



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:46 AM GMT

PDB ID : 2TBV
Title : STRUCTURE OF TOMATO BUSHY STUNT VIRUS. V. COAT PROTEIN SEQUENCE DETERMINATION AND ITS STRUCTURAL IMPLICATIONS
Authors : Harrison, S.C.
Deposited on : 1984-06-22
Resolution : 2.90 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

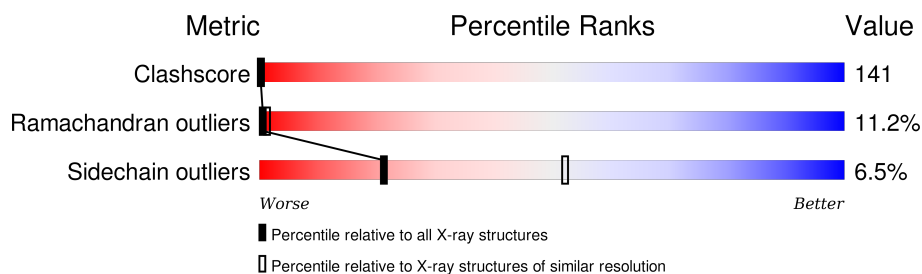
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	387	
1	B	387	
1	C	387	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6648 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 TOMATO BUSHY STUNT VIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	3	1
			2136	1351	360	420	5			
1	B	287	Total	C	N	O	S	0	2	1
			2130	1348	359	418	5			
1	C	321	Total	C	N	O	S	0	3	0
			2376	1502	406	462	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	GLY	SER	CONFLICT	UNP P11795
A	107	SER	GLY	CONFLICT	UNP P11795
B	102	GLY	SER	CONFLICT	UNP P11795
B	107	SER	GLY	CONFLICT	UNP P11795
C	102	GLY	SER	CONFLICT	UNP P11795
C	107	SER	GLY	CONFLICT	UNP P11795

- 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	3	Total	Ca	0	0
			3	3		
2	C	2	Total	Ca	0	0
			2	2		

Note EDS was not executed.

- Molecule 1: TOMATO BUSHY STUNT VIRUS

T365	H304	Y244	K182	F121	LVS	ALA
G366	T305	G245	D183	F122	GLN	MET
S367		G246	S184	V123	GLY	THR
G368	A308	A247	Q185	N124	ASN	THR
G369	T309	G248	D186	G125	GLN	ARG
A370	G310	A249	P187	G126	GLN	ASN
A371	T311	D250	E188	I127	ILE	ASN
L373	F312	A251	P189	V128	ILE	ASN
L374	G313	V252	A190	G129	THR	THR
L375	L314	G253	D191	N130	HIS	VAL
G376	S315	E254	R192	S131	VAL	LEU
G377	G316	L255	V193	L132	GLY	LEU
R378	L318	F256	E194	Q133	GLY	VAL
A379	R319	A258	L195	L134	VAL	SER
R380	G320	R259	A196	N135	GLY	LYS
A381	L321	S260		P136	GLY	LYS
N382	T322	V261	V200	S137	SER	GLN
G383	S323	T262	L201	N138	ILE	LEU
N385	L324	L263	K202	G139	MET	GLY
L386	T325	Y264	E203	T140	ALA	VAL
L387	L326	G265	T204	L141	PRO	LEU
	G327	P266	A205	F142	VAL	ALA
	A328	Q267	P206	S143	ALA	ALA
	T329	P268	W207	W144	VAL	SER
	G330	T269	E209	L145	SER	ALA
	A331	N270	A146	P147	ARG	ALA
	G332	T271	A210	A147	GLN	VAL
	V333	L272	L211		LEU	GLY
	V334	L273	M121		VAL	ALA
	L334	L274	R213	S150	GLY	LEU
	N335	S274	L214	N151	SER	ARG
	D336	S275	P215	F152	LVS	ASN
	L337	K276	T216	D153	PRO	TYR
	L338	R277	T217	Q154	LVS	TYR
	A339	L278	K218	Y155	PHE	GLY
	L340	D279	V219	S156	THR	GLY
	D341	L280	R220	F157	GLY	SER
	N342	T281	R221	N158	ARG	SER
	G343	G282	Y222	S159	THR	PRO
	G344	S283	G223	V160	SER	ALA
	T345	L284	G224	V161	SER	ALA
	A346	A285	R225	L162	LEU	LEU
	S347	D286	S226	D163	LEU	LEU
	D348	A287	A227	Y164	GLN	GLN
	G349	T288	T228	V165	SER	SER
	F350	G289	V229	P166	ALA	ALA
	L351	P290	G229	L167	VAL	VAL
	N352	G291	D230	C168	GLY	GLY
	G353	Y292	Q231	C169	LEU	LEU
	T354	L293	K232	T170	GLY	GLY
	V355	G294	L233	T171	LVS	LVS
	S356	L295	G235	E172	LYS	LYS
	S357	T296	D236	V173	ALA	ALA
	L358	R297	L236	G174	LEU	LEU
	G359	T298	G237	R175	ASN	ASN
	A360	P299	Q238	V176	LVS	LVS
	T361	T300	L239	A177	VAL	VAL
	V362	V301	G240	N178	ARG	ARG
	T363	L302	I241	L179	ASN	ASN
	T364	T202	K242	F180	ARG	ARG
			T243	T181	ARG	ARG

- Molecule 1: TOMATO BUSHY STUNT VIRUS

F121	F122	N123	N124	G125	G126	I127	V128	G129	N130	S131	L132	Q133	L134	N135	P136	S137	N138	G139	T140	L141	F142	S143	W144	L145	P146	A147	L148	A149	S150	M151	F152	D153	Q154	Y155	S156	F157	N158	S159	V160	V161	L162	D163	Y164	V165	P166	L167	C168	G169	T170	T171	E172	V173	G174	R175	V176	A177	L178	Y179	A180
ALA	THR	THR	ASN	GLN	GLN	ILE	ILE	THR	HIS	VAL	GLY	GLY	VAL	GLY	GLY	SER	ILE	MET	ALA	PRO	VAL	ALA	VAL	SER	ALA	ARG	GLN	LEU	VAL	GLY	SER	LYS	PRO	LYS	PHE	THR	GLY	ARG	SER	PRO	ALA	LEU	LEU	GLN	GLN	ALA	VAL	GLY	LEU	LYS	LYS	ALA	ARG	ASN	ALA	ARG			

4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	383.20Å 383.20Å 383.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6648	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.53	29/2165 (1.3%)	2.19	119/2956 (4.0%)
1	B	1.52	29/2171 (1.3%)	2.16	123/2964 (4.1%)
1	C	1.47	32/2409 (1.3%)	2.12	125/3286 (3.8%)
All	All	1.50	90/6745 (1.3%)	2.16	367/9206 (4.0%)

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	2	35
1	B	3	28
1	C	3	32
All	All	8	95

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	138	ASN	N-CA	-24.59	0.97	1.46
1	C	138	ASN	N-CA	-24.56	0.97	1.46
1	A	138	ASN	N-CA	-24.55	0.97	1.46
1	B	137	SER	N-CA	-17.72	1.10	1.46
1	A	137	SER	N-CA	-17.70	1.10	1.46
1	C	137	SER	N-CA	-17.70	1.10	1.46
1	C	280	LEU	N-CA	14.95	1.76	1.46
1	A	280	LEU	N-CA	14.94	1.76	1.46
1	B	280	LEU	N-CA	14.94	1.76	1.46
1	B	362	VAL	N-CA	14.70	1.75	1.46
1	A	362	VAL	N-CA	14.69	1.75	1.46
1	C	362	VAL	N-CA	14.69	1.75	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	107	SER	N-CA	12.25	1.70	1.46
1	A	172	GLU	N-CA	12.13	1.70	1.46
1	B	122	VAL	N-CA	11.02	1.68	1.46
1	A	314	LEU	N-CA	-10.72	1.25	1.46
1	B	314	LEU	N-CA	-10.68	1.25	1.46
1	C	314	LEU	N-CA	-10.66	1.25	1.46
1	C	327	GLY	CA-C	10.48	1.68	1.51
1	A	327	GLY	CA-C	10.45	1.68	1.51
1	B	327	GLY	CA-C	10.42	1.68	1.51
1	B	366	VAL	N-CA	10.24	1.66	1.46
1	A	366	VAL	N-CA	10.22	1.66	1.46
1	C	366	VAL	N-CA	10.20	1.66	1.46
1	A	115	VAL	N-CA	10.15	1.66	1.46
1	A	316	GLY	N-CA	-9.52	1.31	1.46
1	B	316	GLY	N-CA	-9.51	1.31	1.46
1	C	316	GLY	N-CA	-9.51	1.31	1.46
1	C	86	ARG	N-CA	9.45	1.65	1.46
1	A	107	SER	N-CA	8.61	1.63	1.46
1	C	223	CYS	CA-C	8.46	1.75	1.52
1	C	77	SER	N-CA	-7.51	1.31	1.46
1	A	207	TRP	NE1-CE2	-7.36	1.27	1.37
1	C	144	TRP	NE1-CE2	-7.34	1.28	1.37
1	A	144	TRP	NE1-CE2	-7.34	1.28	1.37
1	B	207	TRP	NE1-CE2	-7.33	1.28	1.37
1	B	144	TRP	NE1-CE2	-7.32	1.28	1.37
1	C	207	TRP	NE1-CE2	-7.29	1.28	1.37
1	B	113	THR	CA-C	7.22	1.71	1.52
1	A	123	VAL	CA-C	7.04	1.71	1.52
1	C	352	ASN	N-CA	6.94	1.60	1.46
1	A	352	ASN	N-CA	6.93	1.60	1.46
1	B	115	VAL	CA-C	6.93	1.71	1.52
1	B	352	ASN	N-CA	6.91	1.60	1.46
1	C	263	LEU	CA-C	6.61	1.70	1.52
1	C	238	GLN	CA-C	6.48	1.69	1.52
1	B	238	GLN	CA-C	6.47	1.69	1.52
1	A	238	GLN	CA-C	6.46	1.69	1.52
1	A	324	LEU	N-CA	6.46	1.59	1.46
1	B	324	LEU	N-CA	6.42	1.59	1.46
1	C	324	LEU	N-CA	6.41	1.59	1.46
1	C	126	GLY	CA-C	-6.38	1.41	1.51
1	C	135	ASN	CA-C	-6.36	1.36	1.52
1	B	135	ASN	CA-C	-6.35	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	ASN	CA-C	-6.32	1.36	1.52
1	C	278	LEU	CA-C	5.89	1.68	1.52
1	A	278	LEU	CA-C	5.88	1.68	1.52
1	B	278	LEU	CA-C	5.88	1.68	1.52
1	C	107	SER	N-CA	5.70	1.57	1.46
1	C	79	MET	N-CA	5.68	1.57	1.46
1	B	121	PHE	N-CA	5.42	1.57	1.46
1	B	194	GLU	CD-OE1	-5.32	1.19	1.25
1	A	194	GLU	CD-OE1	-5.29	1.19	1.25
1	A	188	GLU	CD-OE1	-5.28	1.19	1.25
1	C	203	GLU	CD-OE1	-5.27	1.19	1.25
1	C	254	GLU	CD-OE1	-5.26	1.19	1.25
1	B	188	GLU	CD-OE1	-5.25	1.19	1.25
1	B	209	GLU	CD-OE1	-5.24	1.19	1.25
1	A	209	GLU	CD-OE1	-5.24	1.19	1.25
1	B	254	GLU	CD-OE1	-5.23	1.19	1.25
1	C	194	GLU	CD-OE1	-5.22	1.20	1.25
1	C	209	GLU	CD-OE1	-5.22	1.20	1.25
1	B	203	GLU	CD-OE1	-5.21	1.20	1.25
1	A	172	GLU	CD-OE1	-5.21	1.20	1.25
1	C	188	GLU	CD-OE1	-5.20	1.20	1.25
1	A	254	GLU	CD-OE1	-5.20	1.20	1.25
1	A	203	GLU	CD-OE1	-5.19	1.20	1.25
1	C	172	GLU	CD-OE1	-5.18	1.20	1.25
1	B	172	GLU	CD-OE1	-5.17	1.20	1.25
1	A	310	GLY	N-CA	5.12	1.53	1.46
1	B	310	GLY	N-CA	5.12	1.53	1.46
1	C	310	GLY	N-CA	5.12	1.53	1.46
1	C	117	ASN	N-CA	5.05	1.56	1.46
1	A	117	ASN	N-CA	5.04	1.56	1.46
1	B	364	PHE	CA-C	-5.03	1.39	1.52
1	A	364	PHE	CA-C	-5.03	1.39	1.52
1	B	322	THR	CA-C	5.03	1.66	1.52
1	C	322	THR	CA-C	5.03	1.66	1.52
1	A	322	THR	CA-C	5.01	1.66	1.52
1	C	364	PHE	CA-C	-5.01	1.40	1.52

