



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:21 am BST

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

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

with specific help available everywhere you see the ⓘ symbol.

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

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

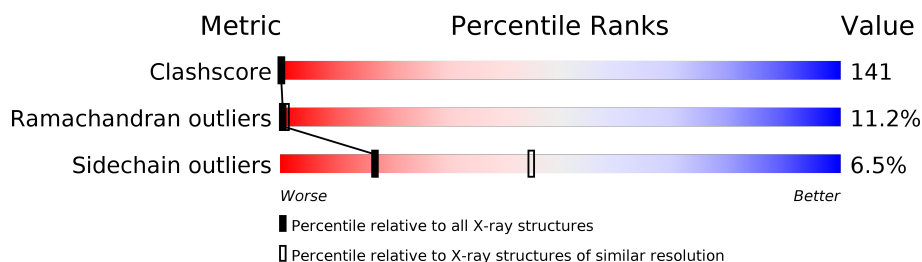
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	387	<div> <div>8%</div> <div>38%</div> <div>21%</div> <div>7%</div> <div>26%</div> </div>
1	B	387	<div> <div>7%</div> <div>37%</div> <div>23%</div> <div>7%</div> <div>26%</div> </div>
1	C	387	<div> <div>8%</div> <div>43%</div> <div>24%</div> <div>7%</div> <div>17%</div> </div>

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:

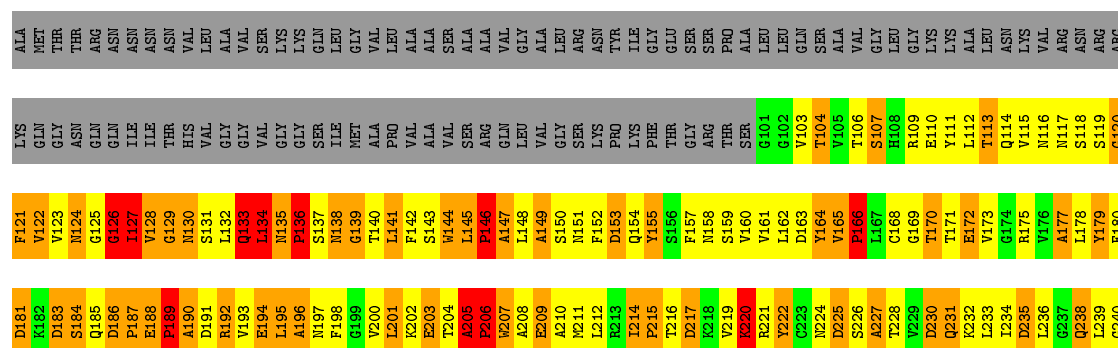
Chain	Residue	Modelled	Actual	Comment	Reference
A	102	GLY	SER	CONFLICT	UNP P11795
A	107	SER	GLY	CONFLICT	UNP P11795
B	102	GLY	SER	CONFLICT	UNP P11795
B	107	SER	GLY	CONFLICT	UNP P11795
C	102	GLY	SER	CONFLICT	UNP P11795
C	107	SER	GLY	CONFLICT	UNP P11795

- 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.

Chain A:



T241	T301	V301	T361
A242	L302	L302	V362
Y244	T303	T303	T363
G245	H304	H304	F364
G246	T305	T305	T365
A247	F306	F306	V366
G248	R307	R307	S367
A249	A308	A308	G368
D250	T309	T309	V369
A251	G310	G310	A370
V252	T311	T311	A371
G253	F312	F312	G372
E254	N313	N313	I373
L255	L314	L314	L374
F256	S315	S315	L375
L257	G316	G316	V376
A258	G317	G317	G377
R259	L318	L318	R378
S260	R319	R319	A379
V261	G320	G320	R380
T262	L321	L321	A381
L263	S322	S322	N382
Y264	G323	G323	V383
F265	L324	L324	R384
P266	T325	T325	N385
Q267	L326	L326	L386
P268	G327	G327	L387
T269	A328	A328	
N270	T269	T269	
T271	G330	G330	
L272	A331	A331	
L273	V332	V332	
S274	V333	V333	
S275	I334	I334	
K276	N335	N335	
R277	D336	D336	
L278	I337	I337	
D279	L338	L338	
L280	A339	A339	
T281	L340	L340	
G282	D341	D341	
S283	N342	N342	
L284	V343	V343	
A285	G344	G344	
D286	T345	T345	
A287	A346	A346	
T288	S347	S347	
G289	D348	D348	
P290	Y349	Y349	
L291	F350	F350	
Y292	L351	L351	
L293	N352	N352	
V294	C353	C353	
L295	T354	T354	
T296	V355	V355	
R297	S356	S356	
T298	S357	S357	
P299	L358	L358	
T300	P359	P359	

• Molecule 1: TOMATO BUSHY STUNT VIRUS

Chain C: 

ALA	ALA	LYS	V123	S184	Y244	T305	T365
PET	PET	GLN	M124	Q185	G245	F306	V366
THR	THR	GLY	G125	D186	G246	R307	S367
ARG	ARG	ASN	G126	P187	A249	A308	G368
ASN	ASN	GLN	I127	E188	D250	G310	V369
ASN	ASN	GLN	V128	P189	A251	T311	A371
ASN	ASN	GLN	G129	A190	V252	F312	G372
ASN	ASN	GLN	M130	D191	G253	N313	I373
ASN	ASN	GLN	S131	R192	E254	L314	L374
VAL	VAL	GLN	L132	V193	L255	S315	L375
LEU	LEU	GLN	Q133	E194	F256	G316	V376
ALA	ALA	GLN	L134	L195	L257	F317	G377
VAL	VAL	GLN	M135	A196	A258	L318	R378
SER	SER	GLN	N136	N197	R259	R319	A379
LYS	LYS	GLN	F136	F198	S260	C320	R380
LYS	LYS	GLN	S137	G199	T261	L321	A381
GLN	GLN	GLN	M138	V200	T262	T322	N382
LEU	LEU	GLN	G139	L201	G263	S323	V383
GLY	GLY	GLN	T140	K202	L263	A328	N384
VAL	VAL	GLN	L141	L203	Y264	G329	R385
LEU	LEU	GLN	F142	E203	N270	G330	L386
ALA	ALA	GLN	S143	T204	T271	V332	L387
ALA	ALA	GLN	M144	A205	L272	V333	
SER	SER	GLN	L145	P206	S273	N335	
ALA	ALA	GLN	R86	N207	K274	D336	
ALA	ALA	GLN	A87	A208	R275	I337	
ALA	ALA	GLN	L88	E209	K276	T337	
VAL	VAL	GLN	H89	A210	R277	L338	
GLY	GLY	GLN	G90	L211	L278	A339	
ALA	ALA	GLN	M91	L212	D279	L340	
LEU	LEU	GLN	S91	K213	T281	D341	
ARG	ARG	GLN	F92	L214	G282	N342	
ASN	ASN	GLN	K93	P215	S283	G344	
ASN	ASN	GLN	K94	T216	A284	T345	
TTR	TTR	GLN	F95	L217	D285	A346	
ILE	ILE	GLN	S96	D217	S286	S347	
GLY	GLY	GLN	G97	N158	T287	D348	
GLU	GLU	GLN	M98	V219	G288	V349	
SER	SER	GLN	T99	K220	G289	F350	
SER	SER	GLN	S100	R221	P290	N351	
PRO	PRO	GLN	G101	Y222	G291	S352	
ALA	ALA	GLN	L102	C223	Y292	C353	
LEU	LEU	GLN	V103	N224	T293	T354	
LEU	LEU	GLN	T104	D225	V294	V355	
GLN	GLN	GLN	V105	S226	L295	S356	
SER	SER	GLN	T106	A227	T296	S357	
ALA	ALA	GLN	S107	T228	R297	L358	
VAL	VAL	GLN	H108	V229	G298	P359	
GLY	GLY	GLN	R109	D230	T299	A360	
LEU	LEU	GLN	E110	Q231	T300	T361	
GLY	GLY	GLN	Y111	K232	T301	V362	
LYS	LYS	GLN	L112	L233	L302	T363	
LYS	LYS	GLN	T113	T234	H304	F364	
ALA	ALA	GLN	Q114	D235			
LEU	LEU	GLN	V115	L236			
ASN	ASN	GLN	N116	G237			
LYS	LYS	GLN	M117	Q238			
VAL	VAL	GLN	L118	L239			
ARG	ARG	GLN	S119	G240			
ASN	ASN	GLN	G120	T241			
ARG	ARG	GLN	F121	L242			
ARG	ARG	GLN	V122	T243			

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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:B:241:ILE:CD1	1:B:255:LEU:HD23	1.42	1.49
1:C:326:LEU:CD2	1:C:337:ILE:HD12	1.43	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:CA	1:A:280:LEU:N	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:147:ALA:CB	1:A:272:LEU:CD2	2.04	1.34
1:A:217:ASP:OD2	1:A:221:ARG:NH2	1.59	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:B:342:ASN:ND2	1:B:346:ALA:O	1.72	1.22
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:A:168:CYS:SG	1:A:252:VAL:HG13	1.80	1.22
1:C:98:ARG:CD	1:C:105:VAL:HG21	1.69	1.21
1:A:221:ARG:HG2	1:A:234:ILE:O	1.37	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:A:164:TYR:CD2	1:A:255:LEU:HD11	1.76	1.20
1:B:289:GLY:CA	1:B:290:PRO:O	1.89	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:277:ARG:CB	1:B:285:ALA:HB3	1.73	1.17
1:B:221:ARG:NH1	1:B:236:LEU:HA	1.59	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:136:PRO:HB2	1:C:145:LEU:HD22	1.20	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: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:275[P]:SER:HA	1:C:375:LEU:HD23	1.20	1.14
1:C:164:TYR:HD2	1:C:255:LEU:CD1	1.59	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:B:317:GLY:HA3	1:B:348:ASP:HA	1.29	1.13
1:C:168:CYS:SG	1:C:252:VAL:HG13	1.88	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:193:VAL:O	1:B:197:ASN:ND2	1.83	1.11
1:B:206:PRO:HB3	1:B:252:VAL:HG11	1.29	1.11
1:B:331:ALA:HB2	1:B:357:SER:HB3	1.28	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

