



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:19 AM UTC

PDB ID : 1SVA / pdb_00001sva
Title : SIMIAN VIRUS 40
Authors : Stehle, T.; Gamblin, S.J.; Harrison, S.C.
Deposited on : 1995-11-27
Resolution : 3.10 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

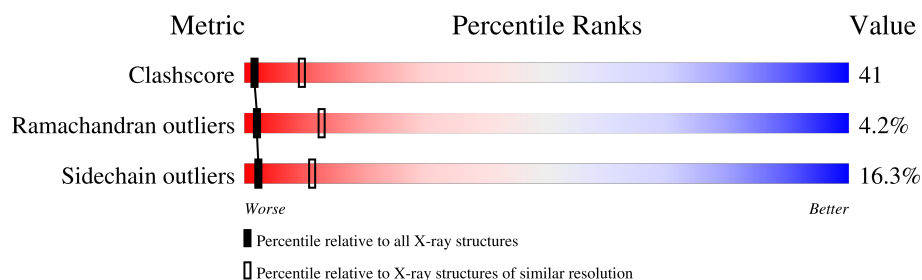
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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	1	361	27% 45% 19% 5% .
1	2	361	28% 50% 16% . .
1	3	361	33% 42% 17% . 5%
1	4	361	29% 46% 14% . 8%
1	5	361	29% 46% 18% . .
1	6	361	38% 43% 13% . 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15983 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 SIMIAN VIRUS 40.

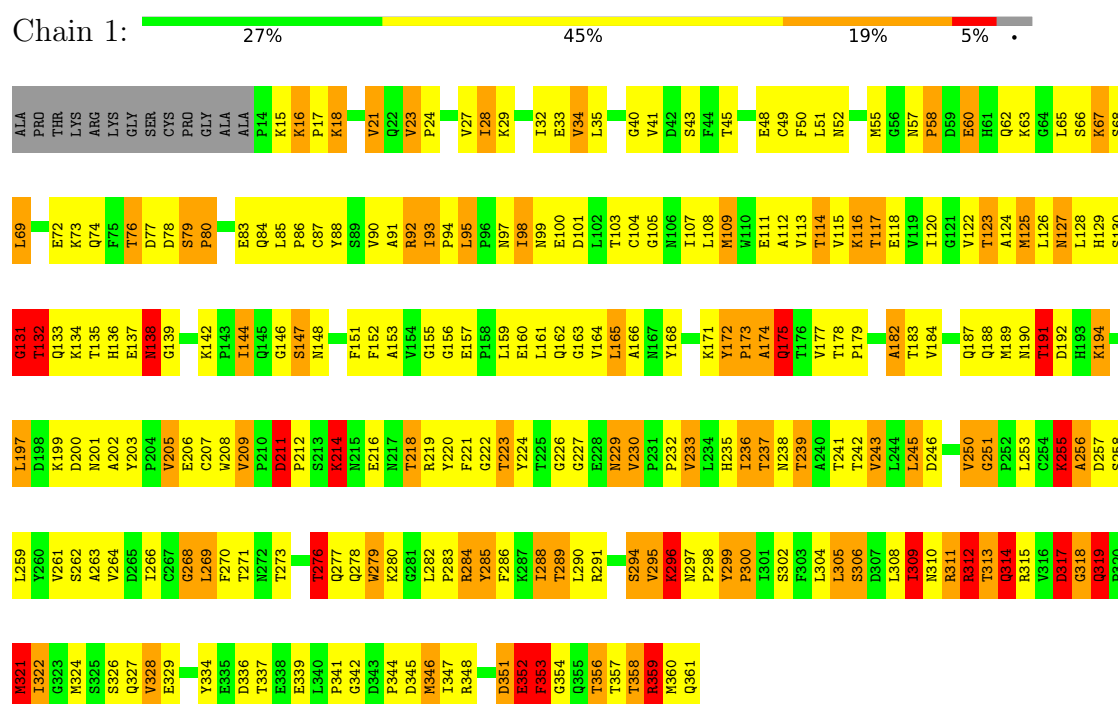
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	348	Total	C	N	O	S	0	0	0
			2707	1703	460	530	14			
1	2	348	Total	C	N	O	S	0	0	0
			2707	1703	460	530	14			
1	3	342	Total	C	N	O	S	0	0	0
			2658	1675	450	520	13			
1	4	331	Total	C	N	O	S	0	0	0
			2560	1612	435	501	12			
1	5	347	Total	C	N	O	S	0	0	0
			2700	1698	459	529	14			
1	6	341	Total	C	N	O	S	0	0	0
			2651	1670	449	519	13			

3 Residue-property plots

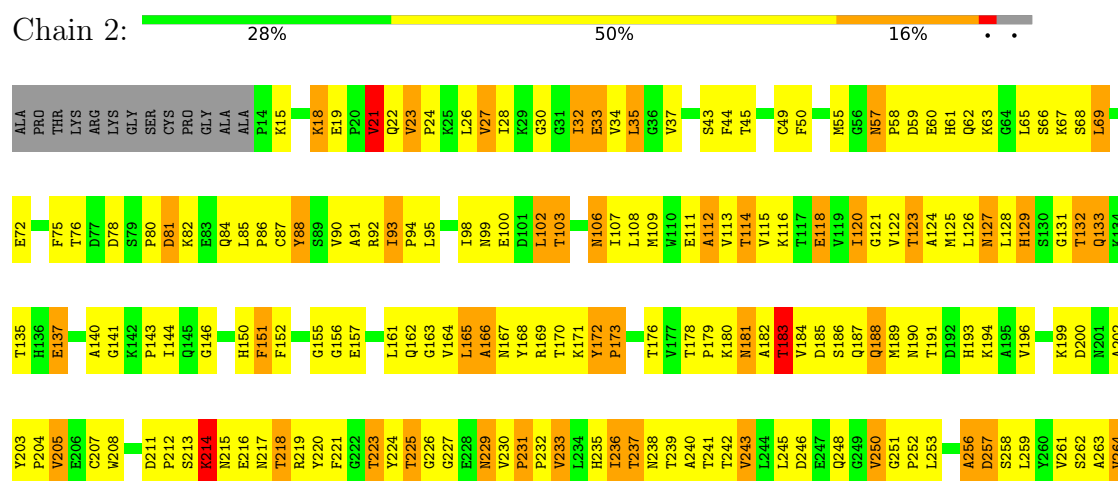
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

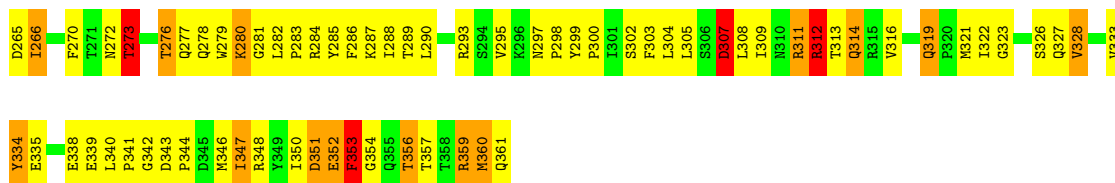
Note EDS was not executed.

• Molecule 1: SIMIAN VIRUS 40

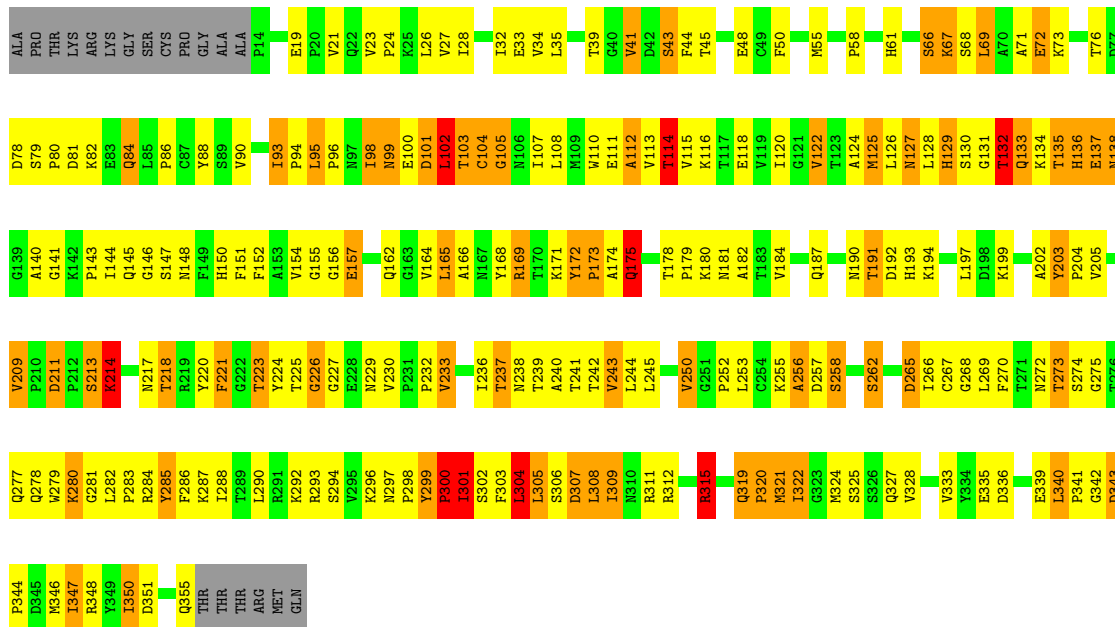


• Molecule 1: SIMIAN VIRUS 40

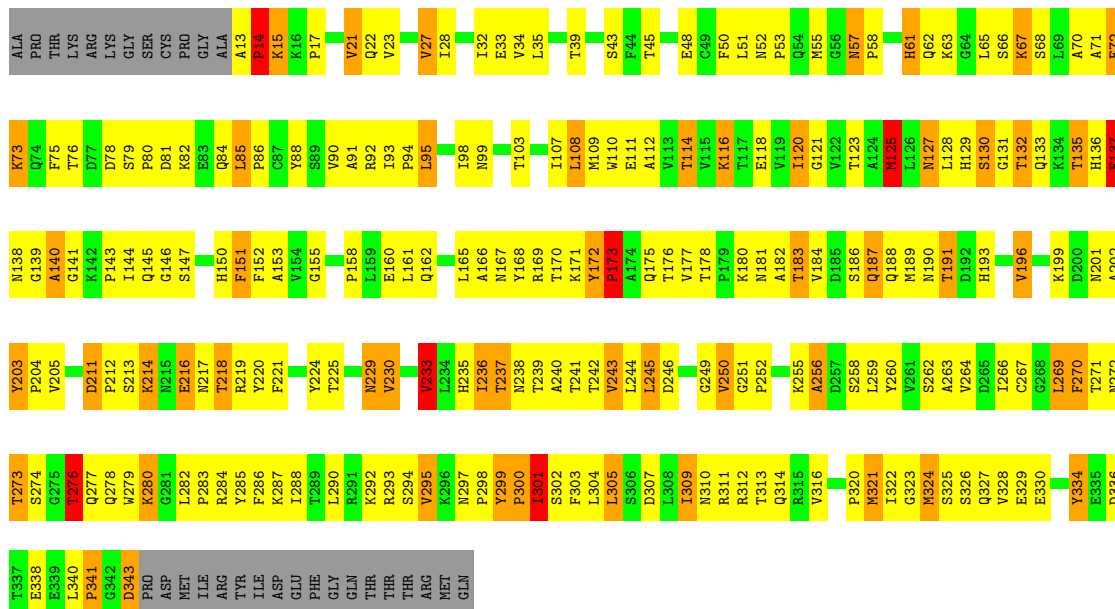




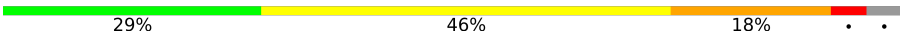
- Molecule 1: SIMIAN VIRUS 40

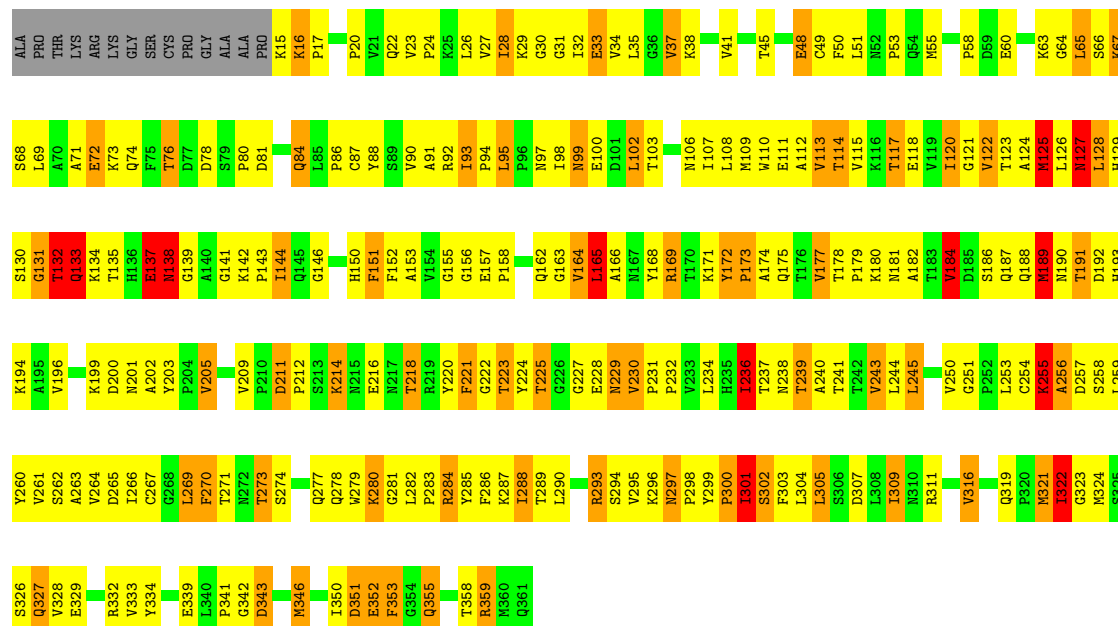


- Molecule 1: SIMIAN VIRUS 40

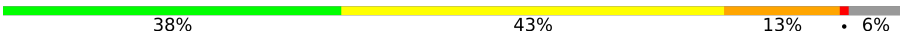


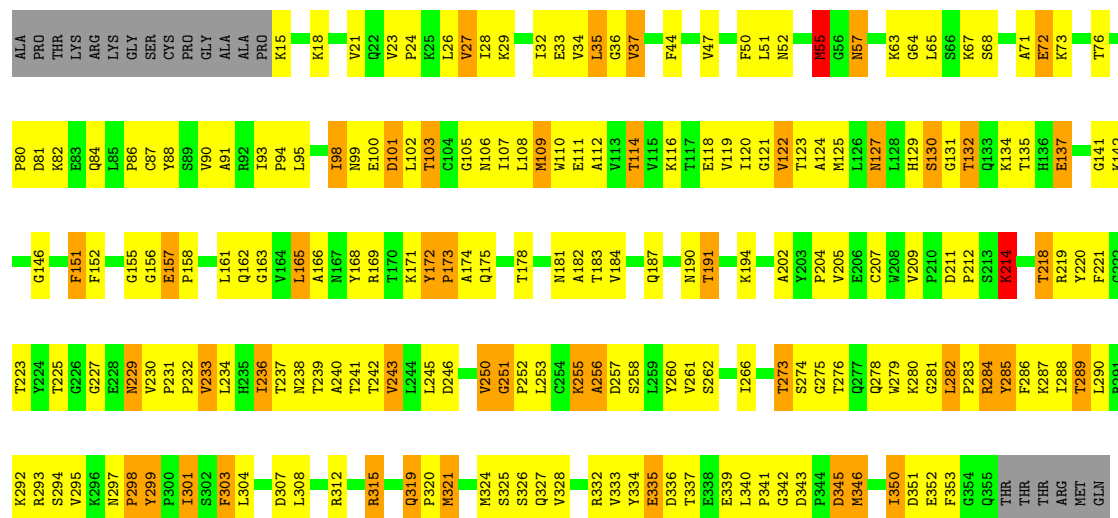
• Molecule 1: SIMIAN VIRUS 40

Chain 5:  29% 46% 18% • •



• Molecule 1: SIMIAN VIRUS 40

Chain 6:  38% 43% 13% • 6%



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	558.00 Å 558.00 Å 558.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.10	Depositor
% Data completeness (in resolution range)	80.2 (12.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.257 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15983	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	1.13	6/2766 (0.2%)	1.60	72/3761 (1.9%)
1	2	1.18	12/2766 (0.4%)	1.48	41/3761 (1.1%)
1	3	1.19	10/2717 (0.4%)	1.65	65/3695 (1.8%)
1	4	1.23	7/2616 (0.3%)	1.55	46/3560 (1.3%)
1	5	1.18	8/2758 (0.3%)	1.57	55/3750 (1.5%)
1	6	1.30	18/2709 (0.7%)	1.55	41/3684 (1.1%)
All	All	1.20	61/16332 (0.4%)	1.57	320/22211 (1.4%)