All (367) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	GLN	C-N-CD	-22.78	70.48	120.60
1	B	165	VAL	C-N-CD	-19.72	77.22	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	145	LEU	C-N-CD	-18.03	80.94	120.60
1	A	135	ASN	CA-C-O	-15.93	86.65	120.10
1	C	135	ASN	CA-C-O	-15.91	86.70	120.10
1	B	135	ASN	CA-C-O	-15.90	86.71	120.10
1	A	165	VAL	C-N-CD	-14.81	88.01	120.60
1	C	165	VAL	C-N-CD	-14.80	88.03	120.60
1	C	137	SER	C-N-CA	14.29	157.43	121.70
1	A	137	SER	C-N-CA	14.29	157.42	121.70
1	B	137	SER	C-N-CA	14.28	157.41	121.70
1	C	206	PRO	CB-CA-C	-14.15	76.63	112.00
1	A	206	PRO	CB-CA-C	-13.91	77.23	112.00
1	B	206	PRO	CB-CA-C	-13.09	79.28	112.00
1	C	266	PRO	CB-CA-C	-12.83	79.93	112.00
1	A	145	LEU	C-N-CD	-12.79	92.46	120.60
1	A	127	ILE	N-CA-C	12.56	144.91	111.00
1	A	136	PRO	CB-CA-C	-12.49	80.78	112.00
1	C	187	PRO	CB-CA-C	-12.47	80.82	112.00
1	C	146	PRO	CB-CA-C	-12.37	81.08	112.00
1	A	187	PRO	CB-CA-C	-12.33	81.18	112.00
1	B	187	PRO	CB-CA-C	-12.33	81.18	112.00
1	B	145	LEU	C-N-CD	-12.20	93.77	120.60
1	C	214	ILE	C-N-CD	-11.85	94.53	120.60
1	A	214	ILE	C-N-CD	-11.85	94.54	120.60
1	A	127	ILE	CB-CA-C	-11.80	88.01	111.60
1	A	126	GLY	N-CA-C	-11.71	83.83	113.10
1	B	135	ASN	CA-C-N	11.36	148.90	117.10
1	C	135	ASN	CA-C-N	11.35	148.89	117.10
1	A	135	ASN	CA-C-N	11.34	148.86	117.10
1	B	214	ILE	C-N-CD	-11.32	95.71	120.60
1	A	352	ASN	N-CA-CB	10.97	130.35	110.60
1	B	352	ASN	N-CA-CB	10.96	130.33	110.60
1	C	352	ASN	N-CA-CB	10.95	130.30	110.60
1	A	137	SER	N-CA-C	10.83	140.25	111.00
1	B	137	SER	N-CA-C	10.82	140.22	111.00
1	C	137	SER	N-CA-C	10.80	140.17	111.00
1	A	215	PRO	CB-CA-C	10.79	138.97	112.00
1	C	215	PRO	CB-CA-C	10.79	138.97	112.00
1	A	137	SER	N-CA-CB	-10.77	94.34	110.50
1	C	137	SER	N-CA-CB	-10.76	94.36	110.50
1	B	137	SER	N-CA-CB	-10.73	94.41	110.50
1	C	295	LEU	CA-C-N	-10.71	93.65	117.20
1	B	295	LEU	CA-C-N	-10.70	93.66	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	LEU	CA-C-N	-10.68	93.70	117.20
1	B	134	LEU	N-CA-C	10.15	138.40	111.00
1	B	166	PRO	CA-CB-CG	-9.84	85.31	104.00
1	A	324	LEU	N-CA-C	9.70	137.20	111.00
1	B	324	LEU	N-CA-C	9.70	137.19	111.00
1	C	324	LEU	N-CA-C	9.70	137.19	111.00
1	C	132	LEU	N-CA-CB	9.62	129.63	110.40
1	C	80	ALA	N-CA-CB	-9.60	96.66	110.10
1	B	352	ASN	N-CA-C	-9.43	85.54	111.00
1	C	352	ASN	N-CA-C	-9.42	85.56	111.00
1	A	352	ASN	N-CA-C	-9.42	85.57	111.00
1	A	189	PRO	CA-CB-CG	-9.19	86.54	104.00
1	C	189	PRO	CA-CB-CG	-9.18	86.56	104.00
1	B	189	PRO	CA-CB-CG	-9.17	86.58	104.00
1	B	220	LYS	N-CA-C	9.12	135.63	111.00
1	C	220	LYS	N-CA-C	9.05	135.43	111.00
1	A	220	LYS	N-CA-C	9.03	135.38	111.00
1	A	138	ASN	N-CA-CB	9.02	126.84	110.60
1	C	138	ASN	N-CA-CB	9.01	126.82	110.60
1	B	138	ASN	N-CA-CB	9.00	126.80	110.60
1	C	327	GLY	CA-C-N	-8.90	97.62	117.20
1	A	327	GLY	CA-C-N	-8.89	97.64	117.20
1	B	327	GLY	CA-C-N	-8.89	97.64	117.20
1	B	220	LYS	CB-CA-C	-8.85	92.71	110.40
1	C	131	SER	C-N-CA	-8.85	99.58	121.70
1	A	220	LYS	CB-CA-C	-8.84	92.72	110.40
1	C	220	LYS	CB-CA-C	-8.84	92.72	110.40
1	B	166	PRO	CB-CA-C	8.66	133.66	112.00
1	B	146	PRO	CB-CA-C	-8.66	90.35	112.00
1	B	136	PRO	C-N-CA	8.61	143.22	121.70
1	A	136	PRO	C-N-CA	8.59	143.18	121.70
1	B	134	LEU	N-CA-CB	-8.56	93.27	110.40
1	C	136	PRO	C-N-CA	8.55	143.08	121.70
1	B	121	PHE	C-N-CA	-8.41	100.67	121.70
1	B	126	GLY	CA-C-O	-8.34	105.59	120.60
1	A	366	VAL	C-N-CA	-8.24	101.09	121.70
1	C	366	VAL	C-N-CA	-8.24	101.09	121.70
1	B	366	VAL	C-N-CA	-8.23	101.12	121.70
1	C	282	GLY	CA-C-O	8.22	135.40	120.60
1	A	282	GLY	CA-C-O	8.21	135.38	120.60
1	B	282	GLY	CA-C-O	8.18	135.33	120.60
1	A	119	SER	N-CA-C	-8.18	88.92	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	PRO	CB-CA-C	8.15	132.37	112.00
1	B	126	GLY	N-CA-C	-8.07	92.93	113.10
1	C	205	ALA	N-CA-C	-8.00	89.41	111.00
1	C	208	ALA	CB-CA-C	-7.85	98.33	110.10
1	A	208	ALA	CB-CA-C	-7.84	98.34	110.10
1	B	208	ALA	CB-CA-C	-7.84	98.34	110.10
1	B	300	THR	CA-C-N	-7.78	100.09	117.20
1	C	300	THR	CA-C-N	-7.76	100.12	117.20
1	C	327	GLY	N-CA-C	-7.75	93.71	113.10
1	A	300	THR	CA-C-N	-7.75	100.14	117.20
1	B	327	GLY	N-CA-C	-7.74	93.75	113.10
1	A	327	GLY	N-CA-C	-7.73	93.77	113.10
1	B	295	LEU	CA-C-O	7.59	136.04	120.10
1	A	295	LEU	CA-C-O	7.59	136.03	120.10
1	C	295	LEU	CA-C-O	7.58	136.03	120.10
1	C	189	PRO	CB-CA-C	7.53	130.82	112.00
1	A	189	PRO	CB-CA-C	7.51	130.77	112.00
1	B	189	PRO	CB-CA-C	7.49	130.72	112.00
1	B	115	VAL	CA-C-N	-7.48	100.74	117.20
1	A	125	GLY	N-CA-C	-7.44	94.50	113.10
1	A	282	GLY	CA-C-N	-7.39	100.94	117.20
1	B	282	GLY	CA-C-N	-7.39	100.94	117.20
1	C	282	GLY	CA-C-N	-7.39	100.93	117.20
1	B	314	LEU	N-CA-C	-7.38	91.07	111.00
1	C	336	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	314	LEU	N-CA-C	-7.37	91.10	111.00
1	C	314	LEU	N-CA-C	-7.37	91.11	111.00
1	A	106	THR	N-CA-C	-7.36	91.12	111.00
1	B	181	ASP	CB-CG-OD1	7.36	124.92	118.30
1	C	191	ASP	CB-CG-OD1	7.36	124.92	118.30
1	C	279	ASP	CB-CG-OD1	7.35	124.91	118.30
1	B	191	ASP	CB-CG-OD1	7.35	124.91	118.30
1	C	153	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	235	ASP	CB-CG-OD1	7.34	124.90	118.30
1	B	250	ASP	CB-CG-OD1	7.34	124.90	118.30
1	B	230	ASP	CB-CG-OD1	7.33	124.90	118.30
1	B	341	ASP	CB-CG-OD1	7.33	124.90	118.30
1	A	186	ASP	CB-CG-OD1	7.33	124.90	118.30
1	A	230	ASP	CB-CG-OD1	7.33	124.90	118.30
1	B	183	ASP	CB-CG-OD1	7.33	124.89	118.30
1	C	186	ASP	CB-CG-OD1	7.33	124.89	118.30
1	A	217	ASP	CB-CG-OD1	7.33	124.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	163	ASP	CB-CG-OD1	7.33	124.89	118.30
1	A	250	ASP	CB-CG-OD1	7.33	124.89	118.30
1	C	225	ASP	CB-CG-OD1	7.32	124.89	118.30
1	C	250	ASP	CB-CG-OD1	7.32	124.89	118.30
1	C	183	ASP	CB-CG-OD1	7.32	124.89	118.30
1	B	279	ASP	CB-CG-OD1	7.32	124.89	118.30
1	A	225	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	279	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	183	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	153	ASP	CB-CG-OD1	7.31	124.88	118.30
1	C	235	ASP	CB-CG-OD1	7.30	124.87	118.30
1	C	348	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	348	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	163	ASP	CB-CG-OD1	7.29	124.87	118.30
1	C	181	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	341	ASP	CB-CG-OD1	7.29	124.86	118.30
1	B	217	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	181	ASP	CB-CG-OD1	7.29	124.86	118.30
1	B	336	ASP	CB-CG-OD1	7.29	124.86	118.30
1	B	186	ASP	CB-CG-OD1	7.29	124.86	118.30
1	C	341	ASP	CB-CG-OD1	7.29	124.86	118.30
1	B	153	ASP	CB-CG-OD1	7.28	124.86	118.30
1	B	133	GLN	C-N-CA	-7.28	103.50	121.70
1	B	348	ASP	CB-CG-OD1	7.28	124.85	118.30
1	B	163	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	336	ASP	CB-CG-OD1	7.27	124.84	118.30
1	C	230	ASP	CB-CG-OD1	7.27	124.84	118.30
1	A	191	ASP	CB-CG-OD1	7.27	124.84	118.30
1	B	225	ASP	CB-CG-OD1	7.26	124.83	118.30
1	C	217	ASP	CB-CG-OD1	7.25	124.82	118.30
1	B	235	ASP	CB-CG-OD1	7.24	124.81	118.30
1	B	358	LEU	C-N-CD	-7.17	104.83	120.60
1	A	358	LEU	C-N-CD	-7.16	104.85	120.60
1	C	134	LEU	N-CA-C	7.16	130.32	111.00
1	C	358	LEU	C-N-CD	-7.15	104.87	120.60
1	C	340	ILE	CA-C-O	-7.02	105.35	120.10
1	A	340	ILE	CA-C-O	-7.02	105.35	120.10
1	B	340	ILE	CA-C-O	-7.02	105.36	120.10
1	C	356	SER	CA-C-N	-7.01	101.78	117.20
1	A	356	SER	CA-C-N	-7.00	101.79	117.20
1	B	356	SER	CA-C-N	-7.00	101.80	117.20
1	A	358	LEU	N-CA-C	-6.82	92.58	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	358	LEU	N-CA-C	-6.81	92.61	111.00
1	B	358	LEU	N-CA-C	-6.80	92.65	111.00
1	B	355	VAL	CA-C-O	-6.75	105.93	120.10
1	C	355	VAL	CA-C-O	-6.74	105.94	120.10
1	A	355	VAL	CA-C-O	-6.74	105.95	120.10
1	A	356	SER	CA-C-O	6.73	134.24	120.10
1	C	189	PRO	N-CD-CG	-6.73	93.11	103.20
1	C	356	SER	CA-C-O	6.72	134.22	120.10
1	B	115	VAL	CA-C-O	6.72	134.21	120.10
1	B	189	PRO	N-CD-CG	-6.71	93.13	103.20
1	A	189	PRO	N-CD-CG	-6.70	93.16	103.20
1	B	356	SER	CA-C-O	6.70	134.16	120.10
1	C	190	ALA	CB-CA-C	-6.69	100.07	110.10
1	A	190	ALA	CB-CA-C	-6.68	100.07	110.10
1	B	190	ALA	CB-CA-C	-6.68	100.08	110.10
1	B	172	GLU	N-CA-C	-6.63	93.09	111.00
1	B	302	LEU	N-CA-CB	-6.61	97.19	110.40
1	B	320	CYS	CB-CA-C	6.61	123.61	110.40
1	A	320	CYS	CB-CA-C	6.60	123.60	110.40
1	C	302	LEU	N-CA-CB	-6.60	97.20	110.40
1	C	320	CYS	CB-CA-C	6.60	123.60	110.40
1	A	302	LEU	N-CA-CB	-6.60	97.20	110.40
1	B	328	ALA	CB-CA-C	-6.57	100.24	110.10
1	A	328	ALA	CB-CA-C	-6.53	100.30	110.10
1	C	328	ALA	CB-CA-C	-6.52	100.32	110.10
1	C	126	GLY	N-CA-C	-6.47	96.93	113.10
1	C	289	GLY	C-N-CD	-6.46	106.40	120.60
1	A	289	GLY	C-N-CD	-6.45	106.41	120.60
1	B	289	GLY	C-N-CD	-6.42	106.47	120.60
1	B	127	ILE	CB-CA-C	-6.41	98.77	111.60
1	C	265	PHE	C-N-CD	-6.36	106.60	120.60
1	B	340	ILE	N-CA-C	-6.35	93.85	111.00
1	C	340	ILE	N-CA-C	-6.34	93.88	111.00
1	A	340	ILE	N-CA-C	-6.34	93.89	111.00
1	B	361	THR	C-N-CA	-6.30	105.94	121.70
1	C	361	THR	C-N-CA	-6.30	105.95	121.70
1	A	361	THR	C-N-CA	-6.29	105.98	121.70
1	B	166	PRO	CA-N-CD	-6.13	102.92	111.50
1	B	227	ALA	CB-CA-C	-6.11	100.93	110.10
1	A	107	SER	N-CA-CB	-6.06	101.42	110.50
1	C	285	ALA	CB-CA-C	-6.03	101.06	110.10
1	A	177	ALA	CB-CA-C	-6.02	101.07	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	GLY	N-CA-C	-6.01	98.06	113.10
1	C	196	ALA	CB-CA-C	-6.01	101.08	110.10
1	A	344	GLY	N-CA-C	-6.01	98.07	113.10
1	A	210	ALA	CB-CA-C	-6.01	101.08	110.10
1	C	344	GLY	N-CA-C	-6.01	98.08	113.10
1	C	93	PRO	CB-CA-C	-6.00	97.00	112.00
1	C	177	ALA	CB-CA-C	-6.00	101.10	110.10
1	A	227	ALA	CB-CA-C	-6.00	101.10	110.10
1	B	196	ALA	CB-CA-C	-6.00	101.10	110.10
1	C	210	ALA	CB-CA-C	-5.99	101.11	110.10
1	A	196	ALA	CB-CA-C	-5.99	101.12	110.10
1	B	285	ALA	CB-CA-C	-5.98	101.13	110.10
1	A	268	PRO	CB-CA-C	5.98	126.95	112.00
1	B	210	ALA	CB-CA-C	-5.98	101.13	110.10
1	C	128	VAL	N-CA-CB	5.98	124.65	111.50
1	A	285	ALA	CB-CA-C	-5.97	101.14	110.10
1	C	227	ALA	CB-CA-C	-5.97	101.14	110.10
1	B	177	ALA	CB-CA-C	-5.97	101.14	110.10
1	B	128	VAL	N-CA-CB	5.97	124.62	111.50
1	C	366	VAL	N-CA-CB	5.94	124.56	111.50
1	C	149	ALA	N-CA-C	-5.92	95.01	111.00
1	A	366	VAL	N-CA-CB	5.92	124.52	111.50
1	B	366	VAL	N-CA-CB	5.91	124.51	111.50
1	A	279	ASP	C-N-CA	-5.85	107.08	121.70
1	C	279	ASP	C-N-CA	-5.85	107.08	121.70
1	B	279	ASP	C-N-CA	-5.84	107.10	121.70
1	A	172	GLU	OE1-CD-OE2	5.82	130.29	123.30
1	A	295	LEU	N-CA-C	-5.82	95.28	111.00
1	B	295	LEU	N-CA-C	-5.82	95.28	111.00
1	C	188	GLU	OE1-CD-OE2	5.82	130.28	123.30
1	C	295	LEU	N-CA-C	-5.81	95.31	111.00
1	A	254	GLU	OE1-CD-OE2	5.80	130.26	123.30
1	C	322	THR	CA-C-N	-5.80	104.43	117.20
1	B	127	ILE	N-CA-C	5.80	126.67	111.00
1	A	322	THR	CA-C-N	-5.80	104.44	117.20
1	A	194	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	B	322	THR	CA-C-N	-5.79	104.46	117.20
1	C	194	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	A	209	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	C	172	GLU	OE1-CD-OE2	5.78	130.24	123.30
1	A	188	GLU	OE1-CD-OE2	5.78	130.24	123.30
1	B	209	GLU	OE1-CD-OE2	5.77	130.23	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	GLU	OE1-CD-OE2	5.77	130.23	123.30
1	A	238	GLN	N-CA-C	-5.77	95.43	111.00
1	C	209	GLU	OE1-CD-OE2	5.76	130.22	123.30
1	B	188	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	A	377	GLY	N-CA-C	-5.76	98.70	113.10
1	B	377	GLY	N-CA-C	-5.76	98.70	113.10
1	C	377	GLY	N-CA-C	-5.76	98.71	113.10
1	B	254	GLU	OE1-CD-OE2	5.75	130.20	123.30
1	C	129	GLY	N-CA-C	-5.75	98.72	113.10
1	C	254	GLU	OE1-CD-OE2	5.75	130.20	123.30
1	C	203	GLU	OE1-CD-OE2	5.75	130.20	123.30
1	A	150	SER	N-CA-C	-5.74	95.51	111.00
1	B	172	GLU	OE1-CD-OE2	5.74	130.19	123.30
1	B	203	GLU	OE1-CD-OE2	5.73	130.18	123.30
1	A	203	GLU	OE1-CD-OE2	5.73	130.18	123.30
1	C	324	LEU	CA-C-O	-5.72	108.09	120.10
1	B	324	LEU	CA-C-O	-5.71	108.11	120.10
1	A	324	LEU	CA-C-O	-5.70	108.14	120.10
1	C	101	GLY	N-CA-C	-5.64	98.99	113.10
1	A	362	VAL	N-CA-CB	-5.64	99.10	111.50
1	C	362	VAL	N-CA-CB	-5.63	99.10	111.50
1	C	364	PHE	CA-C-O	-5.63	108.27	120.10
1	B	362	VAL	N-CA-CB	-5.63	99.12	111.50
1	A	372	GLY	N-CA-C	-5.61	99.06	113.10
1	C	372	GLY	N-CA-C	-5.61	99.07	113.10
1	B	364	PHE	CA-C-O	-5.61	108.33	120.10
1	B	205	ALA	N-CA-C	-5.60	95.87	111.00
1	B	372	GLY	N-CA-C	-5.60	99.09	113.10
1	A	364	PHE	CA-C-O	-5.59	108.37	120.10
1	C	299	PRO	CA-C-O	-5.57	106.84	120.20
1	A	299	PRO	CA-C-O	-5.56	106.85	120.20
1	B	299	PRO	CA-C-O	-5.56	106.85	120.20
1	C	94	LYS	CB-CA-C	-5.56	99.28	110.40
1	B	238	GLN	N-CA-C	-5.43	96.35	111.00
1	C	226	SER	C-N-CA	-5.36	108.29	121.70
1	C	238	GLN	N-CA-C	-5.35	96.56	111.00
1	B	327	GLY	CA-C-O	5.33	130.20	120.60
1	C	326	LEU	N-CA-C	-5.33	96.60	111.00
1	A	326	LEU	N-CA-C	-5.33	96.60	111.00
1	B	326	LEU	N-CA-C	-5.33	96.60	111.00
1	C	327	GLY	CA-C-O	5.33	130.20	120.60
1	A	327	GLY	CA-C-O	5.33	130.19	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	LEU	N-CA-C	5.33	125.39	111.00
1	B	287	ALA	N-CA-CB	-5.29	102.69	110.10
1	A	127	ILE	C-N-CA	-5.28	108.49	121.70
1	A	287	ALA	N-CA-CB	-5.28	102.72	110.10
1	C	287	ALA	N-CA-CB	-5.27	102.73	110.10
1	C	322	THR	CA-C-O	5.26	131.14	120.10
1	A	322	THR	CA-C-O	5.25	131.12	120.10
1	C	290	PRO	CB-CA-C	-5.25	98.88	112.00
1	C	128	VAL	N-CA-C	-5.24	96.85	111.00
1	B	322	THR	CA-C-O	5.23	131.09	120.10
1	A	290	PRO	CB-CA-C	-5.22	98.94	112.00
1	B	290	PRO	CB-CA-C	-5.22	98.95	112.00
1	B	147	ALA	N-CA-CB	-5.20	102.83	110.10
1	C	147	ALA	N-CA-CB	-5.19	102.84	110.10
1	B	209	GLU	CG-CD-OE2	-5.17	107.96	118.30
1	A	254	GLU	CG-CD-OE2	-5.17	107.96	118.30
1	B	188	GLU	CG-CD-OE2	-5.17	107.97	118.30
1	C	254	GLU	CG-CD-OE2	-5.17	107.97	118.30
1	A	194	GLU	CG-CD-OE2	-5.16	107.97	118.30
1	C	188	GLU	CG-CD-OE2	-5.16	107.99	118.30
1	C	194	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	A	188	GLU	CG-CD-OE2	-5.15	107.99	118.30
1	A	172	GLU	CG-CD-OE2	-5.15	108.01	118.30
1	B	194	GLU	CG-CD-OE2	-5.14	108.01	118.30
1	B	254	GLU	CG-CD-OE2	-5.14	108.01	118.30
1	B	203	GLU	CG-CD-OE2	-5.14	108.02	118.30
1	C	209	GLU	CG-CD-OE2	-5.14	108.02	118.30
1	A	349	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	C	292	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	C	172	GLU	CG-CD-OE2	-5.13	108.03	118.30
1	C	126	GLY	CA-C-O	-5.13	111.36	120.60
1	C	203	GLU	CG-CD-OE2	-5.13	108.03	118.30
1	A	209	GLU	CG-CD-OE2	-5.13	108.04	118.30
1	B	129	GLY	N-CA-C	-5.13	100.28	113.10
1	B	172	GLU	CG-CD-OE2	-5.12	108.06	118.30
1	A	203	GLU	CG-CD-OE2	-5.12	108.06	118.30
1	C	164	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	C	289	GLY	N-CA-C	-5.12	100.31	113.10
1	A	264	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	A	226	SER	C-N-CA	-5.11	108.91	121.70
1	B	292	TYR	CB-CG-CD1	-5.11	117.93	121.00
1	C	244	TYR	CB-CG-CD1	-5.10	117.94	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	349	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	C	179	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	A	289	GLY	N-CA-C	-5.09	100.37	113.10
1	B	289	GLY	N-CA-C	-5.09	100.38	113.10
1	A	179	TYR	CB-CG-CD1	-5.09	117.95	121.00
1	C	317	GLY	N-CA-C	-5.09	100.39	113.10
1	B	164	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	C	166	PRO	CB-CA-C	-5.08	99.29	112.00
1	C	264	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	A	222	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	B	317	GLY	N-CA-C	-5.08	100.41	113.10
1	B	222	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	A	292	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	A	317	GLY	N-CA-C	-5.07	100.42	113.10
1	C	155	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	B	179	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	A	146	PRO	CA-CB-CG	-5.06	94.38	104.00
1	A	164	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	A	166	PRO	CB-CA-C	-5.06	99.35	112.00
1	B	155	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	C	222	TYR	CB-CG-CD1	-5.06	117.97	121.00
1	C	75	GLY	N-CA-C	-5.05	100.49	113.10
1	B	264	TYR	CB-CG-CD1	-5.04	117.97	121.00
1	B	244	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	A	244	TYR	CB-CG-CD1	-5.02	117.99	121.00
1	A	155	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	B	349	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	B	368	GLY	N-CA-C	-5.01	100.58	113.10
1	A	368	GLY	N-CA-C	-5.00	100.59	113.10

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	146	PRO	CA
1	A	189	PRO	CA
1	B	146	PRO	CA
1	B	166	PRO	CA
1	B	189	PRO	CA
1	C	132	LEU	CA
1	C	146	PRO	CA
1	C	189	PRO	CA

All (95) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	SER	Peptide
1	A	123	VAL	Mainchain
1	A	124	ASN	Peptide
1	A	126	GLY	Mainchain,Peptide
1	A	127	ILE	Peptide
1	A	136	PRO	Peptide
1	A	220	LYS	Mainchain,Peptide
1	A	225	ASP	Mainchain,Peptide
1	A	227	ALA	Peptide
1	A	273[P]	LEU	Mainchain,Peptide
1	A	274[S]	SER	Peptide
1	A	294	VAL	Mainchain
1	A	295	LEU	Mainchain
1	A	296	THR	Mainchain
1	A	299	PRO	Mainchain
1	A	300	THR	Mainchain,Peptide
1	A	313	ASN	Peptide
1	A	314	LEU	Mainchain
1	A	320	CYS	Mainchain,Peptide
1	A	321	LEU	Peptide
1	A	327	GLY	Mainchain
1	A	338	LEU	Peptide
1	A	340	ILE	Mainchain,Peptide
1	A	345	THR	Mainchain,Peptide
1	A	355	VAL	Mainchain
1	A	361	THR	Peptide
1	A	365	THR	Peptide
1	B	104	THR	Mainchain
1	B	126	GLY	Mainchain,Peptide
1	B	127	ILE	Peptide
1	B	136	PRO	Peptide
1	B	220	LYS	Mainchain,Peptide
1	B	227	ALA	Peptide
1	B	294	VAL	Mainchain
1	B	295	LEU	Mainchain
1	B	296	THR	Mainchain
1	B	299	PRO	Mainchain
1	B	300	THR	Mainchain,Peptide
1	B	313	ASN	Peptide
1	B	314	LEU	Mainchain
1	B	320	CYS	Mainchain,Peptide
1	B	321	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	B	327	GLY	Mainchain
1	B	338	LEU	Peptide
1	B	340	ILE	Mainchain,Peptide
1	B	345	THR	Mainchain,Peptide
1	B	355	VAL	Mainchain
1	B	361	THR	Peptide
1	B	365	THR	Peptide
1	C	127	ILE	Peptide
1	C	131	SER	Peptide
1	C	133	GLN	Peptide
1	C	136	PRO	Peptide
1	C	220	LYS	Mainchain,Peptide
1	C	225	ASP	Mainchain,Peptide
1	C	227	ALA	Peptide
1	C	273[P]	LEU	Mainchain,Peptide
1	C	294	VAL	Mainchain
1	C	295	LEU	Mainchain
1	C	296	THR	Mainchain
1	C	299	PRO	Mainchain
1	C	300	THR	Mainchain,Peptide
1	C	313	ASN	Peptide
1	C	314	LEU	Mainchain
1	C	320	CYS	Mainchain,Peptide
1	C	321	LEU	Peptide
1	C	327	GLY	Mainchain
1	C	338	LEU	Peptide
1	C	340	ILE	Mainchain,Peptide
1	C	345	THR	Mainchain,Peptide
1	C	355	VAL	Mainchain
1	C	361	THR	Peptide
1	C	365	THR	Peptide
1	C	93	PRO	Mainchain

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	2136	0	2111	647	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2130	0	2111	596	2
1	C	2376	0	2374	695	19
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
All	All	6648	0	6596	1878	19

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 141.

