



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:53 PM GMT

PDB ID : 1R1A  
Title : CRYSTAL STRUCTURE OF HUMAN RHINOVIRUS SEROTYPE 1A (HRV1A)  
Authors : Kim, S.; Rossmann, M.G.  
Deposited on : 1989-03-15  
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

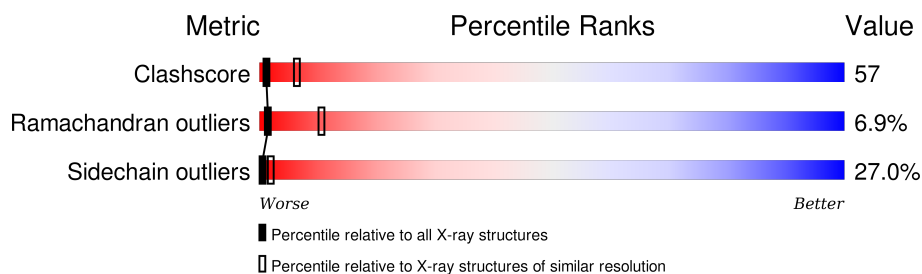
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	287	
2	2	263	
3	3	238	
4	4	44	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SUC	1	288	X	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6246 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 HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	283	Total	C	N	O	S	0	0	0
			2262	1431	389	430	12			

- Molecule 2 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	253	Total	C	N	O	S	0	0	0
			1979	1249	349	371	10			

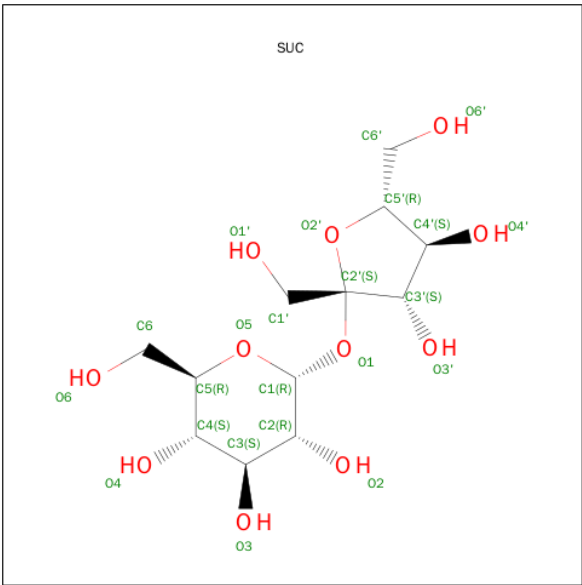
- Molecule 3 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	238	Total	C	N	O	S	0	0	0
			1831	1169	297	348	17			

- Molecule 4 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP4).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	4	19	Total	C	N	O	0	0	0
			151	96	25	30			

- Molecule 5 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: C<sub>12</sub>H<sub>22</sub>O<sub>11</sub>).



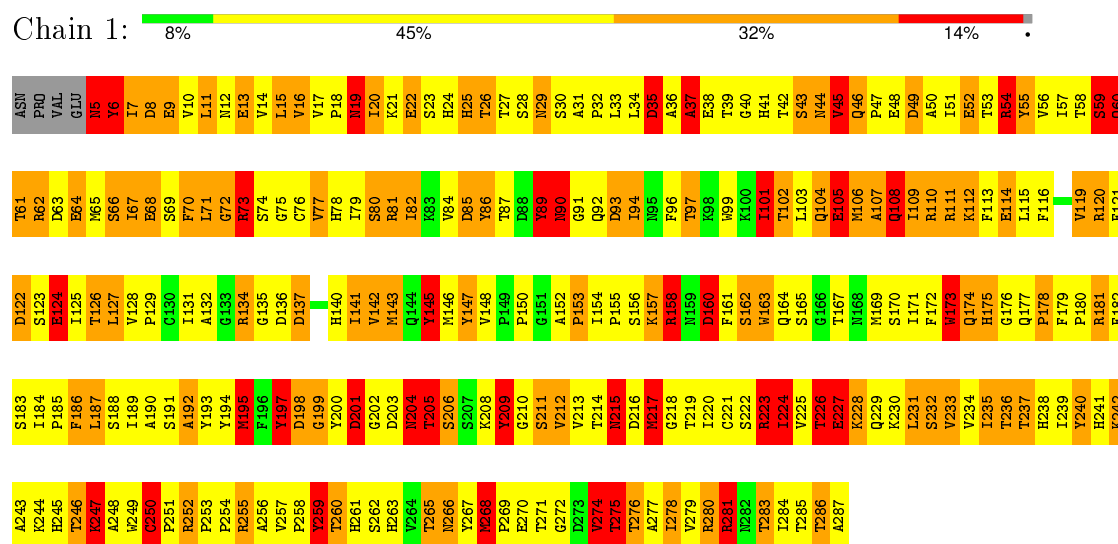
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	1	1	Total	C	O	0	0
			23	12	11		

### 3 Residue-property plots

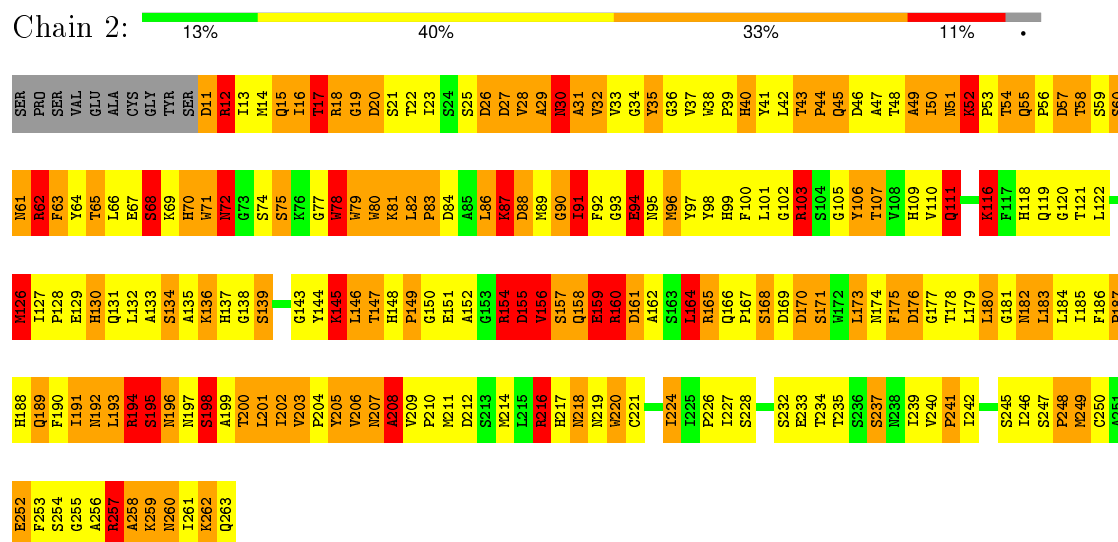
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

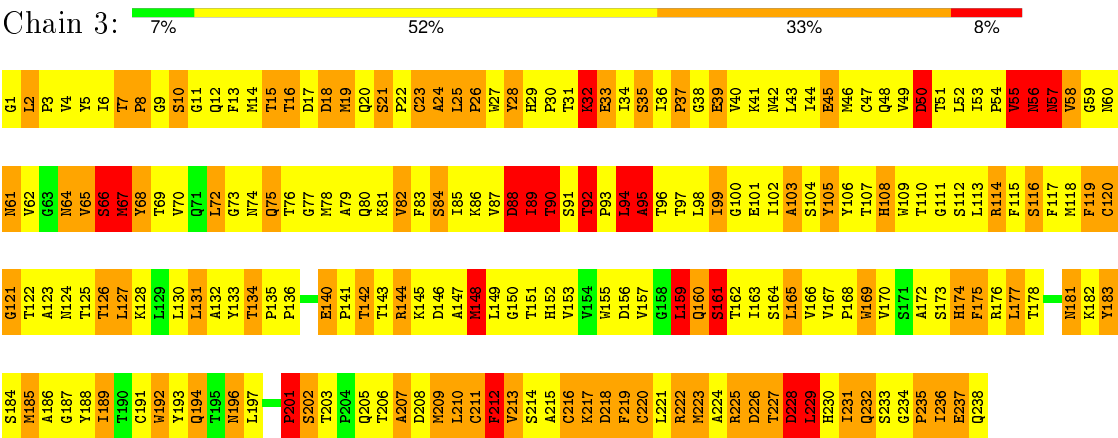
#### • Molecule 1: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP1)



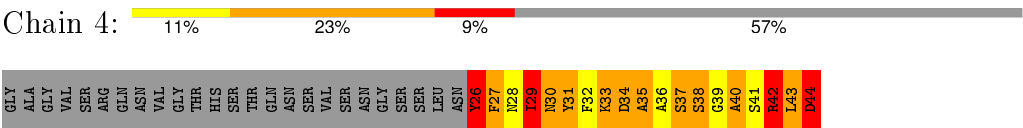
#### • Molecule 2: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP2)



● Molecule 3: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP3)



● Molecule 4: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP4)



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	341.30Å 341.30Å 465.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.293 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6246	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP



## 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: SUC

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	1	0.98	0/2322	2.61	150/3162 (4.7%)
2	2	0.95	0/2033	2.60	151/2770 (5.5%)
3	3	0.93	0/1878	2.47	112/2570 (4.4%)
4	4	1.25	0/154	3.16	21/206 (10.2%)
All	All	0.96	0/6387	2.58	434/8708 (5.0%)

There are no bond length outliers.

All (434) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	62	ARG	CD-NE-CZ	24.80	158.32	123.60
1	1	134	ARG	NE-CZ-NH1	23.96	132.28	120.30
2	2	216	ARG	NE-CZ-NH2	-22.13	109.24	120.30
1	1	280	ARG	NE-CZ-NH2	-20.34	110.13	120.30
1	1	110	ARG	NE-CZ-NH2	-19.11	110.75	120.30
3	3	146	ASP	CB-CG-OD2	-17.24	102.78	118.30
2	2	257	ARG	NE-CZ-NH2	-16.55	112.03	120.30
3	3	222	ARG	CD-NE-CZ	15.89	145.85	123.60
4	4	42	ARG	NE-CZ-NH1	15.16	127.88	120.30
2	2	155	ASP	CB-CG-OD1	-14.68	105.09	118.30
1	1	110	ARG	CD-NE-CZ	14.28	143.59	123.60
1	1	81	ARG	NE-CZ-NH1	14.14	127.37	120.30
1	1	281	ARG	NE-CZ-NH2	-14.08	113.26	120.30
2	2	154	ARG	NE-CZ-NH1	13.91	127.25	120.30
2	2	62	ARG	NE-CZ-NH1	13.84	127.22	120.30
3	3	226	ASP	CB-CG-OD2	13.81	130.73	118.30
1	1	158	ARG	NE-CZ-NH1	13.68	127.14	120.30
3	3	28	TYR	CB-CG-CD1	13.33	129.00	121.00
3	3	228	ASP	CB-CG-OD2	-13.28	106.35	118.30
1	1	110	ARG	NE-CZ-NH1	13.08	126.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	183	TYR	CB-CG-CD1	12.36	128.42	121.00
3	3	144	ARG	CD-NE-CZ	12.32	140.85	123.60
1	1	281	ARG	CA-CB-CG	12.20	140.24	113.40
1	1	227	GLU	OE1-CD-OE2	-12.19	108.67	123.30
1	1	6	TYR	CB-CG-CD2	-12.07	113.76	121.00
1	1	93	ASP	CB-CG-OD2	-11.78	107.70	118.30
3	3	114	ARG	NE-CZ-NH1	-11.75	114.43	120.30
3	3	144	ARG	NE-CZ-NH1	11.39	126.00	120.30
1	1	231	LEU	CA-CB-CG	11.30	141.30	115.30
3	3	50	ASP	CB-CG-OD2	-11.24	108.19	118.30
3	3	225	ARG	NE-CZ-NH1	-11.20	114.70	120.30
3	3	50	ASP	CB-CG-OD1	11.01	128.21	118.30
2	2	67	GLU	OE1-CD-OE2	10.95	136.44	123.30
1	1	255	ARG	CD-NE-CZ	10.89	138.85	123.60
1	1	54	ARG	CG-CD-NE	10.80	134.49	111.80
2	2	35	TYR	CB-CG-CD2	10.79	127.48	121.00
4	4	44	ASP	CB-CG-OD1	-10.74	108.63	118.30
3	3	218	ASP	CB-CG-OD1	-10.33	109.00	118.30
2	2	12	ARG	NE-CZ-NH2	-10.31	115.14	120.30
1	1	106	MET	CA-CB-CG	-10.30	95.79	113.30
2	2	162	ALA	CB-CA-C	10.23	125.44	110.10
2	2	12	ARG	CD-NE-CZ	10.19	137.86	123.60
2	2	205	TYR	CB-CG-CD1	10.13	127.08	121.00
2	2	62	ARG	NH1-CZ-NH2	-9.95	108.46	119.40
2	2	216	ARG	NE-CZ-NH1	9.86	125.23	120.30
2	2	11	ASP	CB-CG-OD1	9.85	127.16	118.30
2	2	31	ALA	N-CA-CB	9.81	123.84	110.10
1	1	223	ARG	NE-CZ-NH2	9.69	125.14	120.30
1	1	223	ARG	NE-CZ-NH1	-9.64	115.48	120.30
3	3	67	MET	N-CA-CB	-9.61	93.30	110.60
1	1	8	ASP	CB-CG-OD1	-9.56	109.70	118.30
2	2	154	ARG	C-N-CA	9.55	145.58	121.70
2	2	29	ALA	N-CA-CB	9.53	123.44	110.10
4	4	42	ARG	CD-NE-CZ	9.45	136.83	123.60
2	2	165	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	1	105	GLU	CA-CB-CG	9.36	133.99	113.40
2	2	176	ASP	CB-CG-OD1	9.36	126.72	118.30
1	1	281	ARG	NE-CZ-NH1	9.35	124.97	120.30
2	2	212	ASP	CB-CG-OD1	9.28	126.65	118.30
1	1	59	SER	N-CA-CB	-9.18	96.73	110.50
1	1	9	GLU	OE1-CD-OE2	9.14	134.27	123.30
3	3	148	MET	CG-SD-CE	9.06	114.70	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	134	ARG	NH1-CZ-NH2	-9.00	109.50	119.40
3	3	18	ASP	CB-CG-OD2	-8.99	110.21	118.30
2	2	165	ARG	NE-CZ-NH2	-8.97	115.81	120.30
2	2	28	VAL	CA-CB-CG1	8.91	124.26	110.90
1	1	227	GLU	CG-CD-OE1	8.80	135.90	118.30
2	2	154	ARG	NE-CZ-NH2	-8.79	115.90	120.30
1	1	60	GLN	O-C-N	8.75	136.70	122.70
2	2	35	TYR	CB-CG-CD1	-8.71	115.78	121.00
3	3	232	GLN	N-CA-CB	8.67	126.21	110.60
2	2	11	ASP	CB-CG-OD2	-8.67	110.50	118.30
1	1	55	TYR	CB-CG-CD2	-8.66	115.80	121.00
1	1	11	LEU	O-C-N	8.62	136.50	122.70
3	3	222	ARG	NE-CZ-NH1	8.47	124.54	120.30
2	2	233	GLU	CG-CD-OE1	8.46	135.21	118.30
1	1	108	GLN	C-N-CA	8.44	142.80	121.70
1	1	68	GLU	CB-CG-CD	8.38	136.82	114.20
3	3	28	TYR	CB-CG-CD2	-8.36	115.98	121.00
1	1	181	ARG	NE-CZ-NH2	8.34	124.47	120.30
1	1	187	LEU	CA-C-O	-8.31	102.66	120.10
2	2	12	ARG	NE-CZ-NH1	8.30	124.45	120.30
2	2	57	ASP	N-CA-CB	-8.29	95.68	110.60
3	3	226	ASP	OD1-CG-OD2	-8.23	107.66	123.30
2	2	97	TYR	CB-CG-CD2	8.19	125.91	121.00
2	2	126	MET	CA-CB-CG	-8.11	99.51	113.30
1	1	120	ARG	NE-CZ-NH2	8.07	124.34	120.30
2	2	12	ARG	CG-CD-NE	8.01	128.62	111.80
2	2	241	PRO	C-N-CA	7.95	141.57	121.70
1	1	111	ARG	CD-NE-CZ	7.94	134.71	123.60
2	2	26	ASP	CB-CG-OD2	7.87	125.38	118.30
2	2	194	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	1	181	ARG	CG-CD-NE	7.85	128.28	111.80
1	1	158	ARG	CD-NE-CZ	7.83	134.56	123.60
2	2	160	ARG	NE-CZ-NH1	-7.82	116.39	120.30
2	2	189	GLN	CA-CB-CG	7.82	130.61	113.40
1	1	211	SER	O-C-N	7.82	135.21	122.70
1	1	49	ASP	CB-CG-OD1	-7.82	111.26	118.30
2	2	161	ASP	N-CA-CB	7.80	124.64	110.60
2	2	61	ASN	CB-CA-C	7.76	125.92	110.40
3	3	56	ASN	C-N-CA	7.75	141.09	121.70
1	1	55	TYR	CB-CG-CD1	7.72	125.63	121.00
3	3	235	PRO	C-N-CA	7.72	141.00	121.70
2	2	94	GLU	OE1-CD-OE2	7.68	132.52	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	93	ASP	CB-CG-OD1	7.64	125.17	118.30
2	2	159	GLU	OE1-CD-OE2	7.64	132.46	123.30
1	1	197	TYR	CB-CG-CD1	7.62	125.58	121.00
1	1	6	TYR	CB-CG-CD1	7.58	125.55	121.00
2	2	71	TRP	CB-CA-C	7.58	125.56	110.40
1	1	134	ARG	CD-NE-CZ	7.57	134.20	123.60
1	1	85	ASP	CB-CG-OD2	-7.56	111.49	118.30
1	1	73	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	1	280	ARG	NH1-CZ-NH2	7.54	127.70	119.40
2	2	161	ASP	CB-CG-OD2	-7.54	111.52	118.30
3	3	207	ALA	O-C-N	7.50	134.69	122.70
1	1	111	ARG	NE-CZ-NH1	-7.47	116.56	120.30
3	3	68	TYR	CB-CG-CD1	7.46	125.48	121.00
2	2	232	SER	N-CA-CB	7.43	121.65	110.50
2	2	252	GLU	OE1-CD-OE2	7.42	132.20	123.30
1	1	61	THR	CA-CB-OG1	-7.40	93.46	109.00
1	1	89	TYR	CB-CG-CD2	-7.34	116.59	121.00
4	4	34	ASP	CB-CG-OD2	-7.34	111.70	118.30
3	3	92	THR	CB-CA-C	7.34	131.41	111.60
3	3	161	SER	CB-CA-C	-7.32	96.19	110.10
4	4	37	SER	O-C-N	7.28	134.34	122.70
2	2	147	THR	N-CA-CB	7.20	123.98	110.30
2	2	233	GLU	CG-CD-OE2	-7.17	103.97	118.30
3	3	95	ALA	CA-C-N	7.16	132.96	117.20
3	3	88	ASP	CB-CG-OD1	7.16	124.74	118.30
1	1	173	TRP	CA-CB-CG	7.16	127.29	113.70
2	2	152	ALA	N-CA-CB	-7.15	100.09	110.10
4	4	40	ALA	O-C-N	7.13	134.11	122.70
1	1	228	LYS	CD-CE-NZ	7.13	128.10	111.70
2	2	78	TRP	CA-CB-CG	7.12	127.23	113.70
2	2	237	SER	CB-CA-C	7.09	123.56	110.10
3	3	232	GLN	O-C-N	7.07	134.01	122.70
2	2	62	ARG	NE-CZ-NH2	7.04	123.82	120.30
3	3	120	CYS	CA-CB-SG	-7.04	101.33	114.00
2	2	164	LEU	O-C-N	7.03	133.94	122.70
1	1	259	TYR	CB-CG-CD2	-7.02	116.79	121.00
3	3	218	ASP	N-CA-CB	-7.01	97.98	110.60
2	2	80	TRP	N-CA-CB	6.99	123.18	110.60
2	2	103	ARG	CD-NE-CZ	6.98	133.37	123.60
2	2	160	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	1	45	VAL	CB-CA-C	6.97	124.64	111.40
4	4	42	ARG	NH1-CZ-NH2	-6.95	111.76	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	31	TYR	CB-CG-CD1	6.92	125.15	121.00
1	1	268	MET	CA-CB-CG	-6.91	101.55	113.30
3	3	222	ARG	NH1-CZ-NH2	-6.87	111.85	119.40
2	2	81	LYS	O-C-N	6.84	133.65	122.70
1	1	164	GLN	OE1-CD-NE2	-6.83	106.19	121.90
2	2	160	ARG	N-CA-CB	-6.83	98.31	110.60
1	1	5	ASN	N-CA-CB	6.81	122.86	110.60
2	2	72	ASN	OD1-CG-ND2	6.81	137.57	121.90
2	2	106	TYR	C-N-CA	6.77	138.63	121.70
3	3	25	LEU	CA-CB-CG	6.77	130.88	115.30
1	1	164	GLN	CG-CD-OE1	6.74	135.08	121.60
1	1	212	VAL	O-C-N	6.73	133.47	122.70
2	2	198	SER	CB-CA-C	-6.73	97.31	110.10
1	1	203	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	1	270	GLU	N-CA-CB	6.70	122.66	110.60
2	2	52	LYS	CA-CB-CG	6.67	128.07	113.40
3	3	26	PRO	O-C-N	6.66	133.36	122.70
3	3	90	THR	N-CA-CB	6.66	122.96	110.30
3	3	193	TYR	O-C-N	6.65	133.34	122.70
3	3	73	GLY	CA-C-O	6.65	132.57	120.60
3	3	218	ASP	CA-CB-CG	-6.64	98.78	113.40
4	4	40	ALA	N-CA-CB	6.62	119.36	110.10
3	3	57	ASN	CB-CG-ND2	-6.60	100.86	116.70
2	2	135	ALA	N-CA-CB	-6.59	100.87	110.10
1	1	37	ALA	N-CA-CB	-6.57	100.90	110.10
1	1	70	PHE	O-C-N	6.57	133.21	122.70
1	1	19	ASN	CB-CG-OD1	-6.56	108.48	121.60
2	2	196	ASN	N-CA-CB	-6.53	98.85	110.60
1	1	5	ASN	O-C-N	6.51	133.12	122.70
1	1	145	TYR	N-CA-CB	6.50	122.30	110.60
3	3	55	VAL	CB-CA-C	6.50	123.75	111.40
2	2	50	ILE	CA-CB-CG2	6.48	123.86	110.90
2	2	187	PRO	CB-CA-C	6.46	128.14	112.00
3	3	16	THR	CA-CB-CG2	6.43	121.40	112.40
2	2	183	LEU	O-C-N	6.42	132.97	122.70
2	2	16	ILE	O-C-N	6.41	132.96	122.70
1	1	64	GLU	CA-CB-CG	6.41	127.50	113.40
2	2	28	VAL	CG1-CB-CG2	-6.41	100.65	110.90
1	1	199	GLY	O-C-N	6.39	132.93	122.70
3	3	172	ALA	CB-CA-C	6.39	119.69	110.10
1	1	13	GLU	O-C-N	6.37	132.89	122.70
1	1	105	GLU	CG-CD-OE2	-6.36	105.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	68	SER	N-CA-CB	6.35	120.02	110.50
3	3	160	GLN	N-CA-CB	6.34	122.01	110.60
3	3	222	ARG	NE-CZ-NH2	6.34	123.47	120.30
2	2	26	ASP	OD1-CG-OD2	-6.33	111.27	123.30
3	3	235	PRO	CA-C-N	-6.32	103.30	117.20
1	1	274	VAL	N-CA-CB	6.30	125.35	111.50
3	3	235	PRO	CA-C-O	6.29	135.31	120.20
1	1	201	ASP	CB-CG-OD2	6.29	123.96	118.30
1	1	275	THR	OG1-CB-CG2	6.29	124.47	110.00
2	2	196	ASN	OD1-CG-ND2	6.29	136.37	121.90
1	1	77	VAL	O-C-N	6.25	132.70	122.70
2	2	248	PRO	N-CA-C	-6.25	95.85	112.10
3	3	37	PRO	N-CA-CB	6.24	110.79	103.30
2	2	161	ASP	O-C-N	6.24	132.68	122.70
1	1	233	VAL	CA-C-N	-6.22	103.51	117.20
4	4	44	ASP	CB-CG-OD2	6.21	123.89	118.30
1	1	233	VAL	CB-CA-C	-6.21	99.61	111.40
2	2	19	GLY	C-N-CA	6.21	137.21	121.70
4	4	30	ASN	CB-CA-C	6.20	122.80	110.40
3	3	33	GLU	CG-CD-OE2	-6.19	105.92	118.30
2	2	94	GLU	CG-CD-OE2	-6.18	105.93	118.30
1	1	86	TYR	CB-CA-C	6.17	122.74	110.40
1	1	211	SER	CA-C-O	-6.17	107.14	120.10
3	3	94	LEU	CA-C-N	6.17	130.76	117.20
3	3	89	ILE	CB-CA-C	-6.16	99.27	111.60
4	4	38	SER	O-C-N	6.16	133.67	123.20
1	1	223	ARG	CA-CB-CG	6.16	126.94	113.40
2	2	155	ASP	N-CA-CB	6.15	121.66	110.60
1	1	16	VAL	CG1-CB-CG2	6.13	120.71	110.90
2	2	205	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	1	175	HIS	N-CA-CB	-6.10	99.62	110.60
1	1	209	TYR	CB-CG-CD1	6.09	124.66	121.00
4	4	35	ALA	CB-CA-C	6.09	119.23	110.10
2	2	154	ARG	CG-CD-NE	6.08	124.58	111.80
1	1	206	SER	O-C-N	6.08	132.42	122.70
2	2	17	THR	CB-CA-C	6.08	128.00	111.60
2	2	155	ASP	CB-CG-OD2	6.06	123.75	118.30
3	3	185	MET	CA-CB-CG	6.05	123.58	113.30
2	2	107	THR	CA-CB-OG1	-6.04	96.33	109.00
1	1	247	LYS	CB-CA-C	-6.03	98.34	110.40
2	2	81	LYS	CA-CB-CG	6.03	126.67	113.40
1	1	227	GLU	CB-CG-CD	6.03	130.48	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	82	LEU	CA-CB-CG	-6.02	101.46	115.30
1	1	35	ASP	CB-CG-OD1	6.01	123.71	118.30
3	3	32	LYS	O-C-N	6.01	132.32	122.70
2	2	57	ASP	CB-CG-OD1	-6.00	112.90	118.30
2	2	57	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	1	187	LEU	CA-C-N	5.99	130.38	117.20
2	2	194	ARG	NH1-CZ-NH2	5.98	125.97	119.40
2	2	262	LYS	CB-CA-C	5.97	122.34	110.40
2	2	160	ARG	CG-CD-NE	5.96	124.32	111.80
3	3	15	THR	N-CA-CB	-5.96	98.98	110.30
2	2	130	HIS	CA-CB-CG	-5.95	103.49	113.60
3	3	183	TYR	CB-CG-CD2	-5.94	117.44	121.00
1	1	231	LEU	CB-CA-C	5.93	121.46	110.20
1	1	82	ILE	CB-CA-C	-5.92	99.75	111.60
3	3	233	SER	CA-C-N	-5.92	104.36	116.20
2	2	130	HIS	O-C-N	5.91	132.15	122.70
2	2	87	LYS	CB-CG-CD	5.90	126.94	111.60
3	3	105	TYR	CB-CG-CD1	5.90	124.54	121.00
1	1	71	LEU	CB-CA-C	5.90	121.41	110.20
1	1	68	GLU	OE1-CD-OE2	-5.89	116.23	123.30
2	2	208	ALA	N-CA-CB	5.89	118.35	110.10
2	2	157	SER	N-CA-CB	5.89	119.33	110.50
2	2	156	VAL	C-N-CA	5.88	136.41	121.70
1	1	217	MET	CB-CA-C	-5.87	98.66	110.40
2	2	49	ALA	CA-C-O	-5.87	107.77	120.10
2	2	91	ILE	N-CA-CB	5.87	124.30	110.80
1	1	20	ILE	O-C-N	5.87	132.09	122.70
2	2	252	GLU	CG-CD-OE2	-5.85	106.59	118.30
1	1	89	TYR	CB-CG-CD1	5.85	124.51	121.00
1	1	55	TYR	O-C-N	5.85	132.06	122.70
3	3	201	PRO	N-CA-C	5.84	127.29	112.10
2	2	97	TYR	CB-CG-CD1	-5.84	117.50	121.00
2	2	257	ARG	NE-CZ-NH1	5.83	123.22	120.30
4	4	26	TYR	CB-CG-CD2	5.83	124.50	121.00
2	2	234	THR	CA-C-O	5.83	132.34	120.10
3	3	68	TYR	CB-CG-CD2	-5.82	117.51	121.00
1	1	215	ASN	O-C-N	5.81	132.00	122.70
2	2	249	MET	CA-CB-CG	5.80	123.16	113.30
1	1	85	ASP	CB-CG-OD1	5.80	123.52	118.30
3	3	185	MET	N-CA-CB	5.79	121.03	110.60
1	1	54	ARG	NE-CZ-NH1	5.79	123.20	120.30
2	2	147	THR	O-C-N	5.79	131.96	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	111	ARG	C-N-CA	5.78	136.15	121.70
1	1	49	ASP	OD1-CG-OD2	5.77	134.26	123.30
1	1	25	HIS	O-C-N	5.76	131.92	122.70
1	1	240	TYR	CB-CG-CD2	-5.76	117.54	121.00
2	2	218	ASN	CA-CB-CG	5.75	126.04	113.40
1	1	216	ASP	CB-CA-C	5.74	121.89	110.40
3	3	24	ALA	N-CA-CB	-5.74	102.06	110.10
1	1	111	ARG	NE-CZ-NH2	5.74	123.17	120.30
2	2	57	ASP	OD1-CG-OD2	5.74	134.20	123.30
1	1	226	THR	N-CA-C	5.73	126.47	111.00
1	1	274	VAL	CA-CB-CG1	5.73	119.49	110.90
1	1	250	CYS	CA-CB-SG	5.72	124.30	114.00
1	1	202	GLY	C-N-CA	5.71	135.98	121.70
2	2	134	SER	CA-C-N	-5.71	104.64	117.20
1	1	16	VAL	CB-CA-C	5.70	122.23	111.40
1	1	81	ARG	NH1-CZ-NH2	-5.69	113.14	119.40
3	3	45	GLU	OE1-CD-OE2	-5.68	116.48	123.30
2	2	83	PRO	C-N-CA	5.67	135.86	121.70
3	3	103	ALA	CB-CA-C	5.66	118.59	110.10
1	1	90	ASN	CB-CA-C	5.66	121.72	110.40
3	3	229	LEU	CA-CB-CG	5.66	128.31	115.30
1	1	232	SER	CB-CA-C	-5.65	99.36	110.10
2	2	249	MET	CG-SD-CE	5.65	109.24	100.20
1	1	204	ASN	CA-C-N	-5.65	104.78	117.20
2	2	139	SER	N-CA-CB	-5.65	102.03	110.50
3	3	77	GLY	CA-C-O	5.64	130.76	120.60
3	3	76	THR	O-C-N	5.63	132.78	123.20
3	3	227	THR	CA-C-O	5.63	131.93	120.10
3	3	160	GLN	O-C-N	5.63	131.70	122.70
3	3	18	ASP	OD1-CG-OD2	5.62	133.97	123.30
2	2	26	ASP	CB-CG-OD1	5.61	123.35	118.30
1	1	198	ASP	CB-CG-OD1	5.61	123.35	118.30
3	3	212	PHE	CA-CB-CG	5.61	127.35	113.90
2	2	49	ALA	CA-C-N	5.60	129.52	117.20
2	2	228	SER	N-CA-CB	5.58	118.86	110.50
1	1	274	VAL	CA-C-N	-5.57	104.94	117.20
3	3	146	ASP	OD1-CG-OD2	5.57	133.89	123.30
1	1	122	ASP	CB-CG-OD2	-5.57	113.29	118.30
3	3	146	ASP	CB-CG-OD1	5.56	123.31	118.30
2	2	220	TRP	CA-C-N	-5.56	104.97	117.20
2	2	83	PRO	CB-CA-C	5.55	125.88	112.00
2	2	134	SER	N-CA-CB	5.55	118.83	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	212	ASP	CB-CG-OD2	-5.55	113.30	118.30
2	2	116	LYS	CB-CA-C	-5.55	99.30	110.40
2	2	149	PRO	CA-C-N	5.55	127.30	116.20
3	3	79	ALA	O-C-N	5.55	131.58	122.70
1	1	68	GLU	CA-CB-CG	5.54	125.59	113.40
2	2	119	GLN	CB-CA-C	5.54	121.47	110.40
1	1	153	PRO	N-CD-CG	-5.53	94.90	103.20
3	3	24	ALA	CA-C-N	5.52	129.35	117.20
3	3	64	ASN	OD1-CG-ND2	5.51	134.56	121.90
1	1	62	ARG	NE-CZ-NH1	-5.50	117.55	120.30
2	2	54	THR	N-CA-CB	5.49	120.74	110.30
2	2	169	ASP	CA-C-O	5.49	131.63	120.10
1	1	260	THR	CA-C-O	-5.49	108.57	120.10
1	1	81	ARG	CD-NE-CZ	5.48	131.28	123.60
2	2	216	ARG	NH1-CZ-NH2	5.46	125.41	119.40
2	2	32	VAL	O-C-N	5.45	131.42	122.70
2	2	90	GLY	CA-C-O	5.45	130.41	120.60
2	2	194	ARG	NE-CZ-NH1	-5.43	117.58	120.30
3	3	228	ASP	CB-CA-C	-5.43	99.55	110.40
1	1	101	ILE	N-CA-CB	-5.42	98.32	110.80
3	3	225	ARG	NE-CZ-NH2	5.42	123.01	120.30
2	2	70	HIS	CB-CA-C	-5.42	99.56	110.40
4	4	40	ALA	N-CA-C	-5.42	96.36	111.00
3	3	169	TRP	CB-CA-C	5.42	121.23	110.40
3	3	58	VAL	CA-CB-CG1	-5.41	102.78	110.90
1	1	270	GLU	O-C-N	5.41	131.36	122.70
3	3	234	GLY	N-CA-C	-5.41	99.58	113.10
3	3	218	ASP	C-N-CA	5.41	135.22	121.70
1	1	124	GLU	CG-CD-OE1	5.39	129.09	118.30
2	2	20	ASP	CB-CG-OD2	-5.39	113.45	118.30
3	3	235	PRO	CB-CA-C	-5.39	98.53	112.00
1	1	147	TYR	O-C-N	5.37	131.30	122.70
3	3	183	TYR	CG-CD2-CE2	5.37	125.60	121.30
3	3	237	GLU	OE1-CD-OE2	5.37	129.75	123.30
3	3	8	PRO	C-N-CA	5.37	133.58	122.30
3	3	175	PHE	CB-CG-CD2	-5.35	117.05	120.80
3	3	203	THR	O-C-N	5.35	131.26	121.10
2	2	150	GLY	O-C-N	5.34	131.25	122.70
1	1	172	PHE	CA-C-O	-5.34	108.88	120.10
3	3	88	ASP	OD1-CG-OD2	-5.34	113.16	123.30
3	3	233	SER	CA-C-O	5.33	131.30	120.10
2	2	161	ASP	CB-CA-C	-5.33	99.74	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	283	THR	O-C-N	5.33	131.22	122.70
3	3	95	ALA	CA-C-O	-5.33	108.92	120.10
3	3	206	THR	N-CA-C	-5.32	96.63	111.00
2	2	87	LYS	CB-CA-C	5.32	121.04	110.40
2	2	165	ARG	C-N-CA	5.32	135.00	121.70
4	4	44	ASP	CA-C-O	5.32	131.26	120.10
2	2	96	MET	CA-C-N	-5.31	105.52	117.20
3	3	206	THR	OG1-CB-CG2	5.31	122.22	110.00
2	2	52	LYS	CG-CD-CE	5.31	127.82	111.90
2	2	111	GLN	CB-CG-CD	5.30	125.39	111.60
4	4	26	TYR	CB-CG-CD1	-5.30	117.82	121.00
3	3	35	SER	N-CA-CB	-5.29	102.57	110.50
4	4	29	ILE	O-C-N	5.28	131.15	122.70
2	2	150	GLY	CA-C-O	-5.28	111.09	120.60
2	2	195	SER	CB-CA-C	5.27	120.11	110.10
1	1	201	ASP	CB-CG-OD1	-5.26	113.56	118.30
2	2	182	ASN	O-C-N	5.26	131.11	122.70
3	3	202	SER	CA-C-N	-5.26	105.63	117.20
3	3	108	HIS	CA-CB-CG	5.25	122.52	113.60
1	1	192	ALA	N-CA-CB	-5.25	102.76	110.10
3	3	10	SER	CB-CA-C	5.24	120.06	110.10
3	3	156	ASP	CB-CG-OD2	-5.23	113.59	118.30
2	2	203	VAL	N-CA-CB	-5.23	100.00	111.50
2	2	82	LEU	N-CA-C	5.22	125.11	111.00
1	1	158	ARG	NH1-CZ-NH2	-5.21	113.67	119.40
1	1	224	ILE	CB-CG1-CD1	-5.21	99.30	113.90
1	1	287	ALA	CA-C-O	-5.21	109.17	120.10
3	3	114	ARG	NE-CZ-NH2	5.21	122.90	120.30
2	2	11	ASP	O-C-N	5.20	131.02	122.70
1	1	242	LYS	CA-C-N	-5.20	105.77	117.20
3	3	92	THR	N-CA-C	-5.19	96.99	111.00
3	3	64	ASN	N-CA-CB	-5.19	101.26	110.60
2	2	12	ARG	CB-CA-C	-5.19	100.03	110.40
2	2	173	LEU	CB-CA-C	5.18	120.04	110.20
3	3	146	ASP	N-CA-CB	5.18	119.92	110.60
3	3	165	LEU	O-C-N	5.17	130.98	122.70
4	4	26	TYR	O-C-N	5.17	130.97	122.70
2	2	30	ASN	N-CA-CB	-5.16	101.31	110.60
1	1	22	GLU	CG-CD-OE1	5.16	128.61	118.30
2	2	19	GLY	CA-C-N	-5.16	105.86	117.20
3	3	24	ALA	CA-C-O	-5.16	109.27	120.10
3	3	76	THR	CA-C-N	-5.15	105.91	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	181	ASN	O-C-N	5.15	130.93	122.70
1	1	120	ARG	NH1-CZ-NH2	-5.13	113.76	119.40
2	2	237	SER	CA-C-O	5.12	130.86	120.10
4	4	42	ARG	C-N-CA	-5.12	108.90	121.70
3	3	72	LEU	CB-CG-CD2	-5.11	102.32	111.00
4	4	38	SER	CA-C-O	-5.11	109.38	120.10
1	1	94	ILE	CA-C-N	-5.09	106.00	117.20
1	1	43	SER	CA-C-N	-5.09	106.00	117.20
1	1	163	TRP	CB-CA-C	5.08	120.57	110.40
2	2	50	ILE	CB-CA-C	5.08	121.76	111.60
1	1	178	PRO	CA-C-N	-5.08	106.03	117.20
1	1	189	ILE	C-N-CA	5.08	134.40	121.70
1	1	205	THR	OG1-CB-CG2	5.08	121.67	110.00
3	3	78	MET	CB-CA-C	5.07	120.54	110.40
1	1	66	SER	O-C-N	5.07	130.80	122.70
2	2	40	HIS	CA-CB-CG	-5.07	104.99	113.60
1	1	46	GLN	O-C-N	5.06	130.72	121.10
2	2	168	SER	C-N-CA	5.06	134.34	121.70
2	2	28	VAL	CB-CA-C	-5.05	101.80	111.40
3	3	227	THR	CA-CB-CG2	-5.05	105.34	112.40
3	3	131	LEU	CA-CB-CG	5.04	126.89	115.30
3	3	223	MET	CG-SD-CE	5.04	108.26	100.20
1	1	212	VAL	CA-C-N	-5.04	106.12	117.20
3	3	64	ASN	CA-CB-CG	-5.04	102.32	113.40
1	1	195	MET	CG-SD-CE	5.03	108.25	100.20
1	1	175	HIS	CB-CA-C	5.03	120.45	110.40
1	1	204	ASN	N-CA-CB	5.03	119.65	110.60
2	2	45	GLN	N-CA-CB	5.03	119.65	110.60
1	1	223	ARG	CG-CD-NE	5.02	122.34	111.80
2	2	79	TRP	CA-CB-CG	5.02	123.24	113.70
3	3	57	ASN	N-CA-CB	-5.01	101.57	110.60
3	3	237	GLU	CA-C-O	5.01	130.63	120.10
2	2	218	ASN	CB-CG-OD1	-5.01	111.58	121.60
1	1	80	SER	CA-C-O	5.01	130.61	120.10
1	1	52	GLU	O-C-N	5.00	130.70	122.70
1	1	235	ILE	CA-C-N	-5.00	106.20	117.20

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	1	2262	0	2193	333	1584
2	2	1979	0	1920	213	840
3	3	1831	0	1809	224	1675
4	4	151	0	136	17	364
5	1	23	0	19	32	7
All	All	6246	0	6077	703	3023

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 57.

