



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:36 PM UTC

PDB ID : 2WB1 / pdb_00002wb1
Title : The complete structure of the archaeal 13-subunit DNA-directed RNA Polymerase
Authors : Korkhin, Y.; Unligil, U.M.; Littlefield, O.; Nelson, P.J.; Stuart, D.I.; Sigler, P.B.; Bell, S.D.; Abrescia, N.G.A.
Deposited on : 2009-02-19
Resolution : 3.52 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:

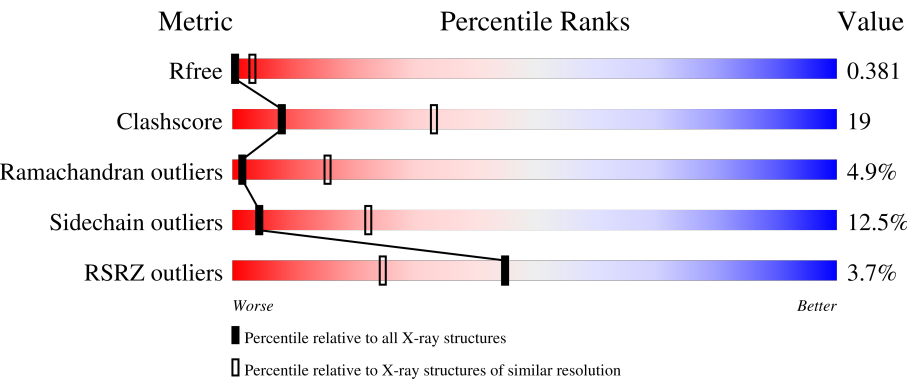
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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	3% 50% 36% 8% • •
1	W	880	2% 49% 38% 8% • •
2	B	1131	4% 50% 38% 8% • •
2	R	1131	4% 48% 38% 9% • •
3	C	395	4% 44% 40% 7% • 7%

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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	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 52739 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 RPO1N SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	841	Total	C	N	O	S	0	0	0
			6691	4256	1183	1226	26			
1	W	841	Total	C	N	O	S	0	0	0
			6691	4256	1183	1226	26			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE RPO2 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1090	Total	C	N	O	S	0	0	0
			8652	5484	1534	1605	29			
2	R	1090	Total	C	N	O	S	0	0	0
			8652	5484	1534	1605	29			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE RPO1C SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	367	Total	C	N	O	S	0	0	0
			2833	1797	481	547	8			
3	Y	367	Total	C	N	O	S	0	0	0
			2833	1797	481	547	8			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASERPO3 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	260	Total	C	N	O	S	0	0	0
			2071	1332	334	392	13			
4	S	260	Total	C	N	O	S	0	0	0
			2071	1332	334	392	13			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE RPO7 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	174	Total	C	N	O	S	0	0	0
			1384	893	232	255	4			
5	T	174	Total	C	N	O	S	0	0	0
			1384	893	232	255	4			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE RPO4 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	91	Total	C	N	O	S	0	0	1
			702	439	115	145	3			
6	U	91	Total	C	N	O	S	0	0	1
			702	439	115	145	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE RPO8 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	113	Total	C	N	O	S	0	0	0
			901	572	152	173	4			
7	V	113	Total	C	N	O	S	0	0	0
			901	572	152	173	4			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE RPO5 SUBUNIT.

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 RPO6 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	82	Total	C	N	O	S	0	0	0
			658	420	121	116	1			
9	K	82	Total	C	N	O	S	0	0	0
			658	420	121	116	1			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASE RPO13 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	35	Total	C	N	O		0	0	0
			301	186	53	62				

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	Q	33	Total	C	N	O	S	0	0	1
			274	172	45	56	1			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE RPO11 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	92	Total	C	N	O	S	0	0	1
			708	454	115	137	2			
11	M	92	Total	C	N	O	S	0	0	1
			708	454	115	137	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASE RPO10 SUBUNIT.

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 DNA-DIRECTED RNA POLYMERASE RPO12 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	P	43	Total	C	N	O	S	0	0	0
			346	230	58	53	5			
13	X	43	Total	C	N	O	S	0	0	0
			346	230	58	53	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	1	Total	Zn	0	0
			1	1		
14	N	1	Total	Zn	0	0
			1	1		
14	O	1	Total	Zn	0	0
			1	1		
14	P	1	Total	Zn	0	0
			1	1		
14	R	1	Total	Zn	0	0
			1	1		

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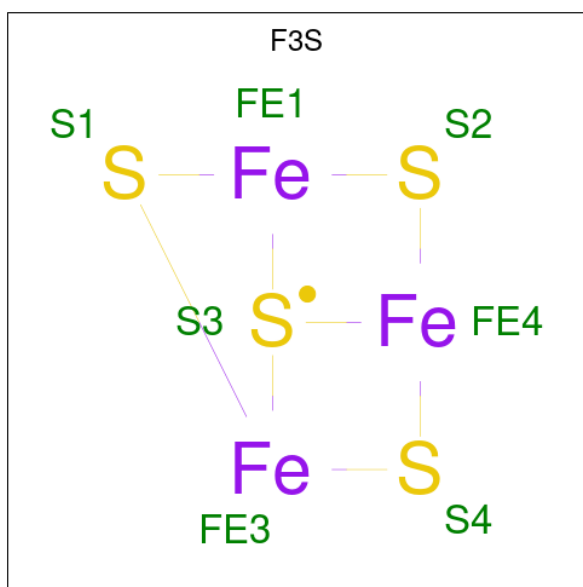
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	W	2	Total	Zn	0	0
			2	2		
14	X	1	Total	Zn	0	0
			1	1		

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

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

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

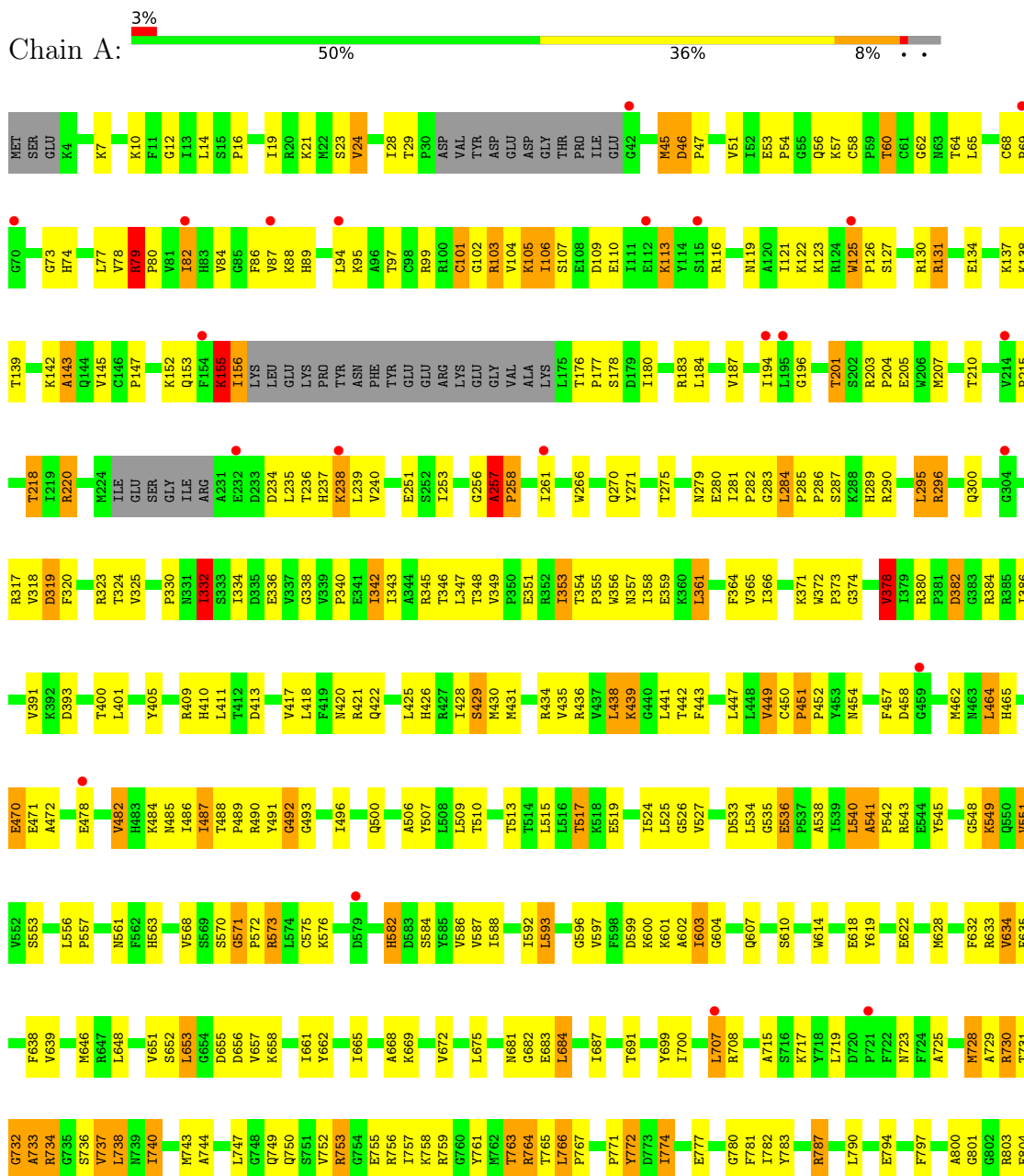


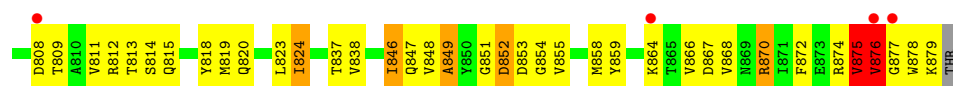
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	D	1	Total	Fe	S	0	0
			7	3	4		
16	S	1	Total	Fe	S	0	0
			7	3	4		

3 Residue-property plots

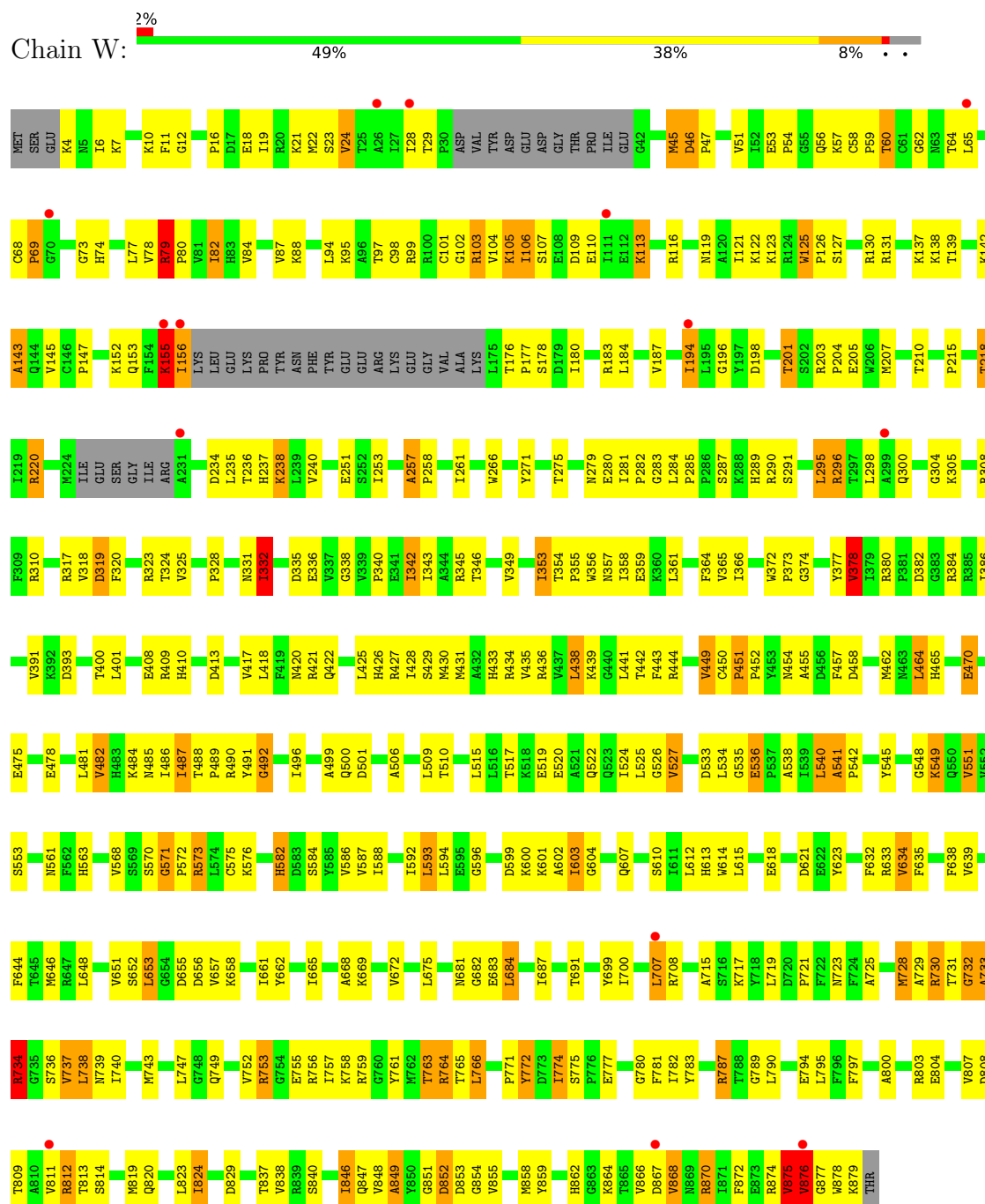
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 RPO1N SUBUNIT

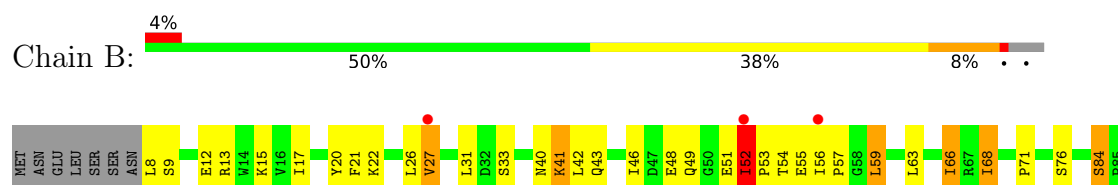


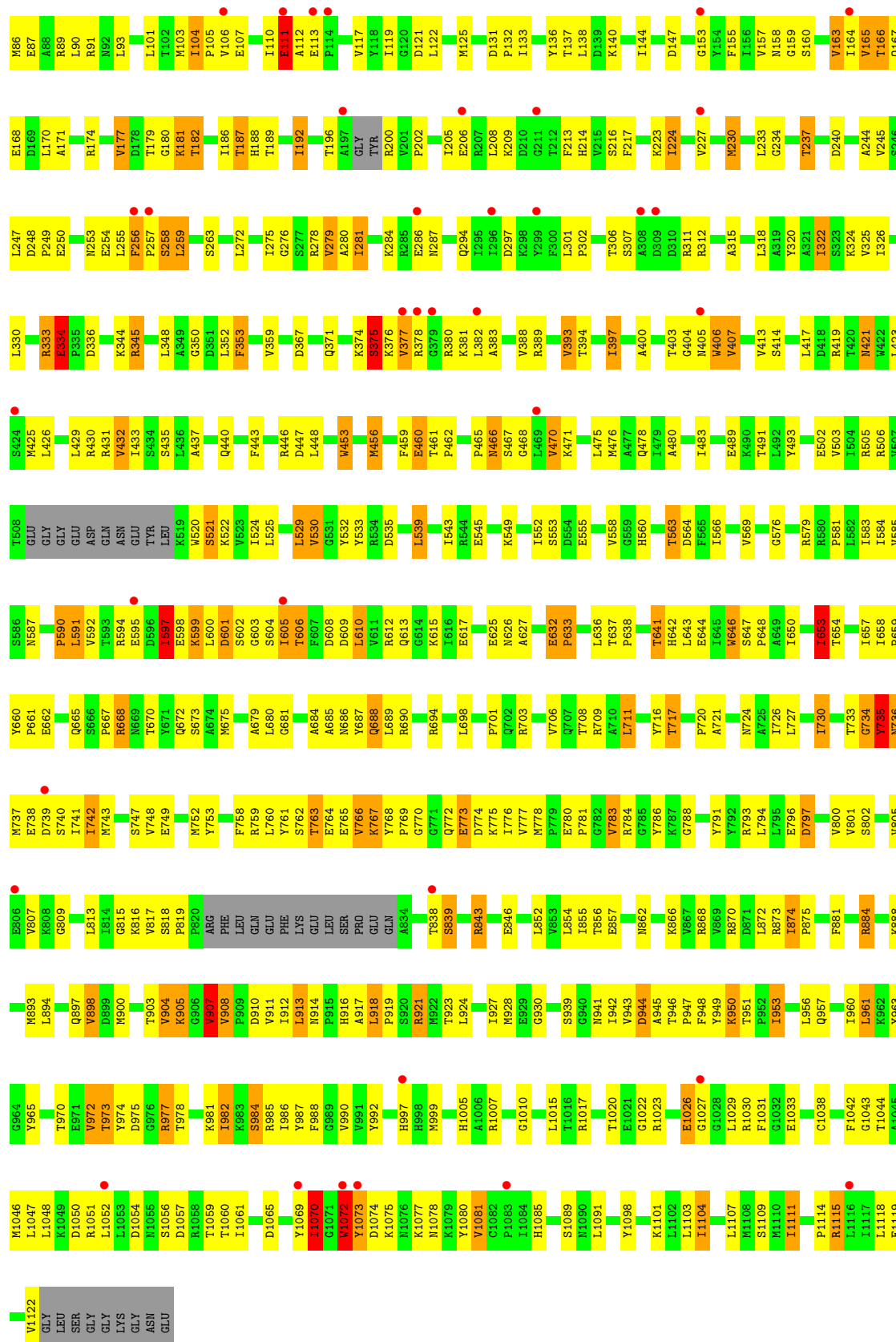


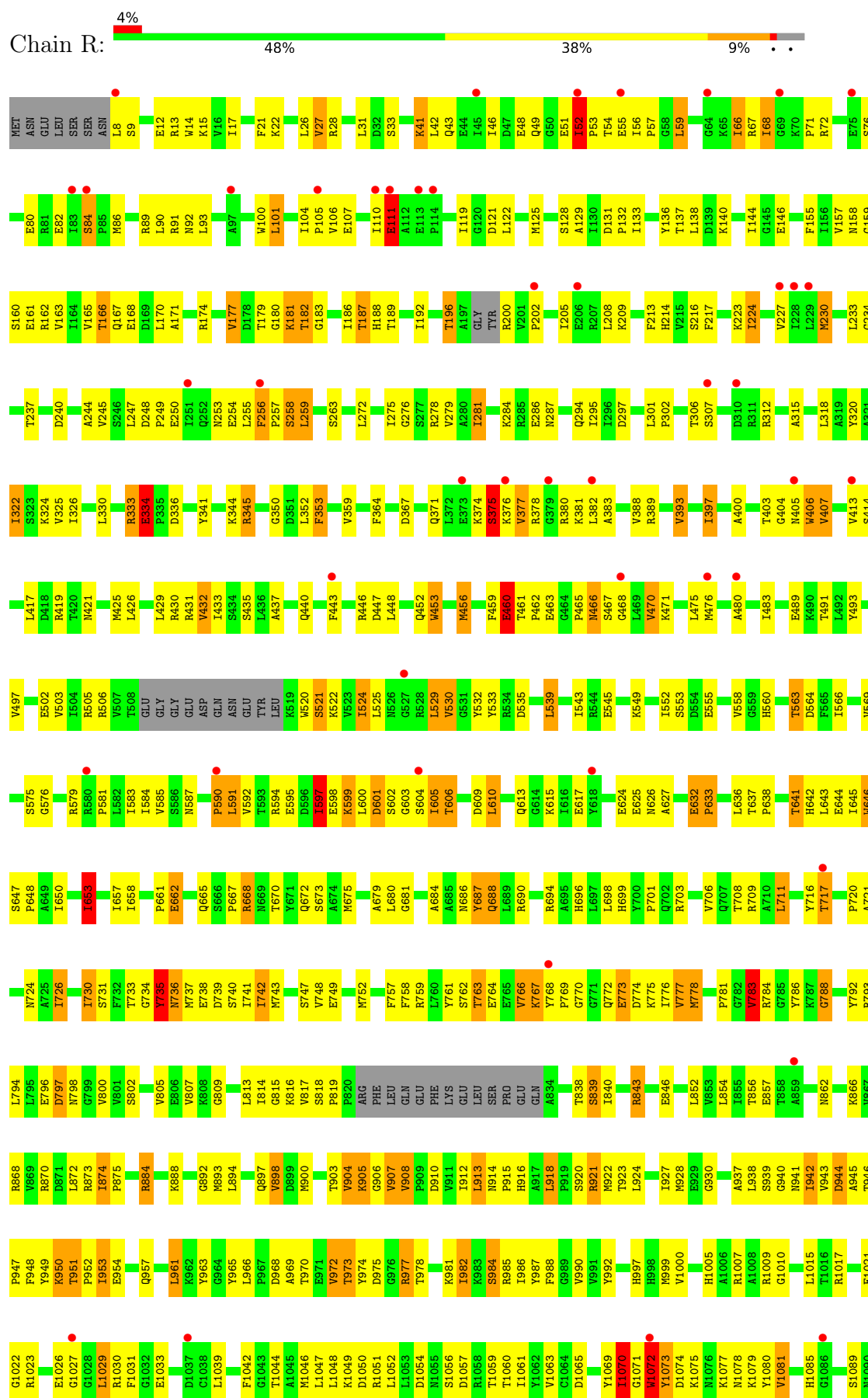
• Molecule 1: DNA-DIRECTED RNA POLYMERASE RPO1N SUBUNIT



• Molecule 2: DNA-DIRECTED RNA POLYMERASE RPO2 SUBUNIT

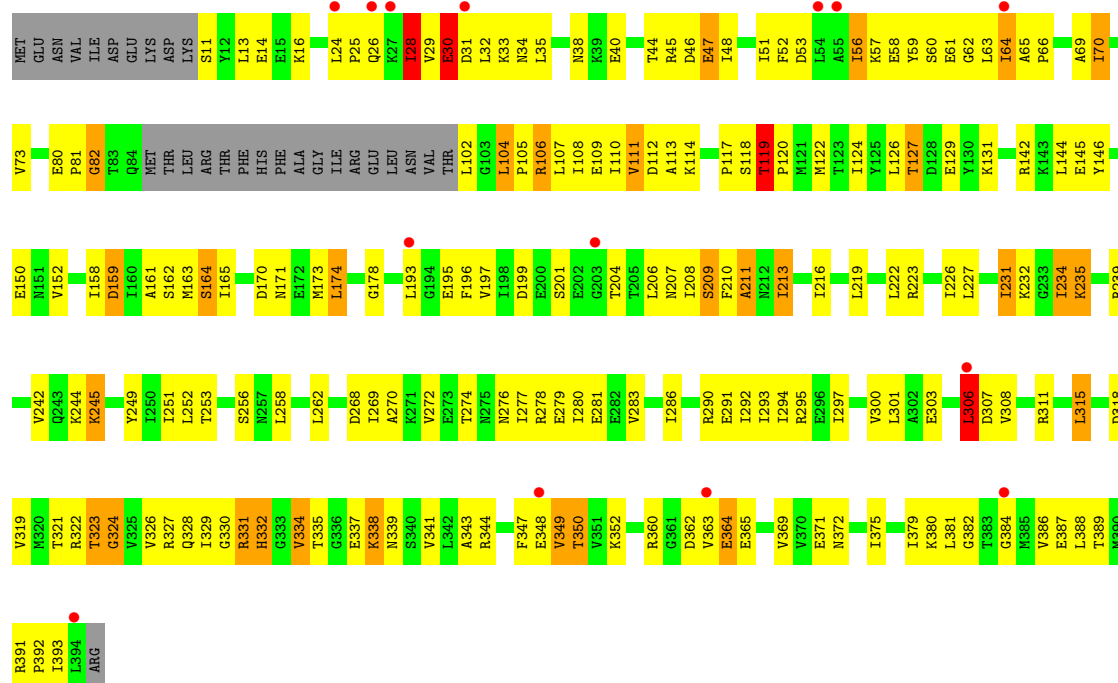
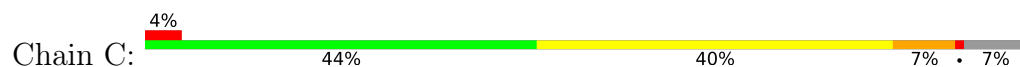




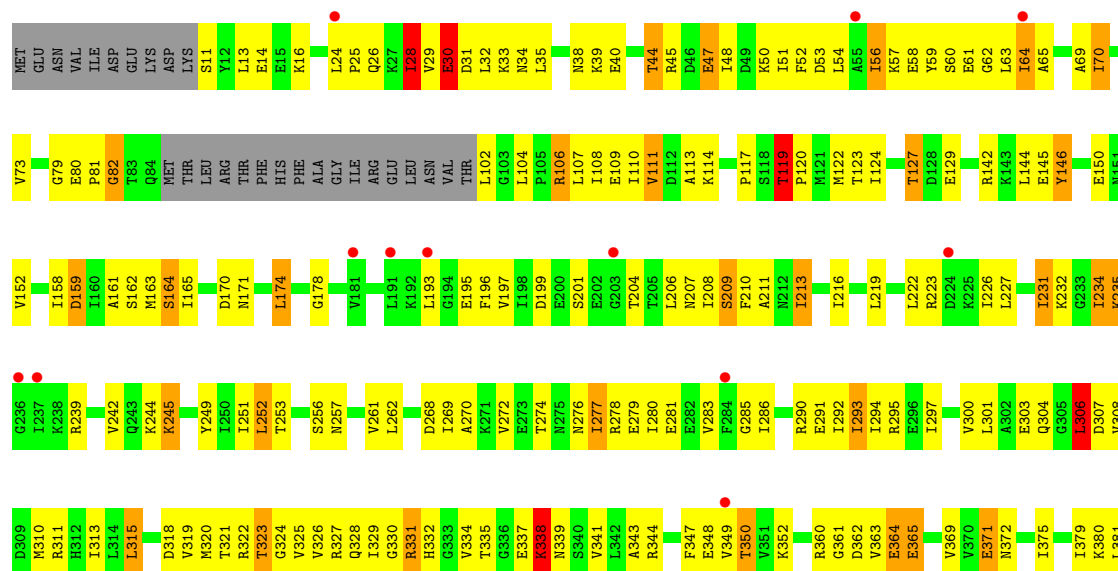
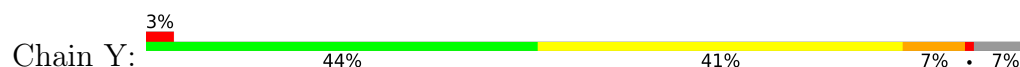




• Molecule 3: DNA-DIRECTED RNA POLYMERASE RPO1C SUBUNIT

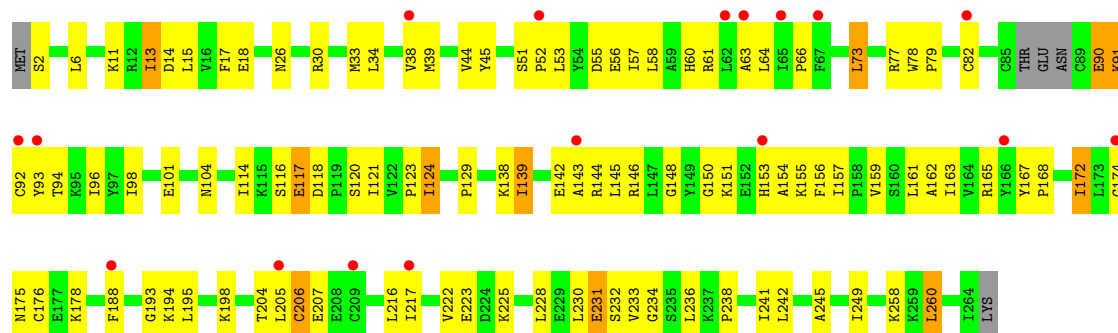


• Molecule 3: DNA-DIRECTED RNA POLYMERASE RPO1C SUBUNIT

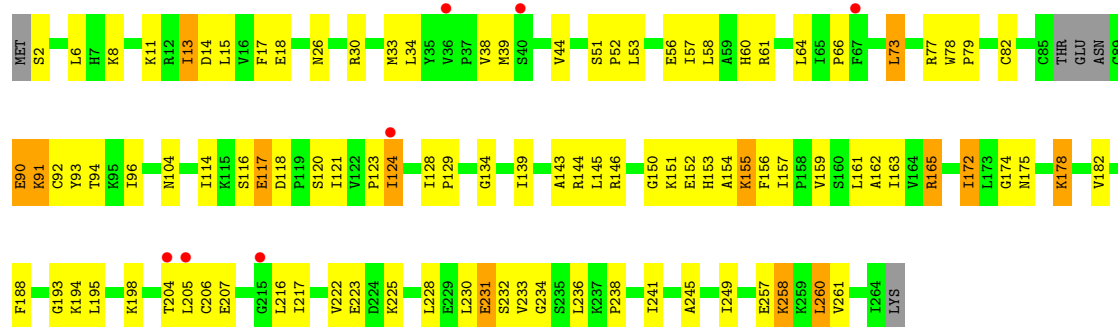




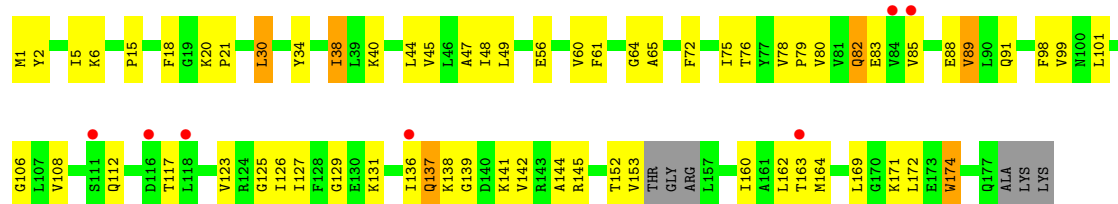
• Molecule 4: DNA-DIRECTED RNA POLYMERASERPO3 SUBUNIT



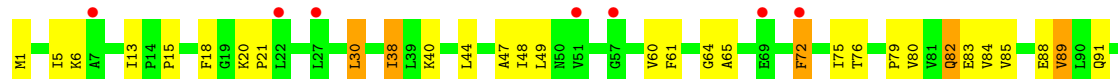
• Molecule 4: DNA-DIRECTED RNA POLYMERASERPO3 SUBUNIT



• Molecule 5: DNA-DIRECTED RNA POLYMERASE RPO7 SUBUNIT

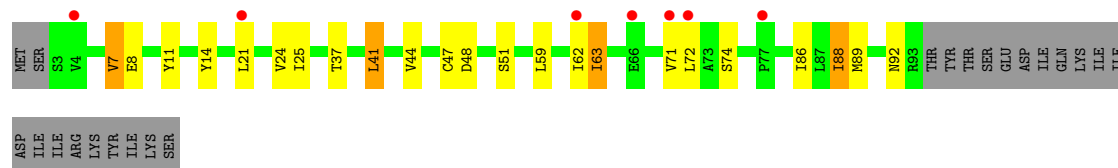


• Molecule 5: DNA-DIRECTED RNA POLYMERASE RPO7 SUBUNIT

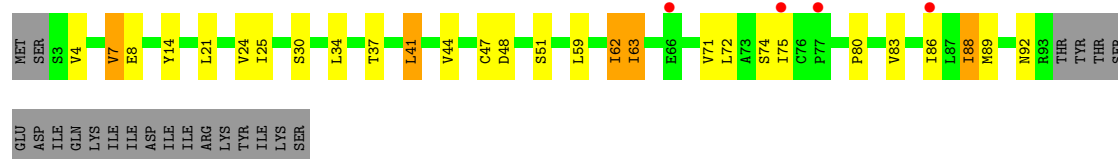




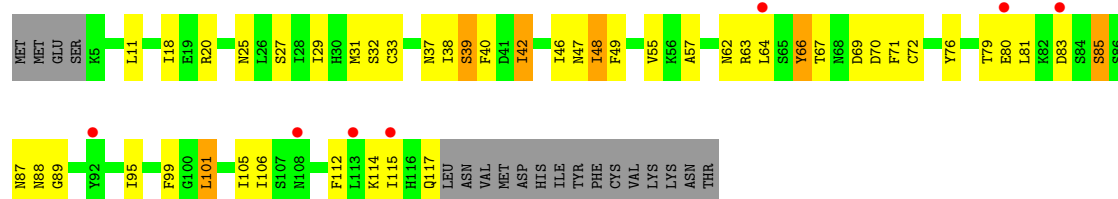
• Molecule 6: DNA-DIRECTED RNA POLYMERASE RPO4 SUBUNIT