All (1878) 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:A:267:GLN:HG3	1:A:268:PRO:CD	1.18	1.59
1:B:122:VAL:CA	1:B:122:VAL:N	1.68	1.56
1:B:107:SER:N	1:B:107:SER:CA	1.70	1.53
1:C:223:CYS:C	1:C:223:CYS:CA	1.75	1.52
1:A:172:GLU:CA	1:A:172:GLU:N	1.70	1.51
1:A:362:VAL:CA	1:A:362:VAL:N	1.75	1.50
1:C:326:LEU:CD2	1:C:337:ILE:HD12	1.43	1.49
1:B:241:ILE:CD1	1:B:255:LEU:HD23	1.42	1.49
1:B:362:VAL:N	1:B:362:VAL:CA	1.75	1.48
1:B:280:LEU:N	1:B:280:LEU:CA	1.76	1.48
1:A:326:LEU:CD2	1:A:337:ILE:HD12	1.43	1.47
1:B:326:LEU:CD2	1:B:337:ILE:HD12	1.43	1.46
1:C:280:LEU:N	1:C:280:LEU:CA	1.76	1.46
1:A:280:LEU:N	1:A:280:LEU:CA	1.76	1.46
1:C:362:VAL:CA	1:C:362:VAL:N	1.75	1.44
1:A:147:ALA:HB2	1:A:272:LEU:CD2	1.49	1.42
1:C:68:ILE:HG21	1:C:70:HIS:CD2	1.54	1.41
1:C:68:ILE:HG21	1:C:70:HIS:NE2	1.37	1.40
1:B:319:ARG:HD2	1:B:371:ALA:CB	1.49	1.40
1:A:319:ARG:HD2	1:A:371:ALA:CB	1.49	1.40
1:B:192:ARG:HH12	1:B:244:TYR:CB	1.35	1.38
1:C:319:ARG:HD2	1:C:371:ALA:CB	1.49	1.37
1:B:324:LEU:CD2	1:B:366:VAL:CG2	2.03	1.37
1:A:267:GLN:CG	1:A:268:PRO:HD2	1.05	1.36
1:A:324:LEU:CD2	1:A:366:VAL:CG2	2.03	1.34
1:A:217:ASP:OD2	1:A:221:ARG:NH2	1.59	1.34
1:A:147:ALA:CB	1:A:272:LEU:CD2	2.04	1.34
1:C:324:LEU:CD2	1:C:366:VAL:CG2	2.03	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ILE:CD1	1:B:255:LEU:CD2	2.03	1.33
1:A:147:ALA:CB	1:A:272:LEU:HD21	1.55	1.33
1:B:241:ILE:HD11	1:B:255:LEU:CD2	1.54	1.32
1:B:324:LEU:CD2	1:B:366:VAL:HG22	1.60	1.32
1:B:225:ASP:OD1	1:B:270:ASN:ND2	1.62	1.31
1:C:217:ASP:OD2	1:C:221:ARG:NH2	1.59	1.31
1:C:324:LEU:CD2	1:C:366:VAL:HG22	1.59	1.31
1:C:68:ILE:CG2	1:C:70:HIS:CD2	2.12	1.31
1:A:289:GLY:HA2	1:A:290:PRO:O	1.16	1.30
1:B:289:GLY:HA2	1:B:290:PRO:O	1.16	1.29
1:C:289:GLY:HA2	1:C:290:PRO:O	1.16	1.29
1:C:164:TYR:CD2	1:C:255:LEU:HD11	1.67	1.28
1:A:152:PHE:CD2	1:A:264:TYR:O	1.87	1.28
1:A:324:LEU:CD2	1:A:366:VAL:HG22	1.60	1.27
1:A:123:VAL:O	1:A:125:GLY:N	1.64	1.27
1:C:138:ASN:O	1:C:140:THR:N	1.66	1.27
1:C:82:VAL:O	1:C:170:THR:HG22	1.29	1.26
1:A:152:PHE:HD2	1:A:264:TYR:O	1.01	1.25
1:B:221:ARG:HG2	1:B:234:ILE:O	1.33	1.25
1:A:228:THR:CG2	1:C:232:LYS:HD2	1.67	1.24
1:A:342:ASN:OD1	1:A:345:THR:HB	1.35	1.24
1:B:133:GLN:NE2	1:B:184:SER:OG	1.68	1.23
1:A:151:ASN:OD1	1:A:269:THR:OG1	1.53	1.23
1:C:342:ASN:ND2	1:C:346:ALA:O	1.72	1.23
1:B:304:HIS:CE1	1:B:374:LEU:HD13	1.74	1.23
1:A:304:HIS:CE1	1:A:374:LEU:HD13	1.74	1.23
1:C:98:ARG:HD2	1:C:105:VAL:CG2	1.70	1.22
1:C:304:HIS:CE1	1:C:374:LEU:HD13	1.74	1.22
1:B:342:ASN:ND2	1:B:346:ALA:O	1.72	1.22
1:A:168:CYS:SG	1:A:252:VAL:HG13	1.80	1.22
1:A:221:ARG:HG2	1:A:234:ILE:O	1.37	1.21
1:C:98:ARG:CD	1:C:105:VAL:HG21	1.69	1.21
1:A:342:ASN:ND2	1:A:346:ALA:O	1.72	1.21
1:A:289:GLY:CA	1:A:290:PRO:O	1.89	1.20
1:B:289:GLY:CA	1:B:290:PRO:O	1.89	1.20
1:A:164:TYR:CD2	1:A:255:LEU:HD11	1.76	1.20
1:B:154:GLN:NE2	1:B:222:TYR:CE1	2.09	1.20
1:C:342:ASN:OD1	1:C:345:THR:HB	1.35	1.20
1:B:342:ASN:OD1	1:B:345:THR:HB	1.35	1.20
1:C:289:GLY:CA	1:C:290:PRO:O	1.89	1.20
1:C:131:SER:O	1:C:133:GLN:N	1.74	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:CYS:SG	1:A:252:VAL:CG1	2.29	1.19
1:C:151:ASN:OD1	1:C:269:THR:OG1	1.61	1.19
1:B:298:THR:OG1	1:B:299:PRO:HD2	1.43	1.19
1:C:190:ALA:HB3	1:C:194:GLU:OE2	1.42	1.19
1:A:298:THR:OG1	1:A:299:PRO:HD2	1.43	1.18
1:C:117:ASN:OD1	1:C:252:VAL:HG21	1.43	1.18
1:B:320:CYS:CB	1:B:366:VAL:HG11	1.74	1.18
1:C:320:CYS:CB	1:C:366:VAL:HG11	1.74	1.18
1:B:221:ARG:HH11	1:B:236:LEU:HA	1.08	1.17
1:A:320:CYS:CB	1:A:366:VAL:HG11	1.74	1.17
1:C:277:ARG:CB	1:C:285:ALA:HB3	1.73	1.17
1:B:221:ARG:NH1	1:B:236:LEU:HA	1.59	1.17
1:B:277:ARG:CB	1:B:285:ALA:HB3	1.73	1.17
1:A:277:ARG:CB	1:A:285:ALA:HB3	1.73	1.17
1:C:326:LEU:HD23	1:C:337:ILE:HD12	1.28	1.16
1:C:221:ARG:HG2	1:C:234:ILE:O	1.40	1.16
1:A:154:GLN:NE2	1:A:222:TYR:CD1	2.12	1.16
1:A:190:ALA:HB3	1:A:194:GLU:OE2	1.46	1.16
1:B:320:CYS:HB2	1:B:366:VAL:CG1	1.75	1.15
1:C:298:THR:OG1	1:C:299:PRO:HD2	1.43	1.15
1:C:154:GLN:NE2	1:C:222:TYR:CD1	2.12	1.15
1:C:320:CYS:HB2	1:C:366:VAL:CG1	1.75	1.15
1:C:136:PRO:HB2	1:C:145:LEU:HD22	1.20	1.15
1:B:168:CYS:SG	1:B:252:VAL:HG13	1.87	1.15
1:C:331:ALA:HB2	1:C:357:SER:HB3	1.28	1.15
1:A:320:CYS:HB2	1:A:366:VAL:CG1	1.75	1.15
1:C:164:TYR:HD2	1:C:255:LEU:CD1	1.59	1.14
1:C:275[P]:SER:HA	1:C:375:LEU:HD23	1.20	1.14
1:C:326:LEU:HD22	1:C:337:ILE:HD12	1.21	1.14
1:B:192:ARG:HH12	1:B:244:TYR:HB2	0.98	1.14
1:B:183:ASP:OD2	1:B:186:ASP:OD2	1.66	1.13
1:C:168:CYS:SG	1:C:252:VAL:HG13	1.88	1.13
1:B:317:GLY:HA3	1:B:348:ASP:HA	1.29	1.13
1:A:104:THR:CG2	1:A:263:LEU:HB2	1.79	1.12
1:A:132:LEU:HD12	1:A:239:LEU:O	1.50	1.12
1:A:276:LYS:HB3	1:A:295:LEU:HD21	1.24	1.12
1:B:206:PRO:HB3	1:B:252:VAL:HG11	1.29	1.11
1:B:193:VAL:O	1:B:197:ASN:ND2	1.83	1.11
1:C:276:LYS:O	1:C:295:LEU:HD11	1.51	1.11
1:B:276:LYS:HB3	1:B:295:LEU:HD21	1.23	1.11
1:B:331:ALA:HB2	1:B:357:SER:HB3	1.28	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275[P]:SER:HA	1:A:375:LEU:HD23	1.20	1.11
1:A:331:ALA:HB2	1:A:357:SER:HB3	1.28	1.11
1:C:103:VAL:HG13	1:C:152:PHE:HE2	1.10	1.10
1:A:326:LEU:HD23	1:A:337:ILE:HD12	1.27	1.10
1:A:147:ALA:CA	1:A:272:LEU:HD21	1.81	1.10
1:C:133:GLN:O	1:C:138:ASN:ND2	1.82	1.10
1:A:317:GLY:HA3	1:A:348:ASP:HA	1.29	1.10
1:A:324:LEU:HD23	1:A:366:VAL:HG22	1.15	1.10
1:C:67:ILE:HG22	1:C:68:ILE:N	1.62	1.09
1:C:164:TYR:CD2	1:C:255:LEU:CD1	2.34	1.09
1:B:275:SER:HA	1:B:375:LEU:HD23	1.20	1.09
1:C:324:LEU:HD23	1:C:366:VAL:HG22	1.15	1.09
1:C:317:GLY:HA3	1:C:348:ASP:HA	1.29	1.09
1:B:221:ARG:CG	1:B:234:ILE:O	2.00	1.09
1:A:276:LYS:O	1:A:295:LEU:HD11	1.51	1.09
1:C:130:ASN:OD1	1:C:188:GLU:OE2	1.70	1.09
1:A:186:ASP:N	1:B:226:SER:OG	1.86	1.09
1:A:225:ASP:CB	1:C:186:ASP:OD1	2.01	1.09
1:B:326:LEU:HD22	1:B:337:ILE:HD12	1.21	1.09
1:B:324:LEU:HD23	1:B:366:VAL:HG22	1.15	1.09
1:A:178:LEU:HD22	1:A:241:ILE:HG12	1.31	1.09
1:B:192:ARG:NH1	1:B:244:TYR:CB	2.15	1.08
1:B:324:LEU:HD21	1:B:366:VAL:HG21	1.35	1.08
1:C:204:THR:HG22	1:C:205:ALA:O	1.51	1.08
1:B:127:ILE:HG22	1:B:128:VAL:N	1.65	1.08
1:A:275[S]:SER:HA	1:A:375:LEU:HD23	1.10	1.08
1:B:152:PHE:CE1	1:B:263:LEU:HD13	1.89	1.08
1:A:324:LEU:HD21	1:A:366:VAL:HG21	1.35	1.08
1:C:324:LEU:HD21	1:C:366:VAL:HG21	1.35	1.08
1:C:103:VAL:HG13	1:C:152:PHE:CE2	1.89	1.08
1:A:335:ASN:CB	1:A:352:ASN:ND2	2.17	1.08
1:B:335:ASN:CB	1:B:352:ASN:ND2	2.17	1.08
1:B:335:ASN:HD22	1:B:353:CYS:CA	1.67	1.08
1:B:276:LYS:O	1:B:295:LEU:HD11	1.51	1.08
1:A:225:ASP:HB2	1:C:186:ASP:OD1	1.51	1.08
1:A:326:LEU:HD22	1:A:337:ILE:HD12	1.21	1.07
1:B:326:LEU:HD23	1:B:337:ILE:HD12	1.27	1.07
1:A:319:ARG:CD	1:A:371:ALA:CB	2.32	1.07
1:A:164:TYR:HD2	1:A:255:LEU:CD1	1.66	1.07
1:C:152:PHE:HD2	1:C:264:TYR:O	1.37	1.07
1:C:335:ASN:CB	1:C:352:ASN:ND2	2.17	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:ARG:CD	1:B:371:ALA:CB	2.32	1.07
1:A:335:ASN:HD22	1:A:353:CYS:CA	1.67	1.07
1:C:276:LYS:HB3	1:C:295:LEU:HD21	1.24	1.07
1:C:241:ILE:HD13	1:C:255:LEU:CD2	1.83	1.07
1:C:319:ARG:CD	1:C:371:ALA:CB	2.32	1.06
1:A:302:LEU:O	1:A:363:THR:HG23	1.55	1.06
1:B:338:LEU:HD23	1:B:339:ALA:N	1.69	1.06
1:C:148:LEU:C	1:C:150:SER:H	1.54	1.06
1:C:335:ASN:HD22	1:C:353:CYS:CA	1.67	1.06
1:C:183:ASP:OD2	1:C:186:ASP:OD2	1.73	1.06
1:A:338:LEU:HD23	1:A:339:ALA:N	1.69	1.06
1:A:123:VAL:O	1:A:126:GLY:N	1.88	1.06
1:C:302:LEU:O	1:C:363:THR:HG23	1.55	1.05
1:A:104:THR:CG2	1:A:263:LEU:HD12	1.86	1.05
1:B:324:LEU:HD21	1:B:366:VAL:CG2	1.84	1.05
1:A:275[S]:SER:HA	1:A:375:LEU:CD2	1.87	1.05
1:C:98:ARG:HD2	1:C:105:VAL:HG21	1.29	1.05
1:B:241:ILE:HD13	1:B:255:LEU:CD2	1.83	1.05
1:B:302:LEU:O	1:B:363:THR:HG23	1.55	1.05
1:B:277:ARG:HB3	1:B:285:ALA:HB3	1.38	1.04
1:C:275[S]:SER:HA	1:C:375:LEU:HD23	1.34	1.04
1:A:331:ALA:HB3	1:A:357:SER:OG	1.57	1.04
1:C:104:THR:HG23	1:C:263:LEU:HD12	1.34	1.04
1:A:335:ASN:ND2	1:A:353:CYS:C	2.10	1.04
1:C:335:ASN:ND2	1:C:353:CYS:C	2.10	1.04
1:C:338:LEU:HD23	1:C:339:ALA:N	1.69	1.04
1:C:331:ALA:HB2	1:C:357:SER:CB	1.88	1.04
1:B:335:ASN:ND2	1:B:353:CYS:C	2.10	1.04
1:A:110:GLU:OE1	1:A:144:TRP:N	1.89	1.04
1:B:331:ALA:HB3	1:B:357:SER:OG	1.56	1.03
1:A:277:ARG:HB3	1:A:285:ALA:HB3	1.38	1.03
1:B:138:ASN:O	1:B:140:THR:N	1.91	1.03
1:A:136:PRO:HB3	1:A:145:LEU:HD22	1.35	1.03
1:A:241:ILE:HD13	1:A:255:LEU:CD2	1.89	1.03
1:B:331:ALA:HB2	1:B:357:SER:CB	1.88	1.03
1:A:104:THR:HG22	1:A:263:LEU:HB2	1.36	1.02
1:A:331:ALA:HB2	1:A:357:SER:CB	1.88	1.02
1:A:271:THR:HG22	1:A:273[S]:LEU:O	1.59	1.02
1:C:277:ARG:HB3	1:C:285:ALA:HB3	1.38	1.02
1:A:201:LEU:HD21	1:A:203:GLU:HG2	1.41	1.02
1:C:179:TYR:CE1	1:C:240:GLY:HA3	1.94	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:THR:HG21	1:C:232:LYS:CD	1.89	1.02
1:A:319:ARG:HD2	1:A:371:ALA:HB2	1.05	1.02
1:C:319:ARG:HD2	1:C:371:ALA:HB2	1.05	1.02
1:C:193:VAL:O	1:C:197:ASN:ND2	1.93	1.01
1:A:178:LEU:CD2	1:A:241:ILE:HG12	1.88	1.01
1:A:164:TYR:CD2	1:A:255:LEU:CD1	2.41	1.01
1:C:331:ALA:HB3	1:C:357:SER:OG	1.57	1.01
1:A:232:LYS:HD2	1:B:228:THR:HG21	1.42	1.01
1:A:335:ASN:ND2	1:A:353:CYS:CA	2.24	1.01
1:B:326:LEU:CD2	1:B:337:ILE:CD1	2.39	1.01
1:C:366:VAL:HG12	1:C:367:SER:N	1.75	1.01
1:B:127:ILE:CG2	1:B:128:VAL:N	2.24	1.01
1:A:326:LEU:CD2	1:A:337:ILE:CD1	2.39	1.00
1:C:200:VAL:O	1:C:200:VAL:HG12	1.57	1.00
1:A:200:VAL:O	1:A:200:VAL:HG12	1.57	1.00
1:C:328:ALA:CB	1:C:362:VAL:HG22	1.91	1.00
1:C:335:ASN:ND2	1:C:353:CYS:CA	2.24	1.00
1:B:335:ASN:ND2	1:B:353:CYS:CA	2.24	1.00
1:B:319:ARG:HD2	1:B:371:ALA:HB2	1.05	1.00
1:A:324:LEU:HD21	1:A:366:VAL:CG2	1.84	1.00
1:B:277:ARG:HB2	1:B:285:ALA:HB3	1.40	1.00
1:A:277:ARG:HB2	1:A:285:ALA:HB3	1.41	1.00
1:B:200:VAL:HG12	1:B:200:VAL:O	1.59	1.00
1:C:98:ARG:NE	1:C:105:VAL:HG21	1.75	1.00
1:A:336:ASP:O	1:A:351:LEU:HA	1.62	1.00
1:B:336:ASP:O	1:B:351:LEU:HA	1.62	1.00
1:C:324:LEU:HD21	1:C:366:VAL:CG2	1.84	1.00
1:B:277:ARG:HB3	1:B:285:ALA:CB	1.92	1.00
1:C:326:LEU:CD2	1:C:337:ILE:CD1	2.39	0.99
1:B:338:LEU:HD23	1:B:339:ALA:H	1.26	0.99
1:A:277:ARG:HB3	1:A:285:ALA:CB	1.92	0.99
1:B:366:VAL:HG12	1:B:367:SER:N	1.75	0.99
1:A:331:ALA:CB	1:A:357:SER:OG	2.10	0.99
1:A:328:ALA:CB	1:A:362:VAL:HG22	1.91	0.99
1:C:136:PRO:HB2	1:C:145:LEU:CD2	1.91	0.99
1:B:206:PRO:HG2	1:B:207:TRP:H	1.24	0.99
1:C:319:ARG:HD2	1:C:371:ALA:HB3	1.41	0.99
1:A:319:ARG:HD2	1:A:371:ALA:HB3	1.41	0.99
1:B:328:ALA:CB	1:B:362:VAL:HG22	1.91	0.99
1:C:68:ILE:CG2	1:C:70:HIS:NE2	2.22	0.99
1:C:277:ARG:HB3	1:C:285:ALA:CB	1.92	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:PRO:O	1:B:269:THR:O	1.81	0.99
1:C:319:ARG:CD	1:C:371:ALA:HB3	1.92	0.98
1:A:132:LEU:CD1	1:A:239:LEU:O	2.11	0.98
1:B:320:CYS:CB	1:B:366:VAL:CG1	2.37	0.98
1:C:103:VAL:HG11	1:C:264:TYR:CA	1.92	0.98
1:B:293:LEU:HD12	1:B:376:VAL:HG21	1.46	0.98
1:A:268:PRO:O	1:A:269:THR:O	1.82	0.98
1:B:154:GLN:NE2	1:B:222:TYR:CD1	2.31	0.98
1:A:320:CYS:CB	1:A:366:VAL:CG1	2.37	0.98
1:A:206:PRO:HB3	1:A:252:VAL:HG11	1.43	0.98
1:A:145:LEU:HD12	1:A:259:ARG:HD3	1.42	0.98
1:C:293:LEU:HD12	1:C:376:VAL:HG21	1.46	0.98
1:B:331:ALA:CB	1:B:357:SER:OG	2.10	0.98
1:B:121:PHE:C	1:B:122:VAL:CA	2.32	0.98
1:C:331:ALA:CB	1:C:357:SER:OG	2.10	0.98
1:B:319:ARG:HD2	1:B:371:ALA:HB3	1.41	0.98
1:C:277:ARG:HB2	1:C:285:ALA:HB3	1.40	0.98
1:C:121:PHE:O	1:C:121:PHE:HD1	1.46	0.98
1:A:293:LEU:HD12	1:A:376:VAL:HG21	1.46	0.97
1:C:320:CYS:CB	1:C:366:VAL:CG1	2.37	0.97
1:C:336:ASP:O	1:C:351:LEU:HA	1.62	0.97
1:A:331:ALA:CB	1:A:357:SER:CB	2.43	0.97
1:B:130:ASN:HD22	1:B:238:GLN:NE2	1.63	0.97
1:A:279:ASP:HB3	1:A:282:GLY:HA3	1.46	0.97
1:B:331:ALA:CB	1:B:357:SER:CB	2.43	0.97
1:B:262:THR:HG22	1:B:264:TYR:CE2	2.00	0.97
1:A:167:LEU:HD23	1:A:167:LEU:H	1.28	0.97
1:A:366:VAL:HG12	1:A:367:SER:N	1.75	0.97
1:C:201:LEU:HD21	1:C:203:GLU:HG2	1.44	0.97
1:B:117:ASN:O	1:B:249:ALA:HA	1.63	0.96
1:C:219:VAL:HB	1:C:221:ARG:HH21	1.28	0.96
1:B:319:ARG:CD	1:B:371:ALA:HB3	1.92	0.96
1:B:269:THR:HG22	1:B:270:ASN:H	1.28	0.96
1:A:145:LEU:HB3	1:A:146:PRO:HD3	1.47	0.96
1:B:241:ILE:HD11	1:B:255:LEU:HD23	1.00	0.96
1:A:319:ARG:CD	1:A:371:ALA:HB2	1.94	0.96
1:C:167:LEU:HD21	1:C:253:GLY:N	1.80	0.96
1:A:168:CYS:SG	1:A:252:VAL:HG12	2.02	0.96
1:A:319:ARG:CD	1:A:371:ALA:HB3	1.92	0.96
1:A:185:GLN:C	1:B:226:SER:OG	2.04	0.96
1:B:279:ASP:HB3	1:B:282:GLY:HA3	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:VAL:HB	1:A:221:ARG:HH21	1.28	0.96
1:C:279:ASP:HB3	1:C:282:GLY:HA3	1.46	0.96
1:C:168:CYS:SG	1:C:252:VAL:CG1	2.52	0.96
1:B:145:LEU:HD12	1:B:259:ARG:HD3	1.47	0.96
1:A:206:PRO:HB3	1:A:252:VAL:CG1	1.94	0.96
1:A:147:ALA:HB2	1:A:272:LEU:HD22	0.96	0.96
1:C:331:ALA:CB	1:C:357:SER:CB	2.43	0.95
1:B:319:ARG:CD	1:B:371:ALA:HB2	1.94	0.95
1:A:262:THR:HG22	1:A:264:TYR:CZ	2.01	0.95
1:A:162:LEU:HD13	1:A:178:LEU:HD13	1.47	0.95
1:A:201:LEU:HD23	1:A:202:LYS:N	1.81	0.95
1:C:103:VAL:HG11	1:C:264:TYR:HA	1.46	0.95
1:C:82:VAL:O	1:C:170:THR:CG2	2.14	0.95
1:B:304:HIS:CE1	1:B:374:LEU:CD1	2.50	0.95
1:A:145:LEU:O	1:A:145:LEU:HD23	1.65	0.95
1:A:183:ASP:OD2	1:A:186:ASP:OD2	1.84	0.95
1:B:262:THR:HG22	1:B:264:TYR:CZ	2.01	0.95
1:C:304:HIS:CE1	1:C:374:LEU:CD1	2.50	0.95
1:B:201:LEU:HD21	1:B:203:GLU:HG2	1.49	0.94
1:C:331:ALA:CB	1:C:357:SER:HB3	1.98	0.94
1:A:103:VAL:HG13	1:A:263:LEU:O	1.66	0.94
1:C:97:GLY:O	1:C:98:ARG:C	2.04	0.94
1:C:319:ARG:CD	1:C:371:ALA:HB2	1.94	0.94
1:A:104:THR:HG23	1:A:263:LEU:HD12	1.46	0.94
1:C:138:ASN:O	1:C:141:LEU:N	2.01	0.94
1:C:338:LEU:HD23	1:C:339:ALA:H	1.26	0.94
1:C:201:LEU:HD23	1:C:202:LYS:N	1.81	0.94
1:B:335:ASN:CB	1:B:352:ASN:HD22	1.80	0.94
1:A:304:HIS:CE1	1:A:374:LEU:CD1	2.50	0.94
1:A:136:PRO:HB3	1:A:145:LEU:CD2	1.98	0.94
1:A:228:THR:HG21	1:C:232:LYS:HD2	0.95	0.94
1:B:178:LEU:HD22	1:B:241:ILE:HG12	1.50	0.94
1:B:201:LEU:C	1:B:201:LEU:HD23	1.88	0.94
1:A:226:SER:HB2	1:C:185:GLN:HB3	1.50	0.94
1:C:138:ASN:OD1	1:C:140:THR:HB	1.66	0.94
1:C:117:ASN:OD1	1:C:252:VAL:CG2	2.16	0.94
1:C:162:LEU:HD13	1:C:178:LEU:HD13	1.50	0.94
1:C:190:ALA:CB	1:C:194:GLU:OE2	2.16	0.94
1:C:68:ILE:HG22	1:C:70:HIS:CD2	2.01	0.93
1:C:241:ILE:HD13	1:C:255:LEU:HD23	1.47	0.93
1:C:324:LEU:HD22	1:C:366:VAL:CG2	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:LEU:HD23	1:C:236:LEU:HD23	1.50	0.93
1:A:110:GLU:CD	1:A:144:TRP:HB3	1.89	0.93
1:C:201:LEU:HD23	1:C:201:LEU:C	1.88	0.93
1:A:183:ASP:O	1:A:185:GLN:N	2.01	0.93
1:A:335:ASN:CB	1:A:352:ASN:HD22	1.80	0.93
1:C:304:HIS:HE1	1:C:374:LEU:HD13	1.13	0.93
1:B:127:ILE:CG2	1:B:128:VAL:H	1.82	0.93
1:A:201:LEU:HD23	1:A:201:LEU:C	1.88	0.93
1:B:331:ALA:CB	1:B:357:SER:HB3	1.98	0.93
1:C:335:ASN:CB	1:C:352:ASN:HD22	1.80	0.93
1:C:81:PRO:O	1:C:170:THR:HG21	1.69	0.92
1:C:183:ASP:O	1:C:185:GLN:N	2.02	0.92
1:A:319:ARG:CG	1:A:371:ALA:HB3	1.99	0.92
1:C:164:TYR:CE2	1:C:255:LEU:HD11	2.05	0.92
1:C:276:LYS:HB3	1:C:295:LEU:CD2	1.99	0.92
1:B:110:GLU:OE1	1:B:144:TRP:N	2.03	0.92
1:A:335:ASN:HB3	1:A:352:ASN:ND2	1.84	0.92
1:C:335:ASN:HB3	1:C:352:ASN:ND2	1.83	0.92
1:A:324:LEU:HD22	1:A:366:VAL:CG2	1.98	0.92
1:C:319:ARG:CG	1:C:371:ALA:HB3	1.99	0.92
1:A:331:ALA:CB	1:A:357:SER:HB3	1.98	0.92
1:C:123:VAL:O	1:C:125:GLY:N	2.03	0.92
1:C:335:ASN:HD21	1:C:353:CYS:C	1.71	0.92
1:C:67:ILE:HG22	1:C:68:ILE:H	1.20	0.92
1:B:319:ARG:CG	1:B:371:ALA:HB3	1.99	0.92
1:A:328:ALA:HB2	1:A:362:VAL:HG22	1.52	0.91
1:A:267:GLN:NE2	1:C:198:PHE:CE1	2.38	0.91
1:B:183:ASP:O	1:B:185:GLN:N	2.01	0.91
1:B:335:ASN:HD21	1:B:353:CYS:C	1.71	0.91
1:B:311:THR:HG22	1:B:379:ALA:O	1.70	0.91
1:B:335:ASN:HB3	1:B:352:ASN:ND2	1.83	0.91
1:B:152:PHE:HD2	1:B:264:TYR:O	1.54	0.91
1:B:276:LYS:HB3	1:B:295:LEU:CD2	1.99	0.91
1:A:276:LYS:HB3	1:A:295:LEU:CD2	1.99	0.91
1:C:195:LEU:CD2	1:C:201:LEU:HD11	2.00	0.91
1:C:296:THR:OG1	1:C:303:THR:HB	1.70	0.91
1:A:278:LEU:HD21	1:A:295:LEU:O	1.70	0.91
1:A:134:LEU:HD23	1:A:236:LEU:HD23	1.52	0.91
1:C:328:ALA:HB2	1:C:362:VAL:HG22	1.52	0.91
1:A:221:ARG:CG	1:A:234:ILE:O	2.18	0.91
1:B:161:VAL:HB	1:B:258:ALA:CB	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:LEU:HD23	1:C:167:LEU:H	1.36	0.91
1:C:311:THR:HG22	1:C:379:ALA:O	1.70	0.91
1:A:311:THR:HG22	1:A:379:ALA:O	1.70	0.91
1:A:338:LEU:HD23	1:A:339:ALA:H	1.26	0.91
1:B:328:ALA:HB2	1:B:362:VAL:HG22	1.52	0.91
1:B:296:THR:OG1	1:B:303:THR:HB	1.70	0.91
1:B:275:SER:CA	1:B:375:LEU:HD23	2.00	0.91
1:A:195:LEU:CD2	1:A:201:LEU:HD11	2.00	0.91
1:C:278:LEU:HD21	1:C:295:LEU:O	1.70	0.90
1:B:324:LEU:HD22	1:B:366:VAL:CG2	1.98	0.90
1:C:262:THR:HG22	1:C:264:TYR:CE2	2.05	0.90
1:C:326:LEU:HD23	1:C:337:ILE:CD1	2.00	0.90
1:C:89:VAL:HG12	1:C:90:GLY:N	1.85	0.90
1:C:97:GLY:O	1:C:99:THR:N	2.04	0.90
1:C:104:THR:HG23	1:C:263:LEU:CD1	2.00	0.90
1:B:241:ILE:HD11	1:B:255:LEU:HD21	1.54	0.90
1:A:147:ALA:CB	1:A:272:LEU:HD22	1.86	0.90
1:A:267:GLN:O	1:C:197:ASN:CB	2.20	0.90
1:B:326:LEU:HD23	1:B:337:ILE:CD1	2.00	0.90
1:B:179:TYR:CE1	1:B:240:GLY:HA3	2.07	0.90
1:A:179:TYR:CE1	1:A:240:GLY:HA3	2.07	0.90
1:A:296:THR:OG1	1:A:303:THR:HB	1.70	0.90
1:A:326:LEU:HD23	1:A:337:ILE:CD1	2.00	0.90
1:A:138:ASN:OD1	1:A:140:THR:HB	1.72	0.89
1:B:278:LEU:HD21	1:B:295:LEU:O	1.70	0.89
1:A:228:THR:CG2	1:C:232:LYS:CD	2.49	0.89
1:B:335:ASN:HB3	1:B:352:ASN:HD22	1.34	0.89
1:B:183:ASP:CB	1:B:186:ASP:OD2	2.20	0.89
1:A:147:ALA:HA	1:A:272:LEU:HD21	1.53	0.89
1:A:304:HIS:HE1	1:A:374:LEU:HD13	1.13	0.89
1:B:161:VAL:HB	1:B:258:ALA:HB3	1.52	0.89
1:A:147:ALA:HB1	1:A:272:LEU:HD11	1.52	0.89
1:A:335:ASN:HB3	1:A:352:ASN:HD22	1.34	0.89
1:B:241:ILE:HD13	1:B:255:LEU:HD23	1.39	0.89
1:A:335:ASN:HD21	1:A:353:CYS:C	1.71	0.89
1:C:164:TYR:HD2	1:C:255:LEU:HD11	1.08	0.89
1:A:271:THR:HG22	1:A:271:THR:O	1.73	0.89
1:C:129:GLY:O	1:C:307:ARG:NH2	2.05	0.89
1:A:324:LEU:CD2	1:A:366:VAL:HG21	1.96	0.89
1:C:195:LEU:HD21	1:C:201:LEU:HD11	1.55	0.89
1:C:221:ARG:CG	1:C:234:ILE:O	2.21	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:HIS:HE1	1:C:374:LEU:CD1	1.85	0.88
1:B:304:HIS:HE1	1:B:374:LEU:HD13	1.13	0.88
1:C:104:THR:HG22	1:C:152:PHE:CZ	2.08	0.88
1:A:274[P]:SER:O	1:A:375:LEU:HA	1.73	0.88
1:A:195:LEU:HD21	1:A:201:LEU:HD11	1.55	0.88
1:B:190:ALA:HB3	1:B:194:GLU:OE2	1.74	0.88
1:A:267:GLN:CD	1:C:198:PHE:CE1	2.46	0.88
1:A:304:HIS:HE1	1:A:374:LEU:CD1	1.85	0.88
1:C:167:LEU:HD23	1:C:252:VAL:O	1.74	0.88
1:B:262:THR:HG21	1:B:264:TYR:OH	1.72	0.88
1:A:241:ILE:HD13	1:A:255:LEU:HD23	1.52	0.88
1:C:351:LEU:HD12	1:C:351:LEU:C	1.94	0.88
1:B:178:LEU:CD2	1:B:241:ILE:HG12	2.02	0.88
1:B:192:ARG:NH1	1:B:244:TYR:HB2	1.82	0.88
1:C:274[P]:SER:O	1:C:375:LEU:HA	1.73	0.88
1:B:133:GLN:NE2	1:B:184:SER:HG	1.68	0.87
1:C:148:LEU:C	1:C:150:SER:N	2.25	0.87
1:A:154:GLN:NE2	1:A:222:TYR:CE1	2.41	0.87
1:A:270:ASN:O	1:A:271:THR:OG1	1.91	0.87
1:A:351:LEU:HD12	1:A:351:LEU:C	1.94	0.87
1:C:154:GLN:NE2	1:C:222:TYR:CE1	2.41	0.87
1:C:267:GLN:HB2	1:C:268:PRO:HD2	1.54	0.87
1:B:271:THR:HG21	1:B:288:THR:HG22	1.56	0.87
1:B:326:LEU:HB2	1:B:337:ILE:HD11	1.57	0.87
1:C:275[P]:SER:HA	1:C:375:LEU:CD2	2.05	0.87
1:A:136:PRO:CB	1:A:145:LEU:HD22	2.04	0.87
1:A:268:PRO:O	1:A:269:THR:C	2.12	0.87
1:B:135:ASN:ND2	1:B:224:ASN:OD1	2.08	0.87
1:A:355:VAL:HG13	1:A:360:ALA:HB2	1.55	0.87
1:B:170:THR:HG22	1:B:170:THR:O	1.73	0.87
1:A:147:ALA:HB1	1:A:272:LEU:HD21	1.56	0.87
1:B:275:SER:HA	1:B:375:LEU:CD2	2.05	0.87
1:A:326:LEU:HB2	1:A:337:ILE:HD11	1.57	0.87
1:A:262:THR:HG21	1:A:264:TYR:OH	1.75	0.87
1:C:121:PHE:O	1:C:121:PHE:CD1	2.27	0.87
1:A:275[P]:SER:HA	1:A:375:LEU:CD2	2.05	0.86
1:C:124:ASN:OD1	1:C:132:LEU:CD1	2.23	0.86
1:B:304:HIS:HE1	1:B:374:LEU:CD1	1.85	0.86
1:C:355:VAL:HG13	1:C:360:ALA:HB2	1.55	0.86
1:C:326:LEU:HB2	1:C:337:ILE:CD1	2.06	0.86
1:B:326:LEU:HB2	1:B:337:ILE:CD1	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:PRO:CG	1:B:207:TRP:H	1.83	0.86
1:B:201:LEU:HD23	1:B:202:LYS:N	1.90	0.86
1:B:351:LEU:C	1:B:351:LEU:HD12	1.94	0.86
1:B:355:VAL:HG13	1:B:360:ALA:HB2	1.55	0.86
1:C:167:LEU:CD2	1:C:252:VAL:C	2.44	0.86
1:A:326:LEU:HB2	1:A:337:ILE:CD1	2.06	0.85
1:B:192:ARG:NH1	1:B:244:TYR:CG	2.44	0.85
1:A:147:ALA:HB1	1:A:272:LEU:CD1	2.05	0.85
1:A:164:TYR:HD2	1:A:255:LEU:HD11	1.16	0.85
1:B:162:LEU:HD13	1:B:178:LEU:HD13	1.56	0.85
1:A:190:ALA:CB	1:A:194:GLU:OE2	2.23	0.85
1:B:269:THR:HG22	1:B:270:ASN:N	1.86	0.85
1:C:319:ARG:HG3	1:C:371:ALA:HB3	1.58	0.85
1:A:279:ASP:HB3	1:A:282:GLY:CA	2.05	0.85
1:B:383:VAL:O	1:B:384:VAL:CG2	2.25	0.85
1:C:383:VAL:O	1:C:384:VAL:CG2	2.25	0.85
1:C:335:ASN:HB3	1:C:352:ASN:HD22	1.34	0.85
1:B:279:ASP:HB3	1:B:282:GLY:CA	2.05	0.85
1:B:342:ASN:OD1	1:B:345:THR:CB	2.23	0.85
1:C:167:LEU:HD21	1:C:252:VAL:C	1.97	0.85
1:A:271:THR:HG21	1:A:288:THR:HG22	1.57	0.84
1:B:335:ASN:HB2	1:B:352:ASN:ND2	1.91	0.84
1:C:96:THR:HG23	1:C:105:VAL:HB	1.56	0.84
1:A:335:ASN:HB2	1:A:352:ASN:ND2	1.91	0.84
1:C:326:LEU:HB2	1:C:337:ILE:HD11	1.57	0.84
1:A:319:ARG:HG3	1:A:371:ALA:HB3	1.58	0.84
1:A:383:VAL:O	1:A:384:VAL:CG2	2.25	0.84
1:C:366:VAL:CG1	1:C:367:SER:N	2.40	0.84
1:B:132:LEU:HD12	1:B:239:LEU:O	1.78	0.84
1:C:178:LEU:HD22	1:C:241:ILE:HG12	1.58	0.84
1:A:226:SER:CB	1:C:185:GLN:HB3	2.07	0.84
1:C:279:ASP:HB3	1:C:282:GLY:CA	2.05	0.84
1:A:164:TYR:CE2	1:A:255:LEU:HD11	2.11	0.84
1:B:221:ARG:CD	1:B:234:ILE:O	2.25	0.84
1:B:269:THR:CG2	1:B:270:ASN:H	1.90	0.84
1:A:104:THR:HG21	1:A:263:LEU:HD12	1.59	0.84
1:C:152:PHE:CD2	1:C:264:TYR:O	2.28	0.84
1:B:319:ARG:HG3	1:B:371:ALA:HB3	1.57	0.84
1:B:298:THR:OG1	1:B:299:PRO:CD	2.26	0.84
1:A:222:TYR:O	1:A:234:ILE:CG2	2.26	0.83
1:C:335:ASN:HB2	1:C:352:ASN:ND2	1.91	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ASN:OD1	1:A:345:THR:CB	2.23	0.83
1:A:147:ALA:HB1	1:A:272:LEU:CD2	2.08	0.83
1:C:342:ASN:OD1	1:C:345:THR:CB	2.24	0.83
1:B:130:ASN:HD22	1:B:238:GLN:CD	1.81	0.83
1:B:321:LEU:O	1:B:322:THR:OG1	1.96	0.83
1:A:186:ASP:N	1:B:226:SER:HG	1.76	0.83
1:C:361:THR:C	1:C:362:VAL:CA	2.47	0.83
1:A:183:ASP:HB3	1:A:186:ASP:OD2	1.79	0.83
1:C:309:THR:HG23	1:C:356:SER:HA	1.60	0.83
1:A:185:GLN:HB3	1:B:226:SER:HB3	1.58	0.83
1:C:96:THR:CG2	1:C:105:VAL:HB	2.09	0.83
1:B:326:LEU:HD12	1:B:327:GLY:N	1.94	0.83
1:B:320:CYS:HB3	1:B:366:VAL:HG11	1.61	0.83
1:C:206:PRO:HG2	1:C:207:TRP:HD1	1.44	0.83
1:A:129:GLY:O	1:A:131:SER:N	2.11	0.83
1:C:326:LEU:HD12	1:C:327:GLY:N	1.94	0.83
1:C:321:LEU:O	1:C:322:THR:OG1	1.96	0.83
1:A:157:PHE:CD2	1:A:261:VAL:HG22	2.14	0.83
1:B:183:ASP:HB3	1:B:186:ASP:OD2	1.79	0.83
1:B:366:VAL:HG12	1:B:367:SER:H	1.44	0.83
1:C:183:ASP:CB	1:C:186:ASP:OD2	2.26	0.82
1:C:157:PHE:O	1:C:158:ASN:ND2	2.11	0.82
1:B:180:PHE:CD1	1:B:214:ILE:HD12	2.14	0.82
1:A:157:PHE:O	1:A:158:ASN:ND2	2.11	0.82
1:B:366:VAL:CG1	1:B:367:SER:N	2.40	0.82
1:C:320:CYS:HB3	1:C:366:VAL:HG11	1.61	0.82
1:B:309:THR:HG23	1:B:356:SER:HA	1.60	0.82
1:B:361:THR:C	1:B:362:VAL:CA	2.47	0.82
1:A:298:THR:OG1	1:A:299:PRO:CD	2.26	0.82
1:A:320:CYS:HB3	1:A:366:VAL:HG11	1.61	0.82
1:C:274[S]:SER:O	1:C:375:LEU:HA	1.79	0.82
1:B:383:VAL:O	1:B:384:VAL:HG23	1.80	0.82
1:A:361:THR:C	1:A:362:VAL:CA	2.47	0.82
1:A:366:VAL:CG1	1:A:367:SER:N	2.40	0.82
1:A:383:VAL:O	1:A:384:VAL:HG23	1.80	0.82
1:C:110:GLU:OE1	1:C:143:SER:N	2.12	0.82
1:C:385:ASN:OD1	1:C:386:LEU:N	2.13	0.82
1:A:309:THR:HG23	1:A:356:SER:HA	1.60	0.82
1:A:321:LEU:O	1:A:322:THR:OG1	1.96	0.82
1:A:326:LEU:HD12	1:A:327:GLY:N	1.94	0.81
1:C:204:THR:C	1:C:205:ALA:O	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:VAL:CG1	1:C:90:GLY:N	2.43	0.81
1:A:122:VAL:HG13	1:A:126:GLY:CA	2.10	0.81
1:B:152:PHE:CD2	1:B:263:LEU:HB3	2.15	0.81
1:C:279:ASP:C	1:C:280:LEU:CA	2.49	0.81
1:B:204:THR:HG22	1:B:205:ALA:O	1.79	0.81
1:B:262:THR:CG2	1:B:264:TYR:CZ	2.63	0.81
1:A:262:THR:CG2	1:A:264:TYR:CZ	2.62	0.81
1:B:206:PRO:CB	1:B:252:VAL:HG11	2.10	0.81
1:C:183:ASP:HB3	1:C:186:ASP:OD2	1.81	0.81
1:B:385:ASN:OD1	1:B:386:LEU:N	2.13	0.81
1:A:366:VAL:HG12	1:A:367:SER:H	1.44	0.81
1:A:385:ASN:OD1	1:A:386:LEU:N	2.13	0.81
1:C:178:LEU:CD2	1:C:241:ILE:HG12	2.11	0.81
1:C:124:ASN:OD1	1:C:132:LEU:HD11	1.81	0.81
1:C:335:ASN:HD22	1:C:353:CYS:N	1.78	0.81
1:C:298:THR:OG1	1:C:299:PRO:CD	2.26	0.81
1:C:383:VAL:O	1:C:384:VAL:HG23	1.80	0.81
1:C:262:THR:HG22	1:C:264:TYR:CZ	2.15	0.81
1:A:231:GLN:O	1:A:235:ASP:OD2	1.99	0.81
1:A:279:ASP:C	1:A:280:LEU:CA	2.49	0.81
1:C:89:VAL:CG1	1:C:90:GLY:H	1.93	0.80
1:A:267:GLN:O	1:C:197:ASN:HB2	1.81	0.80
1:B:189:PRO:HG3	1:B:198:PHE:HE2	1.46	0.80
1:B:342:ASN:ND2	1:B:345:THR:O	2.14	0.80
1:A:145:LEU:HB2	1:A:259:ARG:CZ	2.10	0.80
1:C:130:ASN:ND2	1:C:186:ASP:O	2.14	0.80
1:C:262:THR:HG21	1:C:264:TYR:OH	1.82	0.80
1:A:342:ASN:ND2	1:A:345:THR:O	2.14	0.80
1:C:145:LEU:HB3	1:C:146:PRO:HD3	1.62	0.80
1:B:157:PHE:CD2	1:B:261:VAL:HG22	2.16	0.80
1:A:183:ASP:CB	1:A:186:ASP:OD2	2.29	0.80
1:A:185:GLN:HB3	1:B:226:SER:CB	2.10	0.80
1:B:279:ASP:C	1:B:280:LEU:CA	2.49	0.80
1:A:195:LEU:HD23	1:A:201:LEU:CD1	2.11	0.80
1:B:335:ASN:HD22	1:B:353:CYS:N	1.78	0.80
1:C:195:LEU:HD23	1:C:201:LEU:CD1	2.11	0.80
1:A:335:ASN:HD22	1:A:353:CYS:N	1.78	0.80
1:C:241:ILE:HD13	1:C:255:LEU:HD22	1.63	0.80
1:A:225:ASP:HB3	1:C:186:ASP:OD1	1.79	0.80
1:C:127:ILE:HG22	1:C:128:VAL:N	1.97	0.80
1:C:104:THR:CG2	1:C:263:LEU:HD12	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:TYR:O	1:B:234:ILE:CG2	2.30	0.79
1:B:241:ILE:HD13	1:B:255:LEU:HD22	1.65	0.79
1:C:342:ASN:ND2	1:C:345:THR:O	2.15	0.79
1:C:366:VAL:HG12	1:C:367:SER:H	1.44	0.79
1:B:132:LEU:CD1	1:B:239:LEU:O	2.30	0.79
1:A:267:GLN:O	1:C:197:ASN:HB3	1.82	0.79
1:C:119:SER:HA	1:C:246:GLY:N	1.97	0.79
1:B:180:PHE:HD1	1:B:214:ILE:HD12	1.45	0.79
1:A:186:ASP:CA	1:B:226:SER:OG	2.29	0.79
1:C:217:ASP:CG	1:C:221:ARG:NH2	2.36	0.79
1:A:217:ASP:CG	1:A:221:ARG:NH2	2.36	0.79
1:C:138:ASN:C	1:C:140:THR:N	2.33	0.79
1:C:136:PRO:CB	1:C:145:LEU:HD22	2.10	0.79
1:A:114:GLN:HE21	1:A:251:ALA:HB2	1.46	0.79
1:A:318:LEU:N	1:A:347:SER:O	2.16	0.79
1:A:201:LEU:HD23	1:A:202:LYS:CA	2.13	0.79
1:C:309:THR:HG23	1:C:355:VAL:O	1.82	0.78
1:A:123:VAL:C	1:A:125:GLY:H	1.84	0.78
1:A:267:GLN:HB2	1:C:198:PHE:CD1	2.18	0.78
1:A:104:THR:CG2	1:A:263:LEU:CD1	2.60	0.78
1:A:136:PRO:CB	1:A:145:LEU:CD2	2.61	0.78
1:B:200:VAL:O	1:B:200:VAL:CG1	2.31	0.78
1:A:335:ASN:ND2	1:A:353:CYS:HA	1.98	0.78
1:B:162:LEU:HD12	1:B:212:LEU:HD23	1.64	0.78
1:A:298:THR:HG1	1:A:299:PRO:HD2	1.47	0.78
1:B:309:THR:HG23	1:B:355:VAL:O	1.82	0.78
1:B:228:THR:HG21	1:B:234:ILE:HD11	1.65	0.78
1:A:309:THR:HG23	1:A:355:VAL:O	1.82	0.78
1:C:195:LEU:CD2	1:C:201:LEU:CD1	2.62	0.78
1:C:118:SER:HG	1:C:243:THR:HG1	1.08	0.78
1:C:318:LEU:N	1:C:347:SER:O	2.16	0.78
1:B:168:CYS:SG	1:B:252:VAL:CG1	2.71	0.78
1:B:318:LEU:N	1:B:347:SER:O	2.16	0.78
1:C:114:GLN:HE21	1:C:251:ALA:HB2	1.48	0.77
1:A:167:LEU:CD2	1:A:167:LEU:H	1.95	0.77
1:C:145:LEU:HB3	1:C:146:PRO:CD	2.14	0.77
1:C:266:PRO:O	1:C:266:PRO:HG2	1.82	0.77
1:C:138:ASN:O	1:C:140:THR:CA	2.31	0.77
1:C:201:LEU:HD23	1:C:202:LYS:CA	2.14	0.77
1:B:119:SER:HA	1:B:246:GLY:N	1.99	0.77
1:B:335:ASN:ND2	1:B:353:CYS:HA	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:PHE:HD1	1:B:121:PHE:O	1.67	0.77
1:C:326:LEU:HD22	1:C:337:ILE:CD1	2.10	0.77
1:C:118:SER:O	1:C:119:SER:C	2.23	0.77