All (703) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:102:THR:CA	5:1:288:SUC:H6'1	1.09	1.51
1:1:102:THR:HA	5:1:288:SUC:C6'	0.95	1.40
1:1:23:SER:OG	1:1:53:THR:HG22	1.36	1.24
3:3:42:ASN:HD22	3:3:44:ILE:HG22	1.05	1.20
2:2:18:ARG:NH1	2:2:249:MET:HE2	1.55	1.19
1:1:254:PRO:HG3	3:3:101:GLU:HG2	1.27	1.16
2:2:18:ARG:HH12	2:2:249:MET:HE2	0.99	1.15
3:3:160:GLN:O	3:3:161:SER:HB3	1.48	1.11
1:1:254:PRO:CG	3:3:101:GLU:HG2	1.81	1.09
1:1:46:GLN:HB3	1:1:47:PRO:CD	1.85	1.07
3:3:122:THR:HG22	3:3:123:ALA:H	1.21	1.03
1:1:102:THR:C	5:1:288:SUC:H6'1	1.78	1.03
1:1:7:ILE:HA	1:1:11:LEU:HD23	1.41	1.02
3:3:75:GLN:NE2	3:3:75:GLN:HA	1.75	1.02
1:1:142:VAL:CG1	1:1:225:VAL:HB	1.90	1.01
1:1:45:VAL:H	3:3:114:ARG:NH1	1.59	1.01
1:1:6:TYR:HB3	1:1:7:ILE:HD13	1.42	1.00
1:1:46:GLN:CB	1:1:47:PRO:HD2	1.89	1.00
2:2:185:ILE:HD13	3:3:98:LEU:HD22	1.41	1.00
3:3:42:ASN:ND2	3:3:44:ILE:HG22	1.74	1.00
3:3:75:GLN:HE21	3:3:75:GLN:HA	1.26	0.99
1:1:102:THR:HA	5:1:288:SUC:O6'	1.60	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:83:PRO:HG2	2:2:218:ASN:HA	1.44	0.99
1:1:46:GLN:HB3	1:1:47:PRO:HD2	1.01	0.98
1:1:278:ILE:HD12	3:3:67:MET:CE	1.93	0.97
3:3:117:PHE:CD2	3:3:211:CYS:HB3	2.00	0.97
3:3:117:PHE:HD2	3:3:211:CYS:HB3	1.25	0.97
3:3:51:THR:HG21	3:3:98:LEU:HB2	1.47	0.96
1:1:113:PHE:O	1:1:115:LEU:N	1.99	0.96
1:1:215:ASN:CG	5:1:288:SUC:O3'	2.07	0.92
2:2:185:ILE:HD13	3:3:98:LEU:CD2	2.00	0.91
1:1:35:ASP:O	3:3:162:THR:HB	1.69	0.91
1:1:96:PHE:CE1	1:1:157:LYS:HA	2.06	0.91
1:1:141:ILE:HG12	1:1:141:ILE:O	1.69	0.91
1:1:265:THR:OG1	2:2:133:ALA:HB2	1.69	0.91
1:1:97:THR:HG23	1:1:222:SER:HB3	1.54	0.89
1:1:67:ILE:HD11	3:3:40:VAL:HB	1.54	0.88
1:1:173:TRP:CD1	1:1:180:PRO:HD3	2.08	0.88
2:2:161:ASP:HB2	2:2:164:LEU:HD22	1.55	0.88
3:3:54:PRO:O	3:3:93:PRO:HB2	1.74	0.88
3:3:24:ALA:O	3:3:25:LEU:HB2	1.72	0.87
3:3:82:VAL:HG12	3:3:83:PHE:HD1	1.39	0.87
3:3:231:ILE:HD13	3:3:231:ILE:H	1.39	0.87
2:2:12:ARG:HH11	2:2:12:ARG:HB3	1.36	0.87
1:1:197:TYR:CE1	1:1:214:THR:HG23	2.08	0.86
1:1:142:VAL:HG12	1:1:225:VAL:HB	1.57	0.86
1:1:140:HIS:O	1:1:226:THR:HG21	1.75	0.86
1:1:17:VAL:HG13	1:1:60:GLN:O	1.76	0.86
1:1:75:GLY:O	1:1:77:VAL:HG13	1.74	0.86
3:3:42:ASN:HD22	3:3:44:ILE:CG2	1.87	0.86
1:1:190:ALA:O	3:3:31:THR:HG21	1.75	0.86
1:1:171:ILE:HD11	1:1:180:PRO:HB2	1.58	0.85
3:3:58:VAL:O	3:3:61:ASN:HB2	1.76	0.85
2:2:159:GLU:C	2:2:160:ARG:HG2	1.97	0.85
1:1:254:PRO:HG3	3:3:101:GLU:CG	2.05	0.84
3:3:82:VAL:HG12	3:3:83:PHE:N	1.90	0.84
3:3:51:THR:HG21	3:3:98:LEU:CB	2.07	0.83
1:1:142:VAL:HG11	1:1:225:VAL:HB	1.60	0.83
1:1:129:PRO:HG2	1:1:173:TRP:CE2	2.13	0.83
2:2:161:ASP:HB2	2:2:164:LEU:CD2	2.08	0.83
3:3:102:ILE:HG22	3:3:103:ALA:N	1.92	0.82
1:1:119:VAL:CG1	1:1:121:PHE:HE2	1.93	0.82
1:1:197:TYR:H	2:2:131:GLN:HE21	1.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:168:SER:OG	2:2:170:ASP:HB2	1.79	0.81
3:3:7:THR:O	3:3:10:SER:HB2	1.80	0.81
1:1:173:TRP:HD1	1:1:180:PRO:HD3	1.45	0.80
1:1:215:ASN:H	1:1:215:ASN:ND2	1.77	0.80
1:1:23:SER:CB	1:1:53:THR:HG22	2.11	0.80
1:1:278:ILE:HD12	3:3:67:MET:HE1	1.63	0.79
2:2:146:LEU:HD12	2:2:167:PRO:HD3	1.65	0.78
1:1:7:ILE:O	1:1:11:LEU:HB2	1.84	0.78
2:2:146:LEU:CD1	2:2:166:GLN:HA	2.13	0.78
1:1:103:LEU:N	5:1:288:SUC:H6'1	1.99	0.78
1:1:204:ASN:C	1:1:206:SER:H	1.82	0.78
3:3:160:GLN:O	3:3:161:SER:CB	2.32	0.77
2:2:60:SER:OG	2:2:61:ASN:N	2.14	0.77
2:2:126:MET:HG3	2:2:201:LEU:HD12	1.66	0.77
2:2:18:ARG:HH12	2:2:249:MET:CE	1.90	0.77
3:3:194:GLN:HA	3:3:194:GLN:HE21	1.48	0.77
3:3:231:ILE:CD1	3:3:231:ILE:H	1.97	0.77
2:2:12:ARG:HG3	2:2:13:ILE:N	1.99	0.77
1:1:278:ILE:CD1	3:3:67:MET:CE	2.64	0.76
1:1:45:VAL:H	3:3:114:ARG:HH11	1.31	0.76
1:1:255:ARG:HD3	1:1:259:TYR:CE2	2.20	0.76
3:3:20:GLN:HE22	4:4:30:ASN:HA	1.50	0.76
1:1:127:LEU:HB2	1:1:180:PRO:HG2	1.67	0.75
2:2:173:LEU:O	2:2:174:ASN:HB2	1.83	0.75
3:3:75:GLN:OE1	3:3:80:GLN:HG2	1.87	0.75
3:3:81:LYS:HG3	3:3:82:VAL:N	2.01	0.75
3:3:122:THR:CG2	3:3:123:ALA:H	1.99	0.75
3:3:122:THR:HG22	3:3:123:ALA:N	1.99	0.74
4:4:26:TYR:CD2	4:4:29:ILE:HD11	2.22	0.74
2:2:78:TRP:HZ3	2:2:226:PRO:HD3	1.50	0.74
1:1:223:ARG:HH11	1:1:223:ARG:CG	2.00	0.74
2:2:183:LEU:HD12	2:2:186:PHE:HD1	1.52	0.73
2:2:41:TYR:CD2	2:2:55:GLN:OE1	2.41	0.73
2:2:257:ARG:HG2	2:2:257:ARG:HH11	1.52	0.73
1:1:33:LEU:O	3:3:163:ILE:HD12	1.88	0.73
1:1:119:VAL:HG13	1:1:121:PHE:CE2	2.23	0.73
2:2:12:ARG:CG	2:2:13:ILE:N	2.51	0.73
2:2:146:LEU:HD12	2:2:167:PRO:CD	2.19	0.72
1:1:113:PHE:C	1:1:115:LEU:H	1.93	0.72
1:1:210:GLY:O	1:1:213:VAL:HG23	1.89	0.72
3:3:125:THR:HG22	3:3:126:THR:N	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:173:SER:O	3:3:175:PHE:N	2.22	0.72
2:2:68:SER:C	2:2:69:LYS:HG2	2.07	0.72
1:1:92:GLN:O	1:1:93:ASP:HB2	1.89	0.72
3:3:53:ILE:O	3:3:55:VAL:HG12	1.89	0.72
2:2:148:HIS:N	2:2:149:PRO:CD	2.52	0.72
1:1:123:SER:HB3	1:1:241:HIS:NE2	2.05	0.72
1:1:223:ARG:HH11	1:1:223:ARG:HG2	1.53	0.71
1:1:197:TYR:CD1	1:1:214:THR:HG23	2.24	0.71
2:2:148:HIS:N	2:2:149:PRO:HD3	2.06	0.71
1:1:46:GLN:OE1	3:3:217:LYS:HG3	1.89	0.71
1:1:242:LYS:NZ	3:3:17:ASP:O	2.22	0.71
2:2:78:TRP:HE3	2:2:78:TRP:H	1.39	0.71
3:3:82:VAL:CG1	3:3:83:PHE:HD1	2.04	0.70
1:1:104:GLN:HB3	1:1:110:ARG:HG3	1.72	0.70
1:1:22:GLU:HA	1:1:54:ARG:O	1.91	0.70
1:1:101:ILE:O	5:1:288:SUC:O6'	2.08	0.70
1:1:169:MET:CE	1:1:171:ILE:HB	2.21	0.70
2:2:207:ASN:HD22	2:2:209:VAL:H	1.37	0.70
3:3:42:ASN:HB3	3:3:44:ILE:HG22	1.73	0.70
2:2:37:VAL:HG21	3:3:37:PRO:HB3	1.72	0.70
1:1:124:GLU:OE2	1:1:181:ARG:HD3	1.91	0.70
1:1:127:LEU:O	1:1:180:PRO:HD2	1.92	0.70
2:2:78:TRP:CE3	2:2:78:TRP:N	2.60	0.70
1:1:61:THR:HG22	1:1:63:ASP:OD1	1.90	0.70
1:1:102:THR:OG1	5:1:288:SUC:H5'	1.91	0.69
1:1:14:VAL:HG11	4:4:43:LEU:HB3	1.74	0.69
1:1:44:ASN:HD22	1:1:44:ASN:C	1.95	0.69
1:1:281:ARG:HB3	3:3:57:ASN:O	1.92	0.69
3:3:127:LEU:HG	3:3:128:LYS:N	2.08	0.69
2:2:51:ASN:H	2:2:51:ASN:HD22	1.41	0.69
1:1:7:ILE:CA	1:1:11:LEU:HD23	2.21	0.69
1:1:155:PRO:HB3	1:1:163:TRP:HE1	1.57	0.68
2:2:12:ARG:HD3	2:2:27:ASP:HA	1.74	0.68
1:1:92:GLN:C	1:1:94:ILE:HD12	2.13	0.68
2:2:41:TYR:HD2	2:2:55:GLN:OE1	1.75	0.68
2:2:56:PRO:HB2	2:2:60:SER:HB3	1.76	0.68
2:2:206:VAL:HG12	3:3:37:PRO:HG2	1.75	0.68
3:3:127:LEU:HA	3:3:196:ASN:O	1.93	0.68
3:3:132:ALA:O	3:3:189:ILE:HA	1.93	0.68
1:1:269:PRO:HG2	1:1:272:GLY:O	1.93	0.68
1:1:91:GLY:C	1:1:94:ILE:HD13	2.14	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:171:SER:HA	2:2:175:PHE:CE2	2.28	0.68
1:1:135:GLY:HA3	1:1:231:LEU:HB3	1.76	0.67
1:1:142:VAL:HG13	1:1:143:MET:N	2.07	0.67
2:2:103:ARG:HB3	2:2:211:MET:HG2	1.76	0.67
1:1:38:GLU:O	2:2:189:GLN:HB2	1.93	0.67
1:1:67:ILE:CD1	3:3:40:VAL:HB	2.22	0.67
1:1:92:GLN:C	1:1:94:ILE:CD1	2.63	0.67
1:1:119:VAL:HG13	1:1:121:PHE:HE2	1.60	0.66
3:3:82:VAL:HG12	3:3:83:PHE:CD1	2.25	0.66
3:3:99:ILE:HG22	3:3:100:GLY:N	2.11	0.66
3:3:201:PRO:O	3:3:202:SER:HB2	1.96	0.66
2:2:78:TRP:CZ3	2:2:226:PRO:HD3	2.30	0.66
2:2:12:ARG:HB3	2:2:12:ARG:NH1	2.10	0.65
1:1:45:VAL:H	3:3:114:ARG:HH12	1.45	0.65
3:3:89:ILE:HD11	3:3:109:TRP:CG	2.30	0.65
2:2:78:TRP:N	2:2:78:TRP:HE3	1.92	0.65
1:1:186:PHE:HE2	3:3:31:THR:HG22	1.62	0.65
1:1:160:ASP:H	1:1:163:TRP:HD1	1.44	0.64
3:3:89:ILE:HD11	3:3:109:TRP:CD2	2.33	0.64
2:2:146:LEU:HD12	2:2:166:GLN:HA	1.78	0.64
1:1:19:ASN:HB3	1:1:56:VAL:O	1.97	0.64
1:1:215:ASN:N	1:1:215:ASN:ND2	2.42	0.64
2:2:207:ASN:ND2	2:2:209:VAL:HG22	2.13	0.64
1:1:23:SER:OG	1:1:53:THR:CG2	2.31	0.64
3:3:89:ILE:HA	3:3:94:LEU:HD13	1.80	0.64
3:3:66:SER:C	3:3:68:TYR:H	2.00	0.64
2:2:126:MET:HA	2:2:126:MET:HE3	1.80	0.64
1:1:260:THR:C	1:1:261:HIS:CD2	2.71	0.63
2:2:72:ASN:HB3	2:2:75:SER:N	2.13	0.63
1:1:244:LYS:HE3	4:4:38:SER:O	1.98	0.63
1:1:276:THR:OG1	1:1:277:ALA:N	2.31	0.63
2:2:155:ASP:O	2:2:156:VAL:HB	1.98	0.63
1:1:260:THR:C	1:1:261:HIS:HD2	2.01	0.63
1:1:217:MET:SD	5:1:288:SUC:O3	2.55	0.63
1:1:141:ILE:HA	1:1:226:THR:HG21	1.80	0.63
2:2:174:ASN:C	2:2:175:PHE:HD2	2.02	0.63
3:3:87:VAL:HG22	3:3:189:ILE:HG22	1.79	0.63
1:1:113:PHE:C	1:1:115:LEU:N	2.52	0.63
1:1:215:ASN:CB	5:1:288:SUC:O3'	2.47	0.62
1:1:148:VAL:HG12	1:1:152:ALA:HB3	1.81	0.62
3:3:102:ILE:O	3:3:105:TYR:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:257:ARG:HG2	2:2:257:ARG:NH1	2.14	0.62
1:1:155:PRO:HB3	1:1:163:TRP:NE1	2.15	0.62
1:1:283:THR:HG22	1:1:285:THR:N	2.15	0.62
2:2:30:ASN:HD22	2:2:31:ALA:N	1.97	0.62
1:1:7:ILE:N	1:1:7:ILE:HD13	2.14	0.62
5:1:288:SUC:H6'2	5:1:288:SUC:H5	1.80	0.61
1:1:6:TYR:CB	1:1:7:ILE:HD13	2.25	0.61
2:2:145:LYS:NZ	2:2:263:GLN:HG2	2.15	0.61
1:1:79:ILE:HD13	1:1:238:HIS:CE1	2.35	0.61
1:1:204:ASN:C	1:1:206:SER:N	2.52	0.61
1:1:105:GLU:O	1:1:106:MET:HG3	2.01	0.61
1:1:150:PRO:HG3	1:1:218:GLY:N	2.15	0.61
1:1:281:ARG:NH2	3:3:84:SER:O	2.33	0.61
1:1:94:ILE:N	1:1:94:ILE:HD12	2.16	0.61
3:3:95:ALA:O	3:3:97:THR:N	2.34	0.61
2:2:84:ASP:HB2	2:2:218:ASN:HD21	1.66	0.61
4:4:43:LEU:O	4:4:44:ASP:C	2.38	0.61
3:3:72:LEU:HD11	3:3:209:MET:HB3	1.82	0.61
1:1:91:GLY:O	1:1:157:LYS:CB	2.49	0.61
1:1:223:ARG:HG2	1:1:223:ARG:NH1	2.16	0.61
1:1:14:VAL:HG12	1:1:15:LEU:HD22	1.81	0.61
1:1:140:HIS:O	1:1:226:THR:CG2	2.48	0.60
1:1:200:TYR:CD1	1:1:209:TYR:HB2	2.37	0.60
2:2:84:ASP:OD2	2:2:87:LYS:HE2	2.02	0.60
3:3:91:SER:O	3:3:92:THR:C	2.39	0.60
2:2:91:ILE:O	2:2:92:PHE:C	2.38	0.60
1:1:91:GLY:O	1:1:157:LYS:HB3	2.02	0.60
1:1:119:VAL:CG1	1:1:121:PHE:CE2	2.79	0.60
1:1:108:GLN:HB3	1:1:109:ILE:HG22	1.83	0.60
1:1:249:TRP:HA	3:3:39:GLU:HA	1.84	0.60
1:1:204:ASN:HD22	1:1:205:THR:N	2.00	0.60
1:1:102:THR:CB	5:1:288:SUC:C6'	2.78	0.60
1:1:37:ALA:HB2	3:3:162:THR:HG21	1.83	0.59
1:1:142:VAL:H	1:1:226:THR:HG23	1.67	0.59
2:2:183:LEU:HD12	2:2:186:PHE:CD1	2.34	0.59
1:1:103:LEU:HG	5:1:288:SUC:H61	1.83	0.59
1:1:136:ASP:O	1:1:137:ASP:HB2	2.02	0.59
1:1:22:GLU:CA	1:1:54:ARG:O	2.50	0.59
2:2:207:ASN:HD21	2:2:209:VAL:HG22	1.67	0.59
1:1:215:ASN:H	1:1:215:ASN:HD22	1.51	0.59
2:2:144:TYR:O	2:2:146:LEU:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:85:ASP:OD2	1:1:86:TYR:N	2.36	0.59
3:3:90:THR:OG1	3:3:178:THR:O	2.15	0.58
3:3:42:ASN:ND2	3:3:44:ILE:CG2	2.53	0.58
3:3:44:ILE:O	3:3:47:CYS:HB2	2.02	0.58
2:2:77:GLY:HA2	2:2:78:TRP:CE3	2.37	0.58
1:1:99:TRP:CZ3	1:1:101:ILE:HA	2.39	0.58
1:1:110:ARG:O	1:1:114:GLU:HG3	2.04	0.58
1:1:169:MET:HE2	1:1:171:ILE:HB	1.84	0.58
3:3:46:MET:O	3:3:98:LEU:HD23	2.03	0.58
2:2:154:ARG:HD3	2:2:155:ASP:N	2.19	0.58
1:1:253:PRO:HD3	2:2:185:ILE:CG2	2.34	0.58
3:3:136:PRO:HG3	3:3:176:ARG:NH2	2.19	0.58
1:1:66:SER:O	1:1:68:GLU:N	2.37	0.58
1:1:153:PRO:O	1:1:153:PRO:HG2	2.04	0.58
2:2:49:ALA:O	2:2:50:ILE:HG13	2.04	0.58
1:1:163:TRP:CD2	1:1:223:ARG:HD3	2.39	0.58
1:1:127:LEU:CB	1:1:180:PRO:HG2	2.33	0.58
1:1:253:PRO:HD3	2:2:185:ILE:HG21	1.86	0.58
1:1:199:GLY:HA2	2:2:216:ARG:O	2.04	0.57
1:1:11:LEU:N	1:1:11:LEU:HD22	2.19	0.57
2:2:158:GLN:HG3	2:2:159:GLU:H	1.68	0.57
1:1:278:ILE:HA	3:3:92:THR:HG21	1.85	0.57
3:3:136:PRO:HG3	3:3:176:ARG:HH22	1.68	0.57
3:3:54:PRO:HA	3:3:67:MET:O	2.04	0.57
1:1:67:ILE:HD11	3:3:40:VAL:CB	2.33	0.57
1:1:90:ASN:HD22	1:1:158:ARG:HD3	1.70	0.57
3:3:192:TRP:N	3:3:192:TRP:CD1	2.73	0.57
1:1:7:ILE:HD13	1:1:7:ILE:H	1.67	0.57
1:1:92:GLN:HA	1:1:157:LYS:HG2	1.86	0.57
2:2:120:GLY:HA3	2:2:193:LEU:HD12	1.86	0.57
1:1:261:HIS:H	3:3:237:GLU:H	1.53	0.57
1:1:102:THR:HA	5:1:288:SUC:C5'	2.15	0.57
1:1:54:ARG:CG	1:1:55:TYR:H	2.16	0.57
1:1:111:ARG:NH1	3:3:230:HIS:HB2	2.20	0.56
2:2:57:ASP:O	2:2:58:THR:HG22	2.04	0.56
1:1:102:THR:CA	5:1:288:SUC:HO6'	2.17	0.56
1:1:197:TYR:HD2	1:1:198:ASP:H	1.52	0.56
3:3:7:THR:O	3:3:10:SER:CB	2.53	0.56
3:3:194:GLN:HA	3:3:194:GLN:NE2	2.19	0.56
1:1:44:ASN:ND2	1:1:44:ASN:C	2.58	0.56
2:2:235:THR:C	2:2:237:SER:H	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:92:GLN:N	1:1:94:ILE:CD1	2.68	0.56
3:3:87:VAL:O	3:3:89:ILE:N	2.38	0.56
3:3:104:SER:O	3:3:227:THR:HA	2.06	0.56
3:3:42:ASN:CB	3:3:44:ILE:HG22	2.36	0.56
3:3:14:MET:HG2	3:3:16:THR:HG22	1.88	0.56
3:3:107:THR:O	3:3:177:LEU:HD23	2.06	0.56
1:1:102:THR:CB	5:1:288:SUC:H5'	2.36	0.56
2:2:72:ASN:HB3	2:2:74:SER:H	1.70	0.56
3:3:121:GLY:HA2	3:3:207:ALA:HB1	1.88	0.56
3:3:42:ASN:HB3	3:3:44:ILE:CG2	2.36	0.56
3:3:144:ARG:O	3:3:145:LYS:C	2.44	0.56
1:1:103:LEU:N	5:1:288:SUC:C6'	2.67	0.55
3:3:83:PHE:CE1	3:3:191:CYS:CB	2.89	0.55
1:1:255:ARG:NH2	1:1:259:TYR:HA	2.21	0.55
2:2:173:LEU:O	2:2:174:ASN:CB	2.54	0.55
3:3:228:ASP:HB3	3:3:229:LEU:HD12	1.88	0.55
1:1:124:GLU:HG2	1:1:242:LYS:HB3	1.87	0.55
1:1:129:PRO:HG2	1:1:173:TRP:CZ2	2.40	0.55
2:2:122:LEU:HD22	2:2:224:ILE:HG13	1.87	0.55
1:1:61:THR:CG2	1:1:63:ASP:OD1	2.54	0.55
1:1:66:SER:C	1:1:68:GLU:N	2.60	0.55
3:3:94:LEU:O	3:3:95:ALA:C	2.45	0.55
2:2:57:ASP:O	2:2:58:THR:CB	2.55	0.55
1:1:102:THR:HA	5:1:288:SUC:HO6'	1.71	0.55
3:3:81:LYS:HB2	3:3:192:TRP:CE3	2.41	0.55
2:2:202:ILE:HD13	2:2:249:MET:CE	2.36	0.55
2:2:174:ASN:O	2:2:175:PHE:HB2	2.07	0.55
3:3:173:SER:O	3:3:174:HIS:C	2.43	0.55
1:1:19:ASN:HA	1:1:58:THR:HG23	1.88	0.55
3:3:201:PRO:O	3:3:202:SER:CB	2.53	0.55
1:1:91:GLY:C	1:1:94:ILE:CD1	2.75	0.55
1:1:201:ASP:OD1	1:1:208:LYS:HB2	2.07	0.55
2:2:227:ILE:HG21	3:3:210:LEU:HD11	1.89	0.55
1:1:195:MET:CE	5:1:288:SUC:H1'1	2.37	0.55
1:1:80:SER:HB3	1:1:237:THR:HG23	1.89	0.55
3:3:145:LYS:HA	3:3:148:MET:HE2	1.89	0.55
3:3:165:LEU:HD12	3:3:166:VAL:N	2.21	0.55
2:2:23:ILE:HG21	2:2:109:HIS:CD2	2.42	0.54
2:2:116:LYS:HB2	3:3:124:ASN:ND2	2.21	0.54
1:1:278:ILE:CD1	3:3:67:MET:HE1	2.36	0.54
1:1:17:VAL:CG1	1:1:60:GLN:O	2.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:124:GLU:O	1:1:124:GLU:HG3	2.06	0.54
1:1:84:VAL:HG21	1:1:233:VAL:HG23	1.88	0.54
1:1:72:GLY:C	1:1:73:ARG:HG2	2.27	0.54
2:2:83:PRO:HG2	2:2:218:ASN:CA	2.28	0.54
2:2:127:ILE:HD11	2:2:183:LEU:HD11	1.89	0.54
1:1:96:PHE:HE1	1:1:157:LYS:HA	1.70	0.54
1:1:89:TYR:O	1:1:90:ASN:HB2	2.07	0.54
2:2:103:ARG:CB	2:2:211:MET:HG2	2.38	0.54
1:1:261:HIS:N	1:1:261:HIS:CD2	2.74	0.54
1:1:283:THR:CG2	1:1:285:THR:HB	2.38	0.54
3:3:103:ALA:O	3:3:178:THR:HG21	2.08	0.54
3:3:81:LYS:HB2	3:3:192:TRP:CZ3	2.43	0.54
1:1:61:THR:HG22	1:1:63:ASP:CG	2.28	0.54
3:3:125:THR:CG2	3:3:126:THR:N	2.70	0.54
3:3:80:GLN:NE2	3:3:80:GLN:HA	2.22	0.54
1:1:119:VAL:HG11	1:1:121:PHE:HE2	1.69	0.54
1:1:244:LYS:HZ1	4:4:38:SER:H	1.54	0.54
1:1:84:VAL:HG12	1:1:85:ASP:N	2.22	0.54
1:1:145:TYR:N	1:1:145:TYR:CD2	2.73	0.54
2:2:84:ASP:O	2:2:87:LYS:HD2	2.07	0.54
1:1:257:VAL:HG11	1:1:274:VAL:HG21	1.89	0.54
1:1:200:TYR:HA	1:1:208:LYS:O	2.08	0.54
2:2:102:GLY:HA3	2:2:214:MET:HG3	1.88	0.54
1:1:45:VAL:N	3:3:114:ARG:NH1	2.43	0.53
2:2:40:HIS:HA	2:2:250:CYS:SG	2.47	0.53
3:3:155:TRP:CD2	3:3:163:ILE:CG2	2.90	0.53
2:2:235:THR:OG1	2:2:237:SER:HB3	2.08	0.53
1:1:142:VAL:CG1	1:1:225:VAL:CB	2.76	0.53
1:1:92:GLN:O	1:1:94:ILE:HD11	2.09	0.53
1:1:281:ARG:HH11	3:3:57:ASN:HB3	1.74	0.53
1:1:103:LEU:CG	5:1:288:SUC:H61	2.38	0.53
1:1:106:MET:O	1:1:107:ALA:O	2.27	0.53
1:1:263:HIS:CE1	5:1:288:SUC:O4'	2.61	0.53
1:1:195:MET:HE2	5:1:288:SUC:H1'1	1.90	0.53
3:3:169:TRP:CZ3	3:3:176:ARG:HD2	2.44	0.53
1:1:33:LEU:HB3	3:3:163:ILE:HD11	1.90	0.53
1:1:103:LEU:H	5:1:288:SUC:C5'	2.21	0.53
1:1:89:TYR:HE1	1:1:227:GLU:C	2.12	0.53
2:2:174:ASN:HB3	2:2:176:ASP:OD1	2.08	0.53
2:2:122:LEU:O	2:2:190:PHE:HA	2.08	0.53
1:1:102:THR:CA	5:1:288:SUC:O6'	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:75:GLN:HG2	3:3:80:GLN:HB3	1.91	0.53
3:3:237:GLU:CG	3:3:238:GLN:H	2.20	0.53
1:1:200:TYR:CE1	1:1:209:TYR:HB2	2.44	0.53
2:2:61:ASN:HB2	2:2:248:PRO:O	2.09	0.52
1:1:104:GLN:OE1	1:1:263:HIS:ND1	2.33	0.52
3:3:89:ILE:HA	3:3:94:LEU:CD1	2.38	0.52
4:4:26:TYR:CD2	4:4:29:ILE:CD1	2.91	0.52
1:1:269:PRO:CG	1:1:272:GLY:O	2.56	0.52
2:2:158:GLN:CG	2:2:159:GLU:H	2.21	0.52
1:1:257:VAL:HG21	2:2:173:LEU:HD11	1.91	0.52
2:2:174:ASN:C	2:2:175:PHE:CD2	2.82	0.52
2:2:41:TYR:CE2	2:2:55:GLN:OE1	2.62	0.52
1:1:84:VAL:HG12	1:1:85:ASP:H	1.74	0.52
2:2:18:ARG:HG3	2:2:247:SER:OG	2.09	0.52
1:1:143:MET:HG2	1:1:145:TYR:CE2	2.45	0.52
1:1:284:ILE:HG13	1:1:285:THR:N	2.24	0.52
2:2:65:THR:HG1	2:2:245:SER:HG	1.50	0.52
3:3:173:SER:C	3:3:175:PHE:N	2.63	0.52
1:1:46:GLN:O	1:1:49:ASP:HB2	2.10	0.52
1:1:171:ILE:CD1	1:1:180:PRO:HB2	2.37	0.52
3:3:66:SER:O	3:3:68:TYR:N	2.42	0.52
1:1:271:THR:HG22	1:1:272:GLY:N	2.25	0.52
1:1:215:ASN:OD1	5:1:288:SUC:O3'	2.27	0.52
2:2:185:ILE:HD13	3:3:98:LEU:HD21	1.91	0.51
1:1:215:ASN:CG	5:1:288:SUC:HO3'	2.12	0.51
2:2:202:ILE:HD13	2:2:249:MET:HE3	1.92	0.51
1:1:266:ASN:OD1	2:2:134:SER:N	2.34	0.51
3:3:83:PHE:CE1	3:3:191:CYS:HB3	2.45	0.51
2:2:190:PHE:O	2:2:196:ASN:ND2	2.43	0.51
3:3:136:PRO:HB3	3:3:185:MET:O	2.10	0.51
3:3:102:ILE:O	3:3:105:TYR:N	2.44	0.51
3:3:56:ASN:C	3:3:58:VAL:H	2.12	0.51
2:2:173:LEU:O	2:2:177:GLY:N	2.44	0.51
3:3:110:THR:O	3:3:219:PHE:HA	2.10	0.51
2:2:137:HIS:CD2	2:2:138:GLY:N	2.79	0.51
3:3:181:ASN:OD1	3:3:183:TYR:HB3	2.11	0.51
1:1:46:GLN:CB	1:1:47:PRO:CD	2.57	0.51
1:1:6:TYR:O	1:1:10:VAL:N	2.44	0.51
2:2:154:ARG:CG	2:2:154:ARG:HH11	2.24	0.51
3:3:51:THR:HG21	3:3:98:LEU:HB3	1.92	0.51
2:2:175:PHE:N	2:2:175:PHE:CD2	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:7:ILE:HA	1:1:11:LEU:CD2	2.28	0.50
1:1:92:GLN:C	1:1:94:ILE:HD11	2.31	0.50
3:3:99:ILE:CG2	3:3:100:GLY:N	2.73	0.50
4:4:42:ARG:HH12	4:4:44:ASP:HB3	1.76	0.50
1:1:42:THR:HG22	1:1:43:SER:O	2.12	0.50
2:2:86:LEU:C	2:2:88:ASP:H	2.14	0.50
1:1:19:ASN:N	1:1:19:ASN:ND2	2.57	0.50
1:1:7:ILE:O	1:1:11:LEU:HD23	2.11	0.50
2:2:12:ARG:O	2:2:28:VAL:HG22	2.10	0.50
1:1:186:PHE:CE2	3:3:31:THR:HG22	2.45	0.50
3:3:72:LEU:N	3:3:72:LEU:HD12	2.26	0.50
1:1:123:SER:HB3	1:1:241:HIS:CD2	2.45	0.50
3:3:118:MET:O	3:3:209:MET:HA	2.12	0.50
1:1:7:ILE:H	1:1:7:ILE:CD1	2.17	0.50
1:1:34:LEU:HD23	3:3:162:THR:O	2.12	0.50
1:1:184:ILE:HG22	1:1:185:PRO:O	2.12	0.50
1:1:197:TYR:CD1	1:1:214:THR:CG2	2.94	0.50
1:1:197:TYR:H	2:2:131:GLN:NE2	2.04	0.50
3:3:127:LEU:CG	3:3:128:LYS:N	2.75	0.50
2:2:110:VAL:O	2:2:198:SER:HA	2.10	0.50
1:1:103:LEU:H	5:1:288:SUC:C6'	2.24	0.49
1:1:103:LEU:HG	5:1:288:SUC:C6	2.42	0.49
3:3:62:VAL:HA	3:3:67:MET:HG3	1.94	0.49
2:2:32:VAL:HB	2:2:201:LEU:HD22	1.94	0.49
3:3:117:PHE:CE1	3:3:131:LEU:HG	2.47	0.49
2:2:14:MET:HG2	2:2:15:GLN:N	2.25	0.49
1:1:230:LYS:HD3	1:1:231:LEU:HD22	1.94	0.49
1:1:197:TYR:N	2:2:131:GLN:HE21	2.05	0.49
2:2:159:GLU:HA	2:2:159:GLU:OE1	2.11	0.49
3:3:25:LEU:N	3:3:26:PRO:HD3	2.27	0.49
4:4:26:TYR:O	4:4:27:PHE:HB2	2.12	0.49
2:2:81:LYS:HE2	2:2:132:LEU:HD11	1.94	0.49
1:1:204:ASN:O	1:1:206:SER:N	2.45	0.49
1:1:191:SER:CB	3:3:34:ILE:HG12	2.43	0.49
1:1:65:MET:O	3:3:42:ASN:CG	2.51	0.49
1:1:7:ILE:O	1:1:11:LEU:CB	2.60	0.49
3:3:135:PRO:CB	3:3:136:PRO:HD2	2.42	0.49
2:2:82:LEU:CB	2:2:83:PRO:HD3	2.43	0.49
2:2:12:ARG:CG	2:2:13:ILE:H	2.26	0.49
1:1:197:TYR:HD2	1:1:198:ASP:N	2.11	0.49
2:2:174:ASN:ND2	2:2:178:THR:O	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:141:PRO:HG3	3:3:147:ALA:HB2	1.93	0.49
1:1:7:ILE:N	1:1:7:ILE:CD1	2.76	0.49
1:1:244:LYS:CE	4:4:38:SER:O	2.60	0.49
2:2:145:LYS:HZ2	2:2:263:GLN:HG2	1.77	0.49
1:1:204:ASN:HD22	1:1:205:THR:H	1.61	0.48
1:1:173:TRP:HE3	1:1:173:TRP:O	1.95	0.48
3:3:55:VAL:C	3:3:57:ASN:N	2.67	0.48
3:3:155:TRP:CD2	3:3:163:ILE:HG22	2.48	0.48
3:3:140:GLU:HB3	3:3:188:TYR:CD1	2.48	0.48
3:3:155:TRP:CG	3:3:163:ILE:HG21	2.49	0.48
1:1:261:HIS:H	3:3:237:GLU:N	2.11	0.48
3:3:112:SER:H	3:3:218:ASP:HB3	1.79	0.48
1:1:278:ILE:CD1	3:3:67:MET:HE2	2.42	0.48
1:1:197:TYR:CE1	1:1:214:THR:CG2	2.91	0.48
2:2:70:HIS:ND1	2:2:71:TRP:N	2.60	0.48
3:3:65:VAL:O	3:3:67:MET:N	2.46	0.48
1:1:197:TYR:CD2	1:1:198:ASP:N	2.81	0.48
2:2:174:ASN:C	2:2:176:ASP:H	2.16	0.48
2:2:192:ASN:O	2:2:194:ARG:N	2.46	0.48
1:1:7:ILE:O	1:1:11:LEU:N	2.43	0.48
1:1:141:ILE:CD1	1:1:235:ILE:HG12	2.43	0.48
1:1:93:ASP:N	1:1:94:ILE:HD12	2.28	0.48
3:3:61:ASN:ND2	3:3:66:SER:HB2	2.29	0.48
1:1:38:GLU:C	1:1:40:GLY:H	2.15	0.48
1:1:281:ARG:HH11	3:3:57:ASN:CB	2.26	0.48
2:2:154:ARG:NH2	2:2:167:PRO:HG2	2.28	0.48
1:1:119:VAL:HG13	1:1:121:PHE:CD2	2.49	0.48
1:1:44:ASN:O	1:1:44:ASN:ND2	2.34	0.48
3:3:14:MET:C	3:3:16:THR:H	2.16	0.48
2:2:82:LEU:HD21	2:2:246:ILE:HD13	1.96	0.48
2:2:128:PRO:HD2	2:2:186:PHE:CD2	2.49	0.48
1:1:86:TYR:CZ	1:1:229:GLN:HB2	2.49	0.48
2:2:82:LEU:HD23	2:2:82:LEU:HA	1.55	0.47
1:1:257:VAL:HG21	2:2:173:LEU:CD1	2.44	0.47
2:2:57:ASP:O	2:2:59:SER:N	2.42	0.47
2:2:107:THR:OG1	2:2:249:MET:CE	2.61	0.47
1:1:169:MET:HE2	1:1:171:ILE:CB	2.44	0.47
3:3:131:LEU:CD1	3:3:191:CYS:SG	3.02	0.47
3:3:82:VAL:HG12	3:3:83:PHE:H	1.77	0.47
3:3:155:TRP:CD1	3:3:155:TRP:C	2.87	0.47
2:2:72:ASN:HB3	2:2:75:SER:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:136:PRO:HD3	3:3:186:ALA:O	2.15	0.47
3:3:131:LEU:O	3:3:152:HIS:HB2	2.15	0.47
1:1:84:VAL:CG2	1:1:233:VAL:HG23	2.44	0.47
3:3:124:ASN:H	3:3:124:ASN:HD22	1.63	0.47
1:1:102:THR:CA	5:1:288:SUC:C5'	2.85	0.47
1:1:142:VAL:HG11	1:1:225:VAL:CB	2.39	0.47
1:1:127:LEU:HD12	1:1:239:ILE:HG12	1.95	0.47
1:1:278:ILE:HD12	3:3:67:MET:HE3	1.88	0.47
3:3:231:ILE:CD1	3:3:231:ILE:N	2.70	0.47
2:2:206:VAL:O	2:2:207:ASN:HB2	2.14	0.47
1:1:112:LYS:O	1:1:115:LEU:HB2	2.13	0.47
4:4:27:PHE:O	4:4:28:ASN:HB2	2.14	0.47
1:1:254:PRO:HG2	3:3:101:GLU:HG2	1.83	0.47
2:2:146:LEU:HD11	2:2:166:GLN:HA	1.94	0.47
2:2:78:TRP:CZ2	2:2:242:ILE:HD12	2.50	0.47
1:1:124:GLU:CD	1:1:181:ARG:HH11	2.18	0.47
1:1:15:LEU:CD2	4:4:43:LEU:HD23	2.45	0.47
1:1:42:THR:HG21	3:3:48:GLN:O	2.15	0.47
2:2:253:PHE:O	2:2:254:SER:HB3	2.15	0.47
2:2:116:LYS:HB2	3:3:124:ASN:HD21	1.79	0.47
2:2:130:HIS:CB	2:2:221:CYS:SG	3.03	0.47
2:2:224:ILE:HD11	2:2:242:ILE:HD13	1.96	0.47
3:3:219:PHE:CE2	3:3:221:LEU:HD13	2.50	0.47
3:3:66:SER:C	3:3:68:TYR:N	2.69	0.47
2:2:185:ILE:CD1	3:3:98:LEU:CD2	2.85	0.46
2:2:200:THR:C	2:2:201:LEU:HD23	2.36	0.46
1:1:255:ARG:HH21	1:1:259:TYR:HA	1.80	0.46
1:1:19:ASN:CB	1:1:56:VAL:O	2.63	0.46
2:2:111:GLN:OE1	2:2:245:SER:OG	2.31	0.46
1:1:48:GLU:HA	1:1:53:THR:HG21	1.96	0.46
3:3:57:ASN:HD22	3:3:57:ASN:HA	1.21	0.46
1:1:280:ARG:HG3	3:3:62:VAL:HG21	1.98	0.46
1:1:129:PRO:HA	1:1:237:THR:HA	1.97	0.46
1:1:77:VAL:HG22	1:1:239:ILE:HG22	1.98	0.46
2:2:57:ASP:O	2:2:58:THR:HB	2.15	0.46
1:1:129:PRO:HG2	1:1:173:TRP:NE1	2.31	0.46
2:2:164:LEU:O	2:2:166:GLN:HB2	2.16	0.46
1:1:215:ASN:HB2	5:1:288:SUC:O3'	2.15	0.46
2:2:69:LYS:O	2:2:241:PRO:HA	2.15	0.46
1:1:268:MET:HA	1:1:269:PRO:HD2	1.82	0.46
2:2:66:LEU:HD23	2:2:80:TRP:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:42:ASN:O	3:3:43:LEU:C	2.54	0.46
1:1:188:SER:OG	1:1:190:ALA:HB3	2.16	0.46
2:2:126:MET:HE2	2:2:126:MET:HB3	1.77	0.46
2:2:182:ASN:O	2:2:185:ILE:HG22	2.16	0.46
3:3:46:MET:HE3	3:3:102:ILE:HD11	1.97	0.46
3:3:25:LEU:N	3:3:26:PRO:CD	2.79	0.46
3:3:145:LYS:O	3:3:148:MET:HE3	2.16	0.46
2:2:102:GLY:HA3	2:2:214:MET:CG	2.45	0.46
1:1:90:ASN:ND2	1:1:158:ARG:HD3	2.31	0.45
2:2:127:ILE:HG22	2:2:128:PRO:O	2.16	0.45
1:1:169:MET:HG2	1:1:170:SER:N	2.30	0.45
1:1:254:PRO:CG	3:3:101:GLU:CG	2.72	0.45
3:3:87:VAL:HG22	3:3:189:ILE:CG2	2.45	0.45
1:1:184:ILE:HD13	1:1:184:ILE:HG21	1.62	0.45
1:1:104:GLN:HB3	1:1:104:GLN:HE21	1.64	0.45
1:1:80:SER:O	1:1:236:THR:HA	2.16	0.45
2:2:18:ARG:HA	2:2:18:ARG:HD3	1.56	0.45
3:3:84:SER:OG	3:3:140:GLU:OE1	2.30	0.45
3:3:88:ASP:O	3:3:90:THR:N	2.43	0.45
1:1:97:THR:O	1:1:221:CYS:HA	2.16	0.45
2:2:46:ASP:HB3	3:3:34:ILE:HB	1.98	0.45
1:1:89:TYR:O	1:1:90:ASN:CB	2.62	0.45
3:3:93:PRO:O	3:3:94:LEU:O	2.35	0.45
2:2:121:THR:HG22	2:2:227:ILE:HB	1.98	0.45
3:3:99:ILE:O	3:3:102:ILE:HB	2.16	0.45
2:2:146:LEU:HD12	2:2:167:PRO:HD2	1.95	0.45
2:2:257:ARG:O	2:2:258:ALA:O	2.35	0.45
1:1:124:GLU:OE1	1:1:181:ARG:NH1	2.49	0.45
2:2:15:GLN:HG3	2:2:16:ILE:N	2.29	0.45
1:1:197:TYR:HE2	2:2:217:HIS:CG	2.34	0.45
3:3:237:GLU:HG3	3:3:238:GLN:H	1.81	0.45
1:1:75:GLY:N	1:1:240:TYR:HD2	2.15	0.45
1:1:283:THR:CG2	1:1:285:THR:H	2.29	0.45
2:2:235:THR:HG23	2:2:235:THR:O	2.17	0.45
2:2:80:TRP:NE1	2:2:151:GLU:O	2.50	0.45
3:3:97:THR:O	3:3:98:LEU:C	2.56	0.44
1:1:115:LEU:HA	1:1:115:LEU:HD12	1.76	0.44
1:1:262:SER:O	1:1:263:HIS:HB2	2.18	0.44
4:4:30:ASN:N	4:4:30:ASN:ND2	2.65	0.44
2:2:103:ARG:HD3	2:2:252:GLU:OE2	2.17	0.44
1:1:245:HIS:CE1	4:4:38:SER:OG	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:174:ASN:ND2	2:2:180:LEU:HA	2.32	0.44
2:2:145:LYS:HZ1	2:2:263:GLN:HG2	1.82	0.44
1:1:90:ASN:N	1:1:90:ASN:HD22	2.16	0.44
1:1:260:THR:HB	1:1:261:HIS:CD2	2.53	0.44
1:1:185:PRO:HD3	3:3:23:CYS:SG	2.58	0.44
1:1:104:GLN:O	3:3:236:ILE:HD11	2.17	0.44
3:3:173:SER:C	3:3:175:PHE:H	2.20	0.44
1:1:40:GLY:HA3	2:2:188:HIS:O	2.18	0.44
2:2:192:ASN:C	2:2:194:ARG:H	2.21	0.44
2:2:121:THR:OG1	3:3:120:CYS:HB3	2.17	0.44
3:3:101:GLU:HA	3:3:229:LEU:HD22	1.99	0.44
1:1:142:VAL:H	1:1:226:THR:CG2	2.29	0.44
1:1:156:SER:C	1:1:157:LYS:HG3	2.38	0.44
1:1:194:TYR:OH	2:2:207:ASN:ND2	2.50	0.44
2:2:30:ASN:HD22	2:2:31:ALA:H	1.62	0.44
2:2:79:TRP:CZ3	2:2:81:LYS:HD3	2.52	0.44
3:3:130:LEU:HD23	3:3:130:LEU:C	2.38	0.44
2:2:154:ARG:HG2	2:2:154:ARG:HH11	1.83	0.44
2:2:61:ASN:HD22	2:2:250:CYS:H	1.65	0.44
1:1:283:THR:HG22	1:1:285:THR:H	1.83	0.44
3:3:126:THR:O	3:3:197:LEU:HA	2.18	0.43
2:2:128:PRO:HD3	2:2:220:TRP:CZ3	2.53	0.43
1:1:54:ARG:HG3	1:1:55:TYR:H	1.83	0.43
2:2:29:ALA:O	2:2:30:ASN:C	2.56	0.43
3:3:2:LEU:HD23	3:3:2:LEU:HA	1.80	0.43
2:2:52:LYS:HA	2:2:53:PRO:HD2	1.91	0.43
3:3:1:GLY:O	3:3:3:PRO:HD3	2.18	0.43
3:3:134:THR:HA	3:3:135:PRO:HD2	1.85	0.43
2:2:37:VAL:HG12	2:2:204:PRO:HB3	2.00	0.43
3:3:155:TRP:CD2	3:3:163:ILE:HG21	2.53	0.43
1:1:54:ARG:HD2	1:1:56:VAL:HG22	1.99	0.43
1:1:5:ASN:O	1:1:9:GLU:HB2	2.18	0.43
1:1:244:LYS:NZ	4:4:38:SER:H	2.16	0.43
1:1:74:SER:HB2	3:3:15:THR:HA	2.00	0.43
1:1:96:PHE:CZ	1:1:155:PRO:O	2.71	0.43
1:1:244:LYS:NZ	4:4:38:SER:O	2.52	0.43
1:1:192:ALA:HB3	2:2:208:ALA:HB2	2.01	0.43
2:2:191:ILE:HA	2:2:196:ASN:ND2	2.33	0.43
1:1:66:SER:C	1:1:68:GLU:H	2.21	0.43
1:1:260:THR:HB	1:1:261:HIS:HD2	1.84	0.43
1:1:45:VAL:N	3:3:114:ARG:HH12	2.12	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:72:LEU:CD1	3:3:209:MET:HB3	2.48	0.43
3:3:50:ASP:CA	3:3:214:SER:HB3	2.49	0.43
3:3:43:LEU:O	3:3:44:ILE:C	2.56	0.43
2:2:174:ASN:O	2:2:175:PHE:CB	2.66	0.43
2:2:179:LEU:O	2:2:180:LEU:C	2.56	0.43
2:2:137:HIS:C	2:2:137:HIS:CD2	2.91	0.43
2:2:91:ILE:HG22	2:2:92:PHE:N	2.33	0.43
3:3:149:LEU:HD23	3:3:149:LEU:HA	1.73	0.43
2:2:118:HIS:O	3:3:122:THR:HG23	2.19	0.43
2:2:207:ASN:O	2:2:209:VAL:N	2.51	0.43
3:3:50:ASP:N	3:3:214:SER:HB3	2.34	0.43
3:3:159:LEU:HD23	3:3:159:LEU:HA	1.72	0.43
3:3:103:ALA:C	3:3:105:TYR:H	2.21	0.42
1:1:63:ASP:O	1:1:66:SER:OG	2.27	0.42
1:1:268:MET:O	2:2:137:HIS:HB2	2.19	0.42
2:2:57:ASP:O	2:2:58:THR:CG2	2.67	0.42
1:1:145:TYR:N	1:1:145:TYR:HD2	2.16	0.42
2:2:94:GLU:C	2:2:96:MET:H	2.22	0.42
1:1:197:TYR:HE1	1:1:214:THR:HG23	1.74	0.42
2:2:160:ARG:HD2	2:2:160:ARG:HH11	1.57	0.42
1:1:58:THR:O	1:1:59:SER:HB3	2.19	0.42
1:1:154:ILE:HA	1:1:155:PRO:HD3	1.87	0.42
3:3:53:ILE:HD13	3:3:53:ILE:HG21	1.78	0.42
2:2:147:THR:C	2:2:149:PRO:CD	2.87	0.42
2:2:95:ASN:HB3	2:2:253:PHE:CE2	2.54	0.42
2:2:84:ASP:HB2	2:2:218:ASN:ND2	2.33	0.42
1:1:267:TYR:O	1:1:268:MET:C	2.57	0.42
2:2:65:THR:HA	2:2:245:SER:HA	2.02	0.42
2:2:99:HIS:HA	2:2:255:GLY:O	2.19	0.42
3:3:54:PRO:HA	3:3:68:TYR:CD2	2.54	0.42
2:2:158:GLN:CG	2:2:159:GLU:N	2.83	0.42
2:2:98:TYR:CE2	2:2:259:LYS:HD2	2.54	0.42
2:2:61:ASN:OD1	2:2:61:ASN:N	2.49	0.42
2:2:200:THR:O	2:2:201:LEU:HD23	2.19	0.42
2:2:207:ASN:HD22	2:2:209:VAL:N	2.12	0.42
3:3:219:PHE:O	3:3:220:CYS:HB2	2.20	0.42
2:2:63:PHE:CD2	2:2:247:SER:HB2	2.55	0.42
1:1:145:TYR:HB2	1:1:171:ILE:HG23	2.01	0.42
2:2:136:LYS:HD3	2:2:136:LYS:HA	1.59	0.42
2:2:143:GLY:N	2:2:165:ARG:O	2.48	0.42
2:2:21:SER:OG	2:2:63:PHE:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:7:THR:HA	3:3:8:PRO:HD3	1.78	0.42
1:1:86:TYR:OH	1:1:229:GLN:HB2	2.20	0.42
2:2:111:GLN:H	2:2:111:GLN:HG2	1.29	0.42
2:2:192:ASN:HD22	2:2:192:ASN:HA	1.51	0.41
1:1:165:SER:C	1:1:167:THR:N	2.74	0.41
2:2:43:THR:C	2:2:45:GLN:H	2.22	0.41
1:1:103:LEU:CD2	5:1:288:SUC:H61	2.50	0.41
3:3:122:THR:HB	3:3:125:THR:OG1	2.19	0.41
1:1:90:ASN:C	1:1:91:GLY:O	2.57	0.41
3:3:87:VAL:CG2	3:3:189:ILE:HG22	2.46	0.41
2:2:83:PRO:CG	2:2:218:ASN:HA	2.31	0.41
2:2:171:SER:O	2:2:174:ASN:N	2.38	0.41
1:1:38:GLU:C	1:1:40:GLY:N	2.73	0.41
3:3:14:MET:C	3:3:16:THR:N	2.74	0.41
3:3:141:PRO:CG	3:3:147:ALA:HB2	2.51	0.41
1:1:101:ILE:C	5:1:288:SUC:O6'	2.58	0.41
1:1:145:TYR:O	1:1:170:SER:HA	2.19	0.41
1:1:197:TYR:CE2	2:2:217:HIS:CE1	3.09	0.41
2:2:175:PHE:N	2:2:175:PHE:HD2	2.18	0.41
3:3:91:SER:C	3:3:92:THR:O	2.58	0.41
1:1:74:SER:HA	1:1:241:HIS:O	2.20	0.41
1:1:15:LEU:O	1:1:61:THR:HA	2.21	0.41
1:1:271:THR:O	1:1:272:GLY:C	2.58	0.41
3:3:216:CYS:C	3:3:218:ASP:H	2.22	0.41
1:1:11:LEU:HA	1:1:11:LEU:HD13	1.77	0.41
1:1:143:MET:HG3	1:1:223:ARG:O	2.20	0.41
3:3:83:PHE:CD1	3:3:191:CYS:HB3	2.55	0.41
1:1:70:PHE:O	1:1:112:LYS:HE2	2.20	0.41
1:1:22:GLU:CB	1:1:54:ARG:O	2.69	0.41
2:2:105:GLY:O	2:2:249:MET:N	2.49	0.41
1:1:9:GLU:OE1	4:4:42:ARG:HG3	2.21	0.41
2:2:58:THR:CG2	2:2:59:SER:N	2.83	0.41
1:1:81:ARG:HE	1:1:81:ARG:HB2	1.67	0.41
1:1:235:ILE:HG22	1:1:236:THR:N	2.36	0.41
1:1:92:GLN:N	1:1:94:ILE:HD11	2.35	0.41
3:3:65:VAL:C	3:3:67:MET:N	2.74	0.41
3:3:83:PHE:CD1	3:3:83:PHE:N	2.88	0.41
3:3:191:CYS:C	3:3:192:TRP:CD1	2.94	0.41
2:2:203:VAL:HG22	2:2:220:TRP:CZ2	2.55	0.41
2:2:126:MET:O	2:2:186:PHE:HB3	2.21	0.41
2:2:203:VAL:HA	2:2:204:PRO:HD2	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:147:THR:C	2:2:149:PRO:HD3	2.41	0.41
1:1:110:ARG:NE	1:1:114:GLU:OE1	2.53	0.41
1:1:84:VAL:CG1	1:1:85:ASP:H	2.34	0.41
2:2:54:THR:HG22	2:2:253:PHE:HB2	2.03	0.41
3:3:88:ASP:OD2	3:3:186:ALA:N	2.39	0.40
2:2:192:ASN:HD21	3:3:120:CYS:HA	1.86	0.40
1:1:224:ILE:HG21	1:1:224:ILE:HD13	1.46	0.40
1:1:132:ALA:HB3	1:1:234:VAL:HG13	2.02	0.40
1:1:155:PRO:HG2	1:1:163:TRP:CZ2	2.56	0.40
3:3:53:ILE:HG13	3:3:212:PHE:HA	2.03	0.40
3:3:114:ARG:O	3:3:213:VAL:HA	2.22	0.40
2:2:72:ASN:HD22	2:2:72:ASN:HA	1.54	0.40
3:3:115:PHE:CE2	3:3:167:VAL:HG21	2.57	0.40
3:3:42:ASN:CG	3:3:44:ILE:HG22	2.38	0.40
1:1:77:VAL:HG22	1:1:239:ILE:O	2.21	0.40
2:2:109:HIS:CE1	2:2:198:SER:HB3	2.56	0.40
1:1:7:ILE:C	1:1:11:LEU:HD23	2.42	0.40
1:1:131:ILE:HD13	1:1:141:ILE:HG23	2.02	0.40
3:3:53:ILE:HD11	3:3:213:VAL:HB	2.04	0.40
2:2:61:ASN:HD22	2:2:250:CYS:N	2.19	0.40
3:3:61:ASN:HD22	3:3:61:ASN:HA	1.60	0.40
3:3:155:TRP:HB2	3:3:163:ILE:HG21	2.04	0.40
1:1:260:THR:O	1:1:261:HIS:HB2	2.22	0.40
2:2:58:THR:HG22	2:2:59:SER:N	2.36	0.40
2:2:259:LYS:HG2	2:2:260:ASN:O	2.21	0.40