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	2	0	1
1	6	0	1
All	All	0	2

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4	138	ASN	N-CA	11.49	1.58	1.46
1	6	125	MET	SD-CE	-9.79	1.55	1.79
1	6	27	VAL	CA-CB	-8.36	1.45	1.54
1	4	288	ILE	CA-CB	-8.19	1.44	1.54
1	3	243	VAL	CA-CB	-7.62	1.44	1.54
1	6	119	VAL	CA-CB	-7.53	1.45	1.54
1	2	288	ILE	CA-CB	-7.48	1.45	1.54
1	3	333	VAL	CA-CB	-7.43	1.45	1.54
1	1	109	MET	SD-CE	7.34	1.97	1.79
1	5	125	MET	SD-CE	7.06	1.97	1.79
1	6	240	ALA	CA-CB	-7.00	1.40	1.53
1	6	243	VAL	CA-CB	-6.95	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	243	VAL	CA-CB	-6.81	1.46	1.54
1	6	37	VAL	CA-CB	-6.77	1.47	1.54
1	6	321	MET	SD-CE	-6.68	1.62	1.79
1	5	177	VAL	CA-CB	-6.60	1.46	1.54
1	4	125	MET	SD-CE	6.42	1.95	1.79
1	2	120	ILE	CA-CB	-6.36	1.46	1.54
1	6	233	VAL	CA-CB	-6.36	1.46	1.54
1	5	138	ASN	N-CA	6.33	1.52	1.46
1	3	113	VAL	CA-CB	-6.32	1.47	1.54
1	1	237	THR	CA-CB	-6.26	1.43	1.53
1	5	321	MET	SD-CE	-6.20	1.64	1.79
1	2	347	ILE	CA-CB	-6.09	1.46	1.54
1	6	93	ILE	CA-C	-6.07	1.48	1.53
1	6	55	MET	SD-CE	-6.02	1.64	1.79
1	4	237	THR	CA-CB	-5.87	1.44	1.53
1	2	240	ALA	CA-CB	-5.69	1.44	1.53
1	1	125	MET	SD-CE	5.68	1.93	1.79
1	4	177	VAL	CA-CB	-5.63	1.47	1.54
1	2	21	VAL	CA-CB	-5.62	1.48	1.54
1	5	333	VAL	CA-CB	-5.61	1.46	1.54
1	1	353	PHE	CA-C	5.48	1.60	1.52
1	6	335	GLU	CA-C	-5.47	1.48	1.52
1	6	122	VAL	CA-CB	-5.41	1.48	1.54
1	3	288	ILE	CA-C	-5.41	1.46	1.52
1	1	243	VAL	CA-CB	-5.39	1.47	1.54
1	6	124	ALA	CA-CB	-5.38	1.43	1.53
1	3	112	ALA	CA-CB	-5.36	1.45	1.53
1	3	154	VAL	CA-CB	-5.35	1.47	1.54
1	5	243	VAL	CA-CB	-5.34	1.47	1.54
1	1	113	VAL	CA-CB	-5.33	1.48	1.54
1	2	113	VAL	CA-CB	-5.32	1.49	1.55
1	2	334	TYR	CA-C	-5.25	1.46	1.52
1	4	236	ILE	N-CA	-5.23	1.40	1.46
1	6	236	ILE	CA-CB	5.19	1.60	1.54
1	4	243	VAL	CA-CB	-5.19	1.47	1.54
1	6	161	LEU	CA-C	-5.16	1.46	1.52
1	5	214	LYS	N-CA	-5.16	1.40	1.46
1	2	112	ALA	CA-CB	-5.14	1.46	1.53
1	2	151	PHE	CA-C	-5.12	1.46	1.52
1	3	233	VAL	CA-CB	-5.12	1.48	1.54
1	2	114	THR	CA-C	-5.12	1.46	1.52
1	6	225	THR	CA-CB	-5.11	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3	125	MET	SD-CE	5.11	1.92	1.79
1	6	44	PHE	CA-C	-5.09	1.46	1.52
1	6	93	ILE	CA-CB	-5.08	1.48	1.54
1	2	93	ILE	CA-C	-5.06	1.48	1.53
1	3	288	ILE	CA-CB	-5.06	1.48	1.54
1	5	144	ILE	CA-CB	-5.03	1.48	1.54
1	3	114	THR	CA-C	-5.02	1.46	1.52

All (320) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	256	ALA	N-CA-C	-13.37	89.94	109.59
1	4	256	ALA	N-CA-C	-13.09	91.11	110.48
1	3	256	ALA	N-CA-C	-12.21	90.34	109.76
1	5	93	ILE	CA-C-N	11.62	134.37	119.84
1	5	93	ILE	C-N-CA	11.62	134.37	119.84
1	6	256	ALA	N-CA-C	-11.35	92.27	110.20
1	1	211	ASP	CA-C-N	11.24	132.14	119.32
1	1	211	ASP	C-N-CA	11.24	132.14	119.32
1	3	340	LEU	CA-C-N	11.24	131.97	119.83
1	3	340	LEU	C-N-CA	11.24	131.97	119.83
1	6	93	ILE	CA-C-N	11.19	132.78	120.13
1	6	93	ILE	C-N-CA	11.19	132.78	120.13
1	5	172	TYR	N-CA-C	10.99	124.51	109.24
1	3	343	ASP	CA-C-N	10.93	132.15	119.47
1	3	343	ASP	C-N-CA	10.93	132.15	119.47
1	3	322	ILE	N-CA-C	10.63	122.55	107.88
1	3	335	GLU	CA-C-N	-10.46	111.74	123.04
1	3	335	GLU	C-N-CA	-10.46	111.74	123.04
1	6	319	GLN	CA-C-N	10.39	132.83	119.84
1	6	319	GLN	C-N-CA	10.39	132.83	119.84
1	3	319	GLN	CA-C-N	10.03	132.38	119.84
1	3	319	GLN	C-N-CA	10.03	132.38	119.84
1	2	214	LYS	N-CA-C	10.01	127.23	114.31
1	5	214	LYS	N-CA-C	9.94	125.81	112.30
1	4	336	ASP	N-CA-C	9.87	116.88	108.78
1	4	211	ASP	CA-C-N	9.75	129.87	119.05
1	4	211	ASP	C-N-CA	9.75	129.87	119.05
1	3	105	GLY	N-CA-C	9.59	135.91	113.18
1	5	256	ALA	N-CA-C	-9.48	93.72	109.46
1	4	15	LYS	N-CA-C	-9.47	92.86	108.49
1	5	319	GLN	CA-C-N	9.36	131.54	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	319	GLN	C-N-CA	9.36	131.54	119.84
1	1	322	ILE	N-CA-C	9.20	122.70	108.44
1	3	93	ILE	CA-C-N	9.13	130.45	120.13
1	3	93	ILE	C-N-CA	9.13	130.45	120.13
1	1	312	ARG	N-CA-C	-9.10	98.71	111.81
1	3	321	MET	N-CA-C	-9.01	102.45	112.72
1	3	104	CYS	N-CA-C	8.96	123.14	108.26
1	2	256	ALA	N-CA-C	-8.88	95.05	109.96
1	1	93	ILE	CA-C-N	8.87	129.22	119.90
1	1	93	ILE	C-N-CA	8.87	129.22	119.90
1	5	343	ASP	CA-C-N	8.86	128.89	119.05
1	5	343	ASP	C-N-CA	8.86	128.89	119.05
1	3	214	LYS	N-CA-C	8.73	126.98	113.19
1	4	214	LYS	N-CA-C	8.69	127.56	114.09
1	6	282	LEU	CA-C-N	-8.67	111.94	120.52
1	6	282	LEU	C-N-CA	-8.67	111.94	120.52
1	3	299	TYR	N-CA-C	8.64	125.42	113.16
1	6	209	VAL	N-CA-C	-8.60	99.30	109.01
1	1	359	ARG	N-CA-C	8.53	128.97	110.80
1	5	165	LEU	N-CA-C	8.48	121.60	108.96
1	4	71	ALA	N-CA-C	8.45	121.48	108.30
1	4	137	GLU	CA-C-N	-8.45	108.03	122.14
1	4	137	GLU	C-N-CA	-8.45	108.03	122.14
1	3	237	THR	CB-CA-C	-8.42	96.17	109.72
1	3	98	ILE	N-CA-C	8.25	120.00	111.00
1	3	172	TYR	N-CA-C	8.25	121.58	109.62
1	3	166	ALA	N-CA-C	-8.22	96.88	109.95
1	1	358	THR	N-CA-C	8.17	118.74	108.45
1	1	16	LYS	N-CA-C	-8.11	98.40	110.24
1	5	211	ASP	CA-C-N	8.10	128.04	119.05
1	5	211	ASP	C-N-CA	8.10	128.04	119.05
1	1	269	LEU	N-CA-C	8.07	121.57	108.41
1	1	319	GLN	CA-C-N	8.07	130.16	120.23
1	1	319	GLN	C-N-CA	8.07	130.16	120.23
1	6	183	THR	N-CA-C	-8.04	97.64	108.74
1	5	100	GLU	N-CA-C	-7.99	100.48	112.54
1	5	102	LEU	N-CA-C	7.86	127.53	110.80
1	1	16	LYS	CA-C-N	-7.83	112.70	120.21
1	1	16	LYS	C-N-CA	-7.83	112.70	120.21
1	6	240	ALA	N-CA-C	7.82	121.64	108.90
1	3	71	ALA	N-CA-C	7.81	121.37	108.48
1	1	135	THR	N-CA-C	-7.81	102.70	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	214	LYS	N-CA-C	7.79	125.49	113.19
1	1	172	TYR	N-CA-C	7.67	122.19	108.47
1	6	71	ALA	N-CA-C	7.66	127.11	110.80
1	3	275	GLY	N-CA-C	-7.56	104.64	114.85
1	3	300	PRO	N-CA-C	7.56	128.04	112.47
1	2	316	VAL	N-CA-C	7.54	119.18	108.17
1	2	103	THR	N-CA-C	7.47	126.72	110.80
1	3	211	ASP	CA-C-N	7.47	127.35	119.05
1	3	211	ASP	C-N-CA	7.47	127.35	119.05
1	4	166	ALA	N-CA-C	-7.42	97.49	109.96
1	2	319	GLN	CA-C-N	7.40	128.57	119.98
1	2	319	GLN	C-N-CA	7.40	128.57	119.98
1	5	214	LYS	CA-C-N	-7.33	111.08	122.08
1	5	214	LYS	C-N-CA	-7.33	111.08	122.08
1	5	72	GLU	N-CA-C	7.33	121.64	113.21
1	5	352	GLU	N-CA-C	-7.26	100.44	111.56
1	6	174	ALA	N-CA-C	7.17	119.18	111.36
1	3	315	ARG	N-CA-C	-7.14	97.57	109.07
1	5	236	ILE	N-CA-C	-7.12	98.20	108.17
1	1	321	MET	N-CA-C	-7.08	103.95	112.59
1	3	103	THR	N-CA-C	-7.08	102.69	111.75
1	3	336	ASP	CA-C-O	7.08	122.05	117.94
1	2	166	ALA	N-CA-C	-7.05	97.91	109.40
1	6	103	THR	N-CA-C	7.02	119.04	110.41
1	3	72	GLU	N-CA-C	7.01	120.49	112.57
1	4	336	ASP	CA-C-O	6.98	121.99	117.94
1	1	352	GLU	N-CA-C	-6.96	102.04	112.54
1	2	133	GLN	N-CA-C	-6.95	99.26	110.32
1	4	172	TYR	N-CA-C	6.92	119.66	109.62
1	1	138	ASN	N-CA-C	-6.90	102.47	111.71
1	4	297	ASN	CA-C-N	6.90	126.70	119.05
1	4	297	ASN	C-N-CA	6.90	126.70	119.05
1	1	214	LYS	N-CA-C	6.86	124.72	114.09
1	2	69	LEU	N-CA-C	6.84	120.15	110.50
1	2	21	VAL	CB-CA-C	-6.84	101.84	111.28
1	4	57	ASN	CA-C-N	6.82	126.33	119.24
1	4	57	ASN	C-N-CA	6.82	126.33	119.24
1	3	116	LYS	N-CA-C	-6.80	98.31	109.40
1	6	275	GLY	N-CA-C	-6.80	105.67	114.85
1	5	71	ALA	N-CA-C	6.78	125.24	110.80
1	5	240	ALA	N-CA-C	6.78	119.78	108.73
1	2	314	GLN	N-CA-C	6.78	119.74	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	116	LYS	N-CA-C	-6.77	97.86	108.90
1	5	37	VAL	N-CA-C	6.77	118.42	109.21
1	1	174	ALA	N-CA-C	6.77	125.22	110.80
1	2	266	ILE	CB-CA-C	-6.75	103.93	111.23
1	5	297	ASN	CA-C-N	6.67	126.12	118.85
1	5	297	ASN	C-N-CA	6.67	126.12	118.85
1	6	214	LYS	CA-C-N	-6.67	112.17	122.05
1	6	214	LYS	C-N-CA	-6.67	112.17	122.05
1	1	67	LYS	N-CA-C	-6.67	101.73	110.53
1	5	322	ILE	N-CA-C	6.67	119.62	108.81
1	3	67	LYS	N-CA-C	-6.66	101.74	110.53
1	5	137	GLU	O-C-N	-6.66	113.73	122.59
1	1	60	GLU	N-CA-C	-6.66	105.17	113.55
1	6	266	ILE	CB-CA-C	-6.64	104.11	111.35
1	3	157	GLU	CB-CA-C	-6.62	102.68	110.76