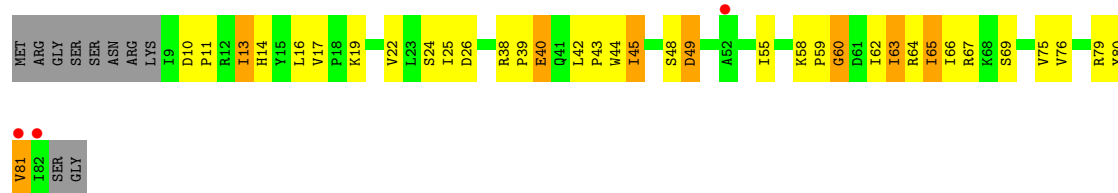


• Molecule 6: DNA-DIRECTED RNA POLYMERASE RPO4 SUBUNIT



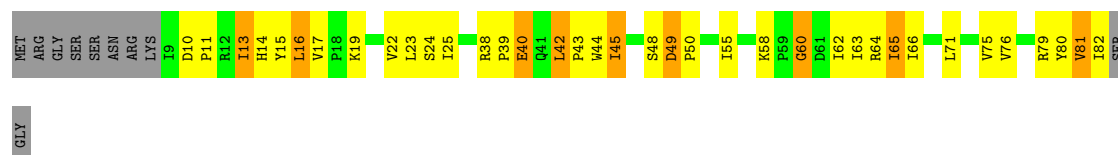
• Molecule 7: DNA-DIRECTED RNA POLYMERASE RPO8 SUBUNIT





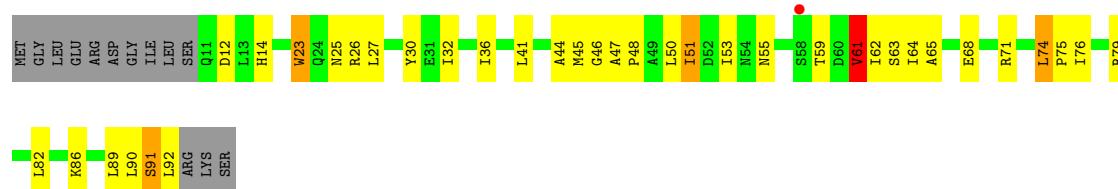
• Molecule 8: DNA-DIRECTED RNA POLYMERASE RPO5 SUBUNIT

Chain Z: 44% 33% 11% 12%



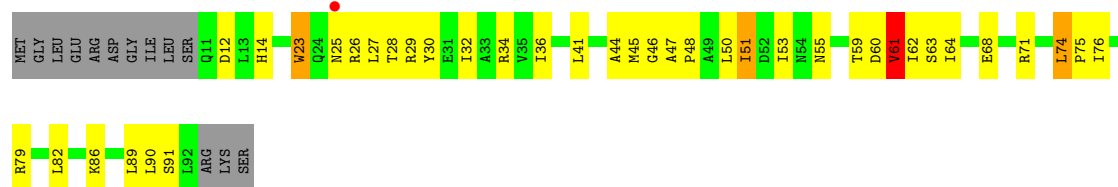
• Molecule 9: DNA-DIRECTED RNA POLYMERASE RPO6 SUBUNIT

Chain I: 47% 34% 14%



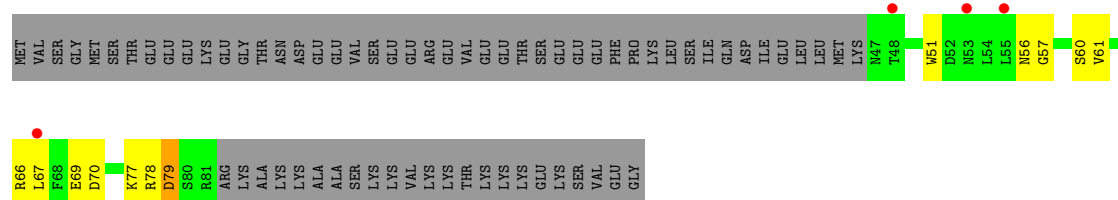
• Molecule 9: DNA-DIRECTED RNA POLYMERASE RPO6 SUBUNIT

Chain K: 45% 37% 14%

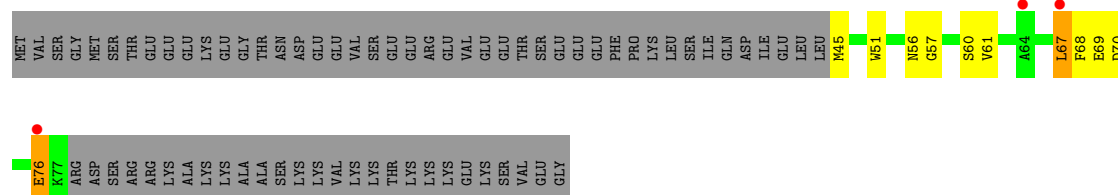


• Molecule 10: DNA-DIRECTED RNA POLYMERASE RPO13 SUBUNIT

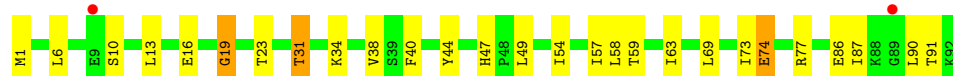
Chain J: 4% 22% 11% 66%



• Molecule 10: DNA-DIRECTED RNA POLYMERASE RPO13 SUBUNIT



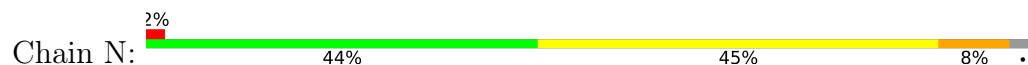
• Molecule 11: DNA-DIRECTED RNA POLYMERASE RPO11 SUBUNIT



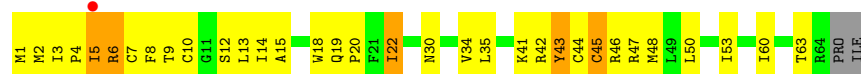
• Molecule 11: DNA-DIRECTED RNA POLYMERASE RPO11 SUBUNIT



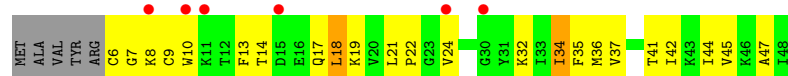
• Molecule 12: DNA-DIRECTED RNA POLYMERASE RPO10 SUBUNIT



• Molecule 12: DNA-DIRECTED RNA POLYMERASE RPO10 SUBUNIT

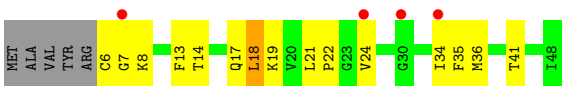


• Molecule 13: DNA-DIRECTED RNA POLYMERASE RPO12 SUBUNIT



• Molecule 13: DNA-DIRECTED RNA POLYMERASE RPO12 SUBUNIT





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	196.09Å 211.87Å 238.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.20 – 3.52 30.20 – 3.52	Depositor EDS
% Data completeness (in resolution range)	92.4 (30.20-3.52) 92.2 (30.20-3.52)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 3.56Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.333 , 0.384 0.332 , 0.381	Depositor DCC
R_{free} test set	5721 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	79.9	Xtrriage
Anisotropy	0.651	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 69.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	52739	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.85 % 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 5.4742e-04. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, 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	0.59	0/6834	0.94	10/9247 (0.1%)
1	W	0.61	1/6834 (0.0%)	0.94	13/9247 (0.1%)
2	B	0.61	0/8816	0.96	18/11926 (0.2%)
2	R	0.61	0/8816	0.96	17/11926 (0.1%)
3	C	0.64	1/2857 (0.0%)	0.94	4/3847 (0.1%)
3	Y	0.69	1/2857 (0.0%)	0.96	4/3847 (0.1%)
4	D	0.53	0/2106	0.81	0/2845
4	S	0.52	0/2106	0.81	1/2845 (0.0%)
5	E	0.61	0/1405	0.92	2/1899 (0.1%)
5	T	0.62	0/1405	0.93	2/1899 (0.1%)
6	F	0.60	1/710 (0.1%)	0.81	0/963
6	U	0.60	1/710 (0.1%)	0.80	0/963
7	G	0.65	0/913	0.86	0/1224
7	V	0.65	0/913	0.87	1/1224 (0.1%)
8	H	0.60	0/623	0.98	2/845 (0.2%)
8	Z	0.61	0/623	1.04	4/845 (0.5%)
9	I	0.65	0/667	0.99	1/903 (0.1%)
9	K	0.64	0/667	0.96	1/903 (0.1%)
10	J	0.66	0/305	0.91	1/408 (0.2%)
10	Q	0.67	1/278 (0.4%)	0.85	0/373
11	L	0.60	1/718 (0.1%)	0.86	0/970
11	M	0.60	1/718 (0.1%)	0.84	0/970
12	N	0.60	0/524	0.83	0/706
12	O	0.58	0/524	0.82	0/706
13	P	0.66	0/354	0.89	0/475
13	X	0.65	0/354	0.86	0/475
All	All	0.61	8/53637 (0.0%)	0.93	81/72481 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	119	THR	CA-CB	8.00	1.58	1.52
6	F	92	ASN	C-N	-7.03	1.23	1.33
10	Q	76	GLU	C-N	-6.94	1.23	1.33
11	M	91	THR	C-N	-6.87	1.23	1.33
6	U	92	ASN	C-N	-6.86	1.23	1.33
11	L	91	THR	C-N	-6.76	1.23	1.33
3	C	119	THR	CA-CB	6.69	1.57	1.52
1	W	499	ALA	CA-C	5.90	1.55	1.52

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	79	ARG	CA-C-N	8.73	128.79	119.89
1	W	79	ARG	C-N-CA	8.73	128.79	119.89
1	A	79	ARG	CA-C-N	8.45	128.51	119.89
1	A	79	ARG	C-N-CA	8.45	128.51	119.89
2	R	56	ILE	CA-C-N	6.95	128.53	119.84
2	R	56	ILE	C-N-CA	6.95	128.53	119.84
2	B	56	ILE	CA-C-N	6.88	128.44	119.84
2	B	56	ILE	C-N-CA	6.88	128.44	119.84
2	R	224	ILE	CA-C-N	6.65	128.15	119.84
2	R	224	ILE	C-N-CA	6.65	128.15	119.84
2	B	224	ILE	CA-C-N	6.36	127.79	119.84
2	B	224	ILE	C-N-CA	6.36	127.79	119.84
2	R	275	ILE	N-CA-C	-6.26	106.86	112.12
1	A	153	GLN	N-CA-C	6.19	118.47	109.07
1	W	153	GLN	N-CA-C	6.14	118.40	109.07
2	B	443	PHE	N-CA-C	-6.14	106.39	114.31
2	R	632	GLU	CA-C-N	5.96	127.29	119.84
2	R	632	GLU	C-N-CA	5.96	127.29	119.84
9	I	90	LEU	N-CA-C	5.96	118.57	110.35
2	R	599	LYS	CB-CA-C	-5.93	109.16	117.23
1	A	113	LYS	N-CA-C	-5.92	107.29	114.75
2	B	632	GLU	CA-C-N	5.89	127.20	119.84
2	B	632	GLU	C-N-CA	5.89	127.20	119.84
3	Y	334	VAL	N-CA-C	5.87	115.99	110.30
3	C	58	GLU	N-CA-C	-5.86	106.13	113.28
3	C	334	VAL	N-CA-C	5.86	116.05	110.42
8	Z	49	ASP	CA-C-N	5.86	126.27	119.47
8	Z	49	ASP	C-N-CA	5.86	126.27	119.47
2	B	40	ASN	N-CA-C	5.84	117.32	111.07
3	Y	364	GLU	N-CA-C	5.80	117.86	108.34
1	W	811	VAL	N-CA-C	5.75	115.62	106.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	PRO	N-CA-C	5.73	117.69	110.70
5	T	138	LYS	CB-CA-C	-5.72	109.96	116.54
2	R	353	PHE	N-CA-C	-5.70	106.16	113.23
2	R	788	GLY	N-CA-C	5.66	119.18	112.33
2	B	599	LYS	CB-CA-C	-5.64	109.56	117.23
3	C	350	THR	N-CA-C	5.63	118.72	109.72
1	A	740	ILE	N-CA-C	-5.60	105.07	110.72
2	R	908	VAL	CA-C-N	-5.59	114.83	120.31
2	R	908	VAL	C-N-CA	-5.59	114.83	120.31
5	E	138	LYS	CB-CA-C	-5.58	110.12	116.54
1	W	113	LYS	N-CA-C	-5.55	107.76	114.75
1	W	862	HIS	N-CA-C	-5.48	99.12	110.80
1	A	257	ALA	CA-C-N	5.48	126.69	119.84
1	A	257	ALA	C-N-CA	5.48	126.69	119.84
3	Y	58	GLU	N-CA-C	-5.48	106.59	113.28
2	B	353	PHE	N-CA-C	-5.47	106.45	113.23
1	A	811	VAL	N-CA-C	5.45	115.16	106.88
1	A	210	THR	N-CA-C	-5.44	106.77	113.41
8	Z	42	LEU	CA-C-N	5.43	126.63	119.84
8	Z	42	LEU	C-N-CA	5.43	126.63	119.84
5	E	126	ILE	N-CA-C	-5.43	107.83	113.10
9	K	90	LEU	N-CA-C	5.43	118.77	110.36
2	B	778	MET	CA-C-N	5.42	126.61	119.84
2	B	778	MET	C-N-CA	5.42	126.61	119.84
1	W	257	ALA	CA-C-N	5.37	126.55	119.84
1	W	257	ALA	C-N-CA	5.37	126.55	119.84
1	W	499	ALA	N-CA-C	5.36	117.32	108.48
8	H	49	ASP	CA-C-N	5.35	125.67	119.47
8	H	49	ASP	C-N-CA	5.35	125.67	119.47
2	B	275	ILE	N-CA-C	-5.28	107.68	112.12
2	R	146	GLU	N-CA-C	5.28	117.22	109.24
3	C	364	GLU	N-CA-C	5.27	116.98	108.34
1	W	210	THR	N-CA-C	-5.21	107.06	113.41
2	B	163	VAL	N-CA-C	5.16	115.34	108.11
2	R	443	PHE	N-CA-C	-5.15	107.67	114.31
2	B	780	GLU	CA-C-N	5.14	126.27	119.84
2	B	780	GLU	C-N-CA	5.14	126.27	119.84
2	R	1071	GLY	N-CA-C	5.14	118.23	111.03
3	Y	350	THR	N-CA-C	5.13	117.93	109.72
2	B	908	VAL	CA-C-N	-5.12	115.29	120.31
2	B	908	VAL	C-N-CA	-5.12	115.29	120.31
4	S	155	LYS	N-CA-C	-5.12	105.89	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	775	SER	CA-C-N	5.11	126.23	119.84
1	W	775	SER	C-N-CA	5.11	126.23	119.84
1	W	451	PRO	N-CA-C	5.07	116.89	110.70
2	R	778	MET	CA-C-N	5.06	126.17	119.84
2	R	778	MET	C-N-CA	5.06	126.17	119.84
7	V	77	ILE	N-CA-C	5.04	115.91	108.45
5	T	72	PHE	N-CA-C	5.04	117.33	109.52
10	J	79	ASP	N-CA-C	5.03	115.78	108.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6691	0	6756	314	0
1	W	6691	0	6760	341	0
2	B	8652	0	8795	377	0
2	R	8652	0	8796	403	0
3	C	2833	0	2992	139	0
3	Y	2833	0	2992	160	0
4	D	2071	0	2116	82	0
4	S	2071	0	2116	80	0
5	E	1384	0	1444	44	0
5	T	1384	0	1444	40	0
6	F	702	0	708	17	0
6	U	702	0	708	21	0
7	G	901	0	912	36	0
7	V	901	0	912	33	0
8	H	609	0	640	28	0
8	Z	609	0	640	35	0
9	I	658	0	692	28	0
9	K	658	0	692	33	0
10	J	301	0	284	10	0
10	Q	274	0	258	9	0
11	L	708	0	739	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	M	708	0	739	26	0
12	N	514	0	528	31	0
12	O	514	0	529	35	0
13	P	346	0	376	23	0
13	X	346	0	374	10	0
14	A	2	0	0	0	0
14	B	1	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	1	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	0	0
16	S	7	0	0	0	0
All	All	52739	0	53942	2067	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 19.

