135:TRP:CE2	1:D:230:MET:SD	2.51	1.03
1:J:656:ILE:HD11	1:J:910:MET:HG3	1.08	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:448:PRO:CB	2:N:529:LEU:HD22	1.88	1.03
1:D:78:TYR:CD1	1:D:78:TYR:O	2.11	1.02
1:F:76:THR:O	1:F:587:LYS:NZ	1.92	1.02
4:P:28:ASN:HA	4:P:42:ALA:CB	1.89	1.02
1:C:34:ALA:HB1	6:W:13:PHE:CB	1.89	1.02
1:B:726:ASP:CB	1:B:900:ALA:H	1.71	1.02
1:D:78:TYR:O	1:D:78:TYR:HD1	1.42	1.02
1:E:439:TRP:O	1:F:280:LEU:HD21	1.60	1.02
1:L:535:PHE:HD2	1:L:704:SER:HB3	1.17	1.02
2:N:448:PRO:HB3	2:N:529:LEU:HD22	1.04	1.02
1:A:793:SER:O	1:A:869:THR:HG21	1.57	1.02
1:K:333:PHE:HE1	1:K:386:MET:O	1.40	1.02
4:P:28:ASN:HA	4:P:42:ALA:HB2	1.41	1.02
4:P:40:LEU:CB	4:P:41:PRO:HD3	1.86	1.01
4:S:48:THR:O	4:S:48:THR:CG2	2.04	1.01
1:A:18:GLN:CB	6:W:10:SER:CB	2.26	1.01
1:D:561:GLN:HB2	1:E:757:ALA:HB2	1.42	1.01
1:E:437:ASN:OD1	1:E:437:ASN:O	1.77	1.01
2:N:141:ASN:ND2	2:N:141:ASN:O	1.94	1.01
1:B:64:LEU:CD1	1:B:619:PHE:O	2.09	1.01
4:P:40:LEU:HB2	4:P:41:PRO:HD2	1.04	1.01
1:K:759:CYS:SG	1:K:864:PHE:HB3	1.99	1.00
1:G:847:PRO:CG	1:I:121:TYR:CD1	2.40	1.00
1:L:757:ALA:HB2	1:L:766:PHE:CZ	1.96	1.00
1:A:176:GLY:H	1:A:219:ALA:CB	1.75	1.00
1:H:874:PRO:CG	1:H:879:PHE:O	2.08	1.00
2:N:457:ILE:O	2:N:457:ILE:HG12	1.59	1.00
1:L:55:ASP:O	1:L:623:ALA:CB	2.08	1.00
1:J:656:ILE:CD1	1:J:910:MET:CG	2.39	0.99
1:G:804:GLN:CG	1:G:850:LEU:HD21	1.90	0.99
1:J:720:LYS:CD	4:Q:22:TRP:CZ3	2.45	0.99
1:A:58:THR:O	1:A:58:THR:HG23	1.61	0.98
1:B:941:LEU:O	1:B:941:LEU:HG	1.62	0.98
1:G:929:HIS:O	1:G:937:GLU:HG2	1.61	0.98
1:J:648:SER:HB3	1:J:922:VAL:O	1.63	0.98
4:P:40:LEU:HB2	4:P:41:PRO:HD3	1.42	0.98
1:G:804:GLN:HG3	1:G:850:LEU:CD2	1.95	0.97
1:J:821:HIS:CG	1:L:244:ASN:O	2.17	0.97
1:G:927:ARG:HB3	1:G:939:VAL:HG23	1.45	0.97
2:N:446:GLN:O	2:N:447:ASP:OD1	1.83	0.97
1:B:347:VAL:HG21	2:N:455:ARG:HG2	1.44	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:712:PHE:O	1:G:867:ASP:O	1.82	0.96
2:N:52:ARG:O	2:N:52:ARG:HG2	1.64	0.96
1:C:747:ARG:HB2	1:C:760:ASN:O	1.65	0.96
1:G:847:PRO:HB2	1:I:121:TYR:HE1	1.28	0.96
1:G:758:GLN:OE1	1:I:549:LEU:HD12	1.66	0.96
1:A:176:GLY:N	1:A:219:ALA:HB2	1.81	0.95
1:G:201:GLN:HB3	1:G:202:PRO:CD	1.95	0.95
1:L:106:VAL:HG21	4:Q:56:PRO:HD2	1.48	0.95
1:J:18:GLN:HG3	1:J:19:ASP:N	1.75	0.95
1:G:804:GLN:HG2	1:G:850:LEU:HD21	1.47	0.95
1:B:81:LYS:NZ	2:N:457:ILE:HG21	1.81	0.95
1:D:135:TRP:CZ2	1:D:230:MET:SD	2.59	0.95
2:N:446:GLN:CB	2:N:532:ARG:NE	2.28	0.95
1:G:689:PRO:HD3	1:G:699:TYR:HD1	1.29	0.95
1:G:713:TYR:HA	1:G:867:ASP:O	1.65	0.95
1:G:804:GLN:CG	1:G:850:LEU:CD2	2.43	0.95
1:J:720:LYS:HD2	4:Q:22:TRP:CE3	2.02	0.94
1:A:269:THR:O	1:C:426:LEU:HA	1.67	0.94
1:E:13:MET:O	1:E:14:HIS:CG	2.21	0.94
1:A:269:THR:O	1:C:425:THR:O	1.86	0.94
1:C:104:ARG:HD3	1:C:612:SER:HG	1.25	0.94
1:J:757:ALA:HB2	1:L:386:MET:CB	1.98	0.94
1:L:824:ASN:CB	1:L:844:ALA:CB	2.43	0.94
1:F:108:ASP:O	1:F:606:ALA:HB1	1.68	0.93
1:C:104:ARG:CD	1:C:612:SER:OG	2.14	0.93
1:H:867:ASP:O	1:H:868:ARG:HB2	1.68	0.93
1:J:720:LYS:CE	4:Q:22:TRP:HZ3	1.72	0.93
1:H:748:SER:HB2	4:R:50:GLU:OE2	1.62	0.93
1:K:333:PHE:CE1	1:K:386:MET:O	2.21	0.93
1:B:941:LEU:CA	1:B:948:GLY:HA2	2.00	0.92
1:C:656:ILE:HG23	1:C:660:ALA:CB	1.99	0.92
1:H:330:ARG:HD2	1:H:708:LEU:CD2	1.97	0.92
1:I:653:LEU:HD23	1:I:653:LEU:H	1.32	0.92
1:G:844:ALA:O	1:I:237:TYR:HB2	1.68	0.92
1:H:874:PRO:HB2	1:H:879:PHE:O	1.68	0.92
2:N:225:LEU:HD22	2:N:285:ALA:HB3	1.49	0.92
1:E:488:SER:HB2	1:E:489:PRO:HD3	1.52	0.92
1:A:174:TYR:HB2	1:A:202:PRO:HB3	1.50	0.92
1:K:201:GLN:HB3	1:K:202:PRO:CD	2.00	0.92
1:A:201:GLN:HG3	1:A:202:PRO:CD	1.97	0.91
1:D:789:ASP:OD2	1:F:382:ARG:NH1	2.03	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:7:ARG:CB	6:W:12:PRO:C	2.39	0.91
1:A:56:VAL:HG23	1:A:56:VAL:O	1.67	0.91
1:A:58:THR:O	1:A:58:THR:CG2	2.18	0.91
1:A:179:ILE:HG12	1:A:218:HIS:HB3	1.52	0.91
1:G:847:PRO:HB2	1:I:121:TYR:CE1	2.04	0.90
1:C:179:ILE:HG22	1:C:180:THR:O	1.70	0.90
1:G:757:ALA:HB2	1:I:386:MET:HG2	1.53	0.90
1:K:759:CYS:HB2	1:K:800:PRO:HB3	1.51	0.90
1:H:570:LYS:O	1:H:643:PHE:CE1	2.24	0.90
1:G:548:MET:HB3	1:H:523:ARG:HB2	1.51	0.90
1:B:532:VAL:O	1:B:534:PRO:HD3	1.71	0.90
1:J:18:GLN:CG	1:J:19:ASP:H	1.85	0.90
1:A:460:MET:HG2	1:B:416:PRO:HA	1.55	0.89
1:G:201:GLN:HB3	1:G:202:PRO:HD3	1.55	0.89
1:K:748:SER:CA	1:K:760:ASN:HD21	1.84	0.89
2:N:446:GLN:HB2	2:N:532:ARG:CZ	2.02	0.89
1:K:201:GLN:HB3	1:K:202:PRO:HD3	1.56	0.88
1:C:656:ILE:CG2	1:C:660:ALA:HB3	2.03	0.88
1:G:847:PRO:HG2	1:I:121:TYR:HD1	0.75	0.88
1:G:201:GLN:O	1:G:203:GLU:HG2	1.72	0.88
1:I:652:MET:HE2	1:I:654:TYR:OH	1.73	0.88
1:I:728:SER:C	1:I:729:VAL:HG23	1.94	0.88
1:C:536:ASN:C	1:C:596:SER:O	2.12	0.88
1:D:269:THR:O	1:D:270:THR:HG22	1.72	0.88
1:G:775:ASN:HD22	1:G:881:SER:HB2	1.39	0.88
4:P:41:PRO:CG	4:P:44:SER:HB2	2.02	0.88
1:I:724:THR:HG23	1:I:729:VAL:O	1.73	0.88
1:B:14:HIS:O	1:B:14:HIS:CD2	2.26	0.87
1:A:476:ASN:O	1:A:537:HIS:NE2	2.07	0.87
1:A:581:TYR:HE2	1:A:583:TRP:HD1	1.21	0.87
1:A:581:TYR:HH	1:A:583:TRP:HE1	1.10	0.87
1:F:533:ASN:CB	1:F:713:TYR:CE2	2.58	0.87
4:S:106:GLN:O	4:S:110:LEU:HG	1.75	0.87
1:A:665:ILE:HG22	1:A:903:MET:HB2	1.56	0.87
1:H:492:VAL:HG11	1:H:506:LYS:HD3	1.54	0.87
2:N:287:LEU:O	2:N:381:PRO:CA	2.22	0.87
1:A:431:PRO:HA	1:A:439:TRP:HD1	1.40	0.87
1:C:824:ASN:HB3	1:C:844:ALA:HB1	1.57	0.87
1:G:712:PHE:C	1:G:867:ASP:O	2.13	0.86
1:J:757:ALA:CB	1:L:386:MET:CB	2.53	0.86
1:H:698:TYR:CD1	4:Q:24:GLY:HA2	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:ASN:HB3	1:B:866:CYS:O	1.74	0.86
1:H:724:THR:O	1:H:902:ASP:O	1.93	0.86
2:N:52:ARG:NH2	2:N:62:PRO:HB2	1.91	0.86
1:J:656:ILE:HD11	1:J:910:MET:HG2	1.54	0.86
1:D:14:HIS:CE1	1:D:24:LEU:HD21	2.09	0.86
2:N:52:ARG:HH21	2:N:63:LEU:N	1.74	0.86
1:A:55:ASP:O	1:A:56:VAL:HG22	1.75	0.86
1:B:726:ASP:O	1:B:726:ASP:OD1	1.93	0.86
1:B:726:ASP:HB3	1:B:900:ALA:H	1.41	0.86
1:H:97:ALA:HB2	1:H:571:ASN:H	1.38	0.86
1:B:13:MET:O	1:B:14:HIS:ND1	2.08	0.86
1:B:922:VAL:HA	1:B:944:PRO:HG2	1.56	0.86
1:A:793:SER:O	1:A:869:THR:HG23	1.74	0.85
1:D:868:ARG:O	1:D:868:ARG:CG	2.24	0.85
1:H:748:SER:HB3	4:R:50:GLU:OE2	1.77	0.85
1:B:184:ILE:O	1:B:195:TYR:HD2	1.59	0.85
1:I:662:ASN:OD1	1:I:906:GLU:HA	1.76	0.85
1:B:252:LYS:CG	1:B:253:GLN:H	1.89	0.85
2:N:52:ARG:HH21	2:N:63:LEU:CA	1.90	0.85
2:N:55:ILE:CG2	2:N:67:THR:OG1	2.24	0.85
1:E:15:ILE:CG2	1:E:15:ILE:O	2.24	0.85
1:J:656:ILE:CD1	1:J:910:MET:HG3	2.00	0.85
1:L:757:ALA:O	1:L:758:GLN:HB2	1.74	0.84
1:L:797:ASN:CB	1:L:867:ASP:O	2.24	0.84
4:S:37:ARG:CB	4:S:38:PRO:HD3	2.02	0.84
1:K:469:TRP:HE1	1:K:516:CYS:HG	1.03	0.84
1:G:929:HIS:CB	1:G:937:GLU:HG3	2.08	0.84
1:B:726:ASP:HB2	1:B:900:ALA:H	1.42	0.84
1:E:724:THR:CG2	1:E:728:SER:O	2.25	0.84
3:M:251:ASP:OD1	3:M:251:ASP:O	1.96	0.84
1:I:724:THR:CG2	1:I:729:VAL:O	2.25	0.84
1:A:927:ARG:O	1:A:938:THR:HG23	1.78	0.84
2:N:52:ARG:NH2	2:N:62:PRO:C	2.31	0.84
4:S:37:ARG:CB	4:S:38:PRO:CD	2.48	0.83
1:G:758:GLN:HA	1:I:559:HIS:CE1	2.13	0.83
1:A:789:ASP:HB3	1:A:796:ARG:HG3	1.59	0.83
1:C:536:ASN:CA	1:C:596:SER:O	2.26	0.83
1:J:201:GLN:HB3	1:J:202:PRO:HD3	1.59	0.83
1:G:856:VAL:O	1:G:856:VAL:HG12	1.76	0.83
1:B:941:LEU:O	1:B:941:LEU:CG	2.26	0.83
1:G:824:ASN:HA	1:G:844:ALA:HB2	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:ARG:HH22	1:B:695:TYR:HE1	1.25	0.83
1:H:732:PRO:HG2	1:H:740:PRO:O	1.78	0.83
4:S:116:VAL:O	4:S:120:GLN:CG	2.27	0.83
1:I:356:ASN:HD21	1:I:940:TYR:HE2	0.85	0.83
1:J:922:VAL:HG12	1:J:944:PRO:HG2	1.60	0.83
4:P:30:MET:HG2	4:P:40:LEU:O	1.79	0.83
4:P:40:LEU:HB3	4:P:41:PRO:HD3	1.60	0.83
1:H:492:VAL:CG2	1:H:506:LYS:HZ3	1.92	0.82
1:I:737:LEU:HD13	1:I:764:ASP:HB2	1.60	0.82
1:J:757:ALA:HB3	1:L:386:MET:HB3	1.60	0.82
1:L:20:ALA:O	1:L:45:PHE:HE2	1.61	0.82
2:N:45:TYR:O	2:N:46:LEU:HG	1.79	0.82
1:J:648:SER:HB2	1:J:922:VAL:O	1.79	0.82
4:S:15:LEU:HD12	4:S:15:LEU:H	1.42	0.82
1:D:478:ALA:HB2	1:D:514:VAL:HG21	1.61	0.82
1:I:652:MET:CE	1:I:654:TYR:CZ	2.62	0.82
1:K:331:ASP:O	1:K:388:ASN:HB3	1.78	0.82
1:J:720:LYS:HE3	4:Q:22:TRP:CZ3	2.13	0.82
1:J:656:ILE:HB	1:J:660:ALA:HB3	1.62	0.82
1:K:755:ASN:CG	1:K:759:CYS:O	2.17	0.82
1:C:597:LEU:HG	1:C:597:LEU:O	1.78	0.81
1:G:204:PRO:HB3	1:H:840:GLN:HB3	1.61	0.81
1:H:513:LEU:O	1:H:518:ILE:HD13	1.80	0.81
1:J:126:PRO:HB3	1:K:461:GLU:HB3	1.62	0.81
1:K:331:ASP:O	1:K:388:ASN:CB	2.27	0.81
2:N:52:ARG:HH21	2:N:63:LEU:C	1.84	0.81
2:N:448:PRO:CA	2:N:529:LEU:HD13	2.11	0.81
1:J:656:ILE:HG13	1:J:656:ILE:O	1.80	0.81
1:B:201:GLN:HB3	1:B:202:PRO:HD3	1.62	0.81
1:G:804:GLN:HG2	1:G:850:LEU:CD2	2.10	0.81
2:N:52:ARG:NE	2:N:63:LEU:O	2.12	0.81
1:A:581:TYR:CE2	1:A:583:TRP:CD1	2.69	0.81
1:I:831:TYR:O	1:I:831:TYR:CE2	2.33	0.81
1:G:804:GLN:NE2	1:G:858:SER:OG	2.14	0.81
1:J:720:LYS:HZ2	4:Q:22:TRP:HZ3	0.81	0.81
1:I:589:VAL:HG22	1:I:602:ARG:HD2	1.63	0.80
1:I:720:LYS:H	1:I:906:GLU:HB2	1.46	0.80
1:J:656:ILE:CD1	1:J:910:MET:HG2	2.10	0.80
1:A:479:LEU:HD21	1:A:505:ASN:HA	1.62	0.80
1:F:242:ASN:O	1:F:242:ASN:OD1	1.98	0.80
1:G:621:PRO:HG2	1:H:878:ASN:OD1	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:497:ASN:OD1	1:K:498:PRO:HD2	1.82	0.80
1:K:842:TYR:CD2	1:K:843:PRO:HD2	2.17	0.80
1:L:757:ALA:HB2	1:L:766:PHE:HZ	1.47	0.80
1:K:493:LYS:O	1:K:494:ILE:CD1	2.30	0.79
1:E:15:ILE:O	1:E:15:ILE:HG22	1.80	0.79
1:J:179:ILE:HG12	1:J:218:HIS:HB3	1.64	0.79
1:G:679:ALA:HB1	1:G:870:LEU:HD22	1.64	0.79
2:N:275:TYR:O	2:N:275:TYR:CD1	2.35	0.79
1:A:833:ALA:O	1:A:835:THR:HG22	1.83	0.79
1:I:349:ALA:CB	1:I:353:SER:O	2.30	0.79
1:C:656:ILE:HG23	1:C:660:ALA:HB3	1.62	0.79
1:H:514:VAL:HA	1:H:518:ILE:HD11	1.62	0.79
1:H:517:TYR:HA	1:H:520:LEU:CD1	2.10	0.79
1:G:928:VAL:HA	1:G:938:THR:HA	1.64	0.79
2:N:247:GLY:HA3	2:N:274:THR:HG23	1.64	0.78
1:D:797:ASN:CB	1:D:867:ASP:O	2.30	0.78
1:G:201:GLN:O	1:G:203:GLU:N	2.16	0.78
1:G:689:PRO:HD3	1:G:699:TYR:CD1	2.18	0.78
1:A:797:ASN:ND2	1:A:869:THR:OG1	2.15	0.78
1:F:533:ASN:CG	1:F:713:TYR:CE2	2.57	0.78
1:G:929:HIS:O	1:G:937:GLU:CG	2.31	0.78
4:S:37:ARG:HB3	4:S:38:PRO:HD2	1.66	0.78
1:H:698:TYR:CD1	4:Q:24:GLY:CA	2.64	0.78
1:K:493:LYS:O	1:K:494:ILE:HD13	1.83	0.78
2:N:123:LEU:HD22	2:N:441:LEU:HD12	1.66	0.78
4:Q:115:ASN:O	4:Q:118:SER:HB3	1.83	0.78
1:C:823:HIS:O	1:C:844:ALA:HA	1.83	0.78
1:G:23:TYR:O	1:G:23:TYR:CD2	2.36	0.78
1:H:698:TYR:CE1	4:Q:24:GLY:N	2.50	0.78
1:L:535:PHE:CD2	1:L:704:SER:HB3	2.10	0.78
1:H:698:TYR:OH	4:Q:26:ARG:HG3	1.84	0.78
4:P:41:PRO:HG2	4:P:44:SER:HB3	0.82	0.78
1:C:215:GLU:O	1:C:216:ILE:HG13	1.85	0.77
1:H:492:VAL:HG22	1:H:506:LYS:HZ3	1.48	0.77
1:J:663:VAL:O	1:J:663:VAL:HG12	1.84	0.77
1:I:728:SER:O	1:I:729:VAL:HG22	1.80	0.77
1:F:533:ASN:CG	1:F:713:TYR:HE2	1.87	0.77
1:J:119:THR:HG23	1:J:297:ASP:HB2	1.66	0.77
4:S:116:VAL:O	4:S:120:GLN:HG3	1.83	0.77
1:K:561:GLN:HB2	1:L:756:VAL:HG13	1.67	0.77
1:A:200:PHE:O	1:A:200:PHE:CD1	2.37	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:726:ASP:HB3	1:H:900:ALA:HB3	1.66	0.77
1:K:204:PRO:C	1:L:826:SER:O	2.22	0.77
1:E:756:VAL:HG22	1:E:757:ALA:H	1.49	0.77
2:N:52:ARG:NH2	2:N:63:LEU:O	2.17	0.77
1:C:33:ARG:HG2	6:W:17:TRP:H	1.49	0.77
1:G:682:ARG:HH21	1:G:907:VAL:HG12	1.49	0.77
1:H:367:GLU:OE2	1:H:708:LEU:HD11	1.84	0.77
1:D:25:SER:O	1:D:29:VAL:HG23	1.84	0.77
1:H:519:ASN:ND2	1:H:803:ARG:HH11	1.82	0.77
1:A:431:PRO:O	1:A:434:GLY:O	2.03	0.76
1:D:76:THR:OG1	1:D:77:ALA:N	2.18	0.76
1:G:722:ALA:HB2	1:G:742:GLU:HB3	1.68	0.76
1:H:332:ASN:H	1:H:388:ASN:HB2	1.50	0.76
1:H:698:TYR:CD1	4:Q:24:GLY:N	2.53	0.76
1:I:356:ASN:O	1:I:356:ASN:OD1	2.03	0.76
1:B:64:LEU:HD12	1:B:619:PHE:O	1.83	0.76
1:J:655:PRO:HG3	1:J:915:LEU:HD23	1.65	0.76
1:K:63:ARG:HG3	1:K:63:ARG:O	1.84	0.76
1:D:201:GLN:HB3	1:D:202:PRO:HD3	1.67	0.76
1:H:790:ARG:HB2	1:H:793:SER:OG	1.86	0.76
1:A:824:ASN:HA	1:A:844:ALA:HB2	1.68	0.76
1:C:84:PHE:HB2	1:C:581:TYR:HB3	1.67	0.76
1:C:533:ASN:HB3	1:C:704:SER:HB2	1.67	0.76
1:H:797:ASN:HB3	1:H:867:ASP:O	1.86	0.76
1:A:411:PRO:HB3	1:C:127:LYS:HG3	1.67	0.76
1:I:722:ALA:HB3	1:I:904:THR:HB	1.66	0.75
1:D:523:ARG:HB2	1:F:548:MET:HB3	1.68	0.75
1:A:472:PHE:O	1:A:476:ASN:CG	2.25	0.75
1:H:272:ALA:O	1:H:280:LEU:CD2	2.34	0.75
2:N:52:ARG:NH2	2:N:63:LEU:N	2.33	0.75
3:M:251:ASP:OD1	3:M:251:ASP:C	2.24	0.75
1:B:756:VAL:HG12	1:B:763:LYS:HG2	1.69	0.75
1:K:755:ASN:HD21	1:K:759:CYS:C	1.89	0.75
1:L:84:PHE:HB2	1:L:581:TYR:HB3	1.69	0.75
1:G:757:ALA:CA	1:I:386:MET:HB3	2.15	0.75
1:J:640:ASP:H	1:L:24:LEU:HD22	1.51	0.75
2:N:445:MET:HB3	2:N:529:LEU:CD1	2.17	0.75
1:I:349:ALA:HB3	1:I:353:SER:O	1.86	0.75
1:D:330:ARG:HG2	1:D:594:GLN:HB2	1.68	0.75
1:H:705:ILE:HG22	1:H:707:TYR:H	1.50	0.75
1:J:546:ARG:HH22	1:J:560:ILE:HG21	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:445:MET:HB3	2:N:529:LEU:HD11	1.67	0.75
1:F:533:ASN:HB2	1:F:713:TYR:CE2	2.22	0.75
1:G:929:HIS:HB2	1:G:937:GLU:CG	2.12	0.75
1:I:653:LEU:H	1:I:653:LEU:CD2	1.98	0.74
2:N:45:TYR:O	2:N:46:LEU:CG	2.35	0.74
1:A:860:THR:HG21	1:C:551:GLY:HA2	1.69	0.74
1:C:10:TRP:HB3	1:C:15:ILE:HB	1.68	0.74
1:C:179:ILE:HG12	1:C:184:ILE:HG23	1.69	0.74
1:C:536:ASN:HA	1:C:596:SER:O	1.86	0.74
1:A:665:ILE:CG2	1:A:903:MET:HB2	2.18	0.74
2:N:52:ARG:HH22	2:N:62:PRO:C	1.87	0.74
3:M:200:ASN:HD21	3:M:235:LEU:HB2	1.50	0.74
1:G:691:LEU:HD13	1:G:692:GLY:N	2.03	0.74
1:H:665:ILE:HG23	1:H:903:MET:HB3	1.70	0.74
1:C:333:PHE:O	1:C:333:PHE:HD1	1.70	0.74
1:H:874:PRO:HG3	1:H:879:PHE:O	1.88	0.74
1:F:481:LEU:HB3	1:F:482:PRO:CD	2.18	0.74
2:N:446:GLN:CB	2:N:532:ARG:HE	1.97	0.74
1:J:656:ILE:HD11	1:J:910:MET:CB	2.18	0.74
1:J:126:PRO:HB3	1:K:461:GLU:CB	2.17	0.74
2:N:446:GLN:HB2	2:N:532:ARG:HE	1.46	0.73
4:S:30:MET:CE	4:S:41:PRO:HB3	2.18	0.73
1:A:748:SER:O	1:A:749:VAL:HG23	1.88	0.73
1:K:776:ILE:HG21	1:K:782:TYR:H	1.53	0.73
3:M:196:LEU:O	5:U:197:TYR:CD1	2.41	0.73
1:C:922:VAL:HG13	1:C:944:PRO:HD2	1.69	0.73
1:K:748:SER:HA	1:K:760:ASN:HD21	1.51	0.73
4:P:28:ASN:CA	4:P:42:ALA:HB2	2.18	0.73
1:A:837:ARG:O	1:A:837:ARG:HG2	1.88	0.73
1:A:581:TYR:HE2	1:A:583:TRP:CD1	2.04	0.73
1:B:798:PHE:HB2	1:B:866:CYS:HA	1.69	0.73
1:D:731:TRP:HB3	1:D:732:PRO:HD3	1.71	0.73
1:I:831:TYR:O	1:I:831:TYR:CE1	2.42	0.73
1:K:493:LYS:O	1:K:494:ILE:HG12	1.88	0.73
4:Q:112:ARG:O	4:Q:116:VAL:HG23	1.88	0.73
4:S:113:GLU:O	4:S:117:VAL:HG23	1.89	0.73
1:J:676:ARG:HB2	1:J:921:GLU:HB3	1.71	0.73
1:D:794:PHE:CD2	1:D:794:PHE:O	2.42	0.72
1:B:13:MET:O	1:B:14:HIS:CG	2.41	0.72
1:C:35:THR:HG23	6:W:5:ALA:HB2	1.71	0.72
1:G:713:TYR:CA	1:G:867:ASP:O	2.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:116:VAL:O	4:S:120:GLN:HG2	1.89	0.72
1:G:775:ASN:ND2	1:G:881:SER:HB2	2.03	0.72
1:J:460:MET:HB3	1:K:416:PRO:HA	1.72	0.72
4:R:42:ALA:O	4:R:46:THR:HG22	1.89	0.72
1:A:267:PHE:HE1	1:A:284:VAL:HB	1.54	0.72
1:I:441:LYS:HG3	1:I:442:ASP:H	1.53	0.72
4:S:18:ARG:HG2	4:S:19:MET:H	1.54	0.72
1:I:730:SER:OG	1:I:740:PRO:HB2	1.90	0.72
1:I:922:VAL:HG13	1:I:944:PRO:HD2	1.71	0.72
2:N:448:PRO:HA	2:N:529:LEU:HD13	1.71	0.72
1:L:10:TRP:HB2	1:L:16:SER:OG	1.89	0.72
1:L:656:ILE:HG23	1:L:660:ALA:HB3	1.70	0.72
2:N:287:LEU:O	2:N:381:PRO:O	2.07	0.72
1:B:941:LEU:HA	1:B:948:GLY:CA	2.13	0.72
1:A:581:TYR:CE2	1:A:583:TRP:HD1	2.02	0.72
1:I:654:TYR:HH	1:I:665:ILE:CD1	2.00	0.72
1:K:823:HIS:HD2	1:K:843:PRO:O	1.72	0.72
1:B:184:ILE:O	1:B:195:TYR:CD2	2.43	0.71
1:E:716:HIS:HB3	1:E:866:CYS:H	1.55	0.71
2:N:448:PRO:HB3	2:N:529:LEU:CG	2.19	0.71
1:H:492:VAL:HG22	1:H:506:LYS:NZ	2.05	0.71
1:I:654:TYR:OH	1:I:665:ILE:HD11	1.90	0.71
4:Q:27:GLN:O	4:Q:29:VAL:HG23	1.91	0.71
4:S:125:ARG:O	4:S:129:SER:OG	2.02	0.71
1:D:98:SER:HB3	1:E:780:GLY:HA2	1.73	0.71
1:D:794:PHE:O	1:D:794:PHE:CG	2.43	0.71
1:I:661:THR:C	1:I:662:ASN:HD22	1.94	0.71
2:N:52:ARG:NH2	2:N:63:LEU:CA	2.54	0.71
1:B:794:PHE:O	1:B:798:PHE:HD2	1.71	0.71
1:D:269:THR:O	1:D:270:THR:CG2	2.38	0.71
1:I:664:PRO:HB3	1:I:905:PHE:H	1.56	0.71
4:P:28:ASN:HA	4:P:42:ALA:HB3	1.72	0.71
1:A:201:GLN:HG2	1:A:202:PRO:CD	2.11	0.71
1:C:18:GLN:O	1:C:19:ASP:OD1	2.08	0.71
1:C:656:ILE:CG2	1:C:660:ALA:CB	2.67	0.71
1:G:508:VAL:HG11	1:G:834:PRO:HD3	1.73	0.71
1:I:793:SER:O	1:I:797:ASN:ND2	2.23	0.71
1:A:837:ARG:O	1:B:456:ASN:ND2	2.24	0.70
1:B:252:LYS:HG2	1:B:253:GLN:H	1.56	0.70
1:I:652:MET:HE2	1:I:654:TYR:CZ	2.25	0.70
1:B:529:MET:O	1:B:532:VAL:HG22	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:PHE:O	1:C:333:PHE:CD1	2.44	0.70
1:G:943:THR:HB	1:G:944:PRO:HD3	1.72	0.70
1:G:201:GLN:HB2	1:G:287:TYR:CZ	2.26	0.70
1:K:493:LYS:O	1:K:494:ILE:CG1	2.38	0.70
4:P:29:VAL:H	4:P:42:ALA:HB2	1.57	0.70
2:N:450:THR:O	2:N:450:THR:OG1	2.09	0.70
1:D:797:ASN:HB3	1:D:867:ASP:O	1.91	0.70
2:N:287:LEU:O	2:N:381:PRO:C	2.29	0.70
1:J:922:VAL:CG1	1:J:944:PRO:HG2	2.22	0.70
3:M:196:LEU:CB	3:M:199:VAL:HG21	2.22	0.70
3:M:200:ASN:HD21	3:M:235:LEU:CA	2.04	0.70
1:G:682:ARG:NH2	1:G:907:VAL:HG12	2.07	0.70
1:E:797:ASN:ND2	1:E:868:ARG:O	2.25	0.69
1:G:927:ARG:HB3	1:G:939:VAL:CG2	2.19	0.69
1:D:757:ALA:O	1:D:758:GLN:HB2	1.92	0.69
1:C:797:ASN:HB2	1:C:867:ASP:O	1.92	0.69
1:E:560:ILE:HG12	1:F:758:GLN:HB3	1.74	0.69
1:K:332:ASN:O	1:K:333:PHE:HB2	1.92	0.69
1:L:535:PHE:HD2	1:L:704:SER:CB	2.01	0.69
1:L:756:VAL:O	1:L:756:VAL:HG12	1.92	0.69
1:K:469:TRP:NE1	1:K:516:CYS:SG	2.53	0.69
2:N:67:THR:O	2:N:563:PRO:CD	2.28	0.69
2:N:243:LEU:HB3	2:N:244:PRO:CD	2.22	0.69
1:A:11:SER:OG	1:A:16:SER:HB2	1.93	0.69
1:G:775:ASN:HD22	1:G:881:SER:CB	2.04	0.69
1:H:46:ARG:HG3	1:I:644:ASN:H	1.57	0.69
1:H:59:ASP:O	1:I:734:ASN:CG	2.30	0.69
1:K:508:VAL:HG11	1:K:834:PRO:HD3	1.75	0.69
1:L:446:PHE:O	1:L:447:SER:O	2.11	0.69
3:M:200:ASN:ND2	3:M:235:LEU:N	2.39	0.69
1:G:929:HIS:C	1:G:937:GLU:CG	2.61	0.69
1:A:431:PRO:HA	1:A:439:TRP:CD1	2.25	0.69
1:B:724:THR:O	1:B:902:ASP:N	2.26	0.69
1:D:758:GLN:HE22	1:F:560:ILE:HA	1.57	0.69
1:G:850:LEU:O	1:G:850:LEU:HG	1.89	0.69
1:B:679:ALA:HB1	1:B:870:LEU:HB3	1.75	0.69
1:L:757:ALA:O	1:L:758:GLN:CB	2.40	0.69
2:N:444:MET:HE1	2:N:561:VAL:HG21	1.73	0.69
4:S:19:MET:HA	4:S:19:MET:CE	2.23	0.69
1:C:318:GLN:HE22	1:C:836:MET:CG	1.99	0.69
1:C:318:GLN:NE2	1:C:836:MET:HG3	2.00	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:929:HIS:C	1:G:937:GLU:HG2	2.13	0.69
1:I:720:LYS:HG3	1:I:906:GLU:HG3	1.73	0.69
4:S:19:MET:HA	4:S:19:MET:HE2	1.74	0.69
1:C:824:ASN:HB3	1:C:844:ALA:CB	2.22	0.69
1:F:330:ARG:HG2	1:F:594:GLN:HB2	1.75	0.69
1:K:332:ASN:HA	1:K:387:TRP:O	1.92	0.69
2:N:446:GLN:HB3	2:N:532:ARG:HG2	1.75	0.69
4:P:41:PRO:HG3	4:P:44:SER:CB	2.20	0.69
1:B:726:ASP:OD1	1:B:726:ASP:C	2.32	0.68
1:E:429:VAL:HG22	1:F:267:PHE:HA	1.73	0.68
1:A:582:GLU:O	1:A:583:TRP:CD1	2.46	0.68
1:E:69:ILE:HG21	1:J:73:ARG:O	1.92	0.68
1:H:514:VAL:HA	1:H:518:ILE:CD1	2.23	0.68
1:F:922:VAL:HG13	1:F:944:PRO:HD2	1.74	0.68
1:H:748:SER:CB	4:R:50:GLU:CD	2.42	0.68
2:N:446:GLN:C	2:N:447:ASP:OD1	2.32	0.68
4:Q:19:MET:O	4:Q:21:PRO:HD3	1.93	0.68
1:H:748:SER:CB	4:R:50:GLU:OE1	2.31	0.68
1:K:759:CYS:CB	1:K:800:PRO:HB3	2.23	0.68
1:A:581:TYR:OH	1:A:583:TRP:NE1	2.11	0.68
1:F:713:TYR:CE1	1:F:714:LEU:HG	2.29	0.68
1:B:837:ARG:HH12	1:C:416:PRO:HD2	1.59	0.68
1:E:184:ILE:HG21	1:E:220:ALA:HB2	1.74	0.68
1:G:135:TRP:HD1	1:G:310:ASN:HB2	1.59	0.68
1:G:931:PRO:HD3	1:G:937:GLU:CD	2.14	0.68
2:N:449:VAL:HG12	2:N:450:THR:HG22	1.75	0.68
1:A:833:ALA:O	1:A:835:THR:N	2.25	0.68
1:E:798:PHE:HB2	1:E:865:LEU:O	1.93	0.68
1:H:367:GLU:OE2	1:H:708:LEU:CD1	2.41	0.68
1:K:700:THR:O	1:K:700:THR:OG1	2.08	0.68
1:C:573:LEU:H	1:C:641:GLN:HE22	1.42	0.68
1:G:119:THR:HG23	1:G:297:ASP:HB2	1.76	0.68
1:G:850:LEU:HD12	1:G:856:VAL:O	1.90	0.68
1:L:513:LEU:HA	1:L:518:ILE:HD11	1.76	0.68
1:G:847:PRO:CB	1:I:121:TYR:CE1	2.77	0.68
1:H:330:ARG:HD2	1:H:708:LEU:HD21	1.75	0.68
4:R:41:PRO:HA	4:R:46:THR:HB	1.75	0.68
1:K:837:ARG:HB2	1:L:459:ALA:HB2	1.75	0.67
1:L:797:ASN:HB3	1:L:867:ASP:O	1.92	0.67
2:N:243:LEU:HB3	2:N:244:PRO:HD2	1.74	0.67
1:L:106:VAL:CG2	4:Q:56:PRO:HD2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:30:MET:HE2	4:S:41:PRO:CA	2.24	0.67
1:F:602:ARG:HG2	4:R:34:ILE:HA	1.75	0.67
1:B:759:CYS:SG	1:B:761:MET:HG3	2.35	0.67
1:D:382:ARG:HH22	1:E:796:ARG:HG3	1.60	0.67
1:K:561:GLN:CB	1:L:756:VAL:HG13	2.24	0.67
1:C:822:GLN:O	1:C:823:HIS:ND1	2.27	0.67
1:L:758:GLN:O	1:L:862:LYS:HD3	1.94	0.67
1:B:184:ILE:HG22	1:B:185:GLN:O	1.94	0.67
1:C:747:ARG:HG2	1:C:762:THR:HB	1.77	0.67
1:H:670:ARG:HB2	1:H:672:TRP:HD1	1.59	0.67
1:I:485:LEU:O	1:I:509:VAL:HG23	1.95	0.67
1:K:748:SER:HA	1:K:760:ASN:ND2	2.10	0.67
1:A:79:SER:HB2	1:A:584:ASN:HD22	1.59	0.67
1:G:568:ALA:HA	1:G:926:VAL:HG11	1.76	0.67
1:A:78:TYR:HB3	1:A:695:TYR:HB2	1.77	0.67
1:B:252:LYS:CG	1:B:253:GLN:N	2.56	0.67
1:B:724:THR:HG22	1:B:725:PHE:N	2.10	0.67
1:B:756:VAL:CG1	1:B:763:LYS:HG2	2.24	0.67
1:D:14:HIS:CE1	1:D:24:LEU:CD2	2.77	0.67
1:E:731:TRP:HB3	1:E:732:PRO:HD3	1.76	0.67
1:I:654:TYR:CE2	1:I:665:ILE:HD12	2.30	0.67
1:J:522:ALA:HB2	1:L:552:ASN:HB2	1.76	0.67
1:C:109:ARG:HH22	1:C:550:LEU:HB2	1.58	0.67
1:J:272:ALA:HB3	1:J:280:LEU:HD21	1.77	0.67
1:A:176:GLY:N	1:A:219:ALA:CB	2.50	0.67
1:A:656:ILE:HG13	1:A:914:THR:O	1.95	0.67
1:G:663:VAL:O	1:G:905:PHE:O	2.13	0.67
1:G:867:ASP:N	1:G:867:ASP:OD1	2.27	0.67
1:I:661:THR:O	1:I:662:ASN:ND2	2.28	0.67
1:I:763:LYS:HA	1:I:766:PHE:HB2	1.77	0.67
1:A:691:LEU:CG	1:A:691:LEU:O	2.41	0.66
1:D:135:TRP:HD1	1:D:310:ASN:HB2	1.60	0.66
1:G:434:GLY:HA2	1:G:438:GLY:O	1.95	0.66
1:H:794:PHE:O	1:H:795:PHE:CD2	2.48	0.66
1:H:330:ARG:HD2	1:H:708:LEU:HD23	1.76	0.66
1:J:840:GLN:HG2	1:L:173:PRO:HD2	1.78	0.66
1:D:269:THR:O	1:D:269:THR:OG1	2.04	0.66
1:I:652:MET:HE1	1:I:654:TYR:OH	1.94	0.66
1:A:52:PRO:HD3	6:W:6:PRO:CB	2.26	0.66
1:A:477:ILE:HA	1:A:537:HIS:CE1	2.31	0.66
1:B:681:THR:HG23	1:B:715:ASN:OD1	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:MET:HB3	1:C:15:ILE:HG13	1.77	0.66
1:I:177:ILE:HG23	1:I:178:ASN:N	2.10	0.66
1:A:267:PHE:CE1	1:A:284:VAL:HB	2.30	0.66
1:B:726:ASP:HB2	1:B:900:ALA:N	2.10	0.66
1:H:772:ALA:O	1:H:881:SER:OG	2.14	0.66
1:I:822:GLN:HA	1:I:845:ASN:HD21	1.61	0.66
1:B:327:ILE:HG21	1:B:601:LEU:HD21	1.78	0.66
1:A:885:LEU:HB2	1:C:51:ALA:HB3	1.77	0.66
1:C:649:ALA:HA	1:C:922:VAL:H	1.59	0.66
1:G:96:MET:HG2	1:G:569:ILE:HG22	1.77	0.66
1:H:272:ALA:O	1:H:280:LEU:HD21	1.95	0.66
1:I:729:VAL:HG12	1:I:730:SER:H	1.60	0.66
1:J:904:THR:HG21	4:Q:20:PRO:HD3	1.77	0.66
1:D:561:GLN:HB2	1:E:757:ALA:CB	2.24	0.66
1:G:121:TYR:O	1:H:824:ASN:ND2	2.29	0.66
4:S:19:MET:HE2	4:S:19:MET:CA	2.19	0.66
1:H:342:THR:HB	1:J:740:PRO:HD2	1.78	0.66
1:J:104:ARG:HG2	1:K:752:GLU:HB2	1.78	0.66
1:A:691:LEU:O	1:A:691:LEU:HG	1.94	0.65
1:A:833:ALA:C	1:A:835:THR:H	2.00	0.65
1:J:561:GLN:H	1:K:757:ALA:HB2	1.61	0.65
3:M:200:ASN:HD21	3:M:235:LEU:CB	2.09	0.65
4:S:57:LEU:HD23	4:S:58:GLU:H	1.59	0.65
1:A:269:THR:CA	1:C:426:LEU:HD23	2.16	0.65
1:G:756:VAL:HG11	1:G:763:LYS:HB3	1.79	0.65
4:S:57:LEU:HD23	4:S:58:GLU:N	2.12	0.65
1:D:222:ARG:H	1:E:840:GLN:HE22	1.43	0.65
1:E:429:VAL:HA	1:E:442:ASP:H	1.62	0.65
1:I:104:ARG:HD3	1:I:612:SER:HB3	1.77	0.65
1:D:350:GLY:HA2	1:D:580:THR:H	1.61	0.65
1:J:821:HIS:CB	1:L:244:ASN:O	2.45	0.65
3:M:200:ASN:HD21	3:M:235:LEU:N	1.94	0.65
1:I:909:PRO:HG3	4:S:45:THR:HA	1.79	0.65
1:K:331:ASP:O	1:K:388:ASN:HB2	1.97	0.65
1:K:548:MET:HB3	1:L:523:ARG:H	1.60	0.65
1:D:110:GLY:HA2	1:D:554:ARG:HE	1.62	0.65
1:E:434:GLY:HA3	1:E:438:GLY:O	1.97	0.65
2:N:225:LEU:HD12	2:N:287:LEU:HD23	1.79	0.65
4:P:41:PRO:CB	4:P:44:SER:HB2	2.27	0.65
1:A:323:ARG:HG3	1:A:479:LEU:HD13	1.78	0.65
1:A:679:ALA:HB3	1:A:919:LEU:HD12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:ARG:O	1:A:837:ARG:CG	2.45	0.65
1:H:877:SER:H	1:H:887:ASP:HB2	1.61	0.65
2:N:256:SER:O	2:N:261:ILE:O	2.14	0.65
1:E:548:MET:HB3	1:F:523:ARG:HB2	1.78	0.64
1:G:23:TYR:O	1:G:23:TYR:CG	2.50	0.64
1:H:300:ILE:HG23	1:H:318:GLN:O	1.97	0.64
1:L:922:VAL:HG13	1:L:944:PRO:HD2	1.79	0.64
4:S:108:ASP:O	4:S:111:THR:N	2.29	0.64
1:A:658:ALA:O	1:A:659:ASN:HB2	1.97	0.64
1:C:716:HIS:HB3	1:C:866:CYS:H	1.62	0.64
1:H:272:ALA:O	1:H:280:LEU:HD22	1.95	0.64
1:D:61:SER:OG	1:E:734:ASN:O	2.13	0.64
1:H:837:ARG:HH22	1:I:415:PHE:HA	1.62	0.64
1:K:332:ASN:CG	1:K:387:TRP:O	2.36	0.64
1:J:184:ILE:HG21	1:J:220:ALA:HB2	1.79	0.64
1:L:109:ARG:HH22	1:L:550:LEU:HB3	1.63	0.64
3:M:80:LEU:HB3	3:M:86:ILE:HG12	1.78	0.64
3:M:196:LEU:O	3:M:199:VAL:HG23	1.98	0.64
3:M:197:GLN:O	3:M:198:THR:HG23	1.96	0.64
1:I:718:PHE:HA	1:I:907:VAL:HA	1.80	0.64
1:L:256:GLY:O	1:L:258:LEU:N	2.31	0.64
2:N:45:TYR:O	2:N:46:LEU:CD2	2.45	0.64
2:N:45:TYR:O	2:N:46:LEU:HD23	1.98	0.64
2:N:445:MET:SD	2:N:529:LEU:HD11	2.38	0.64
1:A:748:SER:O	1:A:749:VAL:CG2	2.45	0.64
1:C:339:TYR:HB2	1:C:367:GLU:HG2	1.79	0.64
1:D:755:ASN:HB3	1:D:759:CYS:O	1.97	0.64
1:G:757:ALA:HB2	1:I:386:MET:CG	2.27	0.64
1:K:92:ARG:H	1:K:576:PRO:HG3	1.63	0.64
5:V:183:ILE:CG2	5:V:184:GLY:O	2.34	0.64
1:A:472:PHE:O	1:A:476:ASN:OD1	2.16	0.64
1:E:722:ALA:HB3	1:E:904:THR:HB	1.78	0.64
1:F:805:VAL:HG12	1:F:806:VAL:H	1.62	0.64
1:H:795:PHE:O	1:H:795:PHE:CD1	2.51	0.64
1:I:202:PRO:HG2	1:I:222:ARG:HH11	1.63	0.64
1:B:342:THR:HB	2:N:92:LEU:HD22	1.80	0.63
1:C:514:VAL:HA	1:C:518:ILE:HD11	1.79	0.63
1:G:771:LEU:O	1:G:880:MET:HA	1.97	0.63
1:H:792:TYR:HD2	1:H:868:ARG:O	1.81	0.63
1:I:127:LYS:HE2	1:I:834:PRO:HB2	1.80	0.63
1:J:216:ILE:HG12	1:L:454:VAL:HB	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:256:GLY:O	1:L:257:LYS:C	2.36	0.63
1:L:756:VAL:O	1:L:756:VAL:CG1	2.47	0.63
1:I:831:TYR:CD2	1:I:831:TYR:C	2.63	0.63
1:A:35:THR:HG23	1:A:38:TYR:HB2	1.80	0.63
1:F:110:GLY:HA3	1:F:606:ALA:HB2	1.81	0.63
1:I:252:LYS:HG3	1:I:253:GLN:H	1.64	0.63
3:M:111:GLN:HA	3:M:114:LEU:HB2	1.81	0.63
1:D:106:VAL:HG12	1:D:557:PRO:HB3	1.81	0.63
1:G:759:CYS:SG	1:G:800:PRO:CB	2.78	0.63
1:I:682:ARG:HH21	1:I:717:THR:HB	1.63	0.63
1:K:493:LYS:C	1:K:494:ILE:HG12	2.19	0.63
2:N:188:ILE:HD11	2:N:208:VAL:HB	1.79	0.63
2:N:448:PRO:CB	2:N:529:LEU:HD13	2.29	0.63
4:S:30:MET:HE2	4:S:41:PRO:HA	1.81	0.63
1:E:583:TRP:HE3	1:E:584:ASN:H	1.45	0.63
1:J:559:HIS:CE1	1:K:756:VAL:O	2.51	0.63
1:J:720:LYS:HE3	4:Q:22:TRP:CH2	2.33	0.63
2:N:462:VAL:HG12	2:N:464:GLY:H	1.64	0.63
1:D:850:LEU:HG	1:F:554:ARG:H	1.64	0.63
1:F:533:ASN:HA	1:F:713:TYR:CD2	2.34	0.63
1:G:44:LYS:HG2	1:H:571:ASN:O	1.99	0.63
1:G:191:GLN:HG2	1:G:191:GLN:O	1.97	0.63
1:G:201:GLN:HB3	1:G:202:PRO:HD2	1.80	0.63
1:I:652:MET:HE3	1:I:654:TYR:CZ	2.32	0.63
1:G:757:ALA:C	1:G:758:GLN:HG3	2.18	0.62
1:I:330:ARG:HD2	1:I:334:ILE:HG22	1.80	0.62
1:B:252:LYS:HG3	1:B:253:GLN:H	1.64	0.62
