



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:38 am BST

PDB ID : 4SBV
Title : The REFINEMENT OF SOUTHERN BEAN MOSAIC VIRUS IN RECIP-
ROCAL SPACE
Authors : Rossmann, M.G.
Deposited on : 1985-04-01
Resolution : 2.80 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

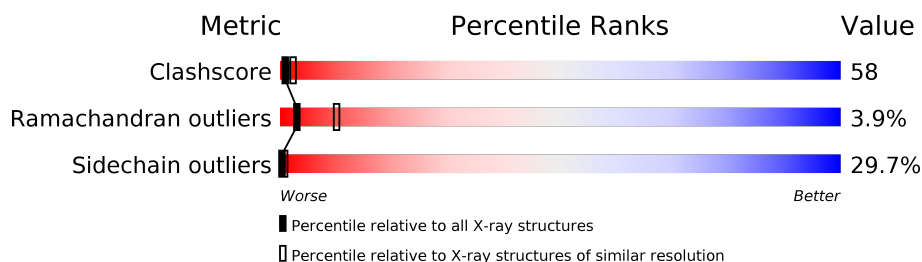
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	260	
1	B	260	
1	C	260	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4723 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 SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	0	0
			1506	956	249	292	9			
1	B	199	Total	C	N	O	S	0	0	0
			1506	956	249	292	9			
1	C	222	Total	C	N	O	S	0	0	0
			1674	1062	281	319	12			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

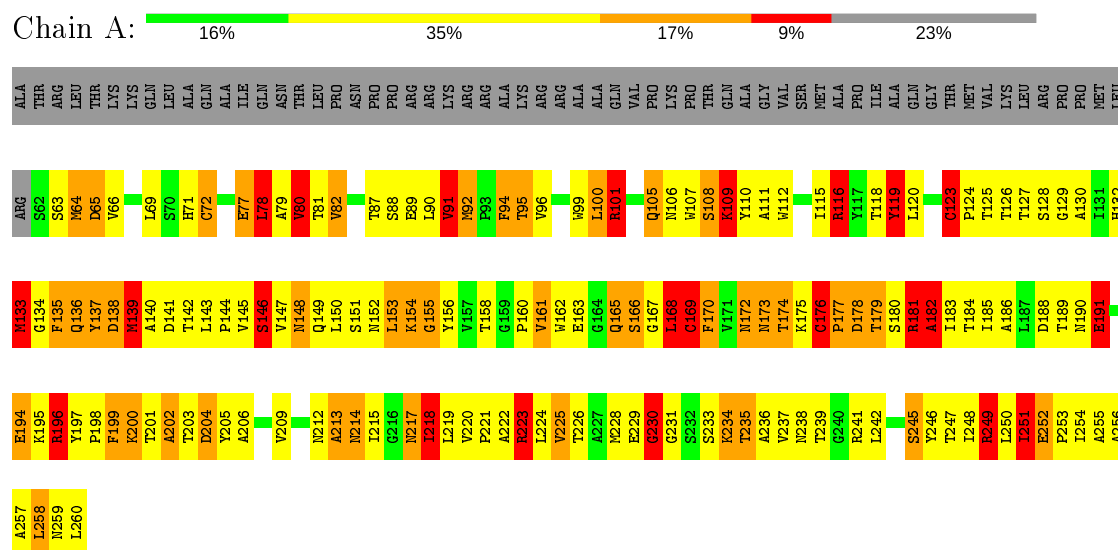
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	10	Total	O	0	0
			10	10		
3	C	9	Total	O	0	0
			9	9		

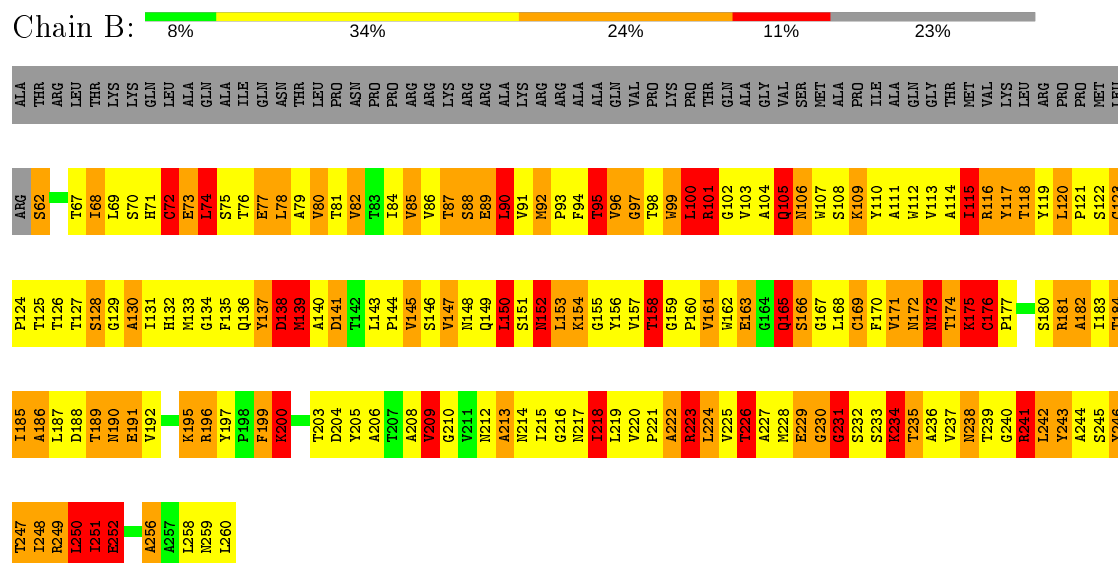
3 Residue-property plots

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.

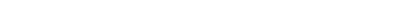
• Molecule 1: SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN

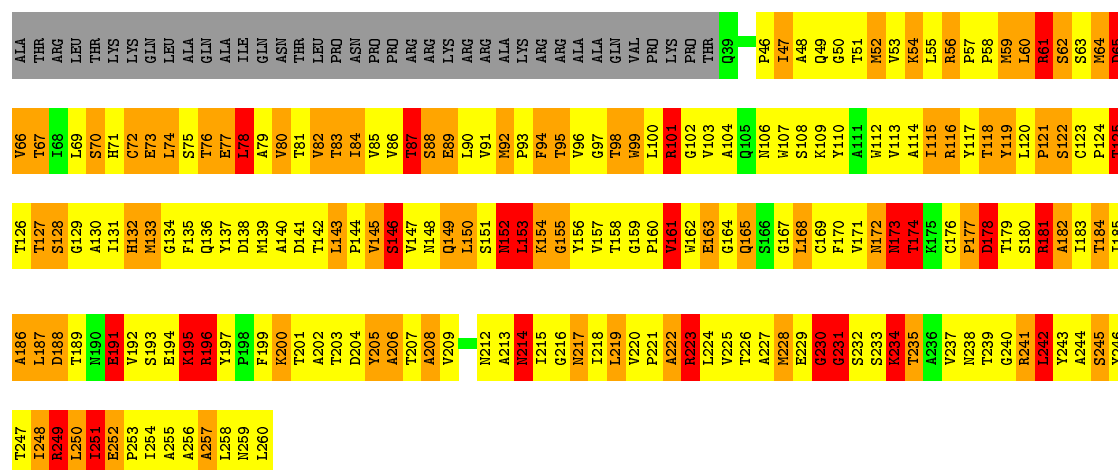


• Molecule 1: SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN



• Molecule 1: SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN

Chain C:  7% 43% 26% 10% 15%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	334.30 Å 334.30 Å 757.50 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.80 142.18 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80) 75.4 (142.18-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.254 , (Not available) 0.504 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.49 , 978.0	EDS
L-test for twinning ¹	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.22	EDS
Total number of atoms	4723	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.47	8/1537 (0.5%)	2.64	103/2104 (4.9%)
1	B	1.43	7/1537 (0.5%)	2.46	106/2104 (5.0%)
1	C	1.48	11/1708 (0.6%)	2.55	96/2335 (4.1%)
All	All	1.46	26/4782 (0.5%)	2.55	305/6543 (4.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	4
All	All	0	10

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	252	GLU	N-CA	10.24	1.66	1.46
1	C	155	GLY	N-CA	9.10	1.59	1.46
1	B	231	GLY	N-CA	-8.86	1.32	1.46
1	C	231	GLY	N-CA	-8.81	1.32	1.46
1	A	230	GLY	N-CA	8.31	1.58	1.46
1	A	155	GLY	N-CA	7.50	1.57	1.46
1	A	252	GLU	N-CA	6.93	1.60	1.46
1	C	251	ILE	C-O	6.72	1.36	1.23
1	C	231	GLY	CA-C	-6.64	1.41	1.51
1	B	251	ILE	C-O	6.62	1.35	1.23
1	A	194	GLU	CB-CG	6.27	1.64	1.52
1	C	231	GLY	C-O	6.05	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	GLU	CD-OE1	-5.74	1.19	1.25
1	A	109	LYS	CA-CB	-5.72	1.41	1.53
1	A	168	LEU	C-O	5.71	1.34	1.23
1	B	252	GLU	CA-CB	-5.67	1.41	1.53
1	B	252	GLU	N-CA	5.65	1.57	1.46
1	B	176	CYS	CB-SG	5.58	1.91	1.82
1	B	137	TYR	C-O	5.52	1.33	1.23
1	C	252	GLU	CA-CB	-5.46	1.42	1.53
1	C	252	GLU	CB-CG	-5.33	1.42	1.52
1	C	64	MET	CA-CB	-5.32	1.42	1.53
1	C	133	MET	CA-CB	-5.32	1.42	1.53
1	B	97	GLY	N-CA	5.14	1.53	1.46
1	C	56	ARG	CZ-NH2	5.06	1.39	1.33
1	A	123	CYS	CB-SG	-5.03	1.73	1.81

All (305) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	ARG	NE-CZ-NH1	31.30	135.95	120.30
1	C	101	ARG	NE-CZ-NH1	26.03	133.32	120.30
1	A	109	LYS	CA-CB-CG	25.72	169.98	113.40
1	A	196	ARG	NE-CZ-NH2	-18.85	110.87	120.30
1	A	125	THR	N-CA-CB	17.78	144.08	110.30
1	B	241	ARG	NE-CZ-NH2	-17.49	111.56	120.30
1	C	231	GLY	N-CA-C	16.71	154.87	113.10
1	C	101	ARG	NE-CZ-NH2	-16.52	112.04	120.30
1	C	252	GLU	CA-CB-CG	15.42	147.32	113.40
1	C	196	ARG	NE-CZ-NH2	-15.35	112.62	120.30
1	C	241	ARG	NE-CZ-NH1	-13.64	113.48	120.30
1	C	56	ARG	NE-CZ-NH1	13.19	126.90	120.30
1	B	231	GLY	N-CA-C	12.93	145.43	113.10
1	A	196	ARG	CD-NE-CZ	12.60	141.25	123.60
1	A	223	ARG	CD-NE-CZ	-12.53	106.06	123.60
1	C	173	ASN	C-N-CA	12.13	152.02	121.70
1	B	252	GLU	OE1-CD-OE2	-11.62	109.36	123.30
1	A	181	ARG	NE-CZ-NH1	11.47	126.03	120.30
1	B	251	ILE	CA-C-N	11.34	142.16	117.20
1	A	101	ARG	NE-CZ-NH1	11.21	125.90	120.30
1	C	249	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	C	241	ARG	NE-CZ-NH2	10.99	125.80	120.30
1	C	252	GLU	CB-CA-C	10.79	131.99	110.40
1	C	251	ILE	CA-C-N	10.78	140.91	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	LEU	N-CA-CB	10.75	131.90	110.40
1	A	168	LEU	CA-C-N	10.61	140.53	117.20
1	A	176	CYS	CA-CB-SG	10.29	132.53	114.00
1	B	251	ILE	CA-C-O	-10.28	98.52	120.10
1	A	178	ASP	C-N-CA	10.18	147.16	121.70
1	C	153	LEU	CA-CB-CG	10.06	138.45	115.30
1	A	168	LEU	CA-C-O	-10.04	99.02	120.10
1	A	169	CYS	CA-CB-SG	9.90	131.83	114.00
1	A	191	GLU	CA-CB-CG	9.90	135.19	113.40
1	C	214	ASN	CB-CA-C	9.85	130.09	110.40
1	B	90	LEU	CA-CB-CG	9.81	137.88	115.30
1	C	133	MET	CA-CB-CG	9.79	129.94	113.30
1	B	72	CYS	CA-CB-SG	-9.76	96.44	114.00
1	A	241	ARG	NE-CZ-NH1	-9.67	115.46	120.30
1	C	178	ASP	CB-CG-OD1	9.56	126.91	118.30
1	B	223	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	B	101	ARG	CG-CD-NE	9.32	131.37	111.80
1	B	74	LEU	O-C-N	9.27	137.53	122.70
1	C	73	GLU	CA-CB-CG	9.21	133.65	113.40
1	C	59	MET	CA-CB-CG	-9.08	97.87	113.30
1	B	138	ASP	O-C-N	8.91	136.95	122.70
1	A	181	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	A	123	CYS	CB-CA-C	-8.63	93.13	110.40
1	C	251	ILE	CA-C-O	-8.62	102.00	120.10
1	C	154	LYS	CA-C-N	8.57	133.35	116.20
1	A	178	ASP	CB-CA-C	8.49	127.37	110.40
1	C	249	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	A	69	LEU	O-C-N	8.42	136.18	122.70
1	A	138	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	A	204	ASP	CB-CG-OD1	8.38	125.84	118.30
1	A	249	ARG	NE-CZ-NH2	8.38	124.49	120.30
1	A	146	SER	N-CA-CB	-8.35	97.97	110.50
1	A	218	ILE	CB-CA-C	-8.30	95.00	111.60
1	B	163	GLU	CG-CD-OE2	-8.26	101.78	118.30
1	C	196	ARG	N-CA-CB	8.15	125.27	110.60
1	B	223	ARG	NE-CZ-NH1	-8.11	116.25	120.30
1	B	176	CYS	CA-CB-SG	-8.05	99.51	114.00
1	B	230	GLY	C-N-CA	8.04	139.19	122.30
1	A	80	VAL	CB-CA-C	-7.97	96.25	111.40
1	B	223	ARG	NH1-CZ-NH2	7.97	128.16	119.40
1	B	252	GLU	CG-CD-OE1	7.95	134.20	118.30
1	B	246	TYR	CB-CG-CD2	7.91	125.75	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	GLN	CA-CB-CG	-7.82	96.20	113.40
1	A	190	ASN	CB-CA-C	-7.79	94.82	110.40
1	C	110	TYR	CB-CG-CD1	7.75	125.65	121.00
1	B	196	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	B	251	ILE	N-CA-C	7.75	131.91	111.00
1	A	251	ILE	CA-C-N	7.73	134.21	117.20
1	C	214	ASN	N-CA-CB	-7.73	96.68	110.60
1	C	65	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	B	158	THR	O-C-N	7.46	135.88	123.20
1	C	95	THR	CA-CB-OG1	-7.39	93.48	109.00
1	C	248	ILE	N-CA-CB	-7.34	93.92	110.80
1	A	111	ALA	N-CA-CB	7.33	120.36	110.10
1	B	252	GLU	CA-CB-CG	7.30	129.46	113.40
1	A	175	LYS	N-CA-CB	7.25	123.65	110.60
1	A	101	ARG	CD-NE-CZ	7.20	133.68	123.60
1	C	154	LYS	CA-C-O	-7.20	104.99	120.10
1	A	252	GLU	CB-CA-C	7.12	124.65	110.40
1	C	230	GLY	N-CA-C	7.11	130.88	113.10
1	B	139	MET	CA-CB-CG	-7.06	101.30	113.30
1	B	241	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	B	141	ASP	CB-CA-C	7.02	124.45	110.40
1	C	196	ARG	CA-CB-CG	7.01	128.83	113.40
1	B	241	ARG	CD-NE-CZ	-7.01	113.79	123.60
1	C	64	MET	CA-CB-CG	7.00	125.19	113.30
1	A	179	THR	CA-C-N	-6.99	101.83	117.20
1	B	150	LEU	CA-CB-CG	6.97	131.34	115.30
1	C	133	MET	CB-CA-C	6.97	124.34	110.40
1	C	61	ARG	CA-CB-CG	6.94	128.68	113.40
1	A	170	PHE	CB-CA-C	6.92	124.24	110.40
1	A	251	ILE	CA-C-O	-6.92	105.58	120.10
1	B	246	TYR	CB-CG-CD1	-6.89	116.87	121.00
1	C	62	SER	N-CA-CB	-6.87	100.20	110.50
1	B	92	MET	CA-CB-CG	6.86	124.96	113.30
1	C	56	ARG	CD-NE-CZ	6.86	133.20	123.60
1	C	217	ASN	CA-C-O	-6.84	105.74	120.10
1	A	168	LEU	CA-CB-CG	6.83	131.00	115.30
1	B	191	GLU	CG-CD-OE1	6.83	131.96	118.30
1	B	243	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	B	252	GLU	N-CA-C	-6.82	92.60	111.00
1	B	185	ILE	CB-CG1-CD1	6.79	132.91	113.90
1	C	213	ALA	C-N-CA	-6.78	104.74	121.70
1	C	73	GLU	CG-CD-OE1	6.77	131.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	GLU	CG-CD-OE1	6.76	131.82	118.30
1	B	115	ILE	CA-CB-CG1	-6.75	98.17	111.00
1	B	130	ALA	CB-CA-C	-6.74	99.99	110.10
1	B	169	CYS	CA-CB-SG	-6.73	101.88	114.00
1	A	153	LEU	CB-CA-C	6.73	122.98	110.20
1	A	178	ASP	CA-C-O	6.70	134.16	120.10
1	A	136	GLN	CB-CA-C	6.69	123.78	110.40
1	A	258	LEU	N-CA-CB	-6.68	97.04	110.40
1	C	146	SER	N-CA-CB	-6.55	100.68	110.50
1	B	105	GLN	CA-CB-CG	6.53	127.77	113.40
1	A	249	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	B	96	VAL	CA-CB-CG1	6.46	120.58	110.90
1	C	73	GLU	CG-CD-OE2	-6.44	105.42	118.30
1	C	242	LEU	CB-CA-C	6.43	122.42	110.20
1	A	116	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	138	ASP	N-CA-C	-6.42	93.65	111.00
1	C	56	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	B	145	VAL	C-N-CA	6.41	137.71	121.70
1	C	188	ASP	CB-CA-C	6.41	123.21	110.40
1	A	194	GLU	CG-CD-OE2	-6.40	105.50	118.30
1	A	154	LYS	CA-C-N	6.37	128.93	116.20
1	B	168	LEU	CA-CB-CG	6.36	129.94	115.30
1	C	251	ILE	CA-CB-CG1	-6.34	98.96	111.00
1	A	178	ASP	CA-CB-CG	6.33	127.33	113.40
1	B	195	LYS	CD-CE-NZ	6.29	126.16	111.70
1	B	117	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	B	138	ASP	CA-CB-CG	6.27	127.20	113.40
1	A	78	LEU	O-C-N	6.26	132.72	122.70
1	A	69	LEU	CA-C-N	-6.24	103.47	117.20
1	A	125	THR	CB-CA-C	-6.24	94.75	111.60
1	B	68	ILE	O-C-N	6.23	132.66	122.70
1	C	206	ALA	N-CA-CB	-6.22	101.39	110.10
1	B	166	SER	O-C-N	6.22	133.78	123.20
1	B	251	ILE	CA-CB-CG1	-6.22	99.19	111.00
1	C	77	GLU	N-CA-CB	6.21	121.78	110.60
1	C	204	ASP	N-CA-CB	6.20	121.77	110.60
1	B	89	GLU	OE1-CD-OE2	-6.19	115.87	123.30
1	A	133	MET	O-C-N	6.18	133.72	123.20
1	C	188	ASP	N-CA-C	-6.18	94.30	111.00
1	C	196	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	A	72	CYS	CA-CB-SG	-6.14	102.94	114.00
1	B	96	VAL	CB-CA-C	6.14	123.07	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	215	ILE	CA-C-O	6.12	132.96	120.10
1	C	94	PHE	CA-C-N	-6.10	103.78	117.20
1	A	169	CYS	O-C-N	6.08	132.44	122.70
1	A	137	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	A	174	THR	CA-CB-CG2	6.05	120.87	112.40
1	A	182	ALA	O-C-N	6.02	132.33	122.70
1	C	173	ASN	CA-CB-CG	6.02	126.64	113.40
1	A	235	THR	CA-CB-OG1	-6.01	96.37	109.00
1	B	89	GLU	CB-CG-CD	6.00	130.39	114.20
1	B	226	THR	CA-CB-CG2	5.98	120.77	112.40
1	B	174	THR	N-CA-C	-5.95	94.94	111.00
1	A	166	SER	N-CA-CB	-5.95	101.58	110.50
1	B	209	VAL	CB-CA-C	5.95	122.70	111.40
1	A	217	ASN	CB-CG-OD1	5.94	133.49	121.60
1	C	252	GLU	N-CA-C	-5.94	94.96	111.00
1	A	251	ILE	N-CA-C	5.92	126.99	111.00
1	B	181	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	109	LYS	CG-CD-CE	5.92	129.66	111.90
1	C	163	GLU	CG-CD-OE2	-5.92	106.47	118.30
1	B	128	SER	N-CA-CB	-5.91	101.63	110.50
1	B	186	ALA	CB-CA-C	5.87	118.90	110.10
1	B	96	VAL	CA-CB-CG2	-5.83	102.15	110.90
1	B	173	ASN	CA-C-N	-5.83	104.37	117.20
1	B	163	GLU	OE1-CD-OE2	5.83	130.29	123.30
1	A	116	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	B	224	LEU	CA-C-O	-5.81	107.89	120.10
1	A	179	THR	CA-C-O	5.81	132.29	120.10
1	C	186	ALA	N-CA-CB	-5.80	101.98	110.10
1	C	76	THR	CA-C-O	-5.78	107.96	120.10
1	A	196	ARG	NH1-CZ-NH2	-5.76	113.06	119.40
1	C	146	SER	CA-CB-OG	5.76	126.76	111.20
1	A	91	VAL	CB-CA-C	5.76	122.34	111.40
1	B	95	THR	CA-CB-CG2	5.74	120.43	112.40
1	B	200	LYS	CD-CE-NZ	5.72	124.85	111.70
1	A	241	ARG	NH1-CZ-NH2	5.71	125.67	119.40
1	A	65	ASP	N-CA-CB	5.70	120.86	110.60
1	B	99	TRP	CA-CB-CG	5.68	124.50	113.70
1	B	138	ASP	CA-C-O	-5.67	108.19	120.10
1	C	152	ASN	CA-CB-CG	5.67	125.86	113.40
1	B	158	THR	N-CA-CB	5.65	121.04	110.30
1	C	119	TYR	N-CA-CB	-5.65	100.42	110.60
1	C	234	LYS	C-N-CA	5.65	135.83	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	SER	CB-CA-C	5.65	120.83	110.10
1	C	154	LYS	C-N-CA	-5.62	110.50	122.30
1	B	234	LYS	CA-CB-CG	5.58	125.68	113.40
1	B	73	GLU	CA-CB-CG	5.57	125.66	113.40
1	A	169	CYS	N-CA-C	-5.57	95.96	111.00
1	C	110	TYR	CB-CG-CD2	-5.56	117.67	121.00
1	A	178	ASP	CB-CG-OD1	5.55	123.30	118.30
1	B	191	GLU	CG-CD-OE2	-5.54	107.22	118.30
1	C	99	TRP	O-C-N	5.52	131.53	122.70
1	B	80	VAL	O-C-N	5.51	131.52	122.70
1	C	143	LEU	CB-CG-CD2	-5.51	101.64	111.00
1	B	99	TRP	CB-CA-C	5.50	121.40	110.40
1	A	230	GLY	N-CA-C	-5.50	99.36	113.10
1	B	246	TYR	O-C-N	5.50	131.50	122.70
1	C	110	TYR	O-C-N	5.49	131.49	122.70
1	B	77	GLU	CG-CD-OE1	5.49	129.28	118.30
1	A	223	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	A	174	THR	CA-CB-OG1	-5.46	97.52	109.00
1	A	252	GLU	CG-CD-OE2	-5.46	107.38	118.30
1	B	184	THR	CA-CB-CG2	-5.45	104.77	112.40
1	B	120	LEU	CB-CA-C	5.45	120.55	110.20
1	A	213	ALA	O-C-N	5.44	131.40	122.70
1	C	95	THR	CA-CB-CG2	5.44	120.01	112.40
1	A	105	GLN	O-C-N	5.44	131.40	122.70
1	A	116	ARG	NH1-CZ-NH2	5.43	125.38	119.40
1	C	138	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	B	243	TYR	CB-CG-CD1	5.41	124.25	121.00
1	B	152	ASN	CA-C-O	-5.40	108.76	120.10
1	C	173	ASN	N-CA-CB	5.39	120.31	110.60
1	C	163	GLU	CG-CD-OE1	5.39	129.08	118.30
1	B	123	CYS	CA-CB-SG	-5.39	104.30	114.00
1	B	174	THR	O-C-N	5.39	131.32	122.70
1	B	182	ALA	O-C-N	5.37	131.29	122.70
1	C	161	VAL	N-CA-CB	-5.37	99.69	111.50
1	C	250	LEU	CB-CA-C	5.37	120.40	110.20
1	A	241	ARG	CD-NE-CZ	-5.37	116.09	123.60
1	A	252	GLU	N-CA-C	-5.37	96.51	111.00
1	A	229	GLU	CA-C-O	-5.36	108.84	120.10
1	C	87	THR	N-CA-CB	-5.36	100.12	110.30
1	A	115	ILE	O-C-N	5.35	131.26	122.70
1	C	101	ARG	NH1-CZ-NH2	-5.35	113.51	119.40
1	C	222	ALA	N-CA-CB	-5.35	102.61	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	GLU	CB-CA-C	5.34	121.09	110.40
1	C	89	GLU	CB-CA-C	-5.34	99.72	110.40
1	C	138	ASP	CB-CA-C	5.34	121.08	110.40
1	B	141	ASP	N-CA-CB	-5.34	101.00	110.60
1	B	100	LEU	O-C-N	5.33	131.23	122.70
1	A	217	ASN	C-N-CA	5.33	135.02	121.70
1	A	247	THR	N-CA-CB	5.33	120.42	110.30
1	A	188	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	191	GLU	CG-CD-OE2	-5.32	107.66	118.30
1	C	230	GLY	O-C-N	-5.31	114.18	123.20
1	B	173	ASN	CA-C-O	5.30	131.24	120.10
1	C	174	THR	CA-CB-CG2	5.30	119.83	112.40
1	A	82	VAL	CA-CB-CG1	5.29	118.84	110.90
1	A	137	TYR	N-CA-CB	-5.28	101.09	110.60
1	B	247	THR	O-C-N	5.28	131.15	122.70
1	C	217	ASN	CB-CG-OD1	-5.28	111.04	121.60
1	C	168	LEU	CA-CB-CG	-5.28	103.16	115.30
1	A	72	CYS	O-C-N	5.28	131.14	122.70
1	A	251	ILE	N-CA-CB	-5.27	98.68	110.80
1	B	256	ALA	CA-C-N	-5.27	105.61	117.20
1	A	111	ALA	O-C-N	5.26	131.11	122.70
1	B	218	ILE	N-CA-CB	5.25	122.88	110.80
1	B	252	GLU	CB-CG-CD	5.25	128.37	114.20
1	A	247	THR	O-C-N	5.24	131.08	122.70
1	A	77	GLU	CG-CD-OE1	5.23	128.77	118.30
1	A	204	ASP	OD1-CG-OD2	-5.22	113.38	123.30
1	B	73	GLU	CA-C-O	-5.22	109.15	120.10
1	B	238	ASN	CA-C-O	-5.21	109.15	120.10
1	C	188	ASP	CA-CB-CG	5.21	124.87	113.40
1	A	116	ARG	N-CA-CB	-5.21	101.22	110.60
1	B	222	ALA	N-CA-CB	-5.20	102.82	110.10
1	C	78	LEU	N-CA-CB	-5.20	100.00	110.40
1	A	135	PHE	O-C-N	5.18	131.00	122.70
1	C	116	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	223	ARG	O-C-N	5.17	130.97	122.70
1	B	204	ASP	CA-CB-CG	-5.17	102.04	113.40
1	C	195	LYS	CA-CB-CG	5.16	124.76	113.40
1	C	132	HIS	O-C-N	5.16	130.95	122.70
1	A	128	SER	CA-C-O	-5.16	109.27	120.10
1	B	77	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	A	95	THR	CB-CA-C	-5.15	97.68	111.60
1	B	250	LEU	O-C-N	5.14	130.92	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	GLU	CA-CB-CG	5.13	124.70	113.40
1	C	208	ALA	CA-C-O	5.13	130.88	120.10
1	B	165	GLN	OE1-CD-NE2	5.12	133.69	121.90
1	B	175	LYS	CB-CA-C	5.12	120.65	110.40
1	A	119	TYR	O-C-N	5.12	130.88	122.70
1	C	216	GLY	O-C-N	5.11	130.88	122.70
1	C	199	PHE	CB-CG-CD1	-5.11	117.22	120.80
1	C	73	GLU	CB-CA-C	5.11	120.61	110.40
1	C	181	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	C	182	ALA	CB-CA-C	5.10	117.76	110.10
1	A	168	LEU	N-CA-C	-5.10	97.23	111.00
1	C	77	GLU	CG-CD-OE2	-5.10	108.10	118.30
1	B	206	ALA	CB-CA-C	5.09	117.74	110.10
1	B	67	THR	CA-CB-OG1	-5.09	98.31	109.00
1	A	133	MET	N-CA-CB	5.09	119.76	110.60
1	A	194	GLU	OE1-CD-OE2	5.08	129.39	123.30
1	B	206	ALA	N-CA-CB	-5.07	103.00	110.10
1	A	213	ALA	CA-C-O	-5.07	109.46	120.10
1	A	218	ILE	O-C-N	5.07	130.81	122.70
1	B	174	THR	N-CA-CB	5.05	119.89	110.30
1	C	116	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	229	GLU	C-N-CA	-5.03	111.73	122.30
1	B	74	LEU	N-CA-C	-5.03	97.42	111.00
1	C	235	THR	CA-CB-OG1	-5.03	98.44	109.00
1	A	77	GLU	OE1-CD-OE2	-5.02	117.27	123.30
1	A	236	ALA	N-CA-CB	-5.02	103.07	110.10
1	A	112	TRP	CA-C-O	-5.01	109.58	120.10
1	A	78	LEU	CA-C-N	-5.01	106.18	117.20
1	B	109	LYS	CB-CA-C	5.01	120.41	110.40

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ARG	Sidechain
1	A	223	ARG	Sidechain
1	A	249	ARG	Sidechain
1	B	101	ARG	Sidechain
1	B	241	ARG	Sidechain
1	B	249	ARG	Sidechain
1	C	101	ARG	Sidechain
1	C	181	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	196	ARG	Sidechain
1	C	223	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1506	0	1504	207	87
1	B	1506	0	1504	182	1771
1	C	1674	0	1691	187	1943
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	15	0	0	1	1
3	B	10	0	0	0	6
3	C	9	0	0	0	15
All	All	4723	0	4699	540	2046

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 58.