1:B:206:PRO:HB3	1:B:252:VAL:CG1	2.11	0.77
1:A:267:GLN:NE2	1:C:198:PHE:CZ	2.53	0.77
1:A:329:THR:O	1:A:361:THR:HG22	1.85	0.77
1:C:335:ASN:ND2	1:C:353:CYS:HA	1.99	0.77
1:B:328:ALA:HB1	1:B:362:VAL:HG22	1.64	0.77
1:A:328:ALA:HB1	1:A:362:VAL:HG22	1.64	0.77
1:C:316:GLY:O	1:C:349:TYR:N	2.17	0.77
1:A:316:GLY:O	1:A:349:TYR:N	2.17	0.77
1:A:200:VAL:CG1	1:A:200:VAL:O	2.29	0.77
1:B:300:THR:O	1:B:366:VAL:O	2.03	0.77
1:C:241:ILE:CD1	1:C:255:LEU:HD23	2.14	0.77
1:B:316:GLY:O	1:B:349:TYR:N	2.17	0.77
1:B:336:ASP:OD2	1:B:385:ASN:HB2	1.85	0.77
1:A:104:THR:HG23	1:A:263:LEU:HB2	1.64	0.77
1:B:183:ASP:CG	1:B:186:ASP:OD2	2.22	0.76
1:A:300:THR:O	1:A:366:VAL:O	2.03	0.76
1:C:329:THR:O	1:C:361:THR:HG22	1.84	0.76
1:C:336:ASP:OD2	1:C:385:ASN:HB2	1.85	0.76
1:C:317:GLY:CA	1:C:348:ASP:HA	2.13	0.76
1:C:67:ILE:CG2	1:C:68:ILE:H	1.92	0.76
1:B:297:ARG:HE	1:B:299:PRO:HA	1.50	0.76
1:A:320:CYS:HB2	1:A:366:VAL:HG12	1.67	0.76
1:A:317:GLY:CA	1:A:348:ASP:HA	2.13	0.76
1:A:195:LEU:CD2	1:A:201:LEU:CD1	2.62	0.76
1:B:329:THR:O	1:B:361:THR:HG22	1.85	0.76
1:C:331:ALA:O	1:C:332:VAL:CG2	2.33	0.76
1:B:183:ASP:C	1:B:185:GLN:H	1.89	0.76
1:C:118:SER:OG	1:C:243:THR:O	2.03	0.76
1:C:297:ARG:HE	1:C:299:PRO:HA	1.50	0.76
1:B:317:GLY:CA	1:B:348:ASP:HA	2.13	0.76
1:A:145:LEU:CB	1:A:146:PRO:HD3	2.16	0.76
1:B:145:LEU:HB3	1:B:146:PRO:HD3	1.68	0.76
1:A:297:ARG:HE	1:A:299:PRO:HA	1.50	0.76
1:B:177:ALA:HB2	1:B:203:GLU:OE1	1.86	0.76
1:C:300:THR:O	1:C:366:VAL:O	2.03	0.76
1:C:320:CYS:HB2	1:C:366:VAL:HG12	1.67	0.76
1:C:289:GLY:CA	1:C:290:PRO:C	2.50	0.76
1:A:321:LEU:HB2	1:A:344:GLY:H	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ASP:OD2	1:A:385:ASN:HB2	1.85	0.76
1:C:328:ALA:HB1	1:C:362:VAL:HG22	1.65	0.75
1:B:331:ALA:O	1:B:332:VAL:CG2	2.33	0.75
1:A:289:GLY:CA	1:A:290:PRO:C	2.50	0.75
1:A:145:LEU:HB3	1:A:146:PRO:CD	2.16	0.75
1:A:232:LYS:HD2	1:B:228:THR:CG2	2.16	0.75
1:B:289:GLY:CA	1:B:290:PRO:C	2.50	0.75
1:A:226:SER:HB3	1:C:185:GLN:C	2.06	0.75
1:C:138:ASN:O	1:C:139:GLY:C	2.25	0.75
1:A:331:ALA:O	1:A:332:VAL:CG2	2.33	0.75
1:B:321:LEU:HB2	1:B:344:GLY:H	1.51	0.75
1:A:183:ASP:C	1:A:185:GLN:H	1.90	0.75
1:B:326:LEU:CB	1:B:337:ILE:CD1	2.65	0.75
1:C:148:LEU:O	1:C:150:SER:N	2.18	0.75
1:C:167:LEU:CD2	1:C:167:LEU:H	2.00	0.74
1:C:121:PHE:C	1:C:121:PHE:CD1	2.59	0.74
1:A:326:LEU:HD22	1:A:337:ILE:CD1	2.10	0.74
1:C:295:LEU:H	1:C:295:LEU:HD23	1.52	0.74
1:C:98:ARG:O	1:C:100:SER:N	2.20	0.74
1:C:321:LEU:HB2	1:C:344:GLY:H	1.51	0.74
1:A:134:LEU:HD23	1:A:236:LEU:CD2	2.16	0.74
1:A:274[S]:SER:O	1:A:375:LEU:HA	1.87	0.74
1:C:168:CYS:CB	1:C:252:VAL:HG13	2.17	0.74
1:C:206:PRO:HB3	1:C:252:VAL:HG11	1.68	0.74
1:C:326:LEU:CB	1:C:337:ILE:CD1	2.65	0.74
1:C:168:CYS:HB3	1:C:252:VAL:HA	1.68	0.74
1:A:317:GLY:HA3	1:A:348:ASP:CA	2.13	0.74
1:C:82:VAL:C	1:C:170:THR:HG22	2.07	0.74
1:B:106:THR:O	1:B:260:SER:HA	1.85	0.74
1:C:134:LEU:CD2	1:C:236:LEU:HD23	2.16	0.74
1:A:123:VAL:HG12	1:A:124:ASN:ND2	2.03	0.74
1:A:230:ASP:O	1:A:232:LYS:N	2.20	0.74
1:C:222:TYR:O	1:C:234:ILE:CG2	2.35	0.74
1:A:326:LEU:CB	1:A:337:ILE:CD1	2.65	0.74
1:A:167:LEU:HD23	1:A:167:LEU:N	2.02	0.74
1:A:241:ILE:HD13	1:A:255:LEU:HD22	1.68	0.74
1:A:123:VAL:CG1	1:A:124:ASN:ND2	2.51	0.74
1:C:230:ASP:O	1:C:232:LYS:N	2.20	0.74
1:B:317:GLY:HA3	1:B:348:ASP:CA	2.13	0.74
1:A:123:VAL:O	1:A:124:ASN:C	2.25	0.73
1:B:152:PHE:CG	1:B:263:LEU:HB3	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ASN:O	1:A:249:ALA:HA	1.88	0.73
1:A:219:VAL:HB	1:A:221:ARG:NH2	2.03	0.73
1:B:300:THR:OG1	1:B:301:VAL:HG23	1.88	0.73
1:A:300:THR:OG1	1:A:301:VAL:HG23	1.88	0.73
1:C:219:VAL:HB	1:C:221:ARG:NH2	2.03	0.73
1:B:112:LEU:HG	1:B:141:LEU:CD1	2.19	0.73
1:C:317:GLY:HA3	1:C:348:ASP:CA	2.13	0.73
1:A:142:PHE:O	1:A:146:PRO:HG2	1.87	0.73
1:C:183:ASP:C	1:C:185:GLN:H	1.91	0.73
1:A:134:LEU:HD13	1:A:239:LEU:HD11	1.71	0.73
1:C:300:THR:OG1	1:C:301:VAL:HG23	1.88	0.73
1:A:295:LEU:HD23	1:A:295:LEU:H	1.52	0.73
1:C:157:PHE:CD2	1:C:261:VAL:HG22	2.23	0.73
1:C:98:ARG:HD2	1:C:105:VAL:HG23	1.69	0.73
1:C:114:GLN:NE2	1:C:251:ALA:HB2	2.02	0.73
1:B:106:THR:C	1:B:107:SER:CA	2.56	0.73
1:C:262:THR:CG2	1:C:264:TYR:CZ	2.72	0.73
1:C:366:VAL:CG1	1:C:367:SER:H	2.01	0.73
1:B:295:LEU:H	1:B:295:LEU:HD23	1.52	0.73
1:A:267:GLN:CB	1:C:198:PHE:CD1	2.72	0.72
1:A:278:LEU:CD2	1:A:295:LEU:O	2.37	0.72
1:C:274[S]:SER:O	1:C:376:VAL:N	2.21	0.72
1:A:366:VAL:CG1	1:A:367:SER:H	2.01	0.72
1:B:366:VAL:CG1	1:B:367:SER:H	2.01	0.72
1:A:341:ASP:OD1	1:A:347:SER:CB	2.38	0.72
1:C:341:ASP:OD1	1:C:347:SER:CB	2.38	0.72
1:C:169:GLY:O	1:C:171:THR:N	2.19	0.72
1:A:271:THR:HG21	1:A:288:THR:CG2	2.19	0.72
1:B:362:VAL:N	1:B:362:VAL:CB	2.52	0.72
1:B:119:SER:HA	1:B:246:GLY:H	1.53	0.72
1:C:98:ARG:HE	1:C:105:VAL:HG21	1.52	0.72
1:C:278:LEU:CD2	1:C:295:LEU:O	2.37	0.72
1:B:278:LEU:CD2	1:B:295:LEU:O	2.37	0.72
1:C:362:VAL:CB	1:C:362:VAL:N	2.52	0.72
1:C:67:ILE:O	1:C:68:ILE:O	2.08	0.72
1:B:341:ASP:OD1	1:B:347:SER:CB	2.38	0.72
1:C:266:PRO:O	1:C:266:PRO:CG	2.29	0.72
1:A:226:SER:OG	1:C:183:ASP:OD2	2.08	0.72
1:B:165:VAL:O	1:B:166:PRO:HB3	1.88	0.72
1:A:151:ASN:CG	1:A:269:THR:OG1	2.27	0.72
1:C:331:ALA:O	1:C:332:VAL:HG23	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:VAL:O	1:C:200:VAL:CG1	2.29	0.72
1:C:124:ASN:OD1	1:C:132:LEU:HD12	1.89	0.71
1:A:123:VAL:C	1:A:125:GLY:N	2.41	0.71
1:A:331:ALA:O	1:A:332:VAL:HG23	1.90	0.71
1:B:127:ILE:HG23	1:B:128:VAL:H	1.55	0.71
1:A:150:SER:O	1:A:269:THR:HA	1.89	0.71
1:B:136:PRO:HB2	1:B:145:LEU:HD22	1.72	0.71
1:B:130:ASN:ND2	1:B:238:GLN:NE2	2.38	0.71
1:C:132:LEU:CD1	1:C:239:LEU:O	2.38	0.71
1:A:103:VAL:CG1	1:A:263:LEU:O	2.39	0.71
1:A:268:PRO:C	1:A:269:THR:O	2.28	0.71
1:B:192:ARG:NH1	1:B:244:TYR:HB3	2.05	0.71
1:A:162:LEU:HD12	1:A:212:LEU:HD23	1.71	0.71
1:A:271:THR:CG2	1:A:273[S]:LEU:O	2.38	0.71
1:B:262:THR:CG2	1:B:264:TYR:OH	2.39	0.71
1:C:162:LEU:HD12	1:C:212:LEU:HD23	1.71	0.71
1:B:326:LEU:HD22	1:B:337:ILE:CD1	2.10	0.71
1:B:320:CYS:HB2	1:B:366:VAL:HG12	1.67	0.71
1:A:117:ASN:HB2	1:A:248:GLY:O	1.91	0.71
1:C:337:ILE:HG23	1:C:337:ILE:O	1.91	0.71
1:A:362:VAL:N	1:A:362:VAL:CB	2.52	0.71
1:C:183:ASP:CG	1:C:186:ASP:OD2	2.30	0.71
1:B:177:ALA:CB	1:B:203:GLU:OE1	2.39	0.71
1:A:355:VAL:CG1	1:A:360:ALA:HB2	2.20	0.71
1:A:186:ASP:OD1	1:B:225:ASP:HB3	1.91	0.70
1:A:262:THR:CG2	1:A:264:TYR:OH	2.39	0.70
1:A:241:ILE:CD1	1:A:255:LEU:HD23	2.20	0.70
1:B:201:LEU:HD23	1:B:202:LYS:CA	2.20	0.70
1:B:123:VAL:O	1:B:126:GLY:N	2.19	0.70
1:B:331:ALA:O	1:B:332:VAL:HG23	1.90	0.70
1:C:355:VAL:CG1	1:C:360:ALA:HB2	2.20	0.70
1:B:355:VAL:CG1	1:B:360:ALA:HB2	2.20	0.70
1:A:172:GLU:C	1:A:172:GLU:N	2.45	0.70
1:B:314:LEU:HD13	1:B:351:LEU:HD11	1.73	0.70
1:C:167:LEU:HD23	1:C:167:LEU:N	2.04	0.70
1:B:340:ILE:O	1:B:347:SER:OG	2.09	0.70
1:A:267:GLN:CG	1:A:268:PRO:CD	1.84	0.70
1:B:138:ASN:O	1:B:141:LEU:N	2.23	0.70
1:C:82:VAL:C	1:C:170:THR:CG2	2.60	0.70
1:C:277:ARG:CB	1:C:285:ALA:CB	2.56	0.70
1:A:355:VAL:HG13	1:A:360:ALA:CB	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LEU:HD13	1:A:351:LEU:HD11	1.73	0.70
1:B:271:THR:HG21	1:B:288:THR:CG2	2.21	0.70
1:C:134:LEU:HD23	1:C:236:LEU:CD2	2.21	0.70
1:A:337:ILE:HG23	1:A:337:ILE:O	1.91	0.70
1:A:169:GLY:O	1:A:171:THR:N	2.21	0.70
1:A:167:LEU:HD21	1:A:253:GLY:N	2.06	0.70
1:C:145:LEU:O	1:C:145:LEU:HD23	1.92	0.70
1:A:104:THR:CG2	1:A:263:LEU:CB	2.65	0.70
1:C:340:ILE:O	1:C:347:SER:OG	2.09	0.70
1:C:355:VAL:HG13	1:C:360:ALA:CB	2.22	0.70
1:A:340:ILE:O	1:A:347:SER:OG	2.09	0.69
1:A:266:PRO:O	1:C:199:GLY:N	2.25	0.69
1:B:231:GLN:O	1:B:235:ASP:OD2	2.09	0.69
1:C:231:GLN:O	1:C:235:ASP:OD2	2.10	0.69
1:C:74:VAL:O	1:C:75:GLY:C	2.30	0.69
1:C:117:ASN:O	1:C:249:ALA:HA	1.93	0.69
1:B:116:ASN:HA	1:B:251:ALA:HA	1.74	0.69
1:B:269:THR:CG2	1:B:270:ASN:N	2.52	0.69
1:A:262:THR:HG22	1:A:264:TYR:CE2	2.27	0.69
1:C:108:HIS:O	1:C:259:ARG:HB3	1.92	0.69
1:B:123:VAL:O	1:B:125:GLY:N	2.25	0.69
1:B:111:TYR:CE2	1:B:254:GLU:HG3	2.27	0.69
1:B:104:THR:HB	1:B:263:LEU:HB2	1.74	0.69
1:C:314:LEU:HD13	1:C:351:LEU:HD11	1.73	0.69
1:B:189:PRO:HG3	1:B:198:PHE:CE2	2.27	0.69
1:A:204:THR:HG22	1:A:205:ALA:O	1.92	0.69
1:C:128:VAL:HG13	1:C:188:GLU:OE1	1.92	0.69
1:C:98:ARG:CD	1:C:105:VAL:CG2	2.43	0.69
1:C:110:GLU:CD	1:C:144:TRP:H	1.95	0.69
1:B:121:PHE:CD1	1:B:121:PHE:C	2.65	0.69
1:B:121:PHE:CD1	1:B:121:PHE:O	2.46	0.69
1:C:183:ASP:OD1	1:C:232:LYS:HE2	1.93	0.69
1:B:103:VAL:HG13	1:B:264:TYR:HA	1.75	0.69
1:B:169:GLY:O	1:B:171:THR:N	2.22	0.69
1:C:351:LEU:C	1:C:351:LEU:CD1	2.61	0.68
1:A:104:THR:HG21	1:A:263:LEU:CD1	2.22	0.68
1:B:152:PHE:CD1	1:B:263:LEU:HD13	2.29	0.68
1:C:100:SER:OG	1:C:101:GLY:N	2.26	0.68
1:B:355:VAL:HG13	1:B:360:ALA:CB	2.22	0.68
1:A:351:LEU:CD1	1:A:351:LEU:C	2.61	0.68
1:C:103:VAL:HG12	1:C:263:LEU:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:THR:O	1:B:346:ALA:O	2.12	0.68
1:B:298:THR:HG1	1:B:299:PRO:HD2	1.56	0.68
1:C:167:LEU:CD2	1:C:253:GLY:N	2.56	0.68
1:B:107:SER:N	1:B:107:SER:CB	2.56	0.68
1:C:111:TYR:HD2	1:C:256:PHE:CE1	2.11	0.68
1:C:297:ARG:HG2	1:C:298:THR:N	2.08	0.68
1:A:277:ARG:HD2	1:A:286:ASP:OD1	1.93	0.68
1:C:274[S]:SER:O	1:C:375:LEU:CA	2.41	0.68
1:B:337:ILE:HG23	1:B:337:ILE:O	1.91	0.68
1:C:164:TYR:HB3	1:C:210:ALA:HB3	1.76	0.68
1:C:201:LEU:C	1:C:201:LEU:CD2	2.61	0.68
1:A:111:TYR:CE2	1:A:254:GLU:OE2	2.46	0.68
1:B:351:LEU:C	1:B:351:LEU:CD1	2.61	0.68
1:A:297:ARG:HG2	1:A:298:THR:N	2.08	0.68
1:A:167:LEU:HD23	1:A:252:VAL:O	1.93	0.68
1:B:204:THR:C	1:B:205:ALA:O	2.22	0.68
1:A:221:ARG:HH11	1:A:236:LEU:HA	1.59	0.68
1:C:277:ARG:HD2	1:C:286:ASP:OD1	1.93	0.68
1:B:222:TYR:O	1:B:234:ILE:HG23	1.95	0.67
1:B:230:ASP:O	1:B:232:LYS:N	2.26	0.67
1:A:345:THR:O	1:A:346:ALA:O	2.12	0.67
1:B:297:ARG:HG2	1:B:298:THR:N	2.08	0.67
1:A:168:CYS:CB	1:A:252:VAL:HG13	2.23	0.67
1:B:277:ARG:HD2	1:B:286:ASP:OD1	1.93	0.67
1:C:309:THR:CG2	1:C:356:SER:HA	2.24	0.67
1:A:117:ASN:OD1	1:A:252:VAL:HG21	1.95	0.67
1:B:309:THR:CG2	1:B:356:SER:HA	2.24	0.67
1:C:262:THR:CG2	1:C:264:TYR:CE2	2.75	0.67
1:C:320:CYS:SG	1:C:366:VAL:HG11	2.35	0.67
1:C:145:LEU:CB	1:C:146:PRO:HD3	2.16	0.67
1:C:104:THR:HG23	1:C:263:LEU:HB2	1.75	0.67
1:C:131:SER:O	1:C:132:LEU:C	2.31	0.67
1:A:320:CYS:SG	1:A:366:VAL:HG11	2.35	0.67
1:A:142:PHE:HB3	1:A:146:PRO:HD2	1.77	0.67
1:C:221:ARG:HH11	1:C:236:LEU:HA	1.60	0.67
1:C:89:VAL:HG12	1:C:90:GLY:H	1.54	0.67
1:A:309:THR:CG2	1:A:356:SER:HA	2.25	0.67
1:B:320:CYS:SG	1:B:366:VAL:HG11	2.35	0.67
1:B:262:THR:CG2	1:B:264:TYR:CE2	2.77	0.67
1:C:206:PRO:CG	1:C:207:TRP:H	2.06	0.67
1:C:129:GLY:O	1:C:130:ASN:C	2.33	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ASP:CB	1:C:282:GLY:HA3	2.22	0.67
1:C:206:PRO:HG2	1:C:207:TRP:H	1.59	0.67
1:A:110:GLU:CD	1:A:144:TRP:CB	2.63	0.66
1:A:267:GLN:HG3	1:A:268:PRO:N	2.05	0.66
1:C:345:THR:O	1:C:346:ALA:O	2.12	0.66
1:B:195:LEU:HD23	1:B:195:LEU:C	2.15	0.66
1:C:110:GLU:O	1:C:257:LEU:HB3	1.95	0.66
1:A:201:LEU:CD2	1:A:202:LYS:N	2.57	0.66
1:B:180:PHE:HB3	1:B:200:VAL:CG1	2.25	0.66
1:A:128:VAL:HG12	1:A:129:GLY:N	2.09	0.66
1:C:206:PRO:HG2	1:C:207:TRP:CD1	2.29	0.66
1:A:158:ASN:HB2	1:A:260:SER:OG	1.96	0.66
1:A:228:THR:HG21	1:A:234:ILE:HD11	1.76	0.66
1:A:104:THR:HG23	1:A:263:LEU:CD1	2.23	0.66
1:C:104:THR:CG2	1:C:263:LEU:CD1	2.73	0.66
1:B:206:PRO:CB	1:B:252:VAL:CG1	2.72	0.66
1:C:324:LEU:CD2	1:C:366:VAL:HG21	1.96	0.66
1:C:164:TYR:CD2	1:C:255:LEU:HD12	2.28	0.66
1:A:146:PRO:O	1:A:150:SER:OG	2.14	0.65
1:B:228:THR:HG21	1:B:234:ILE:CD1	2.25	0.65
1:B:119:SER:O	1:B:120:GLY:O	2.14	0.65
1:B:221:ARG:HH11	1:B:236:LEU:CA	1.98	0.65
1:A:326:LEU:C	1:A:326:LEU:HD12	2.16	0.65
1:A:383:VAL:C	1:A:384:VAL:HG23	2.16	0.65
1:C:127:ILE:CG2	1:C:128:VAL:N	2.58	0.65
1:B:232:LYS:HD2	1:C:228:THR:HG21	1.78	0.65
1:C:326:LEU:HD12	1:C:326:LEU:C	2.16	0.65
1:A:279:ASP:CB	1:A:282:GLY:HA3	2.22	0.65
1:B:383:VAL:C	1:B:384:VAL:HG23	2.17	0.65
1:C:99:THR:HG22	1:C:99:THR:O	1.97	0.65
1:A:222:TYR:O	1:A:234:ILE:HG23	1.94	0.65
1:A:347:SER:OG	1:A:348:ASP:N	2.29	0.65
1:C:88:LEU:CD1	1:C:256:PHE:CE2	2.80	0.65
1:B:335:ASN:HD21	1:B:354:THR:N	1.95	0.65
1:B:279:ASP:CB	1:B:282:GLY:HA3	2.22	0.65
1:A:164:TYR:HB3	1:A:210:ALA:HB3	1.78	0.65
1:C:179:TYR:CZ	1:C:240:GLY:HA3	2.32	0.65
1:A:226:SER:CB	1:C:185:GLN:CB	2.74	0.65
1:B:145:LEU:O	1:B:145:LEU:HD23	1.97	0.65
1:A:138:ASN:O	1:A:141:LEU:N	2.29	0.65
1:A:183:ASP:OD1	1:A:232:LYS:HE2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:LEU:HD23	1:C:252:VAL:C	2.15	0.65
1:A:111:TYR:HE2	1:A:254:GLU:OE2	1.80	0.64
1:A:274[P]:SER:O	1:A:375:LEU:CA	2.44	0.64
1:A:335:ASN:HD21	1:A:354:THR:N	1.95	0.64
1:A:122:VAL:HG13	1:A:126:GLY:HA3	1.79	0.64
1:A:150:SER:O	1:A:269:THR:CA	2.45	0.64
1:B:122:VAL:HG12	1:B:123:VAL:N	2.11	0.64
1:B:110:GLU:CD	1:B:144:TRP:HB3	2.18	0.64
1:C:201:LEU:CD2	1:C:202:LYS:N	2.57	0.64
1:C:383:VAL:C	1:C:384:VAL:HG23	2.17	0.64
1:A:108:HIS:O	1:A:259:ARG:N	2.28	0.64
1:A:180:PHE:O	1:A:180:PHE:HD2	1.79	0.64
1:B:112:LEU:CD2	1:B:113:THR:HG22	2.27	0.64
1:B:121:PHE:O	1:B:122:VAL:HA	1.97	0.64
1:B:192:ARG:CD	1:B:192:ARG:H	2.10	0.64
1:C:133:GLN:HB2	1:C:138:ASN:HD21	1.62	0.64
1:A:338:LEU:HD23	1:A:338:LEU:C	2.18	0.64
1:A:226:SER:HB3	1:C:186:ASP:N	2.13	0.64
1:C:123:VAL:O	1:C:126:GLY:N	2.20	0.64
1:C:335:ASN:HB2	1:C:352:ASN:HD22	1.58	0.64
1:B:326:LEU:C	1:B:326:LEU:HD12	2.16	0.64
1:A:326:LEU:CB	1:A:337:ILE:HD12	2.28	0.64
1:B:129:GLY:O	1:B:131:SER:N	2.30	0.64
1:C:175:ARG:HG2	1:C:244:TYR:CZ	2.33	0.64
1:B:326:LEU:CB	1:B:337:ILE:HD12	2.28	0.64
1:B:338:LEU:HD23	1:B:338:LEU:C	2.18	0.64
1:C:335:ASN:HD21	1:C:354:THR:N	1.95	0.64
1:C:338:LEU:C	1:C:338:LEU:HD23	2.18	0.64
1:B:324:LEU:HD22	1:B:366:VAL:HG23	1.80	0.64
1:A:115:VAL:N	1:A:253:GLY:O	2.29	0.64
1:C:298:THR:O	1:C:300:THR:N	2.31	0.63
1:C:274[P]:SER:O	1:C:375:LEU:CA	2.44	0.63
1:B:347:SER:OG	1:B:348:ASP:N	2.29	0.63
1:A:355:VAL:CG1	1:A:360:ALA:CB	2.77	0.63
1:C:355:VAL:CG1	1:C:360:ALA:CB	2.77	0.63
1:B:118:SER:OG	1:B:122:VAL:HG23	1.97	0.63
1:C:278:LEU:CG	1:C:295:LEU:O	2.47	0.63
1:B:298:THR:O	1:B:300:THR:N	2.31	0.63
1:A:267:GLN:HA	1:C:198:PHE:HA	1.79	0.63
1:C:283:SER:O	1:C:284:LEU:HG	1.98	0.63
1:C:67:ILE:CG2	1:C:68:ILE:N	2.41	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:SER:O	1:B:284:LEU:HG	1.98	0.63
1:A:206:PRO:HB3	1:A:252:VAL:HG12	1.80	0.63
1:C:275[S]:SER:HA	1:C:375:LEU:CD2	2.21	0.63
1:B:132:LEU:O	1:B:141:LEU:CD2	2.46	0.63
1:B:155:TYR:OH	1:B:221:ARG:HD2	1.97	0.63
1:A:180:PHE:CD2	1:A:180:PHE:O	2.51	0.63
1:A:201:LEU:C	1:A:201:LEU:CD2	2.61	0.63
1:B:355:VAL:CG1	1:B:360:ALA:CB	2.77	0.63
1:B:278:LEU:CG	1:B:295:LEU:O	2.47	0.63
1:C:274[S]:SER:HB2	1:C:376:VAL:O	1.99	0.63
1:C:342:ASN:O	1:C:343:VAL:O	2.16	0.63
1:A:298:THR:O	1:A:300:THR:N	2.31	0.63
1:A:278:LEU:CG	1:A:295:LEU:O	2.47	0.63
1:C:228:THR:HG21	1:C:234:ILE:HD11	1.80	0.63
1:C:336:ASP:OD2	1:C:385:ASN:CB	2.47	0.63
1:A:171:THR:C	1:A:172:GLU:CA	2.62	0.63
1:B:335:ASN:HB2	1:B:352:ASN:HD22	1.57	0.63
1:A:147:ALA:CA	1:A:272:LEU:CD2	2.64	0.63
1:B:295:LEU:N	1:B:295:LEU:HD23	2.14	0.63
1:A:164:TYR:CD2	1:A:255:LEU:HD12	2.31	0.63
1:B:314:LEU:HD13	1:B:351:LEU:CD1	2.29	0.63
1:A:283:SER:O	1:A:284:LEU:HG	1.98	0.63
1:A:277:ARG:CB	1:A:285:ALA:CB	2.56	0.63
1:C:145:LEU:HD12	1:C:259:ARG:HD3	1.80	0.63
1:B:321:LEU:HD23	1:B:321:LEU:N	2.14	0.63
1:C:321:LEU:N	1:C:321:LEU:HD23	2.14	0.63
1:A:295:LEU:HD23	1:A:295:LEU:N	2.14	0.62
1:A:314:LEU:HD13	1:A:351:LEU:CD1	2.29	0.62
1:C:114:GLN:HE21	1:C:251:ALA:CB	2.11	0.62
1:A:342:ASN:O	1:A:343:VAL:O	2.16	0.62
1:B:201:LEU:C	1:B:201:LEU:CD2	2.61	0.62
1:C:127:ILE:CD1	1:C:358:LEU:HD13	2.29	0.62
1:C:214:ILE:HD11	1:C:239:LEU:HD21	1.81	0.62
1:C:324:LEU:HD22	1:C:366:VAL:HG23	1.80	0.62
1:B:331:ALA:HB3	1:B:357:SER:CB	2.23	0.62
1:A:321:LEU:N	1:A:321:LEU:HD23	2.14	0.62
1:B:122:VAL:CB	1:B:122:VAL:N	2.60	0.62
1:C:314:LEU:HD13	1:C:351:LEU:CD1	2.29	0.62
1:A:233:LEU:HD21	1:B:234:ILE:HG12	1.82	0.62
1:C:119:SER:HA	1:C:246:GLY:H	1.62	0.62
1:B:180:PHE:HB3	1:B:200:VAL:HG11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:GLU:OE1	1:C:144:TRP:N	2.23	0.62
1:C:132:LEU:HD13	1:C:239:LEU:O	1.98	0.62
1:A:336:ASP:OD2	1:A:385:ASN:CB	2.47	0.62
1:A:168:CYS:HB3	1:A:252:VAL:HA	1.82	0.62
1:C:295:LEU:HD23	1:C:295:LEU:N	2.14	0.62
1:B:336:ASP:OD2	1:B:385:ASN:CB	2.47	0.62
1:A:142:PHE:O	1:A:146:PRO:CG	2.48	0.61
1:B:342:ASN:O	1:B:343:VAL:O	2.16	0.61
1:C:162:LEU:N	1:C:212:LEU:O	2.29	0.61
1:A:123:VAL:HG12	1:A:124:ASN:HD22	1.63	0.61
1:C:222:TYR:O	1:C:234:ILE:HG23	1.99	0.61
1:A:195:LEU:HD23	1:A:195:LEU:C	2.21	0.61
1:C:195:LEU:C	1:C:195:LEU:HD23	2.21	0.61
1:C:154:GLN:HB2	1:C:264:TYR:HB2	1.82	0.61
1:C:108:HIS:CD2	1:C:109:ARG:H	2.18	0.61
1:C:347:SER:OG	1:C:348:ASP:N	2.29	0.61
1:A:234:ILE:HD11	1:C:232:LYS:HD2	1.82	0.61
1:C:351:LEU:CD1	1:C:352:ASN:N	2.64	0.61
1:C:162:LEU:HB2	1:C:212:LEU:HB3	1.82	0.61
1:A:108:HIS:CG	1:A:109:ARG:H	2.18	0.61
1:A:183:ASP:CG	1:A:186:ASP:OD2	2.38	0.61
1:A:271:THR:CG2	1:A:271:THR:O	2.45	0.61
1:B:117:ASN:N	1:B:250:ASP:O	2.33	0.61
1:A:351:LEU:CD1	1:A:352:ASN:N	2.64	0.61
1:A:160:VAL:HA	1:A:258:ALA:O	2.01	0.61
1:B:132:LEU:O	1:B:141:LEU:HD23	2.00	0.61
1:B:135:ASN:OD1	1:B:155:TYR:CE1	2.54	0.61
1:C:338:LEU:HD12	1:C:385:ASN:HA	1.83	0.61
1:A:206:PRO:CB	1:A:252:VAL:HG11	2.28	0.61
1:B:121:PHE:O	1:B:122:VAL:CA	2.49	0.61
1:B:124:ASN:OD1	1:B:132:LEU:CD1	2.48	0.61
1:C:326:LEU:CB	1:C:337:ILE:HD12	2.28	0.61
1:A:300:THR:C	1:A:369:VAL:CG2	2.69	0.61
1:A:331:ALA:HB3	1:A:357:SER:CB	2.23	0.61
1:B:274[S]:SER:N	1:B:376:VAL:O	2.30	0.61
1:B:170:THR:O	1:B:170:THR:CG2	2.45	0.61
1:C:110:GLU:OE1	1:C:142:PHE:C	2.38	0.61
1:A:267:GLN:CD	1:C:198:PHE:HE1	2.04	0.60
1:C:103:VAL:CG1	1:C:263:LEU:O	2.49	0.60
1:C:204:THR:CG2	1:C:205:ALA:O	2.40	0.60
1:A:162:LEU:HD13	1:A:178:LEU:CD1	2.25	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ARG:CB	1:B:285:ALA:CB	2.56	0.60
1:B:107:SER:N	1:B:107:SER:C	2.52	0.60
1:A:226:SER:OG	1:C:185:GLN:HB2	2.00	0.60
1:A:329:THR:N	1:A:361:THR:HG23	2.16	0.60
1:B:160:VAL:HB	1:B:214:ILE:HB	1.83	0.60
1:B:351:LEU:CD1	1:B:352:ASN:N	2.64	0.60
1:C:300:THR:C	1:C:369:VAL:CG2	2.70	0.60
1:A:114:GLN:NE2	1:A:251:ALA:HB2	2.16	0.60
1:C:133:GLN:HE21	1:C:184:SER:HG	1.49	0.60
1:A:180:PHE:CD2	1:A:180:PHE:C	2.74	0.60
1:A:338:LEU:HD12	1:A:385:ASN:HA	1.83	0.60
1:A:114:GLN:HE21	1:A:251:ALA:CB	2.13	0.60
1:B:301:VAL:N	1:B:369:VAL:HG21	2.16	0.60
1:A:161:VAL:HB	1:A:258:ALA:HB3	1.83	0.60
1:A:145:LEU:HD12	1:A:259:ARG:CD	2.25	0.60
1:C:161:VAL:HB	1:C:258:ALA:HB3	1.84	0.60
1:C:70:HIS:HB3	1:C:79:MET:CE	2.32	0.60
1:B:300:THR:C	1:B:369:VAL:CG2	2.69	0.60
1:A:301:VAL:N	1:A:369:VAL:HG21	2.17	0.60
1:C:301:VAL:N	1:C:369:VAL:HG21	2.16	0.60
1:B:155:TYR:OH	1:B:234:ILE:O	2.18	0.60
1:C:274[P]:SER:HB2	1:C:376:VAL:O	2.02	0.60
1:A:274[P]:SER:HB2	1:A:376:VAL:O	2.02	0.60
1:B:338:LEU:HD12	1:B:385:ASN:HA	1.83	0.60
1:C:67:ILE:O	1:C:68:ILE:C	2.40	0.60
1:B:145:LEU:HD21	1:B:149:ALA:HB2	1.84	0.59
1:B:232:LYS:HG3	1:B:233:LEU:N	2.17	0.59
1:A:324:LEU:HD22	1:A:366:VAL:HG23	1.80	0.59
1:C:168:CYS:SG	1:C:252:VAL:HG12	2.40	0.59
1:B:148:LEU:C	1:B:150:SER:H	2.06	0.59
1:B:297:ARG:HG3	1:B:298:THR:O	2.03	0.59
1:A:297:ARG:HG3	1:A:298:THR:O	2.03	0.59
1:A:162:LEU:HB3	1:A:178:LEU:CD1	2.32	0.59
1:A:162:LEU:N	1:A:212:LEU:O	2.28	0.59
1:B:157:PHE:CE2	1:B:261:VAL:HG22	2.37	0.59
1:C:138:ASN:C	1:C:140:THR:H	2.03	0.59
1:A:280:LEU:HB3	1:A:370:ALA:O	2.03	0.59
1:A:162:LEU:HB2	1:A:212:LEU:HB3	1.82	0.59
1:C:383:VAL:O	1:C:384:VAL:HG22	2.02	0.59
1:A:274[P]:SER:O	1:A:376:VAL:N	2.36	0.59
1:C:155:TYR:OH	1:C:221:ARG:HD2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:TYR:CD2	1:A:349:TYR:O	2.56	0.59
1:B:318:LEU:O	1:B:347:SER:N	2.29	0.59
1:B:280:LEU:HB3	1:B:370:ALA:O	2.03	0.59
1:A:383:VAL:O	1:A:384:VAL:HG22	2.02	0.59
1:A:128:VAL:HG12	1:A:129:GLY:H	1.65	0.59
1:C:349:TYR:CD2	1:C:349:TYR:O	2.55	0.59
1:A:112:LEU:CD2	1:A:113:THR:HG22	2.32	0.59
1:B:152:PHE:CD2	1:B:264:TYR:O	2.46	0.59
1:C:103:VAL:CG1	1:C:263:LEU:C	2.71	0.59
1:C:297:ARG:HG3	1:C:298:THR:O	2.03	0.59
1:A:107:SER:HA	1:A:259:ARG:O	2.02	0.59
1:C:167:LEU:HD11	1:C:251:ALA:HB1	1.85	0.59
1:A:155:TYR:OH	1:A:221:ARG:HD2	2.02	0.59
1:B:145:LEU:O	1:B:146:PRO:C	2.41	0.59
1:A:314:LEU:HD22	1:A:351:LEU:HD11	1.85	0.59
1:C:280:LEU:HB3	1:C:370:ALA:O	2.03	0.59
1:B:383:VAL:O	1:B:384:VAL:HG22	2.02	0.59
1:B:111:TYR:HA	1:B:256:PHE:CD1	2.38	0.58
1:A:267:GLN:CG	1:A:268:PRO:N	2.60	0.58
1:C:331:ALA:C	1:C:332:VAL:HG23	2.24	0.58
1:C:132:LEU:HD12	1:C:239:LEU:O	2.03	0.58
1:B:349:TYR:CD2	1:B:349:TYR:O	2.56	0.58
1:A:162:LEU:HD13	1:A:178:LEU:HB3	1.84	0.58
1:B:160:VAL:HA	1:B:258:ALA:O	2.03	0.58
1:C:162:LEU:HB3	1:C:178:LEU:CD1	2.33	0.58
1:B:195:LEU:HD23	1:B:201:LEU:HD12	1.85	0.58
1:A:186:ASP:HA	1:B:226:SER:OG	2.02	0.58
1:B:314:LEU:HD22	1:B:351:LEU:HD11	1.85	0.58
1:B:280:LEU:HA	1:B:370:ALA:O	2.04	0.58
1:B:321:LEU:HB2	1:B:344:GLY:N	2.18	0.58
1:C:114:GLN:NE2	1:C:251:ALA:CB	2.66	0.58
1:B:331:ALA:C	1:B:332:VAL:HG23	2.24	0.58
1:C:103:VAL:HG11	1:C:264:TYR:N	2.18	0.58
1:C:318:LEU:O	1:C:347:SER:N	2.29	0.58
1:A:116:ASN:HA	1:A:250:ASP:O	2.03	0.58
1:A:280:LEU:HA	1:A:370:ALA:O	2.04	0.58
1:C:274[P]:SER:N	1:C:376:VAL:O	2.29	0.58
1:A:331:ALA:C	1:A:332:VAL:HG23	2.24	0.58
1:A:336:ASP:O	1:A:351:LEU:CA	2.45	0.58
1:B:335:ASN:HD22	1:B:353:CYS:HA	1.60	0.58
1:B:161:VAL:CB	1:B:258:ALA:HB3	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:ASN:CG	1:C:345:THR:HB	2.20	0.58
1:A:111:TYR:HE2	1:A:254:GLU:CD	2.08	0.57
1:B:329:THR:N	1:B:361:THR:HG23	2.16	0.57
1:B:336:ASP:O	1:B:351:LEU:CA	2.45	0.57
1:B:280:LEU:CA	1:B:370:ALA:O	2.52	0.57
1:A:329:THR:H	1:A:361:THR:HG23	1.69	0.57
1:C:329:THR:N	1:C:361:THR:HG23	2.16	0.57
1:B:276:LYS:HB2	1:B:374:LEU:HD21	1.86	0.57
1:A:167:LEU:CD2	1:A:252:VAL:C	2.72	0.57
1:B:201:LEU:CD2	1:B:202:LYS:N	2.66	0.57
1:A:132:LEU:HD13	1:A:239:LEU:O	2.00	0.57
1:B:130:ASN:ND2	1:B:238:GLN:CD	2.53	0.57
1:C:98:ARG:C	1:C:100:SER:H	2.07	0.57
1:C:103:VAL:HG12	1:C:263:LEU:C	2.24	0.57
1:B:342:ASN:CG	1:B:345:THR:HB	2.20	0.57
1:C:341:ASP:OD1	1:C:347:SER:HB2	2.04	0.57
1:A:276:LYS:HB2	1:A:374:LEU:CD2	2.34	0.57
1:A:214:ILE:HG22	1:A:215:PRO:N	2.17	0.57
1:A:222:TYR:O	1:A:234:ILE:HG21	2.03	0.57
1:C:112:LEU:HG	1:C:141:LEU:CD1	2.34	0.57
1:A:180:PHE:HB3	1:A:200:VAL:HB	1.87	0.57
1:C:329:THR:H	1:C:361:THR:HG23	1.69	0.57
1:C:314:LEU:HD22	1:C:351:LEU:HD11	1.85	0.57
1:C:276:LYS:HB2	1:C:374:LEU:HD21	1.86	0.57
1:C:280:LEU:HA	1:C:370:ALA:O	2.04	0.57
1:A:147:ALA:CB	1:A:272:LEU:CD1	2.80	0.57
1:B:276:LYS:HB2	1:B:374:LEU:CD2	2.34	0.57
1:C:195:LEU:HD21	1:C:201:LEU:CD1	2.31	0.57
1:B:122:VAL:CG1	1:B:123:VAL:N	2.67	0.57
1:B:145:LEU:HB3	1:B:146:PRO:CD	2.34	0.57
1:A:280:LEU:CA	1:A:370:ALA:O	2.52	0.57
1:A:276:LYS:HB2	1:A:374:LEU:HD21	1.86	0.57
1:C:341:ASP:OD1	1:C:347:SER:OG	2.22	0.57
1:C:336:ASP:O	1:C:351:LEU:CA	2.45	0.57
1:C:82:VAL:CA	1:C:170:THR:HG21	2.35	0.57
1:A:167:LEU:HD21	1:A:252:VAL:C	2.25	0.57
1:B:206:PRO:HG2	1:B:207:TRP:CD1	2.39	0.57
1:B:190:ALA:CB	1:B:194:GLU:OE2	2.51	0.57
1:B:329:THR:H	1:B:361:THR:HG23	1.69	0.57
1:C:280:LEU:CA	1:C:370:ALA:O	2.53	0.57
1:C:311:THR:CG2	1:C:379:ALA:O	2.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LEU:HD12	1:B:259:ARG:CD	2.30	0.57
1:B:132:LEU:HB3	1:B:239:LEU:HB2	1.85	0.57
1:B:165:VAL:HG12	1:B:166:PRO:N	2.20	0.57
1:C:74:VAL:O	1:C:75:GLY:O	2.23	0.57
1:B:183:ASP:OD1	1:B:232:LYS:HE2	2.05	0.56
1:B:317:GLY:HA3	1:B:347:SER:O	2.05	0.56
1:A:341:ASP:OD1	1:A:347:SER:HB2	2.04	0.56
1:C:321:LEU:HB2	1:C:344:GLY:N	2.18	0.56
1:A:157:PHE:CD1	1:A:236:LEU:HD22	2.40	0.56
1:C:274[P]:SER:O	1:C:376:VAL:N	2.36	0.56
1:B:341:ASP:OD1	1:B:347:SER:OG	2.22	0.56
1:A:185:GLN:CB	1:B:226:SER:CB	2.81	0.56
1:C:181:ASP:HB3	1:C:238:GLN:HB3	1.85	0.56
1:A:134:LEU:HD13	1:A:239:LEU:CD1	2.35	0.56
1:C:122:VAL:HG12	1:C:123:VAL:N	2.20	0.56
1:C:276:LYS:HB2	1:C:374:LEU:CD2	2.34	0.56
1:B:300:THR:C	1:B:369:VAL:HG23	2.26	0.56
1:B:341:ASP:OD1	1:B:347:SER:HB2	2.04	0.56
1:A:317:GLY:HA3	1:A:347:SER:O	2.06	0.56
1:B:142:PHE:HB3	1:B:146:PRO:HD2	1.86	0.56
1:A:230:ASP:OD2	1:C:230:ASP:OD2	2.24	0.56
1:C:214:ILE:HG22	1:C:215:PRO:N	2.17	0.56
1:A:335:ASN:HD22	1:A:353:CYS:HA	1.60	0.56
1:B:298:THR:HG22	1:B:301:VAL:O	2.05	0.56
1:C:300:THR:C	1:C:369:VAL:HG23	2.26	0.56
1:C:298:THR:HG22	1:C:301:VAL:O	2.05	0.56
1:C:190:ALA:HB3	1:C:194:GLU:CD	2.23	0.56
1:C:262:THR:CG2	1:C:264:TYR:OH	2.53	0.56
1:B:241:ILE:CD1	1:B:255:LEU:HD21	2.22	0.56
1:C:317:GLY:HA3	1:C:347:SER:O	2.06	0.56
1:A:326:LEU:HB2	1:A:337:ILE:HD12	1.85	0.56
1:A:342:ASN:CG	1:A:345:THR:HB	2.20	0.56
1:A:265:PHE:N	1:A:265:PHE:CD1	2.73	0.56
1:A:168:CYS:HG	1:A:252:VAL:CG1	2.16	0.56
1:A:219:VAL:CB	1:A:221:ARG:HH21	2.11	0.56
1:B:183:ASP:C	1:B:185:GLN:N	2.54	0.56
1:B:328:ALA:HB1	1:B:361:THR:O	2.06	0.56
1:A:298:THR:HG22	1:A:301:VAL:O	2.05	0.56
1:A:341:ASP:OD1	1:A:347:SER:OG	2.22	0.56
1:C:180:PHE:CD2	1:C:180:PHE:C	2.79	0.56
1:A:110:GLU:CG	1:A:144:TRP:HB3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:O	1:A:141:LEU:HD12	2.05	0.56
1:C:180:PHE:CD2	1:C:180:PHE:O	2.59	0.56
1:A:136:PRO:CB	1:A:145:LEU:HD21	2.36	0.55
1:C:328:ALA:HB1	1:C:361:THR:O	2.06	0.55
1:B:180:PHE:CD2	1:B:180:PHE:O	2.59	0.55
1:B:326:LEU:CG	1:B:337:ILE:HD12	2.29	0.55
1:C:82:VAL:HA	1:C:170:THR:HG21	1.88	0.55
1:C:108:HIS:O	1:C:259:ARG:CB	2.54	0.55
1:B:265:PHE:N	1:B:265:PHE:CD1	2.74	0.55
1:C:130:ASN:ND2	1:C:238:GLN:OE1	2.38	0.55
1:C:223:CYS:CA	1:C:224:ASN:N	2.62	0.55
1:A:328:ALA:HB1	1:A:361:THR:O	2.06	0.55
1:C:170:THR:OG1	1:C:170:THR:O	2.24	0.55
1:C:157:PHE:CD1	1:C:236:LEU:HD22	2.41	0.55
1:A:326:LEU:CG	1:A:337:ILE:HD12	2.29	0.55
1:A:267:GLN:CA	1:C:198:PHE:HA	2.36	0.55
1:C:133:GLN:HB2	1:C:138:ASN:ND2	2.21	0.55
1:C:162:LEU:CD1	1:C:178:LEU:HD13	2.32	0.55
1:B:111:TYR:CE2	1:B:254:GLU:CG	2.89	0.55
1:A:300:THR:C	1:A:369:VAL:HG23	2.26	0.55
1:C:160:VAL:HA	1:C:258:ALA:O	2.06	0.55
1:C:326:LEU:CG	1:C:337:ILE:HD12	2.29	0.55
1:A:130:ASN:O	1:A:131:SER:C	2.45	0.55
1:C:118:SER:O	1:C:120:GLY:N	2.40	0.55
1:A:318:LEU:O	1:A:347:SER:N	2.29	0.55
1:B:188:GLU:N	1:B:188:GLU:OE2	2.39	0.55
1:C:91:SER:OG	1:C:108:HIS:CD2	2.60	0.55
1:B:152:PHE:CE2	1:B:263:LEU:HB3	2.41	0.54
1:C:232:LYS:HG3	1:C:233:LEU:N	2.22	0.54
1:B:329:THR:C	1:B:361:THR:HG22	2.25	0.54
1:C:127:ILE:HG22	1:C:128:VAL:H	1.71	0.54
1:B:275:SER:HB2	1:B:375:LEU:HD21	1.88	0.54
1:B:165:VAL:O	1:B:166:PRO:CB	2.55	0.54
1:A:108:HIS:CG	1:A:109:ARG:N	2.76	0.54
1:B:297:ARG:CG	1:B:298:THR:N	2.70	0.54
1:B:152:PHE:CE1	1:B:263:LEU:CD1	2.78	0.54
1:A:319:ARG:HA	1:A:346:ALA:HA	1.90	0.54
1:A:331:ALA:O	1:A:332:VAL:HG22	2.07	0.54
1:A:204:THR:C	1:A:205:ALA:O	2.41	0.54
1:A:228:THR:CG2	1:C:232:LYS:CE	2.85	0.54
1:B:138:ASN:OD1	1:B:140:THR:HB	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ALA:O	1:C:332:VAL:HG22	2.07	0.54
1:B:319:ARG:HA	1:B:346:ALA:HA	1.90	0.54
1:A:297:ARG:CG	1:A:298:THR:N	2.70	0.54
1:C:289:GLY:HA3	1:C:290:PRO:O	1.99	0.54
1:C:151:ASN:O	1:C:267:GLN:N	2.41	0.54
