



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:53 pm BST

PDB ID : 2HWE
Title : A COMPARISON OF THE ANTI-RHINOVIRAL DRUG BINDING
POCKET IN HRV14 AND HRV1A
Authors : Kim, K.H.; Rossmann, M.G.
Deposited on : 1994-01-25
Resolution : 3.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

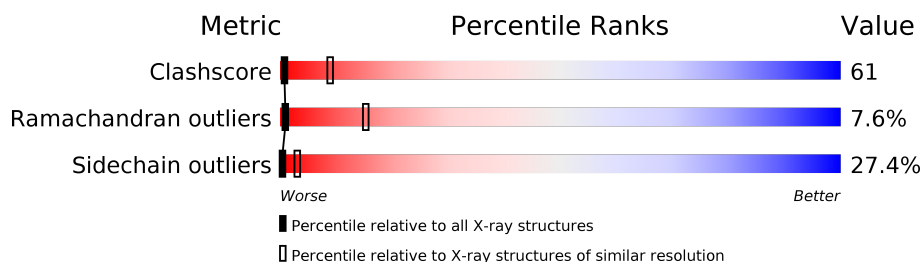
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

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	W54	1	500	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6248 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			

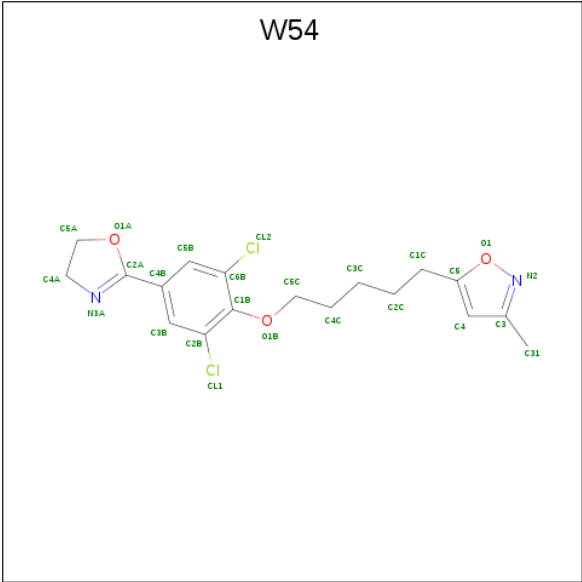
- Molecule 3 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP3).

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 5-(5-(2,6-DICHLORO-4-(4,5-DIHYDRO-2-OXAZOLY)PHENOXY)PENTYL)-3-METHYL ISOXAZOLE (three-letter code: W54) (formula: C₁₈H₂₀Cl₂N₂O₃).



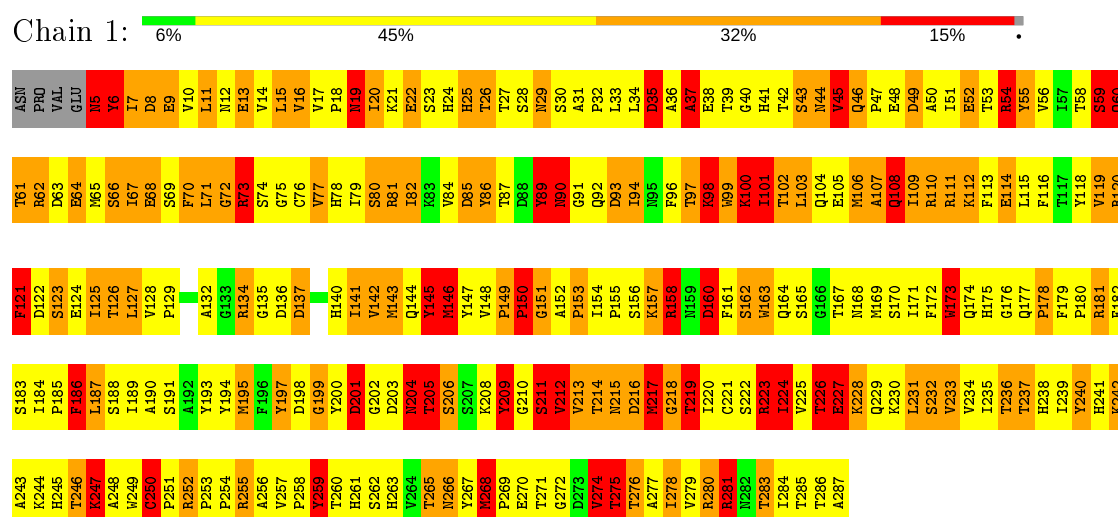
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
5	1	1	25	18	2	2	3	0	0

3 Residue-property plots

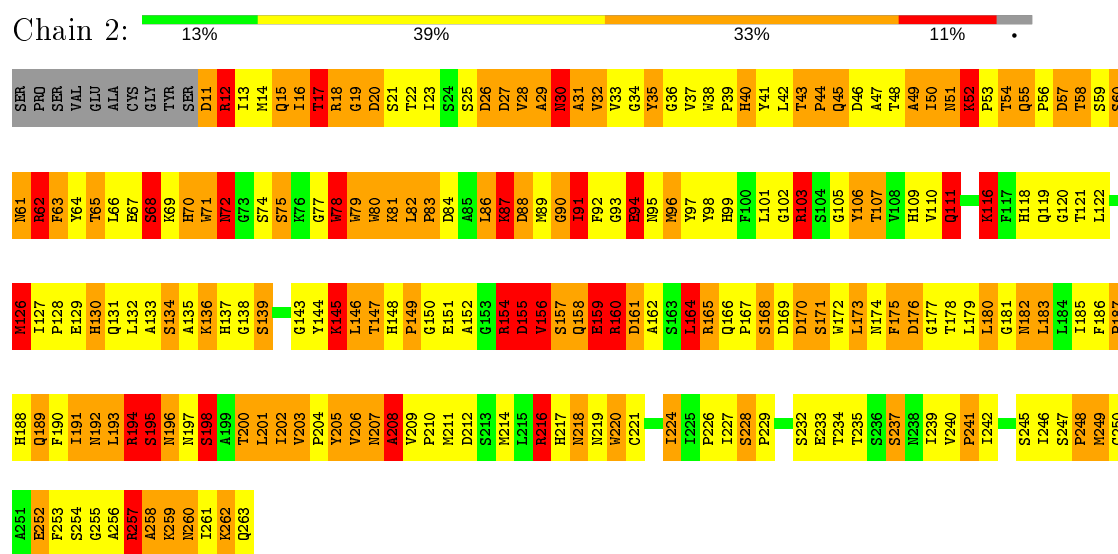
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

S184	G121	M61	G1
M185	T122	V62	L2
A186	A123	G63	P3
I187	M124	M64	V4
G188	T125	V65	V5
I189	T126	S66	I6
T190	L127	M67	T7
C191	K128	V68	P8
W192	L129	T69	G9
A193	L130	V70	S10
Q194	L131	Q71	G11
T195	A132	L72	Q12
M196	Y133	G73	F13
L197	T134	M74	M14
	P135	Q75	T15
	P136	T76	T16
		G77	D17
		M78	D18
	D139	A79	M19
	E140	Q80	Q20
	P141	K81	S21
	T142	V82	P22
	T143	F83	C23
	R144	S84	A24
	K145		A24
	D146	I85	L25
	A147	K86	P26
	M148	V87	W27
	L149	D88	Y28
	G150	I89	H29
	T151	T90	P30
	H152	S91	T31
	V153	T92	R32
	M154	P93	E33
	W155	L94	I34
	D156	A95	S35
	V157	T96	I36
	G158	T97	P37
	L159	L98	G38
	Q160	I99	E39
	S161	G100	V40
	T162	E101	K41
	I163	I102	M42
	S164	A103	L43
	L165	S104	I44
	V166	Y105	E45
	V167	Y106	M46
	P168	T107	C47
	W169	H108	Q48
		W109	V49
	A172	T110	D50
	S173	G111	T51
	H174	S112	L52
	F175	L113	I53
	R176	R114	P54
	T177	F115	V55
	L178	S116	S56
		F117	M57
		M118	V58
	M181	F119	G59
	K182	V120	M60
	Y183		

GLY	ALA	GLY	VAL	SER	ARG	GLN	ASN	VAL	GLY	THR	HIS	SER	THR	GLN	ASN	SER	VAL	SER	ASN	GLY	SER	SER	LEU	ASN	Y26	F27	N28	I29	N30	Y31	F32	K33	D34	A35	A36	S37	S38	G39	A40	S41	R42	L43	D44
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	341.30Å 341.30Å 465.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6248	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: W54

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	1.19	8/2322 (0.3%)	2.59	145/3162 (4.6%)
2	2	0.95	0/2033	2.59	151/2770 (5.5%)
3	3	0.93	0/1878	2.46	110/2570 (4.3%)
4	4	1.25	0/154	3.16	21/206 (10.2%)
All	All	1.05	8/6387 (0.1%)	2.57	427/8708 (4.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	7

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	146	MET	C-N	-15.38	0.98	1.34
1	1	213	VAL	C-N	11.92	1.61	1.34
1	1	98	LYS	C-N	-8.12	1.15	1.34
1	1	218	GLY	CA-C	-6.87	1.40	1.51
1	1	223	ARG	C-N	6.80	1.49	1.34
1	1	118	TYR	C-N	-6.50	1.19	1.34
1	1	145	TYR	C-N	6.34	1.48	1.34
1	1	149	PRO	N-CA	-5.00	1.38	1.47

All (427) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	98	LYS	O-C-N	-28.02	77.86	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	62	ARG	CD-NE-CZ	24.81	158.33	123.60
1	1	134	ARG	NE-CZ-NH1	24.02	132.31	120.30
2	2	216	ARG	NE-CZ-NH2	-22.09	109.26	120.30
1	1	280	ARG	NE-CZ-NH2	-20.40	110.10	120.30
3	3	146	ASP	CB-CG-OD2	-17.24	102.78	118.30
1	1	98	LYS	CA-C-N	16.82	154.19	117.20
1	1	150	PRO	C-N-CA	-16.56	87.53	122.30
2	2	257	ARG	NE-CZ-NH2	-16.46	112.07	120.30
3	3	222	ARG	CD-NE-CZ	15.85	145.79	123.60
4	4	42	ARG	NE-CZ-NH1	15.06	127.83	120.30
2	2	155	ASP	CB-CG-OD2	-14.63	105.13	118.30
1	1	81	ARG	NE-CZ-NH1	14.21	127.41	120.30
1	1	281	ARG	NE-CZ-NH2	-14.15	113.23	120.30
1	1	98	LYS	C-N-CA	14.04	156.81	121.70
2	2	154	ARG	NE-CZ-NH1	13.89	127.25	120.30
2	2	62	ARG	NE-CZ-NH1	13.84	127.22	120.30
3	3	226	ASP	CB-CG-OD1	13.79	130.71	118.30
1	1	158	ARG	NE-CZ-NH1	13.70	127.15	120.30
1	1	218	GLY	O-C-N	13.46	144.24	122.70
3	3	28	TYR	CB-CG-CD2	13.26	128.95	121.00
3	3	228	ASP	CB-CG-OD2	-13.24	106.38	118.30
3	3	183	TYR	CB-CG-CD1	12.39	128.44	121.00
3	3	144	ARG	CD-NE-CZ	12.34	140.88	123.60
1	1	281	ARG	CA-CB-CG	12.20	140.24	113.40
1	1	227	GLU	OE1-CD-OE2	-12.17	108.70	123.30
1	1	6	TYR	CB-CG-CD1	-12.05	113.77	121.00
1	1	93	ASP	CB-CG-OD1	-11.82	107.66	118.30
3	3	114	ARG	NE-CZ-NH1	-11.82	114.39	120.30
3	3	144	ARG	NE-CZ-NH1	11.33	125.96	120.30
1	1	231	LEU	CA-CB-CG	11.29	141.27	115.30
3	3	225	ARG	NE-CZ-NH1	-11.26	114.67	120.30
3	3	50	ASP	CB-CG-OD2	-11.21	108.21	118.30
3	3	50	ASP	CB-CG-OD1	11.00	128.20	118.30
1	1	255	ARG	CD-NE-CZ	10.93	138.90	123.60
2	2	67	GLU	OE1-CD-OE2	10.91	136.39	123.30
1	1	54	ARG	CG-CD-NE	10.81	134.50	111.80
2	2	35	TYR	CB-CG-CD2	10.81	127.48	121.00
4	4	44	ASP	CB-CG-OD2	-10.71	108.66	118.30
1	1	211	SER	C-N-CA	-10.58	95.25	121.70
3	3	218	ASP	CB-CG-OD2	-10.36	108.97	118.30
2	2	12	ARG	NE-CZ-NH2	-10.33	115.14	120.30
2	2	162	ALA	CB-CA-C	10.21	125.41	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	12	ARG	CD-NE-CZ	10.19	137.87	123.60
2	2	205	TYR	CB-CG-CD2	10.18	127.11	121.00
2	2	62	ARG	NH1-CZ-NH2	-9.95	108.45	119.40
2	2	11	ASP	CB-CG-OD1	9.85	127.17	118.30
2	2	31	ALA	N-CA-CB	9.80	123.82	110.10
2	2	216	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	1	8	ASP	CB-CG-OD2	-9.63	109.63	118.30
3	3	67	MET	N-CA-CB	-9.60	93.31	110.60
2	2	154	ARG	C-N-CA	9.54	145.56	121.70
2	2	29	ALA	N-CA-CB	9.52	123.43	110.10
4	4	42	ARG	CD-NE-CZ	9.47	136.86	123.60
2	2	176	ASP	CB-CG-OD2	9.41	126.77	118.30
1	1	281	ARG	NE-CZ-NH1	9.36	124.98	120.30
2	2	165	ARG	NE-CZ-NH1	9.31	124.96	120.30
2	2	212	ASP	CB-CG-OD2	9.29	126.66	118.30
1	1	59	SER	N-CA-CB	-9.16	96.76	110.50
1	1	9	GLU	OE1-CD-OE2	9.15	134.28	123.30
3	3	148	MET	CG-SD-CE	9.04	114.67	100.20
1	1	134	ARG	NH1-CZ-NH2	-9.04	109.46	119.40
3	3	18	ASP	CB-CG-OD1	-8.99	110.21	118.30
2	2	165	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	1	151	GLY	N-CA-C	-8.97	90.67	113.10
1	1	218	GLY	CA-C-N	-8.94	97.53	117.20
2	2	28	VAL	CA-CB-CG1	8.90	124.25	110.90
1	1	146	MET	O-C-N	8.84	136.84	122.70
1	1	227	GLU	CG-CD-OE1	8.79	135.88	118.30
1	1	60	GLN	O-C-N	8.77	136.73	122.70
2	2	154	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	1	214	THR	N-CA-CB	8.73	126.90	110.30
3	3	232	GLN	N-CA-CB	8.67	126.21	110.60
2	2	11	ASP	CB-CG-OD2	-8.66	110.50	118.30
2	2	35	TYR	CB-CG-CD1	-8.65	115.81	121.00
1	1	55	TYR	CB-CG-CD2	-8.63	115.82	121.00
1	1	11	LEU	O-C-N	8.63	136.50	122.70
3	3	222	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	1	214	THR	CB-CA-C	-8.53	88.58	111.60
2	2	233	GLU	CG-CD-OE2	8.45	135.19	118.30
1	1	68	GLU	CB-CG-CD	8.37	136.79	114.20
3	3	28	TYR	CB-CG-CD1	-8.36	115.99	121.00
2	2	57	ASP	N-CA-CB	-8.30	95.66	110.60
1	1	187	LEU	CA-C-O	-8.30	102.67	120.10
2	2	12	ARG	NE-CZ-NH1	8.25	124.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	226	ASP	OD1-CG-OD2	-8.22	107.69	123.30
2	2	97	TYR	CB-CG-CD2	8.21	125.93	121.00
2	2	126	MET	CA-CB-CG	-8.10	99.53	113.30
2	2	12	ARG	CG-CD-NE	8.00	128.61	111.80
1	1	111	ARG	CD-NE-CZ	8.00	134.80	123.60
2	2	241	PRO	C-N-CA	7.94	141.56	121.70
2	2	194	ARG	NE-CZ-NH2	-7.87	116.36	120.30
2	2	160	ARG	NE-CZ-NH1	-7.85	116.37	120.30
1	1	49	ASP	CB-CG-OD1	-7.84	111.24	118.30
2	2	189	GLN	CA-CB-CG	7.84	130.65	113.40
1	1	120	ARG	NE-CZ-NH2	7.84	124.22	120.30
2	2	26	ASP	CB-CG-OD2	7.84	125.35	118.30
1	1	158	ARG	CD-NE-CZ	7.81	134.54	123.60
2	2	161	ASP	N-CA-CB	7.79	124.63	110.60
2	2	61	ASN	CB-CA-C	7.77	125.94	110.40
1	1	55	TYR	CB-CG-CD1	7.76	125.65	121.00
3	3	56	ASN	C-N-CA	7.76	141.09	121.70
3	3	235	PRO	C-N-CA	7.73	141.03	121.70
1	1	93	ASP	CB-CG-OD2	7.68	125.21	118.30
2	2	94	GLU	OE1-CD-OE2	7.68	132.51	123.30
1	1	213	VAL	C-N-CA	-7.64	102.59	121.70
1	1	6	TYR	CB-CG-CD2	7.62	125.57	121.00
2	2	159	GLU	OE1-CD-OE2	7.61	132.44	123.30
1	1	85	ASP	CB-CG-OD1	-7.60	111.46	118.30
1	1	111	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	1	134	ARG	CD-NE-CZ	7.57	134.19	123.60
2	2	71	TRP	CB-CA-C	7.57	125.53	110.40
2	2	161	ASP	CB-CG-OD2	-7.56	111.49	118.30
1	1	280	ARG	NH1-CZ-NH2	7.55	127.70	119.40
1	1	216	ASP	CB-CA-C	7.52	125.44	110.40
3	3	207	ALA	O-C-N	7.50	134.69	122.70
1	1	73	ARG	NE-CZ-NH1	7.49	124.04	120.30
2	2	252	GLU	OE1-CD-OE2	7.47	132.26	123.30
3	3	68	TYR	CB-CG-CD2	7.46	125.48	121.00
1	1	181	ARG	NE-CZ-NH2	7.44	124.02	120.30
2	2	232	SER	N-CA-CB	7.43	121.64	110.50
1	1	111	ARG	C-N-CA	7.40	140.20	121.70
1	1	61	THR	CA-CB-OG1	-7.39	93.48	109.00
4	4	34	ASP	CB-CG-OD1	-7.39	111.65	118.30
1	1	89	TYR	CB-CG-CD1	-7.38	116.57	121.00
3	3	92	THR	CB-CA-C	7.33	131.40	111.60
3	3	161	SER	CB-CA-C	-7.33	96.18	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	37	SER	O-C-N	7.28	134.34	122.70
1	1	223	ARG	NE-CZ-NH2	7.24	123.92	120.30
2	2	147	THR	N-CA-CB	7.20	123.98	110.30
3	3	95	ALA	CA-C-N	7.18	132.99	117.20
3	3	88	ASP	CB-CG-OD2	7.17	124.75	118.30
1	1	173	TRP	CA-CB-CG	7.15	127.29	113.70
2	2	233	GLU	CG-CD-OE1	-7.15	104.00	118.30
1	1	228	LYS	CD-CE-NZ	7.14	128.11	111.70
1	1	213	VAL	O-C-N	7.13	134.12	122.70
2	2	152	ALA	N-CA-CB	-7.13	100.11	110.10
2	2	78	TRP	CA-CB-CG	7.12	127.22	113.70
2	2	237	SER	CB-CA-C	7.11	123.62	110.10
4	4	40	ALA	O-C-N	7.11	134.08	122.70
2	2	62	ARG	NE-CZ-NH2	7.07	123.83	120.30
3	3	120	CYS	CA-CB-SG	-7.05	101.31	114.00
3	3	218	ASP	N-CA-CB	-7.03	97.94	110.60
3	3	232	GLN	O-C-N	7.03	133.95	122.70
2	2	164	LEU	O-C-N	7.03	133.94	122.70
2	2	80	TRP	N-CA-CB	6.99	123.17	110.60
2	2	103	ARG	CD-NE-CZ	6.97	133.36	123.60
2	2	160	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	1	45	VAL	CB-CA-C	6.95	124.60	111.40
4	4	42	ARG	NH1-CZ-NH2	-6.92	111.79	119.40
4	4	31	TYR	CB-CG-CD1	6.91	125.15	121.00
1	1	259	TYR	CB-CG-CD2	-6.91	116.86	121.00
1	1	268	MET	CA-CB-CG	-6.90	101.57	113.30
3	3	222	ARG	NH1-CZ-NH2	-6.89	111.82	119.40
2	2	81	LYS	O-C-N	6.87	133.69	122.70
1	1	164	GLN	OE1-CD-NE2	-6.85	106.15	121.90
2	2	160	ARG	N-CA-CB	-6.83	98.31	110.60
2	2	72	ASN	OD1-CG-ND2	6.82	137.59	121.90
1	1	5	ASN	N-CA-CB	6.82	122.88	110.60
3	3	25	LEU	CA-CB-CG	6.79	130.92	115.30
2	2	106	TYR	C-N-CA	6.78	138.65	121.70
1	1	203	ASP	CB-CG-OD1	-6.75	112.23	118.30
2	2	198	SER	CB-CA-C	-6.74	97.29	110.10
1	1	164	GLN	CG-CD-OE1	6.74	135.08	121.60
1	1	270	GLU	N-CA-CB	6.69	122.65	110.60
2	2	52	LYS	CA-CB-CG	6.68	128.10	113.40
3	3	73	GLY	CA-C-O	6.68	132.63	120.60
3	3	90	THR	N-CA-CB	6.67	122.97	110.30
3	3	218	ASP	CA-CB-CG	-6.66	98.74	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	26	PRO	O-C-N	6.65	133.34	122.70
3	3	193	TYR	O-C-N	6.63	133.32	122.70
4	4	40	ALA	N-CA-CB	6.61	119.35	110.10
1	1	19	ASN	CB-CG-OD1	-6.59	108.41	121.60
1	1	70	PHE	O-C-N	6.59	133.25	122.70
2	2	135	ALA	N-CA-CB	-6.59	100.87	110.10
3	3	57	ASN	CB-CG-ND2	-6.58	100.89	116.70
1	1	37	ALA	N-CA-CB	-6.57	100.90	110.10
3	3	55	VAL	CB-CA-C	6.51	123.78	111.40
1	1	5	ASN	O-C-N	6.50	133.10	122.70
2	2	196	ASN	N-CA-CB	-6.50	98.91	110.60
2	2	50	ILE	CA-CB-CG2	6.49	123.87	110.90
1	1	213	VAL	CA-C-N	-6.46	102.98	117.20
2	2	187	PRO	CB-CA-C	6.45	128.13	112.00
2	2	16	ILE	O-C-N	6.45	133.01	122.70
2	2	183	LEU	O-C-N	6.42	132.97	122.70
3	3	16	THR	CA-CB-CG2	6.42	121.39	112.40
2	2	28	VAL	CG1-CB-CG2	-6.41	100.65	110.90
1	1	64	GLU	CA-CB-CG	6.40	127.47	113.40
1	1	199	GLY	O-C-N	6.37	132.89	122.70
1	1	13	GLU	O-C-N	6.37	132.88	122.70
3	3	160	GLN	N-CA-CB	6.36	122.05	110.60
3	3	172	ALA	CB-CA-C	6.36	119.64	110.10
2	2	68	SER	N-CA-CB	6.34	120.01	110.50
2	2	26	ASP	OD1-CG-OD2	-6.31	111.32	123.30
1	1	201	ASP	CB-CG-OD2	6.31	123.98	118.30
1	1	274	VAL	N-CA-CB	6.31	125.37	111.50
2	2	196	ASN	OD1-CG-ND2	6.31	136.40	121.90
3	3	235	PRO	CA-C-N	-6.30	103.33	117.20
3	3	222	ARG	NE-CZ-NH2	6.30	123.45	120.30
3	3	235	PRO	CA-C-O	6.30	135.32	120.20
1	1	146	MET	CA-C-N	-6.29	103.36	117.20
1	1	275	THR	OG1-CB-CG2	6.28	124.45	110.00
1	1	106	MET	CG-SD-CE	6.26	110.22	100.20
2	2	248	PRO	N-CA-C	-6.26	95.83	112.10
3	3	37	PRO	N-CA-CB	6.25	110.80	103.30
1	1	77	VAL	O-C-N	6.25	132.70	122.70
2	2	161	ASP	O-C-N	6.24	132.68	122.70
4	4	44	ASP	CB-CG-OD1	6.24	123.91	118.30
3	3	33	GLU	CG-CD-OE2	-6.23	105.83	118.30
1	1	233	VAL	CB-CA-C	-6.22	99.58	111.40
2	2	19	GLY	C-N-CA	6.22	137.25	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	233	VAL	CA-C-N	-6.21	103.54	117.20
1	1	211	SER	CA-C-O	-6.19	107.10	120.10
2	2	94	GLU	CG-CD-OE1	-6.18	105.94	118.30
4	4	30	ASN	CB-CA-C	6.18	122.75	110.40
2	2	155	ASP	N-CA-CB	6.17	121.70	110.60
1	1	86	TYR	CB-CA-C	6.16	122.72	110.40
3	3	94	LEU	CA-C-N	6.16	130.75	117.20
4	4	38	SER	O-C-N	6.16	133.67	123.20
3	3	89	ILE	CB-CA-C	-6.16	99.29	111.60
2	2	205	TYR	CB-CG-CD1	-6.15	117.31	121.00
1	1	16	VAL	CG1-CB-CG2	6.13	120.72	110.90
1	1	195	MET	CG-SD-CE	6.13	110.00	100.20
1	1	175	HIS	N-CA-CB	-6.12	99.58	110.60
1	1	209	TYR	CB-CG-CD1	6.10	124.66	121.00
1	1	206	SER	O-C-N	6.09	132.44	122.70
4	4	35	ALA	CB-CA-C	6.08	119.21	110.10
2	2	154	ARG	CG-CD-NE	6.07	124.56	111.80
2	2	17	THR	CB-CA-C	6.07	127.98	111.60
3	3	185	MET	CA-CB-CG	6.05	123.59	113.30
1	1	227	GLU	CB-CG-CD	6.04	130.51	114.20
2	2	155	ASP	CB-CG-OD1	6.04	123.73	118.30
2	2	82	LEU	CA-CB-CG	-6.03	101.43	115.30
2	2	107	THR	CA-CB-OG1	-6.03	96.34	109.00
2	2	81	LYS	CA-CB-CG	6.03	126.66	113.40
1	1	247	LYS	CB-CA-C	-6.02	98.36	110.40
2	2	57	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	1	35	ASP	CB-CG-OD2	6.01	123.71	118.30
3	3	32	LYS	O-C-N	6.01	132.31	122.70
1	1	187	LEU	CA-C-N	5.99	130.39	117.20
2	2	57	ASP	CB-CG-OD1	-5.99	112.91	118.30
3	3	15	THR	N-CA-CB	-5.97	98.97	110.30
2	2	194	ARG	NH1-CZ-NH2	5.96	125.95	119.40
2	2	160	ARG	CG-CD-NE	5.95	124.29	111.80
2	2	262	LYS	CB-CA-C	5.95	122.29	110.40
1	1	82	ILE	CB-CA-C	-5.94	99.71	111.60
1	1	146	MET	CG-SD-CE	5.93	109.68	100.20
2	2	130	HIS	CA-CB-CG	-5.92	103.53	113.60
1	1	71	LEU	CB-CA-C	5.92	121.44	110.20
4	4	26	TYR	CB-CG-CD1	5.92	124.55	121.00
3	3	105	TYR	CB-CG-CD2	5.91	124.55	121.00
3	3	233	SER	CA-C-N	-5.91	104.39	116.20
3	3	183	TYR	CB-CG-CD2	-5.90	117.46	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	217	MET	CG-SD-CE	5.90	109.64	100.20
2	2	87	LYS	CB-CG-CD	5.90	126.93	111.60
2	2	130	HIS	O-C-N	5.89	132.13	122.70
2	2	156	VAL	C-N-CA	5.89	136.43	121.70
2	2	208	ALA	N-CA-CB	5.89	118.35	110.10
1	1	89	TYR	CB-CG-CD2	5.89	124.53	121.00
2	2	91	ILE	N-CA-CB	5.88	124.33	110.80
1	1	231	LEU	CB-CA-C	5.88	121.38	110.20
2	2	252	GLU	CG-CD-OE1	-5.88	106.54	118.30
2	2	157	SER	N-CA-CB	5.87	119.31	110.50
2	2	49	ALA	CA-C-O	-5.86	107.79	120.10
1	1	68	GLU	OE1-CD-OE2	-5.86	116.27	123.30
1	1	100	LYS	O-C-N	5.86	132.07	122.70
2	2	97	TYR	CB-CG-CD1	-5.84	117.50	121.00
3	3	201	PRO	N-CA-C	5.84	127.29	112.10
1	1	55	TYR	O-C-N	5.84	132.04	122.70
3	3	68	TYR	CB-CG-CD1	-5.84	117.50	121.00
1	1	20	ILE	O-C-N	5.83	132.03	122.70
3	3	185	MET	N-CA-CB	5.82	121.08	110.60
2	2	234	THR	CA-C-O	5.82	132.31	120.10
1	1	85	ASP	CB-CG-OD2	5.80	123.52	118.30
2	2	147	THR	O-C-N	5.80	131.97	122.70
1	1	240	TYR	CB-CG-CD1	-5.79	117.53	121.00
1	1	49	ASP	OD1-CG-OD2	5.77	134.26	123.30
2	2	249	MET	CA-CB-CG	5.77	123.10	113.30
3	3	24	ALA	N-CA-CB	-5.77	102.03	110.10
1	1	25	HIS	O-C-N	5.75	131.91	122.70
2	2	57	ASP	OD1-CG-OD2	5.74	134.20	123.30
1	1	274	VAL	CA-CB-CG1	5.73	119.49	110.90
1	1	54	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	1	250	CYS	CA-CB-SG	5.72	124.30	114.00
1	1	226	THR	N-CA-C	5.72	126.44	111.00
2	2	218	ASN	CA-CB-CG	5.72	125.98	113.40
2	2	257	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	1	81	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
1	1	16	VAL	CB-CA-C	5.71	122.25	111.40
1	1	202	GLY	C-N-CA	5.71	135.97	121.70
2	2	134	SER	CA-C-N	-5.71	104.65	117.20
1	1	90	ASN	CB-CA-C	5.66	121.72	110.40
3	3	45	GLU	OE1-CD-OE2	-5.66	116.51	123.30
3	3	77	GLY	CA-C-O	5.66	130.79	120.60
1	1	204	ASN	CA-C-N	-5.66	104.75	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	111	ARG	NE-CZ-NH2	5.66	123.13	120.30
3	3	103	ALA	CB-CA-C	5.65	118.57	110.10
2	2	139	SER	N-CA-CB	-5.65	102.03	110.50
2	2	83	PRO	C-N-CA	5.64	135.80	121.70
3	3	229	LEU	CA-CB-CG	5.64	128.27	115.30
3	3	227	THR	CA-C-O	5.64	131.94	120.10
1	1	232	SER	CB-CA-C	-5.63	99.39	110.10
2	2	249	MET	CG-SD-CE	5.63	109.21	100.20
1	1	121	PHE	CB-CA-C	-5.62	99.15	110.40
3	3	18	ASP	OD1-CG-OD2	5.62	133.98	123.30
3	3	160	GLN	O-C-N	5.62	131.69	122.70
3	3	76	THR	O-C-N	5.62	132.75	123.20
3	3	212	PHE	CA-CB-CG	5.60	127.33	113.90
3	3	146	ASP	OD1-CG-OD2	5.59	133.93	123.30
2	2	26	ASP	CB-CG-OD1	5.59	123.33	118.30
1	1	62	ARG	NE-CZ-NH1	-5.59	117.51	120.30
2	2	49	ALA	CA-C-N	5.58	129.48	117.20
2	2	228	SER	N-CA-CB	5.57	118.85	110.50
1	1	274	VAL	CA-C-N	-5.57	104.96	117.20
2	2	220	TRP	CA-C-N	-5.56	104.96	117.20
2	2	134	SER	N-CA-CB	5.56	118.83	110.50
1	1	153	PRO	N-CD-CG	-5.55	94.87	103.20
2	2	116	LYS	CB-CA-C	-5.55	99.31	110.40
2	2	83	PRO	CB-CA-C	5.54	125.86	112.00
3	3	79	ALA	O-C-N	5.54	131.56	122.70
2	2	212	ASP	CB-CG-OD1	-5.53	113.32	118.30
1	1	68	GLU	CA-CB-CG	5.53	125.56	113.40
2	2	119	GLN	CB-CA-C	5.53	121.46	110.40
2	2	149	PRO	CA-C-N	5.52	127.24	116.20
3	3	146	ASP	CB-CG-OD1	5.51	123.26	118.30
3	3	24	ALA	CA-C-N	5.51	129.32	117.20
3	3	64	ASN	OD1-CG-ND2	5.50	134.56	121.90
2	2	54	THR	N-CA-CB	5.50	120.75	110.30
2	2	216	ARG	NH1-CZ-NH2	5.49	125.44	119.40
2	2	169	ASP	CA-C-O	5.48	131.61	120.10
1	1	81	ARG	CD-NE-CZ	5.46	131.25	123.60
2	2	90	GLY	CA-C-O	5.44	130.39	120.60
3	3	183	TYR	CG-CD2-CE2	5.44	125.65	121.30
4	4	40	ALA	N-CA-C	-5.43	96.35	111.00
2	2	32	VAL	O-C-N	5.42	131.38	122.70
3	3	169	TRP	CB-CA-C	5.42	121.25	110.40
2	2	20	ASP	CB-CG-OD2	-5.42	113.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	218	ASP	C-N-CA	5.41	135.23	121.70
3	3	228	ASP	CB-CA-C	-5.41	99.58	110.40
3	3	58	VAL	CA-CB-CG1	-5.41	102.79	110.90
2	2	70	HIS	CB-CA-C	-5.40	99.60	110.40
3	3	234	GLY	N-CA-C	-5.40	99.61	113.10
1	1	270	GLU	O-C-N	5.39	131.33	122.70
3	3	235	PRO	CB-CA-C	-5.39	98.52	112.00
3	3	8	PRO	C-N-CA	5.38	133.60	122.30
2	2	150	GLY	O-C-N	5.38	131.30	122.70
2	2	194	ARG	NE-CZ-NH1	-5.38	117.61	120.30
3	3	225	ARG	NE-CZ-NH2	5.36	122.98	120.30
3	3	114	ARG	NE-CZ-NH2	5.35	122.98	120.30
1	1	283	THR	O-C-N	5.35	131.26	122.70
3	3	95	ALA	CA-C-O	-5.35	108.87	120.10
3	3	88	ASP	OD1-CG-OD2	-5.34	113.14	123.30
3	3	233	SER	CA-C-O	5.33	131.29	120.10
4	4	44	ASP	CA-C-O	5.32	131.28	120.10
2	2	161	ASP	CB-CA-C	-5.32	99.76	110.40
1	1	172	PHE	CA-C-O	-5.32	108.93	120.10
3	3	203	THR	O-C-N	5.32	131.21	121.10
3	3	206	THR	OG1-CB-CG2	5.31	122.22	110.00
2	2	96	MET	CA-C-N	-5.31	105.52	117.20
3	3	175	PHE	CB-CG-CD1	-5.31	117.08	120.80
3	3	206	THR	N-CA-C	-5.31	96.66	111.00
2	2	87	LYS	CB-CA-C	5.31	121.02	110.40
2	2	111	GLN	CB-CG-CD	5.30	125.39	111.60
2	2	150	GLY	CA-C-O	-5.30	111.06	120.60
4	4	26	TYR	CB-CG-CD2	-5.30	117.82	121.00
2	2	165	ARG	C-N-CA	5.29	134.93	121.70
4	4	29	ILE	O-C-N	5.29	131.17	122.70
2	2	52	LYS	CG-CD-CE	5.29	127.77	111.90
3	3	35	SER	N-CA-CB	-5.29	102.57	110.50
1	1	201	ASP	CB-CG-OD1	-5.28	113.55	118.30
2	2	182	ASN	O-C-N	5.27	131.14	122.70
2	2	195	SER	CB-CA-C	5.27	120.11	110.10
3	3	202	SER	CA-C-N	-5.27	105.61	117.20
1	1	216	ASP	O-C-N	5.26	131.11	122.70
3	3	108	HIS	CA-CB-CG	5.25	122.53	113.60
2	2	203	VAL	N-CA-CB	-5.23	99.99	111.50
1	1	211	SER	O-C-N	5.22	131.06	122.70
1	1	224	ILE	CB-CG1-CD1	-5.22	99.27	113.90
3	3	10	SER	CB-CA-C	5.22	120.02	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	11	ASP	O-C-N	5.22	131.05	122.70
2	2	82	LEU	N-CA-C	5.22	125.09	111.00
1	1	287	ALA	CA-C-O	-5.21	109.17	120.10
4	4	26	TYR	O-C-N	5.19	131.01	122.70
1	1	158	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
1	1	242	LYS	CA-C-N	-5.19	105.79	117.20
3	3	92	THR	N-CA-C	-5.19	96.99	111.00
3	3	156	ASP	CB-CG-OD1	-5.18	113.64	118.30
2	2	12	ARG	CB-CA-C	-5.18	100.04	110.40
3	3	165	LEU	O-C-N	5.17	130.98	122.70
3	3	146	ASP	N-CA-CB	5.17	119.90	110.60
3	3	64	ASN	N-CA-CB	-5.17	101.30	110.60
2	2	19	GLY	CA-C-N	-5.17	105.84	117.20
2	2	173	LEU	CB-CA-C	5.16	120.00	110.20
1	1	22	GLU	CG-CD-OE2	5.16	128.61	118.30
2	2	30	ASN	N-CA-CB	-5.16	101.32	110.60
3	3	76	THR	CA-C-N	-5.15	105.90	116.20
3	3	24	ALA	CA-C-O	-5.14	109.30	120.10
3	3	181	ASN	O-C-N	5.13	130.91	122.70
2	2	237	SER	CA-C-O	5.12	130.86	120.10
4	4	38	SER	CA-C-O	-5.12	109.36	120.10
3	3	72	LEU	CB-CG-CD2	-5.11	102.31	111.00
4	4	42	ARG	C-N-CA	-5.10	108.94	121.70
1	1	43	SER	CA-C-N	-5.10	105.98	117.20
1	1	163	TRP	CB-CA-C	5.10	120.59	110.40
1	1	94	ILE	CA-C-N	-5.09	106.00	117.20
1	1	178	PRO	CA-C-N	-5.08	106.02	117.20
2	2	50	ILE	CB-CA-C	5.08	121.77	111.60
1	1	205	THR	OG1-CB-CG2	5.08	121.68	110.00
3	3	78	MET	CB-CA-C	5.08	120.55	110.40
1	1	66	SER	O-C-N	5.07	130.81	122.70
2	2	28	VAL	CB-CA-C	-5.07	101.78	111.40
1	1	189	ILE	C-N-CA	5.05	134.34	121.70
2	2	40	HIS	CA-CB-CG	-5.05	105.01	113.60
2	2	168	SER	C-N-CA	5.05	134.33	121.70
3	3	64	ASN	CA-CB-CG	-5.04	102.31	113.40
3	3	227	THR	CA-CB-CG2	-5.04	105.34	112.40
1	1	46	GLN	O-C-N	5.04	130.67	121.10
2	2	218	ASN	CB-CG-OD1	-5.03	111.53	121.60
2	2	45	GLN	N-CA-CB	5.03	119.66	110.60
3	3	223	MET	CG-SD-CE	5.03	108.24	100.20
1	1	175	HIS	CB-CA-C	5.02	120.44	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	131	LEU	CA-CB-CG	5.01	126.83	115.30
1	1	52	GLU	O-C-N	5.01	130.72	122.70
1	1	80	SER	CA-C-O	5.01	130.61	120.10
1	1	204	ASN	N-CA-CB	5.01	119.61	110.60
2	2	79	TRP	CA-CB-CG	5.01	123.21	113.70
3	3	57	ASN	N-CA-CB	-5.00	101.59	110.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	110	ARG	Mainchain
1	1	150	PRO	Peptide
1	1	186	PHE	Mainchain
1	1	211	SER	Mainchain
1	1	223	ARG	Mainchain
1	1	98	LYS	Mainchain,Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2262	0	2191	387	1486
2	2	1979	0	1920	211	738
3	3	1831	0	1809	234	1610
4	4	151	0	136	16	345
5	1	25	0	20	3	49
All	All	6248	0	6076	756	2841

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 61.