All (540) 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:C:212:ASN:ND2	1:C:214:ASN:H	1.42	1.15
1:C:145:VAL:H	1:C:149:GLN:NE2	1.46	1.11
1:C:161:VAL:HG22	1:C:239:THR:CG2	1.82	1.08
1:C:161:VAL:HG22	1:C:239:THR:HG21	1.09	1.07
1:C:131:ILE:HG13	1:C:228:MET:HE2	1.34	1.06
1:A:168:LEU:O	1:A:169:CYS:HB2	1.57	1.04
1:A:165:GLN:HE21	1:A:165:GLN:HA	1.21	1.03
1:C:187:LEU:HD22	1:C:188:ASP:H	1.19	1.02
1:A:201:THR:HG22	1:A:260:LEU:OXT	1.61	1.01
1:C:54:LYS:H	1:C:172:ASN:HD21	0.99	0.95
1:A:105:GLN:HA	1:A:199:PHE:CE1	2.01	0.95
1:C:119:TYR:OH	1:C:239:THR:HG22	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:VAL:H	1:C:149:GLN:HE22	1.07	0.93
1:C:139:MET:H	1:C:217:ASN:HD21	0.93	0.92
1:C:125:THR:HG22	1:C:162:TRP:CE3	2.04	0.92
1:C:212:ASN:HD22	1:C:214:ASN:N	1.66	0.91
1:A:251:ILE:HG23	1:A:252:GLU:HG2	1.52	0.91
1:B:150:LEU:HA	1:B:153:LEU:HD12	1.53	0.90
1:C:195:LYS:HZ3	1:C:195:LYS:HB3	1.36	0.90
1:A:178:ASP:HB2	1:A:180:SER:OG	1.72	0.90
1:A:168:LEU:O	1:A:169:CYS:CB	2.20	0.89
1:B:248:ILE:HD12	1:B:250:LEU:HD13	1.52	0.89
1:C:187:LEU:CD2	1:C:188:ASP:H	1.86	0.89
1:C:187:LEU:HD22	1:C:188:ASP:N	1.87	0.89
1:C:115:ILE:HG23	1:C:187:LEU:HB2	1.54	0.89
1:C:161:VAL:CG2	1:C:239:THR:HG21	2.01	0.89
1:A:205:TYR:CE2	1:A:209:VAL:HG21	2.08	0.88
1:A:148:ASN:O	1:A:151:SER:HB3	1.75	0.87
1:A:137:TYR:CE1	1:B:252:GLU:HG3	2.10	0.87
1:C:195:LYS:NZ	1:C:195:LYS:HB3	1.90	0.87
1:C:90:LEU:HB2	1:C:95:THR:HG21	1.57	0.87
1:B:82:VAL:HG22	1:B:234:LYS:HA	1.57	0.86
1:C:139:MET:H	1:C:217:ASN:ND2	1.74	0.85
1:A:136:GLN:HE21	1:A:223:ARG:HH11	1.25	0.85
1:C:129:GLY:HA2	1:C:230:GLY:HA3	1.58	0.84
1:B:103:VAL:O	1:B:106:ASN:ND2	2.11	0.84
1:C:129:GLY:O	1:C:161:VAL:HB	1.77	0.83
1:B:78:LEU:HB2	1:B:228:MET:HE2	1.61	0.82
1:B:140:ALA:O	1:C:260:LEU:HD12	1.79	0.82
1:B:131:ILE:O	1:B:158:THR:HG23	1.80	0.80
1:C:145:VAL:N	1:C:149:GLN:NE2	2.29	0.80
1:C:146:SER:H	1:C:149:GLN:HE21	1.28	0.80
1:A:105:GLN:HA	1:A:199:PHE:HE1	1.42	0.80
1:B:120:LEU:HD11	1:B:171:VAL:HG21	1.64	0.80
1:C:139:MET:N	1:C:217:ASN:HD21	1.77	0.80
1:A:90:LEU:HD13	1:A:92:MET:HE1	1.63	0.79
1:A:165:GLN:NE2	1:A:165:GLN:HA	1.97	0.79
1:A:92:MET:O	1:A:96:VAL:HG23	1.83	0.79
1:B:212:ASN:ND2	1:B:214:ASN:HB2	1.98	0.78
1:B:151:SER:HA	1:B:156:TYR:CD2	2.18	0.78
1:C:212:ASN:ND2	1:C:214:ASN:N	2.25	0.78
1:C:212:ASN:HD22	1:C:214:ASN:H	0.81	0.78
1:B:100:LEU:HG	1:B:246:TYR:CE2	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:LYS:H	1:C:172:ASN:ND2	1.81	0.77
1:B:124:PRO:HD2	1:B:127:THR:OG1	1.82	0.77
1:C:119:TYR:OH	1:C:239:THR:CG2	2.32	0.77
1:B:214:ASN:HD21	1:C:200:LYS:NZ	1.82	0.77
1:B:117:TYR:HB3	1:B:242:LEU:HD21	1.65	0.77
1:A:144:PRO:HA	1:B:258:LEU:HD11	1.66	0.77
1:C:163:GLU:HG3	1:C:164:GLY:N	1.99	0.77
1:A:105:GLN:CA	1:A:199:PHE:HE1	1.97	0.76
1:A:181:ARG:O	1:A:181:ARG:HG2	1.84	0.76
1:C:131:ILE:CG1	1:C:228:MET:HE2	2.14	0.76
1:C:49:GLN:NE2	1:C:165:GLN:HG2	2.00	0.76
1:A:161:VAL:HB	1:A:239:THR:OG1	1.86	0.75
1:A:123:CYS:HB3	1:A:124:PRO:HD2	1.67	0.75
1:A:143:LEU:HD12	1:A:143:LEU:N	2.00	0.75
1:C:169:CYS:O	1:C:173:ASN:N	2.20	0.74
1:A:136:GLN:HE21	1:A:223:ARG:NH1	1.86	0.74
1:A:109:LYS:HE3	1:A:252:GLU:OE1	1.88	0.74
1:C:60:LEU:HD12	1:C:69:LEU:HD13	1.70	0.74
1:A:129:GLY:HA2	1:A:230:GLY:CA	2.18	0.73
1:A:79:ALA:HA	1:A:237:VAL:O	1.89	0.73
1:C:150:LEU:HD13	1:C:150:LEU:O	1.89	0.73
1:C:125:THR:HG22	1:C:162:TRP:CD2	2.24	0.72
1:A:205:TYR:CZ	1:A:209:VAL:HG21	2.24	0.72
1:C:66:VAL:HG12	1:C:251:ILE:HD11	1.70	0.72
1:B:146:SER:OG	1:B:148:ASN:HB2	1.89	0.71
1:A:129:GLY:HA2	1:A:230:GLY:HA2	1.72	0.71
1:C:101:ARG:HG2	1:C:102:GLY:N	2.03	0.71
1:A:200:LYS:HE3	1:A:260:LEU:C	2.11	0.70
1:A:105:GLN:HA	1:A:199:PHE:CD1	2.26	0.70
1:B:195:LYS:HE3	1:C:195:LYS:HZ1	1.56	0.70
1:A:258:LEU:HD11	1:C:144:PRO:HA	1.74	0.69
1:C:116:ARG:HH21	1:C:184:THR:HG21	1.57	0.69
1:A:155:GLY:HA3	1:A:185:ILE:HG13	1.74	0.69
1:C:234:LYS:HE3	1:C:234:LYS:H	1.58	0.69
1:B:110:TYR:HB2	1:B:248:ILE:HD11	1.74	0.69
1:C:239:THR:HG22	1:C:240:GLY:N	2.06	0.69
1:B:118:THR:O	1:B:242:LEU:HD23	1.92	0.69
1:C:81:THR:HG23	1:C:83:THR:O	1.92	0.68
1:B:138:ASP:HA	1:B:217:ASN:HD21	1.58	0.68
1:C:145:VAL:N	1:C:149:GLN:HE22	1.88	0.68
1:A:94:PHE:HB2	1:A:199:PHE:HE2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:MET:H	1:B:217:ASN:HD21	1.40	0.68
1:C:205:TYR:O	1:C:209:VAL:HG23	1.93	0.68
1:B:174:THR:HG22	1:B:175:LYS:H	1.58	0.68
1:C:118:THR:HB	1:C:184:THR:OG1	1.94	0.67
1:A:201:THR:HG22	1:A:260:LEU:C	2.14	0.67
1:B:94:PHE:CE1	1:B:101:ARG:HD2	2.29	0.67
1:C:69:LEU:HD12	1:C:70:SER:N	2.10	0.67
1:A:116:ARG:NE	1:A:170:PHE:HD1	1.92	0.67
1:C:163:GLU:HG3	1:C:164:GLY:H	1.58	0.67
1:B:218:ILE:HG12	1:B:219:LEU:CD1	2.25	0.67
1:A:218:ILE:HD11	1:B:218:ILE:HD12	1.77	0.66
1:B:166:SER:O	1:B:176:CYS:SG	2.53	0.66
1:A:148:ASN:C	1:A:148:ASN:HD22	1.98	0.66
1:B:175:LYS:O	1:B:177:PRO:HD3	1.94	0.66
1:B:119:TYR:O	1:B:120:LEU:HD23	1.96	0.66
1:A:108:SER:HB2	1:A:252:GLU:O	1.96	0.66
1:A:66:VAL:HG21	1:A:249:ARG:HH21	1.61	0.66
1:B:125:THR:O	1:B:125:THR:HG22	1.95	0.66
1:B:71:HIS:HD2	1:B:99:TRP:CZ3	2.13	0.66
1:C:92:MET:O	1:C:96:VAL:HG23	1.94	0.66
1:B:137:TYR:CD1	1:C:252:GLU:HG3	2.31	0.66
1:C:78:LEU:HG	1:C:228:MET:HE3	1.77	0.66
1:C:124:PRO:O	1:C:127:THR:OG1	2.14	0.66
1:A:110:TYR:CD1	1:A:248:ILE:HD11	2.32	0.65
1:A:71:HIS:HB3	1:A:246:TYR:CZ	2.31	0.65
1:B:138:ASP:O	1:B:141:ASP:HB2	1.97	0.65
1:A:81:THR:O	1:A:231:GLY:HA2	1.95	0.65
1:C:195:LYS:NZ	1:C:195:LYS:CB	2.57	0.65
1:A:160:PRO:HG2	1:A:163:GLU:HB2	1.78	0.65
1:B:150:LEU:HA	1:B:153:LEU:CD1	2.25	0.65
1:C:115:ILE:CG2	1:C:187:LEU:HB2	2.27	0.64
1:B:189:THR:HA	1:B:192:VAL:HG23	1.79	0.64
1:B:73:GLU:OE1	1:B:99:TRP:HB3	1.96	0.64
1:B:248:ILE:HD13	1:B:249:ARG:H	1.63	0.64
1:A:174:THR:HG22	1:A:176:CYS:SG	2.38	0.64
1:B:136:GLN:HE22	1:B:143:LEU:HD23	1.61	0.64
1:B:106:ASN:H	1:B:106:ASN:ND2	1.94	0.64
1:A:155:GLY:O	1:A:156:TYR:C	2.36	0.63
1:B:115:ILE:HG13	1:B:246:TYR:HB3	1.79	0.63
1:B:135:PHE:HE2	1:B:187:LEU:HA	1.64	0.63
1:A:215:ILE:O	1:A:219:LEU:HD12	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:LEU:HG	1:C:228:MET:CE	2.28	0.63
1:A:100:LEU:HG	1:A:246:TYR:CE2	2.34	0.62
1:C:146:SER:H	1:C:149:GLN:NE2	1.97	0.62
1:A:92:MET:HE2	1:A:220:VAL:CG1	2.29	0.62
1:A:144:PRO:CA	1:B:258:LEU:HD11	2.29	0.62
1:C:169:CYS:O	1:C:173:ASN:HA	1.99	0.62
1:B:81:THR:O	1:B:231:GLY:HA3	2.00	0.62
1:C:125:THR:CG2	1:C:162:TRP:CE3	2.81	0.62
1:C:144:PRO:CG	1:C:150:LEU:HD23	2.29	0.62
1:B:78:LEU:N	1:B:78:LEU:HD12	2.15	0.62
1:C:169:CYS:O	1:C:173:ASN:CA	2.48	0.62
1:C:155:GLY:HA3	1:C:185:ILE:HG13	1.82	0.61
1:B:79:ALA:HB1	1:B:237:VAL:O	2.00	0.61
1:A:71:HIS:CG	1:A:72:CYS:H	2.18	0.61
1:B:78:LEU:HB2	1:B:228:MET:CE	2.29	0.61
1:A:116:ARG:NE	1:A:170:PHE:CD1	2.68	0.61
1:A:260:LEU:N	1:A:260:LEU:HD23	2.16	0.61
1:A:109:LYS:CE	1:A:252:GLU:OE1	2.49	0.61
1:B:139:MET:CE	1:B:223:ARG:HB3	2.31	0.60
1:A:135:PHE:CE1	1:A:185:ILE:HG12	2.37	0.60
1:A:138:ASP:O	1:A:140:ALA:N	2.35	0.60
1:C:74:LEU:HD12	1:C:75:SER:N	2.16	0.60
1:B:158:THR:HG22	1:B:159:GLY:H	1.66	0.60
1:A:137:TYR:CE2	1:B:252:GLU:OE1	2.55	0.60
1:B:74:LEU:HD12	1:B:74:LEU:H	1.67	0.60
1:C:187:LEU:CD2	1:C:188:ASP:N	2.56	0.60
1:A:129:GLY:C	1:A:161:VAL:HG13	2.21	0.59
1:C:192:VAL:HG13	1:C:197:TYR:OH	2.01	0.59
1:C:133:MET:HA	1:C:225:VAL:O	2.03	0.59
1:C:66:VAL:CG1	1:C:251:ILE:HD11	2.31	0.59
1:A:200:LYS:CE	1:A:260:LEU:OXT	2.51	0.59
1:B:71:HIS:HB3	1:B:246:TYR:CZ	2.38	0.59
1:B:195:LYS:HE3	1:C:195:LYS:CE	2.32	0.59
1:A:123:CYS:CB	1:A:124:PRO:CD	2.79	0.58
1:B:71:HIS:ND1	1:B:72:CYS:N	2.49	0.58
1:C:80:VAL:HG13	1:C:81:THR:N	2.19	0.58
1:A:92:MET:HE2	1:A:220:VAL:HG12	1.84	0.58
1:B:195:LYS:HE3	1:C:195:LYS:NZ	2.18	0.58
1:A:137:TYR:CD1	1:B:252:GLU:HG3	2.39	0.58
1:A:196:ARG:N	1:A:196:ARG:HD2	2.18	0.58
1:B:218:ILE:HG12	1:B:219:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:GLY:O	1:B:219:LEU:N	2.37	0.58
1:A:141:ASP:HB3	1:B:258:LEU:O	2.04	0.58
1:A:135:PHE:HE1	1:A:185:ILE:HG12	1.67	0.58
1:A:251:ILE:HG23	1:A:252:GLU:CG	2.31	0.58
1:B:139:MET:H	1:B:217:ASN:ND2	2.01	0.58
1:C:114:ALA:O	1:C:246:TYR:HA	2.04	0.58
1:C:52:MET:SD	1:C:52:MET:N	2.76	0.58
1:A:248:ILE:HG23	1:A:250:LEU:HD13	1.85	0.57
1:B:155:GLY:O	1:B:157:VAL:HG23	2.04	0.57
1:A:212:ASN:OD1	1:A:214:ASN:HB2	2.02	0.57
1:B:212:ASN:HD21	1:B:214:ASN:HB2	1.67	0.57
1:B:82:VAL:HG21	1:B:234:LYS:HG3	1.86	0.57
1:A:138:ASP:C	1:A:140:ALA:N	2.57	0.57
1:B:139:MET:N	1:B:217:ASN:HD21	2.03	0.57
1:B:246:TYR:N	1:B:246:TYR:CD1	2.72	0.57
1:A:129:GLY:HA2	1:A:230:GLY:HA3	1.85	0.57
1:A:71:HIS:HD2	1:A:99:TRP:CE3	2.23	0.57
1:A:200:LYS:HE3	1:A:260:LEU:OXT	2.05	0.57
1:B:131:ILE:O	1:B:158:THR:CG2	2.53	0.57
1:B:94:PHE:O	1:B:101:ARG:NH1	2.35	0.57
1:C:135:PHE:O	1:C:153:LEU:HG	2.05	0.57
1:C:256:ALA:O	1:C:257:ALA:C	2.43	0.57
1:A:91:VAL:HG13	1:A:222:ALA:O	2.05	0.56
1:C:144:PRO:HG3	1:C:150:LEU:CD2	2.35	0.56
1:A:143:LEU:N	1:A:143:LEU:CD1	2.68	0.56
1:A:248:ILE:HG23	1:A:250:LEU:CD1	2.35	0.56
1:B:135:PHE:CE2	1:B:187:LEU:HA	2.40	0.56
1:B:73:GLU:OE1	1:B:99:TRP:N	2.29	0.56
1:C:234:LYS:H	1:C:234:LYS:CD	2.19	0.56
1:A:195:LYS:C	1:A:196:ARG:HD2	2.26	0.56
1:B:136:GLN:NE2	1:B:143:LEU:HD23	2.19	0.56
1:B:158:THR:HG22	1:B:159:GLY:N	2.20	0.56
1:B:189:THR:HA	1:B:192:VAL:CG2	2.35	0.56
1:A:142:THR:HB	1:B:258:LEU:HD22	1.87	0.56
1:A:137:TYR:CZ	1:B:252:GLU:OE1	2.58	0.56
1:B:156:TYR:C	1:B:157:VAL:HG23	2.26	0.56
1:B:251:ILE:HG23	1:B:252:GLU:OE2	2.06	0.56
1:A:116:ARG:HG3	1:A:186:ALA:HB2	1.86	0.56
1:B:70:SER:OG	1:B:247:THR:HG23	2.06	0.56
1:A:179:THR:O	1:A:180:SER:C	2.43	0.56
1:A:71:HIS:CG	1:A:72:CYS:N	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:CYS:HB3	1:A:124:PRO:CD	2.34	0.56
1:B:248:ILE:HD13	1:B:249:ARG:N	2.20	0.56
1:A:199:PHE:O	1:A:200:LYS:HD2	2.05	0.56
1:A:155:GLY:HA3	1:A:185:ILE:CG1	2.36	0.56
1:A:160:PRO:O	1:A:162:TRP:N	2.39	0.55
1:C:60:LEU:CD1	1:C:69:LEU:HD13	2.36	0.55
1:B:195:LYS:HE3	1:C:195:LYS:HE3	1.89	0.55
1:A:138:ASP:C	1:A:140:ALA:H	2.09	0.55
1:B:106:ASN:N	1:B:106:ASN:ND2	2.54	0.55
1:B:82:VAL:CG2	1:B:234:LYS:HA	2.33	0.55
1:A:251:ILE:CG2	1:A:252:GLU:HG2	2.32	0.55
1:C:49:GLN:CD	1:C:165:GLN:HG2	2.26	0.55
1:C:234:LYS:CE	1:C:234:LYS:H	2.19	0.55
1:C:101:ARG:CG	1:C:102:GLY:N	2.69	0.55
1:C:90:LEU:CB	1:C:95:THR:HG21	2.35	0.55
1:C:90:LEU:HD11	1:C:205:TYR:CE1	2.41	0.55
1:A:119:TYR:O	1:A:120:LEU:HD23	2.06	0.55
1:B:161:VAL:HB	1:B:239:THR:HB	1.89	0.55
1:B:169:CYS:HA	1:B:172:ASN:HB2	1.89	0.55
1:B:150:LEU:O	1:B:150:LEU:HD12	2.07	0.54
1:B:138:ASP:HA	1:B:217:ASN:ND2	2.21	0.54
1:A:200:LYS:HZ2	1:C:140:ALA:HB3	1.72	0.54
1:C:144:PRO:HG3	1:C:150:LEU:HD23	1.89	0.54
1:A:259:ASN:C	1:A:260:LEU:HD23	2.27	0.54
1:B:199:PHE:CD2	1:B:199:PHE:C	2.80	0.54
1:C:80:VAL:CG1	1:C:81:THR:N	2.70	0.54
1:A:223:ARG:HG2	1:A:223:ARG:O	2.07	0.54
1:C:205:TYR:CE1	1:C:209:VAL:HG21	2.43	0.54
1:B:199:PHE:HD2	1:B:199:PHE:C	2.10	0.54
1:C:101:ARG:HG2	1:C:102:GLY:H	1.73	0.54
1:B:214:ASN:HD21	1:C:200:LYS:HZ1	1.56	0.54
1:A:123:CYS:HB2	1:A:124:PRO:O	2.07	0.54
1:C:146:SER:N	1:C:149:GLN:NE2	2.56	0.53
1:A:139:MET:HG3	1:A:205:TYR:OH	2.08	0.53
1:B:123:CYS:HB2	1:B:124:PRO:CD	2.38	0.53
1:B:145:VAL:N	1:B:149:GLN:OE1	2.33	0.53
1:A:81:THR:O	1:A:231:GLY:CA	2.56	0.53
1:B:106:ASN:HD22	1:B:106:ASN:H	1.57	0.53
1:B:137:TYR:CE1	1:C:252:GLU:HG3	2.43	0.53
1:C:218:ILE:O	1:C:220:VAL:N	2.41	0.53
1:C:233:SER:HA	1:C:234:LYS:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:LEU:O	1:C:95:THR:CG2	2.57	0.53
1:A:204:ASP:O	1:A:205:TYR:C	2.46	0.53
1:A:147:VAL:HG12	1:A:148:ASN:N	2.24	0.53
1:A:105:GLN:CA	1:A:199:PHE:CE1	2.77	0.53
1:A:71:HIS:ND1	1:A:72:CYS:N	2.51	0.53
1:C:131:ILE:HG12	1:C:132:HIS:N	2.24	0.53
1:A:139:MET:N	1:A:217:ASN:OD1	2.40	0.53
1:A:124:PRO:HB2	1:A:126:THR:HG22	1.90	0.52
1:A:218:ILE:CD1	1:B:218:ILE:HD12	2.38	0.52
1:B:80:VAL:HG22	1:B:239:THR:CG2	2.39	0.52
1:C:178:ASP:OD1	1:C:180:SER:HB2	2.08	0.52
1:A:134:GLY:HA3	1:A:153:LEU:HB3	1.91	0.52
1:A:63:SER:HA	1:A:66:VAL:O	2.09	0.52
1:A:78:LEU:HB2	1:A:228:MET:CE	2.38	0.52
1:A:165:GLN:O	1:A:167:GLY:N	2.38	0.52
1:A:200:LYS:CG	1:A:219:LEU:HD23	2.39	0.52
1:A:218:ILE:O	1:A:218:ILE:HG22	2.09	0.52
1:B:73:GLU:OE1	1:B:99:TRP:CB	2.57	0.52
1:A:195:LYS:HB3	1:A:196:ARG:HD2	1.92	0.52
1:B:248:ILE:HG23	1:B:250:LEU:HD22	1.91	0.52
1:A:212:ASN:OD1	1:A:213:ALA:N	2.42	0.52
1:A:250:LEU:N	1:A:250:LEU:CD1	2.72	0.52
1:A:123:CYS:CB	1:A:124:PRO:HD2	2.35	0.51
1:A:212:ASN:C	1:A:212:ASN:OD1	2.48	0.51
1:A:92:MET:CE	1:A:220:VAL:HG11	2.39	0.51
1:A:201:THR:CG2	1:A:260:LEU:HA	2.41	0.51
1:C:107:TRP:CE3	1:C:250:LEU:HD23	2.45	0.51
1:C:84:ILE:HG23	1:C:85:VAL:N	2.24	0.51
1:A:194:GLU:HB2	1:A:197:TYR:CZ	2.45	0.51
1:A:132:HIS:CE1	1:A:147:VAL:CG2	2.93	0.51
1:C:116:ARG:NH2	1:C:184:THR:HG21	2.24	0.51
1:B:118:THR:HG23	1:B:184:THR:HB	1.93	0.51
1:B:129:GLY:HA2	1:B:230:GLY:CA	2.40	0.51
1:B:214:ASN:HD22	1:C:219:LEU:HD11	1.76	0.51
1:B:62:SER:HA	1:B:68:ILE:CD1	2.41	0.51
1:C:169:CYS:HB3	1:C:174:THR:HG22	1.93	0.51
1:A:94:PHE:HB2	1:A:199:PHE:CE2	2.43	0.51
1:B:131:ILE:O	1:B:158:THR:HA	2.11	0.51
1:B:175:LYS:O	1:B:177:PRO:CD	2.58	0.51
1:C:218:ILE:O	1:C:219:LEU:C	2.49	0.51
1:B:103:VAL:HG12	1:B:107:TRP:HZ3	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:MET:HG3	1:C:185:ILE:HG21	1.92	0.50
1:C:73:GLU:OE1	1:C:99:TRP:N	2.32	0.50
1:A:258:LEU:HD11	1:C:144:PRO:CA	2.40	0.50
1:B:138:ASP:CA	1:B:217:ASN:HD21	2.23	0.50
1:A:142:THR:HG22	1:A:143:LEU:O	2.11	0.50
1:A:129:GLY:CA	1:A:230:GLY:HA3	2.41	0.50
1:A:228:MET:HE3	1:A:239:THR:HG21	1.94	0.50
1:B:139:MET:HE1	1:B:223:ARG:HB3	1.94	0.50
1:C:131:ILE:O	1:C:158:THR:HA	2.11	0.50
1:A:201:THR:HG22	1:A:260:LEU:CA	2.41	0.50
1:B:205:TYR:O	1:B:208:ALA:HB3	2.11	0.50
1:B:185:ILE:HG23	1:B:185:ILE:O	2.11	0.50
1:C:113:VAL:HB	1:C:247:THR:O	2.12	0.50
1:C:196:ARG:NH1	1:C:249:ARG:HH21	2.10	0.49
1:A:200:LYS:HE3	1:A:260:LEU:O	2.10	0.49
1:B:213:ALA:O	1:B:214:ASN:C	2.50	0.49
1:A:249:ARG:NH2	1:C:191:GLU:OE1	2.45	0.49
1:A:107:TRP:CZ3	1:A:250:LEU:HD23	2.47	0.49
1:C:116:ARG:NE	1:C:170:PHE:CE2	2.80	0.49
1:A:124:PRO:HD2	1:A:127:THR:OG1	2.11	0.49
1:B:72:CYS:HA	1:B:244:ALA:O	2.12	0.49
1:A:133:MET:HA	1:A:225:VAL:O	2.13	0.49
1:A:139:MET:N	1:A:139:MET:SD	2.80	0.49
1:C:56:ARG:HG2	1:C:57:PRO:HD2	1.95	0.49
1:C:69:LEU:HD12	1:C:70:SER:H	1.77	0.49
1:A:124:PRO:HG2	1:A:126:THR:HG22	1.95	0.49
1:A:215:ILE:HG22	1:A:219:LEU:HD11	1.95	0.49
1:B:138:ASP:OD2	1:B:140:ALA:HB3	2.11	0.49
1:C:167:GLY:O	1:C:168:LEU:C	2.51	0.49
1:A:200:LYS:HG3	1:A:219:LEU:HD23	1.95	0.49
1:C:76:THR:CG2	1:C:77:GLU:N	2.75	0.49
1:A:199:PHE:HD2	1:A:200:LYS:N	2.11	0.48
1:B:72:CYS:O	1:B:73:GLU:HB2	2.13	0.48
1:C:201:THR:HG23	1:C:260:LEU:HA	1.94	0.48
1:B:62:SER:HA	1:B:68:ILE:HD12	1.95	0.48
1:C:194:GLU:HB2	1:C:197:TYR:CE2	2.48	0.48
1:B:105:GLN:HA	1:B:199:PHE:CE1	2.48	0.48
1:B:78:LEU:H	1:B:78:LEU:HD12	1.77	0.48
1:B:69:LEU:HB3	1:B:248:ILE:HG22	1.95	0.48
1:C:151:SER:HA	1:C:156:TYR:CD2	2.49	0.48
1:C:99:TRP:O	1:C:100:LEU:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASN:N	1:A:238:ASN:HD22	2.11	0.48
1:A:79:ALA:CA	1:A:237:VAL:O	2.61	0.48
1:B:101:ARG:O	1:B:105:GLN:HB2	2.13	0.48
1:A:89:GLU:OE2	1:A:89:GLU:HA	2.14	0.48
1:A:177:PRO:O	1:A:178:ASP:HB3	2.14	0.48
1:A:200:LYS:HE2	1:A:260:LEU:OXT	2.12	0.48
1:B:69:LEU:HB3	1:B:248:ILE:CG2	2.43	0.48
1:C:150:LEU:HD22	1:C:153:LEU:HD22	1.95	0.48
1:B:213:ALA:O	1:B:216:GLY:N	2.40	0.48
1:B:214:ASN:HD21	1:C:200:LYS:HZ2	1.60	0.48
1:C:116:ARG:CZ	1:C:170:PHE:CE2	2.97	0.47
1:B:188:ASP:OD1	1:B:191:GLU:HB2	2.13	0.47
1:A:155:GLY:HA3	1:A:185:ILE:CD1	2.44	0.47
1:A:169:CYS:N	1:A:172:ASN:HB2	2.30	0.47
1:A:124:PRO:C	1:A:126:THR:H	2.18	0.47
1:A:138:ASP:HB3	1:A:141:ASP:OD2	2.15	0.47
1:A:200:LYS:HZ2	1:C:140:ALA:CB	2.27	0.47
1:B:117:TYR:HB3	1:B:242:LEU:CD2	2.41	0.47
1:A:138:ASP:HB3	1:A:141:ASP:CG	2.35	0.47
1:A:92:MET:CE	1:A:220:VAL:CG1	2.93	0.47
1:C:251:ILE:O	1:C:252:GLU:HB3	2.15	0.47
1:A:181:ARG:O	1:A:182:ALA:HB2	2.14	0.47
1:A:94:PHE:O	1:A:101:ARG:NH1	2.41	0.47
1:B:169:CYS:HB2	1:B:174:THR:HB	1.96	0.47
1:B:70:SER:HA	1:B:246:TYR:O	2.14	0.47
1:C:116:ARG:HE	1:C:184:THR:HG21	1.79	0.47
1:C:116:ARG:HD3	1:C:170:PHE:CD2	2.50	0.47
1:A:64:MET:HA	3:A:262:HOH:O	2.15	0.47
1:C:197:TYR:CZ	1:C:221:PRO:HB3	2.50	0.47
1:A:142:THR:CG2	1:B:258:LEU:HD22	2.45	0.46
1:A:133:MET:CE	1:A:242:LEU:HD11	2.45	0.46
1:A:66:VAL:CG2	1:A:249:ARG:HH21	2.27	0.46
1:A:90:LEU:HD13	1:A:92:MET:CE	2.40	0.46
1:B:110:TYR:HB2	1:B:248:ILE:CD1	2.43	0.46
1:B:71:HIS:HD2	1:B:99:TRP:CH2	2.33	0.46
1:A:203:THR:O	1:A:206:ALA:HB3	2.16	0.46
1:C:119:TYR:C	1:C:119:TYR:CD1	2.89	0.46
1:A:252:GLU:OE2	1:C:137:TYR:CZ	2.67	0.46
1:C:150:LEU:HA	1:C:150:LEU:HD22	1.63	0.46
1:B:93:PRO:CB	1:B:100:LEU:HD13	2.45	0.46
1:C:223:ARG:HG3	1:C:223:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLY:O	1:A:160:PRO:HA	2.15	0.46
1:C:123:CYS:HB2	1:C:127:THR:OG1	2.15	0.46
1:C:200:LYS:HA	1:C:200:LYS:HD2	1.62	0.46
1:C:145:VAL:CG2	1:C:149:GLN:HE22	2.28	0.46
1:A:71:HIS:HB3	1:A:246:TYR:OH	2.15	0.46
1:A:133:MET:HB2	1:A:224:LEU:HD11	1.98	0.46
1:B:219:LEU:O	1:B:220:VAL:HG23	2.16	0.46
1:B:78:LEU:HD22	1:B:228:MET:CE	2.46	0.46
1:C:84:ILE:O	1:C:85:VAL:HG23	2.14	0.46
1:C:90:LEU:O	1:C:95:THR:HG21	2.16	0.46
1:A:201:THR:HG21	1:A:260:LEU:HA	1.98	0.46
1:A:82:VAL:HA	1:A:231:GLY:HA3	1.96	0.46
1:C:168:LEU:O	1:C:169:CYS:C	2.54	0.46
1:A:146:SER:HB3	1:A:149:GLN:HG3	1.97	0.45
1:A:78:LEU:HB2	1:A:228:MET:HE1	1.97	0.45
1:C:91:VAL:O	1:C:91:VAL:HG12	2.16	0.45
1:B:172:ASN:HD22	1:B:172:ASN:HA	1.20	0.45
1:B:212:ASN:HD22	1:B:214:ASN:HB2	1.77	0.45
1:A:132:HIS:CE1	1:A:147:VAL:HG22	2.51	0.45
1:C:196:ARG:HH11	1:C:249:ARG:HH21	1.63	0.45
1:A:150:LEU:HD12	1:A:150:LEU:O	2.17	0.45
1:C:131:ILE:HD12	1:C:228:MET:HE1	1.99	0.45
1:C:59:MET:HG2	1:C:60:LEU:N	2.31	0.45
1:A:233:SER:CB	1:A:235:THR:OG1	2.65	0.45
1:C:139:MET:HA	1:C:139:MET:CE	2.46	0.45
1:C:205:TYR:O	1:C:208:ALA:N	2.50	0.45
1:C:82:VAL:HB	1:C:234:LYS:HA	1.99	0.45
1:A:138:ASP:O	1:A:139:MET:C	2.56	0.45
1:A:72:CYS:SG	1:A:245:SER:OG	2.75	0.45
1:C:155:GLY:O	1:C:156:TYR:C	2.55	0.45
1:B:146:SER:OG	1:B:147:VAL:N	2.49	0.45
1:B:170:PHE:HE1	1:B:184:THR:HG21	1.82	0.45
1:B:139:MET:HE2	1:B:223:ARG:HB3	1.99	0.45
1:B:92:MET:HG2	1:B:94:PHE:H	1.82	0.45
1:C:201:THR:CG2	1:C:260:LEU:HA	2.46	0.45
1:A:191:GLU:HG3	1:B:251:ILE:CD1	2.48	0.44
1:A:179:THR:C	1:A:181:ARG:N	2.70	0.44
1:A:233:SER:HB3	1:A:235:THR:OG1	2.17	0.44
1:B:145:VAL:HG12	1:B:146:SER:N	2.30	0.44
1:C:176:CYS:HA	1:C:177:PRO:HD3	1.83	0.44
1:A:170:PHE:CD2	1:A:170:PHE:N	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:TYR:C	1:B:110:TYR:CD1	2.90	0.44
1:C:116:ARG:CD	1:C:170:PHE:CD2	3.00	0.44
1:A:238:ASN:N	1:A:238:ASN:ND2	2.66	0.44
1:B:212:ASN:O	1:B:213:ALA:C	2.55	0.44
1:B:71:HIS:CD2	1:B:99:TRP:CZ3	3.00	0.44
1:A:130:ALA:N	1:A:161:VAL:HG13	2.33	0.44
1:A:200:LYS:HD2	1:A:200:LYS:HA	1.73	0.44
1:B:100:LEU:HG	1:B:246:TYR:CZ	2.51	0.44
1:A:148:ASN:ND2	1:A:148:ASN:C	2.69	0.44
1:B:151:SER:HA	1:B:156:TYR:CE2	2.51	0.44
1:C:179:THR:O	1:C:180:SER:C	2.56	0.44
1:C:195:LYS:CB	1:C:195:LYS:HZ2	2.30	0.44
1:C:248:ILE:O	1:C:248:ILE:HG23	2.18	0.44
1:C:201:THR:HG23	1:C:260:LEU:CA	2.48	0.44
1:A:66:VAL:HG21	1:A:249:ARG:NH2	2.28	0.44
1:C:256:ALA:O	1:C:258:LEU:N	2.50	0.44
1:B:140:ALA:HB2	1:B:214:ASN:OD1	2.18	0.44
1:B:74:LEU:N	1:B:74:LEU:HD12	2.28	0.44
1:C:116:ARG:O	1:C:244:ALA:HA	2.18	0.43
1:A:107:TRP:CE3	1:A:250:LEU:HD23	2.53	0.43
1:B:110:TYR:CD1	1:B:111:ALA:N	2.86	0.43
1:C:212:ASN:ND2	1:C:214:ASN:ND2	2.66	0.43
1:A:132:HIS:CE1	1:A:147:VAL:HG21	2.54	0.43
1:B:156:TYR:C	1:B:157:VAL:CG2	2.86	0.43
1:B:69:LEU:HD21	1:B:99:TRP:HZ3	1.83	0.43
1:C:116:ARG:NE	1:C:170:PHE:CD2	2.86	0.43
1:B:124:PRO:C	1:B:126:THR:H	2.22	0.43
1:C:206:ALA:O	1:C:207:THR:C	2.56	0.43
1:C:231:GLY:O	1:C:232:SER:HB3	2.19	0.43
1:B:165:GLN:HB3	1:B:165:GLN:HE21	1.11	0.43
1:C:227:ALA:C	1:C:228:MET:HG2	2.38	0.43
1:C:78:LEU:HA	1:C:78:LEU:HD12	1.61	0.43
1:A:214:ASN:HD21	1:B:200:LYS:CE	2.31	0.43
1:C:144:PRO:HG2	1:C:150:LEU:HD23	1.99	0.43
1:C:82:VAL:HG12	1:C:83:THR:N	2.34	0.43
1:A:92:MET:HE2	1:A:220:VAL:HG11	2.00	0.43
1:A:80:VAL:HG11	1:A:129:GLY:HA3	2.01	0.43
1:A:82:VAL:HG13	1:A:234:LYS:CA	2.49	0.43
1:B:72:CYS:SG	1:B:171:VAL:HG13	2.59	0.43
1:B:214:ASN:ND2	1:C:200:LYS:HZ1	2.15	0.43
1:B:74:LEU:CD1	1:B:74:LEU:H	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:ALA:O	1:C:205:TYR:HB3	2.19	0.43
1:C:217:ASN:HD22	1:C:217:ASN:HA	1.53	0.43
1:A:153:LEU:HD12	1:A:153:LEU:HA	1.67	0.43
1:A:181:ARG:N	1:A:181:ARG:HD2	2.33	0.43
1:A:82:VAL:HG13	1:A:234:LYS:N	2.34	0.43
1:A:91:VAL:CG1	1:A:222:ALA:O	2.66	0.43
1:B:79:ALA:HB2	1:B:238:ASN:HA	2.01	0.43
1:B:200:LYS:HD2	1:B:260:LEU:O	2.19	0.42
1:B:209:VAL:O	1:B:212:ASN:N	2.51	0.42
1:C:80:VAL:CG1	1:C:231:GLY:HA2	2.49	0.42
1:C:55:LEU:HA	1:C:55:LEU:HD23	1.72	0.42
1:A:135:PHE:O	1:A:153:LEU:HG	2.18	0.42
1:B:167:GLY:C	1:B:169:CYS:N	2.70	0.42
1:B:259:ASN:OD1	1:B:260:LEU:N	2.52	0.42
1:A:116:ARG:HE	1:A:170:PHE:HD1	1.59	0.42
1:B:133:MET:HB2	1:B:133:MET:HE3	1.94	0.42
1:C:54:LYS:N	1:C:172:ASN:HD21	1.84	0.42
1:A:78:LEU:HB2	1:A:228:MET:HE2	2.00	0.42
1:A:90:LEU:HB3	1:A:92:MET:HE3	2.01	0.42
1:C:205:TYR:O	1:C:208:ALA:HB3	2.19	0.42
1:B:129:GLY:HA2	1:B:230:GLY:HA3	2.00	0.42
1:A:92:MET:HE1	1:A:220:VAL:HG11	2.00	0.42
1:B:233:SER:HB3	1:B:235:THR:HB	2.01	0.42
1:B:218:ILE:HG12	1:B:219:LEU:HD13	2.00	0.42
1:A:250:LEU:N	1:A:250:LEU:HD12	2.35	0.42
1:B:113:VAL:HB	1:B:247:THR:O	2.20	0.42
1:C:172:ASN:HA	1:C:172:ASN:HD22	1.62	0.42
1:A:185:ILE:O	1:A:185:ILE:HG23	2.19	0.42
1:A:92:MET:HE2	1:A:92:MET:HB3	1.60	0.42
1:A:219:LEU:HD21	1:C:214:ASN:OD1	2.20	0.42
1:C:187:LEU:HD23	1:C:187:LEU:HA	1.50	0.42
1:A:88:SER:HA	1:A:224:LEU:O	2.19	0.41
1:C:71:HIS:CG	1:C:72:CYS:H	2.38	0.41
1:A:82:VAL:HG13	1:A:233:SER:C	2.41	0.41
1:B:115:ILE:HG12	1:B:116:ARG:N	2.34	0.41
1:A:140:ALA:O	1:B:260:LEU:HD12	2.20	0.41
1:A:170:PHE:HD2	1:A:170:PHE:N	2.18	0.41
1:A:194:GLU:HA	1:A:194:GLU:OE1	2.19	0.41
1:A:233:SER:C	1:A:235:THR:H	2.22	0.41
1:C:109:LYS:HB3	1:C:197:TYR:O	2.19	0.41
1:C:82:VAL:CG1	1:C:83:THR:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:LEU:HB2	1:C:243:TYR:CE2	2.56	0.41
1:A:160:PRO:HG2	1:A:163:GLU:CB	2.49	0.41
1:A:173:ASN:HA	1:A:173:ASN:HD22	1.27	0.41
1:A:221:PRO:O	1:A:222:ALA:HB2	2.20	0.41
1:B:133:MET:HA	1:B:225:VAL:O	2.20	0.41
1:A:142:THR:HG22	1:B:258:LEU:HD22	2.02	0.41
1:A:167:GLY:O	1:A:168:LEU:C	2.59	0.41
1:A:202:ALA:O	1:A:203:THR:C	2.58	0.41
1:A:71:HIS:HB3	1:A:246:TYR:CE2	2.56	0.41
1:B:248:ILE:HD12	1:B:250:LEU:CD1	2.37	0.41
1:C:116:ARG:CZ	1:C:170:PHE:HE2	2.32	0.41
1:B:175:LYS:O	1:B:177:PRO:N	2.53	0.41
1:C:194:GLU:HG3	1:C:218:ILE:HG23	2.01	0.41
1:C:79:ALA:CB	1:C:238:ASN:HA	2.50	0.41
1:B:161:VAL:HG11	1:B:239:THR:HG21	2.03	0.41
1:B:195:LYS:CE	1:C:195:LYS:HE3	2.50	0.41
1:B:235:THR:HG22	1:B:235:THR:O	2.20	0.41
1:C:194:GLU:OE1	1:C:194:GLU:HA	2.20	0.41
1:B:123:CYS:HB2	1:B:124:PRO:HD2	2.02	0.41
1:C:69:LEU:O	1:C:248:ILE:HG22	2.20	0.41
1:A:200:LYS:HG3	1:A:219:LEU:CD2	2.51	0.40
1:B:229:GLU:O	1:B:229:GLU:CG	2.65	0.40
1:A:71:HIS:CD2	1:A:99:TRP:CE3	3.06	0.40
1:B:78:LEU:HD22	1:B:228:MET:HE1	2.03	0.40
1:C:219:LEU:HG	1:C:219:LEU:H	1.50	0.40
1:C:79:ALA:HB2	1:C:238:ASN:HA	2.03	0.40
1:A:82:VAL:HA	1:A:231:GLY:CA	2.52	0.40
1:B:136:GLN:NE2	1:B:143:LEU:CD2	2.84	0.40
1:B:217:ASN:HA	1:B:217:ASN:HD22	1.47	0.40
1:C:76:THR:HG22	1:C:77:GLU:N	2.36	0.40
1:B:141:ASP:OD1	1:C:259:ASN:HA	2.22	0.40
1:B:197:TYR:CE1	1:B:221:PRO:HB3	2.56	0.40
1:B:213:ALA:O	1:B:215:ILE:N	2.54	0.40
1:B:219:LEU:C	1:B:220:VAL:HG23	2.41	0.40
1:B:99:TRP:O	1:B:100:LEU:C	2.59	0.40
1:B:132:HIS:HB2	1:B:227:ALA:HB3	2.04	0.40

