



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:24 PM UTC

PDB ID : 2TBV / pdb_00002tbv
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

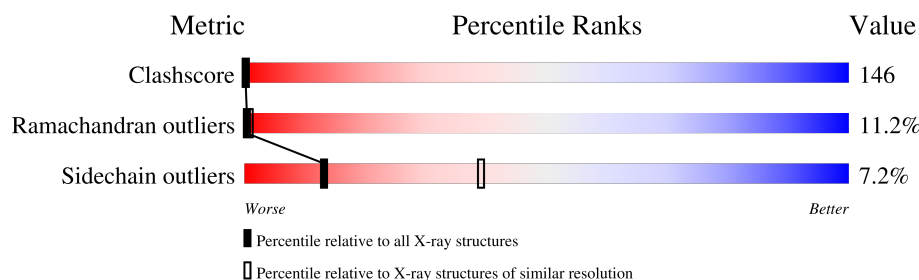
1 Overall quality at a glance

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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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 of 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	
1	B	387	
1	C	387	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6648 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TOMATO BUSHY STUNT VIRUS.

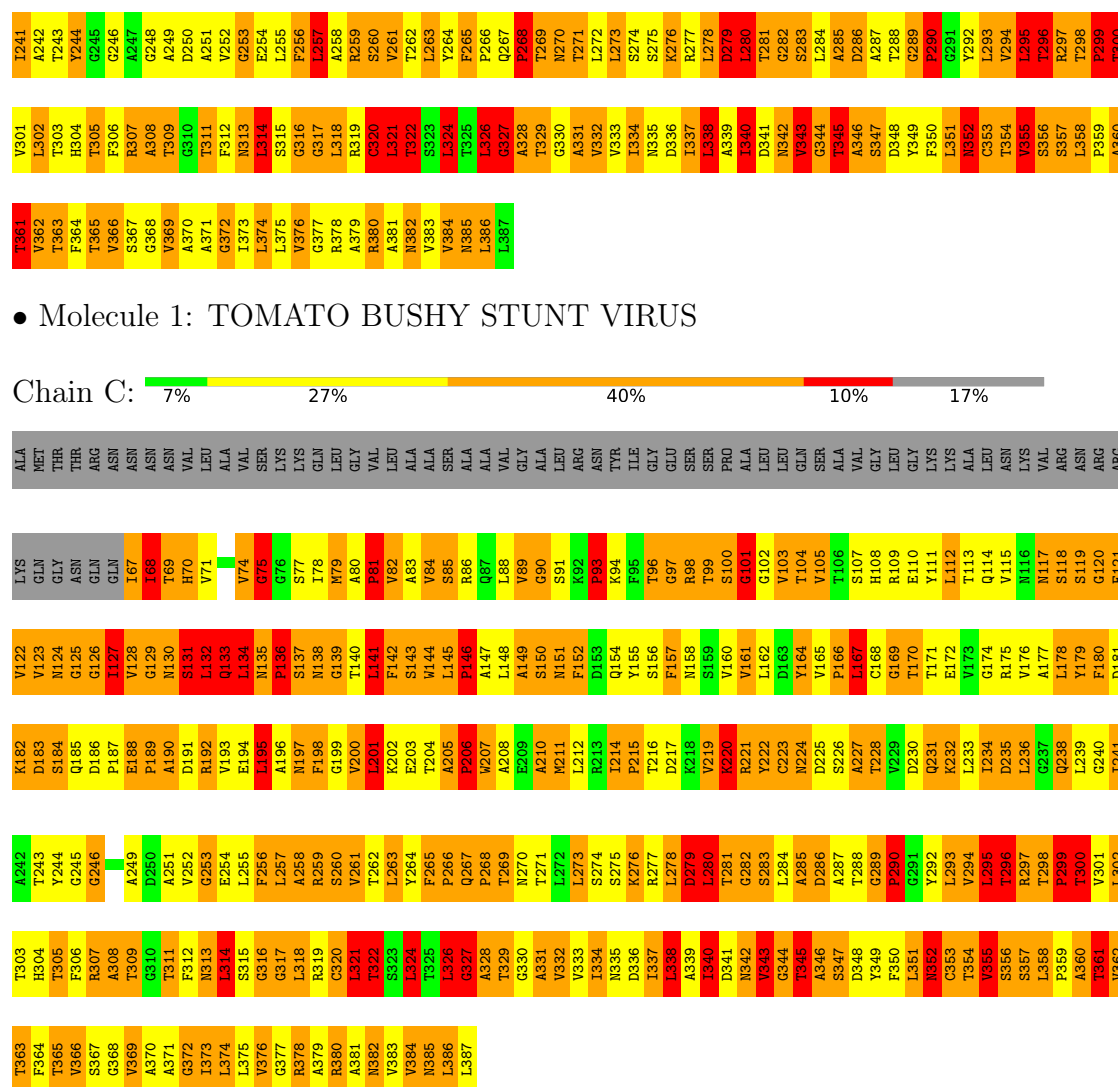
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	3	1
			2136	1351	360	420	5			
1	B	287	Total	C	N	O	S	0	2	1
			2130	1348	359	418	5			
1	C	321	Total	C	N	O	S	0	3	0
			2376	1502	406	462	6			

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ca	0	0
			3	3		
2	B	1	Total	Ca	0	0
			1	1		
2	C	2	Total	Ca	0	0
			2	2		



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 [i](#)

5.1 Standard geometry [i](#)

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	2.23	46/2165 (2.1%)	2.86	211/2956 (7.1%)
1	B	2.25	45/2171 (2.1%)	2.84	221/2964 (7.5%)
1	C	2.16	50/2409 (2.1%)	2.77	237/3286 (7.2%)
All	All	2.21	141/6745 (2.1%)	2.82	669/9206 (7.3%)

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 (141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	138	ASN	N-CA	-40.18	0.97	1.46
1	C	138	ASN	N-CA	-40.14	0.97	1.46
1	A	138	ASN	N-CA	-40.12	0.97	1.46
1	B	137	SER	N-CA	-29.04	1.10	1.46
1	C	137	SER	N-CA	-29.00	1.10	1.46
1	A	137	SER	N-CA	-29.00	1.10	1.46
1	B	362	VAL	N-CA	26.79	1.75	1.46
1	C	362	VAL	N-CA	26.77	1.75	1.46
1	A	362	VAL	N-CA	25.85	1.75	1.46
1	C	280	LEU	N-CA	25.81	1.76	1.46
1	A	280	LEU	N-CA	25.79	1.76	1.46
1	B	280	LEU	N-CA	25.79	1.76	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	327	GLY	CA-C	20.20	1.68	1.52
1	A	327	GLY	CA-C	20.14	1.68	1.52
1	B	327	GLY	CA-C	20.07	1.68	1.52
1	B	107	SER	N-CA	19.00	1.70	1.46
1	B	122	VAL	N-CA	18.99	1.68	1.46
1	A	172	GLU	N-CA	18.14	1.70	1.45
1	A	314	LEU	N-CA	-17.50	1.25	1.46
1	B	314	LEU	N-CA	-17.43	1.25	1.46
1	C	314	LEU	N-CA	-17.41	1.25	1.46
1	A	115	VAL	N-CA	17.07	1.66	1.46
1	B	366	VAL	N-CA	16.39	1.66	1.46
1	A	366	VAL	N-CA	16.35	1.66	1.46
1	C	366	VAL	N-CA	16.32	1.66	1.46
1	B	113	THR	CA-C	15.87	1.71	1.52
1	B	115	VAL	CA-C	15.86	1.71	1.53
1	C	223	CYS	CA-C	15.71	1.75	1.53
1	C	86	ARG	N-CA	15.47	1.65	1.45
1	C	135	ASN	CA-C	-15.38	1.36	1.52
1	B	135	ASN	CA-C	-15.37	1.36	1.52
1	A	135	ASN	CA-C	-15.28	1.36	1.52
1	A	123	VAL	CA-C	14.57	1.71	1.52
1	C	238	GLN	CA-C	14.44	1.69	1.52
1	B	238	GLN	CA-C	14.06	1.69	1.52
1	A	238	GLN	CA-C	14.03	1.69	1.52
1	A	316	GLY	N-CA	-13.88	1.31	1.45
1	B	316	GLY	N-CA	-13.88	1.31	1.45
1	C	316	GLY	N-CA	-13.87	1.31	1.45
1	A	107	SER	N-CA	13.40	1.63	1.46
1	C	263	LEU	CA-C	13.02	1.70	1.52
1	C	278	LEU	CA-C	12.63	1.68	1.52
1	A	278	LEU	CA-C	12.62	1.68	1.52
1	B	278	LEU	CA-C	12.61	1.68	1.52
1	C	352	ASN	N-CA	12.10	1.60	1.46
1	A	352	ASN	N-CA	12.08	1.60	1.46
1	B	352	ASN	N-CA	12.04	1.60	1.46
1	C	77	SER	N-CA	-11.11	1.31	1.45
1	B	364	PHE	CA-C	-10.42	1.39	1.52
1	A	364	PHE	CA-C	-10.41	1.39	1.52
1	C	364	PHE	CA-C	-10.37	1.40	1.52
1	A	355	VAL	CA-C	10.20	1.64	1.52
1	B	355	VAL	CA-C	10.20	1.64	1.52
1	C	355	VAL	CA-C	10.15	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	LEU	N-CA	10.13	1.59	1.46
1	B	324	LEU	N-CA	10.08	1.59	1.46
1	C	324	LEU	N-CA	10.07	1.59	1.46
1	B	322	THR	CA-C	9.89	1.66	1.52
1	C	322	THR	CA-C	9.89	1.66	1.52
1	A	322	THR	CA-C	9.86	1.66	1.52
1	C	79	MET	N-CA	9.63	1.57	1.46
1	C	260	SER	CA-C	9.45	1.63	1.53
1	C	107	SER	N-CA	9.41	1.57	1.46
1	A	207	TRP	NE1-CE2	-8.60	1.27	1.37
1	C	144	TRP	NE1-CE2	-8.59	1.28	1.37
1	A	144	TRP	NE1-CE2	-8.58	1.28	1.37
1	B	207	TRP	NE1-CE2	-8.57	1.28	1.37
1	B	144	TRP	NE1-CE2	-8.56	1.28	1.37
1	C	207	TRP	NE1-CE2	-8.53	1.28	1.37
1	C	117	ASN	N-CA	8.17	1.56	1.45
1	C	228	THR	N-CA	-8.10	1.36	1.46
1	A	228	THR	N-CA	-8.08	1.36	1.46
1	B	300	THR	CA-C	7.95	1.62	1.52
1	B	121	PHE	N-CA	7.94	1.57	1.46
1	A	300	THR	CA-C	7.91	1.62	1.52
1	C	300	THR	CA-C	7.89	1.62	1.52
1	A	117	ASN	N-CA	7.79	1.56	1.45
1	B	105	VAL	CA-C	7.78	1.62	1.52
1	B	227	ALA	N-CA	7.64	1.54	1.45
1	A	354	THR	CA-C	7.46	1.60	1.52
1	B	354	THR	CA-C	7.45	1.60	1.52
1	C	354	THR	CA-C	7.44	1.60	1.52
1	B	132	LEU	N-CA	7.41	1.55	1.46
1	A	128	VAL	N-CA	7.33	1.54	1.46
1	C	227	ALA	N-CA	7.32	1.54	1.45
1	A	287	ALA	N-CA	-7.28	1.36	1.45
1	C	287	ALA	N-CA	-7.26	1.36	1.45
1	B	287	ALA	N-CA	-7.25	1.36	1.45
1	C	126	GLY	CA-C	-7.11	1.41	1.51
1	A	296	THR	CA-C	6.90	1.61	1.52
1	C	296	THR	CA-C	6.86	1.61	1.52
1	C	293	LEU	CA-C	-6.84	1.44	1.52
1	B	296	THR	CA-C	6.82	1.61	1.52
1	B	293	LEU	CA-C	-6.80	1.44	1.52
1	A	293	LEU	CA-C	-6.78	1.44	1.52
1	B	228	THR	N-CA	-6.70	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	227	ALA	N-CA	6.58	1.53	1.45
1	B	318	LEU	N-CA	5.98	1.53	1.46
1	C	318	LEU	N-CA	5.96	1.53	1.46
1	C	94	LYS	CA-C	5.95	1.60	1.52
1	A	318	LEU	N-CA	5.93	1.53	1.46
1	B	285	ALA	N-CA	5.72	1.53	1.46
1	A	108	HIS	CA-C	5.67	1.60	1.52
1	A	285	ALA	N-CA	5.66	1.53	1.46
1	C	302	LEU	N-CA	-5.65	1.38	1.45
1	A	286	ASP	CG-OD2	5.63	1.36	1.25
1	C	285	ALA	N-CA	5.63	1.53	1.46
1	A	369	VAL	N-CA	-5.63	1.39	1.46
1	C	369	VAL	N-CA	-5.63	1.39	1.46
1	B	369	VAL	N-CA	-5.62	1.39	1.46
1	C	84	VAL	CA-C	5.62	1.59	1.52
1	C	286	ASP	CG-OD2	5.61	1.36	1.25
1	B	286	ASP	CG-OD2	5.58	1.35	1.25
1	A	302	LEU	N-CA	-5.57	1.38	1.45
1	B	302	LEU	N-CA	-5.57	1.38	1.45
1	C	78	ILE	N-CA	5.54	1.52	1.46
1	A	326	LEU	N-CA	-5.54	1.39	1.46
1	B	326	LEU	N-CA	-5.50	1.39	1.46
1	B	307	ARG	CA-C	5.49	1.60	1.52
1	A	307	ARG	CA-C	5.49	1.60	1.52
1	C	326	LEU	N-CA	-5.47	1.39	1.46
1	C	307	ARG	CA-C	5.46	1.60	1.52
1	C	93	PRO	CA-C	5.34	1.59	1.52
1	B	220	LYS	CA-C	-5.33	1.45	1.52
1	C	220	LYS	CA-C	-5.32	1.45	1.52
1	A	112	LEU	CG-CD2	5.29	1.70	1.52
1	C	112	LEU	CG-CD2	5.27	1.70	1.52
1	A	220	LYS	CA-C	-5.26	1.45	1.52
1	B	112	LEU	CG-CD2	5.26	1.70	1.52
1	C	308	ALA	CA-C	5.19	1.59	1.52
1	A	132	LEU	N-CA	5.18	1.53	1.46
1	A	308	ALA	CA-C	5.18	1.59	1.52
1	B	308	ALA	CA-C	5.13	1.58	1.52
1	C	84	VAL	N-CA	-5.13	1.40	1.46
1	B	104	THR	CA-C	5.09	1.59	1.52
1	A	105	VAL	CA-C	5.07	1.58	1.52
1	B	364	PHE	N-CA	5.06	1.52	1.46
1	A	364	PHE	N-CA	5.06	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	CYS	CA-C	5.05	1.59	1.53
1	B	320	CYS	CA-C	5.03	1.59	1.53
1	C	364	PHE	N-CA	5.01	1.52	1.46