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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:A:317:GLY:HA3	1:A:348:ASP:HA	1.29	1.10
1:C:133:GLN:O	1:C:138:ASN:ND2	1.82	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:B:275:SER:HA	1:B:375:LEU:HD23	1.20	1.09
1:C:164:TYR:CD2	1:C:255:LEU:CD1	2.34	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:A:276:LYS:O	1:A:295:LEU:HD11	1.51	1.09
1:B:221:ARG:CG	1:B:234:ILE:O	2.00	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:178:LEU:HD22	1:A:241:ILE:HG12	1.31	1.09
1:B:324:LEU:HD23	1:B:366:VAL:HG22	1.15	1.09
1:B:326:LEU:HD22	1:B:337:ILE:HD12	1.21	1.09
1:A:225:ASP:CB	1:C:186:ASP:OD1	2.01	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: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: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:B:276:LYS:O	1:B:295:LEU:HD11	1.51	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: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: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:164:TYR:HD2	1:A:255:LEU:CD1	1.66	1.07
1:A:319:ARG:CD	1:A:371:ALA:CB	2.32	1.07
1:B:319:ARG:CD	1:B:371:ALA:CB	2.32	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:C:152:PHE:HD2	1:C:264:TYR:O	1.37	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:A:302:LEU:O	1:A:363:THR:HG23	1.55	1.06
1:C:319:ARG:CD	1:C:371:ALA:CB	2.32	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:A:338:LEU:HD23	1:A:339:ALA:N	1.69	1.06
1:C:183:ASP:OD2	1:C:186:ASP:OD2	1.73	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: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:C:98:ARG:HD2	1:C:105:VAL:HG21	1.29	1.05
1:B:277:ARG:HB3	1:B:285:ALA:HB3	1.38	1.04
1:A:331:ALA:HB3	1:A:357:SER:OG	1.57	1.04
1:C:275[S]:SER:HA	1:C:375:LEU:HD23	1.34	1.04
1:C:104:THR:HG23	1:C:263:LEU:HD12	1.34	1.04
1:C:335:ASN:ND2	1:C:353:CYS:C	2.10	1.04
1:A:335:ASN:ND2	1:A:353:CYS:C	2.10	1.04
1:C:338:LEU:HD23	1:C:339:ALA:N	1.69	1.04
1:B:335:ASN:ND2	1:B:353:CYS:C	2.10	1.04
1:C:331:ALA:HB2	1:C:357:SER:CB	1.88	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:201:LEU:HD21	1:A:203:GLU:HG2	1.41	1.02
1:A:271:THR:HG22	1:A:273[S]:LEU:O	1.59	1.02
1:C:179:TYR:CE1	1:C:240:GLY:HA3	1.94	1.02
1:C:277:ARG:HB3	1:C:285:ALA:HB3	1.38	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:B:326:LEU:CD2	1:B:337:ILE:CD1	2.39	1.01
1:C:331:ALA:HB3	1:C:357:SER:OG	1.57	1.01
1:C:366:VAL:HG12	1:C:367:SER:N	1.75	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: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:A:200:VAL:HG12	1:A:200:VAL:O	1.57	1.00
1:C:200:VAL:O	1:C:200:VAL:HG12	1.57	1.00
1:B:335:ASN:ND2	1:B:353:CYS:CA	2.24	1.00
1:C:328:ALA:CB	1:C:362:VAL:HG22	1.91	1.00
1:A:277:ARG:HB2	1:A:285:ALA:HB3	1.41	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:B:319:ARG:HD2	1:B:371:ALA:HB2	1.05	1.00
1:C:335:ASN:ND2	1:C:353:CYS:CA	2.24	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:A:277:ARG:HB3	1:A:285:ALA:CB	1.92	0.99
1:B:338:LEU:HD23	1:B:339:ALA:H	1.26	0.99
1:C:326:LEU:CD2	1:C:337:ILE:CD1	2.39	0.99
1:A:331:ALA:CB	1:A:357:SER:OG	2.10	0.99
1:B:366:VAL:HG12	1:B:367:SER:N	1.75	0.99
1:A:328:ALA:CB	1:A:362:VAL:HG22	1.91	0.99
1:B:206:PRO:HG2	1:B:207:TRP:H	1.24	0.99
1:C:136:PRO:HB2	1:C:145:LEU:CD2	1.91	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:277:ARG:HB3	1:C:285:ALA:CB	1.92	0.99
1:C:68:ILE:CG2	1:C:70:HIS:NE2	2.22	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:B:293:LEU:HD12	1:B:376:VAL:HG21	1.46	0.98
1:C:103:VAL:HG11	1:C:264:TYR:CA	1.92	0.98
1:A:206:PRO:HB3	1:A:252:VAL:HG11	1.43	0.98
1:A:268:PRO:O	1:A:269:THR:O	1.82	0.98
1:A:320:CYS:CB	1:A:366:VAL:CG1	2.37	0.98
1:B:154:GLN:NE2	1:B:222:TYR:CD1	2.31	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:B:319:ARG:HD2	1:B:371:ALA:HB3	1.41	0.98
1:C:121:PHE:O	1:C:121:PHE:HD1	1.46	0.98
1:C:277:ARG:HB2	1:C:285:ALA:HB3	1.40	0.98
1:C:331:ALA:CB	1:C:357:SER:OG	2.10	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:A:331:ALA:CB	1:A:357:SER:CB	2.43	0.97
1:C:336:ASP:O	1:C:351:LEU:HA	1.62	0.97
1:A:279:ASP:HB3	1:A:282:GLY:HA3	1.46	0.97
1:B:130:ASN:HD22	1:B:238:GLN:NE2	1.63	0.97
1:B:331:ALA:CB	1:B:357:SER:CB	2.43	0.97
1:A:167:LEU:HD23	1:A:167:LEU:H	1.28	0.97
1:B:262:THR:HG22	1:B:264:TYR:CE2	2.00	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:B:319:ARG:CD	1:B:371:ALA:HB3	1.92	0.96
1:C:219:VAL:HB	1:C:221:ARG:HH21	1.28	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:A:168:CYS:SG	1:A:252:VAL:HG12	2.02	0.96
1:A:319:ARG:CD	1:A:371:ALA:HB2	1.94	0.96
1:B:241:ILE:HD11	1:B:255:LEU:HD23	1.00	0.96
1:C:167:LEU:HD21	1:C:253:GLY:N	1.80	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:168:CYS:SG	1:C:252:VAL:CG1	2.52	0.96
1:C:279:ASP:HB3	1:C:282:GLY:HA3	1.46	0.96
1:A:206:PRO:HB3	1:A:252:VAL:CG1	1.94	0.96
1:B:145:LEU:HD12	1:B:259:ARG:HD3	1.47	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:A:162:LEU:HD13	1:A:178:LEU:HD13	1.47	0.95
1:A:262:THR:HG22	1:A:264:TYR:CZ	2.01	0.95
1:B:319:ARG:CD	1:B:371:ALA:HB2	1.94	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:B:304:HIS:CE1	1:B:374:LEU:CD1	2.50	0.95
1:C:82:VAL:O	1:C:170:THR:CG2	2.14	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:A:103:VAL:HG13	1:A:263:LEU:O	1.66	0.94
1:C:331:ALA:CB	1:C:357:SER:HB3	1.98	0.94
1:C:97:GLY:O	1:C:98:ARG:C	2.04	0.94
1:A:104:THR:HG23	1:A:263:LEU:HD12	1.46	0.94
1:C:319:ARG:CD	1:C:371:ALA:HB2	1.94	0.94
1:C:138:ASN:O	1:C:141:LEU:N	2.01	0.94
1:C:201:LEU:HD23	1:C:202:LYS:N	1.81	0.94
1:C:338:LEU:HD23	1:C:339:ALA:H	1.26	0.94
1:A:304:HIS:CE1	1:A:374:LEU:CD1	2.50	0.94
1:B:335:ASN:CB	1:B:352:ASN:HD22	1.80	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:201:LEU:C	1:B:201:LEU:HD23	1.88	0.94
1:B:178:LEU:HD22	1:B:241:ILE:HG12	1.50	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: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:117:ASN:OD1	1:C:252:VAL:CG2	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:A:110:GLU:CD	1:A:144:TRP:HB3	1.89	0.93
1:C:134:LEU:HD23	1:C:236:LEU:HD23	1.50	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:A:201:LEU:HD23	1:A:201:LEU:C	1.88	0.93
1:B:127:ILE:CG2	1:B:128:VAL:H	1.82	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:A:324:LEU:HD22	1:A:366:VAL:CG2	1.98	0.92
1:A:335:ASN:HB3	1:A:352:ASN:ND2	1.84	0.92
1:B:110:GLU:OE1	1:B:144:TRP:N	2.03	0.92
1:C:335:ASN:HB3	1:C:352:ASN:ND2	1.83	0.92
1:A:331:ALA:CB	1:A:357:SER:HB3	1.98	0.92
1:C:319:ARG:CG	1:C:371:ALA:HB3	1.99	0.92
1:C:123:VAL:O	1:C:125:GLY:N	2.03	0.92
1:B:319:ARG:CG	1:B:371:ALA:HB3	1.99	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: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:A:276:LYS:HB3	1:A:295:LEU:CD2	1.99	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:C:195:LEU:CD2	1:C:201:LEU:HD11	2.00	0.91
1:A:278:LEU:HD21	1:A:295:LEU:O	1.70	0.91
1:C:296:THR:OG1	1:C:303:THR:HB	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:A:311:THR:HG22	1:A:379:ALA:O	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:VAL:HB	1:B:258:ALA:CB	2.00	0.91
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:195:LEU:CD2	1:A:201:LEU:HD11	2.00	0.91
1:A:338:LEU:HD23	1:A:339:ALA:H	1.26	0.91
1:B:275:SER:CA	1:B:375:LEU:HD23	2.00	0.91
1:B:296:THR:OG1	1:B:303:THR:HB	1.70	0.91
1:B:328:ALA:HB2	1:B:362:VAL:HG22	1.52	0.91
1:B:324:LEU:HD22	1:B:366:VAL:CG2	1.98	0.90
1:C:278:LEU:HD21	1:C:295:LEU:O	1.70	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:A:147:ALA:CB	1:A:272:LEU:HD22	1.86	0.90
1:B:241:ILE:HD11	1:B:255:LEU:HD21	1.54	0.90
1:C:104:THR:HG23	1:C:263:LEU:CD1	2.00	0.90
1:B:179:TYR:CE1	1:B:240:GLY:HA3	2.07	0.90
1:B:326:LEU:HD23	1:B:337:ILE:CD1	2.00	0.90
1:A:267:GLN:O	1:C:197:ASN:CB	2.20	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:B:335:ASN:HB3	1:B:352:ASN:HD22	1.34	0.89
1:A:228:THR:CG2	1:C:232:LYS:CD	2.49	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:183:ASP:CB	1:B:186:ASP:OD2	2.20	0.89
1:A:147:ALA:HB1	1:A:272:LEU:HD11	1.52	0.89
1:B:161:VAL:HB	1:B:258:ALA:HB3	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: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:129:GLY:O	1:C:307:ARG:NH2	2.05	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:B:304:HIS:HE1	1:B:374:LEU:HD13	1.13	0.88
1:C:304:HIS:HE1	1:C:374:LEU:CD1	1.85	0.88
1:C:104:THR:HG22	1:C:152:PHE:CZ	2.08	0.88
1:A:195:LEU:HD21	1:A:201:LEU:HD11	1.55	0.88
1:A:274[P]:SER:O	1:A:375:LEU:HA	1.73	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:A:241:ILE:HD13	1:A:255:LEU:HD23	1.52	0.88
1:B:262:THR:HG21	1:B:264:TYR:OH	1.72	0.88
1:B:178:LEU:CD2	1:B:241:ILE:HG12	2.02	0.88
1:C:351:LEU:HD12	1:C:351:LEU:C	1.94	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:A:355:VAL:HG13	1:A:360:ALA:HB2	1.55	0.87
1:B:135:ASN:ND2	1:B:224:ASN:OD1	2.08	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:262:THR:HG21	1:A:264:TYR:OH	1.75	0.87