1:H:59:ASP:O	1:I:734:ASN:ND2	2.32	0.62
1:K:300:ILE:HG21	1:K:303:MET:HB2	1.81	0.62
1:K:416:PRO:HD2	1:K:458:PHE:O	1.99	0.62
3:M:200:ASN:ND2	3:M:235:LEU:HB2	2.14	0.62
1:A:324:PRO:HG2	1:A:538:HIS:HB2	1.80	0.62
1:I:65:THR:C	1:I:66:LEU:HG	2.20	0.62
1:K:929:HIS:HB2	1:K:937:GLU:HB2	1.82	0.62
1:L:930:ARG:N	1:L:931:PRO:HD2	2.14	0.62
1:E:420:VAL:HG22	1:E:457:ASN:HB3	1.80	0.62
1:H:719:LYS:NZ	4:R:47:LEU:O	2.26	0.62
1:K:755:ASN:ND2	1:K:760:ASN:C	2.53	0.62
1:C:598:GLY:HA2	1:C:703:GLY:HA3	1.81	0.62
1:D:566:PHE:HB2	1:D:569:ILE:HG22	1.82	0.62
2:N:52:ARG:CZ	2:N:63:LEU:O	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:30:MET:HE1	4:S:41:PRO:HB3	1.82	0.62
1:A:429:VAL:HG13	1:B:266:PHE:HD1	1.64	0.62
1:G:324:PRO:HG2	1:G:538:HIS:HB2	1.82	0.62
1:I:429:VAL:HB	1:I:439:TRP:CD1	2.35	0.62
1:K:755:ASN:OD1	1:K:759:CYS:O	2.17	0.62
2:N:275:TYR:O	2:N:275:TYR:CG	2.53	0.62
1:H:790:ARG:O	1:H:793:SER:HB2	1.99	0.62
1:I:797:ASN:CG	1:I:867:ASP:O	2.38	0.62
2:N:446:GLN:HB3	2:N:532:ARG:NE	2.11	0.62
4:P:40:LEU:CB	4:P:41:PRO:HD2	1.99	0.62
1:H:475:SER:O	1:H:479:LEU:HG	2.00	0.62
1:L:683:LEU:HB3	1:L:706:PRO:HG2	1.81	0.62
4:P:40:LEU:HD12	4:P:46:THR:OG1	2.00	0.62
4:R:40:LEU:O	4:R:46:THR:HA	2.00	0.62
1:A:748:SER:C	1:A:749:VAL:CG2	2.68	0.61
1:C:661:THR:HG23	1:C:662:ASN:ND2	2.15	0.61
1:I:221:GLY:HA3	1:I:286:LEU:HD23	1.81	0.61
1:J:252:LYS:HG3	1:J:253:GLN:H	1.65	0.61
1:B:354:GLN:HG3	2:N:446:GLN:HA	1.83	0.61
1:B:602:ARG:NH2	1:B:695:TYR:HE1	1.98	0.61
3:M:193:ARG:HB2	3:M:195:GLY:O	1.99	0.61
1:G:923:PHE:O	1:G:941:LEU:HD23	2.01	0.61
4:S:106:GLN:O	4:S:110:LEU:CG	2.48	0.61
1:A:670:ARG:HH12	1:A:947:ALA:HB2	1.65	0.61
1:I:825:ASN:CG	1:I:825:ASN:O	2.37	0.61
1:J:922:VAL:HG11	1:J:944:PRO:HB2	1.81	0.61
1:L:685:THR:HG23	1:L:915:LEU:HD21	1.83	0.61
3:M:196:LEU:HB2	3:M:199:VAL:HG21	1.81	0.61
1:D:119:THR:HG23	1:D:297:ASP:HB2	1.83	0.61
1:J:413:TYR:HB2	1:J:415:PHE:CE2	2.36	0.61
1:B:590:ASN:ND2	1:B:602:ARG:HB3	2.16	0.61
1:G:844:ALA:O	1:I:237:TYR:CB	2.47	0.61
1:H:32:ALA:O	1:H:36:GLU:HB3	2.01	0.61
1:H:455:GLY:O	1:I:173:PRO:HB3	2.01	0.61
1:J:426:LEU:CA	1:K:268:SER:O	2.39	0.61
1:J:650:ALA:HB3	1:J:920:PHE:HB2	1.83	0.61
1:E:575:LEU:HG	1:E:930:ARG:HG3	1.82	0.61
1:H:328:ALA:HB1	1:H:546:ARG:HB2	1.82	0.61
1:I:661:THR:HB	1:I:909:PRO:HA	1.82	0.61
1:D:840:GLN:HG2	1:F:173:PRO:HD2	1.82	0.61
1:H:519:ASN:HD21	1:H:803:ARG:HH11	1.44	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:111:THR:HA	4:Q:114:LEU:HD22	1.83	0.61
1:A:439:TRP:HZ2	1:B:180:THR:O	1.83	0.61
1:B:681:THR:OG1	1:B:870:LEU:HD23	2.00	0.61
1:D:166:THR:N	1:F:447:SER:HG	1.98	0.61
1:E:331:ASP:HA	1:E:388:ASN:HB2	1.81	0.61
1:F:793:SER:O	1:F:869:THR:OG1	2.19	0.61
1:C:33:ARG:HB3	6:W:16:ASN:CA	2.31	0.61
1:C:836:MET:O	1:C:838:GLU:HG3	2.01	0.61
1:F:772:ALA:HB3	1:F:872:ARG:HB3	1.83	0.61
1:D:133:CYS:HB2	1:D:224:LEU:HD12	1.82	0.60
1:I:909:PRO:CG	4:S:45:THR:HA	2.31	0.60
1:A:350:GLY:HA2	1:A:579:TYR:HA	1.82	0.60
1:B:922:VAL:HG12	1:B:923:PHE:H	1.66	0.60
1:E:797:ASN:HB3	1:E:867:ASP:O	2.01	0.60
1:J:124:LEU:HD21	1:K:467:ASN:HB2	1.83	0.60
1:A:384:PHE:HB3	1:A:387:TRP:O	2.01	0.60
1:B:562:VAL:HB	1:B:563:PRO:HD2	1.82	0.60
1:D:94:LEU:HD13	1:D:574:LEU:HD12	1.84	0.60
1:G:924:ASP:HA	1:G:941:LEU:HB3	1.83	0.60
1:K:748:SER:CB	1:K:760:ASN:HD21	2.13	0.60
3:M:196:LEU:HB3	3:M:199:VAL:HG21	1.82	0.60
1:C:756:VAL:HG12	1:C:757:ALA:H	1.66	0.60
1:G:677:GLY:HA2	1:G:874:PRO:HA	1.83	0.60
2:N:283:ILE:HG21	2:N:403:TYR:HB2	1.82	0.60
3:M:196:LEU:HD11	5:U:207:HIS:O	2.00	0.60
1:B:14:HIS:O	1:B:14:HIS:HD2	1.80	0.60
1:E:101:PHE:HB2	1:E:562:VAL:HG22	1.83	0.60
1:E:724:THR:HG23	1:E:728:SER:O	2.00	0.60
1:J:233:CYS:SG	1:K:841:ALA:HB1	2.41	0.60
1:K:415:PHE:HA	1:K:459:ALA:HA	1.83	0.60
3:M:220:ASP:O	3:M:221:ARG:C	2.39	0.60
1:B:354:GLN:HG3	2:N:446:GLN:O	2.01	0.60
1:E:837:ARG:HH22	1:F:415:PHE:HA	1.66	0.60
1:G:464:LEU:HD12	1:I:467:ASN:HD21	1.67	0.60
1:A:439:TRP:CZ2	1:B:180:THR:O	2.54	0.60
1:F:225:LYS:HG3	1:F:226:LYS:H	1.66	0.60
4:Q:113:GLU:O	4:Q:117:VAL:HG23	2.02	0.60
4:S:108:ASP:O	4:S:111:THR:HB	2.02	0.60
1:L:15:ILE:O	1:L:48:PRO:HB3	2.01	0.60
1:A:572:LEU:HD13	1:A:928:VAL:HG11	1.84	0.60
1:E:715:ASN:HD22	1:E:866:CYS:HB3	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:661:THR:C	1:I:662:ASN:ND2	2.54	0.60
1:I:908:ASP:OD1	4:S:48:THR:HG21	2.02	0.60
1:J:817:VAL:HG22	1:J:818:GLY:N	2.16	0.60
1:H:850:LEU:H	1:H:851:ILE:HD12	1.67	0.60
2:N:242:LEU:HD21	2:N:248:VAL:HG22	1.84	0.60
2:N:445:MET:CB	2:N:529:LEU:HD11	2.32	0.60
4:S:40:LEU:HD13	4:S:46:THR:OG1	2.01	0.60
1:A:201:GLN:CB	1:A:202:PRO:HD2	2.32	0.59
1:E:634:LEU:HD12	1:E:639:ASN:HB3	1.84	0.59
1:I:724:THR:HG22	1:I:729:VAL:O	2.00	0.59
1:C:132:PRO:HB3	1:C:170:GLY:HA2	1.84	0.59
1:D:568:ALA:HA	1:D:926:VAL:HG11	1.85	0.59
1:G:869:THR:O	1:G:869:THR:HG23	2.02	0.59
1:B:354:GLN:CG	2:N:446:GLN:O	2.51	0.59
1:F:431:PRO:HA	1:F:439:TRP:HD1	1.67	0.59
1:H:134:GLU:HB3	1:H:167:HIS:HD2	1.67	0.59
1:K:748:SER:HA	1:K:760:ASN:OD1	2.02	0.59
1:K:245:GLY:HA3	1:L:821:HIS:HB3	1.83	0.59
2:N:52:ARG:NH2	2:N:63:LEU:C	2.54	0.59
1:F:132:PRO:HB3	1:F:170:GLY:HA2	1.84	0.59
1:I:719:LYS:HB2	1:I:906:GLU:HB3	1.83	0.59
1:I:806:VAL:HG11	1:I:811:TYR:HE1	1.67	0.59
1:K:270:THR:O	1:K:270:THR:OG1	2.17	0.59
1:L:17:GLY:O	1:L:18:GLN:HG2	2.02	0.59
1:H:492:VAL:CG1	1:H:506:LYS:HZ3	2.15	0.59
1:J:301:SER:HB3	1:J:320:MET:HB2	1.85	0.59
1:K:824:ASN:HB3	1:K:844:ALA:CB	2.32	0.59
1:B:947:ALA:HA	2:N:109:GLN:HB2	1.85	0.59
1:I:380:ARG:HE	1:I:391:VAL:HG11	1.66	0.59
1:K:759:CYS:HB2	1:K:800:PRO:CB	2.29	0.59
1:I:831:TYR:O	1:I:831:TYR:CZ	2.55	0.59
1:A:269:THR:HA	1:C:426:LEU:CD2	2.20	0.59
1:A:748:SER:C	1:A:749:VAL:HG22	2.23	0.59
1:B:354:GLN:NE2	2:N:446:GLN:O	2.34	0.59
1:E:249:ILE:HG12	1:E:260:SER:HA	1.85	0.59
1:H:173:PRO:HD2	1:H:220:ALA:O	2.03	0.59
1:K:678:TRP:HB2	1:K:873:ILE:HD12	1.83	0.59
1:A:280:LEU:HB3	1:C:429:VAL:HG11	1.84	0.58
1:B:772:ALA:HA	1:B:874:PRO:HG3	1.85	0.58
1:D:800:PRO:HG2	1:F:385:SER:HB2	1.82	0.58
1:J:266:PHE:HB3	1:J:285:VAL:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:446:GLN:HB2	2:N:532:ARG:NH2	2.18	0.58
1:G:691:LEU:HD13	1:G:692:GLY:H	1.67	0.58
1:I:349:ALA:HB1	1:I:353:SER:O	2.02	0.58
1:L:632:ALA:HA	1:L:635:ARG:HG2	1.85	0.58
4:S:30:MET:CE	4:S:41:PRO:CB	2.81	0.58
1:F:241:THR:HG22	1:F:242:ASN:H	1.68	0.58
1:B:184:ILE:HG22	1:B:185:GLN:N	2.18	0.58
1:H:689:PRO:HB3	1:H:699:TYR:HB2	1.85	0.58
1:K:755:ASN:ND2	1:K:756:VAL:H	2.01	0.58
1:D:300:ILE:HG21	1:D:317:GLN:HG2	1.85	0.58
1:D:798:PHE:HD1	1:D:866:CYS:HB2	1.67	0.58
1:H:428:LYS:HG2	1:I:267:PHE:HB3	1.85	0.58
1:L:716:HIS:HB3	1:L:866:CYS:H	1.68	0.58
1:A:58:THR:O	1:A:60:ARG:N	2.36	0.58
1:D:101:PHE:HB2	1:D:562:VAL:HG23	1.86	0.58
1:F:399:ARG:CZ	1:F:534:PRO:HG2	2.34	0.58
1:G:388:ASN:HB3	1:G:546:ARG:HH11	1.68	0.58
1:J:794:PHE:HA	1:J:869:THR:HG21	1.84	0.58
1:J:821:HIS:HB3	1:L:244:ASN:O	2.03	0.58
1:K:754:TYR:HB3	1:K:762:THR:HG23	1.85	0.58
1:E:200:PHE:CG	1:E:200:PHE:O	2.55	0.58
1:G:323:ARG:HD3	1:G:479:LEU:HB3	1.85	0.58
1:A:844:ALA:HB3	1:C:121:TYR:HD2	1.67	0.58
1:B:373:LEU:HD22	1:B:646:TYR:H	1.67	0.58
1:B:756:VAL:HB	1:B:763:LYS:HE2	1.85	0.58
1:G:757:ALA:CB	1:I:386:MET:HG2	2.29	0.58
1:A:110:GLY:H	1:A:554:ARG:HG3	1.68	0.58
1:A:338:TYR:HB3	1:A:341:SER:HB3	1.85	0.58
1:B:594:GLN:HE22	1:B:704:SER:HA	1.68	0.58
1:B:924:ASP:HA	1:B:941:LEU:O	2.04	0.58
1:D:833:ALA:HB3	1:D:835:THR:HG23	1.85	0.58
1:H:25:SER:H	1:I:639:ASN:HD22	1.52	0.58
1:H:708:LEU:HG	1:H:708:LEU:O	2.04	0.58
4:Q:107:LEU:HD23	4:Q:110:LEU:HD22	1.86	0.58
1:K:823:HIS:HB3	1:K:845:ASN:N	2.19	0.57
1:L:757:ALA:CB	1:L:766:PHE:HZ	2.16	0.57
4:S:109:SER:O	4:S:113:GLU:HG2	2.04	0.57
1:A:837:ARG:HE	1:B:458:PHE:HA	1.69	0.57
1:E:681:THR:HG21	1:E:712:PHE:HB3	1.86	0.57
1:G:412:ASN:HD21	1:I:462:ILE:HD11	1.69	0.57
1:G:562:VAL:HB	1:G:585:PHE:HE2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:10:ILE:HG23	4:S:11:VAL:N	2.19	0.57
1:C:182:GLU:C	1:C:264:MET:SD	2.80	0.57
2:N:278:LEU:HD22	2:N:406:TRP:HA	1.86	0.57
1:B:794:PHE:O	1:B:798:PHE:CD2	2.55	0.57
1:H:20:ALA:HB2	1:H:48:PRO:HD2	1.86	0.57
1:A:323:ARG:HG3	1:A:479:LEU:HD22	1.86	0.57
1:C:173:PRO:HB2	1:C:207:GLY:HA2	1.87	0.57
1:G:201:GLN:CB	1:G:202:PRO:CD	2.75	0.57
1:H:84:PHE:HB2	1:H:581:TYR:HB3	1.87	0.57
2:N:230:VAL:HG12	2:N:231:TYR:H	1.70	0.57
1:D:94:LEU:HB3	1:D:574:LEU:HB2	1.87	0.57
1:G:794:PHE:HA	1:G:869:THR:HG21	1.86	0.57
1:H:590:ASN:HD21	1:H:602:ARG:HD2	1.70	0.57
1:J:664:PRO:HG2	4:P:15:LEU:HA	1.87	0.57
1:E:90:ASP:HA	1:E:576:PRO:HB3	1.87	0.57
1:J:572:LEU:HG	1:J:573:LEU:O	2.04	0.57
1:J:624:HIS:HA	1:J:627:ALA:HB2	1.85	0.57
1:L:329:PHE:HB2	1:L:546:ARG:HG2	1.86	0.57
2:N:70:TYR:H	2:N:111:ILE:HD12	1.70	0.57
1:A:204:PRO:HD2	1:B:823:HIS:CE1	2.40	0.57
1:G:621:PRO:CG	1:H:878:ASN:OD1	2.51	0.57
1:G:689:PRO:HG3	1:G:699:TYR:HB2	1.86	0.57
1:G:757:ALA:HA	1:I:386:MET:CB	2.24	0.57
1:I:47:ASN:H	1:I:48:PRO:HD3	1.68	0.57
1:B:179:ILE:CG2	1:B:182:GLU:O	2.53	0.57
1:E:184:ILE:HD12	1:E:186:ILE:HD11	1.87	0.57
1:E:850:LEU:HD21	1:E:858:SER:HB3	1.86	0.57
1:H:867:ASP:O	1:H:867:ASP:CG	2.43	0.57
1:K:102:ASP:HB2	1:K:616:TYR:HE1	1.70	0.57
2:N:227:MET:HB2	2:N:228:PRO:HD3	1.86	0.57
1:A:26:PRO:HD3	3:M:19:SER:HB2	1.87	0.57
1:A:201:GLN:CB	1:A:202:PRO:CD	2.83	0.57
1:A:211:TRP:HZ3	1:A:417:LEU:HB3	1.69	0.57
1:H:792:TYR:CD2	1:H:868:ARG:O	2.58	0.57
1:I:179:ILE:HG23	1:I:218:HIS:CG	2.40	0.57
1:J:113:PHE:HE2	1:J:552:ASN:HA	1.70	0.57
1:J:127:LYS:HD2	1:K:411:PRO:HG3	1.86	0.57
1:G:553:GLY:HA3	1:H:850:LEU:HG	1.87	0.56
1:I:797:ASN:HB3	1:I:867:ASP:O	2.05	0.56
1:L:731:TRP:HB3	1:L:732:PRO:HD3	1.87	0.56
1:G:171:GLN:HA	1:I:452:ILE:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:723:ILE:HG23	1:I:903:MET:HG2	1.87	0.56
1:A:840:GLN:HE21	1:C:204:PRO:HA	1.70	0.56
1:G:713:TYR:N	1:G:867:ASP:O	2.37	0.56
1:H:252:LYS:HG3	1:H:253:GLN:H	1.70	0.56
1:I:589:VAL:HB	1:I:593:LEU:HD12	1.86	0.56
1:J:106:VAL:HG12	1:J:557:PRO:HB3	1.87	0.56
1:L:184:ILE:HG12	1:L:220:ALA:HB2	1.87	0.56
1:L:824:ASN:HB2	1:L:844:ALA:HB2	1.84	0.56
2:N:446:GLN:HB3	2:N:532:ARG:CD	2.36	0.56
4:Q:110:LEU:O	4:Q:114:LEU:HD13	2.05	0.56
1:A:752:GLU:HA	1:A:755:ASN:HD22	1.70	0.56
1:B:15:ILE:O	1:B:15:ILE:HG22	2.06	0.56
1:B:182:GLU:HB2	1:B:195:TYR:CD2	2.40	0.56
1:G:849:PRO:O	1:G:851:ILE:N	2.38	0.56
1:H:876:SER:OG	1:H:880:MET:O	2.12	0.56
1:J:648:SER:O	1:J:922:VAL:O	2.23	0.56
1:C:88:VAL:HG23	1:C:577:GLY:H	1.70	0.56
1:G:758:GLN:HG3	1:I:385:SER:HG	1.71	0.56
1:G:774:TYR:HB3	1:G:788:LYS:HD3	1.88	0.56
1:H:691:LEU:O	4:Q:21:PRO:HB2	2.06	0.56
1:B:81:LYS:NZ	2:N:457:ILE:CG2	2.65	0.56
1:B:795:PHE:O	1:B:796:ARG:O	2.22	0.56
1:H:685:THR:HG23	4:Q:26:ARG:HH11	1.71	0.56
1:L:509:VAL:HG13	1:L:510:ALA:H	1.71	0.56
2:N:134:VAL:HG12	2:N:172:GLU:HG2	1.88	0.56
2:N:141:ASN:O	2:N:141:ASN:CG	2.42	0.56
1:A:316:GLY:HA3	1:C:210:GLN:HB2	1.88	0.56
1:B:726:ASP:CB	1:B:900:ALA:N	2.56	0.56
1:D:681:THR:HG21	1:D:712:PHE:HB3	1.88	0.56
1:H:519:ASN:HD21	1:H:803:ARG:NH1	2.03	0.56
1:H:828:PHE:O	1:H:836:MET:O	2.24	0.56
1:A:56:VAL:CG1	6:W:4:LEU:O	2.54	0.56
1:B:447:SER:HB2	1:C:167:HIS:HB3	1.88	0.56
1:F:110:GLY:H	1:F:554:ARG:HG3	1.70	0.56
1:L:224:LEU:HD23	1:L:289:GLU:HB3	1.88	0.56
3:M:158:GLN:HB2	3:M:213:GLY:HA3	1.87	0.56
1:D:723:ILE:HB	1:D:731:TRP:HB2	1.87	0.56
1:G:759:CYS:HG	1:G:800:PRO:HB3	1.69	0.56
1:H:323:ARG:CZ	1:H:504:MET:O	2.53	0.56
1:K:447:SER:HB2	1:L:167:HIS:HB3	1.86	0.56
1:K:549:LEU:HD12	1:L:800:PRO:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ILE:HG22	1:B:260:SER:HA	1.86	0.56
1:B:797:ASN:HB3	1:B:867:ASP:O	2.06	0.56
1:C:35:THR:HG23	6:W:5:ALA:CB	2.36	0.56
1:L:763:LYS:HA	1:L:766:PHE:HB2	1.88	0.56
1:E:731:TRP:HE1	1:E:879:PHE:HZ	1.52	0.55
1:G:559:HIS:CE1	1:H:756:VAL:HA	2.41	0.55
1:H:341:SER:HA	1:H:362:GLN:HG2	1.88	0.55
1:K:97:ALA:HB2	1:K:570:LYS:O	2.06	0.55
2:N:231:TYR:CZ	2:N:284:PRO:O	2.59	0.55
4:P:10:ILE:HG12	4:Q:26:ARG:O	2.06	0.55
1:C:332:ASN:O	1:C:333:PHE:CD2	2.59	0.55
1:H:97:ALA:CB	1:H:571:ASN:H	2.14	0.55
1:H:323:ARG:NE	1:H:504:MET:O	2.40	0.55
4:S:50:GLU:HG3	4:S:52:VAL:HG13	1.88	0.55
1:J:329:PHE:H	1:J:546:ARG:HG2	1.71	0.55
1:K:756:VAL:HG21	1:K:766:PHE:CD1	2.42	0.55
1:C:34:ALA:CB	6:W:13:PHE:CB	2.77	0.55
1:C:333:PHE:CD1	1:C:333:PHE:C	2.79	0.55
1:F:533:ASN:CA	1:F:713:TYR:CE2	2.89	0.55
1:L:19:ASP:O	1:L:48:PRO:HG2	2.07	0.55
1:B:590:ASN:HB3	1:B:699:TYR:CD2	2.42	0.55
1:H:887:ASP:O	1:H:891:ASN:HB2	2.06	0.55
1:J:204:PRO:HB3	1:K:840:GLN:HB2	1.89	0.55
2:N:225:LEU:HD22	2:N:285:ALA:CB	2.31	0.55
1:G:847:PRO:HG2	1:I:121:TYR:CE1	2.31	0.55
1:H:245:GLY:HA3	1:I:821:HIS:HB3	1.89	0.55
1:J:340:ASN:HB3	1:J:366:THR:H	1.72	0.55
1:L:930:ARG:N	1:L:931:PRO:CD	2.69	0.55
2:N:455:ARG:HH21	2:N:540:ARG:HB2	1.71	0.55
1:A:431:PRO:CA	1:A:439:TRP:CD1	2.90	0.55
1:B:14:HIS:O	1:B:14:HIS:CG	2.57	0.55
1:H:364:ARG:HH22	1:H:940:TYR:HE2	1.53	0.55
1:H:705:ILE:HG22	1:H:707:TYR:N	2.20	0.55
1:L:20:ALA:HA	1:L:48:PRO:HD2	1.88	0.55
1:I:130:PRO:HG2	1:I:315:MET:HA	1.88	0.55
1:B:252:LYS:HG2	1:B:253:GLN:N	2.18	0.55
1:C:669:SER:HB2	1:K:664:PRO:HG2	1.88	0.55
1:G:716:HIS:HB3	1:G:866:CYS:H	1.70	0.55
1:J:323:ARG:HG3	1:J:479:LEU:HD13	1.88	0.55
1:K:350:GLY:H	1:K:353:SER:HB3	1.72	0.55
1:K:384:PHE:HB2	1:K:389:GLN:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:53:THR:O	1:L:57:THR:OG1	2.16	0.55
1:B:327:ILE:HD13	1:B:601:LEU:HD21	1.89	0.55
1:D:23:TYR:O	1:D:23:TYR:CD2	2.60	0.55
1:J:171:GLN:HB3	1:K:840:GLN:HG2	1.88	0.55
1:B:748:SER:HB3	1:B:760:ASN:HD21	1.72	0.54
1:E:829:VAL:HG22	1:E:830:GLY:H	1.71	0.54
1:J:121:TYR:OH	1:K:849:PRO:HG3	2.07	0.54
1:G:655:PRO:HB3	1:G:915:LEU:HD23	1.89	0.54
1:G:937:GLU:HG3	1:G:937:GLU:O	2.07	0.54
1:I:730:SER:O	1:I:732:PRO:HD2	2.07	0.54
1:J:850:LEU:HG	1:L:554:ARG:H	1.72	0.54
1:L:824:ASN:HD22	1:L:824:ASN:H	1.54	0.54
1:E:724:THR:HB	1:E:902:ASP:HB3	1.89	0.54
1:I:797:ASN:CB	1:I:867:ASP:O	2.55	0.54
1:J:41:LEU:HD13	1:J:44:LYS:HD2	1.89	0.54
1:J:112:THR:HG21	1:J:599:ASN:HD21	1.73	0.54
4:Q:115:ASN:O	4:Q:118:SER:CB	2.54	0.54
1:B:942:ARG:HB3	1:B:947:ALA:HB3	1.90	0.54
1:C:807:ASP:HB2	1:C:858:SER:HA	1.89	0.54
1:E:943:THR:HB	1:E:944:PRO:HD3	1.87	0.54
1:F:242:ASN:O	1:F:242:ASN:CG	2.46	0.54
1:F:533:ASN:CB	1:F:713:TYR:HE2	2.15	0.54
1:H:716:HIS:HB3	1:H:866:CYS:SG	2.47	0.54
1:K:705:ILE:HB	1:K:708:LEU:HD12	1.88	0.54
4:Q:28:ASN:HA	4:Q:42:ALA:HB3	1.88	0.54
4:R:119:GLN:HA	4:R:122:LEU:HG	1.88	0.54
1:G:79:SER:HB2	1:G:584:ASN:HD22	1.73	0.54
1:H:492:VAL:HG11	1:H:506:LYS:CD	2.32	0.54
1:J:415:PHE:HA	1:L:837:ARG:HH22	1.72	0.54
1:A:678:TRP:HB2	1:A:873:ILE:HD12	1.90	0.54
1:B:649:ALA:HA	1:B:922:VAL:H	1.72	0.54
1:C:332:ASN:O	1:C:333:PHE:CG	2.60	0.54
1:H:524:TRP:HD1	1:H:801:MET:HB3	1.71	0.54
1:I:656:ILE:HD13	1:I:907:VAL:HG21	1.90	0.54
1:J:756:VAL:HG21	1:J:766:PHE:CB	2.37	0.54
3:M:155:PRO:HG2	3:M:159:GLU:HG3	1.90	0.54
1:A:775:ASN:HD22	1:A:779:GLN:HE22	1.56	0.54
1:B:325:ASN:HA	1:B:596:SER:HB3	1.89	0.54
1:C:198:LYS:HB3	1:C:262:VAL:HB	1.89	0.54
1:D:824:ASN:HA	1:D:844:ALA:HB2	1.89	0.54
1:H:724:THR:HB	1:H:902:ASP:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:201:GLN:HB3	1:J:202:PRO:CD	2.35	0.54
1:K:478:ALA:HB2	1:K:514:VAL:HG21	1.90	0.54
1:L:252:LYS:HG2	1:L:253:GLN:H	1.72	0.54
2:N:283:ILE:CG2	2:N:283:ILE:O	2.55	0.54
1:A:548:MET:HB3	1:B:523:ARG:H	1.72	0.54
1:B:188:VAL:HG23	1:B:188:VAL:O	2.06	0.54
1:D:96:MET:HG3	1:D:572:LEU:HB3	1.89	0.54
1:D:368:LEU:HD21	1:D:917:TYR:OH	2.08	0.54
1:F:323:ARG:HG2	1:F:479:LEU:HD13	1.89	0.54
1:L:649:ALA:HA	1:L:922:VAL:H	1.73	0.54
5:V:47:ILE:HA	5:V:50:HIS:HB2	1.90	0.54
1:C:113:PHE:HD1	1:C:327:ILE:HB	1.72	0.54
1:I:474:TYR:HA	1:I:478:ALA:HB3	1.90	0.54
1:I:728:SER:O	1:I:728:SER:OG	2.25	0.54
1:A:720:LYS:HG2	1:A:744:GLU:HG2	1.90	0.54
1:D:794:PHE:CD2	1:D:794:PHE:C	2.74	0.54
1:E:422:ASN:HB3	1:E:453:ARG:HB2	1.90	0.54
1:G:847:PRO:CG	1:I:121:TYR:CE1	2.90	0.54
1:I:132:PRO:HG3	1:I:171:GLN:HB2	1.90	0.54
2:N:139:PHE:HB3	2:N:253:SER:O	2.08	0.54
1:E:332:ASN:H	1:E:388:ASN:HB2	1.73	0.53
1:L:797:ASN:HB2	1:L:867:ASP:O	2.06	0.53
4:P:30:MET:HA	4:P:40:LEU:O	2.08	0.53
1:D:269:THR:C	1:D:270:THR:HG22	2.28	0.53
1:F:365:ASN:HB3	1:F:368:LEU:HB2	1.89	0.53
1:F:533:ASN:HA	1:F:713:TYR:CE2	2.44	0.53
1:H:350:GLY:HA2	1:H:579:TYR:HA	1.90	0.53
1:I:339:TYR:HB2	1:I:367:GLU:HG3	1.91	0.53
1:J:233:CYS:CB	1:K:841:ALA:HB1	2.39	0.53
1:J:821:HIS:ND1	1:L:244:ASN:O	2.41	0.53
1:A:119:THR:HG21	1:A:235:GLY:HA2	1.91	0.53
1:A:328:ALA:HB2	1:A:547:SER:HB2	1.90	0.53
1:C:728:SER:O	1:C:729:VAL:C	2.46	0.53
1:J:425:THR:O	1:K:269:THR:HA	2.09	0.53
4:P:16:THR:HA	4:R:13:SER:HB2	1.89	0.53
4:S:108:ASP:O	4:S:111:THR:CB	2.57	0.53
1:B:340:ASN:HA	1:B:360:ASP:HB3	1.89	0.53
1:G:202:PRO:HG3	1:G:220:ALA:HB1	1.91	0.53
1:G:771:LEU:O	1:G:880:MET:C	2.44	0.53
1:J:281:THR:HA	1:L:439:TRP:HZ3	1.73	0.53
4:P:29:VAL:N	4:P:42:ALA:HB2	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:102:ASP:HB3	1:G:614:CYS:H	1.72	0.53
1:G:204:PRO:HB3	1:H:840:GLN:CB	2.36	0.53
1:H:324:PRO:HD3	1:H:479:LEU:HD22	1.89	0.53
1:H:722:ALA:HB3	1:H:904:THR:HB	1.90	0.53
1:J:906:GLU:OE2	4:Q:22:TRP:CD1	2.62	0.53
1:K:828:PHE:HA	1:K:837:ARG:HG2	1.88	0.53
1:A:772:ALA:HB1	1:A:872:ARG:HB2	1.90	0.53
1:B:64:LEU:HD11	1:B:619:PHE:O	2.01	0.53
1:C:659:ASN:O	1:C:659:ASN:ND2	2.42	0.53
1:D:113:PHE:HB2	1:D:327:ILE:HD12	1.91	0.53
1:F:572:LEU:HD22	1:F:641:GLN:HB3	1.91	0.53
1:I:177:ILE:CG2	1:I:178:ASN:N	2.71	0.53
1:I:205:GLN:HG3	1:I:206:ILE:HG13	1.91	0.53
1:J:461:GLU:HB2	1:L:126:PRO:HB3	1.91	0.53
1:B:724:THR:CG2	1:B:725:PHE:N	2.71	0.53
1:C:430:LYS:HB2	1:C:442:ASP:HA	1.91	0.53
1:D:184:ILE:HD12	1:D:186:ILE:HD11	1.90	0.53
1:D:780:GLY:H	1:F:98:SER:HB2	1.74	0.53
1:G:757:ALA:O	1:G:758:GLN:CG	2.44	0.53
1:H:126:PRO:HB2	1:H:129:ALA:HB2	1.89	0.53
1:J:132:PRO:HB2	1:J:223:VAL:HG23	1.90	0.53
1:L:54:HIS:O	1:L:54:HIS:CG	2.61	0.53
1:E:672:TRP:HE1	1:E:899:HIS:HB2	1.73	0.53
1:G:758:GLN:HG3	1:I:385:SER:OG	2.08	0.53
1:I:333:PHE:HZ	1:I:563:PRO:HD2	1.74	0.53
1:I:752:GLU:HG2	1:I:755:ASN:HB2	1.89	0.53
1:L:594:GLN:NE2	1:L:705:ILE:H	2.07	0.53
1:A:559:HIS:CE1	1:B:755:ASN:O	2.58	0.53
1:A:848:TYR:HB3	1:A:856:VAL:HG21	1.91	0.53
1:B:941:LEU:HD11	1:B:943:THR:OG1	2.09	0.53
1:D:365:ASN:H	1:D:651:ASN:HD21	1.55	0.53
2:N:446:GLN:HB3	2:N:532:ARG:CG	2.39	0.53
1:A:383:TYR:HA	1:A:389:GLN:HB3	1.89	0.53
1:A:745:ILE:HG23	1:A:765:TRP:CE2	2.44	0.53
1:B:722:ALA:HB3	1:B:904:THR:HB	1.91	0.53
1:E:384:PHE:HB2	1:E:389:GLN:HB3	1.90	0.53
1:E:757:ALA:O	1:E:758:GLN:HB2	2.09	0.53
1:J:173:PRO:HG3	1:K:840:GLN:HG3	1.91	0.53
1:J:749:VAL:HG21	4:Q:50:GLU:HA	1.91	0.53
3:M:291:GLY:HA2	3:M:294:GLU:HB2	1.91	0.53
1:E:238:ALA:HB2	1:F:843:PRO:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:621:PRO:HD2	1:H:878:ASN:OD1	2.09	0.52
1:G:678:TRP:HD1	1:G:920:PHE:HA	1.74	0.52
1:I:730:SER:C	1:I:732:PRO:HD2	2.29	0.52
1:J:112:THR:HG21	1:J:599:ASN:ND2	2.24	0.52
1:K:430:LYS:HB2	1:K:442:ASP:HA	1.92	0.52
1:A:840:GLN:HE22	1:C:221:GLY:HA2	1.74	0.52
1:H:514:VAL:CA	1:H:518:ILE:HD11	2.34	0.52
1:H:671:ASN:HD21	1:H:946:SER:HB2	1.74	0.52
1:H:732:PRO:CG	1:H:740:PRO:O	2.56	0.52
1:E:333:PHE:HB2	1:E:563:PRO:HD2	1.91	0.52
1:G:760:ASN:HD22	1:G:863:LYS:HA	1.74	0.52
1:H:719:LYS:HZ3	1:H:746:LYS:HD3	1.74	0.52
1:L:594:GLN:HE21	1:L:705:ILE:HG13	1.74	0.52
3:M:252:THR:HG23	3:M:254:LEU:H	1.74	0.52
6:W:2:ALA:O	6:W:12:PRO:CB	2.58	0.52
1:G:104:ARG:HD3	1:G:612:SER:HB3	1.91	0.52
1:G:336:LEU:HB2	1:G:562:VAL:HG11	1.92	0.52
1:I:223:VAL:HB	1:I:286:LEU:HD22	1.90	0.52
2:N:455:ARG:O	2:N:455:ARG:HG3	2.07	0.52
1:A:735:ASP:HB2	1:C:61:SER:HB2	1.92	0.52
1:B:888:LEU:HA	1:B:891:ASN:HB2	1.91	0.52
1:C:850:LEU:H	1:C:851:ILE:HD12	1.73	0.52
1:D:78:TYR:CD1	1:D:78:TYR:C	2.81	0.52
1:D:231:LYS:HE2	1:D:236:SER:HA	1.91	0.52
1:G:201:GLN:HB2	1:G:287:TYR:CE2	2.45	0.52
1:I:63:ARG:HB2	1:I:66:LEU:HD21	1.92	0.52
1:J:906:GLU:HG3	4:Q:20:PRO:HG2	1.91	0.52
1:K:133:CYS:HB3	1:K:230:MET:HG2	1.89	0.52
1:L:132:PRO:HB2	1:L:223:VAL:HA	1.92	0.52
1:B:867:ASP:O	1:B:868:ARG:HB3	2.09	0.52
1:C:174:TYR:HB2	1:C:220:ALA:H	1.73	0.52
1:J:252:LYS:HB3	1:J:257:LYS:HA	1.91	0.52
1:L:747:ARG:HB2	1:L:755:ASN:HD21	1.75	0.52
1:L:824:ASN:CB	1:L:844:ALA:HB1	2.24	0.52
5:V:183:ILE:HG22	5:V:184:GLY:N	2.24	0.52
1:B:765:TRP:HZ2	1:B:871:TRP:HB3	1.74	0.52
1:C:747:ARG:HG3	1:C:762:THR:CB	2.21	0.52
1:E:524:TRP:CD1	1:E:803:ARG:HB3	2.45	0.52
1:F:104:ARG:HB3	1:F:612:SER:HB3	1.91	0.52
1:G:440:GLU:O	1:G:441:LYS:HG3	2.10	0.52
1:G:719:LYS:HB3	1:G:906:GLU:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:117:SER:HB3	1:I:324:PRO:HG3	1.90	0.52
1:J:405:GLY:HA2	1:J:520:LEU:HD21	1.92	0.52
4:S:20:PRO:HB2	4:S:25:VAL:HG21	1.90	0.52
1:A:107:LEU:HB3	1:A:556:VAL:HG23	1.91	0.52
1:B:338:TYR:HB2	1:B:341:SER:HB3	1.92	0.52
1:B:925:VAL:H	1:B:941:LEU:HD23	1.75	0.52
1:F:84:PHE:HB2	1:F:581:TYR:HB3	1.91	0.52
1:H:121:TYR:CD2	1:H:237:TYR:HA	2.45	0.52
1:J:756:VAL:HG21	1:J:766:PHE:HB2	1.91	0.52
1:K:687:GLU:HA	1:K:701:TYR:HB3	1.92	0.52
1:L:348:LEU:HD21	1:L:569:ILE:HD13	1.91	0.52
1:C:112:THR:HG22	1:C:501:TYR:HB2	1.91	0.52
1:H:225:LYS:HE3	1:H:290:ASP:HB2	1.91	0.52
1:I:718:PHE:HD1	1:I:907:VAL:HG12	1.75	0.52
3:M:80:LEU:HG	3:M:85:ALA:HB3	1.92	0.52
1:A:200:PHE:O	1:A:200:PHE:HD1	1.91	0.52
1:A:830:GLY:HA3	1:A:835:THR:HG23	1.91	0.52
1:D:328:ALA:HB1	1:D:546:ARG:HG3	1.91	0.52
1:G:121:TYR:HA	1:H:824:ASN:ND2	2.24	0.52
1:H:517:TYR:CB	1:H:847:PRO:HG3	2.40	0.52
1:H:660:ALA:HB1	4:Q:11:VAL:HG11	1.92	0.52
1:J:119:THR:HG22	1:J:120:ALA:H	1.75	0.52
1:K:24:LEU:HD22	1:L:639:ASN:HD22	1.75	0.52
1:A:17:GLY:C	1:A:48:PRO:HG2	2.31	0.51
1:B:403:ASN:HB3	1:B:520:LEU:HD23	1.90	0.51
1:B:532:VAL:O	1:B:532:VAL:HG23	2.10	0.51
1:B:590:ASN:HB3	1:B:699:TYR:HD2	1.74	0.51
1:B:933:ARG:HH12	3:M:93:LEU:HD23	1.74	0.51
1:D:173:PRO:HG3	1:E:840:GLN:HG3	1.91	0.51
1:H:324:PRO:HG3	1:H:479:LEU:HD13	1.92	0.51
1:H:655:PRO:HA	1:H:915:LEU:HA	1.93	0.51
1:J:655:PRO:HG3	1:J:915:LEU:CD2	2.39	0.51
1:K:732:PRO:O	1:K:733:GLY:C	2.49	0.51
1:B:119:THR:HG22	1:B:121:TYR:H	1.75	0.51
1:B:940:TYR:HB3	2:N:108:THR:HB	1.92	0.51
1:C:113:PHE:CD1	1:C:327:ILE:HB	2.45	0.51
1:D:52:PRO:HG2	1:D:55:ASP:HB2	1.91	0.51
1:G:738:LEU:HD11	1:G:763:LYS:HE3	1.92	0.51
1:J:575:LEU:HD21	1:J:635:ARG:HE	1.74	0.51
1:B:725:PHE:O	1:B:900:ALA:O	2.28	0.51
1:E:429:VAL:HG12	1:E:441:LYS:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:428:LYS:HD2	1:J:446:PHE:CD1	2.44	0.51
1:L:328:ALA:HB2	1:L:547:SER:HB2	1.92	0.51
1:L:755:ASN:HA	1:L:762:THR:HA	1.92	0.51
1:A:356:ASN:HD22	1:A:356:ASN:H	1.59	0.51
1:C:249:ILE:HG12	1:C:290:ASP:HB2	1.93	0.51
1:D:61:SER:CB	1:E:734:ASN:O	2.59	0.51
1:I:823:HIS:HB2	1:I:844:ALA:HA	1.91	0.51
2:N:196:GLY:O	2:N:200:GLY:O	2.28	0.51
1:C:80:TYR:HB3	1:C:585:PHE:HB2	1.92	0.51
1:C:428:LYS:HB2	1:C:446:PHE:H	1.75	0.51
1:F:501:TYR:O	1:F:505:ASN:HB3	2.10	0.51
1:F:664:PRO:HA	1:F:904:THR:HA	1.91	0.51
1:I:732:PRO:HB2	1:I:734:ASN:O	2.09	0.51
1:J:904:THR:HG21	4:Q:20:PRO:CD	2.40	0.51
1:L:20:ALA:O	1:L:45:PHE:CE2	2.51	0.51
1:A:202:PRO:HG3	1:A:220:ALA:HB3	1.93	0.51
1:B:776:ILE:HG12	1:B:782:TYR:HB2	1.93	0.51
1:J:639:ASN:HD21	1:L:25:SER:HB2	1.75	0.51
1:K:429:VAL:HG12	1:K:441:LYS:HA	1.92	0.51
1:L:656:ILE:O	1:L:913:PRO:HA	2.11	0.51
1:L:768:VAL:HG13	1:L:873:ILE:HB	1.93	0.51
4:Q:85:LEU:HB3	4:Q:92:ARG:HH12	1.76	0.51
1:H:798:PHE:HB3	1:H:866:CYS:HA	1.91	0.51
1:H:823:HIS:HB2	1:H:845:ASN:HB2	1.93	0.51
1:I:272:ALA:HB3	1:I:280:LEU:HB3	1.92	0.51
1:I:349:ALA:O	1:I:350:GLY:O	2.29	0.51
1:K:755:ASN:HD21	1:K:760:ASN:CA	2.24	0.51
1:A:855:ALA:HB2	1:C:554:ARG:HD3	1.92	0.51
1:B:66:LEU:HD12	1:B:92:ARG:HH22	1.76	0.51
1:D:752:GLU:HB3	1:F:559:HIS:HE1	1.76	0.51
1:E:705:ILE:HB	1:E:708:LEU:HB2	1.93	0.51
1:I:172:ALA:CB	1:I:284:VAL:HG11	2.40	0.51
1:J:720:LYS:CE	4:Q:22:TRP:CH2	2.90	0.51
1:K:329:PHE:O	1:K:330:ARG:O	2.28	0.51
1:L:369:SER:HA	1:L:647:LEU:HB3	1.93	0.51
1:F:713:TYR:CD1	1:F:714:LEU:HG	2.45	0.51
1:J:929:HIS:HB2	1:J:937:GLU:HB2	1.93	0.51
1:A:238:ALA:HB2	1:B:843:PRO:HB2	1.93	0.51
1:D:135:TRP:HE1	1:D:230:MET:CG	2.24	0.51
1:H:200:PHE:HA	1:H:246:GLY:HA3	1.93	0.51
1:I:676:ARG:HB3	1:I:921:GLU:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:205:GLN:HG3	1:J:206:ILE:HG13	1.93	0.51
4:R:110:LEU:O	4:R:110:LEU:HD22	2.11	0.51
1:B:225:LYS:HG3	1:B:288:SER:HB3	1.93	0.50
1:B:636:ASN:ND2	3:M:16:SER:HB2	2.26	0.50
1:E:179:ILE:O	1:E:179:ILE:HG22	2.12	0.50
1:E:245:GLY:H	1:F:821:HIS:HB3	1.75	0.50
1:G:552:ASN:H	1:H:804:GLN:HB2	1.75	0.50
1:K:386:MET:SD	1:L:756:VAL:O	2.69	0.50
4:S:41:PRO:HG2	4:S:44:SER:HB2	1.93	0.50
1:D:522:ALA:HB2	1:F:552:ASN:HB2	1.93	0.50
1:E:121:TYR:HD2	1:F:844:ALA:HB3	1.75	0.50
1:F:683:LEU:HD13	1:F:707:TYR:HB2	1.92	0.50
1:G:18:GLN:CD	1:G:22:GLU:HB3	2.31	0.50
1:K:798:PHE:HB3	1:K:866:CYS:HA	1.93	0.50
3:M:214:VAL:O	3:M:251:ASP:O	2.29	0.50
1:G:706:PRO:HA	1:G:711:THR:HG23	1.93	0.50
1:G:929:HIS:C	1:G:937:GLU:HG3	2.31	0.50
1:H:723:ILE:HA	1:H:903:MET:HG3	1.93	0.50
1:H:748:SER:OG	4:R:47:LEU:HD23	2.10	0.50
1:A:19:ASP:OD1	6:W:8:HIS:O	2.28	0.50
1:A:179:ILE:HG22	1:A:184:ILE:HA	1.93	0.50
1:A:225:LYS:HD2	1:A:290:ASP:HB2	1.93	0.50
1:A:683:LEU:O	1:A:914:THR:HA	2.12	0.50
1:B:28:LEU:HD12	1:C:633:MET:HB3	1.94	0.50
1:F:600:ASP:HA	1:F:702:SER:HB2	1.94	0.50
1:I:219:ALA:HB3	1:I:284:VAL:HG22	1.94	0.50
1:I:680:PHE:HB3	1:I:918:VAL:HG22	1.94	0.50
1:K:549:LEU:HD21	1:L:758:GLN:HE22	1.77	0.50
1:K:824:ASN:HB3	1:K:844:ALA:HB2	1.92	0.50
2:N:149:VAL:O	2:N:200:GLY:HA3	2.10	0.50
1:C:14:HIS:CD2	1:C:14:HIS:O	2.64	0.50
1:E:334:ILE:HG21	1:E:708:LEU:HG	1.94	0.50
1:F:301:SER:HB3	1:F:320:MET:HB2	1.94	0.50
1:F:566:PHE:HB2	1:F:569:ILE:HG22	1.93	0.50
1:G:798:PHE:HE1	1:G:864:PHE:HB2	1.75	0.50
1:G:824:ASN:HA	1:G:844:ALA:CB	2.35	0.50
1:G:926:VAL:HA	1:G:939:VAL:O	2.12	0.50
1:H:648:SER:HB2	1:H:924:ASP:HB3	1.94	0.50
1:K:388:ASN:O	1:K:389:GLN:C	2.50	0.50
1:A:582:GLU:O	1:A:583:TRP:CG	2.65	0.50
1:B:240:PRO:HD3	1:C:845:ASN:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:ARG:O	1:B:474:TYR:HB3	2.11	0.50
1:C:479:LEU:HD21	1:C:508:VAL:HG12	1.94	0.50
1:D:53:THR:O	1:D:56:VAL:CG1	2.45	0.50
1:F:431:PRO:HA	1:F:439:TRP:CD1	2.46	0.50
1:G:650:ALA:HB2	1:G:922:VAL:HG21	1.93	0.50
1:J:96:MET:HB2	1:J:572:LEU:H	1.75	0.50
1:J:265:GLN:HE22	1:L:431:PRO:HD2	1.76	0.50
1:K:755:ASN:ND2	1:K:760:ASN:CA	2.75	0.50
2:N:149:VAL:HG22	2:N:191:HIS:HE1	1.75	0.50
1:A:24:LEU:HD21	1:A:45:PHE:CZ	2.47	0.50