All (669) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ASN	CA-C-O	-32.39	86.65	119.69
1	C	135	ASN	CA-C-O	-32.34	86.70	119.69
1	B	135	ASN	CA-C-O	-32.34	86.71	119.69
1	A	127	ILE	N-CA-C	25.31	144.91	108.96
1	C	266	PRO	CB-CA-C	-24.45	79.93	111.71
1	C	137	SER	CA-C-N	22.77	157.43	122.37
1	C	137	SER	C-N-CA	22.77	157.43	122.37
1	A	137	SER	CA-C-N	22.76	157.42	122.37
1	A	137	SER	C-N-CA	22.76	157.42	122.37
1	B	137	SER	CA-C-N	22.75	157.41	122.37
1	B	137	SER	C-N-CA	22.75	157.41	122.37
1	A	126	GLY	N-CA-C	-21.28	83.83	115.32
1	C	206	PRO	CB-CA-C	-21.17	76.63	111.56
1	A	206	PRO	CB-CA-C	-20.80	77.23	111.56
1	B	206	PRO	CB-CA-C	-19.56	79.28	111.56
1	A	137	SER	N-CA-C	19.27	140.25	108.26
1	B	137	SER	N-CA-C	19.25	140.22	108.26
1	C	137	SER	N-CA-C	19.22	140.17	108.26
1	A	136	PRO	CB-CA-C	-18.65	80.78	111.56
1	C	187	PRO	CB-CA-C	-18.63	80.82	111.56
1	C	146	PRO	CB-CA-C	-18.48	81.08	111.56
1	A	187	PRO	CB-CA-C	-18.41	81.18	111.56
1	B	187	PRO	CB-CA-C	-18.41	81.18	111.56
1	A	119	SER	N-CA-C	-16.93	88.92	112.45
1	A	127	ILE	CB-CA-C	-16.92	88.01	111.19
1	A	215	PRO	CB-CA-C	16.61	138.97	111.56
1	C	215	PRO	CB-CA-C	16.61	138.97	111.56
1	B	121	PHE	CA-C-N	-15.90	100.67	122.77
1	B	121	PHE	C-N-CA	-15.90	100.67	122.77
1	B	136	PRO	CA-C-N	14.07	143.22	122.39
1	B	136	PRO	C-N-CA	14.07	143.22	122.39
1	A	136	PRO	CA-C-N	14.05	143.18	122.39
1	A	136	PRO	C-N-CA	14.05	143.18	122.39
1	C	136	PRO	CA-C-N	13.98	143.08	122.39
1	C	136	PRO	C-N-CA	13.98	143.08	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	ASN	N-CA-C	-13.89	85.54	108.32
1	C	352	ASN	N-CA-C	-13.88	85.56	108.32
1	A	352	ASN	N-CA-C	-13.87	85.57	108.32
1	B	166	PRO	CB-CA-C	13.39	133.66	111.56
1	A	150	SER	N-CA-C	-13.39	95.51	114.12
1	B	172	GLU	N-CA-C	-13.37	93.09	110.33
1	A	267	GLN	C-N-CD	-13.30	70.48	125.00
1	B	134	LEU	N-CA-C	12.96	138.40	110.80
1	B	146	PRO	CB-CA-C	-12.85	90.35	111.56
1	B	355	VAL	CA-C-O	-12.76	105.93	121.11
1	C	355	VAL	CA-C-O	-12.75	105.94	121.11
1	A	355	VAL	CA-C-O	-12.74	105.95	121.11
1	B	215	PRO	CB-CA-C	12.61	132.37	111.56
1	A	324	LEU	N-CA-C	12.39	137.20	110.80
1	B	324	LEU	N-CA-C	12.39	137.19	110.80
1	C	324	LEU	N-CA-C	12.39	137.19	110.80
1	C	340	ILE	CA-C-O	-12.34	105.35	121.02
1	A	340	ILE	CA-C-O	-12.34	105.35	121.02
1	B	340	ILE	CA-C-O	-12.34	105.36	121.02
1	B	126	GLY	CA-C-O	-12.03	105.59	120.03
1	C	282	GLY	CA-C-O	11.97	135.40	122.47
1	A	282	GLY	CA-C-O	11.96	135.38	122.47
1	B	282	GLY	CA-C-O	11.90	135.33	122.47
1	A	366	VAL	CA-C-N	-11.85	101.09	121.94
1	A	366	VAL	C-N-CA	-11.85	101.09	121.94
1	C	366	VAL	CA-C-N	-11.85	101.09	121.94
1	C	366	VAL	C-N-CA	-11.85	101.09	121.94
1	B	366	VAL	CA-C-N	-11.83	101.12	121.94
1	B	366	VAL	C-N-CA	-11.83	101.12	121.94
1	A	352	ASN	N-CA-CB	11.71	130.35	110.57
1	B	352	ASN	N-CA-CB	11.69	130.33	110.57
1	C	352	ASN	N-CA-CB	11.68	130.30	110.57
1	C	189	PRO	CB-CA-C	11.67	130.82	111.56
1	B	220	LYS	N-CA-C	11.66	135.63	110.80
1	B	165	VAL	C-N-CD	-11.65	77.22	125.00
1	A	189	PRO	CB-CA-C	11.64	130.77	111.56
1	B	189	PRO	CB-CA-C	11.62	130.72	111.56
1	B	126	GLY	N-CA-C	-11.57	92.93	113.76
1	C	220	LYS	N-CA-C	11.56	135.43	110.80
1	A	220	LYS	N-CA-C	11.54	135.38	110.80
1	B	295	LEU	CA-C-O	11.53	136.04	120.47
1	C	131	SER	CA-C-N	-11.49	99.58	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	131	SER	C-N-CA	-11.49	99.58	121.54
1	B	127	ILE	N-CA-C	11.42	126.67	108.97
1	C	327	GLY	N-CA-C	-11.34	93.71	111.18
1	C	132	LEU	N-CA-CB	11.33	129.63	110.49
1	B	327	GLY	N-CA-C	-11.32	93.75	111.18
1	A	327	GLY	N-CA-C	-11.30	93.77	111.18
1	A	106	THR	N-CA-C	-11.22	91.12	109.40
1	C	93	PRO	CB-CA-C	-11.21	97.00	111.46
1	B	314	LEU	N-CA-C	-11.18	91.07	109.07
1	A	314	LEU	N-CA-C	-11.16	91.10	109.07
1	A	295	LEU	CA-C-O	11.16	136.03	120.52
1	C	295	LEU	CA-C-O	11.16	136.03	120.52
1	C	314	LEU	N-CA-C	-11.15	91.11	109.07
1	B	214	ILE	N-CA-C	11.10	119.99	107.89
1	B	115	VAL	CA-C-O	10.94	134.21	120.76
1	C	364	PHE	CA-C-O	-10.86	108.27	120.54
1	B	364	PHE	CA-C-O	-10.81	108.33	120.54
1	A	364	PHE	CA-C-O	-10.77	108.37	120.54
1	C	145	LEU	C-N-CD	-10.75	80.94	125.00
1	B	361	THR	CA-C-N	-10.59	105.94	122.68
1	B	361	THR	C-N-CA	-10.59	105.94	122.68
1	C	361	THR	CA-C-N	-10.59	105.95	122.68
1	C	361	THR	C-N-CA	-10.59	105.95	122.68
1	C	126	GLY	N-CA-C	-10.57	96.93	114.48
1	B	125	GLY	N-CA-C	-10.49	100.85	115.32
1	A	127	ILE	CA-C-N	-10.27	108.49	122.77
1	A	127	ILE	C-N-CA	-10.27	108.49	122.77
1	A	281	THR	N-CA-C	-10.21	100.94	113.50
1	C	281	THR	N-CA-C	-10.19	100.97	113.50
1	B	134	LEU	N-CA-CB	-10.19	93.27	110.49
1	B	281	THR	N-CA-C	-10.19	100.97	113.50
1	A	172	GLU	N-CA-C	-10.12	97.96	110.41
1	B	150	SER	N-CA-C	-10.11	100.06	114.12
1	B	166	PRO	CA-CB-CG	-10.10	85.31	104.50
1	A	137	SER	N-CA-CB	-10.08	94.34	110.77
1	C	137	SER	N-CA-CB	-10.07	94.36	110.77
1	A	361	THR	CA-C-N	-10.05	105.98	122.57
1	A	361	THR	C-N-CA	-10.05	105.98	122.57
1	B	137	SER	N-CA-CB	-10.04	94.41	110.77
1	B	340	ILE	N-CA-C	-9.88	93.85	108.87
1	A	279	ASP	CA-C-N	-9.86	107.08	120.79
1	A	279	ASP	C-N-CA	-9.86	107.08	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	279	ASP	CA-C-N	-9.86	107.08	120.79
1	C	279	ASP	C-N-CA	-9.86	107.08	120.79
1	C	340	ILE	N-CA-C	-9.86	93.88	108.87
1	A	340	ILE	N-CA-C	-9.86	93.89	108.87
1	B	279	ASP	CA-C-N	-9.85	107.10	120.79
1	B	279	ASP	C-N-CA	-9.85	107.10	120.79
1	C	172	GLU	N-CA-C	-9.74	98.43	110.41
1	A	138	ASN	N-CA-CB	9.61	126.84	110.98
1	C	138	ASN	N-CA-CB	9.60	126.82	110.98
1	B	138	ASN	N-CA-CB	9.59	126.80	110.98
1	A	189	PRO	CA-CB-CG	-9.46	86.54	104.50
1	B	133	GLN	CA-C-N	-9.44	103.50	121.54
1	B	133	GLN	C-N-CA	-9.44	103.50	121.54
1	C	189	PRO	CA-CB-CG	-9.44	86.56	104.50
1	B	189	PRO	CA-CB-CG	-9.43	86.58	104.50
1	C	332	VAL	N-CA-C	9.43	120.14	108.06
1	B	105	VAL	N-CA-C	9.43	122.50	108.46
1	A	332	VAL	N-CA-C	9.42	120.11	108.06
1	B	332	VAL	N-CA-C	9.39	120.08	108.06
1	A	268	PRO	CB-CA-C	9.32	126.95	111.56
1	B	302	LEU	N-CA-CB	-9.27	97.19	110.44
1	C	302	LEU	N-CA-CB	-9.26	97.20	110.44
1	A	302	LEU	N-CA-CB	-9.26	97.20	110.44
1	C	195	LEU	N-CA-C	-9.24	101.18	111.07
1	C	205	ALA	N-CA-C	-9.23	89.41	109.81
1	A	195	LEU	N-CA-C	-9.20	101.23	111.07
1	C	94	LYS	N-CA-C	9.20	124.27	107.99
1	C	134	LEU	N-CA-C	9.17	130.32	110.80
1	A	117	ASN	N-CA-C	9.14	121.65	110.41
1	A	238	GLN	N-CA-C	-9.13	95.43	109.85
1	A	356	SER	CA-C-O	9.10	134.24	122.31
1	C	356	SER	CA-C-O	9.09	134.22	122.31
1	B	356	SER	CA-C-O	9.05	134.16	122.31
1	A	165	VAL	C-N-CD	-9.02	88.01	125.00
1	C	165	VAL	C-N-CD	-9.02	88.03	125.00
1	B	120	GLY	CA-C-N	8.96	133.87	121.33
1	B	120	GLY	C-N-CA	8.96	133.87	121.33
1	B	354	THR	N-CA-C	8.94	123.17	107.61
1	C	354	THR	N-CA-C	8.94	123.17	107.61
1	A	354	THR	N-CA-C	8.94	123.16	107.61
1	A	362	VAL	N-CA-C	8.93	122.93	108.99
1	B	220	LYS	CB-CA-C	-8.90	92.71	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	LYS	CB-CA-C	-8.90	92.72	110.42
1	C	220	LYS	CB-CA-C	-8.89	92.72	110.42
1	A	114	GLN	CA-C-N	-8.87	111.29	122.37
1	A	114	GLN	C-N-CA	-8.87	111.29	122.37
1	B	109	ARG	N-CA-C	8.75	123.34	108.02
1	C	324	LEU	CA-C-O	-8.69	108.09	120.51
1	B	324	LEU	CA-C-O	-8.67	108.11	120.51
1	B	236	LEU	N-CA-C	8.65	120.40	110.97
1	A	324	LEU	CA-C-O	-8.65	108.14	120.51
1	C	307	ARG	CA-C-O	8.65	128.64	118.69
1	B	307	ARG	CA-C-O	8.64	128.63	118.69
1	A	307	ARG	CA-C-O	8.64	128.63	118.69
1	A	357	SER	N-CA-C	8.61	120.02	107.88
1	B	357	SER	N-CA-C	8.61	120.01	107.88
1	C	190	ALA	N-CA-C	8.58	120.41	111.14
1	C	357	SER	N-CA-C	8.58	119.98	107.88
1	A	190	ALA	N-CA-C	8.57	120.39	111.14
1	A	293	LEU	CA-C-O	-8.55	111.47	120.70
1	B	238	GLN	N-CA-C	-8.55	96.35	109.85
1	C	293	LEU	CA-C-O	-8.53	111.49	120.70
1	C	211	MET	N-CA-C	8.52	122.43	109.23
1	B	293	LEU	CA-C-O	-8.50	111.52	120.70
1	A	294	VAL	CA-C-O	-8.49	111.04	120.72
1	B	294	VAL	CA-C-O	-8.47	111.06	120.72
1	C	362	VAL	N-CA-C	8.46	122.92	108.95
1	B	362	VAL	N-CA-C	8.46	122.91	108.95
1	C	294	VAL	CA-C-O	-8.45	111.08	120.72
1	C	238	GLN	N-CA-C	-8.42	96.56	109.95
1	A	140	THR	N-CA-C	8.39	120.05	111.07
1	C	80	ALA	N-CA-CB	-8.36	96.66	110.12
1	B	347	SER	N-CA-C	8.36	120.27	108.74
1	A	347	SER	N-CA-C	8.33	120.23	108.74
1	B	190	ALA	N-CA-C	8.33	120.36	111.28
1	C	347	SER	N-CA-C	8.32	120.22	108.74
1	B	115	VAL	CB-CA-C	-8.31	102.25	111.23
1	C	226	SER	CA-C-N	-8.31	108.29	122.92
1	C	226	SER	C-N-CA	-8.31	108.29	122.92
1	B	272	LEU	N-CA-C	-8.31	100.00	112.54
1	B	127	ILE	CB-CA-C	-8.30	98.77	111.31
1	A	236	LEU	N-CA-C	8.29	120.01	110.97
1	C	97	GLY	N-CA-C	8.28	125.57	115.31
1	C	117	ASN	N-CA-C	8.23	121.66	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	GLY	CA-C-O	8.19	130.20	121.76
1	C	327	GLY	CA-C-O	8.19	130.20	121.76
1	A	327	GLY	CA-C-O	8.18	130.19	121.76
1	A	103	VAL	N-CA-C	8.15	119.44	107.37
1	C	366	VAL	N-CA-CB	8.08	124.56	111.23
1	A	366	VAL	N-CA-CB	8.06	124.52	111.23
1	B	366	VAL	N-CA-CB	8.05	124.51	111.23
1	A	261	VAL	N-CA-C	7.96	120.32	108.46
1	A	362	VAL	N-CA-CB	-7.96	99.10	112.47
1	A	226	SER	CA-C-N	-7.96	108.91	122.92
1	A	226	SER	C-N-CA	-7.96	108.91	122.92
1	C	362	VAL	N-CA-CB	-7.94	99.10	112.44
1	A	145	LEU	C-N-CD	-7.94	92.46	125.00
1	C	263	LEU	N-CA-C	-7.94	97.70	110.32
1	C	127	ILE	N-CA-C	7.93	120.03	108.53
1	B	328	ALA	N-CA-C	7.93	120.20	108.14
1	B	362	VAL	N-CA-CB	-7.93	99.12	112.44
1	C	78	ILE	N-CA-C	7.92	120.01	108.53
1	A	328	ALA	N-CA-C	7.91	120.16	108.14
1	C	328	ALA	N-CA-C	7.90	120.15	108.14
1	A	125	GLY	N-CA-C	-7.88	94.50	113.18
1	A	105	VAL	N-CA-C	7.84	119.42	108.12
1	A	358	LEU	N-CA-C	-7.79	92.58	109.81
1	C	358	LEU	N-CA-C	-7.78	92.61	109.81
1	B	358	LEU	N-CA-C	-7.76	92.65	109.81
1	B	261	VAL	N-CA-C	7.75	120.01	108.46
1	B	145	LEU	C-N-CD	-7.62	93.77	125.00
1	C	83	ALA	CA-C-O	7.59	129.24	120.89
1	A	276	LYS	N-CA-C	7.58	119.90	107.23
1	C	71	VAL	N-CA-C	7.58	120.01	108.71
1	B	276	LYS	N-CA-C	7.58	119.89	107.23
1	C	276	LYS	N-CA-C	7.57	119.87	107.23
1	C	299	PRO	CA-C-O	-7.56	106.84	120.60
1	B	299	PRO	CA-C-O	-7.56	106.85	120.60
1	A	299	PRO	CA-C-O	-7.56	106.85	120.60
1	C	103	VAL	N-CA-C	7.55	120.37	108.89
1	B	321	LEU	N-CA-C	7.54	120.02	107.20
1	A	321	LEU	N-CA-C	7.53	120.01	107.20
1	C	321	LEU	N-CA-C	7.52	119.99	107.20
1	A	148	LEU	N-CA-C	-7.50	102.07	112.12
1	B	263	LEU	N-CA-C	-7.46	98.86	110.42
1	A	326	LEU	N-CA-C	-7.44	96.60	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	LEU	N-CA-C	-7.44	96.60	108.73
1	C	326	LEU	N-CA-C	-7.44	96.60	108.73
1	C	166	PRO	CB-CA-C	-7.44	99.29	111.56
1	C	214	ILE	C-N-CD	-7.43	94.53	125.00
1	C	322	THR	CA-C-O	7.43	131.14	120.51
1	A	214	ILE	C-N-CD	-7.43	94.54	125.00
1	A	322	THR	CA-C-O	7.42	131.12	120.51
1	C	149	ALA	N-CA-C	-7.41	95.01	110.80
1	A	166	PRO	CB-CA-C	-7.40	99.35	111.56
1	B	322	THR	CA-C-O	7.40	131.09	120.51
1	B	198	PHE	CA-CB-CG	7.39	121.19	113.80
1	B	376	VAL	N-CA-C	7.38	118.95	108.17
1	C	128	VAL	N-CA-C	-7.38	96.85	108.81
1	A	308	ALA	N-CA-C	-7.37	98.20	109.85
1	C	376	VAL	N-CA-C	7.37	118.93	108.17
1	A	376	VAL	N-CA-C	7.35	118.91	108.17
1	B	156	SER	N-CA-C	7.35	120.38	108.32
1	C	308	ALA	N-CA-C	-7.35	98.23	109.85
1	C	188	GLU	N-CA-C	7.34	120.02	110.40
1	C	236	LEU	N-CA-C	7.34	119.97	111.02
1	B	308	ALA	N-CA-C	-7.34	98.26	109.85
1	A	258	ALA	N-CA-C	7.33	120.03	108.67
1	B	157	PHE	N-CA-C	-7.33	99.96	110.59
1	A	188	GLU	N-CA-C	7.32	119.99	110.40
1	A	132	LEU	N-CA-C	7.31	121.78	113.01
1	B	244	TYR	N-CA-C	7.30	120.51	109.41
1	B	214	ILE	CB-CA-C	-7.30	102.56	110.37
1	A	316	GLY	N-CA-C	7.30	120.48	110.56
1	C	269	THR	N-CA-C	7.30	119.98	108.67
1	C	316	GLY	N-CA-C	7.29	120.48	110.56
1	B	316	GLY	N-CA-C	7.29	120.48	110.56
1	C	179	TYR	N-CA-C	7.25	119.47	109.18
1	B	179	TYR	N-CA-C	7.23	119.45	109.18
1	B	188	GLU	N-CA-C	7.18	119.98	110.36
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	358	LEU	C-N-CD	-7.15	104.87	120.60
1	B	214	ILE	C-N-CD	-7.14	95.71	125.00
1	B	256	PHE	N-CA-C	7.14	119.98	109.69
1	B	171	THR	N-CA-C	-7.14	103.59	114.16
1	B	180	PHE	N-CA-C	7.14	120.03	107.61
1	C	180	PHE	N-CA-C	7.12	120.00	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	PHE	N-CA-C	7.11	119.98	109.24
1	C	270	ASN	N-CA-C	7.11	120.02	110.35
1	C	83	ALA	N-CA-C	7.10	119.98	108.76
1	C	232	LYS	N-CA-C	7.07	120.03	111.40
1	C	94	LYS	CB-CA-C	-7.06	99.28	110.79
1	B	110	GLU	N-CA-C	7.05	120.74	109.24
1	C	283	SER	N-CA-C	7.05	120.00	111.40
1	A	232	LYS	N-CA-C	7.04	119.99	111.40
1	A	283	SER	N-CA-C	7.04	119.99	111.40
1	B	283	SER	N-CA-C	7.04	119.99	111.40
1	C	192	ARG	N-CA-C	7.03	119.55	111.11
1	A	176	VAL	N-CA-C	-7.03	98.03	108.99
1	A	226	SER	N-CA-C	7.02	120.03	110.55
1	B	142	PHE	CA-CB-CG	7.02	120.82	113.80
1	B	232	LYS	N-CA-C	7.02	119.97	111.40
1	C	226	SER	N-CA-C	7.01	120.01	110.55
1	A	192	ARG	N-CA-C	7.01	119.52	111.11
1	C	152	PHE	N-CA-C	6.99	120.03	109.41
1	B	108	HIS	N-CA-C	-6.96	98.58	108.96
1	C	268	PRO	CB-CA-C	6.95	123.03	111.56
1	B	211	MET	N-CA-C	6.95	120.00	109.23
1	A	178	LEU	N-CA-C	6.94	119.99	108.96
1	B	176	VAL	N-CA-C	-6.88	99.19	108.96
1	C	317	GLY	N-CA-C	-6.87	100.39	111.59
1	B	317	GLY	N-CA-C	-6.86	100.41	111.59
1	C	190	ALA	CB-CA-C	-6.86	100.07	110.90
1	A	190	ALA	CB-CA-C	-6.85	100.07	110.90
1	A	317	GLY	N-CA-C	-6.85	100.42	111.59
1	C	126	GLY	CA-C-O	-6.85	111.36	119.72
1	C	132	LEU	N-CA-C	6.85	125.39	110.80
1	A	152	PHE	N-CA-C	6.83	119.32	109.14
1	B	164	TYR	N-CA-C	6.82	121.40	107.69
1	B	224	ASN	N-CA-C	6.82	119.85	109.62
1	A	365	THR	N-CA-C	6.81	120.04	109.07
1	C	128	VAL	N-CA-CB	6.81	124.65	111.92
1	C	365	THR	N-CA-C	6.80	120.02	109.07
1	B	106	THR	N-CA-C	6.80	120.48	109.40
1	B	365	THR	N-CA-C	6.79	120.01	109.07
1	B	128	VAL	N-CA-CB	6.79	124.62	111.92
1	A	208	ALA	N-CA-C	6.79	121.11	110.32
1	A	179	TYR	N-CA-C	6.79	119.46	109.69
1	B	210	ALA	N-CA-C	6.77	120.01	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	ALA	N-CA-C	6.76	120.00	109.52
1	B	208	ALA	N-CA-C	6.76	121.08	110.32
1	C	208	ALA	N-CA-C	6.76	121.07	110.32
1	A	141	LEU	N-CA-C	6.76	119.96	111.24
1	C	210	ALA	N-CA-C	6.74	119.96	109.52
