



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:18 PM UTC

PDB ID : 2Y0S / pdb_00002y0s
Title : Crystal structure of Sulfolobus shibatae RNA polymerase in P21 space group
Authors : Wojtas, M.; Peralta, B.; Ondiviela, M.; Mogni, M.; Bell, S.D.; Abrescia, N.G.A.
Deposited on : 2010-12-07
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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

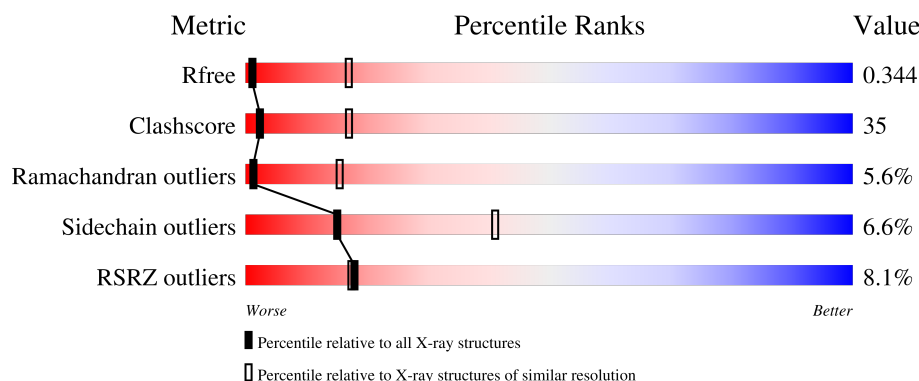
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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 ≥ 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	880	
1	W	880	
2	B	1131	
2	R	1131	
3	C	395	

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Mol	Chain	Length	Quality of chain
3	Y	395	
4	D	265	
4	S	265	
5	E	180	
5	T	180	
6	F	113	
6	U	113	
7	G	132	
7	V	132	
8	H	84	
8	Z	84	
9	I	95	
9	K	95	
10	J	104	
10	Q	104	
11	L	92	
11	M	92	
12	N	66	
12	O	66	
13	P	48	
13	X	48	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	F3S	D	1001	-	-	X	-
16	F3S	S	1001	-	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 52472 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 DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	831	Total	C	N	O	S	0	0	0
			6620	4211	1170	1212	27			
1	W	831	Total	C	N	O	S	0	0	0
			6620	4211	1170	1212	27			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1085	Total	C	N	O	S	0	0	0
			8615	5461	1526	1599	29			
2	R	1085	Total	C	N	O	S	0	0	0
			8615	5461	1526	1599	29			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT A’.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	368	Total	C	N	O	S	0	0	0
			2845	1803	486	548	8			
3	Y	368	Total	C	N	O	S	0	0	0
			2845	1803	486	548	8			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	262	Total	C	N	O	S	0	0	0
			2081	1338	336	394	13			
4	S	262	Total	C	N	O	S	0	0	0
			2081	1338	336	394	13			

- Molecule 5 is a protein called RNA POLYMERASE SUBUNIT 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	164	Total	C	N	O	S	0	0	0
			1297	833	219	240	5			
5	T	164	Total	C	N	O	S	0	0	0
			1297	833	219	240	5			

- Molecule 6 is a protein called RNA POLYMERASE SUBUNIT 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	90	Total	C	N	O	S	0	0	0
			701	439	114	145	3			
6	U	90	Total	C	N	O	S	0	0	0
			701	439	114	145	3			

- Molecule 7 is a protein called RNA POLYMERASE SUBUNIT 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	110	Total	C	N	O	S	0	0	0
			878	558	147	169	4			
7	V	110	Total	C	N	O	S	0	0	0
			878	558	147	169	4			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT H.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	74	Total	C	N	O	0	0	0
			609	396	108	105			
8	Z	74	Total	C	N	O	0	0	0
			609	396	108	105			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	82	Total	C	N	O	S	0	0	0
			653	419	117	116	1			
9	K	82	Total	C	N	O	S	0	0	0
			653	419	117	116	1			

- Molecule 10 is a protein called RNA POLYMERASE SUBUNIT 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	39	Total	C	N	O	S	0	0	0
			332	210	54	67	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	Q	39	Total	C	N	O	S	0	0	0
			332	210	54	67	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	40	ASN	ASP	conflict	UNP B8YB65
Q	40	ASN	ASP	conflict	UNP B8YB65

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	91	Total	C	N	O	S	0	0	0
			707	454	114	137	2			
11	M	91	Total	C	N	O	S	0	0	0
			707	454	114	137	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	N	64	Total	C	N	O	S	0	0	0
			514	327	93	87	7			
12	O	64	Total	C	N	O	S	0	0	0
			514	327	93	87	7			

- Molecule 13 is a protein called RNA POLYMERASE SUBUNIT 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	P	45	Total	C	N	O	S	0	0	0
			369	245	63	56	5			
13	X	45	Total	C	N	O	S	0	0	0
			369	245	63	56	5			

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	2	Total	Zn	0	0
			2	2		
14	B	3	Total	Zn	0	0
			3	3		
14	N	1	Total	Zn	0	0
			1	1		

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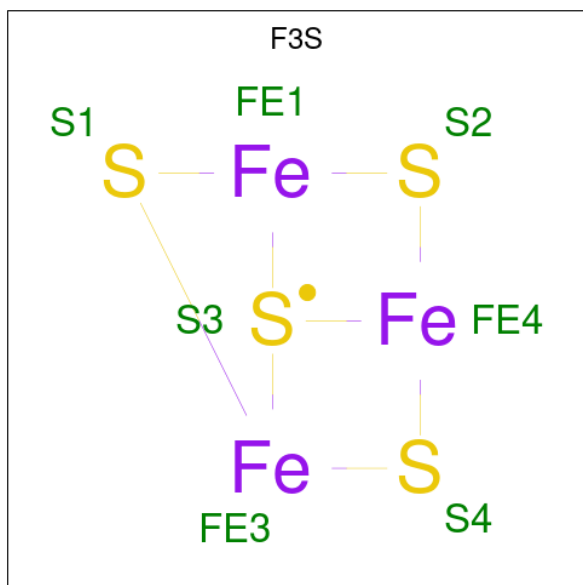
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	O	1	Total 1	Zn 1	0	0
14	P	1	Total 1	Zn 1	0	0
14	R	3	Total 3	Zn 3	0	0
14	W	2	Total 2	Zn 2	0	0
14	X	1	Total 1	Zn 1	0	0

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total 1	Mg 1	0	0
15	W	1	Total 1	Mg 1	0	0

- Molecule 16 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄).

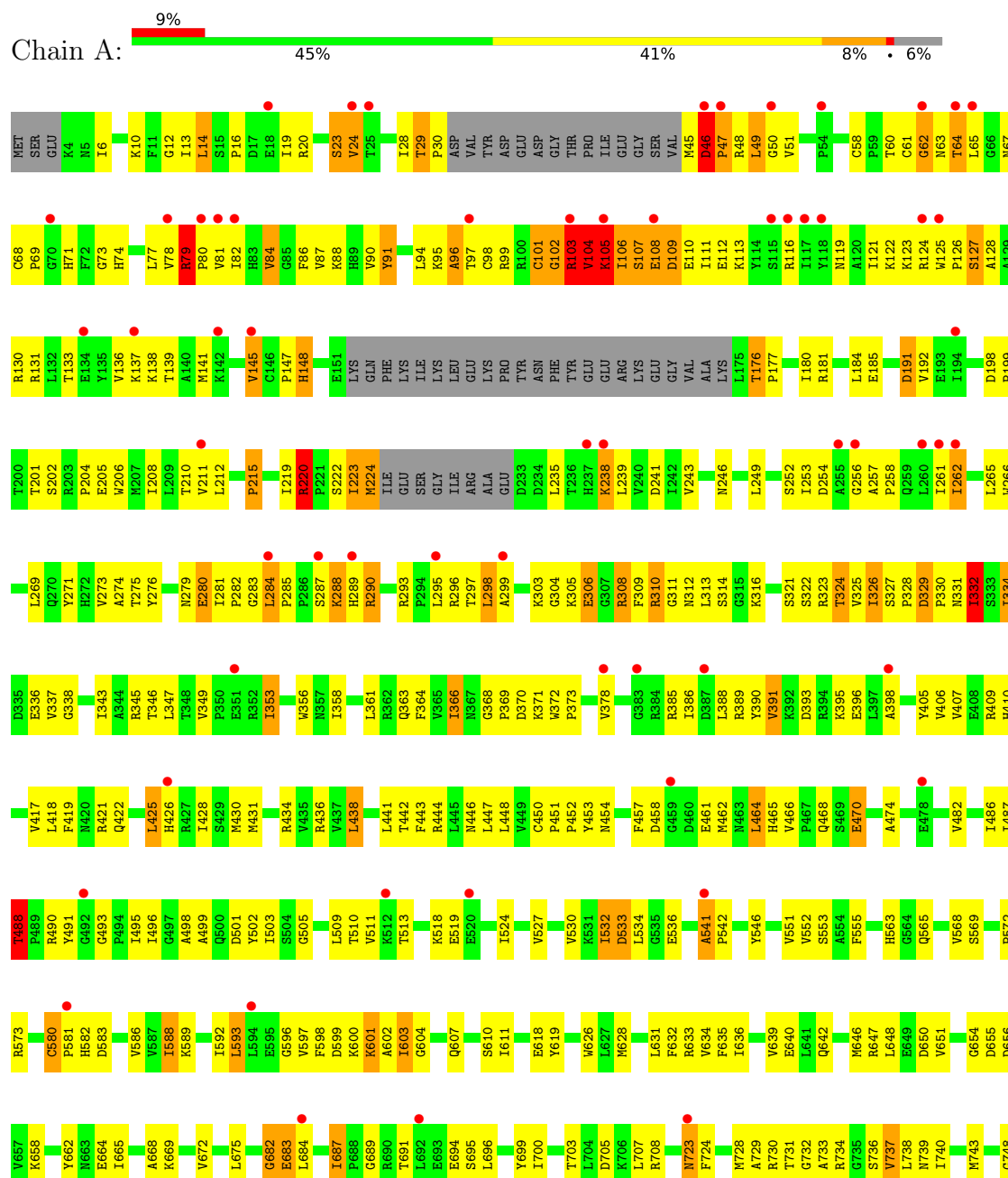


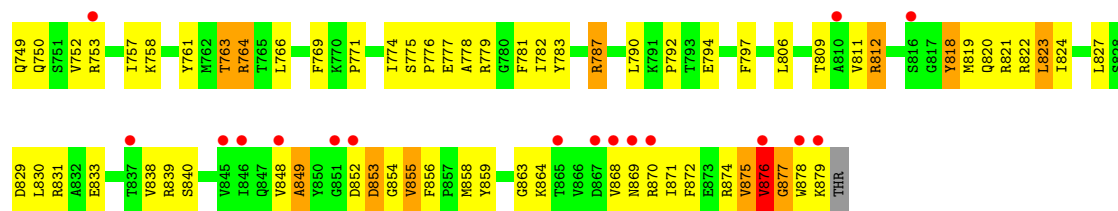
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	D	1	Total 7	Fe 3	S 4	0	0
16	S	1	Total 7	Fe 3	S 4	0	0

3 Residue-property plots

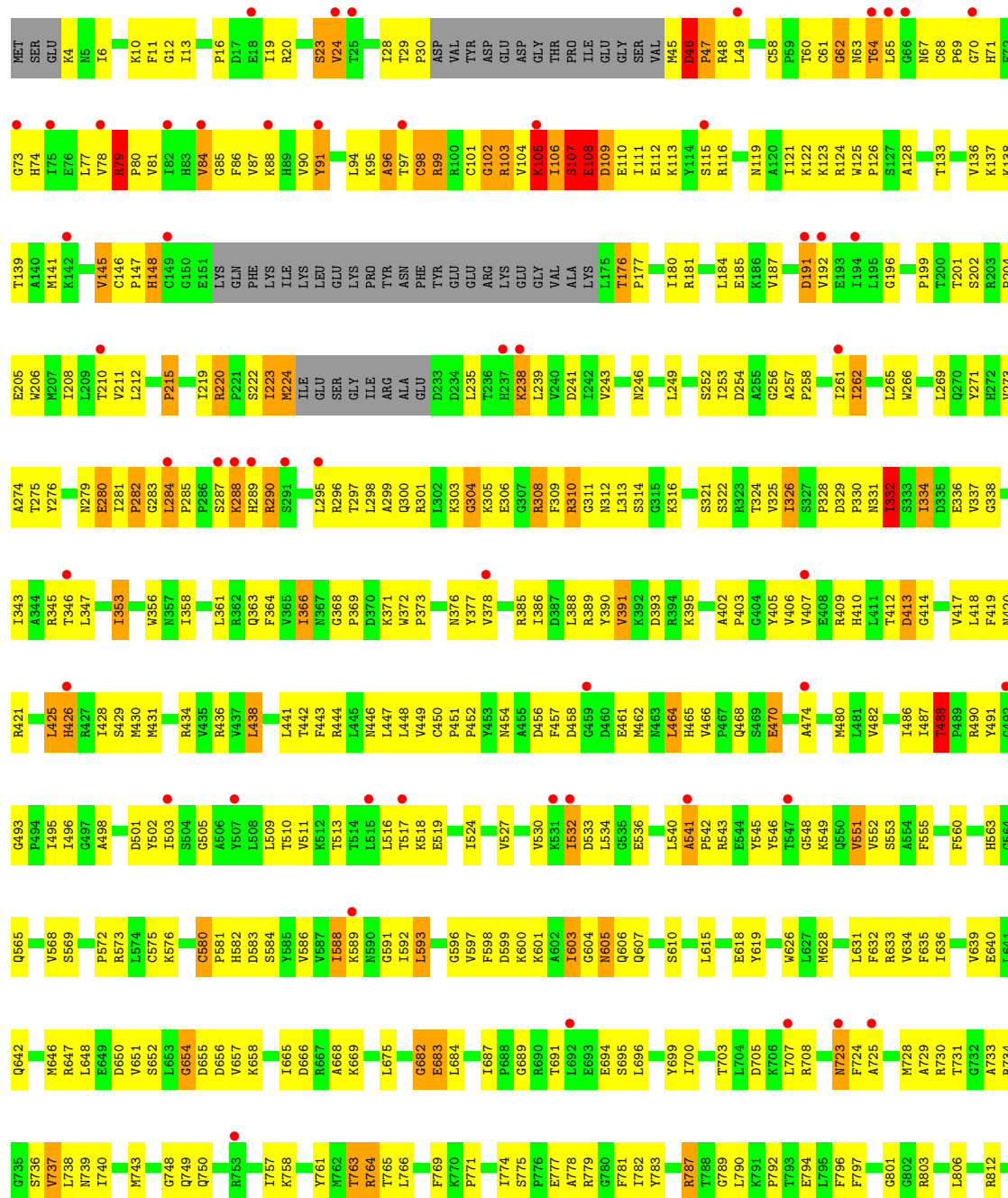
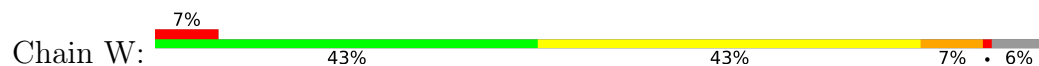
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

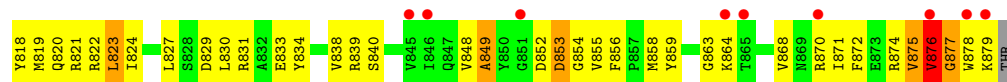
• Molecule 1: DNA-DIRECTED RNA POLYMERASE



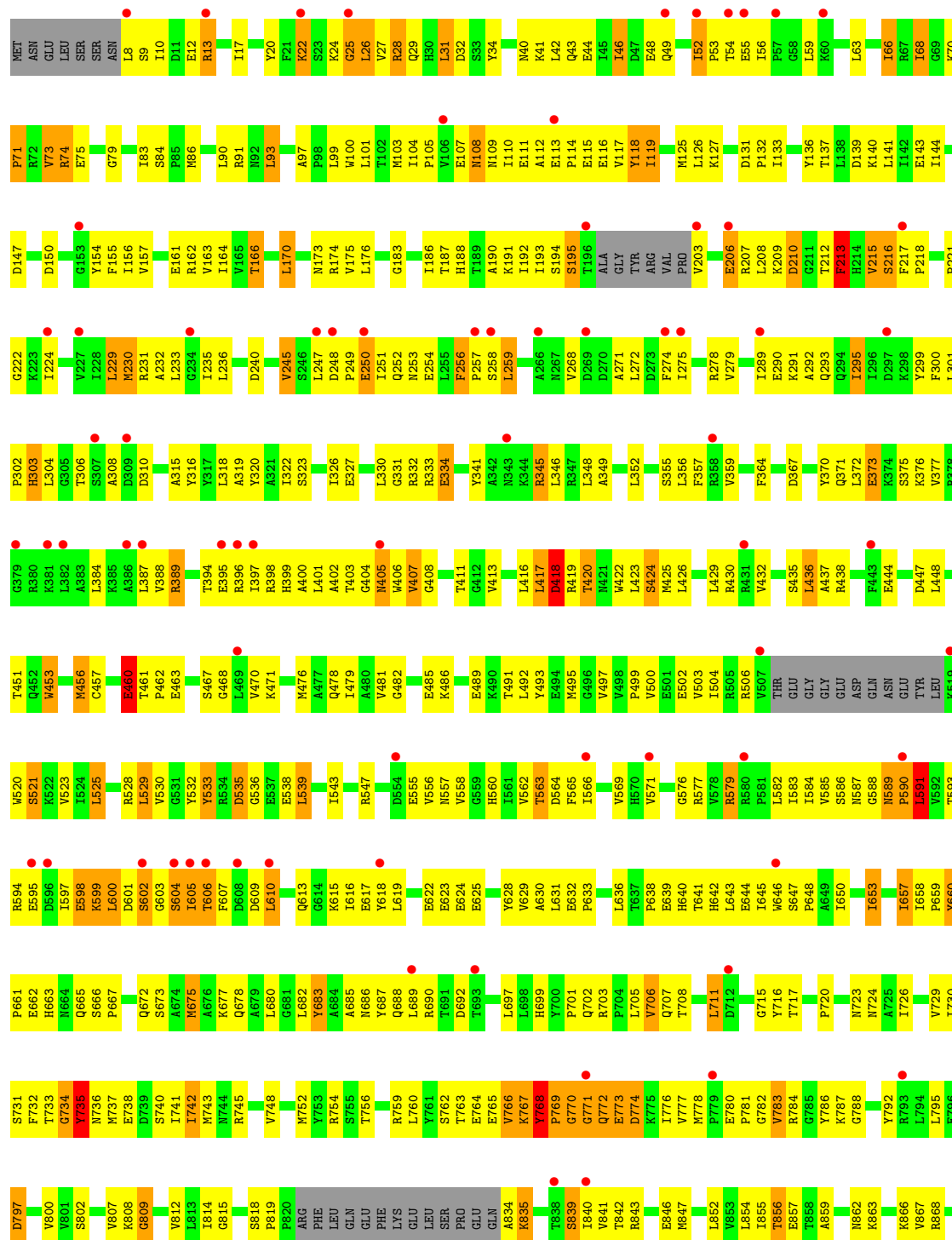


Molecule 1: DNA-DIRECTED RNA POLYMERASE

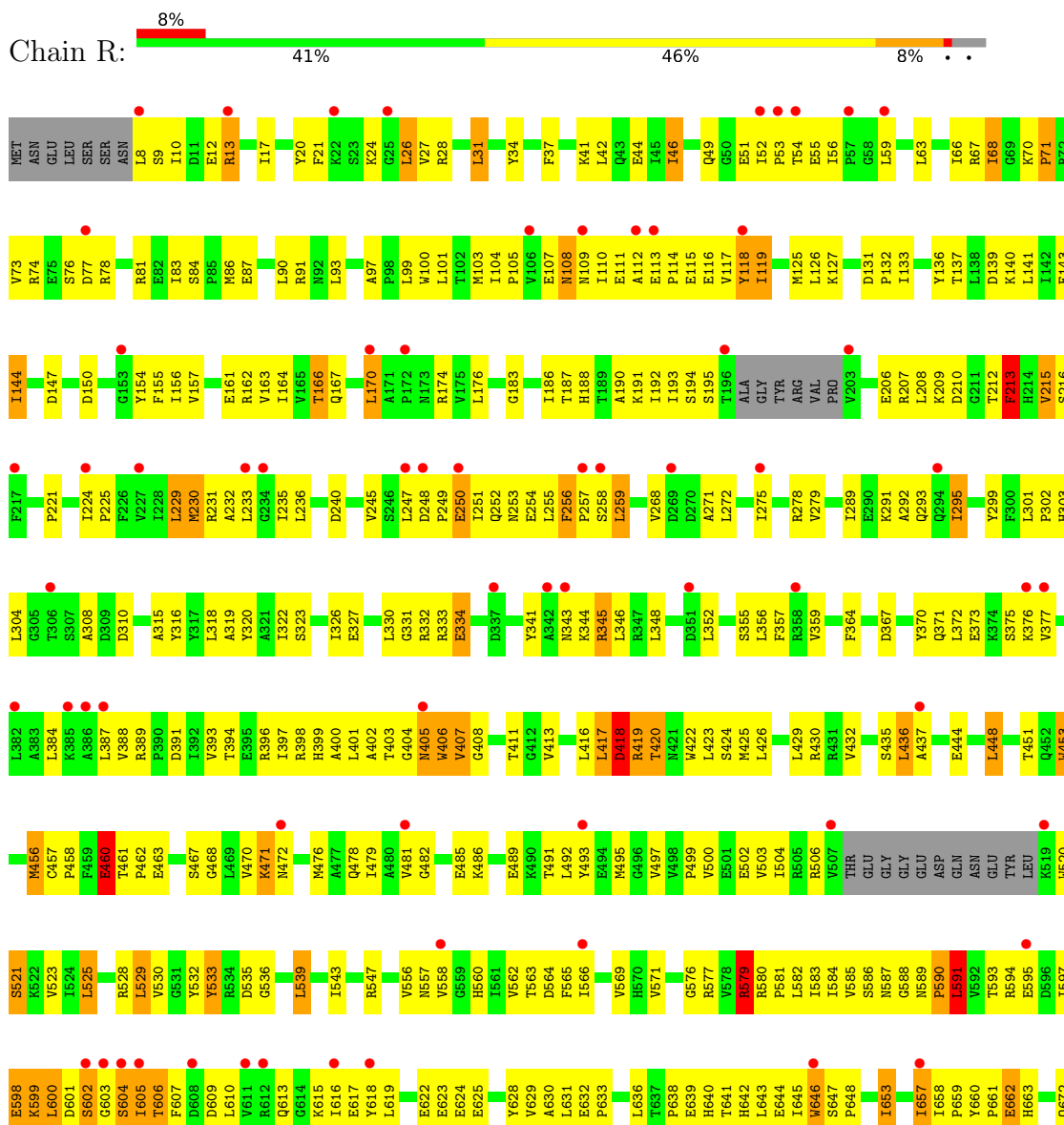




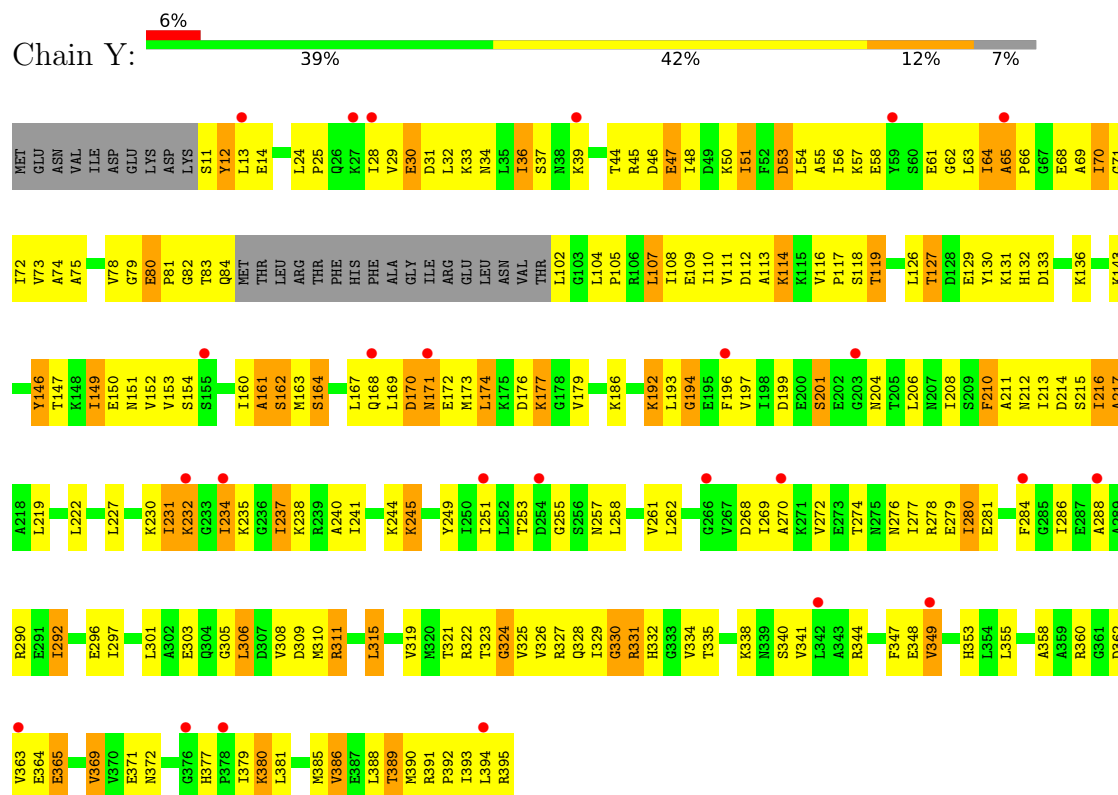
● Molecule 2: DNA-DIRECTED RNA POLYMERASE



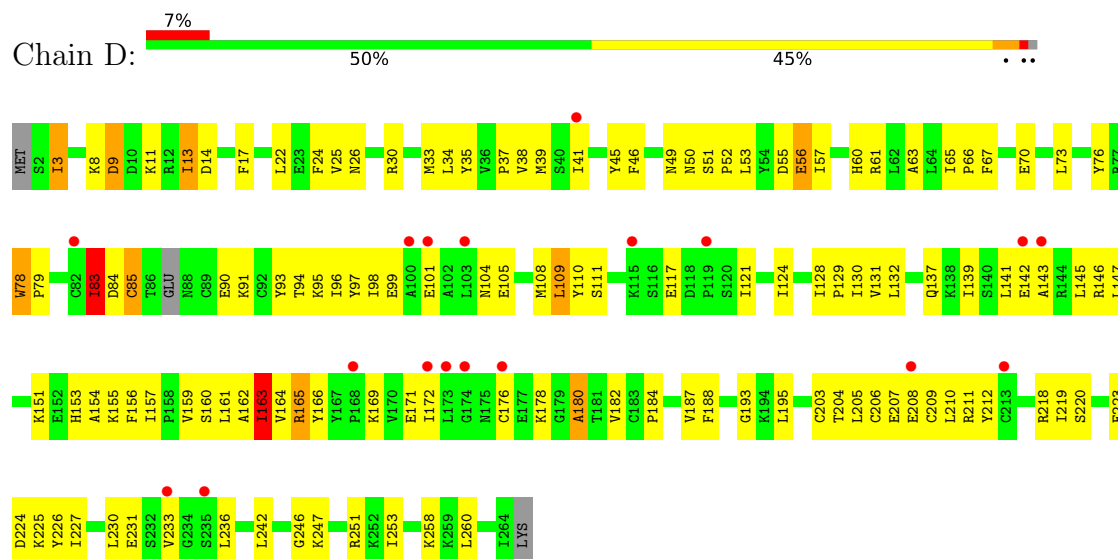
● Molecule 2: DNA-DIRECTED RNA POLYMERASE



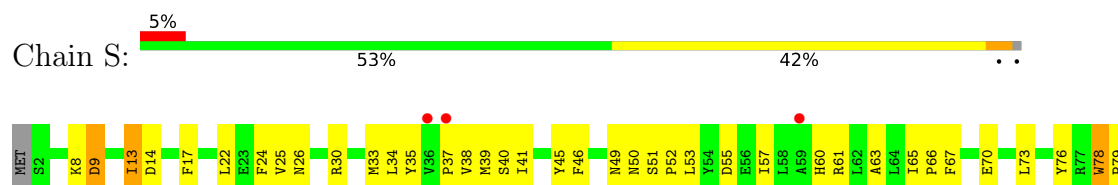
• Molecule 3: DNA-DIRECTED RNA POLYMERASE SUBUNIT A”

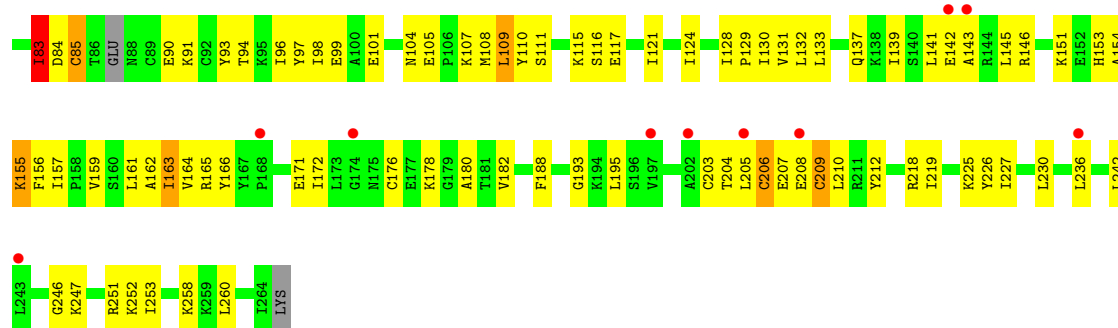


• Molecule 4: DNA-DIRECTED RNA POLYMERASE SUBUNIT D

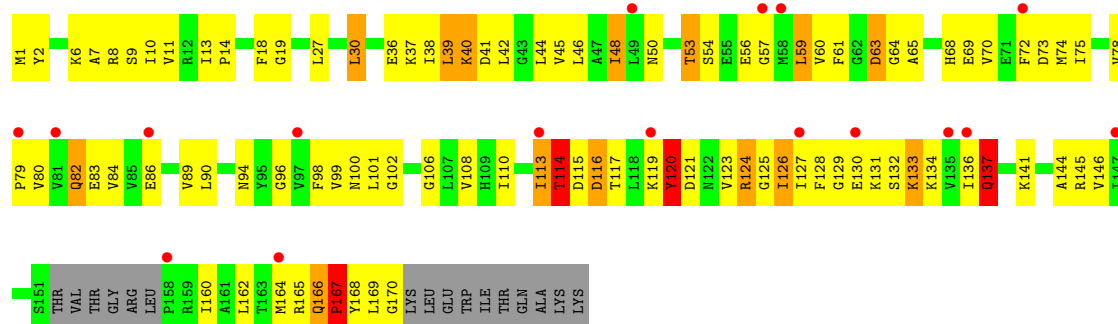


• Molecule 4: DNA-DIRECTED RNA POLYMERASE SUBUNIT D

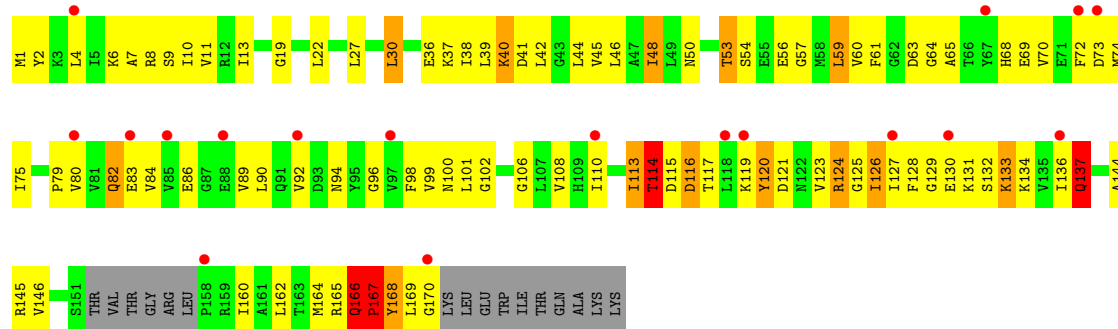




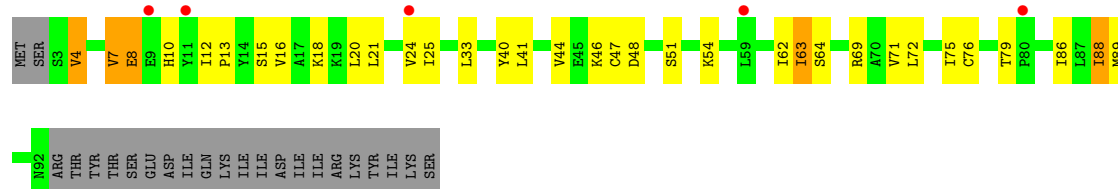
• Molecule 5: RNA POLYMERASE SUBUNIT 4



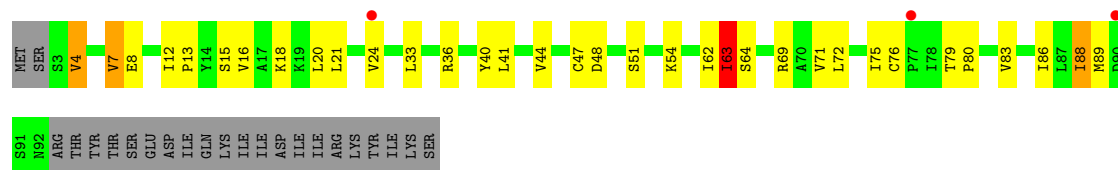
• Molecule 5: RNA POLYMERASE SUBUNIT 4



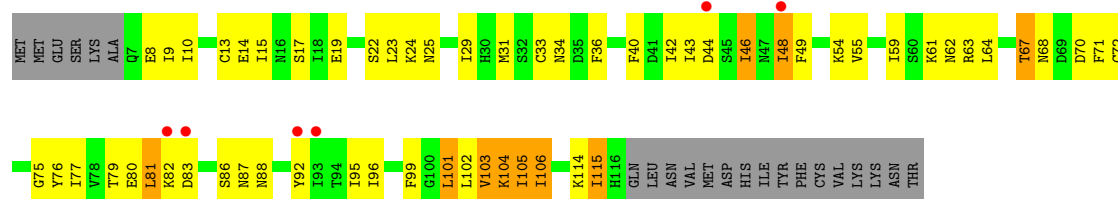
• Molecule 6: RNA POLYMERASE SUBUNIT 7



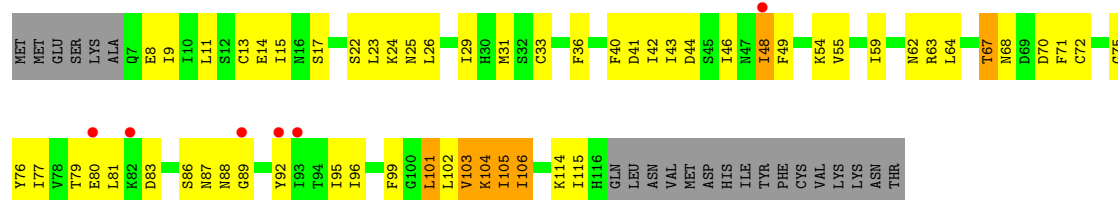
• Molecule 6: RNA POLYMERASE SUBUNIT 7



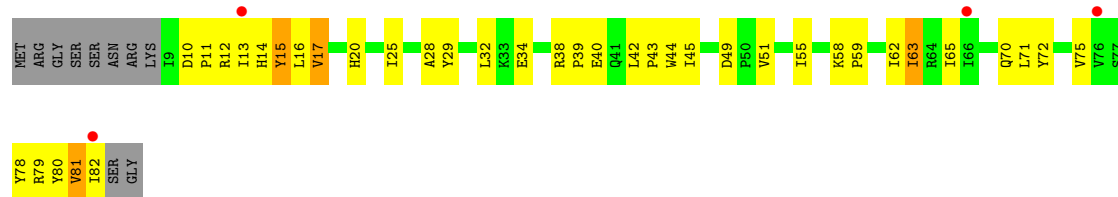
• Molecule 7: RNA POLYMERASE SUBUNIT 8



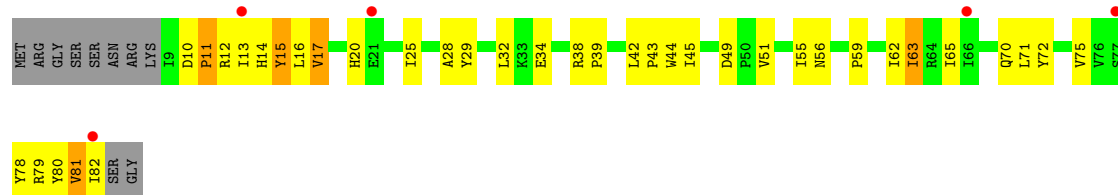
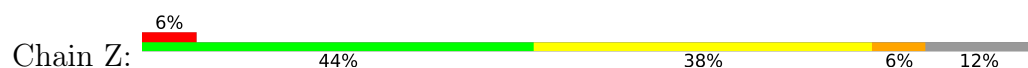
• Molecule 7: RNA POLYMERASE SUBUNIT 8



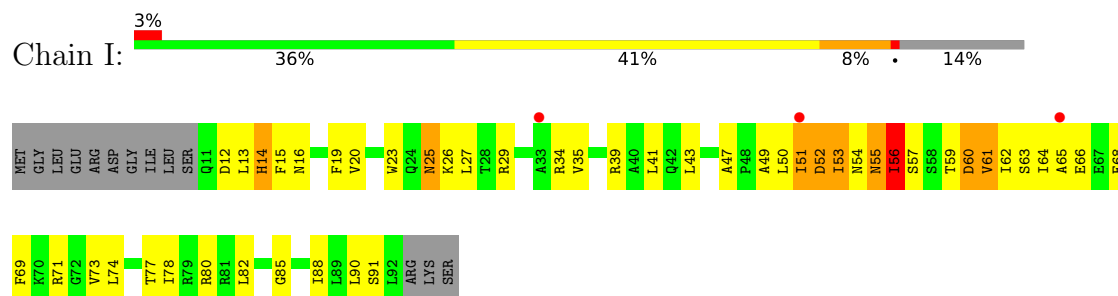
• Molecule 8: DNA-DIRECTED RNA POLYMERASE SUBUNIT H



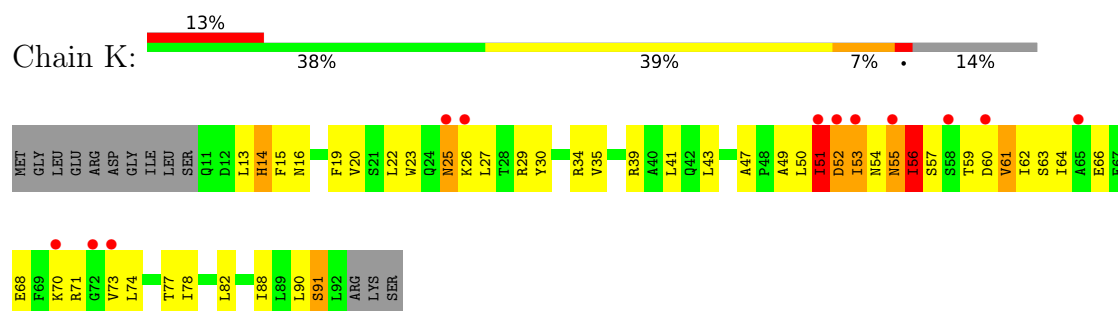
• Molecule 8: DNA-DIRECTED RNA POLYMERASE SUBUNIT H



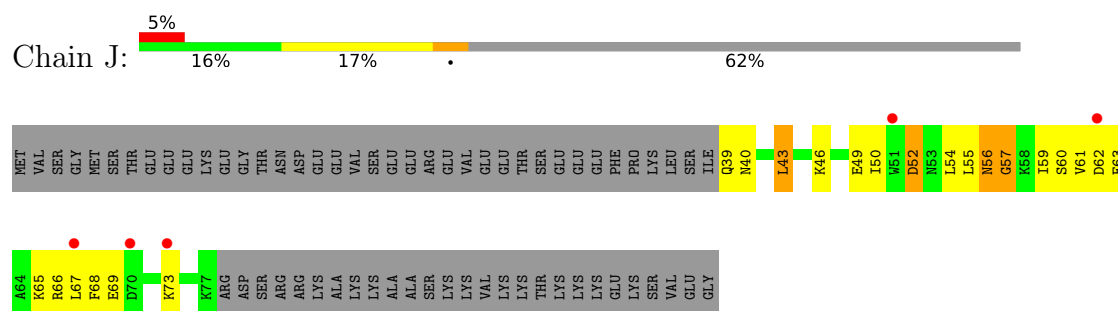
- Molecule 9: DNA-DIRECTED RNA POLYMERASE SUBUNIT K



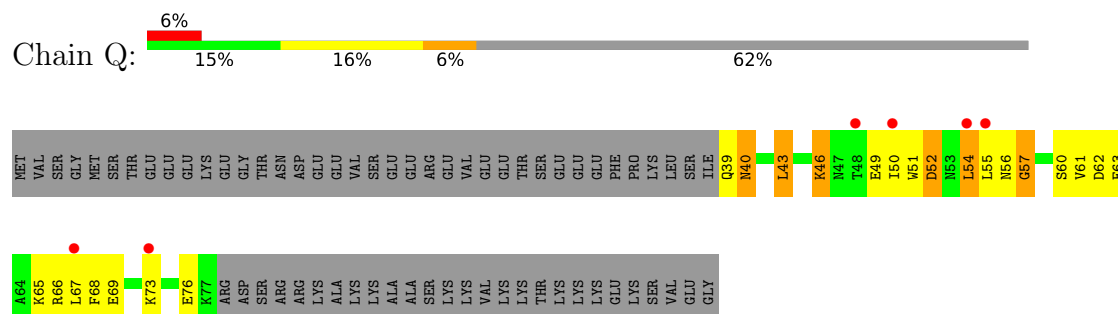
- Molecule 9: DNA-DIRECTED RNA POLYMERASE SUBUNIT K



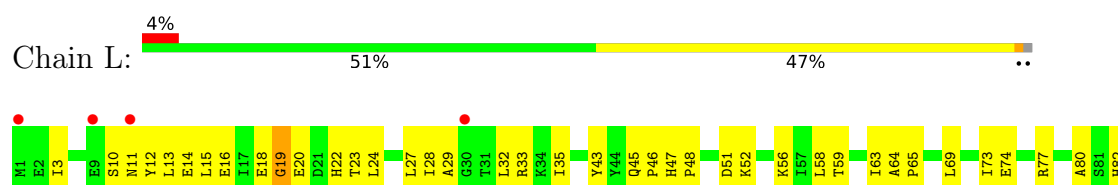
- Molecule 10: RNA POLYMERASE SUBUNIT 13



- Molecule 10: RNA POLYMERASE SUBUNIT 13



- Molecule 11: DNA-DIRECTED RNA POLYMERASE SUBUNIT L

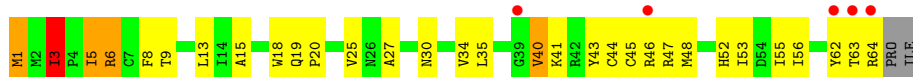




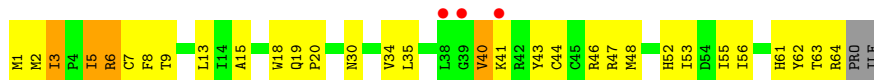
• Molecule 11: DNA-DIRECTED RNA POLYMERASE SUBUNIT L



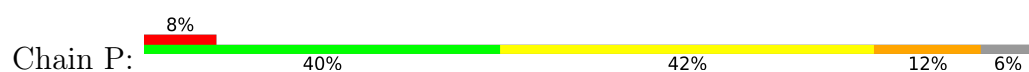
• Molecule 12: DNA-DIRECTED RNA POLYMERASE SUBUNIT N



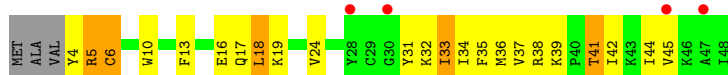
• Molecule 12: DNA-DIRECTED RNA POLYMERASE SUBUNIT N



• Molecule 13: RNA POLYMERASE SUBUNIT 12



• Molecule 13: RNA POLYMERASE SUBUNIT 12



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	129.33Å 195.91Å 212.45Å 90.00° 105.73° 90.00°	Depositor
Resolution (Å)	29.86 – 3.80 29.86 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.86-3.80) 99.0 (29.86-3.80)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 3.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.300 , 0.354 0.288 , 0.344	Depositor DCC
R_{free} test set	5001 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	79.6	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 117.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	52472	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.6829e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, F3S

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	0.67	1/6762 (0.0%)	1.20	55/9151 (0.6%)
1	W	0.55	0/6762	0.95	23/9151 (0.3%)
2	B	0.68	1/8778 (0.0%)	1.17	55/11873 (0.5%)
2	R	0.56	0/8778	0.92	16/11873 (0.1%)
3	C	0.66	0/2869	1.18	18/3862 (0.5%)
3	Y	0.55	0/2869	0.96	10/3862 (0.3%)
4	D	0.51	0/2116	0.97	8/2859 (0.3%)
4	S	0.42	0/2116	0.77	3/2859 (0.1%)
5	E	0.55	1/1316 (0.1%)	1.07	3/1775 (0.2%)
5	T	0.51	1/1316 (0.1%)	0.87	3/1775 (0.2%)
6	F	0.38	0/709	0.94	1/961 (0.1%)
6	U	0.34	0/709	0.71	0/961
7	G	0.53	0/890	0.99	5/1194 (0.4%)
7	V	0.41	0/890	0.76	1/1194 (0.1%)
8	H	0.68	0/623	1.15	2/845 (0.2%)
8	Z	0.55	0/623	0.90	2/845 (0.2%)
9	I	2.28	5/662 (0.8%)	1.27	8/896 (0.9%)
9	K	2.19	5/662 (0.8%)	1.39	10/896 (1.1%)
10	J	0.54	1/336 (0.3%)	0.74	0/450
10	Q	0.68	2/336 (0.6%)	1.04	2/450 (0.4%)
11	L	0.55	0/717	1.10	4/968 (0.4%)
11	M	0.43	0/717	0.85	0/968
12	N	0.58	0/524	1.07	3/706 (0.4%)
12	O	0.48	0/524	0.85	0/706
13	P	0.59	0/378	1.04	1/507 (0.2%)
13	X	0.52	0/378	0.84	0/507
All	All	0.68	17/53360 (0.0%)	1.04	233/72094 (0.3%)

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	A	0	1
5	E	0	1
5	T	0	1
9	I	0	1
9	K	0	1
All	All	0	5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	56	ILE	C-N	-43.24	0.82	1.33
9	K	55	ASN	C-N	37.07	1.84	1.33
9	K	56	ILE	C-N	-35.35	0.84	1.33
9	I	55	ASN	C-N	34.27	1.80	1.33
5	T	57	GLY	C-N	-8.94	1.21	1.33
9	K	70	LYS	N-CA	-8.72	1.36	1.46
9	I	25	ASN	C-N	8.69	1.45	1.33
9	K	25	ASN	C-N	8.64	1.45	1.33
10	Q	39	GLN	C-N	7.61	1.43	1.33
10	Q	40	ASN	C-N	-6.83	1.25	1.33
2	B	774	ASP	CA-CB	-6.42	1.44	1.53
10	J	39	GLN	C-N	6.31	1.41	1.33
1	A	104	VAL	CB-CG2	-5.94	1.32	1.52
9	K	26	LYS	C-N	-5.62	1.25	1.33
5	E	57	GLY	C-N	-5.33	1.26	1.33
9	I	26	LYS	C-N	-5.31	1.25	1.33
9	I	69	PHE	C-N	-5.13	1.27	1.33