1:A:784:PRO:HB3	1:A:788:LYS:HD2	1.92	0.50
1:B:188:VAL:O	1:B:188:VAL:CG2	2.59	0.50
1:B:798:PHE:CB	1:B:866:CYS:HA	2.40	0.50
1:C:310:ASN:HA	1:C:314:LEU:HD12	1.93	0.50
1:D:25:SER:H	1:E:639:ASN:HD21	1.60	0.50
1:E:201:GLN:HB3	1:E:202:PRO:HD2	1.93	0.50
1:H:134:GLU:HB3	1:H:167:HIS:CD2	2.47	0.50
1:H:492:VAL:HG13	1:H:506:LYS:HZ3	1.77	0.50
1:I:96:MET:HG3	1:I:569:ILE:HG13	1.92	0.50
1:I:475:SER:HA	1:I:479:LEU:HD13	1.93	0.50
1:I:661:THR:HB	1:I:909:PRO:CA	2.40	0.50
1:J:561:GLN:N	1:K:757:ALA:HB2	2.26	0.50
1:C:797:ASN:CB	1:C:867:ASP:O	2.60	0.50
1:G:757:ALA:HB1	1:I:385:SER:HB3	1.94	0.50
1:G:804:GLN:CG	1:G:850:LEU:HD23	2.37	0.50
1:J:675:PHE:HB3	1:J:875:PHE:HB2	1.94	0.50
1:L:18:GLN:O	1:L:19:ASP:C	2.49	0.50
1:L:499:ASN:HB3	1:L:599:ASN:HA	1.93	0.50
1:L:600:ASP:HA	1:L:702:SER:OG	2.11	0.50
3:M:196:LEU:CB	3:M:199:VAL:CG2	2.89	0.50
4:S:108:ASP:O	4:S:111:THR:CA	2.60	0.50
1:A:386:MET:HB3	1:B:757:ALA:HB1	1.93	0.50
1:A:737:LEU:HD22	1:A:764:ASP:HA	1.94	0.50
1:A:804:GLN:HB2	1:C:552:ASN:HB3	1.94	0.50
1:D:227:THR:OG1	1:D:290:ASP:OD1	2.28	0.50
1:E:837:ARG:HH21	1:F:413:TYR:HB3	1.76	0.50
1:G:113:PHE:HB2	1:G:327:ILE:HD12	1.94	0.50
1:G:757:ALA:C	1:G:758:GLN:CG	2.80	0.50
1:H:609:LYS:HG2	4:S:58:GLU:HB3	1.92	0.50
1:K:648:SER:HB2	1:K:924:ASP:HB3	1.94	0.50
4:P:39:VAL:O	4:P:40:LEU:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:208:TYR:HB2	5:V:209:PRO:HD2	1.93	0.50
1:A:330:ARG:HH22	1:A:705:ILE:H	1.59	0.49
1:A:691:LEU:O	1:A:691:LEU:HD23	2.12	0.49
1:B:941:LEU:CD1	1:B:943:THR:OG1	2.60	0.49
1:B:943:THR:HB	1:B:944:PRO:HD3	1.94	0.49
1:G:926:VAL:O	1:G:926:VAL:HG13	2.12	0.49
1:K:824:ASN:HB3	1:K:844:ALA:HB1	1.94	0.49
2:N:250:PHE:CE1	2:N:261:ILE:HD12	2.46	0.49
1:A:28:LEU:HD11	1:B:630:LEU:HG	1.94	0.49
1:A:98:SER:HB3	1:B:780:GLY:HA2	1.94	0.49
1:B:339:TYR:HB3	1:B:366:THR:HB	1.93	0.49
1:G:26:PRO:HB2	1:G:30:GLN:HE21	1.77	0.49
1:G:384:PHE:H	1:G:389:GLN:HB3	1.78	0.49
1:H:778:TYR:CZ	1:H:878:ASN:ND2	2.80	0.49
1:I:655:PRO:O	1:I:656:ILE:HG13	2.11	0.49
1:K:65:THR:HA	1:K:618:THR:HG22	1.94	0.49
1:K:127:LYS:HG3	1:L:411:PRO:HB3	1.94	0.49
2:N:52:ARG:HG3	2:N:64:PHE:HA	1.93	0.49
2:N:217:LEU:HB3	2:N:232:THR:HG21	1.93	0.49
2:N:231:TYR:OH	2:N:284:PRO:O	2.23	0.49
1:A:119:THR:HG23	1:A:297:ASP:HB2	1.95	0.49
1:A:321:PRO:HG2	1:B:409:GLU:HG3	1.93	0.49
1:B:704:SER:HB2	1:B:711:THR:HG21	1.93	0.49
1:C:108:ASP:HB2	1:C:607:SER:H	1.77	0.49
1:E:204:PRO:HG3	1:F:842:TYR:HB2	1.94	0.49
1:E:672:TRP:HA	1:E:944:PRO:HB3	1.94	0.49
1:H:663:VAL:HB	1:H:905:PHE:HB3	1.93	0.49
1:I:747:ARG:HB2	1:I:755:ASN:HD21	1.77	0.49
1:L:324:PRO:HG3	1:L:538:HIS:ND1	2.28	0.49
2:N:94:THR:C	2:N:96:ILE:H	2.13	0.49
2:N:286:LEU:O	2:N:382:LEU:HD22	2.12	0.49
5:U:90:VAL:HG13	5:U:168:ILE:HG12	1.94	0.49
1:A:100:TYR:CE1	1:A:616:TYR:HB2	2.47	0.49
1:A:649:ALA:HB1	1:A:919:LEU:HB3	1.93	0.49
1:A:885:LEU:CB	1:C:51:ALA:HB3	2.41	0.49
1:E:83:ARG:HD2	1:E:582:GLU:HB3	1.94	0.49
1:E:323:ARG:HD2	1:E:479:LEU:HD21	1.93	0.49
1:E:684:LYS:HB3	1:E:687:GLU:HB2	1.95	0.49
1:F:10:TRP:HB3	1:F:16:SER:HB2	1.94	0.49
1:G:804:GLN:NE2	1:G:858:SER:O	2.38	0.49
1:H:361:LEU:HD11	1:J:729:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:535:PHE:HZ	1:H:868:ARG:HG3	1.77	0.49
1:K:425:THR:HG23	1:K:448:ASP:HB3	1.94	0.49
3:M:74:LEU:HA	3:M:77:VAL:HG12	1.94	0.49
1:A:27:GLY:HA3	3:M:15:GLN:HA	1.94	0.49
1:A:646:TYR:CE1	6:W:22:THR:O	2.66	0.49
1:C:756:VAL:HG12	1:C:757:ALA:N	2.27	0.49
1:D:384:PHE:HB2	1:D:389:GLN:HB2	1.94	0.49
1:E:455:GLY:H	1:F:173:PRO:HA	1.78	0.49
1:G:633:MET:HG3	1:I:28:LEU:HD13	1.94	0.49
1:I:662:ASN:OD1	1:I:906:GLU:CA	2.55	0.49
1:J:365:ASN:H	1:J:651:ASN:HD21	1.60	0.49
1:J:804:GLN:HB3	1:L:552:ASN:HB3	1.93	0.49
1:L:685:THR:OG1	1:L:913:PRO:HB2	2.13	0.49
2:N:227:MET:HA	2:N:287:LEU:HD11	1.94	0.49
1:A:171:GLN:HA	1:C:452:ILE:HG23	1.93	0.49
1:A:722:ALA:HB2	1:A:742:GLU:HG2	1.95	0.49
1:D:941:LEU:HD13	1:D:949:ASN:HD22	1.78	0.49
1:E:342:THR:HG23	1:E:360:ASP:H	1.78	0.49
1:L:238:ALA:HB1	1:L:291:VAL:HG11	1.94	0.49
1:A:523:ARG:H	1:C:548:MET:HB2	1.78	0.49
1:B:725:PHE:C	1:B:900:ALA:O	2.51	0.49
1:C:383:TYR:CD2	1:C:390:ALA:HA	2.48	0.49
1:D:325:ASN:HB3	1:D:597:LEU:HD13	1.93	0.49
1:E:678:TRP:HB2	1:E:873:ILE:HD12	1.95	0.49
1:E:683:LEU:HD12	1:E:706:PRO:HB2	1.95	0.49
1:F:96:MET:HG2	1:F:569:ILE:HG12	1.95	0.49
1:G:823:HIS:HA	1:G:826:SER:HB3	1.95	0.49
1:J:655:PRO:CG	1:J:915:LEU:HD23	2.38	0.49
2:N:194:LYS:HG3	2:N:195:VAL:HG23	1.95	0.49
1:A:13:MET:HE1	1:B:941:LEU:HB3	1.94	0.49
1:B:549:LEU:HD22	1:C:801:MET:HA	1.95	0.49
1:F:76:THR:HG23	1:F:79:SER:O	2.12	0.49
1:G:25:SER:H	1:H:639:ASN:HD21	1.60	0.49
1:J:654:TYR:O	1:J:654:TYR:HD1	1.96	0.49
1:K:674:ALA:HB1	1:K:923:PHE:CD1	2.48	0.49
1:K:738:LEU:HD11	1:K:763:LYS:HG3	1.94	0.49
1:L:709:ASP:HB2	1:L:711:THR:HG22	1.95	0.49
2:N:176:SER:HB2	2:N:179:MET:HB2	1.95	0.49
3:M:203:GLN:HE21	3:M:206:LYS:HD2	1.78	0.49
1:B:868:ARG:O	1:B:868:ARG:HG2	2.12	0.49
1:D:650:ALA:HB3	1:D:920:PHE:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:LEU:HD22	1:E:44:LYS:HB2	1.93	0.49
1:E:474:TYR:HA	1:E:478:ALA:HB3	1.94	0.49
1:E:579:TYR:CE2	1:E:936:ILE:HG12	2.48	0.49
1:E:724:THR:HG22	1:E:728:SER:O	2.11	0.49
1:G:211:TRP:CE3	1:G:417:LEU:HD22	2.47	0.49
1:H:198:LYS:HB3	1:H:262:VAL:HB	1.94	0.49
1:H:202:PRO:HD2	1:H:222:ARG:HE	1.76	0.49
1:J:57:THR:HG21	1:K:878:ASN:HB3	1.95	0.49
1:J:571:ASN:O	1:L:44:LYS:HD3	2.12	0.49
1:A:13:MET:HE2	1:B:941:LEU:HD22	1.94	0.49
1:A:316:GLY:HA2	1:C:211:TRP:CD1	2.48	0.49
1:B:182:GLU:OE1	1:B:182:GLU:HA	2.13	0.49
1:F:592:VAL:HG13	1:F:593:LEU:HG	1.94	0.49
1:I:130:PRO:HA	1:I:232:PRO:HA	1.93	0.49
1:I:665:ILE:HG23	1:I:903:MET:HB2	1.95	0.49
1:J:299:HIS:HB2	1:J:322:ASN:HD21	1.78	0.49
1:J:682:ARG:HH12	1:J:907:VAL:HB	1.78	0.49
1:L:179:ILE:HG23	1:L:218:HIS:HB3	1.94	0.49
1:A:114:LYS:HB3	1:A:324:PRO:HA	1.95	0.48
1:C:892:LEU:HD23	5:U:217:ASP:HB2	1.95	0.48
1:F:679:ALA:HB3	1:F:919:LEU:HD23	1.95	0.48
1:H:380:ARG:HD3	1:H:391:VAL:HG13	1.95	0.48
1:I:47:ASN:N	1:I:48:PRO:HD3	2.28	0.48
1:J:385:SER:HB3	1:K:758:GLN:HB3	1.95	0.48
1:K:876:SER:HA	1:K:888:LEU:H	1.78	0.48
1:A:204:PRO:HD2	1:B:823:HIS:NE2	2.28	0.48
1:A:280:LEU:HB2	1:C:439:TRP:HB2	1.94	0.48
1:H:235:GLY:O	1:H:298:THR:HG21	2.13	0.48
1:L:545:TYR:O	1:L:549:LEU:HB3	2.13	0.48
1:A:204:PRO:O	1:B:839:GLY:HA3	2.12	0.48
1:C:41:LEU:HB3	1:C:44:LYS:HG3	1.94	0.48
1:F:110:GLY:CA	1:F:606:ALA:HB2	2.42	0.48
1:G:804:GLN:HG3	1:G:850:LEU:HD22	1.91	0.48
1:H:430:LYS:HB2	1:H:442:ASP:HA	1.96	0.48
1:K:332:ASN:OD1	1:K:387:TRP:O	2.31	0.48
1:K:748:SER:N	1:K:760:ASN:HD21	2.11	0.48
1:A:476:ASN:O	1:A:537:HIS:CD2	2.66	0.48
1:B:726:ASP:HB3	1:B:900:ALA:N	2.20	0.48
1:F:589:VAL:HA	1:F:592:VAL:HG12	1.96	0.48
1:H:779:GLN:HE21	1:I:39:PHE:HA	1.78	0.48
1:I:133:CYS:HB2	1:I:230:MET:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:338:TYR:HB3	1:J:341:SER:HB3	1.95	0.48
1:K:132:PRO:HB3	1:K:170:GLY:HA2	1.95	0.48
1:K:896:ASN:HB2	5:U:194:PRO:HG2	1.95	0.48
2:N:231:TYR:CE2	2:N:284:PRO:O	2.67	0.48
2:N:452:ARG:HG2	2:N:453:SER:N	2.27	0.48
1:B:326:TYR:HE1	1:B:543:LEU:HB3	1.78	0.48
1:F:349:ALA:HA	1:F:936:ILE:HD12	1.95	0.48
1:G:632:ALA:HA	1:G:635:ARG:HB2	1.96	0.48
1:J:226:LYS:HB3	1:J:310:ASN:HD21	1.78	0.48
1:K:797:ASN:HD22	1:K:869:THR:HB	1.77	0.48
1:L:24:LEU:O	1:L:26:PRO:HD3	2.14	0.48
2:N:52:ARG:HB2	2:N:64:PHE:HD2	1.77	0.48
4:S:28:ASN:O	4:S:28:ASN:ND2	2.46	0.48
1:A:338:TYR:CZ	1:A:586:ARG:HG2	2.49	0.48
1:B:336:LEU:HD22	1:B:563:PRO:HD2	1.95	0.48
1:G:353:SER:HB3	1:G:355:LEU:HB2	1.95	0.48
1:G:412:ASN:ND2	1:I:462:ILE:HD11	2.28	0.48
1:G:837:ARG:HH11	1:H:459:ALA:HB2	1.77	0.48
1:I:833:ALA:O	1:I:835:THR:N	2.47	0.48
1:J:535:PHE:CE1	1:J:711:THR:HG21	2.48	0.48
1:J:570:LYS:HG3	1:J:571:ASN:HD22	1.79	0.48
1:J:922:VAL:HG11	1:J:944:PRO:CB	2.44	0.48
1:K:493:LYS:C	1:K:494:ILE:CG1	2.81	0.48
1:A:416:PRO:HG3	1:A:458:PHE:HB2	1.96	0.48
1:A:843:PRO:HB2	1:C:238:ALA:HB2	1.96	0.48
1:B:64:LEU:HD13	1:B:621:PRO:HD3	1.96	0.48
1:F:824:ASN:HD21	1:F:847:PRO:HD3	1.79	0.48
1:G:414:CYS:HB2	1:G:460:MET:HB2	1.95	0.48
1:I:663:VAL:HA	1:I:664:PRO:HD3	1.61	0.48
1:J:483:ASP:HA	1:J:486:LYS:HD3	1.95	0.48
1:K:201:GLN:CB	1:K:202:PRO:CD	2.85	0.48
1:K:495:SER:O	1:K:503:TYR:HD1	1.97	0.48
2:N:467:LEU:HB2	2:N:524:THR:HG21	1.96	0.48
1:A:63:ARG:HA	1:B:736:ARG:HA	1.95	0.48
1:A:113:PHE:HB2	1:A:327:ILE:HD12	1.95	0.48
1:A:365:ASN:HB3	1:A:368:LEU:HB3	1.95	0.48
1:B:922:VAL:HG12	1:B:923:PHE:N	2.28	0.48
1:D:23:TYR:O	1:D:23:TYR:CG	2.65	0.48
1:E:798:PHE:CB	1:E:865:LEU:O	2.61	0.48
1:H:863:LYS:NZ	4:R:48:THR:HG22	2.29	0.48
1:I:757:ALA:CB	1:I:766:PHE:HZ	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:748:SER:HA	1:K:760:ASN:CG	2.34	0.48
1:L:478:ALA:HB2	1:L:514:VAL:HG21	1.95	0.48
4:Q:55:THR:O	4:Q:55:THR:OG1	2.25	0.48
5:V:183:ILE:HG23	5:V:187:GLN:HE21	1.79	0.48
1:H:234:TYR:HE2	1:H:321:PRO:HD3	1.79	0.48
1:I:825:ASN:O	1:I:825:ASN:OD1	2.32	0.48
1:J:906:GLU:CD	4:Q:22:TRP:HE1	2.17	0.48
1:L:757:ALA:CB	1:L:766:PHE:CZ	2.83	0.48
1:A:370:TYR:HA	1:A:373:LEU:HD12	1.96	0.48
1:A:754:TYR:HE1	1:E:76:THR:HG21	1.79	0.48
1:B:22:GLU:HA	5:U:176:SER:HB2	1.94	0.48
1:B:548:MET:HB3	1:C:523:ARG:H	1.79	0.48
1:C:949:ASN:HA	1:K:904:THR:HB	1.95	0.48
1:D:212:TYR:CE1	1:E:315:MET:HB3	2.49	0.48
1:G:201:GLN:O	1:G:202:PRO:C	2.51	0.48
1:G:379:ASP:HB3	1:G:381:THR:HG22	1.95	0.48
1:G:641:GLN:O	1:G:927:ARG:HA	2.14	0.48
1:G:851:ILE:HD11	1:I:115:PRO:HD2	1.95	0.48
1:I:648:SER:HB3	1:I:923:PHE:HA	1.95	0.48
1:I:654:TYR:HH	1:I:665:ILE:HD12	1.65	0.48
1:I:654:TYR:O	1:I:915:LEU:HA	2.14	0.48
1:J:682:ARG:HH22	1:J:907:VAL:HG21	1.78	0.48
4:R:19:MET:HA	4:R:20:PRO:HD2	1.70	0.48
1:D:135:TRP:HZ2	1:D:230:MET:SD	2.33	0.47
1:E:572:LEU:HD21	1:E:928:VAL:HG21	1.95	0.47
1:G:550:LEU:HD13	1:H:758:GLN:HE21	1.78	0.47
1:I:386:MET:HG3	1:I:387:TRP:H	1.79	0.47
1:K:386:MET:O	1:K:386:MET:HG2	2.13	0.47
1:K:494:ILE:HG22	1:K:495:SER:N	2.27	0.47
1:K:583:TRP:HE3	1:K:584:ASN:H	1.62	0.47
1:L:225:LYS:HG3	1:L:288:SER:HB2	1.95	0.47
2:N:283:ILE:HG22	2:N:401:THR:HB	1.96	0.47
1:A:429:VAL:HG22	1:A:430:LYS:N	2.28	0.47
1:C:536:ASN:HA	1:C:596:SER:C	2.34	0.47
1:D:430:LYS:HB3	1:D:442:ASP:HA	1.96	0.47
1:D:917:TYR:CE2	1:D:919:LEU:HD11	2.49	0.47
1:E:249:ILE:HG21	1:E:261:GLN:HB2	1.96	0.47
1:E:553:GLY:HA3	1:F:850:LEU:HB3	1.95	0.47
1:E:797:ASN:HD22	1:E:869:THR:HB	1.78	0.47
1:G:88:VAL:HB	1:G:576:PRO:HA	1.96	0.47
1:G:299:HIS:HD2	1:G:322:ASN:HD21	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:469:TRP:CD1	1:I:516:CYS:HB3	2.49	0.47
2:N:88:HIS:HB2	2:N:554:VAL:HB	1.96	0.47
1:A:591:MET:HA	1:A:699:TYR:HE2	1.79	0.47
1:A:712:PHE:HB2	1:A:715:ASN:HD21	1.79	0.47
1:D:928:VAL:HA	1:D:938:THR:HG23	1.95	0.47
1:H:492:VAL:CG1	1:H:506:LYS:HD3	2.37	0.47
1:I:574:LEU:HD23	1:I:930:ARG:HH12	1.79	0.47
1:L:682:ARG:HH21	1:L:916:LEU:HD22	1.80	0.47
4:S:18:ARG:HG2	4:S:19:MET:N	2.26	0.47
1:A:216:ILE:HG21	1:C:454:VAL:HB	1.95	0.47
1:B:241:THR:HA	1:C:813:ASP:HB2	1.95	0.47
1:B:356:ASN:HB3	2:N:455:ARG:HH12	1.79	0.47
1:D:797:ASN:CG	1:D:867:ASP:O	2.52	0.47
1:G:478:ALA:HB2	1:G:514:VAL:HG21	1.95	0.47
1:H:201:GLN:HB3	1:H:202:PRO:HD3	1.97	0.47
1:I:712:PHE:HB2	1:I:868:ARG:HA	1.96	0.47
1:K:842:TYR:CG	1:K:843:PRO:HD2	2.50	0.47
4:Q:14:TYR:HA	4:R:15:LEU:O	2.14	0.47
1:A:94:LEU:HD11	1:A:617:ALA:HB1	1.96	0.47
1:A:665:ILE:HG21	1:A:903:MET:SD	2.55	0.47
1:B:676:ARG:HB3	1:B:921:GLU:HB3	1.97	0.47
1:I:471:ASN:HA	1:I:474:TYR:HB3	1.95	0.47
1:J:654:TYR:HB2	4:P:16:THR:HG22	1.97	0.47
1:K:202:PRO:HD2	1:K:222:ARG:HG3	1.95	0.47
1:C:328:ALA:HB2	1:C:547:SER:HB3	1.96	0.47
1:D:798:PHE:CD1	1:D:866:CYS:HB2	2.49	0.47
1:F:682:ARG:HB3	1:F:714:LEU:HB3	1.97	0.47
1:H:519:ASN:OD1	1:H:805:VAL:HG13	2.14	0.47
1:I:91:ASN:HB3	1:I:624:HIS:HA	1.95	0.47
1:I:361:LEU:HB3	1:I:362:GLN:H	1.61	0.47
1:I:734:ASN:O	1:I:736:ARG:HG2	2.15	0.47
1:K:504:MET:O	1:K:507:ARG:HG2	2.14	0.47
1:L:19:ASP:O	1:L:48:PRO:HD2	2.14	0.47
1:A:201:GLN:CG	1:A:202:PRO:HD3	2.12	0.47
1:A:414:CYS:HB3	1:C:414:CYS:HB2	1.79	0.47
1:C:35:THR:CG2	6:W:5:ALA:HB2	2.41	0.47
1:D:268:SER:O	1:F:426:LEU:HD23	2.13	0.47
1:E:13:MET:O	1:E:14:HIS:CE1	2.58	0.47
1:F:247:GLN:HB2	1:F:291:VAL:HG21	1.97	0.47
1:G:747:ARG:HE	1:G:750:ASP:HB3	1.78	0.47
1:G:823:HIS:CE1	1:I:204:PRO:HD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:925:VAL:H	1:G:941:LEU:HB2	1.80	0.47
1:H:127:LYS:HG3	1:I:411:PRO:HB3	1.96	0.47
1:H:517:TYR:CG	1:H:847:PRO:HG3	2.50	0.47
1:H:662:ASN:HB2	4:Q:11:VAL:HB	1.95	0.47
1:I:544:ARG:O	1:I:548:MET:HG2	2.14	0.47
1:I:653:LEU:CD2	1:I:653:LEU:N	2.71	0.47
1:I:831:TYR:HD2	1:I:838:GLU:OE2	1.97	0.47
1:J:330:ARG:HE	1:J:594:GLN:HG3	1.79	0.47
1:J:817:VAL:HG22	1:J:818:GLY:H	1.77	0.47
1:K:504:MET:O	1:K:507:ARG:CG	2.63	0.47
1:L:19:ASP:O	1:L:48:PRO:CG	2.62	0.47
1:L:112:THR:HG22	1:L:501:TYR:HB2	1.95	0.47
1:L:683:LEU:HD12	1:L:915:LEU:HD12	1.96	0.47
2:N:79:VAL:HG12	2:N:81:SER:H	1.79	0.47
2:N:90:ASN:HD21	2:N:457:ILE:HD12	1.80	0.47
2:N:185:ASN:HD21	2:N:499:PHE:HE1	1.63	0.47
4:P:28:ASN:CA	4:P:42:ALA:CB	2.77	0.47
4:P:135:SER:OG	4:P:136:PRO:HD3	2.14	0.47
1:A:46:ARG:HH21	1:B:923:PHE:HZ	1.63	0.47
1:C:179:ILE:HG23	1:C:183:GLY:O	2.15	0.47
1:D:323:ARG:HD2	1:D:479:LEU:HB3	1.96	0.47
1:F:180:THR:HG23	1:F:182:GLU:H	1.80	0.47
1:H:517:TYR:CD2	1:H:517:TYR:N	2.82	0.47
1:H:775:ASN:HB3	1:H:880:MET:SD	2.54	0.47
1:J:602:ARG:HB3	4:P:34:ILE:HA	1.96	0.47
1:B:420:VAL:HG11	1:B:453:ARG:HB2	1.96	0.47
1:D:223:VAL:HB	1:D:286:LEU:HD22	1.96	0.47
1:E:756:VAL:HG22	1:E:757:ALA:N	2.25	0.47
1:G:681:THR:HG21	1:G:712:PHE:HB3	1.97	0.47
1:G:735:ASP:HB3	1:I:63:ARG:HE	1.80	0.47
1:H:388:ASN:HB3	1:H:546:ARG:HG2	1.97	0.47
1:J:758:GLN:HE21	1:J:862:LYS:HE3	1.79	0.47
1:K:824:ASN:HA	1:K:844:ALA:HA	1.96	0.47
2:N:250:PHE:CZ	2:N:261:ILE:HD12	2.50	0.47
1:A:676:ARG:HB2	1:A:921:GLU:HB3	1.97	0.47
1:A:840:GLN:HA	1:B:457:ASN:HD21	1.79	0.47
1:F:931:PRO:HD2	1:F:932:HIS:CD2	2.50	0.47
1:G:135:TRP:CD1	1:G:310:ASN:HB2	2.46	0.47
1:G:486:LYS:HB3	1:G:507:ARG:HB3	1.97	0.47
1:J:266:PHE:HB2	1:J:282:PRO:HB3	1.97	0.47
1:J:824:ASN:HA	1:J:844:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:110:GLY:HA2	1:K:554:ARG:HE	1.78	0.47
1:K:824:ASN:CB	1:K:844:ALA:HB2	2.45	0.47
2:N:440:SER:C	2:N:442:PRO:HD3	2.35	0.47
1:B:687:GLU:O	1:B:699:TYR:HE1	1.98	0.46
1:D:486:LYS:HB3	1:D:507:ARG:HG2	1.96	0.46
1:D:536:ASN:HA	1:D:596:SER:O	2.14	0.46
1:E:15:ILE:O	1:E:15:ILE:HG23	2.11	0.46
1:G:848:TYR:O	1:G:850:LEU:N	2.48	0.46
1:H:602:ARG:HH21	4:Q:34:ILE:HG13	1.80	0.46
1:I:429:VAL:HB	1:I:439:TRP:HD1	1.80	0.46
1:J:663:VAL:HG13	4:P:16:THR:HB	1.95	0.46
1:K:426:LEU:HD23	1:L:269:THR:HA	1.98	0.46
1:K:575:LEU:HG	1:K:930:ARG:HH11	1.80	0.46
1:L:595:SER:H	1:L:703:GLY:HA2	1.80	0.46
2:N:445:MET:HB3	2:N:529:LEU:HD12	1.97	0.46
3:M:86:ILE:HG21	3:M:94:VAL:HG21	1.96	0.46
5:V:183:ILE:CG2	5:V:184:GLY:N	2.78	0.46
1:D:620:PHE:HB3	1:D:622:MET:HG3	1.97	0.46
1:J:428:LYS:HD2	1:J:446:PHE:HD1	1.79	0.46
1:J:573:LEU:HD13	1:J:573:LEU:HA	1.72	0.46
2:N:449:VAL:C	2:N:450:THR:HG22	2.36	0.46
4:P:10:ILE:CG1	4:Q:26:ARG:O	2.63	0.46
5:V:59:ALA:HA	5:V:193:VAL:HB	1.97	0.46
1:A:58:THR:C	1:A:60:ARG:H	2.18	0.46
1:A:800:PRO:HG2	1:C:549:LEU:HD21	1.97	0.46
1:B:124:LEU:HG	1:C:828:PHE:CD2	2.51	0.46
1:C:822:GLN:HB3	1:C:824:ASN:OD1	2.15	0.46
1:D:269:THR:HG23	1:D:271:GLU:HG3	1.96	0.46
1:D:413:TYR:HB2	1:F:837:ARG:HD2	1.97	0.46
1:G:18:GLN:OE1	1:G:22:GLU:HB3	2.15	0.46
1:H:64:LEU:HD13	1:H:621:PRO:HD3	1.97	0.46
1:J:393:SER:HB3	1:J:541:ALA:HB3	1.97	0.46
1:K:837:ARG:HH12	1:L:419:GLY:HA2	1.79	0.46
2:N:52:ARG:O	2:N:52:ARG:CG	2.46	0.46
1:A:350:GLY:H	1:A:353:SER:HB3	1.80	0.46
1:C:591:MET:HA	1:C:699:TYR:CE2	2.50	0.46
1:K:428:LYS:HG3	1:K:446:PHE:HB2	1.97	0.46
1:K:723:ILE:HA	1:K:903:MET:HB3	1.97	0.46
1:L:446:PHE:O	1:L:447:SER:C	2.54	0.46
2:N:488:GLN:HE21	2:N:507:ARG:HB3	1.80	0.46
1:A:833:ALA:C	1:A:835:THR:N	2.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:TYR:HB2	1:B:587:LYS:HE3	1.96	0.46
1:B:761:MET:HB2	1:B:766:PHE:HD1	1.80	0.46
1:B:941:LEU:CB	1:B:948:GLY:HA2	2.44	0.46
1:D:20:ALA:HA	1:D:47:ASN:HB3	1.98	0.46
1:D:722:ALA:HB3	1:D:904:THR:HB	1.98	0.46
1:G:927:ARG:CB	1:G:939:VAL:HG23	2.31	0.46
1:H:116:TYR:HE2	1:I:851:ILE:HD13	1.80	0.46
1:I:349:ALA:HB1	1:I:353:SER:HG	1.80	0.46
1:J:426:LEU:HB3	1:K:267:PHE:HB3	1.96	0.46
1:L:429:VAL:HB	1:L:439:TRP:HB2	1.96	0.46
5:U:9:TYR:HB3	5:U:23:ALA:HB1	1.97	0.46
1:D:130:PRO:HD2	1:F:418:GLY:HA2	1.98	0.46
1:D:204:PRO:HB3	1:E:840:GLN:HB2	1.97	0.46
1:D:757:ALA:HA	1:F:386:MET:HB3	1.95	0.46
1:G:13:MET:HB2	1:G:15:ILE:HG23	1.98	0.46
1:G:682:ARG:HH22	1:G:718:PHE:HA	1.80	0.46
1:I:654:TYR:HD1	1:I:916:LEU:O	1.98	0.46
1:A:646:TYR:CD1	6:W:22:THR:O	2.69	0.46
1:A:677:GLY:HA3	1:A:873:ILE:O	2.15	0.46
1:I:659:ASN:O	1:I:659:ASN:OD1	2.34	0.46
1:K:422:ASN:HB2	1:K:453:ARG:HB2	1.98	0.46
1:L:96:MET:HB2	1:L:572:LEU:H	1.80	0.46
1:L:353:SER:HB2	1:L:935:VAL:HG22	1.96	0.46
1:L:930:ARG:H	1:L:931:PRO:CD	2.28	0.46
3:M:96:ASP:HA	3:M:99:LEU:HB2	1.98	0.46
1:A:121:TYR:HB3	1:B:844:ALA:HB3	1.97	0.46
1:A:476:ASN:C	1:A:537:HIS:NE2	2.68	0.46
1:A:555:TYR:H	1:B:850:LEU:HD23	1.80	0.46
1:B:554:ARG:H	1:C:850:LEU:HG	1.81	0.46
1:C:179:ILE:CG2	1:C:180:THR:O	2.54	0.46
1:D:428:LYS:HG3	1:D:446:PHE:HB2	1.98	0.46
1:D:672:TRP:CZ2	1:D:901:LEU:HB2	2.51	0.46
1:E:179:ILE:HG13	1:E:184:ILE:HA	1.98	0.46
1:F:135:TRP:HA	1:F:135:TRP:CE3	2.51	0.46
1:F:657:PRO:HB2	1:F:660:ALA:HB3	1.97	0.46
1:G:333:PHE:CD2	1:G:562:VAL:HG22	2.51	0.46
1:G:592:VAL:HG13	1:G:593:LEU:HD13	1.96	0.46
1:I:180:THR:OG1	1:I:181:LYS:N	2.48	0.46
1:J:328:ALA:HB3	1:J:543:LEU:HD22	1.98	0.46
5:V:194:PRO:HB2	5:V:196:VAL:HG13	1.97	0.46
1:A:269:THR:OG1	1:A:283:LYS:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:535:PHE:CG	1:E:711:THR:HG23	2.51	0.46
1:H:833:ALA:HB1	1:H:834:PRO:HD2	1.97	0.46
1:J:592:VAL:HG13	1:J:593:LEU:HD12	1.98	0.46
1:K:249:ILE:HG22	1:K:260:SER:HA	1.96	0.46
1:K:266:PHE:HB3	1:K:282:PRO:HG2	1.98	0.46
1:L:679:ALA:HB3	1:L:919:LEU:HB3	1.98	0.46
3:M:196:LEU:HB3	3:M:199:VAL:CG2	2.45	0.46
1:B:726:ASP:HA	1:B:900:ALA:O	2.16	0.46
1:D:104:ARG:HA	1:E:752:GLU:HB2	1.98	0.46
1:D:923:PHE:HD2	1:D:942:ARG:HA	1.81	0.46
1:G:824:ASN:CA	1:G:844:ALA:HB2	2.39	0.46
1:I:832:LEU:HD23	1:I:832:LEU:O	2.16	0.46
1:K:683:LEU:HD11	1:K:688:THR:HG22	1.96	0.46
1:L:636:ASN:HB2	1:L:639:ASN:HB3	1.98	0.46
4:S:18:ARG:CG	4:S:19:MET:H	2.26	0.46
5:V:37:GLY:O	5:V:41:ILE:N	2.49	0.46
1:A:21:SER:O	1:A:29:VAL:HG22	2.16	0.45
1:A:56:VAL:HG13	6:W:4:LEU:O	2.15	0.45
1:A:561:GLN:HE22	1:B:756:VAL:HB	1.80	0.45
1:B:332:ASN:H	1:B:388:ASN:HB2	1.80	0.45
1:E:732:PRO:HG3	1:E:743:PHE:CE1	2.51	0.45
1:F:513:LEU:HD21	1:F:819:ILE:HG12	1.97	0.45
1:G:114:LYS:HB2	1:G:325:ASN:H	1.80	0.45
1:G:461:GLU:HB2	1:I:126:PRO:HB3	1.98	0.45
1:H:455:GLY:C	1:I:173:PRO:HB3	2.36	0.45
1:I:589:VAL:HG22	1:I:602:ARG:CD	2.42	0.45
1:K:267:PHE:O	1:K:282:PRO:HB3	2.16	0.45
2:N:448:PRO:HB3	2:N:529:LEU:CD1	2.45	0.45
3:M:230:PRO:HA	3:M:233:ARG:HB3	1.98	0.45
1:A:205:GLN:HG3	1:A:206:ILE:HG13	1.98	0.45
1:B:711:THR:HG22	1:B:713:TYR:HD2	1.81	0.45
1:C:178:ASN:O	1:C:185:GLN:HB2	2.17	0.45
1:D:19:ASP:HB2	1:D:22:GLU:HB2	1.98	0.45
1:D:922:VAL:HB	1:D:944:PRO:HG2	1.97	0.45
1:F:577:GLY:HA3	1:F:934:GLY:HA2	1.97	0.45
1:H:403:ASN:HA	1:H:469:TRP:HZ2	1.81	0.45
1:K:90:ASP:HA	1:K:576:PRO:HB3	1.98	0.45
1:L:924:ASP:HB3	1:L:942:ARG:HG2	1.98	0.45
3:M:134:GLN:C	3:M:136:ASN:H	2.19	0.45
1:B:14:HIS:O	1:B:48:PRO:HG3	2.16	0.45
1:C:249:ILE:HD12	1:C:261:GLN:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:SER:H	1:D:314:LEU:HD12	1.81	0.45
1:E:673:ALA:HB3	1:E:943:THR:HG22	1.99	0.45
1:E:689:PRO:HB3	1:E:698:TYR:HB2	1.98	0.45
1:G:650:ALA:N	1:G:922:VAL:HG22	2.31	0.45
1:G:746:LYS:HG3	1:G:760:ASN:OD1	2.15	0.45
1:H:349:ALA:HA	1:H:355:LEU:HB2	1.98	0.45
1:H:437:ASN:OD1	1:I:179:ILE:HD11	2.16	0.45
1:H:644:ASN:HB3	1:H:925:VAL:HA	1.98	0.45
1:I:572:LEU:HD22	1:I:641:GLN:HB3	1.98	0.45
1:J:136:ASP:HA	1:J:166:THR:HA	1.98	0.45
1:J:654:TYR:O	1:J:654:TYR:CD1	2.69	0.45
1:L:10:TRP:HB2	1:L:16:SER:CB	2.46	0.45
1:A:653:LEU:HD22	1:A:915:LEU:HD13	1.99	0.45
1:A:677:GLY:HA2	1:A:875:PHE:HD1	1.81	0.45
1:B:795:PHE:O	1:B:796:ARG:C	2.55	0.45
1:C:722:ALA:HB3	1:C:904:THR:HB	1.99	0.45
1:D:67:ARG:HH21	1:E:763:LYS:HB2	1.82	0.45
1:E:428:LYS:HG3	1:E:446:PHE:HB2	1.98	0.45
1:E:828:PHE:CZ	1:E:841:ALA:HA	2.52	0.45
1:I:179:ILE:HG23	1:I:218:HIS:HB3	1.98	0.45
1:I:732:PRO:HD3	1:I:743:PHE:CZ	2.51	0.45
1:K:716:HIS:HB3	1:K:866:CYS:H	1.82	0.45
1:L:32:ALA:O	1:L:36:GLU:CB	2.36	0.45
1:L:722:ALA:HB3	1:L:904:THR:HB	1.99	0.45
3:M:154:VAL:N	3:M:155:PRO:HD3	2.31	0.45
4:S:48:THR:O	4:S:49:TYR:CD2	2.70	0.45
1:A:109:ARG:HB2	1:A:554:ARG:HA	1.98	0.45
1:A:581:TYR:CZ	1:A:583:TRP:NE1	2.84	0.45
1:A:691:LEU:O	1:A:691:LEU:CD2	2.65	0.45
1:B:103:ILE:HG13	1:B:562:VAL:HG21	1.99	0.45
1:D:70:PRO:HA	1:D:84:PHE:HB3	1.99	0.45
1:D:77:ALA:O	1:D:78:TYR:CG	2.69	0.45
1:E:174:TYR:HB2	1:E:220:ALA:H	1.82	0.45
1:F:714:LEU:HD23	1:F:714:LEU:HA	1.71	0.45
1:G:172:ALA:HA	1:G:221:GLY:HA2	1.99	0.45
1:G:678:TRP:CD1	1:G:920:PHE:HA	2.51	0.45
1:G:719:LYS:HG2	1:G:720:LYS:HD3	1.98	0.45
1:I:10:TRP:HB3	1:I:15:ILE:HB	1.98	0.45
1:I:93:VAL:HB	1:I:573:LEU:HD22	1.98	0.45
1:J:656:ILE:HD11	1:J:910:MET:HB2	1.97	0.45
1:K:122:ASN:HA	1:L:825:ASN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:2:SER:HA	4:R:3:THR:HA	1.66	0.45
1:A:56:VAL:HG11	6:W:4:LEU:O	2.17	0.45
1:A:167:HIS:HE1	1:A:223:VAL:HG21	1.82	0.45
1:C:804:GLN:HE21	1:C:858:SER:HB2	1.81	0.45
1:E:201:GLN:HB3	1:E:202:PRO:CD	2.46	0.45
1:H:74:GLU:HG2	1:L:69:ILE:HD12	1.99	0.45
1:H:670:ARG:HB2	1:H:672:TRP:CD1	2.47	0.45
1:I:720:LYS:N	1:I:906:GLU:HB2	2.25	0.45
1:L:71:VAL:HG13	1:L:72:ASP:H	1.82	0.45
1:L:184:ILE:H	1:L:184:ILE:HG13	1.59	0.45
1:L:804:GLN:HG2	1:L:860:THR:HA	1.99	0.45
2:N:450:THR:O	2:N:451:PHE:CG	2.69	0.45
1:A:323:ARG:NH2	1:A:474:TYR:O	2.43	0.45
1:C:323:ARG:HG2	1:C:479:LEU:HD13	1.98	0.45
1:E:420:VAL:HG12	1:E:453:ARG:HB3	1.99	0.45
1:F:517:TYR:HB2	1:F:847:PRO:HG3	1.98	0.45
1:F:533:ASN:HB2	1:F:713:TYR:CZ	2.52	0.45
1:G:631:GLU:HB2	1:G:635:ARG:CZ	2.46	0.45
1:I:732:PRO:HD3	1:I:743:PHE:HZ	1.82	0.45
1:J:566:PHE:HB3	1:J:569:ILE:HG22	1.98	0.45
1:K:83:ARG:HA	1:K:582:GLU:HG3	1.99	0.45
1:K:674:ALA:HB1	1:K:923:PHE:HD1	1.81	0.45
2:N:271:PHE:HE2	2:N:273:ILE:HG12	1.81	0.45
2:N:283:ILE:CG2	2:N:403:TYR:HB2	2.47	0.45
3:M:208:LEU:HD21	3:M:236:LEU:HD11	1.98	0.45
1:D:731:TRP:HB3	1:D:732:PRO:CD	2.45	0.45
1:E:626:THR:HG22	1:E:630:LEU:HB2	1.99	0.45
1:E:706:PRO:HA	1:E:711:THR:HB	1.99	0.45
1:F:721:VAL:HG23	1:F:745:ILE:HD11	1.99	0.45
1:G:18:GLN:CG	1:G:22:GLU:HB3	2.47	0.45
1:G:561:GLN:HE22	1:H:757:ALA:H	1.65	0.45
1:G:896:ASN:HD22	1:G:896:ASN:N	2.15	0.45
1:H:69:ILE:HA	1:H:70:PRO:HD3	1.84	0.45
1:H:561:GLN:HB2	1:I:756:VAL:HG22	1.98	0.45
1:J:25:SER:HA	1:J:26:PRO:HD3	1.84	0.45
1:K:550:LEU:HG	1:K:556:VAL:HG11	1.99	0.45
1:L:594:GLN:HA	1:L:702:SER:O	2.17	0.45
2:N:171:PRO:HG2	2:N:183:LEU:HD13	1.98	0.45
3:M:197:GLN:HG2	5:U:66:ARG:NH1	2.32	0.45
4:S:30:MET:HE2	4:S:41:PRO:CB	2.46	0.45
1:C:524:TRP:CG	1:C:803:ARG:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:765:TRP:C	1:C:767:LEU:H	2.20	0.45
1:D:33:ARG:O	1:D:36:GLU:HG3	2.15	0.45
1:D:481:LEU:HD12	1:D:509:VAL:HG11	1.98	0.45
1:D:590:ASN:HB3	1:D:699:TYR:CD2	2.52	0.45
1:F:426:LEU:HB2	1:F:450:ASN:HD21	1.82	0.45
1:G:679:ALA:HB3	1:G:919:LEU:HB2	1.98	0.45
1:I:719:LYS:HA	1:I:746:LYS:HB2	1.98	0.45
1:J:374:LEU:HA	1:J:377:ILE:HG22	1.98	0.45
1:J:772:ALA:HA	1:J:879:PHE:O	2.17	0.45
1:K:63:ARG:HA	1:L:735:ASP:O	2.16	0.45
1:L:628:SER:HB3	5:V:92:PRO:HG3	1.99	0.45
1:A:716:HIS:HB3	1:A:866:CYS:H	1.82	0.45
1:B:104:ARG:HA	1:B:559:HIS:HD2	1.82	0.45
1:D:403:ASN:HD21	1:D:516:CYS:HA	1.81	0.45
1:G:267:PHE:HA	1:I:428:LYS:HA	1.99	0.45
1:G:682:ARG:NH2	1:G:718:PHE:HA	2.32	0.45
1:H:104:ARG:HG3	1:H:559:HIS:CD2	2.52	0.45
1:H:611:ASP:OD2	4:S:57:LEU:HD22	2.17	0.45
1:H:719:LYS:H	1:H:907:VAL:HA	1.81	0.45
1:I:394:TYR:OH	1:I:867:ASP:HB3	2.17	0.45
1:I:867:ASP:O	1:I:869:THR:N	2.50	0.45
1:K:656:ILE:HD12	1:K:914:THR:O	2.16	0.45
1:K:718:PHE:HB3	1:K:745:ILE:HD13	1.99	0.45
1:K:755:ASN:HD21	1:K:760:ASN:C	2.21	0.45
1:L:241:THR:OG1	1:L:248:GLY:HA3	2.17	0.45
2:N:89:SER:HA	2:N:543:ILE:HD12	1.98	0.45
3:M:197:GLN:HA	5:U:197:TYR:CD1	2.52	0.45
1:A:500:THR:HA	1:A:599:ASN:HB2	2.00	0.44
1:B:171:GLN:HB3	1:C:840:GLN:HG3	1.98	0.44
1:D:533:ASN:HD21	1:D:706:PRO:HG3	1.82	0.44
1:G:711:THR:HA	1:G:868:ARG:HG3	1.99	0.44
1:H:49:THR:HB	1:I:883:GLY:HA2	1.99	0.44
1:H:95:ASP:H	1:H:619:PHE:HB3	1.82	0.44
1:I:422:ASN:HB3	1:I:453:ARG:HB2	1.99	0.44
1:K:401:ILE:HD12	1:K:525:SER:HA	1.99	0.44
5:V:44:VAL:O	5:V:48:ARG:HB3	2.16	0.44
1:B:333:PHE:HB3	1:B:563:PRO:HG3	1.98	0.44
1:D:84:PHE:CE1	1:D:581:TYR:HB3	2.52	0.44
1:D:330:ARG:HB2	1:D:334:ILE:HG22	1.98	0.44
1:F:668:PRO:HD2	1:H:726:ASP:O	2.17	0.44
1:G:537:HIS:HB3	1:G:540:ASN:HD21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:849:PRO:C	1:G:851:ILE:H	2.20	0.44
1:J:115:PRO:HD3	1:K:851:ILE:HG21	1.99	0.44
1:J:566:PHE:CE2	1:J:568:ALA:HB3	2.53	0.44
1:J:720:LYS:HE2	1:J:747:ARG:HD2	1.98	0.44
1:L:59:ASP:HB3	5:V:102:THR:HB	2.00	0.44
1:L:575:LEU:HD22	1:L:631:GLU:HB2	1.99	0.44
1:L:783:ILE:H	1:L:783:ILE:HG13	1.62	0.44
1:L:865:LEU:HD23	1:L:865:LEU:HA	1.71	0.44
1:E:524:TRP:HH2	1:E:863:LYS:HD3	1.82	0.44
1:F:655:PRO:HA	1:F:915:LEU:HA	1.99	0.44
1:F:867:ASP:O	1:F:868:ARG:HB2	2.17	0.44
1:G:771:LEU:O	1:G:880:MET:CA	2.66	0.44
1:H:867:ASP:O	1:H:868:ARG:CB	2.47	0.44
1:J:347:VAL:HG13	1:J:356:ASN:HB3	2.00	0.44
1:J:922:VAL:HG12	1:J:944:PRO:CG	2.39	0.44
1:K:486:LYS:HB3	1:K:507:ARG:HB2	1.98	0.44
1:K:649:ALA:HB1	1:K:920:PHE:O	2.17	0.44
2:N:271:PHE:CE2	2:N:273:ILE:HG12	2.52	0.44
2:N:285:ALA:CB	2:N:393:LEU:HD22	2.46	0.44
2:N:443:ASP:HB2	2:N:539:GLN:HG2	2.00	0.44
3:M:212:TRP:HD1	3:M:254:LEU:HD11	1.83	0.44
4:S:19:MET:CE	4:S:19:MET:CA	2.88	0.44
1:B:524:TRP:CD1	1:B:803:ARG:HB3	2.53	0.44
1:C:325:ASN:HB3	1:C:597:LEU:HB3	1.98	0.44
1:D:799:GLN:HA	1:D:800:PRO:HD3	1.83	0.44
1:E:266:PHE:HB3	1:E:282:PRO:HG3	1.99	0.44
1:G:325:ASN:HB3	1:G:597:LEU:HB2	1.99	0.44
1:G:513:LEU:HG	1:G:518:ILE:HD12	1.98	0.44
1:G:682:ARG:HD2	1:G:714:LEU:HB3	1.99	0.44
1:H:611:ASP:CG	4:S:57:LEU:HD22	2.38	0.44
1:K:132:PRO:HB2	1:K:223:VAL:HA	2.00	0.44
1:K:426:LEU:HB2	1:K:450:ASN:HD21	1.82	0.44
1:L:676:ARG:HB3	1:L:921:GLU:HB3	2.00	0.44
1:L:723:ILE:HA	1:L:903:MET:HG2	1.99	0.44