1	C	189	PRO	N-CD-CG	-6.73	93.11	103.20
1	B	189	PRO	N-CD-CG	-6.71	93.13	103.20
1	B	235	ASP	N-CA-C	6.70	120.01	109.96
1	A	189	PRO	N-CD-CG	-6.70	93.16	103.20
1	C	235	ASP	N-CA-C	6.69	120.00	109.96
1	C	256	PHE	N-CA-C	6.68	120.04	109.81
1	A	235	ASP	N-CA-C	6.68	119.98	109.96
1	A	164	TYR	N-CA-C	6.64	121.05	107.69
1	A	256	PHE	N-CA-C	6.64	119.98	109.81
1	A	224	ASN	N-CA-C	6.64	119.91	110.68
1	B	198	PHE	N-CA-C	6.64	120.00	110.24
1	B	103	VAL	CA-C-O	6.63	129.83	121.40
1	C	164	TYR	N-CA-C	6.62	121.00	107.69
1	A	263	LEU	N-CA-C	-6.62	100.16	110.42
1	C	315	SER	N-CA-C	6.59	120.03	108.75
1	C	261	VAL	N-CA-C	6.59	118.99	108.85
1	A	198	PHE	N-CA-C	6.58	120.03	110.42
1	B	204	THR	N-CA-C	6.58	120.25	109.72
1	C	198	PHE	N-CA-C	6.57	120.01	110.42
1	C	285	ALA	N-CA-C	6.57	121.22	111.96
1	B	315	SER	N-CA-C	6.56	119.97	108.75
1	A	356	SER	N-CA-C	6.56	121.63	109.24
1	A	315	SER	N-CA-C	6.55	119.96	108.75
1	B	226	SER	N-CA-C	-6.55	101.70	110.55
1	B	356	SER	N-CA-C	6.55	121.61	109.24
1	A	285	ALA	N-CA-C	6.54	121.18	111.96
1	C	356	SER	N-CA-C	6.54	121.61	109.24
1	C	208	ALA	CB-CA-C	-6.54	98.33	109.51
1	C	122	VAL	N-CA-C	6.54	119.19	108.99
1	A	208	ALA	CB-CA-C	-6.53	98.34	109.51
1	B	208	ALA	CB-CA-C	-6.53	98.34	109.51
1	B	285	ALA	N-CA-C	6.53	121.17	111.96
1	A	180	PHE	N-CA-C	6.51	120.00	107.44
1	B	166	PRO	CA-N-CD	-6.49	102.92	112.00
1	C	222	TYR	N-CA-C	6.48	120.85	109.96
1	C	289	GLY	C-N-CD	-6.46	106.40	120.60
1	A	385	ASN	N-CA-C	6.45	120.02	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	GLY	C-N-CD	-6.45	106.41	120.60
1	B	190	ALA	CB-CA-C	-6.45	100.08	110.79
1	B	345	THR	CB-CA-C	6.45	121.32	109.71
1	B	354	THR	CB-CA-C	-6.45	101.83	110.79
1	A	354	THR	CB-CA-C	-6.45	101.83	110.79
1	A	207	TRP	N-CA-C	6.45	120.00	111.75
1	B	385	ASN	N-CA-C	6.44	120.00	109.24
1	C	354	THR	CB-CA-C	-6.44	101.84	110.79
1	C	207	TRP	N-CA-C	6.44	119.99	111.75
1	A	345	THR	CB-CA-C	6.43	121.29	109.71
1	B	207	TRP	N-CA-C	6.43	119.99	111.75
1	C	329	THR	N-CA-C	6.43	120.00	109.06
1	A	329	THR	N-CA-C	6.43	119.99	109.06
1	C	345	THR	CB-CA-C	6.43	121.28	109.71
1	B	289	GLY	C-N-CD	-6.42	106.47	120.60
1	C	385	ASN	N-CA-C	6.42	119.97	109.24
1	B	329	THR	N-CA-C	6.42	119.97	109.06
1	C	224	ASN	N-CA-C	6.42	119.60	110.68
1	A	182	LYS	N-CA-C	6.42	120.21	112.38
1	B	313	ASN	N-CA-C	6.40	120.02	108.69
1	C	313	ASN	N-CA-C	6.40	120.02	108.69
1	A	313	ASN	N-CA-C	6.38	119.99	108.69
1	B	344	GLY	N-CA-C	-6.38	98.06	113.18
1	A	344	GLY	N-CA-C	-6.38	98.07	113.18
1	C	344	GLY	N-CA-C	-6.37	98.08	113.18
1	C	201	LEU	N-CA-C	6.36	120.00	110.14
1	C	178	LEU	N-CA-C	6.36	120.02	109.46
1	A	201	LEU	N-CA-C	6.36	120.00	110.14
1	B	115	VAL	N-CA-C	6.35	117.57	107.98
1	B	178	LEU	N-CA-C	6.35	120.00	109.46
1	C	176	VAL	N-CA-C	-6.33	99.97	108.96
1	B	205	ALA	N-CA-C	-6.31	95.87	109.81
1	B	201	LEU	N-CA-C	6.30	119.97	109.95
1	B	259	ARG	N-CA-C	6.30	119.97	109.95
1	B	295	LEU	N-CA-C	-6.30	95.28	107.44
1	C	84	VAL	N-CA-C	6.29	119.33	108.95
1	B	350	PHE	N-CA-C	-6.28	99.97	109.95
1	C	350	PHE	N-CA-C	-6.28	99.97	109.95
1	A	196	ALA	N-CA-C	6.26	120.02	112.38
1	B	187	PRO	N-CA-C	-6.26	99.57	112.47
1	C	259	ARG	N-CA-C	6.26	120.03	109.76
1	C	182	LYS	N-CA-C	6.25	120.01	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350	PHE	N-CA-C	-6.25	100.01	109.95
1	C	196	ALA	N-CA-C	6.25	120.00	112.38
1	C	100	SER	N-CA-C	6.25	119.16	109.60
1	C	150	SER	N-CA-C	-6.24	105.44	114.12
1	B	182	LYS	N-CA-C	6.24	119.99	112.38
1	A	122	VAL	N-CA-C	6.22	118.34	108.89
1	C	118	SER	N-CA-C	6.19	120.74	107.67
1	A	314	LEU	N-CA-CB	6.18	120.28	110.57
1	C	74	VAL	N-CA-C	-6.16	99.48	108.11
1	C	183	ASP	N-CA-C	6.15	119.26	108.56
1	B	195	LEU	N-CA-C	-6.15	104.27	110.97
1	C	314	LEU	N-CA-CB	6.14	120.21	110.57
1	B	183	ASP	N-CA-C	6.13	119.22	108.56
1	B	163	ASP	N-CA-C	6.13	118.39	108.41
1	A	259	ARG	N-CA-C	6.12	120.03	110.17
1	C	157	PHE	N-CA-C	-6.12	100.34	109.94
1	A	157	PHE	N-CA-C	-6.11	100.35	109.94
1	A	377	GLY	N-CA-C	-6.11	98.70	113.18
1	B	377	GLY	N-CA-C	-6.11	98.70	113.18
1	B	314	LEU	N-CA-CB	6.11	120.16	110.57
1	C	377	GLY	N-CA-C	-6.11	98.71	113.18
1	C	129	GLY	N-CA-C	-6.10	98.72	113.18
1	B	216	THR	N-CA-C	6.10	119.18	109.24
1	C	356	SER	CB-CA-C	-6.10	101.95	112.44
1	A	356	SER	CB-CA-C	-6.09	101.96	112.44
1	B	356	SER	CB-CA-C	-6.09	101.97	112.44
1	C	147	ALA	N-CA-C	6.08	119.99	111.30
1	B	147	ALA	N-CA-C	6.06	119.96	111.30
1	B	268	PRO	N-CA-C	-6.06	99.99	112.47
1	C	151	ASN	N-CA-C	-6.06	105.07	112.88
1	C	258	ALA	N-CA-C	6.05	118.31	108.63
1	B	382	ASN	N-CA-C	6.04	120.11	109.96
1	C	268	PRO	N-CA-C	-6.04	100.02	112.47
1	A	382	ASN	N-CA-C	6.04	120.11	109.96
1	C	382	ASN	N-CA-C	6.03	120.09	109.96
1	A	126	GLY	CA-C-O	-6.02	111.84	119.19
1	C	125	GLY	N-CA-C	-6.02	106.66	115.63
1	A	167	LEU	N-CA-C	6.01	118.80	111.82
1	C	142	PHE	N-CA-C	6.01	118.57	107.99
1	C	123	VAL	N-CA-C	-6.01	100.03	108.80
1	B	222	TYR	N-CA-C	6.00	120.04	109.96
1	A	222	TYR	N-CA-C	5.99	120.02	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	138	ASN	N-CA-C	-5.99	104.50	112.94
1	C	101	GLY	N-CA-C	-5.99	98.99	113.18
1	C	167	LEU	N-CA-C	5.98	118.76	111.82
1	A	221	ARG	N-CA-C	-5.98	100.54	110.17
1	B	121	PHE	CA-CB-CG	-5.98	107.82	113.80
1	A	121	PHE	CA-CB-CG	-5.98	107.82	113.80
1	C	221	ARG	N-CA-C	-5.97	100.55	110.17
1	A	372	GLY	N-CA-C	-5.96	99.06	113.18
1	C	372	GLY	N-CA-C	-5.95	99.07	113.18
1	B	360	ALA	N-CA-C	-5.95	99.96	109.96
1	C	360	ALA	N-CA-C	-5.95	99.96	109.96
1	B	132	LEU	N-CA-C	5.95	123.47	110.80
1	B	328	ALA	CB-CA-C	-5.95	100.24	110.95
1	C	121	PHE	CA-CB-CG	-5.95	107.85	113.80
1	B	372	GLY	N-CA-C	-5.94	99.09	113.18
1	A	295	LEU	N-CA-C	-5.94	95.28	107.70
1	B	103	VAL	N-CA-C	5.93	117.91	108.89
1	C	295	LEU	N-CA-C	-5.93	95.31	107.70
1	A	328	ALA	CB-CA-C	-5.92	100.30	110.95
1	B	142	PHE	N-CA-C	5.92	119.10	107.98
1	B	345	THR	N-CA-C	-5.91	100.98	110.14
1	C	328	ALA	CB-CA-C	-5.91	100.32	110.95
1	A	360	ALA	N-CA-C	-5.91	100.04	109.96
1	C	85	SER	CA-C-N	-5.91	112.48	123.05
1	C	85	SER	C-N-CA	-5.91	112.48	123.05
1	C	96	THR	N-CA-C	-5.91	99.77	109.40
1	C	289	GLY	N-CA-C	-5.90	100.31	112.34
1	A	106	THR	CB-CA-C	5.89	120.63	109.37
1	A	345	THR	N-CA-C	-5.87	101.03	110.14
1	C	345	THR	N-CA-C	-5.87	101.04	110.14
1	A	289	GLY	N-CA-C	-5.87	100.37	112.34
1	C	143	SER	N-CA-C	5.87	120.05	113.01
1	B	289	GLY	N-CA-C	-5.87	100.38	112.34
1	C	219	VAL	N-CA-C	-5.86	99.96	108.87
1	A	219	VAL	N-CA-C	-5.85	99.98	108.87
1	C	104	THR	N-CA-C	5.84	119.17	110.52
1	B	147	ALA	N-CA-CB	-5.81	102.83	111.43
1	A	143	SER	N-CA-C	5.81	119.98	113.01
1	B	143	SER	N-CA-C	5.81	119.98	113.01
1	C	147	ALA	N-CA-CB	-5.80	102.84	111.43
1	B	298	THR	N-CA-C	-5.80	100.08	109.82
1	A	187	PRO	N-CA-C	-5.79	100.54	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	ASN	N-CA-C	-5.77	104.07	113.19
1	B	113	THR	N-CA-C	-5.77	99.37	108.14
1	A	298	THR	N-CA-C	-5.77	100.13	109.82
1	C	298	THR	N-CA-C	-5.76	100.14	109.82
1	C	342	ASN	N-CA-C	-5.76	104.09	113.19
1	B	374	LEU	N-CA-C	5.75	117.53	108.96
1	B	241	ILE	N-CA-C	-5.75	99.77	108.17
1	A	342	ASN	N-CA-C	-5.75	104.11	113.19
1	A	197	ASN	N-CA-C	5.75	120.02	112.89
1	C	374	LEU	N-CA-C	5.74	117.51	108.96
1	B	169	GLY	N-CA-C	5.73	120.00	111.18
1	B	123	VAL	N-CA-C	-5.73	100.35	108.65
1	C	197	ASN	N-CA-C	5.72	119.99	112.89
1	A	374	LEU	N-CA-C	5.71	117.47	108.96
1	C	286	ASP	N-CA-C	-5.69	100.66	109.14
1	B	286	ASP	N-CA-C	-5.67	100.68	109.14
1	A	286	ASP	N-CA-C	-5.67	100.69	109.14
1	B	128	VAL	N-CA-C	-5.66	99.64	108.81
1	A	211	MET	N-CA-C	5.66	118.00	109.23
1	C	293	LEU	N-CA-C	5.65	118.61	109.40
1	A	241	ILE	N-CA-C	-5.65	99.92	108.17
1	A	293	LEU	N-CA-C	5.65	118.60	109.40
1	B	293	LEU	N-CA-C	5.65	118.60	109.40
1	C	80	ALA	O-C-N	5.65	126.82	120.83
1	A	311	THR	N-CA-C	-5.64	99.98	109.07
1	C	311	THR	N-CA-C	-5.64	99.99	109.07
1	C	241	ILE	N-CA-C	-5.63	99.95	108.17
1	B	311	THR	N-CA-C	-5.62	100.02	109.07
1	B	287	ALA	N-CA-CB	-5.61	102.69	111.56
1	C	82	VAL	N-CA-C	5.60	116.33	110.62
1	A	287	ALA	N-CA-CB	-5.60	102.72	111.56
1	C	266	PRO	N-CA-C	5.60	120.02	110.95
1	B	266	PRO	N-CA-C	5.59	120.00	110.95
1	C	287	ALA	N-CA-CB	-5.59	102.73	111.56
1	B	280	LEU	N-CA-C	5.57	117.81	111.02
1	A	280	LEU	N-CA-C	5.56	117.80	111.02
1	A	106	THR	CA-C-N	-5.55	114.14	122.47
1	A	106	THR	C-N-CA	-5.55	114.14	122.47
1	C	280	LEU	N-CA-C	5.55	117.79	111.02
1	C	285	ALA	CB-CA-C	-5.55	101.06	110.88
1	C	333	VAL	CA-C-O	-5.53	114.70	120.51
1	B	230	ASP	N-CA-C	-5.53	105.20	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	VAL	CA-C-O	-5.52	114.72	120.51
1	A	333	VAL	CA-C-O	-5.51	114.72	120.51
1	C	141	LEU	N-CA-C	5.51	120.00	111.56
1	A	107	SER	N-CA-CB	-5.51	101.42	110.95
1	B	285	ALA	CB-CA-C	-5.51	101.13	110.88
1	B	309	THR	N-CA-C	5.51	118.44	109.24
1	A	285	ALA	CB-CA-C	-5.50	101.14	110.88
1	C	105	VAL	N-CA-C	5.48	116.62	108.46
1	C	309	THR	N-CA-C	5.48	118.39	109.24
1	A	309	THR	N-CA-C	5.46	118.36	109.24
1	B	135	ASN	N-CA-C	5.45	118.13	109.40
1	A	131	SER	CA-C-N	-5.45	110.39	121.18
1	A	131	SER	C-N-CA	-5.45	110.39	121.18
1	B	129	GLY	N-CA-C	-5.44	100.28	113.18
1	A	321	LEU	CB-CA-C	-5.44	104.68	111.43
1	B	321	LEU	CB-CA-C	-5.43	104.69	111.43
1	C	127	ILE	CB-CA-C	-5.42	102.57	110.81
1	C	321	LEU	CB-CA-C	-5.41	104.72	111.43
1	C	142	PHE	CA-CB-CG	5.41	119.21	113.80
1	B	253	GLY	N-CA-C	5.38	119.13	110.90
1	A	253	GLY	N-CA-C	5.37	119.12	110.90
1	B	121	PHE	N-CA-C	5.37	116.33	107.20
1	C	253	GLY	N-CA-C	5.36	119.10	110.90
1	C	75	GLY	N-CA-C	-5.36	100.49	113.18
1	A	146	PRO	CA-CB-CG	-5.33	94.38	104.50
1	B	300	THR	CB-CA-C	5.33	117.66	109.03
1	A	183	ASP	N-CA-C	5.32	117.87	108.24
1	A	112	LEU	N-CA-CB	-5.32	101.50	110.49
1	A	269	THR	N-CA-C	-5.32	99.47	110.80
1	B	368	GLY	N-CA-C	-5.32	100.58	113.18
1	A	368	GLY	N-CA-C	-5.31	100.59	113.18
1	B	127	ILE	CA-C-N	-5.31	114.72	122.58
1	B	127	ILE	C-N-CA	-5.31	114.72	122.58
1	C	368	GLY	N-CA-C	-5.31	100.60	113.18
1	A	300	THR	CB-CA-C	5.30	117.62	109.03
1	A	105	VAL	CA-C-O	5.30	125.97	120.36
1	A	161	VAL	N-CA-C	-5.29	100.44	108.17
1	B	192	ARG	N-CA-C	5.29	116.73	111.07
1	C	161	VAL	N-CA-C	-5.29	100.44	108.17
1	C	112	LEU	N-CA-CB	-5.29	101.55	110.49
1	A	169	GLY	N-CA-C	5.29	120.00	111.38
1	C	118	SER	CB-CA-C	-5.29	104.29	111.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	THR	CB-CA-C	5.28	117.16	109.08
1	B	112	LEU	N-CA-CB	-5.28	101.57	110.49
1	C	169	GLY	N-CA-C	5.28	119.99	111.38
1	C	300	THR	CB-CA-C	5.28	117.58	109.03
1	B	200	VAL	N-CA-C	5.27	120.30	109.34
1	A	298	THR	CB-CA-C	5.26	117.13	109.08
1	A	353	CYS	N-CA-C	-5.26	101.13	108.96
1	C	298	THR	CB-CA-C	5.26	117.12	109.08
1	B	353	CYS	N-CA-C	-5.25	101.14	108.96
1	C	290	PRO	CB-CA-C	-5.25	98.88	112.00
1	C	353	CYS	N-CA-C	-5.24	101.15	108.96
1	C	85	SER	N-CA-C	-5.24	100.06	108.55
1	C	119	SER	N-CA-C	-5.23	99.67	110.80
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	A	305	THR	N-CA-C	-5.22	98.89	108.02
1	C	305	THR	N-CA-C	-5.22	98.89	108.02
1	B	257	LEU	N-CA-C	5.21	118.58	107.70
1	B	305	THR	N-CA-C	-5.21	98.91	108.02
1	B	363	THR	N-CA-CB	-5.20	101.82	111.13
1	C	331	ALA	N-CA-C	-5.19	99.74	110.80
1	B	331	ALA	N-CA-C	-5.18	99.76	110.80
1	C	81	PRO	N-CA-C	5.18	119.18	111.41
1	C	363	THR	N-CA-CB	-5.18	101.86	111.13
1	A	132	LEU	N-CA-CB	-5.18	101.33	110.39
1	A	331	ALA	N-CA-C	-5.18	99.77	110.80
1	A	363	THR	N-CA-CB	-5.18	101.86	111.13
1	C	200	VAL	N-CA-C	5.18	120.11	109.34
1	A	174	GLY	N-CA-C	5.17	120.01	111.59
1	A	135	ASN	N-CA-C	5.16	117.66	109.40
1	B	234	ILE	CA-CB-CG2	-5.16	101.72	110.50
1	A	234	ILE	CA-CB-CG2	-5.16	101.72	110.50
1	B	340	ILE	CA-CB-CG2	-5.16	101.72	110.50
1	A	200	VAL	N-CA-C	5.16	120.07	109.34
1	B	174	GLY	N-CA-C	5.16	120.00	111.59
1	C	174	GLY	N-CA-C	5.16	120.00	111.59
1	A	214	ILE	N-CA-C	5.16	120.02	108.88
1	A	241	ILE	CA-CB-CG2	-5.16	101.73	110.50
1	B	203	GLU	N-CA-C	5.16	117.20	108.02
1	C	334	ILE	CA-CB-CG2	-5.16	101.74	110.50
1	A	337	ILE	CA-CB-CG2	-5.15	101.74	110.50
1	A	127	ILE	CA-CB-CG2	-5.15	101.74	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	ILE	CA-CB-CG2	-5.15	101.74	110.50
1	B	241	ILE	CA-CB-CG2	-5.15	101.74	110.50
1	C	337	ILE	CA-CB-CG2	-5.15	101.75	110.50
1	A	340	ILE	CA-CB-CG2	-5.15	101.75	110.50
1	C	340	ILE	CA-CB-CG2	-5.14	101.76	110.50
1	A	373	ILE	CA-CB-CG2	-5.14	101.77	110.50
1	B	373	ILE	CA-CB-CG2	-5.14	101.77	110.50
1	C	67	ILE	CA-CB-CG2	-5.13	101.77	110.50
1	C	234	ILE	CA-CB-CG2	-5.13	101.77	110.50
1	C	343	VAL	N-CA-C	5.13	120.02	109.34
1	C	214	ILE	N-CA-C	5.13	119.97	108.88
1	A	214	ILE	CA-CB-CG2	-5.13	101.78	110.50
1	C	373	ILE	CA-CB-CG2	-5.13	101.78	110.50
1	B	334	ILE	CA-CB-CG2	-5.13	101.78	110.50
1	A	306	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	334	ILE	CA-CB-CG2	-5.13	101.78	110.50
1	B	337	ILE	CA-CB-CG2	-5.13	101.78	110.50
1	C	127	ILE	CA-CB-CG2	-5.13	101.78	110.50
1	B	127	ILE	CA-CB-CG2	-5.12	101.79	110.50
1	C	68	ILE	CA-CB-CG2	-5.12	101.79	110.50
1	B	214	ILE	CA-CB-CG2	-5.12	101.80	110.50
1	C	214	ILE	CA-CB-CG2	-5.12	101.80	110.50
1	A	343	VAL	N-CA-C	5.11	119.97	109.34
1	C	89	VAL	N-CA-C	5.11	119.97	109.34
1	B	343	VAL	N-CA-C	5.11	119.97	109.34
1	A	206	PRO	CA-CB-CG	-5.09	94.82	104.50
1	B	340	ILE	CB-CA-C	5.09	118.19	111.21
1	C	267	GLN	N-CA-C	5.09	118.53	110.58
1	C	355	VAL	CB-CA-C	5.08	118.56	111.34
1	B	355	VAL	CB-CA-C	5.08	118.56	111.34
1	A	340	ILE	CB-CA-C	5.08	118.16	111.21
1	B	270	ASN	N-CA-C	-5.06	100.01	110.80
1	B	306	PHE	CA-CB-CG	5.06	118.86	113.80
1	B	161	VAL	N-CA-C	-5.06	100.97	108.45
1	C	340	ILE	CB-CA-C	5.06	118.14	111.21
1	A	355	VAL	CB-CA-C	5.05	118.50	111.34
1	B	297	ARG	N-CA-C	5.04	118.24	110.42
1	C	191	ASP	N-CA-C	5.04	114.80	108.45
1	A	243	THR	N-CA-C	-5.03	100.25	108.76
1	C	84	VAL	CB-CA-C	-5.03	102.91	110.55
1	C	306	PHE	CA-CB-CG	5.03	118.83	113.80
1	C	297	ARG	N-CA-C	5.03	118.21	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ARG	N-CA-C	5.02	118.20	110.42
1	A	142	PHE	CA-CB-CG	5.01	118.81	113.80
1	A	191	ASP	N-CA-C	5.01	114.76	108.45
1	A	119	SER	CB-CA-C	5.00	119.57	110.11