1:A:321:LEU:HB2	1:A:344:GLY:N	2.18	0.54
1:A:274[P]:SER:N	1:A:376:VAL:O	2.30	0.54
1:B:104:THR:HG1	1:B:152:PHE:HZ	1.54	0.54
1:C:127:ILE:CG2	1:C:128:VAL:H	2.19	0.54
1:A:326:LEU:HD21	1:A:334:ILE:HD13	1.90	0.54
1:B:180:PHE:C	1:B:180:PHE:CD2	2.81	0.54
1:C:297:ARG:CG	1:C:298:THR:N	2.70	0.54
1:C:267:GLN:O	1:C:268:PRO:C	2.46	0.54
1:B:311:THR:CG2	1:B:379:ALA:O	2.50	0.54
1:B:216:THR:HG22	1:B:217:ASP:O	2.07	0.54
1:C:183:ASP:C	1:C:185:GLN:N	2.56	0.54
1:B:180:PHE:HD2	1:B:180:PHE:O	1.91	0.54
1:B:326:LEU:HD21	1:B:334:ILE:HD13	1.90	0.54
1:B:274[P]:SER:N	1:B:376:VAL:O	2.30	0.54
1:A:183:ASP:HB2	1:B:153:ASP:OD2	2.08	0.54
1:B:124:ASN:OD1	1:B:132:LEU:HD12	2.07	0.54
1:C:91:SER:HB2	1:C:109:ARG:NE	2.23	0.54
1:B:275:SER:HB2	1:B:375:LEU:CD2	2.38	0.54
1:C:131:SER:HB2	1:C:140:THR:HG21	1.89	0.54
1:C:329:THR:C	1:C:361:THR:HG22	2.24	0.54
1:B:192:ARG:CD	1:B:192:ARG:N	2.71	0.53
1:C:274[S]:SER:CB	1:C:376:VAL:O	2.56	0.53
1:B:164:TYR:HE2	1:B:253:GLY:HA3	1.73	0.53
1:B:138:ASN:O	1:B:139:GLY:C	2.44	0.53
1:B:145:LEU:CD1	1:B:259:ARG:HD3	2.28	0.53
1:A:228:THR:HA	1:C:230:ASP:OD1	2.09	0.53
1:C:319:ARG:HA	1:C:346:ALA:HA	1.90	0.53
1:C:180:PHE:O	1:C:180:PHE:HD2	1.90	0.53
1:A:180:PHE:HD1	1:A:214:ILE:HD12	1.72	0.53
1:C:275[S]:SER:N	1:C:375:LEU:HD23	2.23	0.53
1:A:311:THR:CG2	1:A:379:ALA:O	2.50	0.53
1:B:232:LYS:HG3	1:B:233:LEU:H	1.71	0.53
1:C:300:THR:CB	1:C:301:VAL:HG23	2.39	0.53
1:C:289:GLY:HA3	1:C:290:PRO:C	2.28	0.53
1:A:329:THR:C	1:A:361:THR:HG22	2.25	0.53
1:A:201:LEU:CD2	1:A:203:GLU:HG2	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LYS:HG3	1:A:233:LEU:N	2.23	0.53
1:B:111:TYR:HE2	1:B:254:GLU:HG3	1.72	0.53
1:B:204:THR:O	1:B:205:ALA:O	2.26	0.53
1:A:150:SER:O	1:A:270:ASN:N	2.42	0.53
1:C:132:LEU:O	1:C:141:LEU:CD2	2.56	0.53
1:B:328:ALA:HB2	1:B:362:VAL:CG2	2.34	0.53
1:A:168:CYS:HG	1:A:252:VAL:HG13	1.69	0.53
1:B:118:SER:OG	1:B:122:VAL:CG2	2.56	0.53
1:B:232:LYS:HD2	1:C:228:THR:CG2	2.38	0.53
1:A:300:THR:CB	1:A:301:VAL:HG23	2.39	0.53
1:C:328:ALA:HB2	1:C:362:VAL:CG2	2.34	0.53
1:B:168:CYS:HB3	1:B:252:VAL:HA	1.91	0.53
1:A:183:ASP:C	1:A:185:GLN:N	2.56	0.53
1:A:351:LEU:HD12	1:A:352:ASN:N	2.24	0.53
1:B:164:TYR:CE2	1:B:253:GLY:HA3	2.44	0.53
1:B:103:VAL:HG13	1:B:264:TYR:CA	2.36	0.52
1:C:214:ILE:CG2	1:C:215:PRO:N	2.71	0.52
1:B:300:THR:CB	1:B:301:VAL:HG23	2.39	0.52
1:B:316:GLY:O	1:B:349:TYR:O	2.26	0.52
1:A:316:GLY:O	1:A:349:TYR:O	2.26	0.52
1:B:330:GLY:HA3	1:B:359:PRO:O	2.09	0.52
1:C:330:GLY:HA3	1:C:359:PRO:O	2.09	0.52
1:A:328:ALA:HB2	1:A:362:VAL:CG2	2.34	0.52
1:C:316:GLY:O	1:C:349:TYR:O	2.26	0.52
1:B:351:LEU:HD12	1:B:352:ASN:N	2.25	0.52
1:A:309:THR:CG2	1:A:355:VAL:O	2.56	0.52
1:A:267:GLN:CB	1:C:198:PHE:HA	2.40	0.52
1:C:326:LEU:HD21	1:C:334:ILE:HD13	1.90	0.52
1:A:200:VAL:HG13	1:A:212:LEU:HD11	1.90	0.52
1:A:330:GLY:HA3	1:A:359:PRO:O	2.09	0.52
1:A:228:THR:HG21	1:A:234:ILE:CD1	2.38	0.52
1:C:112:LEU:HG	1:C:141:LEU:HD11	1.90	0.52
1:C:297:ARG:HE	1:C:299:PRO:CA	2.22	0.52
1:A:162:LEU:CD1	1:A:178:LEU:HD13	2.32	0.52
1:C:115:VAL:HG23	1:C:255:LEU:HD22	1.91	0.52
1:B:276:LYS:O	1:B:374:LEU:HD23	2.10	0.52
1:B:111:TYR:HB2	1:B:256:PHE:CE1	2.45	0.52
1:B:185:GLN:C	1:B:186:ASP:O	2.46	0.52
1:C:351:LEU:HD12	1:C:352:ASN:N	2.24	0.52
1:C:297:ARG:NE	1:C:299:PRO:HA	2.22	0.52
1:C:115:VAL:CG2	1:C:255:LEU:HD22	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:VAL:HG13	1:C:212:LEU:HD11	1.90	0.52
1:A:276:LYS:O	1:A:374:LEU:HD23	2.10	0.52
1:B:331:ALA:O	1:B:332:VAL:HG22	2.07	0.52
1:C:219:VAL:CB	1:C:221:ARG:HH21	2.11	0.52
1:C:221:ARG:NH1	1:C:236:LEU:HA	2.25	0.52
1:A:195:LEU:HD23	1:A:201:LEU:HD12	1.91	0.52
1:A:221:ARG:CD	1:A:234:ILE:O	2.58	0.52
1:A:267:GLN:HB3	1:C:198:PHE:CD1	2.45	0.52
1:C:160:VAL:HG12	1:C:214:ILE:HD12	1.90	0.52
1:B:162:LEU:HB2	1:B:212:LEU:HB3	1.92	0.52
1:A:342:ASN:HD21	1:A:345:THR:C	2.13	0.52
1:A:221:ARG:NH1	1:A:236:LEU:HA	2.25	0.51
1:A:276:LYS:CB	1:A:295:LEU:CD2	2.83	0.51
1:B:121:PHE:CD2	1:B:192:ARG:HD2	2.45	0.51
1:C:68:ILE:CG2	1:C:70:HIS:HD2	2.06	0.51
1:C:383:VAL:C	1:C:384:VAL:CG2	2.77	0.51
1:A:289:GLY:HA3	1:A:290:PRO:C	2.28	0.51
1:C:103:VAL:CG1	1:C:152:PHE:CE2	2.78	0.51
1:C:157:PHE:HD1	1:C:236:LEU:HD22	1.75	0.51
1:A:172:GLU:CB	1:A:172:GLU:N	2.68	0.51
1:C:342:ASN:HD21	1:C:345:THR:C	2.13	0.51
1:C:118:SER:OG	1:C:243:THR:OG1	1.95	0.51
1:A:175:ARG:O	1:A:243:THR:HA	2.09	0.51
1:C:70:HIS:CB	1:C:79:MET:HE3	2.41	0.51
1:C:115:VAL:CG2	1:C:241:ILE:HG21	2.41	0.51
1:C:201:LEU:CD2	1:C:203:GLU:HG2	2.29	0.51
1:B:165:VAL:HA	1:B:209:GLU:HG3	1.92	0.51
1:A:226:SER:OG	1:C:185:GLN:CB	2.59	0.51
1:B:342:ASN:HD21	1:B:345:THR:C	2.13	0.51
1:C:84:VAL:HG12	1:C:85:SER:N	2.26	0.51
1:A:274[P]:SER:O	1:A:375:LEU:HD23	2.10	0.51
1:C:265:PHE:N	1:C:265:PHE:CD1	2.79	0.51
1:C:82:VAL:C	1:C:170:THR:HG21	2.32	0.51
1:B:138:ASN:C	1:B:140:THR:N	2.60	0.51
1:C:135:ASN:OD1	1:C:155:TYR:CE1	2.64	0.51
1:A:154:GLN:NE2	1:A:222:TYR:CG	2.72	0.50
1:B:135:ASN:HB2	1:B:235:ASP:OD1	2.11	0.50
1:B:221:ARG:HD3	1:B:234:ILE:O	2.06	0.50
1:B:114:GLN:HE21	1:B:251:ALA:HB2	1.76	0.50
1:B:112:LEU:HD22	1:B:113:THR:HG22	1.93	0.50
1:C:122:VAL:CG1	1:C:123:VAL:N	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ARG:O	1:C:243:THR:HA	2.12	0.50
1:C:115:VAL:N	1:C:253:GLY:O	2.45	0.50
1:C:274[P]:SER:O	1:C:375:LEU:HD23	2.10	0.50
1:A:289:GLY:HA3	1:A:290:PRO:O	1.99	0.50
1:B:145:LEU:HB2	1:B:259:ARG:NH1	2.26	0.50
1:C:179:TYR:CD1	1:C:240:GLY:HA3	2.45	0.50
1:C:309:THR:CG2	1:C:355:VAL:O	2.56	0.50
1:B:217:ASP:OD1	1:B:236:LEU:CD1	2.58	0.50
1:B:289:GLY:HA3	1:B:290:PRO:O	1.99	0.50
1:B:275:SER:CA	1:B:375:LEU:CD2	2.78	0.50
1:A:157:PHE:HD1	1:A:236:LEU:HD22	1.75	0.50
1:C:221:ARG:CD	1:C:234:ILE:O	2.60	0.50
1:C:276:LYS:O	1:C:374:LEU:HD23	2.10	0.50
1:C:70:HIS:HB3	1:C:79:MET:HE1	1.92	0.50
1:B:380:ARG:HB2	1:B:382:ASN:OD1	2.11	0.50
1:A:380:ARG:HB2	1:A:382:ASN:OD1	2.11	0.50
1:A:121:PHE:C	1:A:121:PHE:CD1	2.84	0.50
1:B:112:LEU:HD23	1:B:113:THR:HG22	1.94	0.50
1:C:185:GLN:C	1:C:186:ASP:O	2.46	0.50
1:C:135:ASN:ND2	1:C:224:ASN:OD1	2.45	0.50
1:B:297:ARG:HG2	1:B:298:THR:C	2.32	0.50
1:B:277:ARG:HB3	1:B:285:ALA:HB2	1.89	0.50
1:A:277:ARG:HB3	1:A:285:ALA:HB2	1.89	0.50
1:A:135:ASN:ND2	1:A:224:ASN:OD1	2.45	0.50
1:A:259:ARG:HG2	1:A:261:VAL:HG23	1.94	0.50
1:B:112:LEU:CD1	1:B:141:LEU:HD11	2.41	0.50
1:B:110:GLU:CD	1:B:144:TRP:CB	2.79	0.50
1:B:111:TYR:HE2	1:B:254:GLU:CG	2.25	0.50
1:C:138:ASN:O	1:C:140:THR:C	2.50	0.50
1:C:380:ARG:HB2	1:C:382:ASN:OD1	2.11	0.50
1:A:128:VAL:CG1	1:A:129:GLY:H	2.25	0.49
1:B:192:ARG:HD2	1:B:192:ARG:N	2.27	0.49
1:B:297:ARG:NE	1:B:299:PRO:HA	2.22	0.49
1:B:158:ASN:HB2	1:B:260:SER:OG	2.12	0.49
1:C:118:SER:HB2	1:C:122:VAL:HG23	1.94	0.49
1:C:89:VAL:HG13	1:C:90:GLY:H	1.77	0.49
1:A:118:SER:O	1:A:246:GLY:HA3	2.12	0.49
1:A:297:ARG:HG2	1:A:298:THR:C	2.32	0.49
1:C:162:LEU:HB3	1:C:178:LEU:HD13	1.93	0.49
1:A:214:ILE:CG2	1:A:215:PRO:N	2.71	0.49
1:C:160:VAL:CG1	1:C:214:ILE:HD12	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:LYS:CB	1:C:295:LEU:CD2	2.83	0.49
1:A:279:ASP:O	1:A:280:LEU:CA	2.61	0.49
1:B:171:THR:O	1:B:173:VAL:HG23	2.12	0.49
1:B:140:THR:HG23	1:B:307:ARG:O	2.12	0.49
1:B:181:ASP:OD1	1:B:183:ASP:N	2.43	0.49
1:B:177:ALA:HB1	1:B:203:GLU:OE1	2.13	0.49
1:A:122:VAL:HG12	1:A:123:VAL:N	2.28	0.49
1:B:151:ASN:O	1:B:267:GLN:N	2.40	0.49
1:B:192:ARG:H	1:B:192:ARG:HD3	1.76	0.49
1:A:351:LEU:HD13	1:A:352:ASN:N	2.27	0.49
1:C:279:ASP:O	1:C:280:LEU:CA	2.61	0.49
1:A:297:ARG:NE	1:A:299:PRO:HA	2.22	0.49
1:C:297:ARG:HG2	1:C:298:THR:C	2.32	0.49
1:C:288:THR:C	1:C:289:GLY:O	2.50	0.49
1:B:152:PHE:HA	1:B:267:GLN:HG3	1.95	0.49
1:C:351:LEU:HD13	1:C:352:ASN:N	2.27	0.49
1:B:276:LYS:CB	1:B:295:LEU:CD2	2.83	0.49
1:B:351:LEU:HD13	1:B:352:ASN:N	2.27	0.49
1:C:164:TYR:CE2	1:C:255:LEU:CD1	2.82	0.49
1:A:150:SER:C	1:A:269:THR:HA	2.32	0.49
1:B:279:ASP:O	1:B:280:LEU:CA	2.61	0.49
1:C:206:PRO:HB3	1:C:252:VAL:CG1	2.42	0.49
1:A:195:LEU:HD21	1:A:201:LEU:CD1	2.31	0.49
1:C:142:PHE:HE2	1:C:257:LEU:CD1	2.26	0.49
1:C:228:THR:HG21	1:C:234:ILE:CD1	2.42	0.49
1:B:303:THR:HG22	1:B:305:THR:OG1	2.12	0.49
1:A:111:TYR:OH	1:A:254:GLU:OE2	2.22	0.48
1:A:274[S]:SER:O	1:A:375:LEU:HD23	2.13	0.48
1:B:103:VAL:CG1	1:B:264:TYR:HA	2.42	0.48
1:C:108:HIS:CG	1:C:109:ARG:H	2.31	0.48
1:A:104:THR:HG23	1:A:263:LEU:CB	2.39	0.48
1:C:380:ARG:C	1:C:382:ASN:H	2.16	0.48
1:A:145:LEU:HB2	1:A:259:ARG:NH1	2.27	0.48
1:C:132:LEU:O	1:C:141:LEU:HD22	2.12	0.48
1:C:292:TYR:HB3	1:C:308:ALA:CB	2.43	0.48
1:A:134:LEU:CD2	1:A:236:LEU:HD23	2.32	0.48
1:A:338:LEU:CD2	1:A:338:LEU:C	2.82	0.48
1:C:303:THR:HG22	1:C:305:THR:OG1	2.12	0.48
1:B:338:LEU:C	1:B:338:LEU:CD2	2.82	0.48
1:B:289:GLY:HA3	1:B:290:PRO:C	2.28	0.48
1:A:303:THR:HG22	1:A:305:THR:OG1	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:TYR:HB3	1:B:308:ALA:CB	2.43	0.48
1:A:141:LEU:HD12	1:A:141:LEU:C	2.33	0.48
1:A:274[S]:SER:O	1:A:375:LEU:CA	2.59	0.48
1:A:274[S]:SER:O	1:A:376:VAL:N	2.44	0.48
1:B:155:TYR:CZ	1:B:221:ARG:HB3	2.49	0.48
1:C:184:SER:HB2	1:C:235:ASP:HB2	1.95	0.48
1:A:136:PRO:HB2	1:A:145:LEU:CD2	2.41	0.48
1:B:181:ASP:HB3	1:B:238:GLN:HB3	1.95	0.48
1:C:145:LEU:HB3	1:C:146:PRO:HD2	1.91	0.48
1:A:380:ARG:C	1:A:382:ASN:H	2.16	0.48
1:B:132:LEU:HD13	1:B:239:LEU:O	2.11	0.48
1:B:334:ILE:HG22	1:B:335:ASN:N	2.29	0.48
1:C:267:GLN:HB2	1:C:268:PRO:CD	2.36	0.48
1:C:132:LEU:O	1:C:133:GLN:C	2.52	0.48
1:A:179:TYR:CZ	1:A:240:GLY:HA3	2.46	0.48
1:C:118:SER:C	1:C:120:GLY:N	2.64	0.48
1:B:206:PRO:HG2	1:B:207:TRP:HD1	1.77	0.48
1:B:309:THR:CG2	1:B:355:VAL:O	2.56	0.48
1:B:132:LEU:O	1:B:133:GLN:C	2.52	0.48
1:B:380:ARG:C	1:B:382:ASN:H	2.16	0.48
1:B:179:TYR:CD1	1:B:240:GLY:HA3	2.49	0.48
1:B:171:THR:C	1:B:172:GLU:O	2.46	0.48
1:A:128:VAL:CG1	1:A:129:GLY:N	2.73	0.48
1:A:267:GLN:HB2	1:C:198:PHE:CG	2.47	0.48
1:C:177:ALA:HB3	1:C:195:LEU:HD11	1.95	0.48
1:C:311:THR:HG21	1:C:380:ARG:C	2.35	0.48
1:B:109:ARG:NH2	1:B:256:PHE:CD2	2.80	0.47
1:C:131:SER:O	1:C:133:GLN:HB2	2.14	0.47
1:A:334:ILE:HG22	1:A:335:ASN:N	2.29	0.47
1:B:195:LEU:CD2	1:B:201:LEU:HD12	2.44	0.47
1:A:228:THR:HG23	1:C:232:LYS:HE3	1.96	0.47
1:A:288:THR:C	1:A:289:GLY:O	2.50	0.47
1:B:145:LEU:HB2	1:B:259:ARG:CZ	2.44	0.47
1:C:155:TYR:O	1:C:156:SER:OG	2.32	0.47
1:C:155:TYR:CZ	1:C:221:ARG:HB3	2.49	0.47
1:C:111:TYR:CD2	1:C:256:PHE:CE1	2.98	0.47
1:B:311:THR:HG21	1:B:380:ARG:C	2.35	0.47
1:C:338:LEU:C	1:C:338:LEU:CD2	2.82	0.47
1:A:190:ALA:HB3	1:A:194:GLU:CD	2.28	0.47
1:B:274[S]:SER:H	1:B:376:VAL:C	2.18	0.47
1:A:155:TYR:CZ	1:A:221:ARG:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ASN:ND2	1:B:238:GLN:OE1	2.47	0.47
1:C:104:THR:O	1:C:263:LEU:HB2	2.14	0.47
1:C:295:LEU:CD2	1:C:295:LEU:N	2.77	0.47
1:B:214:ILE:CG2	1:B:215:PRO:N	2.76	0.47
1:B:288:THR:C	1:B:289:GLY:O	2.50	0.47
1:A:311:THR:HG21	1:A:380:ARG:C	2.35	0.47
1:B:173:VAL:O	1:B:246:GLY:HA2	2.14	0.47
1:A:292:TYR:HB3	1:A:308:ALA:CB	2.43	0.47
1:C:331:ALA:HB3	1:C:357:SER:CB	2.23	0.47
1:C:104:THR:HG23	1:C:263:LEU:CB	2.44	0.47
1:A:162:LEU:HB3	1:A:178:LEU:HD12	1.97	0.47
1:C:110:GLU:O	1:C:257:LEU:CB	2.63	0.47
1:A:135:ASN:OD1	1:A:155:TYR:CE1	2.68	0.47
1:B:117:ASN:HB3	1:B:248:GLY:O	2.14	0.47
1:B:110:GLU:CD	1:B:144:TRP:H	2.06	0.47
1:C:278:LEU:HG	1:C:295:LEU:O	2.14	0.47
1:C:70:HIS:CB	1:C:79:MET:CE	2.92	0.47
1:A:358:LEU:HA	1:A:359:PRO:HA	1.61	0.47
1:A:112:LEU:HD22	1:A:113:THR:HG22	1.95	0.47
1:C:232:LYS:HG3	1:C:233:LEU:H	1.80	0.47
1:A:288:THR:O	1:A:289:GLY:O	2.33	0.47
1:B:142:PHE:HE2	1:B:257:LEU:CD1	2.28	0.47
1:B:228:THR:OG1	1:B:234:ILE:HD12	2.14	0.47
1:C:334:ILE:HG22	1:C:335:ASN:N	2.29	0.47
1:B:329:THR:O	1:B:361:THR:N	2.40	0.47
1:A:278:LEU:HG	1:A:295:LEU:O	2.14	0.47
1:A:180:PHE:CD1	1:A:214:ILE:HD12	2.49	0.47
1:C:277:ARG:HB3	1:C:285:ALA:HB2	1.89	0.47
1:C:137:SER:HB3	1:C:146:PRO:HG3	1.96	0.47
1:C:108:HIS:CG	1:C:109:ARG:N	2.82	0.47
1:C:145:LEU:CD2	1:C:146:PRO:HD3	2.45	0.47
1:B:331:ALA:C	1:B:332:VAL:CG2	2.83	0.47
1:B:358:LEU:HA	1:B:359:PRO:HA	1.61	0.47
1:C:195:LEU:HD23	1:C:201:LEU:HD12	1.91	0.47
1:B:179:TYR:CZ	1:B:240:GLY:HA3	2.49	0.47
1:B:130:ASN:ND2	1:B:238:GLN:HE22	2.10	0.47
1:B:288:THR:O	1:B:289:GLY:O	2.33	0.47
1:C:288:THR:O	1:C:289:GLY:O	2.33	0.47
1:B:278:LEU:HG	1:B:295:LEU:O	2.14	0.47
1:B:127:ILE:HG22	1:B:128:VAL:H	1.44	0.47
1:C:84:VAL:CG1	1:C:85:SER:N	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LEU:HD23	1:B:236:LEU:HD23	1.96	0.47
1:B:142:PHE:O	1:B:146:PRO:HG2	2.15	0.47
1:B:262:THR:HG21	1:B:264:TYR:HH	1.78	0.47
1:C:329:THR:O	1:C:361:THR:N	2.40	0.47
1:C:168:CYS:HB3	1:C:252:VAL:HG13	1.94	0.47
1:B:295:LEU:N	1:B:295:LEU:CD2	2.77	0.47
1:C:100:SER:O	1:C:103:VAL:N	2.39	0.47
1:C:119:SER:O	1:C:245:GLY:N	2.45	0.47
1:C:222:TYR:O	1:C:234:ILE:HG21	2.14	0.47
1:A:145:LEU:H	1:A:259:ARG:NH2	2.10	0.46
1:A:108:HIS:O	1:A:259:ARG:CB	2.63	0.46
1:A:158:ASN:HB2	1:A:260:SER:HG	1.80	0.46
1:B:241:ILE:CD1	1:B:255:LEU:HD22	2.22	0.46
1:A:201:LEU:CG	1:A:202:LYS:N	2.78	0.46
1:C:177:ALA:CB	1:C:195:LEU:HD11	2.44	0.46
1:A:321:LEU:N	1:A:321:LEU:CD2	2.77	0.46
1:B:230:ASP:C	1:B:232:LYS:H	2.19	0.46
1:B:146:PRO:O	1:B:150:SER:OG	2.32	0.46
1:A:228:THR:CG2	1:C:232:LYS:HE3	2.46	0.46
1:C:104:THR:CG2	1:C:152:PHE:CZ	2.90	0.46
1:A:297:ARG:HE	1:A:299:PRO:CA	2.22	0.46
1:C:180:PHE:HB3	1:C:200:VAL:HB	1.97	0.46
1:A:117:ASN:N	1:A:250:ASP:O	2.40	0.46
1:B:138:ASN:O	1:B:140:THR:CA	2.63	0.46
1:C:133:GLN:CB	1:C:138:ASN:ND2	2.78	0.46
1:C:321:LEU:N	1:C:321:LEU:CD2	2.77	0.46
1:B:112:LEU:HG	1:B:141:LEU:HD11	1.97	0.46
1:B:152:PHE:CA	1:B:267:GLN:HG3	2.45	0.46
1:A:164:TYR:CE2	1:A:255:LEU:CD1	2.88	0.46
1:C:91:SER:HB3	1:C:109:ARG:NH2	2.31	0.46
1:C:321:LEU:C	1:C:322:THR:OG1	2.54	0.46
1:B:122:VAL:CG1	1:B:123:VAL:H	2.29	0.46
1:C:184:SER:CB	1:C:235:ASP:HB2	2.46	0.46
1:A:335:ASN:HB2	1:A:352:ASN:HD22	1.57	0.46
1:B:297:ARG:HE	1:B:299:PRO:CA	2.22	0.46
1:A:295:LEU:N	1:A:295:LEU:CD2	2.77	0.46
1:B:195:LEU:HD23	1:B:196:ALA:N	2.31	0.46
1:A:308:ALA:HB1	1:A:312:PHE:HZ	1.81	0.46
1:B:321:LEU:O	1:B:321:LEU:HG	2.16	0.46
1:B:175:ARG:O	1:B:243:THR:HA	2.16	0.46
1:A:142:PHE:O	1:A:146:PRO:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:LEU:HD21	1:B:239:LEU:HD12	1.98	0.46
1:C:331:ALA:C	1:C:332:VAL:CG2	2.83	0.46
1:B:159:SER:O	1:B:160:VAL:CG2	2.64	0.46
1:A:331:ALA:HB2	1:A:357:SER:OG	1.95	0.46
1:C:201:LEU:CG	1:C:202:LYS:N	2.78	0.46
1:B:308:ALA:HB1	1:B:312:PHE:HZ	1.81	0.46
1:A:234:ILE:CG1	1:C:233:LEU:HD21	2.46	0.45
1:B:152:PHE:CD1	1:B:263:LEU:HB3	2.49	0.45
1:C:181:ASP:OD1	1:C:183:ASP:N	2.46	0.45
1:A:214:ILE:HA	1:A:215:PRO:HD2	1.56	0.45
1:B:321:LEU:CD2	1:B:321:LEU:N	2.77	0.45
1:A:321:LEU:HG	1:A:321:LEU:O	2.16	0.45
1:A:142:PHE:HE2	1:A:257:LEU:CD1	2.29	0.45
1:B:145:LEU:CB	1:B:146:PRO:HD3	2.38	0.45
1:C:302:LEU:HD21	1:C:304:HIS:NE2	2.32	0.45
1:A:117:ASN:CB	1:A:248:GLY:O	2.61	0.45
1:A:192:ARG:HH11	1:A:192:ARG:HG3	1.81	0.45
1:A:216:THR:HG22	1:A:217:ASP:O	2.17	0.45
1:B:162:LEU:HB3	1:B:178:LEU:CD1	2.46	0.45
1:B:345:THR:O	1:B:346:ALA:C	2.55	0.45
1:C:321:LEU:HG	1:C:321:LEU:O	2.16	0.45
1:A:321:LEU:CB	1:A:344:GLY:H	2.26	0.45
1:A:145:LEU:C	1:A:145:LEU:HD23	2.32	0.45
1:B:186:ASP:HB3	1:B:187:PRO:HD2	1.97	0.45
1:B:297:ARG:HG2	1:B:298:THR:CA	2.47	0.45
1:A:185:GLN:C	1:A:186:ASP:O	2.51	0.45
1:A:222:TYR:OH	1:C:182:LYS:HG3	2.17	0.45
1:B:122:VAL:C	1:B:122:VAL:N	2.60	0.45
1:C:111:TYR:HD2	1:C:256:PHE:CZ	2.34	0.45
1:B:314:LEU:HB2	1:B:351:LEU:HD12	1.99	0.45
1:A:110:GLU:OE1	1:A:144:TRP:CB	2.65	0.45
1:C:216:THR:HG22	1:C:217:ASP:O	2.17	0.45
1:A:314:LEU:HB2	1:A:351:LEU:HD12	1.99	0.45
1:B:385:ASN:C	1:B:385:ASN:OD1	2.55	0.45
1:A:278:LEU:HB2	1:A:372:GLY:HA3	1.98	0.45
1:B:195:LEU:CD2	1:B:201:LEU:CD1	2.94	0.45
1:B:321:LEU:CB	1:B:344:GLY:H	2.26	0.45
1:A:130:ASN:OD1	1:A:186:ASP:O	2.35	0.45
1:C:69:THR:O	1:C:70:HIS:O	2.35	0.45
1:A:345:THR:O	1:A:346:ALA:C	2.55	0.45
1:C:308:ALA:HB1	1:C:312:PHE:HZ	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:GLU:OE2	1:B:144:TRP:HB3	2.17	0.45
1:A:297:ARG:HG2	1:A:298:THR:CA	2.47	0.45
1:B:278:LEU:HB2	1:B:372:GLY:HA3	1.98	0.45
1:A:111:TYR:CD1	1:A:112:LEU:N	2.85	0.45
1:A:124:ASN:OD1	1:A:132:LEU:HD11	2.17	0.45
1:B:181:ASP:O	1:B:238:GLN:N	2.49	0.45
1:C:345:THR:O	1:C:346:ALA:C	2.55	0.45
1:C:137:SER:HB3	1:C:146:PRO:CB	2.47	0.45
1:C:99:THR:CG2	1:C:99:THR:O	2.64	0.44
1:C:278:LEU:HB2	1:C:372:GLY:HA3	1.98	0.44
1:B:297:ARG:CG	1:B:298:THR:O	2.66	0.44
1:C:167:LEU:CD2	1:C:253:GLY:CA	2.94	0.44
1:B:206:PRO:CG	1:B:207:TRP:N	2.47	0.44
1:A:230:ASP:C	1:A:232:LYS:H	2.20	0.44
1:B:116:ASN:HA	1:B:250:ASP:O	2.17	0.44
1:B:117:ASN:OD1	1:B:118:SER:N	2.51	0.44
1:B:192:ARG:HH11	1:B:192:ARG:HG3	1.82	0.44
1:C:157:PHE:CE2	1:C:261:VAL:HG22	2.51	0.44
1:C:314:LEU:HB2	1:C:351:LEU:HD12	1.99	0.44
1:C:385:ASN:C	1:C:385:ASN:OD1	2.55	0.44
1:B:331:ALA:HB2	1:B:357:SER:OG	1.95	0.44
1:B:122:VAL:HG12	1:B:123:VAL:O	2.17	0.44
1:B:231:GLN:HG3	1:B:231:GLN:H	1.55	0.44
1:B:184:SER:HB2	1:B:235:ASP:HB2	1.99	0.44
1:C:214:ILE:HA	1:C:215:PRO:HD2	1.56	0.44
1:A:337:ILE:CG2	1:A:337:ILE:O	2.64	0.44
1:A:297:ARG:CG	1:A:298:THR:O	2.66	0.44
1:C:297:ARG:HG2	1:C:298:THR:CA	2.47	0.44
1:A:302:LEU:HD21	1:A:304:HIS:NE2	2.32	0.44
1:A:118:SER:O	1:A:246:GLY:N	2.46	0.44
1:A:124:ASN:OD1	1:A:132:LEU:CD1	2.65	0.44
1:B:112:LEU:C	1:B:112:LEU:HD23	2.38	0.44
1:C:127:ILE:HD11	1:C:358:LEU:HD13	1.97	0.44
1:B:337:ILE:CG2	1:B:337:ILE:O	2.64	0.44
1:B:302:LEU:HD21	1:B:304:HIS:NE2	2.32	0.44
1:B:205:ALA:HB1	1:B:207:TRP:NE1	2.32	0.44
1:A:384:VAL:O	1:A:384:VAL:HG12	2.17	0.44
1:B:321:LEU:C	1:B:322:THR:OG1	2.54	0.44
1:A:184:SER:CB	1:A:235:ASP:HB2	2.48	0.44
1:B:157:PHE:CE2	1:B:261:VAL:CG2	3.00	0.44
1:C:192:ARG:HH11	1:C:192:ARG:HG3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:SER:CB	1:B:235:ASP:HB2	2.48	0.44
1:A:226:SER:CB	1:C:185:GLN:C	2.82	0.44
1:A:385:ASN:OD1	1:A:385:ASN:C	2.55	0.44
1:A:292:TYR:HB3	1:A:308:ALA:HB2	2.00	0.44
1:B:154:GLN:HB2	1:B:264:TYR:HB2	2.00	0.44
1:C:111:TYR:HB2	1:C:256:PHE:CE1	2.52	0.44
1:C:104:THR:CG2	1:C:263:LEU:HB2	2.44	0.44
1:B:324:LEU:CD2	1:B:366:VAL:HG21	1.96	0.44
1:B:300:THR:C	1:B:369:VAL:HG21	2.38	0.44
1:B:110:GLU:O	1:B:257:LEU:N	2.51	0.44
1:B:153:ASP:OD1	1:B:222:TYR:CD1	2.71	0.44
1:B:144:TRP:HE3	1:B:259:ARG:HH12	1.66	0.44
1:C:230:ASP:C	1:C:232:LYS:H	2.21	0.44
1:C:357:SER:O	1:C:358:LEU:HG	2.18	0.44
1:C:103:VAL:HG11	1:C:263:LEU:C	2.38	0.44
1:C:336:ASP:CG	1:C:385:ASN:HB2	2.38	0.44
1:C:81:PRO:O	1:C:170:THR:CG2	2.55	0.44
1:A:151:ASN:ND2	1:A:269:THR:HG23	2.32	0.44
1:A:147:ALA:HB1	1:A:272:LEU:CG	2.47	0.44
1:A:178:LEU:O	1:A:212:LEU:HD22	2.18	0.44
1:C:292:TYR:HB3	1:C:308:ALA:HB2	2.00	0.44
1:B:292:TYR:HB3	1:B:308:ALA:HB2	2.00	0.44
1:A:232:LYS:HG3	1:A:233:LEU:H	1.81	0.44
1:A:230:ASP:C	1:A:232:LYS:N	2.71	0.44
1:A:111:TYR:HA	1:A:256:PHE:CD1	2.52	0.44
1:B:114:GLN:HE21	1:B:251:ALA:CB	2.30	0.44
1:B:145:LEU:O	1:B:147:ALA:N	2.51	0.44
1:C:358:LEU:HA	1:C:359:PRO:HA	1.61	0.44
1:C:69:THR:O	1:C:70:HIS:C	2.56	0.44
1:B:300:THR:O	1:B:301:VAL:CG2	2.66	0.44
1:C:300:THR:O	1:C:301:VAL:CG2	2.66	0.44
1:B:206:PRO:HB2	1:B:252:VAL:CG1	2.47	0.44
1:B:357:SER:O	1:B:358:LEU:HG	2.18	0.44
1:A:111:TYR:CE2	1:A:254:GLU:CD	2.88	0.43
1:C:231:GLN:HG3	1:C:231:GLN:H	1.55	0.43
1:C:297:ARG:CG	1:C:298:THR:O	2.66	0.43
1:A:151:ASN:HD21	1:A:269:THR:HG23	1.83	0.43
1:C:230:ASP:C	1:C:232:LYS:N	2.71	0.43
1:C:112:LEU:C	1:C:112:LEU:HD23	2.39	0.43
1:C:74:VAL:C	1:C:75:GLY:O	2.57	0.43
1:A:329:THR:O	1:A:361:THR:N	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:SER:HB2	1:A:120:GLY:H	1.84	0.43
1:A:112:LEU:HD23	1:A:113:THR:HG22	2.00	0.43
1:B:217:ASP:OD2	1:B:219:VAL:HB	2.18	0.43
1:A:300:THR:O	1:A:301:VAL:CG2	2.66	0.43
1:C:91:SER:OG	1:C:109:ARG:HB3	2.18	0.43
1:A:184:SER:HB2	1:A:235:ASP:HB2	1.99	0.43
1:B:264:TYR:O	1:B:265:PHE:C	2.57	0.43
1:C:111:TYR:CD1	1:C:112:LEU:N	2.86	0.43
1:A:279:ASP:OD2	1:A:282:GLY:HA3	2.19	0.43
1:B:278:LEU:HD23	1:B:283:SER:O	2.19	0.43
1:A:278:LEU:HD23	1:A:283:SER:O	2.19	0.43
1:B:195:LEU:HD23	1:B:201:LEU:CD1	2.47	0.43
1:C:384:VAL:HG12	1:C:384:VAL:O	2.18	0.43
1:B:355:VAL:HG11	1:B:360:ALA:CB	2.47	0.43
1:A:335:ASN:CG	1:A:352:ASN:ND2	2.72	0.43
1:C:337:ILE:O	1:C:337:ILE:CG2	2.64	0.43
1:B:335:ASN:CG	1:B:352:ASN:ND2	2.72	0.43
1:B:275:SER:CB	1:B:375:LEU:CD2	2.96	0.43
1:A:321:LEU:C	1:A:322:THR:OG1	2.54	0.43
1:A:336:ASP:CG	1:A:385:ASN:HB2	2.38	0.43
1:A:122:VAL:CG1	1:A:123:VAL:N	2.82	0.43
1:A:185:GLN:OE1	1:A:232:LYS:HE3	2.18	0.43
1:B:154:GLN:NE2	1:B:222:TYR:CZ	2.74	0.43
1:B:279:ASP:OD2	1:B:282:GLY:HA3	2.19	0.43
1:B:304:HIS:CE1	1:B:349:TYR:OH	2.72	0.43
1:C:122:VAL:HG13	1:C:126:GLY:CA	2.49	0.43
1:A:300:THR:C	1:A:369:VAL:HG21	2.38	0.43
1:A:304:HIS:CE1	1:A:349:TYR:OH	2.72	0.43
1:B:204:THR:CG2	1:B:205:ALA:N	2.82	0.43
1:A:355:VAL:HG11	1:A:360:ALA:CB	2.47	0.43
1:B:124:ASN:OD1	1:B:132:LEU:HD11	2.19	0.43
1:C:122:VAL:CG1	1:C:126:GLY:N	2.82	0.43
1:A:180:PHE:CE1	1:A:214:ILE:HG23	2.54	0.43
1:B:204:THR:HG22	1:B:205:ALA:N	2.32	0.43
1:B:201:LEU:HD23	1:B:202:LYS:HA	1.99	0.43
1:B:110:GLU:OE1	1:B:143:SER:N	2.51	0.42
1:B:230:ASP:C	1:B:232:LYS:N	2.71	0.42
1:C:96:THR:HG22	1:C:105:VAL:HB	1.98	0.42
1:C:304:HIS:CE1	1:C:349:TYR:OH	2.72	0.42
1:C:321:LEU:CB	1:C:344:GLY:H	2.26	0.42
1:A:175:ARG:HG2	1:A:244:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:PHE:O	1:A:146:PRO:CD	2.67	0.42
1:B:230:ASP:OD1	1:C:228:THR:HA	2.20	0.42
1:C:278:LEU:HD23	1:C:283:SER:O	2.19	0.42
1:B:336:ASP:CG	1:B:385:ASN:HB2	2.38	0.42
1:A:280:LEU:CB	1:A:280:LEU:N	2.73	0.42
1:C:267:GLN:CB	1:C:268:PRO:HD2	2.34	0.42
1:B:384:VAL:HG12	1:B:384:VAL:O	2.18	0.42
1:A:231:GLN:H	1:A:231:GLN:HG3	1.55	0.42
1:C:112:LEU:CD2	1:C:113:THR:HG22	2.49	0.42
1:C:280:LEU:CB	1:C:370:ALA:O	2.67	0.42
1:C:281:THR:HA	1:C:297:ARG:HH12	1.84	0.42
1:B:204:THR:O	1:B:205:ALA:C	2.58	0.42
1:A:357:SER:O	1:A:358:LEU:HG	2.18	0.42
1:A:234:ILE:HD11	1:C:232:LYS:CD	2.47	0.42
1:C:264:TYR:O	1:C:265:PHE:C	2.57	0.42
1:A:264:TYR:O	1:A:265:PHE:C	2.57	0.42
1:A:110:GLU:OE1	1:A:144:TRP:CA	2.63	0.42
1:A:201:LEU:HD23	1:A:202:LYS:HA	1.99	0.42
1:C:355:VAL:HG11	1:C:360:ALA:CB	2.47	0.42
1:C:382:ASN:O	1:C:384:VAL:HG23	2.20	0.42
1:A:143:SER:HB2	1:A:378:ARG:NH2	2.34	0.42
1:A:267:GLN:HA	1:C:197:ASN:O	2.20	0.42
1:B:280:LEU:CB	1:B:370:ALA:O	2.67	0.42
1:B:281:THR:HA	1:B:297:ARG:NH1	2.35	0.42
1:A:180:PHE:CD1	1:A:214:ILE:HG23	2.55	0.42
1:C:204:THR:O	1:C:205:ALA:O	2.35	0.42
1:A:142:PHE:HB3	1:A:146:PRO:CD	2.48	0.42
1:A:111:TYR:CZ	1:A:254:GLU:OE2	2.72	0.42
1:B:123:VAL:O	1:B:124:ASN:C	2.57	0.42
1:C:88:LEU:HD13	1:C:256:PHE:CZ	2.54	0.42
1:A:280:LEU:CB	1:A:370:ALA:O	2.67	0.42
1:B:114:GLN:NE2	1:B:251:ALA:HB2	2.34	0.42
1:A:230:ASP:OD1	1:B:228:THR:HA	2.20	0.42
1:C:88:LEU:HD13	1:C:256:PHE:CE2	2.55	0.42
1:C:96:THR:CG2	1:C:105:VAL:CB	2.91	0.42
1:A:362:VAL:N	1:A:362:VAL:CG2	2.83	0.42
1:B:281:THR:HA	1:B:297:ARG:HH12	1.84	0.42
1:A:180:PHE:CE1	1:A:214:ILE:CG2	3.02	0.42
1:A:382:ASN:O	1:A:384:VAL:HG23	2.20	0.42
1:A:112:LEU:HG	1:A:141:LEU:CD1	2.49	0.42
1:A:132:LEU:O	1:A:133:GLN:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ASN:HB2	1:C:235:ASP:OD1	2.19	0.42
1:B:180:PHE:HB3	1:B:200:VAL:HB	2.01	0.42
1:A:281:THR:HA	1:A:297:ARG:HH12	1.84	0.42
1:C:167:LEU:HD21	1:C:253:GLY:CA	2.50	0.42
1:B:302:LEU:HG	1:B:304:HIS:HD2	1.85	0.42
1:A:302:LEU:HG	1:A:304:HIS:HD2	1.85	0.42
1:A:104:THR:HG22	1:A:263:LEU:CB	2.26	0.42
1:A:226:SER:OG	1:C:232:LYS:CE	2.68	0.42
1:A:314:LEU:HD22	1:A:351:LEU:CD1	2.50	0.42
1:C:68:ILE:HG22	1:C:69:THR:N	2.33	0.42
1:B:298:THR:O	1:B:299:PRO:C	2.58	0.42
1:A:281:THR:HA	1:A:297:ARG:NH1	2.35	0.42
1:B:382:ASN:O	1:B:384:VAL:HG23	2.20	0.42
1:A:179:TYR:CD1	1:A:240:GLY:HA3	2.53	0.42
1:A:109:ARG:HA	1:A:257:LEU:O	2.19	0.41
1:B:107:SER:HA	1:B:259:ARG:O	2.20	0.41
1:B:112:LEU:HG	1:B:141:LEU:HD12	1.99	0.41
1:A:172:GLU:O	1:A:172:GLU:N	2.52	0.41
1:C:302:LEU:HG	1:C:304:HIS:HD2	1.85	0.41
1:C:279:ASP:OD2	1:C:282:GLY:HA3	2.19	0.41
1:C:281:THR:HA	1:C:297:ARG:NH1	2.35	0.41
1:C:168:CYS:HG	1:C:252:VAL:HG13	1.78	0.41
1:C:82:VAL:HA	1:C:170:THR:CG2	2.48	0.41
1:C:145:LEU:O	1:C:146:PRO:C	2.59	0.41
1:A:157:PHE:CE2	1:A:261:VAL:HG22	2.53	0.41
1:B:217:ASP:OD2	1:B:221:ARG:NH2	2.53	0.41
1:C:112:LEU:CD1	1:C:141:LEU:HD11	2.50	0.41
1:B:362:VAL:N	1:B:362:VAL:CG2	2.83	0.41
1:A:298:THR:O	1:A:299:PRO:C	2.58	0.41
1:C:206:PRO:CB	1:C:252:VAL:HG11	2.44	0.41
1:A:169:GLY:C	1:A:171:THR:H	2.18	0.41
1:B:314:LEU:HD22	1:B:351:LEU:CD1	2.50	0.41
1:B:129:GLY:O	1:B:130:ASN:C	2.58	0.41
1:C:97:GLY:O	1:C:99:THR:CA	2.68	0.41
1:C:276:LYS:O	1:C:295:LEU:CD1	2.44	0.41
1:B:161:VAL:HA	1:B:212:LEU:O	2.20	0.41
1:C:298:THR:O	1:C:299:PRO:C	2.58	0.41
1:C:164:TYR:CE2	1:C:253:GLY:HA3	2.55	0.41
1:A:142:PHE:CB	1:A:146:PRO:HD2	2.48	0.41
1:A:267:GLN:HG3	1:A:268:PRO:CG	2.25	0.41
1:C:131:SER:OG	1:C:132:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:VAL:HG21	1:C:241:ILE:HG21	2.02	0.41
1:A:174:GLY:O	1:A:206:PRO:HD3	2.20	0.41
1:B:168:CYS:CB	1:B:252:VAL:HG13	2.50	0.41
1:A:104:THR:HG23	1:A:263:LEU:CG	2.51	0.41
1:B:195:LEU:CD2	1:B:195:LEU:C	2.88	0.41
1:A:133:GLN:O	1:A:138:ASN:ND2	2.48	0.41
1:B:111:TYR:CD1	1:B:112:LEU:N	2.89	0.41
1:C:154:GLN:NE2	1:C:222:TYR:CG	2.72	0.41
1:A:326:LEU:C	1:A:326:LEU:CD1	2.84	0.41
1:C:327:GLY:O	1:C:362:VAL:HG13	2.21	0.41
1:C:278:LEU:HD11	1:C:296:THR:C	2.41	0.41
1:C:362:VAL:CG2	1:C:362:VAL:N	2.83	0.41
1:C:304:HIS:N	1:C:362:VAL:O	2.49	0.41
1:A:114:GLN:NE2	1:A:251:ALA:CB	2.79	0.41
1:C:232:LYS:HB3	1:C:232:LYS:HE2	1.80	0.41
1:C:141:LEU:HD12	1:C:141:LEU:O	2.20	0.41
1:A:123:VAL:CG1	1:A:124:ASN:HD22	2.25	0.41
1:A:150:SER:O	1:A:269:THR:C	2.59	0.41
1:A:121:PHE:HD1	1:A:121:PHE:O	2.04	0.41
1:B:112:LEU:CG	1:B:141:LEU:HD11	2.51	0.41
1:C:96:THR:CG2	1:C:105:VAL:CG1	2.99	0.41
1:C:123:VAL:O	1:C:124:ASN:C	2.58	0.41
1:A:327:GLY:O	1:A:362:VAL:HG13	2.21	0.41
1:C:314:LEU:HD22	1:C:351:LEU:CD1	2.50	0.41
1:C:300:THR:C	1:C:369:VAL:HG21	2.38	0.41
1:A:278:LEU:HD11	1:A:295:LEU:O	2.22	0.41
1:A:112:LEU:C	1:A:112:LEU:HD23	2.41	0.40
1:C:88:LEU:HD11	1:C:256:PHE:CE2	2.54	0.40
1:B:161:VAL:N	1:B:258:ALA:HB3	2.35	0.40
1:A:298:THR:CB	1:A:299:PRO:HD2	2.42	0.40
1:B:205:ALA:HB1	1:B:207:TRP:CD1	2.56	0.40
1:B:201:LEU:CG	1:B:202:LYS:N	2.84	0.40
1:B:165:VAL:CG1	1:B:166:PRO:N	2.83	0.40
1:C:112:LEU:CG	1:C:141:LEU:HD11	2.51	0.40
1:B:214:ILE:HA	1:B:215:PRO:HD2	1.59	0.40
1:B:148:LEU:O	1:B:152:PHE:HD1	2.04	0.40
1:A:228:THR:HG23	1:C:232:LYS:CE	2.52	0.40
1:B:327:GLY:O	1:B:362:VAL:HG13	2.21	0.40
1:C:115:VAL:HG22	1:C:241:ILE:HG21	2.03	0.40
1:A:278:LEU:HD11	1:A:296:THR:C	2.41	0.40
1:A:110:GLU:HG2	1:A:144:TRP:CB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ALA:N	1:B:242:ALA:O	2.55	0.40
1:A:182:LYS:HG3	1:A:182:LYS:O	2.22	0.40
1:B:141:LEU:HD21	1:B:239:LEU:CD1	2.51	0.40
1:C:133:GLN:C	1:C:138:ASN:ND2	2.68	0.40
1:A:297:ARG:HD2	1:A:369:VAL:O	2.21	0.40
1:B:278:LEU:HD11	1:B:296:THR:C	2.41	0.40
1:A:178:LEU:HD21	1:A:255:LEU:CD2	2.52	0.40
1:C:91:SER:CB	1:C:109:ARG:HB3	2.52	0.40