1:A:216:ILE:HD12	1:A:283:LYS:HB3	1.99	0.44
1:A:646:TYR:HA	6:W:22:THR:CB	2.48	0.44
1:C:824:ASN:HA	1:C:844:ALA:HB2	2.00	0.44
1:D:798:PHE:HD1	1:D:866:CYS:CB	2.29	0.44
1:F:430:LYS:HD2	1:F:442:ASP:HA	1.98	0.44
1:G:245:GLY:HA3	1:H:821:HIS:HB3	2.00	0.44
1:G:931:PRO:HD3	1:G:937:GLU:OE2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:938:THR:OG1	1:G:939:VAL:N	2.49	0.44
1:H:487:TYR:HB2	1:H:508:VAL:O	2.16	0.44
1:H:552:ASN:HD22	1:I:851:ILE:HD11	1.82	0.44
1:H:571:ASN:O	1:H:643:PHE:HZ	2.00	0.44
1:J:690:SER:HA	4:P:26:ARG:HH21	1.81	0.44
1:K:253:GLN:H	1:K:253:GLN:HG3	1.63	0.44
1:K:876:SER:HB3	1:K:887:ASP:H	1.83	0.44
1:L:823:HIS:HB3	1:L:843:PRO:O	2.17	0.44
1:A:251:VAL:HG13	1:A:252:LYS:N	2.33	0.44
1:B:602:ARG:NH2	1:B:695:TYR:CE1	2.66	0.44
1:C:35:THR:HG22	1:C:38:TYR:HB3	1.99	0.44
1:G:676:ARG:HG3	1:G:921:GLU:HG2	2.00	0.44
1:H:70:PRO:HG2	1:H:82:ALA:HB1	1.98	0.44
1:J:720:LYS:CD	4:Q:22:TRP:CH2	2.99	0.44
1:K:755:ASN:OD1	1:K:862:LYS:HE2	2.17	0.44
2:N:83:ASN:HB3	2:N:91:PHE:HB2	2.00	0.44
2:N:480:ALA:HB1	2:N:510:ALA:HB3	1.99	0.44
1:A:330:ARG:HH12	1:A:705:ILE:H	1.66	0.44
1:A:513:LEU:HD13	1:A:819:ILE:HG12	2.00	0.44
1:D:211:TRP:CD1	1:E:836:MET:HG3	2.53	0.44
1:D:380:ARG:HE	1:D:391:VAL:HG22	1.83	0.44
1:D:476:ASN:HA	1:D:538:HIS:HD2	1.82	0.44
1:E:513:LEU:O	1:E:518:ILE:HD12	2.17	0.44
1:F:478:ALA:HA	1:F:481:LEU:HG	1.98	0.44
1:G:13:MET:HA	1:H:927:ARG:HD2	2.00	0.44
1:H:428:LYS:HA	1:I:267:PHE:HB3	2.00	0.44
1:J:179:ILE:HG21	1:J:184:ILE:HG22	1.99	0.44
1:L:252:LYS:HB3	1:L:257:LYS:HA	1.98	0.44
1:L:336:LEU:O	1:L:337:MET:HB2	2.18	0.44
1:L:824:ASN:CA	1:L:844:ALA:HB2	2.46	0.44
2:N:139:PHE:HZ	2:N:547:ARG:HE	1.66	0.44
4:Q:114:LEU:N	4:Q:114:LEU:CD1	2.81	0.44
1:B:41:LEU:HD21	1:B:44:LYS:HD2	2.00	0.44
1:B:269:THR:HB	1:B:271:GLU:HG2	2.00	0.44
1:D:848:TYR:HA	1:D:849:PRO:HD3	1.80	0.44
1:E:332:ASN:HA	1:E:387:TRP:HB3	1.99	0.44
1:F:487:TYR:HB2	1:F:508:VAL:O	2.18	0.44
1:H:414:CYS:HB2	1:I:414:CYS:HB3	1.84	0.44
1:I:387:TRP:CE2	1:I:563:PRO:HG3	2.53	0.44
4:S:15:LEU:HD12	4:S:15:LEU:N	2.22	0.44
1:C:69:ILE:HG23	1:C:70:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:198:LYS:HB3	1:F:262:VAL:HG23	1.99	0.44
1:F:648:SER:O	1:F:921:GLU:HA	2.18	0.44
1:G:45:PHE:HD2	1:G:46:ARG:H	1.64	0.44
1:H:837:ARG:HG3	1:I:459:ALA:HB2	1.98	0.44
1:K:186:ILE:HD11	1:K:196:ALA:HB2	2.00	0.44
1:K:748:SER:CA	1:K:760:ASN:ND2	2.64	0.44
1:K:755:ASN:OD1	1:K:760:ASN:HA	2.18	0.44
1:L:299:HIS:HB2	1:L:322:ASN:HD21	1.83	0.44
1:C:635:ARG:HE	1:C:932:HIS:HA	1.83	0.43
1:D:798:PHE:HD1	1:D:866:CYS:SG	2.41	0.43
1:H:926:VAL:HG22	1:H:940:TYR:HA	2.00	0.43
1:J:415:PHE:HZ	1:K:124:LEU:HD23	1.82	0.43
1:J:720:LYS:NZ	4:Q:22:TRP:CE3	2.80	0.43
1:K:348:LEU:HD13	1:K:357:ALA:HB3	1.99	0.43
1:K:383:TYR:HB3	1:K:390:ALA:HB2	2.00	0.43
2:N:53:ASN:O	2:N:119:TRP:CZ2	2.70	0.43
2:N:283:ILE:HD12	2:N:408:LEU:HD11	1.99	0.43
5:U:86:PRO:HG3	5:U:172:GLN:HA	2.00	0.43
1:B:205:GLN:NE2	1:C:826:SER:OG	2.51	0.43
1:D:268:SER:C	1:F:426:LEU:HD23	2.38	0.43
1:F:533:ASN:OD1	1:F:713:TYR:CD2	2.71	0.43
1:G:91:ASN:HB3	1:G:624:HIS:ND1	2.34	0.43
1:H:121:TYR:CD2	1:I:844:ALA:HB3	2.53	0.43
1:H:696:ASP:OD1	4:Q:23:ALA:HB2	2.18	0.43
1:I:96:MET:HG2	1:I:572:LEU:O	2.19	0.43
1:K:537:HIS:H	1:K:540:ASN:HD21	1.65	0.43
1:B:701:TYR:HD2	1:B:703:GLY:H	1.66	0.43
1:E:486:LYS:HB2	1:E:507:ARG:HH11	1.82	0.43
1:F:328:ALA:HB2	1:F:547:SER:HB2	2.00	0.43
1:F:400:ILE:HA	1:F:525:SER:HB2	1.98	0.43
1:G:745:ILE:HG12	1:G:765:TRP:CD1	2.53	0.43
1:K:412:ASN:HB2	1:K:462:ILE:HG23	2.00	0.43
1:L:10:TRP:CG	1:L:16:SER:HB3	2.54	0.43
1:L:252:LYS:H	1:L:257:LYS:HG2	1.83	0.43
2:N:113:LEU:HD22	2:N:119:TRP:HE3	1.83	0.43
4:S:28:ASN:O	4:S:28:ASN:CG	2.57	0.43
5:U:84:PRO:HB3	5:U:174:SER:HB3	2.01	0.43
1:A:414:CYS:HB2	1:B:414:CYS:HB3	1.82	0.43
1:F:224:LEU:HB3	1:F:228:THR:HG23	2.00	0.43
1:G:174:TYR:HB3	1:G:220:ALA:HB3	2.00	0.43
1:I:331:ASP:HB2	1:I:391:VAL:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:183:GLY:HA3	1:J:201:GLN:HE22	1.83	0.43
1:J:653:LEU:HB2	1:J:915:LEU:HD22	1.99	0.43
3:M:197:GLN:OE1	5:U:66:ARG:NH2	2.35	0.43
1:B:489:PRO:HD3	1:B:494:ILE:HD13	1.99	0.43
1:C:237:TYR:HE1	1:C:239:LYS:HG3	1.83	0.43
1:D:14:HIS:HB2	1:D:45:PHE:HZ	1.84	0.43
1:D:523:ARG:CB	1:F:548:MET:HB3	2.41	0.43
1:G:475:SER:HA	1:G:479:LEU:HD12	2.00	0.43
1:I:850:LEU:HD13	1:I:856:VAL:O	2.18	0.43
1:J:829:VAL:HG22	1:J:830:GLY:H	1.82	0.43
1:K:863:LYS:HB3	1:K:864:PHE:H	1.62	0.43
2:N:444:MET:HG2	2:N:531:LEU:HD22	1.99	0.43
3:M:99:LEU:HA	3:M:102:VAL:HG22	1.99	0.43
4:R:50:GLU:OE1	4:R:50:GLU:HA	2.18	0.43
1:A:57:THR:HB	1:B:877:SER:HB2	2.00	0.43
1:A:58:THR:C	1:A:60:ARG:N	2.72	0.43
1:B:211:TRP:CD1	1:C:316:GLY:HA2	2.53	0.43
1:E:113:PHE:HB3	1:E:327:ILE:HD12	1.99	0.43
1:E:871:TRP:HA	1:E:871:TRP:CE3	2.53	0.43
1:I:350:GLY:HA2	1:I:579:TYR:HA	2.00	0.43
1:I:661:THR:HB	1:I:909:PRO:N	2.34	0.43
1:I:730:SER:HB2	1:I:741:ASN:HA	2.00	0.43
1:J:817:VAL:CG2	1:J:818:GLY:N	2.81	0.43
1:K:65:THR:HG23	1:L:763:LYS:HD3	2.01	0.43
1:K:428:LYS:HA	1:L:267:PHE:HB3	2.01	0.43
1:L:825:ASN:O	1:L:825:ASN:OD1	2.36	0.43
4:P:128:VAL:HA	4:P:131:LEU:HD12	2.01	0.43
1:A:82:ALA:HB2	1:A:613:ILE:HD13	2.01	0.43
1:A:429:VAL:O	1:A:442:ASP:OD2	2.36	0.43
1:C:348:LEU:HD23	1:C:569:ILE:HD13	2.01	0.43
1:E:429:VAL:HA	1:E:442:ASP:N	2.33	0.43
1:G:395:ASP:HA	1:G:396:PRO:HD3	1.91	0.43
1:G:517:TYR:CD1	1:G:846:PHE:HD2	2.37	0.43
1:K:223:VAL:HB	1:K:286:LEU:HD22	2.01	0.43
3:M:13:ALA:HB1	3:M:17:GLN:HE21	1.82	0.43
1:B:184:ILE:HG22	1:B:185:GLN:H	1.82	0.43
1:B:601:LEU:HB3	1:B:606:ALA:HB3	2.00	0.43
1:B:648:SER:HB2	1:B:924:ASP:H	1.83	0.43
1:D:689:PRO:HB3	1:D:699:TYR:HD1	1.84	0.43
1:E:429:VAL:HA	1:E:441:LYS:HA	2.01	0.43
1:E:656:ILE:HD11	1:E:916:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:PRO:HB3	1:F:245:GLY:HA2	1.99	0.43
1:K:351:GLN:HB3	1:K:578:SER:HB2	2.00	0.43
1:B:22:GLU:HG2	5:U:177:GLU:HB2	2.01	0.43
1:B:74:GLU:HB2	1:B:81:LYS:HB2	2.00	0.43
1:B:115:PRO:HA	1:B:326:TYR:HD2	1.83	0.43
1:B:413:TYR:HB3	1:B:459:ALA:HB1	2.01	0.43
1:B:426:LEU:HB3	1:C:267:PHE:HD1	1.83	0.43
1:B:725:PHE:HA	1:B:901:LEU:HA	2.00	0.43
1:C:817:VAL:HG11	1:C:846:PHE:HA	2.00	0.43
1:D:64:LEU:HD13	1:D:621:PRO:HD3	2.00	0.43
1:D:126:PRO:HB2	1:D:129:ALA:HB2	2.01	0.43
1:F:635:ARG:HA	1:F:931:PRO:HA	2.01	0.43
1:F:793:SER:HA	1:F:869:THR:HG23	2.01	0.43
1:G:101:PHE:O	1:G:561:GLN:HA	2.18	0.43
1:G:428:LYS:HG2	1:G:446:PHE:HD1	1.84	0.43
1:G:822:GLN:HA	1:G:845:ASN:HD21	1.84	0.43
1:H:492:VAL:HG13	1:H:506:LYS:NZ	2.33	0.43
1:I:334:ILE:HG13	1:I:565:LYS:HZ3	1.83	0.43
1:J:114:LYS:HA	1:J:115:PRO:HD3	1.83	0.43
1:J:720:LYS:CD	4:Q:22:TRP:CE3	2.86	0.43
1:K:64:LEU:HB3	1:L:736:ARG:O	2.19	0.43
1:K:705:ILE:HG22	1:K:707:TYR:H	1.84	0.43
1:L:930:ARG:H	1:L:931:PRO:HD2	1.80	0.43
5:U:49:ALA:HA	5:U:52:ASN:HD22	1.83	0.43
1:B:656:ILE:HD12	1:B:916:LEU:HB2	2.01	0.43
1:C:333:PHE:HE2	1:C:387:TRP:HA	1.82	0.43
1:C:676:ARG:HB3	1:C:921:GLU:HB3	2.01	0.43
1:D:398:VAL:HG21	1:D:539:ARG:HD2	2.01	0.43
1:D:405:GLY:HA2	1:D:520:LEU:HD11	2.01	0.43
1:E:47:ASN:HA	1:E:48:PRO:HD3	1.86	0.43
1:I:654:TYR:CD1	1:I:916:LEU:O	2.72	0.43
1:J:644:ASN:H	1:L:46:ARG:HD3	1.83	0.43
1:K:748:SER:HB3	1:K:760:ASN:HD21	1.82	0.43
1:L:126:PRO:HG2	1:L:129:ALA:HB2	2.00	0.43
1:L:575:LEU:H	1:L:930:ARG:HH21	1.67	0.43
4:S:30:MET:O	4:S:32:SER:N	2.52	0.43
1:A:55:ASP:O	1:A:56:VAL:CG2	2.58	0.42
1:A:836:MET:O	1:A:836:MET:SD	2.77	0.42
1:B:755:ASN:HD21	1:B:862:LYS:HE3	1.84	0.42
1:C:829:VAL:HG12	1:C:830:GLY:N	2.33	0.42
1:F:131:ASN:HA	1:F:132:PRO:HD3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:775:ASN:ND2	1:G:881:SER:CB	2.73	0.42
1:H:834:PRO:HB3	1:I:410:LEU:HD23	2.01	0.42
1:I:656:ILE:O	1:I:657:PRO:O	2.37	0.42
1:J:552:ASN:HB2	1:K:522:ALA:HB2	1.99	0.42
1:K:386:MET:HG3	1:L:758:GLN:HG3	2.00	0.42
1:K:449:LYS:HD3	1:L:312:ARG:HH22	1.84	0.42
1:K:494:ILE:CG2	1:K:495:SER:N	2.82	0.42
1:K:564:GLN:HE22	1:K:583:TRP:HE1	1.66	0.42
1:K:720:LYS:HG3	1:K:906:GLU:HB3	2.00	0.42
1:L:374:LEU:HD21	1:L:389:GLN:HG2	2.01	0.42
1:A:325:ASN:HA	1:A:596:SER:HB2	2.02	0.42
1:C:47:ASN:HA	1:C:48:PRO:HD3	1.89	0.42
1:C:237:TYR:HE2	1:C:294:GLU:HB2	1.83	0.42
1:C:368:LEU:HD22	1:C:708:LEU:HA	2.02	0.42
1:C:632:ALA:HB2	1:C:933:ARG:HH21	1.83	0.42
1:C:648:SER:HB3	1:C:923:PHE:HA	2.01	0.42
1:D:374:LEU:HD21	1:D:389:GLN:HE22	1.84	0.42
1:D:779:GLN:HA	1:F:95:ASP:HB3	2.02	0.42
1:D:840:GLN:HB2	1:F:204:PRO:HB3	2.02	0.42
1:E:420:VAL:HG13	1:E:457:ASN:HA	2.00	0.42
1:G:428:LYS:HE2	1:H:265:GLN:HB3	2.01	0.42
1:H:570:LYS:O	1:H:643:PHE:HE1	1.90	0.42
1:I:369:SER:HA	1:I:647:LEU:HB3	2.02	0.42
1:I:822:GLN:HB2	1:I:824:ASN:OD1	2.19	0.42
1:J:656:ILE:HG12	1:J:914:THR:OG1	2.19	0.42
3:M:134:GLN:HA	3:M:176:PRO:HB2	2.01	0.42
4:P:15:LEU:HD13	4:R:15:LEU:HD12	2.02	0.42
1:A:771:LEU:HB3	1:A:879:PHE:HB2	2.01	0.42
1:B:128:GLY:HA2	1:B:318:GLN:HA	2.01	0.42
1:E:357:ALA:HA	1:E:938:THR:HG21	2.01	0.42
1:E:464:LEU:HD22	1:F:464:LEU:HD21	2.01	0.42
1:J:923:PHE:HB3	1:J:944:PRO:HD3	2.02	0.42
1:K:328:ALA:HB1	1:K:546:ARG:HB2	2.00	0.42
1:K:941:LEU:HB3	5:U:31:ILE:HG23	2.01	0.42
1:L:421:ILE:O	1:L:421:ILE:HG12	2.18	0.42
2:N:137:PHE:CD2	2:N:137:PHE:O	2.73	0.42
1:B:760:ASN:HB3	1:B:864:PHE:HD2	1.83	0.42
1:C:388:ASN:HB2	1:C:546:ARG:HH11	1.84	0.42
1:D:657:PRO:HG2	1:D:660:ALA:HB2	2.01	0.42
1:E:589:VAL:HG12	1:E:601:LEU:HB3	2.01	0.42
1:F:118:GLY:HA2	1:F:321:PRO:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:759:CYS:C	1:G:761:MET:N	2.71	0.42
1:H:415:PHE:HA	1:H:416:PRO:HD3	1.90	0.42
1:I:709:ASP:HB2	1:I:711:THR:HG22	2.02	0.42
1:J:349:ALA:HB1	1:J:354:GLN:HA	2.00	0.42
1:J:862:LYS:H	4:Q:50:GLU:HB2	1.83	0.42
1:K:230:MET:HB2	1:K:314:LEU:HB2	2.01	0.42
1:K:940:TYR:HB2	5:U:32:ASN:HD22	1.84	0.42
1:L:113:PHE:HD1	1:L:327:ILE:HB	1.83	0.42
1:L:444:THR:O	1:L:445:GLU:C	2.56	0.42
1:L:850:LEU:HD13	1:L:856:VAL:O	2.19	0.42
2:N:382:LEU:HB2	2:N:393:LEU:HD23	2.01	0.42
5:V:37:GLY:O	5:V:41:ILE:HB	2.20	0.42
5:V:183:ILE:HD13	5:V:191:GLU:OE1	2.18	0.42
1:A:132:PRO:HB2	1:A:223:VAL:HA	2.01	0.42
1:A:705:ILE:HG22	1:A:708:LEU:H	1.84	0.42
1:B:327:ILE:HG22	1:B:593:LEU:HD23	2.01	0.42
1:B:414:CYS:HB2	1:C:414:CYS:HB3	2.00	0.42
1:C:223:VAL:HB	1:C:286:LEU:HD22	2.01	0.42
1:F:51:ALA:HA	1:F:52:PRO:HD3	1.92	0.42
1:H:222:ARG:HA	1:H:287:TYR:H	1.85	0.42
1:I:730:SER:O	1:I:732:PRO:CD	2.68	0.42
1:A:58:THR:O	1:A:59:ASP:C	2.57	0.42
1:A:97:ALA:HB3	1:B:780:GLY:HA3	2.01	0.42
1:G:69:ILE:HA	1:G:70:PRO:HD2	1.82	0.42
1:G:299:HIS:HB3	1:G:300:ILE:H	1.70	0.42
1:G:523:ARG:H	1:I:548:MET:HB2	1.84	0.42
1:I:63:ARG:H	1:I:63:ARG:HG2	1.71	0.42
1:I:102:ASP:HB2	1:I:616:TYR:HE1	1.84	0.42
1:I:113:PHE:HD1	1:I:327:ILE:HB	1.84	0.42
1:I:681:THR:HG21	1:I:712:PHE:HB3	2.02	0.42
1:K:108:ASP:HB3	1:K:607:SER:HB2	2.02	0.42
1:B:51:ALA:HA	1:B:52:PRO:HD3	1.94	0.42
1:B:681:THR:HB	1:B:712:PHE:CD2	2.55	0.42
1:C:654:TYR:HA	1:C:655:PRO:HD3	1.94	0.42
1:C:799:GLN:HA	1:C:800:PRO:HD3	1.92	0.42
1:D:270:THR:HG23	1:D:270:THR:O	2.20	0.42
1:H:79:SER:HB2	1:H:584:ASN:HD21	1.85	0.42
1:I:326:TYR:H	1:I:596:SER:HB2	1.84	0.42
1:I:589:VAL:HG12	1:I:608:ILE:HD11	2.02	0.42
1:J:323:ARG:H	1:J:505:ASN:HB2	1.83	0.42
1:J:497:ASN:HA	1:J:498:PRO:HD3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:750:ASP:O	1:K:750:ASP:OD1	2.38	0.42
1:L:600:ASP:HB3	1:L:700:THR:O	2.20	0.42
2:N:240:ILE:HD12	2:N:250:PHE:HZ	1.84	0.42
4:S:34:ILE:O	4:S:35:ASP:CB	2.68	0.42
1:A:581:TYR:CZ	1:A:583:TRP:CD1	3.07	0.42
1:D:337:MET:HB2	1:D:339:TYR:CE1	2.55	0.42
1:D:663:VAL:HB	1:D:905:PHE:HB3	2.02	0.42
1:E:589:VAL:HG13	1:E:608:ILE:HD12	2.01	0.42
1:F:653:LEU:O	4:R:19:MET:HB2	2.19	0.42
1:H:90:ASP:HA	1:H:576:PRO:HG2	2.01	0.42
1:H:518:ILE:HG23	1:H:846:PHE:HE2	1.83	0.42
1:I:810:LYS:HE2	1:I:859:ILE:HD12	2.02	0.42
1:K:755:ASN:CG	1:K:760:ASN:HA	2.40	0.42
1:L:179:ILE:HG12	1:L:218:HIS:CE1	2.55	0.42
2:N:441:LEU:N	2:N:442:PRO:HD3	2.35	0.42
4:R:41:PRO:CA	4:R:46:THR:HB	2.48	0.42
1:A:635:ARG:HB3	1:A:931:PRO:O	2.19	0.42
1:B:64:LEU:HD13	1:B:619:PHE:O	2.13	0.42
1:B:684:LYS:HG2	1:B:914:THR:HG22	2.00	0.42
1:C:365:ASN:HB3	1:C:368:LEU:HB2	2.01	0.42
1:C:534:PRO:HA	1:C:537:HIS:CD2	2.54	0.42
1:D:30:GLN:O	1:D:31:PHE:C	2.56	0.42
1:D:111:PRO:HD3	1:D:554:ARG:HH21	1.85	0.42
1:D:574:LEU:HA	1:D:930:ARG:HH12	1.85	0.42
1:E:374:LEU:HA	1:E:377:ILE:HD12	2.02	0.42
1:E:403:ASN:HB3	1:E:520:LEU:HD12	2.01	0.42
1:E:713:TYR:HD1	1:E:714:LEU:HG	1.84	0.42
1:G:848:TYR:C	1:G:850:LEU:H	2.21	0.42
1:H:90:ASP:HA	1:H:576:PRO:HB2	2.02	0.42
1:H:135:TRP:HA	1:H:310:ASN:HB3	2.02	0.42
1:J:41:LEU:HD22	1:J:44:LYS:HE3	2.02	0.42
1:J:742:GLU:OE2	4:Q:22:TRP:HB3	2.20	0.42
1:K:469:TRP:CD1	1:K:516:CYS:SG	3.08	0.42
1:L:684:LYS:HE2	1:L:912:GLU:HB2	2.01	0.42
4:S:55:THR:O	4:S:55:THR:HG23	2.19	0.42
5:V:51:ARG:HA	5:V:54:ILE:HG12	2.02	0.42
5:V:85:ALA:HA	5:V:86:PRO:HD2	1.88	0.42
1:A:414:CYS:HA	1:C:462:ILE:HB	2.02	0.42
1:A:715:ASN:HD22	1:A:869:THR:H	1.67	0.42
1:B:124:LEU:HD13	1:C:466:ALA:HB3	2.02	0.42
1:B:173:PRO:HB3	1:C:839:GLY:HA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:ALA:HA	1:B:293:ILE:HG22	2.02	0.42
1:B:350:GLY:HA2	1:B:579:TYR:HA	2.01	0.42
1:D:557:PRO:HD2	1:E:860:THR:HG22	2.00	0.42
1:E:651:ASN:HD22	1:E:917:TYR:HE1	1.67	0.42
1:F:769:GLN:HE21	1:F:871:TRP:HD1	1.67	0.42
1:G:925:VAL:H	1:G:941:LEU:CB	2.32	0.42
1:I:353:SER:O	1:I:353:SER:OG	2.36	0.42
1:J:792:TYR:HA	1:J:796:ARG:HB2	2.02	0.42
1:K:101:PHE:O	1:K:561:GLN:HG2	2.20	0.42
1:L:365:ASN:HB3	1:L:368:LEU:HG	2.02	0.42
1:L:922:VAL:HG12	1:L:923:PHE:N	2.34	0.42
1:B:799:GLN:HA	1:B:800:PRO:HD3	1.95	0.41
1:B:922:VAL:CG1	1:B:942:ARG:O	2.67	0.41
1:C:215:GLU:C	1:C:216:ILE:HG13	2.40	0.41
1:E:488:SER:HB2	1:E:489:PRO:CD	2.35	0.41
1:G:552:ASN:ND2	1:H:520:LEU:O	2.53	0.41
1:G:763:LYS:HA	1:G:766:PHE:HB3	2.01	0.41
1:H:380:ARG:HB3	1:H:391:VAL:HG22	2.01	0.41
2:N:230:VAL:HG13	2:N:286:LEU:HD21	2.02	0.41
2:N:457:ILE:O	2:N:457:ILE:CG1	2.40	0.41
4:P:27:GLN:O	4:P:42:ALA:HB3	2.20	0.41
1:A:235:GLY:HA3	1:A:298:THR:HB	2.02	0.41
1:A:566:PHE:HD2	1:A:568:ALA:H	1.68	0.41
1:A:811:TYR:HB3	1:A:814:TYR:H	1.85	0.41
1:B:684:LYS:HB2	1:B:687:GLU:HG2	2.02	0.41
1:B:693:SER:HB3	2:N:84:TYR:HB3	2.02	0.41
1:C:228:THR:HA	1:C:229:PRO:HD3	1.86	0.41
1:D:336:LEU:HD23	1:D:562:VAL:HG11	2.02	0.41
1:D:850:LEU:HG	1:F:554:ARG:N	2.34	0.41
1:E:179:ILE:HG23	1:E:183:GLY:O	2.20	0.41
1:G:650:ALA:CB	1:G:922:VAL:HG21	2.50	0.41
1:H:172:ALA:HB1	1:H:219:ALA:HB1	2.02	0.41
1:H:412:ASN:HB2	1:H:462:ILE:O	2.19	0.41
1:I:179:ILE:HG23	1:I:218:HIS:CB	2.50	0.41
1:I:682:ARG:HA	1:I:915:LEU:O	2.20	0.41
1:J:303:MET:HA	1:J:304:PRO:HD3	1.89	0.41
1:J:939:VAL:HG13	1:J:951:THR:HG21	2.01	0.41
1:K:375:ASP:HB3	1:K:790:ARG:HH11	1.84	0.41
1:K:684:LYS:HB2	1:K:687:GLU:HG2	2.02	0.41
1:L:85:THR:HG23	1:L:580:THR:HG22	2.02	0.41
4:P:124:LEU:O	4:P:128:VAL:HG13	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:783:ILE:HA	1:A:784:PRO:HD3	1.84	0.41
1:B:679:ALA:HA	1:B:871:TRP:O	2.21	0.41
1:C:17:GLY:O	1:C:48:PRO:HB2	2.20	0.41
1:C:672:TRP:HA	1:C:944:PRO:HA	2.02	0.41
1:C:771:LEU:HD22	1:C:778:TYR:CE1	2.54	0.41
1:D:720:LYS:HG2	1:D:744:GLU:HG2	2.01	0.41
1:E:907:VAL:HG11	1:E:916:LEU:HD21	2.01	0.41
1:F:536:ASN:HA	1:F:596:SER:O	2.20	0.41
1:G:336:LEU:HD12	1:G:562:VAL:HG21	2.02	0.41
1:G:414:CYS:HB2	1:H:414:CYS:HB3	1.98	0.41
1:G:517:TYR:CE1	1:G:846:PHE:CD2	3.08	0.41
1:H:789:ASP:OD2	1:H:796:ARG:HG2	2.20	0.41
1:J:94:LEU:HD22	1:J:574:LEU:HD12	2.03	0.41
1:K:706:PRO:HA	1:K:711:THR:HB	2.03	0.41
1:K:841:ALA:O	1:K:842:TYR:HD1	2.02	0.41
5:U:189:ILE:H	5:U:189:ILE:HG13	1.57	0.41
1:C:678:TRP:H	1:C:873:ILE:HG23	1.84	0.41
1:C:867:ASP:O	1:C:868:ARG:HG3	2.19	0.41
1:D:338:TYR:HE2	1:D:694:GLY:HA2	1.86	0.41
1:E:222:ARG:HB2	1:F:842:TYR:OH	2.20	0.41
1:E:340:ASN:O	1:E:341:SER:CB	2.68	0.41
1:G:127:LYS:HG3	1:H:411:PRO:HB3	2.01	0.41
1:G:573:LEU:H	1:G:641:GLN:HE22	1.68	0.41
1:H:517:TYR:CA	1:H:520:LEU:CD1	2.93	0.41
1:H:778:TYR:OH	1:H:878:ASN:ND2	2.53	0.41
1:I:186:ILE:HD12	1:I:194:LYS:HB3	2.01	0.41
1:K:179:ILE:HG13	1:K:218:HIS:HB3	2.03	0.41
1:L:134:GLU:HB3	1:L:168:VAL:HG12	2.01	0.41
1:L:386:MET:HB2	1:L:561:GLN:HB3	2.01	0.41
1:L:486:LYS:HG2	1:L:509:VAL:HB	2.01	0.41
1:L:707:TYR:HA	1:L:712:PHE:HE2	1.86	0.41
4:S:18:ARG:CG	4:S:19:MET:N	2.83	0.41
1:B:338:TYR:CE2	1:B:584:ASN:HB3	2.56	0.41
1:E:110:GLY:H	1:E:554:ARG:HD3	1.86	0.41
1:E:553:GLY:HA3	1:F:850:LEU:HD23	2.01	0.41
1:F:80:TYR:HB2	1:F:587:LYS:HE3	2.02	0.41
1:G:173:PRO:HB3	1:H:840:GLN:HB2	2.03	0.41
1:G:353:SER:HB3	1:G:355:LEU:HD12	2.03	0.41
1:H:715:ASN:HB2	1:H:866:CYS:O	2.20	0.41
1:I:811:TYR:HB2	1:I:814:TYR:HB2	2.02	0.41
1:J:415:PHE:HA	1:L:837:ARG:NH2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:549:LEU:HG	1:K:801:MET:HG3	2.02	0.41
1:J:783:ILE:HD11	1:L:377:ILE:HG23	2.02	0.41
1:K:104:ARG:HD2	1:K:612:SER:HB3	2.03	0.41
1:L:350:GLY:HA2	1:L:579:TYR:HA	2.01	0.41
1:L:656:ILE:O	1:L:656:ILE:HG22	2.20	0.41
1:L:677:GLY:H	1:L:921:GLU:HB2	1.84	0.41
4:Q:114:LEU:HD13	4:Q:114:LEU:N	2.34	0.41
1:A:266:PHE:HB3	1:A:285:VAL:HG23	2.02	0.41
1:A:323:ARG:NH1	1:A:475:SER:O	2.54	0.41
1:A:736:ARG:HB2	1:C:64:LEU:HB3	2.03	0.41
1:D:168:VAL:HG21	1:D:312:ARG:HG3	2.03	0.41
1:D:205:GLN:HG3	1:D:206:ILE:HG13	2.02	0.41
1:D:460:MET:HB2	1:E:415:PHE:O	2.21	0.41
1:D:669:SER:HA	1:D:900:ALA:HA	2.01	0.41
1:E:188:VAL:HG12	1:E:193:PRO:HA	2.03	0.41
1:E:684:LYS:HG3	1:E:914:THR:HG22	2.02	0.41
1:E:687:GLU:O	1:E:699:TYR:HE1	2.04	0.41
1:F:15:ILE:HG23	1:F:48:PRO:HA	2.02	0.41
1:F:93:VAL:HB	1:F:573:LEU:HD11	2.01	0.41
1:F:113:PHE:HD1	1:F:327:ILE:HG22	1.86	0.41
1:G:44:LYS:CG	1:H:571:ASN:O	2.67	0.41
1:G:189:GLU:HB3	1:G:190:GLY:H	1.74	0.41
1:G:523:ARG:N	1:I:548:MET:HB2	2.35	0.41
1:G:621:PRO:CD	1:H:878:ASN:OD1	2.67	0.41
1:I:795:PHE:CG	1:I:795:PHE:O	2.73	0.41
1:I:831:TYR:CD1	1:I:831:TYR:C	2.71	0.41
1:K:121:TYR:OH	1:L:849:PRO:HG3	2.21	0.41
1:K:330:ARG:HD3	1:K:708:LEU:HD13	2.01	0.41
3:M:217:PRO:HB2	3:M:218:THR:H	1.05	0.41
4:Q:8:GLY:HA2	4:R:28:ASN:HB2	2.02	0.41
4:S:131:LEU:HD23	4:S:131:LEU:HA	1.82	0.41
1:A:757:ALA:HB1	1:C:560:ILE:HA	2.01	0.41
1:B:347:VAL:HG13	1:B:582:GLU:HB2	2.02	0.41
1:B:680:PHE:HB3	1:B:918:VAL:HG13	2.02	0.41
1:B:796:ARG:O	1:B:797:ASN:C	2.59	0.41
1:C:218:HIS:ND1	1:C:282:PRO:O	2.54	0.41
1:C:224:LEU:HD23	1:C:289:GLU:HB2	2.02	0.41
1:C:320:MET:HA	1:C:321:PRO:HD3	1.97	0.41
1:E:824:ASN:HD22	1:E:847:PRO:HG2	1.86	0.41
1:F:574:LEU:HD23	1:F:930:ARG:HH22	1.86	0.41
1:G:39:PHE:HB3	1:G:44:LYS:NZ	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:113:PHE:HE2	1:H:554:ARG:HG3	1.86	0.41
1:H:492:VAL:CG1	1:H:506:LYS:CD	2.96	0.41
1:I:13:MET:HB3	1:I:15:ILE:HG13	2.01	0.41
1:I:672:TRP:HE1	1:I:899:HIS:H	1.68	0.41
1:J:477:ILE:HA	1:J:480:TYR:HB3	2.02	0.41
1:J:625:ASN:HB3	3:M:287:GLN:HG3	2.02	0.41
1:J:655:PRO:HB3	1:J:914:THR:O	2.20	0.41
1:A:200:PHE:O	1:A:200:PHE:CG	2.71	0.41
1:A:251:VAL:CG1	1:A:252:LYS:N	2.82	0.41
1:B:943:THR:O	1:B:945:PHE:N	2.53	0.41
1:C:180:THR:OG1	1:C:181:LYS:N	2.54	0.41
1:D:837:ARG:HH11	1:E:459:ALA:H	1.69	0.41
1:E:696:ASP:HA	1:E:697:PRO:HD3	1.92	0.41
1:E:731:TRP:HB3	1:E:732:PRO:CD	2.46	0.41
1:I:680:PHE:CB	1:I:918:VAL:HG22	2.50	0.41
1:I:757:ALA:HB2	1:I:766:PHE:HZ	1.86	0.41
1:I:885:LEU:HB3	1:I:890:GLN:HG3	2.03	0.41
1:J:184:ILE:CG2	1:J:220:ALA:HB2	2.49	0.41
1:J:211:TRP:CH2	1:K:318:GLN:HG3	2.55	0.41
1:J:267:PHE:HB3	1:L:426:LEU:HB3	2.03	0.41
1:J:362:GLN:HB3	4:P:21:PRO:HG2	2.03	0.41
1:K:679:ALA:HB3	1:K:919:LEU:HB2	2.02	0.41
1:L:311:SER:H	1:L:314:LEU:HD12	1.85	0.41
1:L:524:TRP:HA	1:L:801:MET:HB2	2.02	0.41
3:M:67:ASN:HA	3:M:68:PRO:HD3	1.92	0.41
1:B:101:PHE:HB2	1:B:562:VAL:HG23	2.03	0.41
1:B:113:PHE:HB3	1:B:327:ILE:HD12	2.02	0.41
1:B:173:PRO:HD2	1:B:220:ALA:O	2.21	0.41
1:B:247:GLN:HB2	1:B:291:VAL:HG11	2.03	0.41
1:C:174:TYR:CB	1:C:220:ALA:H	2.34	0.41
1:C:563:PRO:HG2	1:C:565:LYS:HE3	2.03	0.41
1:C:597:LEU:O	1:C:597:LEU:CG	2.58	0.41
1:D:197:ASP:C	1:D:199:THR:H	2.24	0.41
1:D:230:MET:HE2	1:D:314:LEU:HB3	1.06	0.41
1:D:543:LEU:HD11	1:D:594:GLN:HE21	1.86	0.41
1:D:559:HIS:O	1:E:757:ALA:HA	2.21	0.41
1:D:792:TYR:HB3	1:D:868:ARG:HG2	2.03	0.41
1:E:221:GLY:O	1:E:286:LEU:HA	2.20	0.41
1:E:561:GLN:HB2	1:F:756:VAL:CG1	2.51	0.41
1:F:223:VAL:HB	1:F:286:LEU:HD13	2.02	0.41
1:G:826:SER:HB2	1:I:205:GLN:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:839:GLY:O	1:I:173:PRO:HG2	2.21	0.41
1:H:307:LYS:HD2	1:H:311:SER:HB3	2.03	0.41
1:H:554:ARG:H	1:I:850:LEU:HG	1.86	0.41
1:H:724:THR:HG22	1:H:725:PHE:N	2.36	0.41
1:H:827:GLY:HA3	1:H:839:GLY:HA3	2.03	0.41
1:H:867:ASP:OD1	1:H:867:ASP:N	2.54	0.41
1:I:473:LEU:HG	1:I:477:ILE:HD12	2.03	0.41
1:J:756:VAL:HG11	1:J:766:PHE:CD1	2.55	0.41
1:K:110:GLY:H	1:K:554:ARG:HG3	1.86	0.41
1:L:53:THR:O	1:L:57:THR:CG2	2.68	0.41
1:L:797:ASN:CG	1:L:867:ASP:O	2.59	0.41
1:C:922:VAL:CG1	1:C:942:ARG:HB3	2.51	0.41
1:C:942:ARG:HB2	1:C:945:PHE:HB3	2.03	0.41
1:D:922:VAL:HG23	1:D:923:PHE:H	1.86	0.41
1:E:84:PHE:HB2	1:E:581:TYR:HB3	2.02	0.41
1:E:905:PHE:HE2	1:E:916:LEU:HD22	1.85	0.41
1:H:570:LYS:O	1:H:643:PHE:CZ	2.73	0.41
1:H:748:SER:CA	4:R:50:GLU:OE2	2.63	0.41
1:I:267:PHE:CZ	1:I:284:VAL:HB	2.56	0.41
1:I:334:ILE:HA	1:I:565:LYS:HZ1	1.86	0.41
1:I:486:LYS:HG2	1:I:507:ARG:HB3	2.03	0.41
1:I:730:SER:O	1:I:733:GLY:N	2.44	0.41
1:K:373:LEU:HD11	1:K:645:ASP:HA	2.03	0.41
1:K:519:ASN:HB3	1:K:522:ALA:HB3	2.02	0.41
2:N:62:PRO:O	2:N:63:LEU:HD23	2.21	0.41
2:N:456:GLN:HG3	2:N:540:ARG:HH12	1.85	0.41
4:S:10:ILE:CG2	4:S:11:VAL:N	2.83	0.41
4:S:26:ARG:HA	4:S:26:ARG:HD2	1.53	0.41
1:C:172:ALA:HB3	1:C:284:VAL:HG12	2.01	0.40
1:C:208:GLU:HB3	1:C:209:SER:H	1.77	0.40
1:D:844:ALA:HB3	1:F:121:TYR:HB3	2.02	0.40
1:E:428:LYS:HA	1:F:267:PHE:HB3	2.03	0.40
1:E:794:PHE:HB3	1:E:798:PHE:HE2	1.85	0.40
1:F:494:ILE:HD11	1:F:503:TYR:HA	2.02	0.40
1:G:130:PRO:HA	1:G:232:PRO:HA	2.02	0.40
1:G:849:PRO:C	1:G:851:ILE:N	2.75	0.40
1:H:300:ILE:CG2	1:H:318:GLN:O	2.67	0.40
1:H:338:TYR:HB3	1:H:583:TRP:HZ3	1.86	0.40
1:J:267:PHE:HE1	1:J:286:LEU:HD12	1.86	0.40
1:J:850:LEU:HD13	1:J:856:VAL:H	1.86	0.40
1:K:767:LEU:O	1:K:771:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:20:PRO:HA	4:S:21:PRO:HD3	1.56	0.40
5:V:32:ASN:O	5:V:35:SER:OG	2.39	0.40
5:V:90:VAL:HA	5:V:168:ILE:HG23	2.03	0.40
1:B:203:GLU:HA	1:B:204:PRO:HD2	1.93	0.40
1:B:941:LEU:HB2	1:B:948:GLY:HA2	2.02	0.40
1:B:945:PHE:HA	2:N:101:TYR:CZ	2.56	0.40
1:D:373:LEU:HD11	1:D:646:TYR:H	1.84	0.40
1:D:878:ASN:C	1:D:880:MET:H	2.25	0.40
1:G:414:CYS:HB3	1:I:414:CYS:HB2	1.92	0.40
1:H:211:TRP:HB2	1:I:836:MET:SD	2.61	0.40
1:H:325:ASN:HD22	1:H:599:ASN:HB3	1.85	0.40
1:H:577:GLY:HA3	1:H:934:GLY:HA2	2.03	0.40
1:I:486:LYS:HG3	1:I:509:VAL:HB	2.03	0.40
1:I:497:ASN:HA	1:I:498:PRO:HD3	1.89	0.40
1:I:659:ASN:O	1:I:659:ASN:CG	2.59	0.40
1:I:732:PRO:C	1:I:734:ASN:H	2.25	0.40
1:K:837:ARG:HE	1:L:415:PHE:HD2	1.69	0.40
3:M:196:LEU:H	3:M:196:LEU:HG	1.54	0.40
4:R:108:ASP:HA	4:R:111:THR:HG23	2.04	0.40
1:C:100:TYR:CD1	1:C:561:GLN:HB2	2.56	0.40
1:D:745:ILE:HG12	1:D:765:TRP:NE1	2.37	0.40
1:E:179:ILE:HG12	1:E:184:ILE:HG22	2.04	0.40
1:F:414:CYS:HB2	1:F:460:MET:HB2	2.04	0.40
1:F:731:TRP:HB3	1:F:732:PRO:HD3	2.04	0.40
1:F:732:PRO:C	1:F:734:ASN:H	2.25	0.40
1:G:524:TRP:CB	1:G:803:ARG:HB3	2.52	0.40
1:H:517:TYR:HB2	1:H:847:PRO:HG3	2.02	0.40
1:H:575:LEU:HD12	1:H:930:ARG:HB2	2.02	0.40
1:I:172:ALA:HB1	1:I:284:VAL:HG11	2.03	0.40
1:I:932:HIS:HB3	1:I:935:VAL:H	1.87	0.40
1:J:179:ILE:HG22	1:J:185:GLN:H	1.87	0.40
1:J:654:TYR:CZ	1:J:665:ILE:HG12	2.57	0.40
1:J:684:LYS:HA	1:J:914:THR:HA	2.02	0.40
1:K:656:ILE:HD11	1:K:916:LEU:HB2	2.03	0.40
1:K:842:TYR:HA	1:K:843:PRO:HD3	1.95	0.40
1:A:339:TYR:HD1	1:A:367:GLU:HG2	1.86	0.40
1:B:121:TYR:HD2	1:C:844:ALA:HB3	1.86	0.40
1:C:174:TYR:HD2	1:C:176:GLY:H	1.69	0.40
1:C:922:VAL:HG12	1:C:942:ARG:HB3	2.03	0.40
1:D:365:ASN:H	1:D:651:ASN:ND2	2.20	0.40
1:D:517:TYR:HA	1:D:520:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:LEU:HD13	1:F:44:LYS:HD2	2.04	0.40
1:G:13:MET:HG2	1:H:927:ARG:HB2	2.04	0.40
1:G:334:ILE:HD11	1:G:367:GLU:HB3	2.02	0.40
1:G:758:GLN:NE2	1:I:549:LEU:HD11	2.29	0.40
1:H:103:ILE:HG12	1:H:613:ILE:HG12	2.04	0.40
1:H:696:ASP:HA	1:H:697:PRO:HD2	2.00	0.40
1:I:238:ALA:HA	1:I:293:ILE:HG22	2.02	0.40
1:I:441:LYS:HG3	1:I:442:ASP:N	2.29	0.40
1:I:678:TRP:HB2	1:I:873:ILE:HG23	2.02	0.40
1:I:922:VAL:CG1	1:I:942:ARG:HB3	2.52	0.40
1:J:696:ASP:HB3	1:J:698:TYR:HD1	1.86	0.40
1:K:564:GLN:HE21	1:K:569:ILE:HD13	1.86	0.40
1:L:53:THR:O	1:L:57:THR:HG23	2.22	0.40
1:L:372:LEU:HD12	1:L:647:LEU:HB2	2.03	0.40
2:N:448:PRO:HA	2:N:529:LEU:HB2	2.04	0.40
1:A:429:VAL:CG1	1:B:266:PHE:HD1	2.30	0.40
1:B:20:ALA:HB2	1:B:48:PRO:HD2	2.03	0.40
1:B:245:GLY:H	1:C:821:HIS:HB3	1.86	0.40
1:B:331:ASP:HA	1:B:388:ASN:HB2	2.03	0.40
1:B:440:GLU:HG3	1:B:441:LYS:H	1.87	0.40
1:B:575:LEU:HB2	1:B:930:ARG:HD3	2.03	0.40
1:C:732:PRO:HB3	1:C:736:ARG:HB2	2.03	0.40
1:E:486:LYS:HB3	1:E:507:ARG:HB3	2.02	0.40
1:F:655:PRO:HB3	1:F:915:LEU:HD23	2.03	0.40
1:G:325:ASN:HA	1:G:596:SER:HB3	2.04	0.40
1:I:10:TRP:HB2	1:I:16:SER:HB3	2.04	0.40
1:K:908:ASP:HB3	1:K:909:PRO:HD2	2.02	0.40
2:N:120:GLY:HA2	2:N:531:LEU:HG	2.04	0.40
3:M:54:LEU:HA	3:M:57:ILE:HD12	2.04	0.40
4:S:34:ILE:N	4:S:34:ILE:HD12	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	913/949 (96%)	749 (82%)	143 (16%)	21 (2%)	5	30
1	B	907/949 (96%)	748 (82%)	130 (14%)	29 (3%)	3	25
1	C	917/949 (97%)	745 (81%)	149 (16%)	23 (2%)	4	28
1	D	913/949 (96%)	766 (84%)	124 (14%)	23 (2%)	4	28
1	E	906/949 (96%)	752 (83%)	138 (15%)	16 (2%)	7	34
1	F	910/949 (96%)	748 (82%)	144 (16%)	18 (2%)	6	32
1	G	905/949 (95%)	738 (82%)	144 (16%)	23 (2%)	4	28
1	H	909/949 (96%)	747 (82%)	140 (15%)	22 (2%)	5	29
1	I	913/949 (96%)	756 (83%)	125 (14%)	32 (4%)	3	23
1	J	911/949 (96%)	751 (82%)	149 (16%)	11 (1%)	11	40
1	K	900/949 (95%)	735 (82%)	145 (16%)	20 (2%)	5	30
1	L	914/949 (96%)	759 (83%)	131 (14%)	24 (3%)	4	28
2	N	443/571 (78%)	352 (80%)	77 (17%)	14 (3%)	3	25
3	M	301/585 (52%)	263 (87%)	32 (11%)	6 (2%)	6	32
4	P	91/140 (65%)	74 (81%)	15 (16%)	2 (2%)	5	30
4	Q	131/140 (94%)	113 (86%)	15 (12%)	3 (2%)	5	30
4	R	94/140 (67%)	81 (86%)	11 (12%)	2 (2%)	5	32
4	S	92/140 (66%)	73 (79%)	15 (16%)	4 (4%)	2	20
5	U	167/227 (74%)	141 (84%)	22 (13%)	4 (2%)	5	29
5	V	170/227 (75%)	138 (81%)	26 (15%)	6 (4%)	3	23
6	W	22/24 (92%)	19 (86%)	2 (9%)	1 (4%)	2	19
All	All	12429/13582 (92%)	10248 (82%)	1877 (15%)	304 (2%)	5	29