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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	667	0
1	B	2130	0	2111	615	2
1	C	2376	0	2374	717	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	1936	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 146.

All (1936) 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:N	1:B:122:VAL:CA	1.68	1.56
1:C:223:CYS:CA	1:C:223:CYS:C	1.75	1.55
1:B:107:SER:N	1:B:107:SER:CA	1.70	1.53
1:A:172:GLU:N	1:A:172:GLU:CA	1.70	1.51
1:A:362:VAL:N	1:A:362:VAL:CA	1.75	1.50
1:B:241:ILE:CD1	1:B:255:LEU:HD23	1.42	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:280:LEU:CA	1.76	1.46
1:C:362:VAL:N	1:C:362:VAL:CA	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:A:319:ARG:HD2	1:A:371:ALA:CB	1.49	1.40
1:B:319:ARG:HD2	1:B: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
1:A:147:ALA:CB	1:A:272:LEU:HD21	1.55	1.33
1:B:241:ILE:CD1	1:B:255:LEU:CD2	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ASN:OD1	1:A:345:THR:HB	1.35	1.24
1:A:151:ASN:OD1	1:A:269:THR:OG1	1.53	1.23
1:B:133:GLN:NE2	1:B:184:SER:OG	1.68	1.23
1:C:342:ASN:ND2	1:C:346:ALA:O	1.72	1.23
1:A:304:HIS:CE1	1:A:374:LEU:HD13	1.74	1.23
1:B:304:HIS:CE1	1:B: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: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:C:98:ARG:CD	1:C:105:VAL:HG21	1.69	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
1:A:168:CYS:SG	1:A:252:VAL:CG1	2.29	1.19
1:C:151:ASN:OD1	1:C:269:THR:OG1	1.61	1.19
1:B:298:THR:OG1	1:B:299:PRO:HD2	1.43	1.19
1:C:190:ALA:HB3	1:C:194:GLU:OE2	1.42	1.19
1:A:298:THR:OG1	1:A:299:PRO:HD2	1.43	1.18
1:C:117:ASN:OD1	1:C:252:VAL:HG21	1.43	1.18
1:B:320:CYS:CB	1:B:366:VAL:HG11	1.74	1.18
1:C:320:CYS:CB	1:C:366:VAL:HG11	1.74	1.18
1:B:221:ARG:HH11	1:B:236:LEU:HA	1.08	1.17
1:A:320:CYS:CB	1:A:366:VAL:HG11	1.74	1.17
1:C:277:ARG:CB	1:C:285:ALA:HB3	1.73	1.17
1:B:221:ARG:NH1	1:B:236:LEU:HA	1.59	1.17
1:B:277:ARG:CB	1:B:285:ALA:HB3	1.73	1.17
1:A:277:ARG:CB	1:A:285:ALA:HB3	1.73	1.17
1:C:326:LEU:HD23	1:C:337:ILE:HD12	1.28	1.16
1:C:221:ARG:HG2	1:C:234:ILE:O	1.40	1.16
1:A:154:GLN:NE2	1:A:222:TYR:CD1	2.12	1.16
1:A:190:ALA:HB3	1:A:194:GLU:OE2	1.46	1.16
1:B:320:CYS:HB2	1:B:366:VAL:CG1	1.75	1.15
1:C:298:THR:OG1	1:C:299:PRO:HD2	1.43	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:320:CYS:HB2	1:A:366:VAL:CG1	1.75	1.15
1:C:331:ALA:HB2	1:C:357:SER:HB3	1.28	1.15
1:C:164:TYR:HD2	1:C:255:LEU:CD1	1.59	1.14
1:C:275[P]:SER:HA	1:C:375:LEU:HD23	1.20	1.14
1:C:326:LEU:HD22	1:C:337:ILE:HD12	1.21	1.14
1:B:192:ARG:HH12	1:B:244:TYR:HB2	0.98	1.14
1:B:183:ASP:OD2	1:B:186:ASP:OD2	1.66	1.13
1: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:276:LYS:HB3	1:B:295:LEU:HD21	1.23	1.11
1:B:331:ALA:HB2	1:B:357:SER:HB3	1.28	1.11
1:C:148:LEU:C	1:C:150:SER:H	1.54	1.11
1:C:276:LYS:O	1:C:295:LEU:HD11	1.51	1.11
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:147:ALA:CA	1:A:272:LEU:HD21	1.81	1.10
1:A:326:LEU:HD23	1:A:337:ILE:HD12	1.27	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:B:275:SER:HA	1:B:375:LEU:HD23	1.20	1.09
1:C:67:ILE:HG22	1:C:68:ILE:N	1.62	1.09
1:C:164:TYR:CD2	1:C:255:LEU:CD1	2.34	1.09
1:C:317:GLY:HA3	1:C:348:ASP:HA	1.29	1.09
1:C:324:LEU:HD23	1:C:366:VAL:HG22	1.15	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:335:ASN:ND2	1:C:353:CYS:C	2.10	1.09
1:A:186:ASP:N	1:B:226:SER:OG	1.86	1.09
1:C:130:ASN:OD1	1:C:188:GLU:OE2	1.70	1.09
1:A:178:LEU:HD22	1:A:241:ILE:HG12	1.31	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASP:CB	1:C:186:ASP:OD1	2.01	1.09
1:A:335:ASN:ND2	1:A:353:CYS:C	2.10	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:B:192:ARG:NH1	1:B:244:TYR:CB	2.15	1.08
1:B:324:LEU:HD21	1:B:366:VAL:HG21	1.35	1.08
1:C:204:THR:HG22	1:C:205:ALA:O	1.51	1.08
1:B:127:ILE:HG22	1:B:128:VAL:N	1.65	1.08
1:A:275[S]:SER:HA	1:A:375:LEU:HD23	1.10	1.08
1:A:324:LEU:HD21	1:A:366:VAL:HG21	1.35	1.08
1:B:152:PHE:CE1	1:B:263:LEU:HD13	1.89	1.08
1:C:324:LEU:HD21	1:C:366:VAL:HG21	1.35	1.08
1:A:335:ASN:CB	1:A:352:ASN:ND2	2.17	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:B:335:ASN:ND2	1:B:353:CYS:C	2.10	1.08
1:C:103:VAL:HG13	1:C:152:PHE:CE2	1.89	1.08
1:A:225:ASP:HB2	1:C:186:ASP:OD1	1.51	1.08
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: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:B:319:ARG:CD	1:B:371:ALA:CB	2.32	1.07
1:C:152:PHE:HD2	1:C:264:TYR:O	1.37	1.07
1:C:335:ASN:CB	1:C:352:ASN:ND2	2.17	1.07
1:A:335:ASN:HD22	1:A:353:CYS:CA	1.67	1.07
1:C:241:ILE:HD13	1:C:255:LEU:CD2	1.83	1.07
1:C:276:LYS:HB3	1:C:295:LEU:HD21	1.24	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:331:ALA:HB3	1:A:357:SER:OG	1.57	1.04
1:B:277:ARG:HB3	1:B:285:ALA:HB3	1.38	1.04
1:C:275[S]:SER:HA	1:C:375:LEU:HD23	1.34	1.04
1:C:104:THR:HG23	1:C:263:LEU:HD12	1.34	1.04
1:C:338:LEU:HD23	1:C:339:ALA:N	1.69	1.04
1:C:331:ALA:HB2	1:C:357:SER:CB	1.88	1.04
1: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:B:121:PHE:C	1:B:122:VAL:CA	2.32	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
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:164:TYR:CD2	1:A:255:LEU:CD1	2.41	1.01
1:A:178:LEU:CD2	1:A:241:ILE:HG12	1.88	1.01
1:A:185:GLN:C	1:B:226:SER:OG	2.04	1.01
1:A:232:LYS:HD2	1:B:228:THR:HG21	1.42	1.01
1:A:335:ASN:ND2	1:A:353:CYS:CA	2.24	1.01
1:B:326:LEU:CD2	1:B:337:ILE:CD1	2.39	1.01
1:C: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:B:127:ILE:CG2	1:B:128:VAL:N	2.24	1.01
1:A:200:VAL:O	1:A:200:VAL:HG12	1.57	1.00
1:A:326:LEU:CD2	1:A:337:ILE:CD1	2.39	1.00
1:C:200:VAL:O	1:C:200:VAL:HG12	1.57	1.00
1:A: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:ARG:HD2	1:B:371:ALA:HB2	1.05	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:C:335:ASN:ND2	1:C:353:CYS:CA	2.24	1.00
1:B:200:VAL:O	1:B:200:VAL:HG12	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:97:GLY:O	1:C:98:ARG:C	2.04	0.99
1:C:319:ARG:HD2	1:C:371:ALA:HB3	1.41	0.99
1:A:319:ARG:HD2	1:A:371:ALA:HB3	1.41	0.99
1:B:328:ALA:CB	1:B:362:VAL:HG22	1.91	0.99
1:C:68:ILE:CG2	1:C:70:HIS:NE2	2.22	0.99
1:C:277:ARG:HB3	1:C:285:ALA:CB	1.92	0.99
1:B:268:PRO:O	1:B:269:THR:O	1.81	0.99
1:B:201:LEU:HD23	1:B:201:LEU:C	1.88	0.98
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:110:GLU:CD	1:A:144:TRP:HB3	1.89	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:201:LEU:C	1:C:201:LEU:HD23	1.88	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:319:ARG:HD2	1:B:371:ALA:HB3	1.41	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:201:LEU:HD23	1:A:201:LEU:C	1.88	0.97
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: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:C:335:ASN:HD21	1:C:353:CYS:C	1.71	0.96
1:B:279:ASP:HB3	1:B:282:GLY:HA3	1.46	0.96
1:A:219:VAL:HB	1:A:221:ARG:HH21	1.28	0.96
1:A:366:VAL:HG12	1:A:367:SER:N	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:HD23	1:A:145:LEU:O	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:B:335:ASN:HD21	1:B:353:CYS:C	1.71	0.94
1:C:331:ALA:CB	1:C:357:SER:HB3	1.98	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: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:117:ASN:OD1	1:C:252:VAL:CG2	2.16	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:A:335:ASN:HD21	1:A:353:CYS:C	1.71	0.93
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
1:C:134:LEU:HD23	1:C:236:LEU:HD23	1.50	0.93
1:A:183:ASP:O	1:A:185:GLN:N	2.01	0.93
1:A:335:ASN:CB	1:A:352:ASN:HD22	1.80	0.93
1:C:304:HIS:HE1	1:C:374:LEU:HD13	1.13	0.93
1:B:127:ILE:CG2	1:B:128:VAL:H	1.82	0.93
1:A:267:GLN:CD	1:C:198:PHE:CE1	2.46	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:351:LEU:HD12	1:C:351:LEU:C	1.94	0.92
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:A:351:LEU:C	1:A:351:LEU:HD12	1.94	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:268:PRO:O	1:A:269:THR:C	2.12	0.92
1:B:319:ARG:CG	1:B:371:ALA:HB3	1.99	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: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
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:351:LEU:C	1:B:351:LEU:HD12	1.94	0.91
1:B:324:LEU:HD22	1:B:366:VAL:CG2	1.98	0.90
1:C:167:LEU:CD2	1:C:252:VAL:C	2.44	0.90
1:C:278:LEU:HD21	1:C:295:LEU:O	1.70	0.90
1:C:89:VAL:HG12	1:C:90:GLY:N	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:267:GLN:O	1:C:197:ASN:CB	2.20	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:C:97:GLY:O	1:C:99:THR:N	2.04	0.90
1:A:179:TYR:CE1	1:A:240:GLY:HA3	2.07	0.90
1:A:296:THR:OG1	1:A:303:THR:HB	1.70	0.90
1:A:326:LEU:HD23	1:A:337:ILE:CD1	2.00	0.90
1:A:138:ASN:OD1	1:A:140:THR:HB	1.72	0.89
1:B:278:LEU:HD21	1:B:295:LEU:O	1.70	0.89
1:A:228:THR:CG2	1:C:232:LYS:CD	2.49	0.89
1:B:335:ASN:HB3	1:B:352:ASN:HD22	1.34	0.89
1:C:167:LEU:HD21	1:C:252:VAL:C	1.97	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:C:148:LEU:C	1:C:150:SER:N	2.25	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: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:129:GLY:O	1:C:307:ARG:NH2	2.05	0.89
1:C:195:LEU:HD21	1:C:201:LEU:HD11	1.55	0.89
1:C:221:ARG:CG	1:C:234:ILE:O	2.21	0.88
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:130:ASN:HD22	1:B:238:GLN:CD	1.81	0.88
1:B:190:ALA:HB3	1:B:194:GLU:OE2	1.74	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:C:361:THR:C	1:C:362:VAL:CA	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:LEU:CD2	1:B:241:ILE:HG12	2.02	0.88
1:B:192:ARG:NH1	1:B:244:TYR:HB2	1.82	0.88
1:C:274[P]:SER:O	1:C:375:LEU:HA	1.73	0.88
1: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: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:B:361:THR:C	1:B:362:VAL:CA	2.47	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: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:O	1:B:170:THR:HG22	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:A:361:THR:C	1:A:362:VAL:CA	2.47	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:204:THR:C	1:C:205:ALA:O	2.11	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
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:C:279:ASP:C	1:C:280:LEU:CA	2.49	0.86
1:B:355:VAL:HG13	1:B:360:ALA:HB2	1.55	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:A:279:ASP:C	1:A:280:LEU:CA	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:279:ASP:C	1:B:280:LEU:CA	2.49	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:319:ARG:HG3	1:A:371:ALA:HB3	1.58	0.84
1:A:335:ASN:HB2	1:A:352:ASN:ND2	1.91	0.84
1:A:383:VAL:O	1:A:384:VAL:CG2	2.25	0.84
1:C:96:THR:HG23	1:C:105:VAL:HB	1.56	0.84
1:C:326:LEU:HB2	1:C:337:ILE:HD11	1.57	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:164:TYR:CE2	1:A:255:LEU:HD11	2.11	0.84
1:A:226:SER:CB	1:C:185:GLN:HB3	2.07	0.84
1:C:279:ASP:HB3	1:C:282:GLY:CA	2.05	0.84
1:A: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:C:217:ASP:CG	1:C:221:ARG:NH2	2.36	0.84
1:A:217:ASP:CG	1:A:221:ARG:NH2	2.36	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
1:C:138:ASN:C	1:C:140:THR:N	2.33	0.83
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:321:LEU:O	1:B:322:THR:OG1	1.96	0.83
1:A:123:VAL:C	1:A:125:GLY:H	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:THR:CG2	1:C:105:VAL:HB	2.09	0.83
1:C:206:PRO:HG2	1:C:207:TRP:HD1	1.44	0.83
1:A:129:GLY:O	1:A:131:SER:N	2.11	0.83
1:C: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: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: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:B:133:GLN:NE2	1:B:184:SER:HG	1.74	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:118:SER:O	1:C:119:SER:C	2.23	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:89:VAL:CG1	1:C:90:GLY:N	2.43	0.81
1:A:122:VAL:HG13	1:A:126:GLY:CA	2.10	0.81
1:B:152:PHE:CD2	1:B:263:LEU:HB3	2.15	0.81
1:B:204:THR:HG22	1:B:205:ALA:O	1.79	0.81
1:A:262:THR:CG2	1:A:264:TYR:CZ	2.62	0.81
1:B:183:ASP:CG	1:B:186:ASP:OD2	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ASP:C	1:B:185:GLN:H	1.89	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: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:C:289:GLY:CA	1:C:290:PRO:C	2.50	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:185:GLN:HB3	1:B:226:SER:CB	2.10	0.80
1:A:195:LEU:HD23	1:A:201:LEU:CD1	2.11	0.80
1:A:289:GLY:CA	1:A:290:PRO:C	2.50	0.80
1:B:289:GLY:CA	1:B:290:PRO:C	2.50	0.80
1:B:335:ASN:HD22	1:B:353:CYS:N	1.78	0.80
1:C:195:LEU:HD23	1:C:201:LEU:CD1	2.11	0.80
1:A:335:ASN:HD22	1:A:353:CYS:N	1.78	0.80
1:C:241:ILE:HD13	1:C:255:LEU:HD22	1.63	0.80
1:A:225:ASP:HB3	1:C:186:ASP:OD1	1.79	0.80
1:A:226:SER:HB3	1:C:185:GLN:C	2.06	0.80
1:C:104:THR:CG2	1:C:263:LEU:HD12	2.12	0.80
1:C:127:ILE:HG22	1:C:128:VAL:N	1.97	0.80
1:C:138:ASN:O	1:C:139:GLY:C	2.25	0.80
1:A:183:ASP:C	1:A:185:GLN:H	1.90	0.79
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:A:267:GLN:O	1:C:197:ASN:HB3	1.82	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:C:119:SER:HA	1:C:246:GLY:N	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:PHE:CD1	1:C:121:PHE:C	2.59	0.79