1	2	120	ILE	N-CA-C	6.61	118.10	108.58
1	1	132	THR	N-CA-C	6.60	119.59	110.35
1	1	48	GLU	N-CA-C	-6.58	98.97	109.76
1	1	95	LEU	CA-C-N	6.58	126.81	119.90
1	1	95	LEU	C-N-CA	6.58	126.81	119.90
1	5	135	THR	N-CA-C	-6.57	104.05	111.07
1	6	106	ASN	N-CA-C	6.57	119.11	108.41
1	5	166	ALA	N-CA-C	-6.56	99.01	109.76
1	4	116	LYS	N-CA-C	-6.55	98.72	109.40
1	5	255	LYS	N-CA-C	-6.55	103.83	110.97
1	3	133	GLN	N-CA-C	-6.49	101.19	110.59
1	2	328	VAL	N-CA-C	-6.48	98.31	108.23
1	1	166	ALA	N-CA-C	-6.47	99.09	109.96
1	4	214	LYS	CA-C-N	-6.47	111.90	122.26
1	4	214	LYS	C-N-CA	-6.47	111.90	122.26
1	5	67	LYS	N-CA-C	-6.45	101.84	110.55
1	1	279	TRP	N-CA-C	6.43	118.40	109.15
1	5	99	ASN	N-CA-C	6.38	119.10	108.96
1	3	129	HIS	CA-C-N	-6.34	116.19	123.04
1	3	129	HIS	C-N-CA	-6.34	116.19	123.04
1	5	316	VAL	N-CA-C	6.33	116.98	107.80
1	6	343	ASP	CA-C-N	6.30	127.72	119.84
1	6	343	ASP	C-N-CA	6.30	127.72	119.84
1	5	172	TYR	CA-C-N	6.29	127.70	119.84
1	5	172	TYR	C-N-CA	6.29	127.70	119.84
1	6	52	ASN	N-CA-C	-6.28	101.62	110.29
1	2	19	GLU	N-CA-C	-6.26	102.18	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	67	LYS	N-CA-C	-6.25	102.11	110.55
1	3	102	LEU	N-CA-C	-6.25	104.22	112.72
1	6	251	GLY	N-CA-C	-6.24	99.61	112.34
1	1	264	VAL	CB-CA-C	-6.24	102.19	111.80
1	6	57	ASN	CA-C-N	6.23	126.42	119.32
1	6	57	ASN	C-N-CA	6.23	126.42	119.32
1	1	236	ILE	N-CA-C	-6.23	99.39	108.11
1	2	106	ASN	N-CA-C	-6.22	99.73	109.25
1	5	22	GLN	N-CA-C	6.22	118.58	108.63
1	2	236	ILE	N-CA-C	-6.22	98.57	107.77
1	4	72	GLU	N-CA-C	6.17	123.93	110.80
1	4	95	LEU	CA-C-N	6.15	125.91	119.76
1	4	95	LEU	C-N-CA	6.15	125.91	119.76
1	2	273	THR	N-CA-C	-6.14	104.59	111.28
1	3	174	ALA	N-CA-C	6.12	118.74	111.33
1	6	157	GLU	N-CA-C	-6.11	101.12	108.14
1	2	297	ASN	N-CA-C	-6.05	100.47	109.42
1	1	209	VAL	N-CA-C	-6.04	95.83	108.88
1	6	191	THR	N-CA-C	6.04	120.19	112.34
1	4	172	TYR	CA-C-N	6.03	127.38	119.84
1	4	172	TYR	C-N-CA	6.03	127.38	119.84
1	5	133	GLN	N-CA-C	-6.03	102.76	110.53
1	5	327	GLN	N-CA-C	-6.02	105.86	112.72
1	3	113	VAL	N-CA-C	6.01	116.77	111.90
1	2	312	ARG	N-CA-C	6.00	122.68	113.19
1	2	66	SER	N-CA-C	-5.99	101.59	110.46
1	6	299	TYR	CA-C-N	5.99	127.39	120.98
1	6	299	TYR	C-N-CA	5.99	127.39	120.98
1	5	142	LYS	N-CA-C	-5.97	98.63	109.44
1	5	189	MET	N-CA-C	5.97	118.17	108.63
1	6	236	ILE	N-CA-C	-5.95	99.78	108.11
1	5	269	LEU	N-CA-C	5.95	118.93	109.24
1	5	157	GLU	CB-CA-C	-5.94	102.23	110.37
1	4	187	GLN	N-CA-C	-5.93	105.89	113.01
1	2	135	THR	N-CA-C	-5.92	104.83	111.28
1	1	194	LYS	N-CA-C	-5.92	100.85	110.20
1	5	230	VAL	CA-C-N	5.90	126.45	120.38
1	5	230	VAL	C-N-CA	5.90	126.45	120.38
1	2	335	GLU	N-CA-C	-5.89	99.74	108.99
1	5	184	VAL	CB-CA-C	-5.89	103.02	112.16
1	2	172	TYR	N-CA-C	5.89	118.14	109.42
1	3	113	VAL	CB-CA-C	-5.89	105.64	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	43	SER	N-CA-C	-5.89	103.17	110.41
1	1	268	GLY	N-CA-C	5.88	117.82	110.29
1	1	324	MET	N-CA-C	5.87	119.97	112.34
1	6	135	THR	N-CA-C	-5.85	104.98	111.36
1	3	19	GLU	N-CA-C	-5.82	102.43	109.83
1	3	214	LYS	CA-C-N	-5.82	113.44	122.05
1	3	214	LYS	C-N-CA	-5.82	113.44	122.05
1	3	172	TYR	CA-C-N	5.82	127.11	119.84
1	3	172	TYR	C-N-CA	5.82	127.11	119.84
1	1	142	LYS	CA-C-N	5.81	125.72	119.85
1	1	142	LYS	C-N-CA	5.81	125.72	119.85
1	1	101	ASP	N-CA-C	-5.80	97.54	107.23
1	6	172	TYR	N-CA-C	5.79	117.37	110.07
1	3	351	ASP	CA-C-N	-5.79	115.31	122.84
1	3	351	ASP	C-N-CA	-5.79	115.31	122.84
1	3	304	LEU	N-CA-C	-5.79	104.94	112.23
1	4	236	ILE	N-CA-C	-5.75	99.85	108.12
1	4	85	LEU	N-CA-C	5.74	119.85	108.59
1	5	174	ALA	N-CA-C	5.73	123.00	110.80
1	3	301	ILE	N-CA-C	5.72	121.25	109.34
1	2	347	ILE	N-CA-C	5.70	116.20	107.77
1	1	230	VAL	N-CA-C	-5.68	103.73	109.02
1	4	61	HIS	N-CA-C	-5.68	107.35	114.56
1	3	269	LEU	N-CA-C	5.66	118.18	109.07
1	5	216	GLU	N-CA-C	5.64	119.67	112.34
1	1	302	SER	N-CA-C	5.63	117.62	109.07
1	1	276	THR	N-CA-C	-5.63	103.49	110.41
1	5	309	ILE	CB-CA-C	-5.62	104.68	112.04
1	6	105	GLY	N-CA-C	5.60	126.45	113.18
1	2	57	ASN	CA-C-N	5.59	126.83	119.84
1	2	57	ASN	C-N-CA	5.59	126.83	119.84
1	4	67	LYS	N-CA-C	-5.57	102.04	110.28
1	4	309	ILE	CB-CA-C	-5.54	104.79	112.04
1	1	131	GLY	CA-C-N	5.54	129.56	121.31
1	1	131	GLY	C-N-CA	5.54	129.56	121.31
1	1	251	GLY	N-CA-C	-5.53	105.53	112.23
1	3	268	GLY	N-CA-C	5.53	117.37	110.29
1	4	183	THR	N-CA-C	-5.53	101.11	108.74
1	2	172	TYR	CA-C-N	5.51	126.73	119.84
1	2	172	TYR	C-N-CA	5.51	126.73	119.84
1	4	299	TYR	CA-C-N	5.50	126.71	119.84
1	4	299	TYR	C-N-CA	5.50	126.71	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	69	LEU	N-CA-C	5.49	118.88	110.20
1	1	114	THR	CA-C-N	-5.49	114.45	122.58
1	1	114	THR	C-N-CA	-5.49	114.45	122.58
1	2	67	LYS	N-CA-C	-5.49	102.76	110.50
1	5	342	GLY	CA-C-N	-5.49	115.40	123.30
1	5	342	GLY	C-N-CA	-5.49	115.40	123.30
1	1	314	GLN	N-CA-C	-5.49	98.02	108.17
1	1	305	LEU	N-CA-C	-5.48	105.00	110.97
1	6	142	LYS	N-CA-C	-5.47	99.54	109.44
1	1	191	THR	N-CA-C	5.46	122.43	110.80
1	1	205	VAL	N-CA-C	5.45	116.08	110.36
1	6	351	ASP	N-CA-C	-5.44	105.74	112.38
1	4	203	TYR	CA-C-N	5.44	125.61	119.90
1	4	203	TYR	C-N-CA	5.44	125.61	119.90
1	2	352	GLU	N-CA-C	-5.44	104.60	113.19
1	2	157	GLU	CB-CA-C	-5.41	102.96	110.37
1	2	118	GLU	CA-C-N	-5.41	115.40	122.37
1	2	118	GLU	C-N-CA	-5.41	115.40	122.37
1	4	276	THR	N-CA-C	-5.40	103.26	110.55
1	1	72	GLU	N-CA-C	5.40	122.30	110.80
1	3	175	GLN	N-CA-C	5.39	119.70	113.18
1	4	240	ALA	N-CA-C	5.39	118.26	109.59
1	1	296	LYS	N-CA-C	5.32	122.13	110.80
1	3	240	ALA	N-CA-C	5.32	117.63	109.07
1	4	21	VAL	CB-CA-C	-5.31	103.96	111.28
1	2	237	THR	CB-CA-C	-5.30	100.32	109.86
1	3	164	VAL	N-CA-C	-5.29	101.29	108.06
1	3	203	TYR	CA-C-N	5.29	125.54	119.83
1	3	203	TYR	C-N-CA	5.29	125.54	119.83
1	1	142	LYS	N-CA-C	-5.28	99.18	108.69
1	2	27	VAL	CB-CA-C	-5.27	105.30	111.94
1	4	269	LEU	N-CA-C	5.27	117.99	109.40
1	2	129	HIS	N-CA-C	5.27	117.19	108.49
1	6	73	LYS	N-CA-C	5.27	117.52	110.35
1	1	144	ILE	CB-CA-C	-5.26	103.39	111.71
1	2	183	THR	N-CA-C	-5.25	101.46	109.65
1	3	300	PRO	CA-C-N	5.24	131.40	121.97
1	3	300	PRO	C-N-CA	5.24	131.40	121.97
1	4	73	LYS	N-CA-C	5.23	117.47	110.35
1	4	343	ASP	N-CA-C	5.22	125.62	111.00
1	2	266	ILE	N-CA-C	-5.22	100.10	107.98
1	3	265	ASP	N-CA-C	5.22	119.33	108.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	342	GLY	CA-C-N	-5.21	114.12	123.08
1	1	342	GLY	C-N-CA	-5.21	114.12	123.08
1	1	69	LEU	N-CA-C	5.20	118.42	110.20
1	1	356	THR	N-CA-C	5.20	117.38	108.90
1	4	120	ILE	N-CA-C	5.20	116.19	108.23
1	1	201	ASN	N-CA-C	-5.20	106.02	112.47
1	1	105	GLY	N-CA-C	5.19	125.47	113.18
1	5	120	ILE	N-CA-C	5.17	116.73	108.87
1	4	321	MET	N-CA-C	-5.17	105.72	113.89
1	1	123	THR	CB-CA-C	-5.16	101.08	110.63
1	4	233	VAL	N-CA-C	-5.16	101.53	108.35
1	6	166	ALA	N-CA-C	-5.15	101.30	109.96
1	1	57	ASN	CA-C-N	5.14	126.27	119.84
1	1	57	ASN	C-N-CA	5.14	126.27	119.84
1	6	116	LYS	N-CA-C	-5.13	100.54	108.90
1	5	254	CYS	CA-C-N	5.11	127.39	120.65
1	5	254	CYS	C-N-CA	5.11	127.39	120.65
1	4	237	THR	CB-CA-C	-5.09	100.70	109.86
1	1	317	ASP	N-CA-C	-5.08	99.97	110.80
1	3	95	LEU	CA-C-N	5.08	125.32	119.83
1	3	95	LEU	C-N-CA	5.08	125.32	119.83
1	2	264	VAL	CB-CA-C	-5.08	103.98	111.80
1	3	66	SER	N-CA-C	-5.08	103.98	110.53
1	6	321	MET	N-CA-C	-5.07	106.34	112.88
1	5	329	GLU	N-CA-C	5.07	118.73	112.54
1	1	211	ASP	CA-C-O	5.07	123.62	119.36
1	1	79	SER	CA-C-N	5.06	126.17	119.84
1	1	79	SER	C-N-CA	5.06	126.17	119.84
1	6	72	GLU	N-CA-C	5.06	121.58	110.80
1	1	175	GLN	N-CA-C	5.05	117.52	111.71
1	5	113	VAL	N-CA-CB	-5.05	104.99	111.90
1	4	135	THR	N-CA-C	-5.04	105.69	111.14
1	3	135	THR	N-CA-C	-5.03	105.88	111.36
1	5	293	ARG	N-CA-C	5.02	117.42	109.24
1	2	311	ARG	N-CA-C	-5.01	106.67	112.89
1	1	309	ILE	N-CA-C	5.01	119.75	109.34
1	3	226	GLY	N-CA-C	-5.00	105.92	112.82