All (304) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	A	271	GLU
1	A	388	ASN
1	B	417	LEU
1	B	570	LYS
1	B	791	MET
1	B	796	ARG

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Mol	Chain	Res	Type
1	B	943	THR
1	C	8	PRO
1	C	732	PRO
1	D	173	PRO
1	D	296	PRO
1	D	501	TYR
1	D	731	TRP
1	E	518	ILE
1	E	824	ASN
1	E	829	VAL
1	F	296	PRO
1	F	879	PHE
1	G	77	ALA
1	G	173	PRO
1	G	189	GLU
1	G	296	PRO
1	G	932	HIS
1	H	173	PRO
1	H	296	PRO
1	H	726	ASP
1	H	824	ASN
1	I	624	HIS
1	I	729	VAL
1	J	173	PRO
1	J	180	THR
1	J	270	THR
1	K	201	GLN
1	K	330	ARG
1	L	447	SER
1	L	668	PRO
1	L	704	SER
1	L	732	PRO
2	N	139	PHE
2	N	201	VAL
2	N	381	PRO
3	M	217	PRO
4	P	40	LEU
4	S	37	ARG
1	A	99	THR
1	A	234	TYR
1	A	269	THR
1	A	296	PRO

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Mol	Chain	Res	Type
1	A	694	GLY
1	A	752	GLU
1	B	234	TYR
1	B	296	PRO
1	B	512	GLY
1	B	641	GLN
1	B	735	ASP
1	C	312	ARG
1	C	405	GLY
1	C	605	GLY
1	C	668	PRO
1	C	837	ARG
1	C	871	TRP
1	D	879	PHE
1	D	933	ARG
1	E	668	PRO
1	F	234	TYR
1	F	333	PHE
1	F	343	GLY
1	F	794	PHE
1	G	279	ASN
1	G	850	LEU
1	G	940	TYR
1	H	61	SER
1	H	515	ASP
1	H	532	VAL
1	I	350	GLY
1	I	671	ASN
1	I	731	TRP
1	I	837	ARG
1	J	213	GLU
1	J	816	GLN
1	J	837	ARG
1	K	24	LEU
1	K	392	ASP
1	K	490	SER
1	K	735	ASP
1	K	795	PHE
1	L	257	LYS
1	L	438	GLY
1	L	509	VAL
1	L	603	VAL