All (2046) 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:B:185:ILE:CG1	1:C:118:THR:N[3_555]	0.11	2.09
1:B:130:ALA:CB	1:C:136:GLN:N[3_555]	0.18	2.02
1:B:120:LEU:C	1:C:156:TYR:CE1[3_555]	0.23	1.97
1:B:74:LEU:CB	1:C:130:ALA:CB[3_555]	0.25	1.95
1:B:160:PRO:O	1:C:153:LEU:C[3_555]	0.29	1.91
1:C:103:VAL:N	1:C:106:ASN:CG[2_555]	0.31	1.89
1:C:58:PRO:C	1:C:67:THR:N[2_555]	0.33	1.87
1:B:241:ARG:CA	1:C:132:HIS:ND1[3_555]	0.34	1.86
1:A:253:PRO:CG	1:B:162:TRP:CE2[2_555]	0.35	1.85
1:B:73:GLU:CA	1:C:160:PRO:CB[3_555]	0.37	1.83
1:B:236:ALA:CB	1:C:145:VAL:CG1[3_555]	0.38	1.82
1:B:191:GLU:CA	1:C:55:LEU:N[3_555]	0.41	1.79
1:B:154:LYS:C	1:C:244:ALA:C[3_555]	0.42	1.78
1:B:136:GLN:O	1:C:74:LEU:CG[3_555]	0.42	1.78
1:B:89:GLU:C	1:C:78:LEU:N[3_555]	0.44	1.76
1:B:80:VAL:C	1:C:143:LEU:C[3_555]	0.45	1.75
1:B:155:GLY:N	1:C:245:SER:N[3_555]	0.45	1.75
1:B:112:TRP:C	1:C:51:THR:CA[3_555]	0.47	1.73
1:B:243:TYR:CB	1:C:159:GLY:CA[3_555]	0.47	1.73
1:A:106:ASN:ND2	1:B:126:THR:CB[2_555]	0.47	1.73
1:B:73:GLU:C	1:C:160:PRO:CA[3_555]	0.48	1.72
1:B:241:ARG:CB	1:C:132:HIS:CE1[3_555]	0.48	1.72
1:B:158:THR:C	1:C:135:PHE:CD1[3_555]	0.48	1.72
1:B:103:VAL:CG1	1:C:47:ILE:CD1[3_555]	0.49	1.71
1:B:236:ALA:C	1:C:145:VAL:CG2[3_555]	0.49	1.71
1:B:152:ASN:OD1	1:C:93:PRO:C[3_555]	0.51	1.69
1:B:153:LEU:N	1:C:96:VAL:CG1[3_555]	0.51	1.69
1:B:239:THR:CA	1:C:150:LEU:N[3_555]	0.52	1.68
1:B:119:TYR:CA	1:C:157:VAL:C[3_555]	0.53	1.67
1:C:246:TYR:OH	1:C:253:PRO:CB[2_555]	0.54	1.66
1:B:147:VAL:N	1:C:90:LEU:CB[3_555]	0.55	1.65
1:B:228:MET:SD	1:C:225:VAL:CG1[3_555]	0.55	1.65
1:B:117:TYR:CE1	1:C:119:TYR:CE2[3_555]	0.55	1.65
1:B:98:THR:CB	1:C:128:SER:N[3_555]	0.58	1.62
1:B:120:LEU:O	1:C:156:TYR:CZ[3_555]	0.59	1.61
1:B:89:GLU:CA	1:C:78:LEU:CA[3_555]	0.59	1.61
1:B:135:PHE:CD2	1:C:243:TYR:CB[3_555]	0.60	1.60
1:B:131:ILE:CA	1:C:134:GLY:O[3_555]	0.60	1.60
1:B:150:LEU:CD2	1:C:89:GLU:CG[3_555]	0.61	1.59
1:B:147:VAL:CA	1:C:90:LEU:CA[3_555]	0.61	1.59
1:B:95:THR:CB	1:C:239:THR:N[3_555]	0.61	1.59
1:B:155:GLY:O	1:C:116:ARG:C[3_555]	0.62	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:LYS:O	1:C:244:ALA:CA[3_555]	0.62	1.58
1:C:99:TRP:CZ3	1:C:107:TRP:CD2[2_555]	0.62	1.58
1:B:132:HIS:C	1:C:224:LEU:CG[3_555]	0.62	1.58
1:B:248:ILE:CA	1:C:50:GLY:N[3_555]	0.63	1.57
1:B:136:GLN:N	1:C:75:SER:N[3_555]	0.63	1.57
1:B:162:TRP:N	1:C:153:LEU:N[3_555]	0.63	1.57
1:B:115:ILE:CD1	1:C:121:PRO:N[3_555]	0.63	1.57
1:B:81:THR:O	1:C:142:THR:C[3_555]	0.64	1.56
1:B:112:TRP:CZ2	1:C:121:PRO:O[3_555]	0.64	1.56
1:A:255:ALA:CA	1:B:127:THR:CA[2_555]	0.65	1.55
1:B:80:VAL:CB	1:C:144:PRO:CD[3_555]	0.65	1.55
1:B:133:MET:SD	1:C:133:MET:SD[3_555]	0.66	1.54
1:A:254:ILE:CG1	1:B:128:SER:C[2_555]	0.66	1.54
1:B:100:LEU:CA	1:C:124:PRO:O[3_555]	0.66	1.54
1:C:99:TRP:N	1:C:254:ILE:CG2[2_555]	0.67	1.53
1:C:99:TRP:CG	1:C:107:TRP:CA[2_555]	0.67	1.53
1:B:99:TRP:C	1:C:126:THR:N[3_555]	0.68	1.52
1:B:100:LEU:CA	1:C:124:PRO:C[3_555]	0.68	1.52
1:B:162:TRP:N	1:C:152:ASN:C[3_555]	0.69	1.51
1:B:135:PHE:CD1	1:C:242:LEU:C[3_555]	0.69	1.51
1:B:190:ASN:O	1:C:54:LYS:CA[3_555]	0.69	1.51
1:B:148:ASN:OD1	1:C:220:VAL:CG1[3_555]	0.70	1.50
1:B:158:THR:N	1:C:135:PHE:CZ[3_555]	0.70	1.50
1:B:153:LEU:CG	1:C:96:VAL:O[3_555]	0.70	1.50
1:B:229:GLU:CA	1:C:223:ARG:NE[3_555]	0.71	1.49
1:B:247:THR:CA	1:C:165:GLN:NE2[3_555]	0.71	1.49
1:B:122:SER:N	1:C:151:SER:CB[3_555]	0.71	1.49
1:B:93:PRO:CA	1:C:122:SER:C[3_555]	0.71	1.49
1:B:76:THR:OG1	1:C:228:MET:CA[3_555]	0.72	1.48
1:B:132:HIS:CD2	1:C:223:ARG:C[3_555]	0.72	1.48
1:B:161:VAL:C	1:C:153:LEU:N[3_555]	0.72	1.48
1:B:89:GLU:CB	1:C:78:LEU:CB[3_555]	0.72	1.48
1:B:95:THR:O	1:C:239:THR:CB[3_555]	0.73	1.47
1:C:57:PRO:CD	1:C:249:ARG:CZ[2_555]	0.74	1.46
1:B:73:GLU:O	1:C:160:PRO:N[3_555]	0.74	1.46
1:B:188:ASP:N	1:C:171:VAL:CG1[3_555]	0.75	1.45
1:C:71:HIS:NE2	1:C:251:ILE:C[2_555]	0.75	1.45
1:B:226:THR:OG1	1:C:226:THR:OG1[3_555]	0.76	1.44
1:B:183:ILE:CD1	1:C:155:GLY:CA[3_555]	0.76	1.44
1:B:69:LEU:CD1	1:C:46:PRO:C[3_555]	0.76	1.44
1:B:155:GLY:C	1:C:116:ARG:O[3_555]	0.76	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ALA:N	1:B:127:THR:C[2_555]	0.76	1.44
1:B:242:LEU:CA	1:C:131:ILE:O[3_555]	0.76	1.44
1:B:191:GLU:N	1:C:54:LYS:C[3_555]	0.76	1.44
1:B:184:THR:N	1:C:184:THR:O[3_555]	0.76	1.44
1:C:58:PRO:CD	1:C:250:LEU:O[2_555]	0.78	1.42
1:B:191:GLU:OE1	1:C:55:LEU:C[3_555]	0.78	1.42
1:B:237:VAL:CG1	1:C:149:GLN:CD[3_555]	0.78	1.42
1:B:71:HIS:ND1	1:C:162:TRP:CH2[3_555]	0.78	1.42
1:B:246:TYR:CA	1:C:49:GLN:NE2[3_555]	0.78	1.42
1:B:93:PRO:CA	1:C:123:CYS:N[3_555]	0.79	1.41
1:B:73:GLU:CD	1:C:162:TRP:CD1[3_555]	0.80	1.40
1:B:135:PHE:CD1	1:C:243:TYR:N[3_555]	0.80	1.40
1:B:98:THR:CA	1:C:127:THR:C[3_555]	0.80	1.40
1:B:100:LEU:CD1	1:C:123:CYS:O[3_555]	0.80	1.40
1:B:190:ASN:O	1:C:54:LYS:CB[3_555]	0.80	1.40
1:B:73:GLU:N	1:C:160:PRO:CG[3_555]	0.81	1.39
1:B:93:PRO:O	1:C:123:CYS:CB[3_555]	0.81	1.39
1:C:59:MET:CE	1:C:63:SER:CA[2_555]	0.81	1.39
1:B:117:TYR:CD2	1:C:119:TYR:CB[3_555]	0.81	1.39
1:B:223:ARG:C	1:C:76:THR:O[3_555]	0.81	1.39
1:B:74:LEU:O	1:C:129:GLY:O[3_555]	0.81	1.39
1:C:98:THR:N	1:C:254:ILE:CG1[2_555]	0.82	1.38
1:B:149:GLN:O	1:C:96:VAL:N[3_555]	0.82	1.38
1:B:152:ASN:CG	1:C:93:PRO:CA[3_555]	0.82	1.38
1:B:117:TYR:O	1:C:183:ILE:C[3_555]	0.82	1.38
1:B:190:ASN:N	1:C:172:ASN:ND2[3_555]	0.82	1.38
1:B:238:ASN:C	1:C:146:SER:O[3_555]	0.82	1.38
1:B:87:THR:OG1	1:C:87:THR:CB[3_555]	0.82	1.38
1:B:237:VAL:CB	1:C:149:GLN:OE1[3_555]	0.83	1.37
1:B:80:VAL:CA	1:C:144:PRO:N[3_555]	0.83	1.37
1:B:115:ILE:CG2	1:C:120:LEU:CB[3_555]	0.83	1.37
1:B:132:HIS:O	1:C:224:LEU:CG[3_555]	0.84	1.36
1:B:244:ALA:O	1:C:163:GLU:CB[3_555]	0.84	1.36
1:B:132:HIS:CA	1:C:224:LEU:CB[3_555]	0.84	1.36
1:C:101:ARG:CG	1:C:255:ALA:C[2_555]	0.84	1.36
1:B:161:VAL:CA	1:C:153:LEU:CB[3_555]	0.84	1.36
1:B:87:THR:N	1:C:87:THR:OG1[3_555]	0.84	1.36
1:C:101:ARG:CG	1:C:256:ALA:N[2_555]	0.85	1.35
1:B:76:THR:N	1:C:130:ALA:O[3_555]	0.85	1.35
1:B:93:PRO:CG	1:C:122:SER:O[3_555]	0.85	1.35
1:C:246:TYR:CZ	1:C:253:PRO:CG[2_555]	0.85	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:MET:CG	1:C:62:SER:C[2_555]	0.85	1.35
1:B:237:VAL:C	1:C:149:GLN:NE2[3_555]	0.85	1.35
1:B:93:PRO:CB	1:C:122:SER:O[3_555]	0.85	1.35
1:B:99:TRP:CD2	1:C:125:THR:O[3_555]	0.86	1.34
1:B:77:GLU:CG	1:C:229:GLU:CB[3_555]	0.86	1.34
1:B:97:GLY:CA	1:C:161:VAL:CG1[3_555]	0.87	1.33
1:A:254:ILE:C	1:B:127:THR:O[2_555]	0.87	1.33
1:C:85:VAL:O	3:B:270:HOH:O[2_555]	0.87	1.33
1:B:87:THR:OG1	1:C:87:THR:CG2[3_555]	0.87	1.33
1:A:258:LEU:O	1:B:231:GLY:C[2_555]	0.87	1.33
1:B:95:THR:O	1:C:239:THR:OG1[3_555]	0.87	1.33
1:B:135:PHE:CG	1:C:243:TYR:CA[3_555]	0.88	1.32
1:B:230:GLY:O	1:C:141:ASP:CB[3_555]	0.88	1.32
1:B:135:PHE:C	1:C:75:SER:N[3_555]	0.88	1.32
1:B:95:THR:N	1:C:238:ASN:O[3_555]	0.88	1.32
1:B:80:VAL:O	1:C:143:LEU:O[3_555]	0.88	1.32
1:B:184:THR:C	1:C:184:THR:CA[3_555]	0.88	1.32
1:C:59:MET:CG	1:C:63:SER:N[2_555]	0.89	1.31
1:B:131:ILE:CG2	1:C:134:GLY:CA[3_555]	0.89	1.31
1:C:57:PRO:O	1:C:66:VAL:CB[2_555]	0.89	1.31
1:B:160:PRO:CD	1:C:154:LYS:CB[3_555]	0.90	1.30
1:B:237:VAL:CG1	1:C:149:GLN:CG[3_555]	0.90	1.30
1:B:156:TYR:CB	1:C:115:ILE:CG1[3_555]	0.90	1.30
1:B:77:GLU:CG	1:C:229:GLU:CG[3_555]	0.90	1.30
1:C:58:PRO:O	1:C:67:THR:N[2_555]	0.90	1.30
1:B:115:ILE:CG1	1:C:121:PRO:CD[3_555]	0.90	1.30
1:B:100:LEU:O	1:C:124:PRO:CB[3_555]	0.91	1.29
1:C:99:TRP:CD2	1:C:107:TRP:CB[2_555]	0.91	1.29
1:B:186:ALA:CA	1:C:118:THR:OG1[3_555]	0.91	1.29
1:C:98:THR:N	1:C:254:ILE:CB[2_555]	0.91	1.29
1:C:99:TRP:CZ3	1:C:107:TRP:CE2[2_555]	0.91	1.29
1:B:183:ILE:CG1	1:C:155:GLY:CA[3_555]	0.92	1.28
1:B:239:THR:CB	1:C:150:LEU:CA[3_555]	0.92	1.28
1:C:55:LEU:CD1	1:C:252:GLU:OE1[2_555]	0.92	1.28
1:B:184:THR:CA	1:C:184:THR:C[3_555]	0.92	1.28
1:B:224:LEU:CD1	1:C:242:LEU:CG[3_555]	0.92	1.28
1:B:73:GLU:OE2	1:C:162:TRP:CG[3_555]	0.92	1.28
1:B:187:LEU:CB	1:C:120:LEU:CD1[3_555]	0.92	1.28
1:B:147:VAL:CG2	1:C:90:LEU:CD2[3_555]	0.92	1.28
1:B:186:ALA:N	1:C:118:THR:OG1[3_555]	0.93	1.27
1:A:254:ILE:CD1	1:B:128:SER:C[2_555]	0.93	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:VAL:N	1:C:153:LEU:CB[3_555]	0.93	1.27
1:B:133:MET:O	1:C:117:TYR:CG[3_555]	0.94	1.26
1:A:254:ILE:CA	1:B:127:THR:O[2_555]	0.94	1.26
1:B:98:THR:C	1:C:127:THR:CA[3_555]	0.94	1.26
1:B:161:VAL:CG2	1:C:153:LEU:CD1[3_555]	0.94	1.26
1:B:188:ASP:N	1:C:171:VAL:CB[3_555]	0.94	1.26
1:B:248:ILE:CG2	1:C:48:ALA:C[3_555]	0.94	1.26
1:B:224:LEU:CD1	1:C:242:LEU:CD1[3_555]	0.94	1.26
1:C:101:ARG:CB	1:C:255:ALA:CA[2_555]	0.95	1.25
1:B:229:GLU:CB	1:C:223:ARG:NE[3_555]	0.95	1.25
1:B:184:THR:CA	1:C:184:THR:O[3_555]	0.95	1.25
1:B:73:GLU:OE2	1:C:162:TRP:CD1[3_555]	0.95	1.25
1:B:81:THR:N	1:C:143:LEU:CA[3_555]	0.96	1.24
1:B:147:VAL:N	1:C:90:LEU:CG[3_555]	0.96	1.24
1:B:237:VAL:CB	1:C:149:GLN:CD[3_555]	0.96	1.24
1:B:135:PHE:CG	1:C:243:TYR:N[3_555]	0.97	1.23
1:B:121:PRO:N	1:C:156:TYR:CD1[3_555]	0.97	1.23
1:B:90:LEU:C	1:C:240:GLY:O[3_555]	0.97	1.23
1:B:154:LYS:O	1:C:244:ALA:N[3_555]	0.97	1.23
1:B:95:THR:CB	1:C:238:ASN:C[3_555]	0.97	1.23
1:A:254:ILE:C	1:B:127:THR:C[2_555]	0.97	1.23
1:B:80:VAL:C	1:C:143:LEU:O[3_555]	0.97	1.23
1:B:191:GLU:CD	1:C:56:ARG:N[3_555]	0.97	1.23
1:B:154:LYS:CB	1:C:244:ALA:O[3_555]	0.97	1.23
1:B:148:ASN:CB	1:C:92:MET:SD[3_555]	0.97	1.23
1:B:132:HIS:NE2	1:C:223:ARG:O[3_555]	0.98	1.22
1:B:226:THR:CB	1:C:226:THR:OG1[3_555]	0.98	1.22
1:B:184:THR:C	1:C:184:THR:C[3_555]	0.98	1.22
1:B:227:ALA:CB	1:C:89:GLU:N[3_555]	0.98	1.22
1:B:117:TYR:CE1	1:C:119:TYR:CD2[3_555]	0.98	1.22
1:B:226:THR:OG1	1:C:226:THR:CB[3_555]	0.98	1.22
1:B:157:VAL:C	1:C:135:PHE:CZ[3_555]	0.98	1.22
1:B:247:THR:OG1	1:C:165:GLN:CD[3_555]	0.98	1.22
1:B:162:TRP:CA	1:C:152:ASN:CA[3_555]	0.98	1.22
1:B:247:THR:CB	1:C:165:GLN:NE2[3_555]	0.99	1.21
1:B:236:ALA:O	1:C:145:VAL:CG2[3_555]	0.99	1.21
1:B:162:TRP:CA	1:C:152:ASN:C[3_555]	0.99	1.21
1:B:191:GLU:CB	1:C:55:LEU:CA[3_555]	0.99	1.21
1:B:238:ASN:CA	1:C:146:SER:CA[3_555]	0.99	1.21
1:C:58:PRO:N	1:C:250:LEU:O[2_555]	0.99	1.21
1:C:99:TRP:CE3	1:C:107:TRP:CG[2_555]	0.99	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:THR:O	1:C:185:ILE:N[3_555]	1.00	1.20
1:B:190:ASN:C	1:C:54:LYS:CA[3_555]	1.00	1.20
1:A:255:ALA:N	1:B:127:THR:CA[2_555]	1.00	1.20
1:B:116:ARG:CD	1:C:182:ALA:CB[3_555]	1.01	1.19
1:B:186:ALA:N	1:C:118:THR:CB[3_555]	1.01	1.19
1:B:116:ARG:CD	1:C:182:ALA:CA[3_555]	1.01	1.19
1:B:229:GLU:C	1:C:136:GLN:OE1[3_555]	1.01	1.19
1:B:131:ILE:CB	1:C:134:GLY:O[3_555]	1.02	1.18
1:B:121:PRO:CB	1:C:151:SER:O[3_555]	1.02	1.18
1:A:253:PRO:CB	1:B:162:TRP:NE1[2_555]	1.02	1.18
1:B:89:GLU:OE2	1:C:79:ALA:N[3_555]	1.02	1.18
1:C:99:TRP:CB	1:C:107:TRP:CA[2_555]	1.02	1.18
1:A:259:ASN:N	1:B:232:SER:OG[2_555]	1.02	1.18
1:B:73:GLU:O	1:C:160:PRO:CA[3_555]	1.02	1.18
1:B:238:ASN:CB	1:C:146:SER:CA[3_555]	1.03	1.17
1:B:112:TRP:CA	1:C:51:THR:N[3_555]	1.03	1.17
1:B:152:ASN:OD1	1:C:93:PRO:CA[3_555]	1.03	1.17
1:B:191:GLU:OE1	1:C:55:LEU:O[3_555]	1.03	1.17
1:B:93:PRO:O	1:C:123:CYS:CA[3_555]	1.03	1.17
1:B:225:VAL:CG2	1:C:76:THR:OG1[3_555]	1.03	1.17
1:B:116:ARG:N	1:C:164:GLY:O[3_555]	1.03	1.17
1:C:71:HIS:CE1	1:C:251:ILE:C[2_555]	1.04	1.16
1:B:224:LEU:N	1:C:76:THR:O[3_555]	1.04	1.16
1:C:71:HIS:CE1	1:C:251:ILE:O[2_555]	1.04	1.16
1:C:58:PRO:CD	1:C:250:LEU:C[2_555]	1.05	1.15
1:B:136:GLN:N	1:C:74:LEU:C[3_555]	1.05	1.15
1:B:116:ARG:NE	1:C:182:ALA:CB[3_555]	1.05	1.15
1:B:131:ILE:CG2	1:C:134:GLY:C[3_555]	1.05	1.15
1:B:239:THR:O	1:C:151:SER:N[3_555]	1.06	1.14
1:B:95:THR:C	1:C:239:THR:CA[3_555]	1.06	1.14
1:B:152:ASN:N	1:C:96:VAL:CG2[3_555]	1.06	1.14
1:B:242:LEU:CA	1:C:131:ILE:C[3_555]	1.06	1.14
1:B:69:LEU:CD1	1:C:46:PRO:CA[3_555]	1.06	1.14
1:C:99:TRP:CH2	1:C:107:TRP:CD2[2_555]	1.06	1.14
1:B:191:GLU:CD	1:C:55:LEU:C[3_555]	1.07	1.13
1:B:120:LEU:O	1:C:156:TYR:CE1[3_555]	1.07	1.13
1:B:183:ILE:CD1	1:C:155:GLY:C[3_555]	1.07	1.13
1:C:101:ARG:CB	1:C:255:ALA:C[2_555]	1.07	1.13
1:B:95:THR:CG2	1:C:238:ASN:CA[3_555]	1.08	1.12
1:B:76:THR:CA	1:C:130:ALA:O[3_555]	1.08	1.12
1:C:85:VAL:C	3:B:270:HOH:O[2_555]	1.08	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ILE:CD1	1:C:133:MET:CA[3_555]	1.08	1.12
1:B:154:LYS:CA	1:C:244:ALA:O[3_555]	1.08	1.12
1:B:185:ILE:N	1:C:184:THR:CA[3_555]	1.08	1.12
1:B:147:VAL:O	1:C:90:LEU:O[3_555]	1.08	1.12
1:B:237:VAL:CG2	1:C:149:GLN:OE1[3_555]	1.09	1.11
1:B:119:TYR:CA	1:C:157:VAL:O[3_555]	1.09	1.11
1:B:148:ASN:O	1:C:92:MET:C[3_555]	1.09	1.11
1:B:133:MET:O	1:C:117:TYR:CD1[3_555]	1.09	1.11
1:B:148:ASN:O	1:C:92:MET:CA[3_555]	1.09	1.11
1:C:56:ARG:C	1:C:251:ILE:CD1[2_555]	1.10	1.10
1:B:248:ILE:CA	1:C:49:GLN:C[3_555]	1.10	1.10
1:B:87:THR:C	3:C:265:HOH:O[3_555]	1.10	1.10
1:B:117:TYR:CD2	1:C:119:TYR:CG[3_555]	1.10	1.10
1:B:227:ALA:O	1:C:224:LEU:O[3_555]	1.10	1.10
1:B:246:TYR:CD1	1:C:162:TRP:O[3_555]	1.10	1.10
1:B:123:CYS:O	1:C:152:ASN:OD1[3_555]	1.10	1.10
1:B:89:GLU:CB	1:C:78:LEU:CA[3_555]	1.10	1.10
1:B:161:VAL:CG1	1:C:153:LEU:CD2[3_555]	1.11	1.09
1:B:114:ALA:O	1:C:165:GLN:CB[3_555]	1.11	1.09
1:B:114:ALA:CB	1:C:165:GLN:O[3_555]	1.11	1.09
1:C:98:THR:C	1:C:254:ILE:CG2[2_555]	1.11	1.09
1:B:239:THR:N	1:C:146:SER:O[3_555]	1.11	1.09
1:B:132:HIS:CG	1:C:224:LEU:N[3_555]	1.11	1.09
1:B:98:THR:C	1:C:127:THR:N[3_555]	1.11	1.09
1:B:158:THR:N	1:C:135:PHE:CE1[3_555]	1.12	1.08
1:B:119:TYR:CE1	1:C:156:TYR:CD2[3_555]	1.12	1.08
1:B:78:LEU:CB	1:C:227:ALA:CB[3_555]	1.12	1.08
1:B:226:THR:CG2	1:C:226:THR:CG2[3_555]	1.12	1.08
1:C:101:ARG:NH1	1:C:258:LEU:CB[2_555]	1.12	1.08
1:B:80:VAL:CG1	1:C:144:PRO:CD[3_555]	1.13	1.07
1:B:157:VAL:CG2	1:C:185:ILE:O[3_555]	1.13	1.07
1:C:56:ARG:O	1:C:251:ILE:CG1[2_555]	1.13	1.07
1:C:101:ARG:CD	1:C:255:ALA:O[2_555]	1.13	1.07
1:B:91:VAL:CG2	1:C:241:ARG:CA[3_555]	1.13	1.07
1:B:92:MET:O	1:C:239:THR:O[3_555]	1.13	1.07
1:C:99:TRP:C	1:C:106:ASN:O[2_555]	1.13	1.07
1:B:89:GLU:CA	1:C:78:LEU:N[3_555]	1.13	1.07
1:B:92:MET:C	1:C:122:SER:CB[3_555]	1.14	1.06
1:B:160:PRO:O	1:C:154:LYS:N[3_555]	1.14	1.06
1:B:192:VAL:CG2	1:C:53:VAL:CB[3_555]	1.15	1.05
1:B:154:LYS:C	1:C:244:ALA:CA[3_555]	1.15	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:TRP:O	1:C:51:THR:C[3_555]	1.15	1.05
1:C:55:LEU:CD1	1:C:252:GLU:CD[2_555]	1.15	1.05
1:B:155:GLY:CA	1:C:116:ARG:O[3_555]	1.15	1.05
1:B:241:ARG:N	1:C:132:HIS:ND1[3_555]	1.15	1.05
1:B:243:TYR:CA	1:C:159:GLY:CA[3_555]	1.16	1.04
1:B:136:GLN:CA	1:C:74:LEU:O[3_555]	1.16	1.04
1:B:100:LEU:N	1:C:124:PRO:O[3_555]	1.16	1.04
1:B:132:HIS:CD2	1:C:223:ARG:O[3_555]	1.16	1.04
1:B:92:MET:CA	1:C:122:SER:CB[3_555]	1.16	1.04
1:B:149:GLN:CB	1:C:95:THR:CA[3_555]	1.16	1.04
1:B:237:VAL:CA	1:C:149:GLN:NE2[3_555]	1.16	1.04
1:B:98:THR:CA	1:C:127:THR:CA[3_555]	1.16	1.04
1:A:254:ILE:CG1	1:B:128:SER:CA[2_555]	1.16	1.04
1:B:155:GLY:O	1:C:116:ARG:O[3_555]	1.17	1.03
1:B:137:TYR:CE1	1:C:73:GLU:C[3_555]	1.17	1.03
1:B:146:SER:OG	1:C:90:LEU:CD1[3_555]	1.17	1.03
1:B:97:GLY:O	1:C:127:THR:CB[3_555]	1.17	1.03
1:C:103:VAL:N	1:C:106:ASN:ND2[2_555]	1.17	1.03
1:B:189:THR:OG1	1:C:168:LEU:CD1[3_555]	1.17	1.03
1:B:76:THR:N	1:C:130:ALA:C[3_555]	1.17	1.03
1:B:170:PHE:CD2	1:C:179:THR:O[3_555]	1.17	1.03
1:C:59:MET:CE	1:C:63:SER:C[2_555]	1.17	1.03
1:B:117:TYR:CG	1:C:119:TYR:CG[3_555]	1.17	1.03
1:B:238:ASN:CA	1:C:146:SER:C[3_555]	1.18	1.02
1:C:73:GLU:OE2	1:C:253:PRO:N[2_555]	1.18	1.02
1:B:100:LEU:O	1:C:124:PRO:CA[3_555]	1.18	1.02
1:B:112:TRP:CE2	1:C:121:PRO:O[3_555]	1.18	1.02
1:B:242:LEU:C	1:C:131:ILE:O[3_555]	1.18	1.02
1:B:103:VAL:CB	1:C:47:ILE:CD1[3_555]	1.18	1.02
1:B:238:ASN:N	1:C:146:SER:N[3_555]	1.18	1.02
1:B:73:GLU:C	1:C:160:PRO:CB[3_555]	1.19	1.01
1:B:112:TRP:CZ2	1:C:121:PRO:C[3_555]	1.19	1.01
1:B:112:TRP:O	1:C:51:THR:CA[3_555]	1.19	1.01
1:B:191:GLU:CG	1:C:55:LEU:CA[3_555]	1.19	1.01
1:B:112:TRP:C	1:C:51:THR:N[3_555]	1.19	1.01
1:A:253:PRO:CA	1:B:162:TRP:NE1[2_555]	1.19	1.01
1:C:71:HIS:CE1	1:C:251:ILE:CA[2_555]	1.19	1.01
1:B:239:THR:OG1	1:C:150:LEU:CB[3_555]	1.20	1.00
1:B:229:GLU:OE1	1:C:139:MET:CE[3_555]	1.20	1.00
1:B:99:TRP:CZ3	1:C:125:THR:CB[3_555]	1.20	1.00
1:B:155:GLY:O	1:C:117:TYR:N[3_555]	1.20	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:O	1:C:124:PRO:CG[3_555]	1.20	1.00
1:B:147:VAL:CA	1:C:90:LEU:CB[3_555]	1.20	1.00
1:B:120:LEU:C	1:C:156:TYR:CD1[3_555]	1.20	1.00
1:B:170:PHE:O	1:C:181:ARG:CB[3_555]	1.20	1.00
1:B:242:LEU:O	1:C:131:ILE:N[3_555]	1.20	1.00
1:B:132:HIS:NE2	1:C:223:ARG:C[3_555]	1.20	1.00
1:B:151:SER:CB	1:C:91:VAL:O[3_555]	1.21	0.99
1:B:227:ALA:O	1:C:224:LEU:C[3_555]	1.21	0.99
1:C:99:TRP:CG	1:C:107:TRP:N[2_555]	1.21	0.99
1:B:241:ARG:CA	1:C:132:HIS:CE1[3_555]	1.21	0.99
1:C:246:TYR:OH	1:C:253:PRO:CG[2_555]	1.21	0.99
1:B:103:VAL:CG1	1:C:47:ILE:CG1[3_555]	1.21	0.99
1:B:93:PRO:N	1:C:122:SER:C[3_555]	1.21	0.99
1:A:253:PRO:CG	1:B:162:TRP:CZ2[2_555]	1.21	0.99
1:B:247:THR:OG1	1:C:165:GLN:OE1[3_555]	1.21	0.99
1:B:236:ALA:CA	1:C:145:VAL:CG1[3_555]	1.22	0.98
1:B:135:PHE:CD2	1:C:243:TYR:CA[3_555]	1.22	0.98
1:B:133:MET:C	1:C:117:TYR:CD2[3_555]	1.22	0.98
1:B:246:TYR:CE1	1:C:162:TRP:O[3_555]	1.22	0.98
1:B:248:ILE:CG2	1:C:48:ALA:O[3_555]	1.22	0.98
1:B:242:LEU:CB	1:C:132:HIS:N[3_555]	1.22	0.98
1:C:73:GLU:OE2	1:C:252:GLU:C[2_555]	1.22	0.98
1:B:229:GLU:O	1:C:136:GLN:OE1[3_555]	1.22	0.98
1:C:73:GLU:CD	1:C:252:GLU:O[2_555]	1.22	0.98
1:B:243:TYR:N	1:C:159:GLY:N[3_555]	1.22	0.98
1:C:97:GLY:O	1:C:255:ALA:N[2_555]	1.22	0.98
1:B:246:TYR:CE1	1:C:162:TRP:C[3_555]	1.22	0.98
1:B:99:TRP:CE3	1:C:125:THR:CB[3_555]	1.23	0.97
1:B:161:VAL:N	1:C:153:LEU:CA[3_555]	1.23	0.97
1:B:157:VAL:CG1	1:C:185:ILE:C[3_555]	1.23	0.97
1:B:185:ILE:CB	1:C:117:TYR:O[3_555]	1.23	0.97
1:C:57:PRO:O	1:C:66:VAL:CA[2_555]	1.23	0.97
1:B:241:ARG:CA	1:C:132:HIS:CG[3_555]	1.23	0.97
1:B:187:LEU:C	1:C:171:VAL:CB[3_555]	1.23	0.97
1:B:188:ASP:OD1	1:C:55:LEU:CD2[3_555]	1.23	0.97
1:B:115:ILE:CD1	1:C:121:PRO:CD[3_555]	1.24	0.96
1:B:133:MET:N	1:C:224:LEU:CD2[3_555]	1.24	0.96
1:B:239:THR:OG1	1:C:150:LEU:CA[3_555]	1.24	0.96
1:A:254:ILE:CB	1:B:128:SER:CA[2_555]	1.24	0.96
1:C:102:GLY:C	1:C:106:ASN:CG[2_555]	1.24	0.96
1:B:246:TYR:CB	1:C:49:GLN:NE2[3_555]	1.24	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:TYR:O	1:C:183:ILE:O[3_555]	1.24	0.96
1:B:90:LEU:O	1:C:240:GLY:O[3_555]	1.24	0.96
1:B:221:PRO:CG	1:C:241:ARG:NH2[3_555]	1.24	0.96
1:B:134:GLY:N	1:C:117:TYR:CD2[3_555]	1.25	0.95
1:B:242:LEU:CB	1:C:131:ILE:C[3_555]	1.25	0.95
1:B:132:HIS:CD2	1:C:224:LEU:N[3_555]	1.25	0.95
1:B:137:TYR:CD1	1:C:74:LEU:N[3_555]	1.25	0.95
1:B:132:HIS:CB	1:C:224:LEU:CB[3_555]	1.25	0.95
1:B:237:VAL:N	1:C:145:VAL:CG2[3_555]	1.25	0.95
1:B:99:TRP:O	1:C:126:THR:N[3_555]	1.25	0.95
1:B:170:PHE:CE2	1:C:179:THR:O[3_555]	1.26	0.94
1:B:183:ILE:N	3:C:267:HOH:O[3_555]	1.26	0.94
1:B:156:TYR:O	1:C:115:ILE:C[3_555]	1.26	0.94
1:B:137:TYR:CE1	1:C:74:LEU:N[3_555]	1.26	0.94
1:B:101:ARG:N	1:C:127:THR:OG1[3_555]	1.26	0.94
1:B:117:TYR:CD1	1:C:119:TYR:CD2[3_555]	1.27	0.93
1:B:81:THR:O	1:C:142:THR:CA[3_555]	1.27	0.93
1:C:97:GLY:O	1:C:254:ILE:C[2_555]	1.27	0.93
1:B:242:LEU:N	1:C:131:ILE:O[3_555]	1.27	0.93
1:B:229:GLU:CB	1:C:223:ARG:CD[3_555]	1.27	0.93
1:B:87:THR:CA	1:C:87:THR:OG1[3_555]	1.27	0.93
1:A:253:PRO:CB	1:B:162:TRP:CE2[2_555]	1.27	0.93
1:B:159:GLY:N	1:C:135:PHE:CD1[3_555]	1.27	0.93
1:B:158:THR:CA	1:C:135:PHE:CE1[3_555]	1.27	0.93
1:B:244:ALA:C	1:C:163:GLU:CB[3_555]	1.28	0.92
1:B:238:ASN:CB	1:C:146:SER:C[3_555]	1.28	0.92
1:B:112:TRP:CB	1:C:51:THR:OG1[3_555]	1.28	0.92
1:B:224:LEU:O	1:C:76:THR:CG2[3_555]	1.28	0.92
1:B:90:LEU:CD1	1:C:77:GLU:OE2[3_555]	1.28	0.92
1:B:245:SER:C	1:C:164:GLY:N[3_555]	1.28	0.92
1:B:132:HIS:C	1:C:224:LEU:CD2[3_555]	1.29	0.91
1:B:80:VAL:CB	1:C:144:PRO:N[3_555]	1.29	0.91
1:B:185:ILE:CG1	1:C:117:TYR:C[3_555]	1.29	0.91
1:C:97:GLY:C	1:C:254:ILE:CG1[2_555]	1.29	0.91
1:B:190:ASN:C	1:C:54:LYS:C[3_555]	1.29	0.91
1:B:98:THR:OG1	1:C:128:SER:N[3_555]	1.29	0.91
1:C:56:ARG:O	1:C:251:ILE:CD1[2_555]	1.29	0.91
1:A:254:ILE:CG2	1:B:128:SER:CB[2_555]	1.29	0.91
1:C:100:LEU:N	1:C:106:ASN:O[2_555]	1.29	0.91
1:B:239:THR:CB	1:C:150:LEU:N[3_555]	1.29	0.91
1:B:119:TYR:OH	1:C:150:LEU:O[3_555]	1.29	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:TYR:OH	1:C:253:PRO:CA[2_555]	1.29	0.91
1:B:117:TYR:C	1:C:183:ILE:CB[3_555]	1.30	0.90
1:B:81:THR:C	1:C:142:THR:C[3_555]	1.30	0.90
1:B:117:TYR:C	1:C:183:ILE:CG2[3_555]	1.30	0.90
1:B:74:LEU:CA	1:C:130:ALA:CB[3_555]	1.30	0.90
1:B:191:GLU:OE2	1:C:56:ARG:N[3_555]	1.30	0.90
1:C:57:PRO:N	1:C:251:ILE:CD1[2_555]	1.30	0.90
1:B:131:ILE:CD1	1:C:133:MET:C[3_555]	1.30	0.90
1:B:248:ILE:CB	1:C:49:GLN:C[3_555]	1.30	0.90
1:C:71:HIS:ND1	1:C:251:ILE:O[2_555]	1.30	0.90
1:B:115:ILE:C	1:C:164:GLY:O[3_555]	1.30	0.90
1:C:99:TRP:O	1:C:106:ASN:CA[2_555]	1.30	0.90
1:B:117:TYR:CZ	1:C:119:TYR:CD2[3_555]	1.30	0.90
1:B:117:TYR:CG	1:C:119:TYR:CB[3_555]	1.31	0.89
1:B:158:THR:CA	1:C:135:PHE:CD1[3_555]	1.31	0.89
1:B:69:LEU:CD1	1:C:47:ILE:N[3_555]	1.31	0.89
1:B:152:ASN:ND2	1:C:93:PRO:CA[3_555]	1.31	0.89
1:B:147:VAL:O	1:C:90:LEU:C[3_555]	1.31	0.89
1:B:136:GLN:O	1:C:74:LEU:CD1[3_555]	1.31	0.89
1:B:82:VAL:N	1:C:142:THR:CB[3_555]	1.31	0.89
1:B:184:THR:OG1	1:C:184:THR:N[3_555]	1.31	0.89
1:B:123:CYS:N	1:C:151:SER:OG[3_555]	1.32	0.88
1:C:72:CYS:O	1:C:252:GLU:CB[2_555]	1.32	0.88
1:C:58:PRO:C	1:C:66:VAL:C[2_555]	1.32	0.88
1:C:59:MET:CB	1:C:66:VAL:O[2_555]	1.32	0.88
1:B:246:TYR:O	1:C:49:GLN:CD[3_555]	1.32	0.88
1:B:99:TRP:N	1:C:127:THR:N[3_555]	1.32	0.88
1:B:147:VAL:C	1:C:90:LEU:C[3_555]	1.32	0.88
1:B:236:ALA:C	1:C:145:VAL:CB[3_555]	1.32	0.88
1:B:73:GLU:CA	1:C:160:PRO:CG[3_555]	1.32	0.88
1:B:135:PHE:C	1:C:74:LEU:C[3_555]	1.32	0.88
1:B:150:LEU:CD2	1:C:89:GLU:CB[3_555]	1.32	0.88
1:B:95:THR:CA	1:C:238:ASN:C[3_555]	1.33	0.87
1:B:185:ILE:CB	1:C:117:TYR:C[3_555]	1.33	0.87
1:B:119:TYR:N	1:C:157:VAL:CB[3_555]	1.33	0.87
1:B:149:GLN:CB	1:C:95:THR:N[3_555]	1.33	0.87
1:B:160:PRO:C	1:C:153:LEU:CA[3_555]	1.33	0.87
1:B:98:THR:CA	1:C:128:SER:N[3_555]	1.33	0.87
1:C:71:HIS:NE2	1:C:251:ILE:CA[2_555]	1.33	0.87
1:B:154:LYS:CA	1:C:244:ALA:C[3_555]	1.33	0.87
1:B:155:GLY:N	1:C:244:ALA:C[3_555]	1.33	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ALA:CA	1:C:135:PHE:C[3_555]	1.33	0.87
1:B:243:TYR:CA	1:C:159:GLY:N[3_555]	1.34	0.86
1:B:98:THR:N	1:C:127:THR:C[3_555]	1.34	0.86
1:C:246:TYR:CZ	1:C:253:PRO:CB[2_555]	1.34	0.86
1:B:148:ASN:CA	1:C:92:MET:CB[3_555]	1.34	0.86
1:B:81:THR:N	1:C:143:LEU:C[3_555]	1.34	0.86
1:B:245:SER:O	1:C:165:GLN:N[3_555]	1.35	0.85
1:C:97:GLY:C	1:C:254:ILE:CB[2_555]	1.35	0.85
1:B:98:THR:O	1:C:126:THR:C[3_555]	1.35	0.85
1:B:78:LEU:CG	1:C:227:ALA:CB[3_555]	1.35	0.85
1:B:115:ILE:CD1	1:C:120:LEU:C[3_555]	1.35	0.85
1:B:119:TYR:CA	1:C:157:VAL:CA[3_555]	1.35	0.85
1:B:154:LYS:CG	1:C:72:CYS:CB[3_555]	1.35	0.85
1:B:80:VAL:N	1:C:144:PRO:C[3_555]	1.36	0.84
1:C:102:GLY:C	1:C:106:ASN:OD1[2_555]	1.36	0.84
1:C:59:MET:CE	1:C:63:SER:CB[2_555]	1.36	0.84
1:C:99:TRP:CD2	1:C:107:TRP:CG[2_555]	1.36	0.84
1:B:88:SER:N	3:C:265:HOH:O[3_555]	1.36	0.84
1:B:221:PRO:CG	1:C:241:ARG:CZ[3_555]	1.36	0.84
1:B:183:ILE:CB	1:C:155:GLY:O[3_555]	1.36	0.84
1:B:118:THR:N	1:C:183:ILE:CG2[3_555]	1.36	0.84
1:B:152:ASN:ND2	1:C:93:PRO:N[3_555]	1.36	0.84
1:B:81:THR:O	1:C:143:LEU:N[3_555]	1.36	0.84
1:B:238:ASN:O	1:C:149:GLN:N[3_555]	1.37	0.83
1:B:157:VAL:CG1	1:C:186:ALA:N[3_555]	1.37	0.83
1:C:59:MET:SD	1:C:63:SER:CA[2_555]	1.37	0.83
1:B:146:SER:C	1:C:90:LEU:CB[3_555]	1.37	0.83
1:B:113:VAL:N	1:C:50:GLY:O[3_555]	1.37	0.83
1:A:258:LEU:O	1:B:231:GLY:O[2_555]	1.37	0.83
1:B:76:THR:OG1	1:C:228:MET:CB[3_555]	1.37	0.83
1:B:100:LEU:C	1:C:124:PRO:O[3_555]	1.37	0.83
1:B:81:THR:C	1:C:142:THR:CA[3_555]	1.37	0.83
1:B:119:TYR:C	1:C:157:VAL:C[3_555]	1.37	0.83
1:C:58:PRO:O	1:C:67:THR:CA[2_555]	1.37	0.83
1:C:60:LEU:O	1:C:62:SER:N[2_555]	1.37	0.83
1:B:98:THR:OG1	1:C:128:SER:CA[3_555]	1.37	0.83
1:B:227:ALA:C	1:C:224:LEU:O[3_555]	1.37	0.83
1:B:112:TRP:O	1:C:52:MET:N[3_555]	1.38	0.82
1:B:80:VAL:N	1:C:144:PRO:O[3_555]	1.38	0.82
1:B:123:CYS:C	1:C:152:ASN:OD1[3_555]	1.38	0.82
1:B:160:PRO:O	1:C:153:LEU:O[3_555]	1.38	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:HIS:C	1:C:224:LEU:CB[3_555]	1.39	0.81
1:C:101:ARG:NH2	1:C:258:LEU:N[2_555]	1.39	0.81
1:C:99:TRP:CB	1:C:107:TRP:C[2_555]	1.39	0.81
1:B:132:HIS:N	1:C:224:LEU:CA[3_555]	1.39	0.81
1:B:85:VAL:O	1:C:88:SER:N[3_555]	1.39	0.81
1:B:117:TYR:CA	1:C:183:ILE:CG2[3_555]	1.39	0.81
1:B:245:SER:CA	1:C:163:GLU:CG[3_555]	1.39	0.81
1:B:191:GLU:CB	1:C:55:LEU:CB[3_555]	1.39	0.81
1:B:188:ASP:CB	1:C:171:VAL:O[3_555]	1.39	0.81
1:B:132:HIS:CE1	1:C:223:ARG:N[3_555]	1.39	0.81
1:B:185:ILE:CD1	1:C:118:THR:N[3_555]	1.39	0.81
1:B:160:PRO:C	1:C:153:LEU:C[3_555]	1.39	0.81
1:B:119:TYR:O	1:C:157:VAL:CA[3_555]	1.39	0.81
1:C:99:TRP:CG	1:C:107:TRP:CB[2_555]	1.39	0.81
1:C:101:ARG:NH1	1:C:258:LEU:CG[2_555]	1.39	0.81
1:C:103:VAL:N	1:C:106:ASN:OD1[2_555]	1.39	0.81
1:B:95:THR:CA	1:C:239:THR:N[3_555]	1.39	0.81
1:B:153:LEU:CA	1:C:96:VAL:CG1[3_555]	1.39	0.81
1:B:130:ALA:CB	1:C:136:GLN:CA[3_555]	1.39	0.81
1:C:103:VAL:CG1	1:C:106:ASN:CB[2_555]	1.40	0.80
1:C:97:GLY:C	1:C:254:ILE:CA[2_555]	1.40	0.80
1:B:89:GLU:O	1:C:78:LEU:N[3_555]	1.40	0.80
1:B:87:THR:CB	1:C:87:THR:CG2[3_555]	1.40	0.80
1:B:155:GLY:C	1:C:116:ARG:C[3_555]	1.40	0.80
1:B:86:VAL:CG2	1:C:88:SER:O[3_555]	1.40	0.80
1:B:238:ASN:CA	1:C:146:SER:N[3_555]	1.40	0.80
1:B:154:LYS:C	1:C:245:SER:N[3_555]	1.40	0.80
1:B:95:THR:C	1:C:239:THR:CB[3_555]	1.40	0.80
1:C:73:GLU:OE2	1:C:252:GLU:O[2_555]	1.40	0.80
1:B:117:TYR:CZ	1:C:119:TYR:CE2[3_555]	1.40	0.80
1:B:158:THR:CA	1:C:135:PHE:CZ[3_555]	1.40	0.80
1:B:162:TRP:CB	1:C:152:ASN:CB[3_555]	1.40	0.80
1:B:93:PRO:N	1:C:122:SER:CA[3_555]	1.40	0.80
1:B:149:GLN:CG	1:C:95:THR:OG1[3_555]	1.41	0.79
1:C:71:HIS:NE2	1:C:252:GLU:N[2_555]	1.41	0.79
1:B:96:VAL:CA	1:C:239:THR:CG2[3_555]	1.41	0.79
1:B:191:GLU:N	1:C:55:LEU:N[3_555]	1.41	0.79
1:B:156:TYR:O	1:C:115:ILE:O[3_555]	1.41	0.79
1:A:106:ASN:CG	1:B:126:THR:CG2[2_555]	1.41	0.79
1:B:89:GLU:OE2	1:C:79:ALA:CA[3_555]	1.41	0.79
1:C:59:MET:N	1:C:66:VAL:C[2_555]	1.41	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ASN:C	1:C:54:LYS:N[3_555]	1.41	0.79
1:C:59:MET:CA	1:C:66:VAL:O[2_555]	1.41	0.79
1:C:99:TRP:CE3	1:C:107:TRP:CD2[2_555]	1.41	0.79
1:B:79:ALA:C	1:C:144:PRO:O[3_555]	1.41	0.79
1:B:237:VAL:O	1:C:149:GLN:NE2[3_555]	1.41	0.79
1:B:81:THR:C	1:C:143:LEU:N[3_555]	1.41	0.79
1:B:133:MET:CA	1:C:224:LEU:CD2[3_555]	1.42	0.78
1:B:148:ASN:O	1:C:92:MET:O[3_555]	1.42	0.78
1:B:130:ALA:CB	1:C:135:PHE:C[3_555]	1.42	0.78
1:B:93:PRO:CB	1:C:122:SER:C[3_555]	1.42	0.78
1:C:99:TRP:C	1:C:106:ASN:C[2_555]	1.42	0.78
1:B:99:TRP:CG	1:C:125:THR:O[3_555]	1.42	0.78
1:B:160:PRO:C	1:C:154:LYS:N[3_555]	1.42	0.78
1:A:253:PRO:CG	1:B:162:TRP:NE1[2_555]	1.42	0.78
1:B:152:ASN:OD1	1:C:93:PRO:O[3_555]	1.42	0.78
1:B:243:TYR:CB	1:C:159:GLY:N[3_555]	1.42	0.78
1:B:93:PRO:N	1:C:122:SER:CB[3_555]	1.43	0.77
1:C:205:TYR:CE1	3:B:266:HOH:O[2_555]	1.43	0.77
1:B:223:ARG:CG	1:C:76:THR:C[3_555]	1.43	0.77
1:B:185:ILE:CG1	1:C:118:THR:CA[3_555]	1.43	0.77
1:B:98:THR:O	1:C:127:THR:N[3_555]	1.43	0.77
1:B:133:MET:O	1:C:117:TYR:CD2[3_555]	1.43	0.77
1:B:131:ILE:CB	1:C:134:GLY:C[3_555]	1.43	0.77
1:B:91:VAL:CG2	1:C:241:ARG:CB[3_555]	1.43	0.77
1:B:225:VAL:CB	1:C:76:THR:OG1[3_555]	1.43	0.77
1:C:57:PRO:CD	1:C:249:ARG:NH1[2_555]	1.43	0.77
1:B:162:TRP:CG	1:C:152:ASN:O[3_555]	1.43	0.77
1:C:59:MET:SD	1:C:63:SER:O[2_555]	1.43	0.77
1:B:80:VAL:N	1:C:144:PRO:CA[3_555]	1.43	0.77
1:B:136:GLN:C	1:C:74:LEU:CG[3_555]	1.43	0.77
1:B:99:TRP:CZ3	1:C:125:THR:OG1[3_555]	1.43	0.77
1:A:106:ASN:ND2	1:B:126:THR:CG2[2_555]	1.43	0.77
1:B:93:PRO:C	1:C:123:CYS:CA[3_555]	1.44	0.76
1:B:149:GLN:CB	1:C:95:THR:CB[3_555]	1.44	0.76
1:B:116:ARG:CG	1:C:183:ILE:N[3_555]	1.44	0.76
1:B:191:GLU:CA	1:C:54:LYS:C[3_555]	1.44	0.76
1:A:253:PRO:CD	1:B:162:TRP:CZ2[2_555]	1.44	0.76
1:B:133:MET:C	1:C:117:TYR:CG[3_555]	1.44	0.76
1:B:80:VAL:CA	1:C:143:LEU:C[3_555]	1.44	0.76
1:B:161:VAL:CB	1:C:153:LEU:CD1[3_555]	1.44	0.76
1:C:101:ARG:CZ	1:C:258:LEU:N[2_555]	1.44	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ILE:O	1:B:126:THR:C[2_555]	1.44	0.76
1:B:183:ILE:C	1:C:184:THR:O[3_555]	1.44	0.76
1:B:237:VAL:CG1	1:C:149:GLN:OE1[3_555]	1.44	0.76
1:A:258:LEU:C	1:B:232:SER:OG[2_555]	1.44	0.76
1:B:72:CYS:O	1:C:162:TRP:CZ2[3_555]	1.44	0.76
1:B:241:ARG:CG	1:C:132:HIS:CE1[3_555]	1.44	0.76
1:B:247:THR:CB	1:C:165:GLN:CD[3_555]	1.44	0.76
1:B:130:ALA:N	1:C:136:GLN:CG[3_555]	1.45	0.75
1:B:242:LEU:N	1:C:131:ILE:C[3_555]	1.45	0.75
1:C:57:PRO:CB	1:C:249:ARG:CG[2_555]	1.45	0.75
1:B:99:TRP:CA	1:C:126:THR:CA[3_555]	1.45	0.75
1:B:136:GLN:CA	1:C:74:LEU:C[3_555]	1.45	0.75
1:B:170:PHE:N	1:C:180:SER:O[3_555]	1.45	0.75
1:B:119:TYR:N	1:C:157:VAL:CA[3_555]	1.45	0.75
1:B:101:ARG:NH1	1:C:237:VAL:CG1[3_555]	1.45	0.75
1:B:81:THR:N	1:C:143:LEU:N[3_555]	1.45	0.75
1:B:99:TRP:CE3	1:C:125:THR:O[3_555]	1.45	0.75
1:B:184:THR:CA	1:C:184:THR:CA[3_555]	1.46	0.74
1:B:95:THR:CA	1:C:238:ASN:O[3_555]	1.46	0.74
1:A:254:ILE:CD1	1:B:129:GLY:N[2_555]	1.46	0.74
1:C:73:GLU:OE2	1:C:253:PRO:CA[2_555]	1.46	0.74
1:B:149:GLN:CB	1:C:95:THR:OG1[3_555]	1.46	0.74
1:B:182:ALA:C	3:C:267:HOH:O[3_555]	1.47	0.73
1:B:114:ALA:N	1:C:51:THR:CG2[3_555]	1.47	0.73
1:B:156:TYR:CE2	1:C:91:VAL:CG2[3_555]	1.47	0.73
1:B:148:ASN:CG	1:C:92:MET:SD[3_555]	1.47	0.73
1:C:99:TRP:CH2	1:C:107:TRP:CE3[2_555]	1.47	0.73
1:B:158:THR:CG2	1:C:135:PHE:CD2[3_555]	1.47	0.73
1:C:102:GLY:C	1:C:106:ASN:ND2[2_555]	1.47	0.73
1:A:254:ILE:CD1	1:B:128:SER:O[2_555]	1.48	0.72
1:B:240:GLY:N	1:C:150:LEU:CB[3_555]	1.48	0.72
1:B:151:SER:CB	1:C:91:VAL:C[3_555]	1.48	0.72
1:B:74:LEU:C	1:C:130:ALA:CA[3_555]	1.48	0.72
1:B:245:SER:O	1:C:164:GLY:C[3_555]	1.48	0.72
1:B:131:ILE:CD1	1:C:134:GLY:N[3_555]	1.48	0.72
1:B:95:THR:C	1:C:239:THR:OG1[3_555]	1.48	0.72
1:A:258:LEU:O	1:B:232:SER:N[2_555]	1.48	0.72
1:C:58:PRO:CG	1:C:250:LEU:C[2_555]	1.48	0.72
1:B:243:TYR:O	1:C:183:ILE:CD1[3_555]	1.48	0.72
1:A:106:ASN:ND2	1:B:126:THR:OG1[2_555]	1.48	0.72
1:B:159:GLY:N	1:C:135:PHE:CG[3_555]	1.48	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:PHE:CA	1:C:181:ARG:CA[3_555]	1.48	0.72
1:B:158:THR:CA	1:C:135:PHE:CG[3_555]	1.48	0.72
1:C:101:ARG:CB	1:C:255:ALA:CB[2_555]	1.48	0.72
1:B:239:THR:CA	1:C:150:LEU:CA[3_555]	1.48	0.72
1:B:246:TYR:O	1:C:49:GLN:OE1[3_555]	1.48	0.72
1:B:117:TYR:CD2	1:C:119:TYR:CA[3_555]	1.48	0.72
1:B:183:ILE:CG2	1:C:185:ILE:CG1[3_555]	1.48	0.72
1:B:112:TRP:CA	1:C:51:THR:CA[3_555]	1.48	0.72
1:B:99:TRP:CA	1:C:126:THR:N[3_555]	1.48	0.72
1:C:98:THR:CA	1:C:254:ILE:CG1[2_555]	1.49	0.71
1:B:100:LEU:CG	1:C:123:CYS:O[3_555]	1.49	0.71
1:B:80:VAL:C	1:C:144:PRO:N[3_555]	1.49	0.71
1:B:74:LEU:O	1:C:129:GLY:C[3_555]	1.49	0.71
1:B:154:LYS:CG	1:C:72:CYS:CA[3_555]	1.49	0.71
1:B:238:ASN:CA	1:C:146:SER:O[3_555]	1.49	0.71
1:B:191:GLU:OE1	1:C:56:ARG:N[3_555]	1.49	0.71
1:B:78:LEU:CD2	1:C:227:ALA:N[3_555]	1.49	0.71
1:B:189:THR:O	1:C:53:VAL:C[3_555]	1.50	0.70
1:B:80:VAL:O	1:C:143:LEU:C[3_555]	1.50	0.70
1:B:98:THR:C	1:C:127:THR:C[3_555]	1.50	0.70
1:B:227:ALA:O	1:C:225:VAL:N[3_555]	1.50	0.70
1:B:91:VAL:O	1:C:241:ARG:NH1[3_555]	1.50	0.70
1:B:229:GLU:CB	1:C:223:ARG:CZ[3_555]	1.50	0.70
1:C:99:TRP:CZ3	1:C:107:TRP:CG[2_555]	1.50	0.70
3:B:262:HOH:O	3:C:263:HOH:O[3_555]	1.50	0.70
1:B:87:THR:O	3:C:265:HOH:O[3_555]	1.50	0.70
1:B:189:THR:OG1	1:C:168:LEU:CG[3_555]	1.50	0.70
1:B:120:LEU:O	1:C:156:TYR:OH[3_555]	1.50	0.70
1:B:99:TRP:CA	1:C:126:THR:C[3_555]	1.50	0.70
1:B:153:LEU:N	1:C:96:VAL:CB[3_555]	1.50	0.70
1:B:191:GLU:CB	1:C:55:LEU:N[3_555]	1.50	0.70
1:B:118:THR:OG1	1:C:182:ALA:O[3_555]	1.50	0.70
1:B:119:TYR:CB	1:C:157:VAL:N[3_555]	1.51	0.69
1:B:229:GLU:O	1:C:136:GLN:CD[3_555]	1.51	0.69
1:B:238:ASN:CG	1:C:146:SER:CA[3_555]	1.51	0.69
1:A:254:ILE:CG2	1:B:128:SER:CA[2_555]	1.51	0.69
1:B:98:THR:O	1:C:126:THR:O[3_555]	1.51	0.69
1:B:248:ILE:CB	1:C:49:GLN:N[3_555]	1.51	0.69
1:B:241:ARG:CG	1:C:132:HIS:NE2[3_555]	1.51	0.69
1:B:228:MET:N	1:C:88:SER:CB[3_555]	1.51	0.69
1:B:247:THR:O	1:C:50:GLY:O[3_555]	1.51	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:MET:O	1:C:143:LEU:CD2[3_555]	1.51	0.69
1:B:119:TYR:C	1:C:157:VAL:CA[3_555]	1.51	0.69
1:B:117:TYR:CA	1:C:183:ILE:CB[3_555]	1.51	0.69
1:B:82:VAL:N	1:C:142:THR:CA[3_555]	1.51	0.69
1:B:100:LEU:C	1:C:124:PRO:C[3_555]	1.51	0.69
1:B:80:VAL:CA	1:C:144:PRO:CD[3_555]	1.52	0.68
1:B:191:GLU:N	1:C:54:LYS:O[3_555]	1.52	0.68
1:B:183:ILE:CD1	1:C:155:GLY:N[3_555]	1.52	0.68
1:B:124:PRO:O	1:C:152:ASN:ND2[3_555]	1.52	0.68
1:B:117:TYR:C	1:C:183:ILE:CA[3_555]	1.52	0.68
1:B:238:ASN:N	1:C:146:SER:CB[3_555]	1.52	0.68
1:B:222:ALA:O	1:C:241:ARG:CD[3_555]	1.52	0.68
1:B:184:THR:N	1:C:184:THR:C[3_555]	1.52	0.68
1:B:69:LEU:CG	1:C:46:PRO:CB[3_555]	1.52	0.68
1:B:91:VAL:CG2	1:C:241:ARG:N[3_555]	1.52	0.68
1:B:242:LEU:CD1	1:C:131:ILE:CD1[3_555]	1.52	0.68
1:B:170:PHE:CE2	1:C:179:THR:C[3_555]	1.52	0.68
1:B:228:MET:SD	1:C:225:VAL:CB[3_555]	1.52	0.68
1:B:153:LEU:CD2	1:C:96:VAL:O[3_555]	1.52	0.68
1:B:156:TYR:CZ	1:C:91:VAL:CG1[3_555]	1.52	0.68
1:B:192:VAL:CB	1:C:53:VAL:O[3_555]	1.53	0.67
1:B:81:THR:CA	1:C:143:LEU:N[3_555]	1.53	0.67
1:B:188:ASP:CB	1:C:171:VAL:C[3_555]	1.53	0.67
1:B:248:ILE:CB	1:C:49:GLN:CA[3_555]	1.53	0.67
1:B:149:GLN:CA	1:C:95:THR:N[3_555]	1.53	0.67
1:B:121:PRO:N	1:C:156:TYR:CE1[3_555]	1.53	0.67