All (233) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	55	ASN	O-C-N	12.11	138.56	122.82
9	I	56	ILE	O-C-N	-11.93	107.66	122.57
9	K	55	ASN	O-C-N	11.30	137.52	122.82
9	K	56	ILE	O-C-N	-10.66	109.24	122.57
9	I	56	ILE	CA-C-N	10.62	138.07	121.19
9	I	56	ILE	C-N-CA	10.62	138.07	121.19
1	A	306	GLU	CA-C-N	-10.16	114.74	121.65
1	A	306	GLU	C-N-CA	-10.16	114.74	121.65
1	A	46	ASP	CA-C-N	-9.83	107.56	119.84
1	A	46	ASP	C-N-CA	-9.83	107.56	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	604	SER	N-CA-C	-9.18	101.99	113.01
3	C	51	ILE	N-CA-C	-9.13	101.44	110.30
1	A	368	GLY	CA-C-N	8.59	129.32	120.04
1	A	368	GLY	C-N-CA	8.59	129.32	120.04
3	C	29	VAL	N-CA-C	-8.49	105.64	113.71
9	K	56	ILE	CA-C-N	8.46	137.70	121.54
9	K	56	ILE	C-N-CA	8.46	137.70	121.54
9	K	47	ALA	CA-C-N	8.34	128.10	119.76
9	K	47	ALA	C-N-CA	8.34	128.10	119.76
1	A	740	ILE	N-CA-C	-8.17	102.46	110.72
3	Y	65	ALA	CA-C-N	8.17	130.05	119.84
3	Y	65	ALA	C-N-CA	8.17	130.05	119.84
1	A	79	ARG	CA-C-N	8.16	128.22	119.89
1	A	79	ARG	C-N-CA	8.16	128.22	119.89
1	A	102	GLY	N-CA-C	-8.13	93.91	113.18
3	Y	51	ILE	N-CA-C	-8.10	101.81	110.23
1	W	79	ARG	CA-C-N	8.07	128.12	119.89
1	W	79	ARG	C-N-CA	8.07	128.12	119.89
4	D	3	ILE	N-CA-C	8.06	118.58	106.42
2	B	195	SER	N-CA-C	8.00	122.19	110.59
2	B	768	TYR	CA-C-N	-7.97	109.88	119.84
2	B	768	TYR	C-N-CA	-7.97	109.88	119.84
2	B	52	ILE	CA-C-N	-7.91	112.56	120.31
2	B	52	ILE	C-N-CA	-7.91	112.56	120.31
3	C	65	ALA	CA-C-N	7.66	130.59	120.25
3	C	65	ALA	C-N-CA	7.66	130.59	120.25
2	B	295	ILE	N-CA-C	-7.64	104.34	111.45
2	B	48	GLU	N-CA-C	-7.51	105.03	114.56
1	A	191	ASP	N-CA-C	7.46	119.05	111.07
2	B	773	GLU	N-CA-C	7.38	119.61	107.73
2	R	729	VAL	N-CA-C	7.35	114.07	106.21
5	T	168	TYR	N-CA-C	-7.31	101.28	111.81
3	C	393	ILE	N-CA-C	7.19	119.09	108.45
1	A	853	ASP	N-CA-C	7.17	118.78	110.97
2	B	73	VAL	N-CA-C	7.12	118.39	107.99
3	C	14	GLU	N-CA-C	7.12	119.04	111.28
2	B	895	ILE	CA-C-N	7.10	127.52	119.92
2	B	895	ILE	C-N-CA	7.10	127.52	119.92
2	B	13	ARG	N-CA-C	-7.08	104.12	112.89
9	I	47	ALA	CA-C-N	7.07	127.62	119.99
9	I	47	ALA	C-N-CA	7.07	127.62	119.99
12	N	27	ALA	N-CA-C	-7.03	103.54	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	624	GLU	N-CA-C	-7.01	103.82	112.38
2	B	482	GLY	N-CA-C	6.92	121.06	112.14
1	W	775	SER	CA-C-N	6.88	127.17	119.32
1	W	775	SER	C-N-CA	6.88	127.17	119.32
2	B	729	VAL	N-CA-C	6.88	113.57	106.21
7	G	77	ILE	N-CA-C	6.81	118.53	108.45
1	W	740	ILE	N-CA-C	-6.76	103.72	110.62
1	W	46	ASP	CA-C-N	-6.75	111.40	119.84
1	W	46	ASP	C-N-CA	-6.75	111.40	119.84
1	W	176	THR	CA-C-N	6.70	126.96	119.32
1	W	176	THR	C-N-CA	6.70	126.96	119.32
1	A	50	GLY	N-CA-C	6.68	118.83	112.08
1	A	176	THR	CA-C-N	6.67	126.93	119.32
1	A	176	THR	C-N-CA	6.67	126.93	119.32
11	L	28	ILE	N-CA-C	6.65	116.78	110.53
1	W	877	GLY	N-CA-C	-6.64	107.03	114.40
3	Y	36	ILE	N-CA-C	-6.64	104.02	110.72
3	Y	58	GLU	N-CA-C	-6.63	105.16	113.18
8	H	17	VAL	CA-C-N	6.62	128.12	119.84
8	H	17	VAL	C-N-CA	6.62	128.12	119.84
3	C	61	GLU	N-CA-C	-6.61	104.16	111.82
1	A	775	SER	CA-C-N	6.58	128.07	119.84
1	A	775	SER	C-N-CA	6.58	128.07	119.84
1	A	488	THR	CA-C-N	6.58	126.20	119.56
1	A	488	THR	C-N-CA	6.58	126.20	119.56
9	K	91	SER	N-CA-C	6.53	124.70	110.80
1	W	98	CYS	CA-CB-SG	6.51	129.38	114.40
2	B	373	GLU	N-CA-C	-6.45	104.25	111.28
1	A	329	ASP	CA-C-N	6.43	126.01	119.19
1	A	329	ASP	C-N-CA	6.43	126.01	119.19
1	A	877	GLY	N-CA-C	-6.37	107.66	114.67
1	W	215	PRO	O-C-N	6.37	124.24	121.31
1	W	488	THR	CA-C-N	6.36	125.98	119.56
1	W	488	THR	C-N-CA	6.36	125.98	119.56
3	C	250	ILE	N-CA-C	6.33	116.97	108.11
11	L	45	GLN	CA-C-N	6.27	125.49	118.97
11	L	45	GLN	C-N-CA	6.27	125.49	118.97
1	A	176	THR	N-CA-C	6.25	118.55	109.04
9	I	85	GLY	N-CA-C	-6.20	107.70	115.08
2	B	300	PHE	N-CA-C	6.20	118.27	108.67
11	L	51	ASP	N-CA-C	6.19	119.24	109.39
2	R	604	SER	N-CA-C	-6.19	105.44	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	579	ARG	N-CA-C	6.16	119.06	109.52
1	W	102	GLY	N-CA-C	-6.16	98.58	113.18
2	R	895	ILE	CA-C-N	6.14	126.49	119.92
2	R	895	ILE	C-N-CA	6.14	126.49	119.92
2	B	774	ASP	CA-C-N	-6.14	112.05	122.67
2	B	774	ASP	C-N-CA	-6.14	112.05	122.67
2	B	25	GLY	N-CA-C	6.12	122.48	111.34
7	G	115	ILE	N-CA-C	6.11	116.92	108.12
2	B	579	ARG	N-CA-C	6.09	118.95	109.52
2	B	942	ILE	N-CA-C	6.08	116.86	110.72
2	B	174	ARG	N-CA-C	6.08	118.81	110.24
2	R	1071	GLY	N-CA-C	6.07	118.46	111.36
1	A	580	CYS	CA-C-N	6.06	126.17	119.87
1	A	580	CYS	C-N-CA	6.06	126.17	119.87
1	A	51	VAL	N-CA-C	6.06	116.35	106.72
1	A	198	ASP	N-CA-C	-6.05	102.43	109.93
1	A	298	LEU	N-CA-C	6.05	118.36	111.11
3	C	374	ILE	N-CA-C	6.03	116.77	110.62
2	B	986	ILE	N-CA-C	6.01	116.53	108.11
2	B	589	ASN	CA-C-N	6.00	127.34	119.84
2	B	589	ASN	C-N-CA	6.00	127.34	119.84
3	C	169	LEU	N-CA-C	5.99	118.59	111.71
4	S	78	TRP	CA-C-N	5.96	127.29	119.84
4	S	78	TRP	C-N-CA	5.96	127.29	119.84
2	B	411	THR	N-CA-C	5.95	118.22	110.43
1	A	533	ASP	N-CA-CB	5.94	119.96	111.05
1	A	257	ALA	CA-C-N	5.91	127.23	119.84
1	A	257	ALA	C-N-CA	5.91	127.23	119.84
1	W	368	GLY	CA-C-N	5.89	126.99	120.45
1	W	368	GLY	C-N-CA	5.89	126.99	120.45
2	B	175	VAL	N-CA-C	5.87	117.23	108.54
2	B	213	PHE	N-CA-C	5.87	123.30	110.80
2	B	389	ARG	CB-CA-C	5.86	115.72	110.44
1	A	105	LYS	CA-C-N	-5.83	111.47	121.97
1	A	105	LYS	C-N-CA	-5.83	111.47	121.97
9	K	60	ASP	N-CA-C	5.83	118.15	108.13
2	R	174	ARG	N-CA-C	5.80	117.78	110.24
1	A	215	PRO	O-C-N	5.79	123.98	121.31
4	D	78	TRP	CA-C-N	5.79	127.08	119.84
4	D	78	TRP	C-N-CA	5.79	127.08	119.84
2	B	424	SER	N-CA-C	5.78	117.26	111.07
5	E	14	PRO	N-CA-C	5.78	116.76	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	56	GLU	N-CA-C	5.77	117.37	111.14
1	A	809	THR	N-CA-C	5.76	118.31	111.33
2	B	1104	ILE	N-CA-C	5.76	115.95	110.42
6	F	8	GLU	N-CA-C	5.76	118.60	109.50
1	A	103	ARG	N-CA-C	5.76	123.06	110.80
1	A	305	LYS	N-CA-C	-5.74	105.44	113.37
1	W	257	ALA	CA-C-N	5.73	127.01	119.84
1	W	257	ALA	C-N-CA	5.73	127.01	119.84
2	B	1060	THR	N-CA-C	5.71	119.95	112.92
7	G	10	ILE	N-CA-C	5.68	116.07	108.11
2	R	624	GLU	N-CA-C	-5.67	105.46	112.38
3	C	377	HIS	CA-C-N	5.67	126.92	119.84
3	C	377	HIS	C-N-CA	5.67	126.92	119.84
9	K	15	PHE	N-CA-C	5.66	118.30	111.40
5	E	39	LEU	N-CA-C	5.65	117.61	108.34
2	B	918	LEU	N-CA-C	5.64	122.27	109.81
2	R	1028	GLY	N-CA-C	5.64	118.72	110.38
1	A	855	VAL	N-CA-C	5.63	116.69	108.53
2	B	303	HIS	N-CA-C	-5.62	106.19	113.16
3	Y	80	GLU	N-CA-C	-5.62	105.95	113.25
4	D	180	ALA	N-CA-C	-5.60	104.80	111.69
2	B	306	THR	N-CA-C	-5.59	107.00	113.88
2	B	274	PHE	N-CA-C	-5.59	106.44	113.20
1	W	304	GLY	N-CA-C	5.56	117.86	111.36
2	R	295	ILE	N-CA-C	-5.56	105.43	110.82
1	A	198	ASP	CA-C-N	5.53	126.39	120.47
1	A	198	ASP	C-N-CA	5.53	126.39	120.47
1	A	293	ARG	N-CA-C	-5.50	101.65	109.62
2	B	1100	PHE	N-CA-C	-5.49	105.32	112.23
5	T	166	GLN	CA-C-N	5.49	126.70	119.84
5	T	166	GLN	C-N-CA	5.49	126.70	119.84
3	C	124	ILE	N-CA-C	5.48	116.47	108.58
7	G	61	LYS	N-CA-C	-5.45	107.00	113.97
4	S	155	LYS	N-CA-C	-5.44	106.71	113.19
2	B	1081	VAL	N-CA-C	5.44	115.47	107.75
13	P	37	VAL	N-CA-C	5.43	117.00	109.45
4	D	187	VAL	N-CA-C	5.42	115.90	111.62
3	C	220	PHE	N-CA-C	-5.41	105.55	111.82
3	C	260	GLY	N-CA-C	5.40	119.68	112.77
1	A	14	LEU	N-CA-C	5.39	116.91	109.15
1	A	818	TYR	N-CA-C	-5.38	105.58	111.82
1	W	580	CYS	CA-C-N	5.37	125.45	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	580	CYS	C-N-CA	5.37	125.45	119.87
2	B	206	GLU	N-CA-C	5.37	117.14	108.34
1	A	422	GLN	CB-CA-C	5.35	116.87	108.63
1	A	82	ILE	N-CA-C	5.34	116.47	109.58
2	B	290	GLU	N-CA-C	5.34	117.10	111.28
2	B	893	MET	N-CA-C	5.33	117.49	109.23
2	B	1010	GLY	CA-C-N	5.31	125.31	120.21
2	B	1010	GLY	C-N-CA	5.31	125.31	120.21
3	Y	330	GLY	N-CA-C	5.30	119.23	112.13
7	V	77	ILE	N-CA-C	5.29	116.28	108.45
9	K	55	ASN	N-CA-C	5.26	117.71	107.71
2	B	395	GLU	N-CA-C	5.26	116.82	111.14
2	B	683	TYR	N-CA-C	5.25	119.39	112.89
1	A	349	VAL	N-CA-C	5.24	113.60	107.89
2	B	349	ALA	N-CA-C	5.22	116.97	111.28
2	B	245	VAL	N-CA-C	5.21	115.32	110.42
12	N	3	ILE	N-CA-CB	5.21	114.93	110.08
9	I	60	ASP	N-CA-C	5.19	116.84	108.32
2	R	768	TYR	CA-C-N	-5.19	113.35	119.84
2	R	768	TYR	C-N-CA	-5.19	113.35	119.84
2	B	610	LEU	N-CA-C	-5.18	106.80	113.23
2	B	660	TYR	CA-C-N	5.17	124.97	119.28
2	B	660	TYR	C-N-CA	5.17	124.97	119.28
3	C	361	GLY	N-CA-C	-5.16	107.13	115.08
2	R	411	THR	N-CA-C	5.16	117.19	110.43
2	B	1028	GLY	N-CA-C	5.15	118.01	110.38
2	R	986	ILE	N-CA-C	5.15	115.32	108.11
10	Q	46	LYS	N-CA-C	-5.15	105.36	111.69
1	A	687	ILE	N-CA-C	5.14	112.96	107.76
1	A	869	ASN	N-CA-CB	5.14	117.85	110.40
1	A	324	THR	N-CA-C	5.12	116.59	108.96
4	D	163	ILE	N-CA-C	5.12	116.09	108.46
10	Q	54	LEU	N-CA-C	-5.12	107.19	112.93
8	Z	17	VAL	CA-C-N	5.12	126.24	119.84
8	Z	17	VAL	C-N-CA	5.12	126.24	119.84
7	G	81	LEU	N-CA-C	-5.12	107.71	114.31
2	B	22	LYS	N-CA-C	-5.11	106.14	112.38
3	Y	377	HIS	CA-C-N	5.09	126.20	119.84
3	Y	377	HIS	C-N-CA	5.09	126.20	119.84
1	A	220	ARG	CA-C-N	-5.07	113.51	119.84
1	A	220	ARG	C-N-CA	-5.07	113.51	119.84
1	A	533	ASP	N-CA-C	-5.07	102.06	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	N	25	VAL	N-CA-C	-5.06	105.49	111.00
5	E	63	ASP	N-CA-C	5.05	117.29	108.76
3	C	36	ILE	N-CA-C	-5.04	105.48	110.62
4	D	211	ARG	N-CA-C	5.03	119.54	113.41
1	A	776	PRO	CA-C-N	5.02	126.97	120.44
1	A	776	PRO	C-N-CA	5.02	126.97	120.44
3	Y	280	ILE	N-CA-C	-5.02	105.50	110.62
2	R	13	ARG	N-CA-C	-5.02	106.42	112.54
1	A	127	SER	N-CA-C	-5.01	106.00	111.82
2	B	66	ILE	N-CA-C	5.01	116.74	108.97
2	R	482	GLY	N-CA-C	5.01	119.39	112.37
3	C	179	VAL	N-CA-C	5.01	115.45	108.84
1	W	105	LYS	CG-CD-CE	5.00	122.80	111.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	VAL	Mainchain
5	E	167	PRO	Peptide
9	I	56	ILE	Mainchain
9	K	56	ILE	Mainchain
5	T	167	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6620	0	6690	502	0
1	W	6620	0	6690	523	0
2	B	8615	0	8753	740	0
2	R	8615	0	8754	736	0
3	C	2845	0	3004	252	0
3	Y	2845	0	3004	255	0
4	D	2081	0	2122	135	0
4	S	2081	0	2123	123	0
5	E	1297	0	1348	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	T	1297	0	1348	128	0
6	F	701	0	708	49	0
6	U	701	0	708	47	0
7	G	878	0	886	57	0
7	V	878	0	886	60	0
8	H	609	0	640	45	0
8	Z	609	0	640	37	0
9	I	653	0	688	62	0
9	K	653	0	688	57	0
10	J	332	0	324	23	0
10	Q	332	0	324	30	0
11	L	707	0	739	37	0
11	M	707	0	739	34	0
12	N	514	0	528	33	0
12	O	514	0	528	37	0
13	P	369	0	396	49	0
13	X	369	0	396	52	0
14	A	2	0	0	0	0
14	B	3	0	0	0	0
14	N	1	0	0	0	0
14	O	1	0	0	0	0
14	P	1	0	0	0	0
14	R	3	0	0	0	0
14	W	2	0	0	0	0
14	X	1	0	0	0	0
15	A	1	0	0	0	0
15	W	1	0	0	0	0
16	D	7	0	0	5	0
16	S	7	0	0	9	0
All	All	52472	0	53654	3758	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 35.