All (2067) 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)
2:R:816:LYS:H	2:R:839:SER:HB3	1.13	1.12
2:B:856:THR:HG22	2:B:857:GLU:H	1.14	1.11
2:R:856:THR:HG22	2:R:857:GLU:H	1.17	1.08
3:C:244:LYS:HA	3:C:245:LYS:HB3	1.32	1.07
3:Y:244:LYS:HA	3:Y:245:LYS:HB3	1.33	1.07
2:B:981:LYS:HE2	4:D:205:LEU:HD13	1.37	1.06
2:R:110:ILE:HA	2:R:111:GLU:CB	1.84	1.05
2:B:110:ILE:HA	2:B:111:GLU:HB2	1.10	1.05
2:B:400:ALA:HA	2:B:403:THR:HG22	1.38	1.05
2:B:110:ILE:HA	2:B:111:GLU:CB	1.87	1.04
3:C:62:GLY:O	3:C:63:LEU:HG	1.59	1.02
3:Y:62:GLY:O	3:Y:63:LEU:HG	1.59	1.02
2:B:461:THR:HG21	2:B:468:GLY:H	1.24	1.01
2:R:110:ILE:HA	2:R:111:GLU:HB2	1.04	1.01
2:R:898:VAL:HG21	4:S:34:LEU:HD21	1.38	1.01
2:B:816:LYS:H	2:B:839:SER:HB3	1.22	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:14:TYR:HD2	6:F:74:SER:HG	1.09	1.00
6:U:14:TYR:HD2	6:U:74:SER:HG	1.10	0.98
2:R:110:ILE:CA	2:R:111:GLU:HB2	1.92	0.98
2:R:31:LEU:HA	2:R:125:MET:HE1	1.46	0.97
1:W:573:ARG:HH11	1:W:573:ARG:HG3	1.28	0.96
2:R:1031:PHE:HE1	1:W:430:MET:HE1	1.29	0.95
2:B:873:ARG:HB3	2:B:999:MET:HE1	1.48	0.95
2:B:31:LEU:HA	2:B:125:MET:HE1	1.48	0.94
2:B:665:GLN:HG2	2:B:667:PRO:HD2	1.48	0.94
2:B:110:ILE:CA	2:B:111:GLU:HB2	1.97	0.94
2:R:400:ALA:HA	2:R:403:THR:HG22	1.47	0.94
2:R:893:MET:HE3	2:R:894:LEU:H	1.32	0.94
1:A:573:ARG:HH11	1:A:573:ARG:HG3	1.33	0.93
2:R:953:ILE:HD13	2:R:953:ILE:H	1.34	0.93
2:R:461:THR:HG21	2:R:468:GLY:H	1.29	0.92
2:B:884:ARG:NH1	2:B:992:TYR:HB3	1.84	0.91
2:R:736:ASN:HD22	2:R:736:ASN:H	1.19	0.90
2:R:1074:ASP:HB3	2:R:1075:LYS:HB3	1.53	0.90
3:Y:70:ILE:HA	3:Y:73:VAL:HG22	1.51	0.89
2:B:430:ARG:HD3	2:B:653:ILE:HG12	1.52	0.89
2:B:736:ASN:HD22	2:B:736:ASN:H	1.17	0.89
1:W:235:LEU:HA	1:W:238:LYS:HE3	1.54	0.89
3:C:13:LEU:HD13	3:C:48:ILE:HG12	1.55	0.88
3:C:163:MET:HB2	3:C:164:SER:HA	1.55	0.88
1:A:235:LEU:HA	1:A:238:LYS:HE3	1.53	0.88
2:B:1074:ASP:HB3	2:B:1075:LYS:HB3	1.51	0.88
2:B:953:ILE:HD13	2:B:953:ILE:H	1.38	0.87
2:R:873:ARG:HB3	2:R:999:MET:HE1	1.56	0.87
3:C:70:ILE:HA	3:C:73:VAL:HG22	1.57	0.87
2:R:884:ARG:NH1	2:R:992:TYR:HB3	1.89	0.87
1:A:486:ILE:HA	1:A:496:ILE:HD12	1.56	0.87
1:A:23:SER:HB2	1:A:74:HIS:NE2	1.90	0.86
2:R:816:LYS:N	2:R:839:SER:HB3	1.88	0.86
11:M:69:LEU:HD23	4:S:260:LEU:HD11	1.57	0.86
2:R:665:GLN:HG2	2:R:667:PRO:HD2	1.55	0.86
2:R:430:ARG:HD3	2:R:653:ILE:HG12	1.57	0.86
3:Y:315:LEU:O	3:Y:319:VAL:HG23	1.74	0.86
2:R:245:VAL:HG21	2:R:256:PHE:CE2	2.10	0.85
3:Y:163:MET:HB2	3:Y:164:SER:HA	1.55	0.85
2:B:703:ARG:O	2:B:724:ASN:ND2	2.10	0.85
2:B:106:VAL:HG22	2:B:110:ILE:HG23	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:49:LEU:HD21	2:R:893:MET:HE1	1.59	0.83
1:A:573:ARG:HH11	1:A:573:ARG:CG	1.90	0.83
1:A:69:PRO:HG2	2:B:1101:LYS:HE3	1.61	0.83
1:W:23:SER:HB2	1:W:74:HIS:NE2	1.93	0.83
1:W:573:ARG:HH11	1:W:573:ARG:CG	1.92	0.82
1:W:867:ASP:HA	1:W:870:ARG:NH2	1.94	0.82
2:R:106:VAL:HG22	2:R:110:ILE:HG23	1.61	0.82
2:R:1031:PHE:CE1	1:W:430:MET:HE1	2.14	0.82
3:Y:13:LEU:HD13	3:Y:48:ILE:HG12	1.62	0.82
2:R:703:ARG:O	2:R:724:ASN:ND2	2.12	0.81
2:B:245:VAL:HG21	2:B:256:PHE:CE2	2.15	0.81
3:Y:152:VAL:HG22	3:Y:174:LEU:HD12	1.61	0.81
3:C:327:ARG:HH22	3:C:337:GLU:HB3	1.45	0.81
3:C:16:LYS:HD2	3:C:52:PHE:CE1	2.15	0.81
2:B:419:ARG:HH12	2:B:690:ARG:HH12	1.25	0.81
3:C:152:VAL:HG22	3:C:174:LEU:HD12	1.63	0.81
3:C:163:MET:CB	3:C:164:SER:HA	2.11	0.81
3:Y:327:ARG:HH22	3:Y:337:GLU:HB3	1.46	0.81
9:K:79:ARG:HG2	9:K:89:LEU:HD23	1.63	0.80
2:B:816:LYS:N	2:B:839:SER:HB3	1.97	0.80
1:W:600:LYS:O	1:W:601:LYS:HB2	1.81	0.80
10:J:51:TRP:HE3	8:Z:25:ILE:HG12	1.47	0.80
9:I:79:ARG:HG2	9:I:89:LEU:HD23	1.64	0.79
1:A:106:ILE:HG22	1:A:107:SER:H	1.46	0.79
2:R:856:THR:HG22	2:R:857:GLU:N	1.98	0.79
1:A:324:THR:HG21	1:A:441:LEU:O	1.83	0.79
2:B:480:ALA:HB2	2:B:579:ARG:HD2	1.63	0.79
2:R:9:SER:HB3	2:R:12:GLU:OE1	1.83	0.79
2:B:367:ASP:O	2:B:371:GLN:HB2	1.82	0.79
2:R:480:ALA:HB2	2:R:579:ARG:HD2	1.63	0.79
2:R:31:LEU:HA	2:R:125:MET:CE	2.13	0.79
3:Y:163:MET:CB	3:Y:164:SER:HA	2.11	0.79
5:E:1:MET:HE1	5:E:85:VAL:HB	1.65	0.78
2:B:893:MET:HE3	2:B:894:LEU:H	1.48	0.78
1:W:614:TRP:O	1:W:618:GLU:HG2	1.84	0.78
4:S:66:PRO:HG2	4:S:124:ILE:HG12	1.63	0.78
2:B:31:LEU:HA	2:B:125:MET:CE	2.14	0.77
2:B:400:ALA:HA	2:B:403:THR:CG2	2.13	0.77
3:C:315:LEU:O	3:C:319:VAL:HG23	1.84	0.77
2:R:893:MET:CE	2:R:894:LEU:H	1.97	0.77
3:Y:16:LYS:HD2	3:Y:52:PHE:CE1	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:ILE:HG21	1:A:632:PHE:HE1	1.49	0.77
1:W:486:ILE:HA	1:W:496:ILE:HD12	1.64	0.77
1:A:600:LYS:O	1:A:601:LYS:HB2	1.84	0.77
3:Y:348:GLU:OE1	3:Y:350:THR:HB	1.86	0.76
2:R:367:ASP:O	2:R:371:GLN:HB2	1.86	0.76
2:B:545:GLU:O	2:B:549:LYS:HG2	1.86	0.76
4:D:66:PRO:HG2	4:D:124:ILE:HG12	1.66	0.76
8:H:25:ILE:HG12	10:Q:51:TRP:HE3	1.50	0.76
2:B:856:THR:HG22	2:B:857:GLU:N	1.96	0.76
1:A:652:SER:HB3	1:A:787:ARG:HE	1.51	0.76
1:W:106:ILE:HG22	1:W:107:SER:H	1.51	0.76
1:A:870:ARG:HD2	3:C:57:LYS:CB	2.16	0.75
3:Y:329:ILE:O	3:Y:335:THR:HG22	1.85	0.75
2:R:594:ARG:NH1	2:R:615:LYS:HB2	2.00	0.75
1:W:324:THR:HG21	1:W:441:LEU:O	1.87	0.75
5:E:30:LEU:HD22	5:E:72:PHE:CE1	2.22	0.75
2:R:545:GLU:O	2:R:549:LYS:HG2	1.86	0.75
4:D:73:LEU:HD11	4:D:236:LEU:HD21	1.66	0.75
2:R:627:ALA:HB1	2:R:642:HIS:HD2	1.51	0.75
5:T:30:LEU:HD22	5:T:72:PHE:CE1	2.22	0.75
1:W:725:ALA:HA	1:W:728:MET:HE2	1.69	0.75
1:A:725:ALA:HA	1:A:728:MET:HE2	1.69	0.74
2:B:594:ARG:NH1	2:B:615:LYS:HB2	2.02	0.74
2:B:1065:ASP:HB3	2:B:1089:SER:HB2	1.69	0.74
2:R:563:THR:HG22	2:R:564:ASP:H	1.52	0.74
2:R:245:VAL:HG21	2:R:256:PHE:HE2	1.47	0.74
1:W:431:MET:HE2	1:W:482:VAL:HA	1.70	0.74
1:W:864:LYS:NZ	3:Y:29:VAL:O	2.18	0.74
1:W:876:VAL:C	1:W:878:TRP:H	1.93	0.74
3:C:339:ASN:HB2	3:C:344:ARG:HD3	1.68	0.74
8:H:45:ILE:O	8:H:81:VAL:HA	1.87	0.74
12:N:6:ARG:HA	12:N:12:SER:O	1.87	0.74
2:R:1065:ASP:HB3	2:R:1089:SER:HB2	1.68	0.74
1:A:859:TYR:OH	9:K:29:ARG:HD2	1.87	0.74
2:R:539:LEU:HD12	2:R:569:VAL:HG11	1.69	0.74
2:B:406:TRP:CG	2:B:407:VAL:H	2.06	0.74
2:R:918:LEU:HD13	1:W:646:MET:HG2	1.68	0.74
5:T:1:MET:HE1	5:T:85:VAL:HB	1.68	0.74
5:T:6:LYS:HA	5:T:72:PHE:O	1.88	0.73
1:W:603:ILE:HG21	1:W:632:PHE:HE1	1.52	0.73
1:W:652:SER:HB3	1:W:787:ARG:HE	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:VAL:HG21	2:B:256:PHE:HE2	1.52	0.73
2:B:106:VAL:HG22	2:B:110:ILE:CG2	2.18	0.73
1:A:870:ARG:HD2	3:C:57:LYS:HB3	1.71	0.73
2:B:256:PHE:HB2	2:B:257:PRO:HD3	1.71	0.73
2:B:857:GLU:HG3	13:P:24:VAL:HG11	1.71	0.73
3:C:348:GLU:OE1	3:C:350:THR:HB	1.89	0.73
4:S:73:LEU:HD11	4:S:236:LEU:HD21	1.68	0.73
3:Y:127:THR:H	3:Y:268:ASP:HB2	1.54	0.73
1:A:271:TYR:HE1	1:A:285:PRO:HB3	1.54	0.72
1:A:876:VAL:C	1:A:878:TRP:H	1.97	0.72
8:Z:45:ILE:O	8:Z:81:VAL:HA	1.88	0.72
2:R:783:VAL:HG12	2:R:784:ARG:HB2	1.70	0.72
2:R:749:GLU:O	4:S:60:HIS:HE1	1.72	0.72
2:B:627:ALA:HB1	2:B:642:HIS:HD2	1.55	0.72
1:A:866:VAL:C	1:A:870:ARG:HH22	1.97	0.72
2:R:256:PHE:HB2	2:R:257:PRO:HD3	1.72	0.72
2:R:898:VAL:CG2	4:S:34:LEU:HD21	2.18	0.72
5:E:6:LYS:HA	5:E:72:PHE:O	1.90	0.72
2:R:419:ARG:HH12	2:R:690:ARG:HH12	1.38	0.72
1:A:867:ASP:HA	1:A:870:ARG:NH2	2.05	0.71
2:R:703:ARG:HD2	2:R:717:THR:HG22	1.71	0.71
2:B:733:THR:HG23	2:B:735:TYR:HB2	1.73	0.71
2:B:563:THR:HG22	2:B:564:ASP:H	1.55	0.71
11:M:22:HIS:CG	2:R:977:ARG:HB2	2.26	0.71
1:A:614:TRP:O	1:A:618:GLU:HG2	1.90	0.71
2:B:405:ASN:HB2	2:B:413:VAL:HB	1.73	0.71
2:B:856:THR:CG2	2:B:857:GLU:H	1.98	0.71
3:C:127:THR:H	3:C:268:ASP:HB2	1.56	0.71
1:A:603:ILE:HG21	1:A:632:PHE:CE1	2.26	0.71
1:W:603:ILE:HG21	1:W:632:PHE:CE1	2.26	0.71
3:C:331:ARG:HD3	3:C:331:ARG:H	1.56	0.71
2:R:406:TRP:CG	2:R:407:VAL:H	2.08	0.71
2:B:1010:GLY:HA3	2:B:1027:GLY:HA2	1.71	0.71
2:R:405:ASN:HB2	2:R:413:VAL:HB	1.73	0.71
3:Y:244:LYS:HA	3:Y:245:LYS:CB	2.15	0.71
9:I:82:LEU:HD12	9:I:86:LYS:HB3	1.72	0.70
2:R:856:THR:CG2	2:R:857:GLU:H	2.01	0.70
7:V:88:ASN:HD22	1:W:538:ALA:HB2	1.55	0.70
2:B:711:LEU:HD13	2:B:716:TYR:HB3	1.74	0.70
9:I:26:ARG:HG2	9:I:27:LEU:H	1.56	0.70
1:A:184:LEU:HB3	1:A:204:PRO:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:105:LYS:HE2	1:W:105:LYS:HA	1.71	0.70
3:Y:30:GLU:O	3:Y:33:LYS:HG2	1.92	0.70
1:A:430:MET:HE1	2:B:1031:PHE:HE1	1.56	0.70
2:R:711:LEU:HD13	2:R:716:TYR:HB3	1.74	0.70
1:A:471:GLU:HG3	9:K:41:LEU:HD13	1.73	0.70
2:B:333:ARG:O	2:B:334:GLU:HB3	1.92	0.70
2:B:703:ARG:HD2	2:B:717:THR:HG22	1.72	0.69
2:B:981:LYS:CE	4:D:205:LEU:HD13	2.20	0.69
1:A:549:LYS:HE2	7:G:89:GLY:HA2	1.73	0.69
3:C:158:ILE:HG13	3:C:223:ARG:HH21	1.57	0.69
5:E:5:ILE:HA	6:F:8:GLU:O	1.91	0.69
2:R:904:VAL:O	4:S:163:ILE:HG12	1.92	0.69
12:O:8:PHE:CD1	12:O:48:MET:HE1	2.27	0.69
1:W:599:ASP:H	1:W:602:ALA:HB3	1.57	0.69
1:A:540:LEU:HB3	7:G:66:TYR:CE2	2.28	0.69
2:R:31:LEU:HD23	2:R:125:MET:HE3	1.73	0.69
3:Y:331:ARG:H	3:Y:331:ARG:HD3	1.56	0.69
3:Y:339:ASN:HB2	3:Y:344:ARG:HD3	1.74	0.69
1:A:575:CYS:SG	1:A:584:SER:HB3	2.32	0.69
1:W:184:LEU:HB3	1:W:204:PRO:HB2	1.73	0.69
2:R:694:ARG:HA	2:R:758:PHE:O	1.92	0.69
1:W:651:VAL:HG11	1:W:743:MET:HB3	1.75	0.69
3:C:329:ILE:O	3:C:335:THR:HG22	1.93	0.69
8:H:44:TRP:O	8:H:79:ARG:HD2	1.93	0.69
2:R:106:VAL:HG22	2:R:110:ILE:CG2	2.23	0.69
1:W:99:ARG:HG2	1:W:183:ARG:HH22	1.58	0.68
3:C:144:LEU:O	3:C:235:LYS:HG3	1.93	0.68
2:B:419:ARG:NH1	2:B:690:ARG:HH12	1.89	0.68
1:W:58:CYS:SG	1:W:60:THR:HG23	2.33	0.68
1:A:803:ARG:HG2	2:B:447:ASP:HA	1.76	0.68
3:C:30:GLU:O	3:C:33:LYS:HG2	1.93	0.68
12:N:8:PHE:CD1	12:N:48:MET:HE1	2.29	0.68
2:R:400:ALA:HA	2:R:403:THR:CG2	2.20	0.68
2:R:419:ARG:NH1	2:R:690:ARG:HH12	1.91	0.68
1:W:271:TYR:HE1	1:W:285:PRO:HB3	1.58	0.68
1:W:866:VAL:C	1:W:870:ARG:HH22	2.02	0.68
3:Y:222:LEU:O	3:Y:226:ILE:HG13	1.93	0.68
1:A:573:ARG:HG3	1:A:573:ARG:NH1	2.07	0.68
1:A:852:ASP:CG	8:H:75:VAL:HG21	2.19	0.68
1:W:488:THR:HG22	1:W:490:ARG:H	1.59	0.68
1:A:97:THR:HG22	1:A:99:ARG:H	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:233:VAL:HG21	12:N:6:ARG:NH2	2.09	0.68
1:A:99:ARG:HG2	1:A:183:ARG:HH22	1.58	0.68
2:B:543:ILE:HD13	2:B:558:VAL:HG21	1.75	0.68
1:A:64:THR:HG22	1:A:65:LEU:HG	1.75	0.68
1:A:105:LYS:HE2	1:A:105:LYS:HA	1.75	0.68
2:B:133:ILE:HA	2:B:136:TYR:CD1	2.29	0.68
9:I:41:LEU:HD12	1:W:470:GLU:HG3	1.76	0.68
2:R:560:HIS:HB3	2:R:626:ASN:HD21	1.59	0.68
2:R:733:THR:HG23	2:R:735:TYR:HB2	1.76	0.68
2:B:893:MET:CE	2:B:894:LEU:H	2.06	0.67
4:D:260:LEU:HD11	11:L:69:LEU:HD23	1.74	0.67
6:F:72:LEU:HD11	6:F:86:ILE:HG12	1.77	0.67
1:W:729:ALA:O	1:W:730:ARG:HB2	1.94	0.67
1:A:651:VAL:HG11	1:A:743:MET:HB3	1.76	0.67
2:B:783:VAL:HG12	2:B:784:ARG:HB2	1.74	0.67
1:W:95:LYS:HB3	1:W:138:LYS:HG2	1.75	0.67
1:A:431:MET:HE2	1:A:482:VAL:HA	1.77	0.67
2:B:982:ILE:HD12	2:B:984:SER:H	1.60	0.67
9:K:26:ARG:HG2	9:K:27:LEU:H	1.59	0.67
2:R:333:ARG:O	2:R:334:GLU:HB3	1.92	0.67
2:R:905:LYS:HE2	2:R:905:LYS:H	1.58	0.67
3:Y:158:ILE:HG13	3:Y:223:ARG:HH21	1.59	0.67
2:B:598:GLU:HA	2:B:602:SER:CB	2.25	0.67
2:B:668:ARG:NH1	2:B:921:ARG:HD2	2.10	0.67
10:J:51:TRP:CE3	8:Z:25:ILE:HG12	2.30	0.67
1:W:575:CYS:SG	1:W:584:SER:HB3	2.34	0.67
2:B:461:THR:CG2	2:B:468:GLY:H	2.06	0.66
2:B:560:HIS:HB3	2:B:626:ASN:HD21	1.58	0.66
2:R:974:TYR:CE2	2:R:981:LYS:HB3	2.30	0.66
1:A:95:LYS:HB3	1:A:138:LYS:HG2	1.77	0.66
3:Y:226:ILE:HB	3:Y:227:LEU:HD12	1.76	0.66
2:B:539:LEU:HD12	2:B:569:VAL:HG11	1.76	0.66
3:C:146:TYR:HD1	3:C:235:LYS:H	1.44	0.66
12:O:13:LEU:HD11	4:S:66:PRO:HG3	1.76	0.66
6:U:72:LEU:HD11	6:U:86:ILE:HG12	1.76	0.66
1:A:729:ALA:O	1:A:730:ARG:HB2	1.94	0.66
2:B:972:VAL:HG11	4:D:204:THR:HB	1.78	0.66
5:E:145:ARG:HD3	6:F:88:ILE:HG21	1.78	0.66
3:Y:64:ILE:HG22	3:Y:65:ALA:H	1.60	0.66
2:B:694:ARG:HA	2:B:758:PHE:O	1.95	0.66
3:Y:146:TYR:HD1	3:Y:235:LYS:H	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:15:PRO:HD3	5:T:65:ALA:HB2	1.78	0.66
3:Y:286:ILE:HG12	8:Z:49:ASP:CG	2.21	0.66
2:B:897:GLN:HG3	2:B:908:VAL:HG21	1.78	0.66
9:K:68:GLU:O	9:K:74:LEU:HG	1.95	0.66
2:R:133:ILE:HA	2:R:136:TYR:CD1	2.30	0.66
10:J:51:TRP:HE3	8:Z:25:ILE:CG1	2.09	0.66
1:W:421:ARG:HG3	1:W:462:MET:HG2	1.78	0.66
4:S:17:PHE:O	4:S:225:LYS:HA	1.96	0.65
1:W:838:VAL:HB	1:W:847:GLN:HB2	1.77	0.65
8:H:42:LEU:O	8:H:44:TRP:CD1	2.49	0.65
1:W:97:THR:HG22	1:W:99:ARG:H	1.60	0.65
3:C:64:ILE:HG22	3:C:65:ALA:H	1.60	0.65
1:A:538:ALA:HB2	7:G:88:ASN:HD22	1.62	0.65
1:A:599:ASP:H	1:A:602:ALA:HB3	1.61	0.65
2:B:975:ASP:OD2	2:B:977:ARG:HD3	1.96	0.65
2:R:897:GLN:HG3	2:R:908:VAL:HG21	1.79	0.65
8:Z:43:PRO:HB2	8:Z:79:ARG:HD3	1.79	0.65
4:D:17:PHE:O	4:D:225:LYS:HA	1.97	0.65
1:A:130:ARG:HH11	1:A:196:GLY:HA2	1.62	0.65
9:K:23:TRP:CE3	9:K:23:TRP:HA	2.32	0.65
2:R:972:VAL:HG11	4:S:204:THR:HB	1.79	0.65
1:W:868:VAL:HG22	3:Y:39:LYS:HZ3	1.62	0.65
2:B:768:TYR:HD1	2:B:819:PRO:HG2	1.62	0.64
5:E:15:PRO:HD3	5:E:65:ALA:HB2	1.78	0.64
2:R:446:ARG:HH22	2:R:465:PRO:HA	1.62	0.64
2:R:975:ASP:OD2	2:R:977:ARG:HD3	1.97	0.64
3:Y:53:ASP:HA	3:Y:56:ILE:HG12	1.79	0.64
3:Y:347:PHE:O	3:Y:348:GLU:HB3	1.97	0.64
1:W:868:VAL:HG22	3:Y:39:LYS:NZ	2.12	0.64
2:B:974:TYR:CE2	2:B:981:LYS:HB3	2.31	0.64
3:C:341:VAL:HG12	3:C:344:ARG:HH22	1.61	0.64
4:D:66:PRO:HG3	12:N:13:LEU:HD11	1.80	0.64
9:I:68:GLU:O	9:I:74:LEU:HG	1.97	0.64
2:R:709:ARG:HG3	2:R:944:ASP:OD2	1.97	0.64
2:R:922:MET:HG2	1:W:743:MET:HG3	1.80	0.64
12:O:6:ARG:HA	12:O:12:SER:O	1.97	0.64
3:Y:341:VAL:HG12	3:Y:344:ARG:HH22	1.62	0.64
5:E:108:VAL:HB	5:E:162:LEU:HB2	1.80	0.64
5:T:141:LYS:HB3	5:T:172:LEU:HD13	1.78	0.64
1:W:365:VAL:HG11	1:W:401:LEU:HD11	1.78	0.64
3:Y:150:GLU:HG3	3:Y:227:LEU:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:502:GLU:O	2:B:506:ARG:HB2	1.97	0.64
2:B:168:GLU:O	2:B:435:SER:HB2	1.98	0.64
1:A:430:MET:HE1	2:B:1031:PHE:CE1	2.32	0.64
2:R:359:VAL:HG11	2:R:407:VAL:HG13	1.80	0.64
5:T:40:LYS:HG3	5:T:153:VAL:HB	1.80	0.64
3:Y:69:ALA:HB2	3:Y:381:LEU:HD13	1.80	0.64
3:Y:274:THR:HG22	3:Y:276:ASN:H	1.63	0.64
2:B:1005:HIS:NE2	2:B:1007:ARG:HD2	2.13	0.63
3:C:69:ALA:HB2	3:C:381:LEU:HD13	1.80	0.63
2:R:380:ARG:HD3	2:R:381:LYS:HE3	1.80	0.63
2:B:736:ASN:H	2:B:736:ASN:ND2	1.91	0.63
3:C:53:ASP:HA	3:C:56:ILE:HG12	1.80	0.63
5:E:141:LYS:HB3	5:E:172:LEU:HD13	1.80	0.63
1:A:99:ARG:HG2	1:A:183:ARG:NH2	2.13	0.63
1:A:777:GLU:HG3	1:A:783:TYR:HE2	1.63	0.63
2:B:91:ARG:HD3	2:B:856:THR:HG21	1.78	0.63
2:B:905:LYS:H	2:B:905:LYS:HE2	1.62	0.63
3:C:150:GLU:HG3	3:C:227:LEU:HB3	1.80	0.63
2:R:590:PRO:O	2:R:615:LYS:HD2	1.99	0.63
1:W:99:ARG:HG2	1:W:183:ARG:NH2	2.13	0.63
2:B:1074:ASP:HB3	2:B:1075:LYS:CB	2.28	0.63
2:R:543:ILE:HD13	2:R:558:VAL:HG21	1.80	0.63
2:R:761:TYR:HE2	2:R:843:ARG:HG2	1.64	0.63
2:B:446:ARG:HH22	2:B:465:PRO:HA	1.63	0.63
4:S:155:LYS:HE3	4:S:156:PHE:CE1	2.34	0.63
1:W:78:VAL:O	1:W:79:ARG:HB2	1.99	0.63
1:W:876:VAL:C	1:W:878:TRP:N	2.55	0.63
3:C:347:PHE:C	3:C:349:VAL:H	2.05	0.63
3:Y:347:PHE:C	3:Y:349:VAL:H	2.07	0.63
2:B:52:ILE:N	2:B:53:PRO:HD3	2.14	0.62
2:B:786:TYR:CE2	2:B:788:GLY:HA2	2.34	0.62
3:C:244:LYS:HA	3:C:245:LYS:CB	2.14	0.62
1:W:380:ARG:HH11	1:W:384:ARG:HE	1.47	0.62
2:B:759:ARG:NH1	2:B:846:GLU:OE2	2.31	0.62
12:O:6:ARG:NH2	4:S:233:VAL:HG21	2.14	0.62
2:B:380:ARG:HD3	2:B:381:LYS:HE3	1.81	0.62
2:R:446:ARG:HH11	1:W:807:VAL:HG13	1.64	0.62
2:R:786:TYR:CE2	2:R:788:GLY:HA2	2.34	0.62
2:R:1111:ILE:O	2:R:1111:ILE:HG22	1.99	0.62
7:V:88:ASN:HD22	1:W:538:ALA:CB	2.12	0.62
2:B:31:LEU:HD23	2:B:125:MET:HE3	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:34:LEU:HA	4:D:150:GLY:HA3	1.81	0.62
2:R:51:GLU:HB2	2:R:53:PRO:HD3	1.81	0.62
1:W:573:ARG:HG3	1:W:573:ARG:NH1	2.05	0.62
9:I:47:ALA:HB1	9:I:48:PRO:CD	2.30	0.62
1:W:553:SER:OG	1:W:592:ILE:HA	2.00	0.62
2:R:52:ILE:N	2:R:53:PRO:HD3	2.15	0.62
1:W:879:LYS:HZ3	3:Y:44:THR:HB	1.63	0.62
1:A:78:VAL:O	1:A:79:ARG:HB2	2.00	0.62
1:A:600:LYS:HB2	1:A:732:GLY:CA	2.29	0.62
2:B:709:ARG:HG3	2:B:944:ASP:OD2	1.99	0.62
2:B:800:VAL:HB	13:P:36:MET:HE1	1.81	0.62
3:C:226:ILE:HB	3:C:227:LEU:HD12	1.81	0.62
2:R:1074:ASP:HB3	2:R:1075:LYS:CB	2.28	0.62
2:R:708:THR:O	2:R:711:LEU:HB2	2.00	0.62
1:W:130:ARG:HH11	1:W:196:GLY:HA2	1.63	0.62
2:B:430:ARG:HD3	2:B:653:ILE:CG1	2.28	0.62
5:E:40:LYS:HG3	5:E:153:VAL:HB	1.82	0.62
5:E:47:ALA:HB3	5:E:75:ILE:HD12	1.81	0.62
2:R:982:ILE:HD12	2:R:984:SER:H	1.65	0.62
2:R:502:GLU:O	2:R:506:ARG:HB2	1.99	0.61
1:A:761:TYR:HB3	2:B:625:GLU:OE1	2.00	0.61
1:A:876:VAL:C	1:A:878:TRP:N	2.58	0.61
2:B:43:GLN:HA	2:B:66:ILE:HD11	1.82	0.61
2:B:432:VAL:HG21	2:B:456:MET:HE3	1.81	0.61
3:C:222:LEU:O	3:C:226:ILE:HG13	1.99	0.61
2:R:563:THR:HG22	2:R:564:ASP:N	2.15	0.61
5:T:47:ALA:HB3	5:T:75:ILE:HD12	1.82	0.61
5:T:108:VAL:HB	5:T:162:LEU:HB2	1.81	0.61
1:A:127:SER:HA	1:A:130:ARG:HD2	1.81	0.61
5:E:6:LYS:HB2	6:F:8:GLU:HB2	1.81	0.61
1:W:109:ASP:HB3	1:W:113:LYS:HE3	1.81	0.61
3:Y:276:ASN:ND2	3:Y:279:GLU:OE2	2.31	0.61
1:A:380:ARG:HH11	1:A:384:ARG:HE	1.46	0.61
2:B:584:ILE:HD11	2:B:617:GLU:HB2	1.82	0.61
1:W:867:ASP:HA	1:W:870:ARG:HH21	1.65	0.61
1:A:109:ASP:HB3	1:A:113:LYS:HE3	1.81	0.61
1:A:549:LYS:HD2	1:A:593:LEU:HD22	1.81	0.61
3:C:270:ALA:HA	8:H:14:HIS:HB3	1.81	0.61
2:R:432:VAL:HG21	2:R:456:MET:HE3	1.82	0.61
2:R:893:MET:HE3	2:R:894:LEU:N	2.11	0.61
1:W:64:THR:HG22	1:W:65:LEU:HG	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:541:ALA:HB3	1:W:542:PRO:CD	2.30	0.61
8:Z:42:LEU:O	8:Z:44:TRP:CD1	2.54	0.61
1:A:488:THR:HG22	1:A:490:ARG:H	1.65	0.61
2:B:870:ARG:NH1	4:D:56:GLU:OE2	2.32	0.61
2:R:168:GLU:O	2:R:435:SER:HB2	2.00	0.61
1:A:365:VAL:HG11	1:A:401:LEU:HD11	1.83	0.61
2:R:91:ARG:HD3	2:R:856:THR:HG21	1.82	0.61
2:R:433:ILE:HG12	2:R:470:VAL:HB	1.81	0.61
2:B:9:SER:HB3	2:B:12:GLU:OE1	2.00	0.61
2:B:857:GLU:HA	2:B:862:ASN:O	2.01	0.61
4:D:2:SER:HB2	4:D:18:GLU:HB3	1.83	0.61
12:O:47:ARG:HD2	2:R:724:ASN:O	2.00	0.61
2:R:930:GLY:HA2	2:R:990:VAL:O	2.01	0.61
2:R:984:SER:O	2:R:985:ARG:HB2	2.01	0.61
7:V:79:THR:HG22	7:V:80:GLU:N	2.16	0.61
1:A:449:VAL:HG12	1:A:452:PRO:HG2	1.82	0.61
1:A:854:GLY:O	3:C:64:ILE:CG2	2.49	0.61
7:V:72:CYS:HB3	7:V:114:LYS:HG2	1.82	0.61
3:Y:144:LEU:O	3:Y:235:LYS:HG3	2.00	0.61
3:C:372:ASN:HA	3:C:375:ILE:HG22	1.82	0.61
9:K:47:ALA:HB1	9:K:48:PRO:CD	2.31	0.60
2:R:1005:HIS:NE2	2:R:1007:ARG:HD2	2.16	0.60
1:W:755:GLU:HB3	1:W:758:LYS:NZ	2.15	0.60
1:W:879:LYS:NZ	3:Y:44:THR:O	2.34	0.60
2:R:736:ASN:H	2:R:736:ASN:ND2	1.93	0.60
12:N:64:ARG:HH22	13:P:37:VAL:HG23	1.66	0.60
4:S:188:PHE:HB3	4:S:195:LEU:HD22	1.84	0.60
5:T:6:LYS:HB2	6:U:8:GLU:HB2	1.82	0.60
1:W:421:ARG:HB2	1:W:462:MET:HE3	1.83	0.60
4:D:188:PHE:HB3	4:D:195:LEU:HD22	1.84	0.60
3:C:122:MET:HG2	3:C:274:THR:HG23	1.84	0.60
7:G:18:ILE:HD12	7:G:29:ILE:HG12	1.83	0.60
7:G:79:THR:HG22	7:G:80:GLU:H	1.67	0.60
2:R:110:ILE:CA	2:R:111:GLU:CB	2.68	0.60
7:V:80:GLU:HG3	7:V:81:LEU:H	1.66	0.60
3:Y:328:GLN:HG2	3:Y:330:GLY:H	1.66	0.60
1:A:545:TYR:CD2	7:G:46:ILE:HD11	2.37	0.60
1:A:848:VAL:O	1:A:849:ALA:HB3	2.00	0.60
2:B:984:SER:O	2:B:985:ARG:HB2	2.01	0.60
2:B:1042:PHE:O	9:K:30:TYR:HE2	1.85	0.60
2:R:759:ARG:NH1	2:R:846:GLU:OE2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:708:THR:O	2:B:711:LEU:HB2	2.02	0.60
7:G:79:THR:HG22	7:G:80:GLU:N	2.16	0.60
2:R:768:TYR:HD1	2:R:819:PRO:HG2	1.66	0.60
3:C:281:GLU:OE1	3:C:326:VAL:HG12	2.02	0.60
3:C:328:GLN:HG2	3:C:330:GLY:H	1.66	0.60
12:O:35:LEU:HD13	12:O:46:ARG:HG3	1.83	0.60
4:D:38:VAL:CG1	4:D:39:MET:N	2.65	0.59
1:W:109:ASP:O	1:W:113:LYS:HG3	2.01	0.59
1:W:127:SER:HA	1:W:130:ARG:HD2	1.84	0.59
2:B:91:ARG:CD	2:B:856:THR:HG21	2.33	0.59
1:W:601:LYS:O	1:W:610:SER:HB2	2.02	0.59
1:A:734:ARG:NH1	2:B:916:HIS:O	2.33	0.59
2:B:563:THR:HG22	2:B:564:ASP:N	2.18	0.59
2:B:684:ALA:O	2:B:687:TYR:HB3	2.01	0.59
8:H:65:ILE:HD11	8:H:79:ARG:HG2	1.83	0.59
11:M:33:ARG:HD2	1:W:519:GLU:HG2	1.82	0.59
1:W:325:VAL:O	1:W:442:THR:HB	2.01	0.59
1:A:109:ASP:O	1:A:113:LYS:HG3	2.02	0.59
2:B:371:GLN:O	2:B:375:SER:HB2	2.01	0.59
2:B:406:TRP:CG	2:B:407:VAL:N	2.70	0.59
7:G:80:GLU:HG3	7:G:81:LEU:H	1.67	0.59
4:S:2:SER:HB2	4:S:18:GLU:HB3	1.83	0.59
4:S:34:LEU:HA	4:S:150:GLY:HA3	1.83	0.59
3:Y:262:LEU:HD11	3:Y:283:VAL:HG11	1.84	0.59
2:B:585:VAL:HG21	2:B:636:LEU:HD11	1.85	0.59
2:R:584:ILE:HD11	2:R:617:GLU:HB2	1.84	0.59
4:S:153:HIS:HB3	4:S:155:LYS:HG2	1.83	0.59
3:Y:281:GLU:OE1	3:Y:326:VAL:HG12	2.03	0.59
2:R:43:GLN:HA	2:R:66:ILE:HD11	1.85	0.59
1:W:734:ARG:HB3	1:W:734:ARG:HH11	1.66	0.59
1:W:753:ARG:HG3	1:W:804:GLU:OE1	2.03	0.59
8:Z:44:TRP:HA	8:Z:80:TYR:H	1.68	0.59
1:A:421:ARG:HB2	1:A:462:MET:HE3	1.84	0.59
1:A:875:VAL:O	1:A:877:GLY:N	2.32	0.59
2:R:1117:ILE:HD11	1:W:10:LYS:HG3	1.83	0.59
5:T:5:ILE:HA	6:U:8:GLU:O	2.01	0.59
2:B:1050:ASP:HA	2:B:1054:ASP:HB2	1.84	0.59
4:D:38:VAL:HG12	4:D:39:MET:N	2.18	0.59
5:E:6:LYS:O	6:F:7:VAL:HG12	2.03	0.59
2:R:1046:MET:HE2	2:R:1046:MET:HA	1.85	0.59
1:W:777:GLU:HG3	1:W:783:TYR:HE2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:44:TRP:HA	8:H:80:TYR:H	1.66	0.59
1:A:431:MET:HE3	1:A:485:ASN:HB2	1.84	0.59
1:A:646:MET:HG2	2:B:918:LEU:HD13	1.83	0.59
2:B:1069:TYR:CB	2:B:1070:ILE:HB	2.33	0.59
7:G:72:CYS:HB3	7:G:114:LYS:HG2	1.85	0.59
2:R:598:GLU:HA	2:R:602:SER:CB	2.33	0.58
1:W:281:ILE:HG21	3:Y:352:LYS:NZ	2.18	0.58
1:W:324:THR:HG22	1:W:325:VAL:H	1.68	0.58
4:D:51:SER:HB2	4:D:52:PRO:HD2	1.85	0.58
5:E:123:VAL:HG22	5:E:125:GLY:H	1.68	0.58
11:L:31:THR:HA	11:L:34:LYS:HD2	1.85	0.58
2:R:916:HIS:O	1:W:734:ARG:NH1	2.33	0.58
1:A:58:CYS:SG	1:A:60:THR:HG23	2.43	0.58
1:A:853:ASP:HB3	1:A:855:VAL:H	1.68	0.58
12:N:14:ILE:HG13	12:N:48:MET:HG3	1.85	0.58
2:R:417:LEU:HD21	2:R:425:MET:HG3	1.85	0.58
4:S:38:VAL:CG1	4:S:39:MET:N	2.65	0.58
1:W:755:GLU:HB3	1:W:758:LYS:HZ2	1.67	0.58
1:A:851:GLY:O	1:A:853:ASP:N	2.35	0.58
8:H:25:ILE:HG12	10:Q:51:TRP:CE3	2.37	0.58
2:R:800:VAL:HB	13:X:36:MET:HE1	1.86	0.58
2:R:953:ILE:HG13	1:W:787:ARG:HH12	1.68	0.58
4:S:38:VAL:HG12	4:S:39:MET:N	2.18	0.58
5:T:6:LYS:O	6:U:7:VAL:HG12	2.04	0.58
7:V:79:THR:HG22	7:V:80:GLU:H	1.68	0.58
1:W:715:ALA:O	1:W:719:LEU:HB3	2.03	0.58
1:A:715:ALA:O	1:A:719:LEU:HB3	2.04	0.58
9:K:82:LEU:HD12	9:K:86:LYS:HB3	1.84	0.58
2:R:1047:LEU:HD21	1:W:418:LEU:HD21	1.84	0.58
3:C:219:LEU:HA	3:C:222:LEU:HD13	1.86	0.58
2:R:430:ARG:HD3	2:R:653:ILE:CG1	2.30	0.58
2:R:658:ILE:O	2:R:661:PRO:HG3	2.04	0.58
5:T:123:VAL:HG22	5:T:125:GLY:H	1.68	0.58
11:M:48:PRO:HG2	2:R:735:TYR:CE2	2.38	0.58
1:W:874:ARG:HB2	3:Y:54:LEU:HD21	1.85	0.58
13:X:7:GLY:HA2	13:X:35:PHE:O	2.03	0.58
8:Z:44:TRP:O	8:Z:79:ARG:HD2	2.04	0.58
1:W:870:ARG:HD2	3:Y:57:LYS:CB	2.34	0.58
1:A:542:PRO:HG2	7:G:46:ILE:HD12	1.86	0.58
2:B:598:GLU:HA	2:B:602:SER:HB2	1.85	0.58
2:R:41:LYS:O	2:R:43:GLN:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:812:ARG:HH22	3:Y:304:GLN:HE22	1.52	0.58
2:B:41:LYS:O	2:B:43:GLN:N	2.37	0.58
3:C:199:ASP:HB2	3:C:206:LEU:HB2	1.86	0.58
4:D:155:LYS:HE3	4:D:156:PHE:CE1	2.38	0.58
7:G:31:MET:HE2	7:G:55:VAL:HG11	1.86	0.58
12:N:7:CYS:SG	12:N:45:CYS:HA	2.44	0.58
2:R:731:SER:OG	1:W:644:PHE:HB3	2.04	0.58
4:D:63:ALA:HB2	13:P:47:ALA:HB1	1.86	0.57
2:R:668:ARG:NH1	2:R:921:ARG:HD2	2.19	0.57
3:Y:47:GLU:HG3	3:Y:51:ILE:HG12	1.86	0.57
3:C:64:ILE:O	9:K:23:TRP:HZ2	1.87	0.57
9:I:23:TRP:HA	9:I:23:TRP:CE3	2.39	0.57
13:P:6:CYS:SG	13:P:18:LEU:HG	2.44	0.57
2:B:761:TYR:HE2	2:B:843:ARG:HG2	1.68	0.57
11:M:49:LEU:CD2	2:R:893:MET:HE1	2.32	0.57
8:Z:65:ILE:HD11	8:Z:79:ARG:HG2	1.86	0.57
1:A:122:LYS:HZ3	10:Q:70:ASP:CG	2.12	0.57
2:B:13:ARG:HH12	2:B:647:SER:H	1.51	0.57
3:C:244:LYS:CA	3:C:245:LYS:HB3	2.22	0.57
2:R:393:VAL:O	2:R:397:ILE:HB	2.04	0.57
13:X:17:GLN:C	13:X:19:LYS:H	2.12	0.57
3:Y:341:VAL:H	3:Y:364:GLU:HG2	1.69	0.57
2:R:371:GLN:O	2:R:375:SER:HB2	2.04	0.57
7:V:31:MET:HE2	7:V:55:VAL:HG11	1.87	0.57
1:W:819:MET:SD	3:Y:107:LEU:HD22	2.45	0.57
1:A:177:PRO:HD2	1:A:266:TRP:HZ2	1.69	0.57
1:A:317:ARG:HA	2:B:1030:ARG:HA	1.86	0.57
2:B:590:PRO:O	2:B:615:LYS:HD2	2.05	0.57
2:R:684:ALA:O	2:R:687:TYR:HB3	2.05	0.57
2:R:1104:ILE:HA	2:R:1107:LEU:HD12	1.85	0.57
4:S:161:LEU:HG	4:S:163:ILE:HD13	1.86	0.57
2:R:688:GLN:O	2:R:868:ARG:NH2	2.37	0.57
1:W:177:PRO:HD2	1:W:266:TRP:HZ2	1.70	0.57
6:F:7:VAL:HG13	6:F:8:GLU:HG2	1.86	0.57
6:U:7:VAL:HG13	6:U:8:GLU:HG2	1.87	0.57
7:V:38:ILE:HG22	7:V:39:SER:N	2.20	0.57
1:A:289:HIS:HB2	1:A:295:LEU:HD21	1.85	0.57
2:B:136:TYR:HD2	2:B:140:LYS:HB3	1.70	0.57
3:C:171:ASN:O	3:C:174:LEU:HD22	2.05	0.57
3:C:347:PHE:O	3:C:348:GLU:HB3	2.05	0.57
2:R:973:THR:HG21	2:R:988:PHE:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:245:ALA:O	4:S:249:ILE:HG12	2.05	0.57
1:A:854:GLY:O	3:C:64:ILE:HG12	2.05	0.56
2:B:973:THR:HG21	2:B:988:PHE:CE1	2.40	0.56
4:D:245:ALA:O	4:D:249:ILE:HG12	2.05	0.56
8:H:39:PRO:HG3	10:Q:67:LEU:HD11	1.85	0.56
2:R:857:GLU:HA	2:R:862:ASN:O	2.05	0.56
1:W:431:MET:HE3	1:W:485:ASN:HB2	1.86	0.56
3:Y:199:ASP:HB2	3:Y:206:LEU:HB2	1.87	0.56
2:B:953:ILE:H	2:B:953:ILE:CD1	2.11	0.56
2:B:1104:ILE:HA	2:B:1107:LEU:HD12	1.85	0.56
6:F:71:VAL:HG13	6:F:72:LEU:HD12	1.87	0.56
2:R:761:TYR:CE2	2:R:843:ARG:HG2	2.40	0.56
2:R:1069:TYR:CB	2:R:1070:ILE:HB	2.35	0.56
7:V:18:ILE:HD12	7:V:29:ILE:HG12	1.87	0.56
7:V:46:ILE:HD12	1:W:542:PRO:HG2	1.87	0.56
1:A:220:ARG:HG2	1:A:235:LEU:HB3	1.88	0.56
1:A:549:LYS:CE	7:G:89:GLY:HA2	2.35	0.56
7:G:87:ASN:O	7:G:88:ASN:C	2.47	0.56
13:P:7:GLY:HA2	13:P:35:PHE:O	2.04	0.56
2:R:981:LYS:HE2	4:S:205:LEU:HD13	1.87	0.56
4:S:53:LEU:HD22	4:S:57:ILE:HG21	1.88	0.56
1:W:510:THR:O	1:W:549:LYS:HD3	2.04	0.56
1:W:852:ASP:CG	8:Z:75:VAL:HG21	2.30	0.56
2:B:21:PHE:HZ	2:B:475:LEU:HB3	1.71	0.56
2:B:186:ILE:HD12	2:B:209:LYS:HB3	1.87	0.56
2:B:1007:ARG:HH22	2:B:1022:GLY:N	2.04	0.56
2:R:870:ARG:NH1	4:S:56:GLU:OE2	2.38	0.56
1:W:324:THR:HG22	1:W:325:VAL:N	2.20	0.56
3:Y:29:VAL:HG12	3:Y:61:GLU:HG3	1.87	0.56
1:A:82:ILE:HD12	1:A:156:ILE:HG13	1.86	0.56
1:A:417:VAL:HG13	1:A:465:HIS:O	2.06	0.56
2:B:157:VAL:O	2:B:159:GLY:N	2.38	0.56
3:C:291:GLU:HA	3:C:294:ILE:HD12	1.88	0.56
11:L:6:LEU:HD11	11:L:16:GLU:HB2	1.88	0.56
11:M:31:THR:HA	11:M:34:LYS:HD2	1.88	0.56
11:M:42:SER:HB3	1:W:522:GLN:O	2.05	0.56
3:Y:291:GLU:HA	3:Y:294:ILE:HD12	1.87	0.56
2:R:978:THR:O	4:S:26:ASN:ND2	2.38	0.56
3:Y:372:ASN:HA	3:Y:375:ILE:HG22	1.86	0.56
2:B:522:LYS:HG2	2:B:532:TYR:CE2	2.41	0.56
4:D:53:LEU:HD22	4:D:57:ILE:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:7:CYS:SG	12:O:45:CYS:HA	2.45	0.56
2:B:930:GLY:HA2	2:B:990:VAL:O	2.06	0.56
3:C:301:LEU:HD22	3:C:308:VAL:HG12	1.87	0.56
2:B:393:VAL:O	2:B:397:ILE:HB	2.06	0.56
2:B:600:LEU:O	2:B:601:ASP:HB2	2.05	0.56
8:H:43:PRO:HB2	8:H:79:ARG:HD3	1.88	0.56
3:Y:70:ILE:HA	3:Y:73:VAL:CG2	2.32	0.56
8:H:40:GLU:H	8:H:40:GLU:CD	2.13	0.56
9:I:30:TYR:HE2	2:R:1042:PHE:O	1.89	0.56
10:J:67:LEU:HD11	8:Z:39:PRO:HG3	1.88	0.56
3:Y:219:LEU:HA	3:Y:222:LEU:HD13	1.88	0.56
2:B:583:ILE:HD12	2:B:591:LEU:HD21	1.86	0.55
2:R:583:ILE:HD12	2:R:591:LEU:HD21	1.89	0.55
3:Y:337:GLU:HG3	3:Y:339:ASN:OD1	2.06	0.55
1:A:323:ARG:HH21	1:A:422:GLN:HE21	1.54	0.55
2:R:1010:GLY:HA3	2:R:1027:GLY:HA2	1.86	0.55
4:S:51:SER:HB2	4:S:52:PRO:HD2	1.88	0.55
1:A:854:GLY:O	3:C:64:ILE:HG21	2.05	0.55
3:C:276:ASN:ND2	3:C:279:GLU:OE2	2.37	0.55
2:R:68:ILE:H	2:R:68:ILE:HD12	1.71	0.55
7:V:88:ASN:ND2	1:W:538:ALA:HB2	2.22	0.55
1:W:281:ILE:HG21	3:Y:352:LYS:HZ1	1.72	0.55
3:Y:171:ASN:O	3:Y:174:LEU:HD22	2.05	0.55
1:A:652:SER:HB3	1:A:787:ARG:NE	2.19	0.55
2:B:763:THR:HG21	2:B:816:LYS:HD3	1.87	0.55
7:G:38:ILE:HG22	7:G:39:SER:N	2.22	0.55
7:G:66:TYR:CD1	7:G:66:TYR:N	2.74	0.55
2:R:783:VAL:CG1	2:R:784:ARG:HB2	2.34	0.55
7:V:11:LEU:HB2	7:V:57:ALA:HB3	1.88	0.55
3:C:262:LEU:HD11	3:C:283:VAL:HG11	1.89	0.55
4:D:13:ILE:HG22	4:D:230:LEU:HB2	1.88	0.55
9:I:44:ALA:C	9:I:46:GLY:H	2.15	0.55
11:L:6:LEU:CD1	11:L:16:GLU:HB2	2.36	0.55
2:R:46:ILE:HG13	2:R:66:ILE:HG12	1.88	0.55
1:W:142:LYS:O	1:W:143:ALA:HB3	2.06	0.55
12:N:42:ARG:C	12:N:44:CYS:H	2.13	0.55
1:A:553:SER:OG	1:A:592:ILE:HA	2.06	0.55
2:B:359:VAL:HG11	2:B:407:VAL:HG13	1.89	0.55
4:D:154:ALA:HA	4:D:157:ILE:HG13	1.89	0.55
5:T:38:ILE:HG12	5:T:44:LEU:HD11	1.88	0.55
1:W:652:SER:HB3	1:W:787:ARG:NE	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:737:VAL:HG23	1:W:738:LEU:H	1.72	0.55
1:A:668:ALA:HB2	1:A:707:LEU:HD22	1.89	0.55
1:A:867:ASP:HA	1:A:870:ARG:HH21	1.72	0.55
3:C:25:PRO:HA	3:C:28:ILE:HA	1.89	0.55
3:C:29:VAL:HB	3:C:32:LEU:HD12	1.88	0.55
3:C:328:GLN:HB3	3:C:332:HIS:ND1	2.22	0.55
4:S:57:ILE:O	4:S:61:ARG:HG3	2.07	0.55
1:A:330:PRO:HG3	2:B:734:GLY:CA	2.36	0.55
1:A:864:LYS:NZ	3:C:29:VAL:O	2.34	0.55
1:A:866:VAL:O	1:A:870:ARG:NH2	2.38	0.55
2:B:665:GLN:CG	2:B:667:PRO:HD2	2.31	0.55
2:B:1111:ILE:O	2:B:1111:ILE:HG22	2.06	0.55
12:O:43:TYR:HB3	2:R:938:LEU:HD23	1.89	0.55
2:R:447:ASP:HA	1:W:803:ARG:HG2	1.88	0.55
2:B:724:ASN:O	12:N:47:ARG:HD2	2.07	0.55
9:I:41:LEU:HD23	5:T:64:GLY:N	2.22	0.55
13:P:24:VAL:HG13	13:P:24:VAL:O	2.06	0.55
5:T:18:PHE:HD2	3:Y:392:PRO:HB3	1.72	0.55
7:V:55:VAL:HG23	7:V:117:GLN:HA	1.89	0.55
1:W:600:LYS:HB2	1:W:732:GLY:CA	2.37	0.55
3:C:47:GLU:HG3	3:C:51:ILE:HG12	1.89	0.54
3:C:274:THR:HG22	3:C:276:ASN:H	1.73	0.54
7:V:66:TYR:N	7:V:66:TYR:CD1	2.75	0.54
1:W:10:LYS:HG2	3:Y:363:VAL:HG13	1.89	0.54
3:Y:29:VAL:HB	3:Y:32:LEU:HD12	1.89	0.54
1:A:354:THR:O	1:A:356:TRP:N	2.41	0.54
2:B:51:GLU:HB2	2:B:53:PRO:HD3	1.88	0.54
2:B:583:ILE:HB	2:B:643:LEU:HB3	1.90	0.54
3:C:341:VAL:H	3:C:364:GLU:HG2	1.72	0.54
2:R:1007:ARG:HH22	2:R:1022:GLY:N	2.05	0.54
1:A:655:ASP:O	1:A:657:VAL:N	2.41	0.54
1:A:838:VAL:HB	1:A:847:GLN:HB2	1.89	0.54
11:M:6:LEU:HD11	11:M:16:GLU:HB2	1.88	0.54
4:S:159:VAL:HG23	4:S:231:GLU:H	1.72	0.54
1:W:417:VAL:HG13	1:W:465:HIS:O	2.07	0.54
1:A:421:ARG:HG3	1:A:462:MET:HG2	1.89	0.54
2:R:186:ILE:HD12	2:R:209:LYS:HB3	1.88	0.54
2:R:585:VAL:HG21	2:R:636:LEU:HD11	1.89	0.54
2:R:872:LEU:HD22	2:R:874:ILE:HG13	1.90	0.54
1:A:737:VAL:HG23	1:A:738:LEU:H	1.73	0.54
2:B:783:VAL:CG1	2:B:784:ARG:HB2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:509:LEU:O	1:W:548:GLY:HA3	2.07	0.54
1:W:875:VAL:O	1:W:877:GLY:N	2.36	0.54
2:R:768:TYR:HB2	2:R:773:GLU:H	1.72	0.54
5:T:38:ILE:HG12	5:T:44:LEU:CD1	2.37	0.54
3:Y:244:LYS:CA	3:Y:245:LYS:HB3	2.23	0.54
1:A:155:LYS:CB	1:A:156:ILE:HA	2.38	0.54
1:A:509:LEU:O	1:A:548:GLY:HA3	2.07	0.54
2:B:768:TYR:HB2	2:B:773:GLU:H	1.73	0.54
4:D:120:SER:OG	4:D:121:ILE:HD12	2.08	0.54
5:E:38:ILE:HG12	5:E:44:LEU:HD11	1.90	0.54
5:E:64:GLY:N	9:K:41:LEU:HD23	2.23	0.54
9:K:26:ARG:CG	9:K:27:LEU:H	2.19	0.54
7:V:87:ASN:O	7:V:88:ASN:C	2.50	0.54
1:W:82:ILE:HD12	1:W:156:ILE:HG13	1.89	0.54
3:C:29:VAL:O	3:C:30:GLU:HB2	2.08	0.54
4:D:161:LEU:HG	4:D:163:ILE:HD13	1.90	0.54
2:R:136:TYR:HD2	2:R:140:LYS:HB3	1.72	0.54
2:R:286:GLU:N	2:R:286:GLU:OE1	2.41	0.54
1:A:318:VAL:HG11	2:B:1051:ARG:O	2.07	0.54
2:B:26:LEU:HG	2:B:27:VAL:HG23	1.90	0.54
12:O:42:ARG:C	12:O:44:CYS:H	2.16	0.54
2:R:406:TRP:CG	2:R:407:VAL:N	2.74	0.54
2:R:520:TRP:O	2:R:521:SER:CB	2.56	0.54
2:R:774:ASP:HB3	2:R:817:VAL:O	2.08	0.54
2:R:1102:LEU:HD13	1:W:308:ARG:NH2	2.23	0.54
4:S:154:ALA:HA	4:S:157:ILE:HG13	1.90	0.54