All (756) 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)
1:1:154:ILE:HG23	1:1:221:CYS:SG	1.55	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:101:ILE:H	1:1:101:ILE:CD1	1.07	1.44
1:1:108:GLN:NE2	3:3:226:ASP:OD2	1.69	1.24
1:1:23:SER:OG	1:1:53:THR:HG22	1.36	1.23
1:1:218:GLY:O	1:1:219:THR:CG2	1.89	1.21
1:1:108:GLN:OE1	3:3:226:ASP:OD2	1.59	1.21
3:3:42:ASN:HD22	3:3:44:ILE:HG22	1.05	1.19
1:1:101:ILE:N	1:1:101:ILE:HD13	1.26	1.19
2:2:18:ARG:NH1	2:2:249:MET:HE2	1.55	1.19
1:1:104:GLN:O	3:3:236:ILE:HD11	1.42	1.16
1:1:218:GLY:C	1:1:219:THR:HG22	1.63	1.15
1:1:254:PRO:HG3	3:3:101:GLU:HG2	1.27	1.15
1:1:211:SER:C	1:1:212:VAL:HG12	1.68	1.14
1:1:101:ILE:HG21	1:1:217:MET:O	1.46	1.14
1:1:104:GLN:O	3:3:236:ILE:CD1	1.95	1.14
1:1:108:GLN:CD	3:3:226:ASP:OD2	1.85	1.13
1:1:218:GLY:O	1:1:219:THR:HG22	0.98	1.13
2:2:18:ARG:HH12	2:2:249:MET:HE2	0.99	1.11
1:1:98:LYS:HA	1:1:220:ILE:O	1.50	1.10
3:3:160:GLN:O	3:3:161:SER:HB3	1.48	1.09
1:1:254:PRO:CG	3:3:101:GLU:HG2	1.81	1.09
1:1:154:ILE:CG2	1:1:221:CYS:SG	2.41	1.07
1:1:46:GLN:HB3	1:1:47:PRO:CD	1.85	1.07
1:1:119:VAL:CG1	1:1:121:PHE:HE1	1.70	1.04
1:1:101:ILE:H	1:1:101:ILE:HD12	1.23	1.03
3:3:122:THR:HG22	3:3:123:ALA:H	1.21	1.02
1:1:100:LYS:CA	1:1:101:ILE:HD13	1.89	1.02
3:3:75:GLN:NE2	3:3:75:GLN:HA	1.75	1.01
1:1:7:ILE:HA	1:1:11:LEU:HD23	1.41	1.01
1:1:218:GLY:C	1:1:219:THR:CG2	2.21	1.01
1:1:142:VAL:CG1	1:1:225:VAL:HB	1.91	1.01
1:1:6:TYR:HB3	1:1:7:ILE:HD13	1.42	1.01
1:1:45:VAL:H	3:3:114:ARG:NH1	1.59	1.00
2:2:185:ILE:HD13	3:3:98:LEU:HD22	1.41	1.00
1:1:46:GLN:CB	1:1:47:PRO:HD2	1.89	1.00
3:3:42:ASN:ND2	3:3:44:ILE:HG22	1.74	1.00
1:1:46:GLN:HB3	1:1:47:PRO:HD2	1.01	0.99
3:3:75:GLN:HE21	3:3:75:GLN:HA	1.26	0.99
2:2:83:PRO:HG2	2:2:218:ASN:HA	1.44	0.98
1:1:108:GLN:OE1	3:3:226:ASP:CG	2.00	0.98
1:1:278:ILE:HD12	3:3:67:MET:CE	1.94	0.97
1:1:100:LYS:C	1:1:101:ILE:HD13	1.84	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:117:PHE:CD1	3:3:211:CYS:HB3	2.00	0.97
3:3:117:PHE:HD1	3:3:211:CYS:HB3	1.25	0.96
1:1:100:LYS:HA	1:1:101:ILE:CD1	1.96	0.96
1:1:211:SER:N	1:1:212:VAL:HG12	1.80	0.96
3:3:51:THR:HG21	3:3:98:LEU:HB2	1.47	0.95
1:1:223:ARG:HH11	1:1:223:ARG:HG2	1.29	0.94
1:1:150:PRO:O	1:1:151:GLY:C	1.99	0.94
1:1:163:TRP:CH2	1:1:222:SER:O	2.21	0.93
1:1:100:LYS:HA	1:1:101:ILE:HD13	1.49	0.93
1:1:211:SER:C	1:1:212:VAL:CG1	2.27	0.93
1:1:35:ASP:O	3:3:162:THR:HB	1.69	0.92
2:2:185:ILE:HD13	3:3:98:LEU:CD2	2.00	0.91
1:1:96:PHE:CE2	1:1:157:LYS:HA	2.06	0.91
1:1:265:THR:OG1	2:2:133:ALA:HB2	1.69	0.91
1:1:113:PHE:O	1:1:115:LEU:N	2.04	0.91
1:1:217:MET:O	1:1:217:MET:HG2	1.70	0.91
1:1:141:ILE:HG12	1:1:141:ILE:O	1.69	0.90
1:1:101:ILE:N	1:1:101:ILE:CD1	1.88	0.90
1:1:101:ILE:HD12	1:1:219:THR:HA	1.53	0.89
1:1:97:THR:HG23	1:1:222:SER:HB3	1.53	0.89
1:1:119:VAL:CG1	1:1:121:PHE:CE1	2.56	0.89
3:3:237:GLU:HG2	3:3:238:GLN:H	1.38	0.88
3:3:54:PRO:O	3:3:93:PRO:HB2	1.74	0.88
1:1:173:TRP:CD1	1:1:180:PRO:HD3	2.09	0.88
2:2:161:ASP:HB2	2:2:164:LEU:HD22	1.55	0.88
3:3:231:ILE:HD13	3:3:231:ILE:H	1.39	0.88
1:1:67:ILE:HD11	3:3:40:VAL:HB	1.54	0.87
3:3:82:VAL:HG12	3:3:83:PHE:HD1	1.39	0.87
1:1:119:VAL:HG11	1:1:121:PHE:HE1	1.38	0.87
1:1:140:HIS:O	1:1:226:THR:HG21	1.75	0.86
1:1:127:LEU:HB2	1:1:180:PRO:HG2	1.56	0.86
1:1:190:ALA:O	3:3:31:THR:HG21	1.75	0.86
3:3:42:ASN:HD22	3:3:44:ILE:CG2	1.87	0.86
2:2:12:ARG:HH11	2:2:12:ARG:HB3	1.36	0.86
3:3:24:ALA:O	3:3:25:LEU:HB2	1.71	0.86
3:3:58:VAL:O	3:3:61:ASN:HB2	1.76	0.86
1:1:119:VAL:HG13	1:1:121:PHE:CE1	2.10	0.86
1:1:142:VAL:HG12	1:1:225:VAL:HB	1.57	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
1:1:171:ILE:HD11	1:1:180:PRO:HB2	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:154:ILE:HG23	1:1:221:CYS:HG	1.07	0.84
1:1:254:PRO:HG3	3:3:101:GLU:CG	2.05	0.84
1:1:217:MET:O	1:1:217:MET:CG	2.22	0.84
2:2:159:GLU:C	2:2:160:ARG:HG2	1.96	0.84
3:3:82:VAL:HG12	3:3:83:PHE:N	1.90	0.84
1:1:102:THR:HG23	1:1:103:LEU:N	1.93	0.83
1:1:142:VAL:HG11	1:1:225:VAL:HB	1.60	0.83
3:3:51:THR:HG21	3:3:98:LEU:CB	2.07	0.83
1:1:101:ILE:HG13	1:1:218:GLY:CA	2.09	0.83
2:2:161:ASP:HB2	2:2:164:LEU:CD2	2.08	0.82
1:1:104:GLN:O	3:3:236:ILE:HD13	1.80	0.82
1:1:97:THR:O	1:1:222:SER:N	2.12	0.82
1:1:150:PRO:O	1:1:152:ALA:N	2.13	0.82
2:2:168:SER:OG	2:2:170:ASP:HB2	1.79	0.81
3:3:102:ILE:HG22	3:3:103:ALA:N	1.92	0.81
3:3:7:THR:O	3:3:10:SER:HB2	1.80	0.81
1:1:123:SER:HB3	1:1:241:HIS:NE2	1.96	0.81
1:1:223:ARG:HG2	1:1:223:ARG:NH1	1.90	0.80
1:1:173:TRP:HD1	1:1:180:PRO:HD3	1.45	0.80
1:1:148:VAL:HG11	1:1:154:ILE:HG13	1.63	0.80
1:1:23:SER:CB	1:1:53:THR:HG22	2.11	0.79
1:1:129:PRO:HG2	1:1:173:TRP:CE2	2.18	0.79
1:1:212:VAL:C	1:1:214:THR:N	2.36	0.78
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
1:1:124:GLU:O	1:1:125:ILE:HG12	1.82	0.78
3:3:194:GLN:HA	3:3:194:GLN:HE21	1.48	0.78
2:2:18:ARG:HH12	2:2:249:MET:CE	1.90	0.78
1:1:204:ASN:C	1:1:206:SER:H	1.82	0.77
2:2:146:LEU:CD1	2:2:166:GLN:HA	2.13	0.77
2:2:126:MET:HG3	2:2:201:LEU:HD12	1.66	0.77
2:2:12:ARG:HG3	2:2:13:ILE:N	1.99	0.77
3:3:231:ILE:CD1	3:3:231:ILE:H	1.97	0.77
2:2:60:SER:OG	2:2:61:ASN:N	2.14	0.77
3:3:160:GLN:O	3:3:161:SER:CB	2.32	0.77
3:3:20:GLN:HE22	4:4:30:ASN:HA	1.50	0.76
1:1:255:ARG:HD3	1:1:259:TYR:CE2	2.20	0.76
2:2:173:LEU:O	2:2:174:ASN:HB2	1.83	0.76
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
1:1:211:SER:CA	1:1:212:VAL:HG12	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:122:THR:HG22	3:3:123:ALA:N	1.99	0.75
3:3:81:LYS:HG3	3:3:82:VAL:N	2.01	0.75
1:1:107:ALA:O	1:1:109:ILE:N	2.18	0.75
3:3:75:GLN:OE1	3:3:80:GLN:HG2	1.87	0.75
1:1:99:TRP:CE3	1:1:220:ILE:HD12	2.22	0.75
3:3:237:GLU:CG	3:3:238:GLN:H	1.95	0.75
4:4:26:TYR:CD1	4:4:29:ILE:HD11	2.22	0.75
1:1:96:PHE:HB2	1:1:222:SER:O	1.86	0.74
1:1:101:ILE:HG13	1:1:218:GLY:N	2.02	0.74
1:1:125:ILE:HD13	5:1:500:W54:C2B	2.17	0.74
3:3:122:THR:CG2	3:3:123:ALA:H	1.99	0.74
1:1:261:HIS:HA	3:3:237:GLU:O	1.87	0.74
2:2:183:LEU:HD12	2:2:186:PHE:HD2	1.52	0.74
2:2:78:TRP:HZ3	2:2:226:PRO:HD3	1.50	0.73
2:2:41:TYR:CD2	2:2:55:GLN:OE1	2.41	0.73
1:1:33:LEU:O	3:3:163:ILE:HD12	1.88	0.73
2:2:146:LEU:HD12	2:2:167:PRO:CD	2.19	0.73
2:2:257:ARG:HG2	2:2:257:ARG:HH11	1.53	0.73
2:2:68:SER:C	2:2:69:LYS:HG2	2.07	0.73
1:1:101:ILE:HD12	1:1:219:THR:CA	2.19	0.72
2:2:12:ARG:CG	2:2:13:ILE:N	2.51	0.72
1:1:145:TYR:N	1:1:145:TYR:CD1	2.54	0.72
1:1:215:ASN:O	1:1:215:ASN:CG	2.27	0.72
1:1:211:SER:N	1:1:212:VAL:CG1	2.51	0.72
1:1:212:VAL:H	1:1:214:THR:H	1.37	0.72
1:1:163:TRP:HH2	1:1:222:SER:O	1.73	0.72
2:2:148:HIS:N	2:2:149:PRO:CD	2.52	0.72
1:1:110:ARG:NE	1:1:114:GLU:OE2	2.22	0.72
1:1:197:TYR:H	2:2:131:GLN:HE21	1.36	0.72
3:3:173:SER:O	3:3:175:PHE:N	2.22	0.72
3:3:53:ILE:O	3:3:55:VAL:HG12	1.89	0.72
3:3:125:THR:HG22	3:3:126:THR:N	2.03	0.72
1:1:113:PHE:C	1:1:115:LEU:H	1.94	0.71
2:2:148:HIS:N	2:2:149:PRO:HD3	2.05	0.71
1:1:92:GLN:O	1:1:93:ASP:HB2	1.89	0.71
2:2:207:ASN:HD22	2:2:209:VAL:H	1.37	0.71
1:1:107:ALA:O	1:1:110:ARG:N	2.22	0.71
1:1:124:GLU:O	1:1:125:ILE:CG1	2.37	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
1:1:46:GLN:OE1	3:3:217:LYS:HG3	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:278:ILE:HD12	3:3:67:MET:HE1	1.71	0.71
1:1:22:GLU:HA	1:1:54:ARG:O	1.91	0.71
3:3:82:VAL:CG1	3:3:83:PHE:HD1	2.04	0.71
1:1:97:THR:O	1:1:221:CYS:HA	1.89	0.71
1:1:146:MET:HB2	1:1:169:MET:O	1.91	0.70
1:1:223:ARG:HH11	1:1:223:ARG:CG	2.02	0.70
3:3:42:ASN:HB3	3:3:44:ILE:HG22	1.73	0.70
1:1:99:TRP:HE3	1:1:220:ILE:HD12	1.54	0.70
1:1:61:THR:HG22	1:1:63:ASP:OD1	1.90	0.70
2:2:78:TRP:CE3	2:2:78:TRP:N	2.60	0.70
1:1:14:VAL:HG11	4:4:43:LEU:HB3	1.74	0.69
1:1:169:MET:CE	1:1:171:ILE:HB	2.21	0.69
2:2:37:VAL:HG21	3:3:37:PRO:HB3	1.72	0.69
1:1:123:SER:HB3	1:1:241:HIS:CD2	2.27	0.69
1:1:104:GLN:HB2	1:1:262:SER:HB2	1.73	0.69
3:3:127:LEU:HG	3:3:128:LYS:N	2.08	0.69
2:2:51:ASN:HD22	2:2:51:ASN:H	1.41	0.69
1:1:110:ARG:O	1:1:114:GLU:HG3	1.93	0.69
1:1:281:ARG:HB3	3:3:57:ASN:O	1.92	0.69
1:1:44:ASN:HD22	1:1:44:ASN:C	1.96	0.69
1:1:92:GLN:C	1:1:94:ILE:HD12	2.13	0.69
1:1:155:PRO:HB3	1:1:163:TRP:HE1	1.57	0.69
2:2:12:ARG:HD3	2:2:27:ASP:HA	1.74	0.69
3:3:127:LEU:HA	3:3:196:ASN:O	1.93	0.68
1:1:269:PRO:HG2	1:1:272:GLY:O	1.93	0.68
2:2:56:PRO:HB2	2:2:60:SER:HB3	1.76	0.68
1:1:97:THR:HG23	1:1:222:SER:CB	2.20	0.68
1:1:7:ILE:CA	1:1:11:LEU:HD23	2.21	0.68
3:3:132:ALA:O	3:3:189:ILE:HA	1.93	0.68
1:1:91:GLY:C	1:1:94:ILE:HD13	2.14	0.68
2:2:41:TYR:HD2	2:2:55:GLN:OE1	1.76	0.68
2:2:171:SER:HA	2:2:175:PHE:CE1	2.28	0.67
2:2:206:VAL:HG12	3:3:37:PRO:HG2	1.75	0.67
1:1:38:GLU:O	2:2:189:GLN:HB2	1.93	0.67
1:1:135:GLY:HA3	1:1:231:LEU:HB3	1.76	0.67
2:2:78:TRP:N	2:2:78:TRP:HE3	1.92	0.67
3:3:82:VAL:HG12	3:3:83:PHE:CD1	2.25	0.67
1:1:142:VAL:HG13	1:1:143:MET:N	2.07	0.67
1:1:67:ILE:CD1	3:3:40:VAL:HB	2.22	0.67
2:2:103:ARG:HB3	2:2:211:MET:HG2	1.76	0.67
1:1:92:GLN:C	1:1:94:ILE:CD1	2.63	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:101:ILE:HG13	1:1:217:MET:C	2.15	0.66
3:3:201:PRO:O	3:3:202:SER:HB2	1.96	0.66
2:2:12:ARG:HB3	2:2:12:ARG:NH1	2.10	0.66
3:3:99:ILE:HG22	3:3:100:GLY:N	2.11	0.66
2:2:78:TRP:CZ3	2:2:226:PRO:HD3	2.30	0.65
3:3:89:ILE:HD11	3:3:109:TRP:CG	2.31	0.65
1:1:278:ILE:HD12	3:3:67:MET:HE3	1.77	0.65
1:1:45:VAL:H	3:3:114:ARG:HH12	1.45	0.65
2:2:146:LEU:HD12	2:2:166:GLN:HA	1.77	0.65
1:1:160:ASP:H	1:1:163:TRP:HD1	1.44	0.64
1:1:19:ASN:HB3	1:1:56:VAL:O	1.97	0.64
3:3:66:SER:C	3:3:68:TYR:H	2.00	0.64
3:3:89:ILE:HD11	3:3:109:TRP:CD2	2.33	0.64
2:2:207:ASN:ND2	2:2:209:VAL:HG22	2.13	0.64
1:1:215:ASN:O	1:1:215:ASN:ND2	2.30	0.64
1:1:23:SER:OG	1:1:53:THR:CG2	2.31	0.64
2:2:126:MET:HA	2:2:126:MET:HE3	1.80	0.64
3:3:89:ILE:HA	3:3:94:LEU:HD13	1.80	0.64
2:2:72:ASN:HB3	2:2:75:SER:N	2.13	0.64
3:3:102:ILE:CG2	3:3:103:ALA:N	2.61	0.63
1:1:276:THR:OG1	1:1:277:ALA:N	2.31	0.63
1:1:212:VAL:N	1:1:214:THR:H	1.96	0.63
3:3:87:VAL:HG22	3:3:189:ILE:HG22	1.79	0.63
1:1:186:PHE:HE1	3:3:31:THR:HG22	1.63	0.63
1:1:244:LYS:HE3	4:4:38:SER:O	1.99	0.63
1:1:145:TYR:N	1:1:145:TYR:HD1	1.97	0.63
1:1:163:TRP:CZ3	1:1:223:ARG:HB2	2.33	0.63
1:1:141:ILE:HA	1:1:226:THR:HG21	1.81	0.63
2:2:174:ASN:C	2:2:175:PHE:HD1	2.03	0.63
1:1:127:LEU:O	1:1:180:PRO:HD2	1.98	0.63
2:2:155:ASP:O	2:2:156:VAL:HB	1.98	0.62
3:3:102:ILE:O	3:3:105:TYR:HB2	2.00	0.62
1:1:7:ILE:N	1:1:7:ILE:HD13	2.15	0.62
2:2:30:ASN:HD22	2:2:31:ALA:N	1.97	0.62
1:1:155:PRO:HB3	1:1:163:TRP:NE1	2.15	0.62
1:1:6:TYR:CB	1:1:7:ILE:HD13	2.25	0.62
1:1:146:MET:CE	1:1:162:SER:O	2.48	0.61
2:2:257:ARG:HG2	2:2:257:ARG:NH1	2.14	0.61
1:1:14:VAL:HG12	1:1:15:LEU:HD22	1.81	0.61
1:1:145:TYR:O	1:1:170:SER:HA	2.01	0.61
1:1:283:THR:HG22	1:1:285:THR:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:79:ILE:HD13	1:1:238:HIS:CE1	2.36	0.61
1:1:182:PHE:HA	3:3:21:SER:HB2	1.82	0.61
1:1:113:PHE:C	1:1:115:LEU:N	2.52	0.61
1:1:204:ASN:C	1:1:206:SER:N	2.52	0.61
2:2:145:LYS:NZ	2:2:263:GLN:HG2	2.15	0.61
1:1:104:GLN:HA	1:1:110:ARG:HG3	1.82	0.61
1:1:260:THR:C	1:1:261:HIS:CD2	2.74	0.61
4:4:43:LEU:O	4:4:44:ASP:C	2.38	0.61
1:1:197:TYR:HD1	1:1:198:ASP:H	1.46	0.61
1:1:140:HIS:O	1:1:226:THR:CG2	2.48	0.61
2:2:84:ASP:HB2	2:2:218:ASN:HD21	1.66	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
1:1:155:PRO:HD2	1:1:221:CYS:SG	2.41	0.60
1:1:183:SER:HG	3:3:21:SER:HG	1.49	0.60
1:1:200:TYR:CD2	1:1:209:TYR:HB2	2.37	0.60
2:2:84:ASP:OD1	2:2:87:LYS:HE2	2.02	0.60
2:2:91:ILE:O	2:2:92:PHE:C	2.38	0.60
3:3:72:LEU:HD11	3:3:209:MET:HB3	1.82	0.60
3:3:91:SER:O	3:3:92:THR:C	2.39	0.60
1:1:146:MET:HG2	1:1:146:MET:O	1.96	0.60
1:1:149:PRO:O	1:1:150:PRO:O	2.20	0.60
1:1:91:GLY:O	1:1:157:LYS:CB	2.49	0.60
1:1:91:GLY:O	1:1:157:LYS:HB3	2.02	0.60
1:1:101:ILE:CG2	1:1:217:MET:O	2.35	0.60
3:3:42:ASN:ND2	3:3:44:ILE:CG2	2.53	0.60
2:2:183:LEU:HD12	2:2:186:PHE:CD2	2.34	0.60
1:1:102:THR:C	1:1:103:LEU:HD23	2.22	0.60
1:1:204:ASN:HD22	1:1:205:THR:N	2.00	0.60
1:1:125:ILE:HD12	1:1:182:PHE:HE1	1.66	0.60
1:1:7:ILE:HD13	1:1:7:ILE:H	1.67	0.60
1:1:249:TRP:HA	3:3:39:GLU:HA	1.84	0.59
3:3:90:THR:OG1	3:3:178:THR:O	2.15	0.59
1:1:142:VAL:H	1:1:226:THR:HG23	1.67	0.59
1:1:260:THR:O	1:1:261:HIS:HB2	2.03	0.59
1:1:37:ALA:HB2	3:3:162:THR:HG21	1.83	0.59
1:1:278:ILE:CD1	3:3:67:MET:HE1	2.29	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
1:1:210:GLY:C	1:1:212:VAL:HG13	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:102:THR:CG2	1:1:103:LEU:N	2.62	0.59
1:1:136:ASP:O	1:1:137:ASP:HB2	2.02	0.59
1:1:85:ASP:OD1	1:1:86:TYR:N	2.36	0.59
1:1:254:PRO:HG2	3:3:101:GLU:HG2	1.83	0.59
1:1:146:MET:HE3	1:1:162:SER:O	2.03	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
1:1:153:PRO:O	1:1:153:PRO:HG2	2.04	0.58
2:2:144:TYR:O	2:2:146:LEU:N	2.36	0.58
2:2:154:ARG:HD3	2:2:155:ASP:N	2.19	0.58
1:1:150:PRO:O	1:1:152:ALA:CB	2.51	0.58
1:1:253:PRO:HD3	2:2:185:ILE:CG2	2.34	0.58
1:1:66:SER:O	1:1:68:GLU:N	2.37	0.58
2:2:158:GLN:HG3	2:2:159:GLU:H	1.68	0.58
1:1:169:MET:HE2	1:1:171:ILE:HB	1.85	0.58
3:3:136:PRO:HG3	3:3:176:ARG:NH2	2.19	0.58
3:3:46:MET:O	3:3:98:LEU:HD23	2.03	0.58
2:2:49:ALA:O	2:2:50:ILE:HG13	2.04	0.58
1:1:253:PRO:HD3	2:2:185:ILE:HG21	1.86	0.58
1:1:11:LEU:N	1:1:11:LEU:HD22	2.19	0.57
3:3:54:PRO:HA	3:3:67:MET:O	2.04	0.57
1:1:90:ASN:HD22	1:1:158:ARG:HD3	1.69	0.57
1:1:199:GLY:HA2	2:2:216:ARG:O	2.04	0.57
2:2:57:ASP:O	2:2:58:THR:HG22	2.04	0.57
1:1:92:GLN:HA	1:1:157:LYS:HG2	1.86	0.57
1:1:67:ILE:HD11	3:3:40:VAL:CB	2.33	0.57
2:2:120:GLY:HA3	2:2:193:LEU:HD12	1.86	0.57
3:3:192:TRP:N	3:3:192:TRP:CD1	2.73	0.57
1:1:278:ILE:HA	3:3:92:THR:HG21	1.85	0.57
1:1:54:ARG:CG	1:1:55:TYR:H	2.16	0.57
3:3:136:PRO:HG3	3:3:176:ARG:HH22	1.68	0.57
1:1:44:ASN:ND2	1:1:44:ASN:C	2.58	0.57
1:1:97:THR:H	1:1:222:SER:HB3	1.69	0.56
1:1:150:PRO:O	1:1:152:ALA:HB2	2.05	0.56
1:1:201:ASP:OD1	1:1:213:VAL:HG22	2.05	0.56
3:3:87:VAL:O	3:3:89:ILE:N	2.38	0.56
2:2:72:ASN:HB3	2:2:74:SER:H	1.70	0.56
3:3:7:THR:O	3:3:10:SER:CB	2.53	0.56
3:3:104:SER:O	3:3:227:THR:HA	2.06	0.56
1:1:143:MET:HG2	1:1:145:TYR:CE1	2.41	0.56
3:3:42:ASN:CB	3:3:44:ILE:HG22	2.36	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	2.69	0.56
2:2:235:THR:C	2:2:237:SER:H	2.06	0.56
3:3:14:MET:HG2	3:3:16:THR:HG22	1.88	0.56
1:1:260:THR:HB	1:1:261:HIS:HD2	1.71	0.56
3:3:107:THR:O	3:3:177:LEU:HD23	2.06	0.56
3:3:121:GLY:HA2	3:3:207:ALA:HB1	1.88	0.56
3:3:194:GLN:HA	3:3:194:GLN:NE2	2.19	0.56
3:3:228:ASP:HB3	3:3:229:LEU:HD12	1.88	0.56
3:3:237:GLU:CG	3:3:238:GLN:N	2.69	0.56
3:3:42:ASN:HB3	3:3:44:ILE:CG2	2.36	0.56
1:1:255:ARG:NH2	1:1:259:TYR:HA	2.21	0.56
3:3:144:ARG:O	3:3:145:LYS:C	2.44	0.56
1:1:184:ILE:HG22	1:1:185:PRO:O	2.06	0.55
3:3:83:PHE:CE1	3:3:191:CYS:CB	2.89	0.55
1:1:119:VAL:HG13	1:1:121:PHE:CD1	2.40	0.55
2:2:173:LEU:O	2:2:174:ASN:CB	2.54	0.55
3:3:201:PRO:O	3:3:202:SER:CB	2.53	0.55
1:1:61:THR:CG2	1:1:63:ASP:OD1	2.54	0.55
3:3:81:LYS:HB2	3:3:192:TRP:CE3	2.41	0.55
3:3:94:LEU:O	3:3:95:ALA:C	2.45	0.55
1:1:260:THR:O	1:1:261:HIS:CB	2.53	0.55
1:1:66:SER:C	1:1:68:GLU:N	2.60	0.55
2:2:202:ILE:HD13	2:2:249:MET:CE	2.36	0.55
1:1:45:VAL:N	3:3:114:ARG:NH1	2.43	0.55
2:2:57:ASP:O	2:2:58:THR:CB	2.55	0.55
3:3:145:LYS:HA	3:3:148:MET:HE2	1.88	0.55
3:3:165:LEU:HD12	3:3:166:VAL:N	2.21	0.55
1:1:111:ARG:NH1	3:3:230:HIS:HB2	2.21	0.55
1:1:210:GLY:C	1:1:212:VAL:CG1	2.75	0.55
1:1:91:GLY:C	1:1:94:ILE:CD1	2.75	0.55
2:2:227:ILE:HG21	3:3:210:LEU:HD11	1.89	0.55
1:1:80:SER:HB3	1:1:237:THR:HG23	1.89	0.55
1:1:89:TYR:O	1:1:90:ASN:HB2	2.06	0.55
1:1:201:ASP:OD1	1:1:208:LYS:HB2	2.07	0.55
1:1:19:ASN:HA	1:1:58:THR:HG23	1.89	0.55
2:2:174:ASN:O	2:2:175:PHE:HB2	2.07	0.55
1:1:84:VAL:HG21	1:1:233:VAL:HG23	1.88	0.55
2:2:116:LYS:HB2	3:3:124:ASN:ND2	2.21	0.55
2:2:122:LEU:HD22	2:2:224:ILE:HG13	1.88	0.55
2:2:23:ILE:HG21	2:2:109:HIS:CD2	2.42	0.54
1:1:260:THR:C	1:1:261:HIS:HD2	2.09	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:127:ILE:HD11	2:2:183:LEU:HD11	1.89	0.54
3:3:173:SER:O	3:3:174:HIS:C	2.43	0.54
1:1:46:GLN:CB	1:1:47:PRO:CD	2.57	0.54
1:1:257:VAL:HG11	1:1:274:VAL:HG21	1.89	0.54
2:2:102:GLY:HA3	2:2:214:MET:HG3	1.88	0.54
1:1:283:THR:CG2	1:1:285:THR:HB	2.38	0.54
2:2:103:ARG:CB	2:2:211:MET:HG2	2.38	0.54
3:3:155:TRP:CD2	3:3:163:ILE:CG2	2.90	0.54
3:3:80:GLN:HA	3:3:80:GLN:NE2	2.23	0.54
3:3:125:THR:CG2	3:3:126:THR:N	2.70	0.54
1:1:72:GLY:C	1:1:73:ARG:HG2	2.27	0.54
1:1:84:VAL:HG12	1:1:85:ASP:N	2.22	0.54
3:3:103:ALA:O	3:3:178:THR:HG21	2.08	0.54
3:3:231:ILE:CD1	3:3:231:ILE:N	2.70	0.54
3:3:81:LYS:HB2	3:3:192:TRP:CZ3	2.43	0.54
1:1:200:TYR:HA	1:1:208:LYS:O	2.08	0.54
1:1:142:VAL:CG1	1:1:225:VAL:CB	2.76	0.54
1:1:61:THR:HG22	1:1:63:ASP:CG	2.28	0.54
1:1:96:PHE:HE2	1:1:157:LYS:HA	1.70	0.53
1:1:17:VAL:CG1	1:1:60:GLN:O	2.53	0.53
2:2:84:ASP:O	2:2:87:LYS:HD2	2.07	0.53
3:3:56:ASN:C	3:3:58:VAL:H	2.12	0.53
2:2:158:GLN:CG	2:2:159:GLU:H	2.21	0.53
2:2:40:HIS:HA	2:2:250:CYS:SG	2.47	0.53
1:1:281:ARG:HH11	3:3:57:ASN:HB3	1.74	0.53
1:1:129:PRO:HG2	1:1:173:TRP:NE1	2.24	0.53
2:2:235:THR:OG1	2:2:237:SER:HB3	2.08	0.53
2:2:83:PRO:HG2	2:2:218:ASN:CA	2.28	0.53
1:1:183:SER:O	1:1:184:ILE:HG12	2.08	0.53
1:1:98:LYS:CA	1:1:220:ILE:O	2.40	0.53
1:1:92:GLN:O	1:1:94:ILE:HD11	2.09	0.53
2:2:122:LEU:O	2:2:190:PHE:HA	2.08	0.53
2:2:174:ASN:HB3	2:2:176:ASP:OD2	2.08	0.53
1:1:89:TYR:HE2	1:1:227:GLU:C	2.12	0.53
1:1:33:LEU:HB3	3:3:163:ILE:HD11	1.90	0.53
1:1:200:TYR:CE2	1:1:209:TYR:HB2	2.44	0.53
3:3:169:TRP:CZ3	3:3:176:ARG:HD2	2.44	0.53
3:3:89:ILE:HA	3:3:94:LEU:CD1	2.38	0.53
1:1:101:ILE:CD1	1:1:219:THR:CA	2.87	0.53
1:1:101:ILE:HG13	1:1:218:GLY:C	2.29	0.53
1:1:260:THR:HB	1:1:261:HIS:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:269:PRO:CG	1:1:272:GLY:O	2.56	0.53
2:2:61:ASN:HB2	2:2:248:PRO:O	2.09	0.53
1:1:261:HIS:CD2	1:1:261:HIS:N	2.76	0.52
3:3:75:GLN:HG2	3:3:80:GLN:HB3	1.91	0.52
4:4:26:TYR:CD1	4:4:29:ILE:CD1	2.91	0.52
1:1:257:VAL:HG21	2:2:173:LEU:HD11	1.91	0.52
2:2:65:THR:HG1	2:2:245:SER:HG	1.50	0.52
1:1:46:GLN:O	1:1:49:ASP:HB2	2.10	0.52
2:2:18:ARG:HG3	2:2:247:SER:OG	2.09	0.52
2:2:202:ILE:HD13	2:2:249:MET:HE3	1.91	0.52
2:2:41:TYR:CE2	2:2:55:GLN:OE1	2.62	0.52
1:1:197:TYR:CD1	1:1:198:ASP:N	2.78	0.52
1:1:84:VAL:HG12	1:1:85:ASP:H	1.75	0.52
3:3:173:SER:C	3:3:175:PHE:N	2.63	0.52
2:2:174:ASN:C	2:2:175:PHE:CD1	2.82	0.52
1:1:101:ILE:CD1	1:1:219:THR:N	2.73	0.52
1:1:7:ILE:H	1:1:7:ILE:CD1	2.17	0.52
1:1:271:THR:HG22	1:1:272:GLY:N	2.25	0.51
1:1:284:ILE:HG13	1:1:285:THR:N	2.24	0.51
1:1:197:TYR:HE1	2:2:217:HIS:CG	2.28	0.51
3:3:66:SER:O	3:3:68:TYR:N	2.42	0.51
1:1:102:THR:O	1:1:103:LEU:HD23	2.11	0.51
1:1:171:ILE:CD1	1:1:180:PRO:HB2	2.37	0.51
1:1:266:ASN:OD1	2:2:134:SER:N	2.34	0.51
3:3:102:ILE:O	3:3:105:TYR:N	2.44	0.51
1:1:145:TYR:H	1:1:145:TYR:HD1	1.57	0.51
1:1:197:TYR:HD1	1:1:198:ASP:N	2.07	0.51
2:2:185:ILE:HD13	3:3:98:LEU:HD21	1.91	0.51
2:2:190:PHE:O	2:2:196:ASN:ND2	2.43	0.51
3:3:83:PHE:CE1	3:3:191:CYS:HB3	2.45	0.51
1:1:19:ASN:N	1:1:19:ASN:ND2	2.57	0.51
2:2:173:LEU:O	2:2:177:GLY:N	2.44	0.51
3:3:181:ASN:OD1	3:3:183:TYR:HB3	2.11	0.51
3:3:136:PRO:HB3	3:3:185:MET:O	2.10	0.51
2:2:145:LYS:HZ2	2:2:263:GLN:HG2	1.74	0.51
2:2:12:ARG:O	2:2:28:VAL:HG22	2.10	0.51
1:1:119:VAL:HG11	1:1:121:PHE:CE1	2.30	0.51
2:2:137:HIS:CD2	2:2:138:GLY:N	2.79	0.51
3:3:99:ILE:CG2	3:3:100:GLY:N	2.73	0.51
3:3:110:THR:O	3:3:219:PHE:HA	2.10	0.51
1:1:7:ILE:O	1:1:11:LEU:HD23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:14:MET:HG2	2:2:15:GLN:N	2.25	0.50
2:2:154:ARG:CG	2:2:154:ARG:HH11	2.24	0.50
2:2:175:PHE:N	2:2:175:PHE:CD1	2.79	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
3:3:118:MET:O	3:3:209:MET:HA	2.11	0.50
1:1:6:TYR:O	1:1:10:VAL:N	2.44	0.50
1:1:92:GLN:C	1:1:94:ILE:HD11	2.31	0.50
3:3:72:LEU:N	3:3:72:LEU:HD12	2.26	0.50
3:3:51:THR:HG21	3:3:98:LEU:HB3	1.92	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
1:1:34:LEU:HD23	3:3:162:THR:O	2.12	0.50
3:3:62:VAL:HA	3:3:67:MET:HG3	1.94	0.50
4:4:26:TYR:O	4:4:27:PHE:HB2	2.12	0.50
2:2:32:VAL:HB	2:2:201:LEU:HD22	1.94	0.50
2:2:86:LEU:C	2:2:88:ASP:H	2.14	0.49
1:1:183:SER:C	1:1:184:ILE:CG1	2.80	0.49
3:3:117:PHE:CE2	3:3:131:LEU:HG	2.47	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
1:1:191:SER:CB	3:3:34:ILE:HG12	2.42	0.49
1:1:204:ASN:O	1:1:206:SER:N	2.45	0.49
1:1:230:LYS:HD3	1:1:231:LEU:HD22	1.95	0.49
1:1:38:GLU:C	1:1:40:GLY:H	2.15	0.49
1:1:7:ILE:N	1:1:7:ILE:CD1	2.76	0.49
1:1:163:TRP:CH2	1:1:222:SER:C	2.86	0.49
1:1:173:TRP:HE3	1:1:173:TRP:O	1.95	0.49
1:1:7:ILE:HA	1:1:11:LEU:CD2	2.28	0.49
3:3:141:PRO:HG3	3:3:147:ALA:HB2	1.93	0.49
1:1:104:GLN:HB2	1:1:262:SER:CB	2.41	0.49
1:1:204:ASN:HD22	1:1:205:THR:H	1.61	0.49
1:1:186:PHE:CE1	3:3:31:THR:HG22	2.46	0.49
1:1:244:LYS:CE	4:4:38:SER:O	2.60	0.49
1:1:7:ILE:O	1:1:11:LEU:CB	2.60	0.49
2:2:81:LYS:HE2	2:2:132:LEU:HD11	1.94	0.49
1:1:186:PHE:CD1	1:1:186:PHE:C	2.86	0.48
3:3:135:PRO:CB	3:3:136:PRO:HD2	2.42	0.48
3:3:55:VAL:C	3:3:57:ASN:N	2.67	0.48
1:1:141:ILE:CD1	1:1:235:ILE:HG12	2.43	0.48
1:1:65:MET:O	3:3:42:ASN:CG	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:7:ILE:O	1:1:11:LEU:N	2.43	0.48
2:2:12:ARG:CG	2:2:13:ILE:H	2.26	0.48
2:2:82:LEU:CB	2:2:83:PRO:HD3	2.43	0.48
3:3:140:GLU:HB3	3:3:188:TYR:CD2	2.48	0.48
3:3:155:TRP:CG	3:3:163:ILE:HG21	2.49	0.48
1:1:112:LYS:O	1:1:115:LEU:HB2	2.13	0.48
3:3:112:SER:H	3:3:218:ASP:HB3	1.79	0.48
3:3:237:GLU:HG2	3:3:238:GLN:N	2.18	0.48
2:2:57:ASP:O	2:2:59:SER:N	2.42	0.48
2:2:70:HIS:ND1	2:2:71:TRP:N	2.60	0.48
3:3:155:TRP:CD2	3:3:163:ILE:HG22	2.48	0.48
2:2:107:THR:OG1	2:2:249:MET:CE	2.61	0.48
3:3:88:ASP:OD1	3:3:186:ALA:N	2.39	0.48
1:1:142:VAL:HG11	1:1:225:VAL:CB	2.39	0.48
1:1:257:VAL:HA	1:1:258:PRO:HD2	1.69	0.48
3:3:14:MET:C	3:3:16:THR:H	2.16	0.48
3:3:61:ASN:ND2	3:3:66:SER:HB2	2.29	0.48
2:2:185:ILE:CD1	3:3:98:LEU:CD2	2.85	0.48
1:1:262:SER:O	1:1:263:HIS:HB2	2.14	0.48
2:2:15:GLN:HG3	2:2:16:ILE:N	2.29	0.48
1:1:281:ARG:HH11	3:3:57:ASN:CB	2.26	0.48
3:3:65:VAL:O	3:3:67:MET:N	2.46	0.48
1:1:145:TYR:HE2	1:1:237:THR:HG1	1.62	0.47
3:3:131:LEU:CD1	3:3:191:CYS:SG	3.02	0.47
1:1:146:MET:HE1	1:1:162:SER:O	2.14	0.47
1:1:93:ASP:N	1:1:94:ILE:HD12	2.28	0.47
1:1:257:VAL:HG21	2:2:173:LEU:CD1	2.44	0.47
2:2:174:ASN:ND2	2:2:178:THR:O	2.41	0.47
2:2:128:PRO:HD2	2:2:186:PHE:CD1	2.49	0.47
2:2:192:ASN:O	2:2:194:ARG:N	2.46	0.47
2:2:82:LEU:HD21	2:2:246:ILE:HD13	1.96	0.47
3:3:124:ASN:HD22	3:3:124:ASN:H	1.63	0.47
3:3:155:TRP:CD1	3:3:155:TRP:C	2.87	0.47
1:1:125:ILE:HD12	1:1:182:PHE:CE1	2.47	0.47
1:1:86:TYR:CZ	1:1:229:GLN:HB2	2.49	0.47
3:3:136:PRO:HD3	3:3:186:ALA:O	2.15	0.47
1:1:15:LEU:CD2	4:4:43:LEU:HD23	2.45	0.47
2:2:206:VAL:O	2:2:207:ASN:HB2	2.15	0.47
3:3:131:LEU:O	3:3:152:HIS:HB2	2.15	0.47
1:1:149:PRO:CB	1:1:150:PRO:HD2	2.44	0.47
2:2:154:ARG:NH2	2:2:167:PRO:HG2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:174:ASN:C	2:2:176:ASP:H	2.16	0.47
3:3:57:ASN:HA	3:3:57:ASN:HD22	1.21	0.47
4:4:27:PHE:O	4:4:28:ASN:HB2	2.14	0.47
1:1:48:GLU:HA	1:1:53:THR:HG21	1.96	0.47
1:1:84:VAL:CG2	1:1:233:VAL:HG23	2.44	0.47
2:2:224:ILE:HD11	2:2:242:ILE:HD13	1.96	0.47
2:2:253:PHE:O	2:2:254:SER:HB3	2.15	0.47
1:1:169:MET:HE2	1:1:171:ILE:CB	2.45	0.47
1:1:255:ARG:HH21	1:1:259:TYR:HA	1.80	0.47
1:1:42:THR:HG21	3:3:48:GLN:O	2.15	0.47
1:1:44:ASN:O	1:1:44:ASN:ND2	2.34	0.47
2:2:116:LYS:HB2	3:3:124:ASN:HD21	1.79	0.47
2:2:160:ARG:HD2	2:2:160:ARG:HH11	1.57	0.47
2:2:146:LEU:HD11	2:2:166:GLN:HA	1.94	0.47
3:3:82:VAL:HG12	3:3:83:PHE:H	1.78	0.47
2:2:72:ASN:HB3	2:2:75:SER:H	1.78	0.47
1:1:280:ARG:HG3	3:3:62:VAL:HG21	1.97	0.47
2:2:130:HIS:CB	2:2:221:CYS:SG	3.03	0.47
2:2:111:GLN:OE1	2:2:245:SER:OG	2.31	0.46
2:2:78:TRP:CZ2	2:2:242:ILE:HD12	2.50	0.46
3:3:219:PHE:CE2	3:3:221:LEU:HD13	2.50	0.46
1:1:101:ILE:HD12	1:1:219:THR:N	2.30	0.46
1:1:19:ASN:CB	1:1:56:VAL:O	2.63	0.46
2:2:200:THR:C	2:2:201:LEU:HD23	2.36	0.46
1:1:11:LEU:HA	1:1:11:LEU:HD13	1.77	0.46
1:1:77:VAL:HG22	1:1:239:ILE:HG22	1.98	0.46
2:2:69:LYS:O	2:2:241:PRO:HA	2.15	0.46
2:2:164:LEU:O	2:2:166:GLN:HB2	2.16	0.46
3:3:42:ASN:O	3:3:43:LEU:C	2.54	0.46
1:1:141:ILE:CG1	1:1:141:ILE:O	2.51	0.46
2:2:57:ASP:O	2:2:58:THR:HB	2.15	0.46
3:3:15:THR:HG22	3:3:15:THR:H	1.45	0.46
1:1:148:VAL:HA	1:1:149:PRO:HD2	1.79	0.46
1:1:188:SER:OG	1:1:190:ALA:HB3	2.16	0.46
1:1:101:ILE:CD1	1:1:219:THR:HA	2.35	0.46
1:1:89:TYR:O	1:1:90:ASN:CB	2.62	0.46
2:2:102:GLY:HA3	2:2:214:MET:CG	2.45	0.46
2:2:66:LEU:HD23	2:2:80:TRP:CD1	2.50	0.46
1:1:194:TYR:OH	2:2:207:ASN:ND2	2.49	0.46
1:1:185:PRO:HD3	3:3:23:CYS:SG	2.56	0.46
1:1:90:ASN:ND2	1:1:158:ARG:HD3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:121:THR:HG22	2:2:227:ILE:HB	1.98	0.46
2:2:182:ASN:O	2:2:185:ILE:HG22	2.16	0.46
1:1:197:TYR:CE1	2:2:217:HIS:CE1	3.04	0.46
3:3:46:MET:HE3	3:3:102:ILE:HD11	1.97	0.46
1:1:80:SER:O	1:1:236:THR:HA	2.16	0.45
3:3:25:LEU:N	3:3:26:PRO:CD	2.79	0.45
2:2:171:SER:O	2:2:174:ASN:N	2.38	0.45
2:2:46:ASP:HB3	3:3:34:ILE:HB	1.98	0.45
2:2:127:ILE:HG22	2:2:128:PRO:O	2.16	0.45
2:2:257:ARG:O	2:2:258:ALA:O	2.35	0.45
1:1:169:MET:HG2	1:1:170:SER:N	2.30	0.45
1:1:75:GLY:N	1:1:240:TYR:HD1	2.15	0.45
1:1:122:ASP:OD1	1:1:245:HIS:HB2	2.15	0.45
1:1:103:LEU:HG	5:1:500:W54:C4	2.47	0.45
3:3:87:VAL:HG22	3:3:189:ILE:CG2	2.45	0.45
3:3:93:PRO:O	3:3:94:LEU:O	2.35	0.45
2:2:235:THR:HG23	2:2:235:THR:O	2.17	0.45
3:3:217:LYS:H	3:3:217:LYS:HG3	1.64	0.45
3:3:88:ASP:O	3:3:90:THR:N	2.43	0.45
3:3:99:ILE:O	3:3:102:ILE:HB	2.16	0.45
1:1:268:MET:HA	1:1:269:PRO:HD2	1.82	0.45
2:2:126:MET:HE2	2:2:126:MET:HB3	1.77	0.45
2:2:146:LEU:HD12	2:2:167:PRO:HD2	1.95	0.45
2:2:80:TRP:NE1	2:2:151:GLU:O	2.50	0.45
3:3:82:VAL:CG1	3:3:83:PHE:CD1	2.94	0.45
2:2:121:THR:OG1	3:3:120:CYS:HB3	2.17	0.44
3:3:97:THR:O	3:3:98:LEU:C	2.56	0.44
1:1:23:SER:OG	1:1:53:THR:N	2.49	0.44
3:3:145:LYS:O	3:3:148:MET:HE3	2.17	0.44
1:1:101:ILE:CG1	1:1:217:MET:C	2.84	0.44
1:1:254:PRO:CG	3:3:101:GLU:CG	2.72	0.44
3:3:101:GLU:HA	3:3:229:LEU:HD22	1.99	0.44
1:1:146:MET:CG	1:1:147:TYR:N	2.72	0.44
1:1:90:ASN:N	1:1:90:ASN:HD22	2.16	0.44
2:2:79:TRP:CZ3	2:2:81:LYS:HD3	2.52	0.44
3:3:84:SER:OG	3:3:140:GLU:OE1	2.29	0.44
1:1:156:SER:C	1:1:157:LYS:HG3	2.38	0.44
2:2:103:ARG:HD3	2:2:252:GLU:OE1	2.17	0.44
2:2:174:ASN:ND2	2:2:180:LEU:HA	2.32	0.44
2:2:192:ASN:C	2:2:194:ARG:H	2.21	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)
1:1:40:GLY:HA3	2:2:188:HIS:O	2.18	0.44
2:2:61:ASN:HD22	2:2:250:CYS:H	1.65	0.44
3:3:173:SER:C	3:3:175:PHE:H	2.20	0.44
4:4:30:ASN:ND2	4:4:30:ASN:N	2.65	0.44
1:1:244:LYS:NZ	4:4:38:SER:H	2.16	0.44
1:1:197:TYR:N	2:2:131:GLN:HE21	2.12	0.44
2:2:52:LYS:HA	2:2:53:PRO:HD2	1.91	0.44
3:3:130:LEU:HD23	3:3:130:LEU:C	2.38	0.44
3:3:126:THR:O	3:3:197:LEU:HA	2.18	0.44
1:1:101:ILE:HG13	1:1:218:GLY:HA3	1.97	0.44
2:2:154:ARG:HG2	2:2:154:ARG:HH11	1.83	0.44
3:3:159:LEU:HD23	3:3:159:LEU:HA	1.72	0.44
1:1:283:THR:CG2	1:1:285:THR:H	2.29	0.43
1:1:54:ARG:HD2	1:1:56:VAL:HG22	2.00	0.43
1:1:127:LEU:HD12	1:1:239:ILE:HG12	1.99	0.43
1:1:54:ARG:HG3	1:1:55:TYR:H	1.83	0.43
1:1:45:VAL:N	3:3:114:ARG:HH12	2.12	0.43
1:1:142:VAL:H	1:1:226:THR:CG2	2.29	0.43
1:1:74:SER:HB2	3:3:15:THR:HA	2.00	0.43
1:1:5:ASN:O	1:1:9:GLU:HB2	2.18	0.43
3:3:155:TRP:CD2	3:3:163:ILE:HG21	2.53	0.43
1:1:96:PHE:CZ	1:1:155:PRO:O	2.71	0.43
1:1:283:THR:HG22	1:1:285:THR:H	1.83	0.43
2:2:111:GLN:H	2:2:111:GLN:HG2	1.29	0.43
2:2:37:VAL:HG12	2:2:204:PRO:HB3	2.01	0.43
3:3:7:THR:HA	3:3:8:PRO:HD3	1.78	0.43
1:1:81:ARG:HE	1:1:81:ARG:HB2	1.67	0.43
2:2:179:LEU:O	2:2:180:LEU:C	2.56	0.43
2:2:29:ALA:O	2:2:30:ASN:C	2.56	0.43
3:3:1:GLY:O	3:3:3:PRO:HD3	2.19	0.43
1:1:244:LYS:NZ	4:4:38:SER:O	2.52	0.43
2:2:105:GLY:O	2:2:249:MET:N	2.49	0.43
2:2:91:ILE:HG22	2:2:92:PHE:N	2.32	0.43
3:3:149:LEU:HA	3:3:149:LEU:HD23	1.73	0.43
3:3:50:ASP:CA	3:3:214:SER:HB3	2.49	0.43
2:2:82:LEU:HD23	2:2:82:LEU:HA	1.55	0.43
1:1:115:LEU:HA	1:1:115:LEU:HD12	1.76	0.43
2:2:147:THR:C	2:2:149:PRO:CD	2.87	0.43
2:2:30:ASN:HD22	2:2:31:ALA:H	1.62	0.43
2:2:57:ASP:O	2:2:58:THR:CG2	2.67	0.43
2:2:61:ASN:OD1	2:2:61:ASN:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:103:ALA:C	3:3:105:TYR:H	2.21	0.43
2:2:174:ASN:O	2:2:175:PHE:CB	2.66	0.43
2:2:191:ILE:HA	2:2:196:ASN:ND2	2.33	0.43
2:2:94:GLU:C	2:2:96:MET:H	2.22	0.43
3:3:72:LEU:CD1	3:3:209:MET:HB3	2.48	0.43
1:1:184:ILE:HG23	1:1:185:PRO:HD2	2.01	0.43
2:2:137:HIS:C	2:2:137:HIS:CD2	2.91	0.43
2:2:128:PRO:HD3	2:2:220:TRP:CZ3	2.53	0.43
3:3:50:ASP:N	3:3:214:SER:HB3	2.34	0.43
1:1:218:GLY:C	1:1:219:THR:HG23	2.26	0.42
2:2:143:GLY:N	2:2:165:ARG:O	2.48	0.42
3:3:43:LEU:O	3:3:44:ILE:C	2.56	0.42
1:1:267:TYR:O	1:1:268:MET:C	2.57	0.42
1:1:63:ASP:O	1:1:66:SER:OG	2.27	0.42
2:2:118:HIS:O	3:3:122:THR:HG23	2.19	0.42
2:2:98:TYR:CE2	2:2:259:LYS:HD2	2.54	0.42
2:2:207:ASN:O	2:2:209:VAL:N	2.52	0.42
1:1:268:MET:O	2:2:137:HIS:HB2	2.19	0.42
1:1:66:SER:C	1:1:68:GLU:H	2.21	0.42
2:2:95:ASN:HB3	2:2:253:PHE:CE2	2.54	0.42
1:1:129:PRO:HA	1:1:237:THR:HA	2.01	0.42
2:2:158:GLN:CG	2:2:159:GLU:N	2.83	0.42
2:2:207:ASN:HD22	2:2:209:VAL:N	2.12	0.42
2:2:99:HIS:HA	2:2:255:GLY:O	2.19	0.42
2:2:65:THR:HA	2:2:245:SER:HA	2.02	0.42
3:3:2:LEU:HD23	3:3:2:LEU:HA	1.80	0.42
1:1:148:VAL:C	1:1:149:PRO:O	2.57	0.42
2:2:136:LYS:HD3	2:2:136:LYS:HA	1.59	0.42
2:2:200:THR:O	2:2:201:LEU:HD23	2.19	0.42
2:2:84:ASP:HB2	2:2:218:ASN:ND2	2.33	0.42
3:3:219:PHE:O	3:3:220:CYS:HB2	2.20	0.42
3:3:54:PRO:HA	3:3:68:TYR:CD1	2.54	0.42
1:1:58:THR:O	1:1:59:SER:HB3	2.19	0.42
2:2:21:SER:OG	2:2:63:PHE:HB2	2.20	0.42
3:3:53:ILE:HD13	3:3:53:ILE:HG21	1.78	0.42
1:1:128:VAL:HB	1:1:238:HIS:HB2	2.02	0.42
3:3:216:CYS:C	3:3:218:ASP:H	2.22	0.42
2:2:63:PHE:CD1	2:2:247:SER:HB2	2.55	0.42
1:1:261:HIS:H	3:3:237:GLU:H	1.68	0.42
1:1:165:SER:C	1:1:167:THR:N	2.74	0.41
1:1:145:TYR:HB2	1:1:171:ILE:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:99:TRP:O	1:1:219:THR:HA	2.20	0.41
1:1:86:TYR:OH	1:1:229:GLN:HB2	2.20	0.41
1:1:90:ASN:C	1:1:91:GLY:O	2.57	0.41
2:2:18:ARG:HD3	2:2:18:ARG:HA	1.57	0.41
3:3:87:VAL:CG2	3:3:189:ILE:HG22	2.47	0.41
3:3:66:SER:C	3:3:68:TYR:N	2.69	0.41
2:2:145:LYS:HZ1	2:2:263:GLN:HG2	1.85	0.41
3:3:141:PRO:CG	3:3:147:ALA:HB2	2.51	0.41
3:3:14:MET:C	3:3:16:THR:N	2.74	0.41
1:1:98:LYS:HB3	1:1:221:CYS:SG	2.60	0.41
3:3:122:THR:HB	3:3:125:THR:OG1	2.19	0.41
1:1:15:LEU:O	1:1:61:THR:HA	2.21	0.41
1:1:71:LEU:HD13	1:1:113:PHE:CE1	2.56	0.41
2:2:147:THR:C	2:2:149:PRO:HD3	2.40	0.41
2:2:228:SER:HA	2:2:229:PRO:HD2	1.68	0.41
2:2:58:THR:CG2	2:2:59:SER:N	2.83	0.41
1:1:257:VAL:HG11	1:1:274:VAL:CG2	2.51	0.41
1:1:271:THR:O	1:1:272:GLY:C	2.58	0.41
2:2:203:VAL:HG22	2:2:220:TRP:CZ2	2.55	0.41
2:2:43:THR:C	2:2:45:GLN:H	2.22	0.41
1:1:9:GLU:OE2	4:4:42:ARG:HG3	2.21	0.41
1:1:74:SER:HA	1:1:241:HIS:O	2.20	0.41
2:2:116:LYS:HB3	2:2:116:LYS:HE3	1.34	0.41
2:2:54:THR:HG22	2:2:253:PHE:HB2	2.03	0.41
3:3:83:PHE:CD1	3:3:191:CYS:HB3	2.55	0.41
3:3:83:PHE:CD1	3:3:83:PHE:N	2.88	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
2:2:126:MET:O	2:2:186:PHE:HB3	2.21	0.41
3:3:191:CYS:C	3:3:192:TRP:CD1	2.94	0.41
3:3:61:ASN:HA	3:3:61:ASN:HD22	1.60	0.41
1:1:124:GLU:N	1:1:242:LYS:O	2.41	0.41
1:1:110:ARG:HD3	1:1:259:TYR:CZ	2.56	0.41
1:1:22:GLU:CB	1:1:54:ARG:O	2.69	0.41
1:1:132:ALA:HB3	1:1:234:VAL:HG13	2.02	0.41
1:1:124:GLU:HB3	1:1:242:LYS:HB3	2.02	0.41
2:2:109:HIS:CE1	2:2:198:SER:HB3	2.56	0.41
2:2:18:ARG:NH1	2:2:249:MET:CE	2.50	0.40
2:2:192:ASN:HD21	3:3:120:CYS:HA	1.86	0.40
1:1:182:PHE:CA	3:3:21:SER:HB2	2.47	0.40
1:1:155:PRO:HG2	1:1:163:TRP:CZ2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:125:ILE:HD11	1:1:184:ILE:HD12	2.02	0.40
1:1:224:ILE:HD13	1:1:224:ILE:HG21	1.46	0.40
1:1:195:MET:SD	5:1:500:W54:H312	2.62	0.40
2:2:127:ILE:N	2:2:221:CYS:O	2.53	0.40
2:2:259:LYS:HG2	2:2:260:ASN:O	2.21	0.40
3:3:114:ARG:O	3:3:213:VAL:HA	2.22	0.40
1:1:101:ILE:CD1	1:1:218:GLY:C	2.90	0.40
1:1:34:LEU:HD23	1:1:34:LEU:HA	1.91	0.40
3:3:115:PHE:CE1	3:3:167:VAL:HG21	2.57	0.40
1:1:84:VAL:CG1	1:1:85:ASP:H	2.34	0.40
2:2:61:ASN:HD22	2:2:250:CYS:N	2.19	0.40
3:3:53:ILE:HG13	3:3:212:PHE:HA	2.03	0.40
1:1:7:ILE:C	1:1:11:LEU:HD23	2.42	0.40
1:1:197:TYR:H	2:2:131:GLN:NE2	2.12	0.40
1:1:197:TYR:HE1	2:2:217:HIS:CE1	2.40	0.40
3:3:53:ILE:HD11	3:3:213:VAL:HB	2.04	0.40
3:3:75:GLN:HE21	3:3:76:THR:H	1.69	0.40