All (3758) 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)
9:I:55:ASN:C	9:I:56:ILE:N	1.80	1.37
9:K:55:ASN:C	9:K:56:ILE:N	1.84	1.34
9:I:56:ILE:O	9:I:57:SER:N	1.67	1.24
9:I:56:ILE:C	9:I:57:SER:CA	2.13	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:56:ILE:C	9:K:57:SER:CA	2.14	1.20
9:K:56:ILE:O	9:K:57:SER:N	1.71	1.19
3:Y:168:GLN:HG2	3:Y:204:ASN:OD1	1.42	1.18
2:B:768:TYR:HB3	2:B:769:PRO:HD3	1.30	1.14
3:C:168:GLN:HG2	3:C:204:ASN:OD1	1.48	1.14
2:B:768:TYR:HB3	2:B:769:PRO:CD	1.81	1.11
9:K:56:ILE:CA	9:K:57:SER:N	2.14	1.10
9:I:56:ILE:CA	9:I:57:SER:N	2.14	1.10
2:R:768:TYR:HB3	2:R:769:PRO:CD	1.82	1.09
2:B:767:LYS:CB	2:B:768:TYR:HA	1.90	1.02
1:A:426:HIS:CE1	3:C:80:GLU:OE2	2.13	1.01
4:S:203:CYS:HG	16:S:1001:F3S:FE3	0.70	1.00
2:R:768:TYR:HB3	2:R:769:PRO:HD3	1.42	0.99
2:B:31:LEU:HD23	2:B:125:MET:HE3	1.43	0.98
2:B:767:LYS:HB3	2:B:768:TYR:HA	1.46	0.98
1:W:103:ARG:HB2	1:W:191:ASP:OD1	1.62	0.98
3:C:244:LYS:HA	3:C:245:LYS:HB3	1.46	0.97
1:A:426:HIS:ND1	3:C:80:GLU:OE2	1.98	0.97
1:W:426:HIS:CE1	3:Y:80:GLU:OE2	2.18	0.97
2:R:31:LEU:HD23	2:R:125:MET:HE3	1.47	0.95
1:W:98:CYS:O	1:W:146:CYS:SG	2.25	0.95
3:Y:244:LYS:HA	3:Y:245:LYS:HB3	1.50	0.94
9:K:56:ILE:C	9:K:57:SER:N	0.84	0.93
1:W:103:ARG:HB2	1:W:191:ASP:CG	1.94	0.92
2:B:766:VAL:HG22	2:B:767:LYS:H	1.34	0.92
1:A:99:ARG:NH1	1:A:147:PRO:HG2	1.85	0.91
9:I:56:ILE:C	9:I:57:SER:N	0.82	0.91
2:R:767:LYS:HB3	2:R:768:TYR:CD1	2.03	0.91
2:R:767:LYS:CB	2:R:768:TYR:HA	1.99	0.91
2:B:767:LYS:HB3	2:B:768:TYR:CD1	2.06	0.90
2:B:767:LYS:HB3	2:B:768:TYR:CA	2.01	0.90
2:B:767:LYS:CG	2:B:768:TYR:HA	2.01	0.90
2:B:766:VAL:HG12	2:B:774:ASP:OD2	1.71	0.89
2:R:31:LEU:HA	2:R:125:MET:CE	2.03	0.89
2:B:786:TYR:CE2	2:B:788:GLY:HA2	2.08	0.89
2:B:767:LYS:HB3	2:B:768:TYR:CG	2.08	0.88
1:W:426:HIS:ND1	3:Y:80:GLU:OE2	2.06	0.88
3:C:149:ILE:HD13	3:C:230:LYS:HB3	1.55	0.88
2:B:31:LEU:HA	2:B:125:MET:CE	2.04	0.88
2:B:953:ILE:HD13	2:B:953:ILE:H	1.39	0.87
5:E:30:LEU:HD13	5:E:72:PHE:CZ	2.10	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:767:LYS:CG	2:R:768:TYR:HA	2.05	0.86
13:P:17:GLN:HG3	13:P:19:LYS:HG2	1.58	0.86
2:R:766:VAL:HG12	2:R:774:ASP:OD2	1.76	0.85
2:R:767:LYS:HB3	2:R:768:TYR:HA	1.55	0.85
1:A:104:VAL:O	1:A:104:VAL:CG1	2.21	0.85
2:R:767:LYS:HB3	2:R:768:TYR:CG	2.12	0.85
2:R:786:TYR:CE2	2:R:788:GLY:HA2	2.10	0.85
1:A:103:ARG:HB2	1:A:191:ASP:CG	2.00	0.84
2:R:356:LEU:HA	2:R:407:VAL:HG21	1.56	0.84
2:B:602:SER:HB2	2:B:605:ILE:HG21	1.60	0.84
7:G:114:LYS:C	7:G:115:ILE:HD12	2.03	0.84
2:B:356:LEU:HA	2:B:407:VAL:HG21	1.57	0.84
2:B:46:ILE:HG13	2:B:66:ILE:HD11	1.60	0.83
7:G:83:ASP:HB2	7:G:101:LEU:HG	1.60	0.83
1:A:104:VAL:HG12	1:A:137:LYS:HA	1.60	0.83
1:A:600:LYS:O	1:A:601:LYS:HB2	1.77	0.83
1:A:586:VAL:HA	1:A:596:GLY:HA3	1.60	0.83
2:R:646:TRP:CZ3	2:R:648:PRO:HB2	2.14	0.82
3:C:28:ILE:HD13	9:K:14:HIS:NE2	1.93	0.82
3:C:163:MET:CB	3:C:164:SER:HA	2.08	0.82
2:B:1069:TYR:HA	2:B:1070:ILE:HB	1.59	0.82
2:B:1031:PHE:CD1	2:B:1052:LEU:HD11	2.14	0.82
2:B:213:PHE:HB2	2:B:259:LEU:HD11	1.60	0.81
5:T:30:LEU:HD13	5:T:72:PHE:CZ	2.16	0.81
7:V:83:ASP:HB2	7:V:101:LEU:HG	1.63	0.81
2:R:767:LYS:CE	2:R:767:LYS:HA	2.10	0.81
9:I:14:HIS:CD2	3:Y:28:ILE:HD13	2.15	0.81
2:R:767:LYS:HB3	2:R:768:TYR:CA	2.11	0.81
2:R:1031:PHE:CD1	2:R:1052:LEU:HD11	2.16	0.81
1:A:103:ARG:NE	1:A:191:ASP:OD1	2.14	0.81
9:I:14:HIS:NE2	3:Y:28:ILE:HD13	1.96	0.81
3:Y:163:MET:HB2	3:Y:164:SER:HA	1.62	0.81
3:C:163:MET:HB2	3:C:164:SER:HA	1.63	0.81
5:E:114:THR:CB	5:E:115:ASP:HA	2.11	0.81
1:W:104:VAL:CG1	1:W:137:LYS:CB	2.58	0.81
1:A:474:ALA:HB2	9:K:62:ILE:CD1	2.09	0.81
3:C:64:ILE:HG22	3:C:65:ALA:H	1.46	0.80
2:R:26:LEU:HG	2:R:27:VAL:HG23	1.64	0.80
2:B:113:GLU:HB3	2:B:114:PRO:CD	2.10	0.80
2:R:856:THR:HG23	13:X:32:LYS:O	1.81	0.80
2:B:646:TRP:CZ3	2:B:648:PRO:HB2	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:953:ILE:HD13	2:R:953:ILE:H	1.45	0.80
1:W:600:LYS:O	1:W:601:LYS:HB2	1.81	0.80
2:R:46:ILE:HG13	2:R:66:ILE:HD11	1.64	0.80
2:B:598:GLU:OE2	2:B:605:ILE:HG13	1.83	0.79
2:R:766:VAL:HG22	2:R:767:LYS:H	1.47	0.79
1:A:309:PHE:O	1:A:310:ARG:HG3	1.82	0.79
3:Y:149:ILE:HD13	3:Y:230:LYS:HB3	1.64	0.79
3:Y:163:MET:CB	3:Y:164:SER:HA	2.12	0.79
2:B:371:GLN:HG3	2:B:387:LEU:HD22	1.64	0.79
1:A:258:PRO:HD2	1:A:261:ILE:HD12	1.65	0.79
2:B:873:ARG:HB3	2:B:999:MET:HE1	1.65	0.79
5:T:114:THR:CB	5:T:115:ASP:HA	2.13	0.79
7:V:114:LYS:C	7:V:115:ILE:HD12	2.08	0.78
2:B:26:LEU:HG	2:B:27:VAL:HG23	1.64	0.78
2:B:767:LYS:CB	2:B:768:TYR:CD1	2.65	0.78
2:R:113:GLU:HB3	2:R:114:PRO:CD	2.12	0.78
2:R:213:PHE:HB2	2:R:259:LEU:HD11	1.63	0.78
2:R:371:GLN:HG3	2:R:387:LEU:HD22	1.66	0.78
2:R:602:SER:HB2	2:R:605:ILE:HG21	1.64	0.78
1:A:104:VAL:O	1:A:104:VAL:HG12	1.82	0.78
1:A:238:LYS:NZ	1:A:275:THR:HG22	1.99	0.78
2:R:752:MET:HE1	2:R:910:ASP:HB3	1.66	0.78
1:A:99:ARG:HH12	1:A:147:PRO:HG2	1.48	0.78
2:R:31:LEU:HA	2:R:125:MET:HE1	1.66	0.78
2:R:767:LYS:CB	2:R:768:TYR:CD1	2.67	0.78
1:W:104:VAL:HG12	1:W:137:LYS:CG	2.14	0.78
2:B:1069:TYR:CA	2:B:1070:ILE:HB	2.14	0.78
13:X:5:ARG:CD	13:X:18:LEU:HD13	2.13	0.78
2:B:31:LEU:HA	2:B:125:MET:HE1	1.64	0.77
3:C:274:THR:HG22	3:C:276:ASN:H	1.50	0.77
2:B:774:ASP:OD1	2:B:819:PRO:HD3	1.83	0.77
2:R:101:LEU:HD12	2:R:103:MET:HE3	1.66	0.77
2:R:974:TYR:CE2	2:R:981:LYS:HB3	2.18	0.77
1:W:98:CYS:C	1:W:146:CYS:SG	2.65	0.77
2:B:856:THR:HG23	13:P:32:LYS:O	1.83	0.77
2:R:884:ARG:NH1	2:R:992:TYR:HB3	2.00	0.77
2:R:767:LYS:HA	2:R:767:LYS:HE3	1.66	0.77
2:B:598:GLU:HA	2:B:605:ILE:HD12	1.67	0.77
1:W:586:VAL:HA	1:W:596:GLY:HA3	1.65	0.77
2:B:598:GLU:HA	2:B:605:ILE:CD1	2.15	0.77
5:E:165:ARG:C	5:E:167:PRO:HD2	2.10	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:62:ILE:CD1	1:W:474:ALA:HB2	2.14	0.77
11:M:69:LEU:O	11:M:73:ILE:HG12	1.85	0.77
2:R:742:ILE:HG23	2:R:912:ILE:HB	1.67	0.77
1:W:99:ARG:NH1	1:W:147:PRO:HG2	2.00	0.77
13:X:10:TRP:HB2	13:X:31:TYR:CE2	2.19	0.77
1:A:12:GLY:HA3	1:A:201:THR:HG22	1.66	0.77
13:P:10:TRP:HB2	13:P:31:TYR:CE2	2.20	0.77
3:Y:64:ILE:HG22	3:Y:65:ALA:H	1.46	0.77
2:B:46:ILE:HG13	2:B:66:ILE:CD1	2.15	0.76
11:L:69:LEU:O	11:L:73:ILE:HG12	1.84	0.76
13:X:17:GLN:HG3	13:X:19:LYS:HG2	1.67	0.76
9:I:55:ASN:CA	9:I:56:ILE:N	2.47	0.76
2:R:207:ARG:HB2	2:R:216:SER:HB3	1.66	0.76
2:B:974:TYR:CE2	2:B:981:LYS:HB3	2.21	0.76
4:D:209:CYS:SG	4:D:219:ILE:HD11	2.25	0.76
1:W:104:VAL:CG1	1:W:137:LYS:HB3	2.16	0.76
2:B:207:ARG:HB2	2:B:216:SER:HB3	1.66	0.76
3:Y:30:GLU:HG3	3:Y:31:ASP:N	1.99	0.76
1:A:763:THR:HG21	1:A:771:PRO:HB3	1.69	0.75
1:W:238:LYS:NZ	1:W:275:THR:HG22	2.01	0.75
5:E:113:ILE:HD12	5:E:164:MET:SD	2.26	0.75
2:R:1069:TYR:CA	2:R:1070:ILE:HB	2.17	0.75
2:B:594:ARG:NH1	2:B:615:LYS:HB2	2.01	0.75
9:K:55:ASN:CA	9:K:56:ILE:N	2.49	0.75
1:A:177:PRO:HD2	1:A:266:TRP:HZ2	1.52	0.75
3:C:388:LEU:CD1	9:K:35:VAL:HG12	2.17	0.75
2:R:594:ARG:NH1	2:R:615:LYS:HB2	2.02	0.75
2:B:605:ILE:HG12	2:B:606:THR:H	1.51	0.75
3:C:28:ILE:HD13	9:K:14:HIS:CD2	2.21	0.75
1:A:106:ILE:HG22	1:A:107:SER:H	1.51	0.75
2:B:752:MET:HE1	2:B:910:ASP:HB3	1.67	0.75
3:C:30:GLU:HG3	3:C:31:ASP:N	2.01	0.75
7:G:72:CYS:HB3	7:G:114:LYS:HG2	1.68	0.75
4:S:207:GLU:HG2	4:S:210:LEU:HD12	1.69	0.75
2:B:215:VAL:HG13	2:B:216:SER:N	2.01	0.74
2:R:133:ILE:HA	2:R:136:TYR:CD1	2.22	0.74
1:W:103:ARG:CB	1:W:191:ASP:OD1	2.34	0.74
1:W:141:MET:HA	1:W:148:HIS:CB	2.17	0.74
1:A:421:ARG:HB2	1:A:462:MET:HE3	1.69	0.74
8:Z:45:ILE:O	8:Z:81:VAL:HA	1.86	0.74
2:B:767:LYS:CE	2:B:767:LYS:HA	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:40:VAL:HG11	12:N:46:ARG:HG3	1.68	0.74
1:W:104:VAL:HG13	1:W:104:VAL:O	1.87	0.74
2:B:742:ILE:HG23	2:B:912:ILE:HB	1.70	0.74
2:B:897:GLN:HG3	2:B:908:VAL:HG21	1.68	0.74
2:R:774:ASP:OD1	2:R:819:PRO:HD3	1.88	0.74
1:W:418:LEU:HD23	1:W:430:MET:HE2	1.69	0.74
1:W:820:GLN:O	1:W:824:ILE:HB	1.88	0.74
1:A:103:ARG:HB2	1:A:191:ASP:OD1	1.87	0.74
2:B:31:LEU:CD2	2:B:125:MET:HE3	2.17	0.74
2:B:767:LYS:HA	2:B:767:LYS:HE3	1.69	0.74
1:A:141:MET:HA	1:A:148:HIS:CB	2.18	0.74
2:B:86:MET:HE3	2:B:686:ASN:ND2	2.03	0.74
2:R:113:GLU:HB3	2:R:114:PRO:HD2	1.70	0.74
4:S:206:CYS:HG	16:S:1001:F3S:FE4	1.04	0.74
9:I:35:VAL:HG12	3:Y:388:LEU:CD1	2.18	0.74
2:B:884:ARG:NH1	2:B:992:TYR:HB3	2.03	0.73
2:R:598:GLU:HA	2:R:605:ILE:CD1	2.18	0.73
2:B:86:MET:HE1	2:B:690:ARG:HD2	1.70	0.73
2:R:86:MET:HE1	2:R:690:ARG:HD2	1.70	0.73
3:Y:274:THR:HG22	3:Y:276:ASN:H	1.52	0.73
1:A:651:VAL:HG11	1:A:743:MET:HB3	1.70	0.73
2:B:113:GLU:HB3	2:B:114:PRO:HD2	1.70	0.73
8:H:45:ILE:O	8:H:81:VAL:HA	1.89	0.73
1:W:651:VAL:HG11	1:W:743:MET:HB3	1.70	0.73
1:A:769:PHE:CE2	1:A:778:ALA:HA	2.23	0.73
2:B:157:VAL:HG21	2:B:402:ALA:HB2	1.69	0.73
5:E:136:ILE:HG22	5:E:137:GLN:H	1.53	0.73
8:H:39:PRO:HB2	8:H:80:TYR:CE1	2.23	0.73
2:R:31:LEU:CD2	2:R:125:MET:HE3	2.17	0.73
1:W:421:ARG:HB2	1:W:462:MET:HE3	1.71	0.73
3:Y:80:GLU:HB3	3:Y:81:PRO:HD3	1.70	0.73
2:B:190:ALA:HB3	2:B:208:LEU:HD12	1.69	0.73
2:R:543:ILE:HD12	2:R:558:VAL:HG21	1.71	0.73
8:Z:39:PRO:HB2	8:Z:80:TYR:CE1	2.24	0.73
1:W:854:GLY:O	3:Y:64:ILE:HG12	1.88	0.72
1:A:241:ASP:OD2	1:A:289:HIS:CE1	2.43	0.72
2:R:46:ILE:HG13	2:R:66:ILE:CD1	2.19	0.72
1:A:426:HIS:NE2	3:C:80:GLU:OE1	2.23	0.72
1:A:618:GLU:O	1:A:619:TYR:CG	2.43	0.72
2:B:101:LEU:HD12	2:B:103:MET:HE3	1.70	0.72
2:R:1054:ASP:HA	2:R:1058:ARG:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:X:5:ARG:O	13:X:6:CYS:SG	2.48	0.72
1:W:769:PHE:CE2	1:W:778:ALA:HA	2.25	0.72
2:B:133:ILE:HA	2:B:136:TYR:CD1	2.24	0.72
2:R:215:VAL:HG13	2:R:216:SER:N	2.03	0.72
2:R:563:THR:HG22	2:R:564:ASP:H	1.53	0.72
1:W:95:LYS:HB3	1:W:138:LYS:HG2	1.70	0.72
1:A:271:TYR:CE2	1:A:285:PRO:HB3	2.24	0.72
7:G:103:VAL:HG13	7:G:104:LYS:HD2	1.72	0.72
7:V:72:CYS:SG	7:V:114:LYS:HB3	2.30	0.72
1:W:648:LEU:HD21	1:W:787:ARG:NH1	2.05	0.72
2:B:207:ARG:HB2	2:B:216:SER:CB	2.20	0.71
2:B:563:THR:HG22	2:B:564:ASP:H	1.54	0.71
13:P:5:ARG:CD	13:P:18:LEU:HD13	2.19	0.71
10:Q:46:LYS:HE2	10:Q:50:ILE:HD11	1.71	0.71
2:R:605:ILE:HG12	2:R:606:THR:H	1.55	0.71
1:W:107:SER:O	1:W:109:ASP:N	2.23	0.71
1:A:447:LEU:HD13	2:B:737:MET:SD	2.30	0.71
2:B:194:SER:HB2	2:B:303:HIS:HB3	1.72	0.71
9:K:50:LEU:O	9:K:51:ILE:O	2.08	0.71
2:R:897:GLN:HG3	2:R:908:VAL:HG21	1.72	0.71
1:A:648:LEU:HD21	1:A:787:ARG:NH1	2.05	0.71
1:W:12:GLY:HA3	1:W:201:THR:HG22	1.71	0.71
1:A:304:GLY:C	1:A:306:GLU:H	1.98	0.71
2:B:289:ILE:O	2:B:293:GLN:HG3	1.90	0.71
2:R:663:HIS:CE1	2:R:928:MET:HE1	2.25	0.71
2:R:1110:MET:HE2	1:W:298:LEU:HB3	1.70	0.71
5:T:113:ILE:HD12	5:T:164:MET:SD	2.29	0.71
1:W:258:PRO:HD2	1:W:261:ILE:HD12	1.71	0.71
1:W:324:THR:HG21	1:W:441:LEU:O	1.90	0.71
1:A:105:LYS:NZ	1:A:133:THR:HG23	2.05	0.71
2:B:208:LEU:HD23	2:B:215:VAL:HG23	1.72	0.71
3:C:53:ASP:HA	3:C:56:ILE:HG12	1.73	0.71
2:R:207:ARG:HB2	2:R:216:SER:CB	2.21	0.71
1:W:241:ASP:OD2	1:W:289:HIS:CE1	2.44	0.71
2:B:1017:ARG:HD3	2:B:1098:TYR:CD2	2.26	0.71
3:C:30:GLU:HG3	3:C:31:ASP:H	1.54	0.71
3:C:270:ALA:HA	8:H:14:HIS:HB3	1.73	0.71
1:W:98:CYS:O	1:W:99:ARG:HB2	1.89	0.71
2:B:213:PHE:HB2	2:B:259:LEU:CD1	2.21	0.71
1:W:104:VAL:HG12	1:W:137:LYS:HG2	1.73	0.71
2:B:663:HIS:CE1	2:B:928:MET:HE1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:859:TYR:HE2	3:C:65:ALA:HB2	1.56	0.70
2:B:1074:ASP:HB3	2:B:1075:LYS:HB3	1.73	0.70
1:W:105:LYS:HZ2	1:W:133:THR:HG23	1.55	0.70
1:A:107:SER:O	1:A:109:ASP:N	2.23	0.70
4:D:51:SER:HB2	4:D:52:PRO:HD2	1.73	0.70
5:E:165:ARG:C	5:E:167:PRO:CD	2.63	0.70
2:R:208:LEU:HD23	2:R:215:VAL:HG23	1.73	0.70
2:R:1069:TYR:HA	2:R:1070:ILE:HB	1.72	0.70
5:T:165:ARG:C	5:T:167:PRO:HD2	2.15	0.70
1:A:668:ALA:CB	1:A:707:LEU:HD13	2.21	0.70
1:A:820:GLN:O	1:A:824:ILE:HB	1.92	0.70
3:C:186:LYS:HB3	3:C:230:LYS:HE2	1.72	0.70
2:R:734:GLY:HA3	2:R:735:TYR:CG	2.26	0.70
1:W:426:HIS:NE2	3:Y:80:GLU:OE1	2.25	0.70
2:R:873:ARG:HB3	2:R:999:MET:HE1	1.72	0.70
1:W:308:ARG:HA	1:W:312:ASN:HB2	1.73	0.70
1:W:618:GLU:O	1:W:619:TYR:CG	2.44	0.70
1:W:763:THR:HG21	1:W:771:PRO:HB3	1.73	0.70
1:W:271:TYR:CE2	1:W:285:PRO:HB3	2.27	0.70
1:W:184:LEU:HB3	1:W:204:PRO:HB2	1.73	0.70
1:A:324:THR:HG21	1:A:441:LEU:O	1.91	0.70
7:G:103:VAL:HG22	7:G:104:LYS:H	1.56	0.70
1:A:95:LYS:HB3	1:A:138:LYS:HE2	1.72	0.69
2:R:856:THR:HG22	2:R:857:GLU:H	1.55	0.69
1:W:589:LYS:HD3	1:W:877:GLY:O	1.92	0.69
3:C:277:ILE:HG22	3:C:278:ARG:H	1.55	0.69
2:R:406:TRP:CG	2:R:407:VAL:H	2.10	0.69
2:R:598:GLU:OE2	2:R:605:ILE:HG13	1.92	0.69
1:A:103:ARG:HB2	1:A:191:ASP:OD2	1.92	0.69
1:A:308:ARG:HA	1:A:312:ASN:HB2	1.74	0.69
1:A:872:PHE:CD2	1:A:876:VAL:HG11	2.27	0.69
3:C:340:SER:HB3	3:C:371:GLU:HG2	1.74	0.69
2:R:598:GLU:HA	2:R:605:ILE:HD12	1.74	0.69
2:B:9:SER:HB3	2:B:12:GLU:HB3	1.74	0.69
1:W:177:PRO:HD2	1:W:266:TRP:HZ2	1.57	0.69
2:B:84:SER:OG	2:B:144:ILE:HG23	1.92	0.69
2:B:768:TYR:CB	2:B:769:PRO:CD	2.66	0.69
2:R:157:VAL:HG21	2:R:402:ALA:HB2	1.75	0.69
2:R:249:PRO:CB	2:R:252:GLN:HB2	2.22	0.69
3:C:231:ILE:HG23	3:C:232:LYS:N	2.08	0.69
2:R:928:MET:HE3	2:R:953:ILE:HD12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:618:GLU:O	1:W:619:TYR:CD2	2.45	0.69
1:A:184:LEU:HB3	1:A:204:PRO:HB2	1.74	0.69
3:C:244:LYS:HA	3:C:245:LYS:CB	2.16	0.69
1:A:95:LYS:HB3	1:A:138:LYS:HG2	1.75	0.69
2:B:66:ILE:HG13	2:B:101:LEU:HD23	1.74	0.69
2:R:658:ILE:HG12	2:R:672:GLN:HG2	1.75	0.69
5:T:144:ALA:HA	5:T:169:LEU:HD23	1.75	0.69
2:B:787:LYS:HE3	2:B:841:VAL:CG2	2.23	0.68
1:W:668:ALA:CB	1:W:707:LEU:HD13	2.22	0.68
1:A:792:PRO:HG3	2:B:948:PHE:CE1	2.28	0.68
2:B:396:ARG:NH2	2:B:406:TRP:CH2	2.61	0.68
12:O:40:VAL:HG11	12:O:46:ARG:HG3	1.75	0.68
1:A:854:GLY:O	3:C:64:ILE:HG12	1.93	0.68
2:B:543:ILE:HD12	2:B:558:VAL:HG21	1.74	0.68
3:C:340:SER:HA	3:C:364:GLU:HG2	1.75	0.68
2:R:212:THR:O	2:R:213:PHE:HB2	1.92	0.68
3:C:388:LEU:HD13	9:K:35:VAL:HG12	1.75	0.68
7:V:103:VAL:HG13	7:V:104:LYS:HD2	1.74	0.68
5:E:114:THR:OG1	5:E:115:ASP:HA	1.93	0.68
6:F:48:ASP:HB3	6:F:51:SER:HB2	1.74	0.68
2:R:84:SER:OG	2:R:144:ILE:HG23	1.93	0.68
1:A:875:VAL:HG12	1:A:876:VAL:H	1.59	0.68
2:R:984:SER:O	2:R:985:ARG:HB2	1.94	0.68
2:B:1017:ARG:HD3	2:B:1098:TYR:CE2	2.29	0.68
5:E:144:ALA:HA	5:E:169:LEU:HD23	1.75	0.68
1:W:105:LYS:NZ	1:W:133:THR:HG23	2.09	0.68
2:B:660:TYR:HD1	2:B:950:LYS:HE3	1.58	0.68
3:C:393:ILE:HG22	5:E:19:GLY:H	1.57	0.68
1:A:311:GLY:HA2	2:B:1030:ARG:HH22	1.59	0.68
1:W:78:VAL:O	1:W:79:ARG:HB2	1.93	0.68
1:W:224:MET:C	1:W:224:MET:HE2	2.18	0.68
1:W:304:GLY:C	1:W:306:GLU:H	2.02	0.68
2:B:186:ILE:HD12	2:B:209:LYS:HD3	1.76	0.67
2:B:252:GLN:HB3	2:B:326:ILE:HD12	1.74	0.67
9:I:50:LEU:O	9:I:51:ILE:O	2.11	0.67
1:A:848:VAL:O	1:A:849:ALA:HB3	1.94	0.67
5:E:7:ALA:HA	6:F:7:VAL:HG13	1.76	0.67
2:B:330:LEU:O	2:B:332:ARG:HG2	1.94	0.67
2:B:658:ILE:HG12	2:B:672:GLN:HG2	1.75	0.67
2:B:686:ASN:O	2:B:690:ARG:HG2	1.93	0.67
2:R:86:MET:HE3	2:R:686:ASN:ND2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:252:GLN:HB3	2:R:326:ILE:HD12	1.76	0.67
5:T:114:THR:OG1	5:T:115:ASP:HA	1.94	0.67
1:W:309:PHE:O	1:W:310:ARG:HG3	1.95	0.67
1:W:848:VAL:O	1:W:849:ALA:HB3	1.94	0.67
1:A:330:PRO:HG3	2:B:734:GLY:HA2	1.76	0.67
1:A:474:ALA:HB2	9:K:62:ILE:HD12	1.76	0.67
2:R:213:PHE:HB2	2:R:259:LEU:CD1	2.24	0.67
1:A:418:LEU:HD23	1:A:430:MET:HE2	1.76	0.67
2:R:1047:LEU:HD21	1:W:418:LEU:HD21	1.77	0.67
2:R:1074:ASP:HB3	2:R:1075:LYS:HB3	1.77	0.67
13:X:31:TYR:CE2	13:X:33:ILE:HB	2.29	0.67
2:R:1017:ARG:HD3	2:R:1098:TYR:CD2	2.30	0.67
1:W:104:VAL:CG1	1:W:137:LYS:HG2	2.25	0.67
3:C:277:ILE:C	3:C:279:GLU:H	2.02	0.67
9:K:82:LEU:HD11	9:K:88:ILE:HD11	1.76	0.67
2:R:161:GLU:OE2	2:R:690:ARG:NH2	2.28	0.67
13:P:31:TYR:CE2	13:P:33:ILE:HB	2.30	0.67
13:X:5:ARG:HG2	13:X:18:LEU:HB2	1.75	0.67
2:B:401:LEU:HG	2:B:401:LEU:O	1.94	0.67
5:E:6:LYS:O	6:F:7:VAL:HG22	1.95	0.67
11:L:74:GLU:HG2	11:L:77:ARG:NH2	2.09	0.67
12:O:47:ARG:CZ	12:O:48:MET:HE2	2.25	0.67
1:W:97:THR:HG23	1:W:102:GLY:HA2	1.76	0.67
1:A:372:TRP:CD1	1:A:372:TRP:C	2.73	0.67
2:B:348:LEU:O	2:B:352:LEU:HB2	1.94	0.67
2:B:584:ILE:HD11	2:B:617:GLU:HB2	1.76	0.67
5:T:30:LEU:HD22	5:T:72:PHE:CE2	2.30	0.67
13:X:5:ARG:HD2	13:X:18:LEU:HD13	1.75	0.67
2:R:190:ALA:HB3	2:R:208:LEU:HD12	1.76	0.66
1:A:603:ILE:HG21	1:A:632:PHE:HE1	1.60	0.66
1:A:792:PRO:HG3	2:B:948:PHE:CD1	2.30	0.66
2:B:641:THR:HG22	2:B:642:HIS:CE1	2.31	0.66
2:B:893:MET:HG3	2:B:894:LEU:N	2.09	0.66
3:C:340:SER:HA	3:C:364:GLU:CG	2.25	0.66
1:W:603:ILE:HG21	1:W:632:PHE:HE1	1.59	0.66
13:X:17:GLN:CG	13:X:19:LYS:HG2	2.25	0.66
2:B:1054:ASP:HA	2:B:1058:ARG:HD2	1.78	0.66
3:C:163:MET:O	3:C:208:ILE:HA	1.95	0.66
5:E:60:VAL:HG22	5:E:61:PHE:H	1.60	0.66
8:H:25:ILE:HG22	10:Q:55:LEU:CD2	2.24	0.66
5:T:165:ARG:C	5:T:167:PRO:CD	2.68	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:123:LYS:HA	1:W:126:PRO:CG	2.26	0.66
2:B:432:VAL:HG21	2:B:456:MET:HE3	1.78	0.66
4:D:45:TYR:HB3	13:P:42:ILE:HD11	1.78	0.66
13:P:31:TYR:HE2	13:P:33:ILE:HB	1.61	0.66
1:A:502:TYR:CE2	2:B:737:MET:HE1	2.31	0.66
2:B:622:GLU:O	2:B:625:GLU:HB3	1.96	0.66
3:C:277:ILE:HG22	3:C:278:ARG:N	2.11	0.66
2:R:417:LEU:HD21	2:R:425:MET:HG3	1.76	0.66
1:W:703:THR:HG22	1:W:707:LEU:HD12	1.78	0.66
3:Y:163:MET:O	3:Y:208:ILE:HA	1.96	0.66
3:Y:168:GLN:CG	3:Y:204:ASN:OD1	2.34	0.66
3:Y:231:ILE:HG23	3:Y:232:LYS:N	2.09	0.66
9:I:82:LEU:HD11	9:I:88:ILE:HD11	1.75	0.66
10:J:46:LYS:HE2	10:J:50:ILE:HD11	1.78	0.66
1:W:125:TRP:N	1:W:126:PRO:HD2	2.11	0.66
13:X:18:LEU:HD12	13:X:18:LEU:O	1.95	0.66
3:Y:270:ALA:HA	8:Z:14:HIS:HB3	1.76	0.66
1:A:238:LYS:CE	1:A:276:TYR:HA	2.26	0.66
5:E:83:GLU:HA	6:F:89:MET:HE3	1.76	0.66
12:N:3:ILE:HG23	12:N:52:HIS:CD2	2.30	0.66
2:R:584:ILE:HD11	2:R:617:GLU:HB2	1.76	0.66
2:B:322:ILE:O	2:B:326:ILE:HG12	1.95	0.66
2:B:734:GLY:HA3	2:B:735:TYR:CG	2.31	0.66
5:E:114:THR:HB	5:E:115:ASP:CA	2.25	0.66
13:P:18:LEU:HD12	13:P:18:LEU:O	1.95	0.66
4:D:207:GLU:HG2	4:D:210:LEU:HD12	1.77	0.66
2:R:737:MET:HE1	1:W:502:TYR:CE2	2.31	0.66
2:R:1007:ARG:NH1	2:R:1028:GLY:C	2.54	0.66
1:W:872:PHE:CD2	1:W:876:VAL:HG11	2.30	0.66
3:C:147:THR:HB	3:C:232:LYS:HB2	1.77	0.66
3:Y:244:LYS:HA	3:Y:245:LYS:CB	2.16	0.66
3:Y:340:SER:HA	3:Y:364:GLU:CG	2.26	0.66
3:Y:340:SER:HB3	3:Y:371:GLU:HG2	1.77	0.66
1:A:430:MET:HE1	2:B:1031:PHE:HE2	1.61	0.65
2:B:105:PRO:HD2	2:B:112:ALA:HB3	1.79	0.65
3:C:169:LEU:HD23	3:C:174:LEU:CD2	2.26	0.65
3:C:327:ARG:HG3	3:C:334:VAL:HG23	1.78	0.65
7:G:80:GLU:HG3	7:G:81:LEU:H	1.61	0.65
2:R:1017:ARG:HD3	2:R:1098:TYR:CE2	2.31	0.65
1:W:103:ARG:HB2	1:W:191:ASP:OD2	1.96	0.65
1:W:104:VAL:CG1	1:W:137:LYS:HA	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:238:LYS:CE	1:W:276:TYR:HA	2.26	0.65
1:W:875:VAL:HG12	1:W:876:VAL:H	1.61	0.65
2:B:815:GLY:HA2	2:B:839:SER:OG	1.96	0.65
7:G:25:ASN:HA	7:G:44:ASP:OD2	1.96	0.65
2:R:322:ILE:O	2:R:326:ILE:HG12	1.95	0.65
2:R:815:GLY:HA2	2:R:839:SER:OG	1.96	0.65
1:A:642:GLN:OE1	1:A:642:GLN:HA	1.97	0.65
4:D:108:MET:HG2	4:D:110:TYR:CZ	2.31	0.65
5:E:114:THR:CB	5:E:115:ASP:CA	2.75	0.65
2:R:66:ILE:HG13	2:R:101:LEU:HD23	1.78	0.65
1:W:104:VAL:HG12	1:W:137:LYS:CB	2.25	0.65
1:A:125:TRP:N	1:A:126:PRO:HD2	2.12	0.65
1:A:736:SER:HB3	1:A:739:ASN:CG	2.22	0.65
2:B:1007:ARG:NH1	2:B:1028:GLY:C	2.55	0.65
2:R:432:VAL:HG21	2:R:456:MET:HE3	1.77	0.65
4:S:51:SER:HB2	4:S:52:PRO:HD2	1.78	0.65
3:Y:168:GLN:HG2	3:Y:204:ASN:CG	2.21	0.65
1:A:703:THR:HG22	1:A:707:LEU:HD12	1.78	0.65
2:R:622:GLU:O	2:R:625:GLU:HB3	1.96	0.65
2:R:874:ILE:H	2:R:874:ILE:HD12	1.62	0.65
4:S:111:SER:HB3	4:S:128:ILE:HB	1.78	0.65
5:T:114:THR:CB	5:T:115:ASP:CA	2.75	0.65
5:T:114:THR:HB	5:T:115:ASP:CA	2.27	0.65
1:W:103:ARG:NE	1:W:191:ASP:OD1	2.30	0.65
1:W:104:VAL:HG11	1:W:137:LYS:HB3	1.79	0.65
1:A:13:ILE:HD12	1:A:202:SER:HB2	1.78	0.65
1:A:589:LYS:HD3	1:A:877:GLY:O	1.97	0.65
2:B:46:ILE:O	2:B:46:ILE:HG22	1.96	0.65
2:B:253:ASN:O	2:B:257:PRO:HD2	1.96	0.65
2:B:974:TYR:CE2	4:D:165:ARG:HA	2.30	0.65
12:N:47:ARG:CZ	12:N:48:MET:HE2	2.26	0.65
2:R:289:ILE:O	2:R:293:GLN:HG3	1.97	0.65
7:V:80:GLU:HG3	7:V:81:LEU:H	1.62	0.65
3:C:169:LEU:HD23	3:C:174:LEU:HD21	1.78	0.65
2:R:46:ILE:O	2:R:46:ILE:HG22	1.95	0.65
5:T:83:GLU:HA	6:U:89:MET:HE3	1.77	0.65
4:D:53:LEU:HD12	4:D:131:VAL:HG23	1.79	0.65
3:Y:340:SER:HA	3:Y:364:GLU:HG2	1.77	0.65
4:D:17:PHE:O	4:D:225:LYS:HA	1.97	0.65
4:S:33:MET:HE3	4:S:162:ALA:HB3	1.78	0.65
1:A:106:ILE:H	1:A:106:ILE:HD12	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:GLU:O	1:A:619:TYR:CD2	2.50	0.64
5:E:136:ILE:HG22	5:E:137:GLN:N	2.11	0.64
1:W:426:HIS:CG	3:Y:80:GLU:OE2	2.51	0.64
1:A:682:GLY:O	1:A:684:LEU:N	2.30	0.64
2:B:212:THR:O	2:B:213:PHE:HB2	1.96	0.64
4:D:33:MET:HE3	4:D:162:ALA:HB3	1.79	0.64
8:H:25:ILE:HG22	10:Q:55:LEU:HD21	1.80	0.64
2:R:660:TYR:HD1	2:R:950:LYS:HE3	1.62	0.64
12:O:8:PHE:CD2	12:O:48:MET:HE1	2.32	0.64
2:R:253:ASN:O	2:R:257:PRO:HD2	1.96	0.64
4:S:45:TYR:HB3	13:X:42:ILE:HD11	1.79	0.64
4:S:159:VAL:HG21	4:S:230:LEU:HD22	1.78	0.64
1:A:426:HIS:CG	3:C:80:GLU:OE2	2.50	0.64
2:B:86:MET:HE3	2:B:686:ASN:HD22	1.61	0.64
5:E:123:VAL:HG22	5:E:127:ILE:HG12	1.80	0.64
2:R:737:MET:SD	1:W:447:LEU:HD13	2.37	0.64
1:A:78:VAL:O	1:A:79:ARG:HB2	1.96	0.64
1:A:311:GLY:HA2	2:B:1030:ARG:NH2	2.13	0.64
1:A:426:HIS:CD2	3:C:80:GLU:CD	2.75	0.64
2:B:405:ASN:HB2	2:B:413:VAL:HB	1.79	0.64
4:D:99:GLU:HA	4:D:139:ILE:O	1.97	0.64
8:H:29:TYR:HE1	10:Q:60:SER:CB	2.11	0.64
13:P:5:ARG:O	13:P:6:CYS:SG	2.56	0.64
2:R:641:THR:HG22	2:R:642:HIS:CE1	2.32	0.64
1:W:426:HIS:CD2	3:Y:80:GLU:CD	2.75	0.64
1:A:177:PRO:HD2	1:A:266:TRP:CZ2	2.32	0.64
1:A:474:ALA:HB2	9:K:62:ILE:HD11	1.78	0.64
2:B:1104:ILE:HD13	2:B:1116:LEU:HD11	1.80	0.64
5:E:30:LEU:HD13	5:E:72:PHE:CE2	2.33	0.64
13:P:5:ARG:O	13:P:6:CYS:CB	2.45	0.64
2:R:731:SER:HB2	1:W:501:ASP:OD2	1.98	0.64
2:R:742:ILE:CG2	2:R:912:ILE:HB	2.27	0.64
4:S:17:PHE:O	4:S:225:LYS:HA	1.98	0.64
1:W:418:LEU:HB3	1:W:430:MET:HE2	1.78	0.64
1:A:108:GLU:O	1:A:111:ILE:N	2.30	0.64
1:A:603:ILE:HG21	1:A:632:PHE:CE1	2.32	0.64
3:C:168:GLN:HG2	3:C:204:ASN:CG	2.22	0.64
5:T:7:ALA:HA	6:U:7:VAL:HG13	1.80	0.64
6:U:48:ASP:HB3	6:U:51:SER:HB2	1.79	0.64
7:V:25:ASN:HA	7:V:44:ASP:OD2	1.97	0.64
1:A:654:GLY:HA2	1:A:658:LYS:HE3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:GLU:OE2	2:B:690:ARG:NH2	2.31	0.64
9:I:56:ILE:O	9:I:57:SER:CA	2.33	0.64
11:M:74:GLU:HG2	11:M:77:ARG:NH2	2.12	0.64
2:R:396:ARG:NH2	2:R:406:TRP:CH2	2.66	0.64
2:R:462:PRO:O	2:R:467:SER:HA	1.98	0.64
5:T:123:VAL:HG13	5:T:127:ILE:HG12	1.80	0.64
3:C:216:ILE:O	3:C:217:ALA:CB	2.45	0.64
2:R:170:LEU:HD21	2:R:176:LEU:CD1	2.28	0.64
2:R:686:ASN:O	2:R:690:ARG:HG2	1.98	0.64
5:T:136:ILE:HG22	5:T:137:GLN:N	2.12	0.64
4:S:99:GLU:HA	4:S:139:ILE:O	1.98	0.63
4:S:206:CYS:SG	16:S:1001:F3S:FE4	1.89	0.63
1:A:238:LYS:HZ2	1:A:275:THR:HG22	1.61	0.63
1:A:309:PHE:O	1:A:310:ARG:CG	2.45	0.63
1:A:856:PHE:CE2	1:A:858:MET:HB3	2.33	0.63
4:D:55:ASP:HB3	13:P:45:VAL:HG21	1.79	0.63
4:D:203:CYS:SG	16:D:1001:F3S:FE3	1.89	0.63
9:I:62:ILE:HD12	1:W:474:ALA:HB2	1.79	0.63
11:M:20:GLU:HG3	11:M:24:LEU:HD23	1.80	0.63
3:Y:143:LYS:O	3:Y:234:ILE:HG12	1.98	0.63
1:A:568:VAL:HG22	1:A:731:THR:HG22	1.79	0.63
3:C:286:ILE:HG12	8:H:49:ASP:CG	2.24	0.63
9:K:51:ILE:O	9:K:52:ASP:CB	2.45	0.63
2:R:10:ILE:HA	2:R:13:ARG:HG2	1.79	0.63
2:R:212:THR:O	2:R:259:LEU:HD11	1.98	0.63
2:R:235:ILE:HG23	2:R:240:ASP:HB3	1.80	0.63
2:R:583:ILE:HD12	2:R:591:LEU:HD21	1.80	0.63
2:R:974:TYR:CE2	4:S:165:ARG:HA	2.33	0.63
1:A:418:LEU:HB3	1:A:430:MET:HE2	1.80	0.63
1:A:505:GLY:HA3	1:A:639:VAL:HG22	1.80	0.63
1:W:249:LEU:HG	1:W:265:LEU:HB3	1.80	0.63
3:Y:216:ILE:O	3:Y:217:ALA:CB	2.46	0.63
12:N:3:ILE:HD13	12:N:15:ALA:HA	1.79	0.63
2:R:734:GLY:HA2	1:W:330:PRO:HG3	1.79	0.63
3:Y:154:SER:OG	3:Y:170:ASP:HB2	1.99	0.63
1:A:123:LYS:HA	1:A:126:PRO:CG	2.28	0.63
1:A:252:SER:HB2	1:A:261:ILE:HG21	1.81	0.63
2:B:646:TRP:CD2	2:B:648:PRO:HD2	2.34	0.63
3:C:70:ILE:HA	3:C:73:VAL:HG22	1.80	0.63
2:R:954:GLU:HA	2:R:957:GLN:HB2	1.80	0.63
4:S:108:MET:HG2	4:S:110:TYR:CZ	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:324:THR:HG22	1:W:325:VAL:H	1.64	0.63
1:W:436:ARG:O	1:W:438:LEU:HD22	1.99	0.63
3:C:237:ILE:HD12	3:C:253:THR:HB	1.81	0.63
3:C:327:ARG:HG3	3:C:334:VAL:CG2	2.28	0.63
11:L:20:GLU:HG3	11:L:24:LEU:HD23	1.81	0.63
2:R:63:LEU:CD2	2:R:103:MET:HE2	2.28	0.63
2:R:105:PRO:HD2	2:R:112:ALA:HB3	1.80	0.63
4:S:203:CYS:SG	16:S:1001:F3S:S1	2.96	0.63
7:V:103:VAL:HG22	7:V:104:LYS:H	1.62	0.63
1:W:95:LYS:HB3	1:W:138:LYS:HE2	1.78	0.63
1:W:568:VAL:HG22	1:W:731:THR:HG22	1.81	0.63
1:A:436:ARG:O	1:A:438:LEU:HD22	1.99	0.63
1:A:864:LYS:HE2	8:H:71:LEU:O	1.98	0.63
2:B:63:LEU:CD2	2:B:103:MET:HE2	2.29	0.63
2:B:583:ILE:HD12	2:B:591:LEU:HD21	1.81	0.63
2:B:834:ALA:O	2:B:835:LYS:HB2	1.98	0.63
2:R:401:LEU:HG	2:R:401:LEU:O	1.98	0.63
5:T:60:VAL:HG22	5:T:61:PHE:H	1.63	0.63
1:A:353:ILE:HG21	1:A:358:ILE:HD13	1.81	0.63
2:B:406:TRP:O	2:B:408:GLY:N	2.31	0.63
2:B:462:PRO:O	2:B:467:SER:HA	1.99	0.63
2:B:1007:ARG:NH1	2:B:1028:GLY:O	2.32	0.63
2:R:330:LEU:O	2:R:332:ARG:HG2	1.98	0.63
1:W:222:SER:C	1:W:223:ILE:HG22	2.24	0.63
3:Y:277:ILE:HG22	3:Y:278:ARG:N	2.14	0.63
3:C:174:LEU:HB3	3:C:179:VAL:HG13	1.81	0.62
3:C:310:MET:HE2	8:H:70:GLN:OE1	1.99	0.62
4:D:159:VAL:HG21	4:D:230:LEU:HD22	1.81	0.62
1:W:104:VAL:CG1	1:W:137:LYS:CA	2.76	0.62
13:X:5:ARG:HG2	13:X:18:LEU:CB	2.29	0.62
3:Y:174:LEU:HB3	3:Y:179:VAL:HG13	1.80	0.62
1:A:353:ILE:CG2	1:A:358:ILE:HD13	2.29	0.62
2:B:320:TYR:CD1	2:B:529:LEU:HD12	2.33	0.62
9:I:35:VAL:HG12	3:Y:388:LEU:HD11	1.81	0.62
2:R:348:LEU:O	2:R:352:LEU:HB2	1.98	0.62
5:T:6:LYS:O	6:U:7:VAL:HG22	2.00	0.62
1:W:104:VAL:HG13	1:W:137:LYS:HA	1.79	0.62
2:B:10:ILE:HA	2:B:13:ARG:HG2	1.81	0.62
2:B:417:LEU:HD21	2:B:425:MET:HG3	1.79	0.62
2:R:834:ALA:O	2:R:835:LYS:HB2	1.98	0.62
2:R:1015:LEU:HD13	2:R:1102:LEU:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:1069:TYR:CB	2:R:1070:ILE:HB	2.30	0.62
4:S:57:ILE:O	4:S:61:ARG:HG3	1.99	0.62
1:W:856:PHE:CE2	1:W:858:MET:HB3	2.34	0.62
1:A:870:ARG:NH2	3:C:36:ILE:HD13	2.14	0.62
5:E:165:ARG:O	5:E:167:PRO:HD2	2.00	0.62
1:W:505:GLY:HA3	1:W:639:VAL:HG22	1.82	0.62
11:M:18:GLU:HG2	11:M:18:GLU:O	1.99	0.62
3:Y:70:ILE:HA	3:Y:73:VAL:HG22	1.81	0.62
2:B:766:VAL:CG1	2:B:774:ASP:OD2	2.47	0.62
12:N:30:ASN:O	12:N:34:VAL:HG23	1.99	0.62
1:W:603:ILE:HG21	1:W:632:PHE:CE1	2.34	0.62
2:B:683:TYR:CZ	2:B:687:TYR:HB2	2.34	0.62
13:P:17:GLN:CG	13:P:19:LYS:HG2	2.29	0.62
2:R:1081:VAL:HG22	2:R:1085:HIS:HA	1.81	0.62
1:W:450:CYS:HB2	1:W:451:PRO:HD3	1.82	0.62
1:W:870:ARG:CZ	1:W:870:ARG:HB2	2.29	0.62
3:Y:30:GLU:HG3	3:Y:31:ASP:H	1.64	0.62
1:A:249:LEU:HG	1:A:265:LEU:HB3	1.82	0.62
2:B:874:ILE:H	2:B:874:ILE:HD12	1.64	0.62
2:R:147:ASP:HB3	2:R:685:ALA:HB3	1.82	0.62
13:X:5:ARG:O	13:X:6:CYS:CB	2.48	0.62
2:B:742:ILE:CG2	2:B:912:ILE:HB	2.29	0.62
2:B:957:GLN:HA	2:B:960:ILE:HD11	1.82	0.62
3:C:13:LEU:HD13	3:C:48:ILE:HG12	1.81	0.62
4:S:155:LYS:HE3	4:S:156:PHE:CZ	2.35	0.62
1:W:104:VAL:CG1	1:W:137:LYS:CG	2.78	0.62
2:B:783:VAL:HG13	2:B:784:ARG:HB2	1.82	0.62
5:E:89:VAL:HG23	5:E:98:PHE:O	2.00	0.62
2:R:9:SER:HB3	2:R:12:GLU:HB3	1.80	0.62
2:R:1031:PHE:HE2	1:W:430:MET:HE1	1.65	0.62
1:A:84:VAL:HG13	1:A:274:ALA:HB1	1.80	0.61
1:A:104:VAL:CG1	1:A:137:LYS:HA	2.29	0.61
2:B:767:LYS:HB3	2:B:768:TYR:CB	2.30	0.61
2:B:1069:TYR:HA	2:B:1070:ILE:CB	2.30	0.61
8:H:65:ILE:HD11	8:H:79:ARG:HG2	1.81	0.61
9:K:43:LEU:HD13	9:K:64:ILE:HG22	1.82	0.61
12:N:64:ARG:NH2	13:P:37:VAL:HG23	2.14	0.61
12:O:3:ILE:HG23	12:O:52:HIS:CD2	2.35	0.61
1:W:13:ILE:HD12	1:W:202:SER:HB2	1.81	0.61
3:Y:262:LEU:HD22	3:Y:269:ILE:HD12	1.82	0.61
3:Y:277:ILE:HG22	3:Y:278:ARG:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:THR:O	2:B:259:LEU:HD11	2.00	0.61
2:B:984:SER:O	2:B:985:ARG:HB2	2.00	0.61
12:O:64:ARG:NH2	13:X:37:VAL:HG23	2.15	0.61
2:R:783:VAL:HG13	2:R:784:ARG:HB2	1.83	0.61
3:Y:176:ASP:O	3:Y:177:LYS:CB	2.48	0.61
2:B:147:ASP:HB3	2:B:685:ALA:HB3	1.80	0.61
7:G:72:CYS:HB3	7:G:114:LYS:CG	2.30	0.61
9:K:56:ILE:O	9:K:57:SER:CA	2.38	0.61
2:R:582:LEU:HD12	2:R:619:LEU:HD12	1.82	0.61
3:Y:147:THR:HB	3:Y:232:LYS:HB2	1.82	0.61
1:A:141:MET:HG3	1:A:148:HIS:HB3	1.82	0.61
3:C:274:THR:HB	3:C:280:ILE:HD11	1.82	0.61
3:C:297:ILE:O	3:C:301:LEU:HD12	2.01	0.61
9:I:35:VAL:HG12	3:Y:388:LEU:HD13	1.81	0.61
10:Q:66:ARG:HG2	10:Q:66:ARG:HH11	1.66	0.61
2:R:743:MET:HE1	2:R:875:PRO:HB2	1.83	0.61
7:V:102:LEU:HA	7:V:106:ILE:HG22	1.83	0.61
1:W:642:GLN:HA	1:W:642:GLN:OE1	2.00	0.61
1:A:418:LEU:HD21	2:B:1047:LEU:HD21	1.82	0.61
1:A:792:PRO:N	2:B:948:PHE:HE1	1.98	0.61
2:B:191:LYS:HE2	2:B:193:ILE:HD11	1.83	0.61
2:B:981:LYS:HE2	4:D:205:LEU:HB2	1.81	0.61
1:W:99:ARG:HH12	1:W:147:PRO:HG2	1.64	0.61
1:W:177:PRO:HD2	1:W:266:TRP:CZ2	2.36	0.61
1:W:353:ILE:CG2	1:W:358:ILE:HD13	2.30	0.61
1:A:854:GLY:O	3:C:64:ILE:CG2	2.48	0.61
2:B:170:LEU:HD21	2:B:176:LEU:CD1	2.30	0.61
2:B:356:LEU:HD12	2:B:407:VAL:HG21	1.83	0.61
3:C:143:LYS:O	3:C:234:ILE:HG12	1.98	0.61
3:C:210:PHE:O	3:C:211:ALA:HB3	2.01	0.61
4:S:209:CYS:SG	4:S:219:ILE:HD11	2.40	0.61
1:W:252:SER:HB2	1:W:261:ILE:HG21	1.82	0.61
1:A:874:ARG:HB2	3:C:54:LEU:HD21	1.80	0.61
2:B:884:ARG:HB2	2:B:884:ARG:HH11	1.65	0.61
3:C:174:LEU:H	3:C:174:LEU:HD12	1.65	0.61
4:D:60:HIS:C	4:D:60:HIS:CD2	2.78	0.61
12:N:8:PHE:CD2	12:N:48:MET:HE1	2.35	0.61
3:Y:53:ASP:HA	3:Y:56:ILE:HG12	1.81	0.61
2:B:767:LYS:CD	2:B:768:TYR:HA	2.30	0.61
2:B:1081:VAL:HG22	2:B:1085:HIS:HA	1.81	0.61
11:L:18:GLU:HG2	11:L:18:GLU:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:3:ILE:HD13	12:O:15:ALA:HA	1.83	0.61
2:R:787:LYS:HE3	2:R:841:VAL:CG2	2.31	0.61
2:R:951:THR:O	2:R:951:THR:HG22	2.01	0.61
3:Y:327:ARG:HG3	3:Y:334:VAL:CG2	2.31	0.61
3:C:174:LEU:HD12	3:C:174:LEU:N	2.15	0.61
5:E:2:TYR:HB2	6:F:12:ILE:O	2.01	0.61
8:H:82:ILE:O	8:H:82:ILE:HG22	2.01	0.61
2:R:194:SER:HB2	2:R:303:HIS:HB3	1.82	0.61
4:S:210:LEU:HD11	4:S:219:ILE:HB	1.83	0.61
1:W:104:VAL:HG12	1:W:137:LYS:HB3	1.83	0.61
1:W:418:LEU:HD23	1:W:430:MET:CE	2.31	0.61
8:Z:65:ILE:HD11	8:Z:79:ARG:HG2	1.81	0.61
2:B:372:LEU:CD2	2:B:376:LYS:HE2	2.31	0.60
2:B:783:VAL:CG1	2:B:784:ARG:HB2	2.31	0.60
9:I:52:ASP:O	9:I:53:ILE:HB	2.01	0.60
2:R:68:ILE:HG13	2:R:99:LEU:HD23	1.82	0.60
2:R:323:SER:O	2:R:327:GLU:HB2	2.01	0.60
2:R:741:ILE:HD11	2:R:911:VAL:HG13	1.83	0.60
1:W:84:VAL:HG13	1:W:274:ALA:HB1	1.83	0.60
1:W:864:LYS:HE2	8:Z:71:LEU:O	2.01	0.60
1:A:222:SER:C	1:A:223:ILE:HG22	2.26	0.60
8:H:28:ALA:HB1	8:H:62:ILE:HD11	1.83	0.60
5:T:101:LEU:HD12	5:T:101:LEU:N	2.17	0.60
7:V:9:ILE:HD13	7:V:104:LYS:HE3	1.82	0.60
4:D:67:PHE:HB3	4:D:121:ILE:HG23	1.82	0.60
4:D:97:TYR:CE1	4:D:142:GLU:HG3	2.36	0.60
9:I:51:ILE:O	9:I:52:ASP:CB	2.49	0.60
13:P:5:ARG:HG2	13:P:18:LEU:CB	2.31	0.60
3:Y:210:PHE:O	3:Y:211:ALA:HB3	2.00	0.60
2:B:86:MET:O	2:B:90:LEU:HG	2.01	0.60
2:B:249:PRO:CB	2:B:252:GLN:HB2	2.31	0.60
3:C:199:ASP:HB2	3:C:206:LEU:HB2	1.81	0.60
3:C:340:SER:CB	3:C:371:GLU:HG2	2.30	0.60
4:D:154:ALA:C	4:D:156:PHE:H	2.09	0.60
7:G:8:GLU:C	7:G:9:ILE:HG13	2.25	0.60
2:R:256:PHE:H	2:R:257:PRO:HD2	1.65	0.60
2:R:743:MET:HE3	2:R:748:VAL:CG2	2.32	0.60
3:Y:176:ASP:O	3:Y:177:LYS:HB2	2.00	0.60
1:A:238:LYS:HG3	1:A:238:LYS:O	1.99	0.60
2:B:743:MET:HE1	2:B:875:PRO:HB2	1.83	0.60
7:G:102:LEU:HA	7:G:106:ILE:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:43:LEU:HD12	10:J:43:LEU:H	1.67	0.60
13:P:5:ARG:HD3	13:P:18:LEU:HD13	1.83	0.60
2:R:703:ARG:HD2	2:R:717:THR:HG22	1.82	0.60
2:R:1074:ASP:HB3	2:R:1075:LYS:CA	2.32	0.60
2:R:1104:ILE:HD13	2:R:1116:LEU:HD11	1.84	0.60
1:W:331:ASN:O	1:W:332:ILE:HG12	2.02	0.60
1:A:97:THR:HG23	1:A:102:GLY:HA2	1.83	0.60
1:A:848:VAL:O	1:A:849:ALA:CB	2.50	0.60
2:B:951:THR:O	2:B:951:THR:HG22	2.02	0.60
2:R:430:ARG:HH11	2:R:653:ILE:HG13	1.66	0.60
2:R:1008:ALA:HB2	1:W:346:THR:O	2.01	0.60
13:X:31:TYR:HE2	13:X:33:ILE:HB	1.65	0.60
2:B:933:GLY:HA3	2:B:990:VAL:HB	1.84	0.60
3:C:154:SER:OG	3:C:170:ASP:HB2	2.02	0.60
2:R:91:ARG:HG3	13:X:33:ILE:HD11	1.83	0.60
2:R:208:LEU:CD2	2:R:215:VAL:HG23	2.32	0.60
3:Y:174:LEU:N	3:Y:174:LEU:HD12	2.16	0.60
2:B:767:LYS:HD3	2:B:768:TYR:HA	1.84	0.60
3:C:168:GLN:CG	3:C:204:ASN:OD1	2.36	0.60
5:E:123:VAL:HG13	5:E:127:ILE:HG12	1.83	0.60
11:M:47:HIS:ND1	11:M:48:PRO:HD2	2.16	0.60
2:R:46:ILE:HG21	2:R:66:ILE:HD11	1.83	0.60
2:R:984:SER:HB2	1:W:642:GLN:O	2.01	0.60
1:W:682:GLY:O	1:W:684:LEU:N	2.34	0.60
1:A:224:MET:C	1:A:224:MET:HE2	2.26	0.60
2:B:601:ASP:O	2:B:602:SER:CB	2.50	0.60
2:B:928:MET:HE3	2:B:953:ILE:HD12	1.83	0.60
4:D:111:SER:HB3	4:D:128:ILE:HB	1.83	0.60
10:Q:43:LEU:H	10:Q:43:LEU:HD12	1.66	0.60
2:R:418:ASP:OD1	2:R:424:SER:OG	2.19	0.60
2:R:601:ASP:O	2:R:602:SER:CB	2.50	0.60
2:R:856:THR:HG21	13:X:33:ILE:HD12	1.84	0.60
1:W:63:ASN:HB2	1:W:68:CYS:HB2	1.82	0.60
3:Y:47:GLU:HB3	3:Y:50:LYS:HB2	1.84	0.60
1:A:141:MET:HA	1:A:148:HIS:HB3	1.83	0.60
2:B:235:ILE:HG23	2:B:240:ASP:HB3	1.82	0.60
2:B:430:ARG:HH11	2:B:653:ILE:HG13	1.67	0.60
2:B:1046:MET:HG2	5:E:61:PHE:CD1	2.36	0.60
7:G:9:ILE:HD13	7:G:104:LYS:HE3	1.83	0.60
2:R:320:TYR:CD1	2:R:529:LEU:HD12	2.37	0.60
2:R:451:THR:HG22	1:W:761:TYR:CD1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:1060:THR:O	2:R:1061:ILE:C	2.45	0.60
1:W:123:LYS:HA	1:W:126:PRO:HG2	1.84	0.60
3:Y:186:LYS:HB3	3:Y:230:LYS:HE2	1.84	0.60
2:B:702:GLN:HB2	2:B:723:ASN:HA	1.84	0.59
3:C:309:ASP:OD2	3:C:311:ARG:HB2	2.01	0.59
2:R:405:ASN:HB2	2:R:413:VAL:HB	1.83	0.59
2:R:406:TRP:CG	2:R:407:VAL:N	2.66	0.59
4:S:209:CYS:SG	16:S:1001:F3S:S2	2.89	0.59
5:T:164:MET:SD	5:T:170:GLY:HA2	2.41	0.59
2:B:46:ILE:HG21	2:B:66:ILE:HD11	1.84	0.59
2:B:100:TRP:CZ3	2:B:118:TYR:HB2	2.36	0.59
2:B:978:THR:HG23	2:B:980:GLN:HG2	1.84	0.59
5:E:36:GLU:HB3	6:F:33:LEU:HD22	1.84	0.59
5:E:119:LYS:HB3	5:E:120:TYR:HB2	1.85	0.59
5:E:164:MET:SD	5:E:170:GLY:HA2	2.42	0.59
7:G:36:PHE:CD1	7:G:96:ILE:HD11	2.37	0.59
13:P:5:ARG:HG2	13:P:18:LEU:HB2	1.84	0.59
2:R:536:GLY:HA3	2:R:560:HIS:CE1	2.37	0.59
2:R:630:ALA:HB3	2:R:636:LEU:CD1	2.32	0.59
2:R:683:TYR:CZ	2:R:687:TYR:HB2	2.37	0.59
5:T:166:GLN:N	5:T:167:PRO:CD	2.65	0.59
1:W:58:CYS:HB3	1:W:62:GLY:N	2.18	0.59
2:B:603:GLY:C	2:B:605:ILE:H	2.06	0.59
2:R:31:LEU:HA	2:R:125:MET:HE3	1.83	0.59
2:R:898:VAL:HG21	4:S:34:LEU:HD21	1.85	0.59
1:W:45:MET:HG2	1:W:45:MET:O	2.01	0.59
1:A:426:HIS:CE1	3:C:80:GLU:CD	2.79	0.59
2:B:954:GLU:HA	2:B:957:GLN:HB2	1.85	0.59
2:B:1060:THR:O	2:B:1061:ILE:C	2.46	0.59
9:I:41:LEU:HD23	5:T:64:GLY:N	2.17	0.59
2:R:520:TRP:O	2:R:521:SER:CB	2.51	0.59
1:A:109:ASP:O	1:A:113:LYS:HG3	2.01	0.59
2:R:42:LEU:HD21	2:R:68:ILE:HD11	1.83	0.59
2:R:372:LEU:CD2	2:R:376:LYS:HE2	2.33	0.59
2:R:767:LYS:HG3	2:R:768:TYR:HD1	1.67	0.59
5:T:136:ILE:HG22	5:T:137:GLN:H	1.64	0.59
1:W:372:TRP:C	1:W:372:TRP:CD1	2.79	0.59
3:Y:277:ILE:C	3:Y:279:GLU:H	2.09	0.59
3:Y:297:ILE:O	3:Y:301:LEU:HD12	2.02	0.59
3:Y:305:GLY:O	3:Y:306:LEU:HB3	2.00	0.59
1:A:501:ASP:OD2	2:B:731:SER:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:THR:HG23	2:B:432:VAL:HG12	1.85	0.59
2:B:855:ILE:HD11	13:P:36:MET:HE3	1.85	0.59
3:C:176:ASP:O	3:C:177:LYS:CB	2.50	0.59
2:R:418:ASP:OD1	2:R:418:ASP:O	2.21	0.59
1:W:109:ASP:O	1:W:113:LYS:HG3	2.02	0.59
1:W:378:VAL:HG13	1:W:386:ILE:HB	1.85	0.59
1:W:654:GLY:HA2	1:W:658:LYS:HE3	1.84	0.59
3:Y:13:LEU:HD13	3:Y:48:ILE:HG12	1.85	0.59
3:Y:169:LEU:HD23	3:Y:174:LEU:HD21	1.83	0.59
2:B:279:VAL:HG12	2:B:291:LYS:HD3	1.83	0.59
3:C:80:GLU:HB3	3:C:81:PRO:HD3	1.84	0.59
10:J:66:ARG:HD3	1:W:121:ILE:HG21	1.84	0.59
2:R:17:ILE:HG13	2:R:476:MET:SD	2.43	0.59
4:S:67:PHE:HB3	4:S:121:ILE:HG23	1.83	0.59
4:S:97:TYR:CE1	4:S:142:GLU:HG3	2.38	0.59
1:W:108:GLU:O	1:W:111:ILE:N	2.35	0.59
8:Z:82:ILE:HG22	8:Z:82:ILE:O	2.02	0.59
1:A:687:ILE:HD12	1:A:695:SER:HB2	1.83	0.59
2:B:834:ALA:O	2:B:835:LYS:CB	2.51	0.59
2:B:898:VAL:HG21	4:D:34:LEU:HD21	1.85	0.59
5:E:64:GLY:N	9:K:41:LEU:HD23	2.17	0.59
5:E:166:GLN:N	5:E:167:PRO:CD	2.65	0.59
13:P:5:ARG:HG3	13:P:6:CYS:H	1.67	0.59
2:R:91:ARG:CG	13:X:33:ILE:HD11	2.33	0.59
2:R:783:VAL:CG1	2:R:784:ARG:HB2	2.33	0.59
5:T:165:ARG:O	5:T:167:PRO:HD2	2.01	0.59
1:W:364:PHE:CE2	1:W:409:ARG:HD2	2.38	0.59
1:A:870:ARG:CZ	1:A:870:ARG:HB2	2.32	0.59
2:B:68:ILE:HG13	2:B:99:LEU:HD23	1.85	0.59
2:B:256:PHE:H	2:B:257:PRO:HD2	1.68	0.59
3:C:262:LEU:HD22	3:C:269:ILE:HD12	1.84	0.59
2:R:186:ILE:HD12	2:R:209:LYS:HD3	1.83	0.59
2:R:1071:GLY:HA3	2:R:1073:TYR:HE1	1.67	0.59
5:T:89:VAL:HG23	5:T:98:PHE:O	2.03	0.59
1:W:426:HIS:CD2	3:Y:80:GLU:OE1	2.56	0.59
3:Y:169:LEU:HD23	3:Y:174:LEU:CD2	2.33	0.59
3:Y:274:THR:HB	3:Y:280:ILE:HD11	1.85	0.59
1:A:736:SER:O	1:A:737:VAL:C	2.46	0.59
1:A:821:ARG:HA	1:A:824:ILE:HG22	1.84	0.59
2:B:703:ARG:HD2	2:B:717:THR:HG22	1.84	0.59
4:D:155:LYS:HE3	4:D:156:PHE:CZ	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:161:LEU:HD12	4:D:163:ILE:HD13	1.85	0.59
5:E:136:ILE:CG2	5:E:137:GLN:H	2.15	0.59
2:R:646:TRP:CD2	2:R:648:PRO:HD2	2.37	0.59
2:R:928:MET:CE	2:R:953:ILE:HD12	2.32	0.59
7:V:8:GLU:C	7:V:9:ILE:HG13	2.27	0.59
1:W:600:LYS:HE2	1:W:607:GLN:OE1	2.03	0.59
1:W:822:ARG:HH22	3:Y:108:ILE:HG23	1.67	0.59
2:B:557:ASN:OD1	2:B:577:ARG:NH1	2.35	0.58
2:B:950:LYS:O	2:B:951:THR:HB	2.03	0.58
2:B:975:ASP:HB3	2:B:978:THR:HG22	1.85	0.58
2:B:1071:GLY:HA3	2:B:1073:TYR:HE1	1.68	0.58
2:R:701:PRO:HB2	2:R:720:PRO:HG2	1.85	0.58
2:R:797:ASP:CG	13:X:4:TYR:HB3	2.28	0.58
2:R:1072:TRP:CZ3	1:W:67:ASN:OD1	2.56	0.58
1:W:353:ILE:HG21	1:W:358:ILE:HD13	1.84	0.58
1:W:555:PHE:HD1	1:W:626:TRP:CH2	2.21	0.58
1:A:555:PHE:HD1	1:A:626:TRP:CH2	2.21	0.58
2:B:157:VAL:HG11	2:B:401:LEU:HD23	1.85	0.58
2:B:520:TRP:O	2:B:521:SER:CB	2.50	0.58
2:B:582:LEU:HD12	2:B:619:LEU:HD12	1.85	0.58
5:E:80:VAL:HG12	5:E:83:GLU:OE2	2.03	0.58
2:R:532:TYR:O	2:R:533:TYR:HB2	2.02	0.58
2:R:957:GLN:HA	2:R:960:ILE:HD11	1.83	0.58
6:U:72:LEU:HD11	6:U:86:ILE:HG12	1.85	0.58
1:W:104:VAL:HG11	1:W:137:LYS:CB	2.33	0.58
1:A:856:PHE:CD2	1:A:858:MET:HB3	2.38	0.58
2:B:187:THR:HG22	2:B:188:HIS:CD2	2.38	0.58
2:B:236:LEU:HD21	2:B:268:VAL:HG22	1.86	0.58
2:B:418:ASP:OD1	2:B:418:ASP:O	2.22	0.58
2:B:683:TYR:CE1	2:B:687:TYR:HB2	2.39	0.58
2:B:703:ARG:HD2	2:B:717:THR:CG2	2.33	0.58
2:B:754:ARG:NH1	4:D:60:HIS:HD1	2.01	0.58
3:C:315:LEU:O	3:C:319:VAL:HG23	2.04	0.58
2:R:486:LYS:HA	2:R:489:GLU:HG2	1.86	0.58
2:R:766:VAL:HG22	2:R:767:LYS:N	2.18	0.58
2:R:834:ALA:O	2:R:835:LYS:CB	2.51	0.58
2:R:1015:LEU:HD13	2:R:1015:LEU:C	2.27	0.58
5:T:30:LEU:HD13	5:T:72:PHE:CE2	2.38	0.58
1:W:553:SER:OG	1:W:592:ILE:HA	2.03	0.58
1:W:603:ILE:HG22	1:W:604:GLY:H	1.68	0.58
1:W:870:ARG:NH2	3:Y:36:ILE:HD13	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PRO:HG2	1:A:220:ARG:HD2	1.86	0.58
2:B:856:THR:HG22	2:B:857:GLU:H	1.68	0.58
4:D:253:ILE:HG13	11:L:73:ILE:HG23	1.85	0.58
11:M:27:LEU:HD13	4:S:24:PHE:HA	1.85	0.58
2:R:1105:GLN:HB3	1:W:219:ILE:HD11	1.85	0.58
5:T:115:ASP:O	5:T:116:ASP:CB	2.50	0.58
5:T:132:SER:O	5:T:133:LYS:CB	2.51	0.58
2:B:394:THR:O	2:B:397:ILE:HG22	2.04	0.58
2:B:486:LYS:HA	2:B:489:GLU:HG2	1.86	0.58
2:B:786:TYR:CD2	2:B:788:GLY:HA2	2.38	0.58
11:L:47:HIS:ND1	11:L:48:PRO:HD2	2.19	0.58
2:R:653:ILE:HD12	2:R:653:ILE:H	1.68	0.58
2:R:672:GLN:NE2	2:R:884:ARG:HG3	2.18	0.58
2:R:703:ARG:HD2	2:R:717:THR:CG2	2.34	0.58
2:R:1007:ARG:NH1	2:R:1028:GLY:O	2.36	0.58
1:A:45:MET:O	1:A:45:MET:HG2	2.02	0.58
2:B:17:ILE:HG13	2:B:476:MET:SD	2.43	0.58
2:B:532:TYR:O	2:B:533:TYR:HB2	2.04	0.58
2:R:100:TRP:CZ3	2:R:118:TYR:HB2	2.39	0.58
2:R:249:PRO:HB3	2:R:252:GLN:HB2	1.86	0.58
1:A:313:LEU:HD21	2:B:1099:ALA:C	2.29	0.58
2:B:1074:ASP:HB3	2:B:1075:LYS:CA	2.34	0.58
1:A:530:VAL:HG11	1:A:555:PHE:CE1	2.38	0.58
2:B:46:ILE:CG1	2:B:66:ILE:HD11	2.33	0.58
2:B:136:TYR:HD2	2:B:140:LYS:HB3	1.69	0.58
2:R:9:SER:HB3	2:R:12:GLU:CB	2.34	0.58
2:R:356:LEU:HD21	2:R:397:ILE:HG13	1.86	0.58
2:R:394:THR:O	2:R:397:ILE:HG22	2.03	0.58
2:R:978:THR:CG2	2:R:980:GLN:HG2	2.34	0.58
2:R:981:LYS:HE2	4:S:205:LEU:HB2	1.86	0.58
8:Z:15:TYR:CD2	8:Z:16:LEU:HG	2.39	0.58
1:A:665:ILE:O	1:A:669:LYS:HG3	2.03	0.58
2:B:53:PRO:HD2	2:B:59:LEU:O	2.03	0.58
4:D:210:LEU:HD11	4:D:219:ILE:HB	1.86	0.58
5:E:102:GLY:HA2	6:F:40:TYR:CG	2.39	0.58
2:R:364:PHE:HE1	2:R:388:VAL:HG13	1.67	0.58
2:R:950:LYS:O	2:R:951:THR:HB	2.03	0.58
1:W:859:TYR:HE2	3:Y:65:ALA:HB2	1.68	0.58
13:X:5:ARG:HG3	13:X:6:CYS:H	1.68	0.58
13:X:6:CYS:CB	13:X:37:VAL:HG12	2.34	0.58
1:A:642:GLN:O	2:B:984:SER:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:328:GLN:OE1	3:C:331:ARG:NH1	2.37	0.58
4:D:203:CYS:HG	16:D:1001:F3S:FE3	1.18	0.58
2:R:191:LYS:HE2	2:R:193:ILE:HD11	1.86	0.58
2:R:500:VAL:O	2:R:504:ILE:HG12	2.04	0.58
2:R:759:ARG:HG3	2:R:760:LEU:H	1.69	0.58
2:R:797:ASP:OD2	13:X:4:TYR:HB3	2.04	0.58
7:V:36:PHE:CD1	7:V:96:ILE:HD11	2.39	0.58
2:B:251:ILE:CD1	2:B:330:LEU:HD11	2.34	0.57
2:B:603:GLY:C	2:B:605:ILE:N	2.60	0.57
2:B:660:TYR:CD1	2:B:950:LYS:HE3	2.38	0.57
2:B:978:THR:CG2	2:B:980:GLN:HG2	2.33	0.57
3:C:219:LEU:HA	3:C:222:LEU:HD13	1.86	0.57
3:C:231:ILE:CG2	3:C:232:LYS:N	2.66	0.57
12:O:30:ASN:O	12:O:34:VAL:HG23	2.03	0.57
2:R:99:LEU:O	2:R:119:ILE:HB	2.04	0.57
2:B:741:ILE:HD11	2:B:911:VAL:HG13	1.85	0.57
6:F:72:LEU:HD11	6:F:86:ILE:HG12	1.85	0.57
5:T:114:THR:HB	5:T:115:ASP:C	2.29	0.57
1:W:309:PHE:O	1:W:310:ARG:CB	2.52	0.57
1:W:820:GLN:OE1	3:Y:79:GLY:HA3	2.04	0.57
1:W:874:ARG:HB2	3:Y:54:LEU:HD21	1.85	0.57
1:A:326:ILE:HG13	1:A:457:PHE:CE1	2.39	0.57
2:B:157:VAL:HG22	2:B:162:ARG:HB2	1.86	0.57
3:C:176:ASP:O	3:C:177:LYS:HG3	2.04	0.57
8:H:63:ILE:HG22	8:H:65:ILE:HD11	1.86	0.57
2:R:333:ARG:O	2:R:334:GLU:HB3	2.03	0.57
1:W:223:ILE:HG12	1:W:224:MET:N	2.19	0.57
1:W:326:ILE:HG13	1:W:457:PHE:CE1	2.38	0.57
1:W:534:LEU:CB	1:W:546:TYR:CE2	2.88	0.57
1:W:848:VAL:O	1:W:849:ALA:CB	2.51	0.57
3:Y:174:LEU:HD12	3:Y:174:LEU:H	1.67	0.57
1:A:553:SER:OG	1:A:592:ILE:HA	2.04	0.57
5:E:82:GLN:HB3	6:F:88:ILE:HB	1.87	0.57
5:E:101:LEU:HD12	5:E:101:LEU:N	2.19	0.57