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	88	TYR	Sidechain
1	6	285	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2707	0	2676	268	0
1	2	2707	0	2676	259	0
1	3	2658	0	2625	228	0
1	4	2560	0	2535	250	0
1	5	2700	0	2668	273	0
1	6	2651	0	2617	193	0
All	All	15983	0	15797	1318	0

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 41.

All (1318) 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)
1:2:121:GLY:HA2	1:3:209:VAL:HG11	1.28	1.12
1:4:27:VAL:HG12	1:4:28:ILE:HG22	1.31	1.12
1:1:27:VAL:HG12	1:1:28:ILE:HG22	1.26	1.10
1:6:237:THR:HG22	1:6:239:THR:H	1.14	1.09
1:5:165:LEU:HD11	1:5:168:TYR:HA	1.39	1.05
1:1:79:SER:HB2	1:1:171:LYS:HB2	1.37	1.01
1:2:22:GLN:HG3	1:6:337:THR:HB	1.43	1.01
1:3:243:VAL:HG12	1:3:245:LEU:H	1.21	1.00
1:2:237:THR:HG22	1:2:239:THR:H	1.24	0.99
1:2:15:LYS:HD3	1:3:41:VAL:HB	1.45	0.98
1:4:132:THR:HG21	1:4:141:GLY:HA3	1.44	0.98
1:1:237:THR:HG22	1:1:239:THR:H	1.30	0.96
1:3:237:THR:HG22	1:3:239:THR:H	1.28	0.96
1:6:168:TYR:HB2	1:6:182:ALA:HB1	1.45	0.95
1:5:199:LYS:HG3	1:5:202:ALA:HB2	1.48	0.94
1:3:132:THR:HG21	1:3:141:GLY:HA3	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:69:LEU:HD12	1:5:278:GLN:HA	1.49	0.94
1:3:55:MET:HE1	1:3:266:ILE:HG13	1.50	0.93
1:1:73:LYS:HD3	1:1:78:ASP:HA	1.48	0.93
1:4:233:VAL:HG13	1:5:225:THR:HG23	1.48	0.93
1:3:140:ALA:H	1:4:277:GLN:HE21	1.17	0.91
1:4:120:ILE:HB	1:4:283:PRO:HG2	1.52	0.91
1:4:121:GLY:HA2	1:5:209:VAL:HG11	1.48	0.91
1:1:162:GLN:HB2	1:1:211:ASP:HB2	1.50	0.90
1:2:155:GLY:HA3	1:2:218:THR:HB	1.50	0.90
1:1:298:PRO:HG2	1:1:299:TYR:CE1	2.06	0.90
1:4:127:ASN:ND2	1:4:130:SER:H	1.70	0.89
1:2:45:THR:HG22	1:6:333:VAL:HG22	1.54	0.89
1:1:155:GLY:HA3	1:1:218:THR:HB	1.56	0.88
1:3:99:ASN:ND2	1:3:108:LEU:H	1.72	0.88
1:6:127:ASN:HD21	1:6:130:SER:H	1.22	0.88
1:3:99:ASN:HD22	1:3:108:LEU:H	1.22	0.87
1:6:321:MET:HE3	1:6:328:VAL:HG23	1.54	0.86
1:5:237:THR:HG22	1:5:239:THR:H	1.40	0.85
1:6:237:THR:HG22	1:6:239:THR:N	1.92	0.84
1:4:155:GLY:HA3	1:4:218:THR:HB	1.60	0.84
1:4:165:LEU:HD11	1:4:168:TYR:HA	1.57	0.84
1:1:92:ARG:HG3	1:1:258:SER:HB3	1.59	0.84
1:4:132:THR:CG2	1:4:141:GLY:HA3	2.07	0.83
1:1:347:ILE:HB	1:1:358:THR:HG23	1.60	0.83
1:3:155:GLY:HA3	1:3:218:THR:HB	1.60	0.83
1:6:27:VAL:HG12	1:6:28:ILE:HG22	1.58	0.82
1:3:125:MET:HE3	1:3:144:ILE:HB	1.60	0.82
1:2:120:ILE:HB	1:2:283:PRO:HG2	1.60	0.82
1:3:175:GLN:HA	1:3:175:GLN:HE21	1.43	0.82
1:4:98:ILE:HD13	1:4:292:LYS:HG2	1.62	0.82
1:5:155:GLY:HA3	1:5:218:THR:HB	1.62	0.81
1:4:127:ASN:HD21	1:4:130:SER:H	1.26	0.81
1:5:270:PHE:HD1	1:5:271:THR:N	1.78	0.81
1:1:88:TYR:HE1	1:1:205:VAL:HA	1.46	0.81
1:2:243:VAL:HG12	1:2:245:LEU:H	1.46	0.81
1:1:55:MET:HE3	1:1:279:TRP:HB3	1.63	0.81
1:2:168:TYR:HB2	1:2:182:ALA:HB1	1.61	0.81
1:2:61:HIS:HD2	1:3:168:TYR:OH	1.64	0.80
1:1:108:LEU:HD23	1:1:294:SER:HA	1.62	0.79
1:5:243:VAL:HG12	1:5:245:LEU:H	1.43	0.79
1:5:23:VAL:HB	1:5:24:PRO:HD2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:99:ASN:HD22	1:2:102:LEU:HD23	1.47	0.79
1:1:151:PHE:HE2	1:1:220:TYR:HB2	1.48	0.79
1:2:165:LEU:O	1:2:187:GLN:HA	1.83	0.79
1:5:98:ILE:HD11	1:5:110:TRP:CE2	2.18	0.79
1:5:120:ILE:HB	1:5:283:PRO:HG2	1.64	0.79
1:5:165:LEU:O	1:5:187:GLN:HA	1.82	0.79
1:2:28:ILE:HG21	1:2:37:VAL:HG21	1.65	0.79
1:5:88:TYR:HE1	1:5:205:VAL:HA	1.48	0.79
1:1:284:ARG:HD3	1:1:286:PHE:CZ	2.17	0.78
1:3:98:ILE:HD11	1:3:110:TRP:CE2	2.19	0.78
1:5:321:MET:HE1	1:5:327:GLN:HB2	1.64	0.78
1:4:298:PRO:HG2	1:4:299:TYR:CD2	2.18	0.78
1:6:28:ILE:HG21	1:6:37:VAL:HG21	1.65	0.78
1:2:237:THR:HG22	1:2:239:THR:N	1.98	0.78
1:5:31:GLY:O	1:5:34:VAL:HG23	1.84	0.77
1:1:163:GLY:O	1:1:164:VAL:HG23	1.84	0.77
1:1:112:ALA:HA	1:1:290:LEU:HD23	1.67	0.77
1:3:227:GLY:HA3	1:3:230:VAL:HG13	1.66	0.77
1:1:98:ILE:HD11	1:1:108:LEU:HD12	1.67	0.76
1:4:132:THR:O	1:4:273:THR:HG23	1.85	0.76
1:6:55:MET:HE3	1:6:55:MET:HA	1.66	0.76
1:1:172:TYR:CG	1:1:178:THR:HG21	2.19	0.76
1:2:33:GLU:CD	1:2:33:GLU:H	1.93	0.76
1:4:168:TYR:HB2	1:4:182:ALA:HB1	1.68	0.76
1:5:55:MET:HE1	1:5:266:ILE:HG13	1.66	0.76
1:2:322:ILE:HG22	1:2:323:GLY:H	1.51	0.76
1:5:351:ASP:CG	1:5:352:GLU:H	1.93	0.76
1:5:28:ILE:HG13	1:5:29:LYS:N	1.99	0.76
1:1:88:TYR:CE1	1:1:205:VAL:HA	2.20	0.76
1:1:235:HIS:CD2	1:2:223:THR:HB	2.21	0.76
1:3:132:THR:CG2	1:3:141:GLY:HA3	2.16	0.76
1:4:165:LEU:O	1:4:187:GLN:HA	1.84	0.76
1:5:80:PRO:O	1:5:173:PRO:HG3	1.86	0.76
1:4:137:GLU:CD	1:4:137:GLU:H	1.94	0.76
1:2:109:MET:HE2	1:2:295:VAL:HG21	1.67	0.75
1:1:227:GLY:HA3	1:1:230:VAL:CG1	2.17	0.75
1:5:88:TYR:CE1	1:5:205:VAL:HA	2.21	0.75
1:5:350:ILE:HG12	1:5:355:GLN:HG3	1.68	0.75
1:2:68:SER:HB3	1:2:276:THR:HG21	1.69	0.74
1:3:237:THR:HG23	1:4:220:TYR:O	1.87	0.74
1:6:32:ILE:CD1	1:6:35:LEU:HD12	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:162:GLN:CB	1:1:211:ASP:HB2	2.18	0.74
1:1:256:ALA:O	1:1:258:SER:N	2.21	0.74
1:3:118:GLU:CD	1:3:236:ILE:HG13	2.13	0.73
1:5:51:LEU:HD11	1:5:261:VAL:HG12	1.68	0.73
1:5:359:ARG:CZ	1:5:359:ARG:HB3	2.16	0.73
1:6:112:ALA:HA	1:6:290:LEU:HD23	1.70	0.73
1:1:243:VAL:HG12	1:1:245:LEU:H	1.51	0.73
1:4:237:THR:HG22	1:4:239:THR:H	1.53	0.73
1:6:127:ASN:ND2	1:6:130:SER:H	1.86	0.73
1:1:298:PRO:HG2	1:1:299:TYR:CD1	2.23	0.73
1:3:27:VAL:HG12	1:3:28:ILE:HG22	1.68	0.73
1:2:321:MET:CE	1:2:328:VAL:HG23	2.18	0.73
1:4:139:GLY:HA3	1:5:277:GLN:HE21	1.54	0.73
1:1:32:ILE:HD12	1:1:35:LEU:HD12	1.70	0.73
1:1:209:VAL:HG11	1:5:121:GLY:HA2	1.71	0.73
1:1:299:TYR:CD1	1:1:299:TYR:N	2.54	0.73
1:3:88:TYR:CE1	1:3:205:VAL:HA	2.23	0.73
1:1:165:LEU:O	1:1:187:GLN:HA	1.87	0.73
1:3:73:LYS:HD2	1:3:78:ASP:HA	1.70	0.73
1:4:55:MET:HE1	1:4:266:ILE:HA	1.71	0.72
1:6:80:PRO:HG2	1:6:173:PRO:HD3	1.71	0.72
1:2:322:ILE:HG22	1:2:323:GLY:N	2.04	0.72
1:4:88:TYR:CE1	1:4:205:VAL:HA	2.24	0.72
1:2:109:MET:CE	1:2:295:VAL:HG21	2.20	0.72
1:2:121:GLY:CA	1:3:209:VAL:HG11	2.16	0.72
1:2:123:THR:OG1	1:3:209:VAL:HG12	1.89	0.72
1:5:165:LEU:CD1	1:5:168:TYR:HA	2.19	0.72
1:2:342:GLY:O	1:2:344:PRO:HD3	1.90	0.72
1:3:168:TYR:HD1	1:3:187:GLN:HE21	1.37	0.72
1:1:80:PRO:O	1:1:173:PRO:HG3	1.90	0.71
1:3:132:THR:O	1:3:273:THR:HG23	1.89	0.71
1:4:121:GLY:HA2	1:5:209:VAL:CG1	2.20	0.71
1:5:128:LEU:HD13	1:5:141:GLY:O	1.91	0.71
1:6:32:ILE:HD11	1:6:35:LEU:HD12	1.71	0.71
1:2:321:MET:HE3	1:2:328:VAL:HG23	1.73	0.71
1:5:99:ASN:HD21	1:5:108:LEU:N	1.87	0.71
1:2:34:VAL:O	1:2:37:VAL:HG23	1.90	0.71
1:3:172:TYR:CG	1:3:178:THR:HG21	2.26	0.71
1:4:13:ALA:HB1	1:4:14:PRO:HD2	1.72	0.71
1:1:227:GLY:HA3	1:1:230:VAL:HG13	1.72	0.70
1:2:112:ALA:HA	1:2:290:LEU:HD23	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:112:ALA:HA	1:5:290:LEU:HD23	1.73	0.70
1:2:49:CYS:HB2	1:6:321:MET:HE2	1.74	0.70
1:3:237:THR:HG22	1:3:239:THR:N	2.06	0.70
1:1:99:ASN:HD21	1:1:108:LEU:H	1.39	0.70
1:3:120:ILE:HD11	1:3:285:TYR:HB2	1.72	0.70
1:4:127:ASN:HD21	1:4:130:SER:N	1.89	0.70
1:6:80:PRO:O	1:6:173:PRO:HG3	1.91	0.70
1:1:299:TYR:HD1	1:1:299:TYR:H	1.40	0.70
1:6:98:ILE:HD13	1:6:292:LYS:HG2	1.74	0.70
1:5:26:LEU:HD12	1:5:27:VAL:H	1.54	0.70
1:2:43:SER:HB3	1:6:335:GLU:HG3	1.73	0.70
1:2:55:MET:HE1	1:2:266:ILE:HA	1.71	0.70
1:3:168:TYR:HB2	1:3:182:ALA:HB1	1.74	0.70
1:6:99:ASN:HD21	1:6:107:ILE:HG23	1.55	0.70
1:1:97:ASN:ND2	1:1:99:ASN:H	1.90	0.69
1:3:347:ILE:HB	1:6:299:TYR:OH	1.92	0.69
1:5:120:ILE:O	1:5:282:LEU:HD22	1.92	0.69
1:5:298:PRO:HG2	1:5:299:TYR:CD2	2.28	0.69
1:2:233:VAL:HG13	1:3:225:THR:HG23	1.74	0.69
1:3:140:ALA:H	1:4:277:GLN:NE2	1.88	0.69
1:4:99:ASN:HD22	1:4:108:LEU:H	1.41	0.69
1:6:227:GLY:HA3	1:6:230:VAL:HG13	1.75	0.68
1:3:237:THR:HG21	1:3:239:THR:OG1	1.92	0.68
1:3:281:GLY:O	1:3:282:LEU:HD23	1.93	0.68
1:4:17:PRO:HB3	1:5:108:LEU:HD21	1.76	0.68
1:3:233:VAL:HG22	1:4:225:THR:HG23	1.74	0.68
1:2:125:MET:HE3	1:2:144:ILE:HB	1.75	0.68
1:6:32:ILE:O	1:6:35:LEU:HB2	1.93	0.68
1:2:121:GLY:HA2	1:3:209:VAL:CG1	2.15	0.68
1:4:55:MET:HE2	1:4:280:LYS:C	2.19	0.67
1:6:81:ASP:HB2	1:6:84:GLN:HG3	1.76	0.67
1:1:178:THR:HB	1:1:179:PRO:HD2	1.75	0.67
1:3:284:ARG:HD3	1:3:286:PHE:CZ	2.29	0.67
1:4:99:ASN:ND2	1:4:107:ILE:HA	2.09	0.67
1:1:233:VAL:HG13	1:2:225:THR:HG23	1.75	0.67
1:6:120:ILE:HB	1:6:283:PRO:HG2	1.76	0.67
1:3:88:TYR:HE1	1:3:205:VAL:HA	1.60	0.67
1:4:109:MET:HE3	1:4:295:VAL:HG21	1.76	0.67
1:1:41:VAL:H	1:5:15:LYS:HD2	1.59	0.67
1:4:94:PRO:C	1:4:95:LEU:HD23	2.19	0.67
1:6:162:GLN:NE2	1:6:194:LYS:HD3	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:16:LYS:HG2	1:5:17:PRO:O	1.95	0.67
1:1:86:PRO:O	1:1:205:VAL:HG22	1.95	0.67
1:6:155:GLY:HA3	1:6:218:THR:HB	1.75	0.66
1:1:172:TYR:CB	1:1:178:THR:HG21	2.25	0.66
1:2:55:MET:HE1	1:2:266:ILE:HG13	1.77	0.66
1:2:60:GLU:O	1:3:184:VAL:HG21	1.95	0.66
1:4:237:THR:HG23	1:5:220:TYR:O	1.95	0.66
1:6:127:ASN:C	1:6:127:ASN:HD22	2.03	0.66
1:4:273:THR:CG2	1:5:72:GLU:HB3	2.26	0.66
1:4:118:GLU:OE2	1:4:236:ILE:HG13	1.96	0.66
1:6:243:VAL:HG12	1:6:245:LEU:H	1.60	0.66
1:1:90:VAL:HG22	1:1:91:ALA:N	2.11	0.66
1:5:95:LEU:HD12	1:5:110:TRP:CG	2.31	0.66
1:1:184:VAL:HG12	1:5:63:LYS:HB2	1.76	0.66
1:6:109:MET:CE	1:6:295:VAL:HG21	2.26	0.66
1:4:93:ILE:N	1:4:93:ILE:HD12	2.10	0.66
1:6:28:ILE:HD13	1:6:34:VAL:HG13	1.76	0.65
1:1:28:ILE:HG12	1:1:34:VAL:HG13	1.77	0.65
1:2:21:VAL:HG21	1:3:293:ARG:HH21	1.62	0.65
1:1:120:ILE:HD11	1:1:285:TYR:HB2	1.78	0.65
1:6:175:GLN:HE21	1:6:175:GLN:HA	1.60	0.65
1:6:237:THR:HG21	1:6:239:THR:OG1	1.96	0.65
1:5:32:ILE:HD12	1:5:35:LEU:HD12	1.79	0.65
1:3:112:ALA:HA	1:3:290:LEU:HD23	1.78	0.65
1:4:118:GLU:CD	1:4:236:ILE:HG13	2.21	0.65
1:2:359:ARG:HB3	1:2:359:ARG:CZ	2.27	0.65
1:4:98:ILE:CD1	1:4:292:LYS:HG2	2.26	0.65
1:2:129:HIS:O	1:2:129:HIS:CD2	2.51	0.65
1:6:127:ASN:HD21	1:6:130:SER:N	1.92	0.65
1:1:125:MET:HE3	1:1:144:ILE:HB	1.77	0.64
1:2:132:THR:O	1:3:72:GLU:HG2	1.97	0.64
1:3:342:GLY:CA	1:6:109:MET:HE1	2.26	0.64
1:5:284:ARG:HG2	1:5:285:TYR:N	2.11	0.64
1:6:256:ALA:O	1:6:258:SER:N	2.30	0.64
1:1:156:GLY:HA3	1:1:253:LEU:O	1.98	0.64
1:3:344:PRO:HD2	1:6:255:LYS:HD2	1.78	0.64