1:A:186:ASP:CA	1:B:226:SER:OG	2.29	0.79
1:C:82:VAL:C	1:C:170:THR:HG22	2.07	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:267:GLN:HB2	1:C:198:PHE:CD1	2.18	0.78
1:A:123:VAL:O	1:A:124:ASN:C	2.25	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:B:106:THR:C	1:B:107:SER:CA	2.56	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:183:ASP:C	1:C:185:GLN:H	1.91	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:H	1:A:167:LEU:CD2	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:HG2	1:C:266:PRO:O	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
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:A:267:GLN:NE2	1:C:198:PHE:CZ	2.53	0.77
1:A:329:THR:O	1:A:361:THR:HG22	1.85	0.77
1:B:328:ALA:HB1	1:B:362:VAL:HG22	1.64	0.77
1:C:335:ASN:ND2	1:C:353:CYS:HA	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:VAL:O	1:A:200:VAL:CG1	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:300:THR:O	1:B:366:VAL:O	2.03	0.77
1:B:316:GLY:O	1:B:349:TYR:N	2.17	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:A:151:ASN:CG	1:A:269:THR:OG1	2.27	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:317:GLY:CA	1:A:348:ASP:HA	2.13	0.76
1:A:320:CYS:HB2	1:A:366:VAL:HG12	1.67	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:A:123:VAL:C	1:A:125:GLY:N	2.41	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: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:A:268:PRO:C	1:A:269:THR:O	2.28	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:300:THR:O	1:C:366:VAL:O	2.03	0.76
1:C:320:CYS:HB2	1:C:366:VAL:HG12	1.67	0.76
1: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:183:ASP:CG	1:C:186:ASP:OD2	2.30	0.75
1:C:328:ALA:HB1	1:C:362:VAL:HG22	1.65	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:A:172:GLU:N	1:A:172:GLU:C	2.45	0.75
1:A:331:ALA:O	1:A:332:VAL:CG2	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:LEU:HB2	1:B:344:GLY:H	1.51	0.75
1:B:326:LEU:CB	1:B:337:ILE:CD1	2.65	0.75
1:C:82:VAL:C	1:C:170:THR:CG2	2.60	0.75
1:C:148:LEU:O	1:C:150:SER:N	2.18	0.75
1:C:167:LEU:H	1:C:167:LEU:CD2	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:98:ARG:O	1:C:100:SER:N	2.20	0.74
1:C:321:LEU:HB2	1:C:344:GLY:H	1.51	0.74
1:A:134:LEU:HD23	1:A:236:LEU:CD2	2.16	0.74
1:A:274[S]:SER:O	1:A:375:LEU:HA	1.87	0.74
1:C:168:CYS:CB	1:C:252:VAL:HG13	2.17	0.74
1:C:206:PRO:HB3	1:C:252:VAL:HG11	1.68	0.74
1:A:317:GLY:HA3	1:A:348:ASP:CA	2.13	0.74
1:C:74:VAL:O	1:C:75:GLY:C	2.30	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: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:C:110:GLU:CD	1:C:144:TRP:H	1.95	0.73
1:A:117:ASN:O	1:A:249:ALA:HA	1.88	0.73
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:121:PHE:C	1:B:121:PHE:CD1	2.65	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:A:351:LEU:C	1:A:351:LEU:CD1	2.61	0.73
1:A:134:LEU:HD13	1:A:239:LEU:HD11	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:98:ARG:HD2	1:C:105:VAL:HG23	1.69	0.73
1:C:114:GLN:NE2	1:C:251:ALA:HB2	2.02	0.73
1:C:157:PHE:CD2	1:C:261:VAL:HG22	2.23	0.73
1:B:295:LEU:HD23	1:B:295:LEU:H	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:267:GLN:CB	1:C:198:PHE:CD1	2.72	0.72
1:A:278:LEU:CD2	1:A:295:LEU:O	2.37	0.72
1:B:351:LEU:C	1:B:351:LEU:CD1	2.61	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:204:THR:C	1:B:205:ALA:O	2.22	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:C:351:LEU:C	1:C:351:LEU:CD1	2.61	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:67:ILE:O	1:C:68:ILE:O	2.08	0.72
1:C:266:PRO:O	1:C:266:PRO:CG	2.29	0.72
1:C:362:VAL:N	1:C:362:VAL:CB	2.52	0.72
1:A:226:SER:OG	1:C:183:ASP:OD2	2.08	0.72
1:B:165:VAL:O	1:B:166:PRO:HB3	1.88	0.72
1:C:131:SER:O	1:C:132:LEU:C	2.31	0.72
1:C:200:VAL:O	1:C:200:VAL:CG1	2.29	0.72
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: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:130:ASN:ND2	1:B:238:GLN:NE2	2.38	0.71
1:B:136:PRO:HB2	1:B:145:LEU:HD22	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:LEU:CD1	1:C:239:LEU:O	2.38	0.71
1:C:129:GLY:O	1:C:130:ASN:C	2.33	0.71
1:A:162:LEU:HD12	1:A:212:LEU:HD23	1.71	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:195:LEU:HD23	1:B:195:LEU:C	2.15	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:A:186:ASP:OD1	1:B:225:ASP:HB3	1.91	0.70
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: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:B:314:LEU:HD13	1:B:351:LEU:HD11	1.73	0.70
1:B:383:VAL:C	1:B:384:VAL:HG23	2.17	0.70
1:C:167:LEU:HD23	1:C:167:LEU:N	2.04	0.70
1:A:110:GLU:CD	1:A:144:TRP:CB	2.63	0.70
1:A:383:VAL:C	1:A:384:VAL:HG23	2.16	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:326:LEU:HD12	1:A:326:LEU:C	2.16	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:277:ARG:CB	1:C:285:ALA:CB	2.56	0.70
1:A:314:LEU:HD13	1:A:351:LEU:HD11	1.73	0.70
1:B:271:THR:HG21	1:B:288:THR:CG2	2.21	0.70
1:C:326:LEU:HD12	1:C:326:LEU:C	2.16	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:167:LEU:HD21	1:A:253:GLY:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLY:O	1:A:171:THR:N	2.21	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:266:PRO:O	1:C:199:GLY:N	2.25	0.69
1:A:340:ILE:O	1:A:347:SER:OG	2.09	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:117:ASN:O	1:C:249:ALA:HA	1.93	0.69
1:C:167:LEU:HD23	1:C:252:VAL:C	2.15	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:110:GLU:CD	1:B:144:TRP:HB3	2.18	0.69
1:B:111:TYR:CE2	1:B:254:GLU:HG3	2.27	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:C:314:LEU:HD13	1:C:351:LEU:HD11	1.73	0.69
1:C:383:VAL:C	1:C:384:VAL:HG23	2.17	0.69
1:A:338:LEU:HD23	1:A:338:LEU:C	2.18	0.69
1:C:98:ARG:CD	1:C:105:VAL:CG2	2.43	0.69
1:C:128:VAL:HG13	1:C:188:GLU:OE1	1.92	0.69
1:A:171:THR:C	1:A:172:GLU:CA	2.62	0.69
1:B:121:PHE:O	1:B:121:PHE:CD1	2.46	0.69
1:C:183:ASP:OD1	1:C:232:LYS:HE2	1.93	0.69
1:B:103:VAL:HG13	1:B:264:TYR:HA	1.75	0.69
1:B:169:GLY:O	1:B:171:THR:N	2.22	0.69
1:A:104:THR:HG21	1:A:263:LEU:CD1	2.22	0.68
1:B:326:LEU:HD12	1:B:326:LEU:C	2.16	0.68
1:B:338:LEU:HD23	1:B:338:LEU:C	2.18	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:338:LEU:HD23	1:C:338:LEU:C	2.18	0.68
1:C:103:VAL:HG12	1:C:263:LEU:O	1.92	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:274[S]:SER:O	1:C:375:LEU:CA	2.41	0.68
1:C:297:ARG:HG2	1:C:298:THR:N	2.08	0.68
1:B:337:ILE:HG23	1:B:337:ILE:O	1.91	0.68
1:C:164:TYR:HB3	1:C:210:ALA:HB3	1.76	0.68
1: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: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:222:TYR:O	1:B:234:ILE:HG23	1.95	0.67
1:B:230:ASP:O	1:B:232:LYS:N	2.26	0.67
1:A: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: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: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:A:342:ASN:CG	1:A:345:THR:HB	2.20	0.67
1:B:130:ASN:ND2	1:B:238:GLN:CD	2.53	0.67
1:C:89:VAL:HG12	1:C:90:GLY:H	1.54	0.67
1:C:221:ARG:HH11	1:C:236:LEU:HA	1.60	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:A:201:LEU:C	1:A:201:LEU:CD2	2.61	0.67
1:C:145:LEU:CB	1:C:146:PRO:HD3	2.16	0.67
1:B:201:LEU:C	1:B:201:LEU:CD2	2.61	0.67
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:267:GLN:HG3	1:A:268:PRO:N	2.05	0.66
1:C:100:SER:OG	1:C:101:GLY:N	2.26	0.66
1:C:110:GLU:O	1:C:257:LEU:HB3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:195:LEU:HD23	1:A:195:LEU:C	2.21	0.66
1:C:195:LEU:HD23	1:C:195:LEU:C	2.21	0.66
1:C:206:PRO:HG2	1:C:207:TRP:CD1	2.29	0.66
1:A:104:THR:HG23	1:A:263:LEU:CD1	2.23	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: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:183:ASP:CG	1:A:186:ASP:OD2	2.38	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:C:110:GLU:OE1	1:C:142:PHE:C	2.38	0.65
1:A:300:THR:C	1:A:369:VAL:CG2	2.69	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:B:107:SER:N	1:B:107:SER:C	2.52	0.65
1:C:300:THR:C	1:C:369:VAL:CG2	2.70	0.65
1:C:99:THR:HG22	1:C:99:THR:O	1.97	0.65
1:A:180:PHE:C	1:A:180:PHE:CD2	2.74	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:88:LEU:CD1	1:C:256:PHE:CE2	2.80	0.65
1:C:179:TYR:CZ	1:C:240:GLY:HA3	2.32	0.65
1:A:226:SER:CB	1:C:185:GLN:CB	2.74	0.65
1:B:145:LEU:O	1:B:145:LEU:HD23	1.97	0.65
1:A:138:ASN:O	1:A:141:LEU:N	2.29	0.65
1:A:183:ASP:OD1	1:A:232:LYS:HE2	1.96	0.65
1:C:321:LEU:C	1:C:322:THR:HG1	2.05	0.65
1:A:111:TYR:HE2	1:A:254:GLU:OE2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:THR:C	1:B:369:VAL:CG2	2.69	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:C:67:ILE:O	1:C:68:ILE:C	2.40	0.64
1:A:122:VAL:HG13	1:A:126:GLY:HA3	1.79	0.64
1:A:150:SER:O	1:A:269:THR:CA	2.45	0.64
1:B:122:VAL:HG12	1:B:123:VAL:N	2.11	0.64
1:C:201:LEU:CD2	1:C:202:LYS:N	2.57	0.64
1:A:108:HIS:O	1:A:259:ARG:N	2.28	0.64
1:A:180:PHE:HD2	1:A:180:PHE:O	1.79	0.64
1:B:112:LEU:CD2	1:B:113:THR:HG22	2.27	0.64
1:B:121:PHE:O	1:B:122:VAL:HA	1.97	0.64
1:B:148:LEU:C	1:B:150:SER:H	2.06	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:A:267:GLN:CD	1:C:198:PHE:HE1	2.04	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:C:138:ASN:C	1:C:140:THR:H	2.03	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:103:VAL:CG1	1:C:263:LEU:C	2.71	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:145:LEU:O	1:B:146:PRO:C	2.41	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
1:C:275[S]:SER:HA	1:C:375:LEU:CD2	2.21	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:SER:O	1:C:284:LEU:HG	1.98	0.63
1:A:180:PHE:CD2	1:A:180:PHE:O	2.51	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:C:331:ALA:C	1:C:332:VAL:HG23	2.24	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:A:331:ALA:C	1:A:332:VAL:HG23	2.24	0.63
1:C:342:ASN:O	1:C:343:VAL:O	2.16	0.63
1:B:331:ALA:C	1:B:332:VAL:HG23	2.24	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:164:TYR:CD2	1:A:255:LEU:HD12	2.31	0.63
1:B:295:LEU:HD23	1:B:295:LEU:N	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:167:LEU:CD2	1:A:252:VAL:C	2.72	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:C:342:ASN:CG	1:C:345:THR:HB	2.20	0.62
1:C:127:ILE:CD1	1:C:358:LEU:HD13	2.29	0.62
1:C:214:ILE:HD11	1:C:239:LEU:HD21	1.81	0.62
1:A:321:LEU:HD23	1:A:321:LEU:N	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:N	1:B:122:VAL:CB	2.60	0.62
1:B:342:ASN:CG	1:B:345:THR:HB	2.20	0.62
1:C:98:ARG:C	1:C:100:SER:H	2.07	0.62
1:C:103:VAL:HG12	1:C:263:LEU:C	2.24	0.62
1:C:314:LEU:HD13	1:C:351:LEU:CD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:LEU:HD21	1:B:234:ILE:HG12	1.82	0.62
1:B:180:PHE:HB3	1:B:200:VAL:HG11	1.82	0.62
1:C:110:GLU:OE1	1:C:144:TRP:N	2.23	0.62
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:A:167:LEU:HD21	1:A:252:VAL:C	2.25	0.61
1:B:342:ASN:O	1:B:343:VAL:O	2.16	0.61
1:C:162:LEU:N	1:C:212:LEU:O	2.29	0.61
1:A:123:VAL:HG12	1:A:124:ASN:HD22	1.63	0.61
1:C:222:TYR:O	1:C:234:ILE:HG23	1.99	0.61
1: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:C:190:ALA:HB3	1:C:194:GLU:CD	2.23	0.61
1:A:108:HIS:CG	1:A:109:ARG:H	2.18	0.61
1:A:111:TYR:HE2	1:A:254:GLU:CD	2.08	0.61
1:B:300:THR:C	1:B:369:VAL:HG23	2.26	0.61
1:C:300:THR:C	1:C:369:VAL:HG23	2.26	0.61
1:A:160:VAL:HA	1:A:258:ALA:O	2.01	0.61
1:A:271:THR:O	1:A:271:THR:CG2	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: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:326:LEU:CB	1:C:337:ILE:HD12	2.28	0.61
1:C:103:VAL:CG1	1:C:263:LEU:O	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:THR:CG2	1:C:205:ALA:O	2.40	0.60
1:A:162:LEU:HD13	1:A:178:LEU:CD1	2.25	0.60
1:B:277:ARG:CB	1:B:285:ALA:CB	2.56	0.60
1:A:114:GLN:NE2	1:A:251:ALA:HB2	2.16	0.60
1:A:226:SER:OG	1:C:185:GLN:HB2	2.00	0.60
1:A:329:THR:N	1:A:361:THR:HG23	2.16	0.60
1:B:160:VAL:HB	1:B:214:ILE:HB	1.83	0.60
1:B:351:LEU:CD1	1:B:352:ASN:N	2.64	0.60
1:C:180:PHE:C	1:C:180:PHE:CD2	2.79	0.60
1:A:114:GLN:HE21	1:A:251:ALA:CB	2.13	0.60
1:A:300:THR:C	1:A:369:VAL:HG23	2.26	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:186:ASP:CA	1:B:226:SER:HG	2.14	0.60
1:A:301:VAL:N	1:A:369:VAL:HG21	2.17	0.60
1:C:70:HIS:HB3	1:C:79:MET:CE	2.32	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: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: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:130:ASN:O	1:A:131:SER:C	2.45	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: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:383:VAL:O	1:C:384:VAL:HG22	2.02	0.59
1:A:274[P]:SER:O	1:A:376:VAL:N	2.36	0.59
1:A:349:TYR:CD2	1:A:349:TYR:O	2.56	0.59
1:B:318:LEU:O	1:B:347:SER:N	2.29	0.59
1:C:155:TYR:OH	1:C:221:ARG:HD2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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:B:329:THR:C	1:B:361:THR:HG22	2.25	0.59
1:A:128:VAL:HG12	1:A:129:GLY:H	1.65	0.59
1:C:349:TYR:O	1:C:349:TYR:CD2	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: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:A:204:THR:C	1:A:205:ALA:O	2.41	0.59