1:A:326:LEU:HB2	1:A:337:ILE:HD11	1.57	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:201:LEU:HD23	1:B:202:LYS:N	1.90	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:326:LEU:HB2	1:B:337:ILE:CD1	2.06	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: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:192:ARG:NH1	1:B:244:TYR:CG	2.44	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:B:279:ASP:HB3	1:B:282:GLY:CA	2.05	0.85
1:C:335:ASN:HB3	1:C:352:ASN:HD22	1.34	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:A:335:ASN:HB2	1:A:352:ASN:ND2	1.91	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:326:LEU:HB2	1:C:337:ILE:HD11	1.57	0.84
1:C:96:THR:HG23	1:C:105:VAL:HB	1.56	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:A:164:TYR:CE2	1:A:255:LEU:HD11	2.11	0.84
1:C:279:ASP:HB3	1:C:282:GLY:CA	2.05	0.84
1:A:104:THR:HG21	1:A:263:LEU:HD12	1.59	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:B:298:THR:OG1	1:B:299:PRO:CD	2.26	0.84
1:B:319:ARG:HG3	1:B:371:ALA:HB3	1.57	0.84
1:C:152:PHE:CD2	1:C:264:TYR:O	2.28	0.84
1:A:222:TYR:O	1:A:234:ILE:CG2	2.26	0.83
1:A:342:ASN:OD1	1:A:345:THR:CB	2.23	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ASN:HB2	1:C:352:ASN:ND2	1.91	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:B:320:CYS:HB3	1:B:366:VAL:HG11	1.61	0.83
1:B:326:LEU:HD12	1:B:327:GLY:N	1.94	0.83
1:C:206:PRO:HG2	1:C:207:TRP:HD1	1.44	0.83
1:C:96:THR:CG2	1:C:105:VAL:HB	2.09	0.83
1:A:129:GLY:O	1:A:131:SER:N	2.11	0.83
1:C:321:LEU:O	1:C:322:THR:OG1	1.96	0.83
1:C:326:LEU:HD12	1:C:327:GLY:N	1.94	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:B:180:PHE:CD1	1:B:214:ILE:HD12	2.14	0.82
1:C:157:PHE:O	1:C:158:ASN:ND2	2.11	0.82
1:C:183:ASP:CB	1:C:186:ASP:OD2	2.26	0.82
1:A:157:PHE:O	1:A:158:ASN:ND2	2.11	0.82
1:B:309:THR:HG23	1:B:356:SER:HA	1.60	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:A:298:THR:OG1	1:A:299:PRO:CD	2.26	0.82
1:B:361:THR:C	1:B:362:VAL:CA	2.47	0.82
1:A:320:CYS:HB3	1:A:366:VAL:HG11	1.61	0.82
1:B:383:VAL:O	1:B:384:VAL:HG23	1.80	0.82
1:C:274[S]:SER:O	1:C:375:LEU:HA	1.79	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: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:C:385:ASN:OD1	1:C:386:LEU:N	2.13	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:B:204:THR:HG22	1:B:205:ALA:O	1.79	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:A:262:THR:CG2	1:A:264:TYR:CZ	2.62	0.81
1:B:262:THR:CG2	1:B:264:TYR:CZ	2.63	0.81
1:B:206:PRO:CB	1:B:252:VAL:HG11	2.10	0.81
1:A:366:VAL:HG12	1:A:367:SER:H	1.44	0.81
1:B:385:ASN:OD1	1:B:386:LEU:N	2.13	0.81
1:C:183:ASP:HB3	1:C:186:ASP:OD2	1.81	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:298:THR:OG1	1:C:299:PRO:CD	2.26	0.81
1:C:335:ASN:HD22	1:C:353:CYS:N	1.78	0.81
1:C:383:VAL:O	1:C:384:VAL:HG23	1.80	0.81
1:A:231:GLN:O	1:A:235:ASP:OD2	1.99	0.81
1:C:262:THR:HG22	1:C:264:TYR:CZ	2.15	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:B:157:PHE:CD2	1:B:261:VAL:HG22	2.16	0.80
1:C:145:LEU:HB3	1:C:146:PRO:HD3	1.62	0.80
1:A:183:ASP:CB	1:A:186:ASP:OD2	2.29	0.80
1:A:195:LEU:HD23	1:A:201:LEU:CD1	2.11	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: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:C:127:ILE:HG22	1:C:128:VAL:N	1.97	0.80
1:A:225:ASP:HB3	1:C:186:ASP:OD1	1.79	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:B:180:PHE:HD1	1:B:214:ILE:HD12	1.45	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: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:A:114:GLN:HE21	1:A:251:ALA:HB2	1.46	0.79
1:C:136:PRO:CB	1:C:145:LEU:HD22	2.10	0.79
1:A:201:LEU:HD23	1:A:202:LYS:CA	2.13	0.79
1:A:318:LEU:N	1:A:347:SER:O	2.16	0.79
1:C:309:THR:HG23	1:C:355:VAL:O	1.82	0.78
1:A:104:THR:CG2	1:A:263:LEU:CD1	2.60	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: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:298:THR:HG1	1:A:299:PRO:HD2	1.47	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:B:309:THR:HG23	1:B:355:VAL:O	1.82	0.78
1:A:309:THR:HG23	1:A:355:VAL:O	1.82	0.78
1:B:228:THR:HG21	1:B:234:ILE:HD11	1.65	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:A:167:LEU:CD2	1:A:167:LEU:H	1.95	0.77
1:C:114:GLN:HE21	1:C:251:ALA:HB2	1.48	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:B:119:SER:HA	1:B:246:GLY:N	1.99	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: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:B:206:PRO:HB3	1:B:252:VAL:CG1	2.11	0.77
1:C:118:SER:O	1:C:119:SER:C	2.23	0.77
1:A:329:THR:O	1:A:361:THR:HG22	1.85	0.77
1:B:328:ALA:HB1	1:B:362:VAL:HG22	1.64	0.77
1:A:267:GLN:NE2	1:C:198:PHE:CZ	2.53	0.77
1:C:335:ASN:ND2	1:C:353:CYS:HA	1.99	0.77
1:A:200:VAL:CG1	1:A:200:VAL:O	2.29	0.77
1:A:316:GLY:O	1:A:349:TYR:N	2.17	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:B:316:GLY:O	1:B:349:TYR:N	2.17	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:A:104:THR:HG23	1:A:263:LEU:HB2	1.64	0.77
1:B:336:ASP:OD2	1:B:385:ASN:HB2	1.85	0.77
1:A:300:THR:O	1:A:366:VAL:O	2.03	0.76
1:B:183:ASP:CG	1:B:186:ASP:OD2	2.22	0.76
1:C:317:GLY:CA	1:C:348:ASP:HA	2.13	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:A:195:LEU:CD2	1:A:201:LEU:CD1	2.62	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:B:297:ARG:HE	1:B:299:PRO:HA	1.50	0.76
1:C:67:ILE:CG2	1:C:68:ILE:H	1.92	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:A:297:ARG:HE	1:A:299:PRO:HA	1.50	0.76
1:B:145:LEU:HB3	1:B:146:PRO:HD3	1.68	0.76
1:B:177:ALA:HB2	1:B:203:GLU:OE1	1.86	0.76
1:A:321:LEU:HB2	1:A:344:GLY:H	1.51	0.76
1:C:289:GLY:CA	1:C:290:PRO:C	2.50	0.76
1:C:320:CYS:HB2	1:C:366:VAL:HG12	1.67	0.76
1:C:300:THR:O	1:C:366:VAL:O	2.03	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:B:331:ALA:O	1:B:332:VAL:CG2	2.33	0.75
1:C:328:ALA:HB1	1:C:362:VAL:HG22	1.65	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: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:C:138:ASN:O	1:C:139:GLY:C	2.25	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:121:PHE:C	1:C:121:PHE:CD1	2.59	0.74
1:C:167:LEU:CD2	1:C:167:LEU:H	2.00	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:321:LEU:HB2	1:C:344:GLY:H	1.51	0.74
1:C:98:ARG:O	1:C:100:SER:N	2.20	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:206:PRO:HB3	1:C:252:VAL:HG11	1.68	0.74
1:C:168:CYS:CB	1:C:252:VAL:HG13	2.17	0.74
1:A:317:GLY:HA3	1:A:348:ASP:CA	2.13	0.74
1:C:168:CYS:HB3	1:C:252:VAL:HA	1.68	0.74
1:C:326:LEU:CB	1:C:337:ILE:CD1	2.65	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: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:326:LEU:CB	1:A:337:ILE:CD1	2.65	0.74
1:A:123:VAL:CG1	1:A:124:ASN:ND2	2.51	0.74
1:B:317:GLY:HA3	1:B:348:ASP:CA	2.13	0.74
1:C:230:ASP:O	1:C:232:LYS:N	2.20	0.74
1:A:117:ASN:O	1:A:249:ALA:HA	1.88	0.73
1:A:123:VAL:O	1:A:124:ASN:C	2.25	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:PHE:CG	1:B:263:LEU:HB3	2.23	0.73
1:A:219:VAL:HB	1:A:221:ARG:NH2	2.03	0.73
1:A:300:THR:OG1	1:A:301:VAL:HG23	1.88	0.73
1:B:300:THR:OG1	1:B: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:A:295:LEU:HD23	1:A:295:LEU:H	1.52	0.73
1:C:300:THR:OG1	1:C:301:VAL:HG23	1.88	0.73
1:C:114:GLN:NE2	1:C:251:ALA:HB2	2.02	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:B:106:THR:C	1:B:107:SER:CA	2.56	0.73
1:B:295:LEU:H	1:B:295:LEU:HD23	1.52	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:A:278:LEU:CD2	1:A:295:LEU:O	2.37	0.72
1:A:267:GLN:CB	1:C:198:PHE:CD1	2.72	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:A:341:ASP:OD1	1:A:347:SER:CB	2.38	0.72
1:B:366:VAL:CG1	1:B:367:SER:H	2.01	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:119:SER:HA	1:B:246:GLY:H	1.53	0.72
1:B:362:VAL:N	1:B:362:VAL:CB	2.52	0.72
1:B:278:LEU:CD2	1:B:295:LEU:O	2.37	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:341:ASP:OD1	1:B:347:SER:CB	2.38	0.72
1:C:266:PRO:CG	1:C:266:PRO:O	2.29	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:165:VAL:O	1:B:166:PRO:HB3	1.88	0.72
1:A:226:SER:OG	1:C:183:ASP:OD2	2.08	0.72
1:A:151:ASN:CG	1:A:269:THR:OG1	2.27	0.72
1:C:200:VAL:O	1:C:200:VAL:CG1	2.29	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ALA:O	1:C:332:VAL:HG23	1.90	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:103:VAL:CG1	1:A:263:LEU:O	2.39	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:162:LEU:HD12	1:A:212:LEU:HD23	1.71	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: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:A:117:ASN:HB2	1:A:248:GLY:O	1.91	0.71
1:B:320:CYS:HB2	1:B:366:VAL:HG12	1.67	0.71
1:B:326:LEU:HD22	1:B:337:ILE:CD1	2.10	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:A:355:VAL:CG1	1:A:360:ALA:HB2	2.20	0.71
1:B:177:ALA:CB	1:B:203:GLU:OE1	2.39	0.71
1:C:183:ASP:CG	1:C:186:ASP:OD2	2.30	0.71
1:A:241:ILE:CD1	1:A:255:LEU:HD23	2.20	0.70
1:A:262:THR:CG2	1:A:264:TYR:OH	2.39	0.70
1:B:201:LEU:HD23	1:B:202:LYS:CA	2.20	0.70
1:A:186:ASP:OD1	1:B:225:ASP:HB3	1.91	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:A:355:VAL:HG13	1:A:360:ALA:CB	2.22	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