All (2841) 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)
1:1:39:THR:N	3:3:30:PRO:CD[12_555]	0.04	2.16
1:1:25:HIS:C	1:1:223:ARG:N[12_555]	0.17	2.03
1:1:243:ALA:N	3:3:215:ALA:N[12_555]	0.21	1.99
2:2:38:TRP:CE3	2:2:210:PRO:CG[12_555]	0.26	1.94
3:3:10:SER:CB	3:3:140:GLU:CA[12_555]	0.32	1.88
3:3:38:GLY:O	3:3:38:GLY:O[12_555]	0.36	1.84
1:1:47:PRO:C	1:1:239:ILE:CG1[12_555]	0.36	1.84
1:1:10:VAL:N	1:1:277:ALA:CA[12_555]	0.37	1.83
1:1:42:THR:CB	1:1:121:PHE:O[12_555]	0.38	1.82
3:3:12:GLN:CG	3:3:187:GLY:CA[12_555]	0.39	1.81
3:3:23:CYS:C	3:3:163:ILE:N[12_555]	0.39	1.81
1:1:241:HIS:NE2	3:3:114:ARG:NH2[12_555]	0.39	1.81
1:1:73:ARG:NH2	3:3:103:ALA:CA[12_555]	0.39	1.81
3:3:118:MET:CG	4:4:34:ASP:CA[12_555]	0.39	1.81
2:2:41:TYR:CE2	2:2:41:TYR:CE2[12_555]	0.40	1.80
1:1:62:ARG:NH1	1:1:109:ILE:O[12_555]	0.40	1.80
1:1:182:PHE:N	3:3:165:LEU:CA[12_555]	0.41	1.79
1:1:14:VAL:CG1	1:1:255:ARG:C[12_555]	0.42	1.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:21:SER:CA	2:2:101:LEU:CD1[2_555]	0.43	1.77
2:2:43:THR:OG1	2:2:106:TYR:CA[12_555]	0.44	1.76
1:1:244:LYS:O	3:3:50:ASP:CA[12_555]	0.44	1.76
1:1:47:PRO:CB	1:1:239:ILE:CA[12_555]	0.46	1.74
1:1:71:LEU:N	3:3:47:CYS:SG[12_555]	0.46	1.74
1:1:72:GLY:C	3:3:99:ILE:CD1[12_555]	0.47	1.73
3:3:106:TYR:CB	3:3:224:ALA:CA[12_555]	0.48	1.72
2:2:89:MET:O	2:2:98:TYR:CD1[2_555]	0.48	1.72
1:1:23:SER:CB	1:1:80:SER:OG[12_555]	0.48	1.72
2:2:17:THR:CA	2:2:49:ALA:C[2_555]	0.48	1.72
1:1:12:ASN:O	3:3:230:HIS:N[12_555]	0.49	1.71
2:2:45:GLN:CA	2:2:107:THR:CA[12_555]	0.50	1.70
1:1:182:PHE:CG	3:3:164:SER:O[12_555]	0.50	1.70
3:3:26:PRO:C	3:3:160:GLN:O[12_555]	0.51	1.69
1:1:12:ASN:CB	3:3:229:LEU:CA[12_555]	0.51	1.69
3:3:212:PHE:CZ	4:4:35:ALA:C[12_555]	0.51	1.69
1:1:5:ASN:O	1:1:276:THR:CB[12_555]	0.52	1.68
2:2:201:LEU:CA	3:3:32:LYS:CE[12_555]	0.54	1.66
2:2:54:THR:C	2:2:57:ASP:O[3_555]	0.54	1.66
1:1:76:CYS:N	3:3:218:ASP:CG[12_555]	0.54	1.66
1:1:27:THR:O	1:1:163:TRP:CB[12_555]	0.54	1.66
1:1:126:THR:CB	3:3:167:VAL:N[12_555]	0.54	1.66
3:3:68:TYR:N	4:4:28:ASN:CA[12_555]	0.54	1.66
1:1:176:GLY:C	3:3:149:LEU:C[12_555]	0.55	1.65
3:3:69:THR:O	4:4:29:ILE:CA[12_555]	0.55	1.65
1:1:48:GLU:CD	1:1:78:HIS:CB[12_555]	0.56	1.64
2:2:89:MET:N	2:2:258:ALA:O[2_555]	0.57	1.63
1:1:75:GLY:C	3:3:218:ASP:CB[12_555]	0.57	1.63
1:1:18:PRO:C	1:1:106:MET:CB[12_555]	0.58	1.62
1:1:19:ASN:CB	1:1:106:MET:CE[12_555]	0.58	1.62
2:2:32:VAL:CB	3:3:32:LYS:C[12_555]	0.58	1.62
2:2:187:PRO:CA	3:3:33:GLU:CD[12_555]	0.59	1.61
1:1:116:PHE:CG	3:3:45:GLU:OE1[12_555]	0.59	1.61
2:2:62:ARG:CZ	2:2:101:LEU:O[2_555]	0.59	1.61
3:3:37:PRO:CG	3:3:37:PRO:CD[12_555]	0.59	1.61
2:2:46:ASP:CG	2:2:203:VAL:N[12_555]	0.60	1.60
1:1:77:VAL:O	3:3:217:LYS:NZ[12_555]	0.60	1.60
3:3:57:ASN:C	4:4:26:TYR:CA[12_555]	0.61	1.59
3:3:209:MET:CG	4:4:32:PHE:N[12_555]	0.61	1.59
2:2:54:THR:N	2:2:58:THR:N[3_555]	0.61	1.59
1:1:177:GLN:CB	3:3:148:MET:O[12_555]	0.61	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:13:GLU:OE2	3:3:231:ILE:CG1[12_555]	0.61	1.59
1:1:41:HIS:C	1:1:186:PHE:CB[12_555]	0.62	1.58
3:3:16:THR:OG1	3:3:89:ILE:CG1[12_555]	0.62	1.58
3:3:23:CYS:SG	3:3:162:THR:CB[12_555]	0.63	1.57
1:1:73:ARG:CB	3:3:219:PHE:CZ[12_555]	0.63	1.57
2:2:40:HIS:N	2:2:103:ARG:NE[12_555]	0.65	1.55
1:1:17:VAL:CA	1:1:107:ALA:O[12_555]	0.65	1.55
2:2:44:PRO:CG	2:2:247:SER:C[12_555]	0.65	1.55
1:1:42:THR:OG1	1:1:121:PHE:C[12_555]	0.66	1.54
3:3:119:PHE:C	4:4:33:LYS:CG[12_555]	0.66	1.54
1:1:63:ASP:OD1	1:1:111:ARG:CZ[12_555]	0.66	1.54
1:1:55:TYR:CB	1:1:81:ARG:NH2[12_555]	0.66	1.54
1:1:191:SER:OG	2:2:33:VAL:N[12_555]	0.66	1.54
1:1:245:HIS:CB	3:3:50:ASP:O[12_555]	0.67	1.53
2:2:18:ARG:CB	2:2:51:ASN:ND2[2_555]	0.67	1.53
3:3:119:PHE:O	4:4:33:LYS:CG[12_555]	0.67	1.53
2:2:35:TYR:CA	3:3:36:ILE:CD1[12_555]	0.68	1.52
1:1:246:THR:O	2:2:185:ILE:CD1[12_555]	0.68	1.52
1:1:181:ARG:N	3:3:165:LEU:CD1[12_555]	0.68	1.52
3:3:211:CYS:O	4:4:38:SER:CA[12_555]	0.68	1.52
1:1:67:ILE:CG2	3:3:46:MET:CG[12_555]	0.68	1.52
1:1:48:GLU:OE2	1:1:78:HIS:CB[12_555]	0.69	1.51
1:1:69:SER:OG	3:3:102:ILE:CA[12_555]	0.69	1.51
3:3:119:PHE:CA	4:4:33:LYS:CB[12_555]	0.69	1.51
3:3:11:GLY:O	3:3:134:THR:CA[12_555]	0.69	1.51
3:3:211:CYS:C	4:4:38:SER:CA[12_555]	0.69	1.51
1:1:124:GLU:CG	3:3:114:ARG:C[12_555]	0.70	1.50
1:1:71:LEU:CD2	3:3:44:ILE:CA[12_555]	0.70	1.50
3:3:106:TYR:C	3:3:223:MET:C[12_555]	0.70	1.50
3:3:16:THR:O	3:3:89:ILE:N[12_555]	0.71	1.49
1:1:128:VAL:CG2	3:3:168:PRO:CB[12_555]	0.71	1.49
2:2:88:ASP:O	2:2:259:LYS:CB[2_555]	0.71	1.49
2:2:178:THR:CB	4:4:44:ASP:CB[12_555]	0.71	1.49
3:3:9:GLY:C	3:3:188:TYR:CE1[12_555]	0.72	1.48
1:1:52:GLU:CA	1:1:237:THR:CG2[12_555]	0.73	1.47
3:3:18:ASP:N	3:3:94:LEU:CG[12_555]	0.73	1.47
1:1:12:ASN:ND2	3:3:229:LEU:CG[12_555]	0.73	1.47
1:1:64:GLU:CG	3:3:105:TYR:N[12_555]	0.73	1.47
1:1:6:TYR:O	1:1:276:THR:C[12_555]	0.74	1.46
2:2:64:TYR:CD2	2:2:256:ALA:C[2_555]	0.74	1.46
1:1:63:ASP:OD1	1:1:111:ARG:NH1[12_555]	0.74	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:179:LEU:CB	4:4:42:ARG:CG[12_555]	0.75	1.45
1:1:67:ILE:CG1	3:3:46:MET:SD[12_555]	0.75	1.45
1:1:18:PRO:CA	1:1:106:MET:CA[12_555]	0.75	1.45
2:2:62:ARG:CB	2:2:254:SER:C[2_555]	0.76	1.44
1:1:183:SER:OG	3:3:116:SER:N[12_555]	0.76	1.44
3:3:13:PHE:CB	3:3:133:TYR:CZ[12_555]	0.76	1.44
3:3:13:PHE:CD1	3:3:167:VAL:CG1[12_555]	0.77	1.43
2:2:53:PRO:C	2:2:58:THR:N[3_555]	0.77	1.43
2:2:52:LYS:NZ	2:2:252:GLU:CD[10_555]	0.77	1.43
2:2:178:THR:CG2	4:4:44:ASP:C[12_555]	0.77	1.43
1:1:76:CYS:N	3:3:218:ASP:OD1[12_555]	0.78	1.42
2:2:64:TYR:CD2	2:2:257:ARG:N[2_555]	0.78	1.42
1:1:18:PRO:N	1:1:106:MET:C[12_555]	0.79	1.41
1:1:70:PHE:CD2	3:3:43:LEU:CB[12_555]	0.79	1.41
1:1:24:HIS:O	1:1:222:SER:OG[12_555]	0.79	1.41
2:2:11:ASP:N	2:2:26:ASP:OD2[11_555]	0.79	1.41
2:2:32:VAL:CG2	3:3:31:THR:O[12_555]	0.79	1.41
3:3:67:MET:C	4:4:28:ASN:N[12_555]	0.79	1.41
1:1:53:THR:CB	1:1:237:THR:O[12_555]	0.80	1.40
1:1:250:CYS:N	3:3:39:GLU:CA[12_555]	0.80	1.40
2:2:42:LEU:O	2:2:249:MET:C[12_555]	0.80	1.40
1:1:178:PRO:CD	3:3:147:ALA:O[12_555]	0.81	1.39
3:3:26:PRO:CB	3:3:161:SER:N[12_555]	0.81	1.39
1:1:41:HIS:CD2	1:1:186:PHE:CE1[12_555]	0.81	1.39
2:2:58:THR:O	2:2:253:PHE:C[2_555]	0.81	1.39
3:3:222:ARG:N	3:3:225:ARG:O[12_555]	0.81	1.39
3:3:21:SER:C	3:3:117:PHE:CD2[12_555]	0.81	1.39
1:1:75:GLY:O	3:3:218:ASP:CB[12_555]	0.81	1.39
1:1:62:ARG:CA	3:3:105:TYR:OH[12_555]	0.82	1.38
1:1:182:PHE:CA	3:3:165:LEU:N[12_555]	0.82	1.38
2:2:38:TRP:CG	2:2:210:PRO:C[12_555]	0.82	1.38
3:3:53:ILE:CG1	4:4:39:GLY:CA[12_555]	0.82	1.38
1:1:21:LYS:O	1:1:79:ILE:C[12_555]	0.82	1.38
1:1:113:PHE:CZ	3:3:48:GLN:CD[12_555]	0.82	1.38
1:1:179:PHE:CA	3:3:151:THR:CB[12_555]	0.82	1.38
2:2:17:THR:CB	2:2:49:ALA:N[2_555]	0.82	1.38
1:1:122:ASP:CB	3:3:50:ASP:OD1[12_555]	0.82	1.38
1:1:27:THR:CG2	1:1:223:ARG:NH2[12_555]	0.83	1.37
1:1:71:LEU:CA	3:3:47:CYS:CB[12_555]	0.83	1.37
3:3:212:PHE:N	4:4:38:SER:N[12_555]	0.83	1.37
1:1:17:VAL:N	1:1:107:ALA:C[12_555]	0.84	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:36:GLY:O	2:2:208:ALA:N[12_555]	0.84	1.36
2:2:40:HIS:NE2	2:2:205:TYR:CB[12_555]	0.84	1.36
1:1:39:THR:CA	3:3:30:PRO:N[12_555]	0.84	1.36
2:2:46:ASP:O	2:2:202:ILE:CG2[12_555]	0.84	1.36
3:3:16:THR:O	3:3:89:ILE:CA[12_555]	0.84	1.36
1:1:22:GLU:CD	1:1:81:ARG:CB[12_555]	0.84	1.36
3:3:57:ASN:CA	4:4:26:TYR:C[12_555]	0.84	1.36
3:3:222:ARG:CA	3:3:225:ARG:O[12_555]	0.85	1.35
1:1:181:ARG:CA	3:3:165:LEU:CD1[12_555]	0.85	1.35
1:1:39:THR:C	3:3:30:PRO:CB[12_555]	0.85	1.35
3:3:68:TYR:O	4:4:30:ASN:ND2[12_555]	0.85	1.35
3:3:13:PHE:CE1	3:3:167:VAL:CG1[12_555]	0.85	1.35
2:2:45:GLN:NE2	2:2:246:ILE:CG2[12_555]	0.85	1.35
3:3:11:GLY:CA	3:3:134:THR:CB[12_555]	0.85	1.35
1:1:6:TYR:N	1:1:276:THR:CG2[12_555]	0.86	1.34
3:3:9:GLY:C	3:3:188:TYR:CD1[12_555]	0.86	1.34
2:2:19:GLY:O	2:2:211:MET:CE[2_555]	0.86	1.34
3:3:18:ASP:CA	3:3:94:LEU:CD2[12_555]	0.86	1.34
2:2:15:GLN:O	2:2:15:GLN:O[11_555]	0.86	1.34
1:1:64:GLU:CD	3:3:104:SER:C[12_555]	0.86	1.34
3:3:11:GLY:O	3:3:134:THR:C[12_555]	0.87	1.33
3:3:17:ASP:C	3:3:94:LEU:CD1[12_555]	0.87	1.33
1:1:68:GLU:OE2	3:3:51:THR:OG1[12_555]	0.87	1.33
1:1:22:GLU:CG	1:1:81:ARG:CA[12_555]	0.87	1.33
2:2:11:ASP:N	2:2:26:ASP:CG[11_555]	0.87	1.33
2:2:41:TYR:OH	2:2:55:GLN:OE1[12_555]	0.87	1.33
2:2:34:GLY:CA	3:3:34:ILE:O[12_555]	0.87	1.33
1:1:244:LYS:NZ	3:3:212:PHE:O[12_555]	0.87	1.33
1:1:60:GLN:CB	1:1:108:GLN:CG[12_555]	0.87	1.33
1:1:18:PRO:N	1:1:106:MET:O[12_555]	0.88	1.32
2:2:32:VAL:CB	3:3:32:LYS:O[12_555]	0.88	1.32
1:1:247:LYS:CD	2:2:185:ILE:O[12_555]	0.88	1.32
2:2:18:ARG:CD	2:2:51:ASN:CA[2_555]	0.88	1.32
1:1:115:LEU:O	3:3:41:LYS:CA[12_555]	0.89	1.31
2:2:62:ARG:NH2	2:2:101:LEU:O[2_555]	0.89	1.31
2:2:182:ASN:ND2	4:4:42:ARG:O[12_555]	0.89	1.31
1:1:251:PRO:CA	3:3:40:VAL:O[12_555]	0.89	1.31
1:1:25:HIS:CG	1:1:224:ILE:N[12_555]	0.90	1.30
1:1:49:ASP:OD1	1:1:220:ILE:CD1[12_555]	0.90	1.30
3:3:6:ILE:CD1	3:3:142:THR:CA[12_555]	0.90	1.30
1:1:14:VAL:CB	1:1:255:ARG:O[12_555]	0.90	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:19:ASN:N	1:1:106:MET:CB[12_555]	0.90	1.30
1:1:17:VAL:CA	1:1:107:ALA:C[12_555]	0.90	1.30
3:3:58:VAL:N	4:4:26:TYR:CA[12_555]	0.91	1.29
1:1:47:PRO:CG	1:1:239:ILE:O[12_555]	0.91	1.29
3:3:9:GLY:O	3:3:188:TYR:CD1[12_555]	0.91	1.29
3:3:12:GLN:CA	3:3:134:THR:O[12_555]	0.91	1.29
1:1:25:HIS:CB	1:1:223:ARG:C[12_555]	0.91	1.29
3:3:23:CYS:C	3:3:162:THR:C[12_555]	0.91	1.29
2:2:44:PRO:CB	2:2:247:SER:CB[12_555]	0.92	1.28
3:3:212:PHE:CZ	4:4:35:ALA:O[12_555]	0.92	1.28
1:1:47:PRO:N	1:1:239:ILE:CG2[12_555]	0.92	1.28
2:2:178:THR:OG1	4:4:44:ASP:CG[12_555]	0.92	1.28
2:2:43:THR:CB	2:2:105:GLY:C[12_555]	0.93	1.27
1:1:74:SER:OG	3:3:113:LEU:CA[12_555]	0.93	1.27
2:2:89:MET:CB	2:2:257:ARG:O[12_555]	0.93	1.27
1:1:241:HIS:CA	3:3:216:CYS:CB[12_555]	0.93	1.27
1:1:181:ARG:NH1	3:3:115:PHE:CE1[12_555]	0.93	1.27
2:2:178:THR:CG2	4:4:44:ASP:CA[12_555]	0.93	1.27
3:3:18:ASP:N	3:3:94:LEU:CD1[12_555]	0.93	1.27
1:1:116:PHE:CE2	3:3:42:ASN:O[12_555]	0.94	1.26
2:2:178:THR:OG1	4:4:44:ASP:CB[12_555]	0.94	1.26
2:2:52:LYS:NZ	2:2:252:GLU:CG[10_555]	0.94	1.26
1:1:249:TRP:O	3:3:39:GLU:O[12_555]	0.94	1.26
3:3:161:SER:O	4:4:34:ASP:OD2[12_555]	0.94	1.26
1:1:71:LEU:CD1	3:3:44:ILE:C[12_555]	0.94	1.26
3:3:210:LEU:N	4:4:32:PHE:O[12_555]	0.94	1.26
1:1:249:TRP:NE1	2:2:35:TYR:CD1[12_555]	0.95	1.25
1:1:5:ASN:C	1:1:276:THR:CB[12_555]	0.95	1.25
3:3:26:PRO:O	3:3:160:GLN:O[12_555]	0.95	1.25
1:1:181:ARG:C	3:3:165:LEU:CB[12_555]	0.95	1.25
3:3:6:ILE:CD1	3:3:142:THR:N[12_555]	0.95	1.25
3:3:106:TYR:C	3:3:224:ALA:N[12_555]	0.95	1.25
3:3:212:PHE:CA	4:4:38:SER:O[12_555]	0.95	1.25
1:1:183:SER:OG	3:3:115:PHE:C[12_555]	0.96	1.24
1:1:31:ALA:CB	1:1:169:MET:N[12_555]	0.96	1.24
2:2:47:ALA:O	2:2:202:ILE:CD1[12_555]	0.96	1.24
1:1:177:GLN:O	3:3:150:GLY:O[12_555]	0.97	1.23
1:1:17:VAL:CG1	1:1:108:GLN:CA[12_555]	0.97	1.23
3:3:68:TYR:O	4:4:30:ASN:CG[12_555]	0.97	1.23
2:2:40:HIS:CA	2:2:103:ARG:NE[12_555]	0.97	1.23
1:1:22:GLU:CG	1:1:81:ARG:CB[12_555]	0.97	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:44:ASN:OD1	5:1:500:W54:C2C[12_555]	0.98	1.22
1:1:13:GLU:CD	3:3:231:ILE:CD1[12_555]	0.98	1.22
2:2:11:ASP:CG	2:2:26:ASP:O[11_555]	0.98	1.22
1:1:73:ARG:CB	3:3:219:PHE:CE1[12_555]	0.98	1.22
2:2:11:ASP:OD2	2:2:26:ASP:O[11_555]	0.98	1.22
1:1:45:VAL:C	5:1:500:W54:CL1[12_555]	0.98	1.22
1:1:42:THR:CB	1:1:121:PHE:C[12_555]	0.98	1.22
1:1:240:TYR:CB	3:3:112:SER:CB[12_555]	0.98	1.22
3:3:106:TYR:CA	3:3:224:ALA:N[12_555]	0.98	1.22
3:3:23:CYS:SG	3:3:162:THR:CG2[12_555]	0.99	1.21
2:2:29:ALA:CB	3:3:29:HIS:CB[12_555]	0.99	1.21
1:1:9:GLU:CD	2:2:179:LEU:CD1[12_555]	0.99	1.21
1:1:115:LEU:O	3:3:41:LYS:CB[12_555]	0.99	1.21
1:1:66:SER:O	3:3:102:ILE:CD1[12_555]	0.99	1.21
1:1:8:ASP:OD2	1:1:258:PRO:CD[12_555]	0.99	1.21
1:1:126:THR:N	3:3:166:VAL:CB[12_555]	0.99	1.21
2:2:40:HIS:N	2:2:103:ARG:CZ[12_555]	0.99	1.21
1:1:53:THR:O	1:1:80:SER:O[12_555]	1.00	1.20
3:3:9:GLY:CA	3:3:188:TYR:CE1[12_555]	1.00	1.20
1:1:181:ARG:CB	3:3:165:LEU:CG[12_555]	1.00	1.20
2:2:178:THR:CB	4:4:44:ASP:CA[12_555]	1.00	1.20
1:1:39:THR:CA	3:3:30:PRO:CA[12_555]	1.00	1.20
1:1:247:LYS:CE	2:2:185:ILE:C[12_555]	1.00	1.20
1:1:6:TYR:C	1:1:276:THR:O[12_555]	1.00	1.20
3:3:19:MET:CG	3:3:85:ILE:CG1[12_555]	1.00	1.20
1:1:25:HIS:O	1:1:222:SER:C[12_555]	1.01	1.19
1:1:65:MET:N	3:3:105:TYR:CD2[12_555]	1.01	1.19
2:2:40:HIS:CB	2:2:103:ARG:CG[12_555]	1.01	1.19
2:2:39:PRO:CG	2:2:42:LEU:CD1[12_555]	1.01	1.19
3:3:56:ASN:OD1	4:4:29:ILE:CG2[12_555]	1.01	1.19
2:2:13:ILE:N	2:2:13:ILE:CG1[11_555]	1.01	1.19
3:3:21:SER:CA	3:3:117:PHE:CE2[12_555]	1.02	1.18
1:1:48:GLU:OE2	1:1:78:HIS:CA[12_555]	1.02	1.18
1:1:124:GLU:C	3:3:114:ARG:CG[12_555]	1.02	1.18
2:2:45:GLN:OE1	2:2:106:TYR:CB[12_555]	1.02	1.18
1:1:177:GLN:N	3:3:149:LEU:CA[12_555]	1.02	1.18
2:2:63:PHE:N	2:2:255:GLY:CA[2_555]	1.02	1.18
1:1:32:PRO:CD	1:1:147:TYR:CB[12_555]	1.02	1.18
1:1:72:GLY:CA	3:3:99:ILE:CG1[12_555]	1.02	1.18
2:2:12:ARG:N	2:2:13:ILE:CD1[11_555]	1.02	1.18
3:3:12:GLN:N	3:3:134:THR:O[12_555]	1.02	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:244:LYS:O	3:3:50:ASP:N[12_555]	1.02	1.18
3:3:67:MET:O	4:4:28:ASN:N[12_555]	1.02	1.18
3:3:66:SER:O	4:4:28:ASN:O[12_555]	1.02	1.18
1:1:28:SER:C	1:1:146:MET:CE[12_555]	1.03	1.17
2:2:194:ARG:NH1	3:3:27:TRP:CE2[12_555]	1.03	1.17
1:1:124:GLU:CB	3:3:114:ARG:C[12_555]	1.03	1.17
1:1:183:SER:CB	3:3:116:SER:CA[12_555]	1.03	1.17
1:1:178:PRO:O	3:3:151:THR:C[12_555]	1.03	1.17
1:1:45:VAL:CA	5:1:500:W54:C1B[12_555]	1.03	1.17
1:1:48:GLU:N	1:1:239:ILE:CG1[12_555]	1.04	1.16
1:1:240:TYR:CD1	3:3:112:SER:N[12_555]	1.04	1.16
1:1:5:ASN:C	1:1:276:THR:CG2[12_555]	1.04	1.16
1:1:126:THR:O	3:3:166:VAL:CG1[12_555]	1.04	1.16
1:1:247:LYS:CE	2:2:186:PHE:N[12_555]	1.04	1.16
1:1:44:ASN:C	5:1:500:W54:O1B[12_555]	1.04	1.16
2:2:91:ILE:CD1	2:2:95:ASN:CA[2_555]	1.04	1.16
1:1:182:PHE:CD1	3:3:164:SER:O[12_555]	1.04	1.16
2:2:182:ASN:OD1	4:4:41:SER:C[12_555]	1.04	1.16
1:1:113:PHE:CE1	3:3:48:GLN:NE2[12_555]	1.04	1.16
2:2:18:ARG:CA	2:2:51:ASN:ND2[2_555]	1.05	1.15
2:2:31:ALA:O	3:3:31:THR:OG1[12_555]	1.05	1.15
1:1:46:GLN:N	5:1:500:W54:CL1[12_555]	1.05	1.15
1:1:124:GLU:CA	3:3:114:ARG:CG[12_555]	1.05	1.15
1:1:10:VAL:CA	1:1:277:ALA:O[12_555]	1.05	1.15
1:1:250:CYS:N	3:3:39:GLU:C[12_555]	1.05	1.15
1:1:240:TYR:CG	3:3:112:SER:OG[12_555]	1.05	1.15
2:2:17:THR:CA	2:2:49:ALA:CA[2_555]	1.05	1.15
1:1:64:GLU:C	3:3:105:TYR:CD2[12_555]	1.05	1.15
2:2:35:TYR:C	3:3:36:ILE:CD1[12_555]	1.05	1.15
3:3:56:ASN:ND2	4:4:29:ILE:CD1[12_555]	1.05	1.15
1:1:125:ILE:O	3:3:166:VAL:N[12_555]	1.05	1.15
2:2:32:VAL:CA	3:3:32:LYS:O[12_555]	1.05	1.15
3:3:119:PHE:C	4:4:33:LYS:CB[12_555]	1.06	1.14
1:1:67:ILE:CG2	3:3:46:MET:CB[12_555]	1.06	1.14
1:1:69:SER:C	3:3:102:ILE:CG2[12_555]	1.06	1.14
2:2:41:TYR:OH	2:2:55:GLN:CD[12_555]	1.06	1.14
1:1:41:HIS:CG	1:1:186:PHE:CD1[12_555]	1.06	1.14
1:1:12:ASN:O	3:3:230:HIS:CA[12_555]	1.06	1.14
3:3:22:PRO:N	3:3:117:PHE:CD2[12_555]	1.06	1.14
1:1:19:ASN:CA	1:1:106:MET:SD[12_555]	1.06	1.14
2:2:36:GLY:O	2:2:207:ASN:C[12_555]	1.06	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:24:ALA:C	3:3:162:THR:O[12_555]	1.07	1.13
2:2:12:ARG:CA	2:2:13:ILE:CD1[11_555]	1.07	1.13
1:1:42:THR:O	1:1:193:TYR:OH[12_555]	1.07	1.13
3:3:57:ASN:CA	4:4:26:TYR:O[12_555]	1.07	1.13
1:1:124:GLU:O	3:3:114:ARG:CD[12_555]	1.07	1.13
2:2:33:VAL:CG1	3:3:34:ILE:CD1[12_555]	1.07	1.13
1:1:122:ASP:CB	3:3:50:ASP:CG[12_555]	1.07	1.13
2:2:89:MET:CG	2:2:258:ALA:N[2_555]	1.07	1.13
1:1:9:GLU:C	1:1:277:ALA:CB[12_555]	1.07	1.13
2:2:45:GLN:CA	2:2:107:THR:N[12_555]	1.07	1.13
2:2:45:GLN:N	2:2:107:THR:N[12_555]	1.07	1.13
1:1:14:VAL:CG2	1:1:256:ALA:CA[12_555]	1.07	1.13
3:3:43:LEU:CD1	3:3:43:LEU:CD1[12_555]	1.07	1.13
2:2:62:ARG:CA	2:2:255:GLY:N[2_555]	1.08	1.12
3:3:20:GLN:C	3:3:117:PHE:CE1[12_555]	1.08	1.12
2:2:43:THR:CG2	2:2:105:GLY:C[12_555]	1.08	1.12
1:1:77:VAL:CB	3:3:217:LYS:CD[12_555]	1.08	1.12
2:2:17:THR:C	2:2:50:ILE:N[2_555]	1.08	1.12
1:1:126:THR:OG1	3:3:167:VAL:N[12_555]	1.08	1.12
1:1:176:GLY:O	3:3:149:LEU:C[12_555]	1.08	1.12
2:2:58:THR:O	2:2:253:PHE:O[2_555]	1.08	1.12
3:3:38:GLY:C	3:3:38:GLY:O[12_555]	1.08	1.12
1:1:244:LYS:C	3:3:50:ASP:CA[12_555]	1.08	1.12
2:2:54:THR:O	2:2:57:ASP:O[3_555]	1.09	1.11
3:3:107:THR:CG2	3:3:223:MET:CE[12_555]	1.09	1.11
3:3:212:PHE:CE2	4:4:35:ALA:O[12_555]	1.09	1.11
1:1:44:ASN:CG	5:1:500:W54:C4C[12_555]	1.09	1.11
2:2:18:ARG:CD	2:2:51:ASN:N[2_555]	1.09	1.11
2:2:42:LEU:O	2:2:249:MET:CA[12_555]	1.09	1.11
1:1:182:PHE:C	3:3:165:LEU:N[12_555]	1.09	1.11
1:1:71:LEU:CA	3:3:47:CYS:SG[12_555]	1.09	1.11
1:1:249:TRP:CE2	2:2:35:TYR:CD1[12_555]	1.09	1.11
1:1:116:PHE:CB	3:3:45:GLU:OE2[12_555]	1.10	1.10
2:2:178:THR:O	4:4:42:ARG:NH1[12_555]	1.10	1.10
1:1:62:ARG:C	3:3:105:TYR:OH[12_555]	1.10	1.10
3:3:56:ASN:C	4:4:27:PHE:N[12_555]	1.10	1.10
2:2:41:TYR:CB	2:2:250:CYS:O[12_555]	1.10	1.10
1:1:52:GLU:CD	1:1:143:MET:CE[12_555]	1.10	1.10
1:1:244:LYS:CB	3:3:213:VAL:O[12_555]	1.10	1.10
2:2:54:THR:CA	2:2:57:ASP:C[3_555]	1.10	1.10
3:3:56:ASN:CB	4:4:29:ILE:CG1[12_555]	1.11	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:47:PRO:CB	1:1:239:ILE:C[12_555]	1.11	1.09
2:2:38:TRP:CB	2:2:210:PRO:C[12_555]	1.11	1.09
1:1:12:ASN:CA	3:3:229:LEU:O[12_555]	1.11	1.09
1:1:7:ILE:CG1	1:1:275:THR:OG1[12_555]	1.11	1.09
1:1:241:HIS:CA	3:3:216:CYS:SG[12_555]	1.11	1.09
1:1:32:PRO:N	1:1:147:TYR:CB[12_555]	1.11	1.09
3:3:119:PHE:O	4:4:33:LYS:CD[12_555]	1.11	1.09
2:2:62:ARG:NH2	2:2:101:LEU:C[2_555]	1.11	1.09
3:3:97:THR:CB	4:4:40:ALA:CB[12_555]	1.11	1.09
1:1:47:PRO:CG	1:1:239:ILE:C[12_555]	1.11	1.09
1:1:35:ASP:CB	3:3:25:LEU:CD1[12_555]	1.12	1.08
1:1:28:SER:O	1:1:146:MET:SD[12_555]	1.12	1.08
1:1:176:GLY:C	3:3:149:LEU:O[12_555]	1.12	1.08
2:2:90:GLY:C	2:2:98:TYR:CB[2_555]	1.12	1.08
3:3:23:CYS:O	3:3:162:THR:C[12_555]	1.12	1.08
1:1:247:LYS:CG	2:2:185:ILE:O[12_555]	1.12	1.08
1:1:73:ARG:CA	3:3:219:PHE:CE1[12_555]	1.12	1.08
1:1:8:ASP:CG	1:1:258:PRO:CD[12_555]	1.12	1.08
3:3:13:PHE:CB	3:3:133:TYR:CE1[12_555]	1.12	1.08
1:1:9:GLU:OE2	2:2:179:LEU:CD1[12_555]	1.12	1.08
1:1:42:THR:N	1:1:186:PHE:CB[12_555]	1.13	1.07
1:1:71:LEU:CD1	3:3:44:ILE:O[12_555]	1.13	1.07
2:2:187:PRO:N	3:3:33:GLU:OE2[12_555]	1.13	1.07
3:3:37:PRO:CG	3:3:37:PRO:CG[12_555]	1.13	1.07
3:3:67:MET:C	4:4:28:ASN:CA[12_555]	1.13	1.07
3:3:120:CYS:SG	4:4:33:LYS:O[12_555]	1.13	1.07
2:2:200:THR:O	3:3:32:LYS:CB[12_555]	1.13	1.07
3:3:58:VAL:CG2	4:4:26:TYR:CG[12_555]	1.13	1.07
2:2:38:TRP:CG	2:2:210:PRO:CA[12_555]	1.13	1.07
1:1:116:PHE:CE1	3:3:40:VAL:CG1[12_555]	1.13	1.07
2:2:46:ASP:OD1	2:2:203:VAL:N[12_555]	1.13	1.07
1:1:20:ILE:CG2	1:1:78:HIS:O[12_555]	1.13	1.07
1:1:126:THR:C	3:3:166:VAL:CG1[12_555]	1.13	1.07
1:1:39:THR:CB	3:3:30:PRO:CA[12_555]	1.13	1.07
1:1:45:VAL:N	5:1:500:W54:O1B[12_555]	1.13	1.07
3:3:13:PHE:CA	3:3:133:TYR:CE1[12_555]	1.13	1.07
3:3:26:PRO:CB	3:3:161:SER:CA[12_555]	1.13	1.07
1:1:177:GLN:CA	3:3:148:MET:C[12_555]	1.13	1.07
1:1:74:SER:CA	3:3:112:SER:O[12_555]	1.13	1.07
1:1:67:ILE:CB	3:3:46:MET:SD[12_555]	1.13	1.07
3:3:209:MET:CB	4:4:32:PHE:CA[12_555]	1.14	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:182:ASN:ND2	4:4:42:ARG:C[12_555]	1.14	1.06
1:1:62:ARG:CZ	1:1:109:ILE:C[12_555]	1.14	1.06
1:1:247:LYS:NZ	2:2:186:PHE:CA[12_555]	1.14	1.06
2:2:40:HIS:O	2:2:40:HIS:O[12_555]	1.14	1.06
3:3:13:PHE:CE2	3:3:168:PRO:O[12_555]	1.14	1.06
1:1:26:THR:N	1:1:223:ARG:N[12_555]	1.14	1.06
1:1:65:MET:SD	1:1:112:LYS:CD[12_555]	1.15	1.05
2:2:46:ASP:OD2	2:2:203:VAL:O[12_555]	1.15	1.05
1:1:52:GLU:C	1:1:237:THR:CB[12_555]	1.15	1.05
3:3:118:MET:CB	4:4:34:ASP:CA[12_555]	1.16	1.04
1:1:177:GLN:CB	3:3:148:MET:C[12_555]	1.16	1.04
2:2:62:ARG:C	2:2:255:GLY:N[2_555]	1.16	1.04
1:1:75:GLY:C	3:3:218:ASP:CG[12_555]	1.16	1.04
1:1:73:ARG:O	3:3:219:PHE:CD1[12_555]	1.16	1.04
1:1:18:PRO:CA	1:1:106:MET:C[12_555]	1.16	1.04
1:1:124:GLU:CB	3:3:114:ARG:O[12_555]	1.17	1.03
3:3:18:ASP:CA	3:3:94:LEU:CG[12_555]	1.17	1.03
1:1:62:ARG:NH2	1:1:109:ILE:CB[12_555]	1.17	1.03
1:1:10:VAL:CG2	1:1:278:ILE:N[12_555]	1.17	1.03
1:1:176:GLY:O	3:3:150:GLY:N[12_555]	1.17	1.03
1:1:48:GLU:C	1:1:239:ILE:CD1[12_555]	1.17	1.03
2:2:91:ILE:CG1	2:2:95:ASN:ND2[2_555]	1.17	1.03
1:1:17:VAL:CB	1:1:107:ALA:O[12_555]	1.17	1.03
1:1:62:ARG:NH2	1:1:109:ILE:CG1[12_555]	1.17	1.03
1:1:250:CYS:CA	3:3:39:GLU:CB[12_555]	1.17	1.03
2:2:18:ARG:CB	2:2:51:ASN:CG[2_555]	1.17	1.03
2:2:37:VAL:CA	2:2:207:ASN:O[12_555]	1.17	1.03
3:3:27:TRP:CZ3	3:3:158:GLY:O[12_555]	1.17	1.03
1:1:27:THR:CG2	1:1:223:ARG:CZ[12_555]	1.17	1.03
1:1:46:GLN:N	5:1:500:W54:C2B[12_555]	1.17	1.03
1:1:17:VAL:O	1:1:107:ALA:N[12_555]	1.17	1.03
1:1:245:HIS:CD2	3:3:51:THR:C[12_555]	1.17	1.03
1:1:124:GLU:CG	3:3:115:PHE:N[12_555]	1.17	1.03
2:2:54:THR:OG1	2:2:56:PRO:C[3_555]	1.17	1.03
2:2:43:THR:CB	2:2:106:TYR:N[12_555]	1.18	1.02
1:1:17:VAL:CG1	1:1:108:GLN:C[12_555]	1.18	1.02
2:2:38:TRP:CD2	2:2:210:PRO:CB[12_555]	1.18	1.02
1:1:64:GLU:OE1	3:3:104:SER:O[12_555]	1.18	1.02
1:1:64:GLU:CD	3:3:105:TYR:N[12_555]	1.18	1.02
1:1:23:SER:CA	1:1:80:SER:OG[12_555]	1.18	1.02
1:1:10:VAL:CB	1:1:277:ALA:O[12_555]	1.18	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:12:ASN:CA	3:3:229:LEU:C[12_555]	1.19	1.01
2:2:201:LEU:C	3:3:32:LYS:CE[12_555]	1.19	1.01
3:3:57:ASN:C	4:4:26:TYR:N[12_555]	1.19	1.01
3:3:67:MET:SD	4:4:27:PHE:CE2[12_555]	1.19	1.01
3:3:211:CYS:C	4:4:38:SER:N[12_555]	1.19	1.01
2:2:44:PRO:CD	2:2:247:SER:O[12_555]	1.19	1.01
1:1:41:HIS:CB	1:1:186:PHE:CD1[12_555]	1.19	1.01
1:1:27:THR:N	1:1:163:TRP:CE3[12_555]	1.19	1.01
2:2:178:THR:C	4:4:42:ARG:NH1[12_555]	1.19	1.01
2:2:13:ILE:O	2:2:13:ILE:CG2[11_555]	1.19	1.01
1:1:122:ASP:CG	3:3:50:ASP:OD1[12_555]	1.20	1.00
3:3:222:ARG:N	3:3:225:ARG:C[12_555]	1.20	1.00
1:1:21:LYS:CE	1:1:105:GLU:OE2[12_555]	1.20	1.00
2:2:13:ILE:N	2:2:13:ILE:CB[11_555]	1.20	1.00
3:3:209:MET:O	4:4:30:ASN:C[12_555]	1.20	1.00
3:3:26:PRO:CG	3:3:161:SER:N[12_555]	1.20	1.00
3:3:6:ILE:CG1	3:3:142:THR:CA[12_555]	1.20	1.00
2:2:46:ASP:OD2	2:2:203:VAL:C[12_555]	1.20	1.00
1:1:73:ARG:CG	3:3:219:PHE:CZ[12_555]	1.20	1.00
2:2:43:THR:CB	2:2:105:GLY:O[12_555]	1.20	1.00
3:3:58:VAL:CG2	4:4:26:TYR:CD2[12_555]	1.20	1.00
3:3:56:ASN:O	4:4:27:PHE:N[12_555]	1.20	1.00
1:1:115:LEU:CB	3:3:42:ASN:CB[12_555]	1.20	1.00
1:1:24:HIS:N	1:1:97:THR:CG2[12_555]	1.20	1.00
1:1:33:LEU:O	3:3:24:ALA:CB[12_555]	1.21	0.99
2:2:91:ILE:CD1	2:2:95:ASN:N[2_555]	1.21	0.99
1:1:251:PRO:CB	3:3:40:VAL:O[12_555]	1.21	0.99
1:1:64:GLU:OE1	3:3:104:SER:C[12_555]	1.21	0.99
2:2:47:ALA:CB	2:2:249:MET:CE[12_555]	1.21	0.99
1:1:63:ASP:CB	1:1:111:ARG:NH2[12_555]	1.21	0.99
3:3:26:PRO:CA	3:3:161:SER:N[12_555]	1.21	0.99
1:1:244:LYS:NZ	3:3:212:PHE:C[12_555]	1.21	0.99
1:1:35:ASP:CA	3:3:25:LEU:CG[12_555]	1.21	0.99
1:1:52:GLU:OE2	1:1:143:MET:CE[12_555]	1.21	0.99
2:2:39:PRO:C	2:2:103:ARG:CZ[12_555]	1.21	0.99
3:3:57:ASN:N	4:4:26:TYR:C[12_555]	1.21	0.99
1:1:44:ASN:ND2	5:1:500:W54:C4C[12_555]	1.21	0.99
1:1:63:ASP:CG	1:1:111:ARG:NH1[12_555]	1.21	0.99
2:2:44:PRO:CB	2:2:247:SER:OG[12_555]	1.22	0.98
2:2:41:TYR:CB	2:2:250:CYS:C[12_555]	1.22	0.98
3:3:24:ALA:O	3:3:162:THR:O[12_555]	1.22	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:32:VAL:CG1	3:3:33:GLU:N[12_555]	1.22	0.98
1:1:7:ILE:N	1:1:276:THR:O[12_555]	1.22	0.98
1:1:13:GLU:C	3:3:230:HIS:ND1[12_555]	1.22	0.98
2:2:187:PRO:CA	3:3:33:GLU:OE1[12_555]	1.22	0.98
2:2:91:ILE:CG1	2:2:95:ASN:CG[2_555]	1.22	0.98
1:1:25:HIS:CB	1:1:223:ARG:O[12_555]	1.22	0.98
3:3:15:THR:CA	3:3:109:TRP:CH2[12_555]	1.22	0.98
1:1:35:ASP:CA	3:3:25:LEU:CD1[12_555]	1.22	0.98
1:1:63:ASP:CG	1:1:111:ARG:CZ[12_555]	1.22	0.98
3:3:65:VAL:O	4:4:28:ASN:CG[12_555]	1.22	0.98
3:3:118:MET:O	4:4:33:LYS:N[12_555]	1.22	0.98
1:1:249:TRP:C	3:3:39:GLU:O[12_555]	1.23	0.97
3:3:67:MET:CG	4:4:27:PHE:CD2[12_555]	1.23	0.97
3:3:212:PHE:CE1	4:4:37:SER:N[12_555]	1.23	0.97
1:1:36:ALA:CB	3:3:28:TYR:CB[12_555]	1.23	0.97
1:1:181:ARG:NH1	3:3:115:PHE:CD1[12_555]	1.23	0.97
2:2:189:GLN:NE2	3:3:30:PRO:O[12_555]	1.23	0.97
1:1:69:SER:OG	3:3:102:ILE:N[12_555]	1.23	0.97
1:1:183:SER:N	3:3:164:SER:CA[12_555]	1.23	0.97
2:2:58:THR:C	2:2:253:PHE:O[2_555]	1.23	0.97
2:2:57:ASP:CG	2:2:57:ASP:OD1[11_555]	1.23	0.97
3:3:6:ILE:CG2	3:3:140:GLU:O[12_555]	1.23	0.97
1:1:65:MET:O	1:1:115:LEU:CD2[12_555]	1.24	0.96
2:2:44:PRO:CG	2:2:247:SER:CA[12_555]	1.24	0.96
2:2:179:LEU:CB	4:4:42:ARG:CD[12_555]	1.24	0.96
1:1:65:MET:CB	1:1:70:PHE:CZ[12_555]	1.24	0.96
1:1:182:PHE:N	3:3:165:LEU:CB[12_555]	1.24	0.96
2:2:38:TRP:CB	2:2:210:PRO:CA[12_555]	1.24	0.96
1:1:254:PRO:CG	4:4:43:LEU:CG[12_555]	1.24	0.96
1:1:40:GLY:N	3:3:30:PRO:CG[12_555]	1.24	0.96
1:1:62:ARG:CZ	1:1:109:ILE:O[12_555]	1.24	0.96
1:1:45:VAL:CB	1:1:125:ILE:CD1[12_555]	1.24	0.96
1:1:22:GLU:CD	1:1:81:ARG:CG[12_555]	1.24	0.96
3:3:37:PRO:CB	3:3:37:PRO:CD[12_555]	1.24	0.96
1:1:15:LEU:CB	1:1:111:ARG:CD[12_555]	1.24	0.96
2:2:17:THR:C	2:2:49:ALA:C[2_555]	1.24	0.96
3:3:70:VAL:CG1	4:4:31:TYR:CG[12_555]	1.25	0.95
1:1:177:GLN:CA	3:3:148:MET:O[12_555]	1.25	0.95
1:1:177:GLN:N	3:3:149:LEU:C[12_555]	1.25	0.95
2:2:19:GLY:CA	2:2:254:SER:OG[2_555]	1.25	0.95
2:2:18:ARG:CG	2:2:51:ASN:CB[2_555]	1.25	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:126:THR:CA	3:3:166:VAL:C[12_555]	1.25	0.95
1:1:113:PHE:CZ	3:3:48:GLN:CG[12_555]	1.25	0.95
1:1:72:GLY:CA	3:3:99:ILE:CD1[12_555]	1.25	0.95
1:1:113:PHE:CD1	3:3:48:GLN:NE2[12_555]	1.25	0.95
1:1:181:ARG:CA	3:3:165:LEU:CG[12_555]	1.25	0.95
1:1:21:LYS:O	1:1:79:ILE:CA[12_555]	1.25	0.95
1:1:66:SER:O	3:3:102:ILE:CG1[12_555]	1.25	0.95
1:1:124:GLU:CB	3:3:114:ARG:CA[12_555]	1.25	0.95
1:1:76:CYS:CA	3:3:218:ASP:OD2[12_555]	1.25	0.95
1:1:17:VAL:C	1:1:107:ALA:N[12_555]	1.25	0.95
2:2:32:VAL:CG1	3:3:32:LYS:C[12_555]	1.26	0.94
1:1:242:LYS:C	3:3:215:ALA:N[12_555]	1.26	0.94
2:2:38:TRP:CD2	2:2:210:PRO:CG[12_555]	1.26	0.94
3:3:21:SER:N	3:3:117:PHE:CE1[12_555]	1.26	0.94
3:3:107:THR:N	3:3:223:MET:O[12_555]	1.26	0.94
1:1:52:GLU:CA	1:1:237:THR:CB[12_555]	1.26	0.94
1:1:77:VAL:C	3:3:217:LYS:NZ[12_555]	1.26	0.94
3:3:57:ASN:O	4:4:26:TYR:N[12_555]	1.26	0.94
1:1:6:TYR:C	1:1:276:THR:C[12_555]	1.26	0.94
1:1:23:SER:OG	1:1:80:SER:CB[12_555]	1.26	0.94
2:2:35:TYR:CB	3:3:36:ILE:CB[12_555]	1.26	0.94
3:3:6:ILE:CG1	3:3:142:THR:N[12_555]	1.27	0.93
2:2:40:HIS:CA	2:2:103:ARG:CD[12_555]	1.27	0.93
1:1:29:ASN:O	1:1:168:ASN:CB[12_555]	1.27	0.93
3:3:24:ALA:N	3:3:163:ILE:CA[12_555]	1.27	0.93
2:2:204:PRO:CD	3:3:35:SER:O[12_555]	1.27	0.93
1:1:27:THR:CB	1:1:223:ARG:NE[12_555]	1.27	0.93
1:1:53:THR:CA	1:1:237:THR:C[12_555]	1.27	0.93
2:2:57:ASP:OD1	2:2:57:ASP:OD2[11_555]	1.27	0.93
1:1:6:TYR:O	1:1:276:THR:O[12_555]	1.27	0.93
1:1:48:GLU:CA	1:1:239:ILE:CD1[12_555]	1.27	0.93
1:1:191:SER:CB	2:2:33:VAL:O[12_555]	1.27	0.93
1:1:10:VAL:CA	1:1:277:ALA:C[12_555]	1.27	0.93
1:1:42:THR:OG1	1:1:122:ASP:N[12_555]	1.27	0.93
1:1:241:HIS:O	3:3:216:CYS:N[12_555]	1.27	0.93
1:1:249:TRP:NE1	2:2:35:TYR:CE1[12_555]	1.27	0.93
1:1:25:HIS:O	1:1:222:SER:O[12_555]	1.28	0.92
1:1:126:THR:N	3:3:166:VAL:CA[12_555]	1.28	0.92
1:1:113:PHE:CE1	3:3:48:GLN:CD[12_555]	1.28	0.92
1:1:49:ASP:C	5:1:500:W54:C4A[12_555]	1.28	0.92
1:1:49:ASP:OD1	1:1:220:ILE:CG1[12_555]	1.28	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:71:LEU:C	3:3:47:CYS:CB[12_555]	1.28	0.92
1:1:18:PRO:C	1:1:106:MET:CA[12_555]	1.28	0.92
2:2:46:ASP:CB	2:2:203:VAL:N[12_555]	1.28	0.92
1:1:14:VAL:CG1	1:1:256:ALA:N[12_555]	1.28	0.92
3:3:69:THR:C	4:4:30:ASN:N[12_555]	1.28	0.92
3:3:27:TRP:CZ3	3:3:158:GLY:C[12_555]	1.28	0.92
1:1:112:LYS:O	3:3:42:ASN:ND2[12_555]	1.28	0.92
1:1:183:SER:CB	3:3:116:SER:CB[12_555]	1.28	0.92
1:1:44:ASN:ND2	5:1:500:W54:C5C[12_555]	1.28	0.92
2:2:46:ASP:C	2:2:202:ILE:CG2[12_555]	1.28	0.92
1:1:13:GLU:OE2	3:3:231:ILE:CD1[12_555]	1.28	0.92
1:1:52:GLU:N	1:1:237:THR:CB[12_555]	1.28	0.92
1:1:126:THR:CG2	3:3:167:VAL:CA[12_555]	1.29	0.91
1:1:52:GLU:C	1:1:237:THR:CA[12_555]	1.29	0.91
2:2:187:PRO:CB	3:3:33:GLU:CG[12_555]	1.29	0.91
1:1:25:HIS:C	1:1:222:SER:C[12_555]	1.29	0.91
1:1:29:ASN:N	1:1:162:SER:O[12_555]	1.29	0.91
2:2:89:MET:C	2:2:98:TYR:CD1[2_555]	1.29	0.91
1:1:12:ASN:CB	3:3:229:LEU:C[12_555]	1.29	0.91
1:1:18:PRO:CB	1:1:106:MET:N[12_555]	1.29	0.91
1:1:244:LYS:CB	3:3:213:VAL:C[12_555]	1.29	0.91
3:3:212:PHE:CD1	4:4:37:SER:N[12_555]	1.29	0.91
1:1:116:PHE:CB	3:3:45:GLU:CD[12_555]	1.29	0.91
1:1:12:ASN:C	3:3:230:HIS:N[12_555]	1.29	0.91
3:3:26:PRO:CA	3:3:161:SER:CA[12_555]	1.29	0.91
1:1:45:VAL:C	5:1:500:W54:C2B[12_555]	1.29	0.91
1:1:13:GLU:CG	3:3:231:ILE:N[12_555]	1.29	0.91
1:1:124:GLU:CA	3:3:114:ARG:CB[12_555]	1.29	0.91
2:2:62:ARG:C	2:2:255:GLY:CA[2_555]	1.29	0.91
1:1:67:ILE:CA	3:3:46:MET:CE[12_555]	1.29	0.91
2:2:36:GLY:CA	2:2:208:ALA:CA[12_555]	1.30	0.90
2:2:44:PRO:CG	2:2:247:SER:O[12_555]	1.30	0.90
1:1:53:THR:CA	1:1:237:THR:O[12_555]	1.30	0.90
2:2:204:PRO:CG	3:3:35:SER:O[12_555]	1.30	0.90
1:1:243:ALA:CB	3:3:48:GLN:CA[12_555]	1.30	0.90
1:1:47:PRO:O	1:1:239:ILE:CG1[12_555]	1.30	0.90
1:1:65:MET:CG	1:1:70:PHE:CE1[12_555]	1.30	0.90
1:1:126:THR:CB	3:3:166:VAL:C[12_555]	1.30	0.90
1:1:242:LYS:C	3:3:214:SER:C[12_555]	1.30	0.90
2:2:46:ASP:N	2:2:106:TYR:O[12_555]	1.30	0.90
1:1:240:TYR:CA	3:3:112:SER:CB[12_555]	1.30	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:41:HIS:CA	1:1:186:PHE:CB[12_555]	1.30	0.90
1:1:8:ASP:OD2	1:1:258:PRO:N[12_555]	1.30	0.90
1:1:71:LEU:CD1	3:3:45:GLU:N[12_555]	1.30	0.90
1:1:73:ARG:NH2	3:3:103:ALA:CB[12_555]	1.31	0.89
2:2:45:GLN:C	2:2:107:THR:CA[12_555]	1.31	0.89
1:1:23:SER:CB	1:1:80:SER:CB[12_555]	1.31	0.89
3:3:67:MET:CA	4:4:27:PHE:O[12_555]	1.31	0.89
1:1:125:ILE:C	3:3:166:VAL:CA[12_555]	1.31	0.89
1:1:125:ILE:O	3:3:165:LEU:C[12_555]	1.31	0.89
3:3:51:THR:CG2	4:4:41:SER:OG[12_555]	1.31	0.89
1:1:69:SER:CB	3:3:102:ILE:CA[12_555]	1.31	0.89
1:1:42:THR:CA	1:1:121:PHE:O[12_555]	1.31	0.89
1:1:254:PRO:CG	4:4:43:LEU:CD1[12_555]	1.31	0.89
1:1:62:ARG:NH1	1:1:109:ILE:C[12_555]	1.32	0.88
1:1:250:CYS:N	3:3:39:GLU:N[12_555]	1.32	0.88
1:1:244:LYS:CE	3:3:212:PHE:C[12_555]	1.32	0.88
3:3:17:ASP:OD2	3:3:87:VAL:CB[12_555]	1.32	0.88
1:1:10:VAL:CG2	1:1:278:ILE:CA[12_555]	1.32	0.88
1:1:68:GLU:CG	3:3:98:LEU:CB[12_555]	1.32	0.88
2:2:41:TYR:CZ	2:2:55:GLN:OE1[12_555]	1.32	0.88
1:1:47:PRO:CD	1:1:239:ILE:CG2[12_555]	1.32	0.88
3:3:67:MET:N	4:4:28:ASN:CB[12_555]	1.32	0.88
2:2:182:ASN:CG	4:4:42:ARG:O[12_555]	1.32	0.88
1:1:73:ARG:C	3:3:219:PHE:CD1[12_555]	1.32	0.88
3:3:17:ASP:OD2	3:3:87:VAL:CA[12_555]	1.32	0.88
2:2:89:MET:CG	2:2:257:ARG:C[2_555]	1.32	0.88
2:2:38:TRP:CZ3	2:2:210:PRO:CG[12_555]	1.33	0.87
1:1:17:VAL:C	1:1:106:MET:C[12_555]	1.33	0.87
2:2:32:VAL:CG1	3:3:33:GLU:CA[12_555]	1.33	0.87
3:3:105:TYR:O	3:3:106:TYR:CD1[12_555]	1.33	0.87
2:2:13:ILE:CA	2:2:13:ILE:CB[11_555]	1.33	0.87
3:3:223:MET:N	3:3:225:ARG:CG[12_555]	1.33	0.87
2:2:17:THR:CG2	2:2:48:THR:C[2_555]	1.33	0.87
1:1:74:SER:OG	3:3:113:LEU:N[12_555]	1.33	0.87
1:1:31:ALA:CB	1:1:169:MET:CA[12_555]	1.33	0.87
1:1:49:ASP:O	5:1:500:W54:C4A[12_555]	1.33	0.87
1:1:177:GLN:C	3:3:150:GLY:O[12_555]	1.33	0.87
1:1:71:LEU:CG	3:3:44:ILE:O[12_555]	1.33	0.87
1:1:30:SER:OG	1:1:149:PRO:CD[12_555]	1.33	0.87
3:3:23:CYS:CA	3:3:163:ILE:N[12_555]	1.34	0.86
1:1:65:MET:SD	1:1:112:LYS:CE[12_555]	1.34	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:50:ILE:CG1	2:2:50:ILE:CG1[10_555]	1.34	0.86
2:2:52:LYS:NZ	2:2:252:GLU:OE1[10_555]	1.34	0.86
1:1:10:VAL:N	1:1:277:ALA:CB[12_555]	1.34	0.86
2:2:62:ARG:CB	2:2:254:SER:CA[2_555]	1.34	0.86
1:1:250:CYS:CA	3:3:39:GLU:CA[12_555]	1.34	0.86
1:1:240:TYR:CZ	3:3:169:TRP:CB[12_555]	1.34	0.86
2:2:47:ALA:CA	2:2:249:MET:CE[12_555]	1.34	0.86
2:2:38:TRP:CE3	2:2:210:PRO:CD[12_555]	1.34	0.86
1:1:126:THR:CA	3:3:166:VAL:CA[12_555]	1.34	0.86
1:1:23:SER:N	1:1:80:SER:CA[12_555]	1.34	0.86
1:1:124:GLU:C	3:3:114:ARG:CB[12_555]	1.34	0.86
1:1:116:PHE:CD1	3:3:40:VAL:CG1[12_555]	1.34	0.86
3:3:222:ARG:CA	3:3:225:ARG:C[12_555]	1.34	0.86
1:1:38:GLU:C	3:3:30:PRO:CD[12_555]	1.34	0.86
2:2:37:VAL:CG2	2:2:207:ASN:N[12_555]	1.34	0.86
3:3:107:THR:N	3:3:223:MET:C[12_555]	1.34	0.86
3:3:56:ASN:CG	4:4:29:ILE:CD1[12_555]	1.35	0.85
3:3:212:PHE:CZ	4:4:36:ALA:N[12_555]	1.35	0.85
1:1:245:HIS:CG	3:3:50:ASP:O[12_555]	1.35	0.85
2:2:46:ASP:CG	2:2:203:VAL:CA[12_555]	1.35	0.85
1:1:25:HIS:O	1:1:223:ARG:N[12_555]	1.35	0.85
3:3:16:THR:CB	3:3:89:ILE:CG1[12_555]	1.35	0.85
1:1:6:TYR:O	1:1:277:ALA:N[12_555]	1.35	0.85
1:1:53:THR:CG2	1:1:80:SER:N[12_555]	1.35	0.85
1:1:191:SER:OG	2:2:33:VAL:CA[12_555]	1.35	0.85
1:1:76:CYS:CA	3:3:218:ASP:CG[12_555]	1.35	0.85
2:2:44:PRO:O	2:2:107:THR:CB[12_555]	1.35	0.85
1:1:5:ASN:O	1:1:276:THR:CA[12_555]	1.35	0.85
1:1:5:ASN:ND2	2:2:173:LEU:CD1[12_555]	1.35	0.85
3:3:20:GLN:CD	3:3:211:CYS:SG[12_555]	1.35	0.85
3:3:18:ASP:CB	3:3:94:LEU:CD2[12_555]	1.35	0.85
1:1:48:GLU:N	1:1:239:ILE:CB[12_555]	1.36	0.84
3:3:222:ARG:O	3:3:225:ARG:N[12_555]	1.36	0.84
3:3:20:GLN:O	3:3:117:PHE:CZ[12_555]	1.36	0.84
1:1:30:SER:C	1:1:147:TYR:O[12_555]	1.36	0.84
2:2:53:PRO:CB	2:2:58:THR:OG1[3_555]	1.36	0.84
1:1:178:PRO:C	3:3:151:THR:C[12_555]	1.36	0.84
3:3:26:PRO:C	3:3:160:GLN:C[12_555]	1.36	0.84
1:1:47:PRO:CA	1:1:239:ILE:CA[12_555]	1.36	0.84
1:1:241:HIS:N	3:3:216:CYS:CB[12_555]	1.36	0.84
1:1:12:ASN:CG	3:3:229:LEU:CB[12_555]	1.36	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:14:VAL:CB	1:1:255:ARG:C[12_555]	1.36	0.84
1:1:176:GLY:C	3:3:149:LEU:CA[12_555]	1.36	0.84
1:1:12:ASN:ND2	3:3:229:LEU:CB[12_555]	1.36	0.84
1:1:52:GLU:O	1:1:237:THR:N[12_555]	1.36	0.84
2:2:54:THR:C	2:2:57:ASP:C[3_555]	1.36	0.84
1:1:71:LEU:CB	3:3:47:CYS:CB[12_555]	1.36	0.84
1:1:10:VAL:N	1:1:277:ALA:C[12_555]	1.36	0.84
2:2:43:THR:OG1	2:2:106:TYR:N[12_555]	1.36	0.84
1:1:23:SER:N	1:1:80:SER:C[12_555]	1.36	0.84
1:1:116:PHE:CD2	3:3:45:GLU:OE1[12_555]	1.37	0.83
2:2:187:PRO:CA	3:3:33:GLU:OE2[12_555]	1.37	0.83
2:2:17:THR:N	2:2:49:ALA:C[2_555]	1.37	0.83
1:1:35:ASP:N	3:3:25:LEU:CB[12_555]	1.37	0.83
1:1:68:GLU:CG	3:3:98:LEU:CA[12_555]	1.37	0.83
2:2:17:THR:CG2	2:2:48:THR:O[2_555]	1.37	0.83
1:1:12:ASN:C	3:3:229:LEU:C[12_555]	1.37	0.83
1:1:6:TYR:CZ	3:3:62:VAL:CG1[12_555]	1.37	0.83
2:2:36:GLY:C	2:2:208:ALA:CA[12_555]	1.37	0.83
1:1:69:SER:CB	3:3:102:ILE:N[12_555]	1.37	0.83
1:1:181:ARG:C	3:3:165:LEU:CA[12_555]	1.37	0.83
1:1:250:CYS:CA	3:3:39:GLU:CG[12_555]	1.37	0.83
3:3:57:ASN:N	4:4:27:PHE:N[12_555]	1.37	0.83
2:2:54:THR:N	2:2:57:ASP:C[3_555]	1.37	0.83
1:1:25:HIS:CE1	1:1:224:ILE:CG2[12_555]	1.37	0.83
2:2:179:LEU:CA	4:4:42:ARG:NE[12_555]	1.37	0.83
1:1:179:PHE:CD2	3:3:133:TYR:CD2[12_555]	1.37	0.83
1:1:53:THR:N	1:1:237:THR:CA[12_555]	1.37	0.83
3:3:11:GLY:C	3:3:134:THR:C[12_555]	1.37	0.83
2:2:201:LEU:C	3:3:32:LYS:NZ[12_555]	1.37	0.83
1:1:171:ILE:CD1	3:3:153:VAL:CG2[12_555]	1.37	0.83
3:3:211:CYS:O	4:4:38:SER:C[12_555]	1.38	0.82
2:2:43:THR:CG2	2:2:105:GLY:CA[12_555]	1.38	0.82
1:1:246:THR:CA	3:3:49:VAL:CB[12_555]	1.38	0.82
1:1:63:ASP:CG	1:1:111:ARG:NH2[12_555]	1.38	0.82
1:1:73:ARG:CZ	3:3:103:ALA:CB[12_555]	1.38	0.82
2:2:89:MET:CA	2:2:258:ALA:O[2_555]	1.38	0.82
3:3:70:VAL:CG1	4:4:31:TYR:CB[12_555]	1.38	0.82