All (3023) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:58:VAL:N	4:4:26:TYR:CB[12_555]	0.10	2.10
2:2:187:PRO:CB	3:3:33:GLU:CG[12_555]	0.16	2.04
2:2:91:ILE:CD1	2:2:95:ASN:CA[2_555]	0.18	2.02
2:2:187:PRO:CD	3:3:33:GLU:OE2[12_555]	0.22	1.98
1:1:48:GLU:CD	1:1:78:HIS:CG[12_555]	0.24	1.96
1:1:53:THR:CG2	1:1:80:SER:CA[12_555]	0.24	1.96
1:1:69:SER:C	3:3:102:ILE:CB[12_555]	0.25	1.95
1:1:27:THR:CB	1:1:223:ARG:NE[12_555]	0.28	1.92
2:2:46:ASP:N	2:2:106:TYR:O[12_555]	0.30	1.90
1:1:69:SER:CB	3:3:102:ILE:N[12_555]	0.31	1.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:120:CYS:N	4:4:33:LYS:CB[12_555]	0.34	1.86
3:3:107:THR:OG1	3:3:107:THR:OG1[12_555]	0.35	1.85
1:1:41:HIS:C	1:1:186:PHE:CA[12_555]	0.35	1.85
3:3:209:MET:SD	4:4:32:PHE:CE1[12_555]	0.35	1.85
3:3:209:MET:CE	4:4:32:PHE:CZ[12_555]	0.35	1.85
1:1:6:TYR:OH	3:3:62:VAL:CG1[12_555]	0.36	1.84
3:3:17:ASP:C	3:3:94:LEU:CG[12_555]	0.37	1.83
2:2:43:THR:CG2	2:2:105:GLY:CA[12_555]	0.38	1.82
2:2:17:THR:OG1	2:2:49:ALA:N[2_555]	0.38	1.82
2:2:90:GLY:C	2:2:98:TYR:CB[2_555]	0.39	1.81
1:1:113:PHE:N	3:3:44:ILE:CG2[12_555]	0.40	1.80
3:3:212:PHE:CE1	4:4:37:SER:N[12_555]	0.41	1.79
1:1:244:LYS:NZ	3:3:212:PHE:CA[12_555]	0.42	1.78
1:1:242:LYS:C	3:3:214:SER:C[12_555]	0.44	1.76
3:3:24:ALA:CA	3:3:162:THR:O[12_555]	0.44	1.76
1:1:17:VAL:N	1:1:107:ALA:CA[12_555]	0.44	1.76
1:1:68:GLU:C	3:3:98:LEU:O[12_555]	0.45	1.75
3:3:222:ARG:CB	3:3:226:ASP:C[12_555]	0.45	1.75
1:1:177:GLN:CG	3:3:148:MET:CB[12_555]	0.47	1.73
1:1:182:PHE:CD2	3:3:164:SER:O[12_555]	0.48	1.72
2:2:17:THR:CG2	2:2:48:THR:O[2_555]	0.48	1.72
3:3:15:THR:CG2	3:3:109:TRP:CZ2[12_555]	0.48	1.72
3:3:67:MET:CG	4:4:27:PHE:CG[12_555]	0.48	1.72
3:3:15:THR:OG1	3:3:109:TRP:CZ3[12_555]	0.49	1.71
2:2:42:LEU:O	2:2:249:MET:C[12_555]	0.50	1.70
2:2:58:THR:C	2:2:253:PHE:O[2_555]	0.50	1.70
1:1:191:SER:CB	2:2:33:VAL:O[12_555]	0.51	1.69
2:2:40:HIS:CA	2:2:103:ARG:CD[12_555]	0.52	1.68
1:1:65:MET:N	3:3:105:TYR:CE1[12_555]	0.53	1.67
1:1:5:ASN:ND2	2:2:173:LEU:CD1[12_555]	0.53	1.67
3:3:26:PRO:CA	3:3:161:SER:CB[12_555]	0.54	1.66
3:3:53:ILE:N	4:4:39:GLY:N[12_555]	0.55	1.65
2:2:46:ASP:OD1	2:2:203:VAL:O[12_555]	0.55	1.65
1:1:180:PRO:C	3:3:165:LEU:CD1[12_555]	0.56	1.64
1:1:61:THR:CG2	3:3:230:HIS:CG[12_555]	0.56	1.64
1:1:42:THR:OG1	1:1:121:PHE:O[12_555]	0.57	1.63
1:1:40:GLY:N	3:3:30:PRO:CG[12_555]	0.57	1.63
1:1:240:TYR:CE2	3:3:111:GLY:C[12_555]	0.57	1.63
1:1:64:GLU:CD	3:3:104:SER:O[12_555]	0.57	1.63
2:2:89:MET:N	2:2:258:ALA:C[2_555]	0.57	1.63
1:1:35:ASP:CA	3:3:25:LEU:CG[12_555]	0.57	1.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:76:CYS:CA	3:3:218:ASP:CG[12_555]	0.57	1.63
2:2:41:TYR:CZ	2:2:55:GLN:OE1[12_555]	0.58	1.62
3:3:69:THR:CA	4:4:30:ASN:N[12_555]	0.59	1.61
2:2:44:PRO:CD	2:2:248:PRO:C[12_555]	0.59	1.61
2:2:36:GLY:C	2:2:208:ALA:CA[12_555]	0.59	1.61
1:1:72:GLY:O	3:3:99:ILE:CG2[12_555]	0.59	1.61
1:1:49:ASP:OD1	1:1:220:ILE:CG2[12_555]	0.59	1.61
2:2:54:THR:OG1	2:2:56:PRO:CA[3_555]	0.59	1.61
1:1:182:PHE:CG	3:3:164:SER:C[12_555]	0.60	1.60
1:1:7:ILE:CB	1:1:275:THR:CB[12_555]	0.61	1.59
2:2:47:ALA:CA	2:2:249:MET:CE[12_555]	0.61	1.59
3:3:23:CYS:N	3:3:117:PHE:O[12_555]	0.62	1.58
1:1:29:ASN:N	1:1:162:SER:O[12_555]	0.62	1.58
2:2:45:GLN:CA	2:2:107:THR:N[12_555]	0.62	1.58
3:3:67:MET:CA	4:4:28:ASN:N[12_555]	0.62	1.58
3:3:58:VAL:CB	4:4:26:TYR:CD1[12_555]	0.63	1.57
1:1:250:CYS:CB	3:3:39:GLU:CB[12_555]	0.63	1.57
3:3:15:THR:CB	3:3:109:TRP:CH2[12_555]	0.63	1.57
1:1:115:LEU:O	3:3:41:LYS:CA[12_555]	0.64	1.56
2:2:62:ARG:CB	2:2:254:SER:C[2_555]	0.64	1.56
1:1:32:PRO:CA	1:1:147:TYR:CB[12_555]	0.64	1.56
3:3:70:VAL:CG2	4:4:31:TYR:CD2[12_555]	0.65	1.55
2:2:35:TYR:CB	3:3:36:ILE:CD1[12_555]	0.65	1.55
1:1:9:GLU:C	1:1:277:ALA:N[12_555]	0.65	1.55
1:1:124:GLU:O	3:3:114:ARG:CB[12_555]	0.65	1.55
1:1:41:HIS:O	1:1:186:PHE:N[12_555]	0.65	1.55
2:2:40:HIS:CB	2:2:103:ARG:CG[12_555]	0.65	1.55
2:2:44:PRO:CG	2:2:248:PRO:N[12_555]	0.65	1.55
2:2:58:THR:O	2:2:254:SER:N[2_555]	0.65	1.55
2:2:21:SER:N	2:2:101:LEU:CD1[2_555]	0.66	1.54
2:2:52:LYS:NZ	2:2:252:GLU:CG[10_555]	0.66	1.54
1:1:10:VAL:N	1:1:277:ALA:N[12_555]	0.67	1.53
1:1:35:ASP:C	3:3:25:LEU:CB[12_555]	0.67	1.53
1:1:73:ARG:CZ	3:3:103:ALA:CA[12_555]	0.68	1.52
3:3:209:MET:CA	4:4:32:PHE:CA[12_555]	0.68	1.52
1:1:63:ASP:CA	1:1:111:ARG:CZ[12_555]	0.69	1.51
2:2:88:ASP:O	2:2:259:LYS:CB[2_555]	0.69	1.51
3:3:16:THR:C	3:3:89:ILE:CA[12_555]	0.69	1.51
1:1:39:THR:C	3:3:30:PRO:CB[12_555]	0.69	1.51
3:3:120:CYS:SG	4:4:33:LYS:C[12_555]	0.69	1.51
1:1:244:LYS:O	3:3:50:ASP:C[12_555]	0.70	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:70:VAL:CB	4:4:31:TYR:CB[12_555]	0.70	1.50
1:1:249:TRP:CE2	2:2:35:TYR:CE1[12_555]	0.70	1.50
2:2:17:THR:C	2:2:49:ALA:C[2_555]	0.70	1.50
2:2:37:VAL:CA	2:2:207:ASN:O[12_555]	0.70	1.50
1:1:32:PRO:CD	1:1:147:TYR:N[12_555]	0.71	1.49
2:2:12:ARG:N	2:2:13:ILE:CD1[11_555]	0.71	1.49
2:2:89:MET:N	2:2:258:ALA:O[2_555]	0.71	1.49
2:2:46:ASP:O	2:2:202:ILE:CG2[12_555]	0.71	1.49
3:3:68:TYR:C	4:4:30:ASN:ND2[12_555]	0.71	1.49
3:3:118:MET:CG	4:4:34:ASP:CB[12_555]	0.72	1.48
1:1:183:SER:CA	3:3:116:SER:CB[12_555]	0.72	1.48
2:2:17:THR:O	2:2:50:ILE:N[2_555]	0.72	1.48
3:3:9:GLY:CA	3:3:188:TYR:CZ[12_555]	0.72	1.48
2:2:32:VAL:CG2	3:3:31:THR:O[12_555]	0.73	1.47
1:1:122:ASP:CA	3:3:50:ASP:OD1[12_555]	0.73	1.47
1:1:17:VAL:CG1	1:1:108:GLN:N[12_555]	0.73	1.47
3:3:69:THR:O	4:4:29:ILE:O[12_555]	0.74	1.46
3:3:223:MET:CA	3:3:225:ARG:NE[12_555]	0.74	1.46
1:1:249:TRP:CZ2	2:2:35:TYR:CE1[12_555]	0.74	1.46
2:2:43:THR:CB	2:2:105:GLY:O[12_555]	0.75	1.45
2:2:62:ARG:NH2	2:2:101:LEU:C[2_555]	0.75	1.45
2:2:59:SER:CA	2:2:253:PHE:CB[2_555]	0.75	1.45
1:1:64:GLU:O	3:3:105:TYR:CD1[12_555]	0.76	1.44
2:2:42:LEU:C	2:2:249:MET:O[12_555]	0.76	1.44
1:1:68:GLU:CG	3:3:98:LEU:CA[12_555]	0.76	1.44
2:2:54:THR:N	2:2:57:ASP:C[3_555]	0.76	1.44
1:1:181:ARG:N	3:3:165:LEU:CG[12_555]	0.76	1.44
2:2:38:TRP:CH2	2:2:48:THR:CG2[12_555]	0.77	1.43
3:3:10:SER:CB	3:3:140:GLU:CG[12_555]	0.77	1.43
3:3:26:PRO:CG	3:3:161:SER:N[12_555]	0.77	1.43
1:1:63:ASP:CG	1:1:111:ARG:NH1[12_555]	0.77	1.43
1:1:62:ARG:CZ	1:1:109:ILE:C[12_555]	0.77	1.43
1:1:247:LYS:CD	2:2:185:ILE:O[12_555]	0.77	1.43
1:1:65:MET:SD	1:1:112:LYS:CD[12_555]	0.78	1.42
1:1:252:ARG:CG	3:3:41:LYS:CG[12_555]	0.78	1.42
1:1:18:PRO:CB	1:1:105:GLU:C[12_555]	0.78	1.42
1:1:14:VAL:CG2	1:1:256:ALA:C[12_555]	0.78	1.42
1:1:125:ILE:O	3:3:165:LEU:O[12_555]	0.78	1.42
1:1:250:CYS:N	3:3:39:GLU:CA[12_555]	0.79	1.41
1:1:70:PHE:CD2	3:3:43:LEU:CB[12_555]	0.79	1.41
3:3:16:THR:CA	3:3:89:ILE:CB[12_555]	0.79	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:15:GLN:O	2:2:15:GLN:O[11_555]	0.80	1.40
1:1:27:THR:C	1:1:163:TRP:CG[12_555]	0.80	1.40
1:1:73:ARG:N	3:3:99:ILE:CD1[12_555]	0.80	1.40
1:1:246:THR:C	2:2:185:ILE:CD1[12_555]	0.80	1.40
3:3:66:SER:O	4:4:29:ILE:N[12_555]	0.80	1.40
3:3:105:TYR:O	3:3:106:TYR:CD2[12_555]	0.81	1.39
2:2:43:THR:CB	2:2:105:GLY:C[12_555]	0.81	1.39
3:3:67:MET:CA	4:4:27:PHE:C[12_555]	0.81	1.39
1:1:17:VAL:CG1	1:1:107:ALA:C[12_555]	0.82	1.38
1:1:71:LEU:CA	3:3:47:CYS:SG[12_555]	0.82	1.38
1:1:181:ARG:C	3:3:165:LEU:CB[12_555]	0.82	1.38
1:1:252:ARG:CG	3:3:41:LYS:CD[12_555]	0.82	1.38
3:3:22:PRO:N	3:3:117:PHE:CG[12_555]	0.83	1.37
3:3:52:LEU:CD2	4:4:38:SER:CB[12_555]	0.83	1.37
3:3:21:SER:C	3:3:117:PHE:CG[12_555]	0.83	1.37
2:2:62:ARG:CA	2:2:255:GLY:N[2_555]	0.83	1.37
2:2:58:THR:C	2:2:253:PHE:C[2_555]	0.83	1.37
2:2:44:PRO:CG	2:2:247:SER:C[12_555]	0.83	1.37
1:1:51:ILE:CB	1:1:237:THR:OG1[12_555]	0.83	1.37
3:3:10:SER:CA	3:3:140:GLU:CB[12_555]	0.84	1.36
1:1:47:PRO:N	1:1:239:ILE:CB[12_555]	0.84	1.36
1:1:176:GLY:N	3:3:149:LEU:C[12_555]	0.84	1.36
3:3:36:ILE:CG2	3:3:37:PRO:C[12_555]	0.84	1.36
1:1:39:THR:OG1	3:3:28:TYR:CE2[12_555]	0.84	1.36
1:1:247:LYS:CE	2:2:186:PHE:CA[12_555]	0.84	1.36
1:1:64:GLU:OE2	3:3:104:SER:O[12_555]	0.84	1.36
1:1:70:PHE:N	3:3:102:ILE:CG1[12_555]	0.85	1.35
1:1:14:VAL:CG2	1:1:256:ALA:CA[12_555]	0.85	1.35
1:1:115:LEU:C	3:3:41:LYS:C[12_555]	0.85	1.35
1:1:240:TYR:CE2	3:3:111:GLY:O[12_555]	0.85	1.35
1:1:32:PRO:N	1:1:147:TYR:CA[12_555]	0.86	1.34
3:3:26:PRO:CD	3:3:161:SER:N[12_555]	0.86	1.34
1:1:176:GLY:CA	3:3:149:LEU:CA[12_555]	0.86	1.34
3:3:17:ASP:CA	3:3:94:LEU:CD1[12_555]	0.86	1.34
1:1:246:THR:O	2:2:185:ILE:CG1[12_555]	0.86	1.34
3:3:223:MET:CA	3:3:225:ARG:CD[12_555]	0.86	1.34
3:3:66:SER:O	4:4:28:ASN:C[12_555]	0.86	1.34
3:3:70:VAL:CB	4:4:31:TYR:CG[12_555]	0.86	1.34
3:3:24:ALA:CA	3:3:162:THR:C[12_555]	0.86	1.34
1:1:49:ASP:CG	1:1:220:ILE:CG2[12_555]	0.87	1.33
1:1:47:PRO:CA	1:1:239:ILE:CG1[12_555]	0.87	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:128:VAL:CA	3:3:168:PRO:CG[12_555]	0.87	1.33
1:1:240:TYR:CG	3:3:112:SER:CA[12_555]	0.88	1.32
1:1:50:ALA:C	1:1:145:TYR:CD1[12_555]	0.88	1.32
1:1:51:ILE:CD1	1:1:237:THR:CA[12_555]	0.88	1.32
1:1:181:ARG:CA	3:3:165:LEU:CG[12_555]	0.88	1.32
2:2:89:MET:CG	2:2:258:ALA:N[2_555]	0.88	1.32
1:1:191:SER:CB	2:2:33:VAL:C[12_555]	0.88	1.32
3:3:24:ALA:N	3:3:162:THR:C[12_555]	0.88	1.32
3:3:66:SER:C	4:4:28:ASN:C[12_555]	0.88	1.32
2:2:179:LEU:CA	4:4:42:ARG:CG[12_555]	0.88	1.32
1:1:38:GLU:CB	3:3:28:TYR:O[12_555]	0.88	1.32
2:2:12:ARG:CA	2:2:13:ILE:CD1[11_555]	0.88	1.32
1:1:51:ILE:CG1	1:1:237:THR:OG1[12_555]	0.89	1.31
1:1:176:GLY:N	3:3:149:LEU:O[12_555]	0.89	1.31
1:1:20:ILE:CG2	1:1:79:ILE:N[12_555]	0.89	1.31
2:2:21:SER:CA	2:2:101:LEU:CD1[2_555]	0.89	1.31
3:3:65:VAL:C	4:4:28:ASN:CB[12_555]	0.89	1.31
2:2:62:ARG:CB	2:2:255:GLY:N[2_555]	0.90	1.30
2:2:11:ASP:N	2:2:26:ASP:CG[11_555]	0.90	1.30
2:2:57:ASP:OD2	2:2:57:ASP:OD2[11_555]	0.90	1.30
1:1:241:HIS:CG	3:3:215:ALA:O[12_555]	0.90	1.30
1:1:7:ILE:CG1	1:1:275:THR:OG1[12_555]	0.90	1.30
1:1:177:GLN:N	3:3:149:LEU:N[12_555]	0.90	1.30
1:1:181:ARG:NH1	3:3:115:PHE:CZ[12_555]	0.90	1.30
2:2:36:GLY:CA	2:2:208:ALA:CB[12_555]	0.90	1.30
2:2:58:THR:O	2:2:253:PHE:C[2_555]	0.90	1.30
1:1:244:LYS:CE	3:3:212:PHE:CB[12_555]	0.90	1.30
3:3:9:GLY:CA	3:3:188:TYR:OH[12_555]	0.90	1.30
2:2:64:TYR:CD1	2:2:256:ALA:C[2_555]	0.91	1.29
3:3:14:MET:N	3:3:87:VAL:CB[12_555]	0.91	1.29
1:1:17:VAL:C	1:1:107:ALA:N[12_555]	0.91	1.29
1:1:250:CYS:CA	3:3:39:GLU:CB[12_555]	0.91	1.29
1:1:64:GLU:C	3:3:105:TYR:CE1[12_555]	0.91	1.29
1:1:76:CYS:O	3:3:218:ASP:CA[12_555]	0.91	1.29
1:1:179:PHE:CB	3:3:133:TYR:CB[12_555]	0.92	1.28
1:1:53:THR:C	1:1:80:SER:O[12_555]	0.92	1.28
3:3:67:MET:SD	4:4:27:PHE:CD2[12_555]	0.92	1.28
1:1:181:ARG:CA	3:3:165:LEU:CB[12_555]	0.92	1.28
3:3:106:TYR:N	3:3:224:ALA:CA[12_555]	0.93	1.27
2:2:54:THR:CA	2:2:57:ASP:N[3_555]	0.93	1.27
2:2:38:TRP:N	2:2:209:VAL:O[12_555]	0.93	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:179:LEU:C	4:4:42:ARG:CB[12_555]	0.93	1.27
3:3:9:GLY:C	3:3:188:TYR:CE1[12_555]	0.93	1.27
1:1:124:GLU:CB	3:3:114:ARG:O[12_555]	0.93	1.27
1:1:74:SER:CB	3:3:113:LEU:CG[12_555]	0.93	1.27
3:3:23:CYS:CA	3:3:117:PHE:O[12_555]	0.93	1.27
1:1:52:GLU:N	1:1:237:THR:CG2[12_555]	0.93	1.27
2:2:17:THR:CB	2:2:48:THR:C[2_555]	0.93	1.27
1:1:18:PRO:O	1:1:106:MET:CG[12_555]	0.94	1.26
1:1:124:GLU:CG	3:3:114:ARG:O[12_555]	0.94	1.26
3:3:10:SER:CB	3:3:140:GLU:CB[12_555]	0.94	1.26
1:1:116:PHE:CG	3:3:40:VAL:CG1[12_555]	0.94	1.26
3:3:209:MET:C	4:4:32:PHE:N[12_555]	0.94	1.26
2:2:64:TYR:CE1	2:2:256:ALA:C[2_555]	0.94	1.26
1:1:21:LYS:O	1:1:79:ILE:O[12_555]	0.95	1.25
2:2:43:THR:CA	2:2:105:GLY:O[12_555]	0.95	1.25
2:2:17:THR:O	2:2:49:ALA:C[2_555]	0.95	1.25
3:3:222:ARG:CB	3:3:226:ASP:O[12_555]	0.95	1.25
1:1:41:HIS:CB	1:1:186:PHE:C[12_555]	0.95	1.25
1:1:10:VAL:N	1:1:276:THR:C[12_555]	0.95	1.25
1:1:252:ARG:CD	3:3:41:LYS:CE[12_555]	0.95	1.25
1:1:73:ARG:NE	3:3:103:ALA:CB[12_555]	0.95	1.25
3:3:14:MET:SD	3:3:88:ASP:CB[12_555]	0.96	1.24
1:1:55:TYR:CA	1:1:81:ARG:NH2[12_555]	0.96	1.24
3:3:21:SER:CA	3:3:117:PHE:CD2[12_555]	0.96	1.24
1:1:246:THR:O	2:2:185:ILE:CD1[12_555]	0.97	1.23
3:3:12:GLN:CA	3:3:188:TYR:N[12_555]	0.97	1.23
3:3:68:TYR:O	4:4:30:ASN:ND2[12_555]	0.97	1.23
1:1:251:PRO:CA	3:3:40:VAL:O[12_555]	0.97	1.23
3:3:24:ALA:N	3:3:163:ILE:N[12_555]	0.97	1.23
1:1:122:ASP:CB	3:3:50:ASP:OD1[12_555]	0.98	1.22
2:2:187:PRO:CA	3:3:33:GLU:OE1[12_555]	0.98	1.22
1:1:249:TRP:O	3:3:39:GLU:O[12_555]	0.98	1.22
1:1:116:PHE:CD2	3:3:40:VAL:CG1[12_555]	0.98	1.22
2:2:38:TRP:CZ2	2:2:48:THR:CG2[12_555]	0.98	1.22
3:3:106:TYR:CA	3:3:224:ALA:CA[12_555]	0.98	1.22
1:1:9:GLU:CB	1:1:276:THR:OG1[12_555]	0.98	1.22
1:1:64:GLU:C	3:3:105:TYR:CD1[12_555]	0.98	1.22
1:1:19:ASN:N	1:1:105:GLU:O[12_555]	0.98	1.22
3:3:14:MET:CG	3:3:88:ASP:CA[12_555]	0.98	1.22
3:3:69:THR:N	4:4:30:ASN:N[12_555]	0.98	1.22
2:2:47:ALA:O	2:2:202:ILE:CD1[12_555]	0.98	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:23:SER:OG	1:1:80:SER:OG[12_555]	0.98	1.22
2:2:45:GLN:C	2:2:107:THR:N[12_555]	0.98	1.22
1:1:76:CYS:C	3:3:218:ASP:CG[12_555]	0.98	1.22
2:2:32:VAL:CG1	3:3:32:LYS:O[12_555]	0.98	1.22
2:2:179:LEU:CA	4:4:42:ARG:CB[12_555]	0.98	1.22
1:1:72:GLY:CA	3:3:99:ILE:CG1[12_555]	0.99	1.21
2:2:179:LEU:CB	4:4:42:ARG:CG[12_555]	0.99	1.21
3:3:69:THR:O	4:4:29:ILE:C[12_555]	0.99	1.21
3:3:9:GLY:O	3:3:188:TYR:CD1[12_555]	0.99	1.21
1:1:247:LYS:CD	2:2:185:ILE:C[12_555]	0.99	1.21
3:3:58:VAL:CB	4:4:26:TYR:CG[12_555]	0.99	1.21
3:3:19:MET:SD	3:3:85:ILE:CG1[12_555]	0.99	1.21
3:3:56:ASN:CB	4:4:29:ILE:CG1[12_555]	0.99	1.21
3:3:52:LEU:C	4:4:39:GLY:O[12_555]	1.00	1.20
3:3:53:ILE:N	4:4:39:GLY:CA[12_555]	1.00	1.20
1:1:48:GLU:CG	1:1:78:HIS:CD2[12_555]	1.00	1.20
3:3:16:THR:CB	3:3:89:ILE:CG1[12_555]	1.00	1.20
1:1:16:VAL:N	1:1:259:TYR:CE1[12_555]	1.01	1.19
2:2:195:SER:CB	3:3:27:TRP:CB[12_555]	1.01	1.19
2:2:42:LEU:O	2:2:249:MET:O[12_555]	1.01	1.19
2:2:58:THR:CA	2:2:253:PHE:O[12_555]	1.01	1.19
1:1:64:GLU:CD	3:3:104:SER:C[12_555]	1.01	1.19
3:3:17:ASP:O	3:3:94:LEU:CD2[12_555]	1.01	1.19
1:1:182:PHE:CG	3:3:164:SER:O[12_555]	1.01	1.19
3:3:209:MET:O	4:4:32:PHE:N[12_555]	1.01	1.19
3:3:106:TYR:C	3:3:224:ALA:C[12_555]	1.01	1.19
1:1:183:SER:CB	3:3:116:SER:CB[12_555]	1.01	1.19
2:2:46:ASP:N	2:2:106:TYR:C[12_555]	1.01	1.19
1:1:47:PRO:CA	1:1:239:ILE:CB[12_555]	1.02	1.18
1:1:242:LYS:O	3:3:214:SER:CA[12_555]	1.02	1.18
1:1:115:LEU:C	3:3:41:LYS:CA[12_555]	1.02	1.18
1:1:249:TRP:O	3:3:39:GLU:C[12_555]	1.02	1.18
2:2:40:HIS:NE2	2:2:205:TYR:CB[12_555]	1.02	1.18
3:3:52:LEU:O	4:4:39:GLY:C[12_555]	1.02	1.18
3:3:23:CYS:N	3:3:117:PHE:C[12_555]	1.02	1.18
1:1:62:ARG:NH1	1:1:110:ARG:N[12_555]	1.02	1.18
2:2:41:TYR:OH	2:2:55:GLN:OE1[12_555]	1.02	1.18
1:1:63:ASP:CB	1:1:111:ARG:NH1[12_555]	1.02	1.18
2:2:45:GLN:OE1	2:2:106:TYR:CG[12_555]	1.02	1.18
2:2:187:PRO:CA	3:3:33:GLU:CD[12_555]	1.03	1.17
3:3:15:THR:CB	3:3:109:TRP:CZ3[12_555]	1.03	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:187:PRO:N	3:3:33:GLU:CD[12_555]	1.03	1.17
1:1:124:GLU:C	3:3:114:ARG:CB[12_555]	1.03	1.17
3:3:53:ILE:CA	4:4:39:GLY:CA[12_555]	1.03	1.17
1:1:53:THR:CA	1:1:80:SER:O[12_555]	1.03	1.17
1:1:245:HIS:NE2	3:3:52:LEU:N[12_555]	1.03	1.17
1:1:191:SER:OG	2:2:33:VAL:C[12_555]	1.03	1.17
1:1:126:THR:C	3:3:166:VAL:C[12_555]	1.04	1.16
1:1:17:VAL:C	1:1:106:MET:C[12_555]	1.04	1.16
3:3:23:CYS:O	3:3:162:THR:CA[12_555]	1.04	1.16
1:1:28:SER:N	1:1:163:TRP:CD2[12_555]	1.04	1.16
2:2:37:VAL:CG2	2:2:207:ASN:N[12_555]	1.04	1.16
3:3:52:LEU:CD2	4:4:38:SER:OG[12_555]	1.04	1.16
2:2:32:VAL:CG2	3:3:31:THR:C[12_555]	1.04	1.16
3:3:14:MET:CB	3:3:88:ASP:N[12_555]	1.04	1.16
3:3:58:VAL:CG2	4:4:26:TYR:CD1[12_555]	1.04	1.16
1:1:244:LYS:C	3:3:51:THR:N[12_555]	1.05	1.15
1:1:30:SER:N	1:1:146:MET:CE[12_555]	1.05	1.15
1:1:18:PRO:CA	1:1:105:GLU:C[12_555]	1.05	1.15
1:1:247:LYS:CE	2:2:186:PHE:N[12_555]	1.05	1.15
3:3:22:PRO:N	3:3:117:PHE:CB[12_555]	1.05	1.15
1:1:112:LYS:C	3:3:42:ASN:ND2[12_555]	1.05	1.15
3:3:14:MET:CB	3:3:87:VAL:C[12_555]	1.05	1.15
1:1:248:ALA:O	1:1:251:PRO:CD[12_555]	1.05	1.15
2:2:38:TRP:CD2	2:2:210:PRO:CG[12_555]	1.05	1.15
1:1:70:PHE:CD2	3:3:43:LEU:CG[12_555]	1.05	1.15
1:1:48:GLU:OE1	1:1:78:HIS:CG[12_555]	1.05	1.15
1:1:70:PHE:CE2	3:3:43:LEU:CB[12_555]	1.06	1.14
1:1:177:GLN:N	3:3:148:MET:C[12_555]	1.06	1.14
1:1:42:THR:OG1	1:1:121:PHE:C[12_555]	1.06	1.14
1:1:55:TYR:N	1:1:81:ARG:NH2[12_555]	1.06	1.14
1:1:191:SER:OG	2:2:33:VAL:CA[12_555]	1.06	1.14
3:3:38:GLY:O	3:3:38:GLY:O[12_555]	1.06	1.14
2:2:53:PRO:C	2:2:57:ASP:C[3_555]	1.06	1.14
1:1:18:PRO:CB	1:1:105:GLU:CA[12_555]	1.06	1.14
2:2:89:MET:CB	2:2:257:ARG:C[2_555]	1.06	1.14
2:2:182:ASN:N	4:4:41:SER:CB[12_555]	1.06	1.14
2:2:11:ASP:CG	2:2:26:ASP:O[11_555]	1.07	1.13
1:1:121:PHE:CD1	3:3:48:GLN:O[12_555]	1.07	1.13
3:3:119:PHE:C	4:4:33:LYS:CB[12_555]	1.07	1.13
1:1:68:GLU:CG	3:3:98:LEU:CB[12_555]	1.07	1.13
3:3:209:MET:CG	4:4:32:PHE:CG[12_555]	1.07	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:52:LYS:NZ	2:2:252:GLU:CD[10_555]	1.07	1.13
3:3:52:LEU:C	4:4:39:GLY:C[12_555]	1.07	1.13
1:1:27:THR:OG1	1:1:223:ARG:CD[12_555]	1.07	1.13
1:1:32:PRO:CD	1:1:147:TYR:CA[12_555]	1.07	1.13
1:1:178:PRO:C	3:3:151:THR:O[12_555]	1.07	1.13
3:3:18:ASP:N	3:3:94:LEU:CG[12_555]	1.07	1.13
1:1:68:GLU:O	3:3:98:LEU:O[12_555]	1.08	1.12
2:2:38:TRP:CH2	2:2:48:THR:CB[12_555]	1.08	1.12
1:1:62:ARG:CZ	1:1:110:ARG:N[12_555]	1.08	1.12
3:3:20:GLN:CB	3:3:211:CYS:SG[12_555]	1.08	1.12
3:3:67:MET:SD	4:4:27:PHE:CE2[12_555]	1.08	1.12
3:3:56:ASN:CG	4:4:29:ILE:CD1[12_555]	1.09	1.11
3:3:21:SER:O	3:3:117:PHE:CA[12_555]	1.09	1.11
1:1:27:THR:O	1:1:163:TRP:CG[12_555]	1.09	1.11
1:1:116:PHE:CD2	3:3:40:VAL:CB[12_555]	1.09	1.11
2:2:36:GLY:C	2:2:208:ALA:C[12_555]	1.09	1.11
1:1:64:GLU:OE1	3:3:104:SER:CA[12_555]	1.09	1.11
1:1:115:LEU:CA	3:3:41:LYS:C[12_555]	1.09	1.11
2:2:62:ARG:C	2:2:255:GLY:CA[2_555]	1.09	1.11
1:1:39:THR:O	3:3:30:PRO:CB[12_555]	1.09	1.11
1:1:65:MET:CE	1:1:112:LYS:CG[12_555]	1.09	1.11
3:3:15:THR:CG2	3:3:109:TRP:CE2[12_555]	1.09	1.11
3:3:9:GLY:O	3:3:188:TYR:CG[12_555]	1.09	1.11
3:3:52:LEU:CG	4:4:38:SER:OG[12_555]	1.09	1.11
2:2:45:GLN:OE1	2:2:106:TYR:CD2[12_555]	1.09	1.11
3:3:36:ILE:CG2	3:3:37:PRO:O[12_555]	1.10	1.10
1:1:62:ARG:NE	1:1:109:ILE:C[12_555]	1.10	1.10
1:1:73:ARG:CZ	3:3:103:ALA:CB[12_555]	1.10	1.10
1:1:252:ARG:CD	3:3:41:LYS:CD[12_555]	1.10	1.10
3:3:12:GLN:C	3:3:188:TYR:N[12_555]	1.10	1.10
2:2:202:ILE:N	3:3:32:LYS:CD[12_555]	1.10	1.10
2:2:178:THR:CA	4:4:44:ASP:N[12_555]	1.10	1.10
1:1:71:LEU:CG	3:3:43:LEU:O[12_555]	1.10	1.10
1:1:70:PHE:N	3:3:102:ILE:CB[12_555]	1.10	1.10
1:1:62:ARG:CA	1:1:111:ARG:CG[12_555]	1.10	1.10
1:1:42:THR:CG2	1:1:123:SER:OG[12_555]	1.10	1.10
1:1:18:PRO:C	1:1:105:GLU:O[12_555]	1.10	1.10
1:1:7:ILE:CB	1:1:275:THR:OG1[12_555]	1.10	1.10
2:2:88:ASP:O	2:2:259:LYS:CA[2_555]	1.10	1.10
3:3:69:THR:CA	4:4:30:ASN:CA[12_555]	1.11	1.09
1:1:74:SER:CB	3:3:113:LEU:CD2[12_555]	1.11	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:35:ASP:O	3:3:25:LEU:CB[12_555]	1.11	1.09
3:3:9:GLY:C	3:3:188:TYR:CZ[12_555]	1.11	1.09
2:2:204:PRO:CG	3:3:35:SER:O[12_555]	1.11	1.09
1:1:177:GLN:CB	3:3:148:MET:CA[12_555]	1.11	1.09
3:3:18:ASP:N	3:3:94:LEU:CB[12_555]	1.11	1.09
2:2:38:TRP:CA	2:2:210:PRO:CA[12_555]	1.11	1.09
2:2:178:THR:OG1	4:4:44:ASP:CG[12_555]	1.11	1.09
3:3:119:PHE:O	4:4:33:LYS:CD[12_555]	1.11	1.09
1:1:241:HIS:CD2	3:3:114:ARG:NH2[12_555]	1.12	1.08
2:2:11:ASP:CB	2:2:26:ASP:O[11_555]	1.12	1.08
1:1:6:TYR:C	1:1:276:THR:N[12_555]	1.12	1.08
3:3:16:THR:CA	3:3:89:ILE:CA[12_555]	1.12	1.08
2:2:62:ARG:CZ	2:2:101:LEU:O[2_555]	1.12	1.08
3:3:19:MET:SD	3:3:85:ILE:CB[12_555]	1.12	1.08
3:3:13:PHE:CB	3:3:133:TYR:CE1[12_555]	1.12	1.08
1:1:121:PHE:CB	3:3:49:VAL:CA[12_555]	1.12	1.08
1:1:115:LEU:CB	3:3:42:ASN:CA[12_555]	1.12	1.08
3:3:120:CYS:SG	4:4:33:LYS:O[12_555]	1.13	1.07
2:2:50:ILE:CG1	2:2:50:ILE:CG1[10_555]	1.13	1.07
1:1:128:VAL:N	3:3:168:PRO:CG[12_555]	1.13	1.07
1:1:47:PRO:CB	1:1:239:ILE:N[12_555]	1.13	1.07
2:2:36:GLY:CA	2:2:208:ALA:CA[12_555]	1.13	1.07
2:2:41:TYR:CB	2:2:250:CYS:O[12_555]	1.13	1.07
3:3:65:VAL:O	4:4:28:ASN:CB[12_555]	1.14	1.06
3:3:67:MET:CG	4:4:27:PHE:CB[12_555]	1.14	1.06
1:1:244:LYS:CD	3:3:213:VAL:N[12_555]	1.14	1.06
1:1:182:PHE:CD1	3:3:164:SER:CA[12_555]	1.14	1.06
3:3:15:THR:OG1	3:3:109:TRP:CE3[12_555]	1.14	1.06
2:2:189:GLN:NE2	3:3:30:PRO:O[12_555]	1.14	1.06
2:2:187:PRO:N	3:3:33:GLU:OE1[12_555]	1.14	1.06
3:3:223:MET:N	3:3:225:ARG:CD[12_555]	1.15	1.05
1:1:47:PRO:CD	1:1:239:ILE:CG2[12_555]	1.15	1.05
1:1:62:ARG:NE	1:1:109:ILE:CA[12_555]	1.15	1.05
1:1:69:SER:CB	3:3:101:GLU:C[12_555]	1.16	1.04
1:1:12:ASN:CB	3:3:229:LEU:O[12_555]	1.16	1.04
1:1:74:SER:OG	3:3:113:LEU:CB[12_555]	1.16	1.04
2:2:41:TYR:OH	2:2:55:GLN:CD[12_555]	1.16	1.04
1:1:8:ASP:N	1:1:275:THR:O[12_555]	1.16	1.04
2:2:45:GLN:O	2:2:107:THR:CA[12_555]	1.16	1.04
2:2:90:GLY:CA	2:2:98:TYR:CA[2_555]	1.16	1.04
2:2:64:TYR:CE1	2:2:257:ARG:N[2_555]	1.16	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:38:GLU:O	3:3:30:PRO:CD[12_555]	1.16	1.04
1:1:6:TYR:O	1:1:276:THR:CA[12_555]	1.16	1.04
1:1:27:THR:O	1:1:163:TRP:CB[12_555]	1.16	1.04
1:1:240:TYR:CD2	3:3:112:SER:N[12_555]	1.16	1.04
1:1:178:PRO:O	3:3:151:THR:O[12_555]	1.17	1.03
2:2:176:ASP:OD2	4:4:44:ASP:OD2[12_555]	1.17	1.03
2:2:62:ARG:NH1	2:2:101:LEU:O[2_555]	1.17	1.03
1:1:242:LYS:O	3:3:214:SER:C[12_555]	1.17	1.03
2:2:47:ALA:CB	2:2:249:MET:CE[12_555]	1.17	1.03
1:1:121:PHE:CB	3:3:49:VAL:CB[12_555]	1.17	1.03
1:1:38:GLU:C	3:3:30:PRO:CD[12_555]	1.17	1.03
1:1:47:PRO:N	1:1:239:ILE:CG2[12_555]	1.17	1.03
3:3:69:THR:C	4:4:29:ILE:C[12_555]	1.17	1.03
2:2:17:THR:CB	2:2:48:THR:O[2_555]	1.17	1.03
1:1:181:ARG:N	3:3:165:LEU:CD1[12_555]	1.17	1.03
3:3:22:PRO:CA	3:3:117:PHE:CB[12_555]	1.17	1.03
3:3:118:MET:SD	4:4:34:ASP:CB[12_555]	1.17	1.03
2:2:38:TRP:N	2:2:209:VAL:C[12_555]	1.17	1.03
3:3:14:MET:CE	3:3:88:ASP:CB[12_555]	1.18	1.02
1:1:124:GLU:O	3:3:114:ARG:CA[12_555]	1.18	1.02
3:3:118:MET:CE	4:4:35:ALA:N[12_555]	1.18	1.02
2:2:18:ARG:NH2	2:2:50:ILE:CG2[2_555]	1.18	1.02
2:2:182:ASN:CA	4:4:41:SER:CB[12_555]	1.18	1.02
1:1:173:TRP:NE1	3:3:151:THR:CA[12_555]	1.18	1.02
1:1:18:PRO:CA	1:1:106:MET:N[12_555]	1.18	1.02
1:1:50:ALA:C	1:1:145:TYR:CE1[12_555]	1.18	1.02
3:3:105:TYR:CB	3:3:106:TYR:CE2[12_555]	1.18	1.02
3:3:26:PRO:CB	3:3:161:SER:CB[12_555]	1.18	1.02
2:2:89:MET:O	2:2:98:TYR:CD1[2_555]	1.18	1.02
1:1:242:LYS:C	3:3:215:ALA:N[12_555]	1.18	1.02
1:1:39:THR:C	3:3:30:PRO:CA[12_555]	1.18	1.02
2:2:54:THR:OG1	2:2:56:PRO:CB[3_555]	1.18	1.02
1:1:65:MET:CE	1:1:112:LYS:CD[12_555]	1.19	1.01
1:1:9:GLU:CB	1:1:276:THR:CB[12_555]	1.19	1.01
3:3:209:MET:C	4:4:32:PHE:CA[12_555]	1.19	1.01
1:1:115:LEU:CA	3:3:41:LYS:O[12_555]	1.19	1.01
1:1:32:PRO:C	1:1:147:TYR:CB[12_555]	1.19	1.01
1:1:127:LEU:N	3:3:166:VAL:O[12_555]	1.19	1.01
2:2:53:PRO:C	2:2:58:THR:N[3_555]	1.19	1.01
2:2:53:PRO:CA	2:2:58:THR:N[3_555]	1.19	1.01
1:1:6:TYR:O	1:1:276:THR:N[12_555]	1.19	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:26:PRO:O	3:3:160:GLN:O[12_555]	1.19	1.01
2:2:40:HIS:NE2	2:2:205:TYR:CG[12_555]	1.19	1.01
1:1:48:GLU:OE1	1:1:78:HIS:ND1[12_555]	1.19	1.01
2:2:44:PRO:CD	2:2:248:PRO:CA[12_555]	1.19	1.01
2:2:40:HIS:CB	2:2:103:ARG:CD[12_555]	1.20	1.00
2:2:38:TRP:CA	2:2:210:PRO:N[12_555]	1.20	1.00
1:1:77:VAL:O	3:3:217:LYS:NZ[12_555]	1.20	1.00
3:3:26:PRO:CG	3:3:161:SER:CA[12_555]	1.20	1.00
1:1:48:GLU:CD	1:1:78:HIS:CD2[12_555]	1.20	1.00
3:3:212:PHE:CG	4:4:36:ALA:O[12_555]	1.20	1.00
3:3:19:MET:O	3:3:53:ILE:CD1[12_555]	1.20	1.00
2:2:35:TYR:CA	3:3:36:ILE:CD1[12_555]	1.20	1.00
1:1:61:THR:CB	3:3:230:HIS:CD2[12_555]	1.20	1.00
2:2:17:THR:C	2:2:50:ILE:N[2_555]	1.20	1.00
2:2:39:PRO:CB	2:2:42:LEU:CD1[12_555]	1.20	1.00
1:1:12:ASN:O	3:3:230:HIS:CA[12_555]	1.21	0.99
2:2:40:HIS:CA	2:2:103:ARG:NE[12_555]	1.21	0.99
2:2:43:THR:CG2	2:2:105:GLY:C[12_555]	1.21	0.99
1:1:32:PRO:CA	1:1:147:TYR:CG[12_555]	1.21	0.99
1:1:181:ARG:NH1	3:3:115:PHE:CE2[12_555]	1.21	0.99
3:3:209:MET:SD	4:4:32:PHE:CD1[12_555]	1.21	0.99
1:1:113:PHE:CD1	3:3:44:ILE:CG1[12_555]	1.21	0.99
1:1:5:ASN:OD1	2:2:173:LEU:CG[12_555]	1.21	0.99
1:1:176:GLY:CA	3:3:149:LEU:CB[12_555]	1.21	0.99
1:1:126:THR:CA	3:3:166:VAL:C[12_555]	1.21	0.99
3:3:210:LEU:O	4:4:37:SER:OG[12_555]	1.21	0.99
1:1:124:GLU:C	3:3:114:ARG:CG[12_555]	1.21	0.99
3:3:212:PHE:CD1	4:4:37:SER:CA[12_555]	1.22	0.98
2:2:178:THR:CG2	4:4:44:ASP:C[12_555]	1.22	0.98
1:1:240:TYR:CA	3:3:112:SER:CB[12_555]	1.22	0.98
1:1:26:THR:N	1:1:223:ARG:CA[12_555]	1.22	0.98
1:1:67:ILE:CG2	3:3:46:MET:SD[12_555]	1.22	0.98
1:1:126:THR:CA	3:3:167:VAL:N[12_555]	1.22	0.98
2:2:32:VAL:CB	3:3:31:THR:C[12_555]	1.22	0.98
2:2:43:THR:OG1	2:2:106:TYR:N[12_555]	1.22	0.98
1:1:29:ASN:C	1:1:146:MET:CE[12_555]	1.22	0.98
1:1:62:ARG:CB	1:1:111:ARG:CB[12_555]	1.22	0.98
1:1:72:GLY:C	3:3:99:ILE:CG1[12_555]	1.23	0.97
1:1:17:VAL:O	1:1:107:ALA:N[12_555]	1.23	0.97
1:1:252:ARG:NE	3:3:41:LYS:CE[12_555]	1.23	0.97
1:1:17:VAL:CA	1:1:107:ALA:N[12_555]	1.23	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:69:THR:C	4:4:29:ILE:O[12_555]	1.23	0.97
1:1:48:GLU:CG	1:1:78:HIS:NE2[12_555]	1.24	0.96
2:2:182:ASN:CA	4:4:41:SER:OG[12_555]	1.24	0.96
1:1:53:THR:OG1	1:1:80:SER:N[12_555]	1.24	0.96
2:2:202:ILE:O	3:3:34:ILE:CG2[12_555]	1.24	0.96
1:1:63:ASP:CA	1:1:111:ARG:NH2[12_555]	1.24	0.96
2:2:17:THR:OG1	2:2:48:THR:C[2_555]	1.24	0.96
1:1:127:LEU:N	3:3:166:VAL:C[12_555]	1.24	0.96
1:1:182:PHE:N	3:3:165:LEU:N[12_555]	1.24	0.96
3:3:14:MET:SD	3:3:88:ASP:CA[12_555]	1.24	0.96
3:3:52:LEU:CA	4:4:39:GLY:O[12_555]	1.24	0.96
1:1:35:ASP:C	3:3:25:LEU:CG[12_555]	1.24	0.96
1:1:250:CYS:CA	3:3:39:GLU:CA[12_555]	1.24	0.96
1:1:39:THR:O	3:3:30:PRO:CA[12_555]	1.24	0.96
2:2:17:THR:CB	2:2:49:ALA:N[2_555]	1.24	0.96
2:2:40:HIS:N	2:2:103:ARG:CZ[12_555]	1.24	0.96
3:3:97:THR:CB	4:4:40:ALA:CB[12_555]	1.24	0.96
3:3:26:PRO:CB	3:3:161:SER:CA[12_555]	1.24	0.96
1:1:27:THR:CG2	1:1:223:ARG:CZ[12_555]	1.24	0.96
2:2:195:SER:OG	3:3:27:TRP:CG[12_555]	1.25	0.95
1:1:41:HIS:CA	1:1:186:PHE:CB[12_555]	1.25	0.95
1:1:43:SER:OG	1:1:184:ILE:CD1[12_555]	1.25	0.95
1:1:123:SER:N	3:3:50:ASP:OD2[12_555]	1.25	0.95
1:1:122:ASP:C	3:3:50:ASP:CG[12_555]	1.25	0.95
3:3:67:MET:C	4:4:28:ASN:N[12_555]	1.25	0.95
1:1:63:ASP:CB	1:1:111:ARG:CZ[12_555]	1.25	0.95
1:1:122:ASP:O	3:3:50:ASP:N[12_555]	1.25	0.95
1:1:40:GLY:N	3:3:30:PRO:CB[12_555]	1.25	0.95
1:1:182:PHE:CD1	3:3:164:SER:CB[12_555]	1.25	0.95
2:2:18:ARG:CD	2:2:51:ASN:N[2_555]	1.25	0.95
2:2:13:ILE:N	2:2:13:ILE:CB[11_555]	1.25	0.95
1:1:8:ASP:N	1:1:275:THR:C[12_555]	1.25	0.95
3:3:37:PRO:CG	3:3:37:PRO:CD[12_555]	1.25	0.95
1:1:61:THR:OG1	3:3:230:HIS:CD2[12_555]	1.26	0.94
3:3:106:TYR:CB	3:3:225:ARG:N[12_555]	1.26	0.94
1:1:20:ILE:CG2	1:1:78:HIS:C[12_555]	1.26	0.94
1:1:103:LEU:CD1	3:3:48:GLN:OE1[12_555]	1.26	0.94
2:2:13:ILE:N	2:2:13:ILE:CG1[11_555]	1.26	0.94
2:2:187:PRO:C	3:3:33:GLU:OE1[12_555]	1.26	0.94
1:1:49:ASP:OD1	1:1:220:ILE:CB[12_555]	1.26	0.94
1:1:69:SER:O	3:3:102:ILE:CG2[12_555]	1.26	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:222:ARG:O	3:3:225:ARG:CA[12_555]	1.26	0.94
1:1:35:ASP:CG	3:3:25:LEU:CD1[12_555]	1.26	0.94
1:1:51:ILE:N	1:1:145:TYR:CE1[12_555]	1.27	0.93
2:2:37:VAL:CB	2:2:207:ASN:O[12_555]	1.27	0.93
1:1:24:HIS:N	1:1:97:THR:CG2[12_555]	1.27	0.93
1:1:47:PRO:CB	1:1:239:ILE:CA[12_555]	1.27	0.93
1:1:125:ILE:N	3:3:114:ARG:CG[12_555]	1.27	0.93
3:3:106:TYR:O	3:3:224:ALA:O[12_555]	1.27	0.93
2:2:46:ASP:CA	2:2:106:TYR:O[12_555]	1.27	0.93
3:3:58:VAL:CA	4:4:26:TYR:CG[12_555]	1.27	0.93
3:3:26:PRO:CD	3:3:160:GLN:C[12_555]	1.27	0.93
1:1:9:GLU:OE1	2:2:179:LEU:CD1[12_555]	1.27	0.93
3:3:212:PHE:CZ	4:4:37:SER:N[12_555]	1.27	0.93
1:1:29:ASN:CA	1:1:162:SER:O[12_555]	1.27	0.93
3:3:209:MET:CG	4:4:32:PHE:CD1[12_555]	1.27	0.93
1:1:242:LYS:CA	3:3:214:SER:O[12_555]	1.27	0.93
1:1:12:ASN:CB	3:3:229:LEU:C[12_555]	1.28	0.92
3:3:211:CYS:O	4:4:38:SER:CA[12_555]	1.28	0.92
2:2:59:SER:OG	2:2:253:PHE:CD2[12_555]	1.28	0.92
1:1:76:CYS:CB	3:3:218:ASP:OD2[12_555]	1.28	0.92
3:3:10:SER:OG	3:3:140:GLU:OE2[12_555]	1.28	0.92
2:2:11:ASP:N	2:2:26:ASP:OD2[11_555]	1.28	0.92
3:3:24:ALA:C	3:3:162:THR:O[12_555]	1.28	0.92
1:1:76:CYS:C	3:3:218:ASP:CB[12_555]	1.28	0.92
3:3:12:GLN:CG	3:3:187:GLY:C[12_555]	1.28	0.92
1:1:177:GLN:CD	3:3:148:MET:CB[12_555]	1.28	0.92
2:2:47:ALA:CB	2:2:249:MET:SD[12_555]	1.28	0.92
1:1:41:HIS:CD2	1:1:186:PHE:CE2[12_555]	1.28	0.92
1:1:14:VAL:CG1	1:1:256:ALA:N[12_555]	1.28	0.92
1:1:53:THR:OG1	1:1:79:ILE:C[12_555]	1.28	0.92
3:3:12:GLN:O	3:3:188:TYR:C[12_555]	1.29	0.91
2:2:31:ALA:O	3:3:31:THR:CB[12_555]	1.29	0.91
3:3:70:VAL:N	4:4:31:TYR:N[12_555]	1.29	0.91
1:1:29:ASN:N	1:1:162:SER:C[12_555]	1.29	0.91
2:2:42:LEU:O	2:2:250:CYS:N[12_555]	1.29	0.91
2:2:203:VAL:CG2	3:3:35:SER:N[12_555]	1.29	0.91
1:1:32:PRO:N	1:1:147:TYR:CB[12_555]	1.29	0.91
1:1:48:GLU:CB	1:1:78:HIS:CD2[12_555]	1.29	0.91
3:3:14:MET:N	3:3:87:VAL:CG1[12_555]	1.29	0.91
1:1:126:THR:C	3:3:167:VAL:N[12_555]	1.29	0.91
3:3:23:CYS:C	3:3:162:THR:CA[12_555]	1.29	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:240:TYR:CD2	3:3:112:SER:CA[12_555]	1.29	0.91
2:2:44:PRO:CA	2:2:247:SER:O[12_555]	1.29	0.91
1:1:39:THR:CA	3:3:30:PRO:N[12_555]	1.29	0.91
2:2:195:SER:OG	3:3:27:TRP:CB[12_555]	1.30	0.90
3:3:12:GLN:CG	3:3:187:GLY:O[12_555]	1.30	0.90
2:2:178:THR:CG2	4:4:43:LEU:O[12_555]	1.30	0.90
1:1:9:GLU:OE1	2:2:179:LEU:CG[12_555]	1.30	0.90
1:1:50:ALA:O	1:1:145:TYR:CE1[12_555]	1.30	0.90
1:1:249:TRP:CE2	2:2:35:TYR:CD1[12_555]	1.30	0.90
3:3:22:PRO:CD	3:3:117:PHE:CD1[12_555]	1.30	0.90
1:1:73:ARG:NH2	3:3:104:SER:N[12_555]	1.30	0.90
2:2:220:TRP:NE1	3:3:35:SER:OG[12_555]	1.30	0.90
1:1:5:ASN:CG	2:2:173:LEU:CD1[12_555]	1.30	0.90
1:1:62:ARG:C	1:1:111:ARG:CG[12_555]	1.30	0.90
3:3:97:THR:CA	4:4:40:ALA:CB[12_555]	1.30	0.90
1:1:125:ILE:O	3:3:165:LEU:C[12_555]	1.30	0.90
1:1:176:GLY:CA	3:3:149:LEU:C[12_555]	1.30	0.90
1:1:244:LYS:NZ	3:3:212:PHE:C[12_555]	1.30	0.90
1:1:183:SER:CA	3:3:116:SER:CA[12_555]	1.31	0.89
1:1:241:HIS:ND1	3:3:215:ALA:O[12_555]	1.31	0.89
2:2:91:ILE:CD1	2:2:95:ASN:N[2_555]	1.31	0.89
2:2:60:SER:CA	2:2:99:HIS:NE2[2_555]	1.31	0.89
1:1:76:CYS:CA	3:3:218:ASP:OD2[12_555]	1.31	0.89
1:1:26:THR:OG1	1:1:163:TRP:CZ3[12_555]	1.31	0.89
2:2:45:GLN:C	2:2:106:TYR:C[12_555]	1.31	0.89
3:3:9:GLY:N	3:3:188:TYR:OH[12_555]	1.31	0.89
1:1:48:GLU:CD	1:1:78:HIS:ND1[12_555]	1.31	0.89
2:2:17:THR:CG2	2:2:48:THR:C[2_555]	1.31	0.89
3:3:66:SER:CA	4:4:28:ASN:O[12_555]	1.31	0.89
1:1:18:PRO:N	1:1:106:MET:N[12_555]	1.31	0.89
3:3:212:PHE:CE1	4:4:36:ALA:C[12_555]	1.31	0.89
1:1:126:THR:O	3:3:166:VAL:CG1[12_555]	1.31	0.89
1:1:112:LYS:CA	3:3:42:ASN:ND2[12_555]	1.31	0.89
1:1:123:SER:CA	3:3:214:SER:OG[12_555]	1.32	0.88
1:1:128:VAL:CB	3:3:168:PRO:CG[12_555]	1.32	0.88
3:3:26:PRO:CA	3:3:161:SER:OG[12_555]	1.32	0.88
3:3:222:ARG:O	3:3:225:ARG:C[12_555]	1.32	0.88
2:2:64:TYR:CD1	2:2:256:ALA:O[2_555]	1.32	0.88
2:2:19:GLY:CA	2:2:254:SER:OG[2_555]	1.32	0.88
2:2:51:ASN:OD1	2:2:61:ASN:O[3_555]	1.32	0.88
1:1:6:TYR:OH	3:3:62:VAL:CB[12_555]	1.32	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:42:LEU:C	2:2:249:MET:C[12_555]	1.32	0.88
1:1:68:GLU:CD	3:3:98:LEU:CB[12_555]	1.32	0.88
2:2:52:LYS:CE	2:2:252:GLU:CG[10_555]	1.32	0.88
3:3:62:VAL:CG2	4:4:26:TYR:N[12_555]	1.32	0.88
1:1:37:ALA:CA	1:1:185:PRO:CB[12_555]	1.32	0.88
1:1:47:PRO:C	1:1:239:ILE:CG1[12_555]	1.32	0.88
1:1:113:PHE:CA	3:3:44:ILE:CG2[12_555]	1.32	0.88
3:3:16:THR:O	3:3:89:ILE:C[12_555]	1.32	0.88
3:3:118:MET:CG	4:4:34:ASP:CG[12_555]	1.32	0.88
1:1:180:PRO:O	3:3:165:LEU:CD1[12_555]	1.32	0.88
2:2:40:HIS:N	2:2:103:ARG:NE[12_555]	1.32	0.88
1:1:36:ALA:O	3:3:28:TYR:CD2[12_555]	1.33	0.87
2:2:46:ASP:CG	2:2:203:VAL:O[12_555]	1.33	0.87
1:1:34:LEU:CG	1:1:169:MET:CB[12_555]	1.33	0.87
3:3:223:MET:CB	3:3:225:ARG:CD[12_555]	1.33	0.87
1:1:68:GLU:O	3:3:98:LEU:C[12_555]	1.33	0.87
1:1:124:GLU:OE1	3:3:213:VAL:CG2[12_555]	1.33	0.87
1:1:64:GLU:OE1	3:3:104:SER:C[12_555]	1.33	0.87
3:3:15:THR:CG2	3:3:109:TRP:CH2[12_555]	1.33	0.87
1:1:183:SER:N	3:3:116:SER:CA[12_555]	1.33	0.87
1:1:41:HIS:C	1:1:186:PHE:CB[12_555]	1.33	0.87
1:1:179:PHE:CD2	3:3:133:TYR:CG[12_555]	1.33	0.87
1:1:53:THR:CG2	1:1:80:SER:CB[12_555]	1.33	0.87
1:1:62:ARG:NH2	1:1:109:ILE:CB[12_555]	1.33	0.87
1:1:244:LYS:CE	3:3:212:PHE:CA[12_555]	1.33	0.87
3:3:21:SER:CA	3:3:117:PHE:CE2[12_555]	1.33	0.87
2:2:201:LEU:C	3:3:32:LYS:CD[12_555]	1.33	0.87
1:1:248:ALA:N	1:1:251:PRO:CG[12_555]	1.34	0.86
1:1:124:GLU:OE2	3:3:115:PHE:CG[12_555]	1.34	0.86
3:3:16:THR:O	3:3:89:ILE:CA[12_555]	1.34	0.86
2:2:90:GLY:O	2:2:98:TYR:CB[2_555]	1.34	0.86
1:1:28:SER:N	1:1:163:TRP:CG[12_555]	1.34	0.86
1:1:18:PRO:N	1:1:106:MET:CA[12_555]	1.34	0.86
1:1:13:GLU:CG	3:3:231:ILE:O[12_555]	1.34	0.86
3:3:67:MET:N	4:4:28:ASN:N[12_555]	1.34	0.86
3:3:67:MET:N	4:4:28:ASN:CA[12_555]	1.34	0.86
2:2:44:PRO:CB	2:2:247:SER:C[12_555]	1.34	0.86
3:3:66:SER:C	4:4:28:ASN:O[12_555]	1.34	0.86
2:2:89:MET:CB	2:2:257:ARG:O[2_555]	1.34	0.86
1:1:177:GLN:CA	3:3:148:MET:CA[12_555]	1.34	0.86
2:2:40:HIS:C	2:2:103:ARG:NE[12_555]	1.34	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:173:TRP:CD1	3:3:152:HIS:N[12_555]	1.34	0.86
1:1:26:THR:N	1:1:223:ARG:N[12_555]	1.34	0.86
1:1:23:SER:CB	1:1:80:SER:OG[12_555]	1.34	0.86
3:3:212:PHE:CZ	4:4:36:ALA:C[12_555]	1.34	0.86
1:1:52:GLU:OE2	1:1:82:ILE:CD1[12_555]	1.34	0.86
3:3:212:PHE:CZ	4:4:36:ALA:N[12_555]	1.35	0.85
1:1:37:ALA:N	1:1:185:PRO:CG[12_555]	1.35	0.85
2:2:46:ASP:OD2	2:2:203:VAL:CG1[12_555]	1.35	0.85
1:1:121:PHE:CE1	3:3:48:GLN:O[12_555]	1.35	0.85
3:3:65:VAL:C	4:4:28:ASN:CG[12_555]	1.35	0.85
1:1:241:HIS:NE2	3:3:114:ARG:NH2[12_555]	1.35	0.85
1:1:63:ASP:CA	1:1:111:ARG:NE[12_555]	1.35	0.85
1:1:174:GLN:O	3:3:148:MET:O[12_555]	1.35	0.85
1:1:58:THR:CG2	1:1:106:MET:CE[12_555]	1.35	0.85
1:1:242:LYS:CA	3:3:214:SER:C[12_555]	1.35	0.85
1:1:17:VAL:CA	1:1:106:MET:C[12_555]	1.35	0.85
3:3:19:MET:CE	3:3:85:ILE:CB[12_555]	1.35	0.85
2:2:64:TYR:CD1	2:2:257:ARG:N[2_555]	1.35	0.85
1:1:68:GLU:OE2	3:3:51:THR:CG2[12_555]	1.35	0.85
1:1:51:ILE:CD1	1:1:237:THR:C[12_555]	1.35	0.85
3:3:105:TYR:C	3:3:106:TYR:CD2[12_555]	1.35	0.85
2:2:62:ARG:CZ	2:2:101:LEU:C[2_555]	1.36	0.84
1:1:27:THR:OG1	1:1:223:ARG:CG[12_555]	1.36	0.84
1:1:126:THR:CG2	3:3:167:VAL:CG2[12_555]	1.36	0.84
2:2:54:THR:O	2:2:57:ASP:O[3_555]	1.36	0.84
3:3:17:ASP:C	3:3:94:LEU:CD1[12_555]	1.36	0.84
3:3:17:ASP:C	3:3:94:LEU:CD2[12_555]	1.36	0.84
3:3:15:THR:O	3:3:89:ILE:CG2[12_555]	1.36	0.84
1:1:57:ILE:CG2	3:3:235:PRO:CD[12_555]	1.36	0.84
1:1:44:ASN:ND2	1:1:101:ILE:CG1[12_555]	1.36	0.84
1:1:50:ALA:O	1:1:145:TYR:CD1[12_555]	1.36	0.84
2:2:62:ARG:CB	2:2:254:SER:O[2_555]	1.36	0.84
1:1:177:GLN:O	3:3:150:GLY:O[12_555]	1.36	0.84
1:1:53:THR:CB	1:1:80:SER:N[12_555]	1.36	0.84
2:2:38:TRP:CE3	2:2:210:PRO:CG[12_555]	1.36	0.84
1:1:10:VAL:CA	1:1:277:ALA:CA[12_555]	1.36	0.84
1:1:240:TYR:CD2	3:3:111:GLY:C[12_555]	1.36	0.84
1:1:181:ARG:NH1	3:3:115:PHE:CE1[12_555]	1.36	0.84
1:1:17:VAL:CA	1:1:107:ALA:CA[12_555]	1.36	0.84
1:1:63:ASP:OD1	1:1:111:ARG:NH1[12_555]	1.36	0.84
3:3:23:CYS:SG	3:3:162:THR:CG2[12_555]	1.36	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:48:GLU:OE2	1:1:78:HIS:CG[12_555]	1.36	0.84
1:1:6:TYR:CZ	3:3:62:VAL:CG1[12_555]	1.37	0.83
1:1:71:LEU:CD1	3:3:46:MET:N[12_555]	1.37	0.83
2:2:53:PRO:O	2:2:57:ASP:CA[3_555]	1.37	0.83
3:3:22:PRO:CB	3:3:155:TRP:CZ3[12_555]	1.37	0.83
2:2:59:SER:O	2:2:99:HIS:ND1[2_555]	1.37	0.83
1:1:18:PRO:CB	1:1:106:MET:N[12_555]	1.37	0.83
1:1:17:VAL:CB	1:1:107:ALA:C[12_555]	1.37	0.83
1:1:41:HIS:CA	1:1:186:PHE:CA[12_555]	1.37	0.83
1:1:41:HIS:CB	1:1:186:PHE:O[12_555]	1.37	0.83
3:3:222:ARG:O	3:3:225:ARG:CB[12_555]	1.37	0.83
2:2:41:TYR:CE2	2:2:55:GLN:OE1[12_555]	1.37	0.83
1:1:71:LEU:CB	3:3:47:CYS:N[12_555]	1.37	0.83
2:2:64:TYR:CE1	2:2:256:ALA:CA[2_555]	1.37	0.83
2:2:178:THR:O	4:4:42:ARG:NH1[12_555]	1.37	0.83
1:1:240:TYR:CE1	3:3:169:TRP:CB[12_555]	1.37	0.83
1:1:252:ARG:CB	3:3:41:LYS:CD[12_555]	1.37	0.83
1:1:177:GLN:CG	3:3:148:MET:CA[12_555]	1.37	0.83
2:2:38:TRP:CB	2:2:210:PRO:N[12_555]	1.37	0.83
3:3:212:PHE:CZ	4:4:36:ALA:CA[12_555]	1.37	0.83
1:1:179:PHE:CG	3:3:133:TYR:CD2[12_555]	1.37	0.83
1:1:39:THR:N	3:3:30:PRO:CD[12_555]	1.37	0.83
3:3:212:PHE:CD1	4:4:37:SER:N[12_555]	1.37	0.83
1:1:72:GLY:C	3:3:99:ILE:CB[12_555]	1.37	0.83
1:1:32:PRO:CD	1:1:146:MET:C[12_555]	1.38	0.82
2:2:187:PRO:CB	3:3:33:GLU:CD[12_555]	1.38	0.82
3:3:37:PRO:CD	3:3:37:PRO:CD[12_555]	1.38	0.82
1:1:42:THR:CB	1:1:121:PHE:O[12_555]	1.38	0.82
3:3:105:TYR:O	3:3:106:TYR:CG[12_555]	1.38	0.82
1:1:242:LYS:C	3:3:214:SER:CA[12_555]	1.38	0.82
2:2:187:PRO:CG	3:3:33:GLU:OE2[12_555]	1.38	0.82
3:3:120:CYS:SG	4:4:33:LYS:CA[12_555]	1.38	0.82
1:1:62:ARG:NH1	1:1:110:ARG:CA[12_555]	1.38	0.82
3:3:56:ASN:OD1	4:4:29:ILE:CB[12_555]	1.39	0.81
2:2:190:PHE:CZ	4:4:35:ALA:CB[12_555]	1.39	0.81
3:3:106:TYR:N	3:3:224:ALA:N[12_555]	1.39	0.81
3:3:6:ILE:CD1	3:3:142:THR:CA[12_555]	1.39	0.81
1:1:32:PRO:CA	1:1:147:TYR:CA[12_555]	1.39	0.81
1:1:62:ARG:NH1	1:1:109:ILE:C[12_555]	1.39	0.81
1:1:179:PHE:CG	3:3:133:TYR:CG[12_555]	1.39	0.81
1:1:27:THR:CB	1:1:223:ARG:CD[12_555]	1.39	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:68:GLU:OE1	3:3:51:THR:OG1[12_555]	1.39	0.81
1:1:69:SER:O	3:3:102:ILE:CB[12_555]	1.39	0.81
1:1:247:LYS:CG	2:2:185:ILE:O[12_555]	1.39	0.81
2:2:17:THR:C	2:2:49:ALA:CA[2_555]	1.39	0.81
1:1:116:PHE:CA	3:3:41:LYS:N[12_555]	1.40	0.80
2:2:187:PRO:N	3:3:33:GLU:OE2[12_555]	1.40	0.80