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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:A:337:ILE:HG23	1:A:337:ILE:O	1.91	0.70
1:C:134:LEU:HD23	1:C:236:LEU:CD2	2.21	0.70
1:A:104:THR:CG2	1:A:263:LEU:CB	2.65	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: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:A:204:THR:HG22	1:A:205:ALA:O	1.92	0.69
1:B:104:THR:HB	1:B:263:LEU:HB2	1.74	0.69
1:B:123:VAL:O	1:B:125:GLY:N	2.25	0.69
1:B:189:PRO:HG3	1:B:198:PHE:CE2	2.27	0.69
1:B:111:TYR:CE2	1:B:254:GLU:HG3	2.27	0.69
1:C:314:LEU:HD13	1:C:351:LEU:HD11	1.73	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:C:128:VAL:HG13	1:C:188:GLU:OE1	1.92	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:169:GLY:O	1:B:171:THR:N	2.22	0.69
1:B:103:VAL:HG13	1:B:264:TYR:HA	1.75	0.69
1:A:104:THR:HG21	1:A:263:LEU:CD1	2.22	0.68
1:C:351:LEU:C	1:C:351:LEU:CD1	2.61	0.68
1:B:152:PHE:CD1	1:B:263:LEU:HD13	2.29	0.68
1:B:355:VAL:HG13	1:B:360:ALA:CB	2.22	0.68
1:C:100:SER:OG	1:C:101:GLY:N	2.26	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:298:THR:HG1	1:B:299:PRO:HD2	1.56	0.68
1:B:345:THR:O	1:B:346:ALA:O	2.12	0.68
1:C:167:LEU:CD2	1:C:253:GLY:N	2.56	0.68
1:A:277:ARG:HD2	1:A:286:ASP:OD1	1.93	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: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:201:LEU:C	1:C:201:LEU:CD2	2.61	0.68
1:C:164:TYR:HB3	1:C:210:ALA:HB3	1.76	0.68
1:A:111:TYR:CE2	1:A:254:GLU:OE2	2.46	0.68
1:A:167:LEU:HD23	1:A:252:VAL:O	1.93	0.68
1:A:297:ARG:HG2	1:A:298:THR:N	2.08	0.68
1:B:351:LEU:C	1:B:351:LEU:CD1	2.61	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:A:345:THR:O	1:A:346:ALA:O	2.12	0.67
1:B:230:ASP:O	1:B:232:LYS:N	2.26	0.67
1:B:222:TYR:O	1:B:234:ILE:HG23	1.95	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:B:297:ARG:HG2	1:B:298:THR:N	2.08	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:145:LEU:CB	1:C:146:PRO:HD3	2.16	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:A:320:CYS:SG	1:A:366:VAL:HG11	2.35	0.67
1:C:131:SER:O	1:C:132:LEU:C	2.31	0.67
1:C:104:THR:HG23	1:C:263:LEU:HB2	1.75	0.67
1:A:142:PHE:HB3	1:A:146:PRO:HD2	1.77	0.67
1:A:309:THR:CG2	1:A:356:SER:HA	2.25	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: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:206:PRO:HG2	1:C:207:TRP:H	1.59	0.67
1:C:279:ASP:CB	1:C:282:GLY:HA3	2.22	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: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:C:345:THR:O	1:C:346:ALA:O	2.12	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:B:206:PRO:CB	1:B:252:VAL:CG1	2.72	0.66
1:C:104:THR:CG2	1:C:263:LEU:CD1	2.73	0.66
1:C:164:TYR:CD2	1:C:255:LEU:HD12	2.28	0.66
1:C:324:LEU:CD2	1:C:366:VAL:HG21	1.96	0.66
1:A:146:PRO:O	1:A:150:SER:OG	2.14	0.65
1:B:119:SER:O	1:B:120:GLY:O	2.14	0.65
1:B:228:THR:HG21	1:B:234:ILE:CD1	2.25	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:B:221:ARG:HH11	1:B:236:LEU:CA	1.98	0.65
1:A:279:ASP:CB	1:A:282:GLY:HA3	2.22	0.65
1:B:232:LYS:HD2	1:C:228:THR:HG21	1.78	0.65
1:C:127:ILE:CG2	1:C:128:VAL:N	2.58	0.65
1:C:326:LEU:HD12	1:C:326:LEU:C	2.16	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:A:164:TYR:HB3	1:A:210:ALA:HB3	1.78	0.65
1:B:279:ASP:CB	1:B:282:GLY:HA3	2.22	0.65
1:B:335:ASN:HD21	1:B:354:THR:N	1.95	0.65
1:C:179:TYR:CZ	1:C:240:GLY:HA3	2.32	0.65
1:C:88:LEU:CD1	1:C:256:PHE:CE2	2.80	0.65
1:A:226:SER:CB	1:C:185:GLN:CB	2.74	0.65
1:B:145:LEU:HD23	1:B:145:LEU:O	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:110:GLU:CD	1:B:144:TRP:HB3	2.18	0.64
1:B:122:VAL:HG12	1:B:123:VAL:N	2.11	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:180:PHE:O	1:A:180:PHE:HD2	1.79	0.64
1:A:108:HIS:O	1:A:259:ARG:N	2.28	0.64
1:A:338:LEU:HD23	1:A:338:LEU:C	2.18	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:226:SER:HB3	1:C:186:ASP:N	2.13	0.64
1:B:326:LEU:C	1:B:326:LEU:HD12	2.16	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: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: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:175:ARG:HG2	1:C:244:TYR:CZ	2.33	0.64
1:A:115:VAL:N	1:A:253:GLY:O	2.29	0.64
1:B:324:LEU:HD22	1:B:366:VAL:HG23	1.80	0.64
1:C:338:LEU:C	1:C:338:LEU:HD23	2.18	0.64
1:C:335:ASN:HD21	1:C:354:THR:N	1.95	0.64
1:A:355:VAL:CG1	1:A:360:ALA:CB	2.77	0.63
1:B:347:SER:OG	1:B:348:ASP:N	2.29	0.63
1:C:274[P]:SER:O	1:C:375:LEU:CA	2.44	0.63
1:C:298:THR:O	1:C:300:THR:N	2.31	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:B:298:THR:O	1:B:300:THR:N	2.31	0.63
1:C:278:LEU:CG	1:C:295:LEU:O	2.47	0.63
1:A:206:PRO:HB3	1:A:252:VAL:HG12	1.80	0.63
1:A:267:GLN:HA	1:C:198:PHE:HA	1.79	0.63
1:B:283:SER:O	1:B:284:LEU:HG	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275[S]:SER:HA	1:C:375:LEU:CD2	2.21	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
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: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: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:A:278:LEU:CG	1:A:295:LEU:O	2.47	0.63
1:A:298:THR:O	1:A:300:THR:N	2.31	0.63
1:C:342:ASN:O	1:C:343:VAL:O	2.16	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:147:ALA:CA	1:A:272:LEU:CD2	2.64	0.63
1:A:171:THR:C	1:A:172:GLU:CA	2.62	0.63
1:A:164:TYR:CD2	1:A:255:LEU:HD12	2.31	0.63
1:B:295:LEU:N	1:B:295:LEU:HD23	2.14	0.63
1:B:335:ASN:HB2	1:B:352:ASN:HD22	1.57	0.63
1:A:277:ARG:CB	1:A:285:ALA:CB	2.56	0.63
1:A:283:SER:O	1:A:284:LEU:HG	1.98	0.63
1:B:314:LEU:HD13	1:B:351:LEU:CD1	2.29	0.63
1:B:321:LEU:N	1:B:321:LEU:HD23	2.14	0.63
1:C:145:LEU:HD12	1:C:259:ARG:HD3	1.80	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:CD2	1:B:201:LEU:C	2.61	0.62
1:C:214:ILE:HD11	1:C:239:LEU:HD21	1.81	0.62
1:C:127:ILE:CD1	1:C:358:LEU:HD13	2.29	0.62
1:A:321:LEU:N	1:A:321:LEU:HD23	2.14	0.62
1:B:331:ALA:HB3	1:B:357:SER:CB	2.23	0.62
1:C:324:LEU:HD22	1:C:366:VAL:HG23	1.80	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:B:180:PHE:HB3	1:B:200:VAL:HG11	1.82	0.62
1:A:233:LEU:HD21	1:B:234:ILE:HG12	1.82	0.62
1:C:110:GLU:OE1	1:C:144:TRP:N	2.23	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:SER:HA	1:C:246:GLY:H	1.62	0.62
1:A:168:CYS:HB3	1:A:252:VAL:HA	1.82	0.62
1:A:336:ASP:OD2	1:A:385:ASN:CB	2.47	0.62
1:C:132:LEU:HD13	1:C:239:LEU:O	1.98	0.62
1:B:336:ASP:OD2	1:B:385:ASN:CB	2.47	0.62
1:C:295:LEU:HD23	1:C:295:LEU:N	2.14	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: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:222:TYR:O	1:C:234:ILE:HG23	1.99	0.61
1:C:108:HIS:CD2	1:C:109:ARG:H	2.18	0.61
1:C:154:GLN:HB2	1:C:264:TYR:HB2	1.82	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:162:LEU:HB2	1:C:212:LEU:HB3	1.82	0.61
1:C:351:LEU:CD1	1:C:352:ASN:N	2.64	0.61
1:A:108:HIS:CG	1:A:109:ARG:H	2.18	0.61
1:A:160:VAL:HA	1:A:258:ALA:O	2.01	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:A:351:LEU:CD1	1:A:352:ASN:N	2.64	0.61
1:B:117:ASN:N	1:B:250:ASP:O	2.33	0.61
1:A:206:PRO:CB	1:A:252:VAL:HG11	2.28	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:331:ALA:HB3	1:A:357:SER:CB	2.23	0.61
1:A:300:THR:C	1:A:369:VAL:CG2	2.69	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:B:170:THR:O	1:B:170:THR:CG2	2.45	0.61
1:B:274[S]:SER:N	1:B:376:VAL:O	2.30	0.61
1:C:110:GLU:OE1	1:C:142:PHE:C	2.38	0.61
1:C:326:LEU:CB	1:C:337:ILE:HD12	2.28	0.61
1:A:267:GLN:CD	1:C:198:PHE:HE1	2.04	0.60
1:C:204:THR:CG2	1:C:205:ALA:O	2.40	0.60
1:C:103:VAL:CG1	1:C:263:LEU:O	2.49	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:A:226:SER:OG	1:C:185:GLN:HB2	2.00	0.60