1:1:177:GLN:O	3:3:150:GLY:C[12_555]	1.38	0.82
2:2:62:ARG:CB	2:2:255:GLY:N[2_555]	1.38	0.82
2:2:43:THR:CG2	2:2:106:TYR:N[12_555]	1.38	0.82
3:3:21:SER:C	3:3:117:PHE:CG[12_555]	1.38	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:21:LYS:O	1:1:79:ILE:O[12_555]	1.38	0.82
1:1:23:SER:OG	1:1:80:SER:OG[12_555]	1.38	0.82
1:1:116:PHE:CB	3:3:45:GLU:OE1[12_555]	1.38	0.82
1:1:47:PRO:CA	1:1:239:ILE:CB[12_555]	1.38	0.82
1:1:71:LEU:CG	3:3:44:ILE:C[12_555]	1.39	0.81
3:3:106:TYR:CA	3:3:223:MET:C[12_555]	1.39	0.81
2:2:17:THR:CB	2:2:49:ALA:CA[2_555]	1.39	0.81
1:1:48:GLU:CD	1:1:78:HIS:CG[12_555]	1.39	0.81
1:1:69:SER:CA	3:3:102:ILE:CB[12_555]	1.39	0.81
1:1:44:ASN:CB	5:1:500:W54:C4C[12_555]	1.39	0.81
2:2:32:VAL:CG2	3:3:31:THR:C[12_555]	1.39	0.81
1:1:43:SER:O	1:1:123:SER:OG[12_555]	1.39	0.81
1:1:124:GLU:OE2	3:3:115:PHE:CG[12_555]	1.39	0.81
1:1:247:LYS:CE	2:2:185:ILE:O[12_555]	1.39	0.81
3:3:209:MET:O	4:4:30:ASN:O[12_555]	1.39	0.81
1:1:252:ARG:CB	3:3:41:LYS:CD[12_555]	1.39	0.81
1:1:182:PHE:N	3:3:165:LEU:N[12_555]	1.39	0.81
1:1:49:ASP:N	1:1:239:ILE:CD1[12_555]	1.40	0.80
3:3:26:PRO:O	3:3:160:GLN:C[12_555]	1.40	0.80
1:1:44:ASN:O	5:1:500:W54:O1B[12_555]	1.40	0.80
2:2:41:TYR:CD2	2:2:41:TYR:CZ[12_555]	1.40	0.80
2:2:179:LEU:N	4:4:42:ARG:NH1[12_555]	1.40	0.80
2:2:90:GLY:O	2:2:98:TYR:CB[2_555]	1.40	0.80
1:1:50:ALA:CB	1:1:127:LEU:CD2[12_555]	1.40	0.80
1:1:126:THR:CG2	3:3:167:VAL:N[12_555]	1.40	0.80
1:1:45:VAL:CG1	1:1:125:ILE:CD1[12_555]	1.40	0.80
1:1:65:MET:CE	1:1:112:LYS:CE[12_555]	1.40	0.80
1:1:27:THR:O	1:1:163:TRP:CG[12_555]	1.40	0.80
1:1:41:HIS:NE2	3:3:31:THR:CG2[12_555]	1.40	0.80
3:3:24:ALA:CA	3:3:162:THR:O[12_555]	1.40	0.80
1:1:10:VAL:CB	1:1:277:ALA:C[12_555]	1.41	0.79
2:2:41:TYR:CE2	2:2:41:TYR:CZ[12_555]	1.41	0.79
1:1:54:ARG:CB	1:1:236:THR:OG1[12_555]	1.41	0.79
1:1:51:ILE:C	1:1:237:THR:OG1[12_555]	1.41	0.79
1:1:21:LYS:C	1:1:79:ILE:O[12_555]	1.41	0.79
1:1:62:ARG:CZ	1:1:109:ILE:CA[12_555]	1.41	0.79
3:3:24:ALA:N	3:3:163:ILE:N[12_555]	1.41	0.79
2:2:40:HIS:CB	2:2:103:ARG:CD[12_555]	1.41	0.79
2:2:187:PRO:CG	3:3:33:GLU:OE2[12_555]	1.41	0.79
3:3:19:MET:SD	3:3:85:ILE:CG1[12_555]	1.41	0.79
1:1:243:ALA:N	3:3:214:SER:C[12_555]	1.41	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:9:GLU:CB	1:1:276:THR:OG1[12_555]	1.42	0.78
2:2:31:ALA:O	3:3:31:THR:CB[12_555]	1.42	0.78
1:1:251:PRO:N	3:3:40:VAL:O[12_555]	1.42	0.78
3:3:19:MET:CG	3:3:85:ILE:CD1[12_555]	1.42	0.78
3:3:106:TYR:CB	3:3:224:ALA:CB[12_555]	1.42	0.78
3:3:106:TYR:O	3:3:224:ALA:N[12_555]	1.42	0.78
1:1:52:GLU:N	1:1:237:THR:OG1[12_555]	1.42	0.78
2:2:38:TRP:CH2	2:2:48:THR:CG2[12_555]	1.42	0.78
1:1:39:THR:CA	3:3:30:PRO:CD[12_555]	1.42	0.78
3:3:69:THR:O	4:4:29:ILE:C[12_555]	1.42	0.78
2:2:91:ILE:CD1	2:2:95:ASN:CB[2_555]	1.42	0.78
3:3:209:MET:CG	4:4:31:TYR:C[12_555]	1.42	0.78
1:1:245:HIS:NE2	3:3:51:THR:O[12_555]	1.42	0.78
3:3:222:ARG:C	3:3:225:ARG:CG[12_555]	1.42	0.78
1:1:252:ARG:CG	3:3:41:LYS:CD[12_555]	1.42	0.78
3:3:66:SER:O	4:4:28:ASN:C[12_555]	1.42	0.78
1:1:48:GLU:N	1:1:239:ILE:CD1[12_555]	1.43	0.77
1:1:22:GLU:OE1	1:1:81:ARG:CB[12_555]	1.43	0.77
1:1:49:ASP:CB	5:1:500:W54:N3A[12_555]	1.43	0.77
2:2:90:GLY:N	2:2:98:TYR:CA[2_555]	1.43	0.77
3:3:69:THR:C	4:4:29:ILE:C[12_555]	1.43	0.77
1:1:247:LYS:CD	2:2:185:ILE:C[12_555]	1.43	0.77
2:2:20:ASP:OD2	2:2:103:ARG:N[2_555]	1.43	0.77
1:1:64:GLU:CG	3:3:104:SER:C[12_555]	1.43	0.77
1:1:50:ALA:CA	1:1:127:LEU:CD2[12_555]	1.43	0.77
1:1:249:TRP:CE2	2:2:35:TYR:CE1[12_555]	1.43	0.77
3:3:10:SER:OG	3:3:140:GLU:CA[12_555]	1.43	0.77
1:1:52:GLU:C	1:1:237:THR:N[12_555]	1.43	0.77
2:2:11:ASP:O	2:2:26:ASP:OD1[11_555]	1.43	0.77
1:1:72:GLY:O	3:3:99:ILE:CD1[12_555]	1.43	0.77
3:3:20:GLN:NE2	3:3:211:CYS:SG[12_555]	1.43	0.77
2:2:17:THR:O	2:2:50:ILE:N[2_555]	1.43	0.77
1:1:28:SER:O	1:1:146:MET:CE[12_555]	1.43	0.77
1:1:29:ASN:N	1:1:146:MET:CE[12_555]	1.43	0.77
2:2:37:VAL:N	2:2:207:ASN:O[12_555]	1.43	0.77
1:1:68:GLU:CB	3:3:98:LEU:CG[12_555]	1.44	0.76
1:1:70:PHE:CG	3:3:43:LEU:CB[12_555]	1.44	0.76
1:1:244:LYS:CD	3:3:213:VAL:N[12_555]	1.44	0.76
1:1:245:HIS:CG	3:3:50:ASP:C[12_555]	1.44	0.76
1:1:182:PHE:CB	3:3:164:SER:C[12_555]	1.44	0.76
1:1:69:SER:O	3:3:102:ILE:CG2[12_555]	1.44	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:58:VAL:CG2	4:4:26:TYR:CD1[12_555]	1.44	0.76
2:2:89:MET:O	2:2:98:TYR:CG[2_555]	1.44	0.76
1:1:74:SER:OG	3:3:113:LEU:CB[12_555]	1.44	0.76
1:1:245:HIS:CD2	3:3:51:THR:CA[12_555]	1.44	0.76
2:2:62:ARG:NH1	2:2:101:LEU:O[2_555]	1.44	0.76
1:1:245:HIS:CB	3:3:50:ASP:C[12_555]	1.44	0.76
3:3:10:SER:CB	3:3:140:GLU:CB[12_555]	1.44	0.76
3:3:211:CYS:O	4:4:38:SER:CB[12_555]	1.44	0.76
2:2:89:MET:SD	2:2:257:ARG:CD[2_555]	1.44	0.76
2:2:250:CYS:SG	2:2:252:GLU:OE1[12_555]	1.44	0.76
1:1:245:HIS:N	3:3:51:THR:N[12_555]	1.44	0.76
3:3:67:MET:CE	4:4:27:PHE:CE2[12_555]	1.44	0.76
2:2:181:GLY:O	4:4:41:SER:CB[12_555]	1.44	0.76
2:2:17:THR:CA	2:2:49:ALA:O[2_555]	1.44	0.76
1:1:22:GLU:OE1	1:1:81:ARG:CG[12_555]	1.44	0.76
2:2:42:LEU:N	2:2:250:CYS:CB[12_555]	1.44	0.76
3:3:7:THR:O	3:3:140:GLU:N[12_555]	1.44	0.76
1:1:249:TRP:C	3:3:39:GLU:C[12_555]	1.45	0.75
1:1:32:PRO:CA	1:1:147:TYR:CG[12_555]	1.45	0.75
2:2:64:TYR:CB	2:2:257:ARG:CG[2_555]	1.45	0.75
2:2:29:ALA:CB	3:3:29:HIS:CA[12_555]	1.45	0.75
1:1:112:LYS:C	3:3:44:ILE:CG2[12_555]	1.45	0.75
2:2:34:GLY:CA	3:3:34:ILE:C[12_555]	1.45	0.75
1:1:14:VAL:O	1:1:255:ARG:CG[12_555]	1.45	0.75
2:2:179:LEU:CA	4:4:42:ARG:CZ[12_555]	1.45	0.75
2:2:47:ALA:C	2:2:202:ILE:CD1[12_555]	1.45	0.75
1:1:241:HIS:C	3:3:216:CYS:N[12_555]	1.45	0.75
3:3:26:PRO:CA	3:3:160:GLN:C[12_555]	1.45	0.75
1:1:20:ILE:CD1	1:1:77:VAL:N[12_555]	1.45	0.75
1:1:242:LYS:CA	3:3:215:ALA:CA[12_555]	1.45	0.75
2:2:18:ARG:NE	2:2:51:ASN:N[2_555]	1.45	0.75
3:3:209:MET:CB	4:4:32:PHE:N[12_555]	1.45	0.75
2:2:46:ASP:OD2	2:2:203:VAL:CA[12_555]	1.46	0.74
3:3:21:SER:O	3:3:117:PHE:N[12_555]	1.46	0.74
3:3:209:MET:CG	4:4:32:PHE:CA[12_555]	1.46	0.74
2:2:89:MET:N	2:2:258:ALA:C[2_555]	1.46	0.74
2:2:17:THR:CB	2:2:48:THR:C[2_555]	1.46	0.74
3:3:11:GLY:C	3:3:134:THR:CA[12_555]	1.46	0.74
1:1:22:GLU:CG	1:1:81:ARG:N[12_555]	1.46	0.74
2:2:45:GLN:CA	2:2:107:THR:C[12_555]	1.46	0.74
2:2:17:THR:O	2:2:50:ILE:CA[2_555]	1.46	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:12:ASN:C	3:3:230:HIS:CA[12_555]	1.46	0.74
2:2:18:ARG:NE	2:2:50:ILE:C[2_555]	1.46	0.74
3:3:69:THR:CA	4:4:30:ASN:N[12_555]	1.46	0.74
1:1:113:PHE:CE2	3:3:48:GLN:OE1[12_555]	1.46	0.74
1:1:179:PHE:CA	3:3:151:THR:CG2[12_555]	1.46	0.74
3:3:22:PRO:CG	3:3:131:LEU:CD2[12_555]	1.46	0.74
2:2:44:PRO:N	2:2:247:SER:O[12_555]	1.46	0.74
3:3:70:VAL:CG1	4:4:31:TYR:CD1[12_555]	1.47	0.73
1:1:52:GLU:C	1:1:237:THR:CG2[12_555]	1.47	0.73
1:1:41:HIS:CA	1:1:186:PHE:CG[12_555]	1.47	0.73
1:1:246:THR:CG2	3:3:46:MET:O[12_555]	1.47	0.73
1:1:35:ASP:CA	3:3:25:LEU:CB[12_555]	1.47	0.73
1:1:10:VAL:CG2	1:1:277:ALA:C[12_555]	1.47	0.73
2:2:11:ASP:CB	2:2:26:ASP:O[11_555]	1.47	0.73
1:1:13:GLU:OE2	3:3:231:ILE:CB[12_555]	1.47	0.73
1:1:125:ILE:O	3:3:166:VAL:CA[12_555]	1.47	0.73
3:3:17:ASP:CA	3:3:94:LEU:CD1[12_555]	1.47	0.73
3:3:21:SER:CA	3:3:117:PHE:CD2[12_555]	1.47	0.73
1:1:36:ALA:CB	3:3:28:TYR:CA[12_555]	1.47	0.73
1:1:45:VAL:O	5:1:500:W54:CL1[12_555]	1.47	0.73
1:1:240:TYR:CE2	3:3:169:TRP:CB[12_555]	1.47	0.73
1:1:177:GLN:CG	3:3:148:MET:CG[12_555]	1.47	0.73
1:1:17:VAL:C	1:1:106:MET:O[12_555]	1.48	0.72
3:3:118:MET:C	4:4:34:ASP:N[12_555]	1.48	0.72
3:3:22:PRO:O	3:3:163:ILE:O[12_555]	1.48	0.72
1:1:244:LYS:N	3:3:214:SER:CA[12_555]	1.48	0.72
3:3:118:MET:CB	4:4:34:ASP:C[12_555]	1.48	0.72
2:2:34:GLY:N	3:3:34:ILE:CG1[12_555]	1.48	0.72
1:1:45:VAL:CA	5:1:500:W54:C2B[12_555]	1.48	0.72
1:1:15:LEU:O	1:1:111:ARG:CB[12_555]	1.48	0.72
2:2:187:PRO:C	3:3:33:GLU:OE1[12_555]	1.48	0.72
3:3:16:THR:OG1	3:3:89:ILE:CD1[12_555]	1.48	0.72
2:2:62:ARG:CD	2:2:99:HIS:CB[2_555]	1.48	0.72
1:1:60:GLN:CB	1:1:108:GLN:CD[12_555]	1.48	0.72
2:2:59:SER:OG	2:2:253:PHE:CD2[2_555]	1.48	0.72
1:1:23:SER:N	1:1:81:ARG:N[12_555]	1.48	0.72
2:2:90:GLY:CA	2:2:98:TYR:CB[2_555]	1.48	0.72
1:1:183:SER:OG	3:3:116:SER:CA[12_555]	1.48	0.72
3:3:70:VAL:CG2	4:4:31:TYR:CD2[12_555]	1.48	0.72
2:2:38:TRP:CD1	2:2:210:PRO:O[12_555]	1.48	0.72
1:1:125:ILE:CA	3:3:166:VAL:CG2[12_555]	1.48	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:15:LEU:CD2	1:1:255:ARG:N[12_555]	1.48	0.72
1:1:116:PHE:CG	3:3:45:GLU:CD[12_555]	1.48	0.72
1:1:48:GLU:CG	1:1:78:HIS:CD2[12_555]	1.48	0.72
1:1:12:ASN:CB	3:3:229:LEU:CB[12_555]	1.49	0.71
1:1:9:GLU:OE1	2:2:179:LEU:CD1[12_555]	1.49	0.71
2:2:64:TYR:CE1	2:2:98:TYR:O[2_555]	1.49	0.71
1:1:14:VAL:CG1	1:1:255:ARG:O[12_555]	1.49	0.71
1:1:44:ASN:CG	5:1:500:W54:C3C[12_555]	1.49	0.71
1:1:61:THR:CG2	3:3:230:HIS:CB[12_555]	1.49	0.71
1:1:67:ILE:CD1	3:3:46:MET:SD[12_555]	1.49	0.71
3:3:11:GLY:CA	3:3:134:THR:OG1[12_555]	1.49	0.71
1:1:18:PRO:C	1:1:106:MET:CG[12_555]	1.49	0.71
1:1:120:ARG:O	3:3:49:VAL:CG2[12_555]	1.49	0.71
2:2:36:GLY:O	2:2:208:ALA:CA[12_555]	1.49	0.71
1:1:178:PRO:C	3:3:151:THR:O[12_555]	1.49	0.71
2:2:179:LEU:N	4:4:42:ARG:CZ[12_555]	1.49	0.71
1:1:112:LYS:O	3:3:44:ILE:CG2[12_555]	1.49	0.71
1:1:17:VAL:CB	1:1:109:ILE:N[12_555]	1.49	0.71
2:2:46:ASP:CA	2:2:202:ILE:CA[12_555]	1.49	0.71
2:2:187:PRO:CD	3:3:33:GLU:OE2[12_555]	1.49	0.71
1:1:124:GLU:N	3:3:114:ARG:CG[12_555]	1.49	0.71
2:2:46:ASP:O	2:2:202:ILE:CB[12_555]	1.49	0.71
1:1:19:ASN:CB	1:1:106:MET:SD[12_555]	1.50	0.70
3:3:15:THR:N	3:3:109:TRP:CH2[12_555]	1.50	0.70
1:1:30:SER:CA	1:1:168:ASN:ND2[12_555]	1.50	0.70
1:1:39:THR:N	3:3:30:PRO:N[12_555]	1.50	0.70
1:1:52:GLU:OE1	1:1:143:MET:CE[12_555]	1.50	0.70
1:1:24:HIS:O	1:1:222:SER:CB[12_555]	1.50	0.70
1:1:9:GLU:N	1:1:277:ALA:N[12_555]	1.50	0.70
3:3:10:SER:N	3:3:188:TYR:CD1[12_555]	1.50	0.70
1:1:177:GLN:OE1	3:3:148:MET:CB[12_555]	1.50	0.70
2:2:62:ARG:O	2:2:256:ALA:N[2_555]	1.50	0.70
1:1:25:HIS:C	1:1:223:ARG:CA[12_555]	1.50	0.70
1:1:49:ASP:CB	5:1:500:W54:C2A[12_555]	1.50	0.70
1:1:68:GLU:O	3:3:99:ILE:CA[12_555]	1.50	0.70
3:3:13:PHE:O	3:3:186:ALA:O[12_555]	1.50	0.70
3:3:8:PRO:O	3:3:188:TYR:OH[12_555]	1.50	0.70
1:1:48:GLU:CG	1:1:78:HIS:CG[12_555]	1.50	0.70
1:1:12:ASN:CG	3:3:229:LEU:CA[12_555]	1.50	0.70
1:1:47:PRO:C	1:1:239:ILE:CB[12_555]	1.50	0.70
1:1:17:VAL:N	1:1:108:GLN:N[12_555]	1.50	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:23:CYS:O	3:3:163:ILE:N[12_555]	1.50	0.70
3:3:209:MET:CA	4:4:32:PHE:C[12_555]	1.51	0.69
1:1:109:ILE:CG2	3:3:217:LYS:O[12_555]	1.51	0.69
1:1:115:LEU:O	3:3:41:LYS:C[12_555]	1.51	0.69
2:2:57:ASP:OD1	2:2:57:ASP:OD1[11_555]	1.51	0.69
2:2:44:PRO:CD	2:2:247:SER:C[12_555]	1.51	0.69
1:1:17:VAL:N	1:1:107:ALA:CA[12_555]	1.51	0.69
1:1:19:ASN:CA	1:1:106:MET:CG[12_555]	1.51	0.69
1:1:241:HIS:CD2	3:3:114:ARG:NH2[12_555]	1.51	0.69
3:3:118:MET:CB	4:4:34:ASP:CB[12_555]	1.51	0.69
3:3:57:ASN:CA	4:4:26:TYR:CA[12_555]	1.51	0.69
2:2:38:TRP:CD1	2:2:210:PRO:C[12_555]	1.51	0.69
3:3:27:TRP:N	3:3:160:GLN:O[12_555]	1.51	0.69
1:1:35:ASP:N	3:3:25:LEU:CG[12_555]	1.51	0.69
1:1:22:GLU:OE2	1:1:81:ARG:CG[12_555]	1.51	0.69
1:1:178:PRO:O	3:3:152:HIS:N[12_555]	1.51	0.69
2:2:43:THR:C	2:2:249:MET:CG[12_555]	1.51	0.69
1:1:39:THR:N	3:3:30:PRO:CG[12_555]	1.51	0.69
3:3:118:MET:CG	4:4:34:ASP:CB[12_555]	1.52	0.68
3:3:106:TYR:CA	3:3:224:ALA:CA[12_555]	1.52	0.68
3:3:56:ASN:CA	4:4:29:ILE:CG1[12_555]	1.52	0.68
1:1:41:HIS:CD2	1:1:186:PHE:CD1[12_555]	1.52	0.68
1:1:113:PHE:CZ	3:3:48:GLN:OE1[12_555]	1.52	0.68
1:1:55:TYR:N	1:1:79:ILE:CG2[12_555]	1.52	0.68
1:1:177:GLN:CA	3:3:149:LEU:N[12_555]	1.52	0.68
2:2:182:ASN:OD1	4:4:41:SER:O[12_555]	1.52	0.68
1:1:13:GLU:OE1	3:3:231:ILE:CD1[12_555]	1.52	0.68
2:2:17:THR:OG1	2:2:49:ALA:N[2_555]	1.52	0.68
1:1:62:ARG:NE	1:1:109:ILE:CA[12_555]	1.52	0.68
2:2:39:PRO:C	2:2:103:ARG:NH1[12_555]	1.52	0.68
3:3:117:PHE:CA	4:4:37:SER:CB[12_555]	1.52	0.68
2:2:32:VAL:CB	3:3:32:LYS:CA[12_555]	1.52	0.68
3:3:12:GLN:CG	3:3:187:GLY:C[12_555]	1.52	0.68
1:1:252:ARG:CA	3:3:41:LYS:CD[12_555]	1.52	0.68
3:3:57:ASN:C	4:4:26:TYR:CB[12_555]	1.52	0.68
1:1:179:PHE:N	3:3:151:THR:CA[12_555]	1.52	0.68
1:1:46:GLN:CA	5:1:500:W54:CL1[12_555]	1.52	0.68
1:1:240:TYR:CB	3:3:112:SER:OG[12_555]	1.52	0.68
2:2:52:LYS:CE	2:2:252:GLU:CG[10_555]	1.52	0.68
3:3:67:MET:CA	4:4:27:PHE:C[12_555]	1.52	0.68
1:1:27:THR:O	1:1:163:TRP:CA[12_555]	1.52	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:11:GLY:C	3:3:134:THR:O[12_555]	1.52	0.68
1:1:17:VAL:CG1	1:1:108:GLN:N[12_555]	1.52	0.68
2:2:187:PRO:CB	3:3:33:GLU:CD[12_555]	1.53	0.67
1:1:12:ASN:C	3:3:229:LEU:O[12_555]	1.53	0.67
2:2:54:THR:N	2:2:58:THR:CA[3_555]	1.53	0.67
1:1:126:THR:N	3:3:166:VAL:CG2[12_555]	1.53	0.67
3:3:107:THR:CA	3:3:223:MET:CG[12_555]	1.53	0.67
1:1:50:ALA:C	1:1:127:LEU:CD2[12_555]	1.53	0.67
1:1:240:TYR:OH	3:3:169:TRP:CG[12_555]	1.53	0.67
3:3:223:MET:N	3:3:225:ARG:CD[12_555]	1.53	0.67
2:2:35:TYR:CB	3:3:36:ILE:CG1[12_555]	1.53	0.67
2:2:32:VAL:CG1	3:3:32:LYS:O[12_555]	1.53	0.67
1:1:15:LEU:O	1:1:111:ARG:CG[12_555]	1.53	0.67
2:2:47:ALA:N	2:2:249:MET:CE[12_555]	1.53	0.67
3:3:70:VAL:CG2	4:4:29:ILE:O[12_555]	1.53	0.67
1:1:63:ASP:OD1	1:1:111:ARG:NE[12_555]	1.53	0.67
1:1:19:ASN:N	1:1:106:MET:CG[12_555]	1.53	0.67
2:2:187:PRO:CB	3:3:33:GLU:OE2[12_555]	1.53	0.67
2:2:44:PRO:C	2:2:107:THR:CB[12_555]	1.53	0.67
3:3:14:MET:SD	3:3:88:ASP:OD1[12_555]	1.54	0.66
2:2:44:PRO:C	2:2:107:THR:OG1[12_555]	1.54	0.66
1:1:182:PHE:CB	3:3:164:SER:O[12_555]	1.54	0.66
1:1:65:MET:N	3:3:105:TYR:CE2[12_555]	1.54	0.66
1:1:176:GLY:CA	3:3:149:LEU:O[12_555]	1.54	0.66
1:1:14:VAL:CG1	1:1:255:ARG:CA[12_555]	1.54	0.66
1:1:51:ILE:CG2	1:1:127:LEU:CB[12_555]	1.54	0.66
2:2:59:SER:CA	2:2:253:PHE:CB[2_555]	1.54	0.66
1:1:64:GLU:OE2	3:3:104:SER:CA[12_555]	1.54	0.66
1:1:27:THR:CB	1:1:223:ARG:CZ[12_555]	1.54	0.66
2:2:88:ASP:C	2:2:259:LYS:CB[2_555]	1.54	0.66
2:2:36:GLY:O	2:2:207:ASN:O[12_555]	1.54	0.66
1:1:32:PRO:CD	1:1:147:TYR:CA[12_555]	1.54	0.66
1:1:22:GLU:N	1:1:79:ILE:O[12_555]	1.54	0.66
3:3:10:SER:N	3:3:188:TYR:CE1[12_555]	1.54	0.66
1:1:18:PRO:CG	1:1:103:LEU:O[12_555]	1.55	0.65
1:1:25:HIS:CG	1:1:223:ARG:C[12_555]	1.55	0.65
3:3:209:MET:C	4:4:32:PHE:O[12_555]	1.55	0.65
1:1:26:THR:CG2	1:1:222:SER:CA[12_555]	1.55	0.65
1:1:67:ILE:CG1	3:3:46:MET:CE[12_555]	1.55	0.65
1:1:30:SER:O	1:1:147:TYR:O[12_555]	1.55	0.65
1:1:18:PRO:CA	1:1:106:MET:N[12_555]	1.55	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:9:GLU:C	1:1:277:ALA:CA[12_555]	1.55	0.65
3:3:23:CYS:CB	3:3:117:PHE:O[12_555]	1.55	0.65
1:1:179:PHE:C	3:3:151:THR:CG2[12_555]	1.55	0.65
1:1:40:GLY:N	3:3:30:PRO:CB[12_555]	1.55	0.65
1:1:178:PRO:C	3:3:151:THR:CA[12_555]	1.55	0.65
1:1:42:THR:OG1	1:1:121:PHE:CA[12_555]	1.55	0.65
2:2:201:LEU:CB	3:3:32:LYS:CE[12_555]	1.55	0.65
3:3:15:THR:CB	3:3:109:TRP:CZ3[12_555]	1.56	0.64
1:1:243:ALA:N	3:3:215:ALA:CA[12_555]	1.56	0.64
2:2:55:GLN:N	2:2:57:ASP:O[3_555]	1.56	0.64
2:2:18:ARG:CD	2:2:51:ASN:CB[2_555]	1.56	0.64
2:2:38:TRP:O	2:2:103:ARG:NH1[12_555]	1.56	0.64
1:1:69:SER:OG	3:3:102:ILE:CB[12_555]	1.56	0.64
3:3:68:TYR:N	4:4:28:ASN:CB[12_555]	1.56	0.64
3:3:209:MET:CE	4:4:32:PHE:CE2[12_555]	1.56	0.64
3:3:19:MET:CE	3:3:85:ILE:CB[12_555]	1.56	0.64
2:2:45:GLN:N	2:2:107:THR:CA[12_555]	1.56	0.64
1:1:17:VAL:CG1	1:1:109:ILE:N[12_555]	1.56	0.64
1:1:6:TYR:CE1	3:3:62:VAL:CG1[12_555]	1.56	0.64
1:1:24:HIS:CE1	1:1:82:ILE:CA[12_555]	1.56	0.64
1:1:73:ARG:O	3:3:219:PHE:CG[12_555]	1.56	0.64
2:2:90:GLY:CA	2:2:98:TYR:CG[2_555]	1.56	0.64
1:1:20:ILE:CG2	1:1:78:HIS:C[12_555]	1.56	0.64
1:1:124:GLU:O	3:3:114:ARG:CG[12_555]	1.56	0.64
1:1:126:THR:CA	3:3:166:VAL:CB[12_555]	1.56	0.64
1:1:250:CYS:CB	3:3:39:GLU:CG[12_555]	1.56	0.64
3:3:24:ALA:N	3:3:162:THR:O[12_555]	1.56	0.64
1:1:39:THR:CA	3:3:30:PRO:CB[12_555]	1.57	0.63
3:3:118:MET:O	4:4:32:PHE:C[12_555]	1.57	0.63
1:1:10:VAL:CG2	1:1:278:ILE:C[12_555]	1.57	0.63
3:3:20:GLN:C	3:3:117:PHE:CZ[12_555]	1.57	0.63
1:1:241:HIS:CD2	3:3:114:ARG:CZ[12_555]	1.57	0.63
3:3:15:THR:CB	3:3:109:TRP:CH2[12_555]	1.57	0.63
1:1:253:PRO:C	4:4:43:LEU:O[12_555]	1.57	0.63
2:2:89:MET:CB	2:2:257:ARG:C[2_555]	1.57	0.63
1:1:18:PRO:O	1:1:106:MET:CB[12_555]	1.57	0.63
3:3:24:ALA:N	3:3:162:THR:C[12_555]	1.57	0.63
1:1:125:ILE:C	3:3:166:VAL:CG2[12_555]	1.57	0.63
1:1:73:ARG:N	3:3:99:ILE:CD1[12_555]	1.57	0.63
2:2:186:PHE:CZ	3:3:41:LYS:NZ[12_555]	1.57	0.63
2:2:64:TYR:CE2	2:2:256:ALA:CA[2_555]	1.57	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:178:THR:CA	4:4:44:ASP:CB[12_555]	1.57	0.63
3:3:108:HIS:N	3:3:224:ALA:O[12_555]	1.57	0.63
1:1:122:ASP:CA	3:3:50:ASP:OD1[12_555]	1.57	0.63
3:3:222:ARG:O	3:3:225:ARG:CB[12_555]	1.57	0.63
1:1:5:ASN:O	1:1:276:THR:OG1[12_555]	1.58	0.62
1:1:52:GLU:O	1:1:237:THR:CA[12_555]	1.58	0.62
2:2:22:THR:OG1	2:2:48:THR:CG2[2_555]	1.58	0.62
2:2:42:LEU:C	2:2:249:MET:CB[12_555]	1.58	0.62
1:1:68:GLU:CB	3:3:98:LEU:CB[12_555]	1.58	0.62
1:1:48:GLU:OE1	1:1:78:HIS:CB[12_555]	1.58	0.62
3:3:13:PHE:CE1	3:3:167:VAL:CB[12_555]	1.58	0.62
1:1:25:HIS:CA	1:1:223:ARG:N[12_555]	1.58	0.62
3:3:21:SER:CA	3:3:117:PHE:CZ[12_555]	1.58	0.62
2:2:54:THR:CG2	2:2:60:SER:N[3_555]	1.58	0.62
1:1:182:PHE:CG	3:3:164:SER:C[12_555]	1.58	0.62
3:3:25:LEU:CA	3:3:160:GLN:CG[12_555]	1.58	0.62
2:2:174:ASN:ND2	4:4:44:ASP:OD2[12_555]	1.58	0.62
1:1:70:PHE:C	3:3:47:CYS:SG[12_555]	1.58	0.62
3:3:51:THR:CB	4:4:41:SER:OG[12_555]	1.58	0.62
1:1:8:ASP:OD1	1:1:258:PRO:CD[12_555]	1.58	0.62
3:3:209:MET:SD	4:4:32:PHE:CD1[12_555]	1.58	0.62
1:1:20:ILE:CD1	1:1:76:CYS:C[12_555]	1.58	0.62
1:1:250:CYS:C	3:3:39:GLU:CG[12_555]	1.58	0.62
3:3:20:GLN:CB	3:3:211:CYS:CB[12_555]	1.58	0.62
2:2:31:ALA:O	3:3:31:THR:CA[12_555]	1.58	0.62
3:3:67:MET:SD	4:4:27:PHE:CD2[12_555]	1.58	0.62
3:3:15:THR:CA	3:3:109:TRP:CZ3[12_555]	1.59	0.61
3:3:26:PRO:CD	3:3:160:GLN:CB[12_555]	1.59	0.61
1:1:18:PRO:O	1:1:106:MET:CG[12_555]	1.59	0.61
1:1:74:SER:C	3:3:112:SER:O[12_555]	1.59	0.61
1:1:176:GLY:O	3:3:149:LEU:O[12_555]	1.59	0.61
1:1:180:PRO:N	3:3:151:THR:CG2[12_555]	1.59	0.61
1:1:21:LYS:CB	1:1:78:HIS:CE1[12_555]	1.59	0.61
2:2:36:GLY:C	2:2:208:ALA:N[12_555]	1.59	0.61
1:1:178:PRO:C	3:3:151:THR:N[12_555]	1.59	0.61
1:1:63:ASP:CA	1:1:111:ARG:NH2[12_555]	1.59	0.61
2:2:12:ARG:C	2:2:13:ILE:CD1[11_555]	1.59	0.61
1:1:122:ASP:C	3:3:50:ASP:OD2[12_555]	1.59	0.61
2:2:32:VAL:N	3:3:32:LYS:N[12_555]	1.59	0.61
1:1:113:PHE:N	3:3:44:ILE:CG2[12_555]	1.59	0.61
1:1:41:HIS:CB	1:1:186:PHE:CG[12_555]	1.59	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:10:SER:OG	3:3:140:GLU:C[12_555]	1.59	0.61
3:3:57:ASN:ND2	4:4:26:TYR:O[12_555]	1.59	0.61
2:2:89:MET:CG	2:2:258:ALA:CA[2_555]	1.59	0.61
2:2:35:TYR:N	3:3:36:ILE:CD1[12_555]	1.59	0.61
2:2:42:LEU:O	2:2:250:CYS:N[12_555]	1.60	0.60
1:1:48:GLU:CB	1:1:78:HIS:CD2[12_555]	1.60	0.60
1:1:39:THR:O	3:3:30:PRO:CB[12_555]	1.60	0.60
2:2:202:ILE:O	3:3:34:ILE:CA[12_555]	1.60	0.60
1:1:241:HIS:C	3:3:216:CYS:CB[12_555]	1.60	0.60
1:1:244:LYS:CD	3:3:213:VAL:CA[12_555]	1.60	0.60
1:1:41:HIS:CG	1:1:186:PHE:CE1[12_555]	1.60	0.60
1:1:17:VAL:O	1:1:107:ALA:CA[12_555]	1.60	0.60
1:1:62:ARG:NH2	1:1:109:ILE:CA[12_555]	1.60	0.60
3:3:66:SER:C	4:4:28:ASN:CB[12_555]	1.60	0.60
1:1:177:GLN:C	3:3:150:GLY:N[12_555]	1.60	0.60
3:3:14:MET:CB	3:3:186:ALA:CB[12_555]	1.60	0.60
1:1:54:ARG:C	1:1:79:ILE:CG2[12_555]	1.60	0.60
1:1:34:LEU:O	3:3:25:LEU:CD2[12_555]	1.60	0.60
2:2:36:GLY:C	2:2:207:ASN:O[12_555]	1.60	0.60
1:1:252:ARG:CD	3:3:41:LYS:CE[12_555]	1.60	0.60
2:2:64:TYR:CG	2:2:256:ALA:C[2_555]	1.60	0.60
1:1:121:PHE:CD2	3:3:48:GLN:O[12_555]	1.60	0.60
1:1:182:PHE:C	3:3:164:SER:C[12_555]	1.60	0.60
2:2:58:THR:CA	2:2:253:PHE:O[2_555]	1.60	0.60
1:1:17:VAL:C	1:1:107:ALA:CA[12_555]	1.60	0.60
2:2:20:ASP:CA	2:2:211:MET:SD[2_555]	1.60	0.60
1:1:116:PHE:CD2	3:3:45:GLU:CG[12_555]	1.60	0.60
1:1:183:SER:OG	3:3:115:PHE:O[12_555]	1.60	0.60
2:2:42:LEU:C	2:2:249:MET:C[12_555]	1.60	0.60
1:1:126:THR:CA	3:3:166:VAL:CG1[12_555]	1.60	0.60
1:1:41:HIS:C	1:1:186:PHE:CA[12_555]	1.61	0.59
1:1:240:TYR:CD1	3:3:112:SER:CA[12_555]	1.61	0.59
1:1:128:VAL:CG2	3:3:168:PRO:CG[12_555]	1.61	0.59
2:2:39:PRO:C	2:2:103:ARG:NE[12_555]	1.61	0.59
2:2:41:TYR:CD2	2:2:41:TYR:CE2[12_555]	1.61	0.59
3:3:52:LEU:O	4:4:40:ALA:O[12_555]	1.61	0.59
2:2:43:THR:N	2:2:249:MET:CB[12_555]	1.61	0.59
3:3:27:TRP:N	3:3:161:SER:CB[12_555]	1.61	0.59
1:1:20:ILE:CG1	1:1:76:CYS:SG[12_555]	1.61	0.59
1:1:45:VAL:CA	5:1:500:W54:O1B[12_555]	1.61	0.59
3:3:14:MET:SD	3:3:88:ASP:CA[12_555]	1.61	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:50:ALA:CB	1:1:127:LEU:CD1[12_555]	1.61	0.59
1:1:116:PHE:CD2	3:3:45:GLU:CD[12_555]	1.61	0.59
1:1:73:ARG:C	3:3:219:PHE:CE1[12_555]	1.61	0.59
1:1:250:CYS:CA	3:3:39:GLU:C[12_555]	1.61	0.59
1:1:51:ILE:CA	1:1:145:TYR:CE2[12_555]	1.61	0.59
1:1:125:ILE:C	3:3:166:VAL:CB[12_555]	1.61	0.59
1:1:247:LYS:CE	2:2:186:PHE:CA[12_555]	1.61	0.59
1:1:126:THR:CB	3:3:167:VAL:CA[12_555]	1.61	0.59
1:1:241:HIS:NE2	3:3:114:ARG:CZ[12_555]	1.61	0.59
1:1:27:THR:CA	1:1:144:GLN:OE1[12_555]	1.61	0.59
3:3:21:SER:N	3:3:117:PHE:CZ[12_555]	1.61	0.59
2:2:58:THR:O	2:2:254:SER:N[2_555]	1.61	0.59
3:3:16:THR:C	3:3:89:ILE:N[12_555]	1.62	0.58
2:2:250:CYS:SG	2:2:252:GLU:CD[12_555]	1.62	0.58
3:3:118:MET:CG	4:4:34:ASP:N[12_555]	1.62	0.58
2:2:34:GLY:N	3:3:34:ILE:CA[12_555]	1.62	0.58
2:2:62:ARG:CG	2:2:254:SER:C[2_555]	1.62	0.58
1:1:70:PHE:N	3:3:102:ILE:CG2[12_555]	1.62	0.58
3:3:106:TYR:CE2	3:3:106:TYR:CZ[12_555]	1.62	0.58
1:1:67:ILE:CB	3:3:46:MET:CE[12_555]	1.62	0.58
1:1:34:LEU:O	3:3:25:LEU:CG[12_555]	1.62	0.58
3:3:221:LEU:C	3:3:225:ARG:O[12_555]	1.62	0.58
2:2:17:THR:CB	2:2:49:ALA:O[2_555]	1.62	0.58
1:1:64:GLU:CD	3:3:104:SER:CA[12_555]	1.62	0.58
1:1:241:HIS:CB	3:3:216:CYS:CB[12_555]	1.62	0.58
1:1:181:ARG:C	3:3:165:LEU:CG[12_555]	1.62	0.58
1:1:73:ARG:NH2	3:3:103:ALA:C[12_555]	1.62	0.58
3:3:15:THR:CG2	3:3:109:TRP:CH2[12_555]	1.62	0.58
3:3:117:PHE:CA	4:4:37:SER:OG[12_555]	1.62	0.58
1:1:241:HIS:CE1	3:3:114:ARG:NH2[12_555]	1.62	0.58
1:1:16:VAL:CG2	1:1:107:ALA:CB[12_555]	1.63	0.57
1:1:177:GLN:NE2	3:3:148:MET:CE[12_555]	1.63	0.57
2:2:201:LEU:CA	3:3:32:LYS:CD[12_555]	1.63	0.57
2:2:44:PRO:CD	2:2:248:PRO:C[12_555]	1.63	0.57
3:3:53:ILE:CB	4:4:39:GLY:CA[12_555]	1.63	0.57
2:2:179:LEU:CA	4:4:42:ARG:NH1[12_555]	1.63	0.57
1:1:252:ARG:N	3:3:41:LYS:CD[12_555]	1.63	0.57
2:2:40:HIS:CD2	2:2:205:TYR:CB[12_555]	1.63	0.57
1:1:126:THR:CG2	3:3:166:VAL:O[12_555]	1.63	0.57
1:1:44:ASN:CA	5:1:500:W54:C4C[12_555]	1.63	0.57
1:1:242:LYS:C	3:3:214:SER:O[12_555]	1.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:14:MET:CG	3:3:186:ALA:CB[12_555]	1.63	0.57
1:1:42:THR:OG1	1:1:121:PHE:O[12_555]	1.63	0.57
3:3:23:CYS:O	3:3:162:THR:CA[12_555]	1.63	0.57
2:2:52:LYS:CE	2:2:252:GLU:CD[10_555]	1.63	0.57
2:2:19:GLY:N	2:2:254:SER:OG[2_555]	1.63	0.57
1:1:71:LEU:CD2	3:3:44:ILE:C[12_555]	1.63	0.57
2:2:15:GLN:C	2:2:15:GLN:O[11_555]	1.63	0.57
3:3:68:TYR:CG	4:4:28:ASN:ND2[12_555]	1.63	0.57
3:3:58:VAL:CG2	4:4:26:TYR:CE2[12_555]	1.63	0.57
1:1:122:ASP:CB	3:3:50:ASP:OD2[12_555]	1.64	0.56
1:1:248:ALA:O	1:1:251:PRO:CD[12_555]	1.64	0.56
3:3:222:ARG:CB	3:3:225:ARG:C[12_555]	1.64	0.56
2:2:43:THR:OG1	2:2:106:TYR:C[12_555]	1.64	0.56
2:2:182:ASN:OD1	4:4:42:ARG:N[12_555]	1.64	0.56
3:3:10:SER:CB	3:3:140:GLU:N[12_555]	1.64	0.56
1:1:126:THR:CG2	3:3:166:VAL:C[12_555]	1.64	0.56
3:3:212:PHE:N	4:4:38:SER:O[12_555]	1.64	0.56
1:1:25:HIS:ND1	1:1:224:ILE:N[12_555]	1.64	0.56
2:2:41:TYR:CA	2:2:250:CYS:O[12_555]	1.64	0.56
1:1:177:GLN:OE1	3:3:148:MET:CA[12_555]	1.64	0.56
2:2:62:ARG:NH2	2:2:102:GLY:N[2_555]	1.64	0.56
3:3:26:PRO:CA	3:3:161:SER:CB[12_555]	1.64	0.56
2:2:18:ARG:NH1	2:2:47:ALA:CB[12_555]	1.64	0.56
1:1:121:PHE:CG	3:3:48:GLN:O[12_555]	1.64	0.56
1:1:182:PHE:CA	3:3:164:SER:C[12_555]	1.64	0.56
2:2:52:LYS:CG	2:2:53:PRO:CG[10_555]	1.64	0.56
1:1:10:VAL:CA	1:1:277:ALA:CA[12_555]	1.64	0.56
1:1:243:ALA:CA	3:3:215:ALA:N[12_555]	1.64	0.56
1:1:39:THR:C	3:3:30:PRO:CA[12_555]	1.64	0.56
1:1:182:PHE:CA	3:3:165:LEU:CA[12_555]	1.64	0.56
1:1:60:GLN:CA	1:1:108:GLN:CG[12_555]	1.64	0.56
2:2:54:THR:OG1	2:2:56:PRO:CA[3_555]	1.64	0.56
1:1:53:THR:N	1:1:237:THR:N[12_555]	1.64	0.56
1:1:179:PHE:CD1	3:3:151:THR:OG1[12_555]	1.64	0.56
1:1:242:LYS:CB	3:3:214:SER:O[12_555]	1.65	0.55
1:1:22:GLU:C	1:1:80:SER:CA[12_555]	1.65	0.55
3:3:209:MET:CE	4:4:32:PHE:CZ[12_555]	1.65	0.55
2:2:46:ASP:OD1	2:2:202:ILE:C[12_555]	1.65	0.55
3:3:21:SER:O	3:3:117:PHE:CG[12_555]	1.65	0.55
3:3:222:ARG:O	3:3:225:ARG:CA[12_555]	1.65	0.55
3:3:68:TYR:CE1	4:4:27:PHE:CE1[12_555]	1.65	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:43:THR:CA	2:2:105:GLY:O[12_555]	1.65	0.55
1:1:5:ASN:OD1	2:2:173:LEU:CD2[12_555]	1.65	0.55
2:2:54:THR:O	2:2:59:SER:N[3_555]	1.65	0.55
1:1:249:TRP:NE1	2:2:35:TYR:CG[12_555]	1.65	0.55
1:1:25:HIS:CD2	1:1:224:ILE:N[12_555]	1.65	0.55
3:3:70:VAL:CG2	4:4:31:TYR:CG[12_555]	1.65	0.55
1:1:71:LEU:CD2	3:3:44:ILE:N[12_555]	1.65	0.55
1:1:71:LEU:CB	3:3:47:CYS:N[12_555]	1.65	0.55
1:1:126:THR:OG1	3:3:113:LEU:O[12_555]	1.65	0.55
1:1:241:HIS:N	3:3:216:CYS:SG[12_555]	1.65	0.55
3:3:12:GLN:CB	3:3:187:GLY:CA[12_555]	1.65	0.55
2:2:64:TYR:CB	2:2:257:ARG:CB[2_555]	1.65	0.55
3:3:23:CYS:CB	3:3:162:THR:CG2[12_555]	1.65	0.55
3:3:212:PHE:CD1	4:4:36:ALA:C[12_555]	1.65	0.55
2:2:45:GLN:N	2:2:107:THR:OG1[12_555]	1.65	0.55
3:3:21:SER:N	3:3:117:PHE:CD1[12_555]	1.65	0.55
3:3:12:GLN:CD	3:3:187:GLY:CA[12_555]	1.66	0.54
2:2:17:THR:N	2:2:49:ALA:O[2_555]	1.66	0.54
2:2:11:ASP:CB	2:2:26:ASP:CA[11_555]	1.66	0.54
1:1:245:HIS:CD2	3:3:51:THR:N[12_555]	1.66	0.54
2:2:64:TYR:CE2	2:2:257:ARG:N[2_555]	1.66	0.54
1:1:76:CYS:N	3:3:218:ASP:OD2[12_555]	1.66	0.54
2:2:55:GLN:CG	2:2:57:ASP:OD2[3_555]	1.66	0.54
1:1:179:PHE:CB	3:3:151:THR:CB[12_555]	1.66	0.54
1:1:27:THR:OG1	1:1:223:ARG:CG[12_555]	1.66	0.54
2:2:45:GLN:CB	2:2:107:THR:N[12_555]	1.66	0.54
1:1:74:SER:CB	3:3:112:SER:C[12_555]	1.66	0.54
2:2:63:PHE:N	2:2:255:GLY:N[2_555]	1.66	0.54
3:3:6:ILE:CD1	3:3:142:THR:C[12_555]	1.66	0.54
1:1:60:GLN:O	1:1:108:GLN:CA[12_555]	1.66	0.54
3:3:21:SER:OG	3:3:115:PHE:C[12_555]	1.66	0.54
1:1:124:GLU:CB	3:3:114:ARG:CB[12_555]	1.66	0.54
1:1:253:PRO:O	4:4:43:LEU:O[12_555]	1.66	0.54
3:3:14:MET:CE	3:3:88:ASP:CB[12_555]	1.66	0.54
1:1:37:ALA:CB	4:4:36:ALA:CB[12_555]	1.66	0.54
1:1:240:TYR:CG	3:3:112:SER:CB[12_555]	1.66	0.54
2:2:17:THR:CA	2:2:50:ILE:N[2_555]	1.66	0.54
1:1:245:HIS:NE2	3:3:51:THR:C[12_555]	1.66	0.54
3:3:26:PRO:N	3:3:161:SER:N[12_555]	1.66	0.54
1:1:76:CYS:CA	3:3:218:ASP:OD1[12_555]	1.66	0.54
2:2:59:SER:O	2:2:99:HIS:CE1[2_555]	1.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:15:THR:C	3:3:109:TRP:CZ3[12_555]	1.66	0.54
1:1:124:GLU:CG	3:3:114:ARG:O[12_555]	1.66	0.54
2:2:194:ARG:NH1	3:3:27:TRP:CD2[12_555]	1.66	0.54
1:1:176:GLY:N	3:3:149:LEU:O[12_555]	1.66	0.54
3:3:9:GLY:CA	3:3:188:TYR:CZ[12_555]	1.66	0.54
1:1:42:THR:N	1:1:186:PHE:CA[12_555]	1.66	0.54
3:3:222:ARG:CD	3:3:226:ASP:O[12_555]	1.67	0.53
1:1:181:ARG:O	3:3:165:LEU:CB[12_555]	1.67	0.53
1:1:69:SER:C	3:3:102:ILE:CB[12_555]	1.67	0.53
1:1:178:PRO:CG	3:3:147:ALA:O[12_555]	1.67	0.53
3:3:36:ILE:C	3:3:37:PRO:O[12_555]	1.67	0.53
1:1:22:GLU:CD	1:1:81:ARG:CA[12_555]	1.67	0.53
2:2:88:ASP:O	2:2:259:LYS:CG[2_555]	1.67	0.53
1:1:69:SER:CB	3:3:102:ILE:CB[12_555]	1.67	0.53
1:1:177:GLN:CG	3:3:148:MET:C[12_555]	1.67	0.53
1:1:24:HIS:C	1:1:222:SER:OG[12_555]	1.67	0.53
2:2:54:THR:CA	2:2:57:ASP:CA[3_555]	1.67	0.53
1:1:123:SER:CB	3:3:114:ARG:CZ[12_555]	1.67	0.53
2:2:179:LEU:O	4:4:42:ARG:CB[12_555]	1.67	0.53
2:2:182:ASN:CG	4:4:42:ARG:N[12_555]	1.67	0.53
1:1:179:PHE:CA	3:3:151:THR:CA[12_555]	1.67	0.53
1:1:17:VAL:CB	1:1:107:ALA:C[12_555]	1.67	0.53
2:2:90:GLY:N	2:2:98:TYR:CG[2_555]	1.67	0.53
2:2:33:VAL:C	3:3:34:ILE:CG1[12_555]	1.67	0.53
3:3:26:PRO:CD	3:3:161:SER:N[12_555]	1.67	0.53
3:3:13:PHE:CB	3:3:133:TYR:OH[12_555]	1.67	0.53
1:1:13:GLU:CD	3:3:231:ILE:CG1[12_555]	1.67	0.53
2:2:20:ASP:N	2:2:211:MET:SD[2_555]	1.67	0.53
3:3:107:THR:OG1	3:3:107:THR:OG1[12_555]	1.68	0.52
2:2:38:TRP:CG	2:2:211:MET:N[12_555]	1.68	0.52
1:1:18:PRO:CD	1:1:106:MET:O[12_555]	1.68	0.52
1:1:36:ALA:CB	3:3:28:TYR:N[12_555]	1.68	0.52
3:3:212:PHE:CE1	4:4:35:ALA:C[12_555]	1.68	0.52
1:1:70:PHE:CD2	3:3:43:LEU:CA[12_555]	1.68	0.52
3:3:36:ILE:O	3:3:37:PRO:O[12_555]	1.68	0.52
1:1:50:ALA:C	1:1:127:LEU:CG[12_555]	1.68	0.52
3:3:11:GLY:C	3:3:134:THR:CB[12_555]	1.68	0.52
1:1:241:HIS:CB	3:3:216:CYS:CA[12_555]	1.68	0.52
2:2:44:PRO:CD	2:2:248:PRO:O[12_555]	1.68	0.52
1:1:25:HIS:ND1	1:1:224:ILE:CG2[12_555]	1.68	0.52
1:1:28:SER:C	1:1:146:MET:SD[12_555]	1.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:19:MET:O	3:3:115:PHE:CD2[12_555]	1.68	0.52
2:2:21:SER:N	2:2:101:LEU:CD1[2_555]	1.68	0.52
1:1:39:THR:O	3:3:30:PRO:C[12_555]	1.68	0.52
2:2:16:ILE:CA	2:2:50:ILE:CD1[2_555]	1.68	0.52
1:1:177:GLN:N	3:3:149:LEU:N[12_555]	1.68	0.52
1:1:53:THR:N	1:1:237:THR:C[12_555]	1.68	0.52
2:2:38:TRP:CE3	2:2:210:PRO:CB[12_555]	1.68	0.52
3:3:65:VAL:O	4:4:28:ASN:CB[12_555]	1.68	0.52
3:3:18:ASP:CB	3:3:94:LEU:CA[12_555]	1.69	0.51
2:2:187:PRO:N	3:3:33:GLU:CD[12_555]	1.69	0.51
1:1:68:GLU:CB	3:3:98:LEU:C[12_555]	1.69	0.51
2:2:21:SER:CB	2:2:101:LEU:CD1[2_555]	1.69	0.51
1:1:34:LEU:C	3:3:25:LEU:CG[12_555]	1.69	0.51
2:2:186:PHE:CE1	3:3:41:LYS:NZ[12_555]	1.69	0.51
1:1:13:GLU:O	3:3:230:HIS:CE1[12_555]	1.69	0.51
3:3:222:ARG:CG	3:3:226:ASP:N[12_555]	1.69	0.51
3:3:68:TYR:O	4:4:30:ASN:OD1[12_555]	1.69	0.51
2:2:19:GLY:CA	2:2:254:SER:CB[2_555]	1.69	0.51
1:1:41:HIS:O	1:1:186:PHE:N[12_555]	1.69	0.51
2:2:62:ARG:CG	2:2:254:SER:O[2_555]	1.69	0.51
1:1:46:GLN:C	1:1:239:ILE:CG2[12_555]	1.69	0.51
1:1:13:GLU:O	3:3:230:HIS:ND1[12_555]	1.69	0.51
2:2:52:LYS:NZ	2:2:252:GLU:CB[10_555]	1.69	0.51
2:2:34:GLY:N	3:3:34:ILE:N[12_555]	1.69	0.51
1:1:12:ASN:O	3:3:229:LEU:C[12_555]	1.69	0.51
1:1:32:PRO:CB	1:1:147:TYR:CD1[12_555]	1.69	0.51
2:2:21:SER:CA	2:2:101:LEU:CG[2_555]	1.69	0.51
1:1:26:THR:CA	1:1:163:TRP:CZ3[12_555]	1.69	0.51
3:3:11:GLY:O	3:3:134:THR:N[12_555]	1.69	0.51
1:1:183:SER:CA	3:3:164:SER:OG[12_555]	1.70	0.50
3:3:36:ILE:CG2	3:3:37:PRO:C[12_555]	1.70	0.50
1:1:244:LYS:O	3:3:50:ASP:CB[12_555]	1.70	0.50
1:1:61:THR:OG1	3:3:230:HIS:O[12_555]	1.70	0.50
3:3:23:CYS:C	3:3:163:ILE:CA[12_555]	1.70	0.50
1:1:245:HIS:O	3:3:49:VAL:CG1[12_555]	1.70	0.50
1:1:6:TYR:OH	3:3:62:VAL:CG1[12_555]	1.70	0.50
3:3:22:PRO:O	3:3:163:ILE:C[12_555]	1.70	0.50
2:2:39:PRO:CA	2:2:103:ARG:NH1[12_555]	1.70	0.50
1:1:251:PRO:CA	3:3:40:VAL:C[12_555]	1.70	0.50
1:1:252:ARG:CG	3:3:41:LYS:CG[12_555]	1.70	0.50
2:2:18:ARG:NH2	2:2:50:ILE:CG2[2_555]	1.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:179:LEU:CA	4:4:42:ARG:CD[12_555]	1.70	0.50
1:1:69:SER:CA	3:3:99:ILE:O[12_555]	1.70	0.50
1:1:51:ILE:C	1:1:145:TYR:CE2[12_555]	1.70	0.50
3:3:106:TYR:C	3:3:223:MET:O[12_555]	1.70	0.50
1:1:179:PHE:N	3:3:151:THR:O[12_555]	1.70	0.50
1:1:25:HIS:CB	1:1:224:ILE:N[12_555]	1.70	0.50
1:1:24:HIS:NE2	1:1:81:ARG:O[12_555]	1.70	0.50
3:3:222:ARG:O	3:3:225:ARG:CG[12_555]	1.70	0.50
1:1:115:LEU:C	3:3:41:LYS:CB[12_555]	1.70	0.50
1:1:73:ARG:CZ	3:3:103:ALA:CA[12_555]	1.70	0.50
3:3:212:PHE:CE1	4:4:35:ALA:O[12_555]	1.70	0.50
3:3:51:THR:O	4:4:39:GLY:O[12_555]	1.70	0.50
1:1:245:HIS:CD2	3:3:51:THR:O[12_555]	1.70	0.50
1:1:62:ARG:CG	1:1:108:GLN:O[12_555]	1.70	0.50
3:3:58:VAL:CB	4:4:26:TYR:CD1[12_555]	1.71	0.49
1:1:124:GLU:CG	3:3:114:ARG:CA[12_555]	1.71	0.49
1:1:43:SER:OG	1:1:184:ILE:CG2[12_555]	1.71	0.49
1:1:39:THR:C	3:3:30:PRO:CG[12_555]	1.71	0.49
1:1:68:GLU:C	3:3:98:LEU:O[12_555]	1.71	0.49
1:1:71:LEU:CB	3:3:47:CYS:CA[12_555]	1.71	0.49
3:3:211:CYS:C	4:4:38:SER:C[12_555]	1.71	0.49
1:1:26:THR:O	1:1:144:GLN:CG[12_555]	1.71	0.49
3:3:14:MET:SD	3:3:88:ASP:CB[12_555]	1.71	0.49
1:1:68:GLU:CG	3:3:98:LEU:C[12_555]	1.71	0.49
1:1:46:GLN:N	5:1:500:W54:C3B[12_555]	1.71	0.49
3:3:40:VAL:CG2	3:3:40:VAL:CG2[12_555]	1.71	0.49
1:1:182:PHE:O	3:3:165:LEU:N[12_555]	1.71	0.49
3:3:56:ASN:CA	4:4:29:ILE:CD1[12_555]	1.71	0.49
1:1:9:GLU:O	1:1:277:ALA:CB[12_555]	1.71	0.49
2:2:38:TRP:CD2	2:2:210:PRO:CA[12_555]	1.71	0.49
1:1:12:ASN:CG	3:3:229:LEU:CG[12_555]	1.71	0.49
1:1:22:GLU:CA	1:1:79:ILE:O[12_555]	1.71	0.49
2:2:19:GLY:C	2:2:211:MET:CE[2_555]	1.71	0.49
1:1:75:GLY:CA	3:3:218:ASP:CB[12_555]	1.71	0.49
2:2:202:ILE:O	3:3:34:ILE:CB[12_555]	1.72	0.48
3:3:14:MET:SD	3:3:88:ASP:CG[12_555]	1.72	0.48
1:1:53:THR:CG2	1:1:80:SER:CB[12_555]	1.72	0.48
1:1:177:GLN:OE1	3:3:148:MET:N[12_555]	1.72	0.48
1:1:24:HIS:CA	1:1:97:THR:CG2[12_555]	1.72	0.48
3:3:17:ASP:CB	3:3:87:VAL:C[12_555]	1.72	0.48
2:2:11:ASP:CB	2:2:26:ASP:C[11_555]	1.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:10:VAL:N	1:1:277:ALA:N[12_555]	1.72	0.48
1:1:14:VAL:N	3:3:230:HIS:ND1[12_555]	1.72	0.48
1:1:242:LYS:CA	3:3:215:ALA:C[12_555]	1.72	0.48
2:2:17:THR:CG2	2:2:50:ILE:CG2[12_555]	1.72	0.48
1:1:240:TYR:CA	3:3:112:SER:OG[12_555]	1.72	0.48
2:2:21:SER:C	2:2:101:LEU:CD1[2_555]	1.72	0.48
2:2:41:TYR:OH	2:2:55:GLN:NE2[12_555]	1.72	0.48
1:1:71:LEU:CB	3:3:44:ILE:O[12_555]	1.72	0.48
3:3:107:THR:CB	3:3:107:THR:OG1[12_555]	1.72	0.48
3:3:212:PHE:CE2	4:4:35:ALA:C[12_555]	1.72	0.48
1:1:115:LEU:CG	3:3:41:LYS:O[12_555]	1.72	0.48
2:2:46:ASP:OD1	2:2:203:VAL:CB[12_555]	1.72	0.48
1:1:182:PHE:CD1	3:3:164:SER:C[12_555]	1.72	0.48
2:2:178:THR:CA	4:4:44:ASP:CA[12_555]	1.72	0.48
3:3:19:MET:CE	3:3:85:ILE:C[12_555]	1.72	0.48
3:3:19:MET:CB	3:3:85:ILE:CD1[12_555]	1.72	0.48
2:2:42:LEU:O	2:2:249:MET:CB[12_555]	1.72	0.48
3:3:106:TYR:O	3:3:223:MET:C[12_555]	1.73	0.47
3:3:222:ARG:CB	3:3:226:ASP:N[12_555]	1.73	0.47
3:3:106:TYR:CB	3:3:224:ALA:N[12_555]	1.73	0.47
1:1:245:HIS:CG	3:3:51:THR:N[12_555]	1.73	0.47
1:1:108:GLN:OE1	3:3:220:CYS:SG[12_555]	1.73	0.47
2:2:178:THR:CA	4:4:44:ASP:N[12_555]	1.73	0.47
3:3:23:CYS:SG	3:3:162:THR:CA[12_555]	1.73	0.47
1:1:35:ASP:C	3:3:25:LEU:CB[12_555]	1.73	0.47
1:1:15:LEU:CA	1:1:111:ARG:CD[12_555]	1.73	0.47
3:3:120:CYS:N	4:4:33:LYS:CA[12_555]	1.73	0.47
3:3:12:GLN:CG	3:3:187:GLY:N[12_555]	1.73	0.47
1:1:64:GLU:OE1	3:3:105:TYR:N[12_555]	1.73	0.47
1:1:126:THR:N	3:3:166:VAL:CG1[12_555]	1.73	0.47
1:1:182:PHE:C	3:3:115:PHE:O[12_555]	1.73	0.47
3:3:17:ASP:CG	3:3:87:VAL:CA[12_555]	1.73	0.47
1:1:47:PRO:CB	1:1:239:ILE:N[12_555]	1.73	0.47
1:1:112:LYS:O	3:3:42:ASN:CG[12_555]	1.73	0.47
1:1:254:PRO:CB	4:4:43:LEU:CD2[12_555]	1.73	0.47
1:1:24:HIS:ND1	1:1:82:ILE:CB[12_555]	1.73	0.47
2:2:43:THR:O	2:2:249:MET:CG[12_555]	1.73	0.47
3:3:20:GLN:CG	3:3:211:CYS:SG[12_555]	1.73	0.47
2:2:38:TRP:C	2:2:103:ARG:NH1[12_555]	1.73	0.47
1:1:242:LYS:N	3:3:215:ALA:C[12_555]	1.73	0.47
1:1:250:CYS:N	3:3:39:GLU:O[12_555]	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:12:GLN:CD	3:3:187:GLY:N[12_555]	1.73	0.47
1:1:27:THR:C	1:1:163:TRP:CB[12_555]	1.73	0.47
1:1:241:HIS:CB	3:3:216:CYS:SG[12_555]	1.74	0.46
2:2:194:ARG:NH1	3:3:27:TRP:CZ2[12_555]	1.74	0.46
3:3:26:PRO:CB	3:3:160:GLN:C[12_555]	1.74	0.46
1:1:71:LEU:CG	3:3:43:LEU:O[12_555]	1.74	0.46
1:1:49:ASP:C	5:1:500:W54:N3A[12_555]	1.74	0.46
1:1:244:LYS:CE	3:3:213:VAL:N[12_555]	1.74	0.46
3:3:67:MET:C	4:4:27:PHE:C[12_555]	1.74	0.46
3:3:69:THR:C	4:4:29:ILE:CA[12_555]	1.74	0.46