1:6:132:THR:HG23	1:6:141:GLY:CA	2.26	0.64
1:2:99:ASN:ND2	1:2:108:LEU:H	1.95	0.64
1:5:73:LYS:HD3	1:5:78:ASP:HA	1.80	0.64
1:3:80:PRO:O	1:3:173:PRO:HG3	1.97	0.64
1:5:125:MET:HE3	1:5:144:ILE:HB	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:49:CYS:HA	1:6:328:VAL:HA	1.78	0.64
1:2:359:ARG:HB3	1:2:359:ARG:NH1	2.13	0.64
1:3:131:GLY:HA3	1:4:75:PHE:HE1	1.63	0.64
1:5:125:MET:CE	1:5:144:ILE:HB	2.28	0.64
1:3:340:LEU:HD12	1:3:341:PRO:HD2	1.79	0.64
1:6:99:ASN:ND2	1:6:107:ILE:HA	2.13	0.64
1:2:199:LYS:HG3	1:2:202:ALA:HB2	1.78	0.64
1:3:157:GLU:HG2	1:3:255:LYS:HD2	1.79	0.64
1:1:284:ARG:HG2	1:1:286:PHE:CE1	2.33	0.64
1:5:99:ASN:HD21	1:5:108:LEU:H	1.45	0.64
1:1:118:GLU:OE2	1:1:236:ILE:HG13	1.99	0.63
1:2:49:CYS:HB2	1:6:321:MET:CE	2.28	0.63
1:3:98:ILE:HD13	1:3:292:LYS:HG2	1.79	0.63
1:4:235:HIS:CD2	1:5:223:THR:HB	2.33	0.63
1:2:32:ILE:HD11	1:2:35:LEU:HD12	1.81	0.63
1:1:18:LYS:H	1:1:18:LYS:HD2	1.63	0.63
1:6:98:ILE:CD1	1:6:292:LYS:HG2	2.29	0.63
1:1:184:VAL:HG21	1:5:60:GLU:O	1.98	0.63
1:3:120:ILE:HB	1:3:283:PRO:HG2	1.81	0.63
1:3:342:GLY:HA2	1:6:109:MET:HE1	1.81	0.62
1:4:243:VAL:HG12	1:4:245:LEU:H	1.63	0.62
1:2:308:LEU:O	1:2:312:ARG:HB2	1.98	0.62
1:3:256:ALA:O	1:3:258:SER:N	2.31	0.62
1:1:309:ILE:HD11	1:5:30:GLY:HA2	1.80	0.62
1:2:86:PRO:O	1:2:205:VAL:HG22	2.00	0.62
1:2:127:ASN:HD22	1:2:129:HIS:H	1.46	0.62
1:4:82:LYS:HD2	1:4:176:THR:HG22	1.82	0.62
1:1:73:LYS:HB2	1:5:129:HIS:O	1.98	0.62
1:3:35:LEU:HD13	1:3:96:PRO:HD3	1.80	0.62
1:4:90:VAL:HG22	1:4:91:ALA:N	2.15	0.62
1:2:256:ALA:O	1:2:258:SER:N	2.32	0.62
1:3:32:ILE:HD11	1:3:35:LEU:HD12	1.82	0.62
1:4:130:SER:O	1:4:132:THR:N	2.32	0.62
1:5:150:HIS:HA	1:5:264:VAL:O	2.00	0.62
1:6:127:ASN:ND2	1:6:129:HIS:H	1.98	0.62
1:1:151:PHE:CE2	1:1:220:TYR:HB2	2.32	0.62
1:3:342:GLY:O	1:3:344:PRO:HD3	2.00	0.62
1:4:93:ILE:HB	1:4:259:LEU:HB3	1.82	0.62
1:1:63:LYS:HB2	1:2:184:VAL:HG12	1.81	0.61
1:1:94:PRO:C	1:1:95:LEU:HD23	2.25	0.61
1:1:189:MET:HG2	1:5:50:PHE:CE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:288:ILE:N	1:1:288:ILE:HD12	2.15	0.61
1:4:125:MET:HB3	1:4:144:ILE:HD12	1.80	0.61
1:5:301:ILE:HD12	1:5:301:ILE:N	2.15	0.61
1:6:127:ASN:HD22	1:6:129:HIS:H	1.46	0.61
1:5:227:GLY:HA3	1:5:230:VAL:HG13	1.81	0.61
1:6:321:MET:HE1	1:6:327:GLN:C	2.25	0.61
1:2:50:PHE:CD1	1:2:50:PHE:C	2.78	0.61
1:4:94:PRO:O	1:4:95:LEU:HD23	2.01	0.61
1:2:43:SER:HB2	1:6:334:TYR:O	1.99	0.61
1:1:125:MET:HE2	1:2:224:TYR:CE2	2.36	0.61
1:3:237:THR:HG22	1:3:238:ASN:N	2.15	0.61
1:2:305:LEU:N	1:2:305:LEU:HD23	2.15	0.61
1:4:172:TYR:CG	1:4:178:THR:HG21	2.35	0.61
1:5:95:LEU:HD12	1:5:110:TRP:CD1	2.35	0.61
1:6:107:ILE:HG22	1:6:108:LEU:N	2.15	0.61
1:6:114:THR:HG23	1:6:241:THR:HG23	1.83	0.61
1:1:157:GLU:HG2	1:1:255:LYS:HD3	1.82	0.61
1:2:300:PRO:O	1:2:304:LEU:HG	2.01	0.61
1:3:168:TYR:CE1	1:3:169:ARG:HD2	2.35	0.60
1:4:58:PRO:HG2	1:4:62:GLN:HB2	1.82	0.60
1:1:188:GLN:HG3	1:1:189:MET:N	2.16	0.60
1:1:190:ASN:C	1:1:190:ASN:HD22	2.09	0.60
1:5:237:THR:CG2	1:5:239:THR:OG1	2.49	0.60
1:6:165:LEU:O	1:6:187:GLN:HA	2.01	0.60
1:4:99:ASN:ND2	1:4:108:LEU:N	2.49	0.60
1:4:112:ALA:HA	1:4:290:LEU:HD23	1.82	0.60
1:1:172:TYR:HB3	1:1:178:THR:HG21	1.83	0.60
1:2:214:LYS:O	1:2:216:GLU:N	2.35	0.60
1:3:133:GLN:HA	1:3:273:THR:HA	1.83	0.60
1:5:168:TYR:HB2	1:5:182:ALA:HB1	1.83	0.60
1:5:178:THR:HB	1:5:179:PRO:HD2	1.83	0.60
1:6:99:ASN:HD21	1:6:107:ILE:CG2	2.14	0.60
1:2:28:ILE:HD13	1:2:34:VAL:HG13	1.82	0.60
1:2:94:PRO:O	1:2:95:LEU:HD23	2.02	0.60
1:2:99:ASN:HA	1:2:102:LEU:HB2	1.82	0.60
1:4:55:MET:HE3	1:4:279:TRP:HB3	1.83	0.60
1:6:98:ILE:CG2	1:6:108:LEU:HB3	2.31	0.60
1:1:118:GLU:CD	1:1:236:ILE:HG13	2.26	0.60
1:1:132:THR:O	1:2:72:GLU:HG2	2.02	0.60
1:4:137:GLU:CD	1:4:137:GLU:N	2.56	0.60
1:4:152:PHE:HA	1:4:263:ALA:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:131:GLY:HA3	1:2:75:PHE:CE1	2.37	0.60
1:2:237:THR:HG23	1:3:220:TYR:O	2.01	0.60
1:2:205:VAL:HG11	1:2:264:VAL:HG11	1.84	0.60
1:3:237:THR:CG2	1:3:239:THR:H	2.11	0.60
1:4:334:TYR:N	1:4:334:TYR:CD1	2.69	0.60
1:5:177:VAL:HG11	1:5:203:TYR:CE2	2.36	0.60
1:5:300:PRO:HD2	1:5:303:PHE:HB3	1.83	0.60
1:5:190:ASN:C	1:5:190:ASN:HD22	2.09	0.59
1:4:32:ILE:O	1:4:35:LEU:HB2	2.02	0.59
1:4:237:THR:HG21	1:4:239:THR:OG1	2.01	0.59
1:4:199:LYS:HG3	1:4:202:ALA:HB2	1.84	0.59
1:5:55:MET:CE	1:5:279:TRP:HB3	2.31	0.59
1:2:98:ILE:HD11	1:2:108:LEU:C	2.27	0.59
1:3:61:HIS:HD2	1:4:168:TYR:OH	1.85	0.59
1:5:32:ILE:CD1	1:5:35:LEU:HD12	2.31	0.59
1:5:94:PRO:C	1:5:95:LEU:HD23	2.28	0.59
1:4:28:ILE:HG12	1:4:34:VAL:CG1	2.32	0.59
1:5:165:LEU:CD2	1:5:179:PRO:HG3	2.33	0.59
1:6:33:GLU:HG2	1:6:34:VAL:N	2.17	0.59
1:1:298:PRO:CG	1:1:299:TYR:CE1	2.83	0.59
1:3:82:LYS:HD3	1:3:175:GLN:HB2	1.84	0.59
1:4:82:LYS:HD3	1:4:175:GLN:HB2	1.84	0.59
1:6:132:THR:HG23	1:6:141:GLY:HA3	1.84	0.59
1:1:28:ILE:HG12	1:1:34:VAL:CG1	2.33	0.59
1:5:111:GLU:OE1	1:5:293:ARG:NH1	2.35	0.59
1:5:288:ILE:HD12	1:5:288:ILE:N	2.17	0.59
1:6:112:ALA:HB3	1:6:252:PRO:HD2	1.83	0.59
1:1:65:LEU:HD22	1:1:278:GLN:HG3	1.84	0.59
1:2:123:THR:HB	1:3:205:VAL:O	2.03	0.59
1:2:80:PRO:HD2	1:2:171:LYS:O	2.03	0.58
1:2:44:PHE:HB2	1:2:290:LEU:O	2.03	0.58
1:1:32:ILE:O	1:1:35:LEU:HB2	2.03	0.58
1:1:326:SER:OG	1:1:328:VAL:HG13	2.03	0.58
1:5:163:GLY:O	1:5:164:VAL:HG23	2.03	0.58
1:1:243:VAL:HG12	1:1:245:LEU:N	2.18	0.58
1:2:111:GLU:OE2	1:2:250:VAL:HA	2.03	0.58
1:3:285:TYR:CD1	1:3:285:TYR:C	2.81	0.58
1:2:227:GLY:HA3	1:2:230:VAL:HG13	1.84	0.58
1:3:165:LEU:O	1:3:187:GLN:HA	2.04	0.58
1:6:28:ILE:CD1	1:6:34:VAL:HG13	2.33	0.58
1:1:162:GLN:HE21	1:1:194:LYS:NZ	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:301:ILE:H	1:3:301:ILE:HD13	1.69	0.58
1:4:237:THR:HG22	1:4:239:THR:N	2.17	0.58
1:1:99:ASN:ND2	1:1:107:ILE:HG23	2.18	0.58
1:1:285:TYR:HE2	1:2:213:SER:HA	1.69	0.58
1:3:284:ARG:HG2	1:3:286:PHE:CE1	2.39	0.58
1:3:285:TYR:CE2	1:4:212:PRO:HB2	2.39	0.58
1:1:55:MET:HE2	1:1:280:LYS:C	2.28	0.57
1:1:93:ILE:HG22	1:1:95:LEU:HD21	1.85	0.57
1:4:107:ILE:HG22	1:4:108:LEU:H	1.68	0.57
1:5:113:VAL:HG13	1:5:245:LEU:HD21	1.85	0.57
1:5:221:PHE:N	1:5:221:PHE:CD1	2.70	0.57
1:5:286:PHE:HB3	1:5:288:ILE:HD11	1.85	0.57
1:1:76:THR:O	1:1:171:LYS:HE3	2.03	0.57
1:2:55:MET:HE3	1:2:279:TRP:HB3	1.86	0.57
1:5:245:LEU:N	1:5:245:LEU:CD2	2.67	0.57
1:1:270:PHE:O	1:1:277:GLN:HA	2.05	0.57
1:4:151:PHE:CD1	1:4:151:PHE:C	2.81	0.57
1:4:298:PRO:HG2	1:4:299:TYR:H	1.68	0.57
1:5:65:LEU:HB3	1:5:278:GLN:HE21	1.68	0.57
1:6:301:ILE:O	1:6:304:LEU:HB3	2.04	0.57
1:4:120:ILE:HD11	1:4:285:TYR:HB2	1.85	0.57
1:5:270:PHE:CD1	1:5:271:THR:N	2.68	0.57
1:5:343:ASP:O	1:5:346:MET:HB3	2.05	0.57
1:1:130:SER:C	1:1:132:THR:H	2.13	0.57
1:1:21:VAL:HG21	1:2:293:ARG:HH21	1.70	0.57
1:2:27:VAL:HG12	1:2:28:ILE:HG22	1.86	0.57
1:3:125:MET:HE2	1:4:224:TYR:HE2	1.69	0.57
1:4:109:MET:SD	1:4:255:LYS:HA	2.45	0.57
1:5:137:GLU:CD	1:5:137:GLU:H	2.13	0.57
1:3:221:PHE:N	1:3:221:PHE:CD1	2.73	0.57
1:4:320:PRO:O	1:4:327:GLN:HG3	2.05	0.57
1:5:95:LEU:HD23	1:5:95:LEU:N	2.20	0.57
1:2:32:ILE:O	1:2:35:LEU:HB2	2.05	0.56
1:2:231:PRO:HB2	1:3:226:GLY:O	2.05	0.56
1:3:125:MET:HE2	1:4:224:TYR:CE2	2.40	0.56
1:3:304:LEU:HA	1:3:307:ASP:HB3	1.86	0.56
1:4:259:LEU:HD12	1:4:260:TYR:H	1.70	0.56
1:4:321:MET:HE1	1:4:327:GLN:HB2	1.85	0.56
1:5:303:PHE:CE1	1:5:307:ASP:HB2	2.40	0.56
1:6:112:ALA:O	1:6:251:GLY:HA3	2.05	0.56
1:1:277:GLN:HE21	1:5:139:GLY:CA	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:106:ASN:O	1:5:107:ILE:HD13	2.05	0.56
1:5:133:GLN:O	1:5:141:GLY:HA2	2.05	0.56
1:1:93:ILE:HG22	1:1:95:LEU:CD2	2.36	0.56
1:1:160:GLU:C	1:1:161:LEU:HD23	2.31	0.56
1:1:190:ASN:O	1:1:192:ASP:N	2.39	0.56
1:1:270:PHE:HD1	1:1:271:THR:N	2.04	0.56
1:1:273:THR:HG23	1:2:72:GLU:CG	2.36	0.56
1:2:45:THR:CG2	1:6:333:VAL:HG22	2.30	0.56
1:5:339:GLU:O	1:5:341:PRO:HD3	2.05	0.56
1:2:26:LEU:HD12	1:6:333:VAL:O	2.04	0.56
1:5:118:GLU:CD	1:5:236:ILE:HG13	2.31	0.56
1:1:79:SER:CB	1:1:171:LYS:HB2	2.23	0.56
1:2:321:MET:HE3	1:2:321:MET:HA	1.86	0.56
1:1:269:LEU:HD21	1:1:279:TRP:CE3	2.40	0.56
1:4:107:ILE:HG22	1:4:108:LEU:N	2.21	0.56
1:1:60:GLU:O	1:2:184:VAL:HG11	2.06	0.56
1:1:86:PRO:HG2	1:1:279:TRP:CD1	2.41	0.56
1:5:130:SER:O	1:5:132:THR:N	2.38	0.56
1:1:285:TYR:CD1	1:1:286:PHE:N	2.74	0.56
1:2:307:ASP:O	1:2:311:ARG:HB3	2.06	0.56
1:6:55:MET:CE	1:6:86:PRO:HB3	2.36	0.56
1:2:163:GLY:O	1:2:164:VAL:HG23	2.05	0.56
1:3:131:GLY:HA3	1:4:75:PHE:CE1	2.41	0.56
1:4:259:LEU:HD12	1:4:260:TYR:N	2.21	0.56
1:5:301:ILE:CD1	1:5:302:SER:H	2.19	0.56
1:6:108:LEU:HD23	1:6:294:SER:HA	1.88	0.56
1:3:143:PRO:HG2	1:3:145:GLN:NE2	2.21	0.55
1:4:99:ASN:HD22	1:4:108:LEU:N	2.03	0.55
1:4:150:HIS:CE1	1:4:267:CYS:HA	2.41	0.55
1:3:111:GLU:OE2	1:3:250:VAL:HA	2.07	0.55
1:5:133:GLN:HG3	1:5:134:LYS:H	1.71	0.55
1:6:202:ALA:O	1:6:204:PRO:HD3	2.05	0.55
1:1:310:ASN:CG	1:1:311:ARG:N	2.64	0.55
1:4:129:HIS:HD2	1:5:78:ASP:OD2	1.88	0.55
1:5:211:ASP:OD2	1:5:214:LYS:HG2	2.07	0.55
1:1:120:ILE:N	1:1:120:ILE:HD12	2.21	0.55
1:3:285:TYR:CD2	1:4:212:PRO:HB2	2.42	0.55
1:5:172:TYR:CG	1:5:178:THR:HG21	2.41	0.55
1:5:286:PHE:HB3	1:5:288:ILE:CD1	2.35	0.55
1:1:203:TYR:H	1:1:203:TYR:HD1	1.51	0.55
1:2:99:ASN:HD21	1:2:108:LEU:H	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:231:PRO:O	1:2:231:PRO:HG2	2.06	0.55
1:2:257:ASP:OD2	1:3:350:ILE:HD11	2.07	0.55
1:1:243:VAL:CG1	1:1:245:LEU:H	2.19	0.55
1:6:55:MET:HE3	1:6:86:PRO:HB3	1.89	0.55
1:6:99:ASN:HD21	1:6:107:ILE:HA	1.70	0.55
1:1:139:GLY:HA2	1:2:277:GLN:HE21	1.71	0.55
1:1:168:TYR:HB2	1:1:182:ALA:HB1	1.88	0.55
1:2:32:ILE:O	1:2:32:ILE:HD12	2.07	0.55
1:3:94:PRO:C	1:3:95:LEU:HD23	2.32	0.55
1:3:140:ALA:N	1:4:277:GLN:HE21	1.98	0.55
1:4:186:SER:HA	1:4:190:ASN:HB2	1.89	0.55
1:1:238:ASN:HB3	1:2:220:TYR:CE2	2.42	0.55
1:2:55:MET:HE2	1:2:280:LYS:C	2.32	0.55
1:2:90:VAL:HG22	1:2:91:ALA:N	2.21	0.55
1:2:102:LEU:HD21	1:2:108:LEU:HD12	1.88	0.55
1:3:270:PHE:O	1:3:277:GLN:HA	2.07	0.55