1:W:125:TRP:N	1:W:126:PRO:CD	2.71	0.54
1:W:763:THR:HB	1:W:764:ARG:HD2	1.90	0.54
13:X:24:VAL:HG13	13:X:24:VAL:O	2.08	0.54
1:A:600:LYS:HB2	1:A:732:GLY:HA3	1.90	0.54
2:B:768:TYR:C	2:B:770:GLY:H	2.15	0.54
2:R:985:ARG:HG3	4:S:205:LEU:HD23	1.89	0.54
5:T:89:VAL:HG13	5:T:139:GLY:HA2	1.90	0.54
1:W:848:VAL:O	1:W:849:ALA:HB3	2.07	0.54
1:A:763:THR:HB	1:A:764:ARG:HD2	1.89	0.53
2:B:743:MET:HE1	2:B:875:PRO:HB2	1.88	0.53
3:C:106:ARG:O	3:C:110:ILE:HG22	2.07	0.53
2:R:233:LEU:HD13	2:R:315:ALA:HA	1.89	0.53
2:R:491:THR:HG21	2:R:552:ILE:HD13	1.89	0.53
2:R:662:GLU:O	1:W:789:GLY:HA2	2.09	0.53
1:A:470:GLU:HG3	9:K:41:LEU:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:884:ARG:HH11	2:B:992:TYR:HB3	1.69	0.53
5:E:129:GLY:H	5:E:137:GLN:HB3	1.73	0.53
4:S:13:ILE:HG22	4:S:230:LEU:HB2	1.91	0.53
1:A:541:ALA:HB3	1:A:542:PRO:CD	2.38	0.53
13:P:17:GLN:C	13:P:19:LYS:H	2.16	0.53
2:R:249:PRO:HG2	2:R:253:ASN:OD1	2.09	0.53
4:S:96:ILE:HG12	4:S:145:LEU:HD11	1.90	0.53
1:W:58:CYS:SG	1:W:60:THR:CG2	2.97	0.53
1:W:563:HIS:CE1	1:W:587:VAL:HG13	2.43	0.53
1:W:829:ASP:O	1:W:840:SER:HA	2.09	0.53
3:Y:25:PRO:HA	3:Y:28:ILE:HA	1.91	0.53
1:A:378:VAL:HG13	1:A:386:ILE:HB	1.90	0.53
1:A:848:VAL:O	1:A:849:ALA:CB	2.56	0.53
2:R:493:TYR:OH	2:R:530:VAL:HG13	2.08	0.53
2:R:1050:ASP:HA	2:R:1054:ASP:HB2	1.89	0.53
4:S:96:ILE:HG22	4:S:116:SER:HA	1.91	0.53
1:W:853:ASP:HB3	1:W:855:VAL:H	1.73	0.53
3:Y:122:MET:HG2	3:Y:274:THR:HG23	1.91	0.53
2:B:973:THR:HG21	2:B:988:PHE:HE1	1.74	0.53
3:C:11:SER:HB2	3:C:14:GLU:HB2	1.89	0.53
7:G:11:LEU:HB2	7:G:57:ALA:HB3	1.91	0.53
7:G:29:ILE:O	7:G:39:SER:HA	2.09	0.53
11:M:40:PHE:HB3	11:M:58:LEU:HD23	1.89	0.53
2:R:625:GLU:OE1	1:W:761:TYR:HB3	2.09	0.53
1:W:125:TRP:N	1:W:126:PRO:HD2	2.23	0.53
1:W:490:ARG:HH22	3:Y:306:LEU:HD11	1.73	0.53
2:B:233:LEU:HD13	2:B:315:ALA:HA	1.91	0.53
2:B:665:GLN:HG2	2:B:667:PRO:CD	2.32	0.53
2:R:600:LEU:O	2:R:601:ASP:HB2	2.07	0.53
2:R:627:ALA:HB1	2:R:642:HIS:CD2	2.38	0.53
2:R:927:ILE:HG23	2:R:987:TYR:CE2	2.44	0.53
3:Y:197:VAL:HB	3:Y:208:ILE:HB	1.91	0.53
4:D:242:LEU:HB3	11:L:87:ILE:HD13	1.90	0.53
1:A:755:GLU:HB3	1:A:758:LYS:NZ	2.24	0.53
2:B:59:LEU:HD23	2:B:107:GLU:HG2	1.91	0.53
3:C:337:GLU:HG3	3:C:339:ASN:OD1	2.08	0.53
11:M:44:TYR:CD1	1:W:527:VAL:HA	2.44	0.53
1:W:289:HIS:HB2	1:W:295:LEU:HD21	1.91	0.53
1:W:323:ARG:HH21	1:W:422:GLN:HE21	1.55	0.53
2:B:762:SER:HB3	2:B:866:LYS:HG2	1.91	0.53
12:N:35:LEU:HD13	12:N:46:ARG:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:98:PHE:HA	5:T:106:GLY:O	2.09	0.53
1:W:413:ASP:OD2	1:W:436:ARG:HA	2.08	0.53
3:Y:328:GLN:HB3	3:Y:332:HIS:ND1	2.23	0.53
3:Y:331:ARG:H	3:Y:331:ARG:CD	2.22	0.53
2:B:15:LYS:NZ	2:B:599:LYS:HE3	2.24	0.53
2:B:286:GLU:N	2:B:286:GLU:OE1	2.42	0.53
2:B:627:ALA:HB1	2:B:642:HIS:CD2	2.41	0.53
11:M:6:LEU:CD1	11:M:16:GLU:HB2	2.39	0.53
2:R:459:PHE:HZ	1:W:795:LEU:HD11	1.74	0.53
2:R:916:HIS:CD2	1:W:733:ALA:HB1	2.44	0.53
8:Z:38:ARG:HB3	8:Z:40:GLU:OE1	2.09	0.53
2:R:26:LEU:HG	2:R:27:VAL:HG23	1.89	0.52
2:R:256:PHE:C	2:R:258:SER:H	2.17	0.52
2:R:973:THR:HG21	2:R:988:PHE:HE1	1.74	0.52
6:U:71:VAL:HG13	6:U:72:LEU:HD12	1.91	0.52
1:W:604:GLY:O	1:W:607:GLN:HB2	2.09	0.52
2:B:658:ILE:O	2:B:661:PRO:HG3	2.10	0.52
4:D:38:VAL:CG1	4:D:39:MET:H	2.23	0.52
5:E:38:ILE:HG12	5:E:44:LEU:CD1	2.40	0.52
1:A:457:PHE:CD1	2:B:738:GLU:HB2	2.44	0.52
1:A:542:PRO:HD3	7:G:70:ASP:O	2.08	0.52
2:B:110:ILE:CA	2:B:111:GLU:CB	2.71	0.52
2:B:345:ARG:HG3	2:B:576:GLY:HA3	1.92	0.52
1:W:870:ARG:HD2	3:Y:57:LYS:HB3	1.91	0.52
1:A:220:ARG:HG2	1:A:235:LEU:HD22	1.91	0.52
1:A:258:PRO:HG2	1:A:261:ILE:HD12	1.90	0.52
2:B:189:THR:HA	2:B:208:LEU:O	2.09	0.52
2:B:493:TYR:OH	2:B:530:VAL:HG13	2.10	0.52
2:B:855:ILE:O	13:P:34:ILE:HG23	2.09	0.52
2:B:1046:MET:HE2	2:B:1046:MET:HA	1.91	0.52
2:B:1069:TYR:CA	2:B:1070:ILE:HB	2.40	0.52
4:D:57:ILE:O	4:D:61:ARG:HG3	2.10	0.52
6:F:48:ASP:HB3	6:F:51:SER:HB2	1.91	0.52
10:J:78:ARG:CZ	8:Z:82:ILE:HG22	2.39	0.52
2:R:284:LYS:HB3	2:R:287:ASN:HD22	1.75	0.52
2:R:921:ARG:HH21	1:W:734:ARG:NH2	2.07	0.52
4:S:38:VAL:CG1	4:S:39:MET:H	2.22	0.52
5:T:145:ARG:HD3	6:U:88:ILE:HG21	1.91	0.52
1:W:340:PRO:HD2	1:W:343:ILE:HG13	1.91	0.52
1:W:378:VAL:HG13	1:W:386:ILE:HB	1.90	0.52
1:W:782:ILE:HG23	1:W:794:GLU:CD	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:X:6:CYS:SG	13:X:18:LEU:HG	2.49	0.52
1:A:734:ARG:HH22	2:B:917:ALA:HA	1.74	0.52
2:B:459:PHE:O	2:B:670:THR:HG23	2.08	0.52
9:I:26:ARG:CG	9:I:27:LEU:H	2.20	0.52
1:W:78:VAL:HG21	1:W:253:ILE:HD11	1.92	0.52
1:W:535:GLY:O	1:W:536:GLU:HB2	2.08	0.52
13:X:8:LYS:HD3	13:X:13:PHE:HD2	1.73	0.52
1:A:78:VAL:HG21	1:A:253:ILE:HD11	1.92	0.52
1:A:271:TYR:CE1	1:A:285:PRO:HB3	2.40	0.52
1:A:731:THR:O	1:A:733:ALA:N	2.42	0.52
2:B:761:TYR:CE2	2:B:843:ARG:HG2	2.44	0.52
1:W:431:MET:HE1	1:W:496:ILE:HD11	1.92	0.52
1:W:572:PRO:HG2	1:W:717:LYS:HE2	1.91	0.52
1:A:524:ILE:HD11	1:A:638:PHE:HD1	1.75	0.52
2:R:928:MET:HG2	1:W:648:LEU:HD11	1.91	0.52
1:A:345:ARG:HA	1:A:410:HIS:CD2	2.44	0.52
1:A:682:GLY:C	1:A:684:LEU:H	2.18	0.52
1:A:755:GLU:HB3	1:A:758:LYS:HZ1	1.75	0.52
7:V:29:ILE:O	7:V:39:SER:HA	2.10	0.52
1:W:6:ILE:HD13	3:Y:375:ILE:HD11	1.90	0.52
1:W:428:ILE:HG22	1:W:452:PRO:HB3	1.92	0.52
1:W:449:VAL:HG12	1:W:452:PRO:HG2	1.91	0.52
1:A:542:PRO:HG3	7:G:46:ILE:HG23	1.92	0.52
2:B:742:ILE:HG23	2:B:912:ILE:HB	1.92	0.52
7:G:55:VAL:HG23	7:G:117:GLN:HA	1.91	0.52
13:P:8:LYS:HD3	13:P:13:PHE:HD2	1.74	0.52
2:R:17:ILE:HG13	2:R:476:MET:SD	2.50	0.52
2:R:91:ARG:CD	2:R:856:THR:HG21	2.39	0.52
2:R:105:PRO:O	2:R:111:GLU:HB3	2.09	0.52
5:T:129:GLY:H	5:T:137:GLN:HB3	1.74	0.52
1:A:372:TRP:O	1:A:374:GLY:N	2.42	0.52
4:D:96:ILE:HG22	4:D:116:SER:HA	1.92	0.52
13:P:9:CYS:SG	13:P:10:TRP:N	2.82	0.52
1:W:855:VAL:O	3:Y:311:ARG:NH1	2.42	0.52
1:W:864:LYS:HG3	1:W:864:LYS:O	2.08	0.52
1:W:867:ASP:CA	1:W:870:ARG:HH22	2.23	0.52
3:Y:286:ILE:HG12	8:Z:49:ASP:OD2	2.09	0.52
1:A:125:TRP:N	1:A:126:PRO:CD	2.73	0.51
2:B:46:ILE:HG13	2:B:66:ILE:HG12	1.91	0.51
2:B:807:VAL:HG11	2:B:813:LEU:HD21	1.92	0.51
5:E:98:PHE:HA	5:E:106:GLY:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:213:PHE:HB3	2:R:214:HIS:ND1	2.24	0.51
1:W:357:ASN:C	1:W:357:ASN:OD1	2.53	0.51
1:W:681:ASN:HB2	1:W:683:GLU:HG2	1.91	0.51
1:A:324:THR:HG22	1:A:325:VAL:N	2.25	0.51
2:B:688:GLN:O	2:B:868:ARG:NH2	2.43	0.51
4:D:33:MET:HE3	4:D:162:ALA:HB3	1.91	0.51
5:E:15:PRO:HA	5:E:18:PHE:CE1	2.45	0.51
2:R:187:THR:HB	2:R:188:HIS:CD2	2.45	0.51
2:R:1069:TYR:CA	2:R:1070:ILE:HB	2.40	0.51
4:S:66:PRO:HG2	4:S:124:ILE:CG1	2.36	0.51
1:W:867:ASP:CA	1:W:870:ARG:NH2	2.69	0.51
3:Y:29:VAL:O	3:Y:30:GLU:HB2	2.10	0.51
2:B:320:TYR:CD2	2:B:529:LEU:HD12	2.45	0.51
7:G:76:TYR:O	7:G:85:SER:HB2	2.10	0.51
10:J:78:ARG:NH1	8:Z:82:ILE:HG22	2.26	0.51
4:S:26:ASN:O	4:S:30:ARG:HG3	2.11	0.51
1:W:155:LYS:CB	1:W:156:ILE:HA	2.41	0.51
1:W:450:CYS:N	1:W:451:PRO:CD	2.73	0.51
1:A:672:VAL:HG13	1:A:700:ILE:HG12	1.93	0.51
2:B:371:GLN:O	2:B:375:SER:CB	2.59	0.51
2:B:380:ARG:HH11	2:B:381:LYS:HE3	1.76	0.51
2:B:597:ILE:HD13	2:B:597:ILE:H	1.75	0.51
2:B:730:ILE:HG12	2:B:986:ILE:HG21	1.92	0.51
9:K:23:TRP:C	9:K:25:ASN:H	2.18	0.51
2:R:376:LYS:C	2:R:378:ARG:H	2.18	0.51
1:W:876:VAL:HA	1:W:879:LYS:HB2	1.92	0.51
1:A:450:CYS:HB2	1:A:451:PRO:HD3	1.93	0.51
1:A:572:PRO:HG2	1:A:717:LYS:HE2	1.92	0.51
1:A:851:GLY:HA3	3:C:311:ARG:HG3	1.92	0.51
2:B:15:LYS:HZ1	2:B:599:LYS:HE3	1.74	0.51
2:B:284:LYS:HB3	2:B:287:ASN:HD22	1.75	0.51
3:C:290:ARG:HA	3:C:321:THR:HG21	1.92	0.51
2:R:522:LYS:HG2	2:R:532:TYR:CE2	2.45	0.51
1:W:323:ARG:NH2	1:W:422:GLN:HE21	2.09	0.51
1:W:449:VAL:HG11	1:W:482:VAL:HG11	1.93	0.51
3:Y:122:MET:SD	3:Y:256:SER:HA	2.50	0.51
2:B:898:VAL:HG21	4:D:34:LEU:HD21	1.93	0.51
4:D:78:TRP:HB3	4:D:79:PRO:HD2	1.91	0.51
1:A:68:CYS:N	1:A:69:PRO:HD3	2.26	0.51
1:A:515:LEU:HB3	1:A:545:TYR:CD1	2.46	0.51
3:Y:348:GLU:CD	3:Y:350:THR:HB	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:GLU:HB3	1:A:54:PRO:HD2	1.93	0.51
1:A:879:LYS:HZ1	3:C:46:ASP:HB2	1.75	0.51
4:D:153:HIS:HB3	4:D:155:LYS:HG2	1.92	0.51
4:D:175:ASN:HD21	4:D:194:LYS:HA	1.75	0.51
12:O:15:ALA:HB1	4:S:129:PRO:HD2	1.93	0.51
1:W:668:ALA:HB2	1:W:707:LEU:HD22	1.92	0.51
3:Y:290:ARG:HA	3:Y:321:THR:HG21	1.92	0.51
1:A:604:GLY:O	1:A:607:GLN:HB2	2.11	0.51
2:B:131:ASP:OD2	2:B:132:PRO:HD2	2.10	0.51
9:I:47:ALA:HB1	9:I:48:PRO:HD2	1.92	0.51
1:W:427:ARG:NH1	3:Y:73:VAL:HG11	2.25	0.51
1:W:734:ARG:HH11	1:W:734:ARG:CB	2.23	0.51
2:B:433:ILE:HG12	2:B:470:VAL:HB	1.91	0.51
2:B:668:ARG:HH12	2:B:921:ARG:HD2	1.75	0.51
3:C:29:VAL:HG12	3:C:61:GLU:HG3	1.93	0.51
5:E:89:VAL:HG13	5:E:139:GLY:HA2	1.92	0.51
3:Y:11:SER:O	3:Y:45:ARG:NH2	2.44	0.51
2:B:476:MET:HE3	2:B:581:PRO:HG2	1.92	0.50
2:B:872:LEU:HD22	2:B:874:ILE:HG13	1.92	0.50
2:B:1080:TYR:HB3	2:B:1091:LEU:HD12	1.92	0.50
4:D:45:TYR:HB3	13:P:42:ILE:HD11	1.93	0.50
1:W:428:ILE:HD11	1:W:489:PRO:HD3	1.92	0.50
1:A:123:LYS:C	1:A:126:PRO:HD2	2.35	0.50
2:B:594:ARG:HH11	2:B:610:LEU:HD23	1.76	0.50
12:O:15:ALA:HB3	4:S:128:ILE:HG23	1.92	0.50
2:R:1009:ARG:HA	1:W:319:ASP:OD2	2.11	0.50
1:A:681:ASN:HB2	1:A:683:GLU:HG2	1.94	0.50
5:E:79:PRO:HB2	5:E:160:ILE:HD11	1.94	0.50
9:I:79:ARG:HB2	3:Y:387:GLU:HG3	1.93	0.50
4:S:93:TYR:CD2	4:S:146:ARG:HB3	2.46	0.50
6:U:41:LEU:HA	6:U:44:VAL:HG12	1.92	0.50
1:W:524:ILE:HD11	1:W:638:PHE:HD1	1.75	0.50
1:W:662:TYR:HA	1:W:665:ILE:HG12	1.93	0.50
1:A:125:TRP:N	1:A:126:PRO:HD2	2.26	0.50
1:A:342:ILE:HD13	1:A:345:ARG:HH22	1.77	0.50
1:A:487:ILE:HD12	1:A:858:MET:O	2.11	0.50
1:A:563:HIS:CE1	1:A:587:VAL:HG13	2.46	0.50
1:A:662:TYR:HA	1:A:665:ILE:HG12	1.93	0.50
2:B:774:ASP:HB3	2:B:817:VAL:O	2.12	0.50
4:D:93:TYR:CD2	4:D:146:ARG:HB3	2.47	0.50
2:R:742:ILE:HG23	2:R:912:ILE:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:1046:MET:HE3	5:T:61:PHE:CD2	2.46	0.50
2:R:1080:TYR:HB3	2:R:1091:LEU:HD12	1.93	0.50
5:T:144:ALA:HA	5:T:169:LEU:HD23	1.93	0.50
1:W:125:TRP:CZ3	8:Z:82:ILE:HG21	2.47	0.50
1:W:541:ALA:CB	1:W:542:PRO:CD	2.89	0.50
3:Y:106:ARG:O	3:Y:110:ILE:HG22	2.11	0.50
1:A:102:GLY:O	1:A:103:ARG:HG2	2.11	0.50
1:A:258:PRO:HD2	1:A:261:ILE:HD12	1.94	0.50
3:C:341:VAL:HG12	3:C:344:ARG:NH2	2.27	0.50
2:R:341:TYR:CE1	2:R:452:GLN:HG2	2.46	0.50
2:R:672:GLN:OE1	2:R:884:ARG:HA	2.11	0.50
1:W:600:LYS:HB2	1:W:732:GLY:HA3	1.93	0.50
2:B:155:PHE:N	2:B:155:PHE:CD2	2.79	0.50
1:W:489:PRO:HA	1:W:858:MET:HB2	1.93	0.50
1:W:490:ARG:HH12	3:Y:306:LEU:HG	1.76	0.50
1:A:281:ILE:HG21	3:C:352:LYS:NZ	2.26	0.50
2:B:453:TRP:HZ3	2:B:644:GLU:CD	2.20	0.50
10:J:70:ASP:CG	1:W:122:LYS:HZ3	2.18	0.50
1:W:549:LYS:HD2	1:W:593:LEU:HD22	1.93	0.50
1:W:651:VAL:CG1	1:W:743:MET:HB3	2.42	0.50
1:A:24:VAL:O	1:A:73:GLY:HA2	2.12	0.50
2:B:462:PRO:HG2	2:B:470:VAL:HG13	1.93	0.50
2:B:491:THR:HG21	2:B:552:ILE:HD13	1.94	0.50
2:B:927:ILE:HG23	2:B:987:TYR:CE2	2.47	0.50
9:I:61:VAL:O	9:I:63:SER:N	2.45	0.50
12:O:14:ILE:HG13	12:O:48:MET:HG3	1.93	0.50
2:R:13:ARG:HH12	2:R:647:SER:H	1.59	0.50
2:R:345:ARG:HG3	2:R:576:GLY:HA3	1.94	0.50
2:R:371:GLN:HE22	2:R:389:ARG:NE	2.10	0.50
2:R:598:GLU:HA	2:R:602:SER:HB2	1.94	0.50
2:R:774:ASP:HB2	2:R:818:SER:HA	1.94	0.50
7:V:76:TYR:O	7:V:85:SER:HB2	2.11	0.50
1:W:354:THR:O	1:W:356:TRP:N	2.45	0.50
1:A:753:ARG:HG3	1:A:804:GLU:OE1	2.11	0.50
2:B:205:ILE:H	2:B:205:ILE:HD12	1.76	0.50
2:B:256:PHE:C	2:B:258:SER:H	2.20	0.50
2:B:736:ASN:HD22	2:B:736:ASN:N	1.97	0.50
4:D:124:ILE:HD13	4:D:234:GLY:HA3	1.94	0.50
2:R:605:ILE:HG23	2:R:606:THR:H	1.77	0.50
2:R:939:SER:HA	2:R:963:TYR:CE2	2.47	0.50
2:R:1092:PHE:CD2	1:W:4:LYS:HD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:161:LEU:O	4:D:230:LEU:HA	2.12	0.49
12:O:1:MET:HB2	2:R:699:HIS:O	2.11	0.49
2:R:763:THR:HG21	2:R:816:LYS:HD3	1.94	0.49
2:R:1119:GLU:OE2	1:W:7:LYS:HE2	2.11	0.49
4:S:161:LEU:O	4:S:230:LEU:HA	2.12	0.49
1:W:682:GLY:C	1:W:684:LEU:H	2.20	0.49
1:W:846:ILE:HG22	1:W:847:GLN:HG3	1.93	0.49
1:A:324:THR:HG22	1:A:325:VAL:H	1.77	0.49
1:A:687:ILE:HD11	1:A:699:TYR:CE2	2.47	0.49
2:B:483:ILE:HD12	2:B:555:GLU:HB2	1.93	0.49
3:C:392:PRO:HB3	5:E:18:PHE:HD2	1.76	0.49
2:R:320:TYR:CD2	2:R:529:LEU:HD12	2.47	0.49
2:R:632:GLU:CD	2:R:633:PRO:HD2	2.36	0.49
2:R:1101:LYS:HE3	1:W:69:PRO:HG2	1.94	0.49
2:B:794:LEU:HD22	2:B:805:VAL:HG11	1.93	0.49
2:R:703:ARG:NH2	2:R:942:ILE:HG21	2.27	0.49
2:R:768:TYR:C	2:R:770:GLY:H	2.20	0.49
1:A:450:CYS:N	1:A:451:PRO:CD	2.75	0.49
2:B:376:LYS:C	2:B:378:ARG:H	2.19	0.49
3:C:197:VAL:HB	3:C:208:ILE:HB	1.94	0.49
2:R:272:LEU:O	2:R:276:GLY:N	2.35	0.49
1:W:58:CYS:H	1:W:62:GLY:HA2	1.76	0.49
1:W:220:ARG:HG2	1:W:235:LEU:HB3	1.95	0.49
1:W:851:GLY:O	1:W:853:ASP:N	2.45	0.49
1:W:852:ASP:CB	8:Z:75:VAL:HG21	2.42	0.49
3:Y:146:TYR:HD1	3:Y:235:LYS:N	2.10	0.49
2:B:760:LEU:HD12	2:B:868:ARG:HB3	1.94	0.49
9:K:32:ILE:O	9:K:36:ILE:HG12	2.12	0.49
2:R:597:ILE:HD13	2:R:597:ILE:H	1.76	0.49
2:R:1051:ARG:NE	2:R:1051:ARG:HA	2.27	0.49
3:Y:242:VAL:HG22	3:Y:251:ILE:HG12	1.95	0.49
1:A:94:LEU:HD21	1:A:180:ILE:HG23	1.94	0.49
2:B:417:LEU:HD21	2:B:425:MET:HG3	1.93	0.49
2:B:633:PRO:HD3	2:B:643:LEU:HD11	1.93	0.49
2:B:701:PRO:HB2	2:B:720:PRO:HG2	1.95	0.49
1:A:734:ARG:HB3	1:A:734:ARG:HH11	1.78	0.49
2:B:752:MET:HE1	2:B:910:ASP:HB3	1.95	0.49
7:G:20:ARG:HA	7:G:27:SER:HA	1.94	0.49
1:A:665:ILE:O	1:A:669:LYS:HG3	2.13	0.49
2:B:939:SER:HA	2:B:963:TYR:CE2	2.48	0.49
2:B:1081:VAL:HG22	2:B:1085:HIS:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:96:ILE:HG12	4:D:145:LEU:HD11	1.95	0.49
5:E:89:VAL:HA	5:E:99:VAL:HA	1.93	0.49
9:I:32:ILE:O	9:I:36:ILE:HG12	2.13	0.49
12:N:18:TRP:CE2	12:N:22:ILE:HG12	2.47	0.49
2:R:21:PHE:HZ	2:R:475:LEU:HB3	1.77	0.49
2:R:766:VAL:HG23	2:R:773:GLU:HG3	1.94	0.49
2:R:884:ARG:HH11	2:R:992:TYR:HB3	1.76	0.49
2:R:1092:PHE:CE2	1:W:4:LYS:HD2	2.48	0.49
3:Y:301:LEU:HD22	3:Y:308:VAL:HG12	1.95	0.49
11:M:48:PRO:HG2	2:R:735:TYR:HE2	1.77	0.49
2:R:27:VAL:HG12	2:R:429:LEU:HB2	1.94	0.49
3:Y:11:SER:HB2	3:Y:14:GLU:HB2	1.95	0.49
8:Z:40:GLU:CD	8:Z:40:GLU:H	2.21	0.49
2:B:975:ASP:HB3	2:B:978:THR:CG2	2.43	0.49
2:B:1069:TYR:HB2	2:B:1070:ILE:HB	1.94	0.49
3:C:122:MET:SD	3:C:256:SER:HA	2.53	0.49
4:D:66:PRO:HG2	4:D:124:ILE:CG1	2.40	0.49
8:H:13:ILE:HG21	8:H:19:LYS:NZ	2.28	0.49
11:L:40:PHE:HB3	11:L:58:LEU:HD23	1.95	0.49
4:S:205:LEU:O	4:S:207:GLU:N	2.46	0.49
7:V:20:ARG:HA	7:V:27:SER:HA	1.93	0.49
1:W:68:CYS:N	1:W:69:PRO:HD3	2.28	0.49
1:A:113:LYS:HG2	1:A:116:ARG:CZ	2.43	0.48
1:A:413:ASP:OD2	1:A:436:ARG:HA	2.13	0.48
1:A:764:ARG:H	1:A:764:ARG:HD3	1.78	0.48
2:B:284:LYS:HB3	2:B:287:ASN:HB2	1.95	0.48
2:B:857:GLU:CD	13:P:24:VAL:CG1	2.86	0.48
4:D:233:VAL:HG21	12:N:6:ARG:HH21	1.77	0.48
8:H:25:ILE:HG13	10:Q:51:TRP:HB3	1.94	0.48
9:K:61:VAL:O	9:K:63:SER:N	2.45	0.48
11:M:13:LEU:HD23	11:M:57:ILE:HD13	1.95	0.48
2:R:1081:VAL:HG22	2:R:1085:HIS:HA	1.95	0.48
1:W:24:VAL:O	1:W:73:GLY:HA2	2.13	0.48
1:W:80:PRO:HD2	1:W:178:SER:HB3	1.95	0.48
1:W:332:ILE:O	1:W:332:ILE:HG13	2.11	0.48
1:W:490:ARG:HD2	1:W:491:TYR:HD1	1.78	0.48
3:Y:35:LEU:HD23	3:Y:38:ASN:HD22	1.77	0.48
1:A:541:ALA:HB3	7:G:72:CYS:H	1.77	0.48
2:B:680:LEU:HD21	2:B:997:HIS:HB3	1.95	0.48
2:R:736:ASN:HD22	2:R:736:ASN:N	2.00	0.48
4:S:44:VAL:HA	4:S:143:ALA:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:124:ILE:HD13	4:S:234:GLY:HA3	1.94	0.48
1:A:490:ARG:HD2	1:A:491:TYR:HD1	1.78	0.48
1:A:506:ALA:O	1:A:510:THR:OG1	2.29	0.48
1:A:535:GLY:O	1:A:536:GLU:HB2	2.13	0.48
2:B:749:GLU:O	4:D:60:HIS:HE1	1.96	0.48
2:R:345:ARG:HA	2:R:576:GLY:O	2.14	0.48
1:W:420:ASN:HB2	1:W:430:MET:HG3	1.96	0.48
1:W:731:THR:O	1:W:733:ALA:N	2.46	0.48
3:Y:330:GLY:HA3	3:Y:331:ARG:HH11	1.79	0.48
1:A:142:LYS:O	1:A:143:ALA:HB3	2.13	0.48
2:B:13:ARG:NH1	2:B:647:SER:H	2.11	0.48
2:B:543:ILE:CD1	2:B:558:VAL:HG21	2.42	0.48
2:B:1007:ARG:HE	2:B:1026:GLU:C	2.20	0.48
12:N:42:ARG:C	12:N:44:CYS:N	2.72	0.48
12:O:18:TRP:CE2	12:O:22:ILE:HG12	2.48	0.48
2:R:852:LEU:HB3	2:R:868:ARG:HG2	1.95	0.48
4:S:13:ILE:HB	4:S:238:PRO:HB2	1.96	0.48
5:T:89:VAL:HA	5:T:99:VAL:HA	1.95	0.48
1:W:220:ARG:HG2	1:W:235:LEU:HD22	1.95	0.48
1:W:234:ASP:OD1	1:W:296:ARG:NH1	2.47	0.48
1:W:281:ILE:HD13	3:Y:352:LYS:HZ1	1.77	0.48
1:A:651:VAL:CG1	1:A:743:MET:HB3	2.42	0.48
2:B:105:PRO:O	2:B:111:GLU:HB3	2.13	0.48
3:C:242:VAL:HG22	3:C:251:ILE:HG12	1.95	0.48
3:C:244:LYS:HG3	3:C:249:TYR:HE2	1.79	0.48
11:M:86:GLU:O	11:M:90:LEU:HB2	2.14	0.48
2:R:59:LEU:HD23	2:R:107:GLU:HG2	1.95	0.48
2:R:371:GLN:O	2:R:375:SER:CB	2.61	0.48
2:R:1094:VAL:HG11	1:W:6:ILE:HG13	1.95	0.48
4:S:33:MET:HE3	4:S:162:ALA:HB3	1.96	0.48
1:A:340:PRO:HD2	1:A:343:ILE:HG13	1.94	0.48
1:A:364:PHE:CD1	1:A:409:ARG:HD2	2.49	0.48
1:A:752:VAL:O	1:A:753:ARG:C	2.55	0.48
1:A:801:GLY:O	1:A:804:GLU:HG2	2.14	0.48
2:B:520:TRP:O	2:B:521:SER:CB	2.61	0.48
2:B:904:VAL:HG21	4:D:204:THR:CG2	2.44	0.48
3:C:297:ILE:O	3:C:301:LEU:HD12	2.13	0.48
2:R:119:ILE:HG22	2:R:393:VAL:HG21	1.94	0.48
2:R:404:GLY:HA2	2:R:414:SER:H	1.78	0.48
2:R:772:GLN:O	2:R:773:GLU:HB3	2.13	0.48
2:R:974:TYR:CE2	4:S:165:ARG:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:LYS:HB3	11:L:49:LEU:HD22	1.95	0.48
1:A:764:ARG:HD3	1:A:764:ARG:N	2.28	0.48
1:A:864:LYS:O	1:A:864:LYS:HG3	2.13	0.48
2:B:856:THR:HG23	13:P:32:LYS:O	2.13	0.48
2:B:1103:LEU:O	2:B:1107:LEU:HG	2.13	0.48
12:O:7:CYS:HB3	12:O:10:CYS:SG	2.53	0.48
2:R:648:PRO:HB3	2:R:947:PRO:HG2	1.95	0.48
6:U:48:ASP:HB3	6:U:51:SER:HB2	1.95	0.48
1:W:635:PHE:O	1:W:639:VAL:HG23	2.14	0.48
1:W:749:GLN:HA	1:W:781:PHE:HA	1.95	0.48
1:W:764:ARG:HD3	1:W:764:ARG:N	2.29	0.48
1:A:449:VAL:HG11	1:A:482:VAL:HG11	1.96	0.48
2:B:672:GLN:OE1	2:B:884:ARG:HA	2.13	0.48
4:D:44:VAL:HA	4:D:143:ALA:HA	1.95	0.48
12:O:6:ARG:HB2	4:S:64:LEU:HD22	1.94	0.48
2:R:72:ARG:HG2	2:R:82:GLU:HG2	1.95	0.48
2:R:189:THR:HA	2:R:208:LEU:O	2.14	0.48
1:A:510:THR:O	1:A:549:LYS:HD3	2.13	0.48
2:B:187:THR:HB	2:B:188:HIS:CD2	2.49	0.48
2:B:774:ASP:HB2	2:B:818:SER:HA	1.95	0.48
4:D:13:ILE:HB	4:D:238:PRO:HB2	1.96	0.48
5:E:82:GLN:HB3	6:F:88:ILE:HB	1.95	0.48
2:R:459:PHE:O	2:R:670:THR:HG23	2.14	0.48
4:S:116:SER:O	4:S:118:ASP:N	2.47	0.48
1:A:10:LYS:HG2	3:C:363:VAL:HG13	1.95	0.48
2:B:1051:ARG:NE	2:B:1051:ARG:HA	2.29	0.48
2:R:633:PRO:HD3	2:R:643:LEU:HD11	1.95	0.48
1:W:487:ILE:HD12	1:W:858:MET:O	2.14	0.48
1:W:672:VAL:HG13	1:W:700:ILE:HG12	1.94	0.48
1:W:764:ARG:HD3	1:W:764:ARG:H	1.78	0.48
1:A:482:VAL:C	1:A:484:LYS:H	2.22	0.47
1:A:782:ILE:HG23	1:A:794:GLU:CD	2.38	0.47
3:C:11:SER:O	3:C:45:ARG:NH2	2.47	0.47
3:C:391:ARG:HD2	9:K:75:PRO:HB2	1.96	0.47
2:R:284:LYS:HB3	2:R:287:ASN:HB2	1.96	0.47
2:R:1072:TRP:C	2:R:1073:TYR:HD2	2.22	0.47
1:W:94:LEU:HD21	1:W:180:ILE:HG23	1.94	0.47
1:W:102:GLY:O	1:W:103:ARG:HG2	2.13	0.47
2:B:679:ALA:CB	2:B:721:ALA:HB1	2.44	0.47
12:N:30:ASN:O	12:N:34:VAL:HG23	2.14	0.47
2:R:51:GLU:C	2:R:53:PRO:HD3	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:66:ILE:HG23	2:R:101:LEU:HB2	1.96	0.47
1:W:570:SER:O	1:W:571:GLY:C	2.56	0.47
13:X:21:LEU:HD22	13:X:22:PRO:HA	1.96	0.47
2:R:605:ILE:HG12	2:R:606:THR:H	1.78	0.47
2:R:768:TYR:CD1	2:R:819:PRO:HG2	2.47	0.47
2:R:953:ILE:H	2:R:953:ILE:CD1	2.06	0.47
1:A:457:PHE:HD1	2:B:738:GLU:HB2	1.78	0.47
2:B:157:VAL:C	2:B:159:GLY:N	2.72	0.47
2:B:772:GLN:O	2:B:773:GLU:HB3	2.14	0.47
1:W:198:ASP:HB2	3:Y:361:GLY:HA3	1.96	0.47
3:Y:108:ILE:O	3:Y:111:VAL:HG12	2.13	0.47
1:A:635:PHE:O	1:A:639:VAL:HG23	2.15	0.47
2:B:301:LEU:N	2:B:302:PRO:HD3	2.29	0.47
2:B:659:PRO:O	2:B:660:TYR:C	2.57	0.47
3:C:46:ASP:N	3:C:47:GLU:OE1	2.43	0.47
4:D:159:VAL:HG23	4:D:231:GLU:H	1.78	0.47
7:G:72:CYS:HA	7:G:114:LYS:HA	1.95	0.47
2:R:679:ALA:HB3	2:R:721:ALA:HB1	1.97	0.47
2:R:737:MET:H	2:R:740:SER:HB3	1.79	0.47
6:U:47:CYS:SG	6:U:74:SER:HA	2.55	0.47
1:W:236:THR:O	1:W:240:VAL:HG23	2.15	0.47
1:W:258:PRO:HG2	1:W:261:ILE:HD12	1.95	0.47
1:W:524:ILE:C	1:W:526:GLY:H	2.21	0.47
1:W:525:LEU:HD11	1:W:551:VAL:HG23	1.96	0.47
2:B:658:ILE:HG12	2:B:672:GLN:HG2	1.96	0.47
6:F:41:LEU:HA	6:F:44:VAL:HG12	1.95	0.47
12:N:43:TYR:HA	12:N:46:ARG:HB3	1.96	0.47
1:W:271:TYR:CE1	1:W:285:PRO:HB3	2.43	0.47
1:W:296:ARG:H	1:W:296:ARG:HD2	1.79	0.47
1:W:553:SER:HB2	1:W:593:LEU:H	1.78	0.47
8:Z:13:ILE:HG21	8:Z:19:LYS:HZ1	1.79	0.47
1:A:80:PRO:HD2	1:A:178:SER:HB3	1.96	0.47
1:A:127:SER:HB2	3:C:360:ARG:HH12	1.80	0.47
1:A:431:MET:HE1	1:A:496:ILE:HD11	1.97	0.47
2:B:84:SER:HB2	2:B:144:ILE:HD12	1.97	0.47
2:B:747:SER:HB3	12:N:8:PHE:HB3	1.97	0.47
2:B:1043:GLY:HA3	3:C:382:GLY:HA3	1.95	0.47
7:G:42:ILE:HG21	7:G:48:ILE:HG23	1.97	0.47
10:J:66:ARG:NH1	8:Z:40:GLU:OE1	2.48	0.47
2:R:446:ARG:NH1	1:W:807:VAL:HG13	2.29	0.47
2:R:493:TYR:HD2	2:R:497:VAL:O	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:532:TYR:O	2:R:533:TYR:HB3	2.15	0.47
2:R:1063:VAL:O	2:R:1091:LEU:HA	2.15	0.47
7:V:32:SER:HA	7:V:37:ASN:OD1	2.15	0.47
7:V:72:CYS:HA	7:V:114:LYS:HA	1.97	0.47
1:W:12:GLY:HA3	1:W:201:THR:HG22	1.97	0.47
1:W:345:ARG:HA	1:W:410:HIS:CD2	2.49	0.47
1:W:421:ARG:HG3	1:W:462:MET:CG	2.45	0.47
1:W:421:ARG:HD3	1:W:455:ALA:HB2	1.97	0.47
3:Y:33:LYS:HG3	3:Y:34:ASN:N	2.30	0.47
1:A:281:ILE:HG21	3:C:352:LYS:HZ3	1.77	0.47
1:A:749:GLN:HA	1:A:781:PHE:HA	1.96	0.47
2:B:852:LEU:HB3	2:B:868:ARG:HG2	1.96	0.47
12:O:30:ASN:O	12:O:34:VAL:HG23	2.14	0.47
2:R:555:GLU:HA	2:R:579:ARG:HH22	1.79	0.47
13:X:17:GLN:C	13:X:19:LYS:N	2.72	0.47
3:Y:285:GLY:HA2	8:Z:50:PRO:HG2	1.96	0.47
11:M:38:VAL:HA	11:M:59:THR:HA	1.97	0.47
12:O:43:TYR:HA	12:O:46:ARG:HB3	1.96	0.47
2:R:914:ASN:HD21	1:W:501:ASP:CG	2.23	0.47
2:R:928:MET:HE2	2:R:953:ILE:HG21	1.95	0.47
2:R:975:ASP:HB3	2:R:978:THR:CG2	2.45	0.47
7:V:72:CYS:HB2	1:W:541:ALA:HB2	1.96	0.47
1:W:771:PRO:O	1:W:772:TYR:HB2	2.14	0.47
2:B:742:ILE:CG2	2:B:912:ILE:HB	2.44	0.47
3:C:117:PRO:HG2	3:C:120:PRO:HB3	1.97	0.47
4:D:26:ASN:O	4:D:30:ARG:HG3	2.15	0.47
9:K:23:TRP:HA	9:K:23:TRP:HE3	1.76	0.47
2:R:374:LYS:HD2	2:R:374:LYS:HA	1.74	0.47
2:R:461:THR:CG2	2:R:468:GLY:H	2.15	0.47
2:R:807:VAL:HG11	2:R:813:LEU:HD21	1.96	0.47
2:R:888:LYS:HB3	1:W:458:ASP:HB2	1.96	0.47
3:Y:117:PRO:HG2	3:Y:120:PRO:HB3	1.97	0.47
1:A:846:ILE:HG22	1:A:847:GLN:HG3	1.97	0.46
3:C:25:PRO:O	3:C:28:ILE:HG12	2.15	0.46
3:C:142:ARG:HD2	3:C:178:GLY:HA3	1.97	0.46
9:I:23:TRP:C	9:I:25:ASN:H	2.22	0.46
12:N:44:CYS:SG	12:N:45:CYS:SG	3.13	0.46
2:R:380:ARG:HH11	2:R:381:LYS:HE3	1.79	0.46
7:V:89:GLY:HA2	1:W:549:LYS:NZ	2.31	0.46
1:W:258:PRO:HD2	1:W:261:ILE:HD12	1.96	0.46
1:W:854:GLY:O	3:Y:64:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:VAL:HG11	1:A:464:LEU:CD1	2.45	0.46
1:A:524:ILE:C	1:A:526:GLY:H	2.23	0.46
2:B:171:ALA:HB1	2:B:174:ARG:HD2	1.97	0.46
2:B:788:GLY:O	2:B:791:TYR:HB2	2.16	0.46
3:C:213:ILE:HA	3:C:216:ILE:HD11	1.97	0.46
2:R:624:GLU:OE1	1:W:761:TYR:OH	2.33	0.46
2:R:966:LEU:HD22	2:R:985:ARG:NH2	2.30	0.46
2:R:1069:TYR:HB2	2:R:1070:ILE:HB	1.97	0.46
5:T:79:PRO:HB2	5:T:160:ILE:HD11	1.97	0.46
1:W:490:ARG:HG2	3:Y:308:VAL:HG23	1.98	0.46
1:A:330:PRO:HG3	2:B:734:GLY:HA2	1.96	0.46
2:B:893:MET:HE3	2:B:894:LEU:N	2.24	0.46
2:R:716:TYR:OH	2:R:721:ALA:HB3	2.15	0.46
2:R:970:THR:HG22	2:R:987:TYR:HA	1.96	0.46
5:T:84:VAL:HG22	6:U:75:ILE:HD13	1.96	0.46
1:W:752:VAL:O	1:W:753:ARG:C	2.59	0.46
3:Y:142:ARG:HD2	3:Y:178:GLY:HA3	1.96	0.46
1:A:553:SER:HB2	1:A:593:LEU:H	1.81	0.46
1:A:601:LYS:O	1:A:610:SER:HB2	2.15	0.46
2:B:112:ALA:O	2:B:113:GLU:HB2	2.16	0.46
2:B:249:PRO:HG2	2:B:253:ASN:OD1	2.15	0.46
5:E:144:ALA:HA	5:E:169:LEU:HD23	1.97	0.46
2:R:46:ILE:HG13	2:R:66:ILE:CG1	2.45	0.46
2:R:701:PRO:HB2	2:R:720:PRO:HG2	1.98	0.46
2:R:796:GLU:O	2:R:797:ASP:C	2.58	0.46
4:S:232:SER:HB3	4:S:241:ILE:CD1	2.46	0.46
1:W:837:THR:HG22	1:W:838:VAL:N	2.31	0.46
8:Z:13:ILE:HG21	8:Z:19:LYS:NZ	2.30	0.46
1:A:69:PRO:HB3	1:A:218:THR:HG21	1.96	0.46
1:A:541:ALA:HB3	7:G:71:PHE:HA	1.98	0.46
1:A:851:GLY:O	3:C:311:ARG:HD2	2.15	0.46
2:B:961:LEU:HA	2:B:965:TYR:O	2.14	0.46
3:C:389:THR:O	9:K:76:ILE:HA	2.15	0.46
9:K:44:ALA:C	9:K:46:GLY:H	2.23	0.46
11:L:13:LEU:HD23	11:L:57:ILE:HD13	1.97	0.46
11:M:69:LEU:O	11:M:73:ILE:HG12	2.15	0.46
2:R:453:TRP:HZ3	2:R:644:GLU:CD	2.23	0.46
2:R:605:ILE:HG12	2:R:606:THR:N	2.31	0.46
1:W:491:TYR:O	1:W:492:GLY:C	2.58	0.46
1:W:561:ASN:HA	1:W:588:ILE:O	2.16	0.46
3:Y:213:ILE:HA	3:Y:216:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:VAL:C	2:B:159:GLY:H	2.24	0.46
2:B:371:GLN:HE22	2:B:389:ARG:NE	2.13	0.46
2:B:903:THR:HG22	2:B:904:VAL:H	1.80	0.46
4:D:94:THR:HG23	4:D:145:LEU:HB2	1.97	0.46
11:L:74:GLU:HG2	11:L:77:ARG:HH21	1.81	0.46
11:M:73:ILE:HG21	4:S:257:GLU:HB2	1.98	0.46
2:R:594:ARG:HH11	2:R:610:LEU:HD23	1.81	0.46
2:R:686:ASN:C	2:R:688:GLN:N	2.74	0.46
1:A:296:ARG:H	1:A:296:ARG:HD2	1.81	0.46
1:A:332:ILE:O	1:A:332:ILE:HG13	2.15	0.46
2:B:213:PHE:HB3	2:B:214:HIS:ND1	2.30	0.46
2:B:605:ILE:HG23	2:B:606:THR:H	1.80	0.46
2:B:748:VAL:HG22	2:B:875:PRO:HG2	1.98	0.46
3:C:331:ARG:HD3	3:C:331:ARG:N	2.28	0.46
9:I:53:ILE:HG23	9:I:55:ASN:HD22	1.80	0.46
2:R:322:ILE:C	2:R:324:LYS:H	2.23	0.46
5:T:88:GLU:HG2	5:T:141:LYS:HA	1.97	0.46
3:Y:327:ARG:NH2	3:Y:337:GLU:HB3	2.23	0.46
2:B:648:PRO:HB3	2:B:947:PRO:HG2	1.98	0.46
3:C:35:LEU:HD23	3:C:38:ASN:HD22	1.81	0.46
3:C:201:SER:HB2	3:C:204:THR:HB	1.97	0.46
4:D:205:LEU:O	4:D:207:GLU:N	2.49	0.46
8:H:38:ARG:HB3	8:H:40:GLU:OE1	2.15	0.46
12:O:42:ARG:C	12:O:44:CYS:N	2.74	0.46
10:Q:57:GLY:C	10:Q:61:VAL:HB	2.41	0.46
2:R:322:ILE:O	2:R:326:ILE:HG12	2.15	0.46
2:R:743:MET:HE1	2:R:875:PRO:HB2	1.97	0.46
1:W:655:ASP:O	1:W:657:VAL:N	2.48	0.46
1:W:864:LYS:HE2	8:Z:71:LEU:O	2.16	0.46
1:A:325:VAL:O	1:A:442:THR:HB	2.15	0.46
2:B:374:LYS:HD2	2:B:374:LYS:HA	1.73	0.46
2:B:646:TRP:CZ3	2:B:648:PRO:HB2	2.51	0.46
2:R:968:ASP:O	2:R:969:ALA:HB3	2.16	0.46
4:S:175:ASN:HD21	4:S:194:LYS:HA	1.81	0.46
1:W:69:PRO:HB3	1:W:218:THR:HG21	1.97	0.46
1:W:687:ILE:HD11	1:W:699:TYR:CE2	2.51	0.46
3:Y:170:ASP:O	3:Y:174:LEU:HD21	2.15	0.46
3:Y:244:LYS:HG3	3:Y:249:TYR:HE2	1.80	0.46
3:Y:276:ASN:O	3:Y:280:ILE:HG12	2.16	0.46
1:A:771:PRO:O	1:A:772:TYR:HB2	2.16	0.46
1:A:874:ARG:HG3	3:C:53:ASP:OD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:LYS:HG3	3:C:34:ASN:N	2.30	0.46
2:R:794:LEU:HD22	2:R:805:VAL:HG11	1.97	0.46
1:W:203:ARG:HE	1:W:205:GLU:CD	2.24	0.46
1:W:308:ARG:HD3	1:W:308:ARG:HA	1.70	0.46
1:W:655:ASP:H	1:W:658:LYS:HD2	1.80	0.46
1:W:665:ILE:O	1:W:669:LYS:HG3	2.16	0.46
3:Y:30:GLU:HB3	3:Y:31:ASP:H	1.49	0.46
3:Y:106:ARG:O	3:Y:106:ARG:HG3	2.15	0.46
1:A:58:CYS:SG	1:A:60:THR:CG2	3.03	0.45
1:A:357:ASN:C	1:A:357:ASN:OD1	2.58	0.45
1:A:837:THR:HG22	1:A:838:VAL:N	2.32	0.45
2:B:119:ILE:HG22	2:B:393:VAL:HG21	1.98	0.45
4:D:15:LEU:HD12	4:D:228:LEU:HD22	1.98	0.45
7:G:32:SER:HA	7:G:37:ASN:OD1	2.17	0.45
11:L:1:MET:HA	11:L:19:GLY:HA3	1.97	0.45
2:R:15:LYS:NZ	2:R:599:LYS:HE3	2.31	0.45
2:R:668:ARG:HH11	2:R:921:ARG:HB3	1.80	0.45
2:R:776:ILE:HG23	2:R:815:GLY:O	2.16	0.45
4:S:77:ARG:HD2	4:S:92:CYS:SG	2.56	0.45
1:W:572:PRO:CG	1:W:717:LYS:HE2	2.46	0.45
3:Y:338:LYS:H	3:Y:338:LYS:HE2	1.81	0.45
1:A:372:TRP:HB3	1:A:373:PRO:HD3	1.98	0.45
1:A:549:LYS:NZ	7:G:89:GLY:HA2	2.31	0.45
2:B:27:VAL:HG12	2:B:429:LEU:HB2	1.97	0.45
3:C:276:ASN:O	3:C:280:ILE:HG12	2.16	0.45
9:I:61:VAL:N	9:I:64:ILE:HG13	2.31	0.45
2:R:874:ILE:H	2:R:874:ILE:HD12	1.80	0.45
4:S:114:ILE:HD12	4:S:123:PRO:HG3	1.98	0.45
5:T:131:LYS:HD2	5:T:136:ILE:HD13	1.99	0.45
7:V:42:ILE:HG21	7:V:48:ILE:HG23	1.98	0.45
7:V:66:TYR:CE2	1:W:540:LEU:HB3	2.51	0.45
1:W:16:PRO:HA	1:W:19:ILE:HD12	1.98	0.45
1:W:319:ASP:O	1:W:320:PHE:C	2.59	0.45
1:W:563:HIS:HB2	1:W:872:PHE:HE2	1.81	0.45
3:Y:28:ILE:H	3:Y:28:ILE:HG13	1.51	0.45
3:Y:104:LEU:O	3:Y:108:ILE:HG13	2.17	0.45
2:B:375:SER:C	2:B:377:VAL:H	2.25	0.45
2:R:322:ILE:HD13	2:R:322:ILE:HA	1.88	0.45
7:V:40:PHE:HZ	7:V:115:ILE:HG12	1.81	0.45
1:W:364:PHE:CD1	1:W:409:ARG:HD2	2.51	0.45
1:W:372:TRP:O	1:W:374:GLY:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:CYS:H	1:A:62:GLY:HA2	1.81	0.45
2:B:345:ARG:HA	2:B:576:GLY:O	2.16	0.45
2:B:914:ASN:C	2:B:916:HIS:H	2.22	0.45
3:C:231:ILE:HG22	3:C:232:LYS:H	1.80	0.45
9:I:76:ILE:HA	3:Y:389:THR:O	2.17	0.45
12:N:64:ARG:HH22	13:P:37:VAL:CG2	2.28	0.45
5:T:20:LYS:O	5:T:21:PRO:C	2.60	0.45
5:T:145:ARG:HG3	5:T:169:LEU:HD21	1.99	0.45
1:A:280:GLU:HB2	1:A:300:GLN:NE2	2.31	0.45
1:A:428:ILE:HD11	1:A:489:PRO:HD3	1.97	0.45
1:A:489:PRO:HA	1:A:858:MET:HB2	1.99	0.45
1:A:491:TYR:O	1:A:493:GLY:N	2.50	0.45
2:B:776:ILE:HG23	2:B:815:GLY:O	2.16	0.45
3:C:145:GLU:HG2	3:C:239:ARG:HA	1.98	0.45
3:C:331:ARG:H	3:C:331:ARG:CD	2.22	0.45
6:F:47:CYS:SG	6:F:74:SER:HA	2.56	0.45
8:H:64:ARG:HG2	8:H:64:ARG:O	2.15	0.45
2:R:920:SER:HA	1:W:739:ASN:HD21	1.82	0.45
2:R:921:ARG:NH2	1:W:734:ARG:NH2	2.64	0.45
1:W:113:LYS:HG2	1:W:116:ARG:CZ	2.46	0.45
1:W:541:ALA:HB3	1:W:542:PRO:HD3	1.97	0.45
1:A:561:ASN:HA	1:A:588:ILE:O	2.17	0.45
1:A:570:SER:O	1:A:571:GLY:C	2.59	0.45
3:C:347:PHE:C	3:C:349:VAL:N	2.75	0.45
2:R:67:ARG:HG3	2:R:100:TRP:HB2	1.97	0.45
1:W:421:ARG:NH2	1:W:454:ASN:O	2.50	0.45
1:W:848:VAL:O	1:W:849:ALA:CB	2.64	0.45
3:Y:327:ARG:HH22	3:Y:337:GLU:CB	2.23	0.45
1:A:353:ILE:CG2	1:A:358:ILE:HD13	2.47	0.45
2:B:766:VAL:H	2:B:767:LYS:HE3	1.82	0.45
2:B:970:THR:HG22	2:B:987:TYR:HA	1.98	0.45
3:C:387:GLU:HG3	9:K:79:ARG:HB2	1.99	0.45
5:E:2:TYR:O	6:F:11:TYR:HA	2.17	0.45
5:E:88:GLU:HG2	5:E:141:LYS:HA	1.98	0.45
5:E:91:GLN:O	5:E:98:PHE:HB2	2.17	0.45
2:R:294:GLN:HA	2:R:297:ASP:HB2	1.98	0.45
2:R:961:LEU:HA	2:R:965:TYR:O	2.16	0.45
2:R:981:LYS:O	2:R:981:LYS:HG3	2.16	0.45
2:R:1077:LYS:N	2:R:1078:ASN:HA	2.31	0.45
1:W:275:THR:HG23	1:W:279:ASN:ND2	2.31	0.45
1:W:780:GLY:HA2	1:W:797:PHE:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:145:GLU:HG2	3:Y:239:ARG:HA	1.98	0.45
1:A:490:ARG:HH22	3:C:306:LEU:HD11	1.82	0.45
2:B:322:ILE:C	2:B:324:LYS:H	2.25	0.45
2:B:857:GLU:CD	13:P:24:VAL:HG12	2.41	0.45
2:B:904:VAL:HG21	4:D:204:THR:HG21	1.97	0.45
4:D:11:LYS:O	4:D:231:GLU:HA	2.16	0.45
4:D:45:TYR:HB2	4:D:142:GLU:HB3	1.99	0.45
4:D:77:ARG:HD2	4:D:92:CYS:SG	2.57	0.45
8:H:58:LYS:O	8:H:60:GLY:N	2.48	0.45
11:L:86:GLU:O	11:L:90:LEU:HB2	2.16	0.45
2:R:658:ILE:HG12	2:R:672:GLN:HG2	1.97	0.45
2:R:730:ILE:HG12	2:R:986:ILE:HG21	1.98	0.45
2:R:748:VAL:HG22	2:R:875:PRO:HG2	1.98	0.45
2:R:945:ALA:O	2:R:946:THR:C	2.60	0.45
4:S:78:TRP:HB3	4:S:79:PRO:HD2	1.99	0.45
6:U:80:PRO:O	6:U:83:VAL:HG12	2.17	0.45
1:W:820:GLN:O	1:W:824:ILE:HB	2.16	0.45
3:Y:106:ARG:HH22	3:Y:277:ILE:HD11	1.81	0.45
1:A:280:GLU:C	1:A:282:PRO:HD2	2.41	0.45
1:A:382:ASP:OD1	1:A:382:ASP:N	2.49	0.45
1:A:622:GLU:OE1	1:A:622:GLU:HA	2.17	0.45
2:B:766:VAL:HG23	2:B:773:GLU:HG3	1.98	0.45
3:C:327:ARG:NH2	3:C:337:GLU:HB3	2.24	0.45
4:D:116:SER:O	4:D:118:ASP:N	2.50	0.45
2:R:1065:ASP:CB	2:R:1089:SER:HB2	2.43	0.45
5:T:108:VAL:HG21	5:T:164:MET:HE3	1.98	0.45
1:W:102:GLY:HA3	1:W:187:VAL:HG12	1.97	0.45
1:W:736:SER:O	1:W:738:LEU:N	2.50	0.45
3:Y:341:VAL:HG12	3:Y:344:ARG:NH2	2.29	0.45