1:B:119:TYR:N	1:C:157:VAL:C[3_555]	1.53	0.67
1:B:89:GLU:C	1:C:77:GLU:C[3_555]	1.53	0.67
1:B:161:VAL:CA	1:C:153:LEU:CA[3_555]	1.53	0.67
1:B:158:THR:CB	1:C:135:PHE:CD2[3_555]	1.53	0.67
1:B:87:THR:CB	1:C:87:THR:CB[3_555]	1.53	0.67
1:B:93:PRO:C	1:C:123:CYS:N[3_555]	1.54	0.66
1:C:59:MET:N	1:C:67:THR:N[2_555]	1.54	0.66
1:B:154:LYS:O	1:C:244:ALA:C[3_555]	1.54	0.66
1:B:120:LEU:CA	1:C:156:TYR:CE1[3_555]	1.54	0.66
1:B:154:LYS:C	1:C:244:ALA:O[3_555]	1.54	0.66
1:B:149:GLN:CA	1:C:95:THR:CB[3_555]	1.54	0.66
1:B:230:GLY:N	1:C:136:GLN:OE1[3_555]	1.54	0.66
1:C:99:TRP:O	1:C:106:ASN:C[2_555]	1.54	0.66
1:B:73:GLU:C	1:C:160:PRO:N[3_555]	1.54	0.66
1:B:160:PRO:N	1:C:154:LYS:CB[3_555]	1.54	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:THR:OG1	1:C:150:LEU:CG[3_555]	1.54	0.66
1:B:117:TYR:CE2	1:C:119:TYR:CG[3_555]	1.54	0.66
1:B:161:VAL:O	1:C:150:LEU:O[3_555]	1.55	0.65
1:B:117:TYR:CE1	1:C:119:TYR:CZ[3_555]	1.55	0.65
1:B:136:GLN:N	1:C:75:SER:CA[3_555]	1.55	0.65
1:B:74:LEU:CB	1:C:130:ALA:CA[3_555]	1.55	0.65
1:B:96:VAL:O	1:C:161:VAL:CG2[3_555]	1.55	0.65
1:B:246:TYR:N	1:C:49:GLN:NE2[3_555]	1.55	0.65
1:C:101:ARG:CA	1:C:255:ALA:CA[2_555]	1.55	0.65
1:B:147:VAL:C	1:C:90:LEU:O[3_555]	1.55	0.65
1:C:59:MET:SD	1:C:63:SER:N[2_555]	1.55	0.65
1:B:71:HIS:CE1	1:C:162:TRP:CZ2[3_555]	1.55	0.65
1:B:135:PHE:CB	1:C:243:TYR:CA[3_555]	1.55	0.65
1:A:255:ALA:N	1:B:127:THR:O[2_555]	1.55	0.65
1:B:184:THR:O	1:C:184:THR:C[3_555]	1.55	0.65
1:B:93:PRO:CA	1:C:122:SER:O[3_555]	1.55	0.65
1:B:158:THR:C	1:C:135:PHE:CE1[3_555]	1.55	0.65
1:C:58:PRO:CG	1:C:250:LEU:CA[2_555]	1.55	0.65
1:B:96:VAL:O	1:C:161:VAL:CB[3_555]	1.55	0.65
1:B:101:ARG:NH2	1:C:237:VAL:CG2[3_555]	1.56	0.64
1:B:184:THR:CG2	1:C:184:THR:CG2[3_555]	1.56	0.64
1:B:134:GLY:CA	1:C:117:TYR:CD2[3_555]	1.56	0.64
1:C:57:PRO:CD	1:C:249:ARG:NE[2_555]	1.56	0.64
1:B:74:LEU:N	1:C:160:PRO:CA[3_555]	1.56	0.64
1:B:151:SER:OG	1:C:91:VAL:O[3_555]	1.56	0.64
1:C:101:ARG:CG	1:C:255:ALA:O[2_555]	1.56	0.64
1:B:89:GLU:N	1:C:77:GLU:O[3_555]	1.56	0.64
1:B:185:ILE:C	1:C:118:THR:CB[3_555]	1.56	0.64
1:B:159:GLY:O	1:C:135:PHE:N[3_555]	1.56	0.64
1:B:122:SER:N	1:C:151:SER:OG[3_555]	1.56	0.64
1:B:184:THR:C	1:C:185:ILE:N[3_555]	1.56	0.64
1:B:120:LEU:C	1:C:156:TYR:CZ[3_555]	1.56	0.64
1:B:132:HIS:CG	1:C:223:ARG:C[3_555]	1.56	0.64
1:B:228:MET:CG	1:C:225:VAL:CG1[3_555]	1.56	0.64
1:B:117:TYR:O	1:C:183:ILE:CA[3_555]	1.56	0.64
1:B:73:GLU:O	1:C:159:GLY:C[3_555]	1.56	0.64
1:B:112:TRP:CH2	1:C:121:PRO:O[3_555]	1.56	0.64
1:B:112:TRP:CH2	1:C:121:PRO:C[3_555]	1.57	0.63
1:B:158:THR:CA	1:C:135:PHE:CE2[3_555]	1.57	0.63
1:B:98:THR:CB	1:C:128:SER:CA[3_555]	1.57	0.63
1:B:137:TYR:CE2	1:C:243:TYR:CD2[3_555]	1.57	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ILE:CB	1:C:118:THR:N[3_555]	1.57	0.63
1:C:58:PRO:C	1:C:67:THR:CA[2_555]	1.57	0.63
1:B:245:SER:N	1:C:164:GLY:N[3_555]	1.57	0.63
1:B:146:SER:C	1:C:90:LEU:CG[3_555]	1.57	0.63
1:B:190:ASN:ND2	1:C:172:ASN:CB[3_555]	1.57	0.63
1:B:239:THR:OG1	1:C:150:LEU:CD2[3_555]	1.58	0.62
1:B:248:ILE:CG2	1:C:49:GLN:N[3_555]	1.58	0.62
1:B:131:ILE:CB	1:C:134:GLY:N[3_555]	1.58	0.62
1:B:156:TYR:CB	1:C:115:ILE:CD1[3_555]	1.58	0.62
1:B:93:PRO:CD	1:C:122:SER:O[3_555]	1.58	0.62
1:C:98:THR:CA	1:C:254:ILE:CD1[2_555]	1.58	0.62
1:B:147:VAL:CA	1:C:90:LEU:C[3_555]	1.58	0.62
1:C:98:THR:CB	1:C:254:ILE:CD1[2_555]	1.58	0.62
1:B:241:ARG:CB	1:C:132:HIS:ND1[3_555]	1.58	0.62
1:A:254:ILE:CG1	1:B:129:GLY:N[2_555]	1.58	0.62
1:B:131:ILE:N	1:C:134:GLY:O[3_555]	1.58	0.62
1:B:190:ASN:N	1:C:172:ASN:CG[3_555]	1.58	0.62
1:B:99:TRP:CE3	1:C:125:THR:CA[3_555]	1.58	0.62
1:B:170:PHE:CD2	1:C:180:SER:C[3_555]	1.58	0.62
1:B:242:LEU:CD1	1:C:131:ILE:CG1[3_555]	1.58	0.62
1:B:246:TYR:C	1:C:49:GLN:CD[3_555]	1.59	0.61
1:B:115:ILE:CG2	1:C:120:LEU:CG[3_555]	1.59	0.61
1:B:132:HIS:O	1:C:224:LEU:CD2[3_555]	1.59	0.61
1:B:162:TRP:CB	1:C:152:ASN:CA[3_555]	1.59	0.61
1:B:246:TYR:C	1:C:49:GLN:NE2[3_555]	1.59	0.61
1:B:135:PHE:CZ	1:C:118:THR:O[3_555]	1.59	0.61
1:A:258:LEU:CA	1:B:232:SER:CB[2_555]	1.59	0.61
1:C:101:ARG:NE	1:C:258:LEU:N[2_555]	1.59	0.61
1:B:85:VAL:O	1:C:88:SER:CA[3_555]	1.59	0.61
1:B:73:GLU:O	1:C:160:PRO:C[3_555]	1.59	0.61
1:B:248:ILE:C	1:C:50:GLY:N[3_555]	1.59	0.61
1:B:243:TYR:CA	1:C:159:GLY:C[3_555]	1.59	0.61
1:B:162:TRP:CB	1:C:152:ASN:O[3_555]	1.59	0.61
1:C:101:ARG:N	1:C:254:ILE:O[2_555]	1.60	0.60
1:B:247:THR:OG1	1:C:165:GLN:NE2[3_555]	1.60	0.60
1:B:156:TYR:O	1:C:116:ARG:N[3_555]	1.60	0.60
1:B:148:ASN:C	1:C:92:MET:CB[3_555]	1.60	0.60
1:B:157:VAL:O	1:C:135:PHE:CZ[3_555]	1.60	0.60
1:C:58:PRO:O	1:C:67:THR:C[2_555]	1.60	0.60
1:B:226:THR:CB	1:C:226:THR:CB[3_555]	1.60	0.60
1:B:113:VAL:N	1:C:50:GLY:C[3_555]	1.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ILE:N	1:C:49:GLN:CA[3_555]	1.60	0.60
1:B:130:ALA:CA	1:C:136:GLN:N[3_555]	1.60	0.60
1:B:89:GLU:OE2	1:C:79:ALA:C[3_555]	1.60	0.60
1:B:151:SER:O	1:C:112:TRP:CZ2[3_555]	1.60	0.60
1:B:102:GLY:N	1:C:126:THR:OG1[3_555]	1.61	0.59
1:B:98:THR:CB	1:C:127:THR:C[3_555]	1.61	0.59
1:B:151:SER:O	1:C:112:TRP:CH2[3_555]	1.61	0.59
1:C:103:VAL:CA	1:C:106:ASN:CG[2_555]	1.61	0.59
1:C:64:MET:O	1:C:70:SER:CB[3_555]	1.61	0.59
1:B:158:THR:CA	1:C:135:PHE:CD2[3_555]	1.61	0.59
1:B:99:TRP:N	1:C:127:THR:O[3_555]	1.61	0.59
1:B:245:SER:CA	1:C:164:GLY:N[3_555]	1.61	0.59
1:B:114:ALA:O	1:C:165:GLN:CA[3_555]	1.61	0.59
1:B:96:VAL:CG1	1:C:161:VAL:O[3_555]	1.61	0.59
1:B:130:ALA:CA	1:C:135:PHE:O[3_555]	1.61	0.59
1:B:158:THR:O	1:C:135:PHE:CD1[3_555]	1.61	0.59
1:B:123:CYS:CB	1:C:148:ASN:O[3_555]	1.61	0.59
1:B:245:SER:O	1:C:164:GLY:CA[3_555]	1.61	0.59
1:C:55:LEU:CD1	1:C:252:GLU:OE2[2_555]	1.61	0.59
1:C:59:MET:SD	1:C:63:SER:C[2_555]	1.61	0.59
1:B:131:ILE:CG1	1:C:134:GLY:N[3_555]	1.62	0.58
1:B:95:THR:OG1	1:C:238:ASN:C[3_555]	1.62	0.58
1:B:238:ASN:N	1:C:146:SER:CA[3_555]	1.62	0.58
1:B:118:THR:N	1:C:183:ILE:CB[3_555]	1.62	0.58
1:B:77:GLU:CD	1:C:229:GLU:OE1[3_555]	1.62	0.58
1:B:183:ILE:C	3:C:267:HOH:O[3_555]	1.62	0.58
1:B:160:PRO:O	1:C:153:LEU:CA[3_555]	1.62	0.58
1:A:106:ASN:CG	1:B:126:THR:CB[2_555]	1.62	0.58
1:B:147:VAL:CB	1:C:90:LEU:CA[3_555]	1.62	0.58
1:B:117:TYR:CD1	1:C:119:TYR:CG[3_555]	1.62	0.58
1:B:97:GLY:O	1:C:127:THR:CG2[3_555]	1.62	0.58
1:B:78:LEU:CA	1:C:227:ALA:CB[3_555]	1.62	0.58
1:B:98:THR:OG1	1:C:128:SER:O[3_555]	1.63	0.57
1:B:135:PHE:CE1	1:C:242:LEU:CA[3_555]	1.63	0.57
1:C:99:TRP:CE2	1:C:107:TRP:CB[2_555]	1.63	0.57
1:B:90:LEU:N	1:C:78:LEU:N[3_555]	1.63	0.57
1:B:122:SER:C	1:C:151:SER:OG[3_555]	1.63	0.57
1:B:148:ASN:O	1:C:92:MET:N[3_555]	1.63	0.57
1:B:113:VAL:N	1:C:51:THR:CA[3_555]	1.63	0.57
1:B:186:ALA:C	1:C:118:THR:OG1[3_555]	1.63	0.57
1:C:103:VAL:N	1:C:106:ASN:CB[2_555]	1.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:THR:CA	1:C:157:VAL:CG2[3_555]	1.63	0.57
1:C:102:GLY:O	1:C:106:ASN:OD1[2_555]	1.63	0.57
1:C:99:TRP:CD2	1:C:107:TRP:CA[2_555]	1.63	0.57
1:B:192:VAL:CG2	1:C:53:VAL:CA[3_555]	1.63	0.57
1:C:57:PRO:CD	1:C:249:ARG:NH2[2_555]	1.63	0.57
1:B:183:ILE:CA	3:C:267:HOH:O[3_555]	1.63	0.57
1:B:238:ASN:C	1:C:146:SER:C[3_555]	1.63	0.57
1:B:137:TYR:CE2	1:C:243:TYR:CE2[3_555]	1.64	0.56
1:B:95:THR:CA	1:C:239:THR:CA[3_555]	1.64	0.56
1:B:189:THR:O	1:C:53:VAL:CA[3_555]	1.64	0.56
1:B:238:ASN:CB	1:C:147:VAL:N[3_555]	1.64	0.56
1:B:80:VAL:N	1:C:144:PRO:N[3_555]	1.64	0.56
1:C:246:TYR:CE1	1:C:253:PRO:CG[2_555]	1.64	0.56
1:B:224:LEU:O	1:C:76:THR:CB[3_555]	1.64	0.56
1:B:158:THR:CG2	1:C:135:PHE:CG[3_555]	1.65	0.55
1:B:85:VAL:O	1:C:88:SER:CB[3_555]	1.65	0.55
1:B:81:THR:N	1:C:143:LEU:O[3_555]	1.65	0.55
1:B:113:VAL:N	1:C:51:THR:N[3_555]	1.65	0.55
1:B:158:THR:C	1:C:135:PHE:CG[3_555]	1.65	0.55
1:B:116:ARG:N	1:C:164:GLY:C[3_555]	1.65	0.55
1:C:99:TRP:CH2	1:C:107:TRP:CE2[2_555]	1.65	0.55
1:B:135:PHE:CE1	1:C:243:TYR:N[3_555]	1.65	0.55
1:B:136:GLN:O	1:C:74:LEU:CB[3_555]	1.65	0.55
1:B:190:ASN:CA	1:C:172:ASN:ND2[3_555]	1.65	0.55
1:B:119:TYR:OH	1:C:150:LEU:CD1[3_555]	1.65	0.55
1:A:254:ILE:CG1	1:B:128:SER:O[2_555]	1.65	0.55
1:A:254:ILE:O	1:B:127:THR:N[2_555]	1.65	0.55
1:B:133:MET:SD	1:C:133:MET:CG[3_555]	1.66	0.54
1:B:100:LEU:C	1:C:124:PRO:CA[3_555]	1.66	0.54
1:B:77:GLU:CG	1:C:229:GLU:CD[3_555]	1.66	0.54
1:C:59:MET:CG	1:C:62:SER:CA[2_555]	1.66	0.54
1:B:132:HIS:C	1:C:224:LEU:CD1[3_555]	1.66	0.54
1:B:241:ARG:C	1:C:132:HIS:ND1[3_555]	1.66	0.54
1:B:159:GLY:N	1:C:135:PHE:CB[3_555]	1.66	0.54
1:C:58:PRO:CD	1:C:250:LEU:CA[2_555]	1.66	0.54
1:B:100:LEU:CA	1:C:125:THR:N[3_555]	1.66	0.54
1:B:185:ILE:CB	1:C:118:THR:CA[3_555]	1.66	0.54
1:B:237:VAL:CB	1:C:149:GLN:NE2[3_555]	1.66	0.54
1:B:99:TRP:CE3	1:C:125:THR:C[3_555]	1.66	0.54
1:B:149:GLN:O	1:C:95:THR:C[3_555]	1.66	0.54
1:B:119:TYR:CB	1:C:157:VAL:O[3_555]	1.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:THR:CG2	1:C:238:ASN:C[3_555]	1.66	0.54
1:B:98:THR:C	1:C:126:THR:C[3_555]	1.67	0.53
1:B:81:THR:N	1:C:143:LEU:CB[3_555]	1.67	0.53
1:B:150:LEU:N	1:C:95:THR:CG2[3_555]	1.67	0.53
1:B:132:HIS:CB	1:C:224:LEU:CA[3_555]	1.67	0.53
1:B:119:TYR:N	1:C:157:VAL:CG2[3_555]	1.67	0.53
1:B:156:TYR:CG	1:C:115:ILE:CG1[3_555]	1.67	0.53
1:B:247:THR:N	1:C:165:GLN:CG[3_555]	1.67	0.53
1:B:101:ARG:CZ	1:C:237:VAL:CG1[3_555]	1.67	0.53
1:B:161:VAL:CB	1:C:153:LEU:CG[3_555]	1.67	0.53
1:A:253:PRO:CG	1:B:162:TRP:CD2[2_555]	1.67	0.53
1:C:101:ARG:NH2	1:C:258:LEU:CA[2_555]	1.67	0.53
1:B:160:PRO:CA	1:C:154:LYS:N[3_555]	1.67	0.53
1:B:248:ILE:N	1:C:49:GLN:C[3_555]	1.67	0.53
1:B:160:PRO:CD	1:C:154:LYS:CA[3_555]	1.67	0.53
1:B:132:HIS:CA	1:C:224:LEU:CA[3_555]	1.67	0.53
1:A:255:ALA:CA	1:B:127:THR:CB[2_555]	1.67	0.53
1:B:190:ASN:CB	1:C:54:LYS:CE[3_555]	1.67	0.53
1:B:224:LEU:CD1	1:C:242:LEU:CB[3_555]	1.67	0.53
1:B:102:GLY:CA	1:C:126:THR:OG1[3_555]	1.67	0.53
1:B:245:SER:N	1:C:163:GLU:C[3_555]	1.67	0.53
1:B:135:PHE:CE2	1:C:243:TYR:CB[3_555]	1.67	0.53
1:B:116:ARG:CZ	1:C:182:ALA:CB[3_555]	1.67	0.53
1:B:135:PHE:CD1	1:C:242:LEU:CA[3_555]	1.67	0.53
1:B:97:GLY:N	1:C:161:VAL:CG1[3_555]	1.67	0.53
1:B:185:ILE:C	1:C:118:THR:CA[3_555]	1.67	0.53
1:B:191:GLU:N	1:C:54:LYS:CA[3_555]	1.67	0.53
1:B:243:TYR:CE1	1:C:158:THR:CG2[3_555]	1.67	0.53
1:B:239:THR:C	1:C:147:VAL:O[3_555]	1.68	0.52
1:B:77:GLU:CD	1:C:229:GLU:CD[3_555]	1.68	0.52
1:C:101:ARG:CG	1:C:256:ALA:CA[2_555]	1.68	0.52
1:B:73:GLU:CB	1:C:160:PRO:CB[3_555]	1.68	0.52
1:C:58:PRO:CG	1:C:250:LEU:CB[2_555]	1.68	0.52
1:C:99:TRP:CG	1:C:107:TRP:C[2_555]	1.68	0.52
1:B:226:THR:OG1	1:C:226:THR:CA[3_555]	1.68	0.52
1:B:223:ARG:N	1:C:74:LEU:CD1[3_555]	1.68	0.52
1:C:103:VAL:CA	1:C:106:ASN:OD1[2_555]	1.68	0.52
1:C:99:TRP:NE1	1:C:104:ALA:O[2_555]	1.68	0.52
1:C:73:GLU:CD	1:C:253:PRO:C[2_555]	1.68	0.52
1:B:114:ALA:C	1:C:165:GLN:CA[3_555]	1.69	0.51
1:B:238:ASN:CB	1:C:146:SER:CB[3_555]	1.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:LEU:N	1:C:254:ILE:O[2_555]	1.69	0.51
1:B:73:GLU:OE2	1:C:162:TRP:CB[3_555]	1.69	0.51
1:B:123:CYS:N	1:C:148:ASN:O[3_555]	1.69	0.51
1:B:147:VAL:O	1:C:91:VAL:N[3_555]	1.69	0.51
1:B:239:THR:C	1:C:151:SER:N[3_555]	1.69	0.51
1:B:221:PRO:CB	1:C:241:ARG:NH2[3_555]	1.69	0.51
1:B:89:GLU:N	1:C:78:LEU:CD1[3_555]	1.69	0.51
1:B:160:PRO:CD	1:C:154:LYS:CG[3_555]	1.69	0.51
1:B:158:THR:CB	1:C:135:PHE:CG[3_555]	1.69	0.51
1:B:223:ARG:CA	1:C:76:THR:O[3_555]	1.69	0.51
1:B:73:GLU:CA	1:C:160:PRO:CA[3_555]	1.69	0.51
1:C:86:VAL:CG1	3:B:269:HOH:O[2_555]	1.69	0.51
1:B:161:VAL:N	1:C:153:LEU:CG[3_555]	1.69	0.51
1:B:187:LEU:CG	1:C:120:LEU:CD1[3_555]	1.69	0.51
1:B:69:LEU:CD2	1:C:48:ALA:N[3_555]	1.69	0.51
1:B:98:THR:OG1	1:C:128:SER:C[3_555]	1.70	0.50
1:C:99:TRP:CZ2	1:C:107:TRP:CE3[2_555]	1.70	0.50
1:B:77:GLU:OE1	1:C:229:GLU:OE1[3_555]	1.70	0.50
1:B:246:TYR:CD1	1:C:162:TRP:C[3_555]	1.70	0.50
1:B:71:HIS:CG	1:C:162:TRP:CZ3[3_555]	1.70	0.50
1:B:161:VAL:CG1	1:C:153:LEU:CG[3_555]	1.70	0.50
1:B:82:VAL:CA	1:C:142:THR:CG2[3_555]	1.70	0.50
1:C:99:TRP:CZ3	1:C:107:TRP:NE1[2_555]	1.70	0.50
1:B:241:ARG:CB	1:C:132:HIS:NE2[3_555]	1.70	0.50
1:C:101:ARG:CB	1:C:256:ALA:N[2_555]	1.70	0.50
1:B:152:ASN:OD1	1:C:94:PHE:N[3_555]	1.70	0.50
1:B:154:LYS:CD	1:C:72:CYS:CB[3_555]	1.70	0.50
1:B:99:TRP:O	1:C:126:THR:CA[3_555]	1.70	0.50
1:B:99:TRP:C	1:C:126:THR:CA[3_555]	1.70	0.50
1:B:91:VAL:CG1	1:C:120:LEU:O[3_555]	1.70	0.50
1:B:224:LEU:C	1:C:76:THR:CB[3_555]	1.70	0.50
1:C:101:ARG:CD	1:C:255:ALA:C[2_555]	1.70	0.50
1:B:162:TRP:N	1:C:152:ASN:O[3_555]	1.71	0.49
1:B:135:PHE:O	1:C:74:LEU:C[3_555]	1.71	0.49
1:B:88:SER:C	1:C:77:GLU:O[3_555]	1.71	0.49
1:B:248:ILE:N	1:C:50:GLY:N[3_555]	1.71	0.49
1:B:96:VAL:N	1:C:239:THR:CA[3_555]	1.71	0.49
1:B:246:TYR:OH	1:C:162:TRP:CE3[3_555]	1.71	0.49
1:B:152:ASN:CG	1:C:93:PRO:C[3_555]	1.71	0.49
1:C:58:PRO:CA	1:C:67:THR:N[2_555]	1.71	0.49
1:B:71:HIS:ND1	1:C:162:TRP:CZ3[3_555]	1.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLU:OE1	1:C:162:TRP:CD1[3_555]	1.71	0.49
1:C:97:GLY:O	1:C:254:ILE:CA[2_555]	1.71	0.49
1:B:149:GLN:NE2	1:C:94:PHE:CD2[3_555]	1.71	0.49
1:C:99:TRP:CD1	1:C:107:TRP:O[2_555]	1.71	0.49
1:B:190:ASN:ND2	1:C:172:ASN:CG[3_555]	1.71	0.49
1:B:131:ILE:N	1:C:135:PHE:CA[3_555]	1.71	0.49
1:B:246:TYR:OH	1:C:162:TRP:CD2[3_555]	1.71	0.49
1:B:160:PRO:N	1:C:154:LYS:N[3_555]	1.71	0.49
1:B:237:VAL:C	1:C:146:SER:N[3_555]	1.71	0.49
1:B:111:ALA:O	1:C:50:GLY:CA[3_555]	1.71	0.49
1:B:94:PHE:C	1:C:238:ASN:O[3_555]	1.71	0.49
1:B:230:GLY:CA	1:C:136:GLN:CD[3_555]	1.72	0.48
1:B:74:LEU:CG	1:C:130:ALA:CB[3_555]	1.72	0.48
1:B:183:ILE:CD1	1:C:156:TYR:N[3_555]	1.72	0.48
1:B:227:ALA:CA	1:C:89:GLU:N[3_555]	1.72	0.48
1:B:91:VAL:N	1:C:240:GLY:O[3_555]	1.72	0.48
1:B:148:ASN:C	1:C:92:MET:CG[3_555]	1.72	0.48
1:B:133:MET:O	1:C:117:TYR:CE1[3_555]	1.72	0.48
1:B:153:LEU:CG	1:C:96:VAL:C[3_555]	1.72	0.48
1:C:60:LEU:O	1:C:61:ARG:C[2_555]	1.72	0.48
1:C:73:GLU:OE2	1:C:253:PRO:C[2_555]	1.72	0.48
1:B:237:VAL:O	1:C:145:VAL:N[3_555]	1.72	0.48
1:B:191:GLU:CA	1:C:55:LEU:CA[3_555]	1.72	0.48
1:B:135:PHE:CA	1:C:75:SER:N[3_555]	1.72	0.48
1:B:82:VAL:CA	1:C:142:THR:CB[3_555]	1.72	0.48
1:B:71:HIS:ND1	1:C:162:TRP:CZ2[3_555]	1.72	0.48
1:A:255:ALA:N	1:B:127:THR:CB[2_555]	1.72	0.48
1:B:130:ALA:O	1:C:225:VAL:CG2[3_555]	1.72	0.48
1:B:247:THR:N	1:C:165:GLN:NE2[3_555]	1.72	0.48
1:B:243:TYR:CG	1:C:159:GLY:CA[3_555]	1.72	0.48
1:B:131:ILE:O	1:C:135:PHE:CD2[3_555]	1.72	0.48
1:B:241:ARG:C	1:C:132:HIS:CG[3_555]	1.72	0.48
1:B:132:HIS:CA	1:C:224:LEU:CG[3_555]	1.72	0.48
1:B:190:ASN:C	1:C:54:LYS:O[3_555]	1.72	0.48
1:B:119:TYR:CE1	1:C:156:TYR:CG[3_555]	1.72	0.48
1:B:148:ASN:CB	1:C:92:MET:CG[3_555]	1.73	0.47
1:B:245:SER:O	1:C:164:GLY:N[3_555]	1.73	0.47
1:B:131:ILE:CG2	1:C:134:GLY:N[3_555]	1.73	0.47
1:B:71:HIS:CE1	1:C:162:TRP:CH2[3_555]	1.73	0.47
1:C:99:TRP:CB	1:C:107:TRP:N[2_555]	1.73	0.47
1:A:258:LEU:C	1:B:232:SER:N[2_555]	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ALA:CB	1:C:145:VAL:CA[3_555]	1.73	0.47
1:B:123:CYS:CA	1:C:148:ASN:O[3_555]	1.73	0.47
1:B:112:TRP:C	1:C:51:THR:C[3_555]	1.73	0.47
1:B:98:THR:O	1:C:127:THR:CA[3_555]	1.73	0.47
1:B:89:GLU:N	1:C:77:GLU:C[3_555]	1.73	0.47
1:B:121:PRO:C	1:C:151:SER:CB[3_555]	1.73	0.47
1:B:223:ARG:O	1:C:76:THR:N[3_555]	1.73	0.47
1:B:189:THR:O	1:C:54:LYS:N[3_555]	1.73	0.47
1:B:104:ALA:N	1:C:124:PRO:CB[3_555]	1.74	0.46
1:C:59:MET:CB	1:C:63:SER:N[2_555]	1.74	0.46
1:B:230:GLY:O	1:C:141:ASP:CG[3_555]	1.74	0.46
1:B:231:GLY:CA	1:C:142:THR:O[3_555]	1.74	0.46
1:B:81:THR:O	1:C:142:THR:O[3_555]	1.74	0.46
1:B:77:GLU:CD	1:C:229:GLU:CB[3_555]	1.74	0.46
1:B:188:ASP:CA	1:C:171:VAL:C[3_555]	1.74	0.46
1:B:88:SER:C	1:C:78:LEU:CD1[3_555]	1.74	0.46
1:B:148:ASN:ND2	1:C:92:MET:SD[3_555]	1.74	0.46
1:B:154:LYS:CE	1:C:72:CYS:CB[3_555]	1.74	0.46
1:C:59:MET:N	1:C:66:VAL:O[2_555]	1.74	0.46
1:B:132:HIS:CB	1:C:224:LEU:N[3_555]	1.74	0.46
1:B:227:ALA:O	1:C:225:VAL:CA[3_555]	1.74	0.46
1:B:183:ILE:CG1	1:C:155:GLY:C[3_555]	1.74	0.46
1:B:135:PHE:CD2	1:C:243:TYR:CG[3_555]	1.74	0.46
1:B:132:HIS:NE2	1:C:223:ARG:N[3_555]	1.74	0.46
1:B:183:ILE:O	1:C:157:VAL:CG1[3_555]	1.74	0.46
1:B:237:VAL:CA	1:C:149:GLN:CD[3_555]	1.74	0.46
1:C:60:LEU:O	1:C:61:ARG:CA[2_555]	1.74	0.46
1:B:119:TYR:CD1	1:C:156:TYR:CD2[3_555]	1.75	0.45
1:B:187:LEU:CA	1:C:171:VAL:CG2[3_555]	1.75	0.45
1:B:132:HIS:NE2	1:C:223:ARG:CA[3_555]	1.75	0.45
1:B:230:GLY:N	1:C:223:ARG:NH2[3_555]	1.75	0.45
1:C:59:MET:SD	1:C:62:SER:C[2_555]	1.75	0.45
1:B:121:PRO:CD	1:C:156:TYR:CD1[3_555]	1.75	0.45
1:B:115:ILE:O	1:C:120:LEU:CD2[3_555]	1.75	0.45
1:B:222:ALA:O	1:C:241:ARG:CG[3_555]	1.75	0.45
1:B:88:SER:O	3:C:263:HOH:O[3_555]	1.75	0.45
1:B:243:TYR:CG	1:C:159:GLY:N[3_555]	1.75	0.45
1:B:241:ARG:CD	1:C:229:GLU:OE2[3_555]	1.75	0.45
1:B:117:TYR:CG	1:C:119:TYR:CD2[3_555]	1.75	0.45
1:B:131:ILE:N	1:C:134:GLY:C[3_555]	1.75	0.45
1:A:255:ALA:CB	1:B:127:THR:CG2[2_555]	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:GLU:CB	1:C:229:GLU:CB[3_555]	1.75	0.45
1:B:135:PHE:CG	1:C:242:LEU:C[3_555]	1.75	0.45
1:A:255:ALA:O	1:B:128:SER:N[2_555]	1.75	0.45
1:B:229:GLU:CG	1:C:223:ARG:CG[3_555]	1.75	0.45
1:B:135:PHE:C	1:C:75:SER:CA[3_555]	1.76	0.44
1:B:156:TYR:CE2	1:C:91:VAL:CG1[3_555]	1.76	0.44
1:B:241:ARG:O	1:C:158:THR:CB[3_555]	1.76	0.44
1:B:119:TYR:CG	1:C:133:MET:O[3_555]	1.76	0.44
1:B:144:PRO:CG	1:C:89:GLU:OE1[3_555]	1.76	0.44
1:B:89:GLU:C	1:C:78:LEU:CA[3_555]	1.76	0.44
1:B:133:MET:SD	1:C:133:MET:CE[3_555]	1.76	0.44
1:A:255:ALA:CB	1:B:127:THR:CB[2_555]	1.76	0.44
1:B:229:GLU:O	1:C:136:GLN:CG[3_555]	1.76	0.44
1:B:246:TYR:C	1:C:165:GLN:CG[3_555]	1.76	0.44
1:B:72:CYS:CA	1:C:163:GLU:OE2[3_555]	1.76	0.44
1:B:246:TYR:CG	1:C:162:TRP:O[3_555]	1.76	0.44
1:B:191:GLU:CB	1:C:55:LEU:CG[3_555]	1.76	0.44
1:B:187:LEU:CD1	1:C:243:TYR:CE1[3_555]	1.76	0.44
1:A:258:LEU:N	1:B:232:SER:CB[2_555]	1.76	0.44
1:B:188:ASP:CA	1:C:171:VAL:CG1[3_555]	1.76	0.44
1:B:91:VAL:CG2	1:C:241:ARG:C[3_555]	1.77	0.43
1:B:242:LEU:O	1:C:131:ILE:CA[3_555]	1.77	0.43
1:B:146:SER:CB	1:C:90:LEU:CD1[3_555]	1.77	0.43
1:B:229:GLU:CB	1:C:223:ARG:CG[3_555]	1.77	0.43
1:B:236:ALA:O	1:C:145:VAL:CB[3_555]	1.77	0.43
1:B:72:CYS:N	1:C:162:TRP:CZ3[3_555]	1.77	0.43
1:B:239:THR:O	1:C:147:VAL:O[3_555]	1.77	0.43
1:B:89:GLU:OE2	1:C:79:ALA:O[3_555]	1.77	0.43
1:B:191:GLU:CD	1:C:55:LEU:CA[3_555]	1.77	0.43
1:B:152:ASN:C	1:C:96:VAL:CG1[3_555]	1.77	0.43
1:C:98:THR:N	1:C:254:ILE:CD1[2_555]	1.77	0.43
1:B:119:TYR:CE2	1:C:150:LEU:CD1[3_555]	1.77	0.43
1:B:158:THR:O	1:C:135:PHE:CE1[3_555]	1.77	0.43
1:B:161:VAL:C	1:C:153:LEU:CA[3_555]	1.77	0.43
1:B:119:TYR:CD2	1:C:133:MET:O[3_555]	1.77	0.43
1:B:223:ARG:CG	1:C:77:GLU:N[3_555]	1.77	0.43
1:A:257:ALA:O	1:B:232:SER:CB[2_555]	1.77	0.43
1:B:226:THR:CA	1:C:226:THR:OG1[3_555]	1.77	0.43
1:B:95:THR:O	1:C:239:THR:CA[3_555]	1.77	0.43
1:B:132:HIS:N	1:C:224:LEU:CB[3_555]	1.77	0.43
1:B:89:GLU:CA	1:C:78:LEU:CB[3_555]	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:ASN:ND2	1:C:145:VAL:O[3_555]	1.77	0.43
1:B:156:TYR:CE2	1:C:91:VAL:CB[3_555]	1.77	0.43
1:B:119:TYR:CD1	1:C:156:TYR:CA[3_555]	1.77	0.43
1:B:72:CYS:C	1:C:160:PRO:CG[3_555]	1.77	0.43
1:B:239:THR:CA	1:C:149:GLN:C[3_555]	1.77	0.43
1:B:157:VAL:CB	1:C:185:ILE:O[3_555]	1.77	0.43
1:C:101:ARG:CZ	1:C:258:LEU:CB[2_555]	1.77	0.43
1:B:92:MET:CA	1:C:122:SER:OG[3_555]	1.77	0.43
1:A:258:LEU:CA	1:B:232:SER:OG[2_555]	1.78	0.42
1:B:246:TYR:CG	1:C:49:GLN:NE2[3_555]	1.78	0.42
1:B:84:ILE:CD1	3:C:268:HOH:O[3_555]	1.78	0.42
1:B:152:ASN:C	1:C:96:VAL:CB[3_555]	1.78	0.42
1:B:148:ASN:CG	1:C:220:VAL:CG1[3_555]	1.78	0.42
1:B:133:MET:N	1:C:224:LEU:CG[3_555]	1.78	0.42
1:B:76:THR:OG1	1:C:228:MET:N[3_555]	1.78	0.42
1:A:253:PRO:CB	1:B:162:TRP:CD1[2_555]	1.78	0.42
1:B:80:VAL:C	1:C:143:LEU:CA[3_555]	1.78	0.42
1:B:135:PHE:CD1	1:C:242:LEU:O[3_555]	1.78	0.42
1:B:82:VAL:CA	1:C:142:THR:CA[3_555]	1.78	0.42
1:B:162:TRP:CB	1:C:152:ASN:C[3_555]	1.78	0.42
1:B:162:TRP:CA	1:C:152:ASN:O[3_555]	1.78	0.42
1:C:98:THR:CA	1:C:254:ILE:CG2[2_555]	1.78	0.42
1:B:188:ASP:O	1:C:53:VAL:CG1[3_555]	1.78	0.42
1:B:118:THR:C	1:C:157:VAL:CG2[3_555]	1.78	0.42
1:B:229:GLU:CA	1:C:223:ARG:CZ[3_555]	1.78	0.42
1:B:119:TYR:CZ	1:C:156:TYR:CD2[3_555]	1.78	0.42
1:B:156:TYR:CZ	1:C:91:VAL:CB[3_555]	1.78	0.42
1:B:91:VAL:CG2	1:C:241:ARG:CG[3_555]	1.78	0.42
1:B:243:TYR:O	1:C:183:ILE:CG1[3_555]	1.78	0.42
1:C:101:ARG:CZ	1:C:258:LEU:CG[2_555]	1.78	0.42
1:B:161:VAL:CG1	1:C:153:LEU:CD1[3_555]	1.78	0.42
1:B:189:THR:CB	1:C:168:LEU:CD1[3_555]	1.79	0.41
1:B:78:LEU:N	1:C:227:ALA:CB[3_555]	1.79	0.41
1:B:131:ILE:CA	1:C:134:GLY:C[3_555]	1.79	0.41
1:B:227:ALA:CB	1:C:89:GLU:CA[3_555]	1.79	0.41
1:A:255:ALA:C	1:B:127:THR:CA[2_555]	1.79	0.41
1:A:255:ALA:CA	1:B:127:THR:N[2_555]	1.79	0.41
1:B:161:VAL:CA	1:C:153:LEU:CG[3_555]	1.79	0.41
1:B:227:ALA:CA	1:C:224:LEU:O[3_555]	1.79	0.41
1:B:99:TRP:N	1:C:126:THR:C[3_555]	1.79	0.41
1:B:100:LEU:O	1:C:124:PRO:N[3_555]	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ALA:CB	1:C:145:VAL:CB[3_555]	1.79	0.41
1:B:93:PRO:N	1:C:122:SER:O[3_555]	1.79	0.41
1:B:185:ILE:CA	1:C:117:TYR:O[3_555]	1.79	0.41
1:B:98:THR:N	1:C:127:THR:O[3_555]	1.79	0.41
1:C:99:TRP:O	1:C:106:ASN:O[2_555]	1.79	0.41
1:B:71:HIS:CB	1:C:162:TRP:CZ3[3_555]	1.79	0.41
1:B:135:PHE:CD2	1:C:243:TYR:N[3_555]	1.79	0.41
1:B:100:LEU:N	1:C:126:THR:N[3_555]	1.79	0.41
1:B:163:GLU:O	1:C:156:TYR:CB[3_555]	1.79	0.41
1:C:57:PRO:CA	1:C:251:ILE:CD1[2_555]	1.79	0.41
1:B:99:TRP:CA	1:C:127:THR:N[3_555]	1.79	0.41
1:C:100:LEU:N	1:C:254:ILE:N[2_555]	1.80	0.40
1:B:89:GLU:CB	1:C:78:LEU:CG[3_555]	1.80	0.40
1:B:184:THR:CB	1:C:184:THR:N[3_555]	1.80	0.40
1:B:158:THR:CG2	1:C:135:PHE:CB[3_555]	1.80	0.40
1:B:100:LEU:C	1:C:124:PRO:CG[3_555]	1.80	0.40
1:B:192:VAL:N	1:C:53:VAL:O[3_555]	1.80	0.40
1:C:94:PHE:CZ	1:C:257:ALA:CB[2_555]	1.80	0.40
1:B:170:PHE:CA	1:C:180:SER:O[3_555]	1.80	0.40
1:B:80:VAL:CG2	1:C:144:PRO:N[3_555]	1.80	0.40
1:C:57:PRO:CG	1:C:249:ARG:CD[2_555]	1.80	0.40
1:C:60:LEU:N	1:C:62:SER:CA[2_555]	1.80	0.40
1:B:239:THR:N	1:C:150:LEU:N[3_555]	1.80	0.40
1:B:93:PRO:CA	1:C:123:CYS:CA[3_555]	1.80	0.40
1:B:131:ILE:CB	1:C:134:GLY:CA[3_555]	1.80	0.40
1:A:254:ILE:C	1:B:127:THR:CA[2_555]	1.80	0.40
1:B:75:SER:C	1:C:130:ALA:O[3_555]	1.80	0.40
1:B:115:ILE:CG2	1:C:120:LEU:CA[3_555]	1.80	0.40
1:B:148:ASN:C	1:C:92:MET:CA[3_555]	1.80	0.40
1:B:118:THR:OG1	1:C:183:ILE:CA[3_555]	1.80	0.40
1:B:223:ARG:CG	1:C:76:THR:CA[3_555]	1.80	0.40
1:B:101:ARG:NH2	1:C:237:VAL:CB[3_555]	1.80	0.40
1:B:149:GLN:CA	1:C:95:THR:CA[3_555]	1.80	0.40
1:B:132:HIS:O	1:C:224:LEU:CB[3_555]	1.81	0.39
1:B:80:VAL:CG2	1:C:144:PRO:CD[3_555]	1.81	0.39
1:C:99:TRP:CE3	1:C:107:TRP:CD1[2_555]	1.81	0.39
1:C:57:PRO:CG	1:C:249:ARG:NE[2_555]	1.81	0.39
1:B:190:ASN:OD1	1:C:172:ASN:O[3_555]	1.81	0.39
1:B:100:LEU:CB	1:C:124:PRO:O[3_555]	1.81	0.39
1:B:245:SER:N	1:C:163:GLU:CG[3_555]	1.81	0.39
1:B:147:VAL:N	1:C:90:LEU:CA[3_555]	1.81	0.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:THR:CB	1:C:87:THR:OG1[3_555]	1.81	0.39
1:B:183:ILE:CG2	1:C:185:ILE:CB[3_555]	1.81	0.39
1:B:225:VAL:N	1:C:242:LEU:CD2[3_555]	1.81	0.39
1:B:99:TRP:O	1:C:126:THR:OG1[3_555]	1.81	0.39
1:B:160:PRO:N	1:C:154:LYS:CA[3_555]	1.81	0.39
1:B:227:ALA:CA	1:C:88:SER:CA[3_555]	1.81	0.39
1:B:73:GLU:CD	1:C:162:TRP:NE1[3_555]	1.81	0.39
1:A:253:PRO:N	1:B:162:TRP:NE1[2_555]	1.81	0.39
1:C:59:MET:SD	1:C:62:SER:O[2_555]	1.81	0.39
1:B:69:LEU:CG	1:C:46:PRO:C[3_555]	1.82	0.38
1:B:69:LEU:CA	1:C:46:PRO:CB[3_555]	1.82	0.38
1:B:87:THR:OG1	1:C:87:THR:CA[3_555]	1.82	0.38
1:C:59:MET:CE	1:C:64:MET:N[2_555]	1.82	0.38
1:B:116:ARG:CD	1:C:182:ALA:C[3_555]	1.82	0.38
1:B:131:ILE:N	1:C:135:PHE:N[3_555]	1.82	0.38
1:B:236:ALA:CA	1:C:145:VAL:CB[3_555]	1.82	0.38
1:C:57:PRO:CG	1:C:249:ARG:NH1[2_555]	1.82	0.38
1:C:58:PRO:CD	1:C:250:LEU:N[2_555]	1.82	0.38
1:B:157:VAL:O	1:C:135:PHE:CE2[3_555]	1.82	0.38
1:B:95:THR:N	1:C:238:ASN:C[3_555]	1.82	0.38
1:B:230:GLY:C	1:C:141:ASP:CB[3_555]	1.82	0.38
1:B:131:ILE:CG1	1:C:225:VAL:O[3_555]	1.82	0.38
1:B:135:PHE:CG	1:C:243:TYR:CB[3_555]	1.82	0.38
1:B:73:GLU:N	1:C:160:PRO:CB[3_555]	1.82	0.38
1:B:225:VAL:CA	1:C:76:THR:OG1[3_555]	1.82	0.38
1:B:117:TYR:CE2	1:C:119:TYR:CD2[3_555]	1.83	0.37
1:B:150:LEU:O	1:C:117:TYR:OH[3_555]	1.83	0.37
1:A:253:PRO:CD	1:B:162:TRP:CE2[2_555]	1.83	0.37
1:B:122:SER:CA	1:C:151:SER:OG[3_555]	1.83	0.37
1:B:230:GLY:CA	1:C:136:GLN:NE2[3_555]	1.83	0.37
1:B:239:THR:C	1:C:150:LEU:CA[3_555]	1.83	0.37
1:B:189:THR:C	1:C:53:VAL:CA[3_555]	1.83	0.37
1:A:254:ILE:O	1:B:126:THR:O[2_555]	1.83	0.37
1:C:58:PRO:O	1:C:67:THR:O[2_555]	1.83	0.37
1:B:162:TRP:N	1:C:153:LEU:CA[3_555]	1.83	0.37
1:B:192:VAL:CA	1:C:53:VAL:O[3_555]	1.83	0.37
1:B:119:TYR:CA	1:C:158:THR:N[3_555]	1.83	0.37
1:B:243:TYR:CA	1:C:159:GLY:O[3_555]	1.83	0.37
1:B:190:ASN:C	1:C:54:LYS:CB[3_555]	1.83	0.37
1:B:120:LEU:O	1:C:156:TYR:CE2[3_555]	1.83	0.37
1:B:96:VAL:O	1:C:161:VAL:CA[3_555]	1.83	0.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:VAL:CG2	1:C:86:VAL:O[3_555]	1.83	0.37
1:B:226:THR:CG2	1:C:226:THR:CB[3_555]	1.83	0.37
1:B:170:PHE:CB	1:C:181:ARG:CA[3_555]	1.83	0.37
1:B:229:GLU:N	1:C:223:ARG:NE[3_555]	1.84	0.36
1:B:170:PHE:CD2	1:C:180:SER:O[3_555]	1.84	0.36
1:B:76:THR:O	1:C:132:HIS:CD2[3_555]	1.84	0.36
1:C:58:PRO:O	1:C:66:VAL:C[2_555]	1.84	0.36
1:C:58:PRO:CG	1:C:250:LEU:O[2_555]	1.84	0.36
1:C:246:TYR:OH	1:C:253:PRO:N[2_555]	1.84	0.36
1:B:71:HIS:CG	1:C:162:TRP:CH2[3_555]	1.84	0.36
1:B:89:GLU:CA	1:C:77:GLU:C[3_555]	1.84	0.36
1:C:57:PRO:CG	1:C:249:ARG:CG[2_555]	1.84	0.36
1:C:73:GLU:OE1	1:C:254:ILE:N[2_555]	1.84	0.36
1:B:246:TYR:CE1	1:C:163:GLU:N[3_555]	1.84	0.36
1:B:155:GLY:CA	1:C:245:SER:N[3_555]	1.84	0.36
1:B:136:GLN:C	1:C:74:LEU:CB[3_555]	1.84	0.36
1:B:154:LYS:CG	1:C:244:ALA:O[3_555]	1.84	0.36
1:B:102:GLY:C	1:C:126:THR:OG1[3_555]	1.84	0.36
1:B:131:ILE:C	1:C:134:GLY:O[3_555]	1.84	0.36
1:B:99:TRP:C	1:C:125:THR:C[3_555]	1.85	0.35
1:B:78:LEU:CG	1:C:227:ALA:CA[3_555]	1.85	0.35
1:B:243:TYR:CD1	1:C:158:THR:C[3_555]	1.85	0.35
1:B:85:VAL:C	1:C:88:SER:N[3_555]	1.85	0.35
1:B:74:LEU:CA	1:C:130:ALA:CA[3_555]	1.85	0.35
1:B:103:VAL:N	1:C:126:THR:OG1[3_555]	1.85	0.35
1:B:161:VAL:O	1:C:153:LEU:N[3_555]	1.85	0.35
1:C:101:ARG:C	1:C:256:ALA:N[2_555]	1.85	0.35
1:B:89:GLU:CD	1:C:79:ALA:N[3_555]	1.85	0.35
1:C:98:THR:CG2	1:C:254:ILE:CD1[2_555]	1.85	0.35
1:C:98:THR:CA	1:C:254:ILE:CB[2_555]	1.85	0.35
1:B:85:VAL:CB	3:C:264:HOH:O[3_555]	1.85	0.35
1:C:71:HIS:CD2	1:C:251:ILE:C[2_555]	1.85	0.35
1:B:89:GLU:OE1	1:C:79:ALA:O[3_555]	1.85	0.35
1:B:239:THR:C	1:C:150:LEU:N[3_555]	1.85	0.35
1:B:101:ARG:N	1:C:124:PRO:O[3_555]	1.85	0.35
1:B:245:SER:N	1:C:163:GLU:CB[3_555]	1.86	0.34
1:B:190:ASN:O	1:C:54:LYS:N[3_555]	1.86	0.34
1:B:222:ALA:O	1:C:241:ARG:CB[3_555]	1.86	0.34
1:B:184:THR:CG2	1:C:184:THR:CB[3_555]	1.86	0.34
1:B:136:GLN:N	1:C:74:LEU:O[3_555]	1.86	0.34
1:B:76:THR:N	1:C:131:ILE:N[3_555]	1.86	0.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:ASN:O	1:C:149:GLN:CB[3_555]	1.86	0.34
1:B:184:THR:CA	1:C:184:THR:N[3_555]	1.86	0.34
1:B:98:THR:CG2	1:C:128:SER:OG[3_555]	1.86	0.34
1:B:170:PHE:CA	1:C:181:ARG:N[3_555]	1.86	0.34
1:C:73:GLU:CD	1:C:253:PRO:O[2_555]	1.86	0.34
1:B:132:HIS:CG	1:C:224:LEU:CA[3_555]	1.86	0.34
1:B:114:ALA:CA	1:C:51:THR:CG2[3_555]	1.86	0.34
1:C:246:TYR:OH	1:C:253:PRO:CD[2_555]	1.86	0.34
1:B:95:THR:CG2	1:C:239:THR:N[3_555]	1.86	0.34
1:B:148:ASN:O	1:C:92:MET:CB[3_555]	1.86	0.34
1:B:100:LEU:CB	1:C:124:PRO:C[3_555]	1.87	0.33
1:B:246:TYR:CD2	1:C:49:GLN:CG[3_555]	1.87	0.33
1:B:149:GLN:C	1:C:96:VAL:N[3_555]	1.87	0.33
1:B:70:SER:N	1:C:46:PRO:CG[3_555]	1.87	0.33
1:C:57:PRO:CG	1:C:249:ARG:CZ[2_555]	1.87	0.33
1:B:112:TRP:CG	1:C:51:THR:OG1[3_555]	1.87	0.33
1:B:73:GLU:OE1	1:C:127:THR:O[3_555]	1.87	0.33
1:B:101:ARG:C	1:C:124:PRO:CG[3_555]	1.87	0.33
1:B:117:TYR:CB	1:C:119:TYR:CB[3_555]	1.87	0.33
1:A:255:ALA:N	1:B:128:SER:N[2_555]	1.87	0.33
1:C:101:ARG:CD	1:C:256:ALA:C[2_555]	1.87	0.33
1:B:247:THR:CA	1:C:165:GLN:CD[3_555]	1.87	0.33
1:B:242:LEU:CA	1:C:132:HIS:N[3_555]	1.87	0.33
1:B:101:ARG:O	1:C:124:PRO:CG[3_555]	1.87	0.33
1:B:123:CYS:SG	1:C:149:GLN:O[3_555]	1.87	0.33
1:C:99:TRP:CZ2	1:C:107:TRP:CD2[2_555]	1.87	0.33
1:B:160:PRO:C	1:C:153:LEU:CB[3_555]	1.87	0.33
1:B:170:PHE:CG	1:C:180:SER:O[3_555]	1.87	0.33
1:C:57:PRO:O	1:C:66:VAL:CG1[2_555]	1.87	0.33
1:B:147:VAL:O	1:C:92:MET:N[3_555]	1.88	0.32
1:B:100:LEU:C	1:C:124:PRO:N[3_555]	1.88	0.32
1:A:257:ALA:C	1:B:232:SER:CB[2_555]	1.88	0.32
1:C:97:GLY:CA	1:C:254:ILE:CA[2_555]	1.88	0.32
1:B:223:ARG:O	1:C:76:THR:O[3_555]	1.88	0.32
1:B:189:THR:CA	1:C:53:VAL:CA[3_555]	1.88	0.32
1:B:242:LEU:N	1:C:132:HIS:N[3_555]	1.88	0.32
1:B:149:GLN:C	1:C:95:THR:C[3_555]	1.88	0.32
1:B:90:LEU:O	1:C:240:GLY:C[3_555]	1.88	0.32
1:C:101:ARG:N	1:C:255:ALA:CA[2_555]	1.88	0.32
1:B:161:VAL:CA	1:C:153:LEU:N[3_555]	1.88	0.32
1:B:73:GLU:CG	1:C:162:TRP:CD1[3_555]	1.88	0.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:TYR:CE1	1:C:73:GLU:CA[3_555]	1.88	0.32
1:B:117:TYR:CZ	1:C:119:TYR:CG[3_555]	1.88	0.32
1:B:132:HIS:CE1	1:C:223:ARG:CA[3_555]	1.88	0.32
1:B:191:GLU:C	1:C:55:LEU:N[3_555]	1.88	0.32
1:B:70:SER:O	1:C:46:PRO:CD[3_555]	1.88	0.32
1:C:99:TRP:C	1:C:254:ILE:O[2_555]	1.88	0.32
1:B:69:LEU:CB	1:C:46:PRO:CB[3_555]	1.89	0.31
1:B:97:GLY:C	1:C:127:THR:CB[3_555]	1.89	0.31
1:B:184:THR:C	1:C:184:THR:CB[3_555]	1.89	0.31
1:B:162:TRP:CD1	1:C:152:ASN:O[3_555]	1.89	0.31
1:B:185:ILE:CD1	1:C:243:TYR:O[3_555]	1.89	0.31
1:B:80:VAL:CG2	1:C:144:PRO:CB[3_555]	1.89	0.31
1:B:118:THR:CG2	1:C:157:VAL:CG2[3_555]	1.89	0.31
1:B:246:TYR:CA	1:C:49:GLN:CD[3_555]	1.89	0.31
1:B:191:GLU:OE2	1:C:56:ARG:CA[3_555]	1.89	0.31
1:B:75:SER:N	1:C:130:ALA:CA[3_555]	1.89	0.31
1:B:238:ASN:CA	1:C:146:SER:CB[3_555]	1.89	0.31
1:B:78:LEU:CG	1:C:227:ALA:N[3_555]	1.89	0.31
1:B:183:ILE:CG2	1:C:185:ILE:CD1[3_555]	1.89	0.31
1:B:117:TYR:C	1:C:183:ILE:C[3_555]	1.89	0.31
1:B:99:TRP:N	1:C:127:THR:C[3_555]	1.89	0.31
1:C:99:TRP:CZ3	1:C:107:TRP:CE3[2_555]	1.89	0.31
1:B:74:LEU:C	1:C:129:GLY:O[3_555]	1.89	0.31
1:B:241:ARG:CA	1:C:132:HIS:NE2[3_555]	1.89	0.31
1:B:231:GLY:N	1:C:142:THR:O[3_555]	1.89	0.31
1:B:242:LEU:C	1:C:131:ILE:C[3_555]	1.89	0.31
1:B:119:TYR:CD1	1:C:156:TYR:CG[3_555]	1.89	0.31
1:B:188:ASP:CA	1:C:172:ASN:N[3_555]	1.90	0.30
1:B:131:ILE:CG2	1:C:134:GLY:O[3_555]	1.90	0.30
1:C:100:LEU:C	1:C:254:ILE:O[2_555]	1.90	0.30
1:B:120:LEU:CA	1:C:156:TYR:CD1[3_555]	1.90	0.30
1:B:112:TRP:CZ2	1:C:122:SER:N[3_555]	1.90	0.30
1:A:258:LEU:N	1:B:232:SER:OG[2_555]	1.90	0.30
1:B:119:TYR:C	1:C:158:THR:N[3_555]	1.90	0.30
1:B:132:HIS:CE1	1:C:222:ALA:C[3_555]	1.90	0.30
1:C:73:GLU:CG	1:C:252:GLU:O[2_555]	1.90	0.30
1:B:117:TYR:CE2	1:C:120:LEU:N[3_555]	1.90	0.30
1:B:72:CYS:O	1:C:162:TRP:CH2[3_555]	1.90	0.30
1:B:87:THR:OG1	1:C:87:THR:OG1[3_555]	1.90	0.30
1:B:154:LYS:CD	1:C:72:CYS:SG[3_555]	1.90	0.30
1:B:91:VAL:CA	1:C:240:GLY:C[3_555]	1.90	0.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:LEU:CG	1:C:46:PRO:CA[3_555]	1.90	0.30
1:B:246:TYR:CZ	1:C:162:TRP:O[3_555]	1.90	0.30
1:B:147:VAL:C	1:C:90:LEU:CA[3_555]	1.90	0.30
1:B:155:GLY:N	1:C:245:SER:CA[3_555]	1.90	0.30
1:B:135:PHE:CE1	1:C:242:LEU:C[3_555]	1.90	0.30
1:B:186:ALA:O	1:C:171:VAL:CG2[3_555]	1.90	0.30
1:B:82:VAL:CB	1:C:142:THR:CG2[3_555]	1.90	0.30
1:B:222:ALA:N	1:C:241:ARG:NE[3_555]	1.90	0.30
1:B:185:ILE:CA	1:C:118:THR:CA[3_555]	1.91	0.29
1:B:112:TRP:CB	1:C:51:THR:O[3_555]	1.91	0.29
1:B:224:LEU:CD1	1:C:242:LEU:CD2[3_555]	1.91	0.29
1:A:253:PRO:C	1:B:162:TRP:CD1[2_555]	1.91	0.29
1:B:93:PRO:C	1:C:123:CYS:CB[3_555]	1.91	0.29
1:B:79:ALA:CB	1:C:145:VAL:N[3_555]	1.91	0.29
1:B:161:VAL:C	1:C:152:ASN:C[3_555]	1.91	0.29
1:B:246:TYR:OH	1:C:162:TRP:CG[3_555]	1.91	0.29
1:B:149:GLN:C	1:C:95:THR:CB[3_555]	1.91	0.29
1:B:243:TYR:N	1:C:158:THR:C[3_555]	1.91	0.29
1:A:258:LEU:CA	1:B:232:SER:N[2_555]	1.91	0.29
1:B:243:TYR:CD1	1:C:158:THR:OG1[3_555]	1.91	0.29
1:B:190:ASN:O	1:C:54:LYS:CG[3_555]	1.91	0.29
1:B:80:VAL:CG1	1:C:144:PRO:CG[3_555]	1.91	0.29
1:B:247:THR:CB	1:C:165:GLN:OE1[3_555]	1.91	0.29
1:B:90:LEU:CD1	1:C:77:GLU:CD[3_555]	1.91	0.29
1:B:77:GLU:OE1	1:C:229:GLU:CD[3_555]	1.91	0.29
1:B:119:TYR:CZ	1:C:150:LEU:CD1[3_555]	1.91	0.29
1:A:256:ALA:N	1:B:126:THR:O[2_555]	1.91	0.29
1:B:91:VAL:CB	1:C:241:ARG:CG[3_555]	1.91	0.29
1:C:97:GLY:O	1:C:254:ILE:CG1[2_555]	1.91	0.29
1:B:136:GLN:O	1:C:74:LEU:CD2[3_555]	1.91	0.29
1:B:153:LEU:C	1:C:244:ALA:CB[3_555]	1.91	0.29
1:B:93:PRO:CD	1:C:122:SER:CB[3_555]	1.91	0.29
1:B:156:TYR:OH	1:C:91:VAL:CB[3_555]	1.91	0.29
1:B:163:GLU:N	1:C:153:LEU:O[3_555]	1.92	0.28
1:B:151:SER:C	1:C:96:VAL:CG2[3_555]	1.92	0.28
1:C:99:TRP:CZ3	1:C:107:TRP:CD1[2_555]	1.92	0.28
1:C:99:TRP:CD2	1:C:107:TRP:N[2_555]	1.92	0.28
1:B:122:SER:CA	1:C:151:SER:CB[3_555]	1.92	0.28
1:B:170:PHE:CD2	1:C:179:THR:C[3_555]	1.92	0.28
1:B:238:ASN:ND2	1:C:146:SER:CA[3_555]	1.92	0.28
1:B:244:ALA:CA	1:C:183:ILE:CD1[3_555]	1.92	0.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:TYR:CE1	1:C:91:VAL:CG1[3_555]	1.92	0.28
1:B:248:ILE:CG1	1:C:49:GLN:O[3_555]	1.92	0.28
1:B:99:TRP:N	1:C:127:THR:CA[3_555]	1.92	0.28
1:B:247:THR:N	1:C:165:GLN:CB[3_555]	1.92	0.28
1:B:117:TYR:CD1	1:C:119:TYR:CE2[3_555]	1.92	0.28
1:B:245:SER:OG	1:C:163:GLU:CG[3_555]	1.92	0.28
1:C:99:TRP:CE3	1:C:107:TRP:CB[2_555]	1.92	0.28
1:C:71:HIS:NE2	1:C:251:ILE:O[2_555]	1.92	0.28
1:B:158:THR:N	1:C:135:PHE:CE2[3_555]	1.92	0.28
1:B:133:MET:O	1:C:117:TYR:CE2[3_555]	1.92	0.28
1:B:135:PHE:CE1	1:C:118:THR:O[3_555]	1.92	0.28
1:B:93:PRO:CD	1:C:122:SER:C[3_555]	1.92	0.28