1:4:70:ALA:HB2	1:4:84:GLN:HE22	1.70	0.55
1:3:162:GLN:NE2	1:3:194:LYS:HD3	2.22	0.54
1:3:303:PHE:CE2	1:6:350:ILE:HG12	2.42	0.54
1:6:350:ILE:HD13	1:6:350:ILE:O	2.07	0.54
1:1:282:LEU:HD23	1:1:283:PRO:HD2	1.89	0.54
1:2:284:ARG:HG2	1:2:286:PHE:CE1	2.42	0.54
1:3:299:TYR:N	1:3:300:PRO:HD2	2.22	0.54
1:4:340:LEU:HD12	1:4:341:PRO:N	2.23	0.54
1:5:118:GLU:OE2	1:5:236:ILE:HG13	2.07	0.54
1:5:284:ARG:HD3	1:5:286:PHE:CZ	2.43	0.54
1:3:199:LYS:HG3	1:3:202:ALA:HB2	1.89	0.54
1:4:73:LYS:HD3	1:4:78:ASP:HA	1.90	0.54
1:6:243:VAL:HG12	1:6:245:LEU:N	2.23	0.54
1:3:220:TYR:C	1:3:221:PHE:CG	2.85	0.54
1:6:285:TYR:CD1	1:6:285:TYR:C	2.86	0.54
1:5:28:ILE:HG12	1:5:34:VAL:CG1	2.37	0.54
1:1:32:ILE:CD1	1:1:35:LEU:HD12	2.38	0.54
1:2:137:GLU:H	1:2:137:GLU:CD	2.16	0.54
1:2:188:GLN:HG3	1:2:189:MET:N	2.23	0.54
1:3:220:TYR:C	1:3:221:PHE:CD1	2.85	0.54
1:4:136:HIS:O	1:4:136:HIS:CD2	2.61	0.54
1:6:151:PHE:CD1	1:6:151:PHE:C	2.84	0.54
1:1:73:LYS:HE2	1:1:79:SER:H	1.72	0.54
1:1:203:TYR:CD1	1:1:203:TYR:N	2.75	0.54
1:3:297:ASN:OD1	1:3:300:PRO:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:73:LYS:CD	1:1:78:ASP:HA	2.29	0.53
1:2:352:GLU:C	1:2:353:PHE:CG	2.86	0.53
1:4:61:HIS:CD2	1:5:168:TYR:OH	2.60	0.53
1:4:111:GLU:OE1	1:4:293:ARG:NH1	2.41	0.53
1:1:212:PRO:HB2	1:5:285:TYR:CE2	2.43	0.53
1:2:132:THR:HG21	1:2:141:GLY:HA3	1.90	0.53
1:1:123:THR:O	1:1:126:LEU:HB2	2.09	0.53
1:1:277:GLN:HE21	1:5:139:GLY:HA3	1.74	0.53
1:4:22:GLN:HA	1:4:22:GLN:OE1	2.08	0.53
1:5:164:VAL:HG22	1:5:188:GLN:O	2.08	0.53
1:6:100:GLU:O	1:6:101:ASP:HB3	2.08	0.53
1:6:107:ILE:HG22	1:6:108:LEU:H	1.73	0.53
1:1:339:GLU:O	1:1:341:PRO:HD3	2.07	0.53
1:2:359:ARG:CZ	1:2:359:ARG:CB	2.86	0.53
1:4:98:ILE:HD11	1:4:110:TRP:CE2	2.44	0.53
1:5:156:GLY:HA3	1:5:253:LEU:O	2.09	0.53
1:6:90:VAL:HG22	1:6:91:ALA:N	2.22	0.53
1:6:111:GLU:OE1	1:6:293:ARG:NH1	2.40	0.53
1:6:120:ILE:HD11	1:6:285:TYR:HB2	1.90	0.53
1:6:132:THR:HG23	1:6:141:GLY:HA2	1.88	0.53
1:6:229:ASN:N	1:6:229:ASN:ND2	2.55	0.53
1:6:122:VAL:HG23	1:6:123:THR:N	2.23	0.53
1:6:172:TYR:CG	1:6:178:THR:HG21	2.43	0.53
1:1:23:VAL:HG23	1:1:24:PRO:HG2	1.91	0.53
1:5:113:VAL:C	1:5:244:LEU:HD12	2.33	0.53
1:5:168:TYR:CE1	1:5:169:ARG:HD2	2.43	0.53
1:6:114:THR:HG23	1:6:241:THR:CG2	2.38	0.53
1:6:152:PHE:CD1	1:6:152:PHE:C	2.87	0.53
1:1:139:GLY:CA	1:2:277:GLN:HE21	2.22	0.53
1:3:211:ASP:OD2	1:3:214:LYS:HG2	2.09	0.53
1:3:32:ILE:CD1	1:3:35:LEU:HD12	2.39	0.53
1:5:301:ILE:N	1:5:301:ILE:CD1	2.72	0.53
1:6:219:ARG:NH2	1:6:246:ASP:HB3	2.24	0.53
1:3:297:ASN:CG	1:3:300:PRO:HD3	2.34	0.53
1:4:28:ILE:CD1	1:4:34:VAL:HG13	2.38	0.53
1:4:128:LEU:HD13	1:4:141:GLY:O	2.09	0.53
1:5:26:LEU:HD12	1:5:27:VAL:N	2.23	0.53
1:1:147:SER:O	1:1:268:GLY:HA2	2.09	0.53
1:1:162:GLN:NE2	1:1:194:LYS:HD3	2.23	0.53
1:2:118:GLU:CD	1:2:236:ILE:HG13	2.34	0.53
1:4:90:VAL:HG22	1:4:91:ALA:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:137:GLU:CD	1:6:137:GLU:H	2.17	0.53
1:6:190:ASN:C	1:6:190:ASN:HD22	2.16	0.53
1:4:214:LYS:O	1:4:216:GLU:N	2.42	0.52
1:5:99:ASN:ND2	1:5:107:ILE:HA	2.24	0.52
1:5:237:THR:HG22	1:5:238:ASN:N	2.24	0.52
1:5:300:PRO:C	1:5:301:ILE:HD12	2.33	0.52
1:6:229:ASN:N	1:6:229:ASN:HD22	2.07	0.52
1:1:88:TYR:HB3	1:1:197:LEU:HD21	1.91	0.52
1:1:98:ILE:HD12	1:1:98:ILE:O	2.10	0.52
1:2:298:PRO:HG2	1:2:299:TYR:CD1	2.45	0.52
1:3:111:GLU:OE1	1:3:293:ARG:NH1	2.42	0.52
1:6:297:ASN:OD1	1:6:298:PRO:HD2	2.08	0.52
1:5:266:ILE:N	1:5:266:ILE:HD12	2.24	0.52
1:5:321:MET:CE	1:5:327:GLN:HB2	2.37	0.52
1:1:295:VAL:C	1:5:20:PRO:HG3	2.34	0.52
1:2:33:GLU:CD	1:2:33:GLU:N	2.67	0.52
1:2:112:ALA:HA	1:2:290:LEU:CD2	2.38	0.52
1:2:350:ILE:HG23	1:2:354:GLY:O	2.08	0.52
1:4:112:ALA:O	1:4:251:GLY:HA3	2.09	0.52
1:1:115:VAL:HG22	1:1:117:THR:HG22	1.90	0.52
1:3:32:ILE:O	1:3:35:LEU:HB2	2.09	0.52
1:3:285:TYR:CD1	1:3:286:PHE:N	2.78	0.52
1:3:298:PRO:C	1:3:300:PRO:HD2	2.35	0.52
1:4:139:GLY:HA2	1:5:277:GLN:HG3	1.92	0.52
1:4:270:PHE:O	1:4:277:GLN:HA	2.10	0.52
1:5:321:MET:SD	1:5:328:VAL:HG23	2.50	0.52
1:2:284:ARG:HD3	1:2:286:PHE:CZ	2.45	0.52
1:3:125:MET:CE	1:4:224:TYR:HE2	2.22	0.52
1:1:160:GLU:O	1:1:161:LEU:HD23	2.09	0.52
1:1:237:THR:HG23	1:2:220:TYR:O	2.10	0.52
1:2:162:GLN:NE2	1:2:194:LYS:HD3	2.24	0.52
1:3:98:ILE:HD11	1:3:110:TRP:CD2	2.44	0.52
1:3:130:SER:O	1:3:132:THR:N	2.43	0.52
1:1:321:MET:SD	1:1:327:GLN:HB2	2.50	0.52
1:3:48:GLU:OE2	1:4:213:SER:O	2.28	0.52
1:3:122:VAL:HG23	1:4:224:TYR:HB2	1.91	0.52
1:4:66:SER:O	1:4:278:GLN:NE2	2.42	0.52
1:4:98:ILE:HG21	1:4:108:LEU:HB3	1.91	0.52
1:5:99:ASN:ND2	1:5:108:LEU:H	2.08	0.52
1:1:125:MET:HE2	1:2:224:TYR:HE2	1.73	0.52
1:1:163:GLY:HA2	1:1:207:CYS:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:237:THR:HG22	1:1:238:ASN:N	2.25	0.52
1:1:286:PHE:HB3	1:1:288:ILE:HD11	1.92	0.52
1:2:49:CYS:SG	1:2:286:PHE:HB2	2.50	0.52
1:2:111:GLU:OE1	1:2:293:ARG:NH1	2.43	0.52
1:2:168:TYR:HD1	1:2:187:GLN:HE21	1.58	0.52
1:4:201:ASN:C	1:4:201:ASN:HD22	2.18	0.52
1:1:207:CYS:HB2	1:1:208:TRP:CD1	2.45	0.52
1:3:151:PHE:CE2	1:3:220:TYR:HB2	2.45	0.52
1:5:122:VAL:O	1:5:125:MET:HG3	2.10	0.52
1:5:326:SER:OG	1:5:328:VAL:HB	2.10	0.52
1:5:351:ASP:CG	1:5:352:GLU:N	2.66	0.52
1:6:94:PRO:O	1:6:95:LEU:HD23	2.09	0.52
1:1:153:ALA:HA	1:1:219:ARG:O	2.10	0.51
1:1:285:TYR:CE2	1:2:212:PRO:HB2	2.45	0.51
1:1:311:ARG:C	1:1:313:THR:H	2.16	0.51
1:2:55:MET:CE	1:2:266:ILE:HA	2.40	0.51
1:2:360:MET:HG3	1:2:361:GLN:H	1.74	0.51
1:3:101:ASP:C	1:3:103:THR:H	2.18	0.51
1:3:150:HIS:CE1	1:3:267:CYS:HA	2.45	0.51
1:4:284:ARG:HG2	1:4:286:PHE:CE1	2.45	0.51
1:4:301:ILE:CD1	1:4:301:ILE:H	2.23	0.51
1:5:158:PRO:HB2	1:5:196:VAL:CG2	2.39	0.51
1:1:241:THR:HG22	1:1:242:THR:N	2.26	0.51
1:1:310:ASN:OD1	1:1:311:ARG:HB2	2.10	0.51
1:2:162:GLN:HE21	1:2:194:LYS:NZ	2.09	0.51
1:3:61:HIS:HB3	1:4:169:ARG:NH1	2.24	0.51
1:3:320:PRO:HD2	1:3:327:GLN:NE2	2.26	0.51
1:4:293:ARG:HD2	1:4:294:SER:H	1.76	0.51
1:5:114:THR:N	1:5:244:LEU:HD12	2.25	0.51
1:4:298:PRO:HG2	1:4:299:TYR:N	2.25	0.51
1:6:57:ASN:OD1	1:6:63:LYS:HA	2.11	0.51
1:2:188:GLN:HG3	1:2:189:MET:H	1.76	0.51
1:4:99:ASN:ND2	1:4:108:LEU:H	2.06	0.51
1:1:352:GLU:C	1:1:353:PHE:CG	2.88	0.51
1:2:314:GLN:OE1	1:2:314:GLN:HA	2.10	0.51
1:3:347:ILE:HB	1:6:299:TYR:CZ	2.45	0.51
1:4:48:GLU:HA	1:4:286:PHE:O	2.11	0.51
1:4:145:GLN:HE22	1:5:228:GLU:HB2	1.76	0.51
1:5:133:GLN:HG3	1:5:134:LYS:N	2.26	0.51
1:5:151:PHE:C	1:5:151:PHE:CD1	2.88	0.51
1:5:288:ILE:HG22	1:5:289:THR:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:285:TYR:CD1	1:1:285:TYR:C	2.89	0.51
1:3:107:ILE:O	1:3:108:LEU:HD23	2.11	0.51
1:5:108:LEU:HD23	1:5:294:SER:HA	1.92	0.51
1:5:115:VAL:HG22	1:5:117:THR:HG22	1.92	0.51
1:5:311:ARG:HG2	1:5:311:ARG:HH11	1.74	0.51
1:1:237:THR:CG2	1:1:239:THR:OG1	2.58	0.51
1:2:87:CYS:HA	1:2:204:PRO:HA	1.91	0.51
1:4:301:ILE:H	1:4:301:ILE:HD13	1.75	0.51
1:5:220:TYR:C	1:5:221:PHE:CD1	2.89	0.51
1:6:237:THR:HG22	1:6:238:ASN:N	2.24	0.51
1:6:284:ARG:HD3	1:6:286:PHE:CZ	2.45	0.51
1:1:136:HIS:CE1	1:2:277:GLN:NE2	2.79	0.51
1:2:237:THR:HG21	1:2:239:THR:OG1	2.11	0.51
1:2:281:GLY:O	1:2:282:LEU:HD23	2.11	0.51
1:4:98:ILE:HD11	1:4:110:TRP:CD2	2.46	0.51
1:5:270:PHE:CD1	1:5:270:PHE:C	2.87	0.51
1:6:165:LEU:CD2	1:6:165:LEU:N	2.72	0.51
1:1:90:VAL:HG22	1:1:91:ALA:H	1.74	0.51
1:2:140:ALA:H	1:3:277:GLN:NE2	2.09	0.51
1:2:185:ASP:O	1:2:190:ASN:HB2	2.09	0.51
1:4:146:GLY:C	1:4:230:VAL:HG23	2.36	0.51
1:4:245:LEU:N	1:4:245:LEU:HD23	2.26	0.51
1:5:53:PRO:HD3	1:5:283:PRO:HA	1.92	0.51
1:6:94:PRO:C	1:6:95:LEU:HD23	2.36	0.51
1:1:66:SER:HB3	1:1:279:TRP:HB2	1.93	0.51
1:1:84:GLN:C	1:1:85:LEU:HD23	2.36	0.51
1:1:209:VAL:CG1	1:5:121:GLY:HA2	2.38	0.51
1:1:351:ASP:OD1	1:1:354:GLY:N	2.44	0.51
1:2:84:GLN:C	1:2:85:LEU:HD23	2.36	0.51
1:3:48:GLU:HG2	1:3:285:TYR:OH	2.11	0.51
1:4:266:ILE:HD12	1:4:266:ILE:N	2.25	0.51
1:6:23:VAL:HB	1:6:24:PRO:HD2	1.92	0.51
1:1:107:ILE:HG22	1:1:108:LEU:N	2.26	0.50
1:1:223:THR:HA	1:5:234:LEU:O	2.11	0.50
1:3:50:PHE:CD1	1:3:50:PHE:C	2.89	0.50
1:3:90:VAL:HG23	1:3:262:SER:HB3	1.91	0.50
1:4:205:VAL:HG11	1:4:264:VAL:HG11	1.92	0.50
1:6:190:ASN:C	1:6:190:ASN:ND2	2.69	0.50
1:2:127:ASN:HD22	1:2:127:ASN:C	2.20	0.50
1:3:243:VAL:HG12	1:3:244:LEU:N	2.26	0.50
1:4:121:GLY:CA	1:5:209:VAL:HG11	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:133:GLN:CG	1:5:134:LYS:N	2.75	0.50
1:1:130:SER:O	1:1:132:THR:N	2.45	0.50
1:3:33:GLU:CD	1:3:33:GLU:H	2.18	0.50
1:5:55:MET:HE2	1:5:279:TRP:HB3	1.92	0.50
1:1:229:ASN:N	1:1:229:ASN:ND2	2.60	0.50
1:3:151:PHE:CD1	1:3:151:PHE:C	2.90	0.50
1:3:293:ARG:HD2	1:3:294:SER:H	1.76	0.50
1:4:188:GLN:HG3	1:4:189:MET:N	2.26	0.50
1:5:64:GLY:O	1:5:65:LEU:HG	2.12	0.50
1:5:117:THR:HB	1:5:285:TYR:O	2.12	0.50
1:2:221:PHE:CD1	1:2:221:PHE:N	2.79	0.50
1:3:128:LEU:O	1:3:132:THR:HG21	2.11	0.50
1:4:27:VAL:HG12	1:4:28:ILE:CG2	2.22	0.50
1:5:184:VAL:O	1:5:187:GLN:HB2	2.12	0.50
1:3:69:LEU:HD11	1:3:279:TRP:CD1	2.46	0.50
1:3:81:ASP:O	1:3:84:GLN:HG3	2.12	0.50
1:3:115:VAL:HA	1:3:287:LYS:O	2.11	0.50
1:3:190:ASN:O	1:3:192:ASP:N	2.45	0.50
1:3:340:LEU:HD12	1:3:341:PRO:CD	2.40	0.50
1:5:127:ASN:C	1:5:127:ASN:HD22	2.20	0.50
1:1:229:ASN:N	1:1:229:ASN:HD22	2.09	0.50
1:4:28:ILE:HG12	1:4:34:VAL:HG11	1.93	0.50
1:5:237:THR:CG2	1:5:238:ASN:N	2.73	0.50
1:4:63:LYS:HD2	1:5:184:VAL:HB	1.94	0.50
1:4:79:SER:HB2	1:4:171:LYS:HB2	1.93	0.50
1:5:49:CYS:SG	1:5:50:PHE:N	2.85	0.50
1:6:175:GLN:HA	1:6:175:GLN:NE2	2.24	0.50
1:1:66:SER:O	1:1:278:GLN:NE2	2.45	0.49
1:1:120:ILE:HD11	1:1:285:TYR:CB	2.40	0.49
1:2:69:LEU:HG	1:2:278:GLN:HA	1.93	0.49
1:2:167:ASN:ND2	1:2:170:THR:OG1	2.45	0.49
1:2:151:PHE:CD1	1:2:151:PHE:C	2.90	0.49
1:2:272:ASN:HD22	1:2:276:THR:HB	1.77	0.49
1:2:351:ASP:OD1	1:2:351:ASP:N	2.45	0.49
1:3:138:ASN:O	1:4:276:THR:HA	2.12	0.49
1:3:156:GLY:HA3	1:3:253:LEU:O	2.12	0.49
1:3:178:THR:HB	1:3:179:PRO:HD2	1.94	0.49
1:3:296:LYS:HD3	1:6:339:GLU:HB2	1.93	0.49
1:5:270:PHE:HD1	1:5:270:PHE:C	2.19	0.49
1:4:93:ILE:HG22	1:4:95:LEU:CD2	2.42	0.49