2:R:251:ILE:CD1	2:R:330:LEU:HD11	2.34	0.57
2:R:702:GLN:HB2	2:R:723:ASN:HA	1.85	0.57
1:A:321:SER:HB2	2:B:1029:LEU:HD12	1.87	0.57
1:A:378:VAL:HG13	1:A:386:ILE:HB	1.87	0.57
1:A:820:GLN:OE1	3:C:79:GLY:HA3	2.05	0.57
2:B:630:ALA:HB3	2:B:636:LEU:CD1	2.33	0.57
2:B:699:HIS:CE1	4:D:57:ILE:HD11	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:292:ILE:O	3:C:292:ILE:HD13	2.04	0.57
7:G:48:ILE:HG22	7:G:49:PHE:H	1.69	0.57
2:R:187:THR:HG22	2:R:188:HIS:CD2	2.40	0.57
2:R:605:ILE:HG23	2:R:606:THR:N	2.19	0.57
2:R:855:ILE:HD11	13:X:36:MET:HE3	1.86	0.57
2:R:974:TYR:CD2	2:R:981:LYS:HB3	2.40	0.57
7:V:102:LEU:HA	7:V:106:ILE:CG2	2.34	0.57
1:W:736:SER:O	1:W:737:VAL:C	2.48	0.57
1:W:856:PHE:CD2	1:W:858:MET:HB3	2.39	0.57
3:Y:327:ARG:HG3	3:Y:334:VAL:HG23	1.86	0.57
1:A:458:ASP:O	2:B:880:LYS:HE3	2.05	0.57
2:B:672:GLN:NE2	2:B:884:ARG:HG3	2.20	0.57
3:C:388:LEU:HD11	9:K:35:VAL:HG12	1.86	0.57
7:G:102:LEU:HA	7:G:106:ILE:CG2	2.34	0.57
3:Y:199:ASP:HB2	3:Y:206:LEU:HB2	1.86	0.57
1:A:63:ASN:HB2	1:A:68:CYS:HB2	1.85	0.57
1:A:141:MET:HG3	1:A:141:MET:O	2.04	0.57
1:A:635:PHE:O	1:A:639:VAL:HG23	2.05	0.57
1:A:654:GLY:HA2	1:A:658:LYS:CE	2.34	0.57
2:B:323:SER:O	2:B:327:GLU:HB2	2.03	0.57
2:B:1015:LEU:HD13	2:B:1102:LEU:HD11	1.85	0.57
5:E:6:LYS:H	6:F:8:GLU:HB2	1.69	0.57
5:E:9:SER:O	5:E:70:VAL:HG12	2.04	0.57
2:R:765:GLU:O	2:R:766:VAL:O	2.22	0.57
2:R:884:ARG:HB2	2:R:884:ARG:HH11	1.70	0.57
1:W:238:LYS:HZ2	1:W:275:THR:HG22	1.69	0.57
1:W:859:TYR:O	3:Y:63:LEU:HD13	2.04	0.57
1:A:23:SER:HB2	1:A:74:HIS:CD2	2.40	0.57
1:A:552:VAL:HG11	1:A:598:PHE:CE2	2.39	0.57
2:B:42:LEU:HD21	2:B:68:ILE:HD11	1.86	0.57
2:B:661:PRO:HG2	2:B:947:PRO:HB3	1.87	0.57
3:C:305:GLY:O	3:C:306:LEU:HB3	2.05	0.57
8:H:11:PRO:O	8:H:17:VAL:HG11	2.05	0.57
2:R:136:TYR:HD2	2:R:140:LYS:HB3	1.69	0.57
2:R:451:THR:HG22	1:W:761:TYR:CE1	2.40	0.57
2:R:774:ASP:OD1	2:R:819:PRO:CD	2.52	0.57
2:R:927:ILE:HG21	1:W:648:LEU:HB2	1.87	0.57
2:R:974:TYR:CZ	2:R:981:LYS:HB3	2.40	0.57
2:R:982:ILE:HD12	2:R:983:LYS:N	2.20	0.57
4:S:22:LEU:HB2	4:S:226:TYR:CZ	2.40	0.57
1:W:552:VAL:HG11	1:W:598:PHE:CE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:219:LEU:HA	3:Y:222:LEU:HD13	1.87	0.57
1:A:95:LYS:CB	1:A:138:LYS:HE2	2.35	0.57
1:A:271:TYR:HE2	1:A:285:PRO:HB3	1.66	0.57
1:A:331:ASN:O	1:A:332:ILE:HG12	2.04	0.57
2:B:55:GLU:OE2	2:B:377:VAL:HG12	2.05	0.57
5:E:30:LEU:HD22	5:E:72:PHE:CE2	2.40	0.57
9:K:39:ARG:NE	9:K:68:GLU:OE2	2.38	0.57
9:K:51:ILE:O	9:K:52:ASP:HB2	2.04	0.57
2:R:602:SER:HA	2:R:605:ILE:HD12	1.85	0.57
5:T:80:VAL:HG12	5:T:83:GLU:OE2	2.05	0.57
1:W:141:MET:HA	1:W:148:HIS:HB3	1.86	0.57
1:A:14:LEU:HB3	2:B:1111:ILE:HG23	1.86	0.57
1:A:298:LEU:HB3	2:B:1110:MET:HE2	1.85	0.57
2:B:1069:TYR:CB	2:B:1070:ILE:HB	2.35	0.57
3:C:70:ILE:HD13	3:C:70:ILE:H	1.68	0.57
8:H:20:HIS:CE1	8:H:51:VAL:HG11	2.40	0.57
2:R:251:ILE:HD12	2:R:330:LEU:HD11	1.86	0.57
2:R:683:TYR:CE1	2:R:687:TYR:HB2	2.40	0.57
1:W:541:ALA:HB3	1:W:542:PRO:CD	2.34	0.57
2:B:406:TRP:CG	2:B:407:VAL:H	2.21	0.56
5:E:133:LYS:O	5:E:134:LYS:HG3	2.05	0.56
2:R:978:THR:HG23	2:R:980:GLN:HG2	1.86	0.56
3:Y:231:ILE:CG2	3:Y:232:LYS:N	2.68	0.56
2:B:249:PRO:HD2	2:B:253:ASN:CG	2.30	0.56
2:B:364:PHE:HE1	2:B:388:VAL:HG13	1.69	0.56
2:B:974:TYR:CD2	2:B:981:LYS:HB3	2.40	0.56
8:H:59:PRO:HA	8:H:81:VAL:HG12	1.87	0.56
2:R:41:LYS:HA	2:R:44:GLU:OE1	2.04	0.56
2:R:975:ASP:OD1	2:R:977:ARG:HD3	2.05	0.56
2:R:1030:ARG:HH22	1:W:311:GLY:HA2	1.67	0.56
2:R:1051:ARG:NE	2:R:1051:ARG:HA	2.21	0.56
1:A:107:SER:O	1:A:108:GLU:C	2.46	0.56
2:B:356:LEU:HD21	2:B:397:ILE:HG13	1.86	0.56
2:B:629:VAL:HG22	2:B:642:HIS:HB2	1.86	0.56
2:B:1112:ILE:O	2:B:1114:PRO:HD3	2.05	0.56
3:C:197:VAL:HB	3:C:208:ILE:CG1	2.36	0.56
9:K:52:ASP:O	9:K:53:ILE:HB	2.05	0.56
2:R:86:MET:O	2:R:90:LEU:HG	2.05	0.56
2:R:249:PRO:HB2	2:R:252:GLN:HB2	1.87	0.56
2:R:661:PRO:HG2	2:R:947:PRO:HB3	1.88	0.56
4:S:53:LEU:HD12	4:S:131:VAL:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:55:ASP:HB3	13:X:45:VAL:HG21	1.87	0.56
5:T:123:VAL:HG22	5:T:127:ILE:HG12	1.87	0.56
1:W:104:VAL:HG11	1:W:137:LYS:CA	2.35	0.56
1:W:665:ILE:O	1:W:669:LYS:HG3	2.05	0.56
1:W:750:GLN:HG3	1:W:782:ILE:HD11	1.87	0.56
8:Z:63:ILE:HG22	8:Z:65:ILE:HD11	1.86	0.56
2:B:9:SER:HB3	2:B:12:GLU:CB	2.34	0.56
2:B:41:LYS:HA	2:B:44:GLU:OE1	2.05	0.56
2:B:367:ASP:OD2	2:B:389:ARG:HD2	2.04	0.56
2:B:898:VAL:HG22	4:D:33:MET:SD	2.46	0.56
9:I:39:ARG:NE	9:I:68:GLU:OE2	2.38	0.56
2:R:1004:ILE:HD12	1:W:441:LEU:HD22	1.87	0.56
2:R:1101:LYS:HE3	1:W:69:PRO:HB2	1.87	0.56
3:Y:323:THR:O	3:Y:325:VAL:N	2.39	0.56
1:A:13:ILE:HG13	1:A:202:SER:HB3	1.87	0.56
1:A:28:ILE:HG23	1:A:30:PRO:HD2	1.87	0.56
2:B:155:PHE:CE1	2:B:164:ILE:HD12	2.41	0.56
3:C:69:ALA:HB2	3:C:381:LEU:HD13	1.87	0.56
2:R:249:PRO:HD2	2:R:253:ASN:CG	2.31	0.56
4:S:93:TYR:HE1	4:S:146:ARG:HG2	1.70	0.56
4:S:219:ILE:HD13	16:S:1001:F3S:S3	2.46	0.56
1:A:534:LEU:CB	1:A:546:TYR:CE1	2.89	0.56
2:B:8:LEU:HA	2:B:633:PRO:HG3	1.87	0.56
2:B:249:PRO:HB3	2:B:252:GLN:HB2	1.87	0.56
2:R:398:ARG:C	2:R:400:ALA:H	2.14	0.56
1:W:417:VAL:HG11	1:W:464:LEU:CD1	2.36	0.56
3:Y:310:MET:HE2	8:Z:70:GLN:OE1	2.05	0.56
2:B:208:LEU:CD2	2:B:215:VAL:HG23	2.35	0.56
2:B:500:VAL:O	2:B:504:ILE:HG12	2.05	0.56
2:B:855:ILE:CD1	13:P:36:MET:HE3	2.35	0.56
4:D:93:TYR:CD1	4:D:146:ARG:HB3	2.41	0.56
4:D:104:ASN:O	4:D:105:GLU:C	2.49	0.56
5:E:115:ASP:O	5:E:116:ASP:CB	2.53	0.56
13:P:6:CYS:HB2	13:P:37:VAL:HG12	1.87	0.56
4:S:161:LEU:HD12	4:S:163:ILE:HD13	1.88	0.56
7:V:48:ILE:HG22	7:V:49:PHE:H	1.71	0.56
3:Y:349:VAL:HG13	3:Y:349:VAL:O	2.05	0.56
8:Z:11:PRO:O	8:Z:17:VAL:HG11	2.05	0.56
1:A:249:LEU:HD21	1:A:265:LEU:HB2	1.87	0.56
1:A:281:ILE:N	1:A:282:PRO:CD	2.68	0.56
1:A:498:ALA:HB1	1:A:502:TYR:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:LYS:HE2	1:A:607:GLN:OE1	2.05	0.56
2:B:1057:ASP:OD1	2:B:1057:ASP:N	2.39	0.56
4:D:57:ILE:O	4:D:61:ARG:HG3	2.05	0.56
7:G:96:ILE:HD13	7:G:101:LEU:CD2	2.36	0.56
8:H:15:TYR:CD2	8:H:16:LEU:HG	2.40	0.56
2:R:767:LYS:CB	2:R:768:TYR:CA	2.72	0.56
2:R:922:MET:HG2	1:W:743:MET:CG	2.36	0.56
2:R:1105:GLN:CB	1:W:219:ILE:HD11	2.35	0.56
4:S:60:HIS:C	4:S:60:HIS:CD2	2.83	0.56
1:W:530:VAL:HG11	1:W:555:PHE:CE1	2.40	0.56
1:A:249:LEU:CD2	1:A:265:LEU:HB2	2.36	0.56
13:P:6:CYS:CB	13:P:37:VAL:HG12	2.36	0.56
2:R:157:VAL:HG22	2:R:162:ARG:HB2	1.88	0.56
2:R:786:TYR:CD2	2:R:788:GLY:HA2	2.40	0.56
2:R:809:GLY:O	2:R:842:THR:HB	2.06	0.56
1:W:336:GLU:OE2	1:W:436:ARG:HB2	2.05	0.56
13:X:5:ARG:HD3	13:X:18:LEU:HD13	1.86	0.56
3:Y:64:ILE:HG22	3:Y:65:ALA:N	2.19	0.56
1:A:385:ARG:NH1	2:B:1009:ARG:NH2	2.54	0.56
5:E:132:SER:O	5:E:133:LYS:HG3	2.05	0.56
9:I:54:ASN:ND2	1:W:356:TRP:CE3	2.73	0.56
2:R:1030:ARG:NH2	1:W:311:GLY:HA2	2.22	0.56
5:T:22:LEU:HD21	3:Y:392:PRO:HG2	1.88	0.56
1:W:23:SER:HB2	1:W:74:HIS:CD2	2.41	0.56
1:W:326:ILE:HG13	1:W:457:PHE:CD1	2.41	0.56
8:Z:28:ALA:HB1	8:Z:62:ILE:HD11	1.86	0.56
8:Z:59:PRO:HA	8:Z:81:VAL:HG12	1.88	0.56
1:A:364:PHE:CE2	1:A:409:ARG:HD2	2.42	0.55
1:A:668:ALA:HB1	1:A:707:LEU:HD13	1.88	0.55
1:A:736:SER:HB3	1:A:739:ASN:OD1	2.05	0.55
2:B:765:GLU:O	2:B:766:VAL:O	2.24	0.55
2:B:857:GLU:HA	2:B:862:ASN:O	2.05	0.55
3:C:389:THR:HG21	5:E:56:GLU:OE1	2.06	0.55
11:L:12:TYR:HD1	11:L:58:LEU:HD13	1.71	0.55
4:S:209:CYS:SG	16:S:1001:F3S:S3	3.04	0.55
6:U:4:VAL:HG13	6:U:4:VAL:O	2.06	0.55
1:W:324:THR:HG22	1:W:325:VAL:N	2.20	0.55
3:Y:340:SER:CB	3:Y:371:GLU:HG2	2.36	0.55
1:A:326:ILE:HG13	1:A:457:PHE:CD1	2.41	0.55
2:B:787:LYS:HE3	2:B:841:VAL:HG21	1.88	0.55
2:B:957:GLN:HA	2:B:960:ILE:CD1	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1015:LEU:HD13	2:B:1015:LEU:C	2.31	0.55
2:B:1046:MET:HG2	5:E:61:PHE:CE1	2.41	0.55
3:C:286:ILE:HG12	8:H:49:ASP:OD1	2.06	0.55
2:R:279:VAL:HG12	2:R:291:LYS:HD3	1.87	0.55
2:R:734:GLY:HA3	2:R:735:TYR:CD2	2.41	0.55
4:S:111:SER:HA	4:S:130:ILE:HD11	1.88	0.55
7:V:96:ILE:HD13	7:V:101:LEU:CD2	2.36	0.55
1:W:141:MET:HG3	1:W:148:HIS:HB3	1.87	0.55
1:W:325:VAL:O	1:W:442:THR:HG22	2.07	0.55
3:Y:292:ILE:O	3:Y:292:ILE:HD13	2.07	0.55
1:A:246:ASN:CG	1:A:246:ASN:O	2.50	0.55
1:A:417:VAL:HG11	1:A:464:LEU:CD1	2.37	0.55
1:A:736:SER:O	1:A:738:LEU:N	2.40	0.55
2:B:117:VAL:HG11	2:B:388:VAL:HG21	1.88	0.55
2:B:136:TYR:HB2	2:B:141:LEU:HD11	1.87	0.55
2:B:731:SER:HA	2:B:914:ASN:ND2	2.22	0.55
3:C:29:VAL:HG12	3:C:61:GLU:HG3	1.89	0.55
5:E:132:SER:O	5:E:133:LYS:CB	2.54	0.55
7:G:80:GLU:C	7:G:81:LEU:HD12	2.31	0.55
5:T:130:GLU:HG3	5:T:137:GLN:OE1	2.07	0.55
1:W:246:ASN:CG	1:W:246:ASN:O	2.50	0.55
1:W:853:ASP:CB	3:Y:311:ARG:NH1	2.70	0.55
3:Y:341:VAL:HG12	3:Y:344:ARG:NH2	2.21	0.55
8:Z:44:TRP:O	8:Z:79:ARG:HD2	2.06	0.55
1:A:792:PRO:CG	2:B:948:PHE:CE1	2.89	0.55
2:B:17:ILE:HD12	2:B:476:MET:SD	2.47	0.55
5:E:114:THR:HB	5:E:115:ASP:C	2.32	0.55
2:R:46:ILE:CG1	2:R:66:ILE:HD11	2.36	0.55
2:R:107:GLU:O	2:R:108:ASN:CB	2.54	0.55
2:R:236:LEU:HD21	2:R:268:VAL:HG22	1.88	0.55
2:R:367:ASP:OD1	2:R:389:ARG:HD2	2.07	0.55
7:V:104:LYS:O	7:V:105:ILE:C	2.49	0.55
1:W:736:SER:HB3	1:W:739:ASN:CG	2.31	0.55
3:Y:315:LEU:O	3:Y:319:VAL:HG23	2.05	0.55
2:B:406:TRP:CG	2:B:407:VAL:N	2.71	0.55
2:B:974:TYR:CZ	2:B:981:LYS:HB3	2.41	0.55
2:B:982:ILE:HD12	2:B:983:LYS:N	2.21	0.55
5:T:119:LYS:HB3	5:T:120:TYR:HB2	1.87	0.55
1:W:334:ILE:CD1	1:W:628:MET:HB3	2.36	0.55
1:A:123:LYS:HA	1:A:126:PRO:HG2	1.88	0.55
1:A:603:ILE:HG22	1:A:604:GLY:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:859:TYR:O	3:C:63:LEU:HD13	2.06	0.55
2:B:248:ASP:N	2:B:249:PRO:HD3	2.22	0.55
3:C:170:ASP:HB3	3:C:173:MET:HB2	1.89	0.55
3:C:176:ASP:O	3:C:177:LYS:HB2	2.07	0.55
3:C:323:THR:O	3:C:325:VAL:N	2.40	0.55
2:B:118:TYR:CD1	2:B:118:TYR:C	2.85	0.55
2:B:802:SER:OG	13:P:39:LYS:HB2	2.07	0.55
3:C:70:ILE:HD13	3:C:70:ILE:N	2.21	0.55
3:C:104:LEU:N	3:C:105:PRO:CD	2.69	0.55
3:C:149:ILE:HA	3:C:152:VAL:HG12	1.89	0.55
4:D:49:ASN:OD1	4:D:139:ILE:CD1	2.55	0.55
10:J:55:LEU:HD21	8:Z:25:ILE:HG22	1.89	0.55
2:R:63:LEU:HD22	2:R:101:LEU:HD11	1.89	0.55
2:R:356:LEU:HD12	2:R:407:VAL:HG21	1.87	0.55
2:R:918:LEU:CD1	1:W:646:MET:HG2	2.37	0.55
2:R:1031:PHE:HD2	1:W:465:HIS:CE1	2.24	0.55
4:S:66:PRO:HB2	4:S:124:ILE:HG12	1.89	0.55
3:Y:104:LEU:N	3:Y:105:PRO:CD	2.69	0.55
4:D:97:TYR:CD1	4:D:142:GLU:HG3	2.41	0.55
5:E:130:GLU:HG3	5:E:137:GLN:OE1	2.06	0.55
9:I:62:ILE:HD11	1:W:474:ALA:HB2	1.87	0.55
11:L:80:ALA:O	11:L:84:ILE:HG12	2.06	0.55
2:R:109:ASN:CG	2:R:109:ASN:O	2.50	0.55
2:R:768:TYR:CB	2:R:769:PRO:CD	2.72	0.55
2:R:1057:ASP:OD2	2:R:1097:SER:HB2	2.06	0.55
1:W:121:ILE:HG23	8:Z:38:ARG:NH1	2.21	0.55
1:W:281:ILE:N	1:W:282:PRO:CD	2.69	0.55
1:W:654:GLY:HA2	1:W:658:LYS:CE	2.37	0.55
3:Y:197:VAL:HB	3:Y:208:ILE:CG1	2.37	0.55
1:A:124:ARG:N	1:A:126:PRO:HD2	2.21	0.55
2:B:229:LEU:HD23	2:B:275:ILE:HD11	1.89	0.55
2:B:774:ASP:OD1	2:B:819:PRO:CD	2.54	0.55
4:D:219:ILE:HD13	16:D:1001:F3S:S3	2.47	0.55
4:S:37:PRO:HG3	4:S:78:TRP:CE3	2.41	0.55
4:S:38:VAL:HG12	4:S:39:MET:N	2.21	0.55
4:S:93:TYR:CE1	4:S:146:ARG:HG2	2.42	0.55
1:W:372:TRP:HB3	1:W:373:PRO:HD3	1.88	0.55
1:A:103:ARG:CB	1:A:191:ASP:OD1	2.54	0.55
1:A:418:LEU:HD23	1:A:430:MET:CE	2.36	0.55
1:A:863:GLY:HA2	3:C:311:ARG:NH2	2.22	0.55
2:B:536:GLY:HA3	2:B:560:HIS:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:84:ASP:O	4:D:85:CYS:C	2.49	0.55
9:I:27:LEU:HD23	9:I:78:ILE:CD1	2.37	0.55
12:N:19:GLN:N	12:N:20:PRO:HD2	2.22	0.55
2:R:398:ARG:HG3	2:R:399:HIS:N	2.22	0.55
2:R:855:ILE:CD1	13:X:36:MET:HE3	2.37	0.55
7:V:80:GLU:C	7:V:81:LEU:HD12	2.32	0.55
1:W:309:PHE:O	1:W:310:ARG:CG	2.55	0.55
1:W:425:LEU:H	1:W:425:LEU:HD12	1.70	0.55
1:A:105:LYS:HZ2	1:A:133:THR:HG23	1.72	0.54
1:A:238:LYS:HE2	1:A:297:THR:HG22	1.89	0.54
1:A:655:ASP:H	1:A:658:LYS:HD2	1.72	0.54
1:A:782:ILE:HG21	1:A:790:LEU:CD2	2.37	0.54
2:B:249:PRO:HB2	2:B:253:ASN:H	1.72	0.54
3:C:348:GLU:O	3:C:349:VAL:C	2.50	0.54
4:D:22:LEU:HB2	4:D:226:TYR:CZ	2.41	0.54
2:R:460:GLU:HG2	2:R:673:SER:HB3	1.88	0.54
7:V:72:CYS:HB3	7:V:114:LYS:HG2	1.89	0.54
1:W:107:SER:O	1:W:108:GLU:C	2.48	0.54
1:W:534:LEU:HB2	1:W:546:TYR:CE2	2.41	0.54
1:W:650:ASP:HB3	1:W:723:ASN:ND2	2.22	0.54
1:W:763:THR:HB	1:W:764:ARG:CD	2.37	0.54
1:W:854:GLY:O	3:Y:64:ILE:CG2	2.54	0.54
2:B:1057:ASP:OD2	2:B:1097:SER:HB2	2.07	0.54
3:C:340:SER:HB3	3:C:371:GLU:CG	2.37	0.54
10:J:65:LYS:O	10:J:68:PHE:HB3	2.07	0.54
13:P:5:ARG:HG2	13:P:18:LEU:HD22	1.89	0.54
2:R:70:LYS:HB3	2:R:71:PRO:HD2	1.89	0.54
2:R:73:VAL:HG22	2:R:74:ARG:O	2.07	0.54
2:R:117:VAL:HG11	2:R:388:VAL:HG21	1.88	0.54
2:R:731:SER:HA	2:R:914:ASN:ND2	2.22	0.54
2:R:948:PHE:CE1	1:W:792:PRO:HG3	2.42	0.54
2:R:1098:TYR:CE1	2:R:1101:LYS:HD3	2.43	0.54
1:W:86:PHE:O	1:W:90:VAL:HG23	2.07	0.54
13:X:6:CYS:HB2	13:X:37:VAL:HG12	1.88	0.54
1:A:47:PRO:O	1:A:48:ARG:CB	2.55	0.54
1:A:106:ILE:HD12	1:A:106:ILE:N	2.22	0.54
1:A:253:ILE:HG22	1:A:254:ASP:OD1	2.08	0.54
2:B:418:ASP:OD1	2:B:424:SER:OG	2.22	0.54
2:B:705:LEU:O	2:B:706:VAL:HB	2.07	0.54
2:B:809:GLY:O	2:B:842:THR:HB	2.07	0.54
4:D:38:VAL:HG12	4:D:39:MET:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:30:LEU:CD1	5:E:72:PHE:CE2	2.91	0.54
12:O:46:ARG:HD2	2:R:937:ALA:O	2.06	0.54
2:R:1106:GLU:OE2	1:W:301:ARG:HD3	2.07	0.54
6:U:12:ILE:HG23	6:U:16:VAL:HG13	1.89	0.54
1:W:511:VAL:HA	1:W:583:ASP:OD2	2.07	0.54
1:A:125:TRP:O	1:A:128:ALA:HB3	2.08	0.54
2:B:251:ILE:HD12	2:B:330:LEU:HD11	1.89	0.54
9:I:61:VAL:H	9:I:64:ILE:HD12	1.71	0.54
2:R:166:THR:HG23	2:R:432:VAL:HG12	1.89	0.54
2:R:970:THR:HG22	2:R:987:TYR:HA	1.89	0.54
5:T:19:GLY:H	3:Y:393:ILE:HG22	1.73	0.54
1:W:238:LYS:HE2	1:W:297:THR:HG22	1.88	0.54
1:W:854:GLY:O	3:Y:64:ILE:CG1	2.55	0.54
3:Y:338:LYS:HD3	3:Y:338:LYS:H	1.72	0.54
1:A:98:CYS:SG	1:A:145:VAL:O	2.65	0.54
1:A:113:LYS:HG2	1:A:116:ARG:CZ	2.38	0.54
1:A:450:CYS:HB2	1:A:451:PRO:HD3	1.87	0.54
2:B:359:VAL:HG11	2:B:407:VAL:HG13	1.90	0.54
2:B:707:GLN:CD	2:B:942:ILE:HD12	2.33	0.54
3:C:133:ASP:OD2	3:C:136:LYS:HG2	2.06	0.54
12:O:9:THR:HB	12:O:44:CYS:HB2	1.90	0.54
7:V:70:ASP:O	1:W:541:ALA:HB1	2.08	0.54
1:A:104:VAL:O	1:A:104:VAL:HG13	2.02	0.54
1:A:110:GLU:HA	1:A:113:LYS:HB2	1.90	0.54
2:B:767:LYS:HG3	2:B:768:TYR:HD1	1.72	0.54
2:B:1098:TYR:CE1	2:B:1101:LYS:HD3	2.43	0.54
3:C:25:PRO:HD3	3:C:33:LYS:HD3	1.90	0.54
12:O:53:ILE:HD12	2:R:720:PRO:HG3	1.89	0.54
12:O:55:ILE:HD12	2:R:682:LEU:HD22	1.89	0.54
2:R:957:GLN:HA	2:R:960:ILE:CD1	2.37	0.54
1:W:324:THR:O	1:W:461:GLU:HA	2.08	0.54
1:W:782:ILE:HG21	1:W:790:LEU:HD22	1.89	0.54
3:Y:12:TYR:HB2	3:Y:45:ARG:HH12	1.71	0.54
1:A:425:LEU:HD12	1:A:425:LEU:H	1.72	0.54
2:B:420:THR:HG21	2:B:677:LYS:O	2.08	0.54
2:B:856:THR:HG21	13:P:33:ILE:HD12	1.89	0.54
2:B:1007:ARG:HH21	2:B:1026:GLU:C	2.16	0.54
3:C:286:ILE:HD12	3:C:324:GLY:O	2.08	0.54
4:D:53:LEU:HD12	4:D:131:VAL:CG2	2.37	0.54
4:D:93:TYR:HE1	4:D:146:ARG:HG2	1.72	0.54
1:W:838:VAL:HG13	3:Y:70:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:69:ALA:HB2	3:Y:381:LEU:HD13	1.90	0.54
1:A:58:CYS:HB3	1:A:62:GLY:N	2.23	0.54
2:R:628:TYR:CE2	2:R:640:HIS:CE1	2.96	0.54
2:R:707:GLN:CD	2:R:942:ILE:HD12	2.33	0.54
2:R:1050:ASP:HA	2:R:1054:ASP:HB2	1.90	0.54
4:S:49:ASN:OD1	4:S:139:ILE:CD1	2.55	0.54
1:W:426:HIS:CE1	3:Y:80:GLU:CD	2.86	0.54
1:W:823:LEU:HB3	3:Y:329:ILE:HG12	1.90	0.54
3:Y:29:VAL:HG12	3:Y:61:GLU:HG3	1.89	0.54
8:Z:43:PRO:O	8:Z:44:TRP:HB2	2.07	0.54
1:A:110:GLU:HA	1:A:113:LYS:HD2	1.90	0.54
1:A:346:THR:O	2:B:1008:ALA:HB2	2.07	0.54
1:A:428:ILE:CG2	1:A:452:PRO:HB3	2.38	0.54
2:B:699:HIS:ND1	4:D:57:ILE:HG12	2.22	0.54
4:D:155:LYS:HE3	4:D:156:PHE:CE2	2.43	0.54
11:M:12:TYR:HD1	11:M:58:LEU:HD13	1.71	0.54
10:Q:65:LYS:O	10:Q:68:PHE:HB3	2.07	0.54
2:R:420:THR:HG21	2:R:677:LYS:O	2.08	0.54
2:R:856:THR:HG23	13:X:32:LYS:C	2.33	0.54
7:V:102:LEU:O	7:V:103:VAL:C	2.51	0.54
1:W:486:ILE:HD13	1:W:628:MET:HE2	1.90	0.54
1:A:223:ILE:HG12	1:A:224:MET:N	2.21	0.54
1:A:329:ASP:O	1:A:446:ASN:HA	2.08	0.54
3:C:108:ILE:O	3:C:112:ASP:HB2	2.07	0.54
6:F:12:ILE:HG23	6:F:16:VAL:HG13	1.90	0.54
9:K:49:ALA:O	9:K:50:LEU:C	2.50	0.54
3:Y:237:ILE:HD12	3:Y:253:THR:HB	1.89	0.54
3:Y:301:LEU:HD22	3:Y:308:VAL:CG1	2.37	0.54
8:Z:20:HIS:CE1	8:Z:51:VAL:HG11	2.43	0.54
1:A:299:ALA:O	1:A:303:LYS:HB2	2.08	0.53
1:A:324:THR:O	1:A:461:GLU:HA	2.08	0.53
2:B:762:SER:OG	2:B:866:LYS:HG2	2.08	0.53
5:E:168:TYR:C	5:E:169:LEU:HD12	2.33	0.53
2:R:59:LEU:O	2:R:59:LEU:HD13	2.08	0.53
2:R:136:TYR:HB2	2:R:141:LEU:HD11	1.88	0.53
2:R:629:VAL:HG22	2:R:642:HIS:HB2	1.90	0.53
2:R:660:TYR:CD1	2:R:950:LYS:HE3	2.42	0.53
2:R:699:HIS:CE1	4:S:57:ILE:HG12	2.43	0.53
5:T:75:ILE:HG21	6:U:21:LEU:HD11	1.89	0.53
1:W:498:ALA:HB1	1:W:502:TYR:HB2	1.89	0.53
3:Y:309:ASP:OD2	3:Y:311:ARG:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:LYS:O	1:A:610:SER:HB2	2.08	0.53
2:B:186:ILE:CD1	2:B:209:LYS:HD3	2.38	0.53
2:B:249:PRO:HD2	2:B:253:ASN:OD1	2.08	0.53
2:B:398:ARG:HG3	2:B:399:HIS:N	2.23	0.53
2:B:599:LYS:O	2:B:600:LEU:C	2.50	0.53
2:B:857:GLU:HG3	13:P:24:VAL:HG11	1.90	0.53
4:D:24:PHE:HA	11:L:27:LEU:HD13	1.89	0.53
4:D:66:PRO:HB2	4:D:124:ILE:HG12	1.91	0.53
4:D:260:LEU:HD11	11:L:69:LEU:HD21	1.89	0.53
9:I:52:ASP:O	9:I:53:ILE:CB	2.56	0.53
11:L:77:ARG:NH1	11:L:77:ARG:HB2	2.23	0.53
13:P:5:ARG:O	13:P:6:CYS:HB2	2.08	0.53
2:R:557:ASN:OD1	2:R:577:ARG:NH1	2.41	0.53
5:T:30:LEU:CD2	5:T:72:PHE:CE2	2.91	0.53
5:T:132:SER:O	5:T:133:LYS:HB2	2.08	0.53
1:W:428:ILE:CG2	1:W:452:PRO:HB3	2.38	0.53
1:W:541:ALA:HB3	1:W:542:PRO:HD3	1.90	0.53
3:Y:110:ILE:HD13	3:Y:297:ILE:HG12	1.89	0.53
2:B:486:LYS:HG2	2:B:489:GLU:OE2	2.09	0.53
2:B:701:PRO:HB2	2:B:720:PRO:HG2	1.88	0.53
9:I:51:ILE:O	9:I:52:ASP:CG	2.51	0.53
2:R:768:TYR:HB3	2:R:769:PRO:HD2	1.83	0.53
5:T:115:ASP:O	5:T:116:ASP:HB2	2.06	0.53
1:W:68:CYS:N	1:W:69:PRO:HD3	2.23	0.53
1:W:299:ALA:O	1:W:303:LYS:HB2	2.08	0.53
3:Y:328:GLN:HB3	3:Y:332:HIS:HB3	1.89	0.53
1:A:124:ARG:HD3	1:A:125:TRP:CZ3	2.42	0.53
2:B:99:LEU:O	2:B:119:ILE:HB	2.09	0.53
2:R:416:LEU:O	2:R:418:ASP:N	2.42	0.53
2:R:808:LYS:HE3	2:R:847:MET:CE	2.38	0.53
5:T:84:VAL:HG21	6:U:75:ILE:HD13	1.90	0.53
5:T:133:LYS:O	5:T:134:LYS:HG3	2.08	0.53
7:V:71:PHE:HA	1:W:541:ALA:HB3	1.89	0.53
1:W:145:VAL:O	1:W:146:CYS:SG	2.66	0.53
1:W:280:GLU:H	1:W:282:PRO:HD2	1.73	0.53
3:Y:109:GLU:OE2	3:Y:117:PRO:HA	2.08	0.53
1:A:68:CYS:N	1:A:69:PRO:HD3	2.23	0.53
1:A:782:ILE:HG23	1:A:794:GLU:CD	2.34	0.53
1:A:792:PRO:CA	2:B:948:PHE:CE1	2.92	0.53
2:B:63:LEU:HD22	2:B:101:LEU:HD11	1.91	0.53
2:B:163:VAL:HG21	2:B:429:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:975:ASP:OD1	2:B:977:ARG:HD3	2.09	0.53
3:C:301:LEU:HD22	3:C:308:VAL:CG1	2.38	0.53
4:D:66:PRO:HG2	12:N:13:LEU:HD11	1.90	0.53
2:R:157:VAL:HG11	2:R:401:LEU:HD23	1.89	0.53
2:R:461:THR:HG21	2:R:468:GLY:N	2.24	0.53
4:S:154:ALA:HA	4:S:157:ILE:HG13	1.88	0.53
1:W:782:ILE:HG21	1:W:790:LEU:CD2	2.38	0.53
3:Y:133:ASP:OD2	3:Y:136:LYS:HG2	2.09	0.53
2:B:416:LEU:O	2:B:418:ASP:N	2.41	0.53
2:B:453:TRP:CZ3	2:B:644:GLU:OE2	2.60	0.53
2:B:743:MET:HE3	2:B:748:VAL:CG2	2.39	0.53
3:C:12:TYR:HB2	3:C:45:ARG:HH12	1.72	0.53
4:D:37:PRO:HG3	4:D:78:TRP:CE3	2.43	0.53
2:R:55:GLU:OE2	2:R:377:VAL:HG12	2.09	0.53
2:R:741:ILE:HG23	2:R:891:ILE:HA	1.91	0.53
2:R:743:MET:HE3	2:R:748:VAL:HG22	1.91	0.53
2:R:857:GLU:HA	2:R:862:ASN:O	2.07	0.53
6:U:12:ILE:HG23	6:U:16:VAL:CG1	2.39	0.53
1:W:95:LYS:CB	1:W:138:LYS:HE2	2.39	0.53
1:A:334:ILE:CD1	1:A:628:MET:HB3	2.39	0.53
1:A:448:LEU:O	1:A:496:ILE:HG23	2.08	0.53
1:A:450:CYS:N	1:A:451:PRO:CD	2.72	0.53
1:A:822:ARG:HH22	3:C:108:ILE:HG23	1.74	0.53
2:B:784:ARG:HB3	2:B:835:LYS:O	2.09	0.53
2:B:1082:CYS:HB3	2:B:1091:LEU:HD21	1.91	0.53
2:R:258:SER:O	2:R:259:LEU:HD22	2.09	0.53
2:R:372:LEU:HD21	2:R:376:LYS:HE2	1.91	0.53
2:R:604:SER:O	2:R:605:ILE:O	2.27	0.53
2:R:767:LYS:CD	2:R:768:TYR:HA	2.38	0.53
2:R:802:SER:OG	13:X:39:LYS:HB2	2.09	0.53
2:R:857:GLU:HG3	13:X:24:VAL:HG11	1.90	0.53
4:S:84:ASP:O	4:S:85:CYS:C	2.51	0.53
1:W:238:LYS:HG3	1:W:238:LYS:O	2.07	0.53
1:W:249:LEU:CD2	1:W:265:LEU:HB2	2.39	0.53
2:B:17:ILE:CD1	2:B:476:MET:SD	2.97	0.53
2:B:20:TYR:HD2	2:B:607:PHE:CE2	2.27	0.53
2:B:59:LEU:O	2:B:59:LEU:HD13	2.09	0.53
2:B:229:LEU:CD2	2:B:275:ILE:HD11	2.39	0.53
3:C:126:LEU:HB2	3:C:131:LYS:HG3	1.90	0.53
3:C:160:ILE:O	3:C:161:ALA:C	2.52	0.53
3:C:338:LYS:HD3	3:C:338:LYS:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:104:LYS:O	7:G:105:ILE:C	2.52	0.53
2:R:133:ILE:HD13	2:R:136:TYR:CE1	2.43	0.53
2:R:235:ILE:HD11	2:R:316:TYR:CE1	2.44	0.53
2:R:525:LEU:HD22	2:R:571:VAL:HB	1.91	0.53
1:W:110:GLU:HA	1:W:113:LYS:HB2	1.90	0.53
1:W:113:LYS:HG2	1:W:116:ARG:CZ	2.38	0.53
1:W:668:ALA:HB1	1:W:707:LEU:HD13	1.88	0.53
3:Y:149:ILE:HA	3:Y:152:VAL:HG12	1.91	0.53
3:Y:237:ILE:HD11	3:Y:240:ALA:HB2	1.91	0.53
1:A:821:ARG:HH12	3:C:347:PHE:HA	1.73	0.53
7:G:72:CYS:SG	7:G:114:LYS:HB3	2.49	0.53
2:R:598:GLU:HG3	2:R:605:ILE:HD11	1.91	0.53
1:W:47:PRO:O	1:W:48:ARG:CB	2.56	0.53
1:A:419:PHE:CE1	1:A:464:LEU:HD23	2.44	0.53
2:B:759:ARG:HG3	2:B:760:LEU:H	1.73	0.53
2:B:1074:ASP:HB3	2:B:1075:LYS:CB	2.37	0.53
4:D:111:SER:HA	4:D:130:ILE:HD11	1.91	0.53
2:R:8:LEU:HA	2:R:633:PRO:HG3	1.90	0.53
2:R:491:THR:HG22	2:R:495:MET:HE2	1.91	0.53
2:R:745:ARG:HD2	2:R:896:PRO:HG3	1.91	0.53
4:S:159:VAL:HG22	4:S:161:LEU:H	1.74	0.53
5:T:63:ASP:OD2	5:T:65:ALA:HB3	2.08	0.53
1:W:363:GLN:O	1:W:366:ILE:HG22	2.08	0.53
2:B:233:LEU:HD13	2:B:315:ALA:HB2	1.91	0.52
2:B:934:LYS:O	2:B:938:LEU:HG	2.08	0.52
4:D:8:LYS:HG2	4:D:9:ASP:N	2.23	0.52
5:E:84:VAL:CG2	6:F:75:ILE:HD13	2.39	0.52
7:G:103:VAL:HG13	7:G:104:LYS:CD	2.39	0.52
2:R:86:MET:HE3	2:R:686:ASN:HD22	1.71	0.52
2:R:843:ARG:HB2	2:R:846:GLU:CD	2.34	0.52
4:S:154:ALA:C	4:S:156:PHE:H	2.16	0.52
1:W:125:TRP:N	1:W:126:PRO:CD	2.71	0.52
1:A:288:LYS:HA	1:A:295:LEU:CD2	2.39	0.52
1:A:426:HIS:CD2	3:C:80:GLU:OE1	2.62	0.52
2:B:31:LEU:HA	2:B:125:MET:HE3	1.88	0.52
2:B:235:ILE:HD11	2:B:316:TYR:CE1	2.45	0.52
2:B:345:ARG:NH2	2:B:577:ARG:HG2	2.24	0.52
2:B:372:LEU:HD21	2:B:376:LYS:HE2	1.91	0.52
2:B:525:LEU:O	2:B:528:ARG:HB3	2.10	0.52
3:C:349:VAL:O	3:C:349:VAL:HG13	2.10	0.52
5:E:40:LYS:O	5:E:41:ASP:CG	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:80:ALA:O	11:M:84:ILE:HG12	2.08	0.52
2:R:647:SER:N	2:R:648:PRO:CD	2.72	0.52
4:S:182:VAL:HG11	4:S:212:TYR:HD2	1.73	0.52
1:W:238:LYS:HE3	1:W:276:TYR:HA	1.91	0.52
1:W:534:LEU:HD22	1:W:534:LEU:N	2.24	0.52
1:W:749:GLN:HA	1:W:781:PHE:HA	1.92	0.52
3:Y:176:ASP:O	3:Y:177:LYS:HG3	2.10	0.52
1:A:441:LEU:HD22	2:B:1004:ILE:HD12	1.91	0.52
2:B:491:THR:HG22	2:B:495:MET:HE2	1.90	0.52
2:B:778:MET:HE2	2:B:795:LEU:HB2	1.91	0.52
2:B:970:THR:HG22	2:B:987:TYR:HA	1.90	0.52
9:K:51:ILE:O	9:K:52:ASP:CG	2.51	0.52
2:R:599:LYS:O	2:R:600:LEU:C	2.52	0.52
2:R:797:ASP:OD1	13:X:4:TYR:HB3	2.09	0.52
2:R:933:GLY:HA3	2:R:990:VAL:HB	1.90	0.52
1:A:125:TRP:N	1:A:126:PRO:CD	2.72	0.52
1:A:782:ILE:HG21	1:A:790:LEU:HD22	1.92	0.52
2:B:133:ILE:HD13	2:B:136:TYR:CE1	2.44	0.52
2:B:493:TYR:HD1	2:B:497:VAL:O	1.92	0.52
2:B:602:SER:HA	2:B:605:ILE:HD12	1.92	0.52
2:B:843:ARG:HB2	2:B:846:GLU:CD	2.35	0.52
3:C:162:SER:HA	3:C:210:PHE:HZ	1.75	0.52
5:E:48:ILE:HD12	5:E:74:MET:HE2	1.91	0.52
11:M:13:LEU:HB2	11:M:65:PRO:HB2	1.92	0.52
2:R:107:GLU:O	2:R:108:ASN:HB2	2.09	0.52
2:R:229:LEU:HD23	2:R:275:ILE:HD11	1.90	0.52
2:R:406:TRP:O	2:R:408:GLY:N	2.43	0.52
2:R:705:LEU:O	2:R:706:VAL:HB	2.09	0.52
2:R:874:ILE:HG22	2:R:875:PRO:HD2	1.91	0.52
1:W:271:TYR:HE2	1:W:285:PRO:HB3	1.74	0.52
1:W:304:GLY:C	1:W:306:GLU:N	2.68	0.52
1:W:451:PRO:N	1:W:452:PRO:CD	2.73	0.52
3:Y:160:ILE:O	3:Y:161:ALA:C	2.53	0.52
1:A:86:PHE:O	1:A:90:VAL:HG23	2.09	0.52
1:A:763:THR:HB	1:A:764:ARG:CD	2.40	0.52
2:B:108:ASN:O	2:B:110:ILE:HG12	2.09	0.52
2:B:109:ASN:CG	2:B:109:ASN:O	2.52	0.52
2:B:430:ARG:HD3	2:B:653:ILE:HG12	1.92	0.52
2:B:583:ILE:HD13	2:B:616:ILE:HG12	1.92	0.52
2:B:647:SER:N	2:B:648:PRO:CD	2.73	0.52
2:B:767:LYS:HD3	2:B:768:TYR:CA	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:417:LEU:CD2	2:R:425:MET:HG3	2.38	0.52
2:R:1007:ARG:HD3	2:R:1028:GLY:HA2	1.91	0.52
2:R:1046:MET:HG2	5:T:61:PHE:CD1	2.44	0.52
2:R:1080:TYR:HB3	2:R:1091:LEU:HD12	1.92	0.52
5:T:114:THR:HG21	5:T:117:THR:OG1	2.10	0.52
1:A:426:HIS:CG	3:C:80:GLU:CD	2.88	0.52
1:A:511:VAL:HA	1:A:583:ASP:OD2	2.08	0.52
1:A:534:LEU:HB3	1:A:546:TYR:CE1	2.43	0.52
1:A:541:ALA:HB3	1:A:542:PRO:HD3	1.92	0.52
1:A:818:TYR:CD2	1:A:822:ARG:NH1	2.78	0.52
2:B:752:MET:HB2	12:N:8:PHE:CD2	2.44	0.52
3:C:11:SER:N	3:C:45:ARG:NH2	2.58	0.52
3:C:210:PHE:O	3:C:211:ALA:CB	2.57	0.52
5:E:53:THR:O	5:E:54:SER:C	2.52	0.52
9:I:62:ILE:HD12	1:W:474:ALA:CB	2.39	0.52
11:M:16:GLU:OE2	11:M:52:LYS:HE2	2.10	0.52
2:R:397:ILE:O	2:R:397:ILE:HG12	2.10	0.52
2:R:630:ALA:HB3	2:R:636:LEU:HD12	1.91	0.52
1:W:141:MET:HG3	1:W:141:MET:O	2.07	0.52
1:W:288:LYS:HA	1:W:295:LEU:CD2	2.39	0.52
1:W:289:HIS:O	1:W:290:ARG:HB2	2.09	0.52
1:A:417:VAL:HG11	1:A:464:LEU:HD11	1.91	0.52
2:B:272:LEU:HD22	2:B:292:ALA:O	2.09	0.52
2:B:973:THR:HG21	2:B:988:PHE:CE1	2.45	0.52
3:C:303:GLU:C	3:C:303:GLU:OE1	2.52	0.52
5:E:114:THR:HG21	5:E:117:THR:OG1	2.09	0.52
6:F:64:SER:HB2	6:F:69:ARG:HD3	1.91	0.52
7:G:103:VAL:HG22	7:G:104:LYS:N	2.23	0.52
13:P:10:TRP:CB	13:P:31:TYR:CE2	2.93	0.52
2:R:215:VAL:HG12	2:R:224:ILE:O	2.09	0.52
2:R:873:ARG:HH22	2:R:1002:ASP:CG	2.17	0.52
7:V:103:VAL:HG22	7:V:104:LYS:N	2.24	0.52
1:W:81:VAL:HG21	1:W:269:LEU:HB3	1.92	0.52
3:Y:70:ILE:HD13	3:Y:70:ILE:N	2.23	0.52
1:A:859:TYR:OH	9:K:29:ARG:HD2	2.10	0.52
2:B:107:GLU:O	2:B:108:ASN:CB	2.57	0.52
2:B:333:ARG:O	2:B:334:GLU:HB3	2.10	0.52
2:B:356:LEU:CD1	2:B:407:VAL:HG21	2.40	0.52
2:B:461:THR:HG21	2:B:468:GLY:N	2.25	0.52
2:B:558:VAL:HG22	2:B:571:VAL:HG22	1.92	0.52
2:B:605:ILE:HG23	2:B:606:THR:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:182:VAL:HG11	4:D:212:TYR:HD2	1.73	0.52
4:D:247:LYS:O	4:D:251:ARG:HG3	2.09	0.52
5:E:63:ASP:OD2	5:E:65:ALA:HB3	2.10	0.52
5:E:128:PHE:HB3	5:E:137:GLN:CD	2.35	0.52
6:F:12:ILE:HG23	6:F:16:VAL:CG1	2.39	0.52
10:J:66:ARG:HH11	10:J:66:ARG:HG2	1.75	0.52
12:N:9:THR:HB	12:N:44:CYS:HB2	1.90	0.52
2:R:108:ASN:O	2:R:110:ILE:HG12	2.09	0.52
2:R:233:LEU:HD13	2:R:315:ALA:HB2	1.92	0.52
2:R:1074:ASP:CB	2:R:1075:LYS:HA	2.40	0.52
7:V:15:ILE:HG12	7:V:31:MET:HE2	1.91	0.52
1:W:635:PHE:O	1:W:639:VAL:HG23	2.10	0.52
1:W:736:SER:O	1:W:738:LEU:N	2.43	0.52
1:A:324:THR:HG22	1:A:325:VAL:H	1.74	0.52
2:B:330:LEU:HD22	2:B:332:ARG:HD3	1.92	0.52
2:B:461:THR:CG2	2:B:468:GLY:N	2.72	0.52
2:B:630:ALA:HB3	2:B:636:LEU:HD12	1.92	0.52
3:C:46:ASP:O	3:C:47:GLU:OE1	2.28	0.52
3:C:277:ILE:C	3:C:279:GLU:N	2.67	0.52
9:I:43:LEU:HD13	9:I:64:ILE:HG22	1.90	0.52
2:R:17:ILE:HD12	2:R:476:MET:SD	2.50	0.52
2:R:229:LEU:CD2	2:R:275:ILE:HD11	2.40	0.52
2:R:603:GLY:C	2:R:605:ILE:N	2.66	0.52
2:R:975:ASP:HB3	2:R:978:THR:HG22	1.92	0.52
1:W:192:VAL:CG2	1:W:199:PRO:HB3	2.40	0.52
1:W:223:ILE:CG1	1:W:224:MET:N	2.73	0.52
3:Y:25:PRO:CG	3:Y:33:LYS:HD3	2.40	0.52
1:A:69:PRO:HB2	2:B:1101:LYS:HE3	1.92	0.52
1:A:853:ASP:HB2	3:C:311:ARG:NH1	2.25	0.52
2:B:250:GLU:HG2	2:B:251:ILE:N	2.25	0.52
2:B:1062:TYR:CE2	2:B:1093:PRO:HG3	2.45	0.52
6:F:41:LEU:HA	6:F:44:VAL:HG12	1.90	0.52
8:H:45:ILE:HG23	8:H:81:VAL:HG22	1.92	0.52
9:K:61:VAL:H	9:K:64:ILE:HD12	1.74	0.52
2:R:453:TRP:CZ3	2:R:644:GLU:OE2	2.63	0.52
2:R:630:ALA:CB	2:R:636:LEU:HD12	2.40	0.52
2:R:767:LYS:HB3	2:R:768:TYR:CB	2.39	0.52
2:R:1029:LEU:HD12	1:W:321:SER:HB2	1.92	0.52
2:R:1066:GLN:HG3	2:R:1089:SER:HB3	1.92	0.52
2:R:1099:ALA:C	1:W:313:LEU:HD21	2.35	0.52
5:T:30:LEU:HD22	5:T:72:PHE:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:782:ILE:HG23	1:W:794:GLU:CD	2.35	0.52
1:A:104:VAL:HG12	1:A:137:LYS:CA	2.37	0.51
1:A:220:ARG:HG2	1:A:235:LEU:HD13	1.92	0.51
1:A:309:PHE:O	1:A:310:ARG:CB	2.58	0.51
2:B:258:SER:O	2:B:259:LEU:HD22	2.10	0.51
2:B:594:ARG:CZ	2:B:615:LYS:HG3	2.40	0.51
2:B:657:ILE:HG13	2:B:711:LEU:CD2	2.40	0.51
2:B:949:TYR:O	2:B:950:LYS:HD2	2.10	0.51
9:I:51:ILE:O	9:I:52:ASP:HB2	2.10	0.51
5:T:48:ILE:HD12	5:T:74:MET:HE2	1.91	0.51
1:W:10:LYS:HG2	3:Y:363:VAL:CG1	2.40	0.51
1:W:249:LEU:HD21	1:W:265:LEU:HB2	1.91	0.51
1:A:541:ALA:HB3	7:G:71:PHE:HA	1.92	0.51
2:B:230:MET:HE1	2:B:315:ALA:HB1	1.92	0.51
2:B:957:GLN:HA	2:B:960:ILE:HG12	1.91	0.51
2:B:1062:TYR:HE2	2:B:1093:PRO:HG3	1.74	0.51
5:E:123:VAL:O	5:E:124:ARG:O	2.29	0.51
5:E:128:PHE:HB3	5:E:137:GLN:NE2	2.25	0.51
12:O:13:LEU:HD11	4:S:66:PRO:HG2	1.92	0.51
2:R:699:HIS:ND1	4:S:57:ILE:HG12	2.24	0.51
2:R:877:ILE:HD12	2:R:877:ILE:H	1.75	0.51
1:W:125:TRP:O	1:W:128:ALA:HB3	2.10	0.51
3:Y:237:ILE:HD12	3:Y:253:THR:CG2	2.40	0.51
3:Y:330:GLY:C	3:Y:335:THR:HG22	2.34	0.51
1:A:366:ILE:HG13	1:A:395:LYS:HG3	1.92	0.51
1:A:428:ILE:HG21	1:A:452:PRO:HB3	1.93	0.51
2:B:543:ILE:CD1	2:B:558:VAL:HG21	2.39	0.51
2:B:653:ILE:H	2:B:653:ILE:HD12	1.75	0.51
2:B:773:GLU:HG2	2:B:774:ASP:N	2.26	0.51
2:B:872:LEU:HD23	2:B:873:ARG:N	2.26	0.51
2:B:928:MET:CE	2:B:953:ILE:HD12	2.40	0.51
3:C:237:ILE:HD12	3:C:253:THR:CG2	2.39	0.51
7:G:36:PHE:CE1	7:G:96:ILE:HD11	2.46	0.51
12:O:47:ARG:HD2	2:R:724:ASN:O	2.10	0.51
2:R:301:LEU:N	2:R:302:PRO:HD3	2.25	0.51
2:R:1039:LEU:HD22	2:R:1044:THR:HG21	1.92	0.51
5:T:84:VAL:CG2	6:U:75:ILE:HD13	2.40	0.51
3:Y:126:LEU:HB2	3:Y:131:LYS:HG3	1.91	0.51
1:A:45:MET:O	1:A:45:MET:HE3	2.11	0.51
1:A:356:TRP:CE3	9:K:54:ASN:ND2	2.78	0.51
1:A:534:LEU:HD22	1:A:534:LEU:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:16:GLU:OE2	11:L:52:LYS:HE2	2.09	0.51
2:R:733:THR:HG23	2:R:734:GLY:N	2.25	0.51
2:R:762:SER:OG	2:R:866:LYS:HG2	2.10	0.51
2:R:766:VAL:CG1	2:R:774:ASP:OD2	2.52	0.51
4:S:180:ALA:HA	4:S:188:PHE:HB2	1.91	0.51
5:T:56:GLU:HG2	3:Y:391:ARG:HG2	1.93	0.51
5:T:82:GLN:HB3	6:U:88:ILE:HB	1.92	0.51
5:T:132:SER:O	5:T:133:LYS:HG3	2.11	0.51
6:U:88:ILE:HD13	6:U:88:ILE:H	1.75	0.51
1:A:12:GLY:HA3	1:A:201:THR:CG2	2.40	0.51
1:A:588:ILE:HG13	1:A:593:LEU:HA	1.92	0.51
1:A:879:LYS:NZ	3:C:44:THR:O	2.43	0.51
4:D:56:GLU:HG3	13:P:45:VAL:HG13	1.91	0.51
4:D:154:ALA:HA	4:D:157:ILE:HG13	1.93	0.51
5:E:86:GLU:O	6:F:44:VAL:HG23	2.09	0.51
9:I:29:ARG:HD2	1:W:859:TYR:OH	2.09	0.51
2:R:754:ARG:NH1	4:S:60:HIS:HD1	2.09	0.51
2:R:1015:LEU:CD1	2:R:1102:LEU:HD11	2.40	0.51
2:R:1069:TYR:HA	2:R:1070:ILE:CB	2.38	0.51
5:T:84:VAL:HG13	6:U:75:ILE:HD11	1.92	0.51
1:W:123:LYS:HA	1:W:126:PRO:HG3	1.92	0.51
13:X:5:ARG:HG2	13:X:18:LEU:HD22	1.93	0.51
8:Z:59:PRO:HA	8:Z:81:VAL:CG1	2.41	0.51
1:A:328:PRO:HB3	1:A:457:PHE:CE2	2.46	0.51
2:B:247:LEU:HD11	2:B:503:VAL:HG12	1.93	0.51
2:B:539:LEU:HD12	2:B:569:VAL:HG11	1.93	0.51
3:C:66:PRO:HD3	9:K:23:TRP:CE2	2.45	0.51
3:C:80:GLU:N	3:C:81:PRO:CD	2.73	0.51
12:O:19:GLN:N	12:O:20:PRO:HD2	2.25	0.51
2:R:461:THR:CG2	2:R:468:GLY:N	2.74	0.51
2:R:539:LEU:HD12	2:R:569:VAL:HG11	1.91	0.51
2:R:708:THR:HG23	2:R:946:THR:HA	1.93	0.51
2:R:1056:SER:CB	1:W:316:LYS:HD3	2.40	0.51
5:T:2:TYR:HB2	6:U:12:ILE:O	2.10	0.51
5:T:40:LYS:O	5:T:41:ASP:CG	2.53	0.51
1:W:220:ARG:HG2	1:W:235:LEU:HD22	1.91	0.51
1:W:636:ILE:O	1:W:640:GLU:HG3	2.09	0.51
1:W:864:LYS:HG3	1:W:864:LYS:O	2.10	0.51
3:Y:11:SER:N	3:Y:45:ARG:NH2	2.58	0.51
3:Y:210:PHE:O	3:Y:211:ALA:CB	2.57	0.51
8:Z:12:ARG:NH2	8:Z:55:ILE:HA	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:VAL:HG21	1:A:269:LEU:HB3	1.91	0.51
1:A:474:ALA:CB	9:K:62:ILE:HD12	2.40	0.51
2:B:355:SER:O	2:B:407:VAL:HG11	2.10	0.51
3:C:25:PRO:CG	3:C:33:LYS:HD3	2.41	0.51
3:C:64:ILE:HG22	3:C:65:ALA:N	2.21	0.51
9:I:19:PHE:HE1	3:Y:64:ILE:HG21	1.76	0.51
9:I:53:ILE:HG23	9:I:53:ILE:O	2.11	0.51
9:K:13:LEU:O	9:K:14:HIS:C	2.53	0.51
11:M:46:PRO:HD2	11:M:52:LYS:O	2.11	0.51
2:R:430:ARG:HD3	2:R:653:ILE:HG12	1.91	0.51
2:R:1074:ASP:HB3	2:R:1075:LYS:CB	2.39	0.51
2:R:1082:CYS:HB3	2:R:1091:LEU:HD21	1.92	0.51
4:S:206:CYS:HB3	16:S:1001:F3S:S3	2.51	0.51
1:W:421:ARG:CZ	1:W:454:ASN:O	2.59	0.51
1:A:13:ILE:HG13	1:A:202:SER:CB	2.41	0.51
1:A:324:THR:HG22	1:A:325:VAL:N	2.26	0.51
1:A:363:GLN:O	1:A:366:ILE:HG22	2.10	0.51
2:B:628:TYR:CE2	2:B:640:HIS:CE1	2.98	0.51
2:B:957:GLN:HA	2:B:960:ILE:CG1	2.41	0.51
12:O:62:TYR:HB3	2:R:689:LEU:CD1	2.40	0.51
2:R:1094:VAL:HG11	1:W:6:ILE:CD1	2.41	0.51
5:T:167:PRO:C	5:T:169:LEU:H	2.19	0.51
3:Y:25:PRO:HD3	3:Y:33:LYS:HD3	1.93	0.51
3:Y:286:ILE:HG12	8:Z:49:ASP:CG	2.36	0.51
3:Y:328:GLN:OE1	3:Y:331:ARG:NH1	2.44	0.51
1:A:854:GLY:O	3:C:64:ILE:HG23	2.11	0.51
1:A:864:LYS:O	1:A:864:LYS:HG3	2.10	0.51
2:B:843:ARG:HB2	2:B:846:GLU:CG	2.41	0.51
2:B:1065:ASP:HB3	2:B:1089:SER:HB2	1.93	0.51
11:M:73:ILE:HG23	4:S:253:ILE:HG13	1.92	0.51
12:O:35:LEU:HD13	12:O:46:ARG:CG	2.41	0.51
2:R:112:ALA:O	2:R:113:GLU:CG	2.59	0.51
2:R:356:LEU:CD1	2:R:407:VAL:HG21	2.41	0.51
2:R:699:HIS:CE1	4:S:57:ILE:HD11	2.46	0.51
2:R:732:PHE:O	2:R:733:THR:HG22	2.11	0.51
2:R:772:GLN:HG2	2:R:773:GLU:H	1.76	0.51
2:R:778:MET:HE2	2:R:795:LEU:HB2	1.92	0.51
2:R:856:THR:HG22	2:R:857:GLU:N	2.25	0.51
2:R:918:LEU:HD13	1:W:646:MET:HG2	1.92	0.51
2:R:1065:ASP:HB3	2:R:1089:SER:HB2	1.93	0.51
5:T:136:ILE:CG2	5:T:137:GLN:H	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:150:GLU:HG3	3:Y:227:LEU:HB3	1.92	0.51
1:A:119:ASN:OD1	1:A:126:PRO:HB3	2.11	0.51
1:A:600:LYS:O	1:A:601:LYS:CB	2.53	0.51
2:B:417:LEU:CD2	2:B:425:MET:HG3	2.41	0.51
2:B:720:PRO:HG3	12:N:53:ILE:CD1	2.40	0.51
2:B:877:ILE:H	2:B:877:ILE:HD12	1.76	0.51
4:D:159:VAL:HG22	4:D:161:LEU:H	1.76	0.51
2:R:872:LEU:HD23	2:R:873:ARG:N	2.25	0.51
2:R:984:SER:O	2:R:985:ARG:CB	2.58	0.51
4:S:97:TYR:CD1	4:S:142:GLU:HG3	2.46	0.51
6:U:72:LEU:HD21	6:U:86:ILE:CG1	2.41	0.51
1:W:28:ILE:HG23	1:W:30:PRO:HD2	1.93	0.51
1:W:588:ILE:HG13	1:W:593:LEU:HA	1.92	0.51
3:Y:46:ASP:O	3:Y:47:GLU:OE1	2.29	0.51
1:A:280:GLU:H	1:A:282:PRO:HD2	1.74	0.50
1:A:750:GLN:HG3	1:A:782:ILE:HD11	1.94	0.50
1:A:838:VAL:HG13	3:C:70:ILE:HD11	1.92	0.50
2:B:772:GLN:HG2	2:B:773:GLU:H	1.75	0.50
3:C:257:ASN:O	3:C:261:VAL:HG23	2.11	0.50
3:C:330:GLY:O	3:C:335:THR:HG22	2.12	0.50
5:E:131:LYS:HE3	5:E:136:ILE:HD11	1.93	0.50
9:I:49:ALA:O	9:I:50:LEU:C	2.54	0.50
11:L:63:ILE:HG22	11:L:64:ALA:O	2.10	0.50
10:Q:49:GLU:O	10:Q:52:ASP:HB3	2.11	0.50
2:R:118:TYR:CD1	2:R:118:TYR:C	2.89	0.50
2:R:773:GLU:CG	2:R:774:ASP:N	2.74	0.50
2:R:973:THR:HG21	2:R:988:PHE:CE1	2.46	0.50
2:R:974:TYR:HA	2:R:981:LYS:HA	1.92	0.50
4:S:34:LEU:HD22	4:S:151:LYS:HB2	1.92	0.50
1:W:98:CYS:HB2	1:W:102:GLY:O	2.11	0.50
1:W:124:ARG:N	1:W:126:PRO:HD2	2.26	0.50
1:W:176:THR:O	1:W:180:ILE:HG13	2.11	0.50
1:W:185:GLU:HA	1:W:205:GLU:OE2	2.11	0.50
1:W:450:CYS:N	1:W:451:PRO:CD	2.74	0.50
1:W:737:VAL:HG23	1:W:738:LEU:HD23	1.93	0.50
1:A:80:PRO:HB3	1:A:208:ILE:HG22	1.93	0.50
1:A:177:PRO:CD	1:A:266:TRP:HZ2	2.22	0.50
1:A:488:THR:HG23	1:A:493:GLY:O	2.11	0.50
1:A:777:GLU:HG3	1:A:783:TYR:HE1	1.76	0.50
2:B:12:GLU:HG3	2:B:595:GLU:OE1	2.11	0.50
2:B:1046:MET:HE3	5:E:61:PHE:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:132:SER:O	5:E:133:LYS:CG	2.58	0.50
8:H:12:ARG:O	8:H:14:HIS:N	2.44	0.50
9:K:63:SER:HA	9:K:66:GLU:HB2	1.93	0.50
2:R:53:PRO:HD2	2:R:59:LEU:O	2.10	0.50
2:R:372:LEU:HD22	2:R:376:LYS:HG3	1.94	0.50
2:R:493:TYR:HD1	2:R:497:VAL:O	1.95	0.50
2:R:605:ILE:HG12	2:R:606:THR:N	2.26	0.50
2:R:732:PHE:C	2:R:733:THR:HG22	2.36	0.50
2:R:898:VAL:HG22	4:S:33:MET:SD	2.52	0.50
5:T:9:SER:O	5:T:70:VAL:HG12	2.11	0.50
1:W:253:ILE:HG22	1:W:254:ASP:OD1	2.10	0.50
1:W:366:ILE:HG13	1:W:395:LYS:HG3	1.92	0.50
1:A:185:GLU:HA	1:A:205:GLU:OE2	2.12	0.50
1:A:541:ALA:HB3	1:A:542:PRO:CD	2.40	0.50
2:B:492:LEU:HB3	2:B:497:VAL:HG21	1.93	0.50
3:C:70:ILE:H	3:C:70:ILE:CD1	2.23	0.50
3:C:150:GLU:HG3	3:C:227:LEU:HB3	1.93	0.50
3:C:197:VAL:HB	3:C:208:ILE:HB	1.92	0.50
4:D:96:ILE:HG12	4:D:145:LEU:HD11	1.93	0.50
4:D:161:LEU:O	4:D:230:LEU:HA	2.12	0.50
2:R:767:LYS:HG3	2:R:768:TYR:HA	1.92	0.50
2:R:1074:ASP:HB3	2:R:1075:LYS:HA	1.93	0.50
1:W:687:ILE:HD12	1:W:695:SER:HB2	1.94	0.50
2:B:17:ILE:O	2:B:20:TYR:HB3	2.11	0.50
2:B:112:ALA:O	2:B:113:GLU:CG	2.59	0.50
2:B:605:ILE:CG1	2:B:606:THR:H	2.18	0.50
2:B:1017:ARG:HD3	2:B:1098:TYR:CG	2.47	0.50
7:G:15:ILE:HG12	7:G:31:MET:HE2	1.94	0.50
8:H:29:TYR:HE1	10:Q:60:SER:HB2	1.77	0.50
2:R:448:LEU:CD2	1:W:796:PHE:CZ	2.94	0.50
2:R:597:ILE:HB	2:R:603:GLY:H	1.76	0.50
2:R:767:LYS:HD3	2:R:768:TYR:HA	1.93	0.50
2:R:1007:ARG:HH21	2:R:1026:GLU:C	2.19	0.50
2:R:1044:THR:HG23	2:R:1044:THR:O	2.11	0.50
6:U:64:SER:HB2	6:U:69:ARG:HD3	1.94	0.50
1:W:777:GLU:H	1:W:777:GLU:CD	2.19	0.50
3:Y:80:GLU:CB	3:Y:81:PRO:HD3	2.39	0.50
1:A:642:GLN:OE1	2:B:983:LYS:HD2	2.10	0.50
2:B:478:GLN:HG2	2:B:479:ILE:N	2.27	0.50
2:B:787:LYS:HE3	2:B:841:VAL:HG23	1.93	0.50
3:C:47:GLU:HB3	3:C:50:LYS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:241:ILE:O	3:C:251:ILE:HG23	2.12	0.50
11:M:48:PRO:HG2	2:R:735:TYR:HE2	1.75	0.50
2:R:126:LEU:HD13	2:R:154:TYR:O	2.11	0.50
2:R:332:ARG:HD2	2:R:565:PHE:HB3	1.92	0.50
2:R:741:ILE:HD11	2:R:911:VAL:CG1	2.42	0.50
5:T:128:PHE:HB3	5:T:137:GLN:CD	2.37	0.50
1:W:110:GLU:HA	1:W:113:LYS:HD2	1.93	0.50
1:W:177:PRO:CD	1:W:266:TRP:HZ2	2.22	0.50
8:Z:63:ILE:HG22	8:Z:65:ILE:CD1	2.41	0.50
1:A:316:LYS:HD3	2:B:1056:SER:CB	2.40	0.50
2:B:127:LYS:HE3	2:B:150:ASP:O	2.12	0.50
2:B:657:ILE:HG13	2:B:711:LEU:HD21	1.94	0.50
3:C:341:VAL:HG12	3:C:344:ARG:NH2	2.26	0.50
9:I:77:THR:HG23	9:I:90:LEU:O	2.12	0.50
9:K:52:ASP:O	9:K:53:ILE:CB	2.59	0.50
11:L:14:GLU:OE1	11:L:56:LYS:HG2	2.12	0.50
2:R:17:ILE:CD1	2:R:476:MET:SD	2.99	0.50
2:R:486:LYS:HG2	2:R:489:GLU:OE2	2.11	0.50
2:R:843:ARG:HB2	2:R:846:GLU:CG	2.41	0.50
2:R:1003:LYS:O	2:R:1004:ILE:C	2.54	0.50
2:R:1057:ASP:N	2:R:1057:ASP:OD1	2.44	0.50
2:R:1112:ILE:O	2:R:1114:PRO:HD3	2.11	0.50
1:W:328:PRO:HB3	1:W:457:PHE:CE2	2.46	0.50
1:W:510:THR:O	1:W:597:VAL:HG23	2.11	0.50
3:Y:197:VAL:HB	3:Y:208:ILE:HB	1.94	0.50
3:Y:340:SER:HB3	3:Y:371:GLU:CG	2.41	0.50
2:B:42:LEU:HD12	2:B:357:PHE:CE2	2.47	0.50
2:B:232:ALA:HB2	2:B:271:ALA:HB1	1.94	0.50
2:B:601:ASP:O	2:B:602:SER:HB3	2.12	0.50
2:B:741:ILE:HG23	2:B:891:ILE:HA	1.94	0.50
3:C:176:ASP:O	3:C:177:LYS:CG	2.59	0.50
4:D:93:TYR:CE1	4:D:146:ARG:HG2	2.47	0.50
4:D:180:ALA:HA	4:D:188:PHE:HB2	1.92	0.50
13:P:37:VAL:HG22	13:P:38:ARG:N	2.27	0.50
2:R:493:TYR:CD1	2:R:499:PRO:HD3	2.47	0.50
2:R:543:ILE:CD1	2:R:558:VAL:HG21	2.40	0.50
2:R:767:LYS:HA	2:R:767:LYS:HZ2	1.76	0.50
2:R:1062:TYR:HA	2:R:1092:PHE:O	2.12	0.50
4:S:172:ILE:CD1	4:S:188:PHE:HE1	2.25	0.50
7:V:24:LYS:O	7:V:25:ASN:HB2	2.12	0.50
1:W:49:LEU:N	1:W:49:LEU:HD12	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:ILE:O	1:A:640:GLU:HG3	2.11	0.50
1:A:684:LEU:H	1:A:684:LEU:HD12	1.76	0.50
1:A:819:MET:HG2	1:A:819:MET:O	2.12	0.50
1:A:870:ARG:HH22	3:C:36:ILE:HD13	1.76	0.50
2:B:953:ILE:H	2:B:953:ILE:CD1	2.14	0.50
3:C:66:PRO:HD3	9:K:23:TRP:CZ2	2.46	0.50
3:C:394:LEU:O	3:C:395:ARG:C	2.54	0.50
4:D:203:CYS:SG	16:D:1001:F3S:S1	3.07	0.50
5:E:165:ARG:C	5:E:167:PRO:HD3	2.37	0.50
2:R:20:TYR:HD2	2:R:607:PHE:CE2	2.30	0.50
2:R:593:THR:HG23	2:R:594:ARG:N	2.26	0.50
2:R:628:TYR:CE2	2:R:640:HIS:ND1	2.80	0.50
2:R:732:PHE:CD2	2:R:733:THR:HB	2.47	0.50
5:T:10:ILE:HG23	5:T:68:HIS:O	2.12	0.50
1:W:695:SER:O	1:W:699:TYR:CD2	2.65	0.50
1:A:219:ILE:HD11	2:B:1105:GLN:HB3	1.94	0.50
2:B:192:ILE:O	2:B:206:GLU:HB2	2.12	0.50
2:B:597:ILE:HB	2:B:603:GLY:H	1.76	0.50
3:C:393:ILE:HG22	5:E:19:GLY:N	2.27	0.50
6:F:71:VAL:HG11	6:F:89:MET:HE1	1.94	0.50
7:G:102:LEU:O	7:G:103:VAL:C	2.55	0.50
10:J:60:SER:CB	8:Z:29:TYR:HE1	2.24	0.50
11:L:12:TYR:CD1	11:L:58:LEU:HB2	2.47	0.50
2:R:583:ILE:HD13	2:R:616:ILE:HG12	1.93	0.50
5:T:123:VAL:HA	5:T:127:ILE:HA	1.93	0.50
5:T:128:PHE:HB3	5:T:137:GLN:NE2	2.26	0.50
1:W:329:ASP:O	1:W:446:ASN:HA	2.11	0.50
1:W:682:GLY:O	1:W:683:GLU:C	2.55	0.50
3:Y:348:GLU:O	3:Y:349:VAL:C	2.54	0.50
3:Y:394:LEU:O	3:Y:395:ARG:C	2.54	0.50
1:A:136:VAL:HA	1:A:139:THR:HG22	1.93	0.49
1:A:450:CYS:H	1:A:451:PRO:CD	2.24	0.49
2:B:73:VAL:HG22	2:B:74:ARG:O	2.12	0.49
2:B:107:GLU:O	2:B:108:ASN:HB2	2.12	0.49
2:B:732:PHE:O	2:B:733:THR:HG22	2.12	0.49
9:K:53:ILE:HG23	9:K:53:ILE:O	2.12	0.49
12:O:46:ARG:NH1	2:R:938:LEU:O	2.45	0.49
10:Q:63:GLU:O	10:Q:67:LEU:HB2	2.12	0.49
2:R:192:ILE:O	2:R:206:GLU:HB2	2.11	0.49
2:R:247:LEU:HD11	2:R:503:VAL:HG12	1.93	0.49
2:R:330:LEU:O	2:R:332:ARG:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:653:ILE:H	2:R:653:ILE:CD1	2.24	0.49
5:T:36:GLU:HB3	6:U:33:LEU:HD22	1.94	0.49
1:A:426:HIS:NE2	3:C:80:GLU:CD	2.70	0.49
1:A:518:LYS:HA	1:A:546:TYR:HE2	1.76	0.49
1:A:792:PRO:HA	2:B:948:PHE:CZ	2.47	0.49
1:A:863:GLY:HA2	3:C:311:ARG:HH22	1.77	0.49
2:B:525:LEU:HD22	2:B:571:VAL:HB	1.94	0.49
2:B:630:ALA:CB	2:B:636:LEU:HD12	2.42	0.49
2:B:733:THR:HG23	2:B:735:TYR:HB2	1.94	0.49
2:B:797:ASP:OD2	13:P:4:TYR:HB3	2.11	0.49
2:B:1021:GLU:OE2	2:B:1022:GLY:N	2.45	0.49
2:B:1062:TYR:HA	2:B:1092:PHE:O	2.11	0.49
4:D:172:ILE:CD1	4:D:188:PHE:HE1	2.24	0.49
9:I:61:VAL:O	9:I:62:ILE:C	2.55	0.49
10:J:55:LEU:CD2	8:Z:25:ILE:HG22	2.42	0.49
2:R:248:ASP:N	2:R:249:PRO:HD3	2.26	0.49
2:R:250:GLU:HG2	2:R:251:ILE:N	2.27	0.49
2:R:584:ILE:CD1	2:R:617:GLU:HB2	2.42	0.49
4:S:155:LYS:HE3	4:S:156:PHE:CE2	2.47	0.49
5:T:123:VAL:O	5:T:124:ARG:O	2.30	0.49
6:U:72:LEU:HD21	6:U:86:ILE:HG12	1.94	0.49
1:W:106:ILE:HD12	1:W:106:ILE:H	1.75	0.49
1:W:518:LYS:HA	1:W:546:TYR:HE1	1.76	0.49
3:Y:257:ASN:O	3:Y:261:VAL:HG23	2.12	0.49
1:A:238:LYS:HE3	1:A:276:TYR:HA	1.94	0.49
1:A:502:TYR:O	1:A:503:ILE:C	2.54	0.49
2:B:579:ARG:HD3	2:B:618:TYR:CD2	2.48	0.49
2:B:874:ILE:HG22	2:B:875:PRO:HD2	1.94	0.49
2:B:1007:ARG:HD3	2:B:1028:GLY:HA2	1.95	0.49
3:C:237:ILE:HD11	3:C:240:ALA:HB2	1.95	0.49
3:C:328:GLN:HB3	3:C:332:HIS:HB3	1.94	0.49
4:D:34:LEU:HD22	4:D:151:LYS:HB2	1.95	0.49
10:J:63:GLU:O	10:J:67:LEU:HB2	2.12	0.49
11:L:13:LEU:HB2	11:L:65:PRO:HB2	1.93	0.49
11:L:32:LEU:HD23	11:L:35:ILE:HD12	1.94	0.49
11:M:14:GLU:OE1	11:M:56:LYS:HG2	2.12	0.49