2:2:202:ILE:N	3:3:32:LYS:CD[12_555]	1.74	0.46
3:3:212:PHE:N	4:4:38:SER:CA[12_555]	1.74	0.46
2:2:31:ALA:C	3:3:32:LYS:N[12_555]	1.74	0.46
1:1:241:HIS:C	3:3:216:CYS:CA[12_555]	1.74	0.46
1:1:177:GLN:CD	3:3:148:MET:CB[12_555]	1.74	0.46
1:1:8:ASP:OD2	1:1:257:VAL:C[12_555]	1.74	0.46
3:3:12:GLN:C	3:3:134:THR:O[12_555]	1.74	0.46
1:1:53:THR:C	1:1:80:SER:O[12_555]	1.74	0.46
1:1:21:LYS:C	1:1:79:ILE:C[12_555]	1.74	0.46
2:2:38:TRP:O	2:2:205:TYR:CD2[12_555]	1.74	0.46
2:2:89:MET:C	2:2:98:TYR:CG[2_555]	1.74	0.46
1:1:20:ILE:O	1:1:79:ILE:CG1[12_555]	1.74	0.46
1:1:14:VAL:CA	1:1:255:ARG:O[12_555]	1.74	0.46
1:1:32:PRO:CA	1:1:147:TYR:CB[12_555]	1.74	0.46
1:1:183:SER:CB	3:3:116:SER:N[12_555]	1.74	0.46
1:1:62:ARG:CD	1:1:112:LYS:CB[12_555]	1.74	0.46
3:3:17:ASP:CB	3:3:87:VAL:O[12_555]	1.74	0.46
1:1:180:PRO:CD	3:3:151:THR:CG2[12_555]	1.74	0.46
1:1:68:GLU:CB	3:3:98:LEU:CA[12_555]	1.74	0.46
3:3:58:VAL:N	4:4:26:TYR:N[12_555]	1.74	0.46
3:3:56:ASN:CG	4:4:29:ILE:CG1[12_555]	1.74	0.46
1:1:124:GLU:OE2	3:3:115:PHE:CD2[12_555]	1.74	0.46
2:2:54:THR:CA	2:2:57:ASP:O[3_555]	1.74	0.46
2:2:178:THR:CB	4:4:44:ASP:CG[12_555]	1.74	0.46
2:2:250:CYS:SG	2:2:252:GLU:OE2[12_555]	1.75	0.45
2:2:17:THR:N	2:2:50:ILE:N[2_555]	1.75	0.45
2:2:203:VAL:CG2	3:3:35:SER:N[12_555]	1.75	0.45
1:1:67:ILE:N	3:3:46:MET:CE[12_555]	1.75	0.45
1:1:245:HIS:N	3:3:50:ASP:C[12_555]	1.75	0.45
1:1:180:PRO:CB	3:3:152:HIS:O[12_555]	1.75	0.45
2:2:40:HIS:CB	2:2:103:ARG:NE[12_555]	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:244:LYS:O	3:3:50:ASP:C[12_555]	1.75	0.45
3:3:70:VAL:CB	4:4:31:TYR:CG[12_555]	1.75	0.45
1:1:18:PRO:N	1:1:107:ALA:N[12_555]	1.75	0.45
1:1:44:ASN:C	5:1:500:W54:C5C[12_555]	1.75	0.45
2:2:36:GLY:C	2:2:207:ASN:C[12_555]	1.75	0.45
3:3:120:CYS:N	4:4:33:LYS:CB[12_555]	1.75	0.45
3:3:116:SER:O	4:4:37:SER:CA[12_555]	1.75	0.45
3:3:120:CYS:N	4:4:33:LYS:CG[12_555]	1.75	0.45
3:3:13:PHE:CA	3:3:133:TYR:CZ[12_555]	1.75	0.45
2:2:64:TYR:CD2	2:2:256:ALA:CA[2_555]	1.75	0.45
3:3:223:MET:O	3:3:223:MET:O[12_555]	1.75	0.45
2:2:62:ARG:CZ	2:2:101:LEU:C[2_555]	1.75	0.45
1:1:115:LEU:CB	3:3:42:ASN:CA[12_555]	1.75	0.45
2:2:64:TYR:CD1	2:2:255:GLY:O[2_555]	1.75	0.45
1:1:244:LYS:CG	3:3:213:VAL:C[12_555]	1.75	0.45
2:2:59:SER:CB	2:2:253:PHE:CD2[2_555]	1.75	0.45
3:3:10:SER:CB	3:3:140:GLU:C[12_555]	1.75	0.45
1:1:113:PHE:CE1	3:3:48:GLN:CG[12_555]	1.75	0.45
1:1:41:HIS:CB	1:1:186:PHE:C[12_555]	1.76	0.44
2:2:55:GLN:N	2:2:57:ASP:N[3_555]	1.76	0.44
1:1:32:PRO:CD	1:1:147:TYR:N[12_555]	1.76	0.44
1:1:252:ARG:N	3:3:41:LYS:CG[12_555]	1.76	0.44
2:2:57:ASP:CG	2:2:57:ASP:CG[11_555]	1.76	0.44
2:2:41:TYR:CB	2:2:250:CYS:CA[12_555]	1.76	0.44
2:2:62:ARG:NH1	2:2:254:SER:N[2_555]	1.76	0.44
3:3:20:GLN:CB	3:3:211:CYS:SG[12_555]	1.76	0.44
1:1:39:THR:CA	3:3:30:PRO:CG[12_555]	1.76	0.44
2:2:200:THR:O	3:3:32:LYS:CG[12_555]	1.76	0.44
1:1:47:PRO:CG	1:1:239:ILE:CA[12_555]	1.76	0.44
1:1:122:ASP:CA	3:3:50:ASP:CG[12_555]	1.76	0.44
1:1:39:THR:CB	3:3:30:PRO:N[12_555]	1.76	0.44
1:1:8:ASP:OD2	1:1:257:VAL:CA[12_555]	1.76	0.44
1:1:113:PHE:CE2	3:3:48:GLN:CD[12_555]	1.76	0.44
2:2:21:SER:O	2:2:49:ALA:CB[2_555]	1.76	0.44
1:1:74:SER:CB	3:3:112:SER:O[12_555]	1.76	0.44
2:2:11:ASP:CA	2:2:26:ASP:CG[11_555]	1.76	0.44
3:3:53:ILE:CG1	4:4:39:GLY:N[12_555]	1.76	0.44
1:1:17:VAL:N	1:1:107:ALA:O[12_555]	1.76	0.44
1:1:244:LYS:C	3:3:50:ASP:C[12_555]	1.76	0.44
2:2:35:TYR:CB	3:3:36:ILE:CD1[12_555]	1.76	0.44
3:3:106:TYR:N	3:3:224:ALA:N[12_555]	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:21:SER:OG	3:3:115:PHE:CB[12_555]	1.76	0.44
2:2:188:HIS:N	3:3:33:GLU:OE1[12_555]	1.76	0.44
2:2:58:THR:C	2:2:253:PHE:C[2_555]	1.76	0.44
2:2:194:ARG:NH1	3:3:27:TRP:NE1[12_555]	1.76	0.44
3:3:212:PHE:CD1	4:4:37:SER:CA[12_555]	1.76	0.44
2:2:90:GLY:N	2:2:98:TYR:CB[2_555]	1.76	0.44
1:1:73:ARG:CA	3:3:219:PHE:CZ[12_555]	1.76	0.44
1:1:240:TYR:CE1	3:3:111:GLY:C[12_555]	1.76	0.44
1:1:284:ILE:CG2	4:4:31:TYR:OH[12_555]	1.77	0.43
1:1:182:PHE:O	3:3:115:PHE:O[12_555]	1.77	0.43
3:3:9:GLY:O	3:3:188:TYR:CE1[12_555]	1.77	0.43
3:3:17:ASP:OD2	3:3:87:VAL:CG2[12_555]	1.77	0.43
1:1:182:PHE:N	3:3:165:LEU:C[12_555]	1.77	0.43
1:1:64:GLU:CA	3:3:105:TYR:CD2[12_555]	1.77	0.43
2:2:53:PRO:O	2:2:58:THR:N[3_555]	1.77	0.43
1:1:26:THR:CB	1:1:221:CYS:O[12_555]	1.77	0.43
3:3:15:THR:C	3:3:109:TRP:CH2[12_555]	1.77	0.43
1:1:122:ASP:O	3:3:214:SER:OG[12_555]	1.77	0.43
3:3:13:PHE:C	3:3:186:ALA:O[12_555]	1.77	0.43
3:3:27:TRP:CZ3	3:3:159:LEU:N[12_555]	1.77	0.43
1:1:68:GLU:CD	3:3:51:THR:OG1[12_555]	1.77	0.43
2:2:182:ASN:CB	4:4:42:ARG:O[12_555]	1.77	0.43
1:1:33:LEU:C	3:3:24:ALA:CB[12_555]	1.77	0.43
3:3:16:THR:C	3:3:89:ILE:CA[12_555]	1.77	0.43
2:2:39:PRO:N	2:2:103:ARG:NH1[12_555]	1.77	0.43
2:2:18:ARG:C	2:2:51:ASN:ND2[2_555]	1.77	0.43
2:2:20:ASP:OD2	2:2:102:GLY:C[2_555]	1.77	0.43
3:3:118:MET:CE	4:4:35:ALA:N[12_555]	1.77	0.43
3:3:72:LEU:CD1	4:4:31:TYR:O[12_555]	1.77	0.43
1:1:115:LEU:CG	3:3:42:ASN:OD1[12_555]	1.77	0.43
1:1:123:SER:CB	3:3:114:ARG:NE[12_555]	1.78	0.42
3:3:118:MET:O	4:4:33:LYS:CA[12_555]	1.78	0.42
1:1:244:LYS:N	3:3:214:SER:CB[12_555]	1.78	0.42
1:1:72:GLY:O	3:3:99:ILE:CG2[12_555]	1.78	0.42
2:2:54:THR:OG1	2:2:56:PRO:O[3_555]	1.78	0.42
1:1:242:LYS:C	3:3:215:ALA:CA[12_555]	1.78	0.42
2:2:46:ASP:OD2	2:2:203:VAL:N[12_555]	1.78	0.42
1:1:25:HIS:ND1	1:1:224:ILE:CB[12_555]	1.78	0.42
1:1:17:VAL:O	1:1:106:MET:C[12_555]	1.78	0.42
3:3:22:PRO:CB	3:3:155:TRP:CE3[12_555]	1.78	0.42
1:1:47:PRO:N	1:1:239:ILE:CB[12_555]	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:7:ILE:CA	1:1:276:THR:O[12_555]	1.78	0.42
2:2:39:PRO:CA	2:2:103:ARG:CZ[12_555]	1.78	0.42
1:1:68:GLU:OE1	3:3:51:THR:CG2[12_555]	1.78	0.42
2:2:54:THR:CA	2:2:58:THR:N[3_555]	1.78	0.42
1:1:9:GLU:OE1	2:2:179:LEU:CG[12_555]	1.78	0.42
3:3:15:THR:OG1	3:3:109:TRP:CZ3[12_555]	1.78	0.42
3:3:18:ASP:CB	3:3:94:LEU:CG[12_555]	1.78	0.42
3:3:68:TYR:CB	4:4:28:ASN:ND2[12_555]	1.78	0.42
3:3:20:GLN:O	3:3:117:PHE:CE1[12_555]	1.78	0.42
1:1:14:VAL:CG2	1:1:256:ALA:CB[12_555]	1.78	0.42
1:1:124:GLU:N	3:3:114:ARG:CB[12_555]	1.78	0.42
1:1:116:PHE:CD1	3:3:45:GLU:OE1[12_555]	1.78	0.42
3:3:70:VAL:CB	4:4:31:TYR:N[12_555]	1.78	0.42
3:3:118:MET:CG	4:4:34:ASP:C[12_555]	1.78	0.42
2:2:11:ASP:N	2:2:26:ASP:CB[11_555]	1.78	0.42
2:2:194:ARG:CZ	3:3:27:TRP:CE2[12_555]	1.78	0.42
3:3:10:SER:OG	3:3:140:GLU:CB[12_555]	1.79	0.41
2:2:38:TRP:CG	2:2:210:PRO:O[12_555]	1.79	0.41
3:3:58:VAL:CG2	4:4:26:TYR:CE1[12_555]	1.79	0.41
3:3:107:THR:CB	3:3:223:MET:CG[12_555]	1.79	0.41
2:2:34:GLY:N	3:3:34:ILE:CB[12_555]	1.79	0.41
1:1:53:THR:N	1:1:237:THR:CB[12_555]	1.79	0.41
3:3:54:PRO:CA	4:4:27:PHE:CD1[12_555]	1.79	0.41
1:1:27:THR:N	1:1:163:TRP:CZ3[12_555]	1.79	0.41
3:3:97:THR:CG2	4:4:40:ALA:N[12_555]	1.79	0.41
1:1:44:ASN:O	5:1:500:W54:CL2[12_555]	1.79	0.41
3:3:97:THR:CG2	4:4:40:ALA:CB[12_555]	1.79	0.41
1:1:183:SER:C	3:3:164:SER:CB[12_555]	1.79	0.41
2:2:59:SER:O	2:2:99:HIS:ND1[2_555]	1.79	0.41
1:1:244:LYS:C	3:3:50:ASP:N[12_555]	1.79	0.41
3:3:13:PHE:CZ	3:3:167:VAL:O[12_555]	1.79	0.41
2:2:43:THR:CB	2:2:106:TYR:CA[12_555]	1.79	0.41
1:1:245:HIS:CA	3:3:50:ASP:C[12_555]	1.79	0.41
3:3:161:SER:O	4:4:34:ASP:CG[12_555]	1.79	0.41
1:1:36:ALA:O	3:3:28:TYR:CD1[12_555]	1.79	0.41
2:2:187:PRO:CA	3:3:33:GLU:CG[12_555]	1.79	0.41
2:2:12:ARG:C	2:2:13:ILE:CG1[11_555]	1.79	0.41
3:3:69:THR:N	4:4:28:ASN:O[12_555]	1.79	0.41
1:1:178:PRO:O	3:3:151:THR:CA[12_555]	1.79	0.41
1:1:49:ASP:CG	1:1:220:ILE:CD1[12_555]	1.79	0.41
1:1:44:ASN:CG	5:1:500:W54:C2C[12_555]	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:11:ASP:OD2	2:2:26:ASP:C[11_555]	1.79	0.41
1:1:176:GLY:C	3:3:150:GLY:N[12_555]	1.79	0.41
3:3:19:MET:CE	3:3:86:LYS:N[12_555]	1.79	0.41
2:2:46:ASP:CB	2:2:202:ILE:C[12_555]	1.79	0.41
1:1:76:CYS:N	3:3:218:ASP:CB[12_555]	1.79	0.41
1:1:246:THR:OG1	3:3:46:MET:C[12_555]	1.79	0.41
3:3:53:ILE:N	4:4:39:GLY:N[12_555]	1.79	0.41
1:1:48:GLU:OE2	1:1:78:HIS:N[12_555]	1.80	0.40
3:3:23:CYS:N	3:3:117:PHE:O[12_555]	1.80	0.40
1:1:53:THR:N	1:1:237:THR:O[12_555]	1.80	0.40
2:2:38:TRP:N	2:2:209:VAL:O[12_555]	1.80	0.40
1:1:240:TYR:CB	3:3:112:SER:CA[12_555]	1.80	0.40
3:3:26:PRO:N	3:3:160:GLN:C[12_555]	1.80	0.40
2:2:90:GLY:C	2:2:98:TYR:CG[2_555]	1.80	0.40
2:2:63:PHE:CA	2:2:255:GLY:CA[2_555]	1.80	0.40
2:2:62:ARG:CA	2:2:254:SER:C[2_555]	1.80	0.40
2:2:40:HIS:N	2:2:103:ARG:NH2[12_555]	1.80	0.40
3:3:67:MET:CE	4:4:27:PHE:CD2[12_555]	1.80	0.40
1:1:50:ALA:CB	1:1:127:LEU:CG[12_555]	1.80	0.40
1:1:177:GLN:CD	3:3:148:MET:CA[12_555]	1.80	0.40
2:2:248:PRO:CD	2:2:256:ALA:CB[2_555]	1.80	0.40
1:1:116:PHE:CZ	3:3:42:ASN:O[12_555]	1.80	0.40
2:2:46:ASP:OD1	2:2:203:VAL:CA[12_555]	1.80	0.40
2:2:89:MET:O	2:2:98:TYR:CE1[2_555]	1.80	0.40
1:1:179:PHE:N	3:3:151:THR:CB[12_555]	1.80	0.40
1:1:35:ASP:OD2	1:1:187:LEU:CD2[12_555]	1.80	0.40
1:1:10:VAL:CG2	1:1:277:ALA:O[12_555]	1.80	0.40
1:1:177:GLN:NE2	3:3:148:MET:SD[12_555]	1.80	0.40
1:1:240:TYR:OH	3:3:169:TRP:CD1[12_555]	1.80	0.40
2:2:18:ARG:CG	2:2:51:ASN:CG[2_555]	1.80	0.40
1:1:8:ASP:CB	1:1:256:ALA:O[12_555]	1.80	0.40
3:3:13:PHE:CB	3:3:133:TYR:CE2[12_555]	1.80	0.40
2:2:53:PRO:C	2:2:57:ASP:C[3_555]	1.80	0.40
2:2:41:TYR:CA	2:2:250:CYS:CB[12_555]	1.80	0.40
2:2:52:LYS:CD	2:2:252:GLU:OE2[10_555]	1.80	0.40
1:1:63:ASP:OD2	1:1:111:ARG:NH1[12_555]	1.80	0.40
1:1:179:PHE:N	3:3:151:THR:C[12_555]	1.80	0.40
1:1:22:GLU:OE1	1:1:81:ARG:CD[12_555]	1.80	0.40
3:3:10:SER:CA	3:3:140:GLU:CA[12_555]	1.81	0.39
1:1:250:CYS:CB	3:3:39:GLU:CB[12_555]	1.81	0.39
2:2:38:TRP:CB	2:2:210:PRO:N[12_555]	1.81	0.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:29:ALA:CB	3:3:29:HIS:CG[12_555]	1.81	0.39
3:3:37:PRO:CD	3:3:37:PRO:CD[12_555]	1.81	0.39
1:1:122:ASP:O	3:3:214:SER:CB[12_555]	1.81	0.39
1:1:124:GLU:O	3:3:114:ARG:NE[12_555]	1.81	0.39
1:1:242:LYS:O	3:3:214:SER:C[12_555]	1.81	0.39
1:1:51:ILE:N	1:1:127:LEU:CG[12_555]	1.81	0.39
3:3:10:SER:OG	3:3:141:PRO:N[12_555]	1.81	0.39
3:3:209:MET:CB	4:4:31:TYR:C[12_555]	1.81	0.39
3:3:223:MET:CB	3:3:225:ARG:CG[12_555]	1.81	0.39
1:1:178:PRO:O	3:3:151:THR:O[12_555]	1.81	0.39
2:2:41:TYR:C	2:2:250:CYS:CB[12_555]	1.81	0.39
2:2:202:ILE:N	3:3:32:LYS:NZ[12_555]	1.81	0.39
2:2:55:GLN:CD	2:2:57:ASP:OD2[3_555]	1.81	0.39
1:1:122:ASP:OD1	3:3:50:ASP:OD1[12_555]	1.81	0.39
3:3:97:THR:CG2	4:4:40:ALA:CA[12_555]	1.81	0.39
2:2:45:GLN:O	2:2:201:LEU:O[12_555]	1.81	0.39
2:2:21:SER:N	2:2:101:LEU:CB[2_555]	1.81	0.39
3:3:57:ASN:O	4:4:26:TYR:CA[12_555]	1.81	0.39
1:1:240:TYR:CG	3:3:112:SER:CA[12_555]	1.81	0.39
3:3:26:PRO:O	3:3:160:GLN:CA[12_555]	1.81	0.39
2:2:88:ASP:O	2:2:259:LYS:CA[2_555]	1.81	0.39
1:1:65:MET:CG	1:1:70:PHE:CZ[12_555]	1.81	0.39
3:3:68:TYR:N	4:4:28:ASN:N[12_555]	1.81	0.39
1:1:5:ASN:ND2	2:2:173:LEU:CG[12_555]	1.81	0.39
1:1:128:VAL:CB	3:3:168:PRO:CB[12_555]	1.81	0.39
2:2:38:TRP:CA	2:2:210:PRO:CA[12_555]	1.81	0.39
2:2:17:THR:O	2:2:50:ILE:C[2_555]	1.81	0.39
1:1:47:PRO:CA	1:1:239:ILE:CG1[12_555]	1.81	0.39
3:3:212:PHE:CD1	4:4:37:SER:C[12_555]	1.81	0.39
1:1:19:ASN:N	1:1:106:MET:CA[12_555]	1.82	0.38
1:1:254:PRO:O	4:4:43:LEU:C[12_555]	1.82	0.38
2:2:64:TYR:CE2	2:2:256:ALA:C[2_555]	1.82	0.38
2:2:89:MET:CG	2:2:258:ALA:C[2_555]	1.82	0.38
1:1:115:LEU:CD2	3:3:42:ASN:OD1[12_555]	1.82	0.38
3:3:69:THR:O	4:4:29:ILE:N[12_555]	1.82	0.38
1:1:177:GLN:C	3:3:150:GLY:C[12_555]	1.82	0.38
1:1:56:VAL:N	1:1:79:ILE:CD1[12_555]	1.82	0.38
3:3:57:ASN:C	4:4:26:TYR:C[12_555]	1.82	0.38
2:2:38:TRP:CB	2:2:211:MET:N[12_555]	1.82	0.38
3:3:37:PRO:C	3:3:37:PRO:O[12_555]	1.82	0.38
3:3:118:MET:SD	4:4:35:ALA:N[12_555]	1.82	0.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:183:SER:O	3:3:164:SER:CB[12_555]	1.82	0.38
1:1:32:PRO:CG	1:1:147:TYR:CB[12_555]	1.82	0.38
2:2:36:GLY:N	3:3:36:ILE:CD1[12_555]	1.82	0.38
2:2:53:PRO:C	2:2:58:THR:CA[3_555]	1.82	0.38
1:1:183:SER:C	3:3:164:SER:OG[12_555]	1.82	0.38
2:2:13:ILE:C	2:2:13:ILE:CB[11_555]	1.82	0.38
2:2:62:ARG:CB	2:2:254:SER:O[2_555]	1.82	0.38
1:1:179:PHE:N	3:3:151:THR:N[12_555]	1.82	0.38
1:1:251:PRO:CG	3:3:40:VAL:O[12_555]	1.82	0.38
3:3:212:PHE:C	4:4:38:SER:O[12_555]	1.82	0.38
3:3:223:MET:CA	3:3:225:ARG:CG[12_555]	1.82	0.38
2:2:179:LEU:CB	4:4:42:ARG:NE[12_555]	1.82	0.38
3:3:70:VAL:CB	4:4:31:TYR:CA[12_555]	1.82	0.38
3:3:15:THR:CG2	3:3:109:TRP:CZ2[12_555]	1.82	0.38
1:1:124:GLU:C	3:3:114:ARG:CD[12_555]	1.82	0.38
1:1:240:TYR:CD2	3:3:112:SER:OG[12_555]	1.83	0.37
1:1:123:SER:CA	3:3:214:SER:OG[12_555]	1.83	0.37
2:2:64:TYR:CZ	2:2:98:TYR:O[2_555]	1.83	0.37
3:3:6:ILE:CD1	3:3:142:THR:CB[12_555]	1.83	0.37
1:1:24:HIS:ND1	1:1:82:ILE:CG2[12_555]	1.83	0.37
1:1:249:TRP:CZ2	2:2:35:TYR:CE1[12_555]	1.83	0.37
2:2:45:GLN:N	2:2:107:THR:CB[12_555]	1.83	0.37
1:1:71:LEU:CD1	3:3:45:GLU:CA[12_555]	1.83	0.37
1:1:67:ILE:CB	3:3:46:MET:CG[12_555]	1.83	0.37
1:1:41:HIS:CA	1:1:186:PHE:CD1[12_555]	1.83	0.37
2:2:90:GLY:CA	2:2:98:TYR:CD2[2_555]	1.83	0.37
1:1:243:ALA:C	3:3:214:SER:CA[12_555]	1.83	0.37
1:1:115:LEU:CD1	3:3:42:ASN:OD1[12_555]	1.83	0.37
1:1:75:GLY:C	3:3:218:ASP:CA[12_555]	1.83	0.37
3:3:56:ASN:CB	4:4:29:ILE:CD1[12_555]	1.83	0.37
1:1:14:VAL:CB	1:1:256:ALA:N[12_555]	1.83	0.37
1:1:73:ARG:NH2	3:3:103:ALA:N[12_555]	1.83	0.37
1:1:69:SER:N	3:3:102:ILE:CB[12_555]	1.83	0.37
3:3:67:MET:CG	4:4:27:PHE:CG[12_555]	1.83	0.37
2:2:42:LEU:O	2:2:249:MET:O[12_555]	1.83	0.37
1:1:28:SER:OG	1:1:155:PRO:CG[12_555]	1.83	0.37
2:2:11:ASP:CB	2:2:26:ASP:CB[11_555]	1.83	0.37
3:3:13:PHE:CD2	3:3:168:PRO:O[12_555]	1.83	0.37
3:3:106:TYR:C	3:3:223:MET:CA[12_555]	1.83	0.37
1:1:9:GLU:CG	3:3:96:THR:CG2[12_555]	1.83	0.37
2:2:32:VAL:CB	3:3:33:GLU:N[12_555]	1.83	0.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:17:THR:CB	2:2:49:ALA:C[2_555]	1.83	0.37
2:2:178:THR:OG1	4:4:44:ASP:OD1[12_555]	1.83	0.37
1:1:42:THR:CG2	1:1:121:PHE:O[12_555]	1.83	0.37
1:1:246:THR:OG1	3:3:46:MET:CA[12_555]	1.83	0.37
1:1:44:ASN:O	5:1:500:W54:C5C[12_555]	1.83	0.37
1:1:22:GLU:CB	1:1:81:ARG:CB[12_555]	1.84	0.36
1:1:21:LYS:CB	1:1:78:HIS:ND1[12_555]	1.84	0.36
2:2:62:ARG:NE	2:2:101:LEU:O[2_555]	1.84	0.36
2:2:42:LEU:C	2:2:249:MET:O[12_555]	1.84	0.36
1:1:18:PRO:CA	1:1:106:MET:CB[12_555]	1.84	0.36
2:2:17:THR:CG2	2:2:49:ALA:O[2_555]	1.84	0.36
1:1:27:THR:CG2	1:1:223:ARG:NE[12_555]	1.84	0.36
1:1:177:GLN:CG	3:3:148:MET:O[12_555]	1.84	0.36
2:2:178:THR:CB	4:4:44:ASP:N[12_555]	1.84	0.36
3:3:23:CYS:CA	3:3:163:ILE:O[12_555]	1.84	0.36
2:2:203:VAL:CG2	3:3:35:SER:CB[12_555]	1.84	0.36
2:2:93:GLY:O	2:2:98:TYR:OH[2_555]	1.84	0.36
1:1:62:ARG:NE	1:1:109:ILE:C[12_555]	1.84	0.36
1:1:182:PHE:CB	3:3:165:LEU:N[12_555]	1.84	0.36
2:2:178:THR:OG1	4:4:44:ASP:OD2[12_555]	1.84	0.36
2:2:38:TRP:CG	2:2:210:PRO:CB[12_555]	1.84	0.36
3:3:16:THR:CA	3:3:89:ILE:CG2[12_555]	1.84	0.36
1:1:249:TRP:C	3:3:39:GLU:N[12_555]	1.84	0.36
1:1:5:ASN:OD1	2:2:172:TRP:CZ3[12_555]	1.84	0.36
1:1:14:VAL:CB	1:1:256:ALA:CA[12_555]	1.84	0.36
1:1:7:ILE:N	1:1:276:THR:N[12_555]	1.84	0.36
1:1:43:SER:OG	1:1:184:ILE:CB[12_555]	1.84	0.36
1:1:64:GLU:CG	3:3:102:ILE:O[12_555]	1.84	0.36
3:3:57:ASN:CB	4:4:26:TYR:O[12_555]	1.84	0.36
2:2:29:ALA:CB	3:3:29:HIS:C[12_555]	1.84	0.36
1:1:244:LYS:CG	3:3:214:SER:N[12_555]	1.84	0.36
1:1:177:GLN:CD	3:3:148:MET:C[12_555]	1.84	0.36
1:1:245:HIS:CE1	3:3:212:PHE:CD2[12_555]	1.84	0.36
1:1:180:PRO:C	3:3:165:LEU:CD1[12_555]	1.84	0.36
1:1:55:TYR:CA	1:1:81:ARG:NH2[12_555]	1.84	0.36
2:2:46:ASP:C	2:2:202:ILE:CB[12_555]	1.84	0.36
1:1:75:GLY:O	3:3:218:ASP:CG[12_555]	1.84	0.36
2:2:64:TYR:CG	2:2:257:ARG:N[2_555]	1.84	0.36
3:3:11:GLY:O	3:3:135:PRO:N[12_555]	1.84	0.36
1:1:51:ILE:CG1	1:1:237:THR:OG1[12_555]	1.84	0.36
2:2:194:ARG:CZ	3:3:27:TRP:CZ2[12_555]	1.85	0.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:44:PRO:CB	2:2:247:SER:CA[12_555]	1.85	0.35
1:1:240:TYR:CD2	3:3:169:TRP:N[12_555]	1.85	0.35
3:3:68:TYR:CA	4:4:28:ASN:CA[12_555]	1.85	0.35
1:1:32:PRO:CB	1:1:147:TYR:CG[12_555]	1.85	0.35
1:1:5:ASN:C	1:1:276:THR:CA[12_555]	1.85	0.35
2:2:15:GLN:N	2:2:15:GLN:N[11_555]	1.85	0.35
2:2:45:GLN:OE1	2:2:106:TYR:CG[12_555]	1.85	0.35
1:1:50:ALA:O	1:1:127:LEU:CD2[12_555]	1.85	0.35
2:2:39:PRO:CB	2:2:42:LEU:CD1[12_555]	1.85	0.35
1:1:240:TYR:CD1	3:3:111:GLY:C[12_555]	1.85	0.35
3:3:54:PRO:CB	4:4:27:PHE:CD1[12_555]	1.85	0.35
1:1:56:VAL:CG2	1:1:79:ILE:CD1[12_555]	1.85	0.35
3:3:21:SER:O	3:3:117:PHE:CB[12_555]	1.85	0.35
1:1:125:ILE:CG2	3:3:166:VAL:CG2[12_555]	1.85	0.35
1:1:52:GLU:O	1:1:236:THR:C[12_555]	1.85	0.35
1:1:17:VAL:CA	1:1:107:ALA:CA[12_555]	1.85	0.35
2:2:194:ARG:NH2	3:3:27:TRP:CZ2[12_555]	1.85	0.35
3:3:19:MET:CE	3:3:85:ILE:CG1[12_555]	1.85	0.35
1:1:62:ARG:CB	1:1:112:LYS:N[12_555]	1.85	0.35
2:2:32:VAL:CA	3:3:32:LYS:C[12_555]	1.85	0.35
2:2:182:ASN:ND2	4:4:42:ARG:CA[12_555]	1.85	0.35
1:1:21:LYS:O	1:1:79:ILE:N[12_555]	1.85	0.35
3:3:107:THR:CG2	3:3:223:MET:SD[12_555]	1.85	0.35
2:2:31:ALA:C	3:3:31:THR:OG1[12_555]	1.85	0.35
1:1:62:ARG:C	3:3:105:TYR:CZ[12_555]	1.85	0.35
3:3:36:ILE:CG2	3:3:38:GLY:N[12_555]	1.85	0.35
2:2:91:ILE:CG2	2:2:95:ASN:OD1[2_555]	1.85	0.35
3:3:37:PRO:N	3:3:37:PRO:O[12_555]	1.85	0.35
1:1:47:PRO:CB	1:1:239:ILE:CB[12_555]	1.85	0.35
1:1:244:LYS:CA	3:3:213:VAL:O[12_555]	1.85	0.35
1:1:254:PRO:CB	4:4:43:LEU:CG[12_555]	1.86	0.34
1:1:246:THR:C	2:2:185:ILE:CD1[12_555]	1.86	0.34
1:1:68:GLU:CA	3:3:98:LEU:O[12_555]	1.86	0.34
1:1:74:SER:CB	3:3:113:LEU:N[12_555]	1.86	0.34
1:1:53:THR:CG2	1:1:80:SER:CA[12_555]	1.86	0.34
3:3:17:ASP:CB	3:3:87:VAL:CA[12_555]	1.86	0.34
3:3:18:ASP:CB	3:3:94:LEU:CB[12_555]	1.86	0.34
1:1:64:GLU:C	3:3:105:TYR:CG[12_555]	1.86	0.34
1:1:13:GLU:N	3:3:230:HIS:CA[12_555]	1.86	0.34
3:3:67:MET:CA	4:4:28:ASN:N[12_555]	1.86	0.34
1:1:122:ASP:CA	3:3:50:ASP:OD2[12_555]	1.86	0.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:65:MET:CA	1:1:70:PHE:CZ[12_555]	1.86	0.34
1:1:18:PRO:CA	1:1:106:MET:O[12_555]	1.86	0.34
1:1:182:PHE:C	3:3:164:SER:CA[12_555]	1.86	0.34
1:1:244:LYS:CE	3:3:212:PHE:CA[12_555]	1.86	0.34
1:1:68:GLU:N	3:3:102:ILE:CD1[12_555]	1.86	0.34
1:1:63:ASP:N	3:3:105:TYR:OH[12_555]	1.86	0.34
2:2:13:ILE:O	2:2:13:ILE:CB[11_555]	1.86	0.34
1:1:32:PRO:CB	1:1:147:TYR:CB[12_555]	1.86	0.34
1:1:179:PHE:C	3:3:151:THR:C[12_555]	1.86	0.34
1:1:43:SER:CB	1:1:184:ILE:CB[12_555]	1.86	0.34
2:2:41:TYR:CE1	2:2:55:GLN:OE1[12_555]	1.86	0.34
1:1:64:GLU:CB	3:3:104:SER:C[12_555]	1.86	0.34
3:3:16:THR:CB	3:3:89:ILE:CD1[12_555]	1.86	0.34
1:1:64:GLU:OE2	3:3:103:ALA:O[12_555]	1.86	0.34
2:2:45:GLN:CB	2:2:107:THR:C[12_555]	1.87	0.33
2:2:42:LEU:C	2:2:249:MET:CA[12_555]	1.87	0.33
1:1:72:GLY:C	3:3:99:ILE:CG1[12_555]	1.87	0.33
1:1:22:GLU:C	1:1:81:ARG:N[12_555]	1.87	0.33
1:1:6:TYR:C	1:1:276:THR:CA[12_555]	1.87	0.33
2:2:88:ASP:C	2:2:258:ALA:O[2_555]	1.87	0.33
2:2:55:GLN:NE2	2:2:57:ASP:OD2[3_555]	1.87	0.33
1:1:50:ALA:N	5:1:500:W54:C4A[12_555]	1.87	0.33
2:2:89:MET:CB	2:2:258:ALA:O[2_555]	1.87	0.33
1:1:128:VAL:CG2	3:3:168:PRO:CA[12_555]	1.87	0.33
1:1:126:THR:CA	3:3:167:VAL:N[12_555]	1.87	0.33
1:1:41:HIS:O	1:1:186:PHE:CB[12_555]	1.87	0.33
3:3:14:MET:CA	3:3:186:ALA:CB[12_555]	1.87	0.33
1:1:12:ASN:ND2	3:3:229:LEU:CD2[12_555]	1.87	0.33
1:1:121:PHE:CB	3:3:48:GLN:O[12_555]	1.87	0.33
1:1:124:GLU:CA	3:3:114:ARG:C[12_555]	1.87	0.33
1:1:64:GLU:CB	3:3:105:TYR:N[12_555]	1.87	0.33
3:3:65:VAL:O	4:4:28:ASN:ND2[12_555]	1.87	0.33
1:1:181:ARG:CB	3:3:165:LEU:CD1[12_555]	1.87	0.33
2:2:29:ALA:C	3:3:29:HIS:O[12_555]	1.87	0.33
3:3:67:MET:CA	4:4:28:ASN:CB[12_555]	1.87	0.33
3:3:18:ASP:N	3:3:94:LEU:CD2[12_555]	1.87	0.33
1:1:62:ARG:N	1:1:111:ARG:CG[12_555]	1.87	0.33
2:2:201:LEU:C	3:3:32:LYS:CD[12_555]	1.87	0.33
2:2:54:THR:OG1	2:2:56:PRO:CB[3_555]	1.88	0.32
1:1:177:GLN:CD	3:3:148:MET:SD[12_555]	1.88	0.32
2:2:178:THR:CG2	4:4:44:ASP:O[12_555]	1.88	0.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:177:GLN:CG	3:3:148:MET:CB[12_555]	1.88	0.32
2:2:44:PRO:CG	2:2:247:SER:CB[12_555]	1.88	0.32
2:2:60:SER:O	2:2:99:HIS:NE2[2_555]	1.88	0.32
1:1:27:THR:OG1	1:1:223:ARG:NH1[12_555]	1.88	0.32
3:3:17:ASP:OD2	3:3:87:VAL:CG1[12_555]	1.88	0.32
3:3:26:PRO:CA	3:3:160:GLN:O[12_555]	1.88	0.32
1:1:182:PHE:CD2	3:3:164:SER:O[12_555]	1.88	0.32
2:2:248:PRO:CG	2:2:256:ALA:CB[2_555]	1.88	0.32
3:3:106:TYR:CB	3:3:224:ALA:C[12_555]	1.88	0.32
1:1:116:PHE:CD1	3:3:41:LYS:N[12_555]	1.88	0.32
1:1:19:ASN:CG	1:1:106:MET:CE[12_555]	1.88	0.32
1:1:240:TYR:OH	3:3:169:TRP:CB[12_555]	1.88	0.32
3:3:16:THR:C	3:3:89:ILE:CB[12_555]	1.88	0.32
1:1:109:ILE:CD1	3:3:216:CYS:O[12_555]	1.88	0.32
1:1:244:LYS:CE	3:3:212:PHE:CB[12_555]	1.88	0.32
3:3:209:MET:CB	4:4:31:TYR:O[12_555]	1.88	0.32
3:3:212:PHE:CE1	4:4:36:ALA:C[12_555]	1.88	0.32
3:3:212:PHE:CD2	4:4:35:ALA:O[12_555]	1.88	0.32
2:2:90:GLY:CA	2:2:98:TYR:CA[2_555]	1.88	0.32
3:3:119:PHE:CA	4:4:33:LYS:CG[12_555]	1.88	0.32
3:3:161:SER:OG	4:4:34:ASP:OD1[12_555]	1.88	0.32
3:3:23:CYS:C	3:3:162:THR:O[12_555]	1.88	0.32
1:1:55:TYR:CB	1:1:81:ARG:CZ[12_555]	1.88	0.32
1:1:19:ASN:CA	1:1:106:MET:CE[12_555]	1.88	0.32
1:1:115:LEU:CB	3:3:42:ASN:CG[12_555]	1.88	0.32
1:1:178:PRO:CA	3:3:150:GLY:C[12_555]	1.88	0.32
2:2:89:MET:CG	2:2:257:ARG:O[2_555]	1.88	0.32
1:1:64:GLU:CD	3:3:104:SER:O[12_555]	1.88	0.32
1:1:179:PHE:O	3:3:151:THR:O[12_555]	1.88	0.32
1:1:113:PHE:CA	3:3:44:ILE:CG2[12_555]	1.88	0.32
1:1:44:ASN:CB	5:1:500:W54:C3C[12_555]	1.89	0.31
1:1:25:HIS:CB	1:1:223:ARG:CA[12_555]	1.89	0.31
1:1:17:VAL:C	1:1:107:ALA:C[12_555]	1.89	0.31
1:1:125:ILE:O	3:3:165:LEU:O[12_555]	1.89	0.31
1:1:7:ILE:CB	1:1:275:THR:CG2[12_555]	1.89	0.31
1:1:183:SER:CB	3:3:116:SER:OG[12_555]	1.89	0.31
1:1:44:ASN:OD1	5:1:500:W54:C3C[12_555]	1.89	0.31
3:3:67:MET:CB	4:4:28:ASN:OD1[12_555]	1.89	0.31
3:3:222:ARG:CB	3:3:225:ARG:O[12_555]	1.89	0.31
1:1:47:PRO:C	1:1:239:ILE:CD1[12_555]	1.89	0.31
1:1:116:PHE:CE2	3:3:42:ASN:C[12_555]	1.89	0.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:68:TYR:N	4:4:28:ASN:C[12_555]	1.89	0.31
2:2:44:PRO:CG	2:2:248:PRO:N[12_555]	1.89	0.31
1:1:63:ASP:OD1	1:1:111:ARG:NH2[12_555]	1.89	0.31
3:3:22:PRO:CD	3:3:117:PHE:CD2[12_555]	1.89	0.31
3:3:70:VAL:N	4:4:30:ASN:N[12_555]	1.89	0.31
3:3:19:MET:CE	3:3:85:ILE:CA[12_555]	1.89	0.31
2:2:46:ASP:CG	2:2:202:ILE:C[12_555]	1.90	0.30
1:1:249:TRP:CZ2	2:2:35:TYR:CD1[12_555]	1.90	0.30
3:3:211:CYS:O	4:4:39:GLY:N[12_555]	1.90	0.30
1:1:191:SER:OG	2:2:33:VAL:C[12_555]	1.90	0.30
1:1:28:SER:N	1:1:163:TRP:CE3[12_555]	1.90	0.30
2:2:62:ARG:CG	2:2:255:GLY:N[2_555]	1.90	0.30
3:3:27:TRP:CE3	3:3:158:GLY:O[12_555]	1.90	0.30
1:1:241:HIS:O	3:3:216:CYS:CA[12_555]	1.90	0.30
1:1:177:GLN:CD	3:3:148:MET:CG[12_555]	1.90	0.30
3:3:22:PRO:C	3:3:163:ILE:CG2[12_555]	1.90	0.30
1:1:26:THR:C	1:1:163:TRP:CZ3[12_555]	1.90	0.30
1:1:68:GLU:CB	3:3:98:LEU:O[12_555]	1.90	0.30
2:2:90:GLY:CA	2:2:98:TYR:N[2_555]	1.90	0.30
1:1:62:ARG:N	3:3:105:TYR:OH[12_555]	1.90	0.30
2:2:39:PRO:CA	2:2:103:ARG:NH2[12_555]	1.90	0.30
1:1:247:LYS:NZ	2:2:186:PHE:N[12_555]	1.90	0.30
1:1:27:THR:C	1:1:163:TRP:CG[12_555]	1.90	0.30
3:3:68:TYR:C	4:4:30:ASN:ND2[12_555]	1.90	0.30
3:3:209:MET:SD	4:4:32:PHE:CG[12_555]	1.90	0.30
1:1:64:GLU:OE2	3:3:104:SER:C[12_555]	1.90	0.30
3:3:27:TRP:CE3	3:3:159:LEU:C[12_555]	1.90	0.30
3:3:222:ARG:C	3:3:225:ARG:CB[12_555]	1.90	0.30
3:3:51:THR:CB	4:4:41:SER:N[12_555]	1.90	0.30
3:3:21:SER:C	3:3:117:PHE:CE2[12_555]	1.90	0.30
1:1:240:TYR:CE1	3:3:112:SER:N[12_555]	1.90	0.30
1:1:45:VAL:CG2	5:1:500:W54:C6B[12_555]	1.90	0.30
1:1:251:PRO:O	3:3:39:GLU:OE1[12_555]	1.90	0.30
3:3:212:PHE:CE1	4:4:36:ALA:N[12_555]	1.90	0.30
1:1:32:PRO:N	1:1:147:TYR:CG[12_555]	1.90	0.30
1:1:251:PRO:CD	3:3:40:VAL:O[12_555]	1.90	0.30
1:1:181:ARG:C	3:3:165:LEU:CD1[12_555]	1.90	0.30
3:3:11:GLY:O	3:3:134:THR:O[12_555]	1.90	0.30
1:1:113:PHE:CZ	3:3:48:GLN:NE2[12_555]	1.90	0.30
1:1:124:GLU:O	3:3:114:ARG:CB[12_555]	1.90	0.30
3:3:22:PRO:CB	3:3:163:ILE:CG2[12_555]	1.90	0.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:191:SER:OG	2:2:32:VAL:C[12_555]	1.90	0.30
1:1:191:SER:CB	2:2:33:VAL:C[12_555]	1.90	0.30
3:3:17:ASP:N	3:3:87:VAL:O[12_555]	1.90	0.30
3:3:13:PHE:N	3:3:133:TYR:CE1[12_555]	1.90	0.30
1:1:48:GLU:CG	1:1:78:HIS:CB[12_555]	1.90	0.30
1:1:69:SER:CB	3:3:99:ILE:O[12_555]	1.90	0.30
1:1:54:ARG:O	1:1:79:ILE:O[12_555]	1.91	0.29
1:1:75:GLY:N	3:3:112:SER:O[12_555]	1.91	0.29
1:1:27:THR:C	1:1:163:TRP:CE3[12_555]	1.91	0.29
1:1:44:ASN:C	5:1:500:W54:C4C[12_555]	1.91	0.29
1:1:26:THR:N	1:1:222:SER:C[12_555]	1.91	0.29
3:3:18:ASP:OD2	3:3:97:THR:CG2[12_555]	1.91	0.29
1:1:245:HIS:CA	3:3:51:THR:N[12_555]	1.91	0.29
3:3:118:MET:CB	4:4:34:ASP:N[12_555]	1.91	0.29
2:2:38:TRP:CH2	2:2:48:THR:CB[12_555]	1.91	0.29
3:3:69:THR:N	4:4:28:ASN:C[12_555]	1.91	0.29
1:1:5:ASN:CB	2:2:172:TRP:CH2[12_555]	1.91	0.29
1:1:5:ASN:ND2	2:2:173:LEU:CD2[12_555]	1.91	0.29
3:3:119:PHE:N	4:4:34:ASP:N[12_555]	1.91	0.29
3:3:220:CYS:O	3:3:226:ASP:OD1[12_555]	1.91	0.29
3:3:9:GLY:O	3:3:188:TYR:CG[12_555]	1.91	0.29
3:3:21:SER:OG	3:3:115:PHE:CA[12_555]	1.91	0.29
2:2:201:LEU:N	3:3:32:LYS:CE[12_555]	1.91	0.29
1:1:67:ILE:CG2	3:3:46:MET:SD[12_555]	1.91	0.29
2:2:60:SER:CA	2:2:99:HIS:NE2[12_555]	1.91	0.29
1:1:115:LEU:C	3:3:41:LYS:C[12_555]	1.91	0.29
3:3:58:VAL:CG2	4:4:26:TYR:CZ[12_555]	1.91	0.29
3:3:20:GLN:OE1	3:3:55:VAL:CG1[12_555]	1.91	0.29
1:1:243:ALA:CB	3:3:47:CYS:O[12_555]	1.91	0.29
1:1:12:ASN:CB	3:3:229:LEU:O[12_555]	1.91	0.29
2:2:62:ARG:O	2:2:255:GLY:CA[12_555]	1.92	0.28
3:3:12:GLN:N	3:3:134:THR:C[12_555]	1.92	0.28
3:3:6:ILE:CG2	3:3:140:GLU:C[12_555]	1.92	0.28
3:3:19:MET:SD	3:3:85:ILE:CD1[12_555]	1.92	0.28
2:2:64:TYR:CD2	2:2:256:ALA:O[12_555]	1.92	0.28
2:2:36:GLY:CA	2:2:208:ALA:CB[12_555]	1.92	0.28
1:1:52:GLU:CB	1:1:237:THR:CG2[12_555]	1.92	0.28
1:1:246:THR:OG1	3:3:46:MET:O[12_555]	1.92	0.28
3:3:52:LEU:CD2	4:4:38:SER:CB[12_555]	1.92	0.28
1:1:35:ASP:CG	3:3:25:LEU:CD1[12_555]	1.92	0.28
1:1:21:LYS:O	1:1:80:SER:N[12_555]	1.92	0.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:6:ILE:CG1	3:3:141:PRO:C[12_555]	1.92	0.28
3:3:69:THR:O	4:4:29:ILE:CB[12_555]	1.92	0.28
2:2:220:TRP:NE1	3:3:35:SER:OG[12_555]	1.92	0.28
3:3:65:VAL:O	4:4:28:ASN:OD1[12_555]	1.92	0.28
1:1:71:LEU:CG	3:3:44:ILE:CA[12_555]	1.92	0.28
1:1:24:HIS:CD2	1:1:81:ARG:O[12_555]	1.92	0.28
2:2:202:ILE:O	3:3:34:ILE:CG2[12_555]	1.92	0.28
3:3:67:MET:C	4:4:28:ASN:CB[12_555]	1.92	0.28
2:2:34:GLY:C	3:3:34:ILE:O[12_555]	1.92	0.28
2:2:41:TYR:CD2	2:2:41:TYR:CE1[12_555]	1.92	0.28
1:1:9:GLU:CA	1:1:277:ALA:N[12_555]	1.92	0.28
2:2:203:VAL:CG2	3:3:35:SER:CA[12_555]	1.92	0.28
2:2:182:ASN:CG	4:4:42:ARG:C[12_555]	1.92	0.28
1:1:6:TYR:CA	1:1:276:THR:CG2[12_555]	1.92	0.28
3:3:106:TYR:CE2	3:3:106:TYR:OH[12_555]	1.92	0.28
3:3:14:MET:SD	3:3:88:ASP:N[12_555]	1.92	0.28
1:1:125:ILE:CB	3:3:166:VAL:CG2[12_555]	1.92	0.28
1:1:53:THR:N	1:1:237:THR:CG2[12_555]	1.92	0.28
2:2:21:SER:CB	2:2:101:LEU:CG[2_555]	1.92	0.28
1:1:18:PRO:CB	1:1:106:MET:CA[12_555]	1.93	0.27
1:1:252:ARG:N	3:3:41:LYS:CB[12_555]	1.93	0.27
1:1:177:GLN:CG	3:3:148:MET:SD[12_555]	1.93	0.27
2:2:43:THR:OG1	2:2:106:TYR:CB[12_555]	1.93	0.27
1:1:53:THR:CB	1:1:237:THR:C[12_555]	1.93	0.27
3:3:70:VAL:N	4:4:29:ILE:C[12_555]	1.93	0.27
3:3:119:PHE:CA	4:4:33:LYS:CA[12_555]	1.93	0.27
1:1:27:THR:C	1:1:163:TRP:CD2[12_555]	1.93	0.27
1:1:124:GLU:CA	3:3:114:ARG:CA[12_555]	1.93	0.27
2:2:53:PRO:CB	2:2:58:THR:CB[3_555]	1.93	0.27
3:3:22:PRO:C	3:3:163:ILE:O[12_555]	1.93	0.27
3:3:16:THR:O	3:3:89:ILE:CB[12_555]	1.93	0.27
1:1:50:ALA:N	5:1:500:W54:N3A[12_555]	1.93	0.27
1:1:242:LYS:NZ	3:3:213:VAL:CG2[12_555]	1.93	0.27
1:1:73:ARG:NE	3:3:103:ALA:CB[12_555]	1.93	0.27
2:2:46:ASP:CA	2:2:202:ILE:CG2[12_555]	1.93	0.27
1:1:73:ARG:CB	3:3:219:PHE:CE2[12_555]	1.93	0.27
1:1:39:THR:CB	3:3:30:PRO:CB[12_555]	1.93	0.27
1:1:27:THR:OG1	1:1:223:ARG:CZ[12_555]	1.93	0.27
2:2:20:ASP:OD2	2:2:103:ARG:CA[2_555]	1.93	0.27
1:1:244:LYS:C	3:3:51:THR:N[12_555]	1.93	0.27
3:3:26:PRO:C	3:3:161:SER:CB[12_555]	1.93	0.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:179:LEU:C	4:4:42:ARG:NH1[12_555]	1.93	0.27
1:1:51:ILE:CG2	1:1:127:LEU:C[12_555]	1.93	0.27
1:1:41:HIS:NE2	1:1:186:PHE:CE1[12_555]	1.94	0.26
1:1:35:ASP:OD1	1:1:185:PRO:CG[12_555]	1.94	0.26
1:1:41:HIS:CB	1:1:186:PHE:O[12_555]	1.94	0.26
2:2:52:LYS:NZ	2:2:252:GLU:OE2[10_555]	1.94	0.26
2:2:35:TYR:C	3:3:36:ILE:CG1[12_555]	1.94	0.26
3:3:209:MET:CA	4:4:32:PHE:CA[12_555]	1.94	0.26
2:2:64:TYR:CG	2:2:257:ARG:CG[2_555]	1.94	0.26
3:3:209:MET:O	4:4:30:ASN:CA[12_555]	1.94	0.26
3:3:24:ALA:O	3:3:162:THR:C[12_555]	1.94	0.26
3:3:116:SER:O	4:4:37:SER:OG[12_555]	1.94	0.26
2:2:32:VAL:C	3:3:32:LYS:O[12_555]	1.94	0.26
1:1:68:GLU:CD	3:3:98:LEU:CB[12_555]	1.94	0.26
1:1:12:ASN:CB	3:3:229:LEU:N[12_555]	1.94	0.26
3:3:16:THR:O	3:3:88:ASP:C[12_555]	1.94	0.26
1:1:65:MET:CE	1:1:112:LYS:CD[12_555]	1.94	0.26
2:2:20:ASP:C	2:2:101:LEU:CB[2_555]	1.94	0.26
2:2:20:ASP:CA	2:2:211:MET:CB[2_555]	1.94	0.26
2:2:40:HIS:CE1	2:2:205:TYR:CB[12_555]	1.94	0.26
3:3:52:LEU:C	4:4:39:GLY:O[12_555]	1.94	0.26
1:1:121:PHE:CB	3:3:49:VAL:CA[12_555]	1.94	0.26
1:1:33:LEU:CG	1:1:182:PHE:CZ[12_555]	1.94	0.26
1:1:240:TYR:CE2	3:3:169:TRP:N[12_555]	1.94	0.26
1:1:27:THR:CA	1:1:163:TRP:CE3[12_555]	1.94	0.26
1:1:123:SER:C	3:3:114:ARG:CG[12_555]	1.95	0.25
1:1:5:ASN:CG	2:2:173:LEU:CD2[12_555]	1.95	0.25
1:1:71:LEU:CD1	3:3:45:GLU:C[12_555]	1.95	0.25
1:1:52:GLU:O	1:1:237:THR:CB[12_555]	1.95	0.25
1:1:240:TYR:O	3:3:216:CYS:SG[12_555]	1.95	0.25
1:1:60:GLN:CB	1:1:108:GLN:NE2[12_555]	1.95	0.25
1:1:12:ASN:CA	3:3:229:LEU:CA[12_555]	1.95	0.25
2:2:173:LEU:CD2	4:4:42:ARG:NH2[12_555]	1.95	0.25
3:3:223:MET:CA	3:3:225:ARG:NE[12_555]	1.95	0.25
1:1:35:ASP:O	3:3:25:LEU:CB[12_555]	1.95	0.25
3:3:22:PRO:O	3:3:163:ILE:CG2[12_555]	1.95	0.25
3:3:212:PHE:CA	4:4:38:SER:N[12_555]	1.95	0.25
3:3:58:VAL:N	4:4:26:TYR:CB[12_555]	1.95	0.25
2:2:32:VAL:CG2	3:3:32:LYS:O[12_555]	1.95	0.25
3:3:209:MET:CA	4:4:32:PHE:O[12_555]	1.95	0.25
1:1:41:HIS:CB	1:1:186:PHE:CB[12_555]	1.95	0.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:45:GLN:CB	2:2:107:THR:CA[12_555]	1.95	0.25
1:1:25:HIS:O	1:1:223:ARG:CA[12_555]	1.95	0.25
1:1:124:GLU:OE2	3:3:115:PHE:CD1[12_555]	1.95	0.25
3:3:14:MET:O	3:3:87:VAL:CG1[12_555]	1.95	0.25
1:1:240:TYR:CD1	3:3:112:SER:OG[12_555]	1.95	0.25
1:1:18:PRO:C	1:1:106:MET:C[12_555]	1.95	0.25
2:2:35:TYR:CA	3:3:36:ILE:CG1[12_555]	1.95	0.25
1:1:69:SER:N	3:3:98:LEU:O[12_555]	1.95	0.25
2:2:45:GLN:CA	2:2:107:THR:CB[12_555]	1.95	0.25
3:3:119:PHE:CB	4:4:33:LYS:CB[12_555]	1.95	0.25
3:3:16:THR:CA	3:3:89:ILE:CG1[12_555]	1.95	0.25
2:2:58:THR:O	2:2:253:PHE:CA[2_555]	1.96	0.24
2:2:15:GLN:O	2:2:50:ILE:CD1[2_555]	1.96	0.24
1:1:30:SER:OG	1:1:147:TYR:O[12_555]	1.96	0.24
2:2:179:LEU:CG	4:4:42:ARG:CD[12_555]	1.96	0.24
1:1:74:SER:O	3:3:111:GLY:C[12_555]	1.96	0.24
1:1:64:GLU:CG	3:3:105:TYR:CA[12_555]	1.96	0.24
1:1:6:TYR:N	1:1:276:THR:CB[12_555]	1.96	0.24
1:1:241:HIS:CA	3:3:216:CYS:CA[12_555]	1.96	0.24
1:1:178:PRO:CD	3:3:147:ALA:C[12_555]	1.96	0.24
1:1:16:VAL:CB	3:3:230:HIS:NE2[12_555]	1.96	0.24
1:1:73:ARG:CG	3:3:219:PHE:CE2[12_555]	1.96	0.24
1:1:245:HIS:N	3:3:49:VAL:O[12_555]	1.96	0.24
1:1:49:ASP:OD2	5:1:500:W54:C3B[12_555]	1.96	0.24
3:3:23:CYS:SG	3:3:162:THR:OG1[12_555]	1.96	0.24
2:2:58:THR:CG2	2:2:252:GLU:CA[2_555]	1.96	0.24
1:1:23:SER:CA	1:1:80:SER:CB[12_555]	1.96	0.24
2:2:32:VAL:CG2	3:3:32:LYS:C[12_555]	1.96	0.24
3:3:212:PHE:CA	4:4:38:SER:C[12_555]	1.96	0.24
3:3:56:ASN:CG	4:4:29:ILE:CG2[12_555]	1.96	0.24
1:1:53:THR:CA	1:1:237:THR:CA[12_555]	1.96	0.24
1:1:21:LYS:N	1:1:79:ILE:N[12_555]	1.96	0.24
3:3:119:PHE:N	4:4:33:LYS:CB[12_555]	1.96	0.24
1:1:45:VAL:N	5:1:500:W54:C1B[12_555]	1.96	0.24
2:2:11:ASP:N	2:2:26:ASP:OD1[11_555]	1.96	0.24
1:1:60:GLN:O	1:1:108:GLN:N[12_555]	1.96	0.24
3:3:6:ILE:CB	3:3:142:THR:N[12_555]	1.96	0.24
1:1:244:LYS:CD	3:3:212:PHE:C[12_555]	1.96	0.24
1:1:44:ASN:CA	5:1:500:W54:C3C[12_555]	1.96	0.24
2:2:34:GLY:N	3:3:34:ILE:C[12_555]	1.96	0.24
1:1:180:PRO:O	3:3:166:VAL:O[12_555]	1.96	0.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:242:LYS:C	3:3:215:ALA:O[12_555]	1.96	0.24
1:1:17:VAL:CG1	1:1:108:GLN:CB[12_555]	1.96	0.24
2:2:53:PRO:CA	2:2:58:THR:CA[3_555]	1.96	0.24
2:2:32:VAL:CG2	3:3:32:LYS:N[12_555]	1.96	0.24
2:2:194:ARG:CZ	3:3:27:TRP:NE1[12_555]	1.96	0.24
1:1:19:ASN:CA	1:1:106:MET:CB[12_555]	1.97	0.23
1:1:20:ILE:C	1:1:79:ILE:N[12_555]	1.97	0.23
3:3:21:SER:O	3:3:117:PHE:CD2[12_555]	1.97	0.23
1:1:176:GLY:O	3:3:150:GLY:CA[12_555]	1.97	0.23
1:1:49:ASP:CA	5:1:500:W54:N3A[12_555]	1.97	0.23
3:3:106:TYR:O	3:3:223:MET:CA[12_555]	1.97	0.23
1:1:75:GLY:C	3:3:218:ASP:OD1[12_555]	1.97	0.23
2:2:17:THR:O	2:2:49:ALA:C[2_555]	1.97	0.23
3:3:37:PRO:N	3:3:37:PRO:CB[12_555]	1.97	0.23
1:1:74:SER:OG	3:3:113:LEU:CG[12_555]	1.97	0.23
1:1:53:THR:CA	1:1:237:THR:N[12_555]	1.97	0.23
1:1:47:PRO:CB	1:1:240:TYR:N[12_555]	1.97	0.23
3:3:23:CYS:O	3:3:162:THR:O[12_555]	1.97	0.23
2:2:55:GLN:N	2:2:57:ASP:CA[3_555]	1.97	0.23
1:1:62:ARG:CD	1:1:112:LYS:N[12_555]	1.97	0.23
2:2:11:ASP:C	2:2:13:ILE:CD1[11_555]	1.97	0.23
1:1:67:ILE:CB	3:3:46:MET:CB[12_555]	1.97	0.23
3:3:106:TYR:CA	3:3:223:MET:O[12_555]	1.97	0.23
2:2:38:TRP:CB	2:2:209:VAL:O[12_555]	1.97	0.23
1:1:42:THR:CG2	1:1:121:PHE:C[12_555]	1.97	0.23
1:1:181:ARG:CA	3:3:165:LEU:CB[12_555]	1.97	0.23
1:1:179:PHE:CA	3:3:151:THR:C[12_555]	1.97	0.23
1:1:13:GLU:CA	3:3:230:HIS:CG[12_555]	1.97	0.23
3:3:210:LEU:O	4:4:37:SER:O[12_555]	1.97	0.23
2:2:46:ASP:CA	2:2:202:ILE:CB[12_555]	1.98	0.22
1:1:7:ILE:N	1:1:276:THR:C[12_555]	1.98	0.22
3:3:222:ARG:C	3:3:225:ARG:CA[12_555]	1.98	0.22
3:3:117:PHE:N	4:4:37:SER:CB[12_555]	1.98	0.22
1:1:65:MET:CB	1:1:70:PHE:CE1[12_555]	1.98	0.22
2:2:40:HIS:CD2	2:2:205:TYR:CG[12_555]	1.98	0.22
1:1:52:GLU:N	1:1:237:THR:CG2[12_555]	1.98	0.22
1:1:47:PRO:CD	1:1:239:ILE:O[12_555]	1.98	0.22
3:3:106:TYR:CG	3:3:224:ALA:CA[12_555]	1.98	0.22
3:3:43:LEU:CG	3:3:43:LEU:CD2[12_555]	1.98	0.22
2:2:178:THR:CG2	4:4:44:ASP:CB[12_555]	1.98	0.22
1:1:28:SER:C	1:1:162:SER:O[12_555]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:112:LYS:C	3:3:42:ASN:ND2[12_555]	1.98	0.22
1:1:250:CYS:C	3:3:39:GLU:C[12_555]	1.98	0.22
1:1:178:PRO:N	3:3:150:GLY:O[12_555]	1.98	0.22
3:3:9:GLY:N	3:3:188:TYR:CE1[12_555]	1.98	0.22
1:1:22:GLU:OE2	1:1:81:ARG:CB[12_555]	1.98	0.22
1:1:240:TYR:C	3:3:216:CYS:SG[12_555]	1.98	0.22
1:1:66:SER:C	3:3:102:ILE:CD1[12_555]	1.98	0.22
1:1:24:HIS:ND1	1:1:82:ILE:CG1[12_555]	1.98	0.22
1:1:48:GLU:CD	1:1:78:HIS:CA[12_555]	1.98	0.22
1:1:62:ARG:NE	1:1:109:ILE:O[12_555]	1.98	0.22
3:3:21:SER:O	3:3:117:PHE:CA[12_555]	1.98	0.22
2:2:54:THR:OG1	2:2:57:ASP:N[3_555]	1.98	0.22
1:1:24:HIS:ND1	1:1:82:ILE:CA[12_555]	1.98	0.22
2:2:187:PRO:C	3:3:33:GLU:CD[12_555]	1.98	0.22
1:1:112:LYS:O	3:3:42:ASN:CB[12_555]	1.98	0.22
2:2:91:ILE:CG1	2:2:95:ASN:CB[2_555]	1.98	0.22
1:1:116:PHE:CZ	3:3:42:ASN:C[12_555]	1.98	0.22
1:1:77:VAL:CG1	3:3:217:LYS:CD[12_555]	1.99	0.21
3:3:106:TYR:CG	3:3:224:ALA:CB[12_555]	1.99	0.21
3:3:212:PHE:CZ	4:4:35:ALA:CA[12_555]	1.99	0.21
2:2:45:GLN:CG	2:2:107:THR:O[12_555]	1.99	0.21
3:3:222:ARG:CB	3:3:226:ASP:O[12_555]	1.99	0.21
3:3:118:MET:CA	4:4:34:ASP:N[12_555]	1.99	0.21
1:1:177:GLN:O	3:3:150:GLY:CA[12_555]	1.99	0.21
3:3:17:ASP:C	3:3:94:LEU:CG[12_555]	1.99	0.21