1:A:176:THR:HA	1:A:177:PRO:HD2	1.84	0.45
2:B:552:ILE:HG13	2:B:553:SER:H	1.82	0.45
3:C:348:GLU:CD	3:C:350:THR:HB	2.41	0.45
11:M:22:HIS:ND1	2:R:977:ARG:HB2	2.32	0.45
2:R:543:ILE:CD1	2:R:558:VAL:HG21	2.45	0.45
2:R:736:ASN:CG	2:R:736:ASN:O	2.60	0.45
7:V:83:ASP:HB2	7:V:101:LEU:HG	1.99	0.45
1:W:194:ILE:H	1:W:194:ILE:HG13	1.56	0.45
1:W:353:ILE:CG2	1:W:358:ILE:HD13	2.47	0.45
1:W:875:VAL:HG12	1:W:876:VAL:H	1.82	0.45
3:Y:159:ASP:HB2	3:Y:163:MET:HB2	1.99	0.45
3:Y:231:ILE:HG22	3:Y:232:LYS:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:39:PRO:HB2	8:Z:80:TYR:CD2	2.52	0.45
1:A:563:HIS:HB2	1:A:872:PHE:HE2	1.81	0.44
2:B:686:ASN:C	2:B:688:GLN:N	2.74	0.44
2:B:945:ALA:O	2:B:946:THR:C	2.59	0.44
3:C:66:PRO:HD2	9:K:28:THR:HG22	1.99	0.44
4:D:96:ILE:HD13	4:D:114:ILE:HG23	1.98	0.44
2:R:68:ILE:HD12	2:R:68:ILE:N	2.33	0.44
2:R:798:ASN:HD21	13:X:36:MET:HE2	1.80	0.44
2:R:903:THR:HG22	2:R:904:VAL:H	1.82	0.44
1:W:110:GLU:HA	1:W:113:LYS:HD2	1.99	0.44
3:Y:348:GLU:OE1	3:Y:350:THR:CB	2.62	0.44
1:A:853:ASP:HB2	3:C:311:ARG:NH1	2.32	0.44
2:B:857:GLU:CG	13:P:24:VAL:HG11	2.43	0.44
3:C:384:GLY:HA2	5:E:61:PHE:CZ	2.52	0.44
5:E:60:VAL:HG22	5:E:61:PHE:H	1.81	0.44
2:R:161:GLU:OE1	2:R:419:ARG:NH1	2.51	0.44
2:R:679:ALA:CB	2:R:721:ALA:HB1	2.47	0.44
2:R:1000:VAL:HG21	1:W:442:THR:HG22	2.00	0.44
3:Y:81:PRO:O	3:Y:82:GLY:C	2.60	0.44
3:Y:165:ILE:HG13	3:Y:219:LEU:HD23	2.00	0.44
1:A:203:ARG:HE	1:A:205:GLU:CD	2.25	0.44
1:A:204:PRO:O	1:A:207:MET:HB2	2.17	0.44
1:A:438:LEU:HD12	11:L:47:HIS:CE1	2.53	0.44
2:B:68:ILE:H	2:B:68:ILE:HD12	1.82	0.44
2:B:117:VAL:HG11	2:B:388:VAL:HG21	2.00	0.44
2:B:166:THR:HG23	2:B:431:ARG:O	2.18	0.44
2:B:350:GLY:C	2:B:352:LEU:H	2.26	0.44
10:J:57:GLY:C	10:J:61:VAL:HB	2.43	0.44
9:K:23:TRP:C	9:K:25:ASN:N	2.74	0.44
12:O:1:MET:O	12:O:2:MET:HB2	2.16	0.44
2:R:128:SER:O	2:R:129:ALA:C	2.61	0.44
4:S:120:SER:OG	4:S:121:ILE:HD12	2.17	0.44
1:W:600:LYS:O	1:W:601:LYS:CB	2.57	0.44
8:Z:64:ARG:O	8:Z:64:ARG:HG2	2.17	0.44
1:A:236:THR:O	1:A:240:VAL:HG23	2.16	0.44
1:A:513:THR:HG21	7:G:25:ASN:HB2	1.98	0.44
1:A:517:THR:C	1:A:519:GLU:N	2.75	0.44
1:A:655:ASP:H	1:A:658:LYS:HD2	1.81	0.44
2:B:461:THR:HG21	2:B:468:GLY:N	2.09	0.44
4:D:129:PRO:HD2	12:N:15:ALA:HB1	1.99	0.44
7:G:40:PHE:HZ	7:G:115:ILE:HG12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:63:ILE:CG2	8:H:65:ILE:HG13	2.48	0.44
9:I:91:SER:O	9:I:92:LEU:HB2	2.17	0.44
11:L:38:VAL:HA	11:L:59:THR:HA	1.99	0.44
2:R:28:ARG:HA	2:R:31:LEU:HD12	1.99	0.44
2:R:430:ARG:HH11	2:R:653:ILE:HG13	1.83	0.44
4:S:144:ARG:HE	4:S:144:ARG:HB3	1.61	0.44
7:V:112:PHE:HD2	7:V:114:LYS:HE3	1.81	0.44
1:W:215:PRO:O	1:W:220:ARG:NH1	2.51	0.44
1:W:491:TYR:O	1:W:491:TYR:CG	2.70	0.44
1:W:782:ILE:HG12	1:W:794:GLU:HG2	2.00	0.44
1:W:876:VAL:C	1:W:879:LYS:H	2.24	0.44
3:Y:293:ILE:O	3:Y:297:ILE:HG12	2.18	0.44
8:Z:66:ILE:HG12	8:Z:76:VAL:HG22	1.99	0.44
1:A:102:GLY:HA3	1:A:187:VAL:HG12	1.98	0.44
2:B:255:LEU:C	2:B:259:LEU:HB2	2.42	0.44
3:C:269:ILE:HA	3:C:272:VAL:HG23	2.00	0.44
3:C:286:ILE:HG12	8:H:49:ASP:CG	2.43	0.44
11:M:74:GLU:HG2	11:M:77:ARG:HH21	1.81	0.44
2:R:1069:TYR:OH	2:R:1115:ARG:NH1	2.50	0.44
1:W:280:GLU:C	1:W:282:PRO:HD2	2.42	0.44
1:W:515:LEU:HB3	1:W:545:TYR:CD1	2.52	0.44
1:W:820:GLN:NE2	3:Y:79:GLY:HA3	2.32	0.44
3:Y:320:MET:O	3:Y:327:ARG:HG2	2.17	0.44
8:Z:43:PRO:HB3	8:Z:79:ARG:HH11	1.82	0.44
1:A:436:ARG:O	1:A:438:LEU:HD22	2.18	0.44
1:A:867:ASP:CA	1:A:870:ARG:NH2	2.79	0.44
2:B:284:LYS:HD3	2:B:287:ASN:ND2	2.33	0.44
2:B:380:ARG:HH11	2:B:381:LYS:CE	2.31	0.44
2:B:681:GLY:HA2	2:B:698:LEU:HB3	1.99	0.44
2:B:796:GLU:O	2:B:797:ASP:C	2.60	0.44
2:B:905:LYS:H	2:B:905:LYS:CE	2.30	0.44
3:C:122:MET:HE2	3:C:124:ILE:HD11	2.00	0.44
11:M:1:MET:HA	11:M:19:GLY:HA3	2.00	0.44
2:R:742:ILE:CG2	2:R:912:ILE:HB	2.48	0.44
2:R:1102:LEU:HD22	1:W:308:ARG:HH21	1.83	0.44
6:U:21:LEU:O	6:U:24:VAL:HG12	2.18	0.44
1:W:123:LYS:C	1:W:126:PRO:HD2	2.41	0.44
1:W:582:HIS:CD2	1:W:582:HIS:N	2.85	0.44
1:A:7:LYS:HE2	2:B:1119:GLU:OE2	2.18	0.44
1:A:215:PRO:HB3	2:B:1109:SER:HB3	1.99	0.44
1:A:470:GLU:CG	9:K:41:LEU:HD12	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:LEU:HA	1:A:557:PRO:HD3	1.88	0.44
2:B:432:VAL:HG21	2:B:456:MET:CE	2.47	0.44
2:B:606:THR:HB	2:B:609:ASP:OD1	2.17	0.44
2:B:632:GLU:CD	2:B:633:PRO:HD2	2.43	0.44
2:B:766:VAL:N	2:B:767:LYS:HE3	2.33	0.44
5:E:108:VAL:HG21	5:E:164:MET:HE3	2.00	0.44
7:G:112:PHE:HD2	7:G:114:LYS:HE3	1.83	0.44
11:M:47:HIS:HE1	11:M:49:LEU:HD12	1.83	0.44
12:N:42:ARG:O	12:N:44:CYS:N	2.50	0.44
2:R:240:ASP:O	2:R:244:ALA:HB2	2.17	0.44
2:R:892:GLY:HA2	1:W:328:PRO:HD2	1.98	0.44
1:W:517:THR:H	1:W:520:GLU:HB2	1.83	0.44
3:Y:201:SER:HB2	3:Y:204:THR:HB	1.99	0.44
1:A:582:HIS:CD2	1:A:582:HIS:N	2.86	0.44
2:B:33:SER:HB2	2:B:348:LEU:HD13	2.00	0.44
2:B:51:GLU:C	2:B:53:PRO:HD3	2.43	0.44
2:B:768:TYR:CD1	2:B:819:PRO:HG2	2.46	0.44
2:B:801:VAL:HG21	2:B:813:LEU:HD23	2.00	0.44
12:N:64:ARG:NH2	13:P:37:VAL:HG23	2.32	0.44
13:P:17:GLN:C	13:P:19:LYS:N	2.76	0.44
2:R:224:ILE:HD11	2:R:278:ARG:HD2	1.99	0.44
2:R:686:ASN:O	2:R:688:GLN:N	2.50	0.44
1:W:127:SER:HB2	3:Y:360:ARG:HH12	1.83	0.44
3:Y:47:GLU:HB3	3:Y:50:LYS:HB2	2.00	0.44
3:Y:328:GLN:CB	3:Y:332:HIS:ND1	2.81	0.44
1:A:421:ARG:N	1:A:462:MET:HE3	2.33	0.44
2:B:900:MET:SD	2:B:912:ILE:HD11	2.58	0.44
3:C:28:ILE:H	3:C:28:ILE:HG13	1.59	0.44
4:D:78:TRP:CB	4:D:79:PRO:HD2	2.46	0.44
4:D:98:ILE:HD11	4:D:114:ILE:HG12	2.00	0.44
5:E:131:LYS:HD2	5:E:136:ILE:HD13	2.00	0.44
6:F:14:TYR:HD2	6:F:74:SER:OG	1.86	0.44
2:R:86:MET:HE2	2:R:89:ARG:HH21	1.83	0.44
2:R:1057:ASP:N	2:R:1057:ASP:OD2	2.51	0.44
4:S:90:GLU:HB3	4:S:91:LYS:H	1.54	0.44
6:U:4:VAL:HG13	6:U:4:VAL:O	2.18	0.44
1:W:204:PRO:O	1:W:207:MET:HB2	2.17	0.44
3:Y:122:MET:HE1	3:Y:261:VAL:HG21	1.99	0.44
3:Y:226:ILE:HG13	3:Y:226:ILE:H	1.68	0.44
1:A:447:LEU:HD22	2:B:737:MET:HE2	2.00	0.43
1:A:653:LEU:HD21	1:A:744:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:SER:HB3	2:B:87:GLU:OE2	2.18	0.43
2:B:322:ILE:HD13	2:B:322:ILE:HA	1.85	0.43
3:C:26:GLN:C	3:C:28:ILE:H	2.26	0.43
3:C:327:ARG:HG3	3:C:334:VAL:HG23	2.00	0.43
2:R:460:GLU:HG2	2:R:673:SER:HB3	2.00	0.43
2:R:1119:GLU:HB2	1:W:7:LYS:HB2	1.99	0.43
4:S:178:LYS:O	4:S:182:VAL:HG22	2.18	0.43
5:T:91:GLN:O	5:T:98:PHE:HB2	2.18	0.43
1:W:304:GLY:O	3:Y:349:VAL:HG21	2.18	0.43
3:Y:308:VAL:HG13	3:Y:313:ILE:HD11	2.00	0.43
1:A:215:PRO:O	1:A:220:ARG:NH1	2.51	0.43
1:A:766:LEU:HB3	1:A:767:PRO:HD2	1.99	0.43
3:C:330:GLY:HA3	3:C:331:ARG:HH11	1.83	0.43
4:D:64:LEU:HD22	12:N:6:ARG:HB2	2.00	0.43
9:K:61:VAL:N	9:K:64:ILE:HG13	2.32	0.43
2:R:752:MET:HE1	2:R:910:ASP:HB3	1.99	0.43
2:R:1029:LEU:HB3	2:R:1030:ARG:H	1.59	0.43
1:W:53:GLU:HB3	1:W:54:PRO:HD2	1.99	0.43
1:W:56:GLN:HB3	1:W:57:LYS:H	1.66	0.43
1:W:338:GLY:O	1:W:443:PHE:HA	2.18	0.43
1:W:427:ARG:HH11	3:Y:73:VAL:HG11	1.83	0.43
1:W:506:ALA:O	1:W:510:THR:OG1	2.34	0.43
3:Y:323:THR:O	3:Y:325:VAL:N	2.51	0.43
1:A:600:LYS:C	1:A:602:ALA:H	2.26	0.43
2:B:907:VAL:HG21	12:N:43:TYR:CE2	2.53	0.43
2:B:1065:ASP:CB	2:B:1089:SER:HB2	2.46	0.43
4:D:167:TYR:HA	4:D:168:PRO:HD3	1.85	0.43
2:R:463:GLU:OE1	2:R:463:GLU:N	2.47	0.43
3:Y:330:GLY:HA3	3:Y:331:ARG:NH1	2.34	0.43
1:A:101:CYS:HB2	1:A:102:GLY:H	1.54	0.43
1:A:343:ILE:HG22	1:A:347:LEU:HD12	2.00	0.43
1:A:731:THR:O	1:A:732:GLY:C	2.61	0.43
1:A:855:VAL:HG13	3:C:63:LEU:O	2.19	0.43
2:B:641:THR:HB	2:B:642:HIS:CD2	2.53	0.43
11:M:48:PRO:HD3	1:W:331:ASN:ND2	2.34	0.43
12:O:42:ARG:O	12:O:44:CYS:N	2.51	0.43
12:O:60:ILE:HD11	4:S:134:GLY:N	2.32	0.43
2:R:157:VAL:O	2:R:159:GLY:N	2.51	0.43
3:Y:235:LYS:HZ1	3:Y:257:ASN:HB3	1.84	0.43
8:Z:58:LYS:O	8:Z:60:GLY:N	2.46	0.43
1:A:215:PRO:HG2	1:A:220:ARG:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:PRO:CD	1:A:261:ILE:HD12	2.47	0.43
1:A:418:LEU:HD11	2:B:1047:LEU:HD21	2.01	0.43
1:A:471:GLU:CG	9:K:41:LEU:HD13	2.44	0.43
1:A:541:ALA:HB3	1:A:542:PRO:HD3	1.99	0.43
1:A:557:PRO:HG2	1:A:619:TYR:CE1	2.54	0.43
1:A:561:ASN:HB2	1:A:872:PHE:O	2.18	0.43
1:A:777:GLU:HG3	1:A:783:TYR:CE2	2.49	0.43
1:A:780:GLY:HA2	1:A:797:PHE:CG	2.53	0.43
2:B:460:GLU:HG2	2:B:673:SER:HB3	2.00	0.43
4:D:90:GLU:HB3	4:D:91:LYS:H	1.55	0.43
5:E:83:GLU:HA	6:F:89:MET:HE3	1.99	0.43
8:H:69:SER:HB2	8:H:75:VAL:HG23	1.98	0.43
12:O:44:CYS:SG	12:O:45:CYS:N	2.91	0.43
2:R:13:ARG:NH1	2:R:647:SER:H	2.16	0.43
2:R:177:VAL:HG23	2:R:336:ASP:OD1	2.18	0.43
2:R:179:THR:HG22	2:R:181:LYS:HB2	2.00	0.43
2:R:524:ILE:HG13	2:R:529:LEU:HA	1.99	0.43
2:R:583:ILE:HB	2:R:643:LEU:HB3	2.00	0.43
4:S:8:LYS:HB2	4:S:13:ILE:HG12	1.99	0.43
5:T:15:PRO:HA	5:T:18:PHE:CE1	2.54	0.43
5:T:83:GLU:HA	6:U:89:MET:HE3	2.00	0.43
7:V:48:ILE:HG22	7:V:49:PHE:H	1.83	0.43
8:Z:49:ASP:HA	8:Z:50:PRO:HD2	1.81	0.43
1:A:237:HIS:HE1	1:A:289:HIS:CD2	2.36	0.43
1:A:420:ASN:HB2	1:A:430:MET:HG3	2.00	0.43
1:A:875:VAL:HG12	1:A:876:VAL:H	1.83	0.43
2:B:179:THR:HG22	2:B:181:LYS:HB2	2.01	0.43
2:B:421:ASN:C	2:B:421:ASN:OD1	2.61	0.43
2:B:972:VAL:HG21	4:D:205:LEU:HB3	2.00	0.43
9:K:47:ALA:HB1	9:K:48:PRO:HD2	2.00	0.43
2:R:131:ASP:OD2	2:R:132:PRO:HD2	2.18	0.43
2:R:166:THR:HG23	2:R:431:ARG:O	2.17	0.43
2:R:738:GLU:C	2:R:740:SER:H	2.26	0.43
2:R:1078:ASN:HD22	2:R:1079:LYS:HG2	1.82	0.43
1:A:16:PRO:HA	1:A:19:ILE:HD12	2.01	0.43
1:A:323:ARG:NH2	1:A:422:GLN:HE21	2.15	0.43
1:A:338:GLY:O	1:A:443:PHE:HA	2.18	0.43
1:A:472:ALA:HB1	2:B:1047:LEU:HD12	2.00	0.43
1:A:572:PRO:CG	1:A:717:LYS:HE2	2.48	0.43
2:B:86:MET:HE2	2:B:89:ARG:HH21	1.83	0.43
2:B:279:VAL:HB	2:B:280:ALA:H	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:126:LEU:HB2	3:C:131:LYS:HG3	2.01	0.43
5:E:20:LYS:O	5:E:21:PRO:C	2.61	0.43
5:E:85:VAL:HG23	6:F:14:TYR:OH	2.19	0.43
7:G:83:ASP:HB2	7:G:101:LEU:HG	1.99	0.43
2:R:662:GLU:H	2:R:662:GLU:HG3	1.53	0.43
2:R:777:VAL:HG12	2:R:778:MET:H	1.84	0.43
2:R:914:ASN:C	2:R:916:HIS:H	2.26	0.43
1:W:280:GLU:HB2	1:W:300:GLN:NE2	2.33	0.43
1:W:586:VAL:HA	1:W:596:GLY:HA3	1.99	0.43
1:W:615:LEU:HD22	1:W:623:TYR:OH	2.19	0.43
3:Y:371:GLU:OE2	3:Y:371:GLU:N	2.39	0.43
2:B:163:VAL:O	2:B:414:SER:HA	2.19	0.43
2:B:765:GLU:HA	2:B:767:LYS:HZ2	1.84	0.43
2:B:904:VAL:HG11	4:D:204:THR:HG22	2.01	0.43
2:B:985:ARG:HD2	4:D:206:CYS:HA	2.00	0.43
2:B:1057:ASP:OD2	2:B:1057:ASP:N	2.52	0.43
2:B:1077:LYS:N	2:B:1078:ASN:HA	2.32	0.43
4:D:114:ILE:HD12	4:D:123:PRO:HG3	2.01	0.43
4:D:232:SER:HB3	4:D:241:ILE:CD1	2.48	0.43
2:R:605:ILE:HG23	2:R:606:THR:N	2.34	0.43
4:S:258:LYS:O	4:S:261:VAL:HG22	2.19	0.43
1:W:335:ASP:O	1:W:433:HIS:HA	2.19	0.43
1:W:561:ASN:HB2	1:W:872:PHE:O	2.18	0.43
3:Y:165:ILE:HG22	3:Y:207:ASN:HD22	1.84	0.43
1:A:586:VAL:HA	1:A:596:GLY:HA3	2.01	0.43
2:B:180:GLY:O	2:B:182:THR:N	2.52	0.43
2:B:240:ASP:O	2:B:244:ALA:HB2	2.18	0.43
3:C:81:PRO:HB3	3:C:306:LEU:HD21	2.00	0.43
3:C:170:ASP:O	3:C:174:LEU:HD21	2.19	0.43
9:I:12:ASP:C	9:I:14:HIS:H	2.27	0.43
9:I:23:TRP:C	9:I:25:ASN:N	2.76	0.43
9:I:41:LEU:HD12	1:W:470:GLU:CG	2.45	0.43
9:I:64:ILE:CD1	1:W:356:TRP:CE2	3.02	0.43
12:N:1:MET:O	12:N:2:MET:HB2	2.19	0.43
12:N:7:CYS:HB3	12:N:10:CYS:SG	2.59	0.43
4:S:15:LEU:HD12	4:S:228:LEU:HD22	2.01	0.43
1:A:104:VAL:HG12	1:A:104:VAL:O	2.19	0.43
1:A:740:ILE:HA	1:A:743:MET:HE3	2.00	0.43
2:B:668:ARG:HH11	2:B:921:ARG:HB3	1.84	0.43
2:B:689:LEU:CD1	12:N:62:TYR:HB3	2.49	0.43
2:B:781:PRO:HA	2:B:786:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:913:LEU:HD22	2:B:914:ASN:H	1.84	0.43
2:B:953:ILE:O	2:B:957:GLN:HG3	2.17	0.43
2:B:1005:HIS:CE1	2:B:1007:ARG:HD2	2.54	0.43
5:E:112:GLN:HB3	5:E:163:THR:HG23	2.01	0.43
12:O:5:ILE:HG12	4:S:64:LEU:HB3	2.00	0.43
2:R:14:TRP:CD1	2:R:709:ARG:NH1	2.87	0.43
2:R:284:LYS:HD3	2:R:287:ASN:ND2	2.34	0.43
2:R:476:MET:HE1	2:R:645:ILE:HB	2.01	0.43
2:R:913:LEU:HD22	2:R:914:ASN:H	1.83	0.43
2:R:914:ASN:HA	2:R:915:PRO:HD2	1.82	0.43
2:R:1078:ASN:ND2	2:R:1079:LYS:HG2	2.33	0.43
1:W:417:VAL:HG11	1:W:464:LEU:CD1	2.49	0.43
1:W:421:ARG:N	1:W:462:MET:HE3	2.33	0.43
1:W:524:ILE:CG2	1:W:634:VAL:HG13	2.49	0.43
3:Y:26:GLN:C	3:Y:28:ILE:H	2.26	0.43
1:A:765:THR:HG22	1:A:766:LEU:HD22	2.00	0.42
2:B:46:ILE:HG13	2:B:66:ILE:CG1	2.49	0.42
2:B:86:MET:HE3	2:B:686:ASN:ND2	2.33	0.42
2:B:928:MET:HE2	2:B:953:ILE:HG21	2.01	0.42
3:C:159:ASP:HB2	3:C:163:MET:HB2	2.01	0.42
4:D:222:VAL:O	4:D:223:GLU:C	2.61	0.42
12:O:4:PRO:HA	4:S:61:ARG:HH12	1.84	0.42
2:R:52:ILE:N	2:R:53:PRO:CD	2.81	0.42
2:R:1021:GLU:HG2	1:W:317:ARG:NH2	2.34	0.42
2:R:1046:MET:HB2	1:W:475:GLU:OE2	2.19	0.42
4:S:11:LYS:O	4:S:231:GLU:HA	2.19	0.42
1:W:372:TRP:HB3	1:W:373:PRO:HD3	2.01	0.42
1:W:765:THR:HG22	1:W:766:LEU:HD22	2.02	0.42
1:A:354:THR:C	1:A:356:TRP:H	2.26	0.42
1:A:736:SER:O	1:A:738:LEU:N	2.52	0.42
2:B:180:GLY:C	2:B:182:THR:H	2.27	0.42
2:B:532:TYR:O	2:B:533:TYR:HB3	2.19	0.42
3:C:165:ILE:HG22	3:C:207:ASN:HD22	1.83	0.42
4:D:144:ARG:HE	4:D:144:ARG:HB3	1.63	0.42
10:J:78:ARG:NH2	8:Z:82:ILE:HG22	2.33	0.42
12:O:8:PHE:HB3	2:R:747:SER:HB3	2.00	0.42
2:R:205:ILE:H	2:R:205:ILE:HD12	1.83	0.42
2:R:483:ILE:HD12	2:R:555:GLU:HB2	2.01	0.42
2:R:1046:MET:HB2	1:W:475:GLU:CD	2.45	0.42
2:R:1049:LYS:C	2:R:1051:ARG:H	2.27	0.42
1:W:482:VAL:C	1:W:484:LYS:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:232:LYS:HB2	3:Y:232:LYS:HE3	1.90	0.42
1:A:782:ILE:HG12	1:A:794:GLU:HG2	2.00	0.42
2:B:466:ASN:HD22	2:B:466:ASN:HA	1.59	0.42
4:D:96:ILE:HD13	4:D:114:ILE:CG2	2.49	0.42
5:E:30:LEU:HD22	5:E:72:PHE:HE1	1.82	0.42
12:O:6:ARG:HH21	4:S:233:VAL:HG21	1.85	0.42
2:R:122:LEU:HD11	2:R:353:PHE:CE2	2.54	0.42
2:R:552:ILE:HG13	2:R:553:SER:H	1.85	0.42
6:U:71:VAL:HG11	6:U:89:MET:HE1	2.02	0.42
1:W:176:THR:HA	1:W:177:PRO:HD2	1.83	0.42
1:W:342:ILE:HD13	1:W:345:ARG:HH22	1.84	0.42
1:W:354:THR:C	1:W:356:TRP:H	2.26	0.42
1:W:481:LEU:HD23	1:W:481:LEU:HA	1.90	0.42
1:W:600:LYS:C	1:W:602:ALA:H	2.26	0.42
3:Y:119:THR:N	3:Y:120:PRO:HD3	2.34	0.42
1:A:573:ARG:CG	1:A:573:ARG:NH1	2.61	0.42
2:B:233:LEU:HD22	2:B:311:ARG:O	2.19	0.42
2:B:703:ARG:CD	2:B:717:THR:HG22	2.47	0.42
2:B:981:LYS:O	2:B:981:LYS:HG3	2.18	0.42
3:C:112:ASP:OD1	3:C:329:ILE:HG22	2.19	0.42
3:C:146:TYR:HD1	3:C:235:LYS:N	2.14	0.42
4:D:30:ARG:HB2	11:L:23:THR:HG23	2.02	0.42
8:H:39:PRO:HB2	8:H:80:TYR:CD2	2.54	0.42
11:M:23:THR:HG23	4:S:30:ARG:HB2	2.00	0.42
12:O:46:ARG:HD2	2:R:937:ALA:O	2.19	0.42
2:R:180:GLY:C	2:R:182:THR:H	2.27	0.42
2:R:364:PHE:HE1	2:R:388:VAL:HG13	1.84	0.42
2:R:462:PRO:HG2	2:R:470:VAL:HG13	2.01	0.42
2:R:951:THR:HA	2:R:952:PRO:HD3	1.90	0.42
2:R:1051:ARG:O	1:W:318:VAL:HG11	2.18	0.42
4:S:172:ILE:HG22	4:S:174:GLY:O	2.19	0.42
1:W:289:HIS:O	1:W:291:SER:N	2.49	0.42
1:W:413:ASP:HA	1:W:435:VAL:O	2.19	0.42
1:W:870:ARG:CZ	1:W:870:ARG:HB2	2.44	0.42
3:Y:123:THR:HG22	3:Y:252:LEU:HD22	2.00	0.42
8:Z:24:SER:O	8:Z:25:ILE:C	2.63	0.42
1:A:86:PHE:HA	1:A:89:HIS:HD2	1.83	0.42
1:A:275:THR:HG23	1:A:279:ASN:ND2	2.34	0.42
1:A:490:ARG:HD2	1:A:491:TYR:CD1	2.54	0.42
1:A:728:MET:HE3	2:B:919:PRO:HG3	2.02	0.42
2:B:52:ILE:N	2:B:53:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:MET:HE1	2:B:315:ALA:HB1	2.01	0.42
2:B:1072:TRP:HB3	2:B:1073:TYR:H	1.44	0.42
13:P:21:LEU:HD22	13:P:22:PRO:HA	2.00	0.42
2:R:180:GLY:O	2:R:182:THR:N	2.50	0.42
2:R:301:LEU:N	2:R:302:PRO:HD3	2.34	0.42
2:R:539:LEU:O	2:R:543:ILE:HG13	2.20	0.42
2:R:814:ILE:O	2:R:839:SER:HB2	2.19	0.42
2:R:1103:LEU:O	2:R:1107:LEU:HG	2.19	0.42
4:S:153:HIS:C	4:S:155:LYS:H	2.28	0.42
1:W:438:LEU:HG	1:W:444:ARG:NH1	2.34	0.42
1:W:653:LEU:HB3	1:W:719:LEU:HD12	2.02	0.42
1:W:729:ALA:O	1:W:730:ARG:CB	2.67	0.42
1:W:740:ILE:HA	1:W:743:MET:HE3	2.01	0.42
2:B:125:MET:SD	2:B:153:GLY:HA2	2.60	0.42
2:B:247:LEU:O	2:B:248:ASP:C	2.63	0.42
2:B:605:ILE:HG12	2:B:606:THR:H	1.85	0.42
2:B:679:ALA:HB3	2:B:721:ALA:HB1	2.01	0.42
3:C:81:PRO:O	3:C:82:GLY:C	2.63	0.42
4:D:90:GLU:O	4:D:92:CYS:N	2.53	0.42
5:E:79:PRO:CB	5:E:160:ILE:HD11	2.50	0.42
9:I:65:ALA:HA	9:I:68:GLU:HG2	2.02	0.42
2:R:375:SER:C	2:R:377:VAL:H	2.27	0.42
2:R:632:GLU:OE1	2:R:633:PRO:HD2	2.20	0.42
2:R:668:ARG:HH12	2:R:921:ARG:HD2	1.85	0.42
4:S:222:VAL:O	4:S:223:GLU:C	2.62	0.42
1:W:490:ARG:HD2	1:W:491:TYR:CD1	2.55	0.42
1:W:756:ARG:NH2	1:W:774:ILE:HG22	2.34	0.42
1:A:458:ASP:HB2	2:B:888:LYS:HB3	2.01	0.42
1:A:507:TYR:CD1	1:A:597:VAL:HG21	2.54	0.42
1:A:542:PRO:HD3	7:G:71:PHE:HA	2.02	0.42
2:B:43:GLN:HA	2:B:66:ILE:CD1	2.48	0.42
2:B:104:ILE:HD12	2:B:113:GLU:CD	2.45	0.42
2:B:237:THR:HB	2:B:240:ASP:HB2	2.02	0.42
2:B:600:LEU:O	2:B:601:ASP:CB	2.67	0.42
3:C:108:ILE:O	3:C:111:VAL:HG12	2.20	0.42
3:C:162:SER:HB2	3:C:210:PHE:CZ	2.55	0.42
3:C:210:PHE:HB3	3:C:211:ALA:H	1.53	0.42
3:C:286:ILE:HG23	3:C:324:GLY:O	2.20	0.42
3:C:322:ARG:O	3:C:323:THR:HB	2.19	0.42
10:Q:45:MET:HB3	10:Q:68:PHE:HE1	1.84	0.42
2:R:1113:SER:O	1:W:11:PHE:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:517:THR:N	1:W:520:GLU:HB2	2.35	0.42
2:B:430:ARG:NH1	2:B:653:ILE:HG13	2.35	0.42
3:C:109:GLU:OE2	3:C:118:SER:OG	2.33	0.42
3:C:226:ILE:HG13	3:C:226:ILE:H	1.69	0.42
3:C:343:ALA:HB2	3:C:371:GLU:CD	2.44	0.42
5:E:34:TYR:O	5:E:45:VAL:HG13	2.20	0.42
8:H:24:SER:C	8:H:26:ASP:N	2.77	0.42
2:R:255:LEU:C	2:R:259:LEU:HB2	2.44	0.42
2:R:476:MET:HE3	2:R:581:PRO:HG2	2.02	0.42
4:S:96:ILE:HD13	4:S:114:ILE:HG23	2.01	0.42
5:T:85:VAL:HG23	6:U:14:TYR:OH	2.19	0.42
1:W:104:VAL:O	1:W:137:LYS:HG2	2.20	0.42
1:W:106:ILE:HG22	1:W:107:SER:N	2.28	0.42
3:Y:80:GLU:OE1	3:Y:81:PRO:HD3	2.19	0.42
3:Y:239:ARG:O	3:Y:253:THR:HA	2.19	0.42
1:A:319:ASP:O	1:A:320:PHE:C	2.63	0.42
1:A:421:ARG:NH2	1:A:454:ASN:O	2.53	0.42
2:B:122:LEU:HD11	2:B:353:PHE:CE2	2.55	0.42
2:B:1005:HIS:CE1	2:B:1007:ARG:NH1	2.87	0.42
9:I:44:ALA:C	9:I:46:GLY:N	2.78	0.42
9:K:60:ASP:O	9:K:61:VAL:O	2.37	0.42
4:S:6:LEU:HB3	4:S:14:ASP:HB3	2.02	0.42
1:W:428:ILE:C	1:W:430:MET:H	2.28	0.42
1:W:592:ILE:O	1:W:594:LEU:HD22	2.19	0.42
1:A:14:LEU:HB3	2:B:1111:ILE:HG23	2.02	0.42
1:A:113:LYS:HA	1:A:116:ARG:HB3	2.02	0.42
1:A:156:ILE:HG21	1:A:270:GLN:O	2.19	0.42
1:A:284:LEU:HD23	1:A:286:PRO:HG3	2.02	0.42
1:A:541:ALA:CB	1:A:542:PRO:CD	2.98	0.42
1:A:648:LEU:HD21	1:A:787:ARG:HD3	2.02	0.42
3:C:388:LEU:HD11	9:K:34:ARG:HG3	2.02	0.42
4:D:101:GLU:HB3	4:D:138:LYS:HG3	2.01	0.42
4:D:153:HIS:C	4:D:155:LYS:H	2.27	0.42
8:H:25:ILE:CG1	10:Q:51:TRP:HE3	2.24	0.42
11:L:44:TYR:CE2	11:L:54:ILE:HB	2.55	0.42
12:O:47:ARG:NH1	2:R:726:ILE:HD12	2.34	0.42
2:R:905:LYS:H	2:R:905:LYS:CE	2.27	0.42
2:R:905:LYS:HE3	2:R:965:TYR:HE2	1.85	0.42
2:R:906:GLY:H	4:S:163:ILE:HD11	1.84	0.42
2:R:1074:ASP:HB3	2:R:1075:LYS:CA	2.50	0.42
1:W:58:CYS:HA	1:W:59:PRO:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:258:PRO:CD	1:W:261:ILE:HD12	2.50	0.42
1:W:353:ILE:HG21	1:W:358:ILE:HD13	2.01	0.42
3:Y:13:LEU:HD21	3:Y:48:ILE:HG23	2.01	0.42
3:Y:322:ARG:O	3:Y:323:THR:HB	2.20	0.42
1:A:353:ILE:HD13	1:A:405:TYR:HB2	2.02	0.41
1:A:819:MET:SD	3:C:107:LEU:HD22	2.60	0.41
2:B:322:ILE:O	2:B:326:ILE:HG12	2.19	0.41
2:B:762:SER:HB3	2:B:866:LYS:HA	2.02	0.41
3:C:102:LEU:HD21	3:C:119:THR:OG1	2.20	0.41
6:F:21:LEU:O	6:F:24:VAL:HG12	2.19	0.41
12:O:19:GLN:HB2	12:O:20:PRO:HD3	2.01	0.41
2:R:591:LEU:HB2	2:R:594:ARG:HD2	2.02	0.41
2:R:606:THR:HB	2:R:609:ASP:OD1	2.20	0.41
2:R:922:MET:SD	1:W:739:ASN:HB2	2.60	0.41
5:T:82:GLN:HB3	6:U:88:ILE:HG13	2.01	0.41
1:W:196:GLY:O	3:Y:360:ARG:HD3	2.20	0.41
1:W:573:ARG:NH2	1:W:721:PRO:HB3	2.35	0.41
1:W:868:VAL:HG13	3:Y:39:LYS:HE2	2.01	0.41
3:Y:347:PHE:C	3:Y:349:VAL:N	2.77	0.41
1:A:56:GLN:HB3	1:A:57:LYS:H	1.66	0.41
1:A:256:GLY:O	1:A:257:ALA:HB3	2.20	0.41
1:A:491:TYR:O	1:A:492:GLY:C	2.61	0.41
1:A:653:LEU:HB3	1:A:719:LEU:HD12	2.02	0.41
2:R:196:THR:OG1	2:R:200:ARG:O	2.38	0.41
2:R:440:GLN:OE1	2:R:440:GLN:HA	2.20	0.41
2:R:600:LEU:O	2:R:601:ASP:CB	2.69	0.41
2:R:646:TRP:CZ3	2:R:648:PRO:HB2	2.55	0.41
1:W:46:ASP:H	1:W:47:PRO:CD	2.33	0.41
1:W:142:LYS:O	1:W:143:ALA:CB	2.68	0.41
1:W:851:GLY:HA3	3:Y:311:ARG:HG3	2.02	0.41
3:Y:122:MET:HE2	3:Y:124:ILE:HD11	2.02	0.41
1:A:156:ILE:HD13	1:A:270:GLN:O	2.20	0.41
1:A:351:GLU:HB3	1:A:361:LEU:HD21	2.02	0.41
1:A:815:GLN:O	1:A:818:TYR:HB3	2.20	0.41
2:B:165:VAL:O	2:B:167:GLN:NE2	2.53	0.41
2:B:765:GLU:HA	2:B:767:LYS:NZ	2.35	0.41
2:B:905:LYS:HE3	2:B:965:TYR:HE2	1.86	0.41
2:B:1007:ARG:NH2	2:B:1026:GLU:O	2.39	0.41
5:E:145:ARG:HG3	5:E:169:LEU:HD21	2.02	0.41
7:G:48:ILE:HG22	7:G:49:PHE:H	1.84	0.41
11:M:22:HIS:O	11:M:23:THR:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:84:SER:HB2	2:R:144:ILE:HD12	2.01	0.41
2:R:703:ARG:HH22	2:R:942:ILE:HG21	1.85	0.41
2:R:1047:LEU:HD11	1:W:418:LEU:HD11	2.02	0.41
4:S:38:VAL:HG13	4:S:39:MET:H	1.85	0.41
1:W:877:GLY:C	1:W:878:TRP:CE3	2.98	0.41
3:Y:297:ILE:O	3:Y:301:LEU:HD12	2.20	0.41
2:B:1074:ASP:HB3	2:B:1075:LYS:CA	2.51	0.41
2:R:380:ARG:HH11	2:R:381:LYS:CE	2.33	0.41
2:R:766:VAL:N	2:R:767:LYS:HE3	2.34	0.41
2:R:921:ARG:H	2:R:921:ARG:HG2	1.74	0.41
4:S:90:GLU:O	4:S:92:CYS:N	2.53	0.41
1:W:859:TYR:HB3	3:Y:63:LEU:HB3	2.03	0.41
1:W:864:LYS:HD2	3:Y:32:LEU:HD11	2.03	0.41
1:A:371:LYS:CD	1:A:373:PRO:HD2	2.50	0.41
1:A:820:GLN:O	1:A:824:ILE:HB	2.20	0.41
1:A:879:LYS:NZ	3:C:46:ASP:HB2	2.35	0.41
2:B:404:GLY:HA2	2:B:414:SER:H	1.84	0.41
2:B:627:ALA:CB	2:B:642:HIS:HD2	2.30	0.41
2:B:855:ILE:O	13:P:34:ILE:CG2	2.68	0.41
2:B:1069:TYR:OH	2:B:1115:ARG:NH1	2.53	0.41
11:M:33:ARG:HE	1:W:522:GLN:HB2	1.85	0.41
12:O:42:ARG:NH1	4:S:161:LEU:HD13	2.35	0.41
12:O:50:LEU:CD2	2:R:940:GLY:HA2	2.50	0.41
2:R:762:SER:HB3	2:R:866:LYS:HG2	2.02	0.41
1:W:98:CYS:O	1:W:98:CYS:SG	2.78	0.41
13:X:19:LYS:HD3	13:X:19:LYS:HA	1.83	0.41
3:Y:102:LEU:HD21	3:Y:119:THR:OG1	2.19	0.41
1:A:411:LEU:HD23	1:A:435:VAL:HG21	2.03	0.41
1:A:876:VAL:HA	1:A:879:LYS:HB2	2.03	0.41
2:B:224:ILE:HD11	2:B:278:ARG:HD2	2.02	0.41
2:B:440:GLN:OE1	2:B:440:GLN:HA	2.20	0.41
2:B:727:LEU:HD12	2:B:911:VAL:HB	2.03	0.41
2:B:1098:TYR:CE1	2:B:1101:LYS:HD3	2.54	0.41
12:N:2:MET:HG2	12:N:56:ILE:HD13	2.03	0.41
2:R:155:PHE:CD2	2:R:155:PHE:N	2.87	0.41
2:R:167:GLN:HG2	2:R:352:LEU:HD21	2.03	0.41
2:R:466:ASN:HD22	2:R:466:ASN:HA	1.59	0.41
2:R:641:THR:HB	2:R:642:HIS:CD2	2.55	0.41
2:R:740:SER:HB2	1:W:457:PHE:HB2	2.02	0.41
2:R:766:VAL:H	2:R:767:LYS:HE3	1.85	0.41
7:V:9:ILE:CD1	7:V:104:LYS:HD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:270:ALA:HA	8:Z:14:HIS:HB3	2.01	0.41
1:A:750:GLN:CG	1:A:782:ILE:HD12	2.51	0.41
2:B:423:LEU:HD21	2:B:654:THR:HG23	2.02	0.41
2:B:972:VAL:CG2	4:D:205:LEU:HB3	2.51	0.41
3:C:104:LEU:HB3	3:C:105:PRO:HD3	2.03	0.41
3:C:239:ARG:O	3:C:253:THR:HA	2.20	0.41
3:C:258:LEU:O	3:C:262:LEU:HG	2.21	0.41
9:I:23:TRP:HA	9:I:23:TRP:HE3	1.85	0.41
11:L:69:LEU:O	11:L:73:ILE:HG12	2.21	0.41
12:N:19:GLN:HB2	12:N:20:PRO:HD3	2.02	0.41
2:R:380:ARG:HD3	2:R:381:LYS:CE	2.48	0.41
2:R:781:PRO:HA	2:R:786:TYR:CZ	2.55	0.41
2:R:1102:LEU:HB3	1:W:308:ARG:HH21	1.86	0.41
1:W:757:ILE:HD13	1:W:800:ALA:HB3	2.03	0.41
3:Y:269:ILE:HA	3:Y:272:VAL:HG23	2.01	0.41
3:Y:337:GLU:O	3:Y:339:ASN:N	2.52	0.41
8:Z:23:LEU:HD12	8:Z:62:ILE:HG13	2.03	0.41
1:A:134:GLU:HA	1:A:137:LYS:HD2	2.02	0.41
1:A:543:ARG:HB2	1:A:545:TYR:CE2	2.56	0.41
1:A:756:ARG:NH2	1:A:774:ILE:HG22	2.36	0.41
2:B:394:THR:O	2:B:397:ILE:HG22	2.21	0.41
2:B:737:MET:H	2:B:740:SER:HB3	1.84	0.41
2:R:1069:TYR:HA	2:R:1070:ILE:HB	2.03	0.41
2:R:1072:TRP:HB3	2:R:1073:TYR:H	1.43	0.41
4:S:216:LEU:C	4:S:217:ILE:HG13	2.46	0.41
1:W:104:VAL:O	1:W:104:VAL:HG12	2.20	0.41
1:W:235:LEU:HD11	1:W:298:LEU:HG	2.02	0.41
1:W:336:GLU:HA	1:W:434:ARG:H	1.86	0.41
1:A:46:ASP:H	1:A:47:PRO:CD	2.34	0.41
1:A:131:ARG:NH2	3:C:360:ARG:HH21	2.19	0.41
1:A:134:GLU:HB3	1:A:138:LYS:HE3	2.03	0.41
1:A:285:PRO:HB2	1:A:286:PRO:HA	2.01	0.41
1:A:525:LEU:HD11	1:A:551:VAL:HG23	2.03	0.41
1:A:648:LEU:HD11	2:B:928:MET:HG2	2.03	0.41
1:A:732:GLY:O	1:A:733:ALA:C	2.64	0.41
1:A:757:ILE:HD13	1:A:800:ALA:HB3	2.03	0.41
2:B:167:GLN:HG2	2:B:352:LEU:HD21	2.03	0.41
2:B:196:THR:OG1	2:B:200:ARG:O	2.39	0.41
2:B:294:GLN:HA	2:B:297:ASP:HB2	2.02	0.41
2:B:608:ASP:O	2:B:612:ARG:HG3	2.21	0.41
2:B:767:LYS:NZ	2:B:774:ASP:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1007:ARG:HH22	2:B:1022:GLY:H	1.68	0.41
3:C:119:THR:N	3:C:120:PRO:HD3	2.36	0.41
4:D:44:VAL:HG13	4:D:143:ALA:HB2	2.02	0.41
4:D:148:GLY:HA3	4:D:156:PHE:CE1	2.56	0.41
5:E:78:VAL:HA	5:E:79:PRO:HD3	1.87	0.41
7:G:31:MET:CE	7:G:55:VAL:HG11	2.51	0.41
8:H:62:ILE:HG22	8:H:80:TYR:HD2	1.86	0.41
9:K:12:ASP:C	9:K:14:HIS:H	2.28	0.41
2:R:737:MET:SD	1:W:501:ASP:HB2	2.61	0.41
2:R:857:GLU:HG2	2:R:862:ASN:C	2.46	0.41
2:R:1039:LEU:HD23	2:R:1039:LEU:HA	1.84	0.41
6:U:30:SER:HB2	6:U:34:LEU:HD13	2.03	0.41
7:V:31:MET:CE	7:V:55:VAL:HG11	2.51	0.41
1:W:812:ARG:NH2	3:Y:304:GLN:HE22	2.18	0.41
3:Y:162:SER:HB2	3:Y:210:PHE:CZ	2.56	0.41
3:Y:195:GLU:HB3	3:Y:209:SER:HA	2.02	0.41
3:Y:219:LEU:HG	3:Y:222:LEU:HD22	2.01	0.41
1:A:110:GLU:HA	1:A:113:LYS:HD2	2.03	0.41
2:B:63:LEU:HD23	2:B:103:MET:HG2	2.03	0.41
2:B:122:LEU:HD11	2:B:353:PHE:HE2	1.86	0.41
2:B:177:VAL:HG23	2:B:336:ASP:OD1	2.21	0.41
2:B:192:ILE:HB	2:B:206:GLU:HB2	2.01	0.41
2:B:843:ARG:HB2	2:B:846:GLU:CD	2.46	0.41
3:C:195:GLU:HB3	3:C:209:SER:HA	2.03	0.41
8:H:13:ILE:HG21	8:H:19:LYS:HZ1	1.86	0.41
9:I:75:PRO:HB2	3:Y:391:ARG:HD2	2.02	0.41
12:N:56:ILE:O	12:N:60:ILE:HB	2.21	0.41
12:O:5:ILE:HD12	4:S:128:ILE:HG21	2.02	0.41
10:Q:76:GLU:N	10:Q:76:GLU:OE1	2.54	0.41
2:R:90:LEU:HD22	2:R:854:LEU:CD1	2.51	0.41
2:R:177:VAL:HG13	2:R:325:VAL:HG22	2.01	0.41
2:R:230:MET:HE1	2:R:315:ALA:HB1	2.02	0.41
2:R:247:LEU:O	2:R:248:ASP:C	2.64	0.41
4:S:94:THR:HG23	4:S:145:LEU:HB2	2.02	0.41
1:W:377:TYR:HB2	1:W:408:GLU:HB2	2.03	0.41
3:Y:293:ILE:HD12	3:Y:320:MET:CE	2.51	0.41
1:A:12:GLY:HA3	1:A:201:THR:HG22	2.03	0.40
3:C:30:GLU:HB3	3:C:31:ASP:H	1.51	0.40
5:E:18:PHE:HB2	9:K:48:PRO:HD3	2.03	0.40
2:R:430:ARG:NH1	2:R:653:ILE:HG13	2.35	0.40
5:T:171:LYS:HB2	5:T:174:TRP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:67:THR:C	7:V:69:ASP:N	2.78	0.40
1:W:88:LYS:H	1:W:88:LYS:HD3	1.86	0.40
1:A:88:LYS:HD3	1:A:88:LYS:H	1.85	0.40
1:A:215:PRO:HD2	1:A:239:LEU:HD11	2.04	0.40
1:A:428:ILE:HG22	1:A:452:PRO:HB3	2.02	0.40
1:A:764:ARG:N	1:A:764:ARG:CD	2.84	0.40
1:A:787:ARG:HH12	2:B:953:ILE:HG13	1.86	0.40
2:B:605:ILE:HG12	2:B:606:THR:N	2.35	0.40
3:C:28:ILE:HG21	9:K:14:HIS:NE2	2.36	0.40
4:D:6:LEU:HB3	4:D:14:ASP:HB3	2.02	0.40
4:D:64:LEU:HB3	12:N:5:ILE:HG12	2.02	0.40
4:D:172:ILE:HG22	4:D:174:GLY:O	2.21	0.40
12:O:42:ARG:HD2	2:R:905:LYS:O	2.21	0.40
2:R:163:VAL:O	2:R:414:SER:HA	2.21	0.40
2:R:646:TRP:CD2	2:R:648:PRO:HD2	2.57	0.40
2:R:681:GLY:HA2	2:R:698:LEU:HB3	2.03	0.40
2:R:954:GLU:HA	2:R:957:GLN:HB2	2.02	0.40
5:T:60:VAL:HG22	5:T:61:PHE:H	1.87	0.40
7:V:66:TYR:N	7:V:66:TYR:HD1	2.18	0.40
1:W:305:LYS:HB3	1:W:310:ARG:NH1	2.35	0.40
1:W:732:GLY:O	1:W:733:ALA:C	2.64	0.40
1:W:764:ARG:N	1:W:764:ARG:CD	2.84	0.40
3:Y:53:ASP:HA	3:Y:56:ILE:CG1	2.50	0.40
1:A:106:ILE:HG22	1:A:107:SER:N	2.24	0.40
1:A:234:ASP:OD1	1:A:296:ARG:NH1	2.54	0.40
1:A:348:THR:HG22	1:A:410:HIS:HA	2.03	0.40
1:A:421:ARG:HB2	1:A:462:MET:CE	2.51	0.40
1:A:524:ILE:CG2	1:A:634:VAL:HG13	2.51	0.40
2:B:627:ALA:CB	2:B:642:HIS:CD2	3.04	0.40
2:B:775:LYS:HB3	2:B:776:ILE:H	1.75	0.40
3:C:389:THR:HG21	5:E:56:GLU:HB3	2.03	0.40
4:D:216:LEU:C	4:D:217:ILE:HG13	2.46	0.40
7:G:67:THR:C	7:G:69:ASP:N	2.80	0.40
13:P:19:LYS:HD3	13:P:19:LYS:HA	1.85	0.40
2:R:680:LEU:HD21	2:R:997:HIS:HB3	2.03	0.40
2:R:696:HIS:CE1	2:R:757:PHE:HD1	2.39	0.40
2:R:703:ARG:CD	2:R:717:THR:HG22	2.47	0.40
2:R:900:MET:SD	2:R:912:ILE:HD11	2.61	0.40
6:U:62:ILE:H	6:U:62:ILE:HG13	1.77	0.40
1:W:612:LEU:O	1:W:613:HIS:C	2.63	0.40
1:W:777:GLU:HG3	1:W:783:TYR:CE2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ILE:HD11	1:A:628:MET:HB3	2.03	0.40
1:A:336:GLU:HA	1:A:434:ARG:H	1.85	0.40
2:B:20:TYR:OH	2:B:478:GLN:HG3	2.22	0.40
2:B:90:LEU:HD22	2:B:854:LEU:CD1	2.51	0.40
2:B:147:ASP:HB3	2:B:685:ALA:HB3	2.04	0.40
2:B:164:ILE:O	2:B:164:ILE:HG22	2.21	0.40
2:B:177:VAL:HG13	2:B:325:VAL:HG22	2.03	0.40
2:B:272:LEU:O	2:B:276:GLY:N	2.34	0.40
2:B:753:TYR:CD1	2:B:881:PHE:HE2	2.40	0.40
2:B:907:VAL:HG21	12:N:43:TYR:HE2	1.86	0.40
8:H:24:SER:O	8:H:25:ILE:C	2.65	0.40
9:K:53:ILE:HG23	9:K:55:ASN:HD22	1.86	0.40
2:R:91:ARG:O	2:R:92:ASN:HB2	2.22	0.40
2:R:157:VAL:HG21	2:R:162:ARG:HD3	2.03	0.40
2:R:171:ALA:HB1	2:R:174:ARG:HD2	2.04	0.40
2:R:775:LYS:HB3	2:R:776:ILE:H	1.79	0.40
2:R:1046:MET:HE3	5:T:61:PHE:HD2	1.83	0.40
1:W:237:HIS:HE1	1:W:289:HIS:CD2	2.38	0.40
1:W:451:PRO:O	1:W:452:PRO:C	2.64	0.40
1:W:734:ARG:NH1	1:W:734:ARG:CB	2.84	0.40
3:Y:343:ALA:HB2	3:Y:371:GLU:HG3	2.03	0.40
8:Z:15:TYR:CD2	8:Z:16:LEU:HG	2.56	0.40
1:A:418:LEU:HD21	2:B:1047:LEU:HD21	2.03	0.40
1:A:491:TYR:O	1:A:491:TYR:CG	2.74	0.40
2:B:956:LEU:O	2:B:960:ILE:HG23	2.21	0.40
3:C:290:ARG:NH2	8:H:67:ARG:HE	2.19	0.40
4:D:51:SER:HB3	4:D:139:ILE:HD11	2.02	0.40
4:D:55:ASP:HB3	13:P:45:VAL:HG21	2.03	0.40
5:E:171:LYS:HB2	5:E:174:TRP:HB2	2.03	0.40
8:H:66:ILE:HG12	8:H:76:VAL:HG22	2.03	0.40
12:O:13:LEU:CD1	4:S:66:PRO:HG3	2.48	0.40
2:R:122:LEU:HD11	2:R:353:PHE:HE2	1.86	0.40
2:R:350:GLY:C	2:R:352:LEU:H	2.28	0.40
2:R:520:TRP:O	2:R:521:SER:HB2	2.21	0.40
2:R:788:GLY:H	2:R:792:TYR:HE1	1.68	0.40
4:S:222:VAL:HB	4:S:225:LYS:HB2	2.03	0.40
5:T:13:ILE:O	5:T:65:ALA:HB1	2.21	0.40
5:T:61:PHE:CZ	3:Y:384:GLY:HA2	2.57	0.40
7:V:79:THR:CG2	7:V:80:GLU:N	2.84	0.40
1:W:18:GLU:O	1:W:19:ILE:C	2.65	0.40
1:W:603:ILE:HG22	1:W:612:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:648:LEU:HD21	1:W:787:ARG:HD3	2.02	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	833/880 (95%)	664 (80%)	130 (16%)	39 (5%)	2	17
1	W	833/880 (95%)	666 (80%)	127 (15%)	40 (5%)	2	16
2	B	1082/1131 (96%)	853 (79%)	164 (15%)	65 (6%)	1	12
2	R	1082/1131 (96%)	852 (79%)	160 (15%)	70 (6%)	1	11
3	C	363/395 (92%)	277 (76%)	66 (18%)	20 (6%)	1	13
3	Y	363/395 (92%)	276 (76%)	64 (18%)	23 (6%)	1	12
4	D	256/265 (97%)	226 (88%)	23 (9%)	7 (3%)	4	26
4	S	256/265 (97%)	226 (88%)	22 (9%)	8 (3%)	3	24
5	E	170/180 (94%)	148 (87%)	20 (12%)	2 (1%)	10	42
5	T	170/180 (94%)	148 (87%)	20 (12%)	2 (1%)	10	42
6	F	89/113 (79%)	78 (88%)	10 (11%)	1 (1%)	11	44
6	U	89/113 (79%)	79 (89%)	9 (10%)	1 (1%)	11	44
7	G	111/132 (84%)	92 (83%)	15 (14%)	4 (4%)	2	21
7	V	111/132 (84%)	92 (83%)	15 (14%)	4 (4%)	2	21
8	H	72/84 (86%)	60 (83%)	6 (8%)	6 (8%)	0	7
8	Z	72/84 (86%)	60 (83%)	7 (10%)	5 (7%)	1	10
9	I	80/95 (84%)	61 (76%)	15 (19%)	4 (5%)	1	15
9	K	80/95 (84%)	61 (76%)	15 (19%)	4 (5%)	1	15
10	J	33/104 (32%)	28 (85%)	5 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	Q	31/104 (30%)	27 (87%)	4 (13%)	0	100	100
11	L	90/92 (98%)	80 (89%)	8 (9%)	2 (2%)	5	30
11	M	90/92 (98%)	81 (90%)	7 (8%)	2 (2%)	5	30
12	N	62/66 (94%)	42 (68%)	15 (24%)	5 (8%)	1	8
12	O	62/66 (94%)	42 (68%)	16 (26%)	4 (6%)	1	11
13	P	41/48 (85%)	34 (83%)	6 (15%)	1 (2%)	4	29
13	X	41/48 (85%)	35 (85%)	5 (12%)	1 (2%)	4	29
All	All	6562/7170 (92%)	5288 (81%)	954 (14%)	320 (5%)	1	16