1:A:114:GLN:NE2	1:A:251:ALA:HB2	2.16	0.60
1:A:329:THR:N	1:A:361:THR:HG23	2.16	0.60
1:B:107:SER:N	1:B:107:SER:C	2.52	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: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:114:GLN:HE21	1:A:251:ALA:CB	2.13	0.60
1:A:338:LEU:HD12	1:A:385:ASN:HA	1.83	0.60
1:A:161:VAL:HB	1:A:258:ALA:HB3	1.83	0.60
1:B:301:VAL:N	1:B:369:VAL:HG21	2.16	0.60
1:A:145:LEU:HD12	1:A:259:ARG:CD	2.25	0.60
1:A:301:VAL:N	1:A:369:VAL:HG21	2.17	0.60
1:B:300:THR:C	1:B:369:VAL:CG2	2.69	0.60
1:C:161:VAL:HB	1:C:258:ALA:HB3	1.84	0.60
1:C:301:VAL:N	1:C:369:VAL:HG21	2.16	0.60
1:C:70:HIS:HB3	1:C:79:MET:CE	2.32	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: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:A:297:ARG:HG3	1:A:298:THR:O	2.03	0.59
1:B:148:LEU:C	1:B:150:SER:H	2.06	0.59
1:B:157:PHE:CE2	1:B:261:VAL:HG22	2.37	0.59
1:B:297:ARG:HG3	1:B:298:THR:O	2.03	0.59
1:A:162:LEU:HB2	1:A:212:LEU:HB3	1.82	0.59
1:A:280:LEU:HB3	1:A:370:ALA:O	2.03	0.59
1:C:138:ASN:C	1:C:140:THR:H	2.03	0.59
1:C:383:VAL:O	1:C:384:VAL:HG22	2.02	0.59
1:A:349:TYR:CD2	1:A:349:TYR:O	2.56	0.59
1:A:274[P]:SER:O	1:A:376:VAL:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:LEU:O	1:B:347:SER:N	2.29	0.59
1:C:155:TYR:OH	1:C:221:ARG:HD2	2.02	0.59
1:A:383:VAL:O	1:A:384:VAL:HG22	2.02	0.59
1:B:280:LEU:HB3	1:B:370:ALA:O	2.03	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:A:314:LEU:HD22	1:A:351:LEU:HD11	1.85	0.59
1:B:145:LEU:O	1:B:146:PRO:C	2.41	0.59
1:B:383:VAL:O	1:B:384:VAL:HG22	2.02	0.59
1:C:280:LEU:HB3	1:C:370:ALA:O	2.03	0.59
1:B:111:TYR:HA	1:B:256:PHE:CD1	2.38	0.58
1:A:162:LEU:HD13	1:A:178:LEU:HB3	1.84	0.58
1:A:267:GLN:CG	1:A:268:PRO:N	2.60	0.58
1:B:349:TYR:CD2	1:B:349:TYR:O	2.56	0.58
1:C:132:LEU:HD12	1:C:239:LEU:O	2.03	0.58
1:C:331:ALA:C	1:C:332:VAL:HG23	2.24	0.58
1:B:160:VAL:HA	1:B:258:ALA:O	2.03	0.58
1:B:195:LEU:HD23	1:B:201:LEU:HD12	1.85	0.58
1:C:162:LEU:HB3	1:C:178:LEU:CD1	2.33	0.58
1:A:186:ASP:HA	1:B:226:SER:OG	2.02	0.58
1:B:280:LEU:HA	1:B:370:ALA:O	2.04	0.58
1:B:314:LEU:HD22	1:B:351:LEU:HD11	1.85	0.58
1:B:321:LEU:HB2	1:B:344:GLY:N	2.18	0.58
1:B:331:ALA:C	1:B:332:VAL:HG23	2.24	0.58
1:C:114:GLN:NE2	1:C:251:ALA:CB	2.66	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:331:ALA:C	1:A:332:VAL:HG23	2.24	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: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:336:ASP:O	1:B:351:LEU:CA	2.45	0.57
1:B:329:THR:N	1:B:361:THR:HG23	2.16	0.57
1:B:280:LEU:CA	1:B:370:ALA:O	2.52	0.57
1:A:167:LEU:CD2	1:A:252:VAL:C	2.72	0.57
1:A:329:THR:H	1:A:361:THR:HG23	1.69	0.57
1:B:201:LEU:CD2	1:B:202:LYS:N	2.66	0.57
1:B:276:LYS:HB2	1:B:374:LEU:HD21	1.86	0.57
1:C:329:THR:N	1:C:361:THR:HG23	2.16	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:B:342:ASN:CG	1:B:345:THR:HB	2.20	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:C:341:ASP:OD1	1:C:347:SER:HB2	2.04	0.57
1:A:214:ILE:HG22	1:A:215:PRO:N	2.17	0.57
1:A:276:LYS:HB2	1:A:374:LEU:CD2	2.34	0.57
1:A:180:PHE:HB3	1:A:200:VAL:HB	1.87	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: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:C:276:LYS:HB2	1:C:374:LEU:HD21	1.86	0.57
1:C:314:LEU:HD22	1:C:351:LEU:HD11	1.85	0.57
1:C:329:THR:H	1:C:361:THR:HG23	1.69	0.57
1:C:280:LEU:HA	1:C:370:ALA:O	2.04	0.57
1:A:276:LYS:HB2	1:A:374:LEU:HD21	1.86	0.57
1:A:280:LEU:CA	1:A:370:ALA:O	2.52	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:C:341:ASP:OD1	1:C:347:SER:OG	2.22	0.57
1:A:167:LEU:HD21	1:A:252:VAL:C	2.25	0.57
1:B:190:ALA:CB	1:B:194:GLU:OE2	2.51	0.57
1:B:206:PRO:HG2	1:B:207:TRP:CD1	2.39	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: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:132:LEU:HB3	1:B:239:LEU:HB2	1.85	0.57
1:B:145:LEU:HD12	1:B:259:ARG:CD	2.30	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:A:341:ASP:OD1	1:A:347:SER:HB2	2.04	0.56
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: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:B:341:ASP:OD1	1:B:347:SER:OG	2.22	0.56
1:C:274[P]:SER:O	1:C:376:VAL:N	2.36	0.56
1:A:185:GLN:CB	1:B:226:SER:CB	2.81	0.56
1:C:122:VAL:HG12	1:C:123:VAL:N	2.20	0.56
1:C:181:ASP:HB3	1:C:238:GLN:HB3	1.85	0.56
1:C:276:LYS:HB2	1:C:374:LEU:CD2	2.34	0.56
1:A:134:LEU:HD13	1:A:239:LEU:CD1	2.35	0.56
1:A:317:GLY:HA3	1:A:347:SER:O	2.06	0.56
1:B:341:ASP:OD1	1:B:347:SER:HB2	2.04	0.56
1:B:300:THR:C	1:B:369:VAL:HG23	2.26	0.56
1:A:230:ASP:OD2	1:C:230:ASP:OD2	2.24	0.56
1:A:335:ASN:HD22	1:A:353:CYS:HA	1.60	0.56
1:B:142:PHE:HB3	1:B:146:PRO:HD2	1.86	0.56
1:B:298:THR:HG22	1:B:301:VAL:O	2.05	0.56
1:C:190:ALA:HB3	1:C:194:GLU:CD	2.23	0.56
1:C:214:ILE:HG22	1:C:215:PRO:N	2.17	0.56
1:C:298:THR:HG22	1:C:301:VAL:O	2.05	0.56
1:C:300:THR:C	1:C:369:VAL:HG23	2.26	0.56
1:B:241:ILE:CD1	1:B:255:LEU:HD21	2.22	0.56
1:C:262:THR:CG2	1:C:264:TYR:OH	2.53	0.56
1:C:317:GLY:HA3	1:C:347:SER:O	2.06	0.56
1:A:168:CYS:HG	1:A:252:VAL:CG1	2.16	0.56
1:A:265:PHE:CD1	1:A:265:PHE:N	2.73	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:219:VAL:CB	1:A:221:ARG:HH21	2.11	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: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:110:GLU:CG	1:A:144:TRP:HB3	2.35	0.56
1:C:180:PHE:CD2	1:C:180:PHE:C	2.79	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: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:C:328:ALA:HB1	1:C:361:THR:O	2.06	0.55
1:A:328:ALA:HB1	1:A:361:THR:O	2.06	0.55
1:B:265:PHE:N	1:B:265:PHE:CD1	2.74	0.55
1:C:170:THR:OG1	1:C:170:THR:O	2.24	0.55
1:C:223:CYS:CA	1:C:224:ASN:N	2.62	0.55
1:C:130:ASN:ND2	1:C:238:GLN:OE1	2.38	0.55
1:A:326:LEU:CG	1:A:337:ILE:HD12	2.29	0.55
1:C:157:PHE:CD1	1:C:236:LEU:HD22	2.41	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:A:267:GLN:CA	1:C:198:PHE:HA	2.36	0.55
1:A:300:THR:C	1:A:369:VAL:HG23	2.26	0.55
1:B:111:TYR:CE2	1:B:254:GLU:CG	2.89	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: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:118:SER:O	1:C:120:GLY:N	2.40	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:B:165:VAL:O	1:B:166:PRO:CB	2.55	0.54
1:B:275:SER:HB2	1:B:375:LEU:HD21	1.88	0.54
1:C:127:ILE:HG22	1:C:128:VAL:H	1.71	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:A:204:THR:C	1:A:205:ALA:O	2.41	0.54
1:A:331:ALA:O	1:A:332:VAL:HG22	2.07	0.54
1:A:319:ARG:HA	1:A:346:ALA:HA	1.90	0.54
1:B:152:PHE:CE1	1:B:263:LEU:CD1	2.78	0.54
1:A:297:ARG:CG	1:A:298:THR:N	2.70	0.54
1:A:321:LEU:HB2	1:A:344:GLY:N	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ASN:OD1	1:B:140:THR:HB	2.08	0.54
1:B:319:ARG:HA	1:B:346:ALA:HA	1.90	0.54
1:C:151:ASN:O	1:C:267:GLN:N	2.41	0.54
1:A:228:THR:CG2	1:C:232:LYS:CE	2.85	0.54
1:C:289:GLY:HA3	1:C:290:PRO:O	1.99	0.54
1:C:331:ALA:O	1:C:332:VAL:HG22	2.07	0.54
1:A:326:LEU:HD21	1:A:334:ILE:HD13	1.90	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:B:180:PHE:C	1:B:180:PHE:CD2	2.81	0.54
1:B:311:THR:CG2	1:B:379:ALA:O	2.50	0.54
1:C:127:ILE:CG2	1:C:128:VAL:H	2.19	0.54
1:C:267:GLN:O	1:C:268:PRO:C	2.46	0.54
1:C:297:ARG:CG	1:C:298:THR:N	2.70	0.54
1:B:180:PHE:HD2	1:B:180:PHE:O	1.91	0.54
1:B:216:THR:HG22	1:B:217:ASP:O	2.07	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:C:183:ASP:C	1:C:185:GLN:N	2.56	0.54
1:B:124:ASN:OD1	1:B:132:LEU:HD12	2.07	0.54
1:A:183:ASP:HB2	1:B:153:ASP:OD2	2.08	0.54
1:B:275:SER:HB2	1:B:375:LEU:CD2	2.38	0.54
1:C:91:SER:HB2	1:C:109:ARG:NE	2.23	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:B:164:TYR:HE2	1:B:253:GLY:HA3	1.73	0.53