1:1:242:LYS:N	3:3:216:CYS:N[12_555]	1.99	0.21
1:1:246:THR:CB	3:3:49:VAL:CB[12_555]	1.99	0.21
1:1:75:GLY:CA	3:3:219:PHE:N[12_555]	1.99	0.21
1:1:177:GLN:CG	3:3:148:MET:CA[12_555]	1.99	0.21
2:2:32:VAL:O	3:3:32:LYS:CG[12_555]	1.99	0.21
3:3:211:CYS:CA	4:4:38:SER:CA[12_555]	1.99	0.21
1:1:37:ALA:N	1:1:185:PRO:CB[12_555]	1.99	0.21
2:2:38:TRP:CB	2:2:210:PRO:O[12_555]	1.99	0.21
1:1:47:PRO:CA	1:1:239:ILE:CG2[12_555]	1.99	0.21
1:1:13:GLU:CA	3:3:230:HIS:CA[12_555]	1.99	0.21
2:2:178:THR:C	4:4:42:ARG:CZ[12_555]	1.99	0.21
1:1:75:GLY:O	3:3:218:ASP:CA[12_555]	1.99	0.21
2:2:202:ILE:N	3:3:32:LYS:CE[12_555]	1.99	0.21
2:2:46:ASP:O	2:2:202:ILE:CD1[12_555]	1.99	0.21
1:1:247:LYS:NZ	2:2:185:ILE:O[12_555]	1.99	0.21
2:2:182:ASN:CG	4:4:41:SER:C[12_555]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:179:PHE:CG	3:3:133:TYR:CD2[12_555]	1.99	0.21
3:3:27:TRP:CH2	3:3:158:GLY:O[12_555]	1.99	0.21
1:1:242:LYS:O	3:3:214:SER:O[12_555]	1.99	0.21
1:1:77:VAL:O	3:3:217:LYS:CE[12_555]	1.99	0.21
1:1:242:LYS:CA	3:3:214:SER:O[12_555]	1.99	0.21
3:3:13:PHE:CG	3:3:167:VAL:CG1[12_555]	1.99	0.21
1:1:181:ARG:CB	3:3:165:LEU:CD2[12_555]	1.99	0.21
1:1:33:LEU:CB	1:1:169:MET:SD[12_555]	1.99	0.21
1:1:123:SER:C	3:3:114:ARG:CD[12_555]	1.99	0.21
2:2:201:LEU:O	3:3:32:LYS:NZ[12_555]	1.99	0.21
3:3:37:PRO:N	3:3:37:PRO:CG[12_555]	2.00	0.20
1:1:116:PHE:CD1	3:3:40:VAL:CB[12_555]	2.00	0.20
1:1:31:ALA:CB	1:1:169:MET:CB[12_555]	2.00	0.20
1:1:26:THR:N	1:1:223:ARG:CA[12_555]	2.00	0.20
1:1:27:THR:OG1	1:1:223:ARG:NE[12_555]	2.00	0.20
3:3:209:MET:CB	4:4:32:PHE:C[12_555]	2.00	0.20
2:2:21:SER:N	2:2:101:LEU:CG[2_555]	2.00	0.20
2:2:13:ILE:CA	2:2:13:ILE:CA[11_555]	2.00	0.20
1:1:122:ASP:N	3:3:50:ASP:OD1[12_555]	2.00	0.20
2:2:179:LEU:CA	4:4:42:ARG:CG[12_555]	2.00	0.20
1:1:10:VAL:CG1	1:1:277:ALA:O[12_555]	2.00	0.20
3:3:18:ASP:CG	3:3:94:LEU:CD2[12_555]	2.00	0.20
2:2:18:ARG:N	2:2:49:ALA:CB[2_555]	2.00	0.20
1:1:48:GLU:OE2	1:1:78:HIS:CG[12_555]	2.00	0.20
3:3:212:PHE:N	4:4:38:SER:C[12_555]	2.00	0.20
1:1:71:LEU:C	3:3:47:CYS:SG[12_555]	2.00	0.20
1:1:244:LYS:CE	3:3:212:PHE:O[12_555]	2.00	0.20
2:2:20:ASP:OD2	2:2:103:ARG:CB[2_555]	2.00	0.20
2:2:41:TYR:N	2:2:250:CYS:O[12_555]	2.00	0.20
1:1:16:VAL:C	1:1:107:ALA:CA[12_555]	2.00	0.20
2:2:201:LEU:CA	3:3:32:LYS:NZ[12_555]	2.00	0.20
3:3:119:PHE:C	4:4:33:LYS:CA[12_555]	2.00	0.20
2:2:89:MET:CA	2:2:258:ALA:C[2_555]	2.00	0.20
1:1:244:LYS:C	3:3:49:VAL:O[12_555]	2.00	0.20
1:1:241:HIS:CG	3:3:216:CYS:CA[12_555]	2.00	0.20
1:1:245:HIS:CA	3:3:50:ASP:O[12_555]	2.00	0.20
1:1:244:LYS:NZ	3:3:212:PHE:CA[12_555]	2.00	0.20
1:1:23:SER:N	1:1:80:SER:CB[12_555]	2.00	0.20
2:2:17:THR:CG2	2:2:49:ALA:N[2_555]	2.01	0.19
3:3:68:TYR:CE1	4:4:27:PHE:CZ[12_555]	2.01	0.19
2:2:46:ASP:O	2:2:202:ILE:CG1[12_555]	2.01	0.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:247:LYS:NZ	2:2:186:PHE:C[12_555]	2.01	0.19
1:1:63:ASP:CB	1:1:111:ARG:CZ[12_555]	2.01	0.19
3:3:70:VAL:CB	4:4:31:TYR:CB[12_555]	2.01	0.19
1:1:51:ILE:CG2	1:1:127:LEU:CA[12_555]	2.01	0.19
2:2:40:HIS:NE2	2:2:205:TYR:CA[12_555]	2.01	0.19
3:3:25:LEU:C	3:3:160:GLN:CG[12_555]	2.01	0.19
1:1:20:ILE:O	1:1:79:ILE:CB[12_555]	2.01	0.19
3:3:22:PRO:N	3:3:117:PHE:CG[12_555]	2.01	0.19
3:3:23:CYS:CA	3:3:117:PHE:O[12_555]	2.01	0.19
1:1:33:LEU:CD2	1:1:182:PHE:CE2[12_555]	2.01	0.19
1:1:61:THR:CG2	3:3:230:HIS:CG[12_555]	2.01	0.19
1:1:246:THR:CB	3:3:46:MET:O[12_555]	2.01	0.19
1:1:179:PHE:CE2	3:3:133:TYR:CE2[12_555]	2.01	0.19
2:2:13:ILE:N	2:2:13:ILE:CD1[11_555]	2.01	0.19
3:3:8:PRO:C	3:3:188:TYR:OH[12_555]	2.01	0.19
3:3:175:PHE:CZ	3:3:226:ASP:CB[12_555]	2.01	0.19
1:1:177:GLN:CB	3:3:148:MET:CA[12_555]	2.01	0.19
1:1:10:VAL:CG2	1:1:278:ILE:O[12_555]	2.01	0.19
1:1:39:THR:O	3:3:30:PRO:CA[12_555]	2.01	0.19
1:1:69:SER:CB	3:3:103:ALA:N[12_555]	2.01	0.19
3:3:18:ASP:OD1	3:3:94:LEU:CD2[12_555]	2.01	0.19
3:3:53:ILE:CB	4:4:39:GLY:N[12_555]	2.01	0.19
2:2:62:ARG:O	2:2:255:GLY:C[2_555]	2.01	0.19
2:2:18:ARG:N	2:2:50:ILE:N[2_555]	2.01	0.19
1:1:5:ASN:O	1:1:276:THR:CG2[12_555]	2.01	0.19
2:2:29:ALA:CB	3:3:29:HIS:O[12_555]	2.01	0.19
3:3:15:THR:O	3:3:109:TRP:CZ3[12_555]	2.01	0.19
3:3:209:MET:CE	4:4:32:PHE:CD2[12_555]	2.01	0.19
3:3:16:THR:C	3:3:89:ILE:CG2[12_555]	2.01	0.19
3:3:56:ASN:OD1	4:4:29:ILE:CB[12_555]	2.01	0.19
1:1:115:LEU:O	3:3:41:LYS:N[12_555]	2.01	0.19
1:1:240:TYR:CE2	3:3:169:TRP:CA[12_555]	2.01	0.19
1:1:179:PHE:CB	3:3:151:THR:CG2[12_555]	2.01	0.19
1:1:45:VAL:C	5:1:500:W54:C1B[12_555]	2.01	0.19
1:1:178:PRO:N	3:3:150:GLY:C[12_555]	2.01	0.19
3:3:67:MET:O	4:4:27:PHE:C[12_555]	2.01	0.19
1:1:252:ARG:CG	3:3:41:LYS:CE[12_555]	2.02	0.18
3:3:106:TYR:CD2	3:3:106:TYR:CE1[12_555]	2.02	0.18
3:3:52:LEU:CD2	4:4:38:SER:OG[12_555]	2.02	0.18
3:3:67:MET:O	4:4:27:PHE:CD1[12_555]	2.02	0.18
1:1:8:ASP:OD1	1:1:258:PRO:CG[12_555]	2.02	0.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:42:THR:CB	1:1:122:ASP:N[12_555]	2.02	0.18
3:3:222:ARG:C	3:3:225:ARG:N[12_555]	2.02	0.18
1:1:53:THR:O	1:1:237:THR:N[12_555]	2.02	0.18
2:2:46:ASP:C	2:2:202:ILE:CD1[12_555]	2.02	0.18
1:1:74:SER:CB	3:3:113:LEU:CG[12_555]	2.02	0.18
1:1:44:ASN:O	5:1:500:W54:C1B[12_555]	2.02	0.18
1:1:64:GLU:OE2	3:3:104:SER:N[12_555]	2.02	0.18
2:2:46:ASP:CB	2:2:202:ILE:CG2[12_555]	2.02	0.18
1:1:115:LEU:CB	3:3:42:ASN:OD1[12_555]	2.02	0.18
2:2:182:ASN:CG	4:4:42:ARG:CA[12_555]	2.02	0.18
2:2:179:LEU:CG	4:4:42:ARG:CG[12_555]	2.02	0.18
2:2:62:ARG:NE	2:2:99:HIS:CB[2_555]	2.02	0.18
1:1:22:GLU:CB	1:1:81:ARG:N[12_555]	2.02	0.18
3:3:212:PHE:N	4:4:37:SER:C[12_555]	2.02	0.18
1:1:42:THR:N	1:1:186:PHE:CG[12_555]	2.02	0.18
1:1:49:ASP:OD2	5:1:500:W54:C4B[12_555]	2.02	0.18
2:2:55:GLN:N	2:2:57:ASP:CB[3_555]	2.02	0.18
3:3:56:ASN:C	4:4:26:TYR:C[12_555]	2.02	0.18
1:1:244:LYS:CB	3:3:214:SER:N[12_555]	2.02	0.18
1:1:13:GLU:N	3:3:229:LEU:O[12_555]	2.02	0.18
3:3:107:THR:OG1	3:3:223:MET:CG[12_555]	2.02	0.18
2:2:32:VAL:CB	3:3:32:LYS:N[12_555]	2.02	0.18
2:2:58:THR:CG2	2:2:253:PHE:N[2_555]	2.03	0.17
1:1:70:PHE:CE2	3:3:43:LEU:CB[12_555]	2.03	0.17
3:3:69:THR:O	4:4:30:ASN:N[12_555]	2.03	0.17
1:1:125:ILE:C	3:3:166:VAL:N[12_555]	2.03	0.17
1:1:69:SER:CB	3:3:102:ILE:C[12_555]	2.03	0.17
3:3:12:GLN:CA	3:3:134:THR:C[12_555]	2.03	0.17
2:2:40:HIS:N	2:2:103:ARG:CD[12_555]	2.03	0.17
2:2:45:GLN:C	2:2:107:THR:N[12_555]	2.03	0.17
1:1:8:ASP:C	1:1:256:ALA:O[12_555]	2.03	0.17
2:2:13:ILE:C	2:2:13:ILE:C[11_555]	2.03	0.17
1:1:253:PRO:CB	4:4:43:LEU:O[12_555]	2.03	0.17
2:2:181:GLY:O	4:4:41:SER:CA[12_555]	2.03	0.17
1:1:26:THR:N	1:1:144:GLN:O[12_555]	2.03	0.17
3:3:118:MET:SD	4:4:34:ASP:CA[12_555]	2.03	0.17
3:3:118:MET:CB	4:4:34:ASP:O[12_555]	2.03	0.17
1:1:27:THR:CB	1:1:144:GLN:OE1[12_555]	2.03	0.17
2:2:18:ARG:CG	2:2:51:ASN:CA[2_555]	2.03	0.17
1:1:53:THR:OG1	1:1:237:THR:O[12_555]	2.03	0.17
2:2:42:LEU:CG	2:2:249:MET:SD[12_555]	2.03	0.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:19:ASN:C	1:1:106:MET:SD[12_555]	2.03	0.17
3:3:67:MET:N	4:4:27:PHE:O[12_555]	2.03	0.17
2:2:45:GLN:O	2:2:107:THR:CA[12_555]	2.03	0.17
1:1:60:GLN:CB	1:1:108:GLN:CB[12_555]	2.03	0.17
1:1:52:GLU:OE1	1:1:143:MET:SD[12_555]	2.03	0.17
2:2:15:GLN:OE1	2:2:48:THR:OG1[2_555]	2.03	0.17
1:1:60:GLN:CG	1:1:108:GLN:NE2[12_555]	2.03	0.17
1:1:115:LEU:C	3:3:41:LYS:CA[12_555]	2.03	0.17
1:1:64:GLU:CA	3:3:101:GLU:O[12_555]	2.03	0.17
3:3:10:SER:OG	3:3:141:PRO:CD[12_555]	2.03	0.17
1:1:177:GLN:N	3:3:149:LEU:O[12_555]	2.04	0.16
1:1:247:LYS:CE	2:2:186:PHE:C[12_555]	2.04	0.16
3:3:57:ASN:N	4:4:26:TYR:O[12_555]	2.04	0.16
1:1:243:ALA:CB	3:3:48:GLN:N[12_555]	2.04	0.16
1:1:64:GLU:O	3:3:102:ILE:O[12_555]	2.04	0.16
3:3:223:MET:N	3:3:225:ARG:NE[12_555]	2.04	0.16
3:3:11:GLY:O	3:3:134:THR:CB[12_555]	2.04	0.16
3:3:14:MET:CE	3:3:88:ASP:CG[12_555]	2.04	0.16
1:1:16:VAL:CG1	1:1:259:TYR:CE1[12_555]	2.04	0.16
3:3:38:GLY:CA	3:3:38:GLY:O[12_555]	2.04	0.16
1:1:49:ASP:CB	5:1:500:W54:C4B[12_555]	2.04	0.16
1:1:77:VAL:CB	3:3:217:LYS:CE[12_555]	2.04	0.16
1:1:26:THR:CG2	1:1:221:CYS:O[12_555]	2.04	0.16
2:2:54:THR:CA	2:2:57:ASP:N[3_555]	2.04	0.16
2:2:60:SER:C	2:2:99:HIS:NE2[2_555]	2.04	0.16
1:1:179:PHE:CD2	3:3:133:TYR:CE2[12_555]	2.04	0.16
3:3:222:ARG:CB	3:3:226:ASP:C[12_555]	2.04	0.16
2:2:53:PRO:CA	2:2:58:THR:N[3_555]	2.04	0.16
3:3:9:GLY:C	3:3:188:TYR:CZ[12_555]	2.04	0.16
3:3:116:SER:O	4:4:37:SER:CB[12_555]	2.04	0.16
1:1:67:ILE:C	3:3:102:ILE:CD1[12_555]	2.04	0.16
3:3:43:LEU:CD2	3:3:43:LEU:CD2[12_555]	2.04	0.16
3:3:12:GLN:O	3:3:188:TYR:O[12_555]	2.04	0.16
1:1:75:GLY:C	3:3:218:ASP:OD2[12_555]	2.04	0.16
1:1:178:PRO:C	3:3:150:GLY:C[12_555]	2.04	0.16
1:1:178:PRO:N	3:3:150:GLY:N[12_555]	2.04	0.16
1:1:43:SER:C	1:1:123:SER:OG[12_555]	2.04	0.16
1:1:253:PRO:O	4:4:44:ASP:O[12_555]	2.04	0.16
1:1:62:ARG:O	3:3:105:TYR:OH[12_555]	2.04	0.16
2:2:36:GLY:C	2:2:208:ALA:C[12_555]	2.04	0.16
3:3:57:ASN:CA	4:4:26:TYR:CB[12_555]	2.04	0.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:241:HIS:O	3:3:216:CYS:CB[12_555]	2.04	0.16
2:2:43:THR:CA	2:2:249:MET:CB[12_555]	2.04	0.16
3:3:13:PHE:CA	3:3:133:TYR:OH[12_555]	2.04	0.16
1:1:243:ALA:CB	3:3:48:GLN:C[12_555]	2.04	0.16
1:1:64:GLU:N	3:3:101:GLU:O[12_555]	2.04	0.16
1:1:177:GLN:N	3:3:148:MET:O[12_555]	2.04	0.16
2:2:179:LEU:CD2	4:4:42:ARG:CD[12_555]	2.04	0.16
2:2:11:ASP:CA	2:2:26:ASP:CB[11_555]	2.04	0.16
2:2:182:ASN:OD1	4:4:41:SER:CA[12_555]	2.04	0.16
1:1:124:GLU:CD	3:3:115:PHE:CD1[12_555]	2.04	0.16
2:2:13:ILE:C	2:2:13:ILE:CG2[11_555]	2.04	0.16
3:3:11:GLY:CA	3:3:134:THR:CA[12_555]	2.04	0.16
1:1:245:HIS:CE1	3:3:212:PHE:CB[12_555]	2.04	0.16
1:1:249:TRP:NE1	2:2:35:TYR:CZ[12_555]	2.04	0.16
1:1:25:HIS:CA	1:1:223:ARG:CA[12_555]	2.04	0.16
1:1:6:TYR:CD2	1:1:278:ILE:O[12_555]	2.04	0.16
1:1:53:THR:C	1:1:237:THR:N[12_555]	2.05	0.15
2:2:178:THR:N	4:4:44:ASP:CB[12_555]	2.05	0.15
2:2:38:TRP:CE2	2:2:210:PRO:CB[12_555]	2.05	0.15
3:3:70:VAL:CG1	4:4:31:TYR:CA[12_555]	2.05	0.15
1:1:41:HIS:CE1	1:1:188:SER:O[12_555]	2.05	0.15
1:1:254:PRO:CG	4:4:43:LEU:CD2[12_555]	2.05	0.15
3:3:118:MET:O	4:4:33:LYS:C[12_555]	2.05	0.15
2:2:18:ARG:CB	2:2:51:ASN:CB[2_555]	2.05	0.15
3:3:22:PRO:CD	3:3:131:LEU:CD2[12_555]	2.05	0.15
2:2:174:ASN:CG	4:4:44:ASP:OD2[12_555]	2.05	0.15
1:1:249:TRP:O	3:3:39:GLU:C[12_555]	2.05	0.15
1:1:176:GLY:CA	3:3:149:LEU:C[12_555]	2.05	0.15
2:2:46:ASP:N	2:2:106:TYR:C[12_555]	2.05	0.15
2:2:44:PRO:CD	2:2:248:PRO:N[12_555]	2.05	0.15
3:3:27:TRP:CH2	3:3:158:GLY:C[12_555]	2.05	0.15
3:3:209:MET:C	4:4:32:PHE:C[12_555]	2.05	0.15
2:2:35:TYR:O	3:3:36:ILE:CD1[12_555]	2.05	0.15
2:2:194:ARG:NE	3:3:27:TRP:NE1[12_555]	2.05	0.15
3:3:6:ILE:CD1	3:3:143:THR:N[12_555]	2.05	0.15
1:1:126:THR:OG1	3:3:166:VAL:C[12_555]	2.05	0.15
1:1:244:LYS:O	3:3:49:VAL:C[12_555]	2.05	0.15
2:2:44:PRO:N	2:2:249:MET:CG[12_555]	2.05	0.15
3:3:58:VAL:CB	4:4:26:TYR:CE1[12_555]	2.05	0.15
1:1:8:ASP:N	1:1:276:THR:CA[12_555]	2.05	0.15
1:1:34:LEU:C	3:3:25:LEU:CB[12_555]	2.05	0.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:38:GLU:CB	3:3:28:TYR:O[12_555]	2.05	0.15
2:2:179:LEU:CG	4:4:42:ARG:NE[12_555]	2.05	0.15
2:2:53:PRO:O	2:2:57:ASP:C[3_555]	2.05	0.15
1:1:68:GLU:CG	3:3:99:ILE:N[12_555]	2.06	0.14
1:1:246:THR:O	2:2:185:ILE:CG1[12_555]	2.06	0.14
3:3:13:PHE:CZ	3:3:167:VAL:CG1[12_555]	2.06	0.14
1:1:74:SER:OG	3:3:112:SER:C[12_555]	2.06	0.14
1:1:30:SER:OG	1:1:148:VAL:CA[12_555]	2.06	0.14
1:1:65:MET:CE	1:1:112:LYS:CG[12_555]	2.06	0.14
2:2:89:MET:N	2:2:259:LYS:N[2_555]	2.06	0.14
1:1:124:GLU:CA	3:3:114:ARG:O[12_555]	2.06	0.14
2:2:62:ARG:CG	2:2:255:GLY:C[2_555]	2.06	0.14
1:1:51:ILE:CB	1:1:237:THR:OG1[12_555]	2.06	0.14
1:1:124:GLU:C	3:3:114:ARG:CA[12_555]	2.06	0.14
2:2:17:THR:CB	2:2:48:THR:O[2_555]	2.06	0.14
1:1:55:TYR:CG	1:1:81:ARG:NH2[12_555]	2.06	0.14
1:1:126:THR:OG1	3:3:167:VAL:CA[12_555]	2.06	0.14
1:1:246:THR:CA	3:3:49:VAL:CG1[12_555]	2.06	0.14
2:2:47:ALA:CA	2:2:202:ILE:CD1[12_555]	2.06	0.14
1:1:35:ASP:OD1	1:1:185:PRO:CB[12_555]	2.06	0.14
1:1:22:GLU:OE2	1:1:82:ILE:N[12_555]	2.06	0.14
3:3:68:TYR:C	4:4:30:ASN:CG[12_555]	2.06	0.14
1:1:124:GLU:CD	3:3:114:ARG:C[12_555]	2.06	0.14
3:3:52:LEU:CA	4:4:39:GLY:O[12_555]	2.06	0.14
3:3:6:ILE:CG2	3:3:141:PRO:CA[12_555]	2.06	0.14
3:3:16:THR:CA	3:3:89:ILE:CB[12_555]	2.06	0.14
1:1:116:PHE:CZ	3:3:40:VAL:CG1[12_555]	2.06	0.14
3:3:222:ARG:N	3:3:225:ARG:CA[12_555]	2.06	0.14
1:1:191:SER:CB	2:2:33:VAL:N[12_555]	2.06	0.14
1:1:178:PRO:CA	3:3:151:THR:N[12_555]	2.06	0.14
3:3:97:THR:OG1	4:4:40:ALA:CB[12_555]	2.06	0.14
1:1:7:ILE:CG1	1:1:275:THR:CB[12_555]	2.06	0.14
2:2:187:PRO:N	3:3:33:GLU:OE1[12_555]	2.06	0.14
1:1:62:ARG:NH2	1:1:109:ILE:C[12_555]	2.06	0.14
1:1:26:THR:C	1:1:163:TRP:CE3[12_555]	2.06	0.14
3:3:21:SER:CB	3:3:117:PHE:CE2[12_555]	2.06	0.14
3:3:43:LEU:CG	3:3:43:LEU:CD1[12_555]	2.06	0.14
1:1:6:TYR:O	1:1:276:THR:CA[12_555]	2.06	0.14
2:2:91:ILE:CD1	2:2:95:ASN:CG[2_555]	2.07	0.13
1:1:24:HIS:CG	1:1:82:ILE:CG1[12_555]	2.07	0.13
3:3:23:CYS:C	3:3:162:THR:CA[12_555]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:12:ASN:O	3:3:230:HIS:C[12_555]	2.07	0.13
1:1:35:ASP:O	3:3:25:LEU:O[12_555]	2.07	0.13
3:3:56:ASN:C	4:4:27:PHE:CA[12_555]	2.07	0.13
3:3:210:LEU:C	4:4:37:SER:O[12_555]	2.07	0.13
3:3:210:LEU:N	4:4:32:PHE:C[12_555]	2.07	0.13
1:1:23:SER:C	1:1:80:SER:OG[12_555]	2.07	0.13
1:1:115:LEU:CD2	3:3:42:ASN:CG[12_555]	2.07	0.13
3:3:9:GLY:CA	3:3:188:TYR:OH[12_555]	2.07	0.13
1:1:74:SER:CA	3:3:112:SER:C[12_555]	2.07	0.13
1:1:177:GLN:CA	3:3:149:LEU:CA[12_555]	2.07	0.13
2:2:220:TRP:CZ2	3:3:35:SER:OG[12_555]	2.07	0.13
1:1:108:GLN:OE1	3:3:220:CYS:CB[12_555]	2.07	0.13
3:3:66:SER:C	4:4:28:ASN:O[12_555]	2.07	0.13
3:3:66:SER:O	4:4:28:ASN:CA[12_555]	2.07	0.13
1:1:245:HIS:ND1	3:3:50:ASP:O[12_555]	2.07	0.13
2:2:18:ARG:CG	2:2:51:ASN:N[2_555]	2.07	0.13
3:3:57:ASN:N	4:4:26:TYR:CA[12_555]	2.07	0.13
1:1:17:VAL:CG1	1:1:107:ALA:C[12_555]	2.07	0.13
1:1:116:PHE:CA	3:3:45:GLU:OE2[12_555]	2.07	0.13
3:3:211:CYS:C	4:4:37:SER:C[12_555]	2.07	0.13
1:1:48:GLU:OE1	1:1:78:HIS:CG[12_555]	2.08	0.12
1:1:41:HIS:CD2	1:1:186:PHE:CZ[12_555]	2.08	0.12
1:1:69:SER:N	3:3:102:ILE:CG1[12_555]	2.08	0.12
1:1:45:VAL:CG2	5:1:500:W54:C5B[12_555]	2.08	0.12
3:3:119:PHE:C	4:4:33:LYS:CD[12_555]	2.08	0.12
1:1:177:GLN:NE2	3:3:149:LEU:N[12_555]	2.08	0.12
1:1:50:ALA:CA	1:1:127:LEU:CG[12_555]	2.08	0.12
3:3:12:GLN:NE2	3:3:187:GLY:O[12_555]	2.08	0.12
1:1:45:VAL:CA	5:1:500:W54:C6B[12_555]	2.08	0.12
1:1:75:GLY:N	3:3:112:SER:N[12_555]	2.08	0.12
1:1:5:ASN:CA	1:1:276:THR:CG2[12_555]	2.08	0.12
1:1:64:GLU:N	3:3:105:TYR:CE2[12_555]	2.08	0.12
3:3:17:ASP:O	3:3:94:LEU:CD1[12_555]	2.08	0.12
1:1:34:LEU:CA	3:3:24:ALA:CB[12_555]	2.08	0.12
2:2:36:GLY:O	2:2:208:ALA:C[12_555]	2.08	0.12
1:1:251:PRO:N	3:3:40:VAL:C[12_555]	2.08	0.12
1:1:25:HIS:ND1	1:1:224:ILE:CA[12_555]	2.08	0.12
1:1:126:THR:C	3:3:166:VAL:CB[12_555]	2.08	0.12
1:1:249:TRP:CD1	2:2:35:TYR:CD1[12_555]	2.08	0.12
3:3:67:MET:O	4:4:28:ASN:CA[12_555]	2.08	0.12
2:2:45:GLN:N	2:2:106:TYR:C[12_555]	2.08	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:177:GLN:OE1	3:3:145:LYS:O[12_555]	2.08	0.12
3:3:21:SER:O	3:3:116:SER:C[12_555]	2.08	0.12
1:1:242:LYS:C	3:3:215:ALA:C[12_555]	2.08	0.12
1:1:241:HIS:ND1	3:3:215:ALA:O[12_555]	2.08	0.12
1:1:76:CYS:C	3:3:218:ASP:OD2[12_555]	2.08	0.12
1:1:67:ILE:O	3:3:46:MET:CB[12_555]	2.08	0.12
1:1:183:SER:N	3:3:164:SER:C[12_555]	2.08	0.12
1:1:36:ALA:CA	3:3:28:TYR:CB[12_555]	2.08	0.12
3:3:57:ASN:O	4:4:26:TYR:CB[12_555]	2.08	0.12
1:1:6:TYR:OH	3:3:62:VAL:CG2[12_555]	2.08	0.12
3:3:18:ASP:N	3:3:94:LEU:CB[12_555]	2.08	0.12
1:1:53:THR:CG2	1:1:237:THR:O[12_555]	2.08	0.12
1:1:73:ARG:CA	3:3:219:PHE:CD1[12_555]	2.08	0.12
1:1:22:GLU:CA	1:1:81:ARG:N[12_555]	2.08	0.12
1:1:65:MET:N	3:3:105:TYR:CG[12_555]	2.08	0.12
2:2:32:VAL:O	3:3:32:LYS:CD[12_555]	2.08	0.12
1:1:177:GLN:CD	3:3:149:LEU:N[12_555]	2.08	0.12
1:1:17:VAL:C	1:1:107:ALA:O[12_555]	2.08	0.12
1:1:177:GLN:CA	3:3:149:LEU:C[12_555]	2.09	0.11
1:1:65:MET:C	1:1:115:LEU:CD2[12_555]	2.09	0.11
3:3:37:PRO:C	3:3:37:PRO:C[12_555]	2.09	0.11
3:3:118:MET:O	4:4:34:ASP:N[12_555]	2.09	0.11
1:1:13:GLU:CG	3:3:231:ILE:CA[12_555]	2.09	0.11
2:2:91:ILE:CB	2:2:95:ASN:OD1[2_555]	2.09	0.11
1:1:240:TYR:CE1	3:3:111:GLY:CA[12_555]	2.09	0.11
1:1:60:GLN:C	1:1:108:GLN:CG[12_555]	2.09	0.11
1:1:77:VAL:CG1	3:3:218:ASP:N[12_555]	2.09	0.11
2:2:47:ALA:N	2:2:202:ILE:CD1[12_555]	2.09	0.11
1:1:179:PHE:C	3:3:151:THR:O[12_555]	2.09	0.11
2:2:17:THR:CA	2:2:49:ALA:N[2_555]	2.09	0.11
2:2:64:TYR:CD2	2:2:257:ARG:CA[2_555]	2.09	0.11
2:2:62:ARG:NE	2:2:254:SER:O[2_555]	2.09	0.11
3:3:106:TYR:CE2	3:3:106:TYR:CE2[12_555]	2.09	0.11
1:1:39:THR:OG1	3:3:28:TYR:CE1[12_555]	2.09	0.11
1:1:244:LYS:C	3:3:49:VAL:C[12_555]	2.09	0.11
1:1:124:GLU:CB	3:3:114:ARG:N[12_555]	2.09	0.11
2:2:43:THR:CA	2:2:249:MET:N[12_555]	2.09	0.11
3:3:23:CYS:N	3:3:163:ILE:O[12_555]	2.09	0.11
2:2:18:ARG:CG	2:2:51:ASN:ND2[2_555]	2.09	0.11
3:3:209:MET:CA	4:4:32:PHE:N[12_555]	2.09	0.11
3:3:118:MET:O	4:4:32:PHE:O[12_555]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:30:SER:O	1:1:147:TYR:C[12_555]	2.09	0.11
2:2:179:LEU:CB	4:4:42:ARG:CB[12_555]	2.09	0.11
1:1:44:ASN:O	5:1:500:W54:C4C[12_555]	2.09	0.11
2:2:41:TYR:CB	2:2:250:CYS:CB[12_555]	2.09	0.11
1:1:48:GLU:CA	1:1:239:ILE:CG1[12_555]	2.09	0.11
1:1:30:SER:CA	1:1:147:TYR:O[12_555]	2.09	0.11
3:3:106:TYR:C	3:3:224:ALA:CA[12_555]	2.09	0.11
2:2:18:ARG:NE	2:2:50:ILE:O[2_555]	2.09	0.11
1:1:63:ASP:C	3:3:105:TYR:CE2[12_555]	2.09	0.11
2:2:29:ALA:CA	3:3:29:HIS:O[12_555]	2.09	0.11
1:1:15:LEU:O	1:1:111:ARG:CD[12_555]	2.09	0.11
2:2:178:THR:CB	4:4:44:ASP:C[12_555]	2.09	0.11
1:1:51:ILE:CA	1:1:237:THR:OG1[12_555]	2.09	0.11
3:3:26:PRO:CA	3:3:161:SER:C[12_555]	2.09	0.11
1:1:249:TRP:C	3:3:39:GLU:CA[12_555]	2.09	0.11
3:3:117:PHE:C	4:4:37:SER:CB[12_555]	2.09	0.11
1:1:179:PHE:CE2	3:3:135:PRO:CD[12_555]	2.09	0.11
1:1:74:SER:O	3:3:111:GLY:CA[12_555]	2.09	0.11
1:1:18:PRO:CB	1:1:103:LEU:O[12_555]	2.09	0.11
2:2:54:THR:CG2	2:2:59:SER:C[3_555]	2.09	0.11
1:1:246:THR:N	3:3:49:VAL:O[12_555]	2.09	0.11
1:1:34:LEU:N	3:3:24:ALA:CB[12_555]	2.09	0.11
3:3:58:VAL:CB	4:4:26:TYR:CG[12_555]	2.10	0.10
2:2:37:VAL:CG2	2:2:206:VAL:C[12_555]	2.10	0.10
3:3:16:THR:OG1	3:3:89:ILE:CB[12_555]	2.10	0.10
2:2:55:GLN:N	2:2:57:ASP:C[3_555]	2.10	0.10
1:1:41:HIS:C	1:1:186:PHE:N[12_555]	2.10	0.10
3:3:97:THR:CG2	4:4:40:ALA:O[12_555]	2.10	0.10
1:1:62:ARG:CA	3:3:105:TYR:CZ[12_555]	2.10	0.10
1:1:61:THR:OG1	3:3:230:HIS:CD2[12_555]	2.10	0.10
2:2:46:ASP:CA	2:2:202:ILE:C[12_555]	2.10	0.10
3:3:209:MET:SD	4:4:32:PHE:CE1[12_555]	2.10	0.10
1:1:22:GLU:C	1:1:80:SER:C[12_555]	2.10	0.10
1:1:71:LEU:O	3:3:47:CYS:CB[12_555]	2.10	0.10
1:1:17:VAL:O	1:1:107:ALA:CB[12_555]	2.10	0.10
1:1:115:LEU:CB	3:3:42:ASN:N[12_555]	2.10	0.10
3:3:15:THR:CG2	3:3:109:TRP:CZ3[12_555]	2.10	0.10
2:2:194:ARG:CD	3:3:27:TRP:NE1[12_555]	2.10	0.10
2:2:91:ILE:CB	2:2:95:ASN:CG[2_555]	2.10	0.10
2:2:54:THR:C	2:2:57:ASP:CA[3_555]	2.10	0.10
3:3:8:PRO:CG	3:3:139:ASP:OD1[12_555]	2.10	0.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:109:ILE:CG1	3:3:217:LYS:O[12_555]	2.10	0.10
1:1:126:THR:CA	3:3:166:VAL:O[12_555]	2.10	0.10
3:3:221:LEU:C	3:3:225:ARG:C[12_555]	2.10	0.10
3:3:221:LEU:O	3:3:225:ARG:O[12_555]	2.10	0.10
2:2:38:TRP:O	2:2:205:TYR:CE2[12_555]	2.10	0.10
3:3:68:TYR:CD2	4:4:28:ASN:ND2[12_555]	2.10	0.10
1:1:15:LEU:N	1:1:111:ARG:CD[12_555]	2.10	0.10
1:1:250:CYS:N	3:3:39:GLU:CB[12_555]	2.10	0.10
1:1:75:GLY:O	3:3:218:ASP:OD2[12_555]	2.10	0.10
1:1:183:SER:CA	3:3:164:SER:CA[12_555]	2.10	0.10
1:1:253:PRO:CA	4:4:43:LEU:O[12_555]	2.10	0.10
1:1:47:PRO:CD	1:1:239:ILE:C[12_555]	2.10	0.10
3:3:220:CYS:C	3:3:226:ASP:OD1[12_555]	2.10	0.10
1:1:245:HIS:CD2	3:3:52:LEU:N[12_555]	2.10	0.10
1:1:125:ILE:N	3:3:114:ARG:CA[12_555]	2.10	0.10
1:1:28:SER:CA	1:1:146:MET:SD[12_555]	2.10	0.10
3:3:9:GLY:N	3:3:188:TYR:OH[12_555]	2.10	0.10
3:3:17:ASP:CA	3:3:87:VAL:O[12_555]	2.10	0.10
2:2:52:LYS:O	2:2:61:ASN:CG[3_555]	2.10	0.10
1:1:64:GLU:N	3:3:105:TYR:CD2[12_555]	2.10	0.10
3:3:8:PRO:CB	3:3:139:ASP:OD1[12_555]	2.10	0.10
1:1:41:HIS:C	1:1:186:PHE:CG[12_555]	2.10	0.10
1:1:241:HIS:ND1	3:3:216:CYS:CA[12_555]	2.10	0.10
1:1:7:ILE:C	1:1:276:THR:C[12_555]	2.10	0.10
1:1:122:ASP:C	3:3:50:ASP:CG[12_555]	2.10	0.10
1:1:9:GLU:C	1:1:277:ALA:N[12_555]	2.10	0.10
1:1:47:PRO:CG	1:1:239:ILE:CB[12_555]	2.10	0.10
1:1:44:ASN:O	5:1:500:W54:C6B[12_555]	2.10	0.10
2:2:19:GLY:C	2:2:211:MET:SD[2_555]	2.11	0.09
2:2:35:TYR:OH	3:3:39:GLU:OE2[12_555]	2.11	0.09
1:1:67:ILE:CG2	3:3:46:MET:CA[12_555]	2.11	0.09
1:1:47:PRO:O	1:1:239:ILE:CD1[12_555]	2.11	0.09
3:3:107:THR:OG1	3:3:223:MET:CB[12_555]	2.11	0.09
1:1:39:THR:OG1	3:3:30:PRO:CB[12_555]	2.11	0.09
1:1:41:HIS:CE1	3:3:31:THR:CG2[12_555]	2.11	0.09
2:2:18:ARG:CD	2:2:50:ILE:C[2_555]	2.11	0.09
1:1:61:THR:CB	3:3:230:HIS:CB[12_555]	2.11	0.09
1:1:76:CYS:C	3:3:218:ASP:CG[12_555]	2.11	0.09
2:2:13:ILE:CB	2:2:13:ILE:CB[11_555]	2.11	0.09
3:3:70:VAL:N	4:4:30:ASN:C[12_555]	2.11	0.09
1:1:177:GLN:C	3:3:150:GLY:CA[12_555]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:177:GLN:N	3:3:148:MET:C[12_555]	2.11	0.09
1:1:240:TYR:CD1	3:3:112:SER:CB[12_555]	2.11	0.09
1:1:35:ASP:O	3:3:24:ALA:O[12_555]	2.11	0.09
1:1:47:PRO:CB	1:1:239:ILE:O[12_555]	2.11	0.09
2:2:41:TYR:O	2:2:249:MET:O[12_555]	2.11	0.09
1:1:18:PRO:N	1:1:106:MET:CA[12_555]	2.11	0.09
2:2:62:ARG:CA	2:2:254:SER:CA[2_555]	2.11	0.09
2:2:47:ALA:O	2:2:202:ILE:CG1[12_555]	2.11	0.09
3:3:66:SER:O	4:4:28:ASN:CB[12_555]	2.11	0.09
2:2:35:TYR:CD2	3:3:36:ILE:O[12_555]	2.11	0.09
3:3:43:LEU:CG	3:3:43:LEU:CG[12_555]	2.11	0.09
1:1:13:GLU:C	3:3:230:HIS:CG[12_555]	2.11	0.09
1:1:243:ALA:O	3:3:47:CYS:O[12_555]	2.11	0.09
2:2:62:ARG:CD	2:2:254:SER:O[2_555]	2.12	0.08
2:2:62:ARG:NH2	2:2:102:GLY:CA[2_555]	2.12	0.08
3:3:120:CYS:SG	4:4:33:LYS:C[12_555]	2.12	0.08
2:2:32:VAL:CG2	3:3:32:LYS:CA[12_555]	2.12	0.08
1:1:243:ALA:CA	3:3:214:SER:C[12_555]	2.12	0.08
1:1:18:PRO:O	1:1:106:MET:O[12_555]	2.12	0.08
3:3:209:MET:O	4:4:31:TYR:N[12_555]	2.12	0.08
2:2:11:ASP:CG	2:2:26:ASP:C[11_555]	2.12	0.08
1:1:116:PHE:CD2	3:3:42:ASN:O[12_555]	2.12	0.08
3:3:53:ILE:CA	4:4:39:GLY:CA[12_555]	2.12	0.08
2:2:52:LYS:CE	2:2:252:GLU:OE2[10_555]	2.12	0.08
1:1:15:LEU:C	1:1:111:ARG:CB[12_555]	2.12	0.08
1:1:27:THR:OG1	1:1:223:ARG:CD[12_555]	2.12	0.08
1:1:16:VAL:C	1:1:107:ALA:C[12_555]	2.12	0.08
1:1:242:LYS:CG	3:3:214:SER:O[12_555]	2.12	0.08
2:2:38:TRP:CE3	2:2:210:PRO:N[12_555]	2.12	0.08
2:2:46:ASP:CG	2:2:203:VAL:C[12_555]	2.12	0.08
1:1:181:ARG:CG	3:3:165:LEU:O[12_555]	2.12	0.08
1:1:15:LEU:CB	1:1:111:ARG:CG[12_555]	2.12	0.08
1:1:13:GLU:CA	3:3:230:HIS:ND1[12_555]	2.12	0.08
3:3:211:CYS:CA	4:4:38:SER:N[12_555]	2.12	0.08
2:2:11:ASP:CA	2:2:26:ASP:OD2[11_555]	2.12	0.08
3:3:56:ASN:CG	4:4:29:ILE:CB[12_555]	2.12	0.08
2:2:17:THR:OG1	2:2:49:ALA:CA[2_555]	2.12	0.08
2:2:220:TRP:CE2	3:3:35:SER:OG[12_555]	2.12	0.08
2:2:33:VAL:CA	3:3:34:ILE:CG1[12_555]	2.12	0.08
2:2:91:ILE:CG1	2:2:95:ASN:OD1[2_555]	2.12	0.08
3:3:222:ARG:C	3:3:225:ARG:CD[12_555]	2.12	0.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:13:GLU:C	3:3:230:HIS:CE1[12_555]	2.12	0.08
1:1:71:LEU:CD2	3:3:44:ILE:CB[12_555]	2.12	0.08
3:3:19:MET:CA	3:3:85:ILE:CD1[12_555]	2.12	0.08
1:1:9:GLU:CA	1:1:277:ALA:CB[12_555]	2.12	0.08
1:1:177:GLN:CA	3:3:150:GLY:N[12_555]	2.13	0.07
3:3:20:GLN:CA	3:3:117:PHE:CE1[12_555]	2.13	0.07
2:2:204:PRO:CG	3:3:35:SER:C[12_555]	2.13	0.07
1:1:39:THR:C	3:3:30:PRO:C[12_555]	2.13	0.07
1:1:113:PHE:CG	3:3:48:GLN:NE2[12_555]	2.13	0.07
2:2:64:TYR:CG	2:2:256:ALA:O[2_555]	2.13	0.07
3:3:161:SER:CB	4:4:34:ASP:OD1[12_555]	2.13	0.07
1:1:13:GLU:CA	3:3:230:HIS:CB[12_555]	2.13	0.07
1:1:183:SER:CA	3:3:164:SER:CB[12_555]	2.13	0.07
2:2:64:TYR:CE1	2:2:98:TYR:C[2_555]	2.13	0.07
1:1:69:SER:N	3:3:102:ILE:CD1[12_555]	2.13	0.07
1:1:51:ILE:CD1	1:1:238:HIS:N[12_555]	2.13	0.07
1:1:71:LEU:CD2	3:3:44:ILE:O[12_555]	2.13	0.07
1:1:177:GLN:O	3:3:150:GLY:N[12_555]	2.13	0.07
2:2:45:GLN:CD	2:2:246:ILE:CG2[12_555]	2.13	0.07
1:1:245:HIS:CG	3:3:51:THR:CA[12_555]	2.13	0.07
2:2:186:PHE:O	3:3:33:GLU:OE1[12_555]	2.13	0.07
1:1:31:ALA:CB	1:1:169:MET:C[12_555]	2.13	0.07
2:2:64:TYR:CD1	2:2:98:TYR:O[2_555]	2.13	0.07
3:3:27:TRP:CZ3	3:3:159:LEU:CA[12_555]	2.13	0.07
3:3:118:MET:CA	4:4:34:ASP:CB[12_555]	2.13	0.07
3:3:21:SER:CA	3:3:117:PHE:CG[12_555]	2.13	0.07
1:1:39:THR:CA	3:3:29:HIS:C[12_555]	2.13	0.07
1:1:240:TYR:CZ	3:3:169:TRP:CG[12_555]	2.13	0.07
1:1:71:LEU:CA	3:3:47:CYS:CA[12_555]	2.13	0.07
1:1:245:HIS:CB	3:3:51:THR:N[12_555]	2.13	0.07
2:2:91:ILE:N	2:2:98:TYR:CD2[2_555]	2.13	0.07
2:2:32:VAL:CA	3:3:32:LYS:N[12_555]	2.13	0.07
1:1:245:HIS:N	3:3:50:ASP:CA[12_555]	2.13	0.07
2:2:179:LEU:C	4:4:42:ARG:CB[12_555]	2.13	0.07
1:1:116:PHE:CA	3:3:45:GLU:OE1[12_555]	2.13	0.07
1:1:9:GLU:C	1:1:277:ALA:C[12_555]	2.13	0.07
1:1:26:THR:CA	1:1:222:SER:C[12_555]	2.13	0.07
1:1:69:SER:CA	3:3:102:ILE:CG2[12_555]	2.13	0.07
1:1:77:VAL:CA	3:3:217:LYS:CD[12_555]	2.13	0.07
1:1:241:HIS:C	3:3:215:ALA:C[12_555]	2.13	0.07
1:1:242:LYS:N	3:3:215:ALA:O[12_555]	2.13	0.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:107:THR:N	3:3:224:ALA:N[12_555]	2.13	0.07
1:1:32:PRO:CA	1:1:147:TYR:CD1[12_555]	2.14	0.06
1:1:22:GLU:CG	1:1:81:ARG:C[12_555]	2.14	0.06
1:1:73:ARG:CD	3:3:221:LEU:CD1[12_555]	2.14	0.06
2:2:64:TYR:CZ	2:2:256:ALA:CA[2_555]	2.14	0.06
3:3:57:ASN:CA	4:4:27:PHE:N[12_555]	2.14	0.06
2:2:38:TRP:CB	2:2:209:VAL:C[12_555]	2.14	0.06
2:2:90:GLY:N	2:2:98:TYR:N[2_555]	2.14	0.06
2:2:88:ASP:C	2:2:259:LYS:CA[2_555]	2.14	0.06
3:3:119:PHE:O	4:4:33:LYS:CB[12_555]	2.14	0.06
1:1:39:THR:CG2	3:3:30:PRO:N[12_555]	2.14	0.06
1:1:25:HIS:CA	1:1:223:ARG:C[12_555]	2.14	0.06
3:3:222:ARG:CG	3:3:225:ARG:C[12_555]	2.14	0.06
1:1:61:THR:O	3:3:227:THR:CG2[12_555]	2.14	0.06
1:1:181:ARG:NH1	3:3:115:PHE:CZ[12_555]	2.14	0.06
3:3:15:THR:N	3:3:109:TRP:CZ2[12_555]	2.14	0.06
3:3:17:ASP:CG	3:3:87:VAL:CG1[12_555]	2.14	0.06
1:1:24:HIS:CB	1:1:97:THR:CG2[12_555]	2.14	0.06
1:1:178:PRO:O	3:3:150:GLY:O[12_555]	2.14	0.06
3:3:67:MET:CA	4:4:28:ASN:CA[12_555]	2.14	0.06
1:1:47:PRO:CG	1:1:239:ILE:CG2[12_555]	2.14	0.06
1:1:30:SER:CA	1:1:168:ASN:CG[12_555]	2.14	0.06
2:2:54:THR:C	2:2:57:ASP:N[3_555]	2.14	0.06
1:1:254:PRO:O	4:4:43:LEU:CB[12_555]	2.14	0.06
1:1:240:TYR:C	3:3:112:SER:CB[12_555]	2.14	0.06
1:1:254:PRO:O	4:4:44:ASP:N[12_555]	2.14	0.06
1:1:181:ARG:CZ	3:3:115:PHE:CE1[12_555]	2.14	0.06
1:1:123:SER:N	3:3:50:ASP:OD2[12_555]	2.14	0.06
1:1:13:GLU:OE2	3:3:231:ILE:CA[12_555]	2.14	0.06
3:3:27:TRP:CE3	3:3:159:LEU:CA[12_555]	2.14	0.06
3:3:69:THR:N	4:4:30:ASN:N[12_555]	2.14	0.06
1:1:51:ILE:N	1:1:145:TYR:CE2[12_555]	2.14	0.06
1:1:30:SER:O	1:1:147:TYR:N[12_555]	2.14	0.06
2:2:36:GLY:O	2:2:209:VAL:N[12_555]	2.14	0.06
1:1:39:THR:O	3:3:30:PRO:O[12_555]	2.14	0.06
3:3:175:PHE:CZ	3:3:226:ASP:CG[12_555]	2.14	0.06
3:3:26:PRO:CG	3:3:160:GLN:C[12_555]	2.14	0.06
2:2:18:ARG:CA	2:2:51:ASN:CG[2_555]	2.14	0.06
2:2:194:ARG:NE	4:4:33:LYS:CE[12_555]	2.14	0.06
2:2:246:ILE:O	2:2:256:ALA:O[2_555]	2.14	0.06
2:2:43:THR:O	2:2:249:MET:SD[12_555]	2.14	0.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:161:SER:C	4:4:34:ASP:OD2[12_555]	2.14	0.06
2:2:64:TYR:CE1	2:2:99:HIS:CA[2_555]	2.14	0.06
1:1:41:HIS:O	1:1:186:PHE:CA[12_555]	2.15	0.05
1:1:25:HIS:CA	1:1:223:ARG:O[12_555]	2.15	0.05
1:1:242:LYS:CA	3:3:215:ALA:N[12_555]	2.15	0.05
2:2:20:ASP:CA	2:2:211:MET:CG[2_555]	2.15	0.05
1:1:70:PHE:N	3:3:102:ILE:CB[12_555]	2.15	0.05
1:1:35:ASP:N	3:3:24:ALA:O[12_555]	2.15	0.05
2:2:17:THR:O	2:2:51:ASN:N[2_555]	2.15	0.05
3:3:211:CYS:O	4:4:38:SER:N[12_555]	2.15	0.05
2:2:39:PRO:O	2:2:103:ARG:NH1[12_555]	2.15	0.05
1:1:251:PRO:CB	3:3:40:VAL:C[12_555]	2.15	0.05
3:3:6:ILE:CD1	3:3:141:PRO:C[12_555]	2.15	0.05
1:1:32:PRO:CG	5:1:500:W54:O1A[12_555]	2.15	0.05
3:3:54:PRO:CB	4:4:27:PHE:CE1[12_555]	2.15	0.05
2:2:204:PRO:O	3:3:35:SER:OG[12_555]	2.15	0.05
1:1:30:SER:CB	1:1:147:TYR:O[12_555]	2.15	0.05
1:1:68:GLU:CG	3:3:98:LEU:N[12_555]	2.15	0.05
1:1:241:HIS:CE1	3:3:215:ALA:O[12_555]	2.15	0.05
1:1:31:ALA:N	1:1:147:TYR:O[12_555]	2.15	0.05
1:1:181:ARG:CG	3:3:165:LEU:CG[12_555]	2.15	0.05
2:2:17:THR:C	2:2:49:ALA:CA[2_555]	2.15	0.05
3:3:23:CYS:O	3:3:162:THR:N[12_555]	2.15	0.05
1:1:247:LYS:CG	2:2:185:ILE:C[12_555]	2.15	0.05
3:3:14:MET:N	3:3:87:VAL:CG1[12_555]	2.15	0.05
3:3:118:MET:C	4:4:33:LYS:C[12_555]	2.15	0.05
1:1:31:ALA:CA	1:1:169:MET:O[12_555]	2.15	0.05
1:1:242:LYS:CE	3:3:213:VAL:CG2[12_555]	2.15	0.05
3:3:222:ARG:CG	3:3:226:ASP:O[12_555]	2.15	0.05
3:3:21:SER:OG	3:3:115:PHE:O[12_555]	2.15	0.05
1:1:54:ARG:CG	1:1:236:THR:OG1[12_555]	2.15	0.05
3:3:70:VAL:CG2	4:4:31:TYR:CE2[12_555]	2.15	0.05
1:1:13:GLU:CG	3:3:231:ILE:CD1[12_555]	2.15	0.05
1:1:183:SER:N	3:3:115:PHE:O[12_555]	2.15	0.05
2:2:190:PHE:O	3:3:29:HIS:CE1[12_555]	2.15	0.05
2:2:44:PRO:CB	2:2:247:SER:C[12_555]	2.16	0.04
1:1:54:ARG:CA	1:1:79:ILE:CG2[12_555]	2.16	0.04
3:3:51:THR:C	4:4:39:GLY:O[12_555]	2.16	0.04
1:1:45:VAL:CA	1:1:125:ILE:CD1[12_555]	2.16	0.04
1:1:116:PHE:CD1	3:3:40:VAL:CA[12_555]	2.16	0.04
1:1:182:PHE:CA	3:3:165:LEU:CB[12_555]	2.16	0.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:13:PHE:CG	3:3:133:TYR:CZ[12_555]	2.16	0.04
3:3:13:PHE:CB	3:3:133:TYR:CD1[12_555]	2.16	0.04
2:2:41:TYR:CZ	2:2:55:GLN:CD[12_555]	2.16	0.04
1:1:250:CYS:CA	3:3:39:GLU:O[12_555]	2.16	0.04
3:3:209:MET:CA	4:4:33:LYS:N[12_555]	2.16	0.04
1:1:22:GLU:OE2	1:1:81:ARG:C[12_555]	2.16	0.04
3:3:211:CYS:CA	4:4:37:SER:C[12_555]	2.16	0.04
1:1:115:LEU:CB	3:3:41:LYS:O[12_555]	2.16	0.04
1:1:56:VAL:CB	1:1:79:ILE:CD1[12_555]	2.16	0.04
2:2:29:ALA:CA	3:3:29:HIS:CB[12_555]	2.16	0.04
1:1:246:THR:N	3:3:49:VAL:CB[12_555]	2.16	0.04
1:1:17:VAL:CB	1:1:108:GLN:N[12_555]	2.16	0.04
3:3:211:CYS:C	4:4:38:SER:CB[12_555]	2.16	0.04
1:1:21:LYS:CD	1:1:99:TRP:CD1[12_555]	2.16	0.04
1:1:25:HIS:CG	1:1:223:ARG:CA[12_555]	2.16	0.04
3:3:37:PRO:CA	3:3:37:PRO:O[12_555]	2.16	0.04
1:1:183:SER:O	3:3:164:SER:N[12_555]	2.16	0.04
1:1:125:ILE:N	3:3:114:ARG:CG[12_555]	2.16	0.04
1:1:12:ASN:ND2	3:3:229:LEU:CD1[12_555]	2.16	0.04
1:1:191:SER:OG	2:2:33:VAL:O[12_555]	2.16	0.04
1:1:54:ARG:CA	1:1:236:THR:OG1[12_555]	2.16	0.04
3:3:222:ARG:CA	3:3:225:ARG:CA[12_555]	2.17	0.03
2:2:13:ILE:C	2:2:13:ILE:O[11_555]	2.17	0.03
1:1:21:LYS:CG	1:1:78:HIS:ND1[12_555]	2.17	0.03
1:1:123:SER:CB	3:3:114:ARG:NH1[12_555]	2.17	0.03
1:1:14:VAL:CG2	1:1:256:ALA:N[12_555]	2.17	0.03
3:3:9:GLY:C	3:3:188:TYR:CG[12_555]	2.17	0.03
3:3:209:MET:CE	4:4:32:PHE:CE1[12_555]	2.17	0.03
1:1:249:TRP:CB	3:3:38:GLY:CA[12_555]	2.17	0.03
3:3:20:GLN:NE2	3:3:211:CYS:N[12_555]	2.17	0.03
2:2:45:GLN:CD	2:2:106:TYR:CB[12_555]	2.17	0.03
3:3:12:GLN:NE2	3:3:187:GLY:N[12_555]	2.17	0.03
1:1:243:ALA:CB	3:3:47:CYS:C[12_555]	2.17	0.03
3:3:106:TYR:CZ	3:3:106:TYR:CZ[12_555]	2.17	0.03
3:3:22:PRO:CA	3:3:163:ILE:CG2[12_555]	2.17	0.03
1:1:6:TYR:C	1:1:276:THR:N[12_555]	2.17	0.03
2:2:201:LEU:CB	3:3:32:LYS:NZ[12_555]	2.17	0.03
3:3:209:MET:C	4:4:32:PHE:N[12_555]	2.17	0.03
2:2:40:HIS:NE2	2:2:205:TYR:CG[12_555]	2.17	0.03
2:2:58:THR:OG1	2:2:252:GLU:CG[2_555]	2.17	0.03
2:2:45:GLN:CG	2:2:107:THR:C[12_555]	2.17	0.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:200:THR:C	3:3:32:LYS:CB[12_555]	2.17	0.03
2:2:40:HIS:N	2:2:103:ARG:NH1[12_555]	2.17	0.03
1:1:30:SER:O	1:1:146:MET:CG[12_555]	2.17	0.03
1:1:62:ARG:CZ	1:1:109:ILE:CB[12_555]	2.17	0.03
2:2:44:PRO:CA	2:2:247:SER:O[12_555]	2.17	0.03
1:1:181:ARG:N	3:3:165:LEU:CG[12_555]	2.17	0.03
1:1:53:THR:O	1:1:236:THR:CA[12_555]	2.17	0.03
3:3:6:ILE:CG1	3:3:142:THR:CB[12_555]	2.18	0.02
3:3:13:PHE:N	3:3:186:ALA:O[12_555]	2.18	0.02
1:1:103:LEU:CD1	3:3:217:LYS:CB[12_555]	2.18	0.02
1:1:22:GLU:CD	1:1:81:ARG:C[12_555]	2.18	0.02
2:2:17:THR:C	2:2:49:ALA:O[2_555]	2.18	0.02
1:1:243:ALA:CA	3:3:214:SER:CA[12_555]	2.18	0.02
2:2:46:ASP:CA	2:2:203:VAL:N[12_555]	2.18	0.02
3:3:56:ASN:CB	4:4:29:ILE:CB[12_555]	2.18	0.02
1:1:181:ARG:CZ	3:3:115:PHE:CD1[12_555]	2.18	0.02
3:3:68:TYR:CZ	4:4:27:PHE:CZ[12_555]	2.18	0.02
1:1:177:GLN:N	3:3:150:GLY:N[12_555]	2.18	0.02
1:1:72:GLY:N	3:3:99:ILE:CG1[12_555]	2.18	0.02
1:1:28:SER:CA	1:1:146:MET:CE[12_555]	2.18	0.02
3:3:15:THR:OG1	3:3:111:GLY:O[12_555]	2.18	0.02
1:1:21:LYS:O	1:1:79:ILE:CB[12_555]	2.18	0.02
2:2:17:THR:N	2:2:50:ILE:CG1[2_555]	2.18	0.02
2:2:35:TYR:O	3:3:36:ILE:CG1[12_555]	2.18	0.02
2:2:179:LEU:CD2	4:4:42:ARG:NE[12_555]	2.18	0.02
2:2:32:VAL:N	3:3:32:LYS:CA[12_555]	2.18	0.02
3:3:26:PRO:CD	3:3:160:GLN:C[12_555]	2.18	0.02
3:3:26:PRO:CA	3:3:161:SER:OG[12_555]	2.18	0.02
1:1:23:SER:N	1:1:80:SER:OG[12_555]	2.18	0.02
1:1:72:GLY:N	3:3:47:CYS:CB[12_555]	2.18	0.02
2:2:54:THR:O	2:2:57:ASP:C[3_555]	2.18	0.02
1:1:245:HIS:C	3:3:49:VAL:CG1[12_555]	2.18	0.02
3:3:10:SER:CA	3:3:188:TYR:CD1[12_555]	2.18	0.02
2:2:62:ARG:NH1	2:2:253:PHE:C[2_555]	2.18	0.02
1:1:63:ASP:C	3:3:101:GLU:O[12_555]	2.18	0.02
2:2:43:THR:CG2	2:2:105:GLY:O[12_555]	2.18	0.02
2:2:201:LEU:O	3:3:32:LYS:CE[12_555]	2.18	0.02
2:2:89:MET:CB	2:2:258:ALA:C[2_555]	2.18	0.02
2:2:18:ARG:N	2:2:51:ASN:ND2[2_555]	2.18	0.02
1:1:8:ASP:CB	1:1:275:THR:O[12_555]	2.18	0.02
3:3:56:ASN:N	4:4:29:ILE:CG1[12_555]	2.18	0.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:90:GLY:N	2:2:98:TYR:CD1[2_555]	2.18	0.02
2:2:54:THR:N	2:2:57:ASP:O[3_555]	2.18	0.02
1:1:12:ASN:CA	3:3:230:HIS:N[12_555]	2.18	0.02
1:1:6:TYR:O	1:1:277:ALA:CA[12_555]	2.18	0.02
3:3:70:VAL:CB	4:4:31:TYR:CD1[12_555]	2.18	0.02
1:1:37:ALA:N	1:1:185:PRO:CG[12_555]	2.19	0.01
2:2:38:TRP:CZ2	2:2:48:THR:CG2[12_555]	2.19	0.01
1:1:8:ASP:N	1:1:276:THR:N[12_555]	2.19	0.01
1:1:45:VAL:CB	5:1:500:W54:C1B[12_555]	2.19	0.01
1:1:123:SER:C	3:3:114:ARG:NE[12_555]	2.19	0.01
3:3:23:CYS:N	3:3:163:ILE:N[12_555]	2.19	0.01
3:3:21:SER:N	3:3:117:PHE:CE2[12_555]	2.19	0.01
1:1:250:CYS:O	3:3:39:GLU:CG[12_555]	2.19	0.01
3:3:222:ARG:O	3:3:224:ALA:C[12_555]	2.19	0.01
1:1:179:PHE:C	3:3:151:THR:CB[12_555]	2.19	0.01
2:2:62:ARG:CD	2:2:99:HIS:CG[2_555]	2.19	0.01
2:2:41:TYR:CG	2:2:250:CYS:O[12_555]	2.19	0.01
3:3:54:PRO:CA	4:4:27:PHE:CE1[12_555]	2.19	0.01
3:3:212:PHE:CZ	4:4:36:ALA:CA[12_555]	2.19	0.01
1:1:29:ASN:C	1:1:168:ASN:CB[12_555]	2.19	0.01
1:1:22:GLU:OE2	1:1:81:ARG:CA[12_555]	2.19	0.01
1:1:27:THR:CA	1:1:144:GLN:CD[12_555]	2.19	0.01
1:1:126:THR:CB	3:3:166:VAL:O[12_555]	2.19	0.01
3:3:25:LEU:CD2	3:3:160:GLN:NE2[12_555]	2.19	0.01
3:3:26:PRO:N	3:3:162:THR:N[12_555]	2.19	0.01
2:2:195:SER:CB	3:3:27:TRP:CB[12_555]	2.19	0.01
1:1:62:ARG:CB	3:3:105:TYR:OH[12_555]	2.19	0.01
2:2:11:ASP:OD1	2:2:26:ASP:O[11_555]	2.19	0.01
1:1:39:THR:CA	3:3:30:PRO:C[12_555]	2.19	0.01
1:1:42:THR:CG2	1:1:122:ASP:C[12_555]	2.19	0.01
1:1:64:GLU:O	3:3:105:TYR:CD2[12_555]	2.19	0.01
2:2:34:GLY:N	3:3:34:ILE:O[12_555]	2.19	0.01
3:3:107:THR:CG2	3:3:223:MET:CG[12_555]	2.19	0.01
2:2:34:GLY:O	3:3:36:ILE:CG1[12_555]	2.19	0.01
1:1:103:LEU:CD2	3:3:217:LYS:CG[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%)	206 (73%)	51 (18%)	24 (8%)	1	12
2	2	251/263 (95%)	201 (80%)	35 (14%)	15 (6%)	1	20
3	3	236/238 (99%)	179 (76%)	37 (16%)	20 (8%)	1	12
4	4	17/44 (39%)	9 (53%)	7 (41%)	1 (6%)	1	21
All	All	785/832 (94%)	595 (76%)	130 (17%)	60 (8%)	1	15