1:B:185:ILE:C	1:C:118:THR:OG1[3_555]	1.92	0.28
1:B:77:GLU:CB	1:C:229:GLU:CG[3_555]	1.92	0.28
1:B:118:THR:CB	1:C:157:VAL:CG2[3_555]	1.92	0.28
1:B:149:GLN:C	1:C:95:THR:CA[3_555]	1.92	0.28
1:C:71:HIS:CD2	1:C:252:GLU:N[2_555]	1.93	0.27
1:B:247:THR:N	1:C:165:GLN:CD[3_555]	1.93	0.27
1:B:238:ASN:O	1:C:149:GLN:CA[3_555]	1.93	0.27
1:C:101:ARG:NH2	1:C:258:LEU:CG[2_555]	1.93	0.27
1:B:151:SER:OG	1:C:91:VAL:C[3_555]	1.93	0.27
1:B:170:PHE:CG	1:C:179:THR:O[3_555]	1.93	0.27
1:B:112:TRP:N	1:C:51:THR:O[3_555]	1.93	0.27
1:B:133:MET:N	1:C:224:LEU:CD1[3_555]	1.93	0.27
1:B:241:ARG:CA	1:C:132:HIS:CD2[3_555]	1.93	0.27
1:B:150:LEU:CG	1:C:89:GLU:CG[3_555]	1.93	0.27
1:B:146:SER:CA	1:C:90:LEU:CD1[3_555]	1.93	0.27
1:B:191:GLU:OE2	1:C:56:ARG:CB[3_555]	1.93	0.27
1:B:149:GLN:NE2	1:C:94:PHE:CE2[3_555]	1.93	0.27
1:C:246:TYR:CE2	1:C:253:PRO:CG[2_555]	1.93	0.27
1:B:99:TRP:C	1:C:127:THR:N[3_555]	1.93	0.27
1:B:223:ARG:C	1:C:76:THR:C[3_555]	1.93	0.27
1:C:102:GLY:N	1:C:256:ALA:N[2_555]	1.93	0.27
1:B:90:LEU:O	1:C:240:GLY:N[3_555]	1.93	0.27
1:C:73:GLU:CG	1:C:253:PRO:O[2_555]	1.93	0.27
1:C:98:THR:OG1	1:C:254:ILE:CD1[2_555]	1.94	0.26
1:B:89:GLU:O	1:C:77:GLU:C[3_555]	1.94	0.26
1:B:119:TYR:N	1:C:157:VAL:CG1[3_555]	1.94	0.26
1:B:95:THR:CB	1:C:238:ASN:CA[3_555]	1.94	0.26
1:B:242:LEU:O	1:C:131:ILE:O[3_555]	1.94	0.26
1:B:147:VAL:CB	1:C:90:LEU:CD2[3_555]	1.94	0.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:PRO:C	1:C:66:VAL:CB[2_555]	1.94	0.26
1:A:253:PRO:C	1:B:162:TRP:NE1[2_555]	1.94	0.26
1:C:55:LEU:O	1:C:196:ARG:NH1[2_555]	1.94	0.26
1:B:93:PRO:CD	1:C:122:SER:CA[3_555]	1.94	0.26
1:B:150:LEU:CD1	1:C:117:TYR:OH[3_555]	1.94	0.26
1:B:71:HIS:O	1:C:163:GLU:CD[3_555]	1.94	0.26
1:B:191:GLU:CG	1:C:55:LEU:C[3_555]	1.94	0.26
1:B:149:GLN:C	1:C:92:MET:O[3_555]	1.94	0.26
1:B:117:TYR:CE1	1:C:119:TYR:CG[3_555]	1.94	0.26
1:B:95:THR:CB	1:C:239:THR:CA[3_555]	1.94	0.26
1:B:150:LEU:N	1:C:95:THR:CB[3_555]	1.94	0.26
1:B:92:MET:C	1:C:122:SER:CA[3_555]	1.94	0.26
1:B:228:MET:CE	1:C:225:VAL:CG1[3_555]	1.94	0.26
1:B:87:THR:CA	1:C:87:THR:CB[3_555]	1.94	0.26
1:B:81:THR:CA	1:C:143:LEU:O[3_555]	1.94	0.26
1:B:150:LEU:CD2	1:C:89:GLU:CD[3_555]	1.94	0.26
1:B:119:TYR:OH	1:C:150:LEU:C[3_555]	1.94	0.26
1:B:112:TRP:CB	1:C:51:THR:CB[3_555]	1.94	0.26
1:B:183:ILE:O	1:C:184:THR:O[3_555]	1.94	0.26
1:B:154:LYS:O	1:C:244:ALA:CB[3_555]	1.94	0.26
1:B:100:LEU:O	1:C:124:PRO:CD[3_555]	1.94	0.26
1:B:189:THR:CG2	1:C:168:LEU:CD1[3_555]	1.94	0.26
1:B:134:GLY:CA	1:C:117:TYR:CE2[3_555]	1.95	0.25
1:B:229:GLU:CA	1:C:223:ARG:CD[3_555]	1.95	0.25
1:B:225:VAL:CG1	1:C:89:GLU:OE2[3_555]	1.95	0.25
1:B:85:VAL:CG2	3:C:264:HOH:O[3_555]	1.95	0.25
1:B:248:ILE:CB	1:C:49:GLN:O[3_555]	1.95	0.25
1:B:190:ASN:O	1:C:54:LYS:C[3_555]	1.95	0.25
1:B:225:VAL:CG2	1:C:76:THR:CB[3_555]	1.95	0.25
1:B:78:LEU:CD2	1:C:226:THR:C[3_555]	1.95	0.25
1:B:119:TYR:CB	1:C:157:VAL:CA[3_555]	1.95	0.25
1:B:89:GLU:CG	1:C:78:LEU:CG[3_555]	1.95	0.25
1:B:98:THR:N	1:C:128:SER:N[3_555]	1.95	0.25
1:B:170:PHE:C	1:C:181:ARG:CA[3_555]	1.95	0.25
1:B:147:VAL:O	1:C:91:VAL:CA[3_555]	1.95	0.25
1:B:191:GLU:N	1:C:54:LYS:N[3_555]	1.95	0.25
1:B:233:SER:O	1:C:142:THR:OG1[3_555]	1.95	0.25
1:B:88:SER:CA	3:C:265:HOH:O[3_555]	1.95	0.25
1:B:154:LYS:CG	1:C:72:CYS:SG[3_555]	1.95	0.25
1:B:82:VAL:CG1	1:C:142:THR:CG2[3_555]	1.95	0.25
1:B:243:TYR:CB	1:C:159:GLY:C[3_555]	1.95	0.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ALA:CB	1:C:243:TYR:CZ[3_555]	1.95	0.25
1:B:132:HIS:CD2	1:C:224:LEU:CA[3_555]	1.95	0.25
1:C:99:TRP:CD1	1:C:107:TRP:N[2_555]	1.95	0.25
1:B:154:LYS:CB	1:C:73:GLU:N[3_555]	1.95	0.25
1:B:153:LEU:CB	1:C:96:VAL:O[3_555]	1.95	0.25
1:B:100:LEU:CD1	1:C:123:CYS:C[3_555]	1.95	0.25
1:B:100:LEU:O	1:C:124:PRO:C[3_555]	1.95	0.25
1:B:78:LEU:CB	1:C:227:ALA:CA[3_555]	1.95	0.25
1:B:90:LEU:C	1:C:240:GLY:C[3_555]	1.96	0.24
1:B:95:THR:OG1	1:C:239:THR:N[3_555]	1.96	0.24
1:B:93:PRO:CB	1:C:123:CYS:N[3_555]	1.96	0.24
1:B:156:TYR:CD1	1:C:115:ILE:CG2[3_555]	1.96	0.24
1:B:225:VAL:N	1:C:76:THR:CB[3_555]	1.96	0.24
1:B:99:TRP:CD2	1:C:125:THR:C[3_555]	1.96	0.24
1:A:254:ILE:CD1	1:B:128:SER:CA[2_555]	1.96	0.24
1:B:243:TYR:C	1:C:183:ILE:CD1[3_555]	1.96	0.24
1:B:131:ILE:CD1	1:C:133:MET:CB[3_555]	1.96	0.24
1:B:80:VAL:CA	1:C:144:PRO:CA[3_555]	1.96	0.24
1:C:100:LEU:CA	1:C:254:ILE:O[2_555]	1.96	0.24
1:B:244:ALA:N	1:C:160:PRO:O[3_555]	1.96	0.24
1:B:119:TYR:C	1:C:157:VAL:N[3_555]	1.96	0.24
1:C:73:GLU:CD	1:C:252:GLU:C[2_555]	1.96	0.24
1:B:89:GLU:CG	1:C:78:LEU:CB[3_555]	1.96	0.24
1:B:156:TYR:CZ	1:C:91:VAL:CG2[3_555]	1.96	0.24
1:B:229:GLU:C	1:C:223:ARG:NE[3_555]	1.96	0.24
1:B:190:ASN:CB	1:C:54:LYS:O[3_555]	1.96	0.24
1:B:112:TRP:C	1:C:51:THR:CB[3_555]	1.96	0.24
1:C:59:MET:CE	1:C:63:SER:N[2_555]	1.96	0.24
1:B:95:THR:OG1	1:C:238:ASN:O[3_555]	1.97	0.23
1:C:99:TRP:CA	1:C:107:TRP:N[2_555]	1.97	0.23
1:A:258:LEU:O	1:B:231:GLY:CA[2_555]	1.97	0.23
1:C:56:ARG:CA	1:C:249:ARG:NH2[2_555]	1.97	0.23
1:B:162:TRP:CA	1:C:153:LEU:N[3_555]	1.97	0.23
1:B:170:PHE:CG	1:C:182:ALA:N[3_555]	1.97	0.23
1:B:117:TYR:O	1:C:184:THR:N[3_555]	1.97	0.23
1:C:99:TRP:CA	1:C:106:ASN:C[2_555]	1.97	0.23
1:B:147:VAL:C	1:C:90:LEU:CB[3_555]	1.97	0.23
1:B:73:GLU:N	1:C:160:PRO:CD[3_555]	1.97	0.23
1:C:99:TRP:N	1:C:254:ILE:CB[2_555]	1.97	0.23
1:B:87:THR:N	1:C:87:THR:CB[3_555]	1.97	0.23
1:B:132:HIS:N	1:C:224:LEU:C[3_555]	1.97	0.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ASP:CA	1:C:171:VAL:CB[3_555]	1.97	0.23
1:B:187:LEU:C	1:C:171:VAL:CG1[3_555]	1.97	0.23
1:B:100:LEU:CA	1:C:124:PRO:CA[3_555]	1.97	0.23
1:B:73:GLU:C	1:C:160:PRO:C[3_555]	1.97	0.23
1:B:157:VAL:CB	1:C:185:ILE:C[3_555]	1.97	0.23
1:B:147:VAL:CA	1:C:90:LEU:N[3_555]	1.97	0.23
1:B:118:THR:N	1:C:183:ILE:CA[3_555]	1.97	0.23
1:B:115:ILE:CD1	1:C:121:PRO:CA[3_555]	1.97	0.23
1:A:254:ILE:O	1:B:127:THR:O[2_555]	1.97	0.23
1:B:187:LEU:C	1:C:171:VAL:CG2[3_555]	1.98	0.22
1:B:119:TYR:CD2	1:C:133:MET:N[3_555]	1.98	0.22
1:B:73:GLU:O	1:C:160:PRO:CD[3_555]	1.98	0.22
1:A:254:ILE:CA	1:B:127:THR:C[2_555]	1.98	0.22
1:B:69:LEU:CD1	1:C:46:PRO:O[3_555]	1.98	0.22
1:B:89:GLU:CA	1:C:78:LEU:C[3_555]	1.98	0.22
1:B:244:ALA:O	1:C:163:GLU:CG[3_555]	1.98	0.22
1:B:112:TRP:N	1:C:51:THR:N[3_555]	1.98	0.22
1:B:73:GLU:O	1:C:160:PRO:O[3_555]	1.98	0.22
1:B:115:ILE:CG2	1:C:120:LEU:CD2[3_555]	1.98	0.22
1:B:115:ILE:CG1	1:C:121:PRO:N[3_555]	1.98	0.22
1:B:77:GLU:N	1:C:229:GLU:N[3_555]	1.98	0.22
1:B:100:LEU:N	1:C:124:PRO:C[3_555]	1.98	0.22
1:B:117:TYR:CD2	1:C:119:TYR:CD2[3_555]	1.98	0.22
1:B:119:TYR:CA	1:C:157:VAL:N[3_555]	1.98	0.22
1:B:242:LEU:CB	1:C:131:ILE:CA[3_555]	1.98	0.22
1:B:228:MET:CA	1:C:225:VAL:CG2[3_555]	1.98	0.22
1:B:72:CYS:CB	1:C:163:GLU:OE2[3_555]	1.98	0.22
1:B:81:THR:C	1:C:142:THR:CB[3_555]	1.98	0.22
1:B:170:PHE:O	1:C:181:ARG:CA[3_555]	1.98	0.22
1:B:229:GLU:OE2	1:C:223:ARG:N[3_555]	1.98	0.22
1:B:170:PHE:CB	1:C:180:SER:O[3_555]	1.98	0.22
1:B:89:GLU:CB	1:C:78:LEU:C[3_555]	1.99	0.21
1:B:244:ALA:CB	1:C:163:GLU:O[3_555]	1.99	0.21
1:C:85:VAL:CA	3:B:270:HOH:O[2_555]	1.99	0.21
1:B:153:LEU:CB	1:C:96:VAL:CG1[3_555]	1.99	0.21
1:B:100:LEU:CB	1:C:123:CYS:O[3_555]	1.99	0.21
1:C:59:MET:C	1:C:67:THR:OG1[2_555]	1.99	0.21
1:C:73:GLU:OE1	1:C:252:GLU:O[2_555]	1.99	0.21
1:B:73:GLU:CD	1:C:162:TRP:CG[3_555]	1.99	0.21
1:B:116:ARG:CG	1:C:182:ALA:C[3_555]	1.99	0.21
1:B:69:LEU:CD1	1:C:46:PRO:CB[3_555]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:VAL:N	1:C:240:GLY:C[3_555]	1.99	0.21
1:B:237:VAL:N	1:C:145:VAL:N[3_555]	1.99	0.21
1:A:254:ILE:O	1:B:127:THR:C[2_555]	1.99	0.21
1:B:99:TRP:O	1:C:126:THR:CB[3_555]	1.99	0.21
1:B:162:TRP:N	1:C:152:ASN:CA[3_555]	1.99	0.21
1:B:117:TYR:CZ	1:C:119:TYR:CZ[3_555]	1.99	0.21
1:C:99:TRP:CD1	1:C:107:TRP:CA[2_555]	1.99	0.21
1:B:170:PHE:CA	1:C:180:SER:C[3_555]	1.99	0.21
1:B:248:ILE:CA	1:C:49:GLN:CA[3_555]	1.99	0.21
1:B:80:VAL:CG2	1:C:144:PRO:CA[3_555]	1.99	0.21
1:B:246:TYR:O	1:C:49:GLN:CG[3_555]	1.99	0.21
1:B:183:ILE:O	1:C:157:VAL:CB[3_555]	1.99	0.21
1:B:71:HIS:C	1:C:162:TRP:CZ3[3_555]	1.99	0.21
1:B:95:THR:C	1:C:239:THR:N[3_555]	1.99	0.21
1:B:98:THR:C	1:C:126:THR:O[3_555]	1.99	0.21
1:A:255:ALA:CB	1:B:127:THR:CA[2_555]	1.99	0.21
1:B:148:ASN:CB	1:C:92:MET:CB[3_555]	1.99	0.21
1:B:89:GLU:N	1:C:78:LEU:N[3_555]	1.99	0.21
1:B:149:GLN:O	1:C:96:VAL:CA[3_555]	1.99	0.21
1:B:243:TYR:CE1	1:C:158:THR:OG1[3_555]	1.99	0.21
1:B:237:VAL:CG1	1:C:149:GLN:NE2[3_555]	1.99	0.21
1:C:58:PRO:CA	1:C:250:LEU:O[2_555]	2.00	0.20
1:B:85:VAL:CG1	1:C:143:LEU:CD1[3_555]	2.00	0.20
1:B:149:GLN:CD	1:C:95:THR:OG1[3_555]	2.00	0.20
1:B:222:ALA:CA	1:C:74:LEU:CD2[3_555]	2.00	0.20
1:B:153:LEU:CD1	1:C:96:VAL:O[3_555]	2.00	0.20
1:B:239:THR:C	1:C:150:LEU:CB[3_555]	2.00	0.20
1:B:135:PHE:N	1:C:75:SER:CB[3_555]	2.00	0.20
1:B:116:ARG:NH1	1:C:182:ALA:CB[3_555]	2.00	0.20
1:C:100:LEU:CA	1:C:106:ASN:O[2_555]	2.00	0.20
1:B:152:ASN:CG	1:C:93:PRO:N[3_555]	2.00	0.20
1:B:228:MET:O	1:C:143:LEU:CD1[3_555]	2.00	0.20
1:B:75:SER:C	1:C:130:ALA:C[3_555]	2.00	0.20
1:B:149:GLN:N	1:C:95:THR:CB[3_555]	2.00	0.20
1:B:132:HIS:CE1	1:C:223:ARG:C[3_555]	2.00	0.20
1:B:246:TYR:CD2	1:C:49:GLN:CB[3_555]	2.00	0.20
1:B:80:VAL:N	1:C:144:PRO:CG[3_555]	2.00	0.20
1:B:91:VAL:CB	1:C:241:ARG:N[3_555]	2.00	0.20
1:A:255:ALA:CA	1:B:127:THR:C[2_555]	2.00	0.20
1:B:187:LEU:CD2	1:C:120:LEU:CD1[3_555]	2.00	0.20
1:C:72:CYS:C	1:C:252:GLU:CB[2_555]	2.00	0.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:THR:CB	1:C:226:THR:CG2[3_555]	2.01	0.19
1:B:147:VAL:N	1:C:90:LEU:CD2[3_555]	2.01	0.19
1:B:118:THR:OG1	1:C:182:ALA:C[3_555]	2.01	0.19
1:B:93:PRO:O	1:C:123:CYS:N[3_555]	2.01	0.19
1:A:254:ILE:CB	1:B:128:SER:C[2_555]	2.01	0.19
1:B:227:ALA:CB	1:C:224:LEU:O[3_555]	2.01	0.19
1:B:86:VAL:CB	1:C:88:SER:O[3_555]	2.01	0.19
1:B:155:GLY:O	1:C:117:TYR:CA[3_555]	2.01	0.19
1:B:187:LEU:CD1	1:C:243:TYR:CD1[3_555]	2.01	0.19
1:B:121:PRO:N	1:C:156:TYR:CG[3_555]	2.01	0.19
1:A:258:LEU:C	1:B:232:SER:CA[2_555]	2.01	0.19
1:B:131:ILE:CG2	1:C:135:PHE:N[3_555]	2.01	0.19
1:C:101:ARG:CZ	1:C:258:LEU:CA[2_555]	2.01	0.19
1:C:101:ARG:NH2	1:C:258:LEU:CB[2_555]	2.01	0.19
1:C:60:LEU:C	1:C:62:SER:N[2_555]	2.01	0.19
1:B:243:TYR:CD1	1:C:158:THR:CG2[3_555]	2.01	0.19
1:B:137:TYR:CG	1:C:74:LEU:CB[3_555]	2.01	0.19
1:B:190:ASN:N	1:C:172:ASN:OD1[3_555]	2.01	0.19
1:B:227:ALA:CA	1:C:88:SER:C[3_555]	2.01	0.19
1:B:184:THR:N	3:C:267:HOH:O[3_555]	2.02	0.18
1:B:170:PHE:CZ	1:C:179:THR:O[3_555]	2.02	0.18
1:B:89:GLU:N	1:C:78:LEU:CA[3_555]	2.02	0.18
1:B:112:TRP:CA	1:C:51:THR:C[3_555]	2.02	0.18
1:B:146:SER:O	1:C:90:LEU:CB[3_555]	2.02	0.18
1:B:230:GLY:CA	1:C:136:GLN:OE1[3_555]	2.02	0.18
1:B:135:PHE:O	1:C:75:SER:N[3_555]	2.02	0.18
1:B:76:THR:C	1:C:130:ALA:O[3_555]	2.02	0.18
1:A:253:PRO:O	1:B:162:TRP:CD1[2_555]	2.02	0.18
1:B:99:TRP:CH2	1:C:46:PRO:O[3_555]	2.02	0.18
1:B:221:PRO:CG	1:C:241:ARG:NE[3_555]	2.02	0.18
1:B:238:ASN:N	1:C:149:GLN:NE2[3_555]	2.02	0.18
1:B:152:ASN:CG	1:C:93:PRO:CB[3_555]	2.02	0.18
1:A:258:LEU:C	1:B:231:GLY:C[2_555]	2.02	0.18
1:B:239:THR:C	1:C:150:LEU:C[3_555]	2.02	0.18
1:A:258:LEU:C	1:B:232:SER:CB[2_555]	2.02	0.18
1:C:57:PRO:C	1:C:250:LEU:O[2_555]	2.02	0.18
1:B:161:VAL:O	1:C:152:ASN:N[3_555]	2.02	0.18
1:B:101:ARG:CA	1:C:124:PRO:CG[3_555]	2.02	0.18
1:B:225:VAL:CG1	1:C:89:GLU:OE1[3_555]	2.02	0.18
1:B:229:GLU:C	1:C:136:GLN:CD[3_555]	2.02	0.18
1:B:152:ASN:N	1:C:96:VAL:CB[3_555]	2.02	0.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:THR:C	1:C:54:LYS:N[3_555]	2.02	0.18
1:B:236:ALA:CA	1:C:145:VAL:CG2[3_555]	2.02	0.18
1:B:80:VAL:CB	1:C:144:PRO:CG[3_555]	2.02	0.18
1:B:159:GLY:O	1:C:135:PHE:O[3_555]	2.02	0.18
1:B:72:CYS:O	1:C:162:TRP:CE2[3_555]	2.03	0.17
1:B:72:CYS:N	1:C:162:TRP:CH2[3_555]	2.03	0.17
1:B:150:LEU:C	1:C:96:VAL:CG2[3_555]	2.03	0.17
1:B:119:TYR:CG	1:C:157:VAL:N[3_555]	2.03	0.17
1:B:185:ILE:N	1:C:184:THR:CB[3_555]	2.03	0.17
1:B:115:ILE:CD1	1:C:120:LEU:CA[3_555]	2.03	0.17
1:B:159:GLY:O	1:C:135:PHE:CA[3_555]	2.03	0.17
1:B:96:VAL:C	1:C:161:VAL:O[3_555]	2.03	0.17
1:C:73:GLU:OE1	1:C:253:PRO:C[2_555]	2.03	0.17
1:B:98:THR:N	1:C:127:THR:CA[3_555]	2.03	0.17
1:C:99:TRP:CE2	1:C:107:TRP:CG[2_555]	2.03	0.17
1:B:136:GLN:CG	1:C:75:SER:O[3_555]	2.03	0.17
1:B:157:VAL:C	1:C:135:PHE:CE2[3_555]	2.03	0.17
1:B:135:PHE:O	1:C:74:LEU:O[3_555]	2.03	0.17
1:B:124:PRO:O	1:C:152:ASN:CG[3_555]	2.03	0.17
1:B:103:VAL:CG1	1:C:47:ILE:CB[3_555]	2.03	0.17
1:B:156:TYR:OH	1:C:91:VAL:CG2[3_555]	2.03	0.17
1:C:99:TRP:CD1	1:C:104:ALA:O[2_555]	2.03	0.17
1:A:106:ASN:ND2	1:B:126:THR:CA[2_555]	2.03	0.17
1:C:102:GLY:CA	1:C:256:ALA:CB[2_555]	2.03	0.17
1:C:60:LEU:CD1	1:C:67:THR:OG1[2_555]	2.03	0.17
1:B:190:ASN:CG	1:C:172:ASN:ND2[3_555]	2.03	0.17
1:B:154:LYS:NZ	1:C:245:SER:CB[3_555]	2.03	0.17
1:B:148:ASN:CA	1:C:92:MET:CG[3_555]	2.04	0.16
1:C:71:HIS:ND1	1:C:251:ILE:C[2_555]	2.04	0.16
1:A:106:ASN:CB	1:B:126:THR:CG2[2_555]	2.04	0.16
1:B:157:VAL:CG1	1:C:185:ILE:O[3_555]	2.04	0.16
1:B:95:THR:CB	1:C:238:ASN:O[3_555]	2.04	0.16
1:B:133:MET:CG	1:C:133:MET:SD[3_555]	2.04	0.16
1:B:76:THR:OG1	1:C:228:MET:CG[3_555]	2.04	0.16
1:B:245:SER:CB	1:C:163:GLU:CG[3_555]	2.04	0.16
1:B:249:ARG:N	1:C:50:GLY:CA[3_555]	2.04	0.16
1:B:225:VAL:CG2	1:C:75:SER:O[3_555]	2.04	0.16
1:B:238:ASN:O	1:C:146:SER:O[3_555]	2.04	0.16
1:B:190:ASN:CA	1:C:54:LYS:CG[3_555]	2.04	0.16
1:B:239:THR:O	1:C:151:SER:CA[3_555]	2.04	0.16
1:B:119:TYR:CB	1:C:157:VAL:C[3_555]	2.04	0.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:TYR:CE1	1:C:73:GLU:O[3_555]	2.04	0.16
1:B:161:VAL:CB	1:C:153:LEU:CB[3_555]	2.04	0.16
1:B:103:VAL:CA	1:C:47:ILE:CD1[3_555]	2.04	0.16
1:B:237:VAL:N	1:C:145:VAL:CB[3_555]	2.04	0.16
1:B:154:LYS:O	1:C:243:TYR:C[3_555]	2.04	0.16
1:B:241:ARG:CG	1:C:229:GLU:OE2[3_555]	2.04	0.16
1:B:241:ARG:N	1:C:132:HIS:CG[3_555]	2.04	0.16
1:B:222:ALA:CB	1:C:243:TYR:OH[3_555]	2.04	0.16
1:C:59:MET:N	1:C:67:THR:CA[2_555]	2.04	0.16
1:B:170:PHE:C	1:C:181:ARG:CB[3_555]	2.04	0.16
1:B:148:ASN:C	1:C:92:MET:N[3_555]	2.04	0.16
1:C:59:MET:CG	1:C:62:SER:O[2_555]	2.04	0.16
1:B:85:VAL:O	1:C:87:THR:C[3_555]	2.04	0.16
1:B:121:PRO:CA	1:C:151:SER:O[3_555]	2.04	0.16
1:A:254:ILE:C	1:B:127:THR:N[2_555]	2.04	0.16
1:B:98:THR:CA	1:C:127:THR:O[3_555]	2.04	0.16
1:B:152:ASN:OD1	1:C:93:PRO:CB[3_555]	2.04	0.16
1:B:71:HIS:O	1:C:163:GLU:OE1[3_555]	2.05	0.15
1:B:186:ALA:CB	1:C:167:GLY:CA[3_555]	2.05	0.15
1:C:59:MET:CA	1:C:66:VAL:C[2_555]	2.05	0.15
1:B:133:MET:O	1:C:117:TYR:CZ[3_555]	2.05	0.15
1:B:80:VAL:O	1:C:144:PRO:N[3_555]	2.05	0.15
1:B:134:GLY:C	1:C:75:SER:CB[3_555]	2.05	0.15
1:B:155:GLY:N	1:C:244:ALA:CA[3_555]	2.05	0.15
1:B:242:LEU:CG	1:C:131:ILE:CG1[3_555]	2.05	0.15
1:B:117:TYR:CB	1:C:183:ILE:CG2[3_555]	2.05	0.15
1:B:156:TYR:N	1:C:116:ARG:O[3_555]	2.05	0.15
1:B:246:TYR:OH	1:C:162:TRP:CB[3_555]	2.05	0.15
1:B:242:LEU:N	1:C:132:HIS:CG[3_555]	2.05	0.15
1:B:100:LEU:CD2	1:C:124:PRO:CA[3_555]	2.05	0.15
1:C:99:TRP:CD1	1:C:107:TRP:CB[2_555]	2.05	0.15
1:C:99:TRP:CD2	1:C:107:TRP:CD2[2_555]	2.05	0.15
1:C:101:ARG:NH2	1:C:257:ALA:C[2_555]	2.05	0.15
1:B:114:ALA:C	1:C:165:GLN:CB[3_555]	2.05	0.15
1:B:170:PHE:CB	1:C:182:ALA:N[3_555]	2.05	0.15
1:B:226:THR:OG1	1:C:226:THR:N[3_555]	2.05	0.15
1:B:77:GLU:O	1:C:228:MET:N[3_555]	2.05	0.15
1:B:244:ALA:C	1:C:163:GLU:CG[3_555]	2.05	0.15
1:B:191:GLU:CG	1:C:56:ARG:N[3_555]	2.05	0.15
1:B:112:TRP:CA	1:C:51:THR:O[3_555]	2.05	0.15
1:B:248:ILE:CA	1:C:50:GLY:CA[3_555]	2.06	0.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ALA:CB	1:B:127:THR:OG1[2_555]	2.06	0.14
1:B:183:ILE:CB	1:C:155:GLY:C[3_555]	2.06	0.14
1:B:134:GLY:N	1:C:117:TYR:CE2[3_555]	2.06	0.14
1:B:189:THR:C	1:C:172:ASN:ND2[3_555]	2.06	0.14
1:B:155:GLY:O	1:C:116:ARG:CA[3_555]	2.06	0.14
1:B:80:VAL:N	1:C:144:PRO:CB[3_555]	2.06	0.14
1:B:69:LEU:CG	1:C:47:ILE:N[3_555]	2.06	0.14
1:B:133:MET:C	1:C:117:TYR:CE2[3_555]	2.06	0.14
1:B:96:VAL:C	1:C:239:THR:CG2[3_555]	2.06	0.14
1:A:254:ILE:C	1:B:128:SER:N[2_555]	2.06	0.14
1:B:242:LEU:CB	1:C:131:ILE:CG1[3_555]	2.06	0.14
1:B:91:VAL:CG2	1:C:241:ARG:O[3_555]	2.06	0.14
1:B:237:VAL:C	1:C:149:GLN:CD[3_555]	2.06	0.14
1:B:192:VAL:CG2	1:C:53:VAL:N[3_555]	2.06	0.14
1:A:254:ILE:CG1	1:B:128:SER:N[2_555]	2.06	0.14
1:B:190:ASN:CA	1:C:54:LYS:N[3_555]	2.06	0.14
1:B:159:GLY:CA	1:C:154:LYS:CB[3_555]	2.06	0.14
1:B:93:PRO:CG	1:C:122:SER:C[3_555]	2.06	0.14
1:C:60:LEU:N	1:C:62:SER:CB[2_555]	2.07	0.13
1:B:98:THR:CG2	1:C:128:SER:N[3_555]	2.07	0.13
1:B:243:TYR:CD1	1:C:158:THR:CB[3_555]	2.07	0.13
1:B:130:ALA:N	1:C:136:GLN:CB[3_555]	2.07	0.13
1:C:98:THR:N	1:C:254:ILE:CG2[2_555]	2.07	0.13
1:B:170:PHE:CB	1:C:181:ARG:C[3_555]	2.07	0.13
1:C:101:ARG:CA	1:C:256:ALA:N[2_555]	2.07	0.13
1:B:96:VAL:CG2	1:C:119:TYR:OH[3_555]	2.07	0.13
1:B:244:ALA:C	1:C:163:GLU:CA[3_555]	2.07	0.13
1:B:246:TYR:CG	1:C:49:GLN:CD[3_555]	2.07	0.13
1:B:189:THR:O	1:C:52:MET:O[3_555]	2.07	0.13
1:C:60:LEU:CA	1:C:62:SER:CB[2_555]	2.07	0.13
1:B:86:VAL:CA	1:C:88:SER:N[3_555]	2.07	0.13
1:B:117:TYR:CE2	1:C:119:TYR:CA[3_555]	2.07	0.13
1:B:116:ARG:CA	1:C:164:GLY:O[3_555]	2.07	0.13
1:A:253:PRO:CB	1:B:162:TRP:CD2[2_555]	2.07	0.13
1:B:99:TRP:C	1:C:124:PRO:O[3_555]	2.07	0.13
1:B:192:VAL:N	1:C:53:VAL:C[3_555]	2.07	0.13
1:B:116:ARG:N	1:C:164:GLY:CA[3_555]	2.07	0.13
1:B:86:VAL:C	1:C:87:THR:OG1[3_555]	2.07	0.13
1:B:79:ALA:CB	1:C:144:PRO:C[3_555]	2.07	0.13
1:B:187:LEU:CB	1:C:120:LEU:CG[3_555]	2.07	0.13
1:B:224:LEU:N	1:C:76:THR:C[3_555]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:LEU:CD2	1:C:132:HIS:O[3_555]	2.07	0.13
1:B:136:GLN:CA	1:C:75:SER:N[3_555]	2.07	0.13
1:B:182:ALA:O	3:C:267:HOH:O[3_555]	2.08	0.12
1:B:157:VAL:C	1:C:135:PHE:CE1[3_555]	2.08	0.12
1:C:102:GLY:N	1:C:106:ASN:ND2[2_555]	2.08	0.12
1:B:99:TRP:CE2	1:C:125:THR:O[3_555]	2.08	0.12
1:B:248:ILE:CB	1:C:50:GLY:N[3_555]	2.08	0.12
1:B:184:THR:O	1:C:184:THR:CA[3_555]	2.08	0.12
1:B:187:LEU:O	1:C:168:LEU:O[3_555]	2.08	0.12
1:C:73:GLU:CB	1:C:252:GLU:O[2_555]	2.08	0.12
1:B:151:SER:C	1:C:112:TRP:CZ2[3_555]	2.08	0.12
1:B:225:VAL:CG1	1:C:89:GLU:CD[3_555]	2.08	0.12
1:C:60:LEU:N	1:C:67:THR:OG1[2_555]	2.08	0.12
1:B:229:GLU:OE2	1:C:136:GLN:O[3_555]	2.08	0.12
1:B:243:TYR:CD1	1:C:159:GLY:N[3_555]	2.08	0.12
1:C:97:GLY:C	1:C:254:ILE:C[2_555]	2.08	0.12
1:B:161:VAL:CB	1:C:153:LEU:CD2[3_555]	2.08	0.12
1:B:78:LEU:CD1	1:C:132:HIS:CB[3_555]	2.08	0.12
1:B:224:LEU:C	1:C:242:LEU:CD2[3_555]	2.08	0.12
1:B:159:GLY:C	1:C:154:LYS:CB[3_555]	2.08	0.12
1:B:229:GLU:O	1:C:136:GLN:CB[3_555]	2.08	0.12
1:B:98:THR:OG1	1:C:128:SER:CB[3_555]	2.08	0.12
1:B:117:TYR:CE2	1:C:119:TYR:C[3_555]	2.08	0.12
1:B:223:ARG:CB	1:C:76:THR:C[3_555]	2.08	0.12
1:C:101:ARG:N	1:C:254:ILE:C[2_555]	2.08	0.12
1:B:239:THR:CB	1:C:149:GLN:C[3_555]	2.08	0.12
1:C:246:TYR:CE2	1:C:253:PRO:CB[2_555]	2.08	0.12
1:C:65:ASP:O	1:C:70:SER:O[3_555]	2.08	0.12
1:B:228:MET:O	1:C:143:LEU:CG[3_555]	2.09	0.11
1:A:253:PRO:CD	1:B:162:TRP:NE1[2_555]	2.09	0.11
1:B:93:PRO:N	1:C:123:CYS:N[3_555]	2.09	0.11
1:B:95:THR:O	1:C:239:THR:CG2[3_555]	2.09	0.11
1:B:135:PHE:CA	1:C:75:SER:CB[3_555]	2.09	0.11
1:C:99:TRP:CB	1:C:108:SER:N[2_555]	2.09	0.11
1:B:183:ILE:CG1	1:C:155:GLY:O[3_555]	2.09	0.11
1:B:184:THR:N	1:C:185:ILE:N[3_555]	2.09	0.11
1:B:79:ALA:C	1:C:144:PRO:C[3_555]	2.09	0.11
1:B:149:GLN:OE1	1:C:95:THR:OG1[3_555]	2.09	0.11
1:B:87:THR:OG1	1:C:87:THR:N[3_555]	2.09	0.11
1:B:117:TYR:OH	1:C:119:TYR:CE2[3_555]	2.09	0.11
1:B:158:THR:CB	1:C:135:PHE:CE2[3_555]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:PRO:N	1:C:152:ASN:OD1[3_555]	2.09	0.11
1:B:242:LEU:N	1:C:132:HIS:CA[3_555]	2.09	0.11
1:B:246:TYR:CD1	1:C:163:GLU:N[3_555]	2.09	0.11
1:B:150:LEU:N	1:C:90:LEU:O[3_555]	2.09	0.11
1:B:96:VAL:O	1:C:161:VAL:O[3_555]	2.10	0.10
1:B:79:ALA:CB	1:C:144:PRO:O[3_555]	2.10	0.10
1:B:189:THR:OG1	1:C:168:LEU:CD2[3_555]	2.10	0.10
1:B:147:VAL:N	1:C:90:LEU:CD1[3_555]	2.10	0.10
1:B:241:ARG:N	1:C:156:TYR:OH[3_555]	2.10	0.10
1:C:101:ARG:CA	1:C:255:ALA:C[2_555]	2.10	0.10
1:B:132:HIS:N	1:C:225:VAL:N[3_555]	2.10	0.10
1:A:258:LEU:CA	1:B:232:SER:CA[2_555]	2.10	0.10
1:B:190:ASN:OD1	1:C:172:ASN:C[3_555]	2.10	0.10
1:B:224:LEU:CA	1:C:242:LEU:CD2[3_555]	2.10	0.10
1:B:229:GLU:CD	1:C:139:MET:CE[3_555]	2.10	0.10
1:B:92:MET:N	1:C:122:SER:CB[3_555]	2.10	0.10
1:B:90:LEU:CD1	1:C:77:GLU:CB[3_555]	2.10	0.10
1:B:93:PRO:CA	1:C:122:SER:CA[3_555]	2.10	0.10
1:B:133:MET:CG	1:C:224:LEU:CD1[3_555]	2.10	0.10
1:B:147:VAL:C	1:C:91:VAL:N[3_555]	2.10	0.10
1:B:184:THR:CB	1:C:184:THR:O[3_555]	2.10	0.10
1:B:237:VAL:CA	1:C:149:GLN:OE1[3_555]	2.10	0.10
1:B:152:ASN:ND2	1:C:93:PRO:CB[3_555]	2.10	0.10
1:B:188:ASP:OD2	1:C:171:VAL:CG1[3_555]	2.10	0.10
1:B:185:ILE:CA	1:C:118:THR:CB[3_555]	2.10	0.10
1:B:154:LYS:N	1:C:244:ALA:CB[3_555]	2.10	0.10
1:B:123:CYS:SG	1:C:152:ASN:N[3_555]	2.11	0.09
1:B:96:VAL:C	1:C:161:VAL:CG1[3_555]	2.11	0.09
1:B:134:GLY:O	1:C:75:SER:CB[3_555]	2.11	0.09
1:B:157:VAL:CG1	1:C:185:ILE:CA[3_555]	2.11	0.09
1:B:135:PHE:CD1	1:C:243:TYR:CA[3_555]	2.11	0.09
1:B:153:LEU:O	1:C:244:ALA:CB[3_555]	2.11	0.09
1:B:246:TYR:CD1	1:C:163:GLU:CA[3_555]	2.11	0.09
1:B:114:ALA:C	1:C:51:THR:CG2[3_555]	2.11	0.09
1:B:242:LEU:O	1:C:131:ILE:C[3_555]	2.11	0.09
1:B:95:THR:CG2	1:C:238:ASN:CB[3_555]	2.11	0.09
1:B:237:VAL:C	1:C:145:VAL:N[3_555]	2.11	0.09
1:B:133:MET:CE	1:C:133:MET:CE[3_555]	2.11	0.09
1:B:149:GLN:N	1:C:92:MET:CG[3_555]	2.11	0.09
1:B:90:LEU:CA	1:C:240:GLY:O[3_555]	2.11	0.09
1:B:119:TYR:CD1	1:C:157:VAL:N[3_555]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:THR:OG1	1:C:152:ASN:ND2[3_555]	2.11	0.09
1:A:253:PRO:CA	1:B:162:TRP:CD1[2_555]	2.11	0.09
1:B:151:SER:OG	1:C:92:MET:N[3_555]	2.11	0.09
1:B:87:THR:CG2	1:C:87:THR:CG2[3_555]	2.11	0.09
1:C:101:ARG:CB	1:C:255:ALA:O[2_555]	2.11	0.09
1:C:99:TRP:CG	1:C:107:TRP:O[2_555]	2.11	0.09
1:B:188:ASP:CA	1:C:171:VAL:CA[3_555]	2.11	0.09
1:C:101:ARG:CD	1:C:256:ALA:O[2_555]	2.11	0.09
1:C:60:LEU:C	1:C:62:SER:CB[2_555]	2.11	0.09
1:B:150:LEU:O	1:C:96:VAL:CG2[3_555]	2.11	0.09
1:B:239:THR:CA	1:C:150:LEU:CB[3_555]	2.11	0.09
1:B:184:THR:CB	1:C:184:THR:CA[3_555]	2.11	0.09
1:B:76:THR:CB	1:C:228:MET:CA[3_555]	2.11	0.09
1:B:190:ASN:N	1:C:54:LYS:N[3_555]	2.12	0.08
1:B:146:SER:CA	1:C:90:LEU:CG[3_555]	2.12	0.08
1:B:69:LEU:CG	1:C:46:PRO:CG[3_555]	2.12	0.08
1:C:71:HIS:NE2	1:C:251:ILE:N[2_555]	2.12	0.08
1:B:156:TYR:CA	1:C:115:ILE:CG1[3_555]	2.12	0.08
1:B:185:ILE:O	1:C:183:ILE:O[3_555]	2.12	0.08
1:B:91:VAL:CA	1:C:241:ARG:N[3_555]	2.12	0.08
1:B:147:VAL:CG1	1:C:223:ARG:CA[3_555]	2.12	0.08
1:B:246:TYR:CZ	1:C:162:TRP:CE3[3_555]	2.12	0.08
1:B:242:LEU:O	1:C:159:GLY:O[3_555]	2.12	0.08
1:B:132:HIS:ND1	1:C:223:ARG:C[3_555]	2.12	0.08
1:B:112:TRP:C	1:C:50:GLY:C[3_555]	2.12	0.08
1:C:102:GLY:CA	1:C:106:ASN:ND2[2_555]	2.12	0.08
1:B:121:PRO:CB	1:C:151:SER:C[3_555]	2.12	0.08
1:A:255:ALA:C	1:B:126:THR:O[2_555]	2.12	0.08
1:B:189:THR:C	1:C:172:ASN:OD1[3_555]	2.12	0.08
1:B:119:TYR:O	1:C:157:VAL:N[3_555]	2.12	0.08
1:C:99:TRP:CH2	1:C:107:TRP:CG[2_555]	2.12	0.08
1:B:156:TYR:CD1	1:C:115:ILE:CG1[3_555]	2.12	0.08
1:B:154:LYS:C	1:C:244:ALA:CB[3_555]	2.12	0.08
1:B:228:MET:CB	1:C:225:VAL:CG1[3_555]	2.12	0.08
1:C:99:TRP:CH2	1:C:107:TRP:CZ3[2_555]	2.12	0.08
1:B:188:ASP:N	1:C:171:VAL:CA[3_555]	2.12	0.08
1:B:117:TYR:C	1:C:183:ILE:O[3_555]	2.12	0.08
1:B:116:ARG:NH2	1:C:170:PHE:CE1[3_555]	2.12	0.08
1:B:155:GLY:CA	1:C:245:SER:OG[3_555]	2.12	0.08
1:B:135:PHE:CA	1:C:242:LEU:O[3_555]	2.12	0.08
1:B:119:TYR:CE1	1:C:156:TYR:CB[3_555]	2.12	0.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:SER:OG	1:C:77:GLU:O[3_555]	2.12	0.08
1:C:57:PRO:N	1:C:249:ARG:CZ[2_555]	2.12	0.08
1:B:113:VAL:C	1:C:51:THR:CG2[3_555]	2.12	0.08
1:B:77:GLU:OE2	1:C:229:GLU:CB[3_555]	2.12	0.08
1:B:156:TYR:O	1:C:116:ARG:CA[3_555]	2.12	0.08
1:B:89:GLU:CD	1:C:79:ALA:O[3_555]	2.12	0.08
1:B:228:MET:CG	1:C:226:THR:N[3_555]	2.12	0.08
1:B:73:GLU:CG	1:C:162:TRP:NE1[3_555]	2.12	0.08
1:B:101:ARG:NH2	1:C:237:VAL:CG1[3_555]	2.12	0.08
1:B:158:THR:OG1	1:C:135:PHE:CE2[3_555]	2.13	0.07
1:B:170:PHE:CE2	1:C:180:SER:N[3_555]	2.13	0.07
1:B:243:TYR:CB	1:C:158:THR:C[3_555]	2.13	0.07
1:C:71:HIS:CB	1:C:253:PRO:CD[2_555]	2.13	0.07
1:B:151:SER:N	1:C:96:VAL:CG2[3_555]	2.13	0.07
1:B:187:LEU:O	1:C:171:VAL:CB[3_555]	2.13	0.07
1:C:101:ARG:CG	1:C:256:ALA:C[2_555]	2.13	0.07
1:B:86:VAL:N	1:C:88:SER:N[3_555]	2.13	0.07
1:B:246:TYR:N	1:C:49:GLN:CD[3_555]	2.13	0.07
1:B:160:PRO:CG	1:C:154:LYS:CA[3_555]	2.13	0.07
1:B:86:VAL:CA	1:C:88:SER:O[3_555]	2.13	0.07
1:C:99:TRP:CA	1:C:254:ILE:CG2[2_555]	2.13	0.07
1:B:100:LEU:C	1:C:124:PRO:CB[3_555]	2.13	0.07
1:C:71:HIS:CE1	1:C:251:ILE:CB[2_555]	2.13	0.07
1:B:74:LEU:O	1:C:130:ALA:N[3_555]	2.13	0.07
1:B:156:TYR:CD2	1:C:117:TYR:OH[3_555]	2.13	0.07
1:B:224:LEU:CB	1:C:242:LEU:N[3_555]	2.13	0.07
1:A:254:ILE:N	1:B:127:THR:O[2_555]	2.13	0.07
1:B:77:GLU:CD	1:C:229:GLU:CG[3_555]	2.13	0.07
1:B:137:TYR:CD1	1:C:73:GLU:C[3_555]	2.13	0.07
1:B:225:VAL:CA	1:C:76:THR:CB[3_555]	2.13	0.07
1:B:115:ILE:CA	1:C:164:GLY:O[3_555]	2.13	0.07
1:C:99:TRP:CZ2	1:C:250:LEU:CD2[2_555]	2.13	0.07
1:B:80:VAL:CB	1:C:143:LEU:C[3_555]	2.13	0.07
1:B:151:SER:OG	1:C:92:MET:CA[3_555]	2.13	0.07
1:B:248:ILE:CB	1:C:48:ALA:C[3_555]	2.13	0.07
1:C:94:PHE:CA	1:C:255:ALA:CB[2_555]	2.14	0.06
1:B:92:MET:O	1:C:239:THR:C[3_555]	2.14	0.06
1:B:70:SER:O	1:C:46:PRO:CG[3_555]	2.14	0.06
1:B:134:GLY:O	1:C:242:LEU:CD2[3_555]	2.14	0.06
1:B:152:ASN:ND2	1:C:93:PRO:CD[3_555]	2.14	0.06
1:B:191:GLU:CD	1:C:55:LEU:O[3_555]	2.14	0.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:THR:C	1:C:127:THR:O[3_555]	2.14	0.06
1:B:74:LEU:O	1:C:130:ALA:CA[3_555]	2.14	0.06
1:B:154:LYS:CB	1:C:244:ALA:C[3_555]	2.14	0.06
1:B:73:GLU:O	1:C:160:PRO:CB[3_555]	2.14	0.06
1:B:244:ALA:N	1:C:183:ILE:CD1[3_555]	2.14	0.06
1:B:185:ILE:CA	1:C:184:THR:OG1[3_555]	2.14	0.06
1:B:224:LEU:CB	1:C:242:LEU:CB[3_555]	2.14	0.06
1:C:56:ARG:C	1:C:251:ILE:CG1[2_555]	2.14	0.06
1:C:73:GLU:OE2	1:C:253:PRO:O[2_555]	2.14	0.06
1:B:230:GLY:O	1:C:141:ASP:OD1[3_555]	2.14	0.06
1:B:224:LEU:CA	1:C:242:LEU:N[3_555]	2.14	0.06
1:B:239:THR:CB	1:C:150:LEU:CB[3_555]	2.14	0.06
1:C:59:MET:O	1:C:62:SER:OG[2_555]	2.15	0.05
1:B:229:GLU:N	1:C:223:ARG:CD[3_555]	2.15	0.05
1:B:170:PHE:N	1:C:180:SER:C[3_555]	2.15	0.05
1:C:73:GLU:OE1	1:C:254:ILE:CB[2_555]	2.15	0.05
1:B:192:VAL:CG2	1:C:53:VAL:C[3_555]	2.15	0.05
1:B:236:ALA:C	1:C:145:VAL:CG1[3_555]	2.15	0.05
1:B:242:LEU:CB	1:C:131:ILE:O[3_555]	2.15	0.05
1:B:72:CYS:N	1:C:163:GLU:OE2[3_555]	2.15	0.05
1:B:115:ILE:N	1:C:165:GLN:CA[3_555]	2.15	0.05
1:B:119:TYR:N	1:C:158:THR:N[3_555]	2.15	0.05
1:B:246:TYR:OH	1:C:125:THR:CG2[3_555]	2.15	0.05
1:C:99:TRP:CZ3	1:C:107:TRP:CZ2[2_555]	2.15	0.05
1:B:112:TRP:CB	1:C:51:THR:CA[3_555]	2.15	0.05
1:B:157:VAL:CG2	1:C:117:TYR:N[3_555]	2.15	0.05
1:B:157:VAL:CG2	1:C:185:ILE:C[3_555]	2.15	0.05
1:B:96:VAL:O	1:C:161:VAL:C[3_555]	2.15	0.05
1:B:137:TYR:CD2	1:C:243:TYR:CE2[3_555]	2.15	0.05
1:B:149:GLN:O	1:C:92:MET:O[3_555]	2.15	0.05
1:B:247:THR:C	1:C:165:GLN:NE2[3_555]	2.15	0.05
1:B:181:ARG:NH1	3:A:272:HOH:O[3_555]	2.15	0.05
1:B:96:VAL:CG2	1:C:240:GLY:CA[3_555]	2.15	0.05
1:B:185:ILE:N	1:C:184:THR:N[3_555]	2.15	0.05
1:B:240:GLY:C	1:C:132:HIS:ND1[3_555]	2.15	0.05
1:B:237:VAL:CA	1:C:145:VAL:CG2[3_555]	2.15	0.05
1:B:75:SER:N	1:C:130:ALA:C[3_555]	2.15	0.05
1:B:191:GLU:OE1	1:C:55:LEU:CA[3_555]	2.15	0.05
1:B:79:ALA:CB	1:C:145:VAL:C[3_555]	2.15	0.05
1:C:59:MET:C	1:C:62:SER:CA[2_555]	2.15	0.05
1:B:162:TRP:CA	1:C:152:ASN:N[3_555]	2.15	0.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:TYR:CD2	1:C:119:TYR:C[3_555]	2.15	0.05
1:B:112:TRP:CD2	1:C:121:PRO:O[3_555]	2.15	0.05
1:B:112:TRP:CA	1:C:51:THR:OG1[3_555]	2.15	0.05
1:B:152:ASN:CA	1:C:96:VAL:CB[3_555]	2.15	0.05
1:B:90:LEU:CD1	1:C:77:GLU:CG[3_555]	2.16	0.04
1:B:136:GLN:C	1:C:74:LEU:C[3_555]	2.16	0.04
1:B:240:GLY:N	1:C:147:VAL:O[3_555]	2.16	0.04
1:B:80:VAL:CG2	1:C:144:PRO:CG[3_555]	2.16	0.04
1:C:72:CYS:O	1:C:252:GLU:CA[2_555]	2.16	0.04
1:C:97:GLY:O	1:C:254:ILE:CB[2_555]	2.16	0.04
1:B:154:LYS:O	1:C:244:ALA:O[3_555]	2.16	0.04
1:A:255:ALA:N	1:B:127:THR:N[2_555]	2.16	0.04
1:B:224:LEU:N	1:C:242:LEU:N[3_555]	2.16	0.04
1:B:152:ASN:ND2	1:C:92:MET:C[3_555]	2.16	0.04
1:B:192:VAL:CG2	1:C:53:VAL:O[3_555]	2.16	0.04
1:B:157:VAL:N	1:C:117:TYR:CD1[3_555]	2.16	0.04
1:B:96:VAL:O	1:C:239:THR:CG2[3_555]	2.16	0.04
1:B:75:SER:CA	1:C:161:VAL:CG2[3_555]	2.16	0.04
1:C:72:CYS:O	1:C:252:GLU:CG[2_555]	2.16	0.04
1:C:94:PHE:CE1	1:C:257:ALA:CB[2_555]	2.16	0.04
1:C:101:ARG:NH2	1:C:258:LEU:CD2[2_555]	2.16	0.04
1:B:227:ALA:CB	1:C:88:SER:C[3_555]	2.16	0.04
1:B:224:LEU:CG	1:C:242:LEU:CG[3_555]	2.16	0.04
1:B:74:LEU:CD2	1:C:130:ALA:N[3_555]	2.16	0.04
1:B:81:THR:CA	1:C:142:THR:C[3_555]	2.16	0.04
1:B:223:ARG:O	1:C:74:LEU:CD1[3_555]	2.16	0.04
1:B:243:TYR:C	1:C:159:GLY:CA[3_555]	2.16	0.04
1:B:103:VAL:CG2	1:C:47:ILE:CD1[3_555]	2.17	0.03
1:C:99:TRP:CD1	1:C:107:TRP:C[2_555]	2.17	0.03
1:B:111:ALA:O	1:C:50:GLY:C[3_555]	2.17	0.03
1:B:229:GLU:CB	1:C:223:ARG:NH1[3_555]	2.17	0.03
1:B:250:LEU:CD2	1:C:48:ALA:CB[3_555]	2.17	0.03
1:B:191:GLU:CB	1:C:55:LEU:CD2[3_555]	2.17	0.03
1:B:244:ALA:C	1:C:163:GLU:C[3_555]	2.17	0.03
1:C:57:PRO:C	1:C:66:VAL:CA[2_555]	2.17	0.03
1:B:69:LEU:CB	1:C:48:ALA:O[3_555]	2.17	0.03
1:B:228:MET:N	1:C:88:SER:CA[3_555]	2.17	0.03
1:B:148:ASN:C	1:C:92:MET:C[3_555]	2.17	0.03
1:B:96:VAL:N	1:C:239:THR:CB[3_555]	2.17	0.03
1:B:74:LEU:N	1:C:160:PRO:CB[3_555]	2.17	0.03
1:B:99:TRP:C	1:C:126:THR:C[3_555]	2.17	0.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:ASN:ND2	1:C:145:VAL:C[3_555]	2.17	0.03
1:C:55:LEU:CD2	1:C:252:GLU:OE2[2_555]	2.17	0.03
1:B:76:THR:OG1	1:C:228:MET:C[3_555]	2.17	0.03
1:B:73:GLU:C	1:C:160:PRO:CG[3_555]	2.17	0.03
1:B:114:ALA:CA	1:C:165:GLN:O[3_555]	2.17	0.03
1:B:96:VAL:O	1:C:161:VAL:CG1[3_555]	2.17	0.03
1:B:130:ALA:C	1:C:135:PHE:C[3_555]	2.17	0.03
1:B:115:ILE:C	1:C:164:GLY:C[3_555]	2.17	0.03
1:B:185:ILE:N	1:C:184:THR:C[3_555]	2.17	0.03
1:B:239:THR:CG2	1:C:144:PRO:CB[3_555]	2.17	0.03
1:B:92:MET:C	1:C:239:THR:O[3_555]	2.17	0.03
1:B:186:ALA:N	1:C:118:THR:CA[3_555]	2.17	0.03
1:B:77:GLU:C	1:C:227:ALA:CB[3_555]	2.17	0.03
1:C:99:TRP:NE1	1:C:107:TRP:CB[2_555]	2.18	0.02
1:B:130:ALA:CA	1:C:136:GLN:CA[3_555]	2.18	0.02
1:B:117:TYR:N	1:C:183:ILE:CB[3_555]	2.18	0.02
1:B:245:SER:N	1:C:163:GLU:CA[3_555]	2.18	0.02
1:B:90:LEU:O	1:C:240:GLY:CA[3_555]	2.18	0.02
1:B:116:ARG:NE	1:C:182:ALA:CA[3_555]	2.18	0.02
1:B:189:THR:C	1:C:53:VAL:C[3_555]	2.18	0.02
1:B:79:ALA:CA	1:C:144:PRO:O[3_555]	2.18	0.02
1:B:185:ILE:N	1:C:184:THR:OG1[3_555]	2.18	0.02
1:B:154:LYS:CG	1:C:72:CYS:C[3_555]	2.18	0.02
1:B:184:THR:C	1:C:184:THR:O[3_555]	2.18	0.02
1:B:239:THR:O	1:C:150:LEU:C[3_555]	2.18	0.02
1:B:237:VAL:CG1	1:C:149:GLN:CB[3_555]	2.18	0.02
1:B:96:VAL:CG2	1:C:240:GLY:N[3_555]	2.18	0.02
1:B:80:VAL:N	1:C:144:PRO:CD[3_555]	2.18	0.02
1:B:228:MET:CG	1:C:225:VAL:CA[3_555]	2.18	0.02
1:B:153:LEU:CD1	1:C:96:VAL:CA[3_555]	2.18	0.02
1:B:152:ASN:CG	1:C:93:PRO:O[3_555]	2.18	0.02
1:B:137:TYR:CZ	1:C:73:GLU:C[3_555]	2.18	0.02
1:B:135:PHE:C	1:C:74:LEU:O[3_555]	2.18	0.02
1:B:184:THR:CA	1:C:185:ILE:N[3_555]	2.18	0.02
1:B:93:PRO:CD	1:C:122:SER:OG[3_555]	2.18	0.02
1:B:96:VAL:N	1:C:123:CYS:SG[3_555]	2.18	0.02
1:B:89:GLU:O	1:C:77:GLU:CA[3_555]	2.18	0.02
1:B:154:LYS:C	1:C:244:ALA:N[3_555]	2.18	0.02
1:B:71:HIS:N	1:C:49:GLN:OE1[3_555]	2.18	0.02
1:B:161:VAL:CG2	1:C:153:LEU:CG[3_555]	2.18	0.02
1:B:147:VAL:O	1:C:91:VAL:C[3_555]	2.18	0.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ILE:CD1	1:C:117:TYR:C[3_555]	2.18	0.02
1:B:224:LEU:CG	1:C:242:LEU:CB[3_555]	2.18	0.02
1:B:146:SER:O	1:C:95:THR:CG2[3_555]	2.18	0.02
1:B:247:THR:CG2	1:C:165:GLN:NE2[3_555]	2.18	0.02
1:B:79:ALA:O	1:C:144:PRO:O[3_555]	2.19	0.01
1:B:246:TYR:N	1:C:49:GLN:OE1[3_555]	2.19	0.01
1:B:136:GLN:C	1:C:74:LEU:O[3_555]	2.19	0.01
1:B:137:TYR:CZ	1:C:243:TYR:CD2[3_555]	2.19	0.01
1:B:115:ILE:CB	1:C:121:PRO:CD[3_555]	2.19	0.01
1:B:188:ASP:OD1	1:C:55:LEU:CG[3_555]	2.19	0.01
1:B:190:ASN:CB	1:C:172:ASN:ND2[3_555]	2.19	0.01
1:B:246:TYR:N	1:C:164:GLY:N[3_555]	2.19	0.01
1:C:103:VAL:CB	1:C:106:ASN:CB[2_555]	2.19	0.01
1:B:118:THR:OG1	1:C:183:ILE:N[3_555]	2.19	0.01
1:B:80:VAL:O	1:C:144:PRO:CA[3_555]	2.19	0.01
1:B:237:VAL:N	1:C:149:GLN:NE2[3_555]	2.19	0.01
1:B:135:PHE:CB	1:C:242:LEU:O[3_555]	2.19	0.01
1:B:132:HIS:N	1:C:224:LEU:CG[3_555]	2.19	0.01
1:B:170:PHE:CD2	1:C:180:SER:CA[3_555]	2.19	0.01
1:B:71:HIS:O	1:C:163:GLU:OE2[3_555]	2.19	0.01
1:B:116:ARG:CG	1:C:182:ALA:CA[3_555]	2.19	0.01
1:A:254:ILE:CB	1:B:127:THR:O[2_555]	2.19	0.01
1:C:98:THR:N	1:C:254:ILE:CA[2_555]	2.19	0.01
1:B:161:VAL:C	1:C:153:LEU:CB[3_555]	2.19	0.01
1:B:248:ILE:CG1	1:C:49:GLN:C[3_555]	2.19	0.01
1:B:191:GLU:OE1	1:C:56:ARG:CA[3_555]	2.19	0.01
1:B:243:TYR:CG	1:C:158:THR:C[3_555]	2.19	0.01
1:B:162:TRP:CA	1:C:152:ASN:CB[3_555]	2.19	0.01
1:B:121:PRO:CA	1:C:156:TYR:CD1[3_555]	2.19	0.01
1:C:58:PRO:N	1:C:250:LEU:C[2_555]	2.19	0.01
1:B:224:LEU:CG	1:C:242:LEU:CD1[3_555]	2.19	0.01
1:B:248:ILE:CG2	1:C:48:ALA:CA[3_555]	2.19	0.01
1:B:93:PRO:C	1:C:122:SER:C[3_555]	2.19	0.01
1:C:101:ARG:NE	1:C:255:ALA:O[2_555]	2.19	0.01
1:B:117:TYR:CE2	1:C:119:TYR:CB[3_555]	2.19	0.01
1:B:151:SER:CB	1:C:91:VAL:CG1[3_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	A	197/260 (76%)	160 (81%)	27 (14%)	10 (5%)	2	6
1	B	197/260 (76%)	163 (83%)	29 (15%)	5 (2%)	5	19
1	C	220/260 (85%)	182 (83%)	29 (13%)	9 (4%)	3	9
All	All	614/780 (79%)	505 (82%)	85 (14%)	24 (4%)	3	10