1:C:70:HIS:CB	1:C:79:MET:HE3	2.33	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:180:PHE:C	1:B:180:PHE:CD2	2.81	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:C:267:GLN:O	1:C:268:PRO:C	2.46	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:183:ASP:C	1:C:185:GLN:N	2.56	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:C:329:THR:C	1:C:361:THR:HG22	2.24	0.58
1:C:114:GLN:NE2	1:C:251:ALA:CB	2.66	0.58
1:B:138:ASN:O	1:B:139:GLY:C	2.44	0.58
1:C:103:VAL:HG11	1:C:264:TYR:N	2.18	0.58
1:C:318:LEU:O	1:C:347:SER:N	2.29	0.58
1:A:116:ASN:HA	1:A:250:ASP:O	2.03	0.58
1:A:280:LEU:HA	1:A:370:ALA:O	2.04	0.58
1:A:329:THR:C	1:A:361:THR:HG22	2.25	0.58
1:C:274[P]:SER:N	1:C:376:VAL:O	2.29	0.58
1:C:289:GLY:HA3	1:C:290:PRO:C	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:CYS:HG	1:A:252:VAL:CG1	2.14	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
1:B:280:LEU:CA	1:B:370:ALA:O	2.52	0.57
1:B:329:THR:N	1:B:361:THR:HG23	2.16	0.57
1:B:336:ASP:O	1:B:351:LEU:CA	2.45	0.57
1: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:C:341:ASP:OD1	1:C:347:SER:HB2	2.04	0.57
1:A:186:ASP:N	1:B:226:SER:HG	1.99	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:280:LEU:HA	1:C:370:ALA:O	2.04	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: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: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:82:VAL:CA	1:C:170:THR:HG21	2.35	0.57
1:C:336:ASP:O	1:C:351:LEU:CA	2.45	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
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:B:185:GLN:C	1:B:186:ASP:O	2.46	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:VAL:O	1:C:75:GLY:O	2.23	0.57
1:C:383:VAL:C	1:C:384:VAL:CG2	2.77	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:289:GLY:HA3	1:B:290:PRO:C	2.28	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:A:289:GLY:HA3	1:A:290:PRO:C	2.28	0.56
1:C:274[P]:SER:O	1:C:376:VAL:N	2.36	0.56
1:A:134:LEU:HD13	1:A:239:LEU:CD1	2.35	0.56
1:A:185:GLN:CB	1:B:226:SER:CB	2.81	0.56
1:A:317:GLY:HA3	1:A:347:SER:O	2.06	0.56
1:A:342:ASN:HD21	1:A:345:THR:C	2.13	0.56
1:B:341:ASP:OD1	1:B:347:SER:HB2	2.04	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: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:A:383:VAL:C	1:A:384:VAL:CG2	2.77	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: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:B:341:ASP:OD1	1:B:347:SER:OG	2.22	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:C:342:ASN:HD21	1:C:345:THR:C	2.13	0.56
1:A:265:PHE:N	1:A:265:PHE:CD1	2.73	0.56
1:A:326:LEU:HB2	1:A:337:ILE:HD12	1.85	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:328:ALA:HB1	1:B:361:THR:O	2.06	0.56
1:C:341:ASP:OD1	1:C:347:SER:OG	2.22	0.56
1:A:110:GLU:CG	1:A:144:TRP:HB3	2.35	0.56
1:A:141:LEU:HD12	1:A:141:LEU:O	2.05	0.56
1:A:190:ALA:HB3	1:A:194:GLU:CD	2.28	0.56
1:C:180:PHE:CD2	1:C:180:PHE:O	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:342:ASN:HD21	1:B:345:THR:C	2.13	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:C:82:VAL:C	1:C:170:THR:HG21	2.32	0.55
1:A:328:ALA:HB1	1:A:361:THR:O	2.06	0.55
1:B:138:ASN:C	1:B:140:THR:N	2.60	0.55
1:B:265:PHE:CD1	1:B:265:PHE:N	2.74	0.55
1:C:130:ASN:ND2	1:C:238:GLN:OE1	2.38	0.55
1:C:170:THR:O	1:C:170:THR:OG1	2.24	0.55
1:C:223:CYS:CA	1:C:224:ASN:N	2.62	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:A:267:GLN:CA	1:C:198:PHE:HA	2.36	0.55
1:B:110:GLU:CD	1:B:144:TRP:CB	2.79	0.55
1:C:133:GLN:HB2	1:C:138:ASN:ND2	2.21	0.55
1:C:162:LEU:CD1	1:C:178:LEU:HD13	2.32	0.55
1:B:111:TYR:CE2	1:B:254:GLU:CG	2.89	0.55
1:A:145:LEU:HD23	1:A:145:LEU:C	2.32	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:168:CYS:HG	1:A:252:VAL:HG13	1.68	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:A:297:ARG:HG2	1:A:298:THR:C	2.32	0.55
1:B:383:VAL:C	1:B:384:VAL:CG2	2.77	0.55
1:C:91:SER:OG	1:C:108:HIS:CD2	2.60	0.55
1:C:138:ASN:O	1:C:140:THR:C	2.50	0.55
1:C:185:GLN:C	1:C:186:ASP:O	2.46	0.55
1:B:152:PHE:CE2	1:B:263:LEU:HB3	2.41	0.54
1:B:297:ARG:HG2	1:B:298:THR:C	2.32	0.54
1:C:232:LYS:HG3	1:C:233:LEU:N	2.22	0.54
1:C:201:LEU:C	1:C:201:LEU:CD2	2.61	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:B:297:ARG:CG	1:B:298:THR:N	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PHE:C	1:A:121:PHE:CD1	2.84	0.54
1:A:319:ARG:HA	1:A:346:ALA:HA	1.90	0.54
1:A:331:ALA:O	1:A:332:VAL:HG22	2.07	0.54
1:B:152:PHE:CE1	1:B:263:LEU:CD1	2.78	0.54
1:A:228:THR:CG2	1:C:232:LYS:CE	2.85	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
1:B:138:ASN:OD1	1:B:140:THR:HB	2.08	0.54
1:B:296:THR:HG1	1:B:303:THR:HB	1.72	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:C:331:ALA:O	1:C:332:VAL:HG22	2.07	0.54
1:A:274[P]:SER:N	1:A:376:VAL:O	2.30	0.54
1:A:326:LEU:HD21	1:A:334:ILE:HD13	1.90	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:297:ARG:CG	1:C:298:THR:N	2.70	0.54
1:B:110:GLU:CD	1:B:144:TRP:H	2.06	0.54
1:B:180:PHE:O	1:B:180:PHE:HD2	1.91	0.54
1:B:216:THR:HG22	1:B:217:ASP:O	2.07	0.54
1:B:274[P]:SER:N	1:B:376:VAL:O	2.30	0.54
1:B:326:LEU:HD21	1:B:334:ILE:HD13	1.90	0.54
1:C:297:ARG:HG2	1:C:298:THR:C	2.32	0.54
1:A:183:ASP:HB2	1:B:153:ASP:OD2	2.08	0.54
1:B:124:ASN:OD1	1:B:132:LEU:HD12	2.07	0.54
1: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:A:150:SER:C	1:A:269:THR:HA	2.32	0.53
1:B:164:TYR:HE2	1:B:253:GLY:HA3	1.73	0.53
1:B:192:ARG:CD	1:B:192:ARG:N	2.71	0.53
1:C:274[S]:SER:CB	1:C:376:VAL:O	2.56	0.53
1:A:180:PHE:HD1	1:A:214:ILE:HD12	1.72	0.53
1:A:228:THR:HA	1:C:230:ASP:OD1	2.09	0.53
1:A:267:GLN:CD	1:A:268:PRO:HD2	2.16	0.53
1:A:311:THR:CG2	1:A:379:ALA:O	2.50	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:C:275[S]:SER:N	1:C:375:LEU:HD23	2.23	0.53
1:C:319:ARG:HA	1:C:346:ALA:HA	1.90	0.53
1:A:108:HIS:CG	1:A:109:ARG:N	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LYS:HG3	1:B:233:LEU:H	1.71	0.53
1:C:300:THR:CB	1:C:301:VAL:HG23	2.39	0.53
1:C:380:ARG:C	1:C:382:ASN:H	2.16	0.53
1:A:201:LEU:CD2	1:A:203:GLU:HG2	2.25	0.53
1:A:232:LYS:HG3	1:A:233:LEU:N	2.23	0.53
1:B:111:TYR:HE2	1:B:254:GLU:HG3	1.72	0.53
1:B:204:THR:O	1:B:205:ALA:O	2.26	0.53
1:A:141:LEU:HD12	1:A:141:LEU:C	2.33	0.53
1:A:150:SER:O	1:A:270:ASN:N	2.42	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:A:380:ARG:C	1:A:382:ASN:H	2.16	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:B:338:LEU:C	1:B:338:LEU:CD2	2.82	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:C:132:LEU:O	1:C:133:GLN:C	2.52	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:C:118:SER:C	1:C:120:GLY:N	2.64	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:132:LEU:O	1:B:133:GLN:C	2.52	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:B:380:ARG:C	1:B:382:ASN:H	2.16	0.52
1:C:214:ILE:CG2	1:C:215:PRO:N	2.71	0.52
1:A:309:THR:CG2	1:A:355:VAL:O	2.56	0.52
1:A:328:ALA:HB2	1:A:362:VAL:CG2	2.34	0.52
1:B:351:LEU:HD12	1:B:352:ASN:N	2.25	0.52
1:C:311:THR:HG21	1:C:380:ARG:C	2.35	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:B:311:THR:HG21	1:B:380:ARG:C	2.35	0.52
1:C:326:LEU:HD21	1:C:334:ILE:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:LEU:C	1:C:338:LEU:CD2	2.82	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:A:311:THR:HG21	1:A:380:ARG:C	2.35	0.52
1:A:338:LEU:C	1:A:338:LEU:CD2	2.82	0.52
1:C:112:LEU:HG	1:C:141:LEU:HD11	1.90	0.52
1:C:133:GLN:HE21	1:C:184:SER:HG	1.55	0.52
1:C:297:ARG:HE	1:C:299:PRO:CA	2.22	0.52
1:A:288:THR:C	1:A:289:GLY:O	2.50	0.52
1:B:274[S]:SER:H	1:B:376:VAL:C	2.18	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: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
1:A:276:LYS:O	1:A:374:LEU:HD23	2.10	0.52
1:B:331:ALA:O	1:B:332:VAL:HG22	2.07	0.52
1:C:288:THR:C	1:C:289:GLY:O	2.50	0.52
1:A:195:LEU:HD23	1:A:201:LEU:HD12	1.91	0.52
1:B:335:ASN:HD22	1:B:353:CYS:C	1.96	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:B:331:ALA:C	1:B:332:VAL:CG2	2.83	0.52
1:A:267:GLN:HB3	1:C:198:PHE:CD1	2.45	0.52
1:B:162:LEU:HB2	1:B:212:LEU:HB3	1.92	0.52
1:C:133:GLN:C	1:C:138:ASN:HD22	2.04	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:A:111:TYR:CE2	1:A:254:GLU:CD	2.88	0.51
1:B:121:PHE:CD2	1:B:192:ARG:HD2	2.45	0.51
1:C:68:ILE:CG2	1:C:70:HIS:HD2	2.06	0.51
1:A:111:TYR:OH	1:A:254:GLU:OE2	2.22	0.51
1:A:172:GLU:N	1:A:172:GLU:CB	2.68	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:B:288:THR:C	1:B:289:GLY:O	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:VAL:HA	1:B:209:GLU:HG3	1.92	0.51
1:C:115:VAL:CG2	1:C:241:ILE:HG21	2.41	0.51
1:C:201:LEU:CD2	1:C:203:GLU:HG2	2.29	0.51
1:A:226:SER:OG	1:C:185:GLN:CB	2.59	0.51
1:B:230:ASP:C	1:B:232:LYS:H	2.19	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: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:114:GLN:HE21	1:B:251:ALA:HB2	1.76	0.50
1:B:135:ASN:HB2	1:B:235:ASP:OD1	2.11	0.50
1:B:221:ARG:HD3	1:B:234:ILE:O	2.06	0.50
1:B: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
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:331:ALA:C	1:A:332:VAL:CG2	2.83	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:C:331:ALA:C	1:C:332:VAL:CG2	2.83	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:A:157:PHE:HD1	1:A:236:LEU:HD22	1.75	0.50
1:A:321:LEU:C	1:A:322:THR:OG1	2.54	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: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:C:135:ASN:ND2	1:C:224:ASN:OD1	2.45	0.50
1:A:135:ASN:ND2	1:A:224:ASN:OD1	2.45	0.50
1:A:185:GLN:C	1:A:186:ASP:O	2.51	0.50
1:A:259:ARG:HG2	1:A:261:VAL:HG23	1.94	0.50
1:B:111:TYR:HE2	1:B:254:GLU:CG	2.25	0.50
1:B:112:LEU:CD1	1:B:141:LEU:HD11	2.41	0.50
1:B:122:VAL:N	1:B:122:VAL:C	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:ARG:HB2	1:C:382:ASN:OD1	2.11	0.50
1:A:158:ASN:HB2	1:A:260:SER:HG	1.77	0.50
1:A:128:VAL:CG1	1:A:129:GLY:H	2.25	0.49
1:B:192:ARG:N	1:B:192:ARG:HD2	2.27	0.49
1:B:297:ARG:NE	1:B:299:PRO:HA	2.22	0.49
1:B:345:THR:O	1:B:346:ALA:C	2.55	0.49
1:B:385:ASN:OD1	1:B:385:ASN:C	2.55	0.49
1:A:118:SER:O	1:A:246:GLY:HA3	2.12	0.49
1:A:345:THR:O	1:A:346:ALA:C	2.55	0.49
1:B:158:ASN:HB2	1:B:260:SER:OG	2.12	0.49
1:C:89:VAL:HG13	1:C:90:GLY:H	1.77	0.49
1:C:118:SER:HB2	1:C:122:VAL:HG23	1.94	0.49
1:A:214:ILE:CG2	1:A:215:PRO:N	2.71	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
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:C:345:THR:O	1:C:346:ALA:C	2.55	0.49
1:B:140:THR:HG23	1:B:307:ARG:O	2.12	0.49
1:B:177:ALA:HB1	1:B:203:GLU:OE1	2.13	0.49
1:B:181:ASP:OD1	1:B:183:ASP:N	2.43	0.49
1:A:230:ASP:C	1:A:232:LYS:H	2.20	0.49
1:A:270:ASN:C	1:A:271:THR:OG1	2.54	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:385:ASN:OD1	1:C:385:ASN:C	2.55	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:321:LEU:C	1:B:322:THR:OG1	2.54	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:385:ASN:OD1	1:A:385:ASN:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:274[S]:SER:O	1:A:375:LEU:HD23	2.13	0.48
1:A:300:THR:C	1:A:369:VAL:HG21	2.38	0.48
1:B:103:VAL:CG1	1:B:264:TYR:HA	2.42	0.48
1:C:103:VAL:HG11	1:C:263:LEU:C	2.38	0.48
1:C:108:HIS:CG	1:C:109:ARG:H	2.31	0.48
1:C:336:ASP:CG	1:C:385:ASN:HB2	2.38	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:230:ASP:C	1:A:232:LYS:N	2.71	0.48
1:A:303:THR:HG22	1:A:305:THR:OG1	2.12	0.48
1:A:353:CYS:C	1:A:354:THR:HG1	2.21	0.48
1:B:292:TYR:HB3	1:B:308:ALA:CB	2.43	0.48
1:C:69:THR:O	1:C:70:HIS:C	2.56	0.48
1:C:303:THR:HG22	1:C:305:THR:OG1	2.12	0.48
1:A:274[S]:SER:O	1:A:375:LEU:CA	2.59	0.48
1:A:274[S]:SER:O	1:A:376:VAL:N	2.44	0.48
1:B:155:TYR:CZ	1:B:221:ARG:HB3	2.49	0.48
1:C:184:SER:HB2	1:C:235:ASP:HB2	1.95	0.48
1:A:136:PRO:HB2	1:A:145:LEU:CD2	2.41	0.48
1:B:181:ASP:HB3	1:B:238:GLN:HB3	1.95	0.48
1:C:112:LEU:C	1:C:112:LEU:HD23	2.39	0.48
1:C:145:LEU:HB3	1:C:146:PRO:HD2	1.91	0.48
1:C:230:ASP:C	1:C:232:LYS:N	2.71	0.48
1:C:351:LEU:HD12	1:C:352:ASN:N	2.24	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:230:ASP:C	1:C:232:LYS:H	2.21	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:B:112:LEU:HD23	1:B:112:LEU:C	2.38	0.48
1:A:335:ASN:CG	1:A:352:ASN:ND2	2.72	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:A:336:ASP:CG	1:A:385:ASN:HB2	2.38	0.48
1:B:179:TYR:CD1	1:B:240:GLY:HA3	2.49	0.48
1:B:335:ASN:CG	1:B:352:ASN:ND2	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:GLN:HB2	1:C:198:PHE:CG	2.47	0.48
1:C:177:ALA:HB3	1:C:195:LEU:HD11	1.95	0.48
1: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:B:336:ASP:CG	1:B:385:ASN:HB2	2.38	0.47
1:C:131:SER:O	1:C:133:GLN:HB2	2.14	0.47
1:C:321:LEU:C	1:C:322:THR:OG1	2.54	0.47
1:A:228:THR:HG23	1:C:232:LYS:HE3	1.96	0.47
1:B:145:LEU:HB2	1:B:259:ARG:CZ	2.44	0.47
1:B:264:TYR:O	1:B:265:PHE:C	2.57	0.47
1:B:300:THR:C	1:B:369:VAL:HG21	2.38	0.47
1:C:111:TYR:CD2	1:C:256:PHE:CE1	2.98	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:122:VAL:HG12	1:A:123:VAL:N	2.28	0.47