5:T:168:TYR:C	5:T:169:LEU:HD12	2.36	0.49
1:W:136:VAL:HA	1:W:139:THR:HG22	1.94	0.49
1:W:428:ILE:HG21	1:W:452:PRO:HB3	1.94	0.49
1:A:470:GLU:HG3	9:K:41:LEU:HD12	1.94	0.49
2:B:973:THR:O	2:B:982:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:109:GLU:OE2	3:C:117:PRO:HA	2.12	0.49
3:C:174:LEU:CB	3:C:179:VAL:HG13	2.42	0.49
2:R:230:MET:HE1	2:R:315:ALA:HB1	1.93	0.49
2:R:345:ARG:NH2	2:R:577:ARG:HG2	2.28	0.49
5:T:40:LYS:O	5:T:42:LEU:HD12	2.12	0.49
1:W:601:LYS:O	1:W:610:SER:HB2	2.12	0.49
1:W:827:LEU:O	3:Y:71:GLY:HA3	2.11	0.49
3:Y:330:GLY:O	3:Y:335:THR:HG22	2.13	0.49
1:A:830:LEU:HD23	1:A:840:SER:HB3	1.92	0.49
2:B:136:TYR:CB	2:B:141:LEU:CD1	2.91	0.49
2:B:699:HIS:CE1	4:D:57:ILE:HG12	2.48	0.49
2:B:1091:LEU:O	2:B:1092:PHE:CG	2.66	0.49
5:E:50:ASN:HB2	5:E:73:ASP:HB2	1.93	0.49
7:G:81:LEU:HD12	7:G:81:LEU:N	2.27	0.49
12:O:47:ARG:NH2	12:O:48:MET:HE2	2.28	0.49
10:Q:69:GLU:CD	10:Q:73:LYS:HE3	2.37	0.49
2:R:759:ARG:HG3	2:R:760:LEU:N	2.28	0.49
4:S:8:LYS:HG2	4:S:9:ASP:N	2.27	0.49
1:W:119:ASN:OD1	1:W:126:PRO:HB3	2.12	0.49
1:W:426:HIS:CG	3:Y:80:GLU:CD	2.91	0.49
1:A:13:ILE:CD1	1:A:202:SER:HB2	2.42	0.49
1:A:316:LYS:HZ3	2:B:1097:SER:HB2	1.78	0.49
1:A:505:GLY:HA3	1:A:639:VAL:CG2	2.43	0.49
2:B:776:ILE:HG23	2:B:815:GLY:O	2.13	0.49
4:D:171:GLU:HB2	4:D:218:ARG:HB3	1.93	0.49
10:J:66:ARG:CD	1:W:121:ILE:HG21	2.43	0.49
9:K:55:ASN:HA	9:K:56:ILE:N	2.28	0.49
2:R:163:VAL:HG21	2:R:429:LEU:HD23	1.93	0.49
2:R:767:LYS:HA	2:R:767:LYS:NZ	2.27	0.49
2:R:973:THR:O	2:R:982:ILE:HG13	2.11	0.49
5:T:84:VAL:CG1	6:U:75:ILE:CD1	2.90	0.49
1:W:13:ILE:CD1	1:W:202:SER:HB2	2.43	0.49
1:W:830:LEU:HD23	1:W:840:SER:HB3	1.93	0.49
1:W:879:LYS:NZ	3:Y:44:THR:O	2.45	0.49
13:X:5:ARG:CZ	13:X:6:CYS:O	2.61	0.49
1:A:235:LEU:O	1:A:239:LEU:HB2	2.12	0.49
2:B:502:GLU:O	2:B:506:ARG:HB2	2.12	0.49
2:B:873:ARG:HH22	2:B:1002:ASP:CG	2.20	0.49
2:B:1050:ASP:HA	2:B:1054:ASP:HB2	1.94	0.49
3:C:277:ILE:CG2	3:C:278:ARG:H	2.22	0.49
3:C:284:PHE:HB3	3:C:288:ALA:HB1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:330:GLY:C	3:C:335:THR:HG22	2.37	0.49
5:E:40:LYS:O	5:E:42:LEU:HD12	2.13	0.49
5:E:84:VAL:HG13	6:F:75:ILE:HD11	1.94	0.49
9:I:62:ILE:O	9:I:66:GLU:HG3	2.13	0.49
12:O:43:TYR:HB3	2:R:938:LEU:HD23	1.94	0.49
10:Q:62:ASP:O	10:Q:66:ARG:HB3	2.13	0.49
5:T:36:GLU:CG	6:U:33:LEU:HD22	2.42	0.49
7:V:103:VAL:HG13	7:V:104:LYS:CD	2.41	0.49
3:Y:211:ALA:O	3:Y:212:ASN:HB2	2.13	0.49
3:Y:347:PHE:O	3:Y:348:GLU:HB3	2.12	0.49
8:Z:62:ILE:O	8:Z:62:ILE:HG13	2.11	0.49
1:A:534:LEU:HB2	1:A:546:TYR:CE1	2.48	0.49
2:B:584:ILE:CD1	2:B:617:GLU:HB2	2.42	0.49
2:B:732:PHE:C	2:B:733:THR:HG22	2.37	0.49
2:B:1074:ASP:HB3	2:B:1075:LYS:HA	1.95	0.49
3:C:127:THR:H	3:C:268:ASP:HB2	1.77	0.49
4:D:209:CYS:SG	4:D:219:ILE:CD1	2.99	0.49
5:E:94:ASN:HA	5:E:121:ASP:OD2	2.13	0.49
5:E:115:ASP:O	5:E:116:ASP:CG	2.55	0.49
6:F:4:VAL:O	6:F:4:VAL:HG13	2.12	0.49
6:F:72:LEU:HD21	6:F:86:ILE:CG1	2.43	0.49
9:I:34:ARG:HB2	3:Y:386:VAL:HG11	1.95	0.49
11:M:77:ARG:NH1	11:M:77:ARG:HB2	2.28	0.49
12:N:5:ILE:HA	12:N:15:ALA:HB2	1.94	0.49
2:R:359:VAL:HG11	2:R:407:VAL:HG13	1.93	0.49
2:R:364:PHE:CE1	2:R:388:VAL:HG13	2.47	0.49
2:R:404:GLY:O	2:R:405:ASN:O	2.31	0.49
2:R:659:PRO:HG3	2:R:884:ARG:NH2	2.28	0.49
2:R:934:LYS:O	2:R:938:LEU:HG	2.13	0.49
4:S:93:TYR:CD1	4:S:146:ARG:HB3	2.46	0.49
5:T:132:SER:O	5:T:133:LYS:CG	2.60	0.49
1:W:45:MET:O	1:W:45:MET:HE3	2.12	0.49
1:W:98:CYS:O	1:W:99:ARG:CB	2.59	0.49
13:X:10:TRP:CB	13:X:31:TYR:CE2	2.93	0.49
3:Y:258:LEU:HD11	3:Y:272:VAL:HG11	1.94	0.49
1:A:123:LYS:HA	1:A:126:PRO:HG3	1.93	0.49
1:A:761:TYR:CD1	2:B:451:THR:HG22	2.48	0.49
2:B:291:LYS:C	2:B:293:GLN:H	2.21	0.49
2:B:532:TYR:O	2:B:533:TYR:CB	2.60	0.49
2:B:604:SER:O	2:B:605:ILE:O	2.31	0.49
2:B:659:PRO:HG3	2:B:884:ARG:NH2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1074:ASP:CB	2:B:1075:LYS:HA	2.43	0.49
2:B:1111:ILE:O	2:B:1111:ILE:HG22	2.12	0.49
5:E:115:ASP:O	5:E:116:ASP:HB2	2.13	0.49
7:G:36:PHE:CE1	7:G:96:ILE:HG12	2.48	0.49
8:H:59:PRO:HA	8:H:81:VAL:CG1	2.43	0.49
2:R:272:LEU:HD22	2:R:292:ALA:O	2.13	0.49
1:W:220:ARG:HG2	1:W:235:LEU:HD13	1.95	0.49
1:W:235:LEU:O	1:W:239:LEU:HB2	2.13	0.49
1:W:428:ILE:C	1:W:430:MET:H	2.21	0.49
3:Y:102:LEU:HD11	3:Y:118:SER:HB3	1.95	0.49
3:Y:232:LYS:HA	3:Y:232:LYS:HE3	1.95	0.49
1:A:95:LYS:HD3	1:A:138:LYS:HD3	1.95	0.49
1:A:328:PRO:HD3	1:A:457:PHE:CG	2.47	0.49
1:A:421:ARG:HD3	1:A:453:TYR:O	2.13	0.49
2:B:84:SER:HG	2:B:144:ILE:HG23	1.76	0.49
2:B:398:ARG:C	2:B:400:ALA:H	2.19	0.49
2:B:732:PHE:CD2	2:B:733:THR:HB	2.48	0.49
2:B:808:LYS:HE3	2:B:847:MET:CE	2.43	0.49
2:B:1056:SER:CB	2:B:1057:ASP:OD1	2.60	0.49
8:H:12:ARG:NH2	8:H:55:ILE:HA	2.27	0.49
2:R:230:MET:HE2	2:R:230:MET:HA	1.94	0.49
2:R:957:GLN:HA	2:R:960:ILE:HG12	1.94	0.49
5:T:94:ASN:HA	5:T:121:ASP:OD2	2.13	0.49
5:T:121:ASP:OD1	5:T:129:GLY:HA3	2.13	0.49
1:W:80:PRO:HB3	1:W:208:ILE:HG22	1.95	0.49
3:Y:170:ASP:HB3	3:Y:173:MET:HB2	1.95	0.49
8:Z:12:ARG:O	8:Z:14:HIS:N	2.45	0.49
1:A:695:SER:O	1:A:699:TYR:CD2	2.66	0.48
1:A:763:THR:HB	1:A:764:ARG:HD3	1.94	0.48
2:B:598:GLU:HA	2:B:605:ILE:HD11	1.91	0.48
2:B:772:GLN:O	2:B:773:GLU:HB2	2.13	0.48
3:C:211:ALA:O	3:C:212:ASN:HB2	2.13	0.48
3:C:292:ILE:HD13	3:C:292:ILE:C	2.37	0.48
4:D:246:GLY:HA3	11:L:84:ILE:CD1	2.43	0.48
5:E:10:ILE:HG23	5:E:68:HIS:O	2.13	0.48
7:G:22:SER:O	7:G:23:LEU:C	2.56	0.48
8:H:44:TRP:O	8:H:79:ARG:HD2	2.13	0.48
9:K:77:THR:HG23	9:K:90:LEU:O	2.13	0.48
2:R:601:ASP:O	2:R:602:SER:HB3	2.12	0.48
2:R:1081:VAL:C	2:R:1091:LEU:HD11	2.38	0.48
4:S:104:ASN:O	4:S:105:GLU:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:80:VAL:HG12	5:T:83:GLU:CD	2.38	0.48
7:V:8:GLU:HG2	7:V:9:ILE:H	1.78	0.48
1:W:334:ILE:HD12	1:W:628:MET:CB	2.43	0.48
1:W:431:MET:HE2	1:W:482:VAL:HA	1.94	0.48
1:W:758:LYS:HA	1:W:779:ARG:HH11	1.78	0.48
1:A:45:MET:O	1:A:45:MET:CG	2.61	0.48
1:A:192:VAL:CG2	1:A:199:PRO:HB3	2.43	0.48
1:A:465:HIS:CE1	2:B:1031:PHE:HD2	2.30	0.48
1:A:687:ILE:HD12	1:A:695:SER:CB	2.44	0.48
1:A:853:ASP:CB	3:C:311:ARG:NH1	2.76	0.48
2:B:155:PHE:HE1	2:B:164:ILE:HD12	1.78	0.48
2:B:230:MET:HE2	2:B:230:MET:HA	1.95	0.48
2:B:631:LEU:O	2:B:632:GLU:OE1	2.31	0.48
2:B:734:GLY:HA3	2:B:735:TYR:CD2	2.48	0.48
2:B:766:VAL:HG22	2:B:767:LYS:N	2.15	0.48
2:B:947:PRO:C	2:B:948:PHE:CD2	2.91	0.48
3:C:127:THR:N	3:C:268:ASP:HB2	2.27	0.48
12:O:61:HIS:O	12:O:62:TYR:CG	2.66	0.48
4:S:13:ILE:HD13	4:S:14:ASP:N	2.27	0.48
4:S:182:VAL:HG11	4:S:212:TYR:CD2	2.48	0.48
1:A:486:ILE:HD13	1:A:628:MET:HE2	1.94	0.48
1:A:823:LEU:HB3	3:C:329:ILE:HG12	1.95	0.48
2:B:1040:ILE:HG23	3:C:381:LEU:HD11	1.95	0.48
2:B:1066:GLN:HG3	2:B:1089:SER:HB3	1.94	0.48
4:D:260:LEU:HD11	11:L:69:LEU:CD2	2.42	0.48
8:H:62:ILE:O	8:H:62:ILE:HG13	2.12	0.48
2:R:558:VAL:HG22	2:R:571:VAL:HG22	1.94	0.48
2:R:767:LYS:HD3	2:R:768:TYR:CA	2.43	0.48
2:R:983:LYS:HD2	1:W:642:GLN:OE1	2.13	0.48
1:W:647:ARG:HE	1:W:724:PHE:HE1	1.61	0.48
1:W:723:ASN:C	1:W:723:ASN:HD22	2.21	0.48
1:W:852:ASP:CG	8:Z:75:VAL:HG21	2.39	0.48
1:A:6:ILE:HD13	2:B:1116:LEU:HD23	1.95	0.48
1:A:647:ARG:HE	1:A:724:PHE:HE1	1.60	0.48
1:A:648:LEU:HB2	2:B:927:ILE:HG21	1.94	0.48
2:B:301:LEU:N	2:B:302:PRO:HD3	2.29	0.48
2:B:697:LEU:C	2:B:697:LEU:HD13	2.38	0.48
2:B:745:ARG:HD2	2:B:896:PRO:HG3	1.96	0.48
2:B:1046:MET:HE2	2:B:1046:MET:HA	1.96	0.48
3:C:133:ASP:O	3:C:249:TYR:CD2	2.66	0.48
3:C:147:THR:HB	3:C:232:LYS:CB	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:30:LEU:CD2	5:E:72:PHE:CE2	2.96	0.48
5:E:116:ASP:O	5:E:117:THR:HG23	2.14	0.48
5:E:119:LYS:HG2	5:E:120:TYR:CD2	2.48	0.48
5:E:121:ASP:OD1	5:E:129:GLY:HA3	2.13	0.48
6:F:62:ILE:HG22	6:F:63:ILE:H	1.78	0.48
12:N:47:ARG:NH2	12:N:48:MET:HE2	2.28	0.48
2:R:66:ILE:HG22	2:R:67:ARG:N	2.29	0.48
2:R:301:LEU:HB3	2:R:304:LEU:HD12	1.94	0.48
5:T:30:LEU:CD1	5:T:72:PHE:CE2	2.96	0.48
7:V:75:GLY:C	7:V:76:TYR:CD1	2.91	0.48
1:W:417:VAL:HG11	1:W:464:LEU:HD11	1.95	0.48
1:W:818:TYR:CD2	1:W:822:ARG:NH1	2.81	0.48
13:X:5:ARG:NH1	13:X:6:CYS:O	2.46	0.48
1:A:338:GLY:HA3	1:A:444:ARG:HB2	1.95	0.48
1:A:819:MET:HE2	1:A:819:MET:HB3	1.76	0.48
2:B:215:VAL:HG12	2:B:224:ILE:O	2.12	0.48
2:B:356:LEU:HD12	2:B:407:VAL:CG2	2.43	0.48
2:B:502:GLU:O	2:B:506:ARG:N	2.46	0.48
2:B:908:VAL:O	12:N:9:THR:HG23	2.14	0.48
3:C:186:LYS:CB	3:C:230:LYS:HE2	2.40	0.48
9:I:56:ILE:C	9:I:57:SER:C	2.80	0.48
2:R:249:PRO:HB2	2:R:253:ASN:H	1.79	0.48
2:R:594:ARG:CZ	2:R:615:LYS:HG3	2.43	0.48
2:R:672:GLN:HG2	2:R:884:ARG:O	2.14	0.48
2:R:784:ARG:HB3	2:R:835:LYS:O	2.13	0.48
2:R:957:GLN:HA	2:R:960:ILE:CG1	2.44	0.48
4:S:171:GLU:HB2	4:S:218:ARG:HB3	1.96	0.48
5:T:6:LYS:HA	5:T:72:PHE:O	2.13	0.48
5:T:10:ILE:HG22	5:T:11:VAL:N	2.29	0.48
5:T:116:ASP:O	5:T:117:THR:HG23	2.14	0.48
1:W:13:ILE:CG1	1:W:202:SER:HB2	2.44	0.48
1:W:124:ARG:HD3	1:W:125:TRP:CZ3	2.48	0.48
3:Y:133:ASP:O	3:Y:249:TYR:CD2	2.66	0.48
1:A:73:GLY:O	1:A:74:HIS:ND1	2.47	0.48
1:A:223:ILE:CG1	1:A:224:MET:N	2.76	0.48
1:A:736:SER:HB3	1:A:739:ASN:ND2	2.28	0.48
1:A:859:TYR:CE2	3:C:65:ALA:HB2	2.43	0.48
2:B:735:TYR:HE2	11:L:48:PRO:HG2	1.77	0.48
2:B:946:THR:O	2:B:947:PRO:C	2.57	0.48
5:E:30:LEU:HD13	5:E:72:PHE:HZ	1.70	0.48
5:E:167:PRO:C	5:E:169:LEU:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:27:LEU:HD23	9:I:78:ILE:HD11	1.95	0.48
9:K:56:ILE:C	9:K:57:SER:C	2.80	0.48
12:O:53:ILE:CD1	2:R:720:PRO:HG3	2.44	0.48
2:R:422:TRP:HZ3	2:R:715:GLY:HA3	1.78	0.48
2:R:502:GLU:O	2:R:506:ARG:HB2	2.13	0.48
2:R:703:ARG:NH2	2:R:942:ILE:HG21	2.29	0.48
2:R:734:GLY:HA3	2:R:735:TYR:CB	2.44	0.48
4:S:38:VAL:CG1	4:S:39:MET:N	2.76	0.48
4:S:96:ILE:HG12	4:S:145:LEU:HD11	1.95	0.48
5:T:53:THR:O	5:T:54:SER:C	2.55	0.48
7:V:22:SER:O	7:V:23:LEU:C	2.57	0.48
13:X:5:ARG:HG3	13:X:6:CYS:N	2.27	0.48
3:Y:162:SER:HA	3:Y:210:PHE:HZ	1.78	0.48
1:A:29:THR:HG23	1:A:243:VAL:HB	1.95	0.48
1:A:325:VAL:O	1:A:442:THR:HG22	2.14	0.48
2:B:157:VAL:CG1	2:B:401:LEU:HD23	2.43	0.48
2:B:1044:THR:HG23	2:B:1044:THR:O	2.13	0.48
3:C:237:ILE:HD12	3:C:253:THR:CB	2.43	0.48
5:E:114:THR:CG2	5:E:131:LYS:HD3	2.44	0.48
9:I:13:LEU:O	9:I:14:HIS:C	2.56	0.48
11:M:18:GLU:O	11:M:18:GLU:CG	2.60	0.48
11:M:32:LEU:HD23	11:M:35:ILE:HD12	1.96	0.48
11:M:63:ILE:HG22	11:M:64:ALA:O	2.13	0.48
2:R:502:GLU:O	2:R:506:ARG:N	2.47	0.48
1:W:121:ILE:HD12	8:Z:38:ARG:NH1	2.29	0.48
1:W:215:PRO:HG2	1:W:220:ARG:HD2	1.94	0.48
1:W:337:VAL:HG13	1:W:337:VAL:O	2.14	0.48
1:W:419:PHE:CE1	1:W:464:LEU:HD23	2.49	0.48
1:W:763:THR:HB	1:W:764:ARG:HD3	1.96	0.48
1:W:819:MET:HG2	1:W:819:MET:O	2.13	0.48
13:X:37:VAL:HG22	13:X:38:ARG:N	2.28	0.48
3:Y:213:ILE:O	3:Y:214:ASP:CG	2.57	0.48
3:Y:286:ILE:HD12	3:Y:324:GLY:O	2.12	0.48
1:A:763:THR:CG2	1:A:771:PRO:HB3	2.43	0.48
2:B:359:VAL:HG11	2:B:407:VAL:HG22	1.94	0.48
3:C:386:VAL:HG11	9:K:34:ARG:HB2	1.95	0.48
4:D:129:PRO:HD2	12:N:15:ALA:HB1	1.96	0.48
4:D:161:LEU:CD1	4:D:163:ILE:HD13	2.43	0.48
6:F:51:SER:HA	6:F:54:LYS:HD2	1.95	0.48
6:F:71:VAL:HG11	6:F:89:MET:CE	2.43	0.48
11:M:22:HIS:ND1	2:R:977:ARG:HB2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:34:TYR:HB3	2:R:125:MET:CE	2.43	0.48
2:R:34:TYR:HB3	2:R:125:MET:HE1	1.95	0.48
2:R:417:LEU:CG	2:R:425:MET:HG3	2.43	0.48
2:R:733:THR:HG23	2:R:735:TYR:HB2	1.96	0.48
2:R:1046:MET:HE3	5:T:61:PHE:CD1	2.49	0.48
4:S:53:LEU:HD12	4:S:131:VAL:CG2	2.43	0.48
4:S:153:HIS:O	4:S:154:ALA:HB3	2.13	0.48
1:W:58:CYS:HB3	1:W:62:GLY:H	1.79	0.48
1:W:655:ASP:H	1:W:658:LYS:HD2	1.78	0.48
1:A:640:GLU:OE1	2:B:977:ARG:NH1	2.46	0.48
1:A:739:ASN:HB2	2:B:922:MET:SD	2.54	0.48
2:B:103:MET:SD	2:B:384:LEU:HD13	2.54	0.48
2:B:493:TYR:CD1	2:B:499:PRO:HD3	2.49	0.48
2:B:743:MET:HE3	2:B:748:VAL:HG22	1.95	0.48
3:C:213:ILE:O	3:C:214:ASP:CG	2.57	0.48
4:D:38:VAL:CG1	4:D:39:MET:N	2.77	0.48
6:F:47:CYS:HB3	6:F:76:CYS:SG	2.54	0.48
2:R:103:MET:SD	2:R:384:LEU:HD13	2.54	0.48
2:R:980:GLN:HA	4:S:22:LEU:HD21	1.94	0.48
2:R:1017:ARG:HD3	2:R:1098:TYR:CZ	2.49	0.48
6:U:41:LEU:HA	6:U:44:VAL:HG12	1.96	0.48
1:W:334:ILE:HD12	1:W:628:MET:HB3	1.95	0.48
3:Y:281:GLU:OE1	3:Y:326:VAL:HG12	2.14	0.48
1:A:104:VAL:HG12	1:A:137:LYS:HG2	1.96	0.48
1:A:490:ARG:HD2	1:A:491:TYR:HD1	1.78	0.48
1:A:792:PRO:HA	2:B:948:PHE:CE1	2.48	0.48
2:B:330:LEU:O	2:B:332:ARG:N	2.46	0.48
2:B:893:MET:CG	2:B:894:LEU:N	2.76	0.48
2:B:984:SER:O	2:B:985:ARG:CB	2.61	0.48
4:D:182:VAL:HG11	4:D:212:TYR:CD2	2.49	0.48
5:E:45:VAL:HG21	5:E:74:MET:SD	2.54	0.48
5:E:83:GLU:O	5:E:145:ARG:HA	2.14	0.48
12:O:9:THR:HG23	2:R:908:VAL:O	2.13	0.48
2:R:598:GLU:HA	2:R:605:ILE:HD11	1.92	0.48
2:R:686:ASN:C	2:R:688:GLN:N	2.68	0.48
2:R:927:ILE:CG2	1:W:648:LEU:HB2	2.44	0.48
5:T:59:LEU:HD12	3:Y:390:MET:HB2	1.96	0.48
5:T:136:ILE:CG2	5:T:137:GLN:N	2.76	0.48
1:W:488:THR:HG23	1:W:493:GLY:O	2.14	0.48
1:W:874:ARG:HG3	3:Y:53:ASP:OD2	2.14	0.48
1:A:510:THR:O	1:A:597:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ILE:HG13	1:A:533:ASP:O	2.14	0.47
2:B:115:GLU:O	2:B:117:VAL:HG23	2.14	0.47
2:B:295:ILE:O	2:B:299:TYR:HB2	2.14	0.47
2:B:1061:ILE:H	2:B:1061:ILE:HD12	1.78	0.47
11:M:69:LEU:HD21	4:S:260:LEU:HD11	1.95	0.47
12:N:35:LEU:HD13	12:N:46:ARG:CG	2.44	0.47
2:R:221:PRO:O	2:R:278:ARG:HD2	2.14	0.47
7:V:81:LEU:HD12	7:V:81:LEU:N	2.29	0.47
1:W:854:GLY:O	3:Y:64:ILE:HG23	2.13	0.47
1:A:336:GLU:HA	1:A:434:ARG:O	2.14	0.47
1:A:729:ALA:O	1:A:730:ARG:HB2	2.14	0.47
1:A:743:MET:CG	2:B:922:MET:HG2	2.44	0.47
1:A:792:PRO:N	2:B:948:PHE:CE1	2.80	0.47
2:B:364:PHE:CE1	2:B:388:VAL:HG13	2.48	0.47
2:B:593:THR:HG23	2:B:594:ARG:N	2.29	0.47
2:B:736:ASN:HA	2:B:740:SER:HB3	1.95	0.47
10:J:73:LYS:CE	1:W:115:SER:HB3	2.44	0.47
2:R:186:ILE:CD1	2:R:209:LYS:HD3	2.43	0.47
2:R:230:MET:HE1	2:R:315:ALA:CA	2.44	0.47
2:R:448:LEU:HD21	1:W:796:PHE:CZ	2.48	0.47
2:R:583:ILE:HG23	2:R:591:LEU:HD21	1.96	0.47
2:R:852:LEU:HB3	2:R:868:ARG:HG2	1.96	0.47
2:R:1061:ILE:H	2:R:1061:ILE:HD12	1.78	0.47
7:V:72:CYS:HB3	7:V:114:LYS:CG	2.44	0.47
1:W:586:VAL:CG1	1:W:588:ILE:HD12	2.43	0.47
1:W:818:TYR:O	1:W:822:ARG:HG3	2.14	0.47
3:Y:110:ILE:HD12	3:Y:296:GLU:HB3	1.97	0.47
1:A:28:ILE:CG2	1:A:29:THR:N	2.77	0.47
1:A:121:ILE:HG21	10:Q:66:ARG:HD3	1.96	0.47
1:A:586:VAL:CG1	1:A:588:ILE:HD12	2.43	0.47
1:A:758:LYS:HA	1:A:779:ARG:HH11	1.80	0.47
2:B:230:MET:HE1	2:B:315:ALA:CA	2.45	0.47
5:E:84:VAL:CG1	6:F:75:ILE:CD1	2.92	0.47
10:Q:61:VAL:C	10:Q:63:GLU:N	2.70	0.47
2:R:12:GLU:HG3	2:R:595:GLU:OE1	2.13	0.47
2:R:245:VAL:HG22	2:R:319:ALA:HB1	1.95	0.47
2:R:245:VAL:HA	2:R:319:ALA:HB1	1.96	0.47
2:R:884:ARG:HH12	2:R:992:TYR:HB3	1.79	0.47
2:R:1040:ILE:CG2	3:Y:72:ILE:HG13	2.45	0.47
7:V:36:PHE:CE1	7:V:96:ILE:HD11	2.49	0.47
1:W:29:THR:HB	1:W:30:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:426:HIS:NE2	3:Y:80:GLU:CD	2.72	0.47
1:W:534:LEU:HB3	1:W:546:TYR:CE2	2.49	0.47
13:X:24:VAL:O	13:X:24:VAL:HG22	2.14	0.47
3:Y:70:ILE:HD13	3:Y:70:ILE:H	1.79	0.47
2:B:245:VAL:HG22	2:B:319:ALA:HB1	1.95	0.47
2:B:301:LEU:HB3	2:B:304:LEU:HD12	1.95	0.47
2:B:332:ARG:HD2	2:B:565:PHE:HB3	1.97	0.47
2:B:699:HIS:HD1	4:D:57:ILE:HG12	1.78	0.47
3:C:64:ILE:HG21	9:K:19:PHE:HE1	1.78	0.47
5:E:1:MET:HE3	5:E:83:GLU:HB2	1.96	0.47
12:N:3:ILE:HD13	12:N:15:ALA:CA	2.43	0.47
2:R:598:GLU:O	2:R:599:LYS:C	2.57	0.47
8:Z:45:ILE:HG23	8:Z:81:VAL:HG22	1.96	0.47
1:A:10:LYS:HG2	3:C:363:VAL:CG1	2.45	0.47
1:A:289:HIS:O	1:A:290:ARG:HB2	2.13	0.47
1:A:490:ARG:HH21	3:C:80:GLU:HG2	1.80	0.47
1:A:565:GLN:HB3	1:A:569:SER:HB3	1.96	0.47
2:B:70:LYS:HB3	2:B:71:PRO:HD2	1.96	0.47
2:B:126:LEU:HD13	2:B:154:TYR:O	2.14	0.47
2:B:330:LEU:O	2:B:332:ARG:CG	2.62	0.47
2:B:370:TYR:O	2:B:370:TYR:CG	2.68	0.47
2:B:605:ILE:HG12	2:B:606:THR:N	2.24	0.47
8:H:12:ARG:HH22	8:H:55:ILE:HD12	1.79	0.47
9:I:59:THR:O	9:I:60:ASP:CG	2.57	0.47
9:K:71:ARG:HB3	9:K:73:VAL:HG22	1.96	0.47
2:R:249:PRO:HD2	2:R:253:ASN:OD1	2.14	0.47
2:R:766:VAL:HG13	2:R:767:LYS:N	2.30	0.47
2:R:1017:ARG:HD3	2:R:1098:TYR:CG	2.48	0.47
2:R:1062:TYR:HE2	2:R:1093:PRO:HG3	1.80	0.47
5:T:8:ARG:NE	5:T:69:GLU:OE2	2.48	0.47
6:U:71:VAL:HG11	6:U:89:MET:HE1	1.96	0.47
1:W:95:LYS:O	1:W:138:LYS:HG2	2.14	0.47
3:Y:192:LYS:O	3:Y:194:GLY:N	2.47	0.47
1:A:338:GLY:HA3	1:A:444:ARG:CG	2.45	0.47
1:A:651:VAL:CG1	1:A:743:MET:HB3	2.43	0.47
2:B:1082:CYS:HB2	2:B:1083:PRO:HD2	1.97	0.47
10:J:57:GLY:C	10:J:61:VAL:CG1	2.88	0.47
11:L:11:ASN:HB3	11:L:59:THR:HG23	1.96	0.47
2:R:63:LEU:HD23	2:R:103:MET:HG2	1.96	0.47
2:R:356:LEU:O	2:R:359:VAL:HG12	2.14	0.47
2:R:657:ILE:HG13	2:R:711:LEU:CD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:119:LYS:HG2	5:T:120:TYR:CD2	2.49	0.47
1:W:821:ARG:HA	1:W:824:ILE:HG22	1.96	0.47
1:A:103:ARG:CG	1:A:191:ASP:OD1	2.63	0.47
1:A:316:LYS:HD3	2:B:1056:SER:HB3	1.97	0.47
2:B:136:TYR:HB3	2:B:141:LEU:CD1	2.44	0.47
2:B:330:LEU:HD22	2:B:332:ARG:HH11	1.79	0.47
2:B:372:LEU:CD2	2:B:376:LYS:CE	2.92	0.47
2:B:396:ARG:NH2	2:B:406:TRP:CZ2	2.83	0.47
2:B:520:TRP:O	2:B:521:SER:HB3	2.14	0.47
2:B:1015:LEU:CD1	2:B:1102:LEU:HD11	2.45	0.47
5:E:80:VAL:HG12	5:E:83:GLU:CD	2.40	0.47
9:I:23:TRP:CE2	3:Y:66:PRO:HD3	2.50	0.47
9:K:27:LEU:HD23	9:K:78:ILE:CD1	2.44	0.47
9:K:61:VAL:O	9:K:62:ILE:C	2.52	0.47
2:R:73:VAL:O	2:R:73:VAL:HG13	2.15	0.47
2:R:126:LEU:HD21	2:R:156:ILE:HD11	1.97	0.47
2:R:157:VAL:CG1	2:R:401:LEU:HD23	2.44	0.47
2:R:370:TYR:O	2:R:370:TYR:CG	2.68	0.47
2:R:371:GLN:HG2	2:R:387:LEU:O	2.14	0.47
2:R:457:CYS:SG	2:R:460:GLU:HB2	2.54	0.47
2:R:525:LEU:O	2:R:528:ARG:HB3	2.13	0.47
2:R:603:GLY:C	2:R:605:ILE:H	2.22	0.47
2:R:647:SER:HB2	2:R:648:PRO:HD3	1.97	0.47
2:R:1009:ARG:NH2	1:W:385:ARG:NH1	2.62	0.47
2:R:1025:ARG:O	2:R:1026:GLU:C	2.57	0.47
2:R:1046:MET:HG2	5:T:61:PHE:CE1	2.50	0.47
2:R:1056:SER:CB	2:R:1057:ASP:OD1	2.62	0.47
2:R:1111:ILE:O	2:R:1111:ILE:HG22	2.15	0.47
5:T:83:GLU:O	5:T:145:ARG:HA	2.14	0.47
5:T:114:THR:CG2	5:T:131:LYS:HD3	2.45	0.47
7:V:24:LYS:O	1:W:513:THR:HG21	2.15	0.47
7:V:33:CYS:HB3	7:V:36:PHE:O	2.14	0.47
1:W:450:CYS:C	1:W:452:PRO:HD2	2.39	0.47
1:W:505:GLY:HA3	1:W:639:VAL:CG2	2.44	0.47
3:Y:33:LYS:HG3	3:Y:34:ASN:N	2.30	0.47
3:Y:80:GLU:N	3:Y:81:PRO:CD	2.78	0.47
3:Y:147:THR:HB	3:Y:232:LYS:CB	2.45	0.47
3:Y:241:ILE:O	3:Y:251:ILE:HG23	2.14	0.47
1:A:141:MET:CA	1:A:148:HIS:HB3	2.45	0.47
1:A:241:ASP:OD2	1:A:289:HIS:NE2	2.48	0.47
1:A:749:GLN:HA	1:A:781:PHE:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:LEU:HD23	2:B:376:LYS:HG2	1.97	0.47
2:B:1053:LEU:HD23	2:B:1054:ASP:OD1	2.15	0.47
3:C:277:ILE:CG2	3:C:278:ARG:N	2.77	0.47
5:E:6:LYS:HA	5:E:72:PHE:O	2.14	0.47
6:F:88:ILE:H	6:F:88:ILE:HD13	1.79	0.47
9:I:41:LEU:HD12	1:W:470:GLU:HG3	1.96	0.47
10:J:62:ASP:O	10:J:66:ARG:HB3	2.14	0.47
2:R:166:THR:CG2	2:R:432:VAL:HG12	2.45	0.47
2:R:291:LYS:C	2:R:293:GLN:H	2.22	0.47
2:R:585:VAL:HG13	2:R:589:ASN:H	1.79	0.47
2:R:730:ILE:CG2	2:R:732:PHE:HB2	2.45	0.47
2:R:782:GLY:O	2:R:783:VAL:C	2.58	0.47
2:R:977:ARG:NH1	1:W:640:GLU:OE1	2.48	0.47
2:R:1069:TYR:HB2	2:R:1070:ILE:HB	1.97	0.47
5:T:30:LEU:HD22	5:T:72:PHE:CD2	2.49	0.47
1:W:73:GLY:O	1:W:74:HIS:ND1	2.48	0.47
1:W:855:VAL:HG13	3:Y:63:LEU:O	2.15	0.47
3:Y:215:SER:O	3:Y:216:ILE:HB	2.15	0.47
3:Y:277:ILE:C	3:Y:279:GLU:N	2.71	0.47
3:Y:277:ILE:HG13	3:Y:292:ILE:HD12	1.97	0.47
3:Y:372:ASN:ND2	3:Y:380:LYS:HE3	2.29	0.47
1:A:23:SER:O	1:A:24:VAL:HG13	2.15	0.47
1:A:326:ILE:HG21	1:A:462:MET:SD	2.55	0.47
1:A:390:TYR:O	1:A:391:VAL:C	2.58	0.47
1:A:829:ASP:O	1:A:840:SER:HA	2.15	0.47
2:B:166:THR:CG2	2:B:432:VAL:HG12	2.44	0.47
2:B:422:TRP:HZ3	2:B:715:GLY:HA3	1.80	0.47
2:B:583:ILE:HG23	2:B:591:LEU:HD21	1.97	0.47
2:B:708:THR:HG23	2:B:946:THR:HA	1.97	0.47
2:B:956:LEU:O	2:B:960:ILE:HG12	2.15	0.47
5:E:60:VAL:HG22	5:E:61:PHE:N	2.29	0.47
6:F:12:ILE:CG2	6:F:16:VAL:HG13	2.44	0.47
7:G:33:CYS:HB3	7:G:36:PHE:O	2.15	0.47
13:P:4:TYR:CD1	13:P:4:TYR:O	2.67	0.47
2:R:330:LEU:HD22	2:R:332:ARG:HD3	1.96	0.47
2:R:586:SER:O	2:R:587:ASN:HB2	2.14	0.47
2:R:609:ASP:O	2:R:613:GLN:HB2	2.14	0.47
2:R:657:ILE:HG13	2:R:711:LEU:HD21	1.96	0.47
2:R:787:LYS:HE3	2:R:841:VAL:HG23	1.97	0.47
5:T:115:ASP:O	5:T:116:ASP:CG	2.58	0.47
1:W:95:LYS:HB3	1:W:138:LYS:CG	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:141:MET:HA	1:W:148:HIS:HB2	1.96	0.47
1:W:853:ASP:HB2	3:Y:311:ARG:NH1	2.29	0.47
1:W:863:GLY:HA2	3:Y:311:ARG:NH2	2.30	0.47
3:Y:176:ASP:O	3:Y:177:LYS:CG	2.62	0.47
3:Y:328:GLN:HG2	3:Y:330:GLY:H	1.80	0.47
1:A:49:LEU:N	1:A:49:LEU:HD12	2.30	0.47
1:A:336:GLU:OE2	1:A:436:ARG:HB2	2.15	0.47
2:B:232:ALA:HB2	2:B:271:ALA:CB	2.45	0.47
2:B:724:ASN:O	12:N:47:ARG:HD2	2.15	0.47
3:C:167:LEU:HD12	3:C:167:LEU:N	2.30	0.47
3:C:192:LYS:O	3:C:194:GLY:N	2.48	0.47
3:C:390:MET:HB2	5:E:59:LEU:HD12	1.96	0.47
12:O:5:ILE:HA	12:O:15:ALA:HB2	1.97	0.47
13:P:37:VAL:HG22	13:P:38:ARG:H	1.80	0.47
2:R:492:LEU:HB3	2:R:497:VAL:HG21	1.97	0.47
2:R:532:TYR:O	2:R:533:TYR:CB	2.62	0.47
2:R:787:LYS:HE3	2:R:841:VAL:HG21	1.97	0.47
2:R:893:MET:HG3	2:R:894:LEU:N	2.30	0.47
2:R:928:MET:HG2	1:W:648:LEU:HD11	1.96	0.47
2:R:949:TYR:C	2:R:950:LYS:HG3	2.39	0.47
2:R:1062:TYR:CE2	2:R:1093:PRO:HG3	2.50	0.47
4:S:41:ILE:HB	4:S:63:ALA:HA	1.97	0.47
7:V:95:ILE:C	7:V:96:ILE:HD12	2.40	0.47
1:W:774:ILE:O	1:W:774:ILE:HG22	2.15	0.47
1:A:176:THR:O	1:A:180:ILE:HG13	2.15	0.46
1:A:573:ARG:HA	1:A:582:HIS:CD2	2.50	0.46
2:B:371:GLN:HG2	2:B:387:LEU:O	2.15	0.46
2:B:404:GLY:O	2:B:405:ASN:O	2.32	0.46
2:B:430:ARG:HH11	2:B:653:ILE:CG1	2.28	0.46
2:B:665:GLN:HG2	2:B:667:PRO:HD2	1.98	0.46
2:B:1062:TYR:CE2	2:B:1080:TYR:HE1	2.33	0.46
5:E:1:MET:HE3	5:E:83:GLU:CB	2.46	0.46
7:G:8:GLU:HG2	7:G:9:ILE:H	1.80	0.46
11:L:18:GLU:O	11:L:18:GLU:CG	2.62	0.46
11:L:46:PRO:HD2	11:L:52:LYS:O	2.15	0.46
2:R:430:ARG:NH1	2:R:653:ILE:HG13	2.30	0.46
2:R:580:ARG:HA	2:R:581:PRO:HD3	1.78	0.46
2:R:808:LYS:HE3	2:R:847:MET:HE1	1.98	0.46
1:W:238:LYS:HE2	1:W:297:THR:CG2	2.45	0.46
1:W:419:PHE:HZ	1:W:443:PHE:HB3	1.80	0.46
1:W:451:PRO:HB2	1:W:495:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:127:THR:N	3:Y:268:ASP:HB2	2.30	0.46
1:A:67:ASN:OD1	2:B:1072:TRP:CZ3	2.68	0.46
1:A:321:SER:OG	2:B:1029:LEU:HB2	2.16	0.46
1:A:682:GLY:O	1:A:683:GLU:C	2.57	0.46
2:B:231:ARG:C	2:B:233:LEU:H	2.23	0.46
3:C:171:ASN:CG	3:C:172:GLU:H	2.23	0.46
5:E:132:SER:O	5:E:133:LYS:HB2	2.16	0.46
11:M:11:ASN:HB3	11:M:59:THR:HG23	1.96	0.46
2:R:880:LYS:C	2:R:881:PHE:CD1	2.94	0.46
2:R:1082:CYS:HB2	2:R:1083:PRO:HD2	1.96	0.46
6:U:47:CYS:HB3	6:U:76:CYS:SG	2.55	0.46
1:W:108:GLU:O	1:W:109:ASP:C	2.57	0.46
3:Y:281:GLU:CD	3:Y:326:VAL:HG12	2.39	0.46
1:A:29:THR:HB	1:A:30:PRO:HD3	1.97	0.46
1:A:124:ARG:C	1:A:126:PRO:HD2	2.40	0.46
1:A:646:MET:HG2	2:B:918:LEU:CD1	2.45	0.46
2:B:396:ARG:O	2:B:396:ARG:HG2	2.14	0.46
5:E:84:VAL:HG21	6:F:75:ILE:HD13	1.95	0.46
5:E:90:LEU:HD13	5:E:100:ASN:OD1	2.15	0.46
9:K:90:LEU:HD23	9:K:90:LEU:HA	1.61	0.46
12:O:5:ILE:O	12:O:6:ARG:HB2	2.14	0.46
2:R:42:LEU:HD12	2:R:357:PHE:CE2	2.51	0.46
2:R:562:VAL:O	2:R:566:ILE:O	2.33	0.46
2:R:662:GLU:O	1:W:789:GLY:HA2	2.15	0.46
2:R:947:PRO:C	2:R:948:PHE:CD2	2.93	0.46
2:R:1091:LEU:O	2:R:1092:PHE:CG	2.68	0.46
1:W:13:ILE:HG13	1:W:202:SER:CB	2.46	0.46
1:A:334:ILE:HD12	1:A:628:MET:CB	2.45	0.46
1:A:513:THR:HG21	7:G:24:LYS:O	2.15	0.46
2:B:103:MET:O	2:B:114:PRO:O	2.34	0.46
2:B:131:ASP:OD1	2:B:132:PRO:HD2	2.15	0.46
2:B:399:HIS:O	2:B:403:THR:HG21	2.16	0.46
3:C:277:ILE:HG13	3:C:292:ILE:HD12	1.97	0.46
5:E:123:VAL:HG22	5:E:127:ILE:HG23	1.98	0.46
11:M:84:ILE:CD1	4:S:246:GLY:HA3	2.45	0.46
2:R:767:LYS:HD3	2:R:768:TYR:O	2.15	0.46
2:R:928:MET:HG2	1:W:648:LEU:CD1	2.45	0.46
2:R:948:PHE:HE1	1:W:792:PRO:N	2.13	0.46
2:R:1029:LEU:HD11	1:W:322:SER:C	2.41	0.46
5:T:90:LEU:HD13	5:T:100:ASN:OD1	2.15	0.46
1:W:105:LYS:HE2	1:W:108:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:729:ALA:O	1:W:730:ARG:HB2	2.16	0.46
3:Y:174:LEU:CB	3:Y:179:VAL:HG13	2.44	0.46
3:Y:331:ARG:H	3:Y:331:ARG:HD3	1.80	0.46
1:A:104:VAL:HG11	1:A:137:LYS:O	2.15	0.46
1:A:331:ASN:O	1:A:332:ILE:CG1	2.63	0.46
1:A:498:ALA:H	1:A:604:GLY:H	1.62	0.46
1:A:748:GLY:HA2	1:A:781:PHE:CE1	2.51	0.46
2:B:417:LEU:CG	2:B:425:MET:HG3	2.46	0.46
2:B:460:GLU:HG2	2:B:673:SER:HB3	1.96	0.46
2:B:720:PRO:HG3	12:N:53:ILE:HD12	1.98	0.46
3:C:102:LEU:HD11	3:C:118:SER:HB3	1.97	0.46
5:E:82:GLN:H	5:E:146:VAL:HG13	1.80	0.46
7:G:25:ASN:HA	7:G:44:ASP:CG	2.40	0.46
9:K:27:LEU:CD2	9:K:78:ILE:HD11	2.46	0.46
13:P:5:ARG:CZ	13:P:6:CYS:O	2.63	0.46
2:R:808:LYS:O	2:R:809:GLY:C	2.59	0.46
5:T:39:LEU:O	5:T:40:LYS:C	2.58	0.46
1:W:45:MET:O	1:W:45:MET:CG	2.60	0.46
1:A:220:ARG:HG2	1:A:235:LEU:HD22	1.97	0.46
1:A:337:VAL:HG21	1:A:419:PHE:CE1	2.51	0.46
2:B:27:VAL:O	2:B:29:GLN:N	2.40	0.46
2:B:533:TYR:CE2	2:B:539:LEU:HB2	2.51	0.46
2:B:772:GLN:HG2	2:B:773:GLU:N	2.31	0.46
2:R:232:ALA:HB2	2:R:271:ALA:CB	2.46	0.46
2:R:539:LEU:O	2:R:543:ILE:HG13	2.15	0.46
4:S:83:ILE:HD12	4:S:84:ASP:N	2.30	0.46
4:S:161:LEU:O	4:S:230:LEU:HA	2.16	0.46
7:V:25:ASN:HA	7:V:44:ASP:CG	2.41	0.46
1:W:600:LYS:O	1:W:601:LYS:CB	2.56	0.46
3:Y:286:ILE:HG12	8:Z:49:ASP:OD1	2.16	0.46
1:A:145:VAL:O	1:A:145:VAL:HG13	2.15	0.46
1:A:353:ILE:HD13	1:A:405:TYR:HB2	1.97	0.46
1:A:856:PHE:CE2	1:A:858:MET:CB	2.98	0.46
2:B:245:VAL:HA	2:B:319:ALA:HB1	1.97	0.46
2:B:356:LEU:CA	2:B:407:VAL:HG21	2.38	0.46
2:B:430:ARG:NH1	2:B:653:ILE:HG13	2.30	0.46
2:B:463:GLU:N	2:B:463:GLU:OE1	2.48	0.46
2:B:585:VAL:HG13	2:B:589:ASN:H	1.80	0.46
2:B:646:TRP:CZ2	2:B:946:THR:HG21	2.50	0.46
2:B:730:ILE:CG2	2:B:732:PHE:HB2	2.46	0.46
3:C:215:SER:O	3:C:216:ILE:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:66:ARG:C	10:Q:68:PHE:H	2.23	0.46
2:R:646:TRP:CZ2	2:R:946:THR:HG21	2.51	0.46
2:R:995:LYS:CE	2:R:999:MET:HE3	2.46	0.46
5:T:44:LEU:O	5:T:46:LEU:HD12	2.16	0.46
1:W:141:MET:CA	1:W:148:HIS:HB3	2.46	0.46
1:W:833:GLU:HG3	1:W:839:ARG:CD	2.45	0.46
1:A:181:ARG:NH1	1:A:210:THR:OG1	2.49	0.46
1:A:451:PRO:N	1:A:452:PRO:CD	2.79	0.46
2:B:582:LEU:HD12	2:B:619:LEU:CD1	2.45	0.46
2:B:672:GLN:HG2	2:B:884:ARG:O	2.16	0.46
3:C:372:ASN:ND2	3:C:380:LYS:HE3	2.31	0.46
2:R:71:PRO:HA	2:R:97:ALA:HB2	1.98	0.46
2:R:231:ARG:C	2:R:233:LEU:H	2.24	0.46
2:R:467:SER:OG	1:W:806:LEU:HB3	2.16	0.46
5:T:83:GLU:HA	6:U:89:MET:CE	2.44	0.46
1:W:102:GLY:O	1:W:103:ARG:C	2.58	0.46
1:W:262:ILE:O	1:W:266:TRP:HB3	2.16	0.46
3:Y:30:GLU:O	3:Y:33:LYS:HG2	2.16	0.46
3:Y:133:ASP:O	3:Y:249:TYR:CE2	2.69	0.46
1:A:58:CYS:HB3	1:A:62:GLY:H	1.80	0.46
1:A:249:LEU:HG	1:A:265:LEU:CB	2.46	0.46
2:B:763:THR:HG22	2:B:764:GLU:O	2.16	0.46
2:B:872:LEU:HD23	2:B:873:ARG:H	1.81	0.46
3:C:33:LYS:HG3	3:C:34:ASN:N	2.30	0.46
3:C:340:SER:HB3	3:C:371:GLU:OE2	2.16	0.46
10:J:69:GLU:CD	10:J:73:LYS:HE3	2.41	0.46
10:Q:54:LEU:C	10:Q:55:LEU:HD12	2.41	0.46
10:Q:57:GLY:C	10:Q:61:VAL:CG1	2.89	0.46
2:R:162:ARG:HG2	2:R:402:ALA:HA	1.98	0.46
2:R:232:ALA:HB2	2:R:271:ALA:HB1	1.98	0.46
2:R:476:MET:HE1	2:R:645:ILE:HB	1.97	0.46
2:R:904:VAL:O	4:S:163:ILE:HG12	2.15	0.46
2:R:947:PRO:HB2	2:R:948:PHE:CD2	2.51	0.46
4:S:17:PHE:CD2	4:S:25:VAL:HG22	2.51	0.46
5:T:119:LYS:O	5:T:131:LYS:HA	2.16	0.46
5:T:123:VAL:HG22	5:T:127:ILE:HG23	1.98	0.46
1:W:830:LEU:HD13	3:Y:315:LEU:HD21	1.97	0.46
3:Y:104:LEU:CD1	3:Y:108:ILE:HD11	2.45	0.46
3:Y:108:ILE:O	3:Y:112:ASP:HB2	2.16	0.46
2:B:221:PRO:O	2:B:278:ARG:HD2	2.15	0.46
2:B:254:GLU:O	2:B:254:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:660:TYR:N	2:B:661:PRO:CD	2.79	0.46
2:B:666:SER:N	2:B:667:PRO:HD2	2.31	0.46
2:B:741:ILE:HD11	2:B:911:VAL:CG1	2.46	0.46
2:B:759:ARG:HG3	2:B:760:LEU:N	2.30	0.46
2:B:938:LEU:HD23	12:N:43:TYR:HB3	1.98	0.46
2:B:1007:ARG:CZ	2:B:1028:GLY:N	2.78	0.46
4:D:53:LEU:CD1	4:D:131:VAL:HG23	2.44	0.46
8:H:28:ALA:CB	8:H:62:ILE:HD11	2.46	0.46
2:R:396:ARG:O	2:R:396:ARG:HG2	2.16	0.46
2:R:646:TRP:CH2	2:R:648:PRO:HB2	2.50	0.46
4:S:50:ASN:ND2	4:S:137:GLN:HG2	2.30	0.46
4:S:154:ALA:C	4:S:156:PHE:N	2.74	0.46
1:W:124:ARG:NH2	3:Y:323:THR:HG21	2.31	0.46
1:W:331:ASN:O	1:W:332:ILE:CG1	2.64	0.46
3:Y:32:LEU:O	3:Y:33:LYS:C	2.59	0.46
1:A:108:GLU:O	1:A:109:ASP:C	2.58	0.45
4:D:108:MET:SD	4:D:132:LEU:HD23	2.55	0.45
5:E:8:ARG:NE	5:E:69:GLU:OE2	2.49	0.45
12:O:3:ILE:HG12	12:O:18:TRP:CB	2.46	0.45
2:R:101:LEU:CD1	2:R:103:MET:HE3	2.43	0.45
2:R:493:TYR:OH	2:R:530:VAL:HG13	2.15	0.45
2:R:1021:GLU:OE2	2:R:1022:GLY:N	2.49	0.45
5:T:56:GLU:OE1	3:Y:389:THR:HG21	2.16	0.45
5:T:167:PRO:HA	5:T:169:LEU:HD13	1.98	0.45
1:W:81:VAL:HG11	1:W:269:LEU:O	2.17	0.45
1:W:361:LEU:HD23	1:W:407:VAL:HB	1.98	0.45
1:A:105:LYS:HD3	1:A:136:VAL:HG11	1.97	0.45
1:A:580:CYS:HA	1:A:581:PRO:HD3	1.75	0.45
1:A:687:ILE:HG13	1:A:699:TYR:OH	2.16	0.45
2:B:112:ALA:O	2:B:113:GLU:HG3	2.16	0.45
2:B:476:MET:HE1	2:B:645:ILE:HD12	1.97	0.45
2:B:782:GLY:O	2:B:783:VAL:C	2.59	0.45
2:B:1017:ARG:HD3	2:B:1098:TYR:CZ	2.51	0.45
3:C:107:LEU:O	3:C:110:ILE:HG22	2.15	0.45
3:C:110:ILE:HD13	3:C:297:ILE:HG12	1.97	0.45
6:F:86:ILE:HG23	6:F:89:MET:SD	2.56	0.45
7:G:76:TYR:N	7:G:76:TYR:CD1	2.84	0.45
12:N:3:ILE:HG12	12:N:18:TRP:CB	2.46	0.45
2:R:430:ARG:HH11	2:R:653:ILE:CG1	2.29	0.45
2:R:582:LEU:HD12	2:R:619:LEU:CD1	2.46	0.45
2:R:589:ASN:HA	2:R:590:PRO:HD3	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:1007:ARG:CZ	2:R:1028:GLY:N	2.80	0.45
6:U:12:ILE:CG2	6:U:16:VAL:HG13	2.45	0.45
7:V:36:PHE:CE1	7:V:96:ILE:HG12	2.51	0.45
7:V:75:GLY:HA3	7:V:86:SER:O	2.17	0.45
1:W:505:GLY:CA	1:W:639:VAL:HG22	2.46	0.45
3:Y:81:PRO:O	3:Y:83:THR:N	2.49	0.45
3:Y:151:ASN:O	3:Y:173:MET:HG3	2.17	0.45
1:A:361:LEU:HD23	1:A:407:VAL:HB	1.96	0.45
1:A:451:PRO:HB2	1:A:495:ILE:O	2.16	0.45
1:A:519:GLU:HG2	11:L:33:ARG:HD2	1.99	0.45
2:B:396:ARG:NH2	2:B:406:TRP:CZ3	2.85	0.45
2:B:397:ILE:O	2:B:397:ILE:HG12	2.16	0.45
2:B:594:ARG:NH1	2:B:615:LYS:CB	2.76	0.45
2:B:609:ASP:O	2:B:613:GLN:HB2	2.16	0.45
2:B:1064:CYS:HB3	2:B:1068:GLY:H	1.81	0.45
3:C:133:ASP:O	3:C:249:TYR:CE2	2.69	0.45
3:C:258:LEU:HD11	3:C:272:VAL:HG11	1.98	0.45
3:C:292:ILE:HB	8:H:16:LEU:HD13	1.98	0.45
7:G:29:ILE:CD1	7:G:42:ILE:HG13	2.46	0.45
7:G:67:THR:HG22	7:G:68:ASN:H	1.81	0.45
11:M:33:ARG:HD2	1:W:519:GLU:HG2	1.98	0.45
2:R:127:LYS:HE3	2:R:150:ASP:O	2.16	0.45
2:R:213:PHE:HB2	2:R:259:LEU:CG	2.46	0.45
2:R:520:TRP:O	2:R:521:SER:HB3	2.16	0.45
2:R:752:MET:HG2	2:R:753:TYR:CD2	2.51	0.45
2:R:895:ILE:HG23	2:R:899:ASP:HB2	1.98	0.45
2:R:903:THR:HA	2:R:973:THR:HG22	1.97	0.45
2:R:982:ILE:CD1	2:R:984:SER:H	2.29	0.45
1:W:13:ILE:HG13	1:W:202:SER:HB3	1.98	0.45
1:W:336:GLU:HA	1:W:434:ARG:O	2.16	0.45
1:W:599:ASP:N	1:W:599:ASP:OD1	2.49	0.45
1:W:872:PHE:CZ	1:W:876:VAL:HG21	2.51	0.45
3:Y:284:PHE:HB3	3:Y:288:ALA:HB1	1.98	0.45
1:A:322:SER:C	2:B:1029:LEU:HD11	2.42	0.45
1:A:406:VAL:O	1:A:406:VAL:HG12	2.16	0.45
1:A:777:GLU:H	1:A:777:GLU:CD	2.24	0.45
1:A:874:ARG:HG3	3:C:53:ASP:OD2	2.16	0.45
2:B:126:LEU:HD21	2:B:156:ILE:HD11	1.98	0.45
2:B:493:TYR:OH	2:B:530:VAL:HG13	2.16	0.45
2:B:918:LEU:H	2:B:919:PRO:HD2	1.82	0.45
2:B:974:TYR:HA	2:B:981:LYS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1039:LEU:HD22	2:B:1044:THR:HG21	1.98	0.45
2:B:1042:PHE:C	2:B:1044:THR:H	2.23	0.45
4:D:56:GLU:HG3	13:P:45:VAL:CG1	2.45	0.45
10:Q:40:ASN:HA	10:Q:43:LEU:CD1	2.46	0.45
2:R:136:TYR:CB	2:R:141:LEU:CD1	2.94	0.45
2:R:345:ARG:HG3	2:R:576:GLY:HA3	1.97	0.45
2:R:841:VAL:HG12	2:R:842:THR:O	2.16	0.45
2:R:1042:PHE:HE2	1:W:430:MET:O	1.99	0.45
1:W:12:GLY:HA3	1:W:201:THR:CG2	2.44	0.45
3:Y:112:ASP:O	3:Y:114:LYS:N	2.49	0.45
3:Y:216:ILE:O	3:Y:217:ALA:HB2	2.17	0.45
2:B:46:ILE:CB	2:B:66:ILE:HD11	2.47	0.45
2:B:194:SER:CB	2:B:303:HIS:HB3	2.44	0.45
3:C:201:SER:HB2	3:C:204:ASN:HB2	1.99	0.45
3:C:281:GLU:OE1	3:C:326:VAL:HG12	2.16	0.45
5:E:44:LEU:O	5:E:46:LEU:HD12	2.16	0.45
5:E:145:ARG:HD3	6:F:88:ILE:HG21	1.98	0.45
7:G:75:GLY:HA3	7:G:86:SER:O	2.17	0.45
10:J:54:LEU:C	10:J:55:LEU:HD12	2.42	0.45
2:R:854:LEU:HA	13:X:35:PHE:HA	1.99	0.45
4:S:108:MET:SD	4:S:132:LEU:HD23	2.56	0.45
5:T:1:MET:HE3	5:T:83:GLU:HB2	1.98	0.45
7:V:62:ASN:O	7:V:63:ARG:HB2	2.17	0.45
1:W:328:PRO:HD3	1:W:457:PHE:CG	2.51	0.45
1:W:417:VAL:HG13	1:W:465:HIS:O	2.17	0.45
1:W:490:ARG:HD2	1:W:491:TYR:HD1	1.80	0.45
3:Y:290:ARG:CB	3:Y:321:THR:HG21	2.47	0.45
1:A:13:ILE:CG1	1:A:202:SER:HB2	2.47	0.45
2:B:137:THR:HG22	2:B:140:LYS:HD2	1.99	0.45
2:B:399:HIS:O	2:B:403:THR:CG2	2.65	0.45
2:B:476:MET:HE1	2:B:645:ILE:HB	1.97	0.45
2:B:808:LYS:HE3	2:B:847:MET:HE1	1.99	0.45
3:C:28:ILE:HD13	9:K:14:HIS:CE1	2.51	0.45
4:D:60:HIS:HD2	4:D:60:HIS:O	2.00	0.45
4:D:154:ALA:C	4:D:156:PHE:N	2.72	0.45
5:E:13:ILE:HD12	5:E:68:HIS:CD2	2.51	0.45
10:J:49:GLU:O	10:J:52:ASP:HB3	2.17	0.45
2:R:419:ARG:NH1	2:R:690:ARG:HH12	2.14	0.45
2:R:1059:THR:CG2	2:R:1061:ILE:HD12	2.46	0.45
1:W:23:SER:O	1:W:24:VAL:HG13	2.16	0.45
1:W:196:GLY:O	3:Y:360:ARG:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:777:GLU:HG3	1:W:783:TYR:HE1	1.81	0.45
3:Y:258:LEU:HD22	3:Y:280:ILE:HD13	1.98	0.45
1:A:421:ARG:CZ	1:A:454:ASN:O	2.64	0.45
1:A:728:MET:HG3	1:A:733:ALA:O	2.17	0.45
1:A:870:ARG:HD2	3:C:57:LYS:HB3	1.99	0.45
3:C:110:ILE:HD12	3:C:296:GLU:HB3	1.98	0.45
4:D:153:HIS:O	4:D:153:HIS:CG	2.70	0.45
5:E:10:ILE:HG22	5:E:11:VAL:N	2.32	0.45
8:H:63:ILE:HG22	8:H:65:ILE:CD1	2.46	0.45
2:R:330:LEU:HD22	2:R:332:ARG:HH11	1.82	0.45
2:R:355:SER:O	2:R:407:VAL:HG11	2.16	0.45
2:R:722:GLY:O	2:R:992:TYR:CE1	2.70	0.45
2:R:904:VAL:O	4:S:163:ILE:HG21	2.17	0.45
2:R:1062:TYR:CE2	2:R:1080:TYR:HE1	2.34	0.45
4:S:35:TYR:CE1	4:S:252:LYS:HE3	2.51	0.45
5:T:100:ASN:HD21	6:U:36:ARG:NH1	2.14	0.45
5:T:145:ARG:HD3	6:U:88:ILE:HD12	1.98	0.45
1:W:28:ILE:CG2	1:W:29:THR:N	2.80	0.45
3:Y:292:ILE:HD13	3:Y:292:ILE:C	2.40	0.45
3:Y:303:GLU:OE1	3:Y:303:GLU:C	2.59	0.45
1:A:327:SER:HB2	1:A:328:PRO:HD2	1.99	0.45
2:B:75:GLU:N	2:B:79:GLY:O	2.50	0.45
2:B:91:ARG:CG	13:P:33:ILE:HD11	2.47	0.45
2:B:680:LEU:HD21	2:B:997:HIS:HB3	1.98	0.45
4:D:35:TYR:HE2	11:L:23:THR:HG21	1.82	0.45
4:D:96:ILE:HD11	4:D:143:ALA:HB3	1.98	0.45
5:E:75:ILE:HG21	6:F:21:LEU:HD11	1.97	0.45
7:G:62:ASN:O	7:G:63:ARG:HB2	2.16	0.45
9:K:27:LEU:CD2	9:K:78:ILE:CD1	2.94	0.45
12:O:3:ILE:HD13	12:O:15:ALA:CA	2.47	0.45
12:O:3:ILE:HG12	12:O:18:TRP:HB2	1.99	0.45
12:O:8:PHE:CD2	2:R:752:MET:HB2	2.51	0.45
2:R:295:ILE:O	2:R:299:TYR:HB2	2.16	0.45
2:R:500:VAL:HG12	2:R:504:ILE:HG12	1.99	0.45
2:R:948:PHE:CD1	1:W:792:PRO:HG3	2.52	0.45
4:S:153:HIS:O	4:S:153:HIS:CG	2.69	0.45
6:U:13:PRO:HG2	6:U:16:VAL:HG12	1.98	0.45
1:W:109:ASP:O	1:W:112:GLU:C	2.59	0.45
3:Y:11:SER:HB2	3:Y:14:GLU:HB2	1.99	0.45
3:Y:127:THR:H	3:Y:268:ASP:HB2	1.82	0.45
3:Y:277:ILE:CG2	3:Y:278:ARG:H	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:THR:HG21	1:A:71:HIS:CG	2.52	0.45
1:A:81:VAL:HG11	1:A:269:LEU:O	2.17	0.45
1:A:116:ARG:HA	1:A:130:ARG:NH2	2.31	0.45
1:A:396:GLU:C	1:A:398:ALA:H	2.25	0.45
1:A:486:ILE:HG12	1:A:496:ILE:HD12	1.99	0.45
1:A:792:PRO:CD	2:B:948:PHE:CE1	3.00	0.45
2:B:308:ALA:C	2:B:310:ASP:H	2.24	0.45
2:B:689:LEU:CD1	12:N:62:TYR:HB3	2.47	0.45
2:B:852:LEU:HB3	2:B:868:ARG:HG2	1.98	0.45
2:B:884:ARG:HH12	2:B:992:TYR:HB3	1.80	0.45
3:C:289:ALA:HA	3:C:292:ILE:HG22	1.99	0.45
4:D:83:ILE:HD12	4:D:84:ASP:N	2.31	0.45
6:F:15:SER:HB3	6:F:47:CYS:SG	2.57	0.45
11:M:12:TYR:CD1	11:M:58:LEU:HB2	2.52	0.45
2:R:131:ASP:OD1	2:R:132:PRO:HD2	2.17	0.45
2:R:251:ILE:O	2:R:255:LEU:HD12	2.17	0.45
2:R:594:ARG:O	2:R:597:ILE:HG12	2.17	0.45
2:R:770:GLY:O	2:R:771:GLY:C	2.60	0.45
1:W:406:VAL:O	1:W:406:VAL:HG12	2.16	0.45
1:W:829:ASP:O	1:W:840:SER:HA	2.16	0.45
1:W:879:LYS:NZ	3:Y:44:THR:HG22	2.32	0.45
13:X:17:GLN:HG3	13:X:19:LYS:H	1.82	0.45
3:Y:149:ILE:HG12	3:Y:230:LYS:HD3	1.98	0.45
1:A:20:ARG:NE	1:A:211:VAL:HG21	2.31	0.45
1:A:304:GLY:C	1:A:306:GLU:N	2.65	0.45
1:A:687:ILE:CD1	1:A:695:SER:HB2	2.46	0.45
2:B:594:ARG:O	2:B:597:ILE:HG12	2.17	0.45
2:B:872:LEU:HD22	2:B:874:ILE:HG13	1.99	0.45
5:E:36:GLU:CG	6:F:33:LEU:HD22	2.47	0.45
13:P:5:ARG:HD2	13:P:18:LEU:HD13	1.95	0.45
13:P:6:CYS:HA	13:P:16:GLU:O	2.16	0.45
2:R:903:THR:HG22	2:R:904:VAL:H	1.82	0.45
2:R:966:LEU:CD2	4:S:208:GLU:HG3	2.47	0.45
5:T:131:LYS:HE3	5:T:136:ILE:HD11	1.99	0.45
1:W:871:ILE:CD1	3:Y:39:LYS:O	2.65	0.45
3:Y:244:LYS:CA	3:Y:245:LYS:CB	2.93	0.45
1:A:321:SER:C	2:B:1029:LEU:HD12	2.42	0.44
1:A:345:ARG:HA	1:A:410:HIS:ND1	2.32	0.44
1:A:419:PHE:HZ	1:A:443:PHE:HB3	1.82	0.44
2:B:236:LEU:HD21	2:B:268:VAL:CG2	2.47	0.44
2:B:733:THR:HG23	2:B:734:GLY:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:28:ILE:CD1	9:K:14:HIS:CD2	2.97	0.44
3:C:80:GLU:CB	3:C:81:PRO:HD3	2.46	0.44
4:D:128:ILE:HG21	12:N:5:ILE:HD12	1.99	0.44
4:D:223:GLU:OE1	4:D:223:GLU:HA	2.17	0.44
5:E:84:VAL:HG13	6:F:75:ILE:CD1	2.46	0.44
8:H:40:GLU:OE2	10:Q:66:ARG:NH1	2.50	0.44
10:J:59:ILE:C	10:J:61:VAL:H	2.25	0.44
2:R:8:LEU:C	2:R:8:LEU:HD12	2.42	0.44
2:R:660:TYR:N	2:R:661:PRO:CD	2.80	0.44
1:A:94:LEU:C	1:A:96:ALA:H	2.26	0.44
2:B:91:ARG:HG3	13:P:33:ILE:HD11	1.99	0.44
2:B:435:SER:O	2:B:436:LEU:C	2.60	0.44
2:B:605:ILE:O	2:B:609:ASP:HB2	2.17	0.44
2:B:767:LYS:HD3	2:B:768:TYR:O	2.17	0.44
2:B:1080:TYR:HB3	2:B:1091:LEU:HD12	1.98	0.44
3:C:331:ARG:HD3	3:C:331:ARG:H	1.83	0.44
6:F:18:LYS:C	6:F:20:LEU:H	2.26	0.44
13:P:26:CYS:HB3	13:P:29:CYS:HB2	1.65	0.44
2:R:249:PRO:HB3	2:R:252:GLN:CD	2.42	0.44
6:U:86:ILE:HG23	6:U:89:MET:SD	2.57	0.44
1:W:420:ASN:HB2	1:W:430:MET:HG3	1.99	0.44
1:W:580:CYS:HA	1:W:581:PRO:HD3	1.80	0.44
3:Y:129:GLU:HB3	3:Y:130:TYR:CD2	2.51	0.44
3:Y:167:LEU:N	3:Y:167:LEU:HD12	2.32	0.44
1:A:109:ASP:O	1:A:112:GLU:C	2.60	0.44
1:A:343:ILE:HG22	1:A:347:LEU:HD12	2.00	0.44
1:A:774:ILE:O	1:A:774:ILE:HG22	2.17	0.44
2:B:249:PRO:HB3	2:B:252:GLN:CD	2.42	0.44
2:B:598:GLU:O	2:B:599:LYS:C	2.60	0.44
2:B:903:THR:HA	2:B:973:THR:HG22	2.00	0.44
2:B:981:LYS:HG2	4:D:166:TYR:CE2	2.52	0.44
2:B:1081:VAL:C	2:B:1091:LEU:HD11	2.42	0.44
4:D:50:ASN:ND2	4:D:137:GLN:HG2	2.32	0.44
5:E:79:PRO:HB3	5:E:160:ILE:HD11	2.00	0.44
9:I:43:LEU:HD12	9:I:65:ALA:HB2	2.00	0.44
12:N:40:VAL:O	12:N:40:VAL:HG12	2.15	0.44
2:R:163:VAL:HG13	2:R:163:VAL:O	2.16	0.44
2:R:463:GLU:N	2:R:463:GLU:OE1	2.50	0.44
2:R:1110:MET:C	2:R:1111:ILE:HD12	2.43	0.44
7:V:104:LYS:O	7:V:106:ILE:N	2.50	0.44
1:W:97:THR:CG2	1:W:102:GLY:HA2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:326:ILE:HG21	1:W:462:MET:HG3	2.00	0.44
1:A:691:THR:HB	1:A:694:GLU:CB	2.48	0.44
2:B:259:LEU:HA	2:B:259:LEU:HD13	1.64	0.44
2:B:937:ALA:O	12:N:46:ARG:HD2	2.16	0.44
2:B:982:ILE:CD1	2:B:984:SER:H	2.30	0.44
2:B:1082:CYS:HB2	2:B:1083:PRO:CD	2.47	0.44
10:Q:61:VAL:C	10:Q:63:GLU:H	2.24	0.44
2:R:396:ARG:NH2	2:R:406:TRP:CZ2	2.86	0.44
2:R:595:GLU:O	2:R:595:GLU:CD	2.59	0.44
2:R:605:ILE:O	2:R:609:ASP:HB2	2.18	0.44
2:R:732:PHE:O	2:R:733:THR:CG2	2.66	0.44
2:R:1007:ARG:CZ	2:R:1028:GLY:C	2.91	0.44
2:R:1082:CYS:HB2	2:R:1083:PRO:CD	2.47	0.44
4:S:26:ASN:O	4:S:30:ARG:HG3	2.18	0.44
4:S:96:ILE:HD11	4:S:143:ALA:HB3	1.99	0.44
1:W:145:VAL:O	1:W:145:VAL:HG13	2.18	0.44
1:W:516:LEU:CD2	1:W:524:ILE:HD12	2.47	0.44
3:Y:28:ILE:H	3:Y:28:ILE:HG13	1.53	0.44
3:Y:340:SER:HB3	3:Y:371:GLU:OE2	2.17	0.44
1:A:731:THR:O	1:A:732:GLY:C	2.61	0.44
2:B:780:GLU:O	2:B:782:GLY:N	2.50	0.44
2:B:856:THR:HG23	13:P:32:LYS:C	2.42	0.44
2:B:947:PRO:O	2:B:948:PHE:CD2	2.70	0.44
2:B:1061:ILE:HG13	2:B:1072:TRP:HE1	1.83	0.44
3:C:120:PRO:HB2	3:C:256:SER:HB3	1.99	0.44
3:C:232:LYS:HA	3:C:232:LYS:HE3	1.99	0.44
4:D:26:ASN:O	4:D:30:ARG:HG3	2.17	0.44
7:G:8:GLU:OE2	7:G:64:LEU:HD22	2.18	0.44
9:K:56:ILE:N	9:K:57:SER:N	2.63	0.44
9:K:59:THR:HB	9:K:63:SER:OG	2.17	0.44
2:R:167:GLN:HG2	2:R:352:LEU:HD21	1.99	0.44
2:R:259:LEU:HD13	2:R:259:LEU:HA	1.67	0.44
2:R:457:CYS:HA	2:R:458:PRO:HD3	1.80	0.44
1:W:95:LYS:HD3	1:W:138:LYS:HD3	1.98	0.44
1:W:725:ALA:HA	1:W:728:MET:HE2	1.98	0.44
3:Y:70:ILE:H	3:Y:70:ILE:CD1	2.29	0.44
1:A:334:ILE:HD12	1:A:628:MET:HB3	1.98	0.44
1:A:853:ASP:CG	8:H:71:LEU:HB3	2.43	0.44
2:B:213:PHE:HB2	2:B:259:LEU:CG	2.48	0.44
2:B:341:TYR:OH	2:B:456:MET:HE2	2.17	0.44
2:B:539:LEU:O	2:B:543:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:628:TYR:CE2	2:B:640:HIS:ND1	2.85	0.44
2:B:884:ARG:NH1	2:B:884:ARG:HB2	2.30	0.44
3:C:393:ILE:O	3:C:393:ILE:HG13	2.16	0.44
4:D:108:MET:CG	4:D:110:TYR:CE2	3.00	0.44
4:D:153:HIS:HE2	13:P:48:ILE:HG23	1.82	0.44
6:F:13:PRO:HG2	6:F:16:VAL:HG12	2.00	0.44
8:H:12:ARG:NH2	8:H:55:ILE:HD12	2.33	0.44
2:R:101:LEU:HD13	2:R:103:MET:HG3	1.99	0.44
2:R:435:SER:O	2:R:436:LEU:C	2.60	0.44
2:R:680:LEU:HD21	2:R:997:HIS:HB3	2.00	0.44
2:R:895:ILE:HA	2:R:896:PRO:HD3	1.83	0.44
4:S:40:SER:OG	4:S:156:PHE:CE1	2.66	0.44
6:U:71:VAL:HG11	6:U:89:MET:CE	2.46	0.44
1:W:181:ARG:NH1	1:W:210:THR:OG1	2.51	0.44
1:W:502:TYR:O	1:W:503:ILE:C	2.60	0.44
1:A:672:VAL:HG13	1:A:700:ILE:HG12	2.00	0.44
2:B:1003:LYS:HD2	2:B:1003:LYS:HA	1.70	0.44
3:C:25:PRO:CD	3:C:33:LYS:HD3	2.48	0.44
12:O:1:MET:O	12:O:2:MET:HB2	2.17	0.44
12:O:40:VAL:O	12:O:40:VAL:HG12	2.15	0.44
13:P:24:VAL:O	13:P:24:VAL:HG22	2.18	0.44
13:P:33:ILE:N	13:P:33:ILE:CD1	2.80	0.44
2:R:207:ARG:HB2	2:R:216:SER:HB2	1.98	0.44
2:R:299:TYR:O	2:R:302:PRO:HD3	2.17	0.44
2:R:1042:PHE:C	2:R:1044:THR:H	2.24	0.44
5:T:167:PRO:C	5:T:169:LEU:N	2.76	0.44
7:V:8:GLU:OE2	7:V:64:LEU:HD22	2.18	0.44
7:V:25:ASN:O	7:V:43:ILE:HA	2.17	0.44
1:W:16:PRO:CD	1:W:206:TRP:CD1	3.01	0.44
1:W:77:LEU:HD22	1:W:77:LEU:N	2.33	0.44
1:W:241:ASP:OD2	1:W:289:HIS:NE2	2.50	0.44
1:W:728:MET:HG3	1:W:733:ALA:O	2.17	0.44
3:Y:219:LEU:N	3:Y:219:LEU:HD12	2.33	0.44
1:A:84:VAL:O	1:A:87:VAL:HG12	2.18	0.44
1:A:121:ILE:HG21	10:Q:66:ARG:CD	2.48	0.44
1:A:818:TYR:O	1:A:822:ARG:HG3	2.17	0.44
2:B:162:ARG:HG2	2:B:402:ALA:HA	2.00	0.44
2:B:646:TRP:CH2	2:B:648:PRO:HB2	2.53	0.44
2:B:841:VAL:HG12	2:B:842:THR:O	2.17	0.44
5:E:123:VAL:HA	5:E:127:ILE:HA	2.00	0.44
5:E:145:ARG:HD3	6:F:88:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:75:GLY:C	7:G:76:TYR:CD1	2.96	0.44
11:M:48:PRO:HG2	2:R:735:TYR:CE2	2.52	0.44
2:R:630:ALA:HB2	2:R:640:HIS:CG	2.53	0.44