All (19) 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:C:340:ILE:CD1	1:C:348:ASP:CG[2_555]	1.00	1.20
1:C:340:ILE:CD1	1:C:348:ASP:OD2[2_555]	1.13	1.07
1:C:340:ILE:CG1	1:C:348:ASP:OD2[2_555]	1.24	0.96
1:C:340:ILE:CD1	1:C:348:ASP:OD1[2_555]	1.60	0.60
1:C:373:ILE:CD1	1:C:386:LEU:N[2_555]	1.67	0.53
1:C:373:ILE:CD1	1:C:386:LEU:CA[2_555]	1.70	0.50
1:C:340:ILE:CB	1:C:348:ASP:OD2[2_555]	1.71	0.49
1:C:280:LEU:CD2	1:C:387:LEU:C[2_555]	1.80	0.40
1:B:193:VAL:CG1	1:C:143:SER:OG[2_555]	1.80	0.40
1:C:373:ILE:CD1	1:C:385:ASN:C[2_555]	1.84	0.36
1:C:280:LEU:CD2	1:C:387:LEU:O[2_555]	1.89	0.31
1:C:373:ILE:CD1	1:C:385:ASN:O[2_555]	1.93	0.27
1:C:340:ILE:CG1	1:C:348:ASP:CG[2_555]	1.94	0.26
1:C:271:THR:CG2	1:C:378:ARG:O[2_555]	2.01	0.19
1:C:340:ILE:CD1	1:C:348:ASP:CB[2_555]	2.10	0.10
1:C:148:LEU:CD2	1:C:148:LEU:CD2[2_555]	2.12	0.08
1:B:244:TYR:OH	1:C:254:GLU:OE1[2_555]	2.13	0.07
1:C:340:ILE:CG1	1:C:348:ASP:OD1[2_555]	2.15	0.05
1:C:93:PRO:O	1:C:102:GLY:O[2_555]	2.18	0.02