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	THR
1	B	231	GLY
1	C	219	LEU
1	C	230	GLY
1	C	231	GLY
1	A	161	VAL
1	A	166	SER
1	A	169	CYS
1	B	210	GLY
1	C	177	PRO
1	A	139	MET
1	A	202	ALA
1	B	173	ASN
1	A	94	PHE
1	A	182	ALA
1	B	213	ALA
1	B	256	ALA
1	C	125	THR
1	C	205	TYR
1	C	257	ALA
1	C	173	ASN
1	C	251	ILE
1	A	177	PRO
1	A	230	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	167/217 (77%)	121 (72%)	46 (28%)	0	1
1	B	167/217 (77%)	116 (70%)	51 (30%)	0	1
1	C	185/217 (85%)	128 (69%)	57 (31%)	0	0
All	All	519/651 (80%)	365 (70%)	154 (30%)	0	1

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	MET
1	A	65	ASP
1	A	77	GLU
1	A	78	LEU
1	A	80	VAL
1	A	87	THR
1	A	91	VAL
1	A	92	MET
1	A	95	THR
1	A	100	LEU
1	A	101	ARG
1	A	108	SER
1	A	109	LYS
1	A	116	ARG
1	A	118	THR
1	A	119	TYR
1	A	123	CYS
1	A	133	MET
1	A	139	MET
1	A	145	VAL
1	A	146	SER
1	A	148	ASN
1	A	152	ASN
1	A	154	LYS
1	A	158	THR
1	A	165	GLN