2:R:639:GLU:CD	2:R:639:GLU:N	2.76	0.44
2:R:872:LEU:HD22	2:R:874:ILE:HG13	2.00	0.44
1:W:84:VAL:O	1:W:87:VAL:HG12	2.18	0.44
1:W:124:ARG:C	1:W:126:PRO:HD2	2.43	0.44
1:W:345:ARG:HA	1:W:410:HIS:ND1	2.33	0.44
1:W:353:ILE:HD13	1:W:405:TYR:HB2	1.99	0.44
1:W:369:PRO:CG	1:W:389:ARG:HD2	2.48	0.44
1:W:509:LEU:HD23	1:W:552:VAL:CG2	2.48	0.44
3:Y:25:PRO:HG3	3:Y:33:LYS:HD3	2.00	0.44
3:Y:47:GLU:CB	3:Y:50:LYS:HB2	2.47	0.44
3:Y:129:GLU:HB3	3:Y:130:TYR:CE2	2.53	0.44
1:A:599:ASP:H	1:A:602:ALA:HB3	1.83	0.44
1:A:872:PHE:CZ	1:A:876:VAL:HG21	2.52	0.44
2:B:595:GLU:O	2:B:595:GLU:CD	2.60	0.44
2:B:783:VAL:HA	2:B:784:ARG:HA	1.72	0.44
4:D:60:HIS:C	4:D:60:HIS:HD2	2.26	0.44
7:G:25:ASN:O	7:G:43:ILE:HA	2.18	0.44
2:R:8:LEU:O	2:R:9:SER:HB3	2.18	0.44
2:R:17:ILE:O	2:R:20:TYR:HB3	2.17	0.44
2:R:597:ILE:HD12	2:R:605:ILE:N	2.32	0.44
7:V:76:TYR:CD1	7:V:76:TYR:N	2.85	0.44
1:W:29:THR:HG23	1:W:243:VAL:HB	1.99	0.44
1:W:78:VAL:O	1:W:78:VAL:HG13	2.18	0.44
1:A:29:THR:OG1	1:A:243:VAL:HG12	2.18	0.43
1:A:238:LYS:HE2	1:A:297:THR:CG2	2.47	0.43
1:A:371:LYS:HD3	1:A:372:TRP:N	2.33	0.43
1:A:871:ILE:CD1	3:C:39:LYS:O	2.66	0.43
2:B:28:ARG:HD2	2:B:32:ASP:OD2	2.18	0.43
2:B:493:TYR:CE1	2:B:499:PRO:HD3	2.52	0.43
3:C:244:LYS:CA	3:C:245:LYS:CB	2.93	0.43
3:C:258:LEU:HD22	3:C:280:ILE:HD13	2.00	0.43
4:D:41:ILE:HB	4:D:63:ALA:HA	2.00	0.43
4:D:73:LEU:HD11	4:D:236:LEU:HD21	1.99	0.43
7:G:96:ILE:HD13	7:G:101:LEU:HD22	1.99	0.43
8:H:32:LEU:HD21	8:H:42:LEU:HD11	2.00	0.43
9:I:14:HIS:CE1	3:Y:28:ILE:HD13	2.53	0.43
11:L:77:ARG:HB2	11:L:77:ARG:HH11	1.83	0.43
2:R:137:THR:HG22	2:R:140:LYS:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:330:LEU:O	2:R:332:ARG:CG	2.65	0.43
2:R:460:GLU:OE1	2:R:472:ASN:ND2	2.51	0.43
5:T:102:GLY:HA2	6:U:40:TYR:CG	2.53	0.43
5:T:145:ARG:HD3	6:U:88:ILE:HG21	1.98	0.43
7:V:29:ILE:CD1	7:V:42:ILE:HG13	2.48	0.43
1:W:249:LEU:HG	1:W:265:LEU:CB	2.45	0.43
3:Y:34:ASN:O	3:Y:37:SER:HB3	2.18	0.43
1:A:10:LYS:HA	3:C:363:VAL:HG22	2.00	0.43
1:A:461:GLU:OE2	2:B:1003:LYS:HG3	2.17	0.43
1:A:650:ASP:HB3	1:A:723:ASN:ND2	2.33	0.43
1:A:853:ASP:HA	8:H:72:TYR:HB2	1.99	0.43
1:A:855:VAL:HB	3:C:311:ARG:NH1	2.33	0.43
2:B:17:ILE:CG1	2:B:476:MET:SD	3.06	0.43
2:B:252:GLN:O	2:B:256:PHE:CD2	2.71	0.43
2:B:254:GLU:C	2:B:256:PHE:H	2.26	0.43
2:B:767:LYS:HA	2:B:767:LYS:HZ2	1.83	0.43
2:B:904:VAL:O	4:D:163:ILE:HG12	2.18	0.43
3:C:63:LEU:C	3:C:64:ILE:HG13	2.42	0.43
3:C:219:LEU:O	3:C:222:LEU:HB2	2.18	0.43
4:D:98:ILE:HD13	4:D:141:LEU:HD11	2.00	0.43
10:J:66:ARG:C	10:J:68:PHE:H	2.25	0.43
12:N:1:MET:HA	12:N:56:ILE:HB	1.99	0.43
2:R:46:ILE:CB	2:R:66:ILE:HD11	2.46	0.43
2:R:103:MET:O	2:R:114:PRO:O	2.36	0.43
2:R:372:LEU:CD2	2:R:376:LYS:CE	2.96	0.43
2:R:476:MET:HE1	2:R:645:ILE:HD12	2.00	0.43
2:R:493:TYR:CE1	2:R:499:PRO:HD3	2.52	0.43
2:R:814:ILE:HD11	2:R:867:VAL:HG23	1.99	0.43
2:R:1120:ASP:HA	1:W:4:LYS:HE2	1.99	0.43
6:U:21:LEU:O	6:U:24:VAL:HG12	2.18	0.43
7:V:41:ASP:O	7:V:42:ILE:HD13	2.18	0.43
1:W:281:ILE:C	1:W:282:PRO:O	2.61	0.43
1:W:870:ARG:HD2	3:Y:57:LYS:HB3	1.99	0.43
3:Y:170:ASP:O	3:Y:174:LEU:HD12	2.18	0.43
1:A:98:CYS:HB3	1:A:101:CYS:HB2	1.86	0.43
2:B:108:ASN:C	2:B:110:ILE:N	2.72	0.43
2:B:555:GLU:HG2	2:B:579:ARG:HH12	1.83	0.43
2:B:1056:SER:HB3	2:B:1057:ASP:OD1	2.18	0.43
3:C:286:ILE:HG23	3:C:324:GLY:O	2.18	0.43
4:D:8:LYS:HG3	4:D:13:ILE:CG1	2.48	0.43
4:D:108:MET:CG	4:D:110:TYR:CZ	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:90:LEU:HD23	9:I:90:LEU:HA	1.71	0.43
10:J:40:ASN:HA	10:J:43:LEU:CD1	2.48	0.43
11:L:29:ALA:HB2	11:L:43:TYR:HB3	1.99	0.43
12:O:1:MET:HE2	12:O:1:MET:HA	2.00	0.43
2:R:194:SER:CB	2:R:303:HIS:HB3	2.48	0.43
2:R:212:THR:C	2:R:259:LEU:HD11	2.42	0.43
2:R:675:MET:HG3	2:R:996:LEU:HD21	1.99	0.43
2:R:737:MET:HE1	1:W:502:TYR:CD2	2.53	0.43
2:R:995:LYS:HE2	2:R:999:MET:HE3	2.00	0.43
2:R:1034:MET:O	2:R:1037:ASP:HB2	2.19	0.43
2:R:1037:ASP:OD2	1:W:824:ILE:HD13	2.19	0.43
4:S:65:ILE:HG23	4:S:128:ILE:HD12	2.00	0.43
6:U:18:LYS:C	6:U:20:LEU:H	2.26	0.43
1:W:20:ARG:NE	1:W:211:VAL:HG21	2.33	0.43
1:W:736:SER:HB3	1:W:739:ASN:ND2	2.33	0.43
1:W:856:PHE:CE2	1:W:858:MET:CB	3.01	0.43
1:A:19:ILE:O	1:A:74:HIS:NE2	2.52	0.43
1:A:139:THR:HG23	1:A:139:THR:O	2.18	0.43
2:B:770:GLY:O	2:B:771:GLY:C	2.61	0.43
3:C:34:ASN:O	3:C:37:SER:HB3	2.18	0.43
3:C:129:GLU:HB3	3:C:130:TYR:CD2	2.54	0.43
4:D:153:HIS:O	4:D:154:ALA:HB3	2.18	0.43
8:H:25:ILE:HG22	10:Q:55:LEU:HD22	1.99	0.43
8:H:28:ALA:HB1	8:H:62:ILE:CD1	2.48	0.43
10:J:61:VAL:C	10:J:63:GLU:N	2.72	0.43
11:M:27:LEU:CD1	4:S:24:PHE:HA	2.48	0.43
11:M:29:ALA:HB2	11:M:43:TYR:HB3	2.00	0.43
2:R:136:TYR:HB2	2:R:141:LEU:CD1	2.48	0.43
2:R:391:ASP:C	2:R:393:VAL:N	2.72	0.43
2:R:533:TYR:CE2	2:R:539:LEU:HD23	2.53	0.43
2:R:946:THR:O	2:R:947:PRO:C	2.62	0.43
5:T:60:VAL:HG22	5:T:61:PHE:N	2.32	0.43
5:T:84:VAL:CG2	6:U:75:ILE:CD1	2.97	0.43
7:V:96:ILE:HD13	7:V:101:LEU:HD21	2.00	0.43
1:W:575:CYS:SG	1:W:584:SER:HB3	2.58	0.43
1:A:95:LYS:HB3	1:A:138:LYS:CE	2.45	0.43
1:A:122:LYS:NZ	10:Q:66:ARG:HG3	2.34	0.43
1:A:353:ILE:HG23	1:A:358:ILE:HD13	1.99	0.43
1:A:378:VAL:CG1	1:A:386:ILE:HB	2.49	0.43
1:A:757:ILE:CD1	1:A:797:PHE:HD1	2.31	0.43
1:A:827:LEU:O	3:C:71:GLY:HA3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:859:TYR:HB2	3:C:63:LEU:HB3	2.00	0.43
2:B:808:LYS:O	2:B:809:GLY:C	2.61	0.43
2:B:814:ILE:HD11	2:B:867:VAL:HG23	2.01	0.43
2:B:1103:LEU:O	2:B:1107:LEU:HG	2.18	0.43
3:C:170:ASP:O	3:C:174:LEU:HD12	2.18	0.43
3:C:216:ILE:O	3:C:217:ALA:HB3	2.17	0.43
4:D:76:TYR:HD1	4:D:91:LYS:C	2.26	0.43
4:D:153:HIS:ND1	4:D:155:LYS:HG2	2.33	0.43
7:G:14:GLU:OE2	7:G:54:LYS:HE2	2.19	0.43
2:R:52:ILE:N	2:R:53:PRO:HD3	2.33	0.43
2:R:765:GLU:HB3	2:R:774:ASP:O	2.19	0.43
4:S:98:ILE:HD13	4:S:141:LEU:HD11	2.00	0.43
5:T:70:VAL:CG1	5:T:72:PHE:CE2	3.01	0.43
5:T:136:ILE:O	5:T:137:GLN:CB	2.66	0.43
7:V:67:THR:HG22	7:V:68:ASN:H	1.83	0.43
3:Y:393:ILE:O	3:Y:393:ILE:HG13	2.16	0.43
1:A:16:PRO:CD	1:A:206:TRP:CD1	3.02	0.43
1:A:119:ASN:OD1	1:A:126:PRO:CB	2.67	0.43
2:B:586:SER:O	2:B:587:ASN:HB2	2.17	0.43
2:B:639:GLU:N	2:B:639:GLU:CD	2.75	0.43
2:B:980:GLN:HA	4:D:22:LEU:HD21	1.99	0.43
4:D:41:ILE:HD13	4:D:145:LEU:HG	2.01	0.43
4:D:219:ILE:CD1	16:D:1001:F3S:S3	3.07	0.43
5:E:75:ILE:CD1	6:F:20:LEU:HB3	2.48	0.43
2:R:638:PRO:HG2	2:R:640:HIS:NE2	2.33	0.43
4:S:8:LYS:HA	4:S:13:ILE:HA	2.01	0.43
4:S:41:ILE:HD13	4:S:145:LEU:HG	2.00	0.43
5:T:4:LEU:HB2	6:U:12:ILE:HD11	1.99	0.43
7:V:89:GLY:HA2	1:W:549:LYS:HE2	2.01	0.43
1:W:541:ALA:CB	1:W:542:PRO:CD	2.97	0.43
1:W:565:GLN:HB3	1:W:569:SER:HB3	2.01	0.43
1:W:631:LEU:O	1:W:634:VAL:HB	2.19	0.43
3:Y:24:LEU:N	3:Y:25:PRO:HD2	2.34	0.43
3:Y:146:TYR:HE2	3:Y:231:ILE:HD11	1.83	0.43
8:Z:12:ARG:HH22	8:Z:55:ILE:HD12	1.83	0.43
2:B:113:GLU:CB	2:B:114:PRO:CD	2.89	0.43
2:B:163:VAL:HG21	2:B:429:LEU:CD2	2.49	0.43
2:B:485:GLU:OE1	2:B:528:ARG:NH1	2.52	0.43
2:B:547:ARG:NH1	2:B:556:VAL:O	2.52	0.43
3:C:112:ASP:O	3:C:114:LYS:N	2.51	0.43
3:C:222:LEU:O	3:C:226:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:281:GLU:CD	3:C:326:VAL:HG12	2.44	0.43
5:E:39:LEU:O	5:E:40:LYS:C	2.61	0.43
5:E:39:LEU:HD12	5:E:39:LEU:N	2.34	0.43
5:E:164:MET:O	5:E:167:PRO:HD3	2.19	0.43
2:R:254:GLU:O	2:R:254:GLU:HG2	2.19	0.43
2:R:308:ALA:C	2:R:310:ASP:H	2.26	0.43
2:R:359:VAL:HG11	2:R:407:VAL:HG22	2.00	0.43
2:R:398:ARG:C	2:R:400:ALA:N	2.76	0.43
2:R:448:LEU:HD22	1:W:796:PHE:CZ	2.54	0.43
2:R:856:THR:CG2	2:R:857:GLU:H	2.21	0.43
2:R:922:MET:HG2	1:W:743:MET:HG3	2.00	0.43
2:R:982:ILE:HD12	2:R:982:ILE:C	2.43	0.43
4:S:108:MET:CG	4:S:110:TYR:CE2	3.01	0.43
5:T:79:PRO:HB3	5:T:160:ILE:HD11	2.01	0.43
7:V:8:GLU:O	7:V:9:ILE:HG13	2.19	0.43
1:W:224:MET:HE2	1:W:224:MET:CA	2.49	0.43
1:W:378:VAL:CG1	1:W:386:ILE:HB	2.49	0.43
1:W:648:LEU:HD21	1:W:787:ARG:HH11	1.81	0.43
3:Y:234:ILE:HG22	3:Y:235:LYS:N	2.33	0.43
3:Y:284:PHE:O	3:Y:288:ALA:HB2	2.19	0.43
1:A:618:GLU:C	1:A:619:TYR:CG	2.97	0.43
1:A:631:LEU:O	1:A:634:VAL:HB	2.19	0.43
1:A:753:ARG:NH2	2:B:447:ASP:OD2	2.52	0.43
2:B:893:MET:HE3	2:B:894:LEU:H	1.83	0.43
2:B:904:VAL:O	4:D:163:ILE:HG21	2.19	0.43
2:B:1025:ARG:O	2:B:1026:GLU:C	2.61	0.43
3:C:104:LEU:CD1	3:C:108:ILE:HD11	2.49	0.43
4:D:65:ILE:HG23	4:D:128:ILE:HD12	2.00	0.43
2:R:17:ILE:CG1	2:R:476:MET:SD	3.07	0.43
2:R:703:ARG:HH22	2:R:942:ILE:HG21	1.84	0.43
2:R:729:VAL:HG23	2:R:987:TYR:CD1	2.54	0.43
2:R:876:SER:O	2:R:877:ILE:C	2.62	0.43
2:R:903:THR:HG21	2:R:971:GLU:OE1	2.19	0.43
2:R:1061:ILE:HA	2:R:1072:TRP:NE1	2.34	0.43
4:S:161:LEU:CD1	4:S:163:ILE:HD13	2.48	0.43
4:S:206:CYS:SG	4:S:207:GLU:N	2.91	0.43
1:W:309:PHE:O	1:W:310:ARG:HB2	2.18	0.43
1:W:376:ASN:HB2	1:W:377:TYR:CD1	2.53	0.43
3:Y:11:SER:C	3:Y:45:ARG:NH2	2.77	0.43
3:Y:186:LYS:CB	3:Y:230:LYS:HE2	2.46	0.43
3:Y:237:ILE:HD12	3:Y:253:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:344:ARG:HB3	3:Y:353:HIS:ND1	2.34	0.43
1:A:281:ILE:C	1:A:282:PRO:O	2.62	0.43
1:A:417:VAL:HG13	1:A:465:HIS:O	2.18	0.43
2:B:139:ASP:O	2:B:143:GLU:HG3	2.18	0.43
2:B:230:MET:HE1	2:B:315:ALA:O	2.18	0.43
2:B:638:PRO:HG2	2:B:640:HIS:NE2	2.34	0.43
2:B:699:HIS:CE1	4:D:57:ILE:CD1	3.01	0.43
3:C:28:ILE:H	3:C:28:ILE:HG13	1.51	0.43
3:C:216:ILE:O	3:C:217:ALA:HB2	2.19	0.43
7:G:82:LYS:HD3	7:G:95:ILE:HG12	2.01	0.43
9:I:16:ASN:O	9:I:20:VAL:HG23	2.18	0.43
12:O:1:MET:HA	12:O:56:ILE:HB	2.01	0.43
2:R:208:LEU:HD23	2:R:215:VAL:CG2	2.46	0.43
2:R:547:ARG:NH1	2:R:556:VAL:O	2.51	0.43
2:R:697:LEU:C	2:R:697:LEU:HD13	2.43	0.43
2:R:948:PHE:CE1	1:W:792:PRO:CG	3.02	0.43
4:S:22:LEU:HD13	4:S:226:TYR:CD1	2.54	0.43
5:T:165:ARG:C	5:T:167:PRO:HD3	2.42	0.43
1:W:45:MET:CE	1:W:46:ASP:OD1	2.67	0.43
1:W:64:THR:O	1:W:65:LEU:HB2	2.19	0.43
1:W:122:LYS:O	1:W:126:PRO:HG3	2.18	0.43
3:Y:127:THR:OG1	3:Y:129:GLU:O	2.35	0.43
1:A:184:LEU:HD22	1:A:204:PRO:HB2	2.01	0.43
1:A:372:TRP:HB3	1:A:373:PRO:HD3	2.01	0.43
1:A:563:HIS:CD2	1:A:872:PHE:CE2	3.07	0.43
2:B:500:VAL:HG12	2:B:504:ILE:HG12	2.01	0.43
2:B:533:TYR:CE2	2:B:539:LEU:HD23	2.54	0.43
2:B:562:VAL:O	2:B:566:ILE:O	2.37	0.43
2:B:949:TYR:O	2:B:951:THR:N	2.52	0.43
2:B:1003:LYS:O	2:B:1004:ILE:C	2.60	0.43
3:C:11:SER:HB2	3:C:14:GLU:HB2	2.01	0.43
3:C:149:ILE:O	3:C:153:VAL:HG12	2.19	0.43
3:C:182:ASP:HB2	3:C:232:LYS:HZ2	1.84	0.43
5:E:124:ARG:O	5:E:126:ILE:N	2.52	0.43
6:F:72:LEU:HD21	6:F:86:ILE:HG12	2.01	0.43
7:G:8:GLU:O	7:G:9:ILE:HG13	2.19	0.43
9:I:55:ASN:HA	9:I:56:ILE:N	2.30	0.43
10:J:55:LEU:O	10:J:56:ASN:CB	2.67	0.43
12:O:64:ARG:O	12:O:64:ARG:CG	2.67	0.43
2:R:254:GLU:C	2:R:256:PHE:H	2.27	0.43
2:R:341:TYR:CD1	2:R:344:LYS:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:398:ARG:HD2	2:R:399:HIS:CE1	2.54	0.43
2:R:399:HIS:O	2:R:403:THR:HG21	2.19	0.43
2:R:619:LEU:HD22	2:R:623:GLU:HG2	2.01	0.43
2:R:1105:GLN:HE22	1:W:70:GLY:HA2	1.84	0.43
4:S:108:MET:CG	4:S:110:TYR:CZ	3.02	0.43
1:W:103:ARG:CG	1:W:191:ASP:OD1	2.67	0.43
1:W:192:VAL:HG21	1:W:199:PRO:HB3	2.00	0.43
1:W:337:VAL:HG21	1:W:419:PHE:CE1	2.53	0.43
1:W:412:THR:O	1:W:414:GLY:N	2.52	0.43
1:W:757:ILE:CD1	1:W:797:PHE:HD1	2.32	0.43
8:Z:12:ARG:NH2	8:Z:55:ILE:HD12	2.34	0.43
1:A:646:MET:HG2	2:B:918:LEU:HD13	2.01	0.42
1:A:683:GLU:N	1:A:683:GLU:OE1	2.52	0.42
2:B:162:ARG:HG2	2:B:401:LEU:O	2.18	0.42
2:B:173:ASN:N	2:B:193:ILE:O	2.49	0.42
2:B:453:TRP:CZ3	2:B:644:GLU:CD	2.97	0.42
2:B:947:PRO:O	2:B:948:PHE:HD2	2.01	0.42
3:C:146:TYR:HE2	3:C:231:ILE:HD11	1.84	0.42
11:M:69:LEU:CD2	4:S:260:LEU:HD11	2.48	0.42
12:O:15:ALA:HB1	4:S:129:PRO:HD2	2.01	0.42
10:Q:73:LYS:HA	10:Q:76:GLU:OE2	2.19	0.42
2:R:37:PHE:CZ	2:R:42:LEU:HD13	2.53	0.42
2:R:675:MET:HG2	2:R:882:ALA:CB	2.49	0.42
4:S:219:ILE:CD1	16:S:1001:F3S:S3	3.07	0.42
1:W:736:SER:HB3	1:W:739:ASN:OD1	2.18	0.42
1:W:870:ARG:CZ	1:W:870:ARG:CB	2.96	0.42
13:X:37:VAL:HG22	13:X:38:ARG:H	1.83	0.42
3:Y:171:ASN:CG	3:Y:172:GLU:H	2.27	0.42
3:Y:237:ILE:HD12	3:Y:253:THR:CB	2.48	0.42
1:A:77:LEU:HD22	1:A:77:LEU:N	2.33	0.42
1:A:212:LEU:CD1	1:A:273:VAL:HG13	2.50	0.42
1:A:369:PRO:CG	1:A:389:ARG:HD2	2.48	0.42
1:A:833:GLU:HG3	1:A:839:ARG:CD	2.49	0.42
2:B:355:SER:C	2:B:407:VAL:HG11	2.44	0.42
2:B:372:LEU:O	2:B:373:GLU:C	2.61	0.42
2:B:605:ILE:CG1	2:B:606:THR:N	2.81	0.42
2:B:678:GLN:HG2	2:B:997:HIS:NE2	2.34	0.42
2:B:703:ARG:NH2	2:B:942:ILE:HG21	2.33	0.42
2:B:756:THR:HG23	2:B:871:ASP:O	2.18	0.42
2:B:1007:ARG:CZ	2:B:1028:GLY:C	2.93	0.42
2:B:1051:ARG:NE	2:B:1051:ARG:HA	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:MET:SD	3:C:206:LEU:CD2	3.07	0.42
4:D:13:ILE:HD13	4:D:14:ASP:N	2.34	0.42
9:I:34:ARG:CB	3:Y:386:VAL:HG11	2.49	0.42
13:P:17:GLN:HG3	13:P:19:LYS:H	1.84	0.42
2:R:87:GLU:HG2	13:X:31:TYR:OH	2.19	0.42
2:R:115:GLU:O	2:R:117:VAL:HG23	2.19	0.42
2:R:453:TRP:CZ3	2:R:644:GLU:CD	2.97	0.42
2:R:763:THR:HG22	2:R:764:GLU:O	2.19	0.42
2:R:918:LEU:H	2:R:919:PRO:HD2	1.84	0.42
2:R:956:LEU:O	2:R:960:ILE:HG12	2.19	0.42
4:S:73:LEU:HD11	4:S:236:LEU:HD21	2.02	0.42
5:T:84:VAL:HG13	6:U:75:ILE:CD1	2.49	0.42
6:U:15:SER:HB3	6:U:47:CYS:SG	2.59	0.42
1:W:85:GLY:HA3	3:Y:355:LEU:HD22	2.01	0.42
1:W:222:SER:C	1:W:223:ILE:CG2	2.92	0.42
1:W:353:ILE:HG23	1:W:358:ILE:HD13	1.99	0.42
1:A:64:THR:O	1:A:65:LEU:HB2	2.19	0.42
1:A:91:TYR:C	1:A:91:TYR:CD1	2.97	0.42
1:A:95:LYS:O	1:A:138:LYS:HG2	2.19	0.42
1:A:127:SER:O	1:A:131:ARG:HG3	2.19	0.42
1:A:185:GLU:HG3	1:A:205:GLU:HG2	2.01	0.42
1:A:224:MET:HE2	1:A:224:MET:CA	2.50	0.42
2:B:249:PRO:HB2	2:B:252:GLN:HB2	2.01	0.42
2:B:333:ARG:HB3	2:B:333:ARG:NH1	2.35	0.42
2:B:623:GLU:C	2:B:625:GLU:N	2.75	0.42
2:B:636:LEU:HD13	2:B:643:LEU:HD12	2.01	0.42
2:B:767:LYS:HA	2:B:767:LYS:NZ	2.34	0.42
2:B:774:ASP:OD1	2:B:818:SER:HA	2.19	0.42
2:B:856:THR:CG2	2:B:857:GLU:H	2.29	0.42
4:D:3:ILE:HD12	11:L:86:GLU:OE1	2.20	0.42
4:D:101:GLU:HB2	4:D:137:GLN:O	2.19	0.42
9:I:27:LEU:CD2	9:I:78:ILE:CD1	2.97	0.42
11:M:19:GLY:O	11:M:20:GLU:CD	2.62	0.42
12:O:61:HIS:O	12:O:62:TYR:CD2	2.72	0.42
13:P:6:CYS:HB3	13:P:7:GLY:H	1.67	0.42
2:R:101:LEU:HD13	2:R:101:LEU:C	2.44	0.42
2:R:155:PHE:CE1	2:R:164:ILE:HD12	2.54	0.42
2:R:162:ARG:HG2	2:R:401:LEU:O	2.19	0.42
2:R:478:GLN:HG2	2:R:479:ILE:N	2.34	0.42
2:R:1096:VAL:CG1	2:R:1097:SER:N	2.82	0.42
4:S:247:LYS:O	4:S:251:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:40:LYS:O	5:T:41:ASP:OD1	2.37	0.42
5:T:45:VAL:HG21	5:T:74:MET:SD	2.59	0.42
1:W:81:VAL:CG2	1:W:269:LEU:HB3	2.49	0.42
1:W:212:LEU:CD1	1:W:273:VAL:HG13	2.50	0.42
1:W:450:CYS:H	1:W:451:PRO:CD	2.33	0.42
1:W:801:GLY:C	1:W:803:ARG:N	2.78	0.42
1:W:856:PHE:HB3	1:W:859:TYR:CD2	2.53	0.42
3:Y:201:SER:HB2	3:Y:204:ASN:HB2	2.00	0.42
3:Y:219:LEU:O	3:Y:222:LEU:HB2	2.19	0.42
1:A:101:CYS:HB2	1:A:102:GLY:H	1.67	0.42
1:A:502:TYR:CD2	2:B:737:MET:HE1	2.54	0.42
2:B:34:TYR:HB3	2:B:125:MET:HE1	2.01	0.42
2:B:112:ALA:C	2:B:113:GLU:HG3	2.44	0.42
2:B:217:PHE:HA	2:B:218:PRO:HD3	1.96	0.42
2:B:1046:MET:CG	5:E:61:PHE:HD1	2.32	0.42
2:B:1059:THR:CG2	2:B:1061:ILE:HD12	2.50	0.42
3:C:63:LEU:HD23	3:C:63:LEU:HA	1.89	0.42
3:C:129:GLU:C	3:C:131:LYS:H	2.27	0.42
4:D:70:GLU:OE1	4:D:70:GLU:HA	2.20	0.42
4:D:205:LEU:O	4:D:207:GLU:N	2.52	0.42
8:H:29:TYR:HE1	10:Q:60:SER:HB3	1.84	0.42
9:I:27:LEU:CD2	9:I:78:ILE:HD11	2.48	0.42
9:I:35:VAL:CG1	3:Y:388:LEU:HD11	2.49	0.42
9:K:16:ASN:O	9:K:20:VAL:HG23	2.20	0.42
2:R:736:ASN:OD1	2:R:914:ASN:HB2	2.19	0.42
2:R:854:LEU:HD12	13:X:35:PHE:CE1	2.54	0.42
5:T:37:LYS:O	5:T:44:LEU:HA	2.19	0.42
5:T:123:VAL:O	5:T:123:VAL:HG12	2.18	0.42
1:W:390:TYR:O	1:W:391:VAL:C	2.63	0.42
13:X:24:VAL:O	13:X:24:VAL:HG13	2.19	0.42
1:A:219:ILE:O	1:A:219:ILE:HG22	2.19	0.42
1:A:488:THR:CG2	1:A:493:GLY:O	2.68	0.42
1:A:696:LEU:HD13	1:A:700:ILE:HD12	2.01	0.42
2:B:93:LEU:HD11	2:B:859:ALA:H	1.85	0.42
2:B:249:PRO:HB2	2:B:253:ASN:N	2.34	0.42
2:B:769:PRO:O	2:B:770:GLY:O	2.37	0.42
3:C:289:ALA:O	3:C:293:ILE:HG12	2.20	0.42
5:E:83:GLU:HA	6:F:89:MET:CE	2.48	0.42
5:E:99:VAL:O	5:E:101:LEU:HD12	2.19	0.42
11:M:3:ILE:CG2	11:M:15:LEU:HD11	2.50	0.42
2:R:51:GLU:C	2:R:53:PRO:HD3	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:101:LEU:CD1	2:R:103:MET:HG3	2.49	0.42
4:S:46:PHE:CG	4:S:55:ASP:OD2	2.73	0.42
4:S:206:CYS:O	4:S:207:GLU:HB2	2.20	0.42
1:W:19:ILE:O	1:W:74:HIS:NE2	2.52	0.42
1:W:448:LEU:O	1:W:496:ILE:HG23	2.18	0.42
1:W:488:THR:CG2	1:W:493:GLY:O	2.67	0.42
1:W:573:ARG:HA	1:W:582:HIS:CD2	2.53	0.42
1:W:687:ILE:CD1	1:W:695:SER:HB2	2.49	0.42
1:W:691:THR:HB	1:W:694:GLU:CB	2.50	0.42
3:Y:163:MET:SD	3:Y:206:LEU:CD2	3.08	0.42
8:Z:65:ILE:HD12	8:Z:78:TYR:HA	2.01	0.42
1:A:45:MET:HE2	1:A:46:ASP:OD1	2.20	0.42
1:A:121:ILE:HG23	8:H:38:ARG:NH1	2.35	0.42
1:A:450:CYS:H	1:A:451:PRO:HD2	1.83	0.42
1:A:572:PRO:HD2	1:A:730:ARG:HH12	1.85	0.42
1:A:831:ARG:CZ	3:C:385:MET:HG3	2.49	0.42
1:A:876:VAL:C	1:A:878:TRP:N	2.77	0.42
2:B:525:LEU:CD2	2:B:571:VAL:HB	2.50	0.42
2:B:895:ILE:HG23	2:B:899:ASP:HB2	2.02	0.42
2:B:949:TYR:C	2:B:950:LYS:HG3	2.43	0.42
2:B:995:LYS:CE	2:B:999:MET:HE3	2.49	0.42
2:B:1061:ILE:HA	2:B:1072:TRP:NE1	2.35	0.42
4:D:153:HIS:NE2	13:P:48:ILE:HG23	2.34	0.42
6:F:4:VAL:O	6:F:4:VAL:HG22	2.18	0.42
7:G:36:PHE:CE1	7:G:96:ILE:CG1	3.03	0.42
8:H:58:LYS:NZ	10:Q:51:TRP:CH2	2.88	0.42
11:L:83:TYR:CZ	11:L:87:ILE:HD11	2.55	0.42
12:N:1:MET:HA	12:N:1:MET:HE2	2.00	0.42
2:R:20:TYR:CD1	2:R:20:TYR:C	2.98	0.42
2:R:579:ARG:HD3	2:R:618:TYR:CD2	2.55	0.42
1:W:687:ILE:HD12	1:W:695:SER:CB	2.49	0.42
1:W:819:MET:HE2	1:W:819:MET:HB3	1.76	0.42
3:Y:107:LEU:O	3:Y:110:ILE:HG22	2.19	0.42
3:Y:127:THR:O	3:Y:131:LYS:HD2	2.20	0.42
3:Y:311:ARG:NH2	8:Z:71:LEU:HD22	2.35	0.42
3:Y:327:ARG:HG3	3:Y:334:VAL:HG22	1.99	0.42
1:A:6:ILE:CD1	2:B:1094:VAL:HG11	2.49	0.42
1:A:45:MET:CE	1:A:46:ASP:OD1	2.67	0.42
1:A:388:LEU:HA	1:A:391:VAL:HG22	2.02	0.42
1:A:505:GLY:CA	1:A:639:VAL:HG22	2.47	0.42
1:A:723:ASN:C	1:A:723:ASN:HD22	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:TYR:HD2	1:A:822:ARG:NH1	2.17	0.42
1:A:833:GLU:HG3	1:A:839:ARG:HD2	2.01	0.42
2:B:126:LEU:HD22	2:B:154:TYR:CE2	2.55	0.42
2:B:457:CYS:SG	2:B:460:GLU:HB2	2.60	0.42
2:B:630:ALA:HB2	2:B:640:HIS:CG	2.54	0.42
2:B:938:LEU:O	12:N:46:ARG:NH1	2.52	0.42
3:C:129:GLU:HB3	3:C:130:TYR:CE2	2.55	0.42
4:D:22:LEU:HD13	4:D:226:TYR:CD1	2.55	0.42
8:H:58:LYS:H	8:H:58:LYS:HG3	1.61	0.42
9:I:23:TRP:CZ2	3:Y:66:PRO:HD3	2.55	0.42
11:L:19:GLY:C	11:L:20:GLU:HG2	2.43	0.42
2:R:622:GLU:O	2:R:625:GLU:CB	2.64	0.42
2:R:734:GLY:CA	2:R:735:TYR:CB	2.97	0.42
2:R:855:ILE:O	13:X:34:ILE:CG2	2.68	0.42
2:R:1025:ARG:C	2:R:1026:GLU:O	2.63	0.42
2:R:1039:LEU:HD22	2:R:1044:THR:CG2	2.49	0.42
4:S:37:PRO:HG3	4:S:78:TRP:CZ3	2.54	0.42
4:S:109:LEU:C	4:S:109:LEU:CD2	2.92	0.42
4:S:164:VAL:HA	4:S:227:ILE:O	2.18	0.42
6:U:62:ILE:HG22	6:U:63:ILE:H	1.84	0.42
7:V:31:MET:CE	7:V:55:VAL:HG11	2.50	0.42
7:V:40:PHE:HA	7:V:92:TYR:CD1	2.54	0.42
1:W:326:ILE:HG21	1:W:462:MET:SD	2.60	0.42
1:W:371:LYS:HD3	1:W:372:TRP:N	2.35	0.42
1:W:417:VAL:CG1	1:W:464:LEU:HD13	2.49	0.42
1:W:560:PHE:CZ	1:W:615:LEU:HG	2.55	0.42
1:W:657:VAL:O	1:W:657:VAL:HG12	2.19	0.42
1:W:668:ALA:HB2	1:W:707:LEU:HD13	2.01	0.42
1:W:705:ASP:O	1:W:708:ARG:HG3	2.18	0.42
3:Y:24:LEU:HD11	3:Y:55:ALA:HB1	2.02	0.42
8:Z:28:ALA:CB	8:Z:62:ILE:HD11	2.49	0.42
1:A:224:MET:HE2	1:A:224:MET:HA	2.02	0.42
1:A:262:ILE:O	1:A:266:TRP:HB3	2.20	0.42
1:A:811:VAL:O	1:A:812:ARG:HB2	2.20	0.42
2:B:345:ARG:HG3	2:B:576:GLY:HA3	2.01	0.42
2:B:423:LEU:HB2	2:B:716:TYR:HD1	1.85	0.42
2:B:589:ASN:HA	2:B:590:PRO:HD3	1.70	0.42
3:C:129:GLU:C	3:C:131:LYS:N	2.77	0.42
4:D:37:PRO:HG3	4:D:78:TRP:CZ3	2.54	0.42
4:D:203:CYS:SG	4:D:204:THR:N	2.93	0.42
9:I:63:SER:HA	9:I:66:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:139:ASP:O	2:R:143:GLU:HG3	2.19	0.42
2:R:252:GLN:O	2:R:256:PHE:CD2	2.73	0.42
2:R:356:LEU:HD12	2:R:407:VAL:CG2	2.48	0.42
2:R:675:MET:HE1	2:R:888:LYS:HE3	2.01	0.42
2:R:772:GLN:HG2	2:R:773:GLU:N	2.35	0.42
5:T:13:ILE:HD12	5:T:68:HIS:CD2	2.55	0.42
5:T:92:VAL:HG11	5:T:137:GLN:HA	2.02	0.42
1:W:119:ASN:OD1	1:W:126:PRO:CB	2.67	0.42
1:W:430:MET:O	1:W:480:MET:HE3	2.19	0.42
1:W:543:ARG:HB2	1:W:545:TYR:CE2	2.55	0.42
1:W:831:ARG:CZ	3:Y:385:MET:HG3	2.50	0.42
1:W:853:ASP:HA	8:Z:72:TYR:HB2	2.01	0.42
3:Y:74:ALA:O	3:Y:75:ALA:C	2.61	0.42
3:Y:277:ILE:CG2	3:Y:278:ARG:N	2.80	0.42
1:A:141:MET:O	1:A:141:MET:CG	2.67	0.42
2:B:157:VAL:CG2	2:B:402:ALA:HB2	2.45	0.42
2:B:1100:PHE:CZ	3:C:375:ILE:HD13	2.55	0.42
3:C:65:ALA:HA	3:C:66:PRO:HD3	1.85	0.42
3:C:301:LEU:HD22	3:C:308:VAL:HG12	2.02	0.42
5:E:136:ILE:CG2	5:E:137:GLN:N	2.75	0.42
5:E:141:LYS:HE3	6:F:46:LYS:HZ3	1.85	0.42
11:L:82:HIS:NE2	11:L:86:GLU:OE2	2.52	0.42
10:Q:40:ASN:HA	10:Q:43:LEU:HD11	2.01	0.42
2:R:252:GLN:HA	2:R:255:LEU:HD12	2.02	0.42
2:R:492:LEU:HD13	2:R:523:VAL:HG11	2.02	0.42
2:R:820:PRO:HD3	2:R:835:LYS:HA	2.01	0.42
5:T:96:GLY:HA2	5:T:110:ILE:CD1	2.50	0.42
5:T:99:VAL:O	5:T:101:LEU:HD12	2.20	0.42
1:W:876:VAL:C	1:W:878:TRP:N	2.75	0.42
3:Y:25:PRO:CD	3:Y:33:LYS:HD3	2.50	0.42
3:Y:174:LEU:HB3	3:Y:179:VAL:CG1	2.47	0.42
8:Z:32:LEU:HD21	8:Z:42:LEU:HD11	2.02	0.42
1:A:541:ALA:HB1	7:G:70:ASP:O	2.20	0.42
1:A:696:LEU:HD13	1:A:696:LEU:C	2.45	0.42
2:B:34:TYR:HB3	2:B:125:MET:CE	2.50	0.42
2:B:405:ASN:HB3	2:B:413:VAL:CG2	2.50	0.42
2:B:622:GLU:O	2:B:625:GLU:CB	2.66	0.42
2:B:767:LYS:HG3	2:B:768:TYR:HA	1.97	0.42
4:D:146:ARG:HD2	4:D:147:LEU:O	2.20	0.42
5:E:167:PRO:HA	5:E:169:LEU:N	2.34	0.42
8:H:43:PRO:O	8:H:44:TRP:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:13:LEU:C	9:I:15:PHE:N	2.76	0.42
9:I:80:ARG:HG2	1:W:834:TYR:CE1	2.54	0.42
9:K:22:LEU:HD23	9:K:22:LEU:HA	1.82	0.42
11:M:83:TYR:CZ	11:M:87:ILE:HD11	2.55	0.42
2:R:126:LEU:HD22	2:R:154:TYR:CE2	2.55	0.42
2:R:630:ALA:HB3	2:R:636:LEU:HD13	2.01	0.42
2:R:636:LEU:HD13	2:R:643:LEU:HD12	2.02	0.42
2:R:690:ARG:HB3	2:R:692:ASP:OD1	2.19	0.42
4:S:53:LEU:CD1	4:S:131:VAL:HG23	2.50	0.42
4:S:65:ILE:HG23	4:S:128:ILE:CD1	2.49	0.42
4:S:162:ALA:C	4:S:163:ILE:HD12	2.45	0.42
1:W:29:THR:OG1	1:W:243:VAL:HG12	2.20	0.42
1:W:684:LEU:HD12	1:W:684:LEU:H	1.84	0.42
1:A:283:GLY:O	1:A:284:LEU:C	2.63	0.41
1:A:563:HIS:CD2	1:A:872:PHE:HE2	2.37	0.41
1:A:705:ASP:O	1:A:708:ARG:HG3	2.20	0.41
2:B:40:ASN:O	2:B:44:GLU:HG3	2.20	0.41
2:B:222:GLY:HA3	2:B:278:ARG:NH1	2.35	0.41
2:B:359:VAL:CG1	2:B:407:VAL:HG13	2.49	0.41
2:B:398:ARG:C	2:B:400:ALA:N	2.78	0.41
2:B:735:TYR:CE2	11:L:48:PRO:HG2	2.55	0.41
2:B:930:GLY:HA3	2:B:987:TYR:OH	2.20	0.41
3:C:151:ASN:O	3:C:173:MET:HG3	2.20	0.41
3:C:311:ARG:NH2	8:H:71:LEU:HD22	2.35	0.41
3:C:385:MET:HE2	3:C:385:MET:HB3	1.90	0.41
5:E:30:LEU:HD22	5:E:72:PHE:CZ	2.55	0.41
5:E:40:LYS:O	5:E:41:ASP:OD1	2.38	0.41
9:I:56:ILE:N	9:I:57:SER:N	2.66	0.41
11:M:30:GLY:HA2	11:M:33:ARG:NH1	2.35	0.41
12:O:8:PHE:HE2	2:R:723:ASN:ND2	2.17	0.41
2:R:81:ARG:HA	2:R:81:ARG:HD3	1.87	0.41
2:R:756:THR:HG23	2:R:871:ASP:O	2.20	0.41
2:R:776:ILE:HG23	2:R:815:GLY:O	2.20	0.41
2:R:808:LYS:HE3	2:R:847:MET:HE2	2.01	0.41
2:R:1053:LEU:HD23	2:R:1054:ASP:OD1	2.20	0.41
4:S:176:CYS:O	4:S:195:LEU:HD11	2.19	0.41
6:U:4:VAL:O	6:U:4:VAL:HG22	2.20	0.41
7:V:101:LEU:O	7:V:102:LEU:C	2.63	0.41
1:W:343:ILE:HG22	1:W:347:LEU:HD12	2.01	0.41
1:W:618:GLU:HG3	1:W:619:TYR:CE2	2.55	0.41
1:W:652:SER:HA	1:W:787:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:748:GLY:HA2	1:W:781:PHE:CE2	2.55	0.41
1:A:737:VAL:HG23	1:A:738:LEU:HD23	2.01	0.41
1:A:823:LEU:HD13	3:C:75:ALA:HB1	2.02	0.41
2:B:22:LYS:O	2:B:22:LYS:HG2	2.20	0.41
2:B:765:GLU:OE2	2:B:863:LYS:HB3	2.19	0.41
2:B:808:LYS:NZ	2:B:847:MET:CE	2.83	0.41
2:B:843:ARG:HB2	2:B:846:GLU:HB2	2.01	0.41
2:B:947:PRO:HB2	2:B:948:PHE:CD2	2.55	0.41
2:B:1053:LEU:CD1	3:C:376:GLY:HA3	2.50	0.41
2:B:1112:ILE:O	2:B:1114:PRO:CD	2.68	0.41
3:C:127:THR:OG1	3:C:129:GLU:O	2.39	0.41
3:C:174:LEU:HB3	3:C:179:VAL:CG1	2.46	0.41
8:H:39:PRO:HG3	10:Q:67:LEU:HD11	2.03	0.41
10:J:60:SER:HB2	8:Z:29:TYR:HE1	1.84	0.41
11:L:15:LEU:HD12	11:L:15:LEU:HA	1.93	0.41
12:N:5:ILE:O	12:N:6:ARG:HB2	2.20	0.41
2:R:230:MET:HE1	2:R:315:ALA:O	2.20	0.41
2:R:1065:ASP:OD2	2:R:1118:LEU:HD13	2.20	0.41
4:S:33:MET:CE	4:S:162:ALA:HB3	2.49	0.41
4:S:70:GLU:HA	4:S:70:GLU:OE1	2.19	0.41
4:S:76:TYR:HD1	4:S:91:LYS:C	2.28	0.41
5:T:113:ILE:HG13	5:T:164:MET:HB2	2.02	0.41
1:W:696:LEU:HD22	1:W:696:LEU:O	2.21	0.41
1:W:801:GLY:C	1:W:803:ARG:H	2.28	0.41
13:X:4:TYR:CD1	13:X:4:TYR:O	2.73	0.41
13:X:6:CYS:HA	13:X:16:GLU:O	2.19	0.41
3:Y:50:LYS:O	3:Y:51:ILE:C	2.59	0.41
3:Y:108:ILE:HA	3:Y:111:VAL:HG12	2.02	0.41
1:A:23:SER:CB	1:A:74:HIS:NE2	2.83	0.41
1:A:45:MET:O	1:A:45:MET:CE	2.68	0.41
1:A:78:VAL:O	1:A:78:VAL:HG13	2.20	0.41
1:A:338:GLY:O	1:A:443:PHE:HA	2.20	0.41
1:A:466:VAL:HG12	1:A:468:GLN:NE2	2.36	0.41
1:A:856:PHE:HE2	1:A:858:MET:HB3	1.81	0.41
2:B:207:ARG:HB2	2:B:216:SER:HB2	1.96	0.41
2:B:598:GLU:HG3	2:B:605:ILE:HD11	2.02	0.41
2:B:807:VAL:HG12	2:B:842:THR:HG21	2.01	0.41
4:D:169:LYS:HD2	4:D:220:SER:OG	2.20	0.41
5:E:36:GLU:CB	6:F:33:LEU:HD22	2.50	0.41
5:E:96:GLY:HA2	5:E:110:ILE:CD1	2.51	0.41
7:G:24:LYS:O	7:G:25:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:62:ILE:O	9:K:66:GLU:HG3	2.20	0.41
2:R:115:GLU:HG2	2:R:384:LEU:HD12	2.01	0.41
2:R:176:LEU:CD2	2:R:343:ASN:OD1	2.68	0.41
2:R:453:TRP:HZ3	2:R:644:GLU:OE2	2.03	0.41
2:R:780:GLU:O	2:R:782:GLY:N	2.53	0.41
2:R:786:TYR:CE1	2:R:792:TYR:CE2	3.08	0.41
2:R:981:LYS:HG2	4:S:166:TYR:CE2	2.56	0.41
2:R:1052:LEU:HD12	2:R:1052:LEU:N	2.36	0.41
1:W:139:THR:HG23	1:W:139:THR:O	2.19	0.41
1:W:338:GLY:HA3	1:W:444:ARG:CG	2.51	0.41
1:W:517:THR:HG22	1:W:518:LYS:N	2.35	0.41
1:W:651:VAL:CG1	1:W:743:MET:HB3	2.44	0.41
1:W:757:ILE:HG22	1:W:765:THR:HG21	2.02	0.41
1:W:870:ARG:HH22	3:Y:36:ILE:HD13	1.82	0.41
1:A:81:VAL:CG2	1:A:269:LEU:HB3	2.49	0.41
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.93	0.41
2:B:252:GLN:O	2:B:253:ASN:C	2.64	0.41
2:B:594:ARG:NH1	2:B:615:LYS:CG	2.83	0.41
2:B:647:SER:HB2	2:B:648:PRO:HD3	2.02	0.41
2:B:1110:MET:C	2:B:1111:ILE:HD12	2.45	0.41
3:C:193:LEU:O	3:C:195:GLU:N	2.53	0.41
3:C:320:MET:HG2	3:C:327:ARG:O	2.21	0.41
4:D:46:PHE:CG	4:D:55:ASP:OD2	2.73	0.41
5:E:37:LYS:O	5:E:44:LEU:HA	2.19	0.41
5:E:78:VAL:HA	5:E:79:PRO:HD3	1.92	0.41
7:G:29:ILE:HD12	7:G:42:ILE:HG13	2.01	0.41
9:I:12:ASP:C	9:I:14:HIS:H	2.27	0.41
9:I:62:ILE:HD13	9:I:62:ILE:HA	1.84	0.41
2:R:423:LEU:HB2	2:R:716:TYR:HD1	1.85	0.41
2:R:485:GLU:OE1	2:R:528:ARG:NH1	2.54	0.41
2:R:767:LYS:HG3	2:R:768:TYR:CD1	2.51	0.41
7:V:103:VAL:HG13	7:V:104:LYS:N	2.34	0.41
1:W:605:ASN:O	1:W:606:GLN:C	2.64	0.41
1:W:696:LEU:C	1:W:696:LEU:HD13	2.45	0.41
1:W:863:GLY:HA2	3:Y:311:ARG:HH22	1.85	0.41
1:W:879:LYS:NZ	3:Y:46:ASP:HB3	2.35	0.41
1:A:224:MET:C	1:A:224:MET:SD	3.03	0.41
1:A:428:ILE:C	1:A:430:MET:H	2.27	0.41
1:A:499:ALA:HB3	2:B:737:MET:CE	2.50	0.41
1:A:509:LEU:HD23	1:A:552:VAL:CG2	2.49	0.41
2:B:115:GLU:HG2	2:B:384:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:VAL:HG13	2:B:163:VAL:O	2.20	0.41
2:B:590:PRO:O	2:B:615:LYS:HD2	2.20	0.41
2:B:630:ALA:HB3	2:B:636:LEU:HD13	2.02	0.41
2:B:675:MET:HG2	2:B:882:ALA:CB	2.51	0.41
2:B:732:PHE:O	2:B:733:THR:CG2	2.69	0.41
2:B:1007:ARG:CZ	2:B:1028:GLY:H	2.33	0.41
3:C:327:ARG:HG3	3:C:334:VAL:HG22	2.02	0.41
4:D:8:LYS:HG3	4:D:13:ILE:HG12	2.03	0.41
4:D:49:ASN:OD1	4:D:139:ILE:HD11	2.20	0.41
4:D:160:SER:HB3	4:D:233:VAL:HG12	2.02	0.41
4:D:176:CYS:O	4:D:195:LEU:HD11	2.20	0.41
7:G:115:ILE:HD12	7:G:115:ILE:N	2.34	0.41
2:R:456:MET:HG2	2:R:471:LYS:HD2	2.01	0.41
2:R:727:LEU:HD22	2:R:991:VAL:HG21	2.03	0.41
2:R:783:VAL:HG11	2:R:834:ALA:N	2.36	0.41
2:R:792:TYR:CE1	2:R:812:VAL:HG21	2.55	0.41
2:R:1004:ILE:CD1	1:W:441:LEU:HD22	2.50	0.41
4:S:13:ILE:HG21	4:S:242:LEU:HD11	2.02	0.41
4:S:94:THR:HG23	4:S:94:THR:O	2.20	0.41
4:S:176:CYS:HB3	4:S:195:LEU:HD11	2.02	0.41
1:W:13:ILE:HG12	3:Y:358:ALA:HB1	2.02	0.41
1:W:219:ILE:O	1:W:219:ILE:HG22	2.19	0.41
1:W:569:SER:HA	1:W:573:ARG:O	2.21	0.41
3:Y:62:GLY:O	3:Y:63:LEU:HG	2.20	0.41
1:A:675:LEU:O	1:A:675:LEU:HD23	2.20	0.41
1:A:761:TYR:CE1	2:B:451:THR:HG22	2.56	0.41
2:B:71:PRO:HA	2:B:97:ALA:HB2	2.02	0.41
2:B:73:VAL:O	2:B:73:VAL:HG13	2.20	0.41
2:B:792:TYR:CE1	2:B:812:VAL:HG21	2.55	0.41
2:B:1096:VAL:CG1	2:B:1097:SER:N	2.84	0.41
3:C:347:PHE:O	3:C:348:GLU:HB3	2.20	0.41
4:D:13:ILE:HG21	4:D:242:LEU:HD11	2.03	0.41
9:I:71:ARG:HB3	9:I:73:VAL:HG22	2.02	0.41
2:R:17:ILE:HG12	2:R:21:PHE:CE2	2.56	0.41
2:R:872:LEU:HD23	2:R:873:ARG:H	1.84	0.41
2:R:918:LEU:HD12	1:W:646:MET:HG2	2.02	0.41
4:S:107:LYS:O	4:S:133:LEU:HB2	2.20	0.41
5:T:6:LYS:H	6:U:8:GLU:HB2	1.86	0.41
5:T:98:PHE:HA	5:T:106:GLY:O	2.20	0.41
7:V:87:ASN:O	7:V:88:ASN:C	2.64	0.41
1:W:60:THR:HG21	1:W:71:HIS:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:831:ARG:HA	3:Y:68:GLU:O	2.20	0.41
1:W:876:VAL:C	1:W:878:TRP:H	2.28	0.41
1:A:122:LYS:O	1:A:126:PRO:HG3	2.20	0.41
1:A:323:ARG:HB2	2:B:1029:LEU:HD21	2.02	0.41
1:A:370:ASP:OD1	1:A:389:ARG:NH1	2.51	0.41
1:A:855:VAL:HG13	3:C:63:LEU:O	2.20	0.41
2:B:653:ILE:H	2:B:653:ILE:CD1	2.28	0.41
2:B:682:LEU:HD22	12:N:55:ILE:HD12	2.02	0.41
2:B:734:GLY:HA3	2:B:735:TYR:CB	2.50	0.41
2:B:1049:LYS:C	2:B:1051:ARG:H	2.28	0.41
2:B:1059:THR:HB	2:B:1061:ILE:HD12	2.03	0.41
3:C:120:PRO:HB2	3:C:256:SER:CB	2.51	0.41
4:D:17:PHE:CD2	4:D:25:VAL:HG22	2.54	0.41
4:D:65:ILE:HG23	4:D:128:ILE:CD1	2.51	0.41
4:D:94:THR:O	4:D:94:THR:HG23	2.21	0.41
5:E:36:GLU:O	5:E:37:LYS:HG3	2.20	0.41
5:E:119:LYS:O	5:E:131:LYS:HA	2.20	0.41
6:F:8:GLU:OE1	6:F:10:HIS:ND1	2.54	0.41
9:I:59:THR:HB	9:I:63:SER:OG	2.21	0.41
11:M:19:GLY:C	11:M:20:GLU:HG2	2.45	0.41
13:P:39:LYS:C	13:P:41:THR:H	2.28	0.41
5:T:50:ASN:HB2	5:T:73:ASP:HB2	2.03	0.41
5:T:124:ARG:O	5:T:126:ILE:N	2.54	0.41
1:W:45:MET:HE2	1:W:46:ASP:OD1	2.20	0.41
1:W:46:ASP:H	1:W:47:PRO:CD	2.34	0.41
1:W:412:THR:O	1:W:413:ASP:C	2.63	0.41
1:A:555:PHE:CD2	1:A:631:LEU:HD13	2.56	0.41
2:B:20:TYR:CD1	2:B:20:TYR:C	2.98	0.41
2:B:161:GLU:OE1	2:B:419:ARG:NH1	2.54	0.41
3:C:25:PRO:HG3	3:C:33:LYS:HD3	2.02	0.41
4:D:11:LYS:O	4:D:231:GLU:HA	2.20	0.41
6:F:21:LEU:O	6:F:24:VAL:HG12	2.20	0.41
7:G:13:CYS:O	7:G:55:VAL:HG12	2.20	0.41
7:G:46:ILE:HD12	7:G:46:ILE:HA	1.92	0.41
10:J:59:ILE:C	10:J:61:VAL:N	2.79	0.41
9:K:62:ILE:HA	9:K:62:ILE:HD13	1.78	0.41
13:P:21:LEU:HD22	13:P:22:PRO:HA	2.02	0.41
2:R:236:LEU:HD21	2:R:268:VAL:CG2	2.50	0.41
2:R:807:VAL:HG12	2:R:842:THR:HG21	2.03	0.41
2:R:843:ARG:HB2	2:R:846:GLU:HB2	2.03	0.41
2:R:1006:ALA:C	2:R:1007:ARG:HG3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:82:GLN:H	5:T:146:VAL:HG13	1.85	0.41
5:T:86:GLU:O	6:U:44:VAL:HG23	2.21	0.41
7:V:13:CYS:O	7:V:55:VAL:HG12	2.21	0.41
1:W:45:MET:O	1:W:45:MET:CE	2.68	0.41
1:W:833:GLU:HG3	1:W:839:ARG:HD2	2.02	0.41
1:W:856:PHE:HE2	1:W:858:MET:HB3	1.83	0.41
3:Y:102:LEU:HD21	3:Y:119:THR:OG1	2.19	0.41
3:Y:340:SER:HA	3:Y:364:GLU:HG3	2.02	0.41
1:A:47:PRO:O	1:A:48:ARG:HB2	2.20	0.41
1:A:141:MET:HA	1:A:148:HIS:HB2	2.02	0.41
1:A:271:TYR:CD1	1:A:271:TYR:C	2.98	0.41
1:A:542:PRO:HD3	7:G:70:ASP:O	2.21	0.41
1:A:696:LEU:O	1:A:696:LEU:HD22	2.20	0.41
1:A:830:LEU:HD13	3:C:315:LEU:HD21	2.03	0.41
1:A:852:ASP:CG	8:H:75:VAL:HG21	2.45	0.41
2:B:9:SER:HB3	2:B:12:GLU:OE1	2.21	0.41
2:B:136:TYR:HB2	2:B:141:LEU:CD1	2.51	0.41
2:B:212:THR:O	2:B:213:PHE:CB	2.67	0.41
2:B:675:MET:HG3	2:B:996:LEU:HD21	2.02	0.41
2:B:773:GLU:CG	2:B:774:ASP:N	2.82	0.41
2:B:780:GLU:C	2:B:782:GLY:H	2.29	0.41
2:B:966:LEU:CD2	4:D:208:GLU:HG3	2.51	0.41
2:B:966:LEU:CD2	4:D:184:PRO:HG3	2.51	0.41
2:B:1065:ASP:OD2	2:B:1118:LEU:HD13	2.20	0.41
3:C:122:MET:HB2	3:C:253:THR:OG1	2.21	0.41
3:C:127:THR:O	3:C:131:LYS:HD2	2.21	0.41
3:C:234:ILE:HG22	3:C:235:LYS:N	2.35	0.41
3:C:284:PHE:HB3	3:C:288:ALA:CB	2.51	0.41
4:D:39:MET:HE2	4:D:39:MET:HB2	1.97	0.41
4:D:129:PRO:HG2	12:N:3:ILE:HD11	2.01	0.41
4:D:164:VAL:HA	4:D:227:ILE:O	2.21	0.41
5:E:84:VAL:CG2	6:F:75:ILE:CD1	2.99	0.41
5:E:108:VAL:HB	5:E:162:LEU:HB2	2.03	0.41
5:E:141:LYS:HE3	6:F:46:LYS:NZ	2.35	0.41
6:F:62:ILE:HG22	6:F:63:ILE:N	2.36	0.41
7:G:9:ILE:HB	7:G:59:ILE:O	2.21	0.41
7:G:40:PHE:HA	7:G:92:TYR:CD1	2.56	0.41
7:G:87:ASN:O	7:G:88:ASN:C	2.64	0.41
7:G:101:LEU:O	7:G:102:LEU:C	2.62	0.41
11:L:86:GLU:O	11:L:90:LEU:HB2	2.21	0.41
11:M:82:HIS:NE2	11:M:86:GLU:OE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:66:ARG:C	10:Q:68:PHE:N	2.79	0.41
2:R:66:ILE:CG2	2:R:67:ARG:N	2.83	0.41
2:R:732:PHE:CG	2:R:733:THR:N	2.89	0.41
2:R:902:TYR:CZ	2:R:974:TYR:HB2	2.56	0.41
2:R:1007:ARG:CZ	2:R:1028:GLY:H	2.33	0.41
5:T:82:GLN:OE1	6:U:88:ILE:HB	2.21	0.41
5:T:164:MET:O	5:T:167:PRO:HD3	2.20	0.41
7:V:31:MET:HE1	7:V:55:VAL:HG11	2.03	0.41
1:W:146:CYS:HA	1:W:147:PRO:HD3	1.92	0.41
1:W:271:TYR:CZ	1:W:285:PRO:HB3	2.56	0.41
1:W:326:ILE:HG21	1:W:462:MET:CG	2.50	0.41
1:W:466:VAL:HG12	1:W:468:GLN:NE2	2.35	0.41
1:W:548:GLY:O	1:W:551:VAL:HG13	2.21	0.41
1:A:275:THR:HG23	1:A:279:ASN:OD1	2.21	0.41
1:A:532:ILE:HG13	1:A:533:ASP:N	2.35	0.41
1:A:662:TYR:HA	1:A:665:ILE:HG12	2.03	0.41
2:B:356:LEU:O	2:B:359:VAL:HG12	2.21	0.41
2:B:476:MET:CE	2:B:645:ILE:HD12	2.50	0.41
2:B:619:LEU:HD22	2:B:623:GLU:HG2	2.02	0.41
3:C:103:GLY:O	3:C:106:ARG:HB3	2.21	0.41
4:D:37:PRO:CG	4:D:78:TRP:CZ3	3.04	0.41
5:E:30:LEU:HD22	5:E:72:PHE:CD2	2.56	0.41
5:E:123:VAL:HG13	5:E:127:ILE:CG1	2.49	0.41
2:R:76:SER:HA	2:R:77:ASP:HA	1.83	0.41
2:R:332:ARG:HD2	2:R:565:PHE:CD1	2.56	0.41
2:R:808:LYS:NZ	2:R:847:MET:CE	2.84	0.41
2:R:949:TYR:O	2:R:950:LYS:HD2	2.21	0.41
7:V:96:ILE:HD13	7:V:101:LEU:HD22	2.01	0.41
1:W:106:ILE:O	1:W:107:SER:C	2.63	0.41
1:W:402:ALA:HB1	1:W:403:PRO:HD2	2.03	0.41
1:W:675:LEU:HD23	1:W:675:LEU:O	2.20	0.41
3:Y:104:LEU:HD13	3:Y:108:ILE:CD1	2.51	0.41
3:Y:149:ILE:O	3:Y:153:VAL:HG12	2.21	0.41
3:Y:216:ILE:O	3:Y:217:ALA:HB3	2.21	0.41
1:A:450:CYS:C	1:A:452:PRO:HD2	2.46	0.40
2:B:372:LEU:HD22	2:B:376:LYS:HG3	2.04	0.40
2:B:597:ILE:CD1	2:B:605:ILE:HA	2.51	0.40
2:B:1040:ILE:HD11	3:C:373:ILE:CD1	2.51	0.40
3:C:145:GLU:HG3	3:C:240:ALA:HB3	2.02	0.40
3:C:265:LYS:H	3:C:265:LYS:HD2	1.84	0.40
3:C:383:THR:HA	9:K:30:TYR:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:388:LEU:HD11	9:K:35:VAL:CG1	2.51	0.40
4:D:24:PHE:HA	11:L:27:LEU:CD1	2.50	0.40
4:D:224:ASP:HA	4:D:226:TYR:CZ	2.55	0.40
5:E:98:PHE:HA	5:E:106:GLY:O	2.21	0.40
7:G:114:LYS:O	7:G:115:ILE:HD12	2.20	0.40
13:P:5:ARG:HG3	13:P:6:CYS:N	2.34	0.40
10:Q:52:ASP:O	10:Q:55:LEU:HB2	2.21	0.40
2:R:112:ALA:O	2:R:113:GLU:HG3	2.20	0.40
2:R:224:ILE:HG23	2:R:225:PRO:HD2	2.03	0.40
2:R:734:GLY:H	2:R:735:TYR:HD2	1.69	0.40
2:R:855:ILE:O	13:X:34:ILE:HG23	2.21	0.40
2:R:914:ASN:OD1	2:R:916:HIS:HB2	2.21	0.40
2:R:947:PRO:HB2	2:R:948:PHE:CE2	2.56	0.40
4:S:45:TYR:CE2	13:X:44:ILE:HG23	2.55	0.40
4:S:83:ILE:CD1	4:S:84:ASP:H	2.34	0.40
4:S:109:LEU:C	4:S:109:LEU:HD23	2.46	0.40
5:T:1:MET:HE3	5:T:83:GLU:CB	2.50	0.40
6:U:51:SER:HA	6:U:54:LYS:HD2	2.02	0.40
7:V:14:GLU:OE2	7:V:54:LYS:HE2	2.20	0.40
1:W:47:PRO:O	1:W:48:ARG:HB2	2.21	0.40
1:W:279:ASN:HB3	1:W:300:GLN:OE1	2.22	0.40
1:W:418:LEU:CD2	1:W:430:MET:HE2	2.47	0.40
1:W:503:ILE:HG21	1:W:731:THR:O	2.21	0.40
1:W:572:PRO:HD2	1:W:730:ARG:HH12	1.86	0.40
1:W:575:CYS:O	1:W:576:LYS:HB2	2.22	0.40
1:W:666:ASP:HA	1:W:669:LYS:HD2	2.03	0.40
3:Y:237:ILE:HA	3:Y:255:GLY:HA3	2.03	0.40
3:Y:369:VAL:HG12	3:Y:379:ILE:HG22	2.04	0.40
1:A:98:CYS:O	1:A:99:ARG:HB2	2.21	0.40
1:A:648:LEU:HD21	1:A:787:ARG:HH11	1.82	0.40
1:A:668:ALA:HB2	1:A:707:LEU:HD13	2.00	0.40
1:A:806:LEU:HB3	2:B:467:SER:OG	2.22	0.40
1:A:855:VAL:HB	3:C:311:ARG:HH12	1.86	0.40
2:B:41:LYS:O	2:B:43:GLN:N	2.53	0.40
2:B:46:ILE:CG2	2:B:66:ILE:HD11	2.50	0.40
2:B:209:LYS:O	2:B:210:ASP:HB3	2.20	0.40
2:B:333:ARG:HB3	2:B:333:ARG:HH11	1.86	0.40
2:B:647:SER:O	2:B:650:ILE:HG12	2.21	0.40
2:B:876:SER:O	2:B:877:ILE:C	2.65	0.40
2:B:902:TYR:HD1	2:B:903:THR:O	2.05	0.40
2:B:974:TYR:CZ	4:D:165:ARG:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:995:LYS:HE2	2:B:999:MET:HE3	2.03	0.40
2:B:1057:ASP:O	2:B:1097:SER:HA	2.21	0.40
3:C:232:LYS:HE2	3:C:232:LYS:HB3	1.79	0.40
3:C:392:PRO:HB3	5:E:18:PHE:CD1	2.57	0.40
4:D:109:LEU:C	4:D:109:LEU:CD2	2.94	0.40
4:D:253:ILE:HG13	11:L:73:ILE:CG2	2.49	0.40
2:R:372:LEU:O	2:R:373:GLU:C	2.64	0.40
2:R:525:LEU:CD2	2:R:571:VAL:HB	2.52	0.40
2:R:767:LYS:CG	2:R:768:TYR:CD1	3.04	0.40
2:R:796:GLU:OE2	13:X:39:LYS:HE2	2.21	0.40
5:T:123:VAL:O	5:T:123:VAL:CG1	2.69	0.40
6:U:71:VAL:HG13	6:U:72:LEU:HD12	2.03	0.40
6:U:80:PRO:O	6:U:83:VAL:HG12	2.21	0.40
7:V:9:ILE:HB	7:V:59:ILE:O	2.21	0.40
1:W:11:PHE:HB2	3:Y:362:ASP:O	2.21	0.40
1:W:94:LEU:C	1:W:96:ALA:H	2.29	0.40
1:W:458:ASP:OD1	1:W:458:ASP:C	2.64	0.40
13:X:33:ILE:N	13:X:33:ILE:CD1	2.83	0.40
3:Y:63:LEU:HD23	3:Y:63:LEU:HA	1.96	0.40
3:Y:284:PHE:HB3	3:Y:288:ALA:CB	2.52	0.40
1:A:102:GLY:O	1:A:103:ARG:C	2.64	0.40
1:A:192:VAL:HG21	1:A:199:PRO:HB3	2.03	0.40
1:A:879:LYS:NZ	3:C:44:THR:HG22	2.36	0.40
2:B:25:GLY:O	2:B:27:VAL:N	2.54	0.40
2:B:535:ASP:OD2	2:B:538:GLU:OE2	2.39	0.40
2:B:800:VAL:HG22	2:B:814:ILE:HG23	2.03	0.40
2:B:977:ARG:HB2	11:L:22:HIS:ND1	2.35	0.40
3:C:70:ILE:N	3:C:70:ILE:CD1	2.84	0.40
4:D:95:LYS:HD3	4:D:142:GLU:OE2	2.22	0.40
6:F:71:VAL:HG13	6:F:72:LEU:HD12	2.04	0.40
8:H:65:ILE:HD12	8:H:78:TYR:HA	2.03	0.40
2:R:9:SER:HB3	2:R:12:GLU:OE1	2.21	0.40
2:R:63:LEU:HD21	2:R:103:MET:HE2	2.04	0.40
2:R:399:HIS:O	2:R:403:THR:CG2	2.69	0.40
2:R:631:LEU:O	2:R:632:GLU:OE1	2.37	0.40
2:R:759:ARG:CG	2:R:760:LEU:N	2.83	0.40
2:R:784:ARG:HD3	2:R:785:GLY:H	1.85	0.40
4:S:101:GLU:HB2	4:S:137:GLN:O	2.21	0.40
4:S:115:LYS:O	4:S:116:SER:HB2	2.21	0.40
4:S:203:CYS:SG	4:S:204:THR:N	2.94	0.40
5:T:108:VAL:HB	5:T:162:LEU:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:371:LYS:O	1:W:372:TRP:C	2.64	0.40
1:W:388:LEU:HA	1:W:391:VAL:HG22	2.04	0.40
1:W:532:ILE:HG13	1:W:533:ASP:O	2.22	0.40
1:W:591:GLY:O	1:W:592:ILE:HD13	2.21	0.40
13:X:39:LYS:C	13:X:41:THR:H	2.28	0.40
3:Y:262:LEU:CD2	3:Y:269:ILE:HD12	2.51	0.40
3:Y:286:ILE:HG23	3:Y:324:GLY:O	2.21	0.40
3:Y:322:ARG:O	3:Y:323:THR:CB	2.69	0.40
1:A:141:MET:HA	1:A:148:HIS:CG	2.55	0.40
1:A:431:MET:HE2	1:A:482:VAL:HA	2.03	0.40
1:A:524:ILE:CG2	1:A:634:VAL:HG13	2.52	0.40
1:A:552:VAL:CG1	1:A:598:PHE:CE2	3.04	0.40
1:A:598:PHE:CE1	1:A:611:ILE:CD1	3.05	0.40
1:A:664:GLU:OE2	1:A:707:LEU:HD22	2.22	0.40
1:A:752:VAL:O	1:A:753:ARG:C	2.63	0.40
2:B:453:TRP:CH2	2:B:644:GLU:CD	3.00	0.40
2:B:597:ILE:HB	2:B:603:GLY:HA3	2.03	0.40
2:B:895:ILE:HA	2:B:896:PRO:HD3	1.86	0.40
2:B:1074:ASP:CB	2:B:1075:LYS:CA	2.98	0.40
5:E:167:PRO:HA	5:E:169:LEU:HD13	2.02	0.40
7:G:96:ILE:HD13	7:G:101:LEU:HD21	2.03	0.40
9:I:27:LEU:N	9:I:27:LEU:HD12	2.37	0.40
2:R:176:LEU:HD21	2:R:343:ASN:OD1	2.21	0.40
2:R:699:HIS:CE1	4:S:57:ILE:CD1	3.04	0.40
2:R:942:ILE:O	2:R:943:VAL:HB	2.21	0.40
2:R:947:PRO:O	2:R:948:PHE:CD2	2.75	0.40
7:V:11:LEU:HD23	7:V:33:CYS:SG	2.62	0.40
7:V:70:ASP:O	1:W:541:ALA:CB	2.69	0.40
1:W:184:LEU:HD22	1:W:204:PRO:HB2	2.03	0.40
1:W:283:GLY:O	1:W:284:LEU:C	2.64	0.40
1:W:524:ILE:CG2	1:W:634:VAL:HG13	2.51	0.40
1:W:552:VAL:CG1	1:W:598:PHE:CE2	3.05	0.40
1:W:563:HIS:CD2	1:W:872:PHE:HE2	2.39	0.40
3:Y:81:PRO:HA	3:Y:84:GLN:OE1	2.21	0.40
1:A:503:ILE:HG21	1:A:731:THR:O	2.21	0.40
1:A:648:LEU:HB2	2:B:927:ILE:CG2	2.52	0.40
2:B:212:THR:C	2:B:259:LEU:HD11	2.47	0.40
2:B:256:PHE:C	2:B:258:SER:N	2.78	0.40
2:B:367:ASP:O	2:B:371:GLN:N	2.55	0.40
2:B:492:LEU:HD13	2:B:523:VAL:HG11	2.03	0.40
2:B:690:ARG:HB3	2:B:692:ASP:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1042:PHE:C	2:B:1044:THR:N	2.80	0.40
3:C:163:MET:C	3:C:207:ASN:O	2.64	0.40
5:E:167:PRO:CA	5:E:169:LEU:H	2.34	0.40
12:N:3:ILE:HG12	12:N:18:TRP:HB2	2.03	0.40
12:O:35:LEU:HD13	12:O:46:ARG:HD3	2.03	0.40
2:R:170:LEU:HD21	2:R:176:LEU:HD12	2.00	0.40
2:R:341:TYR:OH	2:R:456:MET:HE2	2.21	0.40
2:R:873:ARG:NH2	2:R:1002:ASP:OD2	2.54	0.40
2:R:1074:ASP:CB	2:R:1075:LYS:CA	2.96	0.40
2:R:1103:LEU:O	2:R:1107:LEU:HG	2.21	0.40
5:T:70:VAL:HG13	5:T:72:PHE:CE2	2.57	0.40
5:T:101:LEU:N	5:T:101:LEU:CD1	2.85	0.40
7:V:72:CYS:HA	7:V:114:LYS:HA	2.02	0.40
1:W:10:LYS:HG2	3:Y:363:VAL:HG13	2.03	0.40
1:W:91:TYR:CE1	1:W:95:LYS:HD2	2.56	0.40
1:W:95:LYS:O	1:W:96:ALA:HB2	2.22	0.40
1:W:187:VAL:HG23	1:W:187:VAL:O	2.21	0.40
1:W:366:ILE:HD13	1:W:366:ILE:O	2.22	0.40
1:W:456:ASP:CG	1:W:458:ASP:OD2	2.65	0.40
1:W:563:HIS:CD2	1:W:872:PHE:CE2	3.10	0.40
1:W:696:LEU:HD13	1:W:700:ILE:HD12	2.04	0.40
3:Y:70:ILE:N	3:Y:70:ILE:CD1	2.84	0.40
3:Y:170:ASP:O	3:Y:174:LEU:CD1	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	823/880 (94%)	669 (81%)	120 (15%)	34 (4%)	2	20
1	W	823/880 (94%)	672 (82%)	111 (14%)	40 (5%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1077/1131 (95%)	887 (82%)	118 (11%)	72 (7%)	1	13
2	R	1077/1131 (95%)	881 (82%)	122 (11%)	74 (7%)	1	12
3	C	364/395 (92%)	278 (76%)	63 (17%)	23 (6%)	1	14
3	Y	364/395 (92%)	282 (78%)	54 (15%)	28 (8%)	1	11
4	D	258/265 (97%)	219 (85%)	31 (12%)	8 (3%)	3	25
4	S	258/265 (97%)	220 (85%)	30 (12%)	8 (3%)	3	25
5	E	160/180 (89%)	127 (79%)	21 (13%)	12 (8%)	1	11
5	T	160/180 (89%)	125 (78%)	24 (15%)	11 (7%)	1	12
6	F	88/113 (78%)	75 (85%)	11 (12%)	2 (2%)	5	30
6	U	88/113 (78%)	77 (88%)	9 (10%)	2 (2%)	5	30
7	G	108/132 (82%)	89 (82%)	15 (14%)	4 (4%)	2	21
7	V	108/132 (82%)	88 (82%)	16 (15%)	4 (4%)	2	21
8	H	72/84 (86%)	59 (82%)	9 (12%)	4 (6%)	1	15
8	Z	72/84 (86%)	59 (82%)	7 (10%)	6 (8%)	0	9
9	I	80/95 (84%)	64 (80%)	9 (11%)	7 (9%)	0	9
9	K	80/95 (84%)	64 (80%)	9 (11%)	7 (9%)	0	9
10	J	37/104 (36%)	27 (73%)	8 (22%)	2 (5%)	1	16
10	Q	37/104 (36%)	27 (73%)	8 (22%)	2 (5%)	1	16
11	L	89/92 (97%)	78 (88%)	9 (10%)	2 (2%)	5	30
11	M	89/92 (97%)	79 (89%)	8 (9%)	2 (2%)	5	30
12	N	62/66 (94%)	50 (81%)	10 (16%)	2 (3%)	3	24
12	O	62/66 (94%)	50 (81%)	9 (14%)	3 (5%)	2	17
13	P	43/48 (90%)	33 (77%)	7 (16%)	3 (7%)	1	12
13	X	43/48 (90%)	33 (77%)	7 (16%)	3 (7%)	1	12
All	All	6522/7170 (91%)	5312 (81%)	845 (13%)	365 (6%)	1	15