All (320) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	VAL
1	A	287	SER
1	A	378	VAL
1	A	732	GLY
1	A	734	ARG
1	A	737	VAL
1	A	876	VAL
2	B	111	GLU
2	B	158	ASN
2	B	521	SER
2	B	590	PRO
2	B	601	ASP
2	B	605	ILE
2	B	797	ASP
2	B	1044	THR
2	B	1070	ILE
2	B	1072	TRP
3	C	28	ILE
3	C	30	GLU
4	D	117	GLU
4	D	206	CYS
7	G	105	ILE
8	H	13	ILE
9	I	61	VAL
9	K	61	VAL
9	K	91	SER
2	R	111	GLU
2	R	158	ASN

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Mol	Chain	Res	Type
2	R	181	LYS
2	R	521	SER
2	R	590	PRO
2	R	601	ASP
2	R	605	ILE
2	R	797	ASP
2	R	1029	LEU
2	R	1070	ILE
2	R	1072	TRP
4	S	91	LYS
4	S	117	GLU
4	S	206	CYS
7	V	105	ILE
1	W	287	SER
1	W	378	VAL
1	W	732	GLY
1	W	734	ARG
1	W	737	VAL
3	Y	28	ILE
3	Y	114	LYS
8	Z	13	ILE
1	A	143	ALA
1	A	332	ILE
1	A	355	PRO
1	A	492	GLY
1	A	753	ARG
1	A	849	ALA
2	B	22	LYS
2	B	42	LEU
2	B	71	PRO
2	B	181	LYS
2	B	250	GLU
2	B	279	VAL
2	B	382	LEU
2	B	453	TRP
2	B	535	ASP
2	B	603	GLY
2	B	606	THR
2	B	735	TYR
2	B	793	ARG
2	B	809	GLY
2	B	1029	LEU