1:C:274[S]:SER:CB	1:C:376:VAL:O	2.56	0.53
1:A:180:PHE:HD1	1:A:214:ILE:HD12	1.72	0.53
1:A:311:THR:CG2	1:A:379:ALA:O	2.50	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:C:180:PHE:O	1:C:180:PHE:HD2	1.90	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:275[S]:SER:N	1:C:375:LEU:HD23	2.23	0.53
1:B:232:LYS:HG3	1:B:233:LEU:H	1.71	0.53
1:C:289:GLY:HA3	1:C:290:PRO:C	2.28	0.53
1:C:300:THR:CB	1:C:301:VAL:HG23	2.39	0.53
1:A:201:LEU:CD2	1:A:203:GLU:HG2	2.25	0.53
1:A:329:THR:C	1:A:361:THR:HG22	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:204:THR:O	1:B:205:ALA:O	2.26	0.53
1:B:111:TYR:HE2	1:B:254:GLU:HG3	1.72	0.53
1:A:150:SER:O	1:A:270:ASN:N	2.42	0.53
1:A:168:CYS:HG	1:A:252:VAL:HG13	1.69	0.53
1:B:328:ALA:HB2	1:B:362:VAL:CG2	2.34	0.53
1:C:132:LEU:O	1:C:141:LEU:CD2	2.56	0.53
1:A:300:THR:CB	1:A:301:VAL:HG23	2.39	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: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:A:316:GLY:O	1:A:349:TYR:O	2.26	0.52
1:B:103:VAL:HG13	1:B:264:TYR:CA	2.36	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:B:330:GLY:HA3	1:B:359:PRO:O	2.09	0.52
1:C:214:ILE:CG2	1:C:215:PRO:N	2.71	0.52
1:A:328:ALA:HB2	1:A:362:VAL:CG2	2.34	0.52
1:A:309:THR:CG2	1:A:355:VAL:O	2.56	0.52
1:B:351:LEU:HD12	1:B:352:ASN:N	2.25	0.52
1:C:316:GLY:O	1:C:349:TYR:O	2.26	0.52
1:C:330:GLY:HA3	1:C:359:PRO:O	2.09	0.52
1:A:200:VAL:HG13	1:A:212:LEU:HD11	1.90	0.52
1:A:267:GLN:CB	1:C:198:PHE:HA	2.40	0.52
1:A:330:GLY:HA3	1:A:359:PRO:O	2.09	0.52
1:C:326:LEU:HD21	1:C:334:ILE:HD13	1.90	0.52
1:A:162:LEU:CD1	1:A:178:LEU:HD13	2.32	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:B:276:LYS:O	1:B:374:LEU:HD23	2.10	0.52
1:C:115:VAL:HG23	1:C:255:LEU:HD22	1.91	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:115:VAL:CG2	1:C:255:LEU:HD22	2.40	0.52
1:C:200:VAL:HG13	1:C:212:LEU:HD11	1.90	0.52
1:C:297:ARG:NE	1:C:299:PRO:HA	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:LEU:HD12	1:C:352:ASN:N	2.24	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:A:195:LEU:HD23	1:A:201:LEU:HD12	1.91	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:221:ARG:CD	1:A:234:ILE:O	2.58	0.52
1:A:342:ASN:HD21	1:A:345:THR:C	2.13	0.52
1:B:162:LEU:HB2	1:B:212:LEU:HB3	1.92	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: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:383:VAL:C	1:C:384:VAL:CG2	2.77	0.51
1:C:68:ILE:CG2	1:C:70:HIS:HD2	2.06	0.51
1:A:172:GLU:CB	1:A:172:GLU:N	2.68	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:C:342:ASN:HD21	1:C:345:THR:C	2.13	0.51
1:A:175:ARG:O	1:A:243:THR:HA	2.09	0.51
1:C:118:SER:OG	1:C:243:THR:OG1	1.95	0.51
1:B:165:VAL:HA	1:B:209:GLU:HG3	1.92	0.51
1:C:201:LEU:CD2	1:C:203:GLU:HG2	2.29	0.51
1:C:115:VAL:CG2	1:C:241:ILE:HG21	2.41	0.51
1:C:70:HIS:CB	1:C:79:MET:HE3	2.41	0.51
1:B:342:ASN:HD21	1:B:345:THR:C	2.13	0.51
1:A:226:SER:OG	1:C:185:GLN:CB	2.59	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:221:ARG:HD3	1:B:234:ILE:O	2.06	0.50
1:B:135:ASN:HB2	1:B:235:ASP:OD1	2.11	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:115:VAL:N	1:C:253:GLY:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:VAL:CG1	1:C:123:VAL:N	2.74	0.50
1:C:175:ARG:O	1:C:243:THR:HA	2.12	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:275:SER:CA	1:B:375:LEU:CD2	2.78	0.50
1:B:289:GLY:HA3	1:B:290:PRO:O	1.99	0.50
1:A:121:PHE:C	1:A:121:PHE:CD1	2.84	0.50
1:A:157:PHE:HD1	1:A:236:LEU:HD22	1.75	0.50
1:A:380:ARG:HB2	1:A:382:ASN:OD1	2.11	0.50
1:B:380:ARG:HB2	1:B:382:ASN:OD1	2.11	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:A:277:ARG:HB3	1:A:285:ALA:HB2	1.89	0.50
1:B:112:LEU:HD23	1:B:113:THR:HG22	1.94	0.50
1:B:277:ARG:HB3	1:B:285:ALA:HB2	1.89	0.50
1:B:297:ARG:HG2	1:B:298:THR:C	2.32	0.50
1:C:135:ASN:ND2	1:C:224:ASN:OD1	2.45	0.50
1:C:185:GLN:C	1:C:186:ASP:O	2.46	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:110:GLU:CD	1:B:144:TRP:CB	2.79	0.50
1:B:112:LEU:CD1	1:B:141:LEU:HD11	2.41	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:A:118:SER:O	1:A:246:GLY:HA3	2.12	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:214:ILE:CG2	1:A:215:PRO:N	2.71	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:279:ASP:O	1:A:280:LEU:CA	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:THR:O	1:B:173:VAL:HG23	2.12	0.49
1:C:160:VAL:CG1	1:C:214:ILE:HD12	2.42	0.49
1:C:276:LYS:CB	1:C:295:LEU:CD2	2.83	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:A:297:ARG:NE	1:A:299:PRO:HA	2.22	0.49
1:A:351:LEU:HD13	1:A:352:ASN:N	2.27	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:C:279:ASP:O	1:C:280:LEU:CA	2.61	0.49
1:C:288:THR:C	1:C:289:GLY:O	2.50	0.49
1:C:297:ARG:HG2	1:C:298:THR:C	2.32	0.49
1:B:152:PHE:HA	1:B:267:GLN:HG3	1.95	0.49
1:B:276:LYS:CB	1:B:295:LEU:CD2	2.83	0.49
1:C:351:LEU:HD13	1:C:352:ASN:N	2.27	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:195:LEU:HD21	1:A:201:LEU:CD1	2.31	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:142:PHE:HE2	1:C:257:LEU:CD1	2.26	0.49
1:C:206:PRO:HB3	1:C:252:VAL:CG1	2.42	0.49
1:B:303:THR:HG22	1:B:305:THR:OG1	2.12	0.49
1:C:228:THR:HG21	1:C:234:ILE:CD1	2.42	0.49
1:A:104:THR:HG23	1:A:263:LEU:CB	2.39	0.48
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: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:303:THR:HG22	1:A:305:THR:OG1	2.12	0.48
1:A:338:LEU:CD2	1:A:338:LEU:C	2.82	0.48
1:B:289:GLY:HA3	1:B:290:PRO:C	2.28	0.48
1:B:292:TYR:HB3	1:B:308:ALA:CB	2.43	0.48
1:B:338:LEU:C	1:B:338:LEU:CD2	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:THR:HG22	1:C:305:THR:OG1	2.12	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:A:380:ARG:C	1:A:382:ASN:H	2.16	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: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:A:179:TYR:CZ	1:A:240:GLY:HA3	2.46	0.48
1:C:132:LEU:O	1:C:133:GLN:C	2.52	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:C:118:SER:C	1:C:120:GLY:N	2.64	0.48
1:B:132:LEU:O	1:B:133:GLN:C	2.52	0.48
1:B:171:THR:C	1:B:172:GLU:O	2.46	0.48
1:B:179:TYR:CD1	1:B:240:GLY:HA3	2.49	0.48
1:B:380:ARG:C	1:B:382:ASN:H	2.16	0.48
1:A:128:VAL:CG1	1:A:129:GLY:N	2.73	0.48
1:C:177:ALA:HB3	1:C:195:LEU:HD11	1.95	0.48
1:A:267:GLN:HB2	1:C:198:PHE:CG	2.47	0.48
1:C:311:THR:HG21	1:C:380:ARG:C	2.35	0.48
1:A:334:ILE:HG22	1:A:335:ASN:N	2.29	0.47
1:B:109:ARG:NH2	1:B:256:PHE:CD2	2.80	0.47
1:B:195:LEU:CD2	1:B:201:LEU:HD12	2.44	0.47
1:C:131:SER:O	1:C:133:GLN:HB2	2.14	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:B:311:THR:HG21	1:B:380:ARG:C	2.35	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:A:228:THR:HG23	1:C:232:LYS:HE3	1.96	0.47
1:C:111:TYR:CD2	1:C:256:PHE:CE1	2.98	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:C:338:LEU:C	1:C:338:LEU:CD2	2.82	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:A:292:TYR:HB3	1:A:308:ALA:CB	2.43	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:B:214:ILE:CG2	1:B:215:PRO:N	2.76	0.47
1:B:130:ASN:ND2	1:B:238:GLN:OE1	2.47	0.47
1:B:288:THR:C	1:B:289:GLY:O	2.50	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:A:162:LEU:HB3	1:A:178:LEU:HD12	1.97	0.47
1:C:104:THR:HG23	1:C:263:LEU:CB	2.44	0.47
1:C:110:GLU:O	1:C:257:LEU:CB	2.63	0.47
1:C:331:ALA:HB3	1:C:357:SER:CB	2.23	0.47
1:A:135:ASN:OD1	1:A:155:TYR:CE1	2.68	0.47
1:A:358:LEU:HA	1:A:359:PRO:HA	1.61	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:112:LEU:HD22	1:A:113:THR:HG22	1.95	0.47
1:A:278:LEU:HG	1:A:295:LEU:O	2.14	0.47