All (60) 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	150	PRO
1	1	158	ARG
1	1	212	VAL
1	1	219	THR
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

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Mol	Chain	Res	Type
1	1	99	TRP
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
1	1	160	ASP
1	1	266	ASN
2	2	260	ASN
1	1	125	ILE
1	1	205	THR
1	1	268	MET
2	2	87	LYS
2	2	259	LYS
3	3	220	CYS
2	2	44	PRO
3	3	121	GLY
1	1	101	ILE
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%)	182 (72%)	72 (28%)	0	2
2	2	219/227 (96%)	159 (73%)	60 (27%)	0	3
3	3	209/209 (100%)	156 (75%)	53 (25%)	0	4
4	4	15/35 (43%)	9 (60%)	6 (40%)	0	0
All	All	697/729 (96%)	506 (73%)	191 (27%)	0	3

All (191) 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
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	100	LYS
1	1	101	ILE
1	1	102	THR
1	1	103	LEU
1	1	108	GLN
1	1	109	ILE
1	1	112	LYS
1	1	119	VAL

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Mol	Chain	Res	Type
1	1	121	PHE
1	1	123	SER
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	146	MET
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	197	TYR
1	1	201	ASP
1	1	204	ASN
1	1	209	TYR
1	1	212	VAL
1	1	215	ASN
1	1	216	ASP
1	1	217	MET
1	1	219	THR
1	1	223	ARG
1	1	224	ILE
1	1	226	THR
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
3	3	217	LYS
3	3	228	ASP
3	3	231	ILE
3	3	236	ILE
3	3	238	GLN
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 (30) such