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Mol	Chain	Res	Type
1	A	168	LEU
1	A	172	ASN
1	A	173	ASN
1	A	176	CYS
1	A	181	ARG
1	A	183	ILE
1	A	184	THR
1	A	191	GLU
1	A	196	ARG
1	A	198	PRO
1	A	199	PHE
1	A	200	LYS
1	A	214	ASN
1	A	218	ILE
1	A	223	ARG
1	A	225	VAL
1	A	226	THR
1	A	234	LYS
1	A	245	SER
1	A	251	ILE
1	B	62	SER
1	B	72	CYS
1	B	74	LEU
1	B	78	LEU
1	B	82	VAL
1	B	85	VAL
1	B	87	THR
1	B	88	SER
1	B	90	LEU
1	B	95	THR
1	B	100	LEU
1	B	105	GLN
1	B	106	ASN
1	B	108	SER
1	B	109	LYS
1	B	115	ILE
1	B	116	ARG
1	B	118	THR
1	B	138	ASP
1	B	139	MET
1	B	147	VAL
1	B	150	LEU

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Mol	Chain	Res	Type
1	B	152	ASN
1	B	153	LEU
1	B	154	LYS
1	B	158	THR
1	B	161	VAL
1	B	165	GLN
1	B	171	VAL
1	B	172	ASN
1	B	173	ASN
1	B	175	LYS
1	B	176	CYS
1	B	180	SER
1	B	189	THR
1	B	190	ASN
1	B	196	ARG
1	B	199	PHE
1	B	200	LYS
1	B	203	THR
1	B	209	VAL
1	B	218	ILE
1	B	223	ARG
1	B	226	THR
1	B	234	LYS
1	B	235	THR
1	B	242	LEU
1	B	248	ILE
1	B	250	LEU
1	B	251	ILE
1	B	252	GLU
1	C	47	ILE
1	C	52	MET
1	C	54	LYS
1	C	60	LEU
1	C	61	ARG
1	C	65	ASP
1	C	66	VAL
1	C	67	THR
1	C	70	SER
1	C	72	CYS
1	C	74	LEU
1	C	78	LEU
1	C	80	VAL