All (365) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	103	ARG
1	A	108	GLU
1	A	683	GLU
1	A	737	VAL

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Mol	Chain	Res	Type
2	B	28	ARG
2	B	108	ASN
2	B	213	PHE
2	B	331	GLY
2	B	405	ASN
2	B	460	GLU
2	B	521	SER
2	B	590	PRO
2	B	591	LEU
2	B	600	LEU
2	B	602	SER
2	B	605	ILE
2	B	735	TYR
2	B	766	VAL
2	B	768	TYR
2	B	770	GLY
2	B	835	LYS
2	B	950	LYS
2	B	1061	ILE
2	B	1070	ILE
3	C	162	SER
3	C	177	LYS
3	C	192	LYS
3	C	193	LEU
3	C	217	ALA
3	C	236	GLY
3	C	324	GLY
4	D	90	GLU
5	E	114	THR
5	E	116	ASP
5	E	124	ARG
5	E	126	ILE
5	E	133	LYS
5	E	167	PRO
7	G	17	SER
7	G	105	ILE
8	H	13	ILE
9	I	51	ILE
9	I	52	ASP
9	I	53	ILE
9	I	56	ILE
10	J	56	ASN

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Mol	Chain	Res	Type
9	K	51	ILE
9	K	52	ASP
9	K	53	ILE
9	K	56	ILE
13	P	6	CYS
10	Q	56	ASN
2	R	108	ASN
2	R	213	PHE
2	R	405	ASN
2	R	460	GLU
2	R	521	SER
2	R	533	TYR
2	R	590	PRO
2	R	591	LEU
2	R	600	LEU
2	R	602	SER
2	R	605	ILE
2	R	735	TYR
2	R	766	VAL
2	R	768	TYR
2	R	835	LYS
2	R	950	LYS
2	R	1026	GLU
2	R	1061	ILE
2	R	1070	ILE
4	S	90	GLU
5	T	114	THR
5	T	116	ASP
5	T	124	ARG
5	T	126	ILE
5	T	133	LYS
5	T	167	PRO
7	V	17	SER
7	V	105	ILE
1	W	23	SER
1	W	103	ARG
1	W	108	GLU
1	W	683	GLU
1	W	737	VAL
13	X	6	CYS
3	Y	177	LYS
3	Y	192	LYS