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Mol	Chain	Res	Type
3	C	114	LYS
3	C	245	LYS
3	C	324	GLY
3	C	362	ASP
3	C	393	ILE
4	D	91	LYS
4	D	231	GLU
6	F	63	ILE
9	I	91	SER
2	R	22	LYS
2	R	42	LEU
2	R	49	GLN
2	R	71	PRO
2	R	250	GLU
2	R	279	VAL
2	R	382	LEU
2	R	453	TRP
2	R	535	ASP
2	R	606	THR
2	R	735	TYR
2	R	793	ARG
2	R	809	GLY
2	R	1026	GLU
2	R	1044	THR
6	U	63	ILE
1	W	45	MET
1	W	143	ALA
1	W	145	VAL
1	W	155	LYS
1	W	290	ARG
1	W	332	ILE
1	W	355	PRO
1	W	541	ALA
1	W	812	ARG
1	W	876	VAL
13	X	18	LEU
3	Y	30	GLU
3	Y	82	GLY
3	Y	245	LYS
3	Y	324	GLY
3	Y	362	ASP
3	Y	393	ILE

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Mol	Chain	Res	Type
1	A	45	MET
1	A	103	ARG
1	A	155	LYS
1	A	290	ARG
1	A	393	ASP
1	A	541	ALA
1	A	656	ASP
1	A	730	ARG
1	A	733	ALA
1	A	812	ARG
1	A	852	ASP
1	A	875	VAL
2	B	41	LYS
2	B	49	GLN
2	B	202	PRO
2	B	256	PHE
2	B	281	ILE
2	B	375	SER
2	B	406	TRP
2	B	437	ALA
2	B	592	VAL
2	B	633	PRO
2	B	949	TYR
2	B	950	LYS
2	B	951	THR
2	B	1026	GLU
2	B	1111	ILE
3	C	113	ALA
3	C	306	LEU
3	C	323	THR
3	C	338	LYS
7	G	63	ARG
7	G	99	PHE
8	H	11	PRO
8	H	81	VAL
11	L	10	SER
11	M	10	SER
12	N	6	ARG
12	N	41	LYS
12	N	43	TYR
12	O	6	ARG
12	O	41	LYS

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Mol	Chain	Res	Type
12	O	43	TYR
13	P	18	LEU
2	R	202	PRO
2	R	256	PHE
2	R	281	ILE
2	R	375	SER
2	R	406	TRP
2	R	603	GLY
2	R	638	PRO
2	R	687	TYR
2	R	949	TYR
2	R	950	LYS
2	R	951	THR
2	R	1111	ILE
4	S	231	GLU
7	V	99	PHE
1	W	103	ARG
1	W	393	ASP
1	W	429	SER
1	W	730	ARG
1	W	733	ALA
1	W	753	ARG
1	W	849	ALA
1	W	852	ASP
1	W	875	VAL
3	Y	113	ALA
3	Y	161	ALA
3	Y	235	LYS
3	Y	306	LEU
3	Y	310	MET
3	Y	323	THR
3	Y	338	LYS
8	Z	11	PRO
8	Z	81	VAL
1	A	79	ARG
1	A	257	ALA
1	A	429	SER
1	A	536	GLU
2	B	57	PRO
2	B	334	GLU
2	B	383	ALA
2	B	563	THR

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Mol	Chain	Res	Type
2	B	587	ASN
2	B	638	PRO
2	B	739	ASP
2	B	773	GLU
2	B	918	LEU
2	B	948	PHE
3	C	127	THR
3	C	161	ALA
3	C	196	PHE
3	C	235	LYS
5	E	82	GLN
8	H	60	GLY
9	I	45	MET
12	O	9	THR
2	R	41	LYS
2	R	57	PRO
2	R	334	GLU
2	R	437	ALA
2	R	563	THR
2	R	587	ASN
2	R	633	PRO
2	R	734	GLY
2	R	739	ASP
2	R	773	GLU
2	R	918	LEU
5	T	82	GLN
7	V	63	ARG
1	W	79	ARG
1	W	257	ALA
1	W	283	GLY
1	W	492	GLY
1	W	536	GLU
1	W	656	ASP
3	Y	127	THR
3	Y	196	PHE
1	A	283	GLY
1	A	772	TYR
2	B	52	ILE
2	B	223	LYS
2	B	734	GLY
2	B	907	VAL
2	B	943	VAL

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Mol	Chain	Res	Type
2	B	1073	TYR
2	B	1114	PRO
3	C	211	ALA
4	D	90	GLU
4	D	104	ASN
7	G	64	LEU
8	H	10	ASP
9	K	51	ILE
12	N	9	THR
12	N	21	PHE
2	R	52	ILE
2	R	196	THR
2	R	383	ALA
2	R	460	GLU
2	R	592	VAL
2	R	907	VAL
2	R	943	VAL
2	R	948	PHE
2	R	1073	TYR
2	R	1114	PRO
4	S	90	GLU
4	S	104	ASN
4	S	152	GLU
7	V	64	LEU
1	W	22	MET
1	W	106	ILE
1	W	772	TYR
3	Y	109	GLU
3	Y	211	ALA
8	Z	10	ASP
1	A	46	ASP
1	A	106	ILE
2	B	653	ILE
2	B	706	VAL
3	C	82	GLY
9	K	45	MET
2	R	223	LYS
2	R	653	ILE
2	R	706	VAL
1	W	46	ASP
3	Y	146	TYR
3	Y	365	GLU

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Mol	Chain	Res	Type
8	Z	60	GLY
1	A	147	PRO
2	B	597	ILE
3	C	234	ILE
4	D	193	GLY
2	R	407	VAL
2	R	783	VAL
1	A	571	GLY
2	B	234	GLY
2	B	377	VAL
2	B	766	VAL
2	B	769	PRO
9	I	51	ILE
2	R	377	VAL
2	R	597	ILE
2	R	766	VAL
2	R	769	PRO
3	Y	234	ILE
1	A	29	THR
1	A	121	ILE
1	A	125	TRP
2	B	407	VAL
1	W	29	THR
1	W	69	PRO
1	W	121	ILE
1	W	125	TRP
1	W	147	PRO
1	W	571	GLY
8	H	59	PRO
11	L	19	GLY
2	R	234	GLY
4	S	193	GLY
5	T	127	ILE
1	A	258	PRO
3	C	56	ILE
3	C	349	VAL
5	E	127	ILE
11	M	19	GLY
2	R	183	GLY
3	Y	56	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	729/766 (95%)	633 (87%)	96 (13%)	4	21
1	W	729/766 (95%)	633 (87%)	96 (13%)	4	21
2	B	941/975 (96%)	799 (85%)	142 (15%)	3	17
2	R	941/975 (96%)	797 (85%)	144 (15%)	3	17
3	C	315/341 (92%)	270 (86%)	45 (14%)	3	18
3	Y	315/341 (92%)	273 (87%)	42 (13%)	4	21
4	D	233/238 (98%)	218 (94%)	15 (6%)	16	43
4	S	233/238 (98%)	219 (94%)	14 (6%)	17	44
5	E	154/158 (98%)	141 (92%)	13 (8%)	10	34
5	T	154/158 (98%)	141 (92%)	13 (8%)	10	34
6	F	84/107 (78%)	76 (90%)	8 (10%)	8	31
6	U	84/107 (78%)	76 (90%)	8 (10%)	8	31
7	G	106/125 (85%)	95 (90%)	11 (10%)	7	28
7	V	106/125 (85%)	95 (90%)	11 (10%)	7	28
8	H	67/75 (89%)	58 (87%)	9 (13%)	4	21
8	Z	67/75 (89%)	58 (87%)	9 (13%)	4	21
9	I	72/83 (87%)	64 (89%)	8 (11%)	6	27
9	K	72/83 (87%)	64 (89%)	8 (11%)	6	27
10	J	33/96 (34%)	28 (85%)	5 (15%)	3	17
10	Q	30/96 (31%)	26 (87%)	4 (13%)	4	21
11	L	79/80 (99%)	76 (96%)	3 (4%)	29	56
11	M	79/80 (99%)	76 (96%)	3 (4%)	29	56
12	N	58/60 (97%)	52 (90%)	6 (10%)	7	29
12	O	58/60 (97%)	52 (90%)	6 (10%)	7	29
13	P	39/43 (91%)	35 (90%)	4 (10%)	7	29
13	X	39/43 (91%)	36 (92%)	3 (8%)	12	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5817/6294 (92%)	5091 (88%)	726 (12%)	4 22