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Mol	Chain	Res	Type
2	N	273	ILE
2	N	457	ILE
4	Q	28	ASN
4	Q	35	ASP
4	Q	68	ALA
4	S	49	TYR
5	V	32	ASN
5	V	90	VAL
1	A	501	TYR
1	A	846	PHE
1	B	173	PRO
1	B	201	GLN
1	B	253	GLN
1	B	440	GLU
1	B	772	ALA
1	B	797	ASN
1	C	296	PRO
1	C	417	LEU
1	D	824	ASN
1	D	837	ARG
1	D	948	GLY
1	F	825	ASN
1	G	390	ALA
1	G	554	ARG
1	G	882	MET
1	G	939	VAL
1	H	596	SER
1	I	52	PRO
1	I	89	GLY
1	I	181	LYS
1	I	296	PRO
1	I	316	GLY
1	I	760	ASN
1	I	786	SER
1	I	791	MET
1	I	868	ARG
1	K	173	PRO
1	K	331	ASP
1	K	343	GLY
1	K	378	GLY
1	K	891	ASN
1	L	19	ASP

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Mol	Chain	Res	Type
1	L	269	THR
1	L	296	PRO
1	L	337	MET
1	L	943	THR
3	M	176	PRO
3	M	177	GLN
4	R	111	THR
4	S	127	GLN
1	A	20	ALA
1	A	173	PRO
1	A	853	LYS
1	B	202	PRO
1	B	386	MET
1	B	909	PRO
1	C	254	GLN
1	C	576	PRO
1	D	132	PRO
1	D	198	LYS
1	D	563	PRO
1	E	181	LYS
1	E	234	TYR
1	E	442	ASP
1	E	488	SER
1	F	513	LEU
1	F	697	PRO
1	G	202	PRO
1	G	824	ASN
1	G	849	PRO
1	H	727	SER
1	H	785	GLU
1	H	896	ASN
1	I	132	PRO
1	I	340	ASN
1	I	780	GLY
1	I	943	THR
1	J	388	ASN
1	J	791	MET
1	K	668	PRO
1	K	805	VAL
1	L	195	TYR
1	L	462	ILE
1	L	536	ASN