1:1:27:THR:C	1:1:163:TRP:CB[12_555]	1.40	0.80
3:3:65:VAL:O	4:4:28:ASN:CG[12_555]	1.40	0.80
1:1:17:VAL:CB	1:1:107:ALA:O[12_555]	1.40	0.80
1:1:249:TRP:C	3:3:39:GLU:CA[12_555]	1.40	0.80
3:3:70:VAL:CG2	4:4:31:TYR:CG[12_555]	1.40	0.80
1:1:73:ARG:NE	3:3:103:ALA:CA[12_555]	1.40	0.80
1:1:8:ASP:O	1:1:256:ALA:O[12_555]	1.40	0.80
1:1:126:THR:CB	3:3:167:VAL:N[12_555]	1.40	0.80
1:1:249:TRP:C	3:3:39:GLU:C[12_555]	1.40	0.80
2:2:43:THR:OG1	2:2:105:GLY:C[12_555]	1.40	0.80
1:1:63:ASP:N	1:1:111:ARG:NE[12_555]	1.40	0.80
1:1:241:HIS:CB	3:3:216:CYS:CA[12_555]	1.40	0.80
1:1:72:GLY:O	3:3:99:ILE:CB[12_555]	1.40	0.80
3:3:67:MET:SD	4:4:27:PHE:CG[12_555]	1.40	0.80
1:1:9:GLU:OE1	2:2:179:LEU:CD2[12_555]	1.40	0.80
2:2:54:THR:N	2:2:58:THR:N[3_555]	1.40	0.80
1:1:26:THR:N	1:1:223:ARG:CB[12_555]	1.40	0.80
1:1:63:ASP:C	1:1:111:ARG:NH2[12_555]	1.40	0.80
1:1:18:PRO:CG	1:1:106:MET:N[12_555]	1.40	0.80
2:2:17:THR:CA	2:2:49:ALA:CA[2_555]	1.40	0.80
2:2:181:GLY:C	4:4:41:SER:CB[12_555]	1.40	0.80
2:2:178:THR:OG1	4:4:44:ASP:CB[12_555]	1.40	0.80
3:3:58:VAL:CA	4:4:26:TYR:CB[12_555]	1.41	0.79
3:3:64:ASN:O	4:4:28:ASN:OD1[12_555]	1.41	0.79
2:2:94:GLU:OE2	2:2:98:TYR:CE2[2_555]	1.41	0.79
2:2:54:THR:OG1	2:2:56:PRO:C[3_555]	1.41	0.79
1:1:61:THR:CG2	3:3:230:HIS:ND1[12_555]	1.41	0.79
2:2:201:LEU:C	3:3:32:LYS:CE[12_555]	1.41	0.79
3:3:211:CYS:O	4:4:38:SER:C[12_555]	1.41	0.79
1:1:10:VAL:CB	1:1:276:THR:O[12_555]	1.41	0.79
2:2:41:TYR:CE2	2:2:41:TYR:CE2[12_555]	1.41	0.79
3:3:120:CYS:CA	4:4:33:LYS:CG[12_555]	1.41	0.79
3:3:21:SER:C	3:3:117:PHE:CB[12_555]	1.41	0.79
1:1:27:THR:C	1:1:163:TRP:CD2[12_555]	1.41	0.79
3:3:211:CYS:O	4:4:38:SER:N[12_555]	1.41	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:69:SER:CA	3:3:102:ILE:N[12_555]	1.41	0.79
1:1:73:ARG:NH2	3:3:103:ALA:C[12_555]	1.41	0.79
1:1:244:LYS:NZ	3:3:212:PHE:N[12_555]	1.41	0.79
2:2:43:THR:OG1	2:2:106:TYR:CA[12_555]	1.41	0.79
1:1:30:SER:O	1:1:146:MET:CG[12_555]	1.41	0.79
1:1:48:GLU:OE2	1:1:78:HIS:CD2[12_555]	1.41	0.79
2:2:52:LYS:CG	2:2:53:PRO:CG[10_555]	1.41	0.79
3:3:58:VAL:CG1	4:4:26:TYR:CE1[12_555]	1.42	0.78
1:1:42:THR:N	1:1:186:PHE:CA[12_555]	1.42	0.78
1:1:46:GLN:OE1	1:1:77:VAL:CG2[12_555]	1.42	0.78
3:3:223:MET:O	3:3:225:ARG:CG[12_555]	1.42	0.78
1:1:244:LYS:O	3:3:50:ASP:CA[12_555]	1.42	0.78
1:1:71:LEU:CD2	3:3:43:LEU:O[12_555]	1.42	0.78
3:3:17:ASP:N	3:3:94:LEU:CD1[12_555]	1.42	0.78
3:3:222:ARG:N	3:3:226:ASP:CA[12_555]	1.42	0.78
1:1:109:ILE:CB	3:3:219:PHE:O[12_555]	1.42	0.78
1:1:77:VAL:O	3:3:217:LYS:CE[12_555]	1.42	0.78
2:2:17:THR:O	2:2:50:ILE:CA[2_555]	1.42	0.78
2:2:91:ILE:N	2:2:98:TYR:CB[2_555]	1.42	0.78
2:2:32:VAL:CB	3:3:32:LYS:O[12_555]	1.43	0.77
3:3:57:ASN:C	4:4:26:TYR:CB[12_555]	1.43	0.77
1:1:128:VAL:CB	3:3:168:PRO:CB[12_555]	1.43	0.77
1:1:244:LYS:C	3:3:50:ASP:C[12_555]	1.43	0.77
1:1:53:THR:CG2	1:1:80:SER:N[12_555]	1.43	0.77
1:1:18:PRO:CG	1:1:105:GLU:N[12_555]	1.43	0.77
2:2:195:SER:CB	3:3:27:TRP:CG[12_555]	1.43	0.77
3:3:106:TYR:C	3:3:224:ALA:O[12_555]	1.43	0.77
1:1:30:SER:CA	1:1:146:MET:CE[12_555]	1.43	0.77
1:1:32:PRO:N	1:1:147:TYR:N[12_555]	1.43	0.77
2:2:187:PRO:CD	3:3:33:GLU:CD[12_555]	1.43	0.77
1:1:76:CYS:CA	3:3:218:ASP:OD1[12_555]	1.43	0.77
2:2:11:ASP:CB	2:2:26:ASP:C[11_555]	1.43	0.77
1:1:73:ARG:NH2	3:3:103:ALA:CA[12_555]	1.43	0.77
3:3:23:CYS:SG	3:3:162:THR:OG1[12_555]	1.43	0.77
2:2:32:VAL:CB	3:3:31:THR:O[12_555]	1.43	0.77
3:3:209:MET:N	4:4:31:TYR:O[12_555]	1.43	0.77
1:1:115:LEU:O	3:3:41:LYS:C[12_555]	1.43	0.77
1:1:254:PRO:O	4:4:43:LEU:CG[12_555]	1.44	0.76
3:3:14:MET:CG	3:3:88:ASP:N[12_555]	1.44	0.76
1:1:41:HIS:O	1:1:186:PHE:CA[12_555]	1.44	0.76
3:3:106:TYR:CA	3:3:224:ALA:C[12_555]	1.44	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:41:HIS:C	1:1:186:PHE:N[12_555]	1.44	0.76
1:1:27:THR:CA	1:1:223:ARG:NE[12_555]	1.44	0.76
2:2:178:THR:CB	4:4:44:ASP:N[12_555]	1.44	0.76
1:1:42:THR:O	1:1:193:TYR:OH[12_555]	1.44	0.76
2:2:178:THR:CB	4:4:43:LEU:C[12_555]	1.44	0.76
1:1:48:GLU:OE1	1:1:78:HIS:CB[12_555]	1.44	0.76
3:3:66:SER:N	4:4:28:ASN:CB[12_555]	1.44	0.76
3:3:65:VAL:CA	4:4:28:ASN:CG[12_555]	1.44	0.76
1:1:5:ASN:N	1:1:274:VAL:CG1[12_555]	1.44	0.76
1:1:245:HIS:NE2	3:3:51:THR:C[12_555]	1.44	0.76
2:2:41:TYR:CD1	2:2:52:LYS:NZ[2_555]	1.44	0.76
1:1:47:PRO:C	1:1:239:ILE:CD1[12_555]	1.44	0.76
3:3:222:ARG:CG	3:3:226:ASP:O[12_555]	1.45	0.75
2:2:45:GLN:C	2:2:107:THR:CA[12_555]	1.45	0.75
1:1:18:PRO:O	1:1:106:MET:CB[12_555]	1.45	0.75
3:3:65:VAL:O	4:4:28:ASN:CA[12_555]	1.45	0.75
2:2:46:ASP:CB	2:2:203:VAL:N[12_555]	1.45	0.75
1:1:183:SER:CB	3:3:116:SER:CA[12_555]	1.45	0.75
1:1:15:LEU:CD2	1:1:255:ARG:N[12_555]	1.45	0.75
1:1:51:ILE:C	1:1:237:THR:CG2[12_555]	1.45	0.75
1:1:171:ILE:CD1	3:3:153:VAL:CG2[12_555]	1.45	0.75
1:1:22:GLU:CG	1:1:81:ARG:CB[12_555]	1.45	0.75
2:2:32:VAL:CG1	3:3:32:LYS:C[12_555]	1.45	0.75
2:2:52:LYS:NZ	2:2:252:GLU:CB[10_555]	1.45	0.75
3:3:52:LEU:O	4:4:39:GLY:O[12_555]	1.45	0.75
1:1:49:ASP:CG	1:1:220:ILE:CB[12_555]	1.45	0.75
3:3:9:GLY:C	3:3:188:TYR:CD1[12_555]	1.45	0.75
1:1:112:LYS:O	3:3:42:ASN:ND2[12_555]	1.45	0.75
3:3:70:VAL:CA	4:4:31:TYR:CG[12_555]	1.46	0.74
1:1:25:HIS:CB	1:1:224:ILE:N[12_555]	1.46	0.74
2:2:29:ALA:CB	3:3:29:HIS:CA[12_555]	1.46	0.74
1:1:182:PHE:C	3:3:115:PHE:O[12_555]	1.46	0.74
3:3:212:PHE:CE2	4:4:36:ALA:CA[12_555]	1.46	0.74
2:2:11:ASP:OD2	2:2:26:ASP:O[11_555]	1.46	0.74
3:3:10:SER:OG	3:3:140:GLU:CD[12_555]	1.46	0.74
1:1:250:CYS:CB	3:3:39:GLU:CG[12_555]	1.46	0.74
1:1:191:SER:CA	2:2:33:VAL:O[12_555]	1.46	0.74
3:3:223:MET:CB	3:3:225:ARG:NE[12_555]	1.46	0.74
1:1:61:THR:CG2	3:3:230:HIS:CD2[12_555]	1.46	0.74
1:1:8:ASP:CG	1:1:258:PRO:CD[12_555]	1.47	0.73
2:2:54:THR:CA	2:2:57:ASP:CA[3_555]	1.47	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:67:MET:CB	4:4:27:PHE:C[12_555]	1.47	0.73
2:2:91:ILE:CG1	2:2:95:ASN:CG[2_555]	1.47	0.73
3:3:21:SER:C	3:3:117:PHE:CD2[12_555]	1.47	0.73
1:1:249:TRP:NE1	2:2:35:TYR:CZ[12_555]	1.47	0.73
2:2:38:TRP:CB	2:2:211:MET:N[12_555]	1.47	0.73
1:1:35:ASP:O	3:3:24:ALA:O[12_555]	1.47	0.73
1:1:65:MET:N	3:3:105:TYR:CZ[12_555]	1.47	0.73
2:2:36:GLY:O	2:2:208:ALA:N[12_555]	1.47	0.73
2:2:176:ASP:CG	4:4:44:ASP:OD2[12_555]	1.47	0.73
2:2:190:PHE:CE1	4:4:35:ALA:CB[12_555]	1.47	0.73
1:1:14:VAL:CG1	1:1:255:ARG:C[12_555]	1.47	0.73
1:1:18:PRO:O	1:1:106:MET:CA[12_555]	1.47	0.73
2:2:35:TYR:CB	3:3:36:ILE:CG1[12_555]	1.48	0.72
1:1:28:SER:O	1:1:146:MET:SD[12_555]	1.48	0.72
2:2:40:HIS:CG	2:2:103:ARG:CG[12_555]	1.48	0.72
3:3:12:GLN:CB	3:3:187:GLY:C[12_555]	1.48	0.72
1:1:77:VAL:CG1	3:3:217:LYS:N[12_555]	1.48	0.72
1:1:25:HIS:ND1	1:1:224:ILE:CG2[12_555]	1.48	0.72
1:1:240:TYR:CB	3:3:113:LEU:N[12_555]	1.48	0.72
1:1:52:GLU:CA	1:1:237:THR:CG2[12_555]	1.48	0.72
3:3:120:CYS:N	4:4:33:LYS:CA[12_555]	1.48	0.72
2:2:90:GLY:CA	2:2:98:TYR:N[2_555]	1.48	0.72
1:1:71:LEU:CD2	3:3:43:LEU:C[12_555]	1.48	0.72
1:1:62:ARG:NE	1:1:109:ILE:N[12_555]	1.48	0.72
1:1:53:THR:O	1:1:80:SER:O[12_555]	1.48	0.72
1:1:179:PHE:N	3:3:151:THR:O[12_555]	1.48	0.72
3:3:209:MET:CA	4:4:32:PHE:N[12_555]	1.48	0.72
1:1:26:THR:CB	1:1:163:TRP:CH2[12_555]	1.48	0.72
1:1:61:THR:CB	3:3:230:HIS:CG[12_555]	1.48	0.72
1:1:27:THR:OG1	1:1:223:ARG:NE[12_555]	1.48	0.72
2:2:89:MET:SD	2:2:257:ARG:CD[2_555]	1.49	0.71
1:1:182:PHE:CD2	3:3:164:SER:C[12_555]	1.49	0.71
3:3:56:ASN:CG	4:4:29:ILE:CG1[12_555]	1.49	0.71
1:1:242:LYS:CA	3:3:215:ALA:N[12_555]	1.49	0.71
2:2:46:ASP:OD2	2:2:203:VAL:CB[12_555]	1.49	0.71
1:1:6:TYR:O	1:1:276:THR:C[12_555]	1.49	0.71
1:1:182:PHE:CG	3:3:164:SER:CA[12_555]	1.49	0.71
1:1:25:HIS:C	1:1:222:SER:O[12_555]	1.49	0.71
2:2:43:THR:N	2:2:249:MET:O[12_555]	1.49	0.71
2:2:62:ARG:NH2	2:2:101:LEU:O[2_555]	1.49	0.71
1:1:181:ARG:N	3:3:165:LEU:CD2[12_555]	1.49	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:176:GLY:O	3:3:150:GLY:N[12_555]	1.49	0.71
2:2:11:ASP:N	2:2:26:ASP:CB[11_555]	1.49	0.71
2:2:44:PRO:C	2:2:247:SER:O[12_555]	1.49	0.71
3:3:9:GLY:O	3:3:188:TYR:CE1[12_555]	1.49	0.71
1:1:240:TYR:CD2	3:3:111:GLY:O[12_555]	1.49	0.71
1:1:179:PHE:CD1	3:3:133:TYR:CD2[12_555]	1.49	0.71
2:2:53:PRO:C	2:2:57:ASP:CA[3_555]	1.49	0.71
3:3:9:GLY:CA	3:3:188:TYR:CE1[12_555]	1.49	0.71
1:1:182:PHE:CE2	3:3:164:SER:O[12_555]	1.49	0.71
1:1:74:SER:OG	3:3:113:LEU:CG[12_555]	1.49	0.71
3:3:24:ALA:CB	3:3:162:THR:O[12_555]	1.49	0.71
1:1:26:THR:CG2	1:1:222:SER:N[12_555]	1.49	0.71
1:1:48:GLU:CB	1:1:78:HIS:NE2[12_555]	1.49	0.71
2:2:54:THR:C	2:2:57:ASP:N[3_555]	1.49	0.71
3:3:118:MET:CG	4:4:34:ASP:CA[12_555]	1.50	0.70
1:1:69:SER:O	3:3:103:ALA:N[12_555]	1.50	0.70
1:1:115:LEU:C	3:3:42:ASN:N[12_555]	1.50	0.70
1:1:39:THR:C	3:3:30:PRO:CG[12_555]	1.50	0.70
2:2:90:GLY:N	2:2:98:TYR:CA[2_555]	1.50	0.70
3:3:67:MET:N	4:4:27:PHE:C[12_555]	1.50	0.70
1:1:240:TYR:CB	3:3:112:SER:CA[12_555]	1.50	0.70
1:1:8:ASP:CA	1:1:275:THR:O[12_555]	1.50	0.70
2:2:38:TRP:CB	2:2:210:PRO:CA[12_555]	1.50	0.70
1:1:65:MET:O	1:1:115:LEU:CD2[12_555]	1.50	0.70
1:1:73:ARG:NH2	3:3:103:ALA:N[12_555]	1.50	0.70
2:2:178:THR:OG1	4:4:44:ASP:OD1[12_555]	1.50	0.70
1:1:30:SER:OG	1:1:148:VAL:CA[12_555]	1.50	0.70
1:1:176:GLY:C	3:3:149:LEU:N[12_555]	1.50	0.70
2:2:44:PRO:CD	2:2:248:PRO:O[12_555]	1.50	0.70
1:1:72:GLY:CA	3:3:99:ILE:CB[12_555]	1.50	0.70
3:3:65:VAL:O	4:4:28:ASN:ND2[12_555]	1.50	0.70
1:1:245:HIS:CD2	3:3:52:LEU:N[12_555]	1.50	0.70
1:1:70:PHE:CE2	3:3:43:LEU:CG[12_555]	1.50	0.70
2:2:89:MET:N	2:2:259:LYS:N[2_555]	1.51	0.69
2:2:178:THR:CG2	4:4:43:LEU:C[12_555]	1.51	0.69
1:1:47:PRO:CD	1:1:239:ILE:CB[12_555]	1.51	0.69
3:3:209:MET:CE	4:4:32:PHE:CE2[12_555]	1.51	0.69
1:1:124:GLU:C	3:3:114:ARG:CA[12_555]	1.51	0.69
2:2:45:GLN:C	2:2:106:TYR:O[12_555]	1.51	0.69
2:2:36:GLY:O	2:2:208:ALA:CA[12_555]	1.51	0.69
3:3:222:ARG:CB	3:3:226:ASP:CA[12_555]	1.51	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:118:MET:CE	4:4:34:ASP:C[12_555]	1.51	0.69
1:1:69:SER:C	3:3:102:ILE:CA[12_555]	1.51	0.69
3:3:211:CYS:C	4:4:38:SER:N[12_555]	1.51	0.69
1:1:174:GLN:N	3:3:152:HIS:CE1[12_555]	1.51	0.69
1:1:9:GLU:N	1:1:276:THR:CA[12_555]	1.51	0.69
1:1:23:SER:N	1:1:81:ARG:N[12_555]	1.51	0.69
3:3:209:MET:SD	4:4:32:PHE:CZ[12_555]	1.51	0.69
1:1:247:LYS:NZ	2:2:186:PHE:CA[12_555]	1.51	0.69
2:2:29:ALA:CB	3:3:29:HIS:N[12_555]	1.51	0.69
2:2:201:LEU:CA	3:3:32:LYS:CB[12_555]	1.51	0.69
2:2:54:THR:CB	2:2:56:PRO:C[3_555]	1.51	0.69
2:2:52:LYS:O	2:2:61:ASN:CG[3_555]	1.51	0.69
1:1:27:THR:CG2	1:1:223:ARG:NE[12_555]	1.51	0.69
2:2:194:ARG:NH1	3:3:27:TRP:CH2[12_555]	1.51	0.69
2:2:90:GLY:C	2:2:98:TYR:CA[2_555]	1.51	0.69
1:1:242:LYS:O	3:3:214:SER:CB[12_555]	1.51	0.69
1:1:10:VAL:N	1:1:277:ALA:CA[12_555]	1.52	0.68
3:3:222:ARG:N	3:3:226:ASP:N[12_555]	1.52	0.68
1:1:64:GLU:CG	3:3:104:SER:C[12_555]	1.52	0.68
2:2:46:ASP:OD1	2:2:203:VAL:C[12_555]	1.52	0.68
2:2:40:HIS:N	2:2:103:ARG:NH1[12_555]	1.52	0.68
2:2:21:SER:N	2:2:101:LEU:CG[2_555]	1.52	0.68
1:1:50:ALA:CB	1:1:127:LEU:CG[12_555]	1.52	0.68
1:1:62:ARG:CZ	1:1:109:ILE:CA[12_555]	1.52	0.68
1:1:51:ILE:CA	1:1:145:TYR:CE1[12_555]	1.52	0.68
1:1:47:PRO:CB	1:1:239:ILE:CB[12_555]	1.52	0.68
1:1:27:THR:CB	1:1:223:ARG:CZ[12_555]	1.52	0.68
1:1:244:LYS:O	3:3:50:ASP:O[12_555]	1.52	0.68
1:1:177:GLN:OE1	3:3:144:ARG:O[12_555]	1.52	0.68
3:3:23:CYS:SG	3:3:162:THR:CB[12_555]	1.52	0.68
3:3:69:THR:CA	4:4:29:ILE:C[12_555]	1.52	0.68
3:3:17:ASP:O	3:3:94:LEU:CG[12_555]	1.52	0.68
2:2:37:VAL:CG2	2:2:207:ASN:CA[12_555]	1.52	0.68
1:1:191:SER:OG	2:2:33:VAL:N[12_555]	1.53	0.67
2:2:41:TYR:CD1	2:2:252:GLU:OE2[12_555]	1.53	0.67
3:3:22:PRO:N	3:3:117:PHE:CD1[12_555]	1.53	0.67
2:2:59:SER:OG	2:2:253:PHE:CG[2_555]	1.53	0.67
2:2:57:ASP:CG	2:2:57:ASP:OD2[11_555]	1.53	0.67
1:1:75:GLY:N	3:3:112:SER:O[12_555]	1.53	0.67
2:2:40:HIS:C	2:2:103:ARG:CD[12_555]	1.53	0.67
1:1:241:HIS:C	3:3:215:ALA:C[12_555]	1.53	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:77:VAL:CG1	3:3:218:ASP:N[12_555]	1.53	0.67
2:2:90:GLY:CA	2:2:98:TYR:CB[2_555]	1.53	0.67
1:1:31:ALA:CB	1:1:169:MET:N[12_555]	1.53	0.67
1:1:245:HIS:CD2	3:3:51:THR:C[12_555]	1.53	0.67
3:3:212:PHE:CD1	4:4:36:ALA:C[12_555]	1.53	0.67
3:3:212:PHE:CE1	4:4:37:SER:CA[12_555]	1.53	0.67
2:2:47:ALA:C	2:2:249:MET:CE[12_555]	1.53	0.67
1:1:20:ILE:CG2	1:1:79:ILE:CA[12_555]	1.53	0.67
1:1:41:HIS:CE1	1:1:188:SER:O[12_555]	1.53	0.67
1:1:128:VAL:N	3:3:168:PRO:CD[12_555]	1.53	0.67
1:1:27:THR:CG2	1:1:223:ARG:NH2[12_555]	1.53	0.67
1:1:18:PRO:N	1:1:106:MET:C[12_555]	1.54	0.66
1:1:62:ARG:NH2	1:1:109:ILE:CG1[12_555]	1.54	0.66
3:3:22:PRO:O	3:3:163:ILE:O[12_555]	1.54	0.66
3:3:212:PHE:CD1	4:4:36:ALA:O[12_555]	1.54	0.66
1:1:39:THR:CA	3:3:30:PRO:CA[12_555]	1.54	0.66
3:3:17:ASP:CA	3:3:94:LEU:CG[12_555]	1.54	0.66
2:2:32:VAL:CB	3:3:32:LYS:N[12_555]	1.54	0.66
1:1:126:THR:CA	3:3:166:VAL:CA[12_555]	1.54	0.66
1:1:14:VAL:CB	1:1:256:ALA:N[12_555]	1.54	0.66
1:1:115:LEU:CB	3:3:42:ASN:N[12_555]	1.54	0.66
3:3:56:ASN:ND2	4:4:29:ILE:CD1[12_555]	1.54	0.66
1:1:69:SER:OG	3:3:101:GLU:C[12_555]	1.54	0.66
1:1:68:GLU:CB	3:3:98:LEU:CG[12_555]	1.54	0.66
3:3:19:MET:SD	3:3:85:ILE:CD1[12_555]	1.54	0.66
2:2:42:LEU:N	2:2:250:CYS:CB[12_555]	1.54	0.66
3:3:58:VAL:CB	4:4:26:TYR:CE1[12_555]	1.54	0.66
2:2:36:GLY:C	2:2:208:ALA:N[12_555]	1.54	0.66
2:2:58:THR:O	2:2:254:SER:CA[2_555]	1.54	0.66
1:1:245:HIS:N	3:3:51:THR:CG2[12_555]	1.54	0.66
2:2:59:SER:CB	2:2:253:PHE:CB[2_555]	1.54	0.66
3:3:21:SER:O	3:3:117:PHE:N[12_555]	1.54	0.66
2:2:43:THR:CG2	2:2:105:GLY:N[12_555]	1.55	0.65
2:2:44:PRO:N	2:2:247:SER:O[12_555]	1.55	0.65
1:1:176:GLY:N	3:3:149:LEU:CA[12_555]	1.55	0.65
1:1:103:LEU:CD1	3:3:48:GLN:CD[12_555]	1.55	0.65
1:1:35:ASP:CB	3:3:25:LEU:CD1[12_555]	1.55	0.65
1:1:247:LYS:CD	2:2:186:PHE:N[12_555]	1.55	0.65
2:2:62:ARG:NH2	2:2:102:GLY:N[2_555]	1.55	0.65
3:3:22:PRO:CB	3:3:155:TRP:CE3[12_555]	1.55	0.65
3:3:21:SER:N	3:3:117:PHE:CD2[12_555]	1.55	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:58:VAL:N	4:4:26:TYR:CA[12_555]	1.55	0.65
2:2:19:GLY:O	2:2:211:MET:CE[2_555]	1.55	0.65
2:2:37:VAL:N	2:2:207:ASN:O[12_555]	1.55	0.65
2:2:194:ARG:CZ	3:3:27:TRP:CZ2[12_555]	1.55	0.65
1:1:23:SER:O	1:1:81:ARG:O[12_555]	1.55	0.65
2:2:91:ILE:CG1	2:2:95:ASN:CA[2_555]	1.55	0.65
1:1:243:ALA:N	3:3:215:ALA:N[12_555]	1.55	0.65
1:1:18:PRO:CA	1:1:105:GLU:O[12_555]	1.55	0.65
3:3:12:GLN:O	3:3:188:TYR:O[12_555]	1.55	0.65
3:3:70:VAL:CG1	4:4:31:TYR:CB[12_555]	1.56	0.64
3:3:12:GLN:CB	3:3:187:GLY:CA[12_555]	1.56	0.64
2:2:54:THR:CA	2:2:56:PRO:C[3_555]	1.56	0.64
1:1:18:PRO:CB	1:1:105:GLU:N[12_555]	1.56	0.64
2:2:37:VAL:O	3:3:34:ILE:CD1[12_555]	1.56	0.64
1:1:41:HIS:CB	1:1:187:LEU:N[12_555]	1.56	0.64
2:2:179:LEU:O	4:4:42:ARG:CB[12_555]	1.56	0.64
1:1:73:ARG:CB	3:3:219:PHE:CZ[12_555]	1.56	0.64
2:2:88:ASP:C	2:2:258:ALA:O[2_555]	1.56	0.64
1:1:28:SER:C	1:1:162:SER:O[12_555]	1.56	0.64
2:2:41:TYR:CA	2:2:250:CYS:O[12_555]	1.56	0.64
3:3:66:SER:O	4:4:29:ILE:CA[12_555]	1.56	0.64
3:3:222:ARG:CA	3:3:226:ASP:C[12_555]	1.56	0.64
1:1:41:HIS:O	1:1:185:PRO:C[12_555]	1.56	0.64
1:1:50:ALA:O	1:1:145:TYR:CZ[12_555]	1.56	0.64
1:1:240:TYR:OH	3:3:169:TRP:CG[12_555]	1.56	0.64
1:1:69:SER:C	3:3:102:ILE:CG2[12_555]	1.56	0.64
1:1:51:ILE:CG1	1:1:237:THR:CB[12_555]	1.56	0.64
1:1:28:SER:OG	1:1:155:PRO:CG[12_555]	1.56	0.64
1:1:245:HIS:CD2	3:3:51:THR:CA[12_555]	1.56	0.64
2:2:176:ASP:OD2	4:4:44:ASP:CG[12_555]	1.56	0.64
1:1:176:GLY:C	3:3:150:GLY:N[12_555]	1.56	0.64
2:2:64:TYR:CG	2:2:257:ARG:CG[2_555]	1.56	0.64
2:2:52:LYS:O	2:2:61:ASN:OD1[3_555]	1.56	0.64
1:1:47:PRO:N	1:1:239:ILE:CG1[12_555]	1.56	0.64
1:1:75:GLY:O	3:3:218:ASP:CB[12_555]	1.57	0.63
3:3:106:TYR:O	3:3:224:ALA:C[12_555]	1.57	0.63
2:2:18:ARG:CB	2:2:51:ASN:ND2[2_555]	1.57	0.63
1:1:18:PRO:CD	1:1:106:MET:N[12_555]	1.57	0.63
3:3:222:ARG:C	3:3:225:ARG:C[12_555]	1.57	0.63
1:1:112:LYS:C	3:3:44:ILE:CG2[12_555]	1.57	0.63
1:1:182:PHE:CB	3:3:164:SER:C[12_555]	1.57	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:17:THR:O	2:2:49:ALA:O[2_555]	1.57	0.63
1:1:251:PRO:O	3:3:39:GLU:OE2[12_555]	1.57	0.63
1:1:243:ALA:CB	3:3:47:CYS:O[12_555]	1.57	0.63
1:1:28:SER:N	1:1:163:TRP:CE3[12_555]	1.57	0.63
1:1:171:ILE:CG1	3:3:153:VAL:CG1[12_555]	1.57	0.63
2:2:187:PRO:CG	3:3:33:GLU:CG[12_555]	1.57	0.63
2:2:38:TRP:CB	2:2:210:PRO:C[12_555]	1.57	0.63
1:1:36:ALA:N	3:3:25:LEU:CB[12_555]	1.57	0.63
2:2:59:SER:O	2:2:99:HIS:CG[2_555]	1.57	0.63
2:2:45:GLN:N	2:2:107:THR:N[12_555]	1.57	0.63
1:1:62:ARG:N	1:1:111:ARG:CG[12_555]	1.57	0.63
1:1:31:ALA:C	1:1:147:TYR:O[12_555]	1.57	0.63
2:2:32:VAL:CA	3:3:31:THR:OG1[12_555]	1.57	0.63
2:2:43:THR:OG1	2:2:105:GLY:O[12_555]	1.58	0.62
2:2:59:SER:N	2:2:253:PHE:C[2_555]	1.58	0.62
1:1:69:SER:N	3:3:98:LEU:O[12_555]	1.58	0.62
2:2:54:THR:N	2:2:57:ASP:CA[3_555]	1.58	0.62
1:1:181:ARG:CD	3:3:115:PHE:CB[12_555]	1.58	0.62
2:2:18:ARG:C	2:2:51:ASN:ND2[2_555]	1.58	0.62
2:2:89:MET:CA	2:2:258:ALA:O[2_555]	1.58	0.62
3:3:212:PHE:CE2	4:4:36:ALA:C[12_555]	1.58	0.62
3:3:24:ALA:O	3:3:162:THR:CB[12_555]	1.58	0.62
1:1:8:ASP:OD2	1:1:258:PRO:CG[12_555]	1.58	0.62
1:1:115:LEU:CA	3:3:42:ASN:N[12_555]	1.58	0.62
2:2:58:THR:O	2:2:253:PHE:O[2_555]	1.58	0.62
1:1:13:GLU:O	1:1:258:PRO:CA[12_555]	1.58	0.62
3:3:18:ASP:CB	3:3:94:LEU:CA[12_555]	1.58	0.62
1:1:76:CYS:C	3:3:218:ASP:CA[12_555]	1.58	0.62
3:3:210:LEU:N	4:4:32:PHE:O[12_555]	1.58	0.62
1:1:41:HIS:CD2	1:1:186:PHE:CD2[12_555]	1.58	0.62
1:1:241:HIS:CD2	3:3:114:ARG:CZ[12_555]	1.58	0.62
1:1:69:SER:O	3:3:102:ILE:C[12_555]	1.58	0.62
1:1:249:TRP:NE1	2:2:35:TYR:CE2[12_555]	1.58	0.62
2:2:179:LEU:N	4:4:43:LEU:N[12_555]	1.58	0.62
2:2:44:PRO:CB	2:2:247:SER:OG[12_555]	1.58	0.62
1:1:116:PHE:CB	3:3:45:GLU:OE2[12_555]	1.58	0.62
2:2:45:GLN:CA	2:2:106:TYR:C[12_555]	1.58	0.62
2:2:53:PRO:CB	2:2:58:THR:CB[3_555]	1.59	0.61
3:3:120:CYS:CA	4:4:33:LYS:CB[12_555]	1.59	0.61
3:3:69:THR:N	4:4:29:ILE:C[12_555]	1.59	0.61
1:1:73:ARG:CZ	3:3:103:ALA:C[12_555]	1.59	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:9:GLY:O	3:3:188:TYR:CD2[12_555]	1.59	0.61
3:3:26:PRO:CG	3:3:160:GLN:C[12_555]	1.59	0.61
2:2:187:PRO:CB	3:3:33:GLU:CB[12_555]	1.59	0.61
2:2:40:HIS:CE1	2:2:205:TYR:CB[12_555]	1.59	0.61
1:1:182:PHE:CD1	3:3:164:SER:C[12_555]	1.59	0.61
2:2:45:GLN:OE1	2:2:106:TYR:CB[12_555]	1.59	0.61
1:1:35:ASP:OD1	1:1:187:LEU:CD2[12_555]	1.59	0.61
3:3:119:PHE:O	4:4:33:LYS:CG[12_555]	1.59	0.61
1:1:177:GLN:NE2	3:3:145:LYS:O[12_555]	1.59	0.61
2:2:62:ARG:N	2:2:255:GLY:N[2_555]	1.59	0.61
1:1:51:ILE:CB	1:1:237:THR:CB[12_555]	1.59	0.61
2:2:89:MET:CA	2:2:258:ALA:C[2_555]	1.59	0.61
3:3:21:SER:CA	3:3:117:PHE:CG[12_555]	1.59	0.61
3:3:12:GLN:N	3:3:188:TYR:CB[12_555]	1.59	0.61
1:1:128:VAL:CG2	3:3:168:PRO:N[12_555]	1.59	0.61
2:2:47:ALA:N	2:2:249:MET:CE[12_555]	1.59	0.61
1:1:17:VAL:N	1:1:107:ALA:CB[12_555]	1.59	0.61
2:2:45:GLN:NE2	2:2:246:ILE:CG2[12_555]	1.59	0.61
3:3:119:PHE:O	4:4:33:LYS:CE[12_555]	1.59	0.61
1:1:39:THR:CB	3:3:28:TYR:CE2[12_555]	1.59	0.61
2:2:12:ARG:C	2:2:13:ILE:CG1[11_555]	1.59	0.61
2:2:201:LEU:CA	3:3:32:LYS:CG[12_555]	1.60	0.60
2:2:52:LYS:NZ	2:2:252:GLU:OE2[10_555]	1.60	0.60
2:2:88:ASP:C	2:2:259:LYS:N[2_555]	1.60	0.60
3:3:70:VAL:O	4:4:31:TYR:CA[12_555]	1.60	0.60
1:1:122:ASP:O	3:3:50:ASP:CA[12_555]	1.60	0.60
2:2:91:ILE:CD1	2:2:95:ASN:C[2_555]	1.60	0.60
1:1:72:GLY:C	3:3:99:ILE:CD1[12_555]	1.60	0.60
1:1:11:LEU:O	3:3:231:ILE:CD1[12_555]	1.60	0.60
1:1:17:VAL:CA	1:1:106:MET:O[12_555]	1.60	0.60
3:3:56:ASN:O	4:4:27:PHE:N[12_555]	1.60	0.60
1:1:243:ALA:CB	3:3:47:CYS:C[12_555]	1.60	0.60
1:1:240:TYR:CB	3:3:112:SER:C[12_555]	1.60	0.60
1:1:71:LEU:CD1	3:3:43:LEU:O[12_555]	1.60	0.60
2:2:59:SER:N	2:2:253:PHE:O[2_555]	1.60	0.60
3:3:105:TYR:CA	3:3:106:TYR:CE2[12_555]	1.60	0.60
2:2:52:LYS:O	2:2:61:ASN:ND2[3_555]	1.60	0.60
1:1:48:GLU:CG	1:1:78:HIS:CG[12_555]	1.60	0.60
1:1:55:TYR:CB	1:1:81:ARG:CZ[12_555]	1.60	0.60
2:2:189:GLN:CD	3:3:30:PRO:O[12_555]	1.60	0.60
2:2:29:ALA:O	3:3:29:HIS:O[12_555]	1.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:121:PHE:CA	3:3:49:VAL:CG1[12_555]	1.61	0.59
1:1:17:VAL:CB	1:1:106:MET:O[12_555]	1.61	0.59
3:3:67:MET:CG	4:4:27:PHE:CD1[12_555]	1.61	0.59
3:3:67:MET:N	4:4:27:PHE:O[12_555]	1.61	0.59
1:1:7:ILE:CA	1:1:275:THR:CB[12_555]	1.61	0.59
1:1:182:PHE:O	3:3:115:PHE:O[12_555]	1.61	0.59
1:1:54:ARG:C	1:1:81:ARG:NE[12_555]	1.61	0.59
2:2:89:MET:CB	2:2:258:ALA:N[2_555]	1.61	0.59
2:2:88:ASP:C	2:2:258:ALA:C[2_555]	1.61	0.59
2:2:59:SER:CB	2:2:253:PHE:CD2[2_555]	1.61	0.59
3:3:20:GLN:O	3:3:117:PHE:CE2[12_555]	1.61	0.59
1:1:73:ARG:NH1	3:3:103:ALA:C[12_555]	1.61	0.59
1:1:55:TYR:C	1:1:81:ARG:NH2[12_555]	1.61	0.59
1:1:249:TRP:C	3:3:39:GLU:N[12_555]	1.61	0.59
1:1:41:HIS:CA	1:1:186:PHE:C[12_555]	1.61	0.59
1:1:25:HIS:C	1:1:223:ARG:CA[12_555]	1.61	0.59
1:1:248:ALA:C	1:1:251:PRO:CD[12_555]	1.61	0.59
1:1:69:SER:OG	3:3:102:ILE:N[12_555]	1.61	0.59
1:1:53:THR:N	1:1:80:SER:O[12_555]	1.61	0.59
1:1:9:GLU:O	1:1:277:ALA:CB[12_555]	1.61	0.59
2:2:41:TYR:CD2	2:2:41:TYR:CE2[12_555]	1.61	0.59
2:2:41:TYR:CE1	2:2:52:LYS:NZ[2_555]	1.61	0.59
1:1:183:SER:OG	3:3:116:SER:O[12_555]	1.61	0.59
1:1:74:SER:OG	3:3:113:LEU:CD2[12_555]	1.61	0.59
1:1:244:LYS:O	3:3:51:THR:N[12_555]	1.61	0.59
2:2:46:ASP:CG	2:2:203:VAL:C[12_555]	1.61	0.59
2:2:62:ARG:NH2	2:2:101:LEU:CA[2_555]	1.61	0.59
2:2:40:HIS:O	2:2:103:ARG:NE[12_555]	1.61	0.59
1:1:68:GLU:CB	3:3:98:LEU:CA[12_555]	1.61	0.59
3:3:58:VAL:N	4:4:26:TYR:CG[12_555]	1.61	0.59
3:3:67:MET:SD	4:4:27:PHE:CZ[12_555]	1.62	0.58
1:1:53:THR:CG2	1:1:80:SER:C[12_555]	1.62	0.58
1:1:116:PHE:CD1	3:3:40:VAL:CG1[12_555]	1.62	0.58
1:1:181:ARG:CD	3:3:115:PHE:CG[12_555]	1.62	0.58
2:2:40:HIS:CB	2:2:103:ARG:CB[12_555]	1.62	0.58
2:2:62:ARG:CG	2:2:255:GLY:CA[2_555]	1.62	0.58
2:2:58:THR:CG2	2:2:253:PHE:N[2_555]	1.62	0.58
1:1:177:GLN:CA	3:3:148:MET:N[12_555]	1.62	0.58
3:3:68:TYR:CA	4:4:30:ASN:ND2[12_555]	1.62	0.58
3:3:52:LEU:C	4:4:39:GLY:CA[12_555]	1.62	0.58
1:1:241:HIS:CD2	3:3:215:ALA:O[12_555]	1.62	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:20:GLN:CB	3:3:211:CYS:CB[12_555]	1.62	0.58
1:1:77:VAL:O	3:3:217:LYS:CD[12_555]	1.62	0.58
1:1:122:ASP:CA	3:3:50:ASP:CG[12_555]	1.62	0.58
2:2:18:ARG:CA	2:2:51:ASN:ND2[2_555]	1.62	0.58
1:1:63:ASP:CB	1:1:111:ARG:NH2[12_555]	1.62	0.58
1:1:108:GLN:CG	3:3:220:CYS:CB[12_555]	1.62	0.58
1:1:34:LEU:CB	1:1:169:MET:CB[12_555]	1.62	0.58
1:1:17:VAL:CG1	1:1:107:ALA:O[12_555]	1.62	0.58
3:3:211:CYS:O	4:4:38:SER:O[12_555]	1.62	0.58
1:1:65:MET:CE	1:1:112:LYS:CE[12_555]	1.62	0.58
1:1:27:THR:N	1:1:223:ARG:CD[12_555]	1.62	0.58
2:2:32:VAL:N	3:3:32:LYS:N[12_555]	1.62	0.58
1:1:7:ILE:N	1:1:275:THR:CA[12_555]	1.62	0.58
3:3:23:CYS:C	3:3:162:THR:C[12_555]	1.62	0.58
1:1:69:SER:CA	3:3:102:ILE:CB[12_555]	1.62	0.58
3:3:12:GLN:O	3:3:188:TYR:CA[12_555]	1.63	0.57
2:2:38:TRP:CA	2:2:209:VAL:C[12_555]	1.63	0.57
3:3:52:LEU:O	4:4:40:ALA:N[12_555]	1.63	0.57
1:1:244:LYS:NZ	3:3:212:PHE:CB[12_555]	1.63	0.57
2:2:176:ASP:OD1	4:4:44:ASP:OD2[12_555]	1.63	0.57
2:2:41:TYR:CE1	2:2:252:GLU:CD[12_555]	1.63	0.57
2:2:178:THR:CG2	4:4:44:ASP:CA[12_555]	1.63	0.57
1:1:254:PRO:C	4:4:43:LEU:CG[12_555]	1.63	0.57
1:1:241:HIS:N	3:3:216:CYS:CB[12_555]	1.63	0.57
1:1:23:SER:O	1:1:81:ARG:C[12_555]	1.63	0.57
1:1:44:ASN:OD1	5:1:288:SUC:O3[12_555]	1.63	0.57
1:1:7:ILE:CD1	1:1:275:THR:OG1[12_555]	1.63	0.57
1:1:7:ILE:CB	1:1:275:THR:CG2[12_555]	1.63	0.57
3:3:53:ILE:N	4:4:38:SER:C[12_555]	1.63	0.57
1:1:179:PHE:CG	3:3:133:TYR:CB[12_555]	1.63	0.57
2:2:13:ILE:C	2:2:13:ILE:O[11_555]	1.63	0.57
3:3:106:TYR:CB	3:3:224:ALA:C[12_555]	1.63	0.57
1:1:64:GLU:OE1	3:3:104:SER:O[12_555]	1.63	0.57
3:3:66:SER:C	4:4:28:ASN:CA[12_555]	1.63	0.57
1:1:9:GLU:CG	1:1:276:THR:OG1[12_555]	1.63	0.57
1:1:68:GLU:CA	3:3:98:LEU:O[12_555]	1.63	0.57
3:3:18:ASP:N	3:3:94:LEU:CA[12_555]	1.63	0.57
3:3:13:PHE:CA	3:3:87:VAL:CG2[12_555]	1.64	0.56
2:2:31:ALA:O	3:3:31:THR:CA[12_555]	1.64	0.56
3:3:66:SER:O	4:4:28:ASN:O[12_555]	1.64	0.56
1:1:14:VAL:CG2	1:1:257:VAL:N[12_555]	1.64	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:54:THR:C	2:2:57:ASP:O[3_555]	1.64	0.56
3:3:222:ARG:CA	3:3:226:ASP:CA[12_555]	1.64	0.56
1:1:15:LEU:CD2	1:1:255:ARG:CB[12_555]	1.64	0.56
2:2:13:ILE:O	2:2:13:ILE:CG2[11_555]	1.64	0.56
3:3:52:LEU:N	4:4:39:GLY:O[12_555]	1.64	0.56
1:1:26:THR:CB	1:1:163:TRP:CZ3[12_555]	1.64	0.56
1:1:41:HIS:NE2	1:1:188:SER:O[12_555]	1.64	0.56
1:1:116:PHE:N	3:3:41:LYS:N[12_555]	1.64	0.56
1:1:246:THR:O	2:2:185:ILE:CB[12_555]	1.64	0.56
1:1:6:TYR:O	1:1:276:THR:O[12_555]	1.64	0.56
1:1:178:PRO:N	3:3:147:ALA:O[12_555]	1.64	0.56
3:3:67:MET:CB	4:4:28:ASN:N[12_555]	1.64	0.56
2:2:202:ILE:C	3:3:34:ILE:CG2[12_555]	1.64	0.56
2:2:174:ASN:CB	4:4:44:ASP:OD1[12_555]	1.64	0.56
1:1:69:SER:CB	3:3:102:ILE:CA[12_555]	1.64	0.56
2:2:195:SER:OG	3:3:27:TRP:CA[12_555]	1.64	0.56
1:1:73:ARG:NH1	3:3:103:ALA:CA[12_555]	1.65	0.55
1:1:68:GLU:CG	3:3:98:LEU:N[12_555]	1.65	0.55
1:1:250:CYS:O	3:3:39:GLU:CG[12_555]	1.65	0.55
3:3:23:CYS:C	3:3:163:ILE:N[12_555]	1.65	0.55
1:1:249:TRP:CE2	2:2:35:TYR:CZ[12_555]	1.65	0.55
2:2:250:CYS:SG	2:2:252:GLU:OE1[12_555]	1.65	0.55
1:1:121:PHE:CD1	3:3:48:GLN:C[12_555]	1.65	0.55
2:2:44:PRO:N	2:2:248:PRO:C[12_555]	1.65	0.55
1:1:38:GLU:OE1	3:3:27:TRP:CA[12_555]	1.65	0.55
1:1:125:ILE:CG1	3:3:114:ARG:CD[12_555]	1.65	0.55
1:1:5:ASN:CG	2:2:173:LEU:CG[12_555]	1.65	0.55
2:2:12:ARG:C	2:2:13:ILE:CB[11_555]	1.65	0.55
2:2:44:PRO:CD	2:2:249:MET:N[12_555]	1.65	0.55
1:1:242:LYS:CB	3:3:214:SER:O[12_555]	1.65	0.55
1:1:122:ASP:CB	3:3:50:ASP:CG[12_555]	1.65	0.55
1:1:9:GLU:O	1:1:277:ALA:CA[12_555]	1.65	0.55
1:1:254:PRO:O	4:4:43:LEU:CB[12_555]	1.65	0.55
1:1:240:TYR:CE2	3:3:112:SER:N[12_555]	1.65	0.55
2:2:187:PRO:CA	3:3:33:GLU:CG[12_555]	1.65	0.55
1:1:29:ASN:O	1:1:146:MET:CE[12_555]	1.65	0.55
1:1:113:PHE:CZ	3:3:48:GLN:CG[12_555]	1.65	0.55
2:2:20:ASP:OD2	2:2:102:GLY:O[2_555]	1.65	0.55
1:1:61:THR:CG2	3:3:230:HIS:CB[12_555]	1.66	0.54
3:3:53:ILE:CA	4:4:39:GLY:N[12_555]	1.66	0.54
1:1:68:GLU:O	3:3:99:ILE:N[12_555]	1.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:26:THR:CG2	1:1:222:SER:CA[12_555]	1.66	0.54
1:1:242:LYS:C	3:3:214:SER:O[12_555]	1.66	0.54
3:3:56:ASN:OD1	4:4:29:ILE:CG2[12_555]	1.66	0.54
2:2:11:ASP:C	2:2:13:ILE:CD1[11_555]	1.66	0.54
1:1:73:ARG:O	3:3:219:PHE:CE1[12_555]	1.66	0.54
1:1:242:LYS:N	3:3:214:SER:O[12_555]	1.66	0.54
1:1:176:GLY:C	3:3:149:LEU:CA[12_555]	1.66	0.54
2:2:54:THR:N	2:2:57:ASP:O[3_555]	1.66	0.54
1:1:240:TYR:OH	3:3:169:TRP:CD2[12_555]	1.66	0.54
1:1:32:PRO:N	1:1:147:TYR:C[12_555]	1.66	0.54
1:1:68:GLU:C	3:3:98:LEU:C[12_555]	1.66	0.54
2:2:46:ASP:CG	2:2:203:VAL:CA[12_555]	1.66	0.54
1:1:16:VAL:CG1	1:1:259:TYR:CD1[12_555]	1.66	0.54
2:2:39:PRO:CG	2:2:42:LEU:CD1[12_555]	1.66	0.54
2:2:203:VAL:CG2	3:3:34:ILE:C[12_555]	1.66	0.54
1:1:69:SER:CA	3:3:102:ILE:CA[12_555]	1.66	0.54
2:2:62:ARG:CG	2:2:254:SER:O[2_555]	1.66	0.54
3:3:17:ASP:C	3:3:94:LEU:CB[12_555]	1.66	0.54
3:3:16:THR:C	3:3:89:ILE:N[12_555]	1.66	0.54
3:3:209:MET:CE	4:4:32:PHE:CE1[12_555]	1.67	0.53
1:1:38:GLU:CA	3:3:28:TYR:O[12_555]	1.67	0.53
1:1:116:PHE:CE2	3:3:40:VAL:CG1[12_555]	1.67	0.53
1:1:32:PRO:C	1:1:147:TYR:CG[12_555]	1.67	0.53
2:2:195:SER:OG	3:3:27:TRP:CD1[12_555]	1.67	0.53
1:1:33:LEU:CD2	1:1:171:ILE:CG2[12_555]	1.67	0.53
2:2:39:PRO:C	2:2:103:ARG:NH1[12_555]	1.67	0.53
1:1:73:ARG:CD	3:3:103:ALA:CB[12_555]	1.67	0.53
3:3:222:ARG:N	3:3:225:ARG:O[12_555]	1.67	0.53
2:2:91:ILE:CD1	2:2:95:ASN:CB[2_555]	1.67	0.53
2:2:59:SER:CB	2:2:253:PHE:CG[2_555]	1.67	0.53
2:2:37:VAL:N	2:2:208:ALA:CA[12_555]	1.67	0.53
1:1:115:LEU:O	3:3:41:LYS:N[12_555]	1.67	0.53
1:1:249:TRP:CZ2	2:2:35:TYR:CD1[12_555]	1.67	0.53
3:3:58:VAL:CG1	4:4:26:TYR:CD1[12_555]	1.67	0.53
3:3:69:THR:CB	4:4:30:ASN:N[12_555]	1.67	0.53
2:2:41:TYR:C	2:2:250:CYS:O[12_555]	1.67	0.53
1:1:32:PRO:CG	1:1:147:TYR:CA[12_555]	1.67	0.53
1:1:7:ILE:N	1:1:276:THR:N[12_555]	1.67	0.53
1:1:180:PRO:C	3:3:165:LEU:CG[12_555]	1.67	0.53
3:3:21:SER:O	3:3:117:PHE:CB[12_555]	1.67	0.53
3:3:65:VAL:CA	4:4:28:ASN:OD1[12_555]	1.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:32:PRO:CB	1:1:147:TYR:CA[12_555]	1.67	0.53
1:1:41:HIS:CA	1:1:186:PHE:CG[12_555]	1.67	0.53
2:2:36:GLY:O	2:2:208:ALA:C[12_555]	1.67	0.53
1:1:127:LEU:C	3:3:168:PRO:CD[12_555]	1.67	0.53
1:1:72:GLY:C	3:3:99:ILE:CG2[12_555]	1.68	0.52
2:2:17:THR:CA	2:2:49:ALA:C[2_555]	1.68	0.52
3:3:16:THR:CB	3:3:89:ILE:CB[12_555]	1.68	0.52
1:1:76:CYS:CA	3:3:218:ASP:CB[12_555]	1.68	0.52
3:3:13:PHE:O	3:3:186:ALA:C[12_555]	1.68	0.52
2:2:179:LEU:CB	4:4:42:ARG:CB[12_555]	1.68	0.52
1:1:124:GLU:CA	3:3:114:ARG:O[12_555]	1.68	0.52
1:1:179:PHE:N	3:3:133:TYR:N[12_555]	1.68	0.52
1:1:8:ASP:CB	1:1:275:THR:O[12_555]	1.68	0.52
3:3:26:PRO:C	3:3:160:GLN:O[12_555]	1.68	0.52
2:2:62:ARG:CA	2:2:255:GLY:CA[2_555]	1.68	0.52
1:1:18:PRO:C	1:1:105:GLU:C[12_555]	1.68	0.52
2:2:189:GLN:NE2	3:3:30:PRO:C[12_555]	1.68	0.52
1:1:26:THR:CG2	1:1:222:SER:C[12_555]	1.68	0.52
1:1:124:GLU:C	3:3:114:ARG:C[12_555]	1.68	0.52
1:1:39:THR:CG2	3:3:28:TYR:CE1[12_555]	1.68	0.52
1:1:50:ALA:O	1:1:145:TYR:CG[12_555]	1.68	0.52
1:1:240:TYR:O	3:3:216:CYS:SG[12_555]	1.68	0.52
1:1:27:THR:O	1:1:163:TRP:CD1[12_555]	1.68	0.52
2:2:194:ARG:NH1	3:3:27:TRP:CZ3[12_555]	1.68	0.52
1:1:35:ASP:CA	3:3:25:LEU:CD1[12_555]	1.68	0.52
1:1:177:GLN:CA	3:3:148:MET:C[12_555]	1.68	0.52
1:1:77:VAL:N	3:3:218:ASP:OD1[12_555]	1.68	0.52
1:1:14:VAL:C	1:1:255:ARG:CG[12_555]	1.68	0.52
1:1:9:GLU:O	1:1:277:ALA:N[12_555]	1.68	0.52
1:1:252:ARG:CG	3:3:41:LYS:CB[12_555]	1.68	0.52
3:3:222:ARG:CA	3:3:225:ARG:O[12_555]	1.69	0.51
1:1:46:GLN:O	1:1:239:ILE:CD1[12_555]	1.69	0.51
2:2:41:TYR:CD1	2:2:252:GLU:CD[12_555]	1.69	0.51
2:2:62:ARG:NH1	2:2:101:LEU:C[2_555]	1.69	0.51
1:1:126:THR:C	3:3:166:VAL:CA[12_555]	1.69	0.51
2:2:37:VAL:N	2:2:208:ALA:C[12_555]	1.69	0.51
3:3:17:ASP:OD1	3:3:87:VAL:CA[12_555]	1.69	0.51
1:1:68:GLU:CB	3:3:98:LEU:CB[12_555]	1.69	0.51
3:3:118:MET:CE	4:4:34:ASP:CA[12_555]	1.69	0.51
1:1:73:ARG:C	3:3:219:PHE:CE1[12_555]	1.69	0.51
1:1:7:ILE:C	1:1:275:THR:CG2[12_555]	1.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:21:SER:N	3:3:117:PHE:CE2[12_555]	1.69	0.51
3:3:222:ARG:N	3:3:225:ARG:C[12_555]	1.69	0.51
1:1:76:CYS:C	3:3:218:ASP:OD1[12_555]	1.69	0.51
1:1:50:ALA:CA	1:1:145:TYR:CD1[12_555]	1.70	0.50
3:3:69:THR:O	4:4:29:ILE:CA[12_555]	1.70	0.50
1:1:115:LEU:N	3:3:42:ASN:CB[12_555]	1.70	0.50
2:2:179:LEU:O	4:4:42:ARG:N[12_555]	1.70	0.50
1:1:53:THR:CB	1:1:80:SER:CA[12_555]	1.70	0.50
1:1:182:PHE:N	3:3:165:LEU:CA[12_555]	1.70	0.50
3:3:210:LEU:N	4:4:32:PHE:C[12_555]	1.70	0.50
1:1:62:ARG:C	1:1:111:ARG:NE[12_555]	1.70	0.50
3:3:22:PRO:CD	3:3:117:PHE:CG[12_555]	1.70	0.50
1:1:64:GLU:CG	3:3:104:SER:O[12_555]	1.70	0.50
2:2:64:TYR:CE2	2:2:255:GLY:O[2_555]	1.70	0.50
1:1:5:ASN:OD1	2:2:173:LEU:CD2[12_555]	1.70	0.50
1:1:180:PRO:CD	3:3:151:THR:CG2[12_555]	1.70	0.50
1:1:179:PHE:CD2	3:3:133:TYR:CD2[12_555]	1.70	0.50
2:2:89:MET:CG	2:2:257:ARG:C[2_555]	1.70	0.50
1:1:182:PHE:CA	3:3:165:LEU:N[12_555]	1.70	0.50
2:2:62:ARG:CG	2:2:255:GLY:C[2_555]	1.70	0.50
1:1:181:ARG:NH1	3:3:115:PHE:CD2[12_555]	1.70	0.50
1:1:242:LYS:N	3:3:215:ALA:CA[12_555]	1.70	0.50
1:1:68:GLU:CB	3:3:98:LEU:CD1[12_555]	1.70	0.50
3:3:70:VAL:CA	4:4:31:TYR:CB[12_555]	1.70	0.50
2:2:44:PRO:CG	2:2:247:SER:O[12_555]	1.70	0.50
1:1:48:GLU:CD	1:1:78:HIS:CB[12_555]	1.70	0.50
2:2:44:PRO:CG	2:2:248:PRO:CA[12_555]	1.71	0.49
1:1:7:ILE:CG1	1:1:275:THR:CB[12_555]	1.71	0.49
1:1:51:ILE:CA	1:1:237:THR:OG1[12_555]	1.71	0.49
1:1:177:GLN:CG	3:3:148:MET:CG[12_555]	1.71	0.49
1:1:62:ARG:NE	1:1:110:ARG:N[12_555]	1.71	0.49
1:1:71:LEU:C	3:3:47:CYS:SG[12_555]	1.71	0.49
1:1:20:ILE:CB	1:1:79:ILE:CG1[12_555]	1.71	0.49
3:3:106:TYR:N	3:3:224:ALA:CB[12_555]	1.71	0.49
3:3:209:MET:CB	4:4:32:PHE:CA[12_555]	1.71	0.49
2:2:201:LEU:CD2	3:3:32:LYS:CA[12_555]	1.71	0.49
3:3:120:CYS:N	4:4:33:LYS:CG[12_555]	1.71	0.49
1:1:10:VAL:CA	1:1:277:ALA:C[12_555]	1.71	0.49
3:3:13:PHE:O	3:3:186:ALA:O[12_555]	1.71	0.49
2:2:179:LEU:O	4:4:42:ARG:CA[12_555]	1.71	0.49
1:1:74:SER:CA	3:3:113:LEU:CD2[12_555]	1.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:251:PRO:N	3:3:40:VAL:O[12_555]	1.71	0.49
3:3:12:GLN:N	3:3:188:TYR:N[12_555]	1.71	0.49
2:2:181:GLY:O	4:4:41:SER:CB[12_555]	1.71	0.49
1:1:177:GLN:C	3:3:147:ALA:O[12_555]	1.71	0.49
1:1:70:PHE:CA	3:3:102:ILE:CG2[12_555]	1.71	0.49
1:1:177:GLN:CA	3:3:147:ALA:O[12_555]	1.71	0.49
1:1:12:ASN:O	3:3:230:HIS:C[12_555]	1.71	0.49
1:1:40:GLY:CA	3:3:30:PRO:CG[12_555]	1.71	0.49
1:1:68:GLU:OE2	3:3:98:LEU:CB[12_555]	1.71	0.49
1:1:46:GLN:C	1:1:239:ILE:CG2[12_555]	1.71	0.49
1:1:254:PRO:CG	4:4:43:LEU:CD1[12_555]	1.71	0.49
3:3:209:MET:N	4:4:31:TYR:C[12_555]	1.71	0.49
2:2:13:ILE:C	2:2:13:ILE:C[11_555]	1.71	0.49
1:1:183:SER:CA	3:3:116:SER:OG[12_555]	1.71	0.49
1:1:240:TYR:N	3:3:112:SER:CB[12_555]	1.71	0.49
1:1:70:PHE:CG	3:3:43:LEU:CD1[12_555]	1.71	0.49
2:2:182:ASN:OD1	4:4:41:SER:N[12_555]	1.72	0.48
1:1:128:VAL:CG2	3:3:168:PRO:CA[12_555]	1.72	0.48
3:3:67:MET:CG	4:4:27:PHE:CD2[12_555]	1.72	0.48
2:2:59:SER:O	2:2:99:HIS:CE1[12_555]	1.72	0.48
1:1:17:VAL:CG1	1:1:108:GLN:CA[12_555]	1.72	0.48
2:2:53:PRO:O	2:2:57:ASP:CG[3_555]	1.72	0.48
1:1:9:GLU:C	1:1:277:ALA:CA[12_555]	1.72	0.48
3:3:118:MET:CB	4:4:34:ASP:CB[12_555]	1.72	0.48
2:2:201:LEU:CA	3:3:32:LYS:CD[12_555]	1.72	0.48
2:2:53:PRO:O	2:2:57:ASP:CB[3_555]	1.72	0.48
2:2:200:THR:O	3:3:32:LYS:CB[12_555]	1.72	0.48
3:3:10:SER:O	3:3:140:GLU:CA[12_555]	1.72	0.48
2:2:41:TYR:CE1	2:2:252:GLU:CG[12_555]	1.72	0.48
1:1:121:PHE:CB	3:3:49:VAL:CG1[12_555]	1.72	0.48
3:3:58:VAL:CG2	4:4:26:TYR:CE1[12_555]	1.72	0.48
3:3:212:PHE:CD2	4:4:36:ALA:O[12_555]	1.72	0.48
3:3:15:THR:CB	3:3:109:TRP:CZ2[12_555]	1.72	0.48
2:2:248:PRO:CG	2:2:256:ALA:CB[2_555]	1.72	0.48
1:1:169:MET:CE	3:3:163:ILE:CD1[12_555]	1.72	0.48
1:1:116:PHE:O	3:3:45:GLU:OE1[12_555]	1.72	0.48
1:1:28:SER:OG	1:1:163:TRP:NE1[12_555]	1.72	0.48
2:2:199:ALA:CA	3:3:29:HIS:NE2[12_555]	1.72	0.48
2:2:29:ALA:C	3:3:29:HIS:O[12_555]	1.72	0.48
3:3:106:TYR:O	3:3:224:ALA:N[12_555]	1.72	0.48
3:3:10:SER:CB	3:3:140:GLU:CD[12_555]	1.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:73:ARG:NH1	3:3:103:ALA:CB[12_555]	1.72	0.48
1:1:126:THR:N	3:3:166:VAL:CA[12_555]	1.72	0.48
1:1:124:GLU:CG	3:3:114:ARG:C[12_555]	1.72	0.48
1:1:49:ASP:CB	1:1:220:ILE:CG1[12_555]	1.73	0.47
1:1:125:ILE:CG2	3:3:166:VAL:CG2[12_555]	1.73	0.47
3:3:19:MET:CG	3:3:85:ILE:CG2[12_555]	1.73	0.47
1:1:176:GLY:C	3:3:149:LEU:C[12_555]	1.73	0.47
3:3:20:GLN:CA	3:3:211:CYS:CB[12_555]	1.73	0.47
1:1:181:ARG:N	3:3:165:LEU:CB[12_555]	1.73	0.47
1:1:67:ILE:CB	3:3:46:MET:SD[12_555]	1.73	0.47
2:2:29:ALA:CB	3:3:29:HIS:CB[12_555]	1.73	0.47
3:3:222:ARG:CB	3:3:227:THR:N[12_555]	1.73	0.47
1:1:240:TYR:CZ	3:3:169:TRP:CB[12_555]	1.73	0.47
1:1:76:CYS:N	3:3:218:ASP:CB[12_555]	1.73	0.47
2:2:187:PRO:CG	3:3:33:GLU:CD[12_555]	1.73	0.47
1:1:183:SER:C	3:3:116:SER:CB[12_555]	1.73	0.47
2:2:40:HIS:CD2	2:2:205:TYR:CD1[12_555]	1.73	0.47
1:1:246:THR:C	2:2:185:ILE:CG1[12_555]	1.73	0.47
1:1:121:PHE:CG	3:3:49:VAL:CA[12_555]	1.73	0.47
3:3:12:GLN:C	3:3:187:GLY:C[12_555]	1.73	0.47
1:1:17:VAL:N	1:1:107:ALA:C[12_555]	1.73	0.47
2:2:47:ALA:CA	2:2:249:MET:SD[12_555]	1.73	0.47
1:1:55:TYR:N	1:1:81:ARG:CZ[12_555]	1.73	0.47
1:1:70:PHE:N	3:3:102:ILE:CD1[12_555]	1.73	0.47
1:1:241:HIS:ND1	3:3:215:ALA:C[12_555]	1.73	0.47
2:2:20:ASP:O	2:2:101:LEU:CD2[12_555]	1.73	0.47
1:1:241:HIS:O	3:3:216:CYS:N[12_555]	1.73	0.47
1:1:76:CYS:CB	3:3:218:ASP:CG[12_555]	1.73	0.47
1:1:14:VAL:CB	1:1:255:ARG:C[12_555]	1.73	0.47
1:1:53:THR:OG1	1:1:79:ILE:CA[12_555]	1.74	0.46
2:2:182:ASN:CG	4:4:41:SER:C[12_555]	1.74	0.46
2:2:13:ILE:CA	2:2:13:ILE:CB[11_555]	1.74	0.46
3:3:24:ALA:C	3:3:162:THR:C[12_555]	1.74	0.46
1:1:171:ILE:CG1	3:3:153:VAL:CB[12_555]	1.74	0.46
1:1:50:ALA:CB	1:1:127:LEU:CD2[12_555]	1.74	0.46
1:1:13:GLU:OE2	3:3:231:ILE:CG1[12_555]	1.74	0.46
1:1:75:GLY:C	3:3:218:ASP:CB[12_555]	1.74	0.46
2:2:173:LEU:CD2	4:4:42:ARG:NE[12_555]	1.74	0.46
1:1:126:THR:OG1	3:3:113:LEU:O[12_555]	1.74	0.46
2:2:31:ALA:O	3:3:31:THR:OG1[12_555]	1.74	0.46
3:3:9:GLY:C	3:3:188:TYR:CE2[12_555]	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:11:ASP:CB	2:2:26:ASP:CA[11_555]	1.74	0.46
1:1:249:TRP:NE1	2:2:35:TYR:CE1[12_555]	1.74	0.46
3:3:23:CYS:O	3:3:162:THR:N[12_555]	1.74	0.46
1:1:181:ARG:O	3:3:165:LEU:CB[12_555]	1.74	0.46
1:1:25:HIS:CB	1:1:223:ARG:C[12_555]	1.74	0.46
1:1:10:VAL:N	1:1:276:THR:O[12_555]	1.74	0.46
2:2:201:LEU:C	3:3:32:LYS:CG[12_555]	1.74	0.46
1:1:246:THR:CG2	3:3:46:MET:O[12_555]	1.74	0.46
3:3:222:ARG:CA	3:3:226:ASP:N[12_555]	1.74	0.46
3:3:69:THR:C	4:4:30:ASN:N[12_555]	1.74	0.46
1:1:124:GLU:O	3:3:114:ARG:N[12_555]	1.74	0.46
2:2:194:ARG:NH1	3:3:27:TRP:CZ2[12_555]	1.74	0.46
1:1:69:SER:O	3:3:102:ILE:CA[12_555]	1.74	0.46
2:2:201:LEU:CA	3:3:32:LYS:CE[12_555]	1.74	0.46
2:2:62:ARG:O	2:2:255:GLY:CA[2_555]	1.74	0.46
1:1:16:VAL:C	1:1:107:ALA:CA[12_555]	1.74	0.46
1:1:241:HIS:C	3:3:216:CYS:N[12_555]	1.74	0.46
1:1:122:ASP:C	3:3:50:ASP:OD1[12_555]	1.75	0.45
3:3:212:PHE:CD2	4:4:36:ALA:C[12_555]	1.75	0.45
1:1:26:THR:C	1:1:163:TRP:CZ3[12_555]	1.75	0.45
3:3:14:MET:C	3:3:87:VAL:O[12_555]	1.75	0.45
3:3:70:VAL:CA	4:4:31:TYR:CD1[12_555]	1.75	0.45
2:2:11:ASP:O	2:2:26:ASP:OD1[11_555]	1.75	0.45
2:2:202:ILE:N	3:3:32:LYS:CG[12_555]	1.75	0.45
3:3:212:PHE:CE2	4:4:35:ALA:O[12_555]	1.75	0.45
2:2:89:MET:CG	2:2:258:ALA:CA[2_555]	1.75	0.45