1:A:152:PHE:HD2	1:A:264:TYR:C	2.04	0.47
1:A:155:TYR:CZ	1:A:221:ARG:HB3	2.49	0.47
1:A:292:TYR:HB3	1:A:308:ALA:CB	2.43	0.47
1:B:130:ASN:ND2	1:B:238:GLN:OE1	2.47	0.47
1:B:173:VAL:O	1:B:246:GLY:HA2	2.14	0.47
1:B:230:ASP:C	1:B:232:LYS:N	2.71	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:A:226:SER:CB	1:C:185:GLN:C	2.82	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:204:THR:O	1:B:205:ALA:C	2.58	0.47
1:C:70:HIS:CB	1:C:79:MET:CE	2.92	0.47
1:C:278:LEU:HG	1:C:295:LEU:O	2.14	0.47
1:A:112:LEU:HD22	1:A:113:THR:HG22	1.95	0.47
1:A:180:PHE:CD1	1:A:214:ILE:HD12	2.49	0.47
1:A:264:TYR:O	1:A:265:PHE:C	2.57	0.47
1:A:278:LEU:HG	1:A:295:LEU:O	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:THR:C	1:B:172:GLU:O	2.46	0.47
1:B:179:TYR:CZ	1:B:240:GLY:HA3	2.49	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:B:358:LEU:HA	1:B:359:PRO:HA	1.61	0.47
1:C:70:HIS:HB3	1:C:79:MET:HE3	1.95	0.47
1:C:108:HIS:CG	1:C:109:ARG:N	2.82	0.47
1:C:137:SER:HB3	1:C:146:PRO:HG3	1.96	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:232:LYS:HG3	1:C:233:LEU:H	1.80	0.47
1:C:264:TYR:O	1:C:265:PHE:C	2.57	0.47
1:C:277:ARG:HB3	1:C:285:ALA:HB2	1.89	0.47
1:C:334:ILE:HG22	1:C:335:ASN:N	2.29	0.47
1:A:128:VAL:CG1	1:A:129:GLY:N	2.73	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:278:LEU:HG	1:B:295:LEU:O	2.14	0.47
1:B:288:THR:O	1:B:289:GLY:O	2.33	0.47
1:C:84:VAL:CG1	1:C:85:SER:N	2.78	0.47
1:C:288:THR:O	1:C:289:GLY:O	2.33	0.47
1:B:123:VAL:O	1:B:124:ASN:C	2.57	0.47
1:B:134:LEU:HD23	1:B:236:LEU:HD23	1.96	0.47
1:B:142:PHE:O	1:B:146:PRO:HG2	2.15	0.47
1:B:289:GLY:HA3	1:B:290:PRO:O	1.99	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:A:129:GLY:O	1:A:130:ASN:C	2.57	0.47
1:C:100:SER:O	1:C:103:VAL:N	2.39	0.47
1:C:119:SER:O	1:C:245:GLY:N	2.45	0.47
1:C:222:TYR:O	1:C:234:ILE:HG21	2.14	0.47
1:A:145:LEU:H	1:A:259:ARG:NH2	2.10	0.46
1:A:108:HIS:O	1:A:259:ARG:CB	2.63	0.46
1:A:132:LEU:O	1:A:133:GLN:C	2.58	0.46
1:A:201:LEU:CG	1:A:202:LYS:N	2.78	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:B:298:THR:O	1:B:299:PRO:C	2.58	0.46
1:C:177:ALA:CB	1:C:195:LEU:HD11	2.44	0.46
1:B:146:PRO:O	1:B:150:SER:OG	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:LEU:O	1:C:146:PRO:C	2.59	0.46
1:C:289:GLY:HA3	1:C:290:PRO:O	1.99	0.46
1:C:300:THR:C	1:C:369:VAL:HG21	2.38	0.46
1:A:117:ASN:N	1:A:250:ASP:O	2.40	0.46
1:A:228:THR:CG2	1:C:232:LYS:HE3	2.46	0.46
1:A:297:ARG:HE	1:A:299:PRO:CA	2.22	0.46
1:A:298:THR:O	1:A:299:PRO:C	2.58	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:A:169:GLY:C	1:A:171:THR:H	2.18	0.46
1:B:129:GLY:O	1:B:130:ASN:C	2.58	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:B:326:LEU:C	1:B:326:LEU:CD1	2.84	0.46
1:C:91:SER:HB3	1:C:109:ARG:NH2	2.31	0.46
1:A:295:LEU:CD2	1:A:295:LEU:N	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:C	1:B:195:LEU:CD2	2.88	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:A:289:GLY:HA3	1:A:290:PRO:O	1.99	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
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:195:LEU:HD23	1:B:196:ALA:N	2.31	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:278:LEU:HD11	1:C:296:THR:C	2.41	0.46
1:A:150:SER:O	1:A:269:THR:C	2.59	0.45
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:O	1:A:321:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LEU:C	1:B:150:SER:N	2.73	0.45
1:B:152:PHE:CD1	1:B:263:LEU:HB3	2.49	0.45
1:B:321:LEU:N	1:B:321:LEU:CD2	2.77	0.45
1:C:181:ASP:OD1	1:C:183:ASP:N	2.46	0.45
1:A:117:ASN:CB	1:A:248:GLY:O	2.61	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: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:C:123:VAL:O	1:C:124:ASN:C	2.58	0.45
1:C:321:LEU:O	1:C:321:LEU:HG	2.16	0.45
1:A:112:LEU:HD23	1:A:112:LEU:C	2.41	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:222:TYR:OH	1:C:182:LYS:HG3	2.17	0.45
1:C:70:HIS:HB2	1:C:79:MET:HE3	1.98	0.45
1:C:111:TYR:HD2	1:C:256:PHE:CZ	2.34	0.45
1:C:169:GLY:C	1:C:171:THR:H	2.19	0.45
1:A:110:GLU:OE1	1:A:144:TRP:CB	2.65	0.45
1:A:278:LEU:HD11	1:A:296:THR:C	2.41	0.45
1:B:314:LEU:HB2	1:B:351:LEU:HD12	1.99	0.45
1:A:278:LEU:HB2	1:A:372:GLY:HA3	1.98	0.45
1:A:314:LEU:HB2	1:A:351:LEU:HD12	1.99	0.45
1:B:195:LEU:CD2	1:B:201:LEU:CD1	2.94	0.45
1:B:278:LEU:HD11	1:B:296:THR:C	2.41	0.45
1:B:321:LEU:CB	1:B:344:GLY:H	2.26	0.45
1:C:133:GLN:C	1:C:138:ASN:ND2	2.68	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:C:69:THR:O	1:C:70:HIS:O	2.35	0.45
1:C:308:ALA:HB1	1:C:312:PHE:HZ	1.81	0.45
1:A:297:ARG:HG2	1:A:298:THR:CA	2.47	0.45
1:B:278:LEU:HB2	1:B:372:GLY:HA3	1.98	0.45
1:A:111:TYR:CD1	1:A:112:LEU:N	2.85	0.45
1:A:124:ASN:OD1	1:A:132:LEU:HD11	2.17	0.45
1:B:181:ASP:O	1:B:238:GLN:N	2.49	0.45
1:C:137:SER:HB3	1:C:146:PRO:CB	2.47	0.45
1:C:335:ASN:CG	1:C:352:ASN:ND2	2.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:GLU:OE2	1:B:144:TRP:HB3	2.17	0.44
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:99:THR:O	1:C:99:THR:CG2	2.64	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: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:185:GLN:O	1:B:186:ASP:C	2.60	0.44
1:B:192:ARG:HG3	1:B:192:ARG:HH11	1.82	0.44
1:B:331:ALA:HB2	1:B:357:SER:OG	1.95	0.44
1:C:74:VAL:C	1:C:75:GLY:O	2.57	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:380:ARG:C	1:C:382:ASN:N	2.75	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:O	1:A:337:ILE:CG2	2.64	0.44
1:B:122:VAL:HG12	1:B:123:VAL:O	2.17	0.44
1:B:169:GLY:C	1:B:171:THR:H	2.20	0.44
1:B:184:SER:HB2	1:B:235:ASP:HB2	1.99	0.44
1:B:231:GLN:H	1:B:231:GLN:HG3	1.55	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:C:298:THR:O	1:C:299:PRO:C	2.58	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:380:ARG:C	1:A:382:ASN:N	2.75	0.44
1:A:384:VAL:HG12	1:A:384:VAL:O	2.17	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:337:ILE:O	1:B:337:ILE:CG2	2.64	0.44
1:B:380:ARG:C	1:B:382:ASN:N	2.75	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
1:A:292:TYR:HB3	1:A:308:ALA:HB2	2.00	0.44
1:B:184:SER:CB	1:B:235:ASP:HB2	2.48	0.44
1:B:154:GLN:HB2	1:B:264:TYR:HB2	2.00	0.44
1:B:183:ASP:C	1:B:185:GLN:N	2.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:LEU:CD2	1:B:366:VAL:HG21	1.96	0.44
1:C:104:THR:CG2	1:C:263:LEU:HB2	2.44	0.44
1:C:111:TYR:HB2	1:C:256:PHE:CE1	2.52	0.44
1:B:110:GLU:O	1:B:257:LEU:N	2.51	0.44
1:B:144:TRP:HE3	1:B:259:ARG:HH12	1.66	0.44
1:B:153:ASP:OD1	1:B:222:TYR:CD1	2.71	0.44
1:C:81:PRO:O	1:C:170:THR:CG2	2.55	0.44
1:C:357:SER:O	1:C:358:LEU:HG	2.18	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:103:VAL:HG11	1:C:264:TYR:C	2.42	0.44
1:C:292:TYR:HB3	1:C:308:ALA:HB2	2.00	0.44
1:A:111:TYR:HA	1:A:256:PHE:CD1	2.52	0.44
1:A:232:LYS:HG3	1:A:233:LEU:H	1.81	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:257:LEU:HD13	1:B:257:LEU:C	2.42	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:B:151:ASN:C	1:B:267:GLN:HB2	2.43	0.43
1:C:185:GLN:O	1:C:186:ASP:C	2.60	0.43
1:C:231:GLN:H	1:C:231:GLN:HG3	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:A:118:SER:HB2	1:A:120:GLY:H	1.84	0.43
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:145:LEU:O	1:B:147:ALA:N	2.51	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:C:300:THR:C	1:C:301:VAL:HG23	2.44	0.43
1:C:321:LEU:HB3	1:C:344:GLY:C	2.44	0.43
1:A:186:ASP:HA	1:B:226:SER:HG	1.82	0.43
1:A:278:LEU:HD23	1:A:283:SER:O	2.19	0.43
1:A:279:ASP:OD2	1:A:282:GLY:HA3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LEU:HB3	1:A:344:GLY:C	2.44	0.43
1:B:195:LEU:HD23	1:B:201:LEU:CD1	2.47	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:O	1:C:384:VAL:HG12	2.18	0.43
1:B:275:SER:CB	1:B:375:LEU:CD2	2.96	0.43
1:C:337:ILE:O	1:C:337:ILE:CG2	2.64	0.43
1:A:122:VAL:CG1	1:A:123:VAL:N	2.82	0.43
1:A:185:GLN:OE1	1:A:232:LYS:HE3	2.18	0.43
1:B:154:GLN:NE2	1:B:222:TYR:CZ	2.74	0.43
1:B:279:ASP:OD2	1:B:282:GLY:HA3	2.19	0.43
1:B:304:HIS:CE1	1:B:349:TYR:OH	2.72	0.43
1:C:124:ASN:CG	1:C:132:LEU:HD12	2.44	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:B:321:LEU:HB3	1:B:344:GLY:C	2.44	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:A:300:THR:C	1:A:301:VAL:HG23	2.44	0.43
1:B:119:SER:HB3	1:B:246:GLY:C	2.43	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:B:300:THR:C	1:B:301:VAL:HG23	2.44	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:A:336:ASP:OD1	1:A:384:VAL:C	2.62	0.42
1:B:110:GLU:OE1	1:B:143:SER:N	2.51	0.42
1:C:96:THR:HG22	1:C:105:VAL:HB	1.98	0.42
1:C:304:HIS:CE1	1:C:349:TYR:OH	2.72	0.42
1:C:321:LEU:CB	1:C:344:GLY:H	2.26	0.42
1:A: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:N	1:A:280:LEU:CB	2.73	0.42
1:B:230:ASP:OD1	1:C:228:THR:HA	2.20	0.42
1:B:384:VAL:O	1:B:384:VAL:HG12	2.18	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:267:GLN:HA	1:C:197:ASN:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:SER:O	1:A:358:LEU:HG	2.18	0.42
1:C:112:LEU:CD2	1:C:113:THR:HG22	2.49	0.42
1:C:280:LEU:CB	1:C:370:ALA:O	2.67	0.42
1:C:281:THR:HA	1:C:297:ARG:HH12	1.84	0.42
1:C:336:ASP:OD1	1:C:384:VAL:C	2.63	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:B:280:LEU:O	1:B:370:ALA:C	2.62	0.42
1:C:280:LEU:O	1:C:370:ALA:C	2.62	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:A:274[S]:SER:C	1:A:375:LEU:HD23	2.44	0.42
1:A:280:LEU:O	1:A:370:ALA:C	2.62	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:280:LEU:CB	1:B:370:ALA:O	2.67	0.42
1:B:281:THR:HA	1:B:297:ARG:NH1	2.35	0.42
1:B:336:ASP:OD1	1:B:384:VAL:C	2.62	0.42
1:A:111:TYR:CZ	1:A:254:GLU:OE2	2.72	0.42
1:A:142:PHE:HB3	1:A:146:PRO:CD	2.48	0.42
1:A:280:LEU:CB	1:A:370:ALA:O	2.67	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:230:ASP:OD1	1:B:228:THR:HA	2.20	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: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
1:A:185:GLN:O	1:A:186:ASP:C	2.63	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:297:ARG:CG	1:B:298:THR:C	2.93	0.42
1:B:302:LEU:HG	1:B:304:HIS:HD2	1.85	0.42
1:C:135:ASN:HB2	1:C:235:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:LEU:HD21	1:C:253:GLY:CA	2.50	0.42
1:A:179:TYR:CD1	1:A:240:GLY:HA3	2.53	0.42
1:A:226:SER:OG	1:C:232:LYS:CE	2.68	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: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:109:ARG:HA	1:A:257:LEU:O	2.19	0.41
1:A:172:GLU:N	1:A:172:GLU:O	2.52	0.41
1:B:107:SER:HA	1:B:259:ARG:O	2.20	0.41
1:B:112:LEU:HG	1:B:141:LEU:HD12	1.99	0.41
1:C:82:VAL:HA	1:C:170:THR:CG2	2.48	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:A:117:ASN:C	1:A:249:ALA:HA	2.44	0.41
1:A:157:PHE:CE2	1:A:261:VAL:HG22	2.53	0.41
1:B:217:ASP:OD2	1:B:221:ARG:NH2	2.53	0.41
1: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:B:275:SER:C	1:B:276:LYS:HG2	2.45	0.41
1:B:314:LEU:HD22	1:B:351:LEU:CD1	2.50	0.41
1:A:297:ARG:CG	1:A:298:THR:C	2.93	0.41
1:B:161:VAL:HA	1:B:212:LEU:O	2.20	0.41
1:C:97:GLY:O	1:C:99:THR:CA	2.68	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: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
1:A:267:GLN:HG3	1:A:268:PRO:CG	2.25	0.41
1:B:111:TYR:HE2	1:B:254:GLU:CD	2.28	0.41
1:B:168:CYS:CB	1:B:252:VAL:HG13	2.50	0.41
1:C:115:VAL:HG21	1:C:241:ILE:HG21	2.02	0.41
1:C:131:SER:OG	1:C:132:LEU:N	2.53	0.41
1:A:133:GLN:O	1:A:138:ASN:ND2	2.48	0.41
1:B:111:TYR:CD1	1:B:112:LEU:N	2.89	0.41
1:C:67:ILE:C	1:C:68:ILE:O	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLN:NE2	1:A:251:ALA:CB	2.79	0.41
1:C:304:HIS:N	1:C:362:VAL:O	2.49	0.41
1:C:362:VAL:N	1:C:362:VAL:CG2	2.83	0.41
1:C:141:LEU:HD12	1:C:141:LEU:O	2.20	0.41
1:C:195:LEU:CD2	1:C:195:LEU:C	2.93	0.41
1:C:232:LYS:HE2	1:C:232:LYS:HB3	1.80	0.41
1:A:110:GLU:CD	1:A:145:LEU:H	2.27	0.41
1:A:121:PHE:O	1:A:121:PHE:HD1	2.04	0.41
1:A:123:VAL:CG1	1:A:124:ASN:HD22	2.25	0.41
1:A:257:LEU:C	1:A:257:LEU:HD13	2.46	0.41
1:C:98:ARG:C	1:C:100:SER:N	2.70	0.41
1:C:141:LEU:HD12	1:C:141:LEU:C	2.46	0.41
1:C:204:THR:O	1:C:205:ALA:O	2.35	0.41
1:C:223:CYS:C	1:C:223:CYS:N	2.63	0.41
1:C:257:LEU:C	1:C:257:LEU:HD13	2.46	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:314:LEU:HD22	1:C:351:LEU:CD1	2.50	0.41
1:A:298:THR:CB	1:A:299:PRO:HD2	2.42	0.40
1:B:161:VAL:N	1:B:258:ALA:HB3	2.35	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: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:B:270:ASN:O	1:B:271:THR:C	2.64	0.40
1:C:112:LEU:CG	1:C:141:LEU:HD11	2.51	0.40
1:C:297:ARG:CG	1:C:298:THR:C	2.93	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:228:THR:HG23	1:C:232:LYS:CE	2.52	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
1:C:115:VAL:HG22	1:C:241:ILE:HG21	2.03	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:183:ASP:O	1:C:184:SER:C	2.63	0.40
1:A:178:LEU:HD21	1:A:255:LEU:CD2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:193:VAL:CG1	1:C:143:SER:OG[2_555]	1.80	0.40
1:C:280:LEU:CD2	1:C:387:LEU:C[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 [i](#)