1:2:229:ASN:N	1:2:229:ASN:ND2	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:128:LEU:O	1:4:132:THR:HG21	2.12	0.49
1:4:139:GLY:CA	1:5:277:GLN:HE21	2.25	0.49
1:2:57:ASN:OD1	1:2:63:LYS:HA	2.12	0.49
1:2:82:LYS:HD2	1:2:176:THR:HG22	1.94	0.49
1:2:220:TYR:C	1:2:221:PHE:CG	2.90	0.49
1:4:125:MET:HE2	1:5:224:TYR:OH	2.13	0.49
1:5:88:TYR:CD1	1:5:205:VAL:HG12	2.47	0.49
1:5:133:GLN:HA	1:5:273:THR:HA	1.95	0.49
1:5:152:PHE:CD1	1:5:152:PHE:C	2.89	0.49
1:6:332:ARG:HD3	1:6:334:TYR:OH	2.13	0.49
1:2:237:THR:HG22	1:2:238:ASN:N	2.26	0.49
1:2:304:LEU:HA	1:6:308:LEU:HD11	1.94	0.49
1:3:23:VAL:HG13	1:3:24:PRO:HD2	1.94	0.49
1:5:162:GLN:NE2	1:5:194:LYS:HD3	2.28	0.49
1:1:60:GLU:O	1:2:184:VAL:CG1	2.61	0.49
1:1:237:THR:HG22	1:1:239:THR:N	2.13	0.49
1:2:248:GLN:HB2	1:2:250:VAL:HG13	1.95	0.49
1:4:28:ILE:HG12	1:4:34:VAL:HG13	1.95	0.49
1:2:203:TYR:N	1:2:203:TYR:CD1	2.81	0.49
1:4:305:LEU:O	1:4:309:ILE:HG13	2.13	0.49
1:5:199:LYS:CG	1:5:202:ALA:HB2	2.34	0.49
1:6:28:ILE:CG1	1:6:29:LYS:N	2.75	0.49
1:1:68:SER:HB3	1:1:276:THR:HG21	1.95	0.49
1:1:120:ILE:HD12	1:1:120:ILE:H	1.78	0.49
1:5:86:PRO:CG	1:5:279:TRP:CD1	2.96	0.49
1:1:348:ARG:HA	1:1:356:THR:O	2.13	0.48
1:2:98:ILE:HD11	1:2:109:MET:N	2.27	0.48
1:2:339:GLU:O	1:2:341:PRO:HD3	2.13	0.48
1:3:115:VAL:HG13	1:3:242:THR:HB	1.94	0.48
1:5:98:ILE:HD11	1:5:110:TRP:CZ2	2.48	0.48
1:6:50:PHE:CD1	1:6:50:PHE:C	2.91	0.48
1:2:353:PHE:CD1	1:2:353:PHE:N	2.80	0.48
1:3:237:THR:CG2	1:3:239:THR:OG1	2.61	0.48
1:5:151:PHE:CG	1:5:152:PHE:N	2.80	0.48
1:6:237:THR:CG2	1:6:239:THR:OG1	2.60	0.48
1:1:23:VAL:HG23	1:1:24:PRO:CD	2.43	0.48
1:1:109:MET:CE	1:1:295:VAL:HG21	2.43	0.48
1:1:146:GLY:C	1:1:230:VAL:HG22	2.38	0.48
1:2:80:PRO:O	1:2:173:PRO:HD3	2.13	0.48
1:2:180:LYS:O	1:2:181:ASN:HB2	2.12	0.48
1:3:321:MET:SD	1:3:328:VAL:HG23	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:84:GLN:O	1:4:86:PRO:HD3	2.13	0.48
1:6:55:MET:SD	1:6:281:GLY:HA3	2.53	0.48
1:6:151:PHE:CG	1:6:152:PHE:N	2.80	0.48
1:1:60:GLU:C	1:1:62:GLN:H	2.22	0.48
1:1:87:CYS:HB3	1:1:203:TYR:O	2.13	0.48
1:3:88:TYR:HB3	1:3:197:LEU:HD21	1.95	0.48
1:5:109:MET:SD	1:5:255:LYS:HA	2.54	0.48
1:1:51:LEU:HD11	1:1:261:VAL:HG12	1.96	0.48
1:2:93:ILE:HB	1:2:259:LEU:HB3	1.95	0.48
1:2:338:GLU:CD	1:2:348:ARG:HH12	2.22	0.48
1:4:211:ASP:HA	1:4:212:PRO:HD2	1.58	0.48
1:4:270:PHE:CD1	1:4:270:PHE:C	2.90	0.48
1:5:92:ARG:O	1:5:94:PRO:HD3	2.13	0.48
1:1:214:LYS:HB3	1:1:214:LYS:HE2	1.72	0.48
1:2:85:LEU:HD23	1:2:85:LEU:N	2.26	0.48
1:2:133:GLN:HA	1:2:273:THR:HA	1.95	0.48
1:3:98:ILE:HD11	1:3:110:TRP:CZ2	2.49	0.48
1:1:35:LEU:HD23	1:1:35:LEU:HA	1.57	0.48
1:2:93:ILE:HG12	1:6:321:MET:HG3	1.96	0.48
1:2:172:TYR:CB	1:2:178:THR:HG21	2.43	0.48
1:2:204:PRO:HG2	1:2:207:CYS:SG	2.54	0.48
1:4:125:MET:HE3	1:4:144:ILE:HB	1.96	0.48
1:5:280:LYS:HG3	1:5:281:GLY:N	2.28	0.48
1:1:40:GLY:HA3	1:5:15:LYS:HE2	1.95	0.48
1:1:69:LEU:HD11	1:1:279:TRP:CD1	2.48	0.48
1:4:220:TYR:C	1:4:221:PHE:CD1	2.92	0.48
1:5:27:VAL:C	1:5:28:ILE:HG22	2.39	0.48
1:5:256:ALA:O	1:5:258:SER:N	2.47	0.48
1:6:98:ILE:HD11	1:6:110:TRP:CE2	2.49	0.48
1:2:322:ILE:CG2	1:2:323:GLY:N	2.75	0.48
1:3:194:LYS:HZ2	1:3:211:ASP:CG	2.22	0.48
1:3:302:SER:HA	1:3:305:LEU:HB2	1.95	0.48
1:2:270:PHE:CD1	1:2:270:PHE:C	2.91	0.48
1:3:241:THR:HG22	1:3:242:THR:N	2.28	0.48
1:4:80:PRO:O	1:4:173:PRO:HG3	2.14	0.48
1:5:28:ILE:HG12	1:5:34:VAL:HG13	1.96	0.48
1:5:90:VAL:HG22	1:5:91:ALA:H	1.78	0.48
1:1:229:ASN:HD22	1:1:229:ASN:H	1.61	0.47
1:1:358:THR:OG1	1:1:359:ARG:N	2.46	0.47
1:4:15:LYS:HA	1:5:41:VAL:HB	1.96	0.47
1:6:130:SER:O	1:6:132:THR:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:35:LEU:HD23	1:3:35:LEU:HA	1.67	0.47
1:4:52:ASN:OD1	1:5:189:MET:HB2	2.14	0.47
1:4:300:PRO:O	1:4:303:PHE:HB3	2.14	0.47
1:5:128:LEU:HD21	1:5:143:PRO:HB3	1.94	0.47
1:5:162:GLN:HA	1:5:193:HIS:O	2.14	0.47
1:5:285:TYR:C	1:5:286:PHE:CD1	2.92	0.47
1:6:237:THR:CG2	1:6:238:ASN:N	2.76	0.47
1:1:15:LYS:HA	1:1:15:LYS:HD3	1.77	0.47
1:1:288:ILE:HG22	1:1:289:THR:N	2.28	0.47
1:1:334:TYR:N	1:1:334:TYR:CD1	2.81	0.47
1:6:118:GLU:OE2	1:6:236:ILE:HG13	2.14	0.47
1:6:158:PRO:HG3	1:6:260:TYR:CE2	2.49	0.47
1:1:17:PRO:HG3	1:2:106:ASN:HB3	1.96	0.47
1:1:90:VAL:CG2	1:1:91:ALA:N	2.76	0.47
1:1:127:ASN:HD22	1:1:129:HIS:H	1.61	0.47
1:1:151:PHE:CG	1:1:152:PHE:N	2.83	0.47
1:3:308:LEU:HG	1:3:309:ILE:N	2.30	0.47
1:4:107:ILE:O	1:4:108:LEU:HD23	2.14	0.47
1:5:146:GLY:C	1:5:230:VAL:HG22	2.40	0.47
1:6:86:PRO:O	1:6:205:VAL:HG22	2.15	0.47
1:2:90:VAL:HG22	1:2:91:ALA:H	1.79	0.47
1:3:130:SER:C	1:3:132:THR:H	2.22	0.47
1:3:180:LYS:O	1:3:181:ASN:HB2	2.13	0.47
1:4:152:PHE:CD1	1:4:152:PHE:C	2.92	0.47
1:4:165:LEU:CD1	1:4:168:TYR:HA	2.36	0.47
1:5:93:ILE:HA	1:5:94:PRO:HD3	1.43	0.47
1:5:162:GLN:HE21	1:5:194:LYS:NZ	2.11	0.47
1:1:165:LEU:HD11	1:1:168:TYR:HA	1.96	0.47
1:1:211:ASP:HA	1:1:212:PRO:HD2	1.43	0.47
1:2:98:ILE:CD1	1:2:108:LEU:HB3	2.45	0.47
1:2:162:GLN:HB2	1:2:211:ASP:HB2	1.97	0.47
1:2:348:ARG:HA	1:2:356:THR:O	2.14	0.47
1:3:133:GLN:CG	1:3:134:LYS:N	2.77	0.47
1:4:50:PHE:CD1	1:4:50:PHE:C	2.93	0.47
1:4:237:THR:CG2	1:4:239:THR:OG1	2.61	0.47
1:1:86:PRO:CG	1:1:279:TRP:CD1	2.98	0.47
1:1:138:ASN:O	1:2:276:THR:HA	2.14	0.47
1:1:199:LYS:O	1:1:202:ALA:HB3	2.15	0.47
1:1:282:LEU:CD2	1:1:283:PRO:HD2	2.43	0.47
1:3:125:MET:HE1	1:3:232:PRO:HG3	1.96	0.47
1:3:148:ASN:HB2	1:3:266:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:190:ASN:HD22	1:3:190:ASN:C	2.22	0.47
1:4:33:GLU:H	1:4:33:GLU:CD	2.22	0.47
1:4:125:MET:HE2	1:5:224:TYR:CE2	2.50	0.47
1:4:220:TYR:C	1:4:221:PHE:CG	2.93	0.47
1:5:30:GLY:HA3	1:5:34:VAL:HG21	1.97	0.47
1:5:74:GLN:HA	1:5:74:GLN:OE1	2.14	0.47
1:5:90:VAL:HG22	1:5:91:ALA:N	2.30	0.47
1:5:95:LEU:CB	1:5:110:TRP:CD1	2.97	0.47
1:6:107:ILE:CD1	1:6:298:PRO:HD2	2.45	0.47
1:1:168:TYR:HD2	1:1:182:ALA:O	1.98	0.47
1:1:220:TYR:C	1:1:221:PHE:CD1	2.93	0.47
1:4:129:HIS:CD2	1:5:78:ASP:OD2	2.67	0.47
1:2:129:HIS:O	1:2:129:HIS:CG	2.65	0.47
1:4:109:MET:CE	1:4:295:VAL:HG21	2.42	0.47
1:5:285:TYR:CE1	1:5:287:LYS:HB2	2.50	0.47
1:6:90:VAL:HG22	1:6:91:ALA:H	1.79	0.47
1:1:28:ILE:CG1	1:1:29:LYS:N	2.78	0.47
1:1:286:PHE:HB3	1:1:288:ILE:CD1	2.45	0.47
1:1:295:VAL:O	1:5:20:PRO:HG3	2.15	0.47
1:5:211:ASP:HA	1:5:212:PRO:HD2	1.72	0.47
1:6:26:LEU:HD11	1:6:28:ILE:O	2.15	0.47
1:6:241:THR:HG22	1:6:242:THR:N	2.28	0.47
1:1:94:PRO:O	1:1:95:LEU:HD23	2.14	0.46
1:1:202:ALA:HB3	1:1:203:TYR:CD1	2.50	0.46
1:1:305:LEU:H	1:1:305:LEU:HD22	1.80	0.46
1:3:126:LEU:HD21	1:4:224:TYR:HE1	1.80	0.46
1:3:127:ASN:C	1:3:127:ASN:HD22	2.23	0.46
1:4:84:GLN:C	1:4:85:LEU:HD23	2.40	0.46
1:4:108:LEU:HA	1:4:293:ARG:O	2.15	0.46
1:5:137:GLU:CD	1:5:137:GLU:N	2.70	0.46
1:1:311:ARG:C	1:1:313:THR:N	2.74	0.46
1:2:15:LYS:HB2	1:3:41:VAL:HB	1.97	0.46
1:3:61:HIS:CD2	1:4:168:TYR:OH	2.66	0.46
1:4:112:ALA:HB3	1:4:252:PRO:HD2	1.97	0.46
1:2:265:ASP:OD1	1:2:284:ARG:NH1	2.49	0.46
1:3:28:ILE:HG12	1:3:34:VAL:CG1	2.45	0.46
1:3:94:PRO:O	1:3:95:LEU:HD23	2.15	0.46
1:4:39:THR:HB	1:4:43:SER:HB3	1.97	0.46
1:4:128:LEU:HD21	1:4:143:PRO:HB3	1.97	0.46
1:4:130:SER:C	1:4:132:THR:H	2.24	0.46
1:4:158:PRO:HB2	1:4:196:VAL:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:48:GLU:HG2	1:5:285:TYR:OH	2.15	0.46
1:5:138:ASN:OD1	1:5:138:ASN:N	2.49	0.46
1:5:269:LEU:HA	1:5:269:LEU:HD23	1.66	0.46
1:6:98:ILE:HG21	1:6:108:LEU:HB3	1.97	0.46
1:2:245:LEU:HD23	1:2:245:LEU:HA	1.67	0.46
1:3:319:GLN:HA	1:3:320:PRO:HD3	1.60	0.46
1:4:39:THR:HB	1:4:43:SER:CB	2.45	0.46
1:4:55:MET:CE	1:4:266:ILE:HA	2.42	0.46
1:4:73:LYS:NZ	1:4:80:PRO:HA	2.30	0.46
1:5:132:THR:CG2	1:5:141:GLY:HA3	2.45	0.46
1:1:120:ILE:HB	1:1:283:PRO:HG2	1.98	0.46
1:1:273:THR:HG23	1:2:72:GLU:HG2	1.98	0.46
1:3:227:GLY:HA3	1:3:230:VAL:CG1	2.41	0.46
1:4:180:LYS:HA	1:4:180:LYS:HD3	1.71	0.46
1:4:270:PHE:C	1:4:270:PHE:HD1	2.24	0.46
1:4:341:PRO:HA	1:4:343:ASP:OD1	2.15	0.46
1:5:23:VAL:HB	1:5:24:PRO:CD	2.38	0.46
1:1:124:ALA:C	1:1:126:LEU:H	2.24	0.46
1:1:211:ASP:OD2	1:1:214:LYS:HG2	2.15	0.46
1:2:68:SER:HB3	1:2:276:THR:CG2	2.42	0.46
1:3:122:VAL:CG2	1:4:224:TYR:HB2	2.46	0.46
1:4:92:ARG:HD2	1:4:258:SER:HB3	1.97	0.46
1:6:325:SER:O	1:6:326:SER:C	2.57	0.46
1:2:35:LEU:HA	1:2:35:LEU:HD23	1.68	0.46
1:3:135:THR:HG22	1:3:136:HIS:ND1	2.30	0.46
1:3:308:LEU:HA	1:3:311:ARG:HD3	1.97	0.46
1:3:339:GLU:O	1:3:341:PRO:HD3	2.16	0.46
1:4:116:LYS:HB2	1:4:287:LYS:HB3	1.97	0.46
1:5:55:MET:O	1:5:66:SER:HA	2.16	0.46
1:5:259:LEU:HD12	1:5:260:TYR:N	2.29	0.46
1:6:107:ILE:HD12	1:6:298:PRO:CD	2.45	0.46
1:1:139:GLY:CA	1:2:277:GLN:NE2	2.79	0.46
1:2:115:VAL:HG22	1:2:116:LYS:N	2.31	0.46
1:2:220:TYR:C	1:2:221:PHE:CD1	2.94	0.46
1:5:284:ARG:HB2	1:5:284:ARG:HH11	1.81	0.46
1:6:80:PRO:HD2	1:6:171:LYS:O	2.15	0.46
1:6:321:MET:CE	1:6:328:VAL:HG23	2.36	0.46
1:2:15:LYS:HD3	1:3:41:VAL:CB	2.31	0.46
1:2:23:VAL:O	1:6:337:THR:HA	2.16	0.46
1:2:152:PHE:HA	1:2:263:ALA:HA	1.97	0.46
1:5:229:ASN:N	1:5:229:ASN:ND2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:123:THR:HG1	1:3:209:VAL:HG12	1.80	0.46
1:2:211:ASP:CG	1:2:214:LYS:HG2	2.40	0.46
1:6:163:GLY:HA2	1:6:207:CYS:O	2.15	0.46
1:6:220:TYR:C	1:6:221:PHE:CG	2.93	0.46
1:6:345:ASP:O	1:6:346:MET:C	2.59	0.46
1:1:49:CYS:SG	1:1:50:PHE:N	2.88	0.45
1:1:200:ASP:C	1:1:202:ALA:N	2.71	0.45
1:1:285:TYR:HE2	1:2:213:SER:CA	2.29	0.45
1:2:49:CYS:CB	1:6:321:MET:HE2	2.45	0.45
1:2:211:ASP:OD2	1:2:214:LYS:HG2	2.16	0.45
1:2:313:THR:HG22	1:2:314:GLN:H	1.81	0.45
1:3:26:LEU:HD12	1:3:27:VAL:N	2.31	0.45
1:4:55:MET:HE2	1:4:280:LYS:O	2.15	0.45
1:4:285:TYR:C	1:4:286:PHE:CD1	2.95	0.45
1:5:175:GLN:HE21	1:5:175:GLN:HA	1.81	0.45
1:5:303:PHE:O	1:5:304:LEU:C	2.59	0.45
1:1:69:LEU:HD11	1:1:279:TRP:NE1	2.32	0.45
1:3:203:TYR:HA	1:3:204:PRO:HD2	1.74	0.45
1:4:152:PHE:CD1	1:4:153:ALA:N	2.84	0.45
1:4:219:ARG:NH2	1:4:246:ASP:HB3	2.31	0.45
1:4:245:LEU:HD13	1:4:249:GLY:C	2.41	0.45
1:6:233:VAL:O	1:6:234:LEU:HD23	2.16	0.45
1:3:44:PHE:CD1	1:3:44:PHE:C	2.94	0.45
1:4:125:MET:HE2	1:5:224:TYR:CZ	2.52	0.45
1:4:270:PHE:HD1	1:4:271:THR:N	2.14	0.45
1:5:30:GLY:HA3	1:5:34:VAL:CG2	2.47	0.45
1:5:304:LEU:HA	1:5:304:LEU:HD23	1.71	0.45
1:6:168:TYR:CE1	1:6:169:ARG:HD2	2.51	0.45
1:3:265:ASP:OD2	1:3:284:ARG:NH1	2.49	0.45
1:4:175:GLN:HA	1:4:175:GLN:HE21	1.82	0.45
1:6:122:VAL:CG2	1:6:123:THR:N	2.80	0.45
1:6:132:THR:O	1:6:273:THR:HG23	2.16	0.45
1:6:334:TYR:N	1:6:334:TYR:CD1	2.84	0.45
1:1:33:GLU:C	1:1:35:LEU:N	2.74	0.45
1:4:17:PRO:CB	1:5:108:LEU:HD21	2.43	0.45
1:6:146:GLY:C	1:6:230:VAL:HG22	2.41	0.45
1:1:55:MET:HE1	1:1:266:ILE:HG13	1.98	0.45
1:1:269:LEU:CD2	1:1:279:TRP:CE3	3.00	0.45
1:2:63:LYS:HB2	1:3:184:VAL:HG12	1.97	0.45
1:2:88:TYR:CE1	1:2:205:VAL:HA	2.51	0.45
1:2:156:GLY:HA3	1:2:253:LEU:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:219:ARG:NH2	1:2:246:ASP:HB3	2.31	0.45
1:2:340:LEU:HA	1:2:341:PRO:HD2	1.82	0.45
1:4:167:ASN:ND2	1:4:170:THR:OG1	2.50	0.45
1:4:301:ILE:O	1:4:302:SER:C	2.59	0.45
1:5:95:LEU:HB2	1:5:110:TRP:CD1	2.52	0.45
1:5:284:ARG:CG	1:5:285:TYR:N	2.79	0.45
1:5:300:PRO:O	1:5:303:PHE:N	2.49	0.45
1:1:310:ASN:HB3	1:5:28:ILE:HD11	1.99	0.45
1:5:30:GLY:CA	1:5:34:VAL:HG21	2.46	0.45
1:6:28:ILE:HG12	1:6:34:VAL:HG11	1.97	0.45
1:6:81:ASP:O	1:6:82:LYS:C	2.58	0.45
1:1:285:TYR:CD2	1:2:212:PRO:HB2	2.52	0.45
1:2:124:ALA:C	1:2:126:LEU:H	2.24	0.45
1:2:168:TYR:CE2	1:2:169:ARG:HG3	2.51	0.45
1:3:293:ARG:HD2	1:3:294:SER:N	2.32	0.45
1:4:151:PHE:CG	1:4:152:PHE:N	2.84	0.45
1:5:109:MET:HG3	1:5:295:VAL:HG21	1.99	0.45
1:1:33:GLU:O	1:1:35:LEU:N	2.50	0.45
1:1:266:ILE:N	1:1:266:ILE:HD12	2.32	0.45
1:2:59:ASP:OD1	1:2:62:GLN:N	2.50	0.45
1:2:179:PRO:HB3	1:2:193:HIS:CG	2.52	0.45
1:3:304:LEU:CA	1:3:307:ASP:HB3	2.47	0.45
1:4:17:PRO:HG3	1:5:106:ASN:HB3	1.99	0.45
1:4:81:ASP:HB2	1:4:84:GLN:HG3	1.99	0.45
1:5:190:ASN:O	1:5:192:ASP:N	2.50	0.45
1:6:107:ILE:HD12	1:6:298:PRO:HD2	1.98	0.45
1:6:108:LEU:HD23	1:6:108:LEU:HA	1.57	0.45
1:1:28:ILE:CD1	1:1:34:VAL:HG13	2.47	0.44
1:1:312:ARG:O	1:1:314:GLN:N	2.49	0.44
1:2:109:MET:HE3	1:2:295:VAL:HG21	1.98	0.44
1:2:140:ALA:H	1:3:277:GLN:HE21	1.64	0.44
1:2:172:TYR:CG	1:2:178:THR:HG21	2.52	0.44
1:2:214:LYS:HE2	1:2:214:LYS:HB3	1.74	0.44
1:3:114:THR:HG23	1:3:115:VAL:N	2.31	0.44
1:3:172:TYR:CD2	1:3:178:THR:HG21	2.51	0.44
1:5:76:THR:O	1:5:171:LYS:HE3	2.17	0.44
1:5:151:PHE:CD1	1:5:152:PHE:N	2.84	0.44
1:5:153:ALA:HB2	1:5:220:TYR:CB	2.47	0.44
1:6:301:ILE:H	1:6:301:ILE:HD12	1.82	0.44
1:1:73:LYS:HD3	1:1:77:ASP:O	2.17	0.44
1:1:111:GLU:CD	1:1:291:ARG:HH21	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:309:ILE:HG12	1:1:310:ASN:HD22	1.81	0.44
1:2:23:VAL:HB	1:2:24:PRO:HD2	1.99	0.44
1:2:93:ILE:CG1	1:6:321:MET:HG3	2.48	0.44
1:3:127:ASN:ND2	1:3:129:HIS:CD2	2.85	0.44
1:3:297:ASN:HA	1:3:298:PRO:HD2	1.83	0.44
1:4:35:LEU:HD23	1:4:35:LEU:HA	1.55	0.44
1:4:65:LEU:HA	1:4:279:TRP:O	2.15	0.44
1:1:133:GLN:HA	1:1:273:THR:HA	1.99	0.44
1:1:144:ILE:HD13	1:1:280:LYS:HB3	1.99	0.44
1:1:148:ASN:HB2	1:1:266:ILE:O	2.17	0.44
1:2:351:ASP:CG	1:2:352:GLU:H	2.24	0.44
1:3:61:HIS:O	1:4:187:GLN:NE2	2.50	0.44
1:3:98:ILE:CG2	1:3:108:LEU:HB2	2.46	0.44
1:3:151:PHE:HE2	1:3:220:TYR:HB2	1.82	0.44
1:3:203:TYR:CD1	1:3:203:TYR:N	2.85	0.44
1:3:319:GLN:NE2	1:3:327:GLN:OE1	2.50	0.44
1:4:180:LYS:O	1:4:181:ASN:HB2	2.17	0.44
1:5:305:LEU:HD12	1:5:309:ILE:HG13	1.99	0.44
1:6:194:LYS:HD2	1:6:211:ASP:OD2	2.16	0.44
1:1:79:SER:HA	1:1:171:LYS:O	2.17	0.44
1:2:32:ILE:CD1	1:2:35:LEU:HD12	2.46	0.44
1:2:172:TYR:HB3	1:2:178:THR:HG21	1.99	0.44
1:3:80:PRO:O	1:3:173:PRO:CG	2.65	0.44
1:4:162:GLN:HB2	1:4:211:ASP:HB2	1.98	0.44
1:4:175:GLN:HA	1:4:175:GLN:NE2	2.32	0.44
1:5:220:TYR:C	1:5:221:PHE:CG	2.95	0.44
1:5:322:ILE:HG23	1:5:323:GLY:N	2.33	0.44
1:1:270:PHE:C	1:1:270:PHE:CD1	2.96	0.44
1:1:309:ILE:HG22	1:1:312:ARG:HB2	2.00	0.44
1:4:133:GLN:HB2	1:4:272:ASN:O	2.17	0.44
1:5:165:LEU:HD23	1:5:179:PRO:HG3	2.00	0.44
1:6:127:ASN:ND2	1:6:127:ASN:C	2.73	0.44
1:6:157:GLU:OE2	1:6:255:LYS:HE3	2.17	0.44
1:5:131:GLY:O	1:5:273:THR:OG1	2.33	0.44
1:5:270:PHE:O	1:5:277:GLN:HA	2.18	0.44
1:5:300:PRO:O	1:5:301:ILE:C	2.61	0.44
1:3:120:ILE:HD12	1:3:120:ILE:H	1.83	0.44
1:4:238:ASN:HB3	1:5:220:TYR:CE2	2.53	0.44
1:4:282:LEU:HA	1:4:282:LEU:HD23	1.73	0.44
1:6:227:GLY:HA3	1:6:230:VAL:CG1	2.46	0.44
1:6:288:ILE:N	1:6:288:ILE:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:28:ILE:HG13	1:1:29:LYS:N	2.31	0.44
1:1:219:ARG:NH2	1:1:246:ASP:HB3	2.32	0.44
1:2:18:LYS:H	1:2:18:LYS:HG3	1.53	0.44
1:4:329:GLU:O	1:4:330:GLU:HB2	2.18	0.44
1:5:120:ILE:HD12	1:5:120:ILE:N	2.32	0.44
1:5:125:MET:HE3	1:5:144:ILE:HD12	2.00	0.44
1:5:162:GLN:OE1	1:5:163:GLY:O	2.35	0.44
1:1:67:LYS:O	1:1:68:SER:C	2.61	0.44
1:1:351:ASP:OD1	1:1:351:ASP:N	2.50	0.44
1:2:24:PRO:HA	1:6:336:ASP:O	2.18	0.44
1:2:127:ASN:ND2	1:2:129:HIS:H	2.15	0.44
1:2:207:CYS:HB2	1:2:208:TRP:CD1	2.52	0.44
1:3:67:LYS:HG2	1:3:68:SER:N	2.33	0.44
1:5:35:LEU:HA	1:5:35:LEU:HD23	1.70	0.44
1:5:214:LYS:HB3	1:5:214:LYS:HE2	1.79	0.44
1:6:88:TYR:CE1	1:6:205:VAL:HA	2.53	0.44
1:6:321:MET:SD	1:6:327:GLN:HB2	2.58	0.44
1:6:350:ILE:C	1:6:352:GLU:N	2.75	0.44
1:1:253:LEU:HA	1:1:253:LEU:HD23	1.41	0.43
1:2:132:THR:CG2	1:2:141:GLY:HA3	2.48	0.43
1:3:282:LEU:HD23	1:3:282:LEU:HA	1.73	0.43
1:4:305:LEU:HD11	1:4:309:ILE:HD11	2.00	0.43
1:5:37:VAL:HG12	1:5:38:LYS:O	2.18	0.43
1:5:146:GLY:O	1:5:230:VAL:HG22	2.18	0.43
1:6:99:ASN:HD21	1:6:107:ILE:CA	2.30	0.43
1:6:168:TYR:HD1	1:6:187:GLN:HE21	1.65	0.43
1:6:231:PRO:HA	1:6:232:PRO:HD2	1.84	0.43
1:1:108:LEU:HD23	1:1:108:LEU:HA	1.82	0.43
1:1:288:ILE:N	1:1:288:ILE:CD1	2.81	0.43
1:3:118:GLU:OE2	1:3:236:ILE:HG13	2.17	0.43
1:3:135:THR:O	1:3:136:HIS:HB3	2.18	0.43
1:4:33:GLU:O	1:4:35:LEU:N	2.51	0.43
1:4:50:PHE:O	1:4:51:LEU:HD23	2.18	0.43
1:4:120:ILE:O	1:4:282:LEU:HD13	2.18	0.43
1:4:237:THR:HG22	1:4:238:ASN:N	2.32	0.43
1:5:285:TYR:CD1	1:5:286:PHE:N	2.87	0.43
1:2:22:GLN:CG	1:6:337:THR:HB	2.30	0.43
1:3:102:LEU:C	1:3:104:CYS:N	2.72	0.43
1:3:152:PHE:CD1	1:3:152:PHE:C	2.96	0.43
1:4:57:ASN:OD1	1:4:63:LYS:HA	2.17	0.43
1:4:303:PHE:O	1:4:304:LEU:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:199:LYS:HG3	1:5:202:ALA:CB	2.34	0.43
1:5:227:GLY:HA3	1:5:230:VAL:CG1	2.47	0.43
1:5:237:THR:CG2	1:5:239:THR:H	2.23	0.43
1:5:267:CYS:SG	1:5:282:LEU:HD12	2.58	0.43
1:1:28:ILE:CG1	1:1:34:VAL:HG13	2.44	0.43
1:2:343:ASP:O	1:2:346:MET:HB3	2.18	0.43
1:3:98:ILE:HG22	1:3:108:LEU:HB2	2.01	0.43
1:3:129:HIS:HD2	1:4:78:ASP:OD2	2.00	0.43
1:3:243:VAL:HG12	1:3:245:LEU:N	2.06	0.43
1:4:84:GLN:O	1:4:85:LEU:HD23	2.19	0.43
1:6:23:VAL:O	1:6:24:PRO:C	2.61	0.43
1:6:87:CYS:HA	1:6:204:PRO:HA	2.00	0.43
1:6:109:MET:HE2	1:6:295:VAL:HG21	1.98	0.43
1:6:286:PHE:CD1	1:6:286:PHE:N	2.85	0.43
1:1:297:ASN:HB3	1:1:300:PRO:CG	2.49	0.43
1:3:343:ASP:HA	1:3:344:PRO:HD3	1.74	0.43
1:4:146:GLY:O	1:4:147:SER:C	2.61	0.43
1:4:284:ARG:HD3	1:4:286:PHE:CZ	2.53	0.43
1:4:293:ARG:HD2	1:4:294:SER:N	2.33	0.43
1:5:265:ASP:CG	1:5:284:ARG:HH12	2.27	0.43
1:5:301:ILE:HD13	1:5:302:SER:H	1.83	0.43
1:6:33:GLU:CG	1:6:34:VAL:N	2.81	0.43
1:2:285:TYR:HE2	1:3:213:SER:HA	1.83	0.43
1:2:304:LEU:HD23	1:2:304:LEU:N	2.32	0.43
1:2:347:ILE:O	1:2:357:THR:HA	2.19	0.43
1:3:307:ASP:O	1:3:311:ARG:HD3	2.19	0.43
1:4:168:TYR:CE1	1:4:169:ARG:HD2	2.53	0.43
1:4:241:THR:HG22	1:4:242:THR:N	2.33	0.43
1:6:99:ASN:ND2	1:6:108:LEU:H	2.16	0.43
1:1:112:ALA:O	1:1:251:GLY:HA3	2.18	0.43
1:3:296:LYS:O	1:3:297:ASN:C	2.62	0.43
1:4:162:GLN:HA	1:4:193:HIS:O	2.18	0.43
1:4:167:ASN:H	1:4:187:GLN:CD	2.27	0.43
1:4:290:LEU:HD23	1:4:290:LEU:HA	1.79	0.43
1:5:50:PHE:O	1:5:51:LEU:HD23	2.18	0.43
1:5:95:LEU:HD12	1:5:110:TRP:CB	2.49	0.43
1:5:288:ILE:N	1:5:288:ILE:CD1	2.82	0.43
1:6:33:GLU:HG2	1:6:34:VAL:H	1.80	0.43
1:2:300:PRO:HG2	1:2:303:PHE:HB2	2.00	0.43
1:4:67:LYS:O	1:4:68:SER:C	2.61	0.43
1:4:162:GLN:CB	1:4:211:ASP:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:67:LYS:O	1:5:68:SER:C	2.61	0.43
1:1:232:PRO:HD2	1:2:226:GLY:O	2.18	0.43
1:2:168:TYR:CG	1:2:183:THR:O	2.71	0.43
1:3:93:ILE:HA	1:3:94:PRO:HD3	1.63	0.43
1:3:127:ASN:HD22	1:3:129:HIS:H	1.66	0.43
1:3:306:SER:O	1:3:307:ASP:C	2.61	0.43
1:4:93:ILE:HA	1:4:94:PRO:HD3	1.80	0.43
1:5:114:THR:HG23	1:5:241:THR:CG2	2.48	0.43
1:5:284:ARG:CD	1:5:286:PHE:CZ	3.02	0.43
1:1:152:PHE:CD1	1:1:152:PHE:C	2.97	0.43
1:1:318:GLY:O	1:1:319:GLN:C	2.61	0.43
1:5:87:CYS:HB3	1:5:203:TYR:O	2.19	0.43
1:5:120:ILE:HD11	1:5:285:TYR:HB2	2.01	0.43
1:1:69:LEU:HD11	1:1:279:TRP:CE2	2.54	0.42
1:1:172:TYR:CD2	1:1:178:THR:HG21	2.54	0.42
1:2:196:VAL:O	1:2:196:VAL:HG13	2.18	0.42
1:3:315:ARG:NH1	1:3:315:ARG:HG2	2.34	0.42
1:4:79:SER:HA	1:4:171:LYS:O	2.18	0.42
1:5:180:LYS:O	1:5:181:ASN:HB2	2.18	0.42
1:5:277:GLN:O	1:5:278:GLN:HB3	2.18	0.42
1:5:288:ILE:CG2	1:5:289:THR:N	2.82	0.42
1:1:352:GLU:O	1:1:353:PHE:CG	2.72	0.42
1:2:280:LYS:HG3	1:2:281:GLY:N	2.35	0.42
1:4:55:MET:HE1	1:4:266:ILE:HG13	2.01	0.42
1:4:136:HIS:CE1	1:5:277:GLN:NE2	2.87	0.42
1:6:288:ILE:HG22	1:6:289:THR:N	2.33	0.42
1:1:107:ILE:N	1:1:107:ILE:HD13	2.34	0.42
1:1:134:LYS:HB2	1:1:134:LYS:HE3	1.71	0.42
1:1:159:LEU:HG	1:1:161:LEU:HD21	2.02	0.42
1:1:222:GLY:C	1:1:223:THR:CG2	2.92	0.42
1:2:78:ASP:O	1:2:170:THR:HG23	2.20	0.42
1:2:112:ALA:O	1:2:251:GLY:HA3	2.19	0.42
1:2:150:HIS:HA	1:2:264:VAL:O	2.19	0.42
1:3:243:VAL:CG1	1:3:244:LEU:N	2.83	0.42
1:4:93:ILE:N	1:4:93:ILE:CD1	2.79	0.42
1:6:64:GLY:C	1:6:65:LEU:HG	2.44	0.42
1:6:146:GLY:HA2	1:6:229:ASN:HA	2.01	0.42
1:6:220:TYR:C	1:6:221:PHE:CD1	2.97	0.42
1:6:307:ASP:O	1:6:308:LEU:C	2.62	0.42
1:6:353:PHE:HD1	1:6:353:PHE:HA	1.73	0.42
1:1:16:LYS:HG2	1:1:17:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:93:ILE:HB	1:1:259:LEU:HB3	2.01	0.42
1:1:175:GLN:H	1:1:175:GLN:HG2	1.51	0.42
1:2:307:ASP:O	1:2:308:LEU:C	2.62	0.42
1:3:220:TYR:C	1:3:220:TYR:CD1	2.98	0.42
1:4:136:HIS:CD2	1:4:136:HIS:C	2.98	0.42
1:6:47:VAL:O	1:6:287:LYS:HA	2.19	0.42
1:6:250:VAL:HG23	1:6:251:GLY:O	2.20