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	288/387 (74%)	208 (72%)	49 (17%)	31 (11%)	0	1
1	B	287/387 (74%)	212 (74%)	43 (15%)	32 (11%)	0	1
1	C	322/387 (83%)	240 (74%)	45 (14%)	37 (12%)	0	1
All	All	897/1161 (77%)	660 (74%)	137 (15%)	100 (11%)	0	1

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	130	ASN
1	A	139	GLY
1	A	166	PRO
1	A	170	THR
1	A	184	SER
1	A	231	GLN
1	A	268	PRO
1	A	269	THR
1	A	272	LEU
1	A	290	PRO
1	A	322	THR
1	A	343	VAL
1	A	346	ALA
1	A	381	ALA
1	A	384	VAL
1	A	386	LEU
1	B	120	GLY
1	B	124	ASN
1	B	130	ASN
1	B	139	GLY
1	B	166	PRO
1	B	170	THR
1	B	184	SER
1	B	231	GLN
1	B	269	THR
1	B	271	THR
1	B	290	PRO
1	B	322	THR
1	B	343	VAL
1	B	346	ALA

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Mol	Chain	Res	Type
1	B	381	ALA
1	B	384	VAL
1	B	386	LEU
1	C	70	HIS
1	C	98	ARG
1	C	99	THR
1	C	101	GLY
1	C	124	ASN
1	C	132	LEU
1	C	134	LEU
1	C	139	GLY
1	C	166	PRO
1	C	170	THR
1	C	184	SER
1	C	231	GLN
1	C	290	PRO
1	C	322	THR
1	C	343	VAL
1	C	346	ALA
1	C	381	ALA
1	C	384	VAL
1	C	386	LEU
1	A	133	GLN
1	A	271	THR
1	B	146	PRO
1	C	68	ILE
1	C	75	GLY
1	C	130	ASN
1	C	133	GLN
1	A	220	LYS
1	A	267	GLN
1	A	279	ASP
1	A	324	LEU
1	B	133	GLN
1	B	134	LEU
1	B	206	PRO
1	B	220	LYS
1	B	279	ASP
1	B	324	LEU
1	C	146	PRO
1	C	149	ALA
1	C	220	LYS