2:2:38:TRP:CG	2:2:211:MET:N[12_555]	1.75	0.45
1:1:171:ILE:CD1	3:3:153:VAL:CG1[12_555]	1.75	0.45
2:2:18:ARG:CZ	2:2:50:ILE:CG2[2_555]	1.75	0.45
1:1:7:ILE:CA	1:1:275:THR:CG2[12_555]	1.75	0.45
2:2:63:PHE:N	2:2:255:GLY:CA[2_555]	1.75	0.45
2:2:195:SER:N	3:3:27:TRP:CD1[12_555]	1.75	0.45
3:3:222:ARG:C	3:3:225:ARG:O[12_555]	1.75	0.45
2:2:45:GLN:CA	2:2:107:THR:CA[12_555]	1.75	0.45
1:1:62:ARG:CB	1:1:111:ARG:CG[12_555]	1.75	0.45
1:1:113:PHE:O	3:3:42:ASN:CB[12_555]	1.75	0.45
1:1:51:ILE:CG1	1:1:237:THR:CA[12_555]	1.75	0.45
3:3:13:PHE:C	3:3:87:VAL:CB[12_555]	1.75	0.45
2:2:32:VAL:N	3:3:31:THR:OG1[12_555]	1.75	0.45
1:1:243:ALA:N	3:3:214:SER:C[12_555]	1.75	0.45
1:1:60:GLN:CB	1:1:108:GLN:NE2[12_555]	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:244:LYS:CA	3:3:51:THR:N[12_555]	1.75	0.45
2:2:31:ALA:C	3:3:31:THR:OG1[12_555]	1.75	0.45
3:3:106:TYR:C	3:3:224:ALA:CA[12_555]	1.75	0.45
3:3:67:MET:CA	4:4:27:PHE:CA[12_555]	1.75	0.45
1:1:68:GLU:OE1	3:3:51:THR:CB[12_555]	1.75	0.45
2:2:187:PRO:O	3:3:33:GLU:OE1[12_555]	1.75	0.45
1:1:242:LYS:CA	3:3:215:ALA:CA[12_555]	1.75	0.45
2:2:64:TYR:CD2	2:2:255:GLY:O[2_555]	1.75	0.45
1:1:242:LYS:CE	3:3:213:VAL:CG1[12_555]	1.76	0.44
3:3:52:LEU:C	4:4:39:GLY:N[12_555]	1.76	0.44
2:2:178:THR:C	4:4:42:ARG:NH1[12_555]	1.76	0.44
1:1:50:ALA:CB	1:1:127:LEU:CD1[12_555]	1.76	0.44
2:2:59:SER:CA	2:2:253:PHE:CA[2_555]	1.76	0.44
2:2:91:ILE:CG1	2:2:95:ASN:CB[2_555]	1.76	0.44
1:1:17:VAL:N	1:1:107:ALA:N[12_555]	1.76	0.44
2:2:38:TRP:C	2:2:210:PRO:CA[12_555]	1.76	0.44
3:3:118:MET:SD	4:4:34:ASP:CA[12_555]	1.76	0.44
1:1:122:ASP:C	3:3:50:ASP:OD2[12_555]	1.76	0.44
2:2:44:PRO:N	2:2:249:MET:N[12_555]	1.76	0.44
2:2:41:TYR:CZ	2:2:55:GLN:CD[12_555]	1.76	0.44
1:1:64:GLU:OE1	3:3:104:SER:CB[12_555]	1.76	0.44
1:1:36:ALA:CB	3:3:28:TYR:CB[12_555]	1.76	0.44
1:1:62:ARG:NH1	1:1:109:ILE:O[12_555]	1.76	0.44
1:1:252:ARG:CD	3:3:41:LYS:CG[12_555]	1.76	0.44
1:1:69:SER:C	3:3:102:ILE:CG1[12_555]	1.76	0.44
1:1:70:PHE:N	3:3:102:ILE:CG2[12_555]	1.76	0.44
2:2:90:GLY:C	2:2:98:TYR:CG[2_555]	1.76	0.44
3:3:14:MET:SD	3:3:88:ASP:N[12_555]	1.76	0.44
1:1:76:CYS:C	3:3:218:ASP:OD2[12_555]	1.76	0.44
2:2:31:ALA:C	3:3:31:THR:CA[12_555]	1.76	0.44
2:2:59:SER:N	2:2:253:PHE:CA[2_555]	1.76	0.44
3:3:14:MET:O	3:3:87:VAL:O[12_555]	1.76	0.44
3:3:68:TYR:N	4:4:28:ASN:CA[12_555]	1.76	0.44
2:2:91:ILE:N	2:2:98:TYR:CG[2_555]	1.76	0.44
1:1:25:HIS:O	1:1:222:SER:O[12_555]	1.76	0.44
1:1:171:ILE:CG1	3:3:153:VAL:CG2[12_555]	1.76	0.44
1:1:74:SER:N	3:3:113:LEU:CD2[12_555]	1.77	0.43
1:1:52:GLU:N	1:1:237:THR:CB[12_555]	1.77	0.43
3:3:16:THR:CA	3:3:89:ILE:CG1[12_555]	1.77	0.43
3:3:70:VAL:N	4:4:31:TYR:CA[12_555]	1.77	0.43
2:2:178:THR:CG2	4:4:44:ASP:N[12_555]	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:15:THR:C	3:3:89:ILE:CG2[12_555]	1.77	0.43
3:3:68:TYR:O	4:4:30:ASN:CG[12_555]	1.77	0.43
2:2:62:ARG:NE	2:2:254:SER:O[2_555]	1.77	0.43
3:3:221:LEU:CA	3:3:226:ASP:OD2[12_555]	1.77	0.43
2:2:45:GLN:CB	2:2:106:TYR:CB[12_555]	1.77	0.43
1:1:67:ILE:CG2	3:3:46:MET:CG[12_555]	1.77	0.43
1:1:128:VAL:CG2	3:3:168:PRO:CG[12_555]	1.77	0.43
2:2:44:PRO:CD	2:2:248:PRO:N[12_555]	1.77	0.43
1:1:53:THR:O	1:1:81:ARG:CA[12_555]	1.77	0.43
1:1:178:PRO:O	3:3:151:THR:C[12_555]	1.77	0.43
3:3:17:ASP:CB	3:3:94:LEU:CD1[12_555]	1.77	0.43
3:3:16:THR:CA	3:3:89:ILE:N[12_555]	1.77	0.43
2:2:43:THR:CA	2:2:249:MET:N[12_555]	1.77	0.43
1:1:17:VAL:C	1:1:106:MET:CA[12_555]	1.77	0.43
2:2:43:THR:O	2:2:249:MET:CG[12_555]	1.77	0.43
3:3:16:THR:OG1	3:3:89:ILE:CG1[12_555]	1.77	0.43
1:1:62:ARG:NH2	1:1:109:ILE:CA[12_555]	1.77	0.43
1:1:240:TYR:CZ	3:3:111:GLY:O[12_555]	1.77	0.43
3:3:209:MET:CA	4:4:32:PHE:C[12_555]	1.77	0.43
2:2:21:SER:CB	2:2:101:LEU:CD1[2_555]	1.77	0.43
2:2:38:TRP:CG	2:2:210:PRO:CA[12_555]	1.77	0.43
3:3:10:SER:OG	3:3:140:GLU:CG[12_555]	1.77	0.43
3:3:12:GLN:CB	3:3:188:TYR:N[12_555]	1.77	0.43
2:2:20:ASP:OD2	2:2:102:GLY:C[2_555]	1.77	0.43
2:2:64:TYR:CZ	2:2:256:ALA:CA[2_555]	1.77	0.43
1:1:178:PRO:CD	3:3:147:ALA:O[12_555]	1.78	0.42
3:3:212:PHE:CG	4:4:36:ALA:C[12_555]	1.78	0.42
1:1:241:HIS:CG	3:3:215:ALA:C[12_555]	1.78	0.42
2:2:173:LEU:CA	4:4:42:ARG:NH2[12_555]	1.78	0.42
1:1:122:ASP:O	3:3:50:ASP:CB[12_555]	1.78	0.42
3:3:70:VAL:N	4:4:30:ASN:C[12_555]	1.78	0.42
3:3:209:MET:O	4:4:31:TYR:C[12_555]	1.78	0.42
1:1:48:GLU:CG	1:1:78:HIS:CE1[12_555]	1.78	0.42
1:1:34:LEU:CG	1:1:169:MET:CG[12_555]	1.78	0.42
2:2:52:LYS:CE	2:2:252:GLU:CD[10_555]	1.78	0.42
3:3:12:GLN:CA	3:3:187:GLY:C[12_555]	1.78	0.42
1:1:62:ARG:CA	1:1:111:ARG:CB[12_555]	1.78	0.42
1:1:71:LEU:CD2	3:3:44:ILE:N[12_555]	1.78	0.42
3:3:18:ASP:N	3:3:94:LEU:CD2[12_555]	1.78	0.42
2:2:36:GLY:O	2:2:209:VAL:N[12_555]	1.78	0.42
3:3:119:PHE:C	4:4:33:LYS:CG[12_555]	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:18:ARG:O	2:2:51:ASN:ND2[2_555]	1.78	0.42
3:3:69:THR:CA	4:4:30:ASN:C[12_555]	1.78	0.42
1:1:23:SER:OG	1:1:80:SER:CB[12_555]	1.78	0.42
3:3:24:ALA:CA	3:3:163:ILE:N[12_555]	1.78	0.42
2:2:179:LEU:CG	4:4:42:ARG:CG[12_555]	1.78	0.42
3:3:107:THR:CB	3:3:107:THR:OG1[12_555]	1.78	0.42
3:3:64:ASN:C	4:4:28:ASN:OD1[12_555]	1.78	0.42
1:1:183:SER:OG	3:3:116:SER:C[12_555]	1.78	0.42
1:1:125:ILE:C	3:3:165:LEU:O[12_555]	1.78	0.42
1:1:39:THR:O	3:3:30:PRO:C[12_555]	1.78	0.42
1:1:124:GLU:OE2	3:3:115:PHE:CD2[12_555]	1.78	0.42
2:2:44:PRO:CB	2:2:247:SER:CA[12_555]	1.78	0.42
3:3:10:SER:C	3:3:140:GLU:CB[12_555]	1.78	0.42
1:1:65:MET:N	3:3:105:TYR:CD1[12_555]	1.78	0.42
3:3:26:PRO:N	3:3:161:SER:OG[12_555]	1.78	0.42
1:1:247:LYS:NZ	2:2:186:PHE:CB[12_555]	1.78	0.42
1:1:124:GLU:CB	3:3:114:ARG:C[12_555]	1.78	0.42
1:1:245:HIS:N	3:3:51:THR:N[12_555]	1.78	0.42
2:2:32:VAL:C	3:3:32:LYS:O[12_555]	1.78	0.42
1:1:113:PHE:N	3:3:44:ILE:CB[12_555]	1.78	0.42
3:3:10:SER:N	3:3:140:GLU:CB[12_555]	1.78	0.42
1:1:183:SER:OG	3:3:116:SER:CA[12_555]	1.79	0.41
2:2:18:ARG:N	2:2:49:ALA:CA[2_555]	1.79	0.41
3:3:209:MET:CB	4:4:32:PHE:CD1[12_555]	1.79	0.41
1:1:73:ARG:CZ	3:3:103:ALA:N[12_555]	1.79	0.41
2:2:178:THR:N	4:4:44:ASP:N[12_555]	1.79	0.41
1:1:123:SER:N	3:3:50:ASP:CG[12_555]	1.79	0.41
1:1:249:TRP:CB	3:3:38:GLY:C[12_555]	1.79	0.41
1:1:39:THR:CG2	3:3:28:TYR:CZ[12_555]	1.79	0.41
1:1:36:ALA:CA	3:3:25:LEU:O[12_555]	1.79	0.41
2:2:201:LEU:CB	3:3:32:LYS:CE[12_555]	1.79	0.41
3:3:106:TYR:CA	3:3:225:ARG:N[12_555]	1.79	0.41
2:2:62:ARG:CD	2:2:254:SER:O[2_555]	1.79	0.41
2:2:93:GLY:O	2:2:98:TYR:OH[2_555]	1.79	0.41
1:1:47:PRO:CG	1:1:239:ILE:CB[12_555]	1.79	0.41
1:1:179:PHE:CZ	3:3:133:TYR:CE2[12_555]	1.79	0.41
1:1:244:LYS:CB	3:3:213:VAL:O[12_555]	1.79	0.41
1:1:171:ILE:CD1	3:3:153:VAL:CB[12_555]	1.79	0.41
3:3:16:THR:CA	3:3:89:ILE:CG2[12_555]	1.79	0.41
2:2:34:GLY:N	3:3:34:ILE:CG1[12_555]	1.79	0.41
1:1:73:ARG:NE	3:3:103:ALA:N[12_555]	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:32:PRO:O	1:1:147:TYR:CG[12_555]	1.79	0.41
1:1:21:LYS:O	1:1:79:ILE:C[12_555]	1.79	0.41
3:3:68:TYR:C	4:4:30:ASN:CG[12_555]	1.79	0.41
2:2:220:TRP:NE1	3:3:35:SER:CB[12_555]	1.79	0.41
1:1:191:SER:OG	2:2:34:GLY:N[12_555]	1.80	0.40
1:1:177:GLN:CD	3:3:148:MET:CA[12_555]	1.80	0.40
3:3:26:PRO:CD	3:3:161:SER:CA[12_555]	1.80	0.40
1:1:182:PHE:CE1	3:3:164:SER:CB[12_555]	1.80	0.40
1:1:181:ARG:CG	3:3:115:PHE:CB[12_555]	1.80	0.40
2:2:186:PHE:C	3:3:33:GLU:OE1[12_555]	1.80	0.40
2:2:55:GLN:N	2:2:57:ASP:N[3_555]	1.80	0.40
1:1:44:ASN:CG	5:1:288:SUC:O4[12_555]	1.80	0.40
1:1:115:LEU:CB	3:3:41:LYS:O[12_555]	1.80	0.40
2:2:38:TRP:CG	2:2:210:PRO:CG[12_555]	1.80	0.40
2:2:38:TRP:CG	2:2:210:PRO:C[12_555]	1.80	0.40
1:1:14:VAL:CB	1:1:256:ALA:CA[12_555]	1.80	0.40
2:2:17:THR:OG1	2:2:49:ALA:CA[2_555]	1.80	0.40
1:1:181:ARG:NH1	3:3:115:PHE:CD1[12_555]	1.80	0.40
2:2:18:ARG:N	2:2:49:ALA:CB[2_555]	1.80	0.40
1:1:9:GLU:C	1:1:276:THR:C[12_555]	1.80	0.40
1:1:250:CYS:CB	3:3:39:GLU:CA[12_555]	1.80	0.40
1:1:65:MET:CG	1:1:112:LYS:CD[12_555]	1.80	0.40
3:3:23:CYS:CB	3:3:162:THR:CG2[12_555]	1.80	0.40
1:1:182:PHE:N	3:3:165:LEU:CB[12_555]	1.80	0.40
2:2:62:ARG:CB	2:2:255:GLY:CA[2_555]	1.80	0.40
2:2:182:ASN:OD1	4:4:41:SER:O[12_555]	1.80	0.40
1:1:31:ALA:CB	1:1:169:MET:O[12_555]	1.80	0.40
3:3:19:MET:C	3:3:53:ILE:CD1[12_555]	1.80	0.40
3:3:13:PHE:CE2	3:3:167:VAL:CG1[12_555]	1.80	0.40
1:1:26:THR:CA	1:1:223:ARG:CB[12_555]	1.80	0.40
1:1:109:ILE:CG2	3:3:219:PHE:O[12_555]	1.80	0.40
1:1:8:ASP:C	1:1:256:ALA:O[12_555]	1.80	0.40
3:3:212:PHE:CZ	4:4:35:ALA:C[12_555]	1.80	0.40
2:2:88:ASP:C	2:2:259:LYS:CB[2_555]	1.81	0.39
2:2:38:TRP:CA	2:2:209:VAL:O[12_555]	1.81	0.39
1:1:37:ALA:CB	4:4:36:ALA:CB[12_555]	1.81	0.39
1:1:48:GLU:N	1:1:239:ILE:CD1[12_555]	1.81	0.39
1:1:54:ARG:O	1:1:81:ARG:NE[12_555]	1.81	0.39
1:1:181:ARG:CB	3:3:165:LEU:CG[12_555]	1.81	0.39
2:2:53:PRO:O	2:2:57:ASP:OD2[3_555]	1.81	0.39
2:2:186:PHE:CZ	3:3:41:LYS:NZ[12_555]	1.81	0.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:15:LEU:CD2	1:1:255:ARG:CA[12_555]	1.81	0.39
1:1:34:LEU:CD1	1:1:169:MET:CB[12_555]	1.81	0.39
1:1:128:VAL:CG2	3:3:168:PRO:CD[12_555]	1.81	0.39
1:1:245:HIS:N	3:3:51:THR:CA[12_555]	1.81	0.39
3:3:223:MET:CB	3:3:225:ARG:CG[12_555]	1.81	0.39
3:3:24:ALA:N	3:3:162:THR:CA[12_555]	1.81	0.39
1:1:55:TYR:CB	1:1:81:ARG:NH2[12_555]	1.81	0.39
3:3:70:VAL:CA	4:4:31:TYR:CA[12_555]	1.81	0.39
3:3:70:VAL:O	4:4:31:TYR:O[12_555]	1.81	0.39
3:3:209:MET:C	4:4:32:PHE:C[12_555]	1.81	0.39
1:1:116:PHE:N	3:3:41:LYS:CA[12_555]	1.81	0.39
1:1:12:ASN:O	3:3:231:ILE:N[12_555]	1.81	0.39
3:3:12:GLN:O	3:3:188:TYR:N[12_555]	1.81	0.39
1:1:241:HIS:C	3:3:215:ALA:CA[12_555]	1.81	0.39
1:1:177:GLN:O	3:3:150:GLY:C[12_555]	1.81	0.39
3:3:22:PRO:C	3:3:117:PHE:O[12_555]	1.81	0.39
3:3:58:VAL:CA	4:4:26:TYR:CD1[12_555]	1.81	0.39
3:3:106:TYR:CB	3:3:224:ALA:CA[12_555]	1.81	0.39
2:2:41:TYR:OH	2:2:55:GLN:NE2[12_555]	1.81	0.39
1:1:68:GLU:CA	3:3:98:LEU:CG[12_555]	1.81	0.39
3:3:70:VAL:CG1	4:4:31:TYR:CG[12_555]	1.81	0.39
2:2:38:TRP:C	2:2:210:PRO:C[12_555]	1.82	0.38
1:1:51:ILE:N	1:1:145:TYR:CD1[12_555]	1.82	0.38
1:1:175:HIS:C	3:3:149:LEU:O[12_555]	1.82	0.38
2:2:44:PRO:CB	2:2:247:SER:O[12_555]	1.82	0.38
2:2:51:ASN:OD1	2:2:61:ASN:C[3_555]	1.82	0.38
1:1:244:LYS:N	3:3:49:VAL:O[12_555]	1.82	0.38
1:1:50:ALA:O	1:1:145:TYR:CE2[12_555]	1.82	0.38
3:3:209:MET:CG	4:4:32:PHE:CD2[12_555]	1.82	0.38
2:2:202:ILE:O	3:3:34:ILE:CB[12_555]	1.82	0.38
2:2:46:ASP:CA	2:2:203:VAL:N[12_555]	1.82	0.38
3:3:67:MET:N	4:4:28:ASN:C[12_555]	1.82	0.38
1:1:51:ILE:CG1	1:1:237:THR:C[12_555]	1.82	0.38
1:1:177:GLN:CD	3:3:148:MET:N[12_555]	1.82	0.38
1:1:35:ASP:CA	3:3:25:LEU:CB[12_555]	1.82	0.38
1:1:42:THR:OG1	1:1:122:ASP:N[12_555]	1.82	0.38
1:1:113:PHE:CD2	3:3:48:GLN:NE2[12_555]	1.82	0.38
3:3:36:ILE:CG2	3:3:38:GLY:N[12_555]	1.82	0.38
2:2:40:HIS:CD2	2:2:205:TYR:CG[12_555]	1.82	0.38
3:3:70:VAL:CB	4:4:31:TYR:CD2[12_555]	1.82	0.38
1:1:62:ARG:CG	1:1:111:ARG:CB[12_555]	1.82	0.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:38:GLU:OE1	3:3:27:TRP:C[12_555]	1.82	0.38
1:1:69:SER:OG	3:3:101:GLU:O[12_555]	1.82	0.38
2:2:53:PRO:CB	2:2:58:THR:OG1[3_555]	1.82	0.38
1:1:62:ARG:C	1:1:111:ARG:CD[12_555]	1.82	0.38
3:3:222:ARG:CA	3:3:225:ARG:C[12_555]	1.82	0.38
3:3:26:PRO:N	3:3:161:SER:CB[12_555]	1.82	0.38
1:1:5:ASN:N	1:1:274:VAL:CB[12_555]	1.82	0.38
1:1:67:ILE:CA	3:3:46:MET:CE[12_555]	1.82	0.38
1:1:182:PHE:CB	3:3:164:SER:CA[12_555]	1.82	0.38
1:1:14:VAL:CG2	1:1:256:ALA:N[12_555]	1.82	0.38
2:2:41:TYR:CD2	2:2:41:TYR:CD2[12_555]	1.82	0.38
2:2:54:THR:OG1	2:2:56:PRO:N[3_555]	1.82	0.38
1:1:52:GLU:O	1:1:237:THR:N[12_555]	1.83	0.37
3:3:210:LEU:CD2	4:4:34:ASP:O[12_555]	1.83	0.37
1:1:250:CYS:N	3:3:39:GLU:C[12_555]	1.83	0.37
1:1:245:HIS:N	3:3:51:THR:CB[12_555]	1.83	0.37
1:1:124:GLU:CD	3:3:213:VAL:CG2[12_555]	1.83	0.37
2:2:179:LEU:CA	4:4:42:ARG:CD[12_555]	1.83	0.37
1:1:9:GLU:CA	1:1:276:THR:OG1[12_555]	1.83	0.37
3:3:56:ASN:OD1	4:4:29:ILE:CD1[12_555]	1.83	0.37
3:3:56:ASN:OD1	4:4:29:ILE:CG1[12_555]	1.83	0.37
2:2:88:ASP:C	2:2:259:LYS:CA[2_555]	1.83	0.37
2:2:204:PRO:CD	3:3:35:SER:O[12_555]	1.83	0.37
2:2:20:ASP:CA	2:2:211:MET:CB[2_555]	1.83	0.37
1:1:63:ASP:N	1:1:111:ARG:CZ[12_555]	1.83	0.37
1:1:243:ALA:CB	3:3:48:GLN:N[12_555]	1.83	0.37
1:1:73:ARG:N	3:3:99:ILE:CG1[12_555]	1.83	0.37
1:1:36:ALA:C	1:1:185:PRO:CG[12_555]	1.83	0.37
3:3:26:PRO:CA	3:3:161:SER:CA[12_555]	1.83	0.37
1:1:77:VAL:CG1	3:3:216:CYS:C[12_555]	1.83	0.37
3:3:58:VAL:CB	4:4:26:TYR:CD2[12_555]	1.83	0.37
1:1:64:GLU:O	3:3:105:TYR:CG[12_555]	1.83	0.37
1:1:115:LEU:C	3:3:41:LYS:N[12_555]	1.83	0.37
1:1:53:THR:C	1:1:80:SER:C[12_555]	1.83	0.37
3:3:20:GLN:C	3:3:117:PHE:CE2[12_555]	1.83	0.37
2:2:194:ARG:CB	3:3:27:TRP:NE1[12_555]	1.83	0.37
1:1:76:CYS:O	3:3:218:ASP:CB[12_555]	1.83	0.37
2:2:54:THR:CA	2:2:57:ASP:C[3_555]	1.83	0.37
1:1:20:ILE:CD1	1:1:78:HIS:N[12_555]	1.83	0.37
1:1:241:HIS:O	3:3:215:ALA:CA[12_555]	1.83	0.37
1:1:62:ARG:CD	1:1:109:ILE:C[12_555]	1.84	0.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:64:TYR:CZ	2:2:98:TYR:O[2_555]	1.84	0.36
1:1:39:THR:CA	3:3:30:PRO:CD[12_555]	1.84	0.36
1:1:68:GLU:O	3:3:99:ILE:CA[12_555]	1.84	0.36
3:3:221:LEU:C	3:3:226:ASP:CA[12_555]	1.84	0.36
2:2:39:PRO:CD	2:2:210:PRO:CB[12_555]	1.84	0.36
1:1:18:PRO:CA	1:1:106:MET:CA[12_555]	1.84	0.36
1:1:47:PRO:CA	1:1:239:ILE:CA[12_555]	1.84	0.36
2:2:46:ASP:OD2	2:2:203:VAL:CA[12_555]	1.84	0.36
1:1:73:ARG:O	3:3:219:PHE:CD1[12_555]	1.84	0.36
1:1:48:GLU:OE1	1:1:78:HIS:CA[12_555]	1.84	0.36
1:1:241:HIS:CB	3:3:216:CYS:N[12_555]	1.84	0.36
3:3:13:PHE:O	3:3:186:ALA:CB[12_555]	1.84	0.36
3:3:223:MET:C	3:3:225:ARG:CG[12_555]	1.84	0.36
3:3:210:LEU:N	4:4:32:PHE:CA[12_555]	1.84	0.36
3:3:18:ASP:CA	3:3:94:LEU:CD2[12_555]	1.84	0.36
1:1:27:THR:CA	1:1:223:ARG:CD[12_555]	1.84	0.36
1:1:30:SER:C	1:1:146:MET:CE[12_555]	1.84	0.36
1:1:247:LYS:N	2:2:185:ILE:CD1[12_555]	1.84	0.36
1:1:179:PHE:N	3:3:133:TYR:O[12_555]	1.84	0.36
1:1:63:ASP:CA	1:1:111:ARG:NH1[12_555]	1.84	0.36
2:2:39:PRO:CA	2:2:103:ARG:NH1[12_555]	1.84	0.36
1:1:250:CYS:N	3:3:39:GLU:N[12_555]	1.84	0.36
3:3:67:MET:CB	4:4:27:PHE:CG[12_555]	1.84	0.36
3:3:24:ALA:O	3:3:162:THR:CA[12_555]	1.84	0.36
3:3:13:PHE:CZ	3:3:167:VAL:CG1[12_555]	1.84	0.36
3:3:14:MET:CB	3:3:87:VAL:O[12_555]	1.84	0.36
3:3:15:THR:OG1	3:3:109:TRP:CH2[12_555]	1.84	0.36
2:2:46:ASP:CG	2:2:203:VAL:N[12_555]	1.84	0.36
1:1:27:THR:OG1	1:1:223:ARG:NH1[12_555]	1.85	0.35
3:3:65:VAL:N	4:4:28:ASN:OD1[12_555]	1.85	0.35
3:3:17:ASP:O	3:3:94:LEU:CD1[12_555]	1.85	0.35
1:1:249:TRP:CZ2	2:2:35:TYR:CZ[12_555]	1.85	0.35
3:3:56:ASN:CB	4:4:29:ILE:CD1[12_555]	1.85	0.35
1:1:240:TYR:C	3:3:216:CYS:SG[12_555]	1.85	0.35
1:1:33:LEU:N	1:1:147:TYR:CB[12_555]	1.85	0.35
2:2:90:GLY:CA	2:2:98:TYR:CG[2_555]	1.85	0.35
1:1:126:THR:CB	3:3:167:VAL:CA[12_555]	1.85	0.35
1:1:27:THR:N	1:1:163:TRP:CE3[12_555]	1.85	0.35
2:2:58:THR:C	2:2:254:SER:N[2_555]	1.85	0.35
1:1:115:LEU:CB	3:3:41:LYS:C[12_555]	1.85	0.35
1:1:32:PRO:CG	1:1:146:MET:O[12_555]	1.85	0.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:194:ARG:C	3:3:27:TRP:NE1[12_555]	1.85	0.35
2:2:47:ALA:C	2:2:202:ILE:CD1[12_555]	1.85	0.35
2:2:46:ASP:OD2	2:2:203:VAL:N[12_555]	1.85	0.35
1:1:5:ASN:O	1:1:276:THR:CB[12_555]	1.85	0.35
2:2:250:CYS:SG	2:2:252:GLU:CD[12_555]	1.85	0.35
3:3:97:THR:CG2	4:4:40:ALA:CB[12_555]	1.85	0.35
2:2:46:ASP:C	2:2:202:ILE:CG2[12_555]	1.85	0.35
3:3:67:MET:SD	4:4:27:PHE:CD1[12_555]	1.85	0.35
1:1:51:ILE:CD1	1:1:238:HIS:N[12_555]	1.85	0.35
1:1:35:ASP:CA	3:3:25:LEU:CD2[12_555]	1.85	0.35
1:1:63:ASP:O	1:1:111:ARG:NH2[12_555]	1.85	0.35
1:1:44:ASN:CB	5:1:288:SUC:O4[12_555]	1.85	0.35
2:2:45:GLN:N	2:2:247:SER:O[12_555]	1.85	0.35
1:1:39:THR:CB	3:3:28:TYR:CZ[12_555]	1.85	0.35
1:1:71:LEU:N	3:3:47:CYS:SG[12_555]	1.85	0.35
1:1:26:THR:C	1:1:163:TRP:CE3[12_555]	1.85	0.35
2:2:38:TRP:C	2:2:210:PRO:O[12_555]	1.85	0.35
1:1:23:SER:C	1:1:81:ARG:O[12_555]	1.85	0.35
3:3:223:MET:CA	3:3:225:ARG:CZ[12_555]	1.85	0.35
1:1:26:THR:CA	1:1:163:TRP:CH2[12_555]	1.85	0.35
1:1:14:VAL:O	1:1:257:VAL:O[12_555]	1.86	0.34
1:1:13:GLU:O	1:1:258:PRO:N[12_555]	1.86	0.34
1:1:14:VAL:CG2	1:1:256:ALA:O[12_555]	1.86	0.34
2:2:13:ILE:O	2:2:13:ILE:CB[11_555]	1.86	0.34
1:1:65:MET:CA	3:3:105:TYR:CE1[12_555]	1.86	0.34
1:1:76:CYS:N	3:3:218:ASP:CG[12_555]	1.86	0.34
2:2:182:ASN:CG	4:4:41:SER:O[12_555]	1.86	0.34
1:1:52:GLU:C	1:1:237:THR:CG2[12_555]	1.86	0.34
1:1:26:THR:N	1:1:222:SER:C[12_555]	1.86	0.34
3:3:222:ARG:O	3:3:225:ARG:CG[12_555]	1.86	0.34
3:3:19:MET:CB	3:3:85:ILE:CD1[12_555]	1.86	0.34
2:2:32:VAL:CB	3:3:32:LYS:C[12_555]	1.86	0.34
2:2:38:TRP:CB	2:2:209:VAL:C[12_555]	1.86	0.34
1:1:121:PHE:CD2	3:3:49:VAL:CG2[12_555]	1.86	0.34
1:1:26:THR:C	1:1:223:ARG:CB[12_555]	1.86	0.34
3:3:21:SER:N	3:3:211:CYS:CB[12_555]	1.86	0.34
1:1:120:ARG:O	3:3:49:VAL:CG2[12_555]	1.86	0.34
2:2:62:ARG:C	2:2:255:GLY:N[2_555]	1.86	0.34
1:1:25:HIS:O	1:1:96:PHE:CB[12_555]	1.86	0.34
1:1:182:PHE:CG	3:3:165:LEU:N[12_555]	1.86	0.34
1:1:240:TYR:CZ	3:3:111:GLY:C[12_555]	1.86	0.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:32:VAL:CA	3:3:32:LYS:O[12_555]	1.86	0.34
2:2:37:VAL:CA	2:2:207:ASN:C[12_555]	1.86	0.34
3:3:12:GLN:N	3:3:188:TYR:CA[12_555]	1.86	0.34
1:1:116:PHE:N	3:3:45:GLU:OE2[12_555]	1.86	0.34
1:1:181:ARG:C	3:3:165:LEU:CA[12_555]	1.86	0.34
1:1:41:HIS:C	1:1:186:PHE:C[12_555]	1.86	0.34
3:3:67:MET:N	4:4:28:ASN:CB[12_555]	1.86	0.34
1:1:17:VAL:CB	1:1:106:MET:C[12_555]	1.86	0.34
1:1:17:VAL:CA	1:1:107:ALA:C[12_555]	1.87	0.33
1:1:62:ARG:CB	1:1:111:ARG:CA[12_555]	1.87	0.33
1:1:26:THR:CA	1:1:163:TRP:CZ3[12_555]	1.87	0.33
3:3:22:PRO:C	3:3:117:PHE:CA[12_555]	1.87	0.33
1:1:240:TYR:CE2	3:3:111:GLY:CA[12_555]	1.87	0.33
1:1:116:PHE:CA	3:3:45:GLU:OE2[12_555]	1.87	0.33
1:1:76:CYS:O	3:3:218:ASP:C[12_555]	1.87	0.33
1:1:247:LYS:CE	2:2:186:PHE:CB[12_555]	1.87	0.33
1:1:180:PRO:CA	3:3:165:LEU:CD1[12_555]	1.87	0.33
3:3:6:ILE:CD1	3:3:142:THR:C[12_555]	1.87	0.33
3:3:52:LEU:O	4:4:40:ALA:O[12_555]	1.87	0.33
1:1:179:PHE:O	3:3:133:TYR:N[12_555]	1.87	0.33
2:2:44:PRO:CB	2:2:247:SER:CB[12_555]	1.87	0.33
1:1:62:ARG:CG	1:1:108:GLN:O[12_555]	1.87	0.33
1:1:7:ILE:CA	1:1:275:THR:OG1[12_555]	1.87	0.33
3:3:66:SER:C	4:4:29:ILE:N[12_555]	1.87	0.33
3:3:13:PHE:N	3:3:187:GLY:C[12_555]	1.87	0.33
2:2:176:ASP:OD1	4:4:44:ASP:CG[12_555]	1.87	0.33
2:2:182:ASN:OD1	4:4:41:SER:C[12_555]	1.87	0.33
1:1:245:HIS:CA	3:3:51:THR:CG2[12_555]	1.87	0.33
1:1:250:CYS:C	3:3:39:GLU:CG[12_555]	1.87	0.33
2:2:178:THR:CB	4:4:44:ASP:CA[12_555]	1.87	0.33
3:3:223:MET:CA	3:3:225:ARG:CG[12_555]	1.87	0.33
1:1:179:PHE:CA	3:3:151:THR:O[12_555]	1.87	0.33
1:1:248:ALA:CA	1:1:251:PRO:CG[12_555]	1.87	0.33
1:1:50:ALA:O	1:1:145:TYR:CD2[12_555]	1.87	0.33
2:2:32:VAL:CG2	3:3:31:THR:CA[12_555]	1.87	0.33
1:1:45:VAL:O	1:1:125:ILE:CD1[12_555]	1.87	0.33
3:3:10:SER:N	3:3:188:TYR:CE1[12_555]	1.88	0.32
1:1:247:LYS:CB	2:2:185:ILE:O[12_555]	1.88	0.32
1:1:109:ILE:CD1	3:3:216:CYS:O[12_555]	1.88	0.32
3:3:53:ILE:N	4:4:39:GLY:C[12_555]	1.88	0.32
1:1:35:ASP:OD2	3:3:25:LEU:CD1[12_555]	1.88	0.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:34:LEU:CD1	1:1:169:MET:CA[12_555]	1.88	0.32
1:1:240:TYR:CE1	3:3:169:TRP:CA[12_555]	1.88	0.32
1:1:247:LYS:CE	2:2:185:ILE:C[12_555]	1.88	0.32
1:1:70:PHE:CD2	3:3:43:LEU:CD1[12_555]	1.88	0.32
3:3:222:ARG:C	3:3:225:ARG:CD[12_555]	1.88	0.32
1:1:36:ALA:CB	3:3:25:LEU:O[12_555]	1.88	0.32
1:1:25:HIS:CA	1:1:223:ARG:CA[12_555]	1.88	0.32
2:2:36:GLY:C	2:2:209:VAL:N[12_555]	1.88	0.32
1:1:240:TYR:CD2	3:3:112:SER:C[12_555]	1.88	0.32
3:3:9:GLY:O	3:3:188:TYR:CZ[12_555]	1.88	0.32
2:2:62:ARG:CZ	2:2:101:LEU:CA[2_555]	1.88	0.32
3:3:24:ALA:N	3:3:162:THR:O[12_555]	1.88	0.32
1:1:125:ILE:N	3:3:114:ARG:CB[12_555]	1.88	0.32
1:1:183:SER:CB	3:3:116:SER:C[12_555]	1.88	0.32
1:1:66:SER:CA	1:1:115:LEU:CD1[12_555]	1.88	0.32
1:1:72:GLY:CA	3:3:99:ILE:CA[12_555]	1.88	0.32
2:2:43:THR:C	2:2:249:MET:N[12_555]	1.88	0.32
1:1:116:PHE:CE1	3:3:42:ASN:O[12_555]	1.88	0.32
3:3:120:CYS:CB	4:4:33:LYS:CA[12_555]	1.88	0.32
2:2:35:TYR:N	3:3:36:ILE:CD1[12_555]	1.88	0.32
1:1:128:VAL:CG2	3:3:168:PRO:CB[12_555]	1.88	0.32
2:2:194:ARG:C	3:3:27:TRP:CD1[12_555]	1.88	0.32
2:2:178:THR:CA	4:4:43:LEU:C[12_555]	1.88	0.32
3:3:13:PHE:CD2	3:3:167:VAL:CG1[12_555]	1.88	0.32
2:2:36:GLY:CA	2:2:208:ALA:C[12_555]	1.89	0.31
2:2:43:THR:CB	2:2:105:GLY:CA[12_555]	1.89	0.31
1:1:179:PHE:CE1	3:3:133:TYR:CD2[12_555]	1.89	0.31
1:1:28:SER:OG	1:1:163:TRP:CE2[12_555]	1.89	0.31
2:2:182:ASN:ND2	4:4:41:SER:O[12_555]	1.89	0.31
1:1:31:ALA:CB	1:1:169:MET:C[12_555]	1.89	0.31
1:1:26:THR:CG2	1:1:221:CYS:C[12_555]	1.89	0.31
2:2:20:ASP:O	2:2:211:MET:O[2_555]	1.89	0.31
1:1:116:PHE:CG	3:3:40:VAL:CB[12_555]	1.89	0.31
1:1:12:ASN:ND2	3:3:229:LEU:CB[12_555]	1.89	0.31
3:3:13:PHE:CB	3:3:133:TYR:CD1[12_555]	1.89	0.31
2:2:181:GLY:C	4:4:41:SER:CA[12_555]	1.89	0.31
2:2:43:THR:C	2:2:105:GLY:O[12_555]	1.89	0.31
1:1:35:ASP:O	3:3:25:LEU:CA[12_555]	1.89	0.31
1:1:115:LEU:C	3:3:41:LYS:CB[12_555]	1.89	0.31
1:1:35:ASP:CB	3:3:25:LEU:CG[12_555]	1.89	0.31
1:1:62:ARG:CD	1:1:111:ARG:N[12_555]	1.89	0.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:18:PRO:C	1:1:106:MET:CA[12_555]	1.89	0.31
1:1:20:ILE:CG2	1:1:78:HIS:O[12_555]	1.89	0.31
1:1:60:GLN:O	1:1:108:GLN:N[12_555]	1.89	0.31
1:1:17:VAL:CG2	1:1:106:MET:C[12_555]	1.89	0.31
3:3:223:MET:C	3:3:225:ARG:NE[12_555]	1.89	0.31
3:3:222:ARG:CG	3:3:226:ASP:C[12_555]	1.89	0.31
3:3:107:THR:N	3:3:224:ALA:C[12_555]	1.89	0.31
1:1:249:TRP:CB	3:3:38:GLY:CA[12_555]	1.89	0.31
1:1:113:PHE:CE1	3:3:44:ILE:O[12_555]	1.89	0.31
1:1:62:ARG:CB	1:1:112:LYS:N[12_555]	1.89	0.31
3:3:9:GLY:N	3:3:188:TYR:CZ[12_555]	1.89	0.31
1:1:246:THR:CG2	3:3:98:LEU:CD2[12_555]	1.89	0.31
1:1:245:HIS:CB	2:2:184:LEU:CB[12_555]	1.89	0.31
2:2:18:ARG:N	2:2:50:ILE:N[2_555]	1.89	0.31
3:3:14:MET:CG	3:3:88:ASP:CB[12_555]	1.89	0.31
3:3:18:ASP:CA	3:3:94:LEU:CA[12_555]	1.89	0.31
3:3:26:PRO:C	3:3:161:SER:CB[12_555]	1.89	0.31
1:1:73:ARG:CA	3:3:99:ILE:CD1[12_555]	1.89	0.31
1:1:9:GLU:CD	2:2:179:LEU:CG[12_555]	1.90	0.30
2:2:90:GLY:O	2:2:98:TYR:CA[2_555]	1.90	0.30
1:1:35:ASP:N	3:3:25:LEU:CG[12_555]	1.90	0.30
1:1:71:LEU:CB	3:3:47:CYS:CA[12_555]	1.90	0.30
1:1:43:SER:CB	1:1:184:ILE:CB[12_555]	1.90	0.30
1:1:177:GLN:CA	3:3:147:ALA:C[12_555]	1.90	0.30
1:1:182:PHE:CB	3:3:164:SER:N[12_555]	1.90	0.30
1:1:8:ASP:OD1	1:1:258:PRO:CD[12_555]	1.90	0.30
3:3:97:THR:CG2	4:4:40:ALA:N[12_555]	1.90	0.30
2:2:40:HIS:N	2:2:103:ARG:CD[12_555]	1.90	0.30
2:2:173:LEU:CD2	4:4:42:ARG:NH2[12_555]	1.90	0.30
1:1:64:GLU:CD	3:3:104:SER:CA[12_555]	1.90	0.30
1:1:62:ARG:CZ	1:1:109:ILE:O[12_555]	1.90	0.30
2:2:194:ARG:CD	3:3:27:TRP:NE1[12_555]	1.90	0.30
2:2:37:VAL:CG2	2:2:207:ASN:C[12_555]	1.90	0.30
2:2:20:ASP:C	2:2:101:LEU:CD1[2_555]	1.90	0.30
3:3:212:PHE:CE2	4:4:36:ALA:N[12_555]	1.90	0.30
2:2:64:TYR:CB	2:2:257:ARG:CG[2_555]	1.90	0.30
1:1:46:GLN:CG	1:1:99:TRP:CZ3[12_555]	1.90	0.30
3:3:22:PRO:C	3:3:117:PHE:CB[12_555]	1.90	0.30
1:1:246:THR:CA	2:2:185:ILE:CD1[12_555]	1.90	0.30
3:3:220:CYS:O	3:3:226:ASP:OD2[12_555]	1.90	0.30
1:1:116:PHE:CG	3:3:45:GLU:OE2[12_555]	1.90	0.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:69:THR:N	4:4:30:ASN:ND2[12_555]	1.90	0.30
3:3:210:LEU:C	4:4:37:SER:OG[12_555]	1.90	0.30
1:1:248:ALA:O	1:1:251:PRO:N[12_555]	1.91	0.29
1:1:9:GLU:CA	1:1:277:ALA:N[12_555]	1.91	0.29
1:1:23:SER:O	1:1:82:ILE:N[12_555]	1.91	0.29
1:1:32:PRO:CD	1:1:146:MET:O[12_555]	1.91	0.29
1:1:65:MET:C	1:1:115:LEU:CD2[12_555]	1.91	0.29
3:3:119:PHE:N	4:4:34:ASP:OD1[12_555]	1.91	0.29
3:3:23:CYS:CB	3:3:117:PHE:O[12_555]	1.91	0.29
2:2:17:THR:CB	2:2:49:ALA:CA[2_555]	1.91	0.29
1:1:252:ARG:NE	3:3:41:LYS:CD[12_555]	1.91	0.29
3:3:7:THR:O	3:3:140:GLU:CG[12_555]	1.91	0.29
1:1:254:PRO:O	4:4:43:LEU:CA[12_555]	1.91	0.29
2:2:190:PHE:O	3:3:29:HIS:ND1[12_555]	1.91	0.29
2:2:18:ARG:NE	2:2:50:ILE:CB[2_555]	1.91	0.29
2:2:178:THR:CB	4:4:43:LEU:O[12_555]	1.91	0.29
1:1:39:THR:OG1	3:3:28:TYR:CZ[12_555]	1.91	0.29
3:3:16:THR:O	3:3:90:THR:N[12_555]	1.91	0.29
3:3:16:THR:C	3:3:89:ILE:C[12_555]	1.91	0.29
2:2:190:PHE:CE2	4:4:35:ALA:CB[12_555]	1.91	0.29
1:1:73:ARG:NH1	3:3:103:ALA:O[12_555]	1.91	0.29
1:1:5:ASN:ND2	2:2:173:LEU:CG[12_555]	1.91	0.29
1:1:77:VAL:N	3:3:218:ASP:CG[12_555]	1.91	0.29
1:1:103:LEU:CG	3:3:48:GLN:OE1[12_555]	1.91	0.29
2:2:176:ASP:CG	4:4:44:ASP:CG[12_555]	1.91	0.29
2:2:62:ARG:CA	2:2:254:SER:C[2_555]	1.91	0.29
1:1:240:TYR:OH	3:3:169:TRP:CB[12_555]	1.91	0.29
2:2:46:ASP:N	2:2:107:THR:N[12_555]	1.91	0.29
2:2:41:TYR:CD1	2:2:252:GLU:CG[12_555]	1.91	0.29
2:2:194:ARG:CZ	3:3:27:TRP:CH2[12_555]	1.91	0.29
1:1:20:ILE:CB	1:1:79:ILE:N[12_555]	1.91	0.29
1:1:52:GLU:C	1:1:237:THR:N[12_555]	1.92	0.28
1:1:182:PHE:CD1	3:3:164:SER:N[12_555]	1.92	0.28
1:1:249:TRP:NE1	2:2:35:TYR:CD2[12_555]	1.92	0.28
2:2:17:THR:C	2:2:49:ALA:O[2_555]	1.92	0.28
1:1:32:PRO:N	1:1:147:TYR:O[12_555]	1.92	0.28
1:1:49:ASP:OD2	1:1:220:ILE:CG2[12_555]	1.92	0.28
2:2:38:TRP:CZ3	2:2:48:THR:CG2[12_555]	1.92	0.28
1:1:55:TYR:CA	1:1:81:ARG:CZ[12_555]	1.92	0.28
2:2:58:THR:CG2	2:2:252:GLU:C[2_555]	1.92	0.28
1:1:191:SER:OG	2:2:33:VAL:O[12_555]	1.92	0.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:126:THR:C	3:3:166:VAL:CG1[12_555]	1.92	0.28
1:1:27:THR:N	1:1:163:TRP:CD2[12_555]	1.92	0.28
1:1:16:VAL:N	1:1:259:TYR:CZ[12_555]	1.92	0.28
1:1:47:PRO:O	1:1:239:ILE:CD1[12_555]	1.92	0.28
2:2:38:TRP:CA	2:2:210:PRO:C[12_555]	1.92	0.28
1:1:245:HIS:NE2	3:3:52:LEU:CA[12_555]	1.92	0.28
3:3:52:LEU:CG	4:4:38:SER:CB[12_555]	1.92	0.28
1:1:64:GLU:O	3:3:105:TYR:CE1[12_555]	1.92	0.28
1:1:16:VAL:CA	1:1:259:TYR:CE1[12_555]	1.92	0.28
1:1:41:HIS:CA	1:1:186:PHE:CD2[12_555]	1.92	0.28
1:1:16:VAL:CG2	3:3:232:GLN:CG[12_555]	1.92	0.28
1:1:76:CYS:O	3:3:218:ASP:CG[12_555]	1.92	0.28
1:1:248:ALA:N	1:1:251:PRO:CD[12_555]	1.92	0.28
2:2:38:TRP:CE3	2:2:210:PRO:CD[12_555]	1.92	0.28
2:2:173:LEU:CB	4:4:42:ARG:NH2[12_555]	1.92	0.28
2:2:182:ASN:ND2	4:4:42:ARG:O[12_555]	1.92	0.28
1:1:112:LYS:O	3:3:42:ASN:CG[12_555]	1.92	0.28
3:3:106:TYR:C	3:3:225:ARG:N[12_555]	1.92	0.28
2:2:45:GLN:O	2:2:107:THR:N[12_555]	1.92	0.28
2:2:194:ARG:NE	4:4:33:LYS:CE[12_555]	1.92	0.28
1:1:124:GLU:OE2	3:3:115:PHE:CB[12_555]	1.92	0.28
1:1:25:HIS:CB	1:1:223:ARG:CA[12_555]	1.92	0.28
2:2:62:ARG:CG	2:2:255:GLY:N[2_555]	1.92	0.28
2:2:178:THR:N	4:4:44:ASP:CB[12_555]	1.92	0.28
1:1:66:SER:CA	1:1:115:LEU:CD2[12_555]	1.92	0.28
1:1:46:GLN:CA	1:1:239:ILE:CG2[12_555]	1.92	0.28
1:1:46:GLN:C	1:1:239:ILE:CD1[12_555]	1.92	0.28
2:2:204:PRO:O	3:3:35:SER:CB[12_555]	1.92	0.28
1:1:33:LEU:CB	1:1:169:MET:SD[12_555]	1.93	0.27
2:2:179:LEU:N	4:4:42:ARG:CG[12_555]	1.93	0.27
1:1:242:LYS:O	3:3:214:SER:O[12_555]	1.93	0.27
3:3:22:PRO:C	3:3:117:PHE:C[12_555]	1.93	0.27
3:3:11:GLY:N	3:3:188:TYR:CB[12_555]	1.93	0.27
1:1:40:GLY:CA	3:3:30:PRO:CB[12_555]	1.93	0.27
3:3:10:SER:C	3:3:140:GLU:CA[12_555]	1.93	0.27
2:2:43:THR:CB	2:2:106:TYR:N[12_555]	1.93	0.27
1:1:18:PRO:C	1:1:106:MET:CG[12_555]	1.93	0.27
1:1:37:ALA:N	1:1:185:PRO:CB[12_555]	1.93	0.27
3:3:118:MET:CG	4:4:34:ASP:OD1[12_555]	1.93	0.27
2:2:18:ARG:N	2:2:49:ALA:C[2_555]	1.93	0.27
2:2:32:VAL:CA	3:3:32:LYS:N[12_555]	1.93	0.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:177:GLN:CB	3:3:148:MET:CB[12_555]	1.93	0.27
3:3:11:GLY:O	3:3:188:TYR:O[12_555]	1.93	0.27
2:2:62:ARG:CG	2:2:254:SER:C[2_555]	1.93	0.27
1:1:12:ASN:CG	3:3:229:LEU:CA[12_555]	1.93	0.27
2:2:34:GLY:N	3:3:34:ILE:N[12_555]	1.93	0.27
1:1:76:CYS:O	3:3:218:ASP:OD2[12_555]	1.93	0.27
3:3:211:CYS:CA	4:4:37:SER:OG[12_555]	1.93	0.27
1:1:242:LYS:O	3:3:214:SER:N[12_555]	1.93	0.27
1:1:182:PHE:CB	3:3:165:LEU:N[12_555]	1.93	0.27
3:3:69:THR:N	4:4:30:ASN:CA[12_555]	1.93	0.27
1:1:173:TRP:CD1	3:3:151:THR:C[12_555]	1.93	0.27
2:2:40:HIS:CA	2:2:103:ARG:CG[12_555]	1.93	0.27
2:2:194:ARG:CD	4:4:33:LYS:CE[12_555]	1.93	0.27
1:1:242:LYS:O	3:3:214:SER:OG[12_555]	1.93	0.27
1:1:16:VAL:CG2	1:1:107:ALA:CB[12_555]	1.93	0.27
1:1:27:THR:OG1	1:1:223:ARG:CZ[12_555]	1.93	0.27
1:1:8:ASP:CG	1:1:258:PRO:CG[12_555]	1.93	0.27
1:1:10:VAL:CA	1:1:277:ALA:N[12_555]	1.93	0.27
1:1:28:SER:CB	1:1:155:PRO:CG[12_555]	1.93	0.27
1:1:113:PHE:CE1	3:3:44:ILE:CG1[12_555]	1.93	0.27
1:1:177:GLN:N	3:3:148:MET:CA[12_555]	1.93	0.27
2:2:45:GLN:CB	2:2:107:THR:N[12_555]	1.93	0.27
2:2:202:ILE:O	3:3:34:ILE:CA[12_555]	1.93	0.27
3:3:67:MET:SD	4:4:27:PHE:CE1[12_555]	1.93	0.27
1:1:65:MET:SD	1:1:112:LYS:CG[12_555]	1.93	0.27
1:1:71:LEU:O	3:3:47:CYS:CB[12_555]	1.93	0.27
2:2:45:GLN:N	2:2:106:TYR:C[12_555]	1.93	0.27
1:1:74:SER:OG	3:3:113:LEU:CA[12_555]	1.93	0.27
1:1:39:THR:CG2	3:3:28:TYR:CD1[12_555]	1.94	0.26
1:1:252:ARG:CZ	3:3:41:LYS:CE[12_555]	1.94	0.26
1:1:7:ILE:N	1:1:275:THR:C[12_555]	1.94	0.26
1:1:62:ARG:N	1:1:111:ARG:CB[12_555]	1.94	0.26
2:2:38:TRP:N	2:2:210:PRO:N[12_555]	1.94	0.26
2:2:20:ASP:C	2:2:101:LEU:CG[2_555]	1.94	0.26
1:1:35:ASP:C	3:3:25:LEU:CD1[12_555]	1.94	0.26
3:3:20:GLN:OE1	3:3:55:VAL:CG1[12_555]	1.94	0.26
3:3:20:GLN:C	3:3:211:CYS:CB[12_555]	1.94	0.26
3:3:16:THR:N	3:3:89:ILE:CG2[12_555]	1.94	0.26
1:1:181:ARG:CZ	3:3:115:PHE:CZ[12_555]	1.94	0.26
1:1:61:THR:CB	3:3:230:HIS:CB[12_555]	1.94	0.26
1:1:182:PHE:N	3:3:115:PHE:O[12_555]	1.94	0.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:52:LYS:CE	2:2:58:THR:OG1[12_555]	1.94	0.26
1:1:36:ALA:O	3:3:28:TYR:CG[12_555]	1.94	0.26
3:3:52:LEU:CB	4:4:38:SER:OG[12_555]	1.94	0.26
2:2:88:ASP:O	2:2:259:LYS:N[2_555]	1.94	0.26
2:2:43:THR:CA	2:2:105:GLY:C[12_555]	1.94	0.26
3:3:26:PRO:N	3:3:160:GLN:C[12_555]	1.94	0.26
1:1:123:SER:C	3:3:214:SER:OG[12_555]	1.94	0.26
3:3:13:PHE:CE1	3:3:167:VAL:CG1[12_555]	1.94	0.26
2:2:178:THR:C	4:4:43:LEU:N[12_555]	1.94	0.26
1:1:119:VAL:CG2	3:3:45:GLU:CB[12_555]	1.94	0.26
1:1:37:ALA:CA	1:1:185:PRO:CG[12_555]	1.94	0.26
3:3:19:MET:CG	3:3:85:ILE:CG1[12_555]	1.94	0.26
3:3:68:TYR:N	4:4:28:ASN:N[12_555]	1.94	0.26
1:1:7:ILE:C	1:1:275:THR:C[12_555]	1.94	0.26
1:1:241:HIS:CB	3:3:216:CYS:CB[12_555]	1.94	0.26
1:1:74:SER:CB	3:3:113:LEU:CB[12_555]	1.94	0.26
3:3:70:VAL:C	4:4:31:TYR:CA[12_555]	1.94	0.26
1:1:70:PHE:CD2	3:3:43:LEU:CD2[12_555]	1.94	0.26
1:1:53:THR:CA	1:1:80:SER:C[12_555]	1.94	0.26
1:1:183:SER:OG	3:3:116:SER:N[12_555]	1.94	0.26
2:2:38:TRP:CD1	2:2:210:PRO:C[12_555]	1.95	0.25
2:2:54:THR:CB	2:2:56:PRO:CA[3_555]	1.95	0.25
1:1:126:THR:CG2	3:3:167:VAL:CB[12_555]	1.95	0.25
1:1:38:GLU:CB	3:3:28:TYR:C[12_555]	1.95	0.25
1:1:249:TRP:CD2	2:2:35:TYR:CD1[12_555]	1.95	0.25
2:2:91:ILE:CG2	2:2:95:ASN:OD1[2_555]	1.95	0.25
1:1:14:VAL:O	1:1:255:ARG:NE[12_555]	1.95	0.25
2:2:50:ILE:CD1	2:2:50:ILE:CD1[10_555]	1.95	0.25
2:2:194:ARG:CG	3:3:27:TRP:NE1[12_555]	1.95	0.25
3:3:21:SER:O	3:3:116:SER:O[12_555]	1.95	0.25
1:1:244:LYS:CD	3:3:212:PHE:C[12_555]	1.95	0.25
2:2:53:PRO:CA	2:2:58:THR:CA[3_555]	1.95	0.25
1:1:116:PHE:CB	3:3:40:VAL:CA[12_555]	1.95	0.25
1:1:39:THR:N	3:3:30:PRO:N[12_555]	1.95	0.25
3:3:23:CYS:O	3:3:161:SER:C[12_555]	1.95	0.25
1:1:39:THR:C	3:3:30:PRO:N[12_555]	1.95	0.25
3:3:6:ILE:CD1	3:3:142:THR:O[12_555]	1.95	0.25
1:1:243:ALA:N	3:3:214:SER:CA[12_555]	1.95	0.25
2:2:15:GLN:C	2:2:15:GLN:O[11_555]	1.95	0.25
1:1:49:ASP:CB	1:1:220:ILE:CD1[12_555]	1.95	0.25
1:1:44:ASN:CA	5:1:288:SUC:O4[12_555]	1.95	0.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:38:TRP:CG	2:2:210:PRO:CB[12_555]	1.95	0.25
1:1:240:TYR:CB	3:3:112:SER:CB[12_555]	1.95	0.25
1:1:39:THR:OG1	3:3:28:TYR:CD2[12_555]	1.95	0.25
1:1:182:PHE:CD1	3:3:164:SER:O[12_555]	1.95	0.25
1:1:179:PHE:CB	3:3:133:TYR:CA[12_555]	1.95	0.25
3:3:21:SER:C	3:3:117:PHE:CA[12_555]	1.95	0.25
1:1:123:SER:O	3:3:116:SER:OG[12_555]	1.95	0.25
1:1:241:HIS:CD2	3:3:114:ARG:NE[12_555]	1.95	0.25
1:1:181:ARG:NH1	3:3:115:PHE:CG[12_555]	1.95	0.25
2:2:64:TYR:CD1	2:2:257:ARG:CA[2_555]	1.96	0.24
3:3:12:GLN:C	3:3:188:TYR:CA[12_555]	1.96	0.24
1:1:14:VAL:CG1	1:1:255:ARG:CA[12_555]	1.96	0.24
1:1:44:ASN:ND2	1:1:101:ILE:CB[12_555]	1.96	0.24
1:1:42:THR:C	1:1:193:TYR:OH[12_555]	1.96	0.24
2:2:62:ARG:CZ	2:2:101:LEU:N[2_555]	1.96	0.24
1:1:52:GLU:CD	1:1:82:ILE:CD1[12_555]	1.96	0.24
3:3:67:MET:CA	4:4:27:PHE:O[12_555]	1.96	0.24
1:1:240:TYR:CG	3:3:112:SER:N[12_555]	1.96	0.24
2:2:18:ARG:CD	2:2:50:ILE:C[2_555]	1.96	0.24
2:2:35:TYR:CG	3:3:36:ILE:CD1[12_555]	1.96	0.24
1:1:30:SER:CB	1:1:148:VAL:CG1[12_555]	1.96	0.24
3:3:106:TYR:O	3:3:224:ALA:CA[12_555]	1.96	0.24
2:2:41:TYR:CE1	2:2:55:GLN:OE1[12_555]	1.96	0.24
3:3:18:ASP:OD2	3:3:97:THR:CG2[12_555]	1.96	0.24
2:2:52:LYS:CD	2:2:252:GLU:OE1[10_555]	1.96	0.24
1:1:14:VAL:O	1:1:255:ARG:CG[12_555]	1.96	0.24
3:3:9:GLY:C	3:3:188:TYR:CG[12_555]	1.96	0.24
3:3:23:CYS:O	3:3:161:SER:O[12_555]	1.96	0.24
3:3:9:GLY:O	3:3:188:TYR:CE2[12_555]	1.96	0.24
3:3:21:SER:O	3:3:116:SER:C[12_555]	1.96	0.24
1:1:126:THR:CG2	3:3:167:VAL:CA[12_555]	1.96	0.24
2:2:90:GLY:O	2:2:98:TYR:C[2_555]	1.96	0.24
1:1:244:LYS:O	3:3:50:ASP:N[12_555]	1.96	0.24
1:1:124:GLU:CA	3:3:114:ARG:CG[12_555]	1.96	0.24
1:1:10:VAL:CA	1:1:276:THR:O[12_555]	1.96	0.24
3:3:209:MET:CB	4:4:32:PHE:CG[12_555]	1.96	0.24
1:1:240:TYR:CA	3:3:112:SER:CA[12_555]	1.96	0.24
3:3:10:SER:CA	3:3:140:GLU:CG[12_555]	1.96	0.24
3:3:209:MET:N	4:4:32:PHE:N[12_555]	1.96	0.24
3:3:107:THR:N	3:3:224:ALA:O[12_555]	1.96	0.24
1:1:46:GLN:C	1:1:239:ILE:CG1[12_555]	1.96	0.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:26:PRO:N	3:3:160:GLN:O[12_555]	1.96	0.24
2:2:199:ALA:CB	3:3:29:HIS:NE2[12_555]	1.96	0.24
1:1:30:SER:OG	1:1:148:VAL:CB[12_555]	1.97	0.23
1:1:180:PRO:O	3:3:166:VAL:O[12_555]	1.97	0.23
1:1:113:PHE:CE1	3:3:44:ILE:CD1[12_555]	1.97	0.23
1:1:182:PHE:CA	3:3:115:PHE:O[12_555]	1.97	0.23
2:2:62:ARG:NE	2:2:101:LEU:N[2_555]	1.97	0.23
1:1:121:PHE:CB	3:3:49:VAL:CG2[12_555]	1.97	0.23
1:1:249:TRP:O	3:3:39:GLU:CA[12_555]	1.97	0.23
2:2:11:ASP:N	2:2:26:ASP:OD1[11_555]	1.97	0.23
2:2:64:TYR:CG	2:2:257:ARG:CB[2_555]	1.97	0.23
1:1:115:LEU:C	3:3:41:LYS:O[12_555]	1.97	0.23
2:2:201:LEU:N	3:3:32:LYS:CB[12_555]	1.97	0.23
1:1:9:GLU:C	1:1:276:THR:OG1[12_555]	1.97	0.23
2:2:41:TYR:OH	2:2:57:ASP:OD1[11_555]	1.97	0.23
1:1:249:TRP:CH2	2:2:35:TYR:CE1[12_555]	1.97	0.23
3:3:67:MET:CE	4:4:27:PHE:CD2[12_555]	1.97	0.23
1:1:62:ARG:NH2	1:1:109:ILE:C[12_555]	1.97	0.23
1:1:116:PHE:N	3:3:42:ASN:N[12_555]	1.97	0.23
1:1:242:LYS:N	3:3:215:ALA:C[12_555]	1.97	0.23
1:1:41:HIS:CG	1:1:186:PHE:CD2[12_555]	1.97	0.23
2:2:38:TRP:O	2:2:210:PRO:O[12_555]	1.97	0.23
3:3:16:THR:C	3:3:89:ILE:CB[12_555]	1.97	0.23
1:1:66:SER:N	1:1:115:LEU:CD2[12_555]	1.97	0.23
1:1:48:GLU:CD	1:1:78:HIS:CE1[12_555]	1.97	0.23
2:2:54:THR:CB	2:2:57:ASP:N[3_555]	1.97	0.23
1:1:63:ASP:OD2	1:1:111:ARG:NH1[12_555]	1.97	0.23
1:1:191:SER:CB	2:2:34:GLY:N[12_555]	1.97	0.23
2:2:59:SER:O	2:2:99:HIS:CD2[2_555]	1.97	0.23
3:3:15:THR:CG2	3:3:109:TRP:CD2[12_555]	1.97	0.23
1:1:77:VAL:N	3:3:218:ASP:CB[12_555]	1.97	0.23
3:3:209:MET:O	4:4:31:TYR:N[12_555]	1.97	0.23
1:1:64:GLU:CG	3:3:105:TYR:N[12_555]	1.97	0.23
1:1:41:HIS:CA	1:1:186:PHE:O[12_555]	1.97	0.23
1:1:25:HIS:C	1:1:223:ARG:N[12_555]	1.98	0.22
1:1:241:HIS:CA	3:3:216:CYS:N[12_555]	1.98	0.22
2:2:62:ARG:CD	2:2:100:PHE:N[2_555]	1.98	0.22
1:1:243:ALA:CB	3:3:48:GLN:CA[12_555]	1.98	0.22
2:2:201:LEU:O	3:3:32:LYS:CE[12_555]	1.98	0.22
1:1:70:PHE:CD1	3:3:43:LEU:CD1[12_555]	1.98	0.22
1:1:113:PHE:CE2	3:3:48:GLN:NE2[12_555]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:14:MET:CA	3:3:87:VAL:C[12_555]	1.98	0.22
2:2:178:THR:CG2	4:4:44:ASP:O[12_555]	1.98	0.22
2:2:94:GLU:OE2	2:2:98:TYR:CD2[2_555]	1.98	0.22
1:1:23:SER:N	1:1:81:ARG:O[12_555]	1.98	0.22
3:3:103:ALA:O	3:3:224:ALA:CB[12_555]	1.98	0.22
2:2:13:ILE:CA	2:2:13:ILE:CA[11_555]	1.98	0.22
1:1:240:TYR:CG	3:3:112:SER:C[12_555]	1.98	0.22
3:3:118:MET:CG	4:4:34:ASP:N[12_555]	1.98	0.22
1:1:28:SER:OG	1:1:155:PRO:CB[12_555]	1.98	0.22
1:1:62:ARG:O	1:1:111:ARG:NE[12_555]	1.98	0.22
2:2:176:ASP:OD2	4:4:44:ASP:CB[12_555]	1.98	0.22
1:1:70:PHE:CG	3:3:43:LEU:CB[12_555]	1.98	0.22
1:1:53:THR:N	1:1:237:THR:N[12_555]	1.98	0.22
3:3:223:MET:C	3:3:225:ARG:CD[12_555]	1.98	0.22
2:2:89:MET:N	2:2:258:ALA:CA[2_555]	1.98	0.22
2:2:64:TYR:CE2	2:2:98:TYR:O[2_555]	1.98	0.22
3:3:70:VAL:CG2	4:4:31:TYR:CE2[12_555]	1.98	0.22
1:1:126:THR:CB	3:3:167:VAL:CB[12_555]	1.98	0.22
2:2:62:ARG:CG	2:2:255:GLY:O[2_555]	1.98	0.22
1:1:247:LYS:CD	2:2:186:PHE:CA[12_555]	1.98	0.22
2:2:44:PRO:CB	2:2:248:PRO:O[12_555]	1.98	0.22
1:1:40:GLY:N	3:3:30:PRO:CD[12_555]	1.98	0.22
1:1:71:LEU:CD1	3:3:45:GLU:C[12_555]	1.98	0.22
1:1:120:ARG:NH2	2:2:188:HIS:O[12_555]	1.98	0.22
3:3:26:PRO:CA	3:3:160:GLN:O[12_555]	1.98	0.22
3:3:11:GLY:O	3:3:134:THR:CA[12_555]	1.99	0.21
3:3:70:VAL:CB	4:4:31:TYR:CA[12_555]	1.99	0.21
1:1:115:LEU:CG	3:3:41:LYS:O[12_555]	1.99	0.21
3:3:58:VAL:CG2	4:4:26:TYR:CG[12_555]	1.99	0.21
1:1:63:ASP:CG	1:1:111:ARG:CZ[12_555]	1.99	0.21
2:2:52:LYS:CD	2:2:58:THR:OG1[12_555]	1.99	0.21
2:2:37:VAL:CG2	2:2:207:ASN:O[12_555]	1.99	0.21
2:2:201:LEU:CD2	3:3:32:LYS:CB[12_555]	1.99	0.21
1:1:126:THR:O	3:3:167:VAL:N[12_555]	1.99	0.21
1:1:71:LEU:CA	3:3:47:CYS:CB[12_555]	1.99	0.21
1:1:241:HIS:CB	3:3:215:ALA:O[12_555]	1.99	0.21
3:3:17:ASP:CA	3:3:94:LEU:CB[12_555]	1.99	0.21
1:1:113:PHE:CD1	3:3:44:ILE:CB[12_555]	1.99	0.21
3:3:13:PHE:CG	3:3:167:VAL:CG1[12_555]	1.99	0.21
1:1:182:PHE:CG	3:3:164:SER:N[12_555]	1.99	0.21
3:3:21:SER:C	3:3:117:PHE:CD1[12_555]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:17:ASP:OD1	3:3:87:VAL:N[12_555]	1.99	0.21
1:1:241:HIS:O	3:3:215:ALA:C[12_555]	1.99	0.21
1:1:38:GLU:CD	3:3:28:TYR:N[12_555]	1.99	0.21