1:B:179:TYR:CZ	1:B:240:GLY:HA3	2.49	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:137:SER:HB3	1:C:146:PRO:HG3	1.96	0.47
1:C:232:LYS:HG3	1:C:233:LEU:H	1.80	0.47
1:C:334:ILE:HG22	1:C:335:ASN:N	2.29	0.47
1:A:180:PHE:CD1	1:A:214:ILE:HD12	2.49	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:B:329:THR:O	1:B:361:THR:N	2.40	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:C:195:LEU:HD23	1:C:201:LEU:HD12	1.91	0.47
1:C:277:ARG:HB3	1:C:285:ALA:HB2	1.89	0.47
1:B:127:ILE:HG22	1:B:128:VAL:H	1.44	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:B:278:LEU:HG	1:B:295:LEU:O	2.14	0.47
1:C:288:THR:O	1:C:289:GLY:O	2.33	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:142:PHE:O	1:B:146:PRO:HG2	2.15	0.47
1:B:134:LEU:HD23	1:B:236:LEU:HD23	1.96	0.47
1:B:262:THR:HG21	1:B:264:TYR:HH	1.78	0.47
1:B:295:LEU:CD2	1:B:295:LEU:N	2.77	0.47
1:C:168:CYS:HB3	1:C:252:VAL:HG13	1.94	0.47
1:C:329:THR:O	1:C:361:THR:N	2.40	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:158:ASN:HB2	1:A:260:SER:HG	1.80	0.46
1:A:201:LEU:CG	1:A:202:LYS:N	2.78	0.46
1:A:108:HIS:O	1:A:259:ARG:CB	2.63	0.46
1:A:321:LEU:N	1:A:321:LEU:CD2	2.77	0.46
1:B:241:ILE:CD1	1:B:255:LEU:HD22	2.22	0.46
1:C:177:ALA:CB	1:C:195:LEU:HD11	2.44	0.46
1:B:230:ASP:C	1:B:232:LYS:H	2.19	0.46
1:A:228:THR:CG2	1:C:232:LYS:HE3	2.46	0.46
1:A:117:ASN:N	1:A:250:ASP:O	2.40	0.46
1:A:297:ARG:HE	1:A:299:PRO:CA	2.22	0.46
1:B:146:PRO:O	1:B:150:SER:OG	2.32	0.46
1:C:104:THR:CG2	1:C:152:PHE:CZ	2.90	0.46
1:C:180:PHE:HB3	1:C:200:VAL:HB	1.97	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:A:164:TYR:CE2	1:A:255:LEU:CD1	2.88	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:C:321:LEU:C	1:C:322:THR:OG1	2.54	0.46
1:C:91:SER:HB3	1:C:109:ARG:NH2	2.31	0.46
1:A:295:LEU:N	1:A:295:LEU:CD2	2.77	0.46
1:A:308:ALA:HB1	1:A:312:PHE:HZ	1.81	0.46
1:A:335:ASN:HB2	1:A:352:ASN:HD22	1.57	0.46
1:B:122:VAL:CG1	1:B:123:VAL:H	2.29	0.46
1:B:195:LEU:HD23	1:B:196:ALA:N	2.31	0.46
1:B:297:ARG:HE	1:B:299:PRO:CA	2.22	0.46
1:C:184:SER:CB	1:C:235:ASP:HB2	2.46	0.46
1:B:175:ARG:O	1:B:243:THR:HA	2.16	0.46
1:B:321:LEU:O	1:B:321:LEU:HG	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:A:331:ALA:HB2	1:A:357:SER:OG	1.95	0.46
1:B:141:LEU:HD21	1:B:239:LEU:HD12	1.98	0.46
1:B:159:SER:O	1:B:160:VAL:CG2	2.64	0.46
1:B:308:ALA:HB1	1:B:312:PHE:HZ	1.81	0.46
1:C:201:LEU:CG	1:C:202:LYS:N	2.78	0.46
1:C:331:ALA:C	1:C:332:VAL:CG2	2.83	0.46
1:A:214:ILE:HA	1:A:215:PRO:HD2	1.56	0.45
1:A:234:ILE:CG1	1:C:233:LEU:HD21	2.46	0.45
1:A:321:LEU:HG	1:A:321:LEU:O	2.16	0.45
1:B:152:PHE:CD1	1:B:263:LEU:HB3	2.49	0.45
1:B:321:LEU:CD2	1:B:321:LEU:N	2.77	0.45
1:C:181:ASP:OD1	1:C:183:ASP:N	2.46	0.45
1:A:142:PHE:HE2	1:A:257:LEU:CD1	2.29	0.45
1:A:192:ARG:HH11	1:A:192:ARG:HG3	1.81	0.45
1:A:117:ASN:CB	1:A:248:GLY:O	2.61	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:216:THR:HG22	1:A:217:ASP:O	2.17	0.45
1:A:321:LEU:CB	1:A:344:GLY:H	2.26	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: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: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:A:222:TYR:OH	1:C:182:LYS:HG3	2.17	0.45
1:A:110:GLU:OE1	1:A:144:TRP:CB	2.65	0.45
1:B:314:LEU:HB2	1:B:351:LEU:HD12	1.99	0.45
1:A:314:LEU:HB2	1:A:351:LEU:HD12	1.99	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:B:385:ASN:OD1	1:B:385:ASN:C	2.55	0.45
1:C:216:THR:HG22	1:C:217:ASP:O	2.17	0.45
1:A:130:ASN:OD1	1:A:186:ASP: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
1:C:69:THR:O	1:C:70:HIS:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ARG:HG2	1:A:298:THR:CA	2.47	0.45
1:B:110:GLU:OE2	1:B:144:TRP:HB3	2.17	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:137:SER:HB3	1:C:146:PRO:CB	2.47	0.45
1:C:345:THR:O	1:C:346:ALA:C	2.55	0.45
1:B:206:PRO:CG	1:B:207:TRP:N	2.47	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:C:278:LEU:HB2	1:C:372:GLY:HA3	1.98	0.44
1:C:99:THR:CG2	1:C:99:THR:O	2.64	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:B:331:ALA:HB2	1:B:357:SER:OG	1.95	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:A:118:SER:O	1:A:246:GLY:N	2.46	0.44
1:A:297:ARG:CG	1:A:298:THR:O	2.66	0.44
1:A:302:LEU:HD21	1:A:304:HIS:NE2	2.32	0.44
1:A:337:ILE:CG2	1:A:337:ILE:O	2.64	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:C:297:ARG:HG2	1:C:298:THR:CA	2.47	0.44
1:A:124:ASN:OD1	1:A:132:LEU:CD1	2.65	0.44
1:A:184:SER:CB	1:A:235:ASP:HB2	2.48	0.44
1:A:384:VAL:O	1:A:384:VAL:HG12	2.17	0.44
1:B:112:LEU:C	1:B:112:LEU:HD23	2.38	0.44
1:B:157:PHE:CE2	1:B:261:VAL:CG2	3.00	0.44
1:B:205:ALA:HB1	1:B:207:TRP:NE1	2.32	0.44
1:B:302:LEU:HD21	1:B:304:HIS:NE2	2.32	0.44
1:B:321:LEU:C	1:B:322:THR:OG1	2.54	0.44
1:B:337:ILE:CG2	1:B:337:ILE:O	2.64	0.44
1:C:127:ILE:HD11	1:C:358:LEU:HD13	1.97	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:A:292:TYR:HB3	1:A:308:ALA:HB2	2.00	0.44
1:A:385:ASN:OD1	1:A:385:ASN:C	2.55	0.44
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:B:154:GLN:HB2	1:B:264:TYR:HB2	2.00	0.44
1:B:300:THR:C	1:B:369:VAL:HG21	2.38	0.44
1:B:324:LEU:CD2	1:B:366:VAL:HG21	1.96	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: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:103:VAL:HG11	1:C:263:LEU:C	2.38	0.44
1:C:357:SER:O	1:C:358:LEU:HG	2.18	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:147:ALA:HB1	1:A:272:LEU:CG	2.47	0.44
1:A:151:ASN:ND2	1:A:269:THR:HG23	2.32	0.44
1:A:178:LEU:O	1:A:212:LEU:HD22	2.18	0.44
1:B:292:TYR:HB3	1:B:308:ALA:HB2	2.00	0.44
1:C:292:TYR:HB3	1:C:308:ALA:HB2	2.00	0.44
1:A:230:ASP:C	1:A:232:LYS:N	2.71	0.44
1:A:232:LYS:HG3	1:A:233:LEU:H	1.81	0.44
1:A:111:TYR:HA	1:A:256:PHE:CD1	2.52	0.44
1:B:145:LEU:O	1:B:147:ALA:N	2.51	0.44
1:B:114:GLN:HE21	1:B:251:ALA:CB	2.30	0.44
1:B:206:PRO:HB2	1:B:252:VAL:CG1	2.47	0.44
1:B:300:THR:O	1:B:301:VAL:CG2	2.66	0.44
1:B:357:SER:O	1:B:358:LEU:HG	2.18	0.44
1:C:300:THR:O	1:C:301:VAL:CG2	2.66	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: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:112:LEU:C	1:C:112:LEU:HD23	2.39	0.43
1:C:230:ASP:C	1:C:232:LYS:N	2.71	0.43
1:C:74:VAL:C	1:C:75:GLY:O	2.57	0.43
1:A:118:SER:HB2	1:A:120:GLY:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:THR:O	1:A:361:THR:N	2.40	0.43
1:A:112:LEU:HD23	1:A:113:THR:HG22	2.00	0.43
1:A:184:SER:HB2	1:A:235:ASP:HB2	1.99	0.43
1:A:300:THR:O	1:A:301:VAL:CG2	2.66	0.43
1:B:217:ASP:OD2	1:B:219:VAL:HB	2.18	0.43
1:C:91:SER:OG	1:C:109:ARG:HB3	2.18	0.43
1:A:279:ASP:OD2	1:A:282:GLY:HA3	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:B:264:TYR:O	1:B:265:PHE:C	2.57	0.43
1:B:278:LEU:HD23	1:B:283:SER:O	2.19	0.43
1:B:355:VAL:HG11	1:B:360:ALA:CB	2.47	0.43
1:C:111:TYR:CD1	1:C:112:LEU:N	2.86	0.43
1:C:384:VAL:HG12	1:C:384:VAL:O	2.18	0.43
1:A:321:LEU:C	1:A:322:THR:OG1	2.54	0.43
1:A:335:ASN:CG	1:A:352:ASN:ND2	2.72	0.43
1:B:275:SER:CB	1:B:375:LEU:CD2	2.96	0.43
1:B:335:ASN:CG	1:B:352:ASN:ND2	2.72	0.43
1:C:337:ILE:O	1:C:337:ILE:CG2	2.64	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: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:A:355:VAL:HG11	1:A:360:ALA:CB	2.47	0.43
1:B:204:THR:CG2	1:B:205:ALA:N	2.82	0.43
1:C:122:VAL:HG13	1:C:126:GLY:CA	2.49	0.43
1:A:180:PHE:CE1	1:A:214:ILE:HG23	2.54	0.43
1:B:124:ASN:OD1	1:B:132:LEU:HD11	2.19	0.43
1:B:201:LEU:HD23	1:B:202:LYS:HA	1.99	0.43
1:B:204:THR:HG22	1:B:205:ALA:N	2.32	0.43
1:C:122:VAL:CG1	1:C:126:GLY:N	2.82	0.43
1:A:175:ARG:HG2	1:A:244:TYR:CZ	2.54	0.42
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