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Mol	Chain	Res	Type
3	Y	193	LEU
3	Y	217	ALA
3	Y	324	GLY
8	Z	13	ILE
1	A	96	ALA
1	A	280	GLU
1	A	310	ARG
1	A	332	ILE
1	A	391	VAL
1	A	734	ARG
1	A	812	ARG
1	A	876	VAL
2	B	24	LYS
2	B	46	ILE
2	B	418	ASP
2	B	533	TYR
2	B	598	GLU
2	B	599	LYS
2	B	771	GLY
2	B	772	GLN
2	B	797	ASP
2	B	809	GLY
2	B	877	ILE
2	B	1026	GLU
2	B	1072	TRP
3	C	12	TYR
3	C	194	GLY
3	C	245	LYS
3	C	365	GLU
4	D	206	CYS
5	E	125	GLY
5	E	137	GLN
7	G	103	VAL
9	I	14	HIS
9	I	61	VAL
9	K	61	VAL
13	P	5	ARG
2	R	24	LYS
2	R	49	GLN
2	R	331	GLY
2	R	418	ASP
2	R	598	GLU

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Mol	Chain	Res	Type
2	R	599	LYS
2	R	770	GLY
2	R	771	GLY
2	R	797	ASP
2	R	809	GLY
2	R	877	ILE
2	R	943	VAL
2	R	1029	LEU
2	R	1072	TRP
4	S	117	GLU
5	T	137	GLN
7	V	99	PHE
7	V	103	VAL
1	W	96	ALA
1	W	256	GLY
1	W	308	ARG
1	W	310	ARG
1	W	332	ILE
1	W	391	VAL
1	W	605	ASN
1	W	734	ARG
1	W	812	ARG
1	W	876	VAL
13	X	13	PHE
3	Y	12	TYR
3	Y	82	GLY
3	Y	162	SER
3	Y	194	GLY
3	Y	245	LYS
3	Y	349	VAL
1	A	109	ASP
1	A	148	HIS
1	A	290	ARG
1	A	532	ILE
1	A	536	GLU
1	A	849	ALA
2	B	49	GLN
2	B	116	GLU
2	B	250	GLU
2	B	256	PHE
2	B	375	SER
2	B	407	VAL

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Mol	Chain	Res	Type
2	B	417	LEU
2	B	606	THR
2	B	734	GLY
2	B	918	LEU
2	B	943	VAL
2	B	982	ILE
2	B	985	ARG
2	B	1029	LEU
3	C	53	ASP
3	C	113	ALA
3	C	114	LYS
3	C	171	ASN
3	C	211	ALA
4	D	83	ILE
4	D	85	CYS
4	D	117	GLU
5	E	40	LYS
7	G	99	PHE
10	J	57	GLY
9	K	14	HIS
9	K	91	SER
11	L	19	GLY
11	M	19	GLY
13	P	13	PHE
10	Q	57	GLY
2	R	26	LEU
2	R	28	ARG
2	R	250	GLU
2	R	256	PHE
2	R	375	SER
2	R	406	TRP
2	R	417	LEU
2	R	453	TRP
2	R	772	GLN
2	R	918	LEU
2	R	985	ARG
4	S	83	ILE
4	S	85	CYS
4	S	206	CYS
5	T	40	LYS
5	T	82	GLN
1	W	107	SER

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Mol	Chain	Res	Type
1	W	109	ASP
1	W	148	HIS
1	W	280	GLU
1	W	290	ARG
1	W	393	ASP
1	W	541	ALA
1	W	682	GLY
1	W	849	ALA
13	X	5	ARG
3	Y	53	ASP
3	Y	114	LYS
3	Y	127	THR
3	Y	170	ASP
3	Y	201	SER
3	Y	365	GLU
8	Z	15	TYR
1	A	79	ARG
1	A	256	GLY
1	A	308	ARG
1	A	393	ASP
1	A	541	ALA
1	A	601	LYS
2	B	26	LEU
2	B	437	ALA
2	B	453	TRP
2	B	738	GLU
2	B	781	PRO
2	B	949	TYR
2	B	951	THR
3	C	161	ALA
3	C	170	ASP
3	C	201	SER
3	C	216	ILE
3	C	234	ILE
4	D	193	GLY
5	E	82	GLN
8	H	15	TYR
8	H	81	VAL
9	I	91	SER
12	N	41	LYS
12	O	41	LYS
2	R	116	GLU

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Mol	Chain	Res	Type
2	R	210	ASP
2	R	437	ALA
2	R	535	ASP
2	R	606	THR
2	R	734	GLY
2	R	738	GLU
2	R	839	SER
2	R	949	TYR
2	R	951	THR
2	R	982	ILE
2	R	1053	LEU
2	R	1073	TYR
5	T	125	GLY
1	W	46	ASP
1	W	79	ARG
1	W	287	SER
1	W	413	ASP
1	W	536	GLU
3	Y	113	ALA
3	Y	171	ASN
3	Y	216	ILE
3	Y	234	ILE
8	Z	81	VAL
1	A	46	ASP
1	A	47	PRO
1	A	287	SER
1	A	682	GLY
2	B	71	PRO
2	B	74	ARG
2	B	183	GLY
2	B	210	ASP
2	B	334	GLU
2	B	535	ASP
2	B	706	VAL
2	B	839	SER
2	B	907	VAL
2	B	1044	THR
3	C	44	THR
3	C	349	VAL
4	D	9	ASP
4	D	79	PRO
5	E	120	TYR

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Mol	Chain	Res	Type
11	L	10	SER
11	M	10	SER
12	N	6	ARG
12	O	6	ARG
2	R	78	ARG
2	R	334	GLU
2	R	706	VAL
2	R	1051	ARG
2	R	1079	LYS
4	S	9	ASP
4	S	193	GLY
1	W	62	GLY
1	W	305	LYS
1	W	429	SER
1	W	656	ASP
3	Y	30	GLU
3	Y	161	ALA
3	Y	196	PHE
3	Y	306	LEU
8	Z	10	ASP
8	Z	56	ASN
1	A	62	GLY
1	A	656	ASP
2	B	56	ILE
2	B	438	ARG
2	B	1079	LYS
5	E	166	GLN
8	H	10	ASP
12	O	63	THR
2	R	56	ILE
2	R	183	GLY
2	R	407	VAL
2	R	781	PRO
2	R	783	VAL
2	R	907	VAL
5	T	166	GLN
6	U	4	VAL
3	Y	132	HIS
3	Y	146	TYR
3	Y	210	PHE
1	A	145	VAL
2	R	46	ILE

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Mol	Chain	Res	Type
2	R	1114	PRO
4	S	79	PRO
1	W	282	PRO
1	W	689	GLY
1	A	689	GLY
2	B	769	PRO
1	W	47	PRO
1	W	145	VAL
1	W	532	ILE
1	W	654	GLY
1	A	29	THR
2	B	588	GLY
2	B	901	PRO
2	B	1114	PRO
6	F	25	ILE
2	R	71	PRO
2	R	588	GLY
2	B	783	VAL
6	F	4	VAL
2	R	769	PRO
2	R	901	PRO
6	U	63	ILE
8	Z	11	PRO
1	W	449	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	723/766 (94%)	676 (94%)	47 (6%)	15	42
1	W	723/766 (94%)	672 (93%)	51 (7%)	13	39
2	B	937/975 (96%)	867 (92%)	70 (8%)	12	38
2	R	937/975 (96%)	866 (92%)	71 (8%)	12	37
3	C	316/341 (93%)	291 (92%)	25 (8%)	11	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Y	316/341 (93%)	293 (93%)	23 (7%)	13	39
4	D	233/238 (98%)	226 (97%)	7 (3%)	36	57
4	S	233/238 (98%)	226 (97%)	7 (3%)	36	57
5	E	144/158 (91%)	134 (93%)	10 (7%)	14	40
5	T	144/158 (91%)	134 (93%)	10 (7%)	14	40
6	F	84/107 (78%)	80 (95%)	4 (5%)	23	47
6	U	84/107 (78%)	80 (95%)	4 (5%)	23	47
7	G	104/125 (83%)	95 (91%)	9 (9%)	9	33
7	V	104/125 (83%)	96 (92%)	8 (8%)	12	37
8	H	67/75 (89%)	65 (97%)	2 (3%)	36	57
8	Z	67/75 (89%)	65 (97%)	2 (3%)	36	57
9	I	72/83 (87%)	69 (96%)	3 (4%)	26	50
9	K	72/83 (87%)	68 (94%)	4 (6%)	19	45
10	J	37/96 (38%)	35 (95%)	2 (5%)	20	45
10	Q	37/96 (38%)	35 (95%)	2 (5%)	20	45
11	L	79/80 (99%)	78 (99%)	1 (1%)	61	71
11	M	79/80 (99%)	77 (98%)	2 (2%)	42	61
12	N	58/60 (97%)	52 (90%)	6 (10%)	7	27
12	O	58/60 (97%)	54 (93%)	4 (7%)	14	40
13	P	41/43 (95%)	38 (93%)	3 (7%)	13	39
13	X	41/43 (95%)	38 (93%)	3 (7%)	13	39
All	All	5790/6294 (92%)	5410 (93%)	380 (7%)	15	41

All (380) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	49	LEU
1	A	61	CYS
1	A	64	THR
1	A	84	VAL
1	A	88	LYS
1	A	91	TYR
1	A	101	CYS
1	A	104	VAL

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Mol	Chain	Res	Type
1	A	105	LYS
1	A	106	ILE
1	A	107	SER
1	A	220	ARG
1	A	223	ILE
1	A	224	MET
1	A	238	LYS
1	A	262	ILE
1	A	284	LEU
1	A	288	LYS
1	A	296	ARG
1	A	314	SER
1	A	326	ILE
1	A	332	ILE
1	A	334	ILE
1	A	353	ILE
1	A	366	ILE
1	A	425	LEU
1	A	438	LEU
1	A	464	LEU
1	A	470	GLU
1	A	487	ILE
1	A	488	THR
1	A	527	VAL
1	A	551	VAL
1	A	588	ILE
1	A	593	LEU
1	A	603	ILE
1	A	633	ARG
1	A	723	ASN
1	A	763	THR
1	A	764	ARG
1	A	766	LEU
1	A	787	ARG
1	A	823	LEU
1	A	868	VAL
1	A	875	VAL
1	A	876	VAL
2	B	31	LEU
2	B	52	ILE
2	B	54	THR
2	B	68	ILE

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Mol	Chain	Res	Type
2	B	83	ILE
2	B	93	LEU
2	B	104	ILE
2	B	111	GLU
2	B	118	TYR
2	B	119	ILE
2	B	166	THR
2	B	170	LEU
2	B	195	SER
2	B	203	VAL
2	B	215	VAL
2	B	216	SER
2	B	229	LEU
2	B	230	MET
2	B	259	LEU
2	B	318	LEU
2	B	345	ARG
2	B	346	LEU
2	B	418	ASP
2	B	420	THR
2	B	426	LEU
2	B	436	LEU
2	B	444	GLU
2	B	448	LEU
2	B	456	MET
2	B	460	GLU
2	B	470	VAL
2	B	471	LYS
2	B	481	VAL
2	B	525	LEU
2	B	529	LEU
2	B	539	LEU
2	B	563	THR
2	B	591	LEU
2	B	610	LEU
2	B	653	ILE
2	B	657	ILE
2	B	662	GLU
2	B	675	MET
2	B	688	GLN
2	B	711	LEU
2	B	726	ILE

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Mol	Chain	Res	Type
2	B	735	TYR
2	B	742	ILE
2	B	767	LYS
2	B	777	VAL
2	B	840	ILE
2	B	854	LEU
2	B	856	THR
2	B	874	ILE
2	B	884	ARG
2	B	903	THR
2	B	905	LYS
2	B	913	LEU
2	B	943	VAL
2	B	950	LYS
2	B	951	THR
2	B	953	ILE
2	B	960	ILE
2	B	973	THR
2	B	977	ARG
2	B	994	GLN
2	B	1013	GLN
2	B	1070	ILE
2	B	1081	VAL
2	B	1104	ILE
3	C	28	ILE
3	C	47	GLU
3	C	64	ILE
3	C	70	ILE
3	C	102	LEU
3	C	107	LEU
3	C	111	VAL
3	C	119	THR
3	C	149	ILE
3	C	164	SER
3	C	174	LEU
3	C	180	THR
3	C	231	ILE
3	C	232	LYS
3	C	237	ILE
3	C	238	LYS
3	C	292	ILE
3	C	311	ARG

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Mol	Chain	Res	Type
3	C	315	LEU
3	C	331	ARG
3	C	365	GLU
3	C	369	VAL
3	C	380	LYS
3	C	389	THR
3	C	393	ILE
4	D	13	ILE
4	D	83	ILE
4	D	109	LEU
4	D	163	ILE
4	D	165	ARG
4	D	178	LYS
4	D	258	LYS
5	E	27	LEU
5	E	30	LEU
5	E	38	ILE
5	E	48	ILE
5	E	53	THR
5	E	59	LEU
5	E	113	ILE
5	E	114	THR
5	E	120	TYR
5	E	137	GLN
6	F	7	VAL
6	F	63	ILE
6	F	79	THR
6	F	88	ILE
7	G	19	GLU
7	G	34	ASN
7	G	46	ILE
7	G	48	ILE
7	G	67	THR
7	G	79	THR
7	G	101	LEU
7	G	104	LYS
7	G	106	ILE
8	H	34	GLU
8	H	63	ILE
9	I	25	ASN
9	I	56	ILE
9	I	74	LEU

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Mol	Chain	Res	Type
10	J	43	LEU
10	J	52	ASP
9	K	25	ASN
9	K	51	ILE
9	K	56	ILE
9	K	74	LEU
11	L	3	ILE
11	M	3	ILE
11	M	5	ILE
12	N	1	MET
12	N	3	ILE
12	N	5	ILE
12	N	40	VAL
12	N	45	CYS
12	N	63	THR
12	O	3	ILE
12	O	5	ILE
12	O	7	CYS
12	O	40	VAL
13	P	18	LEU
13	P	33	ILE
13	P	41	THR
10	Q	43	LEU
10	Q	52	ASP
2	R	31	LEU
2	R	54	THR
2	R	68	ILE
2	R	83	ILE
2	R	93	LEU
2	R	104	ILE
2	R	111	GLU
2	R	118	TYR
2	R	119	ILE
2	R	144	ILE
2	R	166	THR
2	R	170	LEU
2	R	195	SER
2	R	213	PHE
2	R	215	VAL
2	R	229	LEU
2	R	230	MET
2	R	259	LEU

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Mol	Chain	Res	Type
2	R	318	LEU
2	R	345	ARG
2	R	346	LEU
2	R	418	ASP
2	R	419	ARG
2	R	420	THR
2	R	426	LEU
2	R	436	LEU
2	R	444	GLU
2	R	448	LEU
2	R	456	MET
2	R	460	GLU
2	R	470	VAL
2	R	471	LYS
2	R	481	VAL
2	R	525	LEU
2	R	529	LEU
2	R	539	LEU
2	R	579	ARG
2	R	591	LEU
2	R	610	LEU
2	R	646	TRP
2	R	653	ILE
2	R	657	ILE
2	R	662	GLU
2	R	675	MET
2	R	688	GLN
2	R	711	LEU
2	R	726	ILE
2	R	735	TYR
2	R	742	ILE
2	R	767	LYS
2	R	773	GLU
2	R	777	VAL
2	R	840	ILE
2	R	854	LEU
2	R	874	ILE
2	R	884	ARG
2	R	905	LYS
2	R	913	LEU
2	R	924	LEU
2	R	943	VAL

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Mol	Chain	Res	Type
2	R	950	LYS
2	R	951	THR
2	R	953	ILE
2	R	960	ILE
2	R	973	THR
2	R	977	ARG
2	R	994	GLN
2	R	1013	GLN
2	R	1070	ILE
2	R	1081	VAL
2	R	1104	ILE
4	S	13	ILE
4	S	83	ILE
4	S	109	LEU
4	S	163	ILE
4	S	178	LYS
4	S	209	CYS
4	S	258	LYS
5	T	27	LEU
5	T	30	LEU
5	T	38	ILE
5	T	48	ILE
5	T	53	THR
5	T	59	LEU
5	T	113	ILE
5	T	114	THR
5	T	120	TYR
5	T	137	GLN
6	U	7	VAL
6	U	63	ILE
6	U	79	THR
6	U	88	ILE
7	V	26	LEU
7	V	46	ILE
7	V	48	ILE
7	V	67	THR
7	V	79	THR
7	V	101	LEU
7	V	104	LYS
7	V	106	ILE
1	W	24	VAL
1	W	61	CYS

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Mol	Chain	Res	Type
1	W	64	THR
1	W	84	VAL
1	W	88	LYS
1	W	91	TYR
1	W	99	ARG
1	W	101	CYS
1	W	105	LYS
1	W	106	ILE
1	W	107	SER
1	W	108	GLU
1	W	191	ASP
1	W	220	ARG
1	W	223	ILE
1	W	224	MET
1	W	238	LYS
1	W	262	ILE
1	W	284	LEU
1	W	288	LYS
1	W	296	ARG
1	W	314	SER
1	W	326	ILE
1	W	332	ILE
1	W	334	ILE
1	W	353	ILE
1	W	366	ILE
1	W	425	LEU
1	W	426	HIS
1	W	438	LEU
1	W	464	LEU
1	W	470	GLU
1	W	487	ILE
1	W	488	THR
1	W	527	VAL
1	W	540	LEU
1	W	551	VAL
1	W	588	ILE
1	W	593	LEU
1	W	603	ILE
1	W	633	ARG
1	W	723	ASN
1	W	763	THR
1	W	764	ARG

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Mol	Chain	Res	Type
1	W	766	LEU
1	W	787	ARG
1	W	823	LEU
1	W	853	ASP
1	W	868	VAL
1	W	875	VAL
1	W	876	VAL
13	X	18	LEU
13	X	33	ILE
13	X	41	THR
3	Y	47	GLU
3	Y	64	ILE
3	Y	70	ILE
3	Y	78	VAL
3	Y	107	LEU
3	Y	116	VAL
3	Y	119	THR
3	Y	149	ILE
3	Y	164	SER
3	Y	174	LEU
3	Y	231	ILE
3	Y	232	LYS
3	Y	237	ILE
3	Y	238	LYS
3	Y	292	ILE
3	Y	311	ARG
3	Y	315	LEU
3	Y	331	ARG
3	Y	365	GLU
3	Y	369	VAL
3	Y	380	LYS
3	Y	386	VAL
3	Y	389	THR
8	Z	34	GLU
8	Z	63	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	465	HIS
1	A	483	HIS
1	A	550	GLN

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Mol	Chain	Res	Type
1	A	577	ASN
1	A	582	HIS
1	A	698	ASN
1	A	847	GLN
2	B	678	GLN
2	B	887	GLN
2	B	897	GLN
2	B	1013	GLN
2	B	1085	HIS
3	C	189	ASN
5	E	16	ASN
7	G	88	ASN
2	R	665	GLN
2	R	678	GLN
2	R	887	GLN
2	R	897	GLN
2	R	1013	GLN
5	T	100	ASN
1	W	63	ASN
1	W	67	ASN
1	W	483	HIS
1	W	550	GLN
1	W	563	HIS
1	W	577	ASN
1	W	582	HIS
1	W	698	ASN
1	W	847	GLN
3	Y	189	ASN
8	Z	14	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 16 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	F3S	S	1001	4	0,9,9	-	-	-		
16	F3S	D	1001	4	0,9,9	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	F3S	S	1001	4	-	-	0/3/3/3
16	F3S	D	1001	4	-	-	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	S	1001	F3S	9	0
16	D	1001	F3S	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	K	2
9	I	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	55:ASN	C	56:ILE	N	1.84
1	I	55:ASN	C	56:ILE	N	1.80
1	K	56:ILE	C	57:SER	N	0.84
1	I	56:ILE	C	57:SER	N	0.82

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, 95th 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 ²)	Q<0.9
1	A	831/880 (94%)	0.69	77 (9%) 14 16	28, 92, 200, 308	0
1	W	831/880 (94%)	0.67	63 (7%) 20 18	46, 106, 212, 378	0
2	B	1085/1131 (95%)	0.74	91 (8%) 17 17	29, 88, 181, 293	0
2	R	1085/1131 (95%)	0.77	96 (8%) 15 16	55, 93, 190, 334	0
3	C	368/395 (93%)	0.86	43 (11%) 9 12	33, 108, 214, 329	0
3	Y	368/395 (93%)	0.71	25 (6%) 23 20	56, 115, 224, 338	0
4	D	262/265 (98%)	0.72	18 (6%) 23 20	59, 116, 219, 298	0
4	S	262/265 (98%)	0.58	13 (4%) 34 25	77, 134, 209, 265	0
5	E	164/180 (91%)	0.96	17 (10%) 11 14	70, 166, 254, 302	0
5	T	164/180 (91%)	0.96	18 (10%) 10 13	72, 164, 255, 300	0
6	F	90/113 (79%)	0.85	5 (5%) 30 23	98, 188, 257, 327	0
6	U	90/113 (79%)	0.81	3 (3%) 49 34	128, 184, 276, 323	0
7	G	110/132 (83%)	0.74	6 (5%) 30 23	66, 132, 226, 301	0
7	V	110/132 (83%)	0.68	6 (5%) 30 23	75, 145, 228, 295	0
8	H	74/84 (88%)	0.63	4 (5%) 31 24	53, 82, 153, 205	0
8	Z	74/84 (88%)	0.70	5 (6%) 23 20	83, 99, 171, 205	0
9	I	82/95 (86%)	0.64	3 (3%) 45 31	57, 91, 160, 195	0
9	K	82/95 (86%)	0.90	12 (14%) 6 9	35, 84, 181, 219	0
10	J	39/104 (37%)	1.06	5 (12%) 7 11	130, 183, 243, 268	0
10	Q	39/104 (37%)	1.23	6 (15%) 5 8	112, 162, 213, 265	0
11	L	91/92 (98%)	0.45	4 (4%) 39 28	65, 99, 194, 250	0
11	M	91/92 (98%)	0.29	2 (2%) 62 44	95, 121, 175, 247	0
12	N	64/66 (96%)	0.76	5 (7%) 19 17	59, 103, 177, 205	0
12	O	64/66 (96%)	0.42	3 (4%) 36 27	91, 112, 168, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	P	45/48 (93%)	0.89	4 (8%) 15 16	71, 93, 189, 275	0
13	X	45/48 (93%)	0.87	4 (8%) 15 16	85, 105, 197, 249	0
All	All	6610/7170 (92%)	0.73	538 (8%) 18 17	28, 105, 217, 378	0

All (538) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	238	LYS	6.6
2	B	1072	TRP	6.1
1	W	24	VAL	5.9
2	R	1072	TRP	5.8
12	N	64	ARG	5.5
1	A	238	LYS	5.3
2	B	838	THR	5.3
2	B	13	ARG	5.1
1	A	24	VAL	5.1
3	C	234	ILE	4.9
2	R	608	ASP	4.8
1	W	194	ILE	4.8
1	A	115	SER	4.6
1	W	115	SER	4.6
1	W	91	TYR	4.5
3	Y	234	ILE	4.5
1	W	70	GLY	4.4
3	Y	27	LYS	4.4
2	B	387	LEU	4.4
1	A	876	VAL	4.4
1	A	870	ARG	4.4
1	W	870	ARG	4.4
2	R	234	GLY	4.4
10	Q	67	LEU	4.4
3	C	13	LEU	4.2
2	R	838	THR	4.1
7	G	92	TYR	4.1
8	H	13	ILE	4.1
2	R	618	TYR	4.0
10	J	67	LEU	4.0
12	N	39	GLY	4.0
3	C	394	LEU	4.0
2	R	247	LEU	3.9
1	A	50	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
7	G	82	LYS	3.9
2	R	13	ARG	3.9
2	B	57	PRO	3.9
1	W	287	SER	3.9
2	B	309	ASP	3.8
2	B	106	VAL	3.8
2	B	203	VAL	3.8
2	R	57	PRO	3.8
13	X	45	VAL	3.7
1	A	852	ASP	3.7
2	B	1118	LEU	3.7
1	W	878	TRP	3.7
3	C	27	LYS	3.7
1	W	25	THR	3.6
2	R	106	VAL	3.6
9	K	52	ASP	3.6
8	H	66	ILE	3.6
2	R	8	LEU	3.6
1	A	137	LYS	3.6
1	W	876	VAL	3.5
8	Z	66	ILE	3.5
2	B	382	LEU	3.5
2	B	590	PRO	3.5
2	R	203	VAL	3.5
9	K	51	ILE	3.5
2	R	257	PRO	3.5
5	E	81	VAL	3.4
2	B	224	ILE	3.4
2	R	387	LEU	3.4
2	R	1083	PRO	3.4
2	B	381	LYS	3.4
5	E	97	VAL	3.4
2	B	217	PHE	3.4
2	B	269	ASP	3.4
1	W	97	THR	3.3
1	W	532	ILE	3.3
10	J	70	ASP	3.3
2	B	22	LYS	3.3
2	B	153	GLY	3.3
1	W	105	LYS	3.3
2	R	507	VAL	3.3
8	Z	82	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
3	Y	171	ASN	3.3
2	R	196	THR	3.3
3	C	59	TYR	3.3
9	I	51	ILE	3.3
7	V	92	TYR	3.3
2	B	8	LEU	3.2
2	B	689	LEU	3.2
12	N	63	THR	3.2
1	W	82	ILE	3.2
7	G	93	ILE	3.2
3	C	155	SER	3.2
1	A	846	ILE	3.2
1	W	18	GLU	3.2
2	R	342	ALA	3.2
2	B	257	PRO	3.2
2	R	343	ASN	3.2
3	C	363	VAL	3.2
3	Y	394	LEU	3.2
4	S	205	LEU	3.2
2	B	1071	GLY	3.1
3	Y	168	GLN	3.1
1	A	879	LYS	3.1
1	A	118	TYR	3.1
2	B	250	GLU	3.1
3	C	391	ARG	3.1
2	B	1027	GLY	3.1
1	A	97	THR	3.1
3	C	24	LEU	3.1
9	K	55	ASN	3.1
1	W	210	THR	3.1
1	A	878	TRP	3.1
4	D	208	GLU	3.1
7	V	48	ILE	3.1
2	R	25	GLY	3.1
2	B	196	THR	3.1
2	B	693	THR	3.1
9	I	65	ALA	3.0
2	R	779	PRO	3.0
13	P	15	ASP	3.0
2	B	580	ARG	3.0
1	W	851	GLY	3.0
1	A	426	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
2	R	1084	ILE	3.0
1	A	70	GLY	3.0
1	A	845	VAL	3.0
2	B	618	TYR	3.0
11	L	11	ASN	3.0
2	R	248	ASP	3.0
1	A	261	ILE	2.9
2	B	1084	ILE	2.9
10	Q	73	LYS	2.9
1	A	753	ARG	2.9
8	H	76	VAL	2.9
1	W	541	ALA	2.9
2	B	266	ALA	2.9
2	B	1083	PRO	2.9
1	A	851	GLY	2.9
2	R	604	SER	2.9
2	B	275	ILE	2.9
1	W	459	GLY	2.9
4	S	197	VAL	2.9
1	W	879	LYS	2.9
3	Y	39	LYS	2.9
2	R	337	ASP	2.9
1	A	287	SER	2.9
2	R	233	LEU	2.9
1	A	134	GLU	2.9
1	A	383	GLY	2.8
1	A	64	THR	2.8
3	C	65	ALA	2.8
10	Q	48	THR	2.8
13	P	35	PHE	2.8
4	D	168	PRO	2.8
2	B	55	GLU	2.8
1	W	531	LYS	2.8
1	W	753	ARG	2.8
1	A	80	PRO	2.8
1	W	75	ILE	2.8
1	W	78	VAL	2.8
2	B	227	VAL	2.8
2	R	595	GLU	2.8
1	A	867	ASP	2.8
2	R	437	ALA	2.8
13	P	10	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
2	R	22	LYS	2.8
2	R	566	ILE	2.8
1	W	845	VAL	2.8
3	Y	59	TYR	2.8
6	F	9	GLU	2.8
1	A	520	GLU	2.8
1	A	351	GLU	2.8
1	A	142	LYS	2.8
2	R	358	ARG	2.7
2	R	840	ILE	2.7
2	B	307	SER	2.7
2	R	172	PRO	2.7
13	X	28	TYR	2.7
3	C	171	ASN	2.7
1	A	103	ARG	2.7
3	C	28	ILE	2.7
5	T	80	VAL	2.7
1	A	512	LYS	2.7
3	C	314	LEU	2.7
1	W	237	HIS	2.7
2	R	817	VAL	2.7
2	B	247	LEU	2.7
1	W	474	ALA	2.7
2	B	343	ASN	2.7
2	B	566	ILE	2.7
2	R	605	ILE	2.7
2	R	53	PRO	2.7
3	C	360	ARG	2.7
4	S	143	ALA	2.7
5	E	136	ILE	2.7
5	E	119	LYS	2.7
2	R	258	SER	2.7
3	C	332	HIS	2.7
1	W	378	VAL	2.7
4	S	236	LEU	2.7
2	B	431	ARG	2.7
2	B	1087	ASP	2.7
3	C	183	ASP	2.7
1	A	194	ILE	2.7
1	A	398	ALA	2.7
2	R	275	ILE	2.7
4	D	41	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
12	O	39	GLY	2.7
7	V	80	GLU	2.7
2	R	217	PHE	2.7
1	W	289	HIS	2.6
2	B	1081	VAL	2.6
2	R	113	GLU	2.6
2	R	382	LEU	2.6
3	C	48	ILE	2.6
3	C	377	HIS	2.6
2	R	1114	PRO	2.6
2	R	519	LYS	2.6
2	R	771	GLY	2.6
3	C	194	GLY	2.6
4	D	174	GLY	2.6
5	T	73	ASP	2.6
5	E	130	GLU	2.6
2	B	405	ASN	2.6
2	R	405	ASN	2.6
1	W	88	LYS	2.6
3	C	39	LYS	2.6
9	K	70	LYS	2.6
2	R	1099	ALA	2.6
1	A	46	ASP	2.6
3	Y	284	PHE	2.6
2	R	602	SER	2.6
2	R	376	LYS	2.6
1	W	515	LEU	2.6
3	Y	13	LEU	2.6
12	N	62	TYR	2.6
5	T	110	ILE	2.6
3	Y	232	LYS	2.6
3	Y	378	PRO	2.6
3	Y	203	GLY	2.6
4	S	174	GLY	2.6
1	W	261	ILE	2.6
2	R	269	ASP	2.6
1	W	707	LEU	2.6
4	D	173	LEU	2.6
3	C	284	PHE	2.6
1	W	346	THR	2.5
2	B	840	ILE	2.5
7	V	82	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	608	ASP	2.5
2	R	472	ASN	2.5
2	B	469	LEU	2.5
2	R	386	ALA	2.5
3	Y	65	ALA	2.5
5	T	72	PHE	2.5
3	Y	28	ILE	2.5
1	W	507	TYR	2.5
9	K	26	LYS	2.5
10	J	51	TRP	2.5
1	W	284	LEU	2.5
5	E	49	LEU	2.5
2	B	1065	ASP	2.5
2	B	1062	TYR	2.5
2	R	1069	TYR	2.5
1	A	65	LEU	2.5
1	W	295	LEU	2.5
2	R	646	TRP	2.5
2	R	689	LEU	2.5
2	R	904	VAL	2.5
2	R	1081	VAL	2.5
2	R	693	THR	2.5
2	B	395	GLU	2.5
9	K	25	ASN	2.5
1	A	82	ILE	2.5
2	B	289	ILE	2.5
2	R	351	ASP	2.5
2	R	657	ILE	2.5
2	R	1027	GLY	2.5
3	Y	342	LEU	2.5
1	A	289	HIS	2.5
2	B	571	VAL	2.5
10	J	73	LYS	2.5
1	A	692	LEU	2.5
2	R	59	LEU	2.5
5	T	170	GLY	2.5
2	R	306	THR	2.5
2	B	1079	LYS	2.4
1	A	541	ALA	2.4
1	W	65	LEU	2.4
1	W	692	LEU	2.4
1	A	492	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	W	64	THR	2.4
1	W	291	SER	2.4
2	R	1062	TYR	2.4
2	R	224	ILE	2.4
3	C	364	GLU	2.4
2	B	646	TRP	2.4
1	W	547	THR	2.4
9	K	58	SER	2.4
5	E	135	VAL	2.4
3	C	376	GLY	2.4
2	B	606	THR	2.4
9	K	60	ASP	2.4
2	B	113	GLU	2.4
3	C	14	GLU	2.4
4	D	142	GLU	2.4
2	B	49	GLN	2.4
1	W	66	GLY	2.4
2	B	25	GLY	2.4
9	K	72	GLY	2.4
1	W	517	THR	2.4
1	W	503	ILE	2.4
2	B	248	ASP	2.4
2	B	712	ASP	2.4
2	R	1076	ASN	2.4
3	C	266	GLY	2.4
5	T	158	PRO	2.4
2	B	1109	SER	2.4
3	C	196	PHE	2.4
4	D	235	SER	2.4
1	A	387	ASP	2.4
1	W	191	ASP	2.4
1	A	105	LYS	2.4
3	C	339	ASN	2.3
3	C	361	GLY	2.3
13	X	30	GLY	2.3
1	W	192	VAL	2.3
2	B	943	VAL	2.3
2	R	118	TYR	2.3
2	R	385	LYS	2.3
5	T	119	LYS	2.3
2	R	250	GLU	2.3
1	A	256	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	R	52	ILE	2.3
2	R	1109	SER	2.3
2	R	1116	LEU	2.3
4	D	119	PRO	2.3
9	K	53	ILE	2.3
10	Q	50	ILE	2.3
1	W	865	THR	2.3
2	R	77	ASP	2.3
1	A	684	LEU	2.3
2	B	605	ILE	2.3
2	R	1014	ILE	2.3
1	A	47	PRO	2.3
1	A	62	GLY	2.3
2	B	234	GLY	2.3
3	Y	376	GLY	2.3
2	R	905	LYS	2.3
1	A	255	ALA	2.3
13	X	47	ALA	2.3
8	Z	13	ILE	2.3
6	U	90	ASP	2.3
8	Z	77	SER	2.3
2	R	1086	GLY	2.3
2	R	54	THR	2.3
3	C	204	ASN	2.3
11	L	1	MET	2.3
2	B	52	ILE	2.3
2	R	616	ILE	2.3
4	D	101	GLU	2.3
1	A	581	PRO	2.3
1	W	73	GLY	2.3
10	J	62	ASP	2.3
2	R	377	VAL	2.3
2	R	481	VAL	2.3
9	K	73	VAL	2.3
13	P	30	GLY	2.3
4	D	176	CYS	2.3
3	C	387	GLU	2.3
8	Z	21	GLU	2.3
5	E	158	PRO	2.3
5	E	58	MET	2.3
1	A	25	THR	2.2
1	W	723	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	1060	THR	2.2
2	R	1085	HIS	2.2
1	A	284	LEU	2.2
5	E	113	ILE	2.2
7	V	93	ILE	2.2
9	I	33	ALA	2.2
1	A	54	PRO	2.2
2	B	358	ARG	2.2
2	R	558	VAL	2.2
4	S	36	VAL	2.2
4	D	103	LEU	2.2
3	Y	196	PHE	2.2
5	T	136	ILE	2.2
2	R	984	SER	2.2
1	A	478	GLU	2.2
2	B	396	ARG	2.2
1	A	594	LEU	2.2
1	W	492	GLY	2.2
3	C	102	LEU	2.2
3	Y	266	GLY	2.2
5	T	97	VAL	2.2
5	T	4	LEU	2.2
2	B	54	THR	2.2
2	R	1087	ASP	2.2
5	E	127	ILE	2.2
1	W	426	HIS	2.2
1	A	810	ALA	2.2
1	A	81	VAL	2.2
1	A	124	ARG	2.2
1	A	295	LEU	2.2
3	C	167	LEU	2.2
12	O	38	LEU	2.2
3	C	348	GLU	2.2
5	E	57	GLY	2.2
1	A	117	ILE	2.2
5	E	147	ILE	2.2
8	H	82	ILE	2.2
2	B	60	LYS	2.2
1	A	299	ALA	2.2
2	B	386	ALA	2.2
2	R	112	ALA	2.2
4	D	143	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	R	795	LEU	2.2
1	W	846	ILE	2.2
2	B	779	PRO	2.2
3	C	58	GLU	2.2
5	E	86	GLU	2.2
5	T	130	GLU	2.2
6	U	77	PRO	2.2
1	A	723	ASN	2.2
7	G	44	ASP	2.2
1	A	125	TRP	2.2
5	T	118	LEU	2.2
1	A	78	VAL	2.2
1	A	848	VAL	2.2
1	W	84	VAL	2.2
2	R	611	VAL	2.2
3	Y	363	VAL	2.2
1	A	262	ILE	2.2
4	S	142	GLU	2.2
5	T	88	GLU	2.2
1	W	288	LYS	2.2
1	A	260	LEU	2.2
2	B	602	SER	2.1
12	N	46	ARG	2.1
1	A	211	VAL	2.1
2	R	493	TYR	2.1
3	C	349	VAL	2.1
3	Y	251	ILE	2.1
2	B	274	PHE	2.1
2	B	771	GLY	2.1
2	B	1086	GLY	2.1
11	M	40	PHE	2.1
1	A	18	GLU	2.1
2	B	206	GLU	2.1
11	L	9	GLU	2.1
10	Q	55	LEU	2.1
3	Y	155	SER	2.1
2	B	297	ASP	2.1
3	Y	254	ASP	2.1
5	T	127	ILE	2.1
4	D	82	CYS	2.1
1	W	142	LYS	2.1
2	B	519	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	232	LYS	2.1
3	C	30	GLU	2.1
10	Q	54	LEU	2.1
3	C	137	ALA	2.1
7	G	48	ILE	2.1
4	D	115	LYS	2.1
6	F	24	VAL	2.1
6	F	11	TYR	2.1
2	B	1010	GLY	2.1
3	C	310	MET	2.1
1	A	816	SER	2.1
4	D	172	ILE	2.1
11	M	11	ASN	2.1
2	R	294	GLN	2.1
5	T	92	VAL	2.1
2	B	596	ASP	2.1
2	R	153	GLY	2.1
2	R	170	LEU	2.1
5	T	67	TYR	2.1
6	F	59	LEU	2.1
7	G	83	ASP	2.1
1	A	837	THR	2.1
1	W	149	CYS	2.1
2	B	595	GLU	2.1
3	Y	270	ALA	2.1
4	S	202	ALA	2.1
1	A	378	VAL	2.1
2	R	227	VAL	2.1
4	D	233	VAL	2.1
1	W	49	LEU	2.1
1	A	459	GLY	2.1
2	R	603	GLY	2.1
4	S	37	PRO	2.1
4	S	168	PRO	2.1
1	A	108	GLU	2.1
1	A	865	THR	2.1
2	R	1060	THR	2.1
4	S	208	GLU	2.1
2	R	1064	CYS	2.1
2	R	1070	ILE	2.1
1	W	725	ALA	2.1
1	A	145	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	507	VAL	2.1
2	B	610	LEU	2.1
3	C	306	LEU	2.1
3	Y	349	VAL	2.1
1	A	237	HIS	2.0
2	B	379	GLY	2.0
2	B	1080	TYR	2.0
7	V	89	GLY	2.0
11	L	30	GLY	2.0
6	F	80	PRO	2.0
2	B	554	ASP	2.0
1	W	589	LYS	2.0
2	B	397	ILE	2.0
5	T	83	GLU	2.0
4	S	59	ALA	2.0
4	D	213	CYS	2.0
1	A	868	VAL	2.0
6	U	24	VAL	2.0
2	R	109	ASN	2.0
5	E	164	MET	2.0
1	W	864	LYS	2.0
2	R	612	ARG	2.0
5	E	79	PRO	2.0
12	O	41	LYS	2.0
4	D	100	ALA	2.0
4	S	243	LEU	2.0
3	C	386	VAL	2.0
1	A	869	ASN	2.0
1	A	116	ARG	2.0
2	B	793	ARG	2.0
3	C	203	GLY	2.0
2	B	1014	ILE	2.0
2	B	1070	ILE	2.0
3	C	392	PRO	2.0
2	B	443	PHE	2.0
5	E	72	PHE	2.0
2	B	258	SER	2.0
2	B	604	SER	2.0
3	Y	288	ALA	2.0
9	K	65	ALA	2.0
1	W	407	VAL	2.0
5	T	85	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	MG	W	1882	1/1	0.41	0.31	246,246,246,246	0
15	MG	A	1882	1/1	0.42	0.31	246,246,246,246	0
14	ZN	B	2124	1/1	0.46	0.39	246,246,246,246	0
14	ZN	B	2125	1/1	0.52	0.25	246,246,246,246	0
14	ZN	R	2124	1/1	0.54	0.36	246,246,246,246	0
14	ZN	R	2125	1/1	0.67	0.27	246,246,246,246	0
14	ZN	W	1881	1/1	0.79	0.10	246,246,246,246	0
16	F3S	D	1001	7/7	0.82	0.34	232,235,241,245	0
14	ZN	R	2123	1/1	0.84	0.14	246,246,246,246	0
16	F3S	S	1001	7/7	0.85	0.26	247,251,257,260	0
14	ZN	B	2123	1/1	0.86	0.18	246,246,246,246	0
14	ZN	A	1881	1/1	0.89	0.07	246,246,246,246	0
14	ZN	A	1880	1/1	0.90	0.14	246,246,246,246	0
14	ZN	W	1880	1/1	0.94	0.09	246,246,246,246	0
14	ZN	P	1049	1/1	0.96	0.06	142,142,142,142	0
14	ZN	X	1049	1/1	0.96	0.06	157,157,157,157	0
14	ZN	O	1065	1/1	0.99	0.02	165,165,165,165	0
14	ZN	N	1065	1/1	1.00	0.02	130,130,130,130	0

6.5 Other polymers [i](#)

There are no such residues in this entry.