1:1:55:TYR:O	1:1:81:ARG:NH2[12_555]	1.99	0.21
2:2:59:SER:C	2:2:253:PHE:CB[2_555]	1.99	0.21
1:1:25:HIS:C	1:1:222:SER:C[12_555]	1.99	0.21
3:3:16:THR:CB	3:3:89:ILE:CA[12_555]	1.99	0.21
3:3:15:THR:CA	3:3:109:TRP:CH2[12_555]	1.99	0.21
3:3:21:SER:CA	3:3:117:PHE:CZ[12_555]	1.99	0.21
1:1:179:PHE:CB	3:3:133:TYR:CG[12_555]	1.99	0.21
2:2:182:ASN:CB	4:4:41:SER:OG[12_555]	1.99	0.21
2:2:89:MET:CA	2:2:259:LYS:N[2_555]	1.99	0.21
1:1:126:THR:C	3:3:166:VAL:O[12_555]	1.99	0.21
3:3:70:VAL:O	4:4:31:TYR:C[12_555]	1.99	0.21
2:2:36:GLY:C	2:2:208:ALA:CB[12_555]	1.99	0.21
2:2:64:TYR:CD2	2:2:257:ARG:CG[2_555]	1.99	0.21
1:1:8:ASP:OD2	1:1:258:PRO:CD[12_555]	1.99	0.21
3:3:17:ASP:N	3:3:89:ILE:CA[12_555]	1.99	0.21
2:2:44:PRO:CA	2:2:247:SER:C[12_555]	1.99	0.21
1:1:47:PRO:O	1:1:239:ILE:CG1[12_555]	1.99	0.21
2:2:220:TRP:CE2	3:3:35:SER:OG[12_555]	1.99	0.21
1:1:179:PHE:CD2	3:3:133:TYR:CD1[12_555]	1.99	0.21
3:3:119:PHE:O	4:4:33:LYS:CB[12_555]	1.99	0.21
1:1:249:TRP:CD2	2:2:35:TYR:CE1[12_555]	1.99	0.21
2:2:190:PHE:CD1	4:4:35:ALA:CB[12_555]	1.99	0.21
1:1:8:ASP:OD1	1:1:258:PRO:N[12_555]	1.99	0.21
1:1:32:PRO:CB	1:1:147:TYR:CB[12_555]	1.99	0.21
1:1:179:PHE:CE2	3:3:135:PRO:N[12_555]	1.99	0.21
1:1:109:ILE:CA	3:3:219:PHE:O[12_555]	1.99	0.21
2:2:59:SER:N	2:2:253:PHE:CB[2_555]	2.00	0.20
3:3:56:ASN:O	4:4:26:TYR:C[12_555]	2.00	0.20
1:1:31:ALA:CB	1:1:169:MET:CA[12_555]	2.00	0.20
1:1:7:ILE:CA	1:1:275:THR:CA[12_555]	2.00	0.20
1:1:62:ARG:NH2	1:1:109:ILE:CG2[12_555]	2.00	0.20
1:1:6:TYR:CA	1:1:276:THR:CG2[12_555]	2.00	0.20
3:3:13:PHE:CD1	3:3:167:VAL:CG1[12_555]	2.00	0.20
3:3:23:CYS:N	3:3:117:PHE:CA[12_555]	2.00	0.20
1:1:48:GLU:CG	1:1:78:HIS:ND1[12_555]	2.00	0.20
1:1:113:PHE:CZ	3:3:44:ILE:O[12_555]	2.00	0.20
1:1:71:LEU:CB	3:3:47:CYS:SG[12_555]	2.00	0.20
1:1:36:ALA:N	3:3:25:LEU:CD1[12_555]	2.00	0.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:179:PHE:CD2	3:3:133:TYR:C[12_555]	2.00	0.20
1:1:121:PHE:CG	3:3:49:VAL:N[12_555]	2.00	0.20
3:3:67:MET:CE	4:4:27:PHE:CE2[12_555]	2.00	0.20
2:2:53:PRO:O	2:2:57:ASP:C[3_555]	2.00	0.20
1:1:244:LYS:CE	3:3:212:PHE:C[12_555]	2.00	0.20
1:1:47:PRO:CG	1:1:78:HIS:O[12_555]	2.00	0.20
1:1:70:PHE:CA	3:3:102:ILE:CG1[12_555]	2.00	0.20
2:2:36:GLY:N	2:2:208:ALA:CB[12_555]	2.00	0.20
2:2:44:PRO:CG	2:2:248:PRO:CD[12_555]	2.00	0.20
1:1:115:LEU:CB	3:3:42:ASN:CB[12_555]	2.00	0.20
1:1:9:GLU:CD	2:2:179:LEU:CD1[12_555]	2.00	0.20
2:2:64:TYR:CB	2:2:257:ARG:CB[2_555]	2.00	0.20
1:1:245:HIS:CG	3:3:51:THR:CA[12_555]	2.00	0.20
1:1:51:ILE:CD1	1:1:237:THR:CB[12_555]	2.00	0.20
1:1:32:PRO:CG	1:1:147:TYR:N[12_555]	2.00	0.20
3:3:23:CYS:CA	3:3:117:PHE:C[12_555]	2.00	0.20
2:2:29:ALA:CB	3:3:29:HIS:C[12_555]	2.00	0.20
1:1:53:THR:CB	1:1:80:SER:C[12_555]	2.00	0.20
2:2:20:ASP:C	2:2:101:LEU:CD2[2_555]	2.00	0.20
1:1:63:ASP:N	1:1:111:ARG:CD[12_555]	2.01	0.19
3:3:67:MET:CA	4:4:28:ASN:CA[12_555]	2.01	0.19
1:1:49:ASP:CB	1:1:220:ILE:CG2[12_555]	2.01	0.19
1:1:68:GLU:CD	3:3:98:LEU:CA[12_555]	2.01	0.19
1:1:18:PRO:CB	1:1:105:GLU:O[12_555]	2.01	0.19
1:1:67:ILE:CG1	3:3:46:MET:SD[12_555]	2.01	0.19
1:1:10:VAL:C	1:1:277:ALA:CA[12_555]	2.01	0.19
1:1:22:GLU:CG	1:1:81:ARG:CA[12_555]	2.01	0.19
3:3:120:CYS:SG	4:4:34:ASP:N[12_555]	2.01	0.19
1:1:71:LEU:CD2	3:3:44:ILE:CA[12_555]	2.01	0.19
1:1:48:GLU:CD	1:1:78:HIS:NE2[12_555]	2.01	0.19
2:2:42:LEU:O	2:2:249:MET:CA[12_555]	2.01	0.19
1:1:250:CYS:CA	3:3:39:GLU:CG[12_555]	2.01	0.19
3:3:22:PRO:O	3:3:117:PHE:N[12_555]	2.01	0.19
3:3:210:LEU:O	4:4:37:SER:CB[12_555]	2.01	0.19
3:3:69:THR:C	4:4:30:ASN:C[12_555]	2.01	0.19
2:2:89:MET:C	2:2:258:ALA:O[2_555]	2.01	0.19
1:1:112:LYS:O	3:3:42:ASN:CB[12_555]	2.01	0.19
3:3:69:THR:C	4:4:31:TYR:N[12_555]	2.01	0.19
3:3:212:PHE:CE2	4:4:35:ALA:C[12_555]	2.01	0.19
2:2:64:TYR:OH	2:2:98:TYR:O[2_555]	2.01	0.19
3:3:222:ARG:O	3:3:225:ARG:O[12_555]	2.01	0.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:18:ARG:NE	2:2:50:ILE:CA[2_555]	2.01	0.19
1:1:176:GLY:CA	3:3:149:LEU:N[12_555]	2.01	0.19
2:2:182:ASN:OD1	4:4:41:SER:CA[12_555]	2.01	0.19
1:1:112:LYS:O	3:3:42:ASN:C[12_555]	2.01	0.19
2:2:38:TRP:CZ2	2:2:48:THR:CB[12_555]	2.01	0.19
1:1:250:CYS:C	3:3:39:GLU:CB[12_555]	2.01	0.19
2:2:194:ARG:NH1	3:3:27:TRP:CE2[12_555]	2.01	0.19
3:3:14:MET:SD	3:3:88:ASP:CG[12_555]	2.01	0.19
1:1:124:GLU:OE2	3:3:115:PHE:CA[12_555]	2.01	0.19
1:1:122:ASP:O	3:3:50:ASP:CG[12_555]	2.01	0.19
1:1:17:VAL:CA	1:1:107:ALA:O[12_555]	2.01	0.19
1:1:122:ASP:C	3:3:50:ASP:CB[12_555]	2.01	0.19
3:3:16:THR:N	3:3:89:ILE:CB[12_555]	2.01	0.19
1:1:32:PRO:O	1:1:147:TYR:CD2[12_555]	2.01	0.19
1:1:177:GLN:N	3:3:148:MET:O[12_555]	2.01	0.19
3:3:21:SER:O	3:3:117:PHE:CG[12_555]	2.01	0.19
1:1:177:GLN:NE2	3:3:148:MET:CB[12_555]	2.01	0.19
1:1:116:PHE:CD1	3:3:45:GLU:OE2[12_555]	2.01	0.19
2:2:181:GLY:O	4:4:41:SER:CA[12_555]	2.02	0.18
1:1:62:ARG:O	1:1:111:ARG:CG[12_555]	2.02	0.18
1:1:124:GLU:N	3:3:214:SER:OG[12_555]	2.02	0.18
3:3:24:ALA:C	3:3:162:THR:CA[12_555]	2.02	0.18
1:1:71:LEU:O	3:3:47:CYS:SG[12_555]	2.02	0.18
3:3:67:MET:CB	4:4:27:PHE:CB[12_555]	2.02	0.18
2:2:39:PRO:O	2:2:210:PRO:O[12_555]	2.02	0.18
2:2:36:GLY:CA	2:2:208:ALA:O[12_555]	2.02	0.18
1:1:33:LEU:C	1:1:169:MET:SD[12_555]	2.02	0.18
1:1:250:CYS:N	3:3:39:GLU:CB[12_555]	2.02	0.18
1:1:247:LYS:NZ	2:2:186:PHE:CD2[12_555]	2.02	0.18
1:1:15:LEU:CA	1:1:259:TYR:OH[12_555]	2.02	0.18
2:2:41:TYR:CB	2:2:250:CYS:C[12_555]	2.02	0.18
3:3:68:TYR:N	4:4:29:ILE:N[12_555]	2.02	0.18
1:1:126:THR:CB	3:3:167:VAL:CG2[12_555]	2.02	0.18
1:1:28:SER:CA	1:1:163:TRP:CG[12_555]	2.02	0.18
1:1:182:PHE:C	3:3:164:SER:CA[12_555]	2.02	0.18
1:1:16:VAL:CG2	3:3:232:GLN:CB[12_555]	2.02	0.18
1:1:30:SER:C	1:1:146:MET:CG[12_555]	2.02	0.18
3:3:23:CYS:O	3:3:162:THR:C[12_555]	2.02	0.18
1:1:35:ASP:OD1	3:3:25:LEU:CD1[12_555]	2.02	0.18
1:1:249:TRP:O	3:3:40:VAL:N[12_555]	2.02	0.18
2:2:32:VAL:CA	3:3:31:THR:C[12_555]	2.02	0.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:19:MET:CE	3:3:85:ILE:CG2[12_555]	2.02	0.18
1:1:18:PRO:C	1:1:106:MET:N[12_555]	2.02	0.18
1:1:41:HIS:CG	1:1:186:PHE:O[12_555]	2.02	0.18
3:3:223:MET:CG	3:3:225:ARG:NE[12_555]	2.02	0.18
2:2:91:ILE:N	2:2:98:TYR:CD2[2_555]	2.02	0.18
1:1:17:VAL:CG2	1:1:106:MET:O[12_555]	2.02	0.18
2:2:59:SER:O	2:2:99:HIS:NE2[2_555]	2.02	0.18
2:2:31:ALA:C	3:3:31:THR:CB[12_555]	2.02	0.18
1:1:17:VAL:O	1:1:106:MET:C[12_555]	2.03	0.17
2:2:38:TRP:O	2:2:205:TYR:CE1[12_555]	2.03	0.17
1:1:77:VAL:CB	3:3:217:LYS:CD[12_555]	2.03	0.17
2:2:38:TRP:CD1	2:2:211:MET:N[12_555]	2.03	0.17
1:1:70:PHE:CG	3:3:43:LEU:CG[12_555]	2.03	0.17
3:3:53:ILE:CB	4:4:39:GLY:CA[12_555]	2.03	0.17
3:3:16:THR:OG1	3:3:89:ILE:C[12_555]	2.03	0.17
2:2:13:ILE:C	2:2:13:ILE:CB[11_555]	2.03	0.17
2:2:36:GLY:N	2:2:208:ALA:CA[12_555]	2.03	0.17
1:1:61:THR:CA	3:3:230:HIS:CD2[12_555]	2.03	0.17
1:1:9:GLU:CA	1:1:276:THR:CA[12_555]	2.03	0.17
1:1:24:HIS:O	1:1:97:THR:CG2[12_555]	2.03	0.17
1:1:73:ARG:NH2	3:3:102:ILE:C[12_555]	2.03	0.17
1:1:51:ILE:CG2	1:1:237:THR:OG1[12_555]	2.03	0.17
1:1:113:PHE:CD1	3:3:44:ILE:C[12_555]	2.03	0.17
3:3:120:CYS:CA	4:4:33:LYS:CA[12_555]	2.03	0.17
3:3:14:MET:CB	3:3:87:VAL:CA[12_555]	2.03	0.17
1:1:191:SER:CB	2:2:33:VAL:CA[12_555]	2.03	0.17
3:3:209:MET:CB	4:4:32:PHE:CB[12_555]	2.03	0.17
1:1:55:TYR:CB	1:1:81:ARG:NH1[12_555]	2.03	0.17
3:3:65:VAL:C	4:4:28:ASN:ND2[12_555]	2.03	0.17
1:1:244:LYS:CB	3:3:51:THR:N[12_555]	2.03	0.17
1:1:49:ASP:N	1:1:239:ILE:CD1[12_555]	2.03	0.17
2:2:178:THR:N	4:4:44:ASP:CA[12_555]	2.04	0.16
1:1:62:ARG:C	3:3:105:TYR:OH[12_555]	2.04	0.16
1:1:113:PHE:C	3:3:42:ASN:CB[12_555]	2.04	0.16
1:1:45:VAL:C	1:1:125:ILE:CD1[12_555]	2.04	0.16
1:1:12:ASN:C	3:3:230:HIS:CA[12_555]	2.04	0.16
1:1:179:PHE:CE1	3:3:133:TYR:CE2[12_555]	2.04	0.16
2:2:21:SER:CA	2:2:101:LEU:CG[2_555]	2.04	0.16
2:2:37:VAL:C	2:2:209:VAL:C[12_555]	2.04	0.16
2:2:91:ILE:CG1	2:2:95:ASN:OD1[2_555]	2.04	0.16
3:3:9:GLY:C	3:3:188:TYR:CD2[12_555]	2.04	0.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:11:GLY:O	3:3:134:THR:N[12_555]	2.04	0.16
1:1:28:SER:N	1:1:163:TRP:CB[12_555]	2.04	0.16
1:1:52:GLU:O	1:1:236:THR:N[12_555]	2.04	0.16
1:1:76:CYS:N	3:3:112:SER:N[12_555]	2.04	0.16
1:1:26:THR:N	1:1:222:SER:O[12_555]	2.04	0.16
2:2:20:ASP:OD1	2:2:211:MET:SD[2_555]	2.04	0.16
2:2:45:GLN:N	2:2:106:TYR:CA[12_555]	2.04	0.16
2:2:40:HIS:NE2	2:2:205:TYR:CD1[12_555]	2.04	0.16
1:1:49:ASP:OD1	1:1:220:ILE:CA[12_555]	2.04	0.16
3:3:52:LEU:O	4:4:39:GLY:CA[12_555]	2.04	0.16
1:1:108:GLN:OE1	3:3:110:THR:CG2[12_555]	2.04	0.16
1:1:177:GLN:CB	3:3:148:MET:C[12_555]	2.04	0.16
1:1:125:ILE:N	3:3:114:ARG:CA[12_555]	2.04	0.16
1:1:50:ALA:C	1:1:145:TYR:CG[12_555]	2.04	0.16
2:2:18:ARG:NE	2:2:50:ILE:C[2_555]	2.04	0.16
2:2:37:VAL:N	2:2:209:VAL:N[12_555]	2.04	0.16
3:3:106:TYR:CA	3:3:224:ALA:N[12_555]	2.04	0.16
3:3:11:GLY:O	3:3:134:THR:CB[12_555]	2.04	0.16
2:2:39:PRO:N	2:2:210:PRO:CA[12_555]	2.04	0.16
2:2:32:VAL:CB	3:3:32:LYS:CA[12_555]	2.04	0.16
2:2:220:TRP:CZ2	3:3:35:SER:CA[12_555]	2.04	0.16
1:1:24:HIS:CA	1:1:82:ILE:CG1[12_555]	2.04	0.16
1:1:241:HIS:CE1	3:3:215:ALA:O[12_555]	2.04	0.16
1:1:240:TYR:CG	3:3:112:SER:CB[12_555]	2.04	0.16
1:1:36:ALA:N	3:3:25:LEU:CG[12_555]	2.04	0.16
2:2:41:TYR:CD1	2:2:252:GLU:CB[12_555]	2.04	0.16
1:1:41:HIS:ND1	1:1:188:SER:N[12_555]	2.04	0.16
2:2:34:GLY:CA	3:3:34:ILE:O[12_555]	2.04	0.16
1:1:248:ALA:CA	1:1:251:PRO:CD[12_555]	2.04	0.16
1:1:42:THR:N	1:1:186:PHE:CB[12_555]	2.04	0.16
1:1:35:ASP:O	3:3:24:ALA:C[12_555]	2.05	0.15
3:3:58:VAL:CG1	4:4:26:TYR:CZ[12_555]	2.05	0.15
1:1:128:VAL:CG2	3:3:168:PRO:C[12_555]	2.05	0.15
3:3:23:CYS:C	3:3:117:PHE:O[12_555]	2.05	0.15
2:2:44:PRO:CG	2:2:248:PRO:C[12_555]	2.05	0.15
2:2:182:ASN:N	4:4:41:SER:CA[12_555]	2.05	0.15
1:1:128:VAL:CG1	3:3:170:VAL:CG2[12_555]	2.05	0.15
1:1:251:PRO:C	3:3:40:VAL:O[12_555]	2.05	0.15
2:2:179:LEU:CB	4:4:42:ARG:CA[12_555]	2.05	0.15
1:1:124:GLU:C	3:3:114:ARG:O[12_555]	2.05	0.15
3:3:14:MET:CA	3:3:87:VAL:CG1[12_555]	2.05	0.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:22:GLU:CG	1:1:81:ARG:C[12_555]	2.05	0.15
1:1:65:MET:CE	1:1:112:LYS:NZ[12_555]	2.05	0.15
1:1:182:PHE:O	3:3:164:SER:OG[12_555]	2.05	0.15
1:1:112:LYS:C	3:3:42:ASN:CG[12_555]	2.05	0.15
1:1:70:PHE:CD2	3:3:43:LEU:CA[12_555]	2.05	0.15
1:1:177:GLN:N	3:3:149:LEU:CA[12_555]	2.05	0.15
1:1:71:LEU:CD1	3:3:44:ILE:C[12_555]	2.05	0.15
1:1:14:VAL:N	3:3:230:HIS:ND1[12_555]	2.05	0.15
1:1:247:LYS:NZ	2:2:186:PHE:CG[12_555]	2.05	0.15
1:1:56:VAL:CG2	1:1:79:ILE:CD1[12_555]	2.05	0.15
1:1:245:HIS:CB	3:3:50:ASP:O[12_555]	2.05	0.15
2:2:46:ASP:CB	2:2:203:VAL:CA[12_555]	2.05	0.15
1:1:14:VAL:CB	1:1:257:VAL:N[12_555]	2.05	0.15
1:1:241:HIS:CA	3:3:216:CYS:CB[12_555]	2.05	0.15
2:2:54:THR:CB	2:2:56:PRO:CB[3_555]	2.06	0.14
3:3:106:TYR:C	3:3:224:ALA:N[12_555]	2.06	0.14
2:2:22:THR:OG1	2:2:48:THR:CG2[2_555]	2.06	0.14
1:1:178:PRO:CD	3:3:147:ALA:C[12_555]	2.06	0.14
1:1:77:VAL:C	3:3:217:LYS:CD[12_555]	2.06	0.14
2:2:187:PRO:CA	3:3:33:GLU:CB[12_555]	2.06	0.14
2:2:173:LEU:CD2	4:4:42:ARG:CZ[12_555]	2.06	0.14
1:1:121:PHE:CE1	3:3:48:GLN:C[12_555]	2.06	0.14
1:1:62:ARG:CB	1:1:111:ARG:C[12_555]	2.06	0.14
1:1:5:ASN:OD1	2:2:173:LEU:CD1[12_555]	2.06	0.14
1:1:69:SER:OG	3:3:102:ILE:CA[12_555]	2.06	0.14
3:3:14:MET:CB	3:3:88:ASP:CA[12_555]	2.06	0.14
2:2:45:GLN:CD	2:2:106:TYR:CD2[12_555]	2.06	0.14
1:1:255:ARG:N	4:4:43:LEU:CD2[12_555]	2.06	0.14
1:1:76:CYS:N	3:3:218:ASP:OD2[12_555]	2.06	0.14
3:3:221:LEU:N	3:3:226:ASP:OD2[12_555]	2.06	0.14
1:1:16:VAL:CA	1:1:107:ALA:CB[12_555]	2.06	0.14
1:1:249:TRP:O	3:3:39:GLU:N[12_555]	2.06	0.14
1:1:243:ALA:N	3:3:47:CYS:O[12_555]	2.06	0.14
3:3:16:THR:OG1	3:3:89:ILE:CB[12_555]	2.06	0.14
1:1:178:PRO:CB	3:3:132:ALA:CB[12_555]	2.06	0.14
1:1:8:ASP:CB	1:1:258:PRO:CD[12_555]	2.06	0.14
1:1:121:PHE:CG	3:3:49:VAL:CG2[12_555]	2.06	0.14
1:1:31:ALA:CA	1:1:169:MET:O[12_555]	2.06	0.14
1:1:27:THR:C	1:1:163:TRP:CD1[12_555]	2.06	0.14
1:1:18:PRO:CG	1:1:105:GLU:C[12_555]	2.06	0.14
2:2:64:TYR:CD1	2:2:257:ARG:CB[2_555]	2.06	0.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:71:LEU:N	3:3:102:ILE:CD1[12_555]	2.06	0.14
1:1:9:GLU:CD	2:2:179:LEU:CD2[12_555]	2.06	0.14
2:2:194:ARG:NH1	3:3:27:TRP:CE3[12_555]	2.06	0.14
1:1:173:TRP:CB	3:3:152:HIS:O[12_555]	2.06	0.14
1:1:55:TYR:N	1:1:81:ARG:NE[12_555]	2.06	0.14
1:1:16:VAL:N	1:1:259:TYR:CD1[12_555]	2.06	0.14
1:1:181:ARG:CA	3:3:165:LEU:CD2[12_555]	2.06	0.14
3:3:10:SER:CB	3:3:140:GLU:CA[12_555]	2.07	0.13
3:3:9:GLY:CA	3:3:188:TYR:CE2[12_555]	2.07	0.13
3:3:26:PRO:CB	3:3:161:SER:N[12_555]	2.07	0.13
2:2:43:THR:C	2:2:249:MET:CB[12_555]	2.07	0.13
3:3:21:SER:CB	3:3:117:PHE:CZ[12_555]	2.07	0.13
1:1:30:SER:OG	1:1:148:VAL:CG1[12_555]	2.07	0.13
1:1:181:ARG:CA	3:3:165:LEU:CA[12_555]	2.07	0.13
1:1:66:SER:CA	1:1:115:LEU:CG[12_555]	2.07	0.13
1:1:7:ILE:CB	1:1:275:THR:CA[12_555]	2.07	0.13
1:1:124:GLU:CA	3:3:114:ARG:C[12_555]	2.07	0.13
1:1:51:ILE:C	1:1:237:THR:CB[12_555]	2.07	0.13
1:1:128:VAL:CA	3:3:168:PRO:CB[12_555]	2.07	0.13
1:1:71:LEU:C	3:3:47:CYS:CB[12_555]	2.07	0.13
3:3:68:TYR:N	4:4:28:ASN:C[12_555]	2.07	0.13
2:2:38:TRP:CE2	2:2:48:THR:CG2[12_555]	2.07	0.13
3:3:97:THR:CG2	4:4:40:ALA:CA[12_555]	2.07	0.13
1:1:41:HIS:CB	1:1:186:PHE:CA[12_555]	2.07	0.13
2:2:45:GLN:CD	2:2:106:TYR:CB[12_555]	2.07	0.13
1:1:64:GLU:OE2	3:3:104:SER:C[12_555]	2.07	0.13
1:1:62:ARG:NE	1:1:109:ILE:O[12_555]	2.07	0.13
3:3:19:MET:CG	3:3:85:ILE:CD1[12_555]	2.07	0.13
1:1:45:VAL:CA	1:1:125:ILE:CD1[12_555]	2.07	0.13
1:1:52:GLU:O	1:1:236:THR:C[12_555]	2.07	0.13
1:1:68:GLU:OE1	3:3:98:LEU:N[12_555]	2.07	0.13
1:1:12:ASN:CA	3:3:229:LEU:O[12_555]	2.07	0.13
1:1:32:PRO:CD	1:1:147:TYR:C[12_555]	2.07	0.13
2:2:89:MET:C	2:2:98:TYR:CD1[12_555]	2.07	0.13
1:1:249:TRP:NE1	2:2:35:TYR:CD1[12_555]	2.07	0.13
3:3:66:SER:CA	4:4:28:ASN:C[12_555]	2.07	0.13
1:1:181:ARG:CZ	3:3:115:PHE:CE1[12_555]	2.07	0.13
1:1:64:GLU:OE2	3:3:227:THR:CA[12_555]	2.07	0.13
2:2:206:VAL:CG1	3:3:36:ILE:N[12_555]	2.07	0.13
1:1:41:HIS:CG	1:1:188:SER:N[12_555]	2.07	0.13
3:3:15:THR:CB	3:3:109:TRP:CE3[12_555]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:46:ASP:CB	2:2:203:VAL:O[12_555]	2.07	0.13
2:2:58:THR:C	2:2:253:PHE:CA[2_555]	2.07	0.13
1:1:68:GLU:CD	3:3:98:LEU:N[12_555]	2.07	0.13
1:1:44:ASN:OD1	5:1:288:SUC:O4[12_555]	2.08	0.12
2:2:41:TYR:CE1	2:2:252:GLU:OE1[12_555]	2.08	0.12
1:1:250:CYS:C	3:3:39:GLU:C[12_555]	2.08	0.12
2:2:43:THR:OG1	2:2:106:TYR:CB[12_555]	2.08	0.12
1:1:14:VAL:CB	1:1:256:ALA:C[12_555]	2.08	0.12
1:1:71:LEU:CD1	3:3:44:ILE:O[12_555]	2.08	0.12
3:3:107:THR:N	3:3:225:ARG:N[12_555]	2.08	0.12
2:2:59:SER:N	2:2:253:PHE:N[2_555]	2.08	0.12
1:1:7:ILE:CG2	1:1:275:THR:CB[12_555]	2.08	0.12
1:1:41:HIS:ND1	3:3:28:TYR:OH[12_555]	2.08	0.12
3:3:209:MET:N	4:4:32:PHE:CA[12_555]	2.08	0.12
1:1:241:HIS:CB	3:3:215:ALA:C[12_555]	2.08	0.12
1:1:286:THR:CB	3:3:7:THR:CG2[12_555]	2.08	0.12
3:3:15:THR:CG2	3:3:109:TRP:CZ3[12_555]	2.08	0.12
1:1:173:TRP:NE1	3:3:151:THR:C[12_555]	2.08	0.12
3:3:10:SER:OG	3:3:140:GLU:CB[12_555]	2.08	0.12
2:2:18:ARG:NE	2:2:50:ILE:CG2[2_555]	2.08	0.12
3:3:26:PRO:N	3:3:161:SER:CA[12_555]	2.08	0.12
3:3:222:ARG:C	3:3:226:ASP:N[12_555]	2.08	0.12
3:3:16:THR:OG1	3:3:89:ILE:O[12_555]	2.08	0.12
3:3:106:TYR:C	3:3:223:MET:O[12_555]	2.08	0.12
3:3:16:THR:N	3:3:89:ILE:N[12_555]	2.08	0.12
3:3:209:MET:CA	4:4:32:PHE:CB[12_555]	2.08	0.12
1:1:173:TRP:CD1	3:3:151:THR:CA[12_555]	2.08	0.12
1:1:246:THR:CB	3:3:46:MET:O[12_555]	2.08	0.12
3:3:52:LEU:CD2	4:4:38:SER:CA[12_555]	2.08	0.12
2:2:250:CYS:CB	2:2:252:GLU:OE1[12_555]	2.08	0.12
1:1:247:LYS:CG	2:2:185:ILE:C[12_555]	2.08	0.12
1:1:53:THR:O	1:1:80:SER:C[12_555]	2.08	0.12
1:1:181:ARG:CZ	3:3:115:PHE:CE2[12_555]	2.09	0.11
1:1:62:ARG:CD	1:1:109:ILE:O[12_555]	2.09	0.11
2:2:44:PRO:CB	2:2:248:PRO:N[12_555]	2.09	0.11
1:1:46:GLN:O	1:1:239:ILE:CG1[12_555]	2.09	0.11
3:3:210:LEU:CB	4:4:37:SER:O[12_555]	2.09	0.11
1:1:250:CYS:C	3:3:40:VAL:N[12_555]	2.09	0.11
3:3:26:PRO:N	3:3:161:SER:N[12_555]	2.09	0.11
2:2:17:THR:CA	2:2:49:ALA:N[2_555]	2.09	0.11
1:1:46:GLN:C	1:1:239:ILE:CB[12_555]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:124:GLU:O	3:3:114:ARG:CG[12_555]	2.09	0.11
1:1:115:LEU:O	3:3:41:LYS:CB[12_555]	2.09	0.11
1:1:179:PHE:CZ	3:3:135:PRO:CD[12_555]	2.09	0.11
1:1:179:PHE:CE2	3:3:133:TYR:CE2[12_555]	2.09	0.11
3:3:10:SER:N	3:3:188:TYR:CD1[12_555]	2.09	0.11
1:1:32:PRO:CG	1:1:146:MET:C[12_555]	2.09	0.11
1:1:15:LEU:CG	1:1:255:ARG:CB[12_555]	2.09	0.11
1:1:64:GLU:CA	3:3:105:TYR:CE1[12_555]	2.09	0.11
1:1:123:SER:CA	3:3:50:ASP:OD2[12_555]	2.09	0.11
1:1:116:PHE:N	3:3:41:LYS:C[12_555]	2.09	0.11
1:1:111:ARG:O	3:3:42:ASN:OD1[12_555]	2.09	0.11
2:2:177:GLY:C	4:4:44:ASP:CA[12_555]	2.09	0.11
1:1:116:PHE:CA	3:3:40:VAL:C[12_555]	2.09	0.11
2:2:42:LEU:O	2:2:250:CYS:CA[12_555]	2.09	0.11
2:2:91:ILE:CG1	2:2:95:ASN:ND2[2_555]	2.09	0.11
1:1:252:ARG:NE	3:3:41:LYS:NZ[12_555]	2.09	0.11
2:2:44:PRO:CG	2:2:247:SER:CA[12_555]	2.09	0.11
1:1:7:ILE:C	1:1:276:THR:N[12_555]	2.09	0.11
3:3:209:MET:CG	4:4:32:PHE:CE1[12_555]	2.09	0.11
1:1:15:LEU:C	1:1:259:TYR:CE1[12_555]	2.09	0.11
1:1:53:THR:CB	1:1:80:SER:O[12_555]	2.09	0.11
3:3:10:SER:CA	3:3:140:GLU:CA[12_555]	2.09	0.11
2:2:46:ASP:O	2:2:202:ILE:CB[12_555]	2.09	0.11
1:1:240:TYR:OH	3:3:169:TRP:CE3[12_555]	2.09	0.11
1:1:18:PRO:CD	1:1:106:MET:O[12_555]	2.09	0.11
1:1:10:VAL:CG2	1:1:276:THR:O[12_555]	2.09	0.11
3:3:210:LEU:CB	4:4:34:ASP:O[12_555]	2.09	0.11
1:1:7:ILE:CG2	1:1:275:THR:CG2[12_555]	2.09	0.11
1:1:25:HIS:O	1:1:96:PHE:CA[12_555]	2.09	0.11
1:1:73:ARG:O	3:3:219:PHE:CZ[12_555]	2.09	0.11
2:2:46:ASP:CB	2:2:203:VAL:C[12_555]	2.09	0.11
1:1:253:PRO:O	4:4:43:LEU:O[12_555]	2.09	0.11
1:1:103:LEU:CD1	3:3:48:GLN:NE2[12_555]	2.10	0.10
1:1:127:LEU:N	3:3:166:VAL:CA[12_555]	2.10	0.10
1:1:9:GLU:CA	1:1:276:THR:CB[12_555]	2.10	0.10
2:2:39:PRO:CD	2:2:210:PRO:CA[12_555]	2.10	0.10
1:1:41:HIS:N	1:1:186:PHE:O[12_555]	2.10	0.10
1:1:10:VAL:CA	1:1:276:THR:C[12_555]	2.10	0.10
2:2:43:THR:N	2:2:105:GLY:O[12_555]	2.10	0.10
2:2:18:ARG:CD	2:2:51:ASN:CA[2_555]	2.10	0.10
1:1:6:TYR:C	1:1:276:THR:CA[12_555]	2.10	0.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:39:THR:CG2	3:3:28:TYR:CE2[12_555]	2.10	0.10
1:1:15:LEU:C	1:1:259:TYR:OH[12_555]	2.10	0.10
1:1:180:PRO:CB	3:3:153:VAL:CG2[12_555]	2.10	0.10
3:3:223:MET:N	3:3:225:ARG:NE[12_555]	2.10	0.10
1:1:181:ARG:CB	3:3:165:LEU:CD2[12_555]	2.10	0.10
1:1:14:VAL:O	1:1:255:ARG:CD[12_555]	2.10	0.10
2:2:192:ASN:OD1	4:4:33:LYS:CD[12_555]	2.10	0.10
1:1:179:PHE:CE2	3:3:133:TYR:CD2[12_555]	2.10	0.10
3:3:210:LEU:N	4:4:32:PHE:CB[12_555]	2.10	0.10
1:1:10:VAL:CG2	1:1:278:ILE:N[12_555]	2.10	0.10
3:3:14:MET:CA	3:3:87:VAL:CB[12_555]	2.10	0.10
3:3:15:THR:O	3:3:89:ILE:CD1[12_555]	2.10	0.10
1:1:36:ALA:O	3:3:28:TYR:CB[12_555]	2.10	0.10
1:1:5:ASN:O	1:1:276:THR:CA[12_555]	2.10	0.10
1:1:241:HIS:CG	3:3:114:ARG:NH2[12_555]	2.10	0.10
3:3:67:MET:CB	4:4:27:PHE:O[12_555]	2.10	0.10
1:1:38:GLU:OE2	3:3:27:TRP:N[12_555]	2.10	0.10
3:3:13:PHE:O	3:3:186:ALA:CA[12_555]	2.10	0.10
1:1:31:ALA:O	1:1:147:TYR:O[12_555]	2.10	0.10
1:1:183:SER:N	3:3:116:SER:CB[12_555]	2.10	0.10
3:3:58:VAL:CA	4:4:26:TYR:CA[12_555]	2.10	0.10
1:1:38:GLU:OE1	3:3:28:TYR:N[12_555]	2.10	0.10
3:3:22:PRO:C	3:3:117:PHE:N[12_555]	2.10	0.10
3:3:14:MET:C	3:3:87:VAL:CG1[12_555]	2.10	0.10
1:1:126:THR:N	3:3:113:LEU:O[12_555]	2.10	0.10
1:1:244:LYS:C	3:3:51:THR:CA[12_555]	2.10	0.10
1:1:26:THR:CG2	1:1:222:SER:O[12_555]	2.10	0.10
2:2:173:LEU:CA	4:4:42:ARG:CZ[12_555]	2.10	0.10
1:1:244:LYS:NZ	3:3:212:PHE:O[12_555]	2.10	0.10
3:3:10:SER:N	3:3:188:TYR:CZ[12_555]	2.10	0.10
2:2:194:ARG:O	3:3:27:TRP:NE1[12_555]	2.10	0.10
2:2:54:THR:OG1	2:2:56:PRO:CG[3_555]	2.10	0.10
1:1:33:LEU:O	3:3:24:ALA:CB[12_555]	2.10	0.10
3:3:56:ASN:CG	4:4:29:ILE:CB[12_555]	2.10	0.10
2:2:62:ARG:CB	2:2:254:SER:CA[2_555]	2.10	0.10
1:1:66:SER:O	3:3:102:ILE:CG1[12_555]	2.10	0.10
1:1:17:VAL:CB	1:1:107:ALA:CA[12_555]	2.10	0.10
3:3:12:GLN:NE2	3:3:86:LYS:CB[12_555]	2.10	0.10
1:1:63:ASP:C	1:1:111:ARG:CZ[12_555]	2.10	0.10
2:2:60:SER:O	2:2:256:ALA:CB[2_555]	2.11	0.09
2:2:11:ASP:CA	2:2:26:ASP:CG[11_555]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:54:THR:CA	2:2:57:ASP:O[3_555]	2.11	0.09
1:1:53:THR:N	1:1:237:THR:CG2[12_555]	2.11	0.09
3:3:14:MET:CA	3:3:87:VAL:O[12_555]	2.11	0.09
1:1:39:THR:O	3:3:31:THR:N[12_555]	2.11	0.09
2:2:202:ILE:N	3:3:32:LYS:CE[12_555]	2.11	0.09
2:2:200:THR:C	3:3:32:LYS:CB[12_555]	2.11	0.09
3:3:119:PHE:O	4:4:33:LYS:NZ[12_555]	2.11	0.09
1:1:16:VAL:C	1:1:107:ALA:CB[12_555]	2.11	0.09
1:1:8:ASP:N	1:1:276:THR:N[12_555]	2.11	0.09
1:1:27:THR:CA	1:1:163:TRP:CD2[12_555]	2.11	0.09
2:2:21:SER:C	2:2:101:LEU:CD1[2_555]	2.11	0.09
2:2:19:GLY:C	2:2:211:MET:CE[2_555]	2.11	0.09
1:1:179:PHE:N	3:3:133:TYR:C[12_555]	2.11	0.09
3:3:13:PHE:N	3:3:188:TYR:N[12_555]	2.11	0.09
1:1:173:TRP:NE1	3:3:151:THR:N[12_555]	2.11	0.09
1:1:116:PHE:CE1	3:3:40:VAL:CG1[12_555]	2.11	0.09
2:2:195:SER:CB	3:3:27:TRP:CD1[12_555]	2.11	0.09
1:1:240:TYR:CD1	3:3:112:SER:CA[12_555]	2.11	0.09
2:2:43:THR:CG2	2:2:105:GLY:O[12_555]	2.11	0.09
2:2:187:PRO:CB	3:3:33:GLU:OE2[12_555]	2.11	0.09
1:1:48:GLU:OE2	1:1:78:HIS:CB[12_555]	2.11	0.09
2:2:45:GLN:CB	2:2:106:TYR:C[12_555]	2.11	0.09
1:1:245:HIS:CG	3:3:50:ASP:O[12_555]	2.11	0.09
3:3:16:THR:O	3:3:89:ILE:N[12_555]	2.11	0.09
1:1:124:GLU:O	3:3:114:ARG:C[12_555]	2.11	0.09
1:1:250:CYS:CA	3:3:39:GLU:C[12_555]	2.11	0.09
1:1:249:TRP:C	3:3:40:VAL:N[12_555]	2.11	0.09
1:1:116:PHE:C	3:3:45:GLU:OE1[12_555]	2.11	0.09
2:2:34:GLY:CA	3:3:34:ILE:N[12_555]	2.11	0.09
1:1:21:LYS:C	1:1:79:ILE:O[12_555]	2.11	0.09
2:2:36:GLY:C	2:2:208:ALA:O[12_555]	2.11	0.09
2:2:17:THR:CG2	2:2:50:ILE:CG2[12_555]	2.11	0.09
1:1:113:PHE:CD2	3:3:45:GLU:CA[12_555]	2.11	0.09
1:1:51:ILE:O	1:1:237:THR:CG2[12_555]	2.11	0.09
2:2:40:HIS:CB	2:2:103:ARG:NE[12_555]	2.11	0.09
2:2:13:ILE:CA	2:2:13:ILE:O[11_555]	2.11	0.09
2:2:35:TYR:C	3:3:36:ILE:CD1[12_555]	2.11	0.09
3:3:17:ASP:OD1	3:3:86:LYS:O[12_555]	2.11	0.09
1:1:47:PRO:CG	1:1:239:ILE:CA[12_555]	2.11	0.09
1:1:127:LEU:O	3:3:151:THR:CG2[12_555]	2.12	0.08
1:1:53:THR:CB	1:1:80:SER:CB[12_555]	2.12	0.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:116:PHE:CD2	3:3:40:VAL:CA[12_555]	2.12	0.08
2:2:41:TYR:CE2	2:2:55:GLN:CD[12_555]	2.12	0.08
1:1:63:ASP:N	1:1:111:ARG:CG[12_555]	2.12	0.08
2:2:64:TYR:CG	2:2:256:ALA:O[2_555]	2.12	0.08
2:2:43:THR:O	2:2:249:MET:CB[12_555]	2.12	0.08
1:1:17:VAL:CB	1:1:107:ALA:N[12_555]	2.12	0.08
2:2:88:ASP:O	2:2:259:LYS:CG[2_555]	2.12	0.08
3:3:212:PHE:CA	4:4:38:SER:O[12_555]	2.12	0.08
3:3:209:MET:C	4:4:32:PHE:O[12_555]	2.12	0.08
1:1:77:VAL:CG1	3:3:217:LYS:CA[12_555]	2.12	0.08
1:1:126:THR:C	3:3:166:VAL:CB[12_555]	2.12	0.08
1:1:246:THR:OG1	3:3:46:MET:CA[12_555]	2.12	0.08
3:3:70:VAL:CB	4:4:31:TYR:CD1[12_555]	2.12	0.08
2:2:11:ASP:OD2	2:2:26:ASP:C[11_555]	2.12	0.08
1:1:116:PHE:CZ	3:3:40:VAL:CG1[12_555]	2.12	0.08
2:2:37:VAL:N	2:2:207:ASN:C[12_555]	2.12	0.08
2:2:89:MET:O	2:2:98:TYR:CG[2_555]	2.12	0.08
1:1:176:GLY:N	3:3:150:GLY:N[12_555]	2.12	0.08
1:1:8:ASP:N	1:1:275:THR:CG2[12_555]	2.12	0.08
2:2:59:SER:CA	2:2:253:PHE:CG[2_555]	2.12	0.08
1:1:175:HIS:C	3:3:149:LEU:CA[12_555]	2.12	0.08
2:2:59:SER:OG	2:2:253:PHE:CB[2_555]	2.12	0.08
1:1:175:HIS:C	3:3:149:LEU:C[12_555]	2.12	0.08
1:1:7:ILE:CG2	1:1:275:THR:OG1[12_555]	2.12	0.08
2:2:11:ASP:CA	2:2:26:ASP:CB[11_555]	2.12	0.08
1:1:49:ASP:OD2	1:1:101:ILE:CD1[12_555]	2.12	0.08
1:1:29:ASN:CA	1:1:162:SER:C[12_555]	2.12	0.08
2:2:179:LEU:N	4:4:42:ARG:CB[12_555]	2.12	0.08
2:2:37:VAL:CA	2:2:209:VAL:N[12_555]	2.12	0.08
2:2:52:LYS:CG	2:2:58:THR:OG1[12_555]	2.12	0.08
1:1:31:ALA:C	1:1:147:TYR:CB[12_555]	2.12	0.08
2:2:178:THR:CB	4:4:44:ASP:CB[12_555]	2.12	0.08
1:1:12:ASN:CB	3:3:230:HIS:N[12_555]	2.12	0.08
3:3:70:VAL:CG2	4:4:31:TYR:CB[12_555]	2.12	0.08
3:3:24:ALA:O	3:3:162:THR:C[12_555]	2.12	0.08
1:1:15:LEU:N	1:1:255:ARG:CG[12_555]	2.13	0.07
1:1:109:ILE:CD1	3:3:219:PHE:CB[12_555]	2.13	0.07
1:1:243:ALA:C	3:3:49:VAL:O[12_555]	2.13	0.07
3:3:70:VAL:N	4:4:29:ILE:O[12_555]	2.13	0.07
1:1:39:THR:C	3:3:30:PRO:CD[12_555]	2.13	0.07
1:1:122:ASP:N	3:3:50:ASP:OD1[12_555]	2.13	0.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:242:LYS:N	3:3:215:ALA:N[12_555]	2.13	0.07
1:1:113:PHE:CG	3:3:45:GLU:N[12_555]	2.13	0.07
3:3:19:MET:CG	3:3:85:ILE:CB[12_555]	2.13	0.07
1:1:179:PHE:CD2	3:3:133:TYR:CB[12_555]	2.13	0.07
1:1:68:GLU:CD	3:3:51:THR:CG2[12_555]	2.13	0.07
1:1:53:THR:O	1:1:81:ARG:N[12_555]	2.13	0.07
1:1:121:PHE:CD1	3:3:49:VAL:N[12_555]	2.13	0.07
2:2:37:VAL:CB	2:2:207:ASN:C[12_555]	2.13	0.07
1:1:71:LEU:CB	3:3:47:CYS:CB[12_555]	2.13	0.07
1:1:244:LYS:CE	3:3:213:VAL:N[12_555]	2.13	0.07
2:2:189:GLN:NE2	3:3:30:PRO:N[12_555]	2.13	0.07
1:1:179:PHE:N	3:3:133:TYR:CA[12_555]	2.13	0.07
2:2:37:VAL:N	2:2:208:ALA:N[12_555]	2.13	0.07
1:1:128:VAL:N	3:3:168:PRO:CB[12_555]	2.13	0.07
1:1:6:TYR:C	1:1:275:THR:C[12_555]	2.13	0.07
2:2:50:ILE:CG1	2:2:50:ILE:CD1[10_555]	2.13	0.07
1:1:77:VAL:CG1	3:3:217:LYS:C[12_555]	2.13	0.07
3:3:209:MET:CA	4:4:31:TYR:C[12_555]	2.13	0.07
1:1:38:GLU:CG	3:3:28:TYR:O[12_555]	2.13	0.07
1:1:14:VAL:CB	1:1:255:ARG:O[12_555]	2.13	0.07
1:1:39:THR:N	3:3:30:PRO:CG[12_555]	2.13	0.07
2:2:44:PRO:CD	2:2:247:SER:O[12_555]	2.13	0.07
1:1:35:ASP:CG	1:1:187:LEU:CD2[12_555]	2.13	0.07
1:1:31:ALA:C	1:1:147:TYR:CA[12_555]	2.13	0.07
2:2:179:LEU:C	4:4:42:ARG:CA[12_555]	2.13	0.07
2:2:44:PRO:CD	2:2:247:SER:C[12_555]	2.13	0.07
2:2:38:TRP:CD2	2:2:210:PRO:CB[12_555]	2.13	0.07
3:3:222:ARG:O	3:3:226:ASP:N[12_555]	2.13	0.07
1:1:14:VAL:CG2	1:1:256:ALA:CB[12_555]	2.13	0.07
1:1:8:ASP:OD1	1:1:257:VAL:CG1[12_555]	2.13	0.07
3:3:18:ASP:CB	3:3:94:LEU:N[12_555]	2.13	0.07
3:3:12:GLN:CG	3:3:188:TYR:N[12_555]	2.13	0.07
1:1:63:ASP:OD1	1:1:255:ARG:O[12_555]	2.13	0.07
2:2:42:LEU:CA	2:2:249:MET:O[12_555]	2.13	0.07
1:1:44:ASN:O	1:1:101:ILE:CG1[12_555]	2.13	0.07
2:2:37:VAL:C	2:2:209:VAL:O[12_555]	2.14	0.06
2:2:199:ALA:CB	3:3:29:HIS:CE1[12_555]	2.14	0.06
1:1:31:ALA:N	1:1:147:TYR:O[12_555]	2.14	0.06
3:3:23:CYS:N	3:3:118:MET:N[12_555]	2.14	0.06
2:2:17:THR:CA	2:2:48:THR:O[2_555]	2.14	0.06
1:1:46:GLN:NE2	5:1:288:SUC:O6[12_555]	2.14	0.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:10:VAL:CG2	1:1:278:ILE:O[12_555]	2.14	0.06
2:2:42:LEU:CA	2:2:250:CYS:CB[12_555]	2.14	0.06
1:1:65:MET:SD	1:1:112:LYS:CE[12_555]	2.14	0.06
2:2:194:ARG:NE	3:3:27:TRP:CZ2[12_555]	2.14	0.06
1:1:244:LYS:C	3:3:50:ASP:CA[12_555]	2.14	0.06
3:3:67:MET:C	4:4:28:ASN:CA[12_555]	2.14	0.06
3:3:24:ALA:C	3:3:162:THR:N[12_555]	2.14	0.06
1:1:249:TRP:C	3:3:39:GLU:O[12_555]	2.14	0.06
3:3:118:MET:O	4:4:33:LYS:N[12_555]	2.14	0.06
1:1:176:GLY:CA	3:3:150:GLY:N[12_555]	2.14	0.06
3:3:222:ARG:CA	3:3:226:ASP:O[12_555]	2.14	0.06
1:1:53:THR:CB	1:1:237:THR:O[12_555]	2.14	0.06
3:3:68:TYR:C	4:4:30:ASN:N[12_555]	2.14	0.06
1:1:51:ILE:CA	1:1:145:TYR:CZ[12_555]	2.14	0.06
3:3:209:MET:C	4:4:32:PHE:CB[12_555]	2.14	0.06
1:1:15:LEU:CD1	1:1:255:ARG:CB[12_555]	2.14	0.06
2:2:44:PRO:O	2:2:247:SER:CB[12_555]	2.14	0.06
1:1:13:GLU:CD	3:3:231:ILE:O[12_555]	2.14	0.06
1:1:183:SER:CB	3:3:116:SER:OG[12_555]	2.14	0.06
1:1:14:VAL:CG1	1:1:255:ARG:CG[12_555]	2.14	0.06
3:3:222:ARG:CG	3:3:226:ASP:CA[12_555]	2.14	0.06
3:3:212:PHE:CZ	4:4:35:ALA:O[12_555]	2.14	0.06
1:1:32:PRO:CA	1:1:147:TYR:CD2[12_555]	2.14	0.06
3:3:68:TYR:CB	4:4:30:ASN:ND2[12_555]	2.14	0.06
1:1:242:LYS:O	3:3:215:ALA:N[12_555]	2.14	0.06
1:1:46:GLN:CG	1:1:99:TRP:CH2[12_555]	2.14	0.06
1:1:67:ILE:CG2	3:3:46:MET:CB[12_555]	2.14	0.06
1:1:109:ILE:CG2	3:3:218:ASP:C[12_555]	2.14	0.06
1:1:124:GLU:OE2	3:3:115:PHE:CD1[12_555]	2.15	0.05
3:3:24:ALA:N	3:3:163:ILE:CA[12_555]	2.15	0.05
3:3:209:MET:CG	4:4:32:PHE:CB[12_555]	2.15	0.05
1:1:37:ALA:CA	1:1:185:PRO:CA[12_555]	2.15	0.05
1:1:54:ARG:N	1:1:80:SER:O[12_555]	2.15	0.05
1:1:17:VAL:C	1:1:106:MET:O[12_555]	2.15	0.05
2:2:60:SER:C	2:2:99:HIS:NE2[12_555]	2.15	0.05
1:1:246:THR:OG1	3:3:46:MET:O[12_555]	2.15	0.05
1:1:175:HIS:O	3:3:149:LEU:CA[12_555]	2.15	0.05
2:2:43:THR:CG2	2:2:106:TYR:N[12_555]	2.15	0.05
1:1:181:ARG:NE	3:3:115:PHE:CG[12_555]	2.15	0.05
1:1:116:PHE:CE2	3:3:40:VAL:CB[12_555]	2.15	0.05
1:1:245:HIS:ND1	3:3:50:ASP:O[12_555]	2.15	0.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:44:PRO:O	2:2:107:THR:CB[12_555]	2.15	0.05
2:2:173:LEU:O	4:4:42:ARG:NH1[12_555]	2.15	0.05
1:1:243:ALA:CB	3:3:48:GLN:C[12_555]	2.15	0.05
2:2:180:LEU:N	4:4:42:ARG:CB[12_555]	2.15	0.05
2:2:178:THR:OG1	4:4:44:ASP:OD2[12_555]	2.15	0.05
3:3:68:TYR:CB	4:4:30:ASN:OD1[12_555]	2.15	0.05
1:1:25:HIS:CG	1:1:224:ILE:N[12_555]	2.15	0.05
1:1:243:ALA:CB	3:3:49:VAL:N[12_555]	2.15	0.05
1:1:242:LYS:NZ	3:3:213:VAL:CG1[12_555]	2.15	0.05
2:2:41:TYR:N	2:2:103:ARG:CD[12_555]	2.15	0.05
3:3:12:GLN:CG	3:3:187:GLY:CA[12_555]	2.15	0.05
3:3:17:ASP:OD2	3:3:94:LEU:CD1[12_555]	2.15	0.05
1:1:176:GLY:O	3:3:147:ALA:O[12_555]	2.15	0.05
3:3:14:MET:N	3:3:87:VAL:CA[12_555]	2.15	0.05
3:3:18:ASP:CG	3:3:97:THR:CG2[12_555]	2.15	0.05
1:1:49:ASP:CB	1:1:220:ILE:CB[12_555]	2.15	0.05
1:1:28:SER:CA	1:1:163:TRP:CD2[12_555]	2.15	0.05
1:1:183:SER:OG	3:3:116:SER:CB[12_555]	2.15	0.05
2:2:44:PRO:CG	2:2:248:PRO:O[12_555]	2.15	0.05
1:1:251:PRO:CA	3:3:40:VAL:C[12_555]	2.15	0.05
1:1:66:SER:OG	1:1:254:PRO:CB[12_555]	2.15	0.05
2:2:58:THR:N	2:2:253:PHE:O[2_555]	2.15	0.05
1:1:53:THR:CA	1:1:237:THR:N[12_555]	2.15	0.05
2:2:250:CYS:CA	2:2:252:GLU:OE1[12_555]	2.15	0.05
1:1:64:GLU:CA	3:3:101:GLU:O[12_555]	2.15	0.05
1:1:30:SER:O	1:1:146:MET:SD[12_555]	2.15	0.05
2:2:46:ASP:CG	2:2:203:VAL:CG1[12_555]	2.15	0.05
1:1:67:ILE:CB	3:3:46:MET:CE[12_555]	2.16	0.04
3:3:220:CYS:C	3:3:226:ASP:OD2[12_555]	2.16	0.04
1:1:109:ILE:N	3:3:219:PHE:O[12_555]	2.16	0.04
1:1:69:SER:CB	3:3:101:GLU:O[12_555]	2.16	0.04
3:3:67:MET:CB	4:4:27:PHE:CA[12_555]	2.16	0.04
1:1:38:GLU:C	3:3:28:TYR:O[12_555]	2.16	0.04
1:1:23:SER:C	1:1:97:THR:CG2[12_555]	2.16	0.04
1:1:128:VAL:CG2	3:3:168:PRO:O[12_555]	2.16	0.04
1:1:242:LYS:N	3:3:214:SER:C[12_555]	2.16	0.04
1:1:116:PHE:N	3:3:41:LYS:CB[12_555]	2.16	0.04
2:2:187:PRO:C	3:3:33:GLU:CD[12_555]	2.16	0.04
3:3:22:PRO:N	3:3:117:PHE:CD2[12_555]	2.16	0.04
2:2:53:PRO:CA	2:2:57:ASP:C[3_555]	2.16	0.04
2:2:38:TRP:CE2	2:2:210:PRO:CG[12_555]	2.16	0.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:52:GLU:O	1:1:236:THR:CA[12_555]	2.16	0.04
1:1:5:ASN:N	1:1:274:VAL:CG2[12_555]	2.16	0.04
2:2:40:HIS:CG	2:2:103:ARG:NE[12_555]	2.16	0.04
3:3:106:TYR:C	3:3:223:MET:C[12_555]	2.16	0.04
1:1:64:GLU:C	3:3:105:TYR:CZ[12_555]	2.16	0.04
1:1:122:ASP:CG	3:3:50:ASP:OD1[12_555]	2.16	0.04
2:2:17:THR:OG1	2:2:48:THR:CA[2_555]	2.16	0.04
1:1:31:ALA:C	1:1:147:TYR:N[12_555]	2.16	0.04
3:3:14:MET:O	3:3:87:VAL:CG1[12_555]	2.16	0.04
2:2:40:HIS:CE1	2:2:205:TYR:CG[12_555]	2.16	0.04
1:1:243:ALA:CA	3:3:47:CYS:O[12_555]	2.16	0.04
3:3:65:VAL:CA	4:4:28:ASN:ND2[12_555]	2.16	0.04
1:1:179:PHE:CZ	3:3:133:TYR:CD2[12_555]	2.16	0.04
2:2:55:GLN:CD	2:2:57:ASP:OD1[3_555]	2.16	0.04
1:1:33:LEU:CA	1:1:169:MET:SD[12_555]	2.16	0.04
2:2:53:PRO:CB	2:2:58:THR:CA[3_555]	2.16	0.04
3:3:16:THR:CG2	3:3:89:ILE:N[12_555]	2.16	0.04
3:3:13:PHE:CG	3:3:133:TYR:CE1[12_555]	2.16	0.04
1:1:115:LEU:CA	3:3:42:ASN:CA[12_555]	2.16	0.04
1:1:5:ASN:O	1:1:276:THR:N[12_555]	2.16	0.04
3:3:12:GLN:N	3:3:188:TYR:CG[12_555]	2.16	0.04
3:3:222:ARG:CD	3:3:226:ASP:O[12_555]	2.16	0.04
2:2:54:THR:C	2:2:57:ASP:CA[3_555]	2.16	0.04
2:2:43:THR:N	2:2:249:MET:C[12_555]	2.16	0.04
1:1:254:PRO:C	4:4:43:LEU:CD2[12_555]	2.16	0.04
1:1:241:HIS:NE2	3:3:215:ALA:O[12_555]	2.16	0.04
1:1:126:THR:CG2	3:3:167:VAL:N[12_555]	2.16	0.04
1:1:69:SER:CB	3:3:101:GLU:CA[12_555]	2.16	0.04
2:2:20:ASP:N	2:2:101:LEU:CB[2_555]	2.16	0.04
2:2:89:MET:CA	2:2:257:ARG:O[2_555]	2.17	0.03
1:1:26:THR:OG1	1:1:163:TRP:CH2[12_555]	2.17	0.03
1:1:179:PHE:CA	3:3:133:TYR:N[12_555]	2.17	0.03
2:2:250:CYS:SG	2:2:252:GLU:OE2[12_555]	2.17	0.03
3:3:106:TYR:O	3:3:223:MET:C[12_555]	2.17	0.03
2:2:57:ASP:OD1	2:2:57:ASP:OD2[11_555]	2.17	0.03
1:1:250:CYS:SG	3:3:39:GLU:N[12_555]	2.17	0.03
1:1:44:ASN:OD1	5:1:288:SUC:C3[12_555]	2.17	0.03
2:2:64:TYR:CG	2:2:256:ALA:C[2_555]	2.17	0.03
3:3:8:PRO:C	3:3:188:TYR:OH[12_555]	2.17	0.03
1:1:127:LEU:N	3:3:167:VAL:N[12_555]	2.17	0.03
1:1:23:SER:O	1:1:82:ILE:CG1[12_555]	2.17	0.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:71:LEU:CG	3:3:43:LEU:C[12_555]	2.17	0.03
1:1:241:HIS:CA	3:3:215:ALA:C[12_555]	2.17	0.03
1:1:22:GLU:CB	1:1:81:ARG:CB[12_555]	2.17	0.03
1:1:69:SER:N	3:3:102:ILE:CG1[12_555]	2.17	0.03
1:1:76:CYS:CB	3:3:218:ASP:OD1[12_555]	2.17	0.03
2:2:32:VAL:CA	3:3:31:THR:CB[12_555]	2.17	0.03
2:2:36:GLY:O	2:2:207:ASN:C[12_555]	2.17	0.03
1:1:116:PHE:CD1	3:3:42:ASN:O[12_555]	2.17	0.03
2:2:17:THR:CG2	2:2:48:THR:CA[2_555]	2.17	0.03
1:1:17:VAL:CG1	1:1:107:ALA:CA[12_555]	2.17	0.03
2:2:62:ARG:NH2	2:2:101:LEU:N[2_555]	2.17	0.03
2:2:203:VAL:CG2	3:3:34:ILE:CA[12_555]	2.17	0.03
2:2:58:THR:CA	2:2:253:PHE:C[2_555]	2.17	0.03
1:1:176:GLY:CA	3:3:149:LEU:O[12_555]	2.17	0.03
2:2:11:ASP:CG	2:2:26:ASP:C[11_555]	2.17	0.03
1:1:47:PRO:CA	1:1:239:ILE:CD1[12_555]	2.17	0.03
2:2:194:ARG:NH1	3:3:27:TRP:CD2[12_555]	2.17	0.03
3:3:21:SER:CA	3:3:117:PHE:CD1[12_555]	2.17	0.03
3:3:20:GLN:CG	3:3:55:VAL:CG1[12_555]	2.17	0.03
1:1:40:GLY:O	1:1:186:PHE:CB[12_555]	2.17	0.03
3:3:12:GLN:CA	3:3:187:GLY:CA[12_555]	2.17	0.03
2:2:47:ALA:CB	2:2:249:MET:CG[12_555]	2.18	0.02
1:1:124:GLU:OE2	3:3:115:PHE:N[12_555]	2.18	0.02
1:1:181:ARG:NE	3:3:189:ILE:CD1[12_555]	2.18	0.02
1:1:5:ASN:O	1:1:276:THR:CG2[12_555]	2.18	0.02
1:1:37:ALA:N	1:1:185:PRO:CD[12_555]	2.18	0.02
3:3:66:SER:CA	4:4:28:ASN:CB[12_555]	2.18	0.02
3:3:69:THR:O	4:4:29:ILE:CB[12_555]	2.18	0.02
1:1:240:TYR:CA	3:3:112:SER:C[12_555]	2.18	0.02
3:3:13:PHE:N	3:3:187:GLY:CA[12_555]	2.18	0.02
2:2:64:TYR:CE1	2:2:256:ALA:O[2_555]	2.18	0.02
1:1:74:SER:C	3:3:112:SER:O[12_555]	2.18	0.02
2:2:60:SER:CA	2:2:99:HIS:CD2[2_555]	2.18	0.02
1:1:252:ARG:CB	3:3:41:LYS:CG[12_555]	2.18	0.02
3:3:11:GLY:C	3:3:188:TYR:CB[12_555]	2.18	0.02
1:1:12:ASN:CB	3:3:229:LEU:CA[12_555]	2.18	0.02
2:2:52:LYS:NZ	2:2:252:GLU:OE1[10_555]	2.18	0.02
1:1:6:TYR:O	1:1:276:THR:CB[12_555]	2.18	0.02
2:2:186:PHE:CE2	3:3:41:LYS:NZ[12_555]	2.18	0.02
1:1:6:TYR:CE1	1:1:280:ARG:NH1[12_555]	2.18	0.02
2:2:54:THR:CB	2:2:56:PRO:O[3_555]	2.18	0.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:180:PRO:O	3:3:165:LEU:CG[12_555]	2.18	0.02
3:3:17:ASP:OD1	3:3:86:LYS:C[12_555]	2.18	0.02
1:1:245:HIS:ND1	2:2:184:LEU:CD2[12_555]	2.18	0.02
3:3:23:CYS:C	3:3:162:THR:CB[12_555]	2.18	0.02
2:2:42:LEU:CB	2:2:250:CYS:SG[12_555]	2.18	0.02
2:2:38:TRP:CH2	2:2:48:THR:OG1[12_555]	2.18	0.02
3:3:108:HIS:N	3:3:225:ARG:CA[12_555]	2.18	0.02
2:2:20:ASP:CB	2:2:211:MET:CB[2_555]	2.18	0.02
1:1:63:ASP:CG	1:1:255:ARG:O[12_555]	2.18	0.02
1:1:255:ARG:O	4:4:43:LEU:CD2[12_555]	2.18	0.02
1:1:125:ILE:O	3:3:166:VAL:N[12_555]	2.18	0.02
2:2:64:TYR:CZ	2:2:256:ALA:C[2_555]	2.18	0.02
1:1:127:LEU:C	3:3:168:PRO:CG[12_555]	2.18	0.02
3:3:106:TYR:CB	3:3:224:ALA:CB[12_555]	2.18	0.02
2:2:21:SER:CB	2:2:101:LEU:CG[2_555]	2.18	0.02
2:2:17:THR:CA	2:2:49:ALA:O[2_555]	2.18	0.02
1:1:244:LYS:CD	3:3:213:VAL:CA[12_555]	2.18	0.02
3:3:222:ARG:O	3:3:225:ARG:CD[12_555]	2.18	0.02
1:1:116:PHE:CB	3:3:45:GLU:CD[12_555]	2.18	0.02
2:2:204:PRO:O	3:3:35:SER:OG[12_555]	2.18	0.02
2:2:44:PRO:N	2:2:248:PRO:O[12_555]	2.18	0.02
1:1:126:THR:CB	3:3:113:LEU:O[12_555]	2.19	0.01
2:2:29:ALA:CB	3:3:29:HIS:O[12_555]	2.19	0.01
2:2:194:ARG:CD	3:3:27:TRP:CE2[12_555]	2.19	0.01
1:1:252:ARG:CG	3:3:41:LYS:CE[12_555]	2.19	0.01
2:2:34:GLY:O	3:3:34:ILE:CG1[12_555]	2.19	0.01
1:1:109:ILE:CG2	3:3:218:ASP:O[12_555]	2.19	0.01
1:1:52:GLU:OE1	1:1:235:ILE:CD1[12_555]	2.19	0.01
3:3:212:PHE:CE2	4:4:37:SER:N[12_555]	2.19	0.01
1:1:177:GLN:OE1	3:3:148:MET:N[12_555]	2.19	0.01
3:3:11:GLY:O	3:3:134:THR:OG1[12_555]	2.19	0.01
1:1:249:TRP:NE1	2:2:35:TYR:CG[12_555]	2.19	0.01
2:2:62:ARG:O	2:2:255:GLY:C[2_555]	2.19	0.01
2:2:58:THR:CB	2:2:253:PHE:O[2_555]	2.19	0.01
1:1:74:SER:C	3:3:219:PHE:CD1[12_555]	2.19	0.01
3:3:22:PRO:CD	3:3:117:PHE:CE1[12_555]	2.19	0.01
1:1:102:THR:O	3:3:217:LYS:CG[12_555]	2.19	0.01
1:1:31:ALA:C	1:1:147:TYR:C[12_555]	2.19	0.01
1:1:245:HIS:O	2:2:184:LEU:O[12_555]	2.19	0.01
1:1:18:PRO:CB	1:1:105:GLU:CB[12_555]	2.19	0.01
1:1:113:PHE:CE2	3:3:48:GLN:CB[12_555]	2.19	0.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:20:GLN:CA	3:3:211:CYS:SG[12_555]	2.19	0.01
1:1:60:GLN:O	1:1:107:ALA:CB[12_555]	2.19	0.01
1:1:241:HIS:N	3:3:216:CYS:SG[12_555]	2.19	0.01
1:1:76:CYS:N	3:3:111:GLY:CA[12_555]	2.19	0.01
3:3:118:MET:O	4:4:32:PHE:CB[12_555]	2.19	0.01
3:3:22:PRO:CG	3:3:155:TRP:CE3[12_555]	2.19	0.01
3:3:25:LEU:N	3:3:162:THR:O[12_555]	2.19	0.01
1:1:25:HIS:N	1:1:82:ILE:CD1[12_555]	2.19	0.01
1:1:39:THR:CA	3:3:30:PRO:CB[12_555]	2.19	0.01
1:1:61:THR:CG2	3:3:230:HIS:NE2[12_555]	2.19	0.01
1:1:47:PRO:N	1:1:239:ILE:CD1[12_555]	2.19	0.01
3:3:16:THR:CB	3:3:89:ILE:N[12_555]	2.19	0.01
2:2:62:ARG:O	2:2:256:ALA:N[2_555]	2.19	0.01
1:1:12:ASN:CG	3:3:229:LEU:C[12_555]	2.19	0.01
1:1:12:ASN:CG	3:3:229:LEU:O[12_555]	2.19	0.01
2:2:176:ASP:OD1	4:4:44:ASP:OD1[12_555]	2.19	0.01
3:3:209:MET:O	4:4:30:ASN:C[12_555]	2.19	0.01
1:1:61:THR:CG2	3:3:230:HIS:CE1[12_555]	2.19	0.01
2:2:60:SER:N	2:2:99:HIS:NE2[2_555]	2.19	0.01
1:1:115:LEU:CD1	3:3:41:LYS:O[12_555]	2.19	0.01