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Mol	Chain	Res	Type
1	C	265	PHE
1	C	279	ASP
1	C	324	LEU
1	A	206	PRO
1	A	246	GLY
1	A	265	PHE
1	A	378	ARG
1	B	149	ALA
1	B	268	PRO
1	B	378	ARG
1	C	206	PRO
1	C	246	GLY
1	C	378	ARG
1	A	299	PRO
1	A	380	ARG
1	B	205	ALA
1	B	265	PHE
1	B	299	PRO
1	B	380	ARG
1	C	299	PRO
1	C	380	ARG
1	A	136	PRO
1	B	136	PRO
1	C	120	GLY
1	C	136	PRO
1	A	205	ALA
1	C	90	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	232/309 (75%)	217 (94%)	15 (6%)	21	52
1	B	233/309 (75%)	217 (93%)	16 (7%)	19	48
1	C	258/309 (84%)	242 (94%)	16 (6%)	23	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	723/927 (78%)	676 (94%)	47 (6%)	21	52

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	LEU
1	A	146	PRO
1	A	167	LEU
1	A	189	PRO
1	A	195	LEU
1	A	206	PRO
1	A	211	MET
1	A	257	LEU
1	A	260	SER
1	A	295	LEU
1	A	321	LEU
1	A	326	LEU
1	A	338	LEU
1	A	351	LEU
1	A	352	ASN
1	B	141	LEU
1	B	146	PRO
1	B	166	PRO
1	B	189	PRO
1	B	192	ARG
1	B	195	LEU
1	B	201	LEU
1	B	211	MET
1	B	257	LEU
1	B	260	SER
1	B	295	LEU
1	B	321	LEU
1	B	326	LEU
1	B	338	LEU
1	B	351	LEU
1	B	352	ASN
1	C	69	THR
1	C	81	PRO
1	C	141	LEU
1	C	167	LEU
1	C	189	PRO
1	C	195	LEU

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Mol	Chain	Res	Type
1	C	211	MET
1	C	257	LEU
1	C	260	SER
1	C	265	PHE
1	C	295	LEU
1	C	321	LEU
1	C	326	LEU
1	C	338	LEU
1	C	351	LEU
1	C	352	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	130	ASN
1	A	135	ASN
1	A	151	ASN
1	A	158	ASN
1	A	197	ASN
1	A	224	ASN
1	A	304	HIS
1	A	335	ASN
1	A	352	ASN
1	B	114	GLN
1	B	130	ASN
1	B	133	GLN
1	B	238	GLN
1	B	304	HIS
1	B	335	ASN
1	B	352	ASN
1	C	108	HIS
1	C	114	GLN
1	C	130	ASN
1	C	135	ASN
1	C	158	ASN
1	C	197	ASN
1	C	224	ASN
1	C	304	HIS
1	C	335	ASN
1	C	352	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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