All (726) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	24	VAL
1	A	28	ILE
1	A	45	MET
1	A	51	VAL
1	A	60	THR
1	A	77	LEU
1	A	82	ILE
1	A	84	VAL
1	A	87	VAL
1	A	101	CYS
1	A	105	LYS
1	A	119	ASN
1	A	131	ARG
1	A	139	THR
1	A	152	LYS
1	A	155	LYS
1	A	156	ILE
1	A	194	ILE
1	A	201	THR
1	A	218	THR
1	A	220	ARG
1	A	238	LYS
1	A	251	GLU
1	A	284	LEU
1	A	295	LEU
1	A	296	ARG
1	A	319	ASP
1	A	332	ILE
1	A	342	ILE
1	A	346	THR
1	A	349	VAL
1	A	353	ILE
1	A	359	GLU
1	A	361	LEU
1	A	366	ILE
1	A	378	VAL

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Mol	Chain	Res	Type
1	A	382	ASP
1	A	391	VAL
1	A	400	THR
1	A	425	LEU
1	A	426	HIS
1	A	429	SER
1	A	438	LEU
1	A	439	LYS
1	A	449	VAL
1	A	464	LEU
1	A	470	GLU
1	A	478	GLU
1	A	482	VAL
1	A	487	ILE
1	A	500	GLN
1	A	517	THR
1	A	527	VAL
1	A	533	ASP
1	A	534	LEU
1	A	540	LEU
1	A	549	LYS
1	A	551	VAL
1	A	568	VAL
1	A	573	ARG
1	A	576	LYS
1	A	582	HIS
1	A	593	LEU
1	A	603	ILE
1	A	633	ARG
1	A	634	VAL
1	A	653	LEU
1	A	661	ILE
1	A	675	LEU
1	A	684	LEU
1	A	691	THR
1	A	707	LEU
1	A	708	ARG
1	A	723	ASN
1	A	728	MET
1	A	738	LEU
1	A	747	LEU
1	A	759	ARG

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Mol	Chain	Res	Type
1	A	763	THR
1	A	764	ARG
1	A	766	LEU
1	A	774	ILE
1	A	787	ARG
1	A	790	LEU
1	A	808	ASP
1	A	809	THR
1	A	813	THR
1	A	814	SER
1	A	823	LEU
1	A	824	ILE
1	A	846	ILE
1	A	868	VAL
1	A	870	ARG
1	A	875	VAL
1	A	876	VAL
2	B	8	LEU
2	B	17	ILE
2	B	27	VAL
2	B	48	GLU
2	B	52	ILE
2	B	54	THR
2	B	55	GLU
2	B	59	LEU
2	B	66	ILE
2	B	68	ILE
2	B	76	SER
2	B	84	SER
2	B	93	LEU
2	B	101	LEU
2	B	104	ILE
2	B	111	GLU
2	B	121	ASP
2	B	137	THR
2	B	138	LEU
2	B	160	SER
2	B	165	VAL
2	B	166	THR
2	B	170	LEU
2	B	177	VAL
2	B	182	THR

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Mol	Chain	Res	Type
2	B	187	THR
2	B	192	ILE
2	B	216	SER
2	B	217	PHE
2	B	227	VAL
2	B	230	MET
2	B	237	THR
2	B	254	GLU
2	B	258	SER
2	B	259	LEU
2	B	263	SER
2	B	281	ILE
2	B	306	THR
2	B	307	SER
2	B	312	ARG
2	B	318	LEU
2	B	322	ILE
2	B	330	LEU
2	B	333	ARG
2	B	334	GLU
2	B	344	LYS
2	B	345	ARG
2	B	375	SER
2	B	393	VAL
2	B	397	ILE
2	B	421	ASN
2	B	426	LEU
2	B	432	VAL
2	B	448	LEU
2	B	456	MET
2	B	460	GLU
2	B	466	ASN
2	B	467	SER
2	B	470	VAL
2	B	471	LYS
2	B	489	GLU
2	B	503	VAL
2	B	505	ARG
2	B	524	ILE
2	B	525	LEU
2	B	529	LEU
2	B	530	VAL

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Mol	Chain	Res	Type
2	B	539	LEU
2	B	566	ILE
2	B	591	LEU
2	B	595	GLU
2	B	597	ILE
2	B	604	SER
2	B	610	LEU
2	B	613	GLN
2	B	637	THR
2	B	641	THR
2	B	646	TRP
2	B	650	ILE
2	B	653	ILE
2	B	657	ILE
2	B	662	GLU
2	B	668	ARG
2	B	675	MET
2	B	688	GLN
2	B	711	LEU
2	B	717	THR
2	B	726	ILE
2	B	730	ILE
2	B	735	TYR
2	B	736	ASN
2	B	741	ILE
2	B	742	ILE
2	B	763	THR
2	B	764	GLU
2	B	767	LYS
2	B	777	VAL
2	B	783	VAL
2	B	802	SER
2	B	838	THR
2	B	839	SER
2	B	843	ARG
2	B	874	ILE
2	B	884	ARG
2	B	898	VAL
2	B	904	VAL
2	B	905	LYS
2	B	907	VAL
2	B	913	LEU

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Mol	Chain	Res	Type
2	B	921	ARG
2	B	923	THR
2	B	924	LEU
2	B	941	ASN
2	B	942	ILE
2	B	944	ASP
2	B	950	LYS
2	B	953	ILE
2	B	961	LEU
2	B	972	VAL
2	B	973	THR
2	B	977	ARG
2	B	982	ILE
2	B	984	SER
2	B	1015	LEU
2	B	1017	ARG
2	B	1020	THR
2	B	1023	ARG
2	B	1033	GLU
2	B	1038	CYS
2	B	1048	LEU
2	B	1052	LEU
2	B	1056	SER
2	B	1059	THR
2	B	1060	THR
2	B	1061	ILE
2	B	1070	ILE
2	B	1072	TRP
2	B	1081	VAL
2	B	1104	ILE
2	B	1115	ARG
2	B	1118	LEU
2	B	1122	VAL
3	C	24	LEU
3	C	28	ILE
3	C	30	GLU
3	C	40	GLU
3	C	44	THR
3	C	47	GLU
3	C	59	TYR
3	C	60	SER
3	C	64	ILE

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Mol	Chain	Res	Type
3	C	70	ILE
3	C	80	GLU
3	C	104	LEU
3	C	106	ARG
3	C	111	VAL
3	C	119	THR
3	C	129	GLU
3	C	159	ASP
3	C	164	SER
3	C	173	MET
3	C	174	LEU
3	C	193	LEU
3	C	209	SER
3	C	213	ILE
3	C	231	ILE
3	C	234	ILE
3	C	252	LEU
3	C	277	ILE
3	C	278	ARG
3	C	292	ILE
3	C	293	ILE
3	C	295	ARG
3	C	300	VAL
3	C	303	GLU
3	C	306	LEU
3	C	307	ASP
3	C	315	LEU
3	C	318	ASP
3	C	331	ARG
3	C	332	HIS
3	C	338	LYS
3	C	365	GLU
3	C	369	VAL
3	C	379	ILE
3	C	380	LYS
3	C	386	VAL
4	D	13	ILE
4	D	58	LEU
4	D	73	LEU
4	D	82	CYS
4	D	117	GLU
4	D	124	ILE

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Mol	Chain	Res	Type
4	D	139	ILE
4	D	151	LYS
4	D	165	ARG
4	D	172	ILE
4	D	176	CYS
4	D	178	LYS
4	D	198	LYS
4	D	258	LYS
4	D	260	LEU
5	E	30	LEU
5	E	38	ILE
5	E	48	ILE
5	E	49	LEU
5	E	76	THR
5	E	80	VAL
5	E	89	VAL
5	E	101	LEU
5	E	117	THR
5	E	137	GLN
5	E	142	VAL
5	E	152	THR
5	E	174	TRP
6	F	7	VAL
6	F	25	ILE
6	F	37	THR
6	F	41	LEU
6	F	59	LEU
6	F	62	ILE
6	F	63	ILE
6	F	88	ILE
7	G	33	CYS
7	G	39	SER
7	G	42	ILE
7	G	47	ASN
7	G	48	ILE
7	G	62	ASN
7	G	66	TYR
7	G	85	SER
7	G	95	ILE
7	G	101	LEU
7	G	106	ILE
8	H	16	LEU

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Mol	Chain	Res	Type
8	H	17	VAL
8	H	22	VAL
8	H	40	GLU
8	H	45	ILE
8	H	48	SER
8	H	55	ILE
8	H	63	ILE
8	H	65	ILE
9	I	23	TRP
9	I	50	LEU
9	I	51	ILE
9	I	59	THR
9	I	61	VAL
9	I	62	ILE
9	I	71	ARG
9	I	74	LEU
10	J	56	ASN
10	J	60	SER
10	J	69	GLU
10	J	77	LYS
10	J	79	ASP
9	K	23	TRP
9	K	50	LEU
9	K	51	ILE
9	K	59	THR
9	K	61	VAL
9	K	62	ILE
9	K	71	ARG
9	K	74	LEU
11	L	31	THR
11	L	63	ILE
11	L	74	GLU
11	M	31	THR
11	M	63	ILE
11	M	74	GLU
12	N	3	ILE
12	N	5	ILE
12	N	22	ILE
12	N	45	CYS
12	N	53	ILE
12	N	63	THR
12	O	3	ILE

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Mol	Chain	Res	Type
12	O	5	ILE
12	O	22	ILE
12	O	45	CYS
12	O	53	ILE
12	O	63	THR
13	P	14	THR
13	P	34	ILE
13	P	41	THR
13	P	44	ILE
10	Q	56	ASN
10	Q	60	SER
10	Q	67	LEU
10	Q	69	GLU
2	R	8	LEU
2	R	27	VAL
2	R	33	SER
2	R	48	GLU
2	R	52	ILE
2	R	54	THR
2	R	55	GLU
2	R	59	LEU
2	R	66	ILE
2	R	68	ILE
2	R	76	SER
2	R	80	GLU
2	R	84	SER
2	R	93	LEU
2	R	101	LEU
2	R	104	ILE
2	R	111	GLU
2	R	121	ASP
2	R	137	THR
2	R	138	LEU
2	R	160	SER
2	R	165	VAL
2	R	166	THR
2	R	170	LEU
2	R	177	VAL
2	R	182	THR
2	R	187	THR
2	R	192	ILE
2	R	216	SER

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Mol	Chain	Res	Type
2	R	217	PHE
2	R	227	VAL
2	R	230	MET
2	R	237	THR
2	R	254	GLU
2	R	258	SER
2	R	259	LEU
2	R	263	SER
2	R	281	ILE
2	R	295	ILE
2	R	306	THR
2	R	307	SER
2	R	312	ARG
2	R	318	LEU
2	R	322	ILE
2	R	330	LEU
2	R	333	ARG
2	R	334	GLU
2	R	344	LYS
2	R	345	ARG
2	R	375	SER
2	R	393	VAL
2	R	397	ILE
2	R	421	ASN
2	R	426	LEU
2	R	432	VAL
2	R	448	LEU
2	R	456	MET
2	R	460	GLU
2	R	466	ASN
2	R	467	SER
2	R	470	VAL
2	R	471	LYS
2	R	489	GLU
2	R	503	VAL
2	R	505	ARG
2	R	524	ILE
2	R	525	LEU
2	R	529	LEU
2	R	530	VAL
2	R	539	LEU
2	R	566	ILE

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Mol	Chain	Res	Type
2	R	575	SER
2	R	591	LEU
2	R	595	GLU
2	R	597	ILE
2	R	604	SER
2	R	610	LEU
2	R	613	GLN
2	R	637	THR
2	R	641	THR
2	R	646	TRP
2	R	650	ILE
2	R	653	ILE
2	R	657	ILE
2	R	662	GLU
2	R	668	ARG
2	R	675	MET
2	R	688	GLN
2	R	711	LEU
2	R	717	THR
2	R	726	ILE
2	R	730	ILE
2	R	735	TYR
2	R	736	ASN
2	R	741	ILE
2	R	742	ILE
2	R	763	THR
2	R	764	GLU
2	R	767	LYS
2	R	777	VAL
2	R	783	VAL
2	R	802	SER
2	R	838	THR
2	R	839	SER
2	R	840	ILE
2	R	843	ARG
2	R	874	ILE
2	R	884	ARG
2	R	898	VAL
2	R	904	VAL
2	R	905	LYS
2	R	907	VAL
2	R	913	LEU

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Mol	Chain	Res	Type
2	R	921	ARG
2	R	923	THR
2	R	924	LEU
2	R	941	ASN
2	R	942	ILE
2	R	944	ASP
2	R	950	LYS
2	R	953	ILE
2	R	961	LEU
2	R	972	VAL
2	R	973	THR
2	R	977	ARG
2	R	982	ILE
2	R	984	SER
2	R	1015	LEU
2	R	1017	ARG
2	R	1023	ARG
2	R	1033	GLU
2	R	1048	LEU
2	R	1052	LEU
2	R	1056	SER
2	R	1059	THR
2	R	1060	THR
2	R	1061	ILE
2	R	1070	ILE
2	R	1072	TRP
2	R	1081	VAL
2	R	1104	ILE
2	R	1115	ARG
2	R	1118	LEU
2	R	1122	VAL
4	S	13	ILE
4	S	58	LEU
4	S	73	LEU
4	S	82	CYS
4	S	117	GLU
4	S	124	ILE
4	S	139	ILE
4	S	151	LYS
4	S	165	ARG
4	S	172	ILE
4	S	178	LYS

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Mol	Chain	Res	Type
4	S	198	LYS
4	S	258	LYS
4	S	260	LEU
5	T	30	LEU
5	T	38	ILE
5	T	48	ILE
5	T	49	LEU
5	T	76	THR
5	T	80	VAL
5	T	89	VAL
5	T	101	LEU
5	T	117	THR
5	T	137	GLN
5	T	142	VAL
5	T	152	THR
5	T	174	TRP
6	U	7	VAL
6	U	25	ILE
6	U	37	THR
6	U	41	LEU
6	U	59	LEU
6	U	62	ILE
6	U	63	ILE
6	U	88	ILE
7	V	33	CYS
7	V	39	SER
7	V	42	ILE
7	V	47	ASN
7	V	48	ILE
7	V	62	ASN
7	V	66	TYR
7	V	85	SER
7	V	95	ILE
7	V	101	LEU
7	V	106	ILE
1	W	21	LYS
1	W	24	VAL
1	W	28	ILE
1	W	45	MET
1	W	51	VAL
1	W	60	THR
1	W	77	LEU

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Mol	Chain	Res	Type
1	W	82	ILE
1	W	84	VAL
1	W	87	VAL
1	W	101	CYS
1	W	105	LYS
1	W	119	ASN
1	W	131	ARG
1	W	139	THR
1	W	152	LYS
1	W	155	LYS
1	W	156	ILE
1	W	194	ILE
1	W	201	THR
1	W	218	THR
1	W	220	ARG
1	W	238	LYS
1	W	251	GLU
1	W	284	LEU
1	W	295	LEU
1	W	296	ARG
1	W	319	ASP
1	W	332	ILE
1	W	342	ILE
1	W	346	THR
1	W	349	VAL
1	W	353	ILE
1	W	359	GLU
1	W	361	LEU
1	W	366	ILE
1	W	378	VAL
1	W	382	ASP
1	W	391	VAL
1	W	400	THR
1	W	425	LEU
1	W	426	HIS
1	W	438	LEU
1	W	439	LYS
1	W	449	VAL
1	W	464	LEU
1	W	470	GLU
1	W	478	GLU
1	W	482	VAL

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Mol	Chain	Res	Type
1	W	487	ILE
1	W	500	GLN
1	W	527	VAL
1	W	533	ASP
1	W	534	LEU
1	W	540	LEU
1	W	549	LYS
1	W	551	VAL
1	W	568	VAL
1	W	573	ARG
1	W	576	LYS
1	W	582	HIS
1	W	593	LEU
1	W	603	ILE
1	W	621	ASP
1	W	633	ARG
1	W	634	VAL
1	W	653	LEU
1	W	661	ILE
1	W	675	LEU
1	W	684	LEU
1	W	691	THR
1	W	707	LEU
1	W	708	ARG
1	W	723	ASN
1	W	728	MET
1	W	734	ARG
1	W	738	LEU
1	W	747	LEU
1	W	759	ARG
1	W	763	THR
1	W	764	ARG
1	W	766	LEU
1	W	774	ILE
1	W	787	ARG
1	W	790	LEU
1	W	808	ASP
1	W	809	THR
1	W	813	THR
1	W	814	SER
1	W	823	LEU
1	W	824	ILE

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Mol	Chain	Res	Type
1	W	846	ILE
1	W	868	VAL
1	W	870	ARG
1	W	875	VAL
1	W	876	VAL
13	X	14	THR
13	X	34	ILE
13	X	41	THR
3	Y	24	LEU
3	Y	28	ILE
3	Y	30	GLU
3	Y	40	GLU
3	Y	44	THR
3	Y	47	GLU
3	Y	59	TYR
3	Y	60	SER
3	Y	64	ILE
3	Y	70	ILE
3	Y	106	ARG
3	Y	111	VAL
3	Y	119	THR
3	Y	129	GLU
3	Y	159	ASP
3	Y	164	SER
3	Y	174	LEU
3	Y	193	LEU
3	Y	209	SER
3	Y	213	ILE
3	Y	231	ILE
3	Y	234	ILE
3	Y	252	LEU
3	Y	277	ILE
3	Y	278	ARG
3	Y	292	ILE
3	Y	293	ILE
3	Y	295	ARG
3	Y	300	VAL
3	Y	303	GLU
3	Y	306	LEU
3	Y	307	ASP
3	Y	315	LEU
3	Y	318	ASP

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Mol	Chain	Res	Type
3	Y	331	ARG
3	Y	338	LYS
3	Y	365	GLU
3	Y	369	VAL
3	Y	371	GLU
3	Y	379	ILE
3	Y	380	LYS
3	Y	386	VAL
8	Z	16	LEU
8	Z	17	VAL
8	Z	22	VAL
8	Z	40	GLU
8	Z	45	ILE
8	Z	48	SER
8	Z	55	ILE
8	Z	63	ILE
8	Z	65	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	89	HIS
1	A	148	HIS
1	A	237	HIS
1	A	270	GLN
1	A	272	HIS
1	A	279	ASN
1	A	312	ASN
1	A	420	ASN
1	A	422	GLN
1	A	500	GLN
1	A	567	ASN
1	A	820	GLN
2	B	173	ASN
2	B	188	HIS
2	B	261	GLN
2	B	287	ASN
2	B	371	GLN
2	B	415	GLN
2	B	466	ASN
2	B	478	GLN

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Mol	Chain	Res	Type
2	B	560	HIS
2	B	626	ASN
2	B	642	HIS
2	B	678	GLN
2	B	696	HIS
2	B	707	GLN
2	B	723	ASN
2	B	736	ASN
2	B	994	GLN
2	B	1078	ASN
2	B	1085	HIS
3	C	38	ASN
3	C	207	ASN
3	C	228	ASN
3	C	304	GLN
4	D	136	ASN
5	E	137	GLN
6	F	53	GLN
7	G	16	ASN
7	G	47	ASN
7	G	62	ASN
7	G	87	ASN
7	G	88	ASN
7	G	117	GLN
9	I	55	ASN
9	I	84	ASN
10	J	47	ASN
9	K	55	ASN
12	N	61	HIS
12	O	61	HIS
10	Q	47	ASN
2	R	173	ASN
2	R	188	HIS
2	R	261	GLN
2	R	287	ASN
2	R	442	ASN
2	R	466	ASN
2	R	478	GLN
2	R	484	ASN
2	R	560	HIS
2	R	626	ASN
2	R	642	HIS

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Mol	Chain	Res	Type
2	R	696	HIS
2	R	707	GLN
2	R	723	ASN
2	R	736	ASN
2	R	887	GLN
2	R	994	GLN
2	R	1078	ASN
2	R	1085	HIS
4	S	60	HIS
4	S	136	ASN
5	T	137	GLN
6	U	53	GLN
7	V	16	ASN
7	V	47	ASN
7	V	62	ASN
7	V	88	ASN
7	V	117	GLN
1	W	63	ASN
1	W	83	HIS
1	W	89	HIS
1	W	119	ASN
1	W	148	HIS
1	W	279	ASN
1	W	312	ASN
1	W	331	ASN
1	W	420	ASN
1	W	422	GLN
1	W	500	GLN
1	W	567	ASN
1	W	742	GLN
1	W	815	GLN
1	W	820	GLN
3	Y	38	ASN
3	Y	207	ASN
3	Y	228	ASN
3	Y	304	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 12 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	1265	4	0,9,9	-	-	-		
16	F3S	D	1265	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	1265	4	-	-	0/3/3/3
16	F3S	D	1265	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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	841/880 (95%)	0.60	26 (3%)	51	29	65, 91, 152, 185	0
1	W	841/880 (95%)	0.53	14 (1%)	69	41	61, 87, 141, 171	0
2	B	1090/1131 (96%)	0.64	40 (3%)	45	25	64, 87, 129, 155	0
2	R	1090/1131 (96%)	0.63	46 (4%)	40	21	64, 89, 120, 137	0
3	C	367/395 (92%)	0.76	14 (3%)	44	24	82, 106, 147, 155	0
3	Y	367/395 (92%)	0.58	13 (3%)	47	26	62, 89, 145, 160	0
4	D	260/265 (98%)	0.73	17 (6%)	25	15	90, 110, 127, 142	0
4	S	260/265 (98%)	0.56	7 (2%)	56	32	88, 106, 126, 140	0
5	E	174/180 (96%)	0.76	7 (4%)	42	23	98, 132, 196, 214	0
5	T	174/180 (96%)	0.87	12 (6%)	23	14	92, 125, 174, 189	0
6	F	91/113 (80%)	0.66	7 (7%)	19	13	135, 163, 191, 204	0
6	U	91/113 (80%)	0.88	4 (4%)	39	21	131, 160, 202, 216	0
7	G	113/132 (85%)	0.79	7 (6%)	26	16	87, 114, 138, 155	0
7	V	113/132 (85%)	0.83	7 (6%)	26	16	81, 112, 136, 149	0
8	H	74/84 (88%)	0.59	3 (4%)	41	22	75, 96, 118, 145	0
8	Z	74/84 (88%)	0.68	0	100	100	72, 95, 114, 144	0
9	I	82/95 (86%)	0.52	1 (1%)	76	50	61, 79, 103, 126	0
9	K	82/95 (86%)	0.50	1 (1%)	76	50	64, 82, 103, 121	0
10	J	35/104 (33%)	1.07	4 (11%)	10	6	112, 126, 147, 153	0
10	Q	33/104 (31%)	1.15	3 (9%)	15	9	129, 166, 225, 285	0
11	L	92/92 (100%)	0.54	2 (2%)	62	35	75, 97, 136, 181	0
11	M	92/92 (100%)	0.40	1 (1%)	78	52	68, 91, 141, 184	0
12	N	64/66 (96%)	0.65	1 (1%)	70	43	79, 96, 119, 136	0
12	O	64/66 (96%)	0.51	1 (1%)	70	43	74, 89, 103, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	P	43/48 (89%)	1.04	6 (13%) 6 5	80, 105, 127, 141	0
13	X	43/48 (89%)	0.83	4 (9%) 14 9	90, 106, 121, 125	0
All	All	6650/7170 (92%)	0.64	248 (3%) 45 25	61, 96, 153, 285	0

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	GLU	5.9
2	B	382	LEU	5.2
5	T	7	ALA	4.6
2	R	405	ASN	4.6
10	J	55	LEU	4.5
2	R	113	GLU	4.4
13	P	30	GLY	4.4
2	B	379	GLY	3.9
7	V	92	TYR	3.9
2	R	1072	TRP	3.9
2	R	110	ILE	3.8
1	A	864	LYS	3.7
2	B	114	PRO	3.6
11	L	9	GLU	3.6
2	B	52	ILE	3.6
2	B	256	PHE	3.6
1	A	876	VAL	3.5
10	Q	76	GLU	3.5
1	W	867	ASP	3.4
2	B	286	GLU	3.4
7	G	80	GLU	3.4
4	S	36	VAL	3.4
4	D	62	LEU	3.4
11	L	89	GLY	3.3
7	G	92	TYR	3.3
2	B	113	GLU	3.3
2	R	84	SER	3.3
3	C	394	LEU	3.2
13	P	15	ASP	3.2
4	S	215	GLY	3.2
1	W	299	ALA	3.2
5	E	136	ILE	3.2
7	V	80	GLU	3.2
1	A	125	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
4	S	204	THR	3.1
1	W	28	ILE	3.1
1	A	238	LYS	3.0
3	Y	24	LEU	3.0
12	N	64	ARG	3.0
2	R	228	ILE	3.0
2	R	75	GLU	3.0
8	H	82	ILE	3.0
2	R	310	ASP	2.9
2	R	1027	GLY	2.9
2	R	717	THR	2.9
4	D	209	CYS	2.9
2	R	251	ILE	2.9
2	B	378	ARG	2.9
3	C	26	GLN	2.9
1	A	214	VAL	2.9
2	R	227	VAL	2.9
2	R	379	GLY	2.9
2	R	527	GLY	2.8
10	J	67	LEU	2.8
1	A	112	GLU	2.8
5	T	69	GLU	2.8
1	A	261	ILE	2.8
5	T	153	VAL	2.8
2	B	211	GLY	2.8
1	A	82	ILE	2.8
1	A	115	SER	2.8
5	T	57	GLY	2.8
3	C	27	LYS	2.8
2	R	382	LEU	2.8
2	B	1073	TYR	2.8
2	B	405	ASN	2.8
2	R	97	ALA	2.8
2	R	859	ALA	2.8
3	C	55	ALA	2.8
10	J	48	THR	2.8
2	R	476	MET	2.7
2	B	838	THR	2.7
2	R	83	ILE	2.7
1	W	155	LYS	2.7
5	E	111	SER	2.7
4	S	40	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	808	ASP	2.7
2	B	197	ALA	2.7
13	X	30	GLY	2.7
2	R	45	ILE	2.7
4	D	93	TYR	2.7
2	B	111	GLU	2.7
3	Y	284	PHE	2.7
1	W	70	GLY	2.6
3	Y	191	LEU	2.6
2	R	64	GLY	2.6
4	D	188	PHE	2.6
6	F	62	ILE	2.6
3	C	24	LEU	2.6
2	B	299	TYR	2.6
7	V	78	VAL	2.6
1	W	231	ALA	2.6
6	U	77	PRO	2.6
3	C	348	GLU	2.6
2	B	106	VAL	2.6
2	B	257	PRO	2.6
2	B	296	ILE	2.5
2	R	604	SER	2.5
1	A	707	LEU	2.5
4	D	205	LEU	2.5
5	T	158	PRO	2.5
3	Y	237	ILE	2.5
2	B	227	VAL	2.5
2	R	111	GLU	2.5
6	U	66	GLU	2.5
3	C	306	LEU	2.5
2	B	739	ASP	2.5
4	D	174	GLY	2.5
1	A	195	LEU	2.5
2	B	595	GLU	2.5
2	B	1072	TRP	2.5
2	R	373	GLU	2.5
1	A	69	PRO	2.5
2	R	443	PHE	2.5
7	G	83	ASP	2.5
7	V	48	ILE	2.5
1	A	877	GLY	2.5
3	Y	349	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
5	T	72	PHE	2.5
4	D	143	ALA	2.5
4	D	92	CYS	2.5
2	B	377	VAL	2.5
2	R	206	GLU	2.4
5	E	116	ASP	2.4
1	W	876	VAL	2.4
13	X	34	ILE	2.4
4	D	63	ALA	2.4
2	B	424	SER	2.4
2	B	56	ILE	2.4
3	C	64	ILE	2.4
5	T	136	ILE	2.4
2	R	114	PRO	2.4
3	C	31	ASP	2.4
9	K	25	ASN	2.4
13	X	24	VAL	2.4
1	A	579	ASP	2.4
13	P	8	LYS	2.4
3	C	203	GLY	2.4
4	D	217	ILE	2.4
5	E	163	THR	2.4
5	T	51	VAL	2.4
9	I	58	SER	2.3
6	F	72	LEU	2.3
2	B	206	GLU	2.3
2	R	580	ARG	2.3
2	B	1069	TYR	2.3
4	S	67	PHE	2.3
1	A	304	GLY	2.3
2	R	413	VAL	2.3
1	W	26	ALA	2.3
3	Y	64	ILE	2.3
4	D	65	ILE	2.3
5	T	97	ILE	2.3
2	B	309	ASP	2.3
3	C	384	GLY	2.3
6	F	71	VAL	2.3
1	W	707	LEU	2.3
2	R	229	LEU	2.3
1	A	194	ILE	2.3
13	P	24	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
11	M	34	LYS	2.3
2	B	308	ALA	2.3
2	R	768	TYR	2.3
5	T	167	PRO	2.3
6	F	4	VAL	2.3
3	C	54	LEU	2.2
5	T	27	LEU	2.2
7	V	81	LEU	2.2
2	R	618	TYR	2.2
1	A	478	GLU	2.2
1	A	721	PRO	2.2
2	R	69	GLY	2.2
2	R	105	PRO	2.2
13	X	7	GLY	2.2
1	A	94	LEU	2.2
2	B	469	LEU	2.2
2	R	8	LEU	2.2
1	A	154	PHE	2.2
2	B	164	ILE	2.2
2	R	256	PHE	2.2
2	R	468	GLY	2.2
5	E	118	LEU	2.2
6	F	21	LEU	2.2
2	B	997	HIS	2.2
2	R	480	ALA	2.2
13	P	10	TRP	2.2
1	A	42	GLY	2.2
1	A	459	GLY	2.2
2	B	1027	GLY	2.2
2	R	590	PRO	2.2
6	F	77	PRO	2.2
6	U	86	ILE	2.2
7	V	6	ALA	2.2
3	C	363	VAL	2.2
4	S	124	ILE	2.2
2	R	1037	ASP	2.2
2	R	307	SER	2.2
3	Y	236	GLY	2.2
12	O	5	ILE	2.2
2	B	806	GLU	2.2
7	G	108	ASN	2.2
2	B	1052	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	Y	55	ALA	2.1
3	Y	193	LEU	2.2
10	Q	67	LEU	2.2
1	W	811	VAL	2.1
2	B	27	VAL	2.1
1	A	70	GLY	2.1
2	R	55	GLU	2.1
13	P	11	LYS	2.1
5	T	22	LEU	2.1
3	Y	224	ASP	2.1
4	D	82	CYS	2.1
2	R	376	LYS	2.1
4	D	166	TYR	2.1
2	B	153	GLY	2.1
10	J	53	ASN	2.1
10	Q	64	ALA	2.1
6	U	75	ILE	2.1
2	R	1086	GLY	2.1
6	F	66	GLU	2.1
5	E	85	VAL	2.1
2	R	202	PRO	2.1
4	D	52	PRO	2.1
1	W	111	ILE	2.1
2	R	52	ILE	2.1
4	D	67	PHE	2.1
1	A	87	VAL	2.1
3	Y	394	LEU	2.1
4	D	153	HIS	2.1
1	W	156	ILE	2.1
1	W	194	ILE	2.1
3	C	193	LEU	2.1
3	Y	181	VAL	2.1
7	V	116	HIS	2.0
7	G	115	ILE	2.0
1	W	65	LEU	2.0
7	G	64	LEU	2.0
7	G	113	LEU	2.0
3	Y	203	GLY	2.0
2	B	1083	PRO	2.0
2	B	1116	LEU	2.0
4	S	205	LEU	2.0
8	H	52	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	605	ILE	2.0
4	D	38	VAL	2.0
5	E	84	VAL	2.0
8	H	81	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	0.86	0.17	81,81,81,81	0
15	MG	A	1882	1/1	0.87	0.22	79,79,79,79	0
16	F3S	S	1265	7/7	0.95	0.08	86,86,86,86	0
14	ZN	B	2123	1/1	0.96	0.03	75,75,75,75	0
14	ZN	W	1881	1/1	0.97	0.04	81,81,81,81	0
16	F3S	D	1265	7/7	0.97	0.08	88,88,88,88	0
14	ZN	P	1049	1/1	0.97	0.04	87,87,87,87	0
14	ZN	X	1049	1/1	0.98	0.03	91,91,91,91	0
14	ZN	A	1881	1/1	0.98	0.03	79,79,79,79	0
14	ZN	R	2123	1/1	0.98	0.04	76,76,76,76	0
14	ZN	W	1880	1/1	0.98	0.03	81,81,81,81	0
14	ZN	O	1065	1/1	0.98	0.05	81,81,81,81	0
14	ZN	A	1880	1/1	0.99	0.02	79,79,79,79	0
14	ZN	N	1065	1/1	1.00	0.03	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.