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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:A:231:GLN:H	1:A:231:GLN:HG3	1.55	0.42
1:A:280:LEU:CB	1:A:280:LEU:N	2.73	0.42
1:B:384:VAL:HG12	1:B:384:VAL:O	2.18	0.42
1:B:336:ASP:CG	1:B:385:ASN:HB2	2.38	0.42
1:B:230:ASP:OD1	1:C:228:THR:HA	2.20	0.42
1:C:267:GLN:CB	1:C:268:PRO:HD2	2.34	0.42
1:C:278:LEU:HD23	1:C:283:SER:O	2.19	0.42
1:A:357:SER:O	1:A:358:LEU:HG	2.18	0.42
1:B:204:THR:O	1:B:205:ALA:C	2.58	0.42
1:C:112:LEU:CD2	1:C:113:THR:HG22	2.49	0.42
1:C:281:THR:HA	1:C:297:ARG:HH12	1.84	0.42
1:C:280:LEU:CB	1:C:370:ALA:O	2.67	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:A:234:ILE:HD11	1:C:232:LYS:CD	2.47	0.42
1:A:264:TYR:O	1:A:265:PHE:C	2.57	0.42
1:C:264:TYR:O	1:C:265:PHE:C	2.57	0.42
1:C:355:VAL:HG11	1:C:360:ALA:CB	2.47	0.42
1:A:143:SER:HB2	1:A:378:ARG:NH2	2.34	0.42
1:C:382:ASN:O	1:C:384:VAL:HG23	2.20	0.42
1:A:180:PHE:CD1	1:A:214:ILE:HG23	2.55	0.42
1:A:267:GLN:HA	1:C:197:ASN:O	2.20	0.42
1:B:281:THR:HA	1:B:297:ARG:NH1	2.35	0.42
1:B:280:LEU:CB	1:B:370:ALA:O	2.67	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:A:280:LEU:CB	1:A:370:ALA:O	2.67	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:180:PHE:CE1	1:A:214:ILE:CG2	3.02	0.42
1:A:362:VAL:N	1:A:362:VAL:CG2	2.83	0.42
1:A:382:ASN:O	1:A:384:VAL:HG23	2.20	0.42
1:A:230:ASP:OD1	1:B:228:THR:HA	2.20	0.42
1:B:114:GLN:NE2	1:B:251:ALA:HB2	2.34	0.42
1:B:281:THR:HA	1:B:297:ARG:HH12	1.84	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:104:THR:HG22	1:A:263:LEU:CB	2.26	0.42
1:A:112:LEU:HG	1:A:141:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:O	1:A:133:GLN:C	2.58	0.42
1:A:281:THR:HA	1:A:297:ARG:HH12	1.84	0.42
1:A:302:LEU:HG	1:A:304:HIS:HD2	1.85	0.42
1:B:180:PHE:HB3	1:B:200:VAL:HB	2.01	0.42
1:B:302:LEU:HG	1:B:304:HIS:HD2	1.85	0.42
1:C:167:LEU:HD21	1:C:253:GLY:CA	2.50	0.42
1:C:135:ASN:HB2	1:C:235:ASP:OD1	2.19	0.42
1:A:226:SER:OG	1:C:232:LYS:CE	2.68	0.42
1:A:179:TYR:CD1	1:A:240:GLY:HA3	2.53	0.42
1:A:281:THR:HA	1:A:297:ARG:NH1	2.35	0.42
1:A:314:LEU:HD22	1:A:351:LEU:CD1	2.50	0.42
1:B:298:THR:O	1:B:299:PRO:C	2.58	0.42
1:B:382:ASN:O	1:B:384:VAL:HG23	2.20	0.42
1:C:68:ILE:HG22	1:C:69:THR:N	2.33	0.42
1:A:172:GLU:O	1:A:172:GLU:N	2.52	0.41
1:A:109:ARG:HA	1:A:257:LEU:O	2.19	0.41
1:B:112:LEU:HG	1:B:141:LEU:HD12	1.99	0.41
1:B:107:SER:HA	1:B:259:ARG:O	2.20	0.41
1:C:145:LEU:O	1:C:146:PRO:C	2.59	0.41
1:C:168:CYS:HG	1:C:252:VAL:HG13	1.78	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:302:LEU:HG	1:C:304:HIS:HD2	1.85	0.41
1:C:82:VAL:HA	1:C:170:THR:CG2	2.48	0.41
1:A:157:PHE:CE2	1:A:261:VAL:HG22	2.53	0.41
1:A:298:THR:O	1:A:299:PRO:C	2.58	0.41
1:B:217:ASP:OD2	1:B:221:ARG:NH2	2.53	0.41
1:B:362:VAL:N	1:B:362:VAL:CG2	2.83	0.41
1:C:112:LEU:CD1	1:C:141:LEU:HD11	2.50	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:B:161:VAL:HA	1:B:212:LEU:O	2.20	0.41
1:C:164:TYR:CE2	1:C:253:GLY:HA3	2.55	0.41
1:C:276:LYS:O	1:C:295:LEU:CD1	2.44	0.41
1:C:298:THR:O	1:C:299:PRO:C	2.58	0.41
1:C:97:GLY:O	1:C:99:THR:CA	2.68	0.41
1:A:104:THR:HG23	1:A:263:LEU:CG	2.51	0.41
1:A:142:PHE:CB	1:A:146:PRO:HD2	2.48	0.41
1:A:174:GLY:O	1:A:206:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:GLN:HG3	1:A:268:PRO:CG	2.25	0.41
1:B:195:LEU:CD2	1:B:195:LEU:C	2.88	0.41
1:B:168:CYS:CB	1:B:252:VAL:HG13	2.50	0.41
1:C:131:SER:OG	1:C:132:LEU:N	2.53	0.41
1:C:115:VAL:HG21	1:C:241:ILE:HG21	2.02	0.41
1:A:133:GLN:O	1:A:138:ASN:ND2	2.48	0.41
1:A:326:LEU:C	1:A:326:LEU:CD1	2.84	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:C:327:GLY:O	1:C:362:VAL:HG13	2.21	0.41
1:A:114:GLN:NE2	1:A:251:ALA:CB	2.79	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:C:141:LEU:HD12	1:C:141:LEU:O	2.20	0.41
1:C:232:LYS:HB3	1:C:232:LYS:HE2	1.80	0.41
1:A:121:PHE:HD1	1:A:121:PHE:O	2.04	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:278:LEU:HD11	1:A:295:LEU:O	2.22	0.41
1:A:327:GLY:O	1:A:362:VAL:HG13	2.21	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: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:112:LEU:C	1:A:112:LEU:HD23	2.41	0.40
1:A:298:THR:CB	1:A:299:PRO:HD2	2.42	0.40
1:B:165:VAL:CG1	1:B:166:PRO:N	2.83	0.40
1:B:201:LEU:CG	1:B:202:LYS:N	2.84	0.40
1:B:205:ALA:HB1	1:B:207:TRP:CD1	2.56	0.40
1:B:161:VAL:N	1:B:258:ALA:HB3	2.35	0.40
1:C:88:LEU:HD11	1:C:256:PHE:CE2	2.54	0.40
1:B:214:ILE:HA	1:B:215:PRO:HD2	1.59	0.40
1:C:112:LEU:CG	1:C:141:LEU:HD11	2.51	0.40
1:A:110:GLU:HG2	1:A:144:TRP:CB	2.52	0.40
1:A:182:LYS:HG3	1:A:182:LYS:O	2.22	0.40
1:A:278:LEU:HD11	1:A:296:THR:C	2.41	0.40
1:B:148:LEU:O	1:B:152:PHE:HD1	2.04	0.40
1:B:177:ALA:N	1:B:242:ALA:O	2.55	0.40
1:B:327:GLY:O	1:B:362:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:VAL:HG22	1:C:241:ILE:HG21	2.03	0.40
1:A:228:THR:HG23	1:C:232:LYS:CE	2.52	0.40
1:A:297:ARG:HD2	1:A:369:VAL:O	2.21	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:178:LEU:HD21	1:A:255:LEU:CD2	2.52	0.40
1:B:278:LEU:HD11	1:B:296:THR:C	2.41	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%)	17	45
1	B	233/309 (75%)	217 (93%)	16 (7%)	15	41
1	C	258/309 (84%)	242 (94%)	16 (6%)	18	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	723/927 (78%)	676 (94%)	47 (6%)	17	45

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.