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Mol	Chain	Res	Type
2	N	270	GLY
2	N	500	PRO
5	U	84	PRO
1	A	59	ASP
1	B	418	GLY
1	B	436	GLU
1	C	251	VAL
1	C	302	TYR
1	C	450	ASN
1	C	729	VAL
1	D	48	PRO
1	D	122	ASN
1	D	748	SER
1	E	198	LYS
1	F	89	GLY
1	F	749	VAL
1	G	115	PRO
1	G	201	GLN
1	G	852	GLY
1	H	42	ASN
1	H	304	PRO
1	H	605	GLY
1	H	619	PHE
1	I	234	TYR
1	I	356	ASN
1	I	664	PRO
1	I	916	LEU
1	K	807	ASP
1	K	843	PRO
1	L	312	ARG
2	N	275	TYR
2	N	509	PRO
2	N	545	ASP
4	P	34	ILE
4	R	15	LEU
5	U	185	THR
5	V	28	SER
5	V	209	PRO
1	A	834	PRO
1	B	489	PRO
1	B	557	PRO
1	B	605	GLY

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Mol	Chain	Res	Type
1	C	335	GLY
1	E	576	PRO
1	E	756	VAL
1	E	944	PRO
1	F	324	PRO
1	F	664	PRO
1	F	834	PRO
1	G	19	ASP
1	G	358	VAL
1	G	443	ALA
1	G	664	PRO
1	H	190	GLY
1	H	377	ILE
1	H	698	TYR
1	H	740	PRO
1	H	777	GLY
1	I	253	GLN
1	I	563	PRO
1	I	697	PRO
1	I	703	GLY
1	J	749	VAL
1	J	824	ASN
1	L	418	GLY
1	L	825	ASN
6	W	12	PRO
1	A	304	PRO
1	B	843	PRO
1	D	777	GLY
1	D	829	VAL
1	D	849	PRO
1	E	512	GLY
1	H	438	GLY
1	I	47	ASN
1	J	56	VAL
1	K	697	PRO
1	K	909	PRO
2	N	415	PRO
2	N	418	GLY
2	N	559	GLY
3	M	155	PRO
4	S	31	GLY
5	U	204	PRO

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Mol	Chain	Res	Type
1	A	115	PRO
1	C	26	PRO
1	C	692	GLY
1	C	777	GLY
1	D	70	PRO
1	D	694	GLY
1	E	202	PRO
1	F	563	PRO
1	I	438	GLY
1	I	657	PRO
5	V	64	THR
1	B	753	GLY
1	C	183	GLY
1	C	657	PRO
1	F	934	GLY
1	K	207	GLY
2	N	228	PRO
1	A	56	VAL
1	A	207	GLY
1	B	533	ASN
1	B	731	TRP
1	C	805	VAL
1	D	177	ILE
1	D	482	PRO
1	D	494	ILE
1	E	418	GLY
1	E	732	PRO
1	F	316	GLY
1	F	481	LEU
1	G	692	GLY
1	H	256	GLY
1	L	71	VAL
1	L	256	GLY
1	L	749	VAL
1	L	777	GLY
1	L	930	ARG
3	M	213	GLY
5	U	184	GLY
5	V	208	TYR
1	A	240	PRO
1	B	692	GLY
1	I	418	GLY

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Mol	Chain	Res	Type
1	I	849	PRO
1	K	689	PRO
3	M	68	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	799/827 (97%)	740 (93%)	59 (7%)	11	35
1	B	794/827 (96%)	739 (93%)	55 (7%)	13	37
1	C	803/827 (97%)	741 (92%)	62 (8%)	10	34
1	D	799/827 (97%)	738 (92%)	61 (8%)	11	34
1	E	795/827 (96%)	721 (91%)	74 (9%)	7	27
1	F	797/827 (96%)	729 (92%)	68 (8%)	8	31
1	G	794/827 (96%)	722 (91%)	72 (9%)	7	28
1	H	796/827 (96%)	736 (92%)	60 (8%)	11	35
1	I	799/827 (97%)	709 (89%)	90 (11%)	4	21
1	J	797/827 (96%)	724 (91%)	73 (9%)	7	28
1	K	789/827 (95%)	711 (90%)	78 (10%)	6	25
1	L	800/827 (97%)	732 (92%)	68 (8%)	8	31
2	N	404/489 (83%)	366 (91%)	38 (9%)	7	27
3	M	253/500 (51%)	235 (93%)	18 (7%)	12	36
4	P	84/112 (75%)	74 (88%)	10 (12%)	4	20
4	Q	106/112 (95%)	96 (91%)	10 (9%)	7	27
4	R	84/112 (75%)	67 (80%)	17 (20%)	1	6
4	S	84/112 (75%)	69 (82%)	15 (18%)	1	9
5	U	144/186 (77%)	132 (92%)	12 (8%)	9	32
5	V	145/186 (78%)	130 (90%)	15 (10%)	6	23
All	All	10866/11733 (93%)	9911 (91%)	955 (9%)	8	30

All (955) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	49	THR
1	A	50	VAL
1	A	53	THR
1	A	55	ASP
1	A	58	THR
1	A	60	ARG
1	A	68	PHE
1	A	94	LEU
1	A	103	ILE
1	A	116	TYR
1	A	121	TYR
1	A	184	ILE
1	A	201	GLN
1	A	230	MET
1	A	258	LEU
1	A	270	THR
1	A	299	HIS
1	A	356	ASN
1	A	360	ASP
1	A	375	ASP
1	A	413	TYR
1	A	420	VAL
1	A	425	THR
1	A	427	THR
1	A	476	ASN
1	A	477	ILE
1	A	479	LEU
1	A	514	VAL
1	A	546	ARG
1	A	549	LEU
1	A	556	VAL
1	A	562	VAL
1	A	566	PHE
1	A	622	MET
1	A	626	THR
1	A	672	TRP
1	A	683	LEU
1	A	691	LEU
1	A	700	THR
1	A	717	THR
1	A	725	PHE

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Mol	Chain	Res	Type
1	A	735	ASP
1	A	749	VAL
1	A	762	THR
1	A	764	ASP
1	A	778	TYR
1	A	805	VAL
1	A	807	ASP
1	A	817	VAL
1	A	819	ILE
1	A	825	ASN
1	A	850	LEU
1	A	851	ILE
1	A	860	THR
1	A	873	ILE
1	A	875	PHE
1	A	927	ARG
1	A	941	LEU
1	B	24	LEU
1	B	36	GLU
1	B	76	THR
1	B	85	THR
1	B	247	GLN
1	B	266	PHE
1	B	269	THR
1	B	280	LEU
1	B	281	THR
1	B	305	THR
1	B	326	TYR
1	B	344	ASN
1	B	345	MET
1	B	359	VAL
1	B	360	ASP
1	B	361	LEU
1	B	367	GLU
1	B	373	LEU
1	B	381	THR
1	B	439	TRP
1	B	442	ASP
1	B	470	ARG
1	B	474	TYR
1	B	508	VAL
1	B	529	MET

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Mol	Chain	Res	Type
1	B	531	ASN
1	B	546	ARG
1	B	556	VAL
1	B	560	ILE
1	B	604	ASP
1	B	624	HIS
1	B	675	PHE
1	B	681	THR
1	B	701	TYR
1	B	709	ASP
1	B	717	THR
1	B	726	ASP
1	B	737	LEU
1	B	756	VAL
1	B	759	CYS
1	B	798	PHE
1	B	825	ASN
1	B	835	THR
1	B	850	LEU
1	B	866	CYS
1	B	886	THR
1	B	902	ASP
1	B	926	VAL
1	B	930	ARG
1	B	933	ARG
1	B	939	VAL
1	B	941	LEU
1	B	943	THR
1	B	944	PRO
1	B	945	PHE
1	C	15	ILE
1	C	35	THR
1	C	39	PHE
1	C	46	ARG
1	C	64	LEU
1	C	68	PHE
1	C	75	ASP
1	C	95	ASP
1	C	103	ILE
1	C	107	LEU
1	C	177	ILE
1	C	180	THR

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Mol	Chain	Res	Type
1	C	184	ILE
1	C	195	TYR
1	C	241	THR
1	C	242	ASN
1	C	243	GLU
1	C	250	LEU
1	C	254	GLN
1	C	284	VAL
1	C	285	VAL
1	C	295	THR
1	C	305	THR
1	C	306	ILE
1	C	332	ASN
1	C	359	VAL
1	C	381	THR
1	C	391	VAL
1	C	440	GLU
1	C	464	LEU
1	C	518	ILE
1	C	549	LEU
1	C	564	GLN
1	C	569	ILE
1	C	613	ILE
1	C	620	PHE
1	C	624	HIS
1	C	626	THR
1	C	633	MET
1	C	636	ASN
1	C	663	VAL
1	C	672	TRP
1	C	675	PHE
1	C	682	ARG
1	C	724	THR
1	C	747	ARG
1	C	766	PHE
1	C	767	LEU
1	C	770	MET
1	C	774	TYR
1	C	798	PHE
1	C	805	VAL
1	C	824	ASN
1	C	825	ASN

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Mol	Chain	Res	Type
1	C	831	TYR
1	C	867	ASP
1	C	868	ARG
1	C	869	THR
1	C	885	LEU
1	C	886	THR
1	C	893	LEU
1	C	943	THR
1	D	28	LEU
1	D	30	GLN
1	D	35	THR
1	D	41	LEU
1	D	53	THR
1	D	59	ASP
1	D	64	LEU
1	D	73	ARG
1	D	79	SER
1	D	84	PHE
1	D	95	ASP
1	D	107	LEU
1	D	119	THR
1	D	121	TYR
1	D	169	PHE
1	D	180	THR
1	D	184	ILE
1	D	223	VAL
1	D	227	THR
1	D	231	LYS
1	D	268	SER
1	D	269	THR
1	D	299	HIS
1	D	366	THR
1	D	368	LEU
1	D	414	CYS
1	D	439	TRP
1	D	442	ASP
1	D	469	TRP
1	D	473	LEU
1	D	494	ILE
1	D	514	VAL
1	D	527	ASP
1	D	548	MET

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Mol	Chain	Res	Type
1	D	562	VAL
1	D	597	LEU
1	D	613	ILE
1	D	620	PHE
1	D	645	ASP
1	D	651	ASN
1	D	656	ILE
1	D	678	TRP
1	D	681	THR
1	D	683	LEU
1	D	700	THR
1	D	717	THR
1	D	723	ILE
1	D	724	THR
1	D	737	LEU
1	D	739	THR
1	D	749	VAL
1	D	758	GLN
1	D	762	THR
1	D	765	TRP
1	D	804	GLN
1	D	805	VAL
1	D	813	ASP
1	D	815	GLN
1	D	837	ARG
1	D	848	TYR
1	D	901	LEU
1	E	11	SER
1	E	31	PHE
1	E	76	THR
1	E	90	ASP
1	E	112	THR
1	E	133	CYS
1	E	174	TYR
1	E	186	ILE
1	E	200	PHE
1	E	201	GLN
1	E	241	THR
1	E	264	MET
1	E	269	THR
1	E	280	LEU
1	E	291	VAL

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Mol	Chain	Res	Type
1	E	306	ILE
1	E	331	ASP
1	E	336	LEU
1	E	337	MET
1	E	341	SER
1	E	342	THR
1	E	348	LEU
1	E	359	VAL
1	E	372	LEU
1	E	375	ASP
1	E	392	ASP
1	E	430	LYS
1	E	432	LYS
1	E	439	TRP
1	E	441	LYS
1	E	457	ASN
1	E	458	PHE
1	E	468	LEU
1	E	469	TRP
1	E	480	TYR
1	E	481	LEU
1	E	500	THR
1	E	508	VAL
1	E	509	VAL
1	E	514	VAL
1	E	526	LEU
1	E	538	HIS
1	E	549	LEU
1	E	559	HIS
1	E	560	ILE
1	E	562	VAL
1	E	569	ILE
1	E	572	LEU
1	E	574	LEU
1	E	582	GLU
1	E	611	ASP
1	E	624	HIS
1	E	643	PHE
1	E	656	ILE
1	E	675	PHE
1	E	681	THR
1	E	695	TYR

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Mol	Chain	Res	Type
1	E	708	LEU
1	E	724	THR
1	E	727	SER
1	E	728	SER
1	E	730	SER
1	E	742	GLU
1	E	760	ASN
1	E	770	MET
1	E	778	TYR
1	E	871	TRP
1	E	892	LEU
1	E	893	LEU
1	E	908	ASP
1	E	910	MET
1	E	930	ARG
1	E	941	LEU
1	E	943	THR
1	F	9	GLN
1	F	35	THR
1	F	36	GLU
1	F	76	THR
1	F	88	VAL
1	F	107	LEU
1	F	121	TYR
1	F	133	CYS
1	F	181	LYS
1	F	184	ILE
1	F	228	THR
1	F	237	TYR
1	F	273	THR
1	F	280	LEU
1	F	291	VAL
1	F	292	ASP
1	F	295	THR
1	F	305	THR
1	F	306	ILE
1	F	327	ILE
1	F	334	ILE
1	F	337	MET
1	F	360	ASP
1	F	362	GLN
1	F	366	THR

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Mol	Chain	Res	Type
1	F	368	LEU
1	F	383	TYR
1	F	391	VAL
1	F	399	ARG
1	F	425	THR
1	F	429	VAL
1	F	450	ASN
1	F	454	VAL
1	F	464	LEU
1	F	471	ASN
1	F	476	ASN
1	F	509	VAL
1	F	569	ILE
1	F	604	ASP
1	F	613	ILE
1	F	626	THR
1	F	634	LEU
1	F	653	LEU
1	F	681	THR
1	F	683	LEU
1	F	684	LYS
1	F	688	THR
1	F	690	SER
1	F	711	THR
1	F	724	THR
1	F	741	ASN
1	F	756	VAL
1	F	767	LEU
1	F	797	ASN
1	F	829	VAL
1	F	835	THR
1	F	848	TYR
1	F	866	CYS
1	F	867	ASP
1	F	875	PHE
1	F	882	MET
1	F	899	HIS
1	F	908	ASP
1	F	923	PHE
1	F	925	VAL
1	F	929	HIS
1	F	941	LEU

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Mol	Chain	Res	Type
1	F	943	THR
1	G	56	VAL
1	G	78	TYR
1	G	90	ASP
1	G	116	TYR
1	G	119	THR
1	G	122	ASN
1	G	124	LEU
1	G	166	THR
1	G	178	ASN
1	G	188	VAL
1	G	204	PRO
1	G	212	TYR
1	G	241	THR
1	G	249	ILE
1	G	266	PHE
1	G	269	THR
1	G	366	THR
1	G	373	LEU
1	G	375	ASP
1	G	399	ARG
1	G	413	TYR
1	G	417	LEU
1	G	422	ASN
1	G	444	THR
1	G	453	ARG
1	G	477	ILE
1	G	485	LEU
1	G	500	THR
1	G	549	LEU
1	G	556	VAL
1	G	560	ILE
1	G	561	GLN
1	G	614	CYS
1	G	635	ARG
1	G	637	ASP
1	G	639	ASN
1	G	651	ASN
1	G	671	ASN
1	G	685	THR
1	G	691	LEU
1	G	693	SER

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Mol	Chain	Res	Type
1	G	696	ASP
1	G	711	THR
1	G	717	THR
1	G	720	LYS
1	G	726	ASP
1	G	737	LEU
1	G	756	VAL
1	G	758	GLN
1	G	762	THR
1	G	763	LYS
1	G	765	TRP
1	G	774	TYR
1	G	776	ILE
1	G	805	VAL
1	G	806	VAL
1	G	808	ASP
1	G	813	ASP
1	G	814	TYR
1	G	829	VAL
1	G	832	LEU
1	G	835	THR
1	G	848	TYR
1	G	867	ASP
1	G	886	THR
1	G	887	ASP
1	G	891	ASN
1	G	896	ASN
1	G	923	PHE
1	G	939	VAL
1	G	940	TYR
1	G	943	THR
1	H	10	TRP
1	H	13	MET
1	H	35	THR
1	H	46	ARG
1	H	59	ASP
1	H	76	THR
1	H	184	ILE
1	H	199	THR
1	H	236	SER
1	H	270	THR
1	H	276	ASN

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Mol	Chain	Res	Type
1	H	295	THR
1	H	298	THR
1	H	300	ILE
1	H	302	TYR
1	H	336	LEU
1	H	348	LEU
1	H	356	ASN
1	H	381	THR
1	H	391	VAL
1	H	406	THR
1	H	439	TRP
1	H	458	PHE
1	H	469	TRP
1	H	483	ASP
1	H	487	TYR
1	H	492	VAL
1	H	505	ASN
1	H	509	VAL
1	H	516	CYS
1	H	517	TYR
1	H	518	ILE
1	H	520	LEU
1	H	559	HIS
1	H	560	ILE
1	H	569	ILE
1	H	570	LYS
1	H	574	LEU
1	H	587	LYS
1	H	589	VAL
1	H	592	VAL
1	H	600	ASP
1	H	602	ARG
1	H	651	ASN
1	H	665	ILE
1	H	675	PHE
1	H	682	ARG
1	H	725	PHE
1	H	726	ASP
1	H	738	LEU
1	H	766	PHE
1	H	778	TYR
1	H	835	THR

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Mol	Chain	Res	Type
1	H	836	MET
1	H	840	GLN
1	H	871	TRP
1	H	890	GLN
1	H	905	PHE
1	H	916	LEU
1	H	929	HIS
1	I	12	TYR
1	I	19	ASP
1	I	25	SER
1	I	45	PHE
1	I	46	ARG
1	I	50	VAL
1	I	54	HIS
1	I	63	ARG
1	I	66	LEU
1	I	69	ILE
1	I	75	ASP
1	I	121	TYR
1	I	173	PRO
1	I	174	TYR
1	I	180	THR
1	I	185	GLN
1	I	224	LEU
1	I	226	LYS
1	I	280	LEU
1	I	289	GLU
1	I	292	ASP
1	I	313	GLU
1	I	334	ILE
1	I	336	LEU
1	I	340	ASN
1	I	351	GLN
1	I	353	SER
1	I	354	GLN
1	I	370	TYR
1	I	381	THR
1	I	395	ASP
1	I	413	TYR
1	I	415	PHE
1	I	444	THR
1	I	448	ASP

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Mol	Chain	Res	Type
1	I	452	ILE
1	I	471	ASN
1	I	485	LEU
1	I	487	TYR
1	I	508	VAL
1	I	549	LEU
1	I	554	ARG
1	I	565	LYS
1	I	584	ASN
1	I	602	ARG
1	I	604	ASP
1	I	624	HIS
1	I	626	THR
1	I	643	PHE
1	I	651	ASN
1	I	653	LEU
1	I	661	THR
1	I	662	ASN
1	I	683	LEU
1	I	685	THR
1	I	686	LYS
1	I	691	LEU
1	I	701	TYR
1	I	724	THR
1	I	728	SER
1	I	737	LEU
1	I	739	THR
1	I	749	VAL
1	I	756	VAL
1	I	766	PHE
1	I	774	TYR
1	I	776	ILE
1	I	784	PRO
1	I	789	ASP
1	I	808	ASP
1	I	809	THR
1	I	820	LEU
1	I	822	GLN
1	I	824	ASN
1	I	825	ASN
1	I	828	PHE
1	I	829	VAL

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Mol	Chain	Res	Type
1	I	831	TYR
1	I	832	LEU
1	I	836	MET
1	I	869	THR
1	I	893	LEU
1	I	908	ASP
1	I	912	GLU
1	I	917	TYR
1	I	920	PHE
1	I	941	LEU
1	I	942	ARG
1	I	943	THR
1	I	945	PHE
1	J	11	SER
1	J	37	THR
1	J	38	TYR
1	J	45	PHE
1	J	46	ARG
1	J	58	THR
1	J	84	PHE
1	J	112	THR
1	J	119	THR
1	J	121	TYR
1	J	131	ASN
1	J	174	TYR
1	J	227	THR
1	J	230	MET
1	J	241	THR
1	J	264	MET
1	J	299	HIS
1	J	305	THR
1	J	360	ASP
1	J	370	TYR
1	J	372	LEU
1	J	384	PHE
1	J	392	ASP
1	J	413	TYR
1	J	414	CYS
1	J	415	PHE
1	J	430	LYS
1	J	442	ASP
1	J	469	TRP

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Mol	Chain	Res	Type
1	J	481	LEU
1	J	485	LEU
1	J	494	ILE
1	J	505	ASN
1	J	508	VAL
1	J	532	VAL
1	J	547	SER
1	J	554	ARG
1	J	570	LYS
1	J	573	LEU
1	J	581	TYR
1	J	590	ASN
1	J	618	THR
1	J	626	THR
1	J	653	LEU
1	J	665	ILE
1	J	675	PHE
1	J	681	THR
1	J	695	TYR
1	J	700	THR
1	J	724	THR
1	J	735	ASP
1	J	765	TRP
1	J	773	ASN
1	J	797	ASN
1	J	809	THR
1	J	816	GLN
1	J	828	PHE
1	J	832	LEU
1	J	837	ARG
1	J	848	TYR
1	J	882	MET
1	J	890	GLN
1	J	893	LEU
1	J	896	ASN
1	J	904	THR
1	J	907	VAL
1	J	917	TYR
1	J	918	VAL
1	J	919	LEU
1	J	922	VAL
1	J	926	VAL

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Mol	Chain	Res	Type
1	J	932	HIS
1	J	941	LEU
1	K	31	PHE
1	K	76	THR
1	K	85	THR
1	K	94	LEU
1	K	167	HIS
1	K	178	ASN
1	K	184	ILE
1	K	253	GLN
1	K	257	LYS
1	K	268	SER
1	K	280	LEU
1	K	281	THR
1	K	305	THR
1	K	329	PHE
1	K	339	TYR
1	K	340	ASN
1	K	342	THR
1	K	348	LEU
1	K	351	GLN
1	K	361	LEU
1	K	362	GLN
1	K	364	ARG
1	K	368	LEU
1	K	372	LEU
1	K	375	ASP
1	K	383	TYR
1	K	384	PHE
1	K	386	MET
1	K	399	ARG
1	K	416	PRO
1	K	417	LEU
1	K	420	VAL
1	K	442	ASP
1	K	450	ASN
1	K	460	MET
1	K	461	GLU
1	K	472	PHE
1	K	473	LEU
1	K	488	SER
1	K	490	SER

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Mol	Chain	Res	Type
1	K	495	SER
1	K	496	ASP
1	K	504	MET
1	K	520	LEU
1	K	529	MET
1	K	530	ASP
1	K	546	ARG
1	K	549	LEU
1	K	561	GLN
1	K	566	PHE
1	K	570	LYS
1	K	594	GLN
1	K	624	HIS
1	K	656	ILE
1	K	675	PHE
1	K	681	THR
1	K	688	THR
1	K	700	THR
1	K	738	LEU
1	K	748	SER
1	K	749	VAL
1	K	750	ASP
1	K	776	ILE
1	K	801	MET
1	K	805	VAL
1	K	835	THR
1	K	837	ARG
1	K	842	TYR
1	K	848	TYR
1	K	850	LEU
1	K	851	ILE
1	K	866	CYS
1	K	875	PHE
1	K	877	SER
1	K	907	VAL
1	K	916	LEU
1	K	922	VAL
1	K	939	VAL
1	L	35	THR
1	L	37	THR
1	L	60	ARG
1	L	96	MET

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Mol	Chain	Res	Type
1	L	102	ASP
1	L	121	TYR
1	L	184	ILE
1	L	188	VAL
1	L	228	THR
1	L	291	VAL
1	L	292	ASP
1	L	295	THR
1	L	300	ILE
1	L	306	ILE
1	L	355	LEU
1	L	360	ASP
1	L	368	LEU
1	L	373	LEU
1	L	381	THR
1	L	382	ARG
1	L	384	PHE
1	L	391	VAL
1	L	413	TYR
1	L	422	ASN
1	L	429	VAL
1	L	442	ASP
1	L	444	THR
1	L	445	GLU
1	L	454	VAL
1	L	546	ARG
1	L	549	LEU
1	L	550	LEU
1	L	584	ASN
1	L	626	THR
1	L	634	LEU
1	L	639	ASN
1	L	656	ILE
1	L	671	ASN
1	L	672	TRP
1	L	681	THR
1	L	683	LEU
1	L	684	LYS
1	L	685	THR
1	L	707	TYR
1	L	708	LEU
1	L	761	MET

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Mol	Chain	Res	Type
1	L	762	THR
1	L	769	GLN
1	L	774	TYR
1	L	783	ILE
1	L	805	VAL
1	L	806	VAL
1	L	823	HIS
1	L	824	ASN
1	L	825	ASN
1	L	865	LEU
1	L	866	CYS
1	L	867	ASP
1	L	869	THR
1	L	885	LEU
1	L	893	LEU
1	L	902	ASP
1	L	929	HIS
1	L	936	ILE
1	L	941	LEU
1	L	943	THR
1	L	951	THR
1	L	952	THR
2	N	49	THR
2	N	52	ARG
2	N	69	VAL
2	N	84	TYR
2	N	91	PHE
2	N	101	TYR
2	N	135	ASN
2	N	140	THR
2	N	147	VAL
2	N	178	THR
2	N	201	VAL
2	N	211	ASP
2	N	217	LEU
2	N	230	VAL
2	N	251	THR
2	N	262	ARG
2	N	283	ILE
2	N	287	LEU
2	N	397	ASP
2	N	417	THR

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Mol	Chain	Res	Type
2	N	430	VAL
2	N	439	TRP
2	N	447	ASP
2	N	450	THR
2	N	454	THR
2	N	456	GLN
2	N	468	LEU
2	N	474	SER
2	N	477	ASN
2	N	478	ASP
2	N	482	TYR
2	N	499	PHE
2	N	504	ILE
2	N	505	LEU
2	N	529	LEU
2	N	545	ASP
2	N	553	TYR
2	N	554	VAL
3	M	11	ARG
3	M	27	TRP
3	M	35	MET
3	M	95	TYR
3	M	98	LEU
3	M	101	ARG
3	M	114	LEU
3	M	147	LEU
3	M	154	VAL
3	M	155	PRO
3	M	196	LEU
3	M	197	GLN
3	M	198	THR
3	M	218	THR
3	M	231	ASN
3	M	250	ARG
3	M	289	ASP
3	M	297	LEU
4	P	3	THR
4	P	6	PHE
4	P	11	VAL
4	P	15	LEU
4	P	25	VAL
4	P	35	ASP

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Mol	Chain	Res	Type
4	P	39	VAL
4	P	45	THR
4	P	46	THR
4	P	98	ASP
4	Q	5	SER
4	Q	6	PHE
4	Q	10	ILE
4	Q	26	ARG
4	Q	55	THR
4	Q	57	LEU
4	Q	100	LEU
4	Q	110	LEU
4	Q	112	ARG
4	Q	114	LEU
4	R	5	SER
4	R	6	PHE
4	R	7	ASP
4	R	10	ILE
4	R	17	THR
4	R	19	MET
4	R	45	THR
4	R	46	THR
4	R	51	THR
4	R	97	ASP
4	R	104	LEU
4	R	107	LEU
4	R	108	ASP
4	R	110	LEU
4	R	114	LEU
4	R	117	VAL
4	R	121	LEU
4	S	10	ILE
4	S	11	VAL
4	S	13	SER
4	S	15	LEU
4	S	16	THR
4	S	26	ARG
4	S	29	VAL
4	S	30	MET
4	S	33	SER
4	S	34	ILE
4	S	35	ASP