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	281/287 (98%)	217 (77%)	46 (16%)	18 (6%)	2	13
2	2	251/263 (95%)	201 (80%)	35 (14%)	15 (6%)	2	16
3	3	236/238 (99%)	179 (76%)	37 (16%)	20 (8%)	1	6
4	4	17/44 (39%)	9 (53%)	7 (41%)	1 (6%)	2	16
All	All	785/832 (94%)	606 (77%)	125 (16%)	54 (7%)	1	10

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	59	SER
1	1	72	GLY
1	1	107	ALA
1	1	108	GLN
1	1	114	GLU
1	1	158	ARG
1	1	226	THR
2	2	145	LYS
2	2	157	SER
2	2	258	ALA
3	3	57	ASN
3	3	88	ASP
3	3	89	ILE
3	3	94	LEU
3	3	96	THR
1	1	29	ASN
1	1	37	ALA
1	1	67	ILE
1	1	90	ASN
1	1	227	GLU
2	2	91	ILE
2	2	129	GLU
2	2	155	ASP
2	2	193	LEU
2	2	208	ALA
2	2	257	ARG
3	3	59	GLY
3	3	66	SER
3	3	67	MET
3	3	95	ALA
3	3	161	SER
3	3	174	HIS
3	3	184	SER
1	1	6	TYR
1	1	137	ASP
2	2	30	ASN
2	2	156	VAL
3	3	74	ASN
3	3	159	LEU
3	3	201	PRO
3	3	219	PHE
3	3	229	LEU
4	4	27	PHE