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Mol	Chain	Res	Type
1	C	82	VAL
1	C	83	THR
1	C	84	ILE
1	C	87	THR
1	C	88	SER
1	C	92	MET
1	C	98	THR
1	C	115	ILE
1	C	118	THR
1	C	121	PRO
1	C	122	SER
1	C	125	THR
1	C	127	THR
1	C	128	SER
1	C	145	VAL
1	C	146	SER
1	C	149	GLN
1	C	150	LEU
1	C	152	ASN
1	C	153	LEU
1	C	161	VAL
1	C	165	GLN
1	C	172	ASN
1	C	173	ASN
1	C	174	THR
1	C	178	ASP
1	C	181	ARG
1	C	184	THR
1	C	187	LEU
1	C	189	THR
1	C	191	GLU
1	C	193	SER
1	C	195	LYS
1	C	196	ARG
1	C	200	LYS
1	C	203	THR
1	C	214	ASN
1	C	228	MET
1	C	234	LYS
1	C	235	THR
1	C	242	LEU
1	C	245	SER

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Mol	Chain	Res	Type
1	C	249	ARG
1	C	251	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	136	GLN
1	A	148	ASN
1	A	165	GLN
1	A	172	ASN
1	A	173	ASN
1	A	190	ASN
1	A	214	ASN
1	A	238	ASN
1	B	106	ASN
1	B	136	GLN
1	B	152	ASN
1	B	165	GLN
1	B	172	ASN
1	B	173	ASN
1	B	190	ASN
1	B	212	ASN
1	B	214	ASN
1	B	217	ASN
1	B	238	ASN
1	C	49	GLN
1	C	149	GLN
1	C	172	ASN
1	C	173	ASN
1	C	212	ASN
1	C	217	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

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.