sidechains are listed below:

Mol	Chain	Res	Type
1	1	90	ASN
1	1	95	ASN
1	1	140	HIS
1	1	159	ASN
1	1	204	ASN
1	1	215	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
3	3	124	ASN
3	3	194	GLN
4	4	30	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	W54	1	500	-	24,27,27	3.13	5 (20%)	31,36,36	2.84	9 (29%)

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	W54	1	500	-	-	4/12/20/20	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	500	W54	C2A-N3A	12.19	1.43	1.27
5	1	500	W54	C4A-N3A	-6.37	1.36	1.47
5	1	500	W54	O1A-C2A	-4.05	1.29	1.36
5	1	500	W54	C4-C5	-3.66	1.34	1.39
5	1	500	W54	O1A-C5A	-3.13	1.38	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	500	W54	O1A-C2A-N3A	-9.64	109.94	118.23
5	1	500	W54	C4A-N3A-C2A	6.76	112.81	106.77
5	1	500	W54	O1A-C2A-C4B	6.18	124.04	115.85
5	1	500	W54	O1B-C1B-C6B	-4.62	115.18	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	500	W54	O1A-C5A-C4A	3.65	111.72	104.28
5	1	500	W54	O1B-C1B-C2B	3.13	125.22	121.17
5	1	500	W54	C5A-C4A-N3A	-2.42	98.58	104.35
5	1	500	W54	C1C-C5-C4	2.38	134.76	128.60
5	1	500	W54	C5C-O1B-C1B	2.03	120.38	114.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

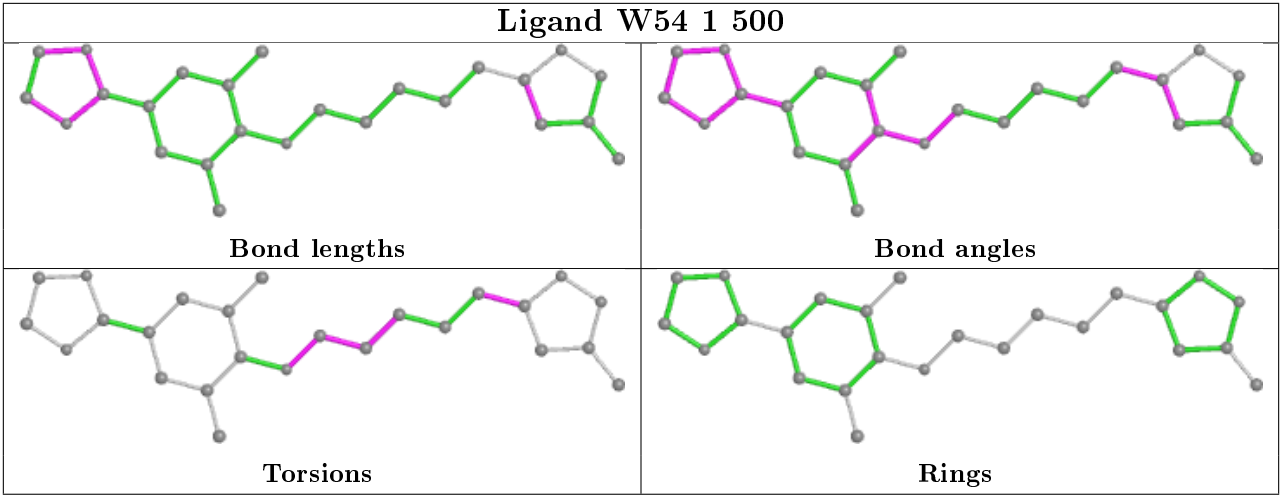
Mol	Chain	Res	Type	Atoms
5	1	500	W54	C2C-C1C-C5-C4
5	1	500	W54	C3C-C4C-C5C-O1B
5	1	500	W54	C2C-C3C-C4C-C5C
5	1	500	W54	C4C-C5C-O1B-C1B

There are no ring outliers.

1 monomer is involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	500	W54	3	49

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	213:VAL	C	214:THR	N	1.61
1	1	118:TYR	C	119:VAL	N	1.19
1	1	98:LYS	C	99:TRP	N	1.15
1	1	146:MET	C	147:TYR	N	0.98

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.