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Mol	Chain	Res	Type
1	1	160	ASP
1	1	266	ASN
2	2	260	ASN
1	1	205	THR
1	1	268	MET
2	2	87	LYS
2	2	259	LYS
3	3	220	CYS
3	3	121	GLY
2	2	44	PRO
3	3	82	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	254/258 (98%)	184 (72%)	70 (28%)	0	1
2	2	219/227 (96%)	159 (73%)	60 (27%)	0	1
3	3	209/209 (100%)	157 (75%)	52 (25%)	1	3
4	4	15/35 (43%)	9 (60%)	6 (40%)	0	0
All	All	697/729 (96%)	509 (73%)	188 (27%)	0	2

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	5	ASN
1	1	6	TYR
1	1	7	ILE
1	1	15	LEU
1	1	19	ASN
1	1	26	THR
1	1	35	ASP
1	1	44	ASN
1	1	45	VAL
1	1	54	ARG

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Mol	Chain	Res	Type
1	1	60	GLN
1	1	73	ARG
1	1	87	THR
1	1	89	TYR
1	1	90	ASN
1	1	97	THR
1	1	101	ILE
1	1	102	THR
1	1	104	GLN
1	1	105	GLU
1	1	108	GLN
1	1	109	ILE
1	1	112	LYS
1	1	119	VAL
1	1	124	GLU
1	1	126	THR
1	1	127	LEU
1	1	134	ARG
1	1	141	ILE
1	1	142	VAL
1	1	143	MET
1	1	145	TYR
1	1	157	LYS
1	1	158	ARG
1	1	160	ASP
1	1	161	PHE
1	1	162	SER
1	1	173	TRP
1	1	174	GLN
1	1	186	PHE
1	1	195	MET
1	1	197	TYR
1	1	201	ASP
1	1	204	ASN
1	1	209	TYR
1	1	211	SER
1	1	212	VAL
1	1	215	ASN
1	1	217	MET
1	1	219	THR
1	1	223	ARG
1	1	224	ILE

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Mol	Chain	Res	Type
1	1	227	GLU
1	1	228	LYS
1	1	232	SER
1	1	236	THR
1	1	237	THR
1	1	246	THR
1	1	247	LYS
1	1	250	CYS
1	1	252	ARG
1	1	259	TYR
1	1	265	THR
1	1	274	VAL
1	1	275	THR
1	1	276	THR
1	1	278	ILE
1	1	279	VAL
1	1	281	ARG
1	1	286	THR
2	2	12	ARG
2	2	15	GLN
2	2	17	THR
2	2	18	ARG
2	2	25	SER
2	2	27	ASP
2	2	30	ASN
2	2	43	THR
2	2	51	ASN
2	2	52	LYS
2	2	55	GLN
2	2	58	THR
2	2	60	SER
2	2	62	ARG
2	2	63	PHE
2	2	65	THR
2	2	68	SER
2	2	72	ASN
2	2	75	SER
2	2	78	TRP
2	2	86	LEU
2	2	87	LYS
2	2	88	ASP
2	2	94	GLU

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Mol	Chain	Res	Type
2	2	103	ARG
2	2	111	GLN
2	2	116	LYS
2	2	126	MET
2	2	136	LYS
2	2	139	SER
2	2	145	LYS
2	2	146	LEU
2	2	154	ARG
2	2	158	GLN
2	2	159	GLU
2	2	160	ARG
2	2	164	LEU
2	2	170	ASP
2	2	171	SER
2	2	175	PHE
2	2	180	LEU
2	2	191	ILE
2	2	192	ASN
2	2	194	ARG
2	2	195	SER
2	2	197	ASN
2	2	198	SER
2	2	200	THR
2	2	201	LEU
2	2	202	ILE
2	2	206	VAL
2	2	207	ASN
2	2	216	ARG
2	2	219	ASN
2	2	224	ILE
2	2	239	ILE
2	2	240	VAL
2	2	257	ARG
2	2	261	ILE
2	2	262	LYS
3	3	2	LEU
3	3	4	VAL
3	3	5	TYR
3	3	7	THR
3	3	19	MET
3	3	21	SER

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Mol	Chain	Res	Type
3	3	23	CYS
3	3	32	LYS
3	3	39	GLU
3	3	50	ASP
3	3	55	VAL
3	3	56	ASN
3	3	60	ASN
3	3	61	ASN
3	3	65	VAL
3	3	66	SER
3	3	75	GLN
3	3	84	SER
3	3	90	THR
3	3	92	THR
3	3	99	ILE
3	3	116	SER
3	3	119	PHE
3	3	126	THR
3	3	127	LEU
3	3	134	THR
3	3	140	GLU
3	3	142	THR
3	3	143	THR
3	3	148	MET
3	3	157	VAL
3	3	159	LEU
3	3	161	SER
3	3	177	LEU
3	3	182	LYS
3	3	189	ILE
3	3	192	TRP
3	3	194	GLN
3	3	196	ASN
3	3	201	PRO
3	3	205	GLN
3	3	208	ASP
3	3	209	MET
3	3	210	LEU
3	3	211	CYS
3	3	212	PHE
3	3	213	VAL
3	3	216	CYS

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Mol	Chain	Res	Type
3	3	217	LYS
3	3	228	ASP
3	3	231	ILE
3	3	236	ILE
4	4	26	TYR
4	4	29	ILE
4	4	33	LYS
4	4	42	ARG
4	4	43	LEU
4	4	44	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	19	ASN
1	1	90	ASN
1	1	95	ASN
1	1	140	HIS
1	1	159	ASN
1	1	168	ASN
1	1	204	ASN
1	1	261	HIS
1	1	282	ASN
2	2	15	GLN
2	2	30	ASN
2	2	51	ASN
2	2	72	ASN
2	2	109	HIS
2	2	111	GLN
2	2	131	GLN
2	2	192	ASN
2	2	197	ASN
2	2	207	ASN
2	2	218	ASN
2	2	219	ASN
3	3	20	GLN
3	3	42	ASN
3	3	56	ASN
3	3	57	ASN
3	3	61	ASN
3	3	75	GLN
3	3	80	GLN

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Mol	Chain	Res	Type
3	3	124	ASN
3	3	194	GLN
4	4	30	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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
5	SUC	1	288	1	24,24,24	1.04	1 (4%)	36,36,36	3.45	16 (44%)

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
5	SUC	1	288	1	1/1/9/9	0/12/51/51	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	288	SUC	O5-C1	-3.19	1.33	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	288	SUC	C3-C4-C5	-4.72	101.97	110.20
5	1	288	SUC	O2-C2-C1	-3.38	102.61	110.02
5	1	288	SUC	C6'-C5'-C4'	-2.91	108.19	115.08
5	1	288	SUC	O2'-C2'-C1'	-2.60	100.91	107.98
5	1	288	SUC	O4-C4-C5	-2.10	103.69	109.24
5	1	288	SUC	O5-C5-C4	2.03	113.48	109.68
5	1	288	SUC	O1-C1-C2	2.40	116.38	108.36
5	1	288	SUC	O1-C2'-C3'	2.41	116.43	108.04
5	1	288	SUC	O1-C2'-O2'	3.13	120.45	110.52
5	1	288	SUC	C2'-O1-C1	4.02	128.12	117.53
5	1	288	SUC	C1-O5-C5	4.11	121.72	113.75
5	1	288	SUC	O5-C5-C6	4.49	117.69	106.36
5	1	288	SUC	O2-C2-C3	5.69	123.14	110.34
5	1	288	SUC	O3'-C3'-C2'	6.01	133.23	113.96
5	1	288	SUC	O5-C1-O1	6.06	130.31	109.96
5	1	288	SUC	O3-C3-C2	12.72	138.98	110.34

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	1	288	SUC	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	288	SUC	32	7

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.