5.3.1 Protein backbone [i](#)

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
1	B	381	ALA
1	B	384	VAL
1	B	386	LEU

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Mol	Chain	Res	Type
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
1	C	265	PHE
1	C	279	ASP
1	C	324	LEU

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Mol	Chain	Res	Type
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%)	215 (93%)	17 (7%)	13	38
1	B	233/309 (75%)	214 (92%)	19 (8%)	10	32
1	C	258/309 (84%)	241 (93%)	17 (7%)	15	43
All	All	723/927 (78%)	670 (93%)	53 (7%)	13	38

All (53) 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	201	LEU
1	A	206	PRO
1	A	211	MET
1	A	257	LEU
1	A	260	SER
1	A	280	LEU
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	273[P]	LEU
1	B	273[S]	LEU
1	B	280	LEU
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
1	C	201	LEU

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Mol	Chain	Res	Type
1	C	211	MET
1	C	257	LEU
1	C	260	SER
1	C	280	LEU
1	C	295	LEU
1	C	321	LEU
1	C	326	LEU
1	C	338	LEU
1	C	351	LEU
1	C	352	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) 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	238	GLN
1	A	304	HIS
1	A	335	ASN
1	A	352	ASN
1	B	114	GLN
1	B	116	ASN
1	B	130	ASN
1	B	133	GLN
1	B	135	ASN
1	B	224	ASN
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	116	ASN
1	C	130	ASN
1	C	135	ASN
1	C	158	ASN
1	C	197	ASN
1	C	224	ASN

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Mol	Chain	Res	Type
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 oligosaccharides 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.