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Mol	Chain	Res	Type
4	S	57	LEU
4	S	98	ASP
4	S	114	LEU
4	S	121	LEU
5	U	7	THR
5	U	15	PRO
5	U	31	ILE
5	U	90	VAL
5	U	91	LEU
5	U	168	ILE
5	U	173	THR
5	U	189	ILE
5	U	193	VAL
5	U	198	PHE
5	U	210	ASP
5	U	217	ASP
5	V	10	MET
5	V	12	SER
5	V	26	ASP
5	V	28	SER
5	V	29	THR
5	V	32	ASN
5	V	40	MET
5	V	51	ARG
5	V	52	ASN
5	V	62	THR
5	V	101	MET
5	V	166	GLN
5	V	168	ILE
5	V	209	PRO
5	V	213	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (228) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	322	ASN
1	A	340	ASN
1	A	351	GLN
1	A	356	ASN
1	A	365	ASN
1	A	403	ASN
1	A	412	ASN

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Mol	Chain	Res	Type
1	A	536	ASN
1	A	540	ASN
1	A	561	GLN
1	A	584	ASN
1	A	636	ASN
1	A	644	ASN
1	A	715	ASN
1	A	755	ASN
1	A	779	GLN
1	A	797	ASN
1	A	840	GLN
1	B	14	HIS
1	B	171	GLN
1	B	210	GLN
1	B	253	GLN
1	B	317	GLN
1	B	322	ASN
1	B	332	ASN
1	B	340	ASN
1	B	437	ASN
1	B	457	ASN
1	B	505	ASN
1	B	533	ASN
1	B	594	GLN
1	B	636	ASN
1	B	651	ASN
1	B	773	ASN
1	C	42	ASN
1	C	62	GLN
1	C	122	ASN
1	C	299	HIS
1	C	318	GLN
1	C	332	ASN
1	C	365	ASN
1	C	371	GLN
1	C	540	ASN
1	C	564	GLN
1	C	624	HIS
1	C	639	ASN
1	C	641	GLN
1	C	659	ASN
1	C	662	ASN

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Mol	Chain	Res	Type
1	C	734	ASN
1	D	14	HIS
1	D	310	ASN
1	D	332	ASN
1	D	389	GLN
1	D	564	GLN
1	D	651	ASN
1	D	715	ASN
1	D	758	GLN
1	D	821	HIS
1	E	122	ASN
1	E	253	GLN
1	E	322	ASN
1	E	332	ASN
1	E	354	GLN
1	E	437	ASN
1	E	465	ASN
1	E	471	ASN
1	E	561	GLN
1	E	639	ASN
1	E	779	GLN
1	E	797	ASN
1	E	824	ASN
1	E	840	GLN
1	E	878	ASN
1	F	122	ASN
1	F	244	ASN
1	F	340	ASN
1	F	362	GLN
1	F	365	ASN
1	F	371	GLN
1	F	412	ASN
1	F	422	ASN
1	F	450	ASN
1	F	538	HIS
1	F	540	ASN
1	F	559	HIS
1	F	584	ASN
1	F	594	GLN
1	F	651	ASN
1	F	769	GLN
1	F	773	ASN

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Mol	Chain	Res	Type
1	F	775	ASN
1	F	779	GLN
1	F	797	ASN
1	F	823	HIS
1	F	932	HIS
1	G	30	GLN
1	G	171	GLN
1	G	299	HIS
1	G	317	GLN
1	G	322	ASN
1	G	465	ASN
1	G	471	ASN
1	G	538	HIS
1	G	540	ASN
1	G	552	ASN
1	G	559	HIS
1	G	561	GLN
1	G	564	GLN
1	G	571	ASN
1	G	584	ASN
1	G	639	ASN
1	G	641	GLN
1	G	662	ASN
1	G	775	ASN
1	G	804	GLN
1	G	821	HIS
1	G	891	ASN
1	G	896	ASN
1	H	14	HIS
1	H	205	GLN
1	H	242	ASN
1	H	299	HIS
1	H	325	ASN
1	H	354	GLN
1	H	365	ASN
1	H	389	GLN
1	H	412	ASN
1	H	422	ASN
1	H	465	ASN
1	H	561	GLN
1	H	590	ASN
1	H	639	ASN

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Mol	Chain	Res	Type
1	H	651	ASN
1	H	671	ASN
1	H	758	GLN
1	H	775	ASN
1	H	779	GLN
1	H	861	GLN
1	H	890	GLN
1	I	14	HIS
1	I	122	ASN
1	I	244	ASN
1	I	317	GLN
1	I	325	ASN
1	I	388	ASN
1	I	404	HIS
1	I	463	ASN
1	I	467	ASN
1	I	471	ASN
1	I	571	ASN
1	I	590	ASN
1	I	639	ASN
1	I	644	ASN
1	I	662	ASN
1	I	734	ASN
1	I	755	ASN
1	I	779	GLN
1	I	822	GLN
1	I	845	ASN
1	J	131	ASN
1	J	201	GLN
1	J	265	GLN
1	J	310	ASN
1	J	317	GLN
1	J	322	ASN
1	J	351	GLN
1	J	536	ASN
1	J	571	ASN
1	J	599	ASN
1	J	639	ASN
1	J	641	GLN
1	J	651	ASN
1	J	734	ASN
1	J	741	ASN

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Mol	Chain	Res	Type
1	J	758	GLN
1	J	797	ASN
1	J	822	GLN
1	K	122	ASN
1	K	244	ASN
1	K	351	GLN
1	K	362	GLN
1	K	471	ASN
1	K	533	ASN
1	K	536	ASN
1	K	540	ASN
1	K	564	GLN
1	K	599	ASN
1	K	641	GLN
1	K	734	ASN
1	K	755	ASN
1	K	760	ASN
1	K	779	GLN
1	K	797	ASN
1	K	799	GLN
1	K	823	HIS
1	L	322	ASN
1	L	332	ASN
1	L	365	ASN
1	L	412	ASN
1	L	465	ASN
1	L	471	ASN
1	L	594	GLN
1	L	671	ASN
1	L	758	GLN
1	L	822	GLN
1	L	824	ASN
2	N	83	ASN
2	N	86	ASN
2	N	90	ASN
2	N	174	ASN
2	N	185	ASN
2	N	191	HIS
2	N	282	ASN
2	N	488	GLN
2	N	497	ASN
3	M	17	GLN

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Mol	Chain	Res	Type
3	M	144	ASN
3	M	190	GLN
3	M	200	ASN
3	M	203	GLN
3	M	231	ASN
4	S	28	ASN
5	U	52	ASN
5	V	25	GLN
5	V	32	ASN
5	V	107	GLN
5	V	187	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	917/949 (96%)	0.29	61 (6%) 25 24	26, 98, 169, 207	0
1	B	911/949 (95%)	0.24	48 (5%) 33 29	34, 97, 163, 200	0
1	C	921/949 (97%)	0.34	72 (7%) 20 20	33, 99, 169, 221	0
1	D	917/949 (96%)	0.22	50 (5%) 32 28	30, 98, 160, 203	0
1	E	910/949 (95%)	0.20	42 (4%) 38 33	33, 95, 163, 224	0
1	F	914/949 (96%)	0.31	63 (6%) 24 23	19, 95, 161, 228	0
1	G	909/949 (95%)	0.24	54 (5%) 29 27	25, 95, 163, 206	0
1	H	913/949 (96%)	0.18	37 (4%) 42 35	29, 94, 159, 208	0
1	I	917/949 (96%)	0.19	47 (5%) 34 30	24, 94, 162, 212	0
1	J	915/949 (96%)	0.42	71 (7%) 20 20	26, 95, 164, 209	0
1	K	904/949 (95%)	0.20	48 (5%) 33 29	27, 95, 162, 217	0
1	L	918/949 (96%)	0.25	56 (6%) 28 26	28, 95, 163, 220	0
2	N	447/571 (78%)	0.20	21 (4%) 37 32	50, 122, 189, 226	0
3	M	303/585 (51%)	0.18	11 (3%) 46 38	16, 110, 183, 229	0
4	P	95/140 (67%)	0.51	8 (8%) 18 18	53, 112, 193, 219	0
4	Q	133/140 (95%)	0.51	16 (12%) 10 14	49, 129, 199, 234	0
4	R	98/140 (70%)	0.34	8 (8%) 19 19	39, 117, 209, 229	0
4	S	96/140 (68%)	0.03	6 (6%) 27 25	48, 112, 187, 220	0
5	U	171/227 (75%)	0.36	12 (7%) 24 23	41, 104, 168, 191	0
5	V	174/227 (76%)	0.19	10 (5%) 30 27	44, 103, 161, 220	0
6	W	24/24 (100%)	0.56	3 (12%) 9 13	47, 137, 201, 219	0
All	All	12507/13582 (92%)	0.26	744 (5%) 29 27	16, 98, 167, 234	0

All (744) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	491	ASN	9.5
1	C	578	SER	7.9
1	B	191	GLN	7.6
1	I	275	GLY	7.2
1	B	215	GLU	7.1
4	P	53	SER	6.9
4	Q	74	GLY	6.5
1	C	448	ASP	6.4
5	V	110	GLY	6.4
1	K	215	GLU	6.3
1	E	351	GLN	6.3
1	J	367	GLU	6.2
1	J	214	THR	6.0
1	L	488	SER	5.9
1	G	214	THR	5.6
3	M	246	GLY	5.5
1	J	607	SER	5.5
1	A	290	ASP	5.4
1	K	465	ASN	5.4
1	I	170	GLY	5.3
4	R	36	GLY	5.1
1	F	242	ASN	5.1
1	L	213	GLU	5.1
1	C	261	GLN	5.0
1	K	637	ASP	5.0
1	G	385	SER	5.0
1	C	406	THR	4.9
1	J	692	GLY	4.9
1	B	214	THR	4.9
1	K	491	ASN	4.8
2	N	569	ARG	4.7
1	G	170	GLY	4.7
3	M	52	ASN	4.7
1	F	189	GLU	4.6
1	F	650	ALA	4.6
1	G	874	PRO	4.6
4	R	35	ASP	4.6
1	D	290	ASP	4.6
6	W	23	SER	4.5
4	Q	134	SER	4.5
1	L	775	ASN	4.4
4	Q	72	ALA	4.4
1	A	727	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	H	488	SER	4.4
1	L	49	THR	4.4
1	J	605	GLY	4.4
1	D	21	SER	4.4
1	E	444	THR	4.4
1	K	213	GLU	4.3
1	A	551	GLY	4.3
1	G	215	GLU	4.3
1	L	308	GLU	4.3
4	P	137	PRO	4.2
1	C	254	GLN	4.2
1	I	274	ALA	4.2
1	K	644	ASN	4.2
1	B	35	THR	4.2
1	I	527	ASP	4.2
1	K	271	GLU	4.2
1	L	931	PRO	4.2
1	B	425	THR	4.1
1	C	255	ASN	4.1
1	F	707	TYR	4.1
1	I	848	TYR	4.1
1	C	897	SER	4.1
1	E	405	GLY	4.1
1	B	21	SER	4.1
1	I	826	SER	4.1
4	Q	4	ASN	4.1
1	H	911	ASP	4.1
1	J	883	GLY	4.1
1	C	424	GLU	4.1
1	L	650	ALA	4.1
1	B	818	GLY	4.1
1	I	16	SER	4.1
1	E	409	GLU	4.1
1	J	606	ALA	4.1
1	H	671	ASN	4.0
1	A	215	GLU	4.0
1	A	489	PRO	4.0
1	G	134	GLU	4.0
1	F	809	THR	4.0
1	B	490	SER	4.0
1	A	729	VAL	3.9
1	I	99	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	773	ASN	3.9
1	D	46	ARG	3.9
4	P	126	GLN	3.9
1	D	692	GLY	3.9
1	A	213	GLU	3.9
1	K	323	ARG	3.9
1	D	499	ASN	3.9
1	I	539	ARG	3.9
1	H	531	ASN	3.8
2	N	537	GLY	3.8
4	R	89	ALA	3.8
1	J	502	ASP	3.8
1	D	435	GLN	3.8
1	D	250	LEU	3.8
1	C	908	ASP	3.8
1	K	772	ALA	3.8
1	G	235	GLY	3.8
1	J	444	THR	3.8
1	L	934	GLY	3.7
1	C	483	ASP	3.7
1	A	37	THR	3.7
1	L	849	PRO	3.7
1	A	16	SER	3.7
1	I	606	ALA	3.7
4	Q	83	SER	3.7
1	K	412	ASN	3.7
4	P	106	GLN	3.7
1	B	598	GLY	3.7
1	I	775	ASN	3.7
1	C	16	SER	3.7
1	B	49	THR	3.7
1	L	489	PRO	3.7
1	G	189	GLU	3.7
1	F	812	LYS	3.6
1	I	890	GLN	3.6
1	A	214	THR	3.6
1	G	290	ASP	3.6
1	J	881	SER	3.6
1	L	808	ASP	3.6
1	L	89	GLY	3.5
6	W	22	THR	3.5
1	A	134	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
4	Q	5	SER	3.5
1	I	276	ASN	3.5
1	J	488	SER	3.5
1	E	385	SER	3.5
1	L	17	GLY	3.5
1	D	25	SER	3.4
1	F	530	ASP	3.4
1	I	483	ASP	3.4
1	J	594	GLN	3.4
1	L	496	ASP	3.4
1	J	674	ALA	3.4
1	J	543	LEU	3.4
1	J	175	SER	3.4
1	F	403	ASN	3.4
1	K	42	ASN	3.4
1	J	261	GLN	3.4
1	J	252	LYS	3.4
1	H	519	ASN	3.4
4	Q	127	GLN	3.4
1	E	197	ASP	3.4
5	U	55	LEU	3.4
1	D	809	THR	3.4
1	G	673	ALA	3.3
1	H	854	THR	3.3
1	C	308	GLU	3.3
1	E	214	THR	3.3
1	A	536	ASN	3.3
1	C	465	ASN	3.3
1	E	671	ASN	3.3
1	E	8	PRO	3.3
2	N	538	VAL	3.3
1	D	582	GLU	3.3
1	L	666	SER	3.3
1	C	617	ALA	3.3
1	H	857	ASP	3.3
2	N	59	GLU	3.3
1	E	580	THR	3.3
1	K	523	ARG	3.3
1	F	254	GLN	3.3
1	J	279	ASN	3.3
1	A	811	TYR	3.3
1	I	273	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	607	SER	3.3
4	Q	84	PRO	3.3
1	C	42	ASN	3.3
1	K	34	ALA	3.3
1	F	407	GLU	3.3
1	G	604	ASP	3.3
1	J	37	THR	3.2
1	A	482	PRO	3.2
1	C	565	LYS	3.2
4	P	37	ARG	3.2
1	A	207	GLY	3.2
1	E	404	HIS	3.2
1	G	493	LYS	3.2
1	J	620	PHE	3.2
1	L	443	ALA	3.2
5	U	166	GLN	3.2
1	I	182	GLU	3.2
1	J	407	GLU	3.2
1	C	444	THR	3.2
1	E	54	HIS	3.2
4	P	35	ASP	3.2
1	D	891	ASN	3.2
1	J	775	ASN	3.2
1	G	706	PRO	3.2
1	H	202	PRO	3.2
1	K	480	TYR	3.1
1	H	515	ASP	3.1
1	E	607	SER	3.1
1	F	612	SER	3.1
1	F	22	GLU	3.1
1	F	128	GLY	3.1
1	F	733	GLY	3.1
2	N	50	GLY	3.1
1	E	555	TYR	3.1
1	L	99	THR	3.1
1	A	376	SER	3.1
1	I	308	GLU	3.1
1	C	292	ASP	3.1
1	C	395	ASP	3.1
1	F	611	ASP	3.1
1	B	779	GLN	3.1
1	L	768	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	219	ALA	3.1
1	D	500	THR	3.1
1	J	693	SER	3.1
1	F	196	ALA	3.1
1	A	55	ASP	3.1
4	Q	82	LEU	3.1
1	C	950	ALA	3.1
1	J	773	ASN	3.1
1	L	517	TYR	3.1
1	J	932	HIS	3.1
1	A	108	ASP	3.0
1	F	898	ALA	3.0
1	C	94	LEU	3.0
1	L	392	ASP	3.0
1	D	215	GLU	3.0
1	F	137	GLU	3.0
2	N	136	GLU	3.0
2	N	269	GLU	3.0
1	G	447	SER	3.0
1	B	177	ILE	3.0
1	A	325	ASN	3.0
1	I	88	VAL	3.0
1	G	256	GLY	3.0
1	I	521	GLY	3.0
1	E	531	ASN	3.0
1	G	479	LEU	3.0
1	A	471	ASN	3.0
1	L	823	HIS	3.0
1	H	553	GLY	3.0
1	J	60	ARG	3.0
1	J	213	GLU	3.0
1	D	766	PHE	3.0
1	H	422	ASN	3.0
1	C	99	THR	3.0
1	C	214	THR	3.0
1	G	49	THR	3.0
1	L	852	GLY	3.0
1	L	948	GLY	3.0
1	F	792	TYR	2.9
1	K	857	ASP	2.9
1	J	369	SER	2.9
5	U	73	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	499	ASN	2.9
1	H	214	THR	2.9
1	K	854	THR	2.9
1	A	271	GLU	2.9
1	D	289	GLU	2.9
1	F	897	SER	2.9
1	D	673	ALA	2.9
1	F	334	ILE	2.9
1	J	816	GLN	2.9
1	C	175	SER	2.9
1	G	367	GLU	2.9
1	E	308	GLU	2.9
1	F	328	ALA	2.9
2	N	392	ASN	2.9
1	D	87	ALA	2.8
1	L	692	GLY	2.8
1	D	292	ASP	2.8
1	H	391	VAL	2.8
1	E	85	THR	2.8
1	J	809	THR	2.8
1	K	773	ASN	2.8
4	P	112	ARG	2.8
1	J	462	ILE	2.8
1	G	190	GLY	2.8
1	J	309	GLY	2.8
1	L	170	GLY	2.8
1	J	108	ASP	2.8
5	U	221	ASP	2.8
1	A	488	SER	2.8
1	B	376	SER	2.8
1	L	353	SER	2.8
4	S	53	SER	2.8
1	B	340	ASN	2.8
1	H	191	GLN	2.8
1	L	182	GLU	2.8
4	Q	58	GLU	2.8
1	G	216	ILE	2.8
1	F	94	LEU	2.8
3	M	230	PRO	2.8
1	D	170	GLY	2.8
5	V	219	VAL	2.8
1	B	778	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	493	LYS	2.8
1	H	30	GLN	2.8
1	K	655	PRO	2.8
1	H	701	TYR	2.8
1	B	72	ASP	2.8
1	G	448	ASP	2.8
1	E	858	SER	2.8
1	G	265	GLN	2.8
1	A	540	ASN	2.8
1	I	277	GLY	2.8
1	C	515	ASP	2.8
1	A	119	THR	2.8
1	F	854	THR	2.8
1	D	781	PHE	2.8
1	I	785	GLU	2.8
1	A	949	ASN	2.8
1	F	531	ASN	2.8
1	K	43	ASN	2.8
2	N	103	PRO	2.8
1	B	554	ARG	2.8
1	G	299	HIS	2.7
5	V	82	GLU	2.7
1	F	47	ASN	2.7
2	N	130	ASN	2.7
1	C	256	GLY	2.7
1	A	49	THR	2.7
1	F	60	ARG	2.7
1	C	690	SER	2.7
1	F	488	SER	2.7
4	R	53	SER	2.7
1	C	242	ASN	2.7
1	F	659	ASN	2.7
1	F	429	VAL	2.7
1	L	750	ASP	2.7
6	W	5	ALA	2.7
1	C	187	GLY	2.7
1	G	79	SER	2.7
1	I	450	ASN	2.7
1	K	915	LEU	2.7
1	I	812	LYS	2.7
1	E	799	GLN	2.7
1	L	215	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
3	M	216	ALA	2.7
5	U	64	THR	2.7
1	H	813	ASP	2.7
1	D	896	ASN	2.7
1	A	696	ASP	2.7
1	E	252	LYS	2.7
1	E	719	LYS	2.7
1	I	599	ASN	2.7
1	J	325	ASN	2.7
4	S	37	ARG	2.7
1	G	466	ALA	2.6
1	J	459	ALA	2.6
1	C	215	GLU	2.6
1	J	277	GLY	2.6
1	C	496	ASP	2.6
5	V	26	ASP	2.6
1	H	467	ASN	2.6
1	E	275	GLY	2.6
1	H	335	GLY	2.6
2	N	528	THR	2.6
1	F	676	ARG	2.6
1	D	59	ASP	2.6
1	G	496	ASP	2.6
1	G	764	ASP	2.6
1	K	578	SER	2.6
1	I	617	ALA	2.6
1	E	110	GLY	2.6
1	J	205	GLN	2.6
1	A	787	TYR	2.6
1	I	108	ASP	2.6
1	B	34	ALA	2.6
1	D	493	LYS	2.6
1	G	539	ARG	2.6
1	F	655	PRO	2.6
1	H	416	PRO	2.6
1	I	496	ASP	2.6
1	A	131	ASN	2.6
1	A	775	ASN	2.6
1	H	649	ALA	2.6
1	L	230	MET	2.6
1	H	559	HIS	2.6
1	L	777	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	294	GLU	2.6
1	B	180	THR	2.6
1	D	495	SER	2.6
1	C	276	ASN	2.6
1	J	217	ASN	2.6
1	C	213	GLU	2.5
1	E	22	GLU	2.5
2	N	432	CYS	2.5
1	E	18	GLN	2.5
1	B	548	MET	2.5
1	I	392	ASP	2.5
1	B	422	ASN	2.5
1	I	412	ASN	2.5
1	C	176	GLY	2.5
1	D	537	HIS	2.5
1	J	263	GLU	2.5
1	H	351	GLN	2.5
1	J	763	LYS	2.5
1	K	812	LYS	2.5
1	B	303	MET	2.5
1	A	292	ASP	2.5
1	H	637	ASP	2.5
3	M	4	ASP	2.5
1	B	178	ASN	2.5
1	J	170	GLY	2.5
1	K	47	ASN	2.5
1	G	182	GLU	2.5
1	K	464	LEU	2.5
1	K	597	LEU	2.5
1	L	50	VAL	2.5
1	E	930	ARG	2.5
1	I	377	ILE	2.5
1	D	123	ALA	2.5
1	B	108	ASP	2.5
1	K	16	SER	2.5
1	C	450	ASN	2.5
1	A	286	LEU	2.5
1	I	550	LEU	2.5
1	D	759	CYS	2.5
1	H	166	THR	2.5
1	D	328	ALA	2.5
1	F	108	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	483	ASP	2.5
1	K	719	LYS	2.5
1	L	209	SER	2.5
1	C	332	ASN	2.5
1	A	285	VAL	2.5
1	D	445	GLU	2.5
1	B	248	GLY	2.5
1	B	59	ASP	2.5
1	J	33	ARG	2.5
4	S	32	SER	2.5
1	B	308	GLU	2.5
5	U	215	ASN	2.5
1	G	101	PHE	2.4
1	L	77	ALA	2.4
1	G	759	CYS	2.4
1	L	935	VAL	2.4
1	D	690	SER	2.4
1	L	197	ASP	2.4
4	R	38	PRO	2.4
1	F	255	ASN	2.4
1	H	617	ALA	2.4
5	U	163	THR	2.4
1	H	751	GLY	2.4
1	J	302	TYR	2.4
1	L	189	GLU	2.4
1	E	641	GLN	2.4
2	N	198	GLN	2.4
1	L	686	LYS	2.4
1	C	661	THR	2.4
3	M	286	GLY	2.4
4	P	24	GLY	2.4
1	C	707	TYR	2.4
1	I	52	PRO	2.4
1	G	308	GLU	2.4
1	C	108	ASP	2.4
1	J	530	ASP	2.4
4	Q	129	SER	2.4
1	D	594	GLN	2.4
1	J	499	ASN	2.4
1	L	244	ASN	2.4
2	N	293	GLN	2.4
1	H	269	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	787	TYR	2.4
2	N	426	CYS	2.4
1	J	621	PRO	2.4
1	F	912	GLU	2.4
1	C	930	ARG	2.4
1	F	816	GLN	2.4
1	J	278	ASP	2.4
1	L	62	GLN	2.4
2	N	290	ASP	2.4
1	H	471	ASN	2.4
1	A	618	THR	2.4
1	E	904	THR	2.4
2	N	270	GLY	2.4
1	A	940	TYR	2.4
1	I	100	TYR	2.4
1	A	74	GLU	2.4
1	C	641	GLN	2.4
1	K	488	SER	2.4
1	L	564	GLN	2.4
1	A	644	ASN	2.4
4	R	115	ASN	2.4
1	A	462	ILE	2.3
4	Q	16	THR	2.3
1	A	234	TYR	2.3
1	L	774	TYR	2.3
1	B	841	ALA	2.3
1	D	833	ALA	2.3
1	L	679	ALA	2.3
2	N	190	GLU	2.3
2	N	548	ARG	2.3
1	B	641	GLN	2.3
1	J	924	ASP	2.3
5	U	174	SER	2.3
1	C	227	THR	2.3
1	D	818	GLY	2.3
1	L	780	GLY	2.3
2	N	229	GLY	2.3
1	B	326	TYR	2.3
1	I	616	TYR	2.3
1	C	657	PRO	2.3
1	J	440	GLU	2.3
1	I	815	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	288	SER	2.3
1	F	728	SER	2.3
1	E	181	LYS	2.3
1	I	47	ASN	2.3
1	C	869	THR	2.3
1	D	119	THR	2.3
1	D	551	GLY	2.3
1	J	49	THR	2.3
4	S	6	PHE	2.3
1	B	480	TYR	2.3
1	C	650	ALA	2.3
1	I	849	PRO	2.3
4	Q	86	ALA	2.3
1	A	594	GLN	2.3
1	B	816	GLN	2.3
1	F	253	GLN	2.3
1	A	256	GLY	2.3
1	A	465	ASN	2.3
1	E	363	ASP	2.3
1	J	187	GLY	2.3
1	K	59	ASP	2.3
1	K	605	GLY	2.3
1	L	643	PHE	2.3
1	E	323	ARG	2.3
1	L	884	ALA	2.3
1	F	779	GLN	2.3
1	C	346	GLY	2.3
1	D	555	TYR	2.3
5	V	73	SER	2.3
1	J	734	ASN	2.3
1	L	491	ASN	2.3
1	C	219	ALA	2.3
1	K	411	PRO	2.3
1	A	806	VAL	2.3
1	F	558	PHE	2.3
1	B	435	GLN	2.3
1	J	371	GLN	2.3
1	A	221	GLY	2.3
1	H	190	GLY	2.3
1	F	37	THR	2.3
1	F	217	ASN	2.3
1	G	197	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
4	Q	35	ASP	2.3
1	C	563	PRO	2.2
1	C	585	PHE	2.2
1	D	850	LEU	2.2
1	B	483	ASP	2.2
1	E	341	SER	2.2
1	E	639	ASN	2.2
1	F	385	SER	2.2
1	H	55	ASP	2.2
1	K	136	ASP	2.2
4	S	98	ASP	2.2
1	F	873	ILE	2.2
1	K	263	GLU	2.2
1	F	551	GLY	2.2
1	G	30	GLN	2.2
1	B	812	LYS	2.2
1	E	305	THR	2.2
1	B	292	ASP	2.2
1	B	385	SER	2.2
1	B	495	SER	2.2
1	C	607	SER	2.2
1	G	319	SER	2.2
1	G	571	ASN	2.2
1	I	515	ASP	2.2
1	B	849	PRO	2.2
1	G	93	VAL	2.2
1	C	74	GLU	2.2
1	G	263	GLU	2.2
1	I	551	GLY	2.2
1	J	561	GLN	2.2
1	K	720	LYS	2.2
1	C	466	ALA	2.2
1	A	136	ASP	2.2
1	D	696	ASP	2.2
1	E	911	ASP	2.2
1	G	547	SER	2.2
1	I	519	ASN	2.2
1	K	539	ARG	2.2
1	G	271	GLU	2.2
1	J	744	GLU	2.2
1	F	883	GLY	2.2
1	L	187	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	191	GLN	2.2
1	G	196	ALA	2.2
1	F	92	ARG	2.2
1	G	396	PRO	2.2
1	J	209	SER	2.2
5	V	205	PRO	2.2
1	B	857	ASP	2.2
1	E	599	ASN	2.2
1	J	764	ASP	2.2
1	K	496	ASP	2.2
1	K	625	ASN	2.2
1	G	259	GLU	2.2
1	L	822	GLN	2.2
1	D	494	ILE	2.2
1	L	673	ALA	2.2
1	A	323	ARG	2.2
1	C	544	ARG	2.2
1	A	464	LEU	2.2
1	E	834	PRO	2.2
1	A	369	SER	2.2
1	C	403	ASN	2.2
1	L	495	SER	2.2
1	J	257	LYS	2.1
1	J	395	ASP	2.2
1	D	424	GLU	2.1
1	F	215	GLU	2.1
1	F	243	GLU	2.1
5	U	177	GLU	2.1
1	E	577	GLY	2.1
4	R	54	GLY	2.1
1	K	778	TYR	2.1
1	F	815	GLN	2.1
1	J	123	ALA	2.1
1	L	660	ALA	2.1
1	G	860	THR	2.1
1	A	175	SER	2.1
1	G	773	ASN	2.1
1	I	911	ASP	2.1
1	K	527	ASP	2.1
1	A	703	GLY	2.1
1	F	87	ALA	2.1
1	C	250	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	396	PRO	2.1
1	K	130	PRO	2.1
1	C	952	THR	2.1
1	G	305	THR	2.1
1	A	612	SER	2.1
1	A	728	SER	2.1
1	I	467	ASN	2.1
1	L	826	SER	2.1
1	K	640	ASP	2.1
1	C	275	GLY	2.1
1	D	380	ARG	2.1
3	M	46	ARG	2.1
5	V	167	ALA	2.1
1	A	821	HIS	2.1
5	U	188	PHE	2.1
5	V	162	PHE	2.1
1	J	768	VAL	2.1
1	K	29	VAL	2.1
1	C	489	PRO	2.1
1	B	166	THR	2.1
1	I	303	MET	2.1
1	D	313	GLU	2.1
1	F	61	SER	2.1
1	F	465	ASN	2.1
1	F	748	SER	2.1
1	H	319	SER	2.1
1	I	744	GLU	2.1
1	A	75	ASP	2.1
1	B	839	GLY	2.1
5	V	72	ARG	2.1
1	E	701	TYR	2.1
1	G	136	ASP	2.1
1	J	645	ASP	2.1
1	D	106	VAL	2.1
4	Q	76	VAL	2.1
4	S	52	VAL	2.1
5	V	204	PRO	2.1
1	E	199	THR	2.1
1	D	676	ARG	2.1
1	G	602	ARG	2.1
1	K	421	ILE	2.1
1	H	74	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	259	GLU	2.1
1	C	78	TYR	2.1
1	C	488	SER	2.1
1	H	487	TYR	2.1
1	H	528	TYR	2.1
1	I	588	ASP	2.1
1	I	637	ASP	2.1
4	Q	47	LEU	2.1
1	D	323	ARG	2.1
1	F	872	ARG	2.1
1	I	405	GLY	2.1
3	M	174	GLU	2.1
3	M	219	GLY	2.1
1	C	660	ALA	2.1
1	L	788	LYS	2.1
1	C	519	ASN	2.1
1	D	802	SER	2.1
1	F	279	ASN	2.1
1	K	659	ASN	2.1
1	L	276	ASN	2.1
1	J	496	ASP	2.0
1	K	290	ASP	2.0
1	K	297	ASP	2.0
5	U	217	ASP	2.0
1	G	594	GLN	2.0
1	J	103	ILE	2.0
1	A	762	THR	2.0
1	D	305	THR	2.0
1	F	938	THR	2.0
1	L	228	THR	2.0
1	C	66	LEU	2.0
1	A	367	GLU	2.0
1	A	436	GLU	2.0
1	B	263	GLU	2.0
1	C	51	ALA	2.0
1	C	480	TYR	2.0
1	F	616	TYR	2.0
1	J	374	LEU	2.0
1	K	207	GLY	2.0
5	U	196	VAL	2.0
1	C	5	SER	2.0
1	E	47	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	98	SER	2.0
1	G	607	SER	2.0
1	J	61	SER	2.0
1	B	750	ASP	2.0
1	J	323	ARG	2.0
4	R	30	MET	2.0
1	A	124	LEU	2.0
1	B	410	LEU	2.0
1	E	258	LEU	2.0
1	G	124	LEU	2.0
1	G	593	LEU	2.0
3	M	24	THR	2.0
1	C	405	GLY	2.0
1	C	695	TYR	2.0
1	G	884	ALA	2.0
1	J	219	ALA	2.0
1	J	673	ALA	2.0
1	J	695	TYR	2.0
2	N	260	GLY	2.0
3	M	184	GLY	2.0
1	A	424	GLU	2.0
1	B	22	GLU	2.0
1	B	294	GLU	2.0
1	F	182	GLU	2.0
1	F	131	ASN	2.0
1	H	353	SER	2.0
1	C	299	HIS	2.0
1	C	890	GLN	2.0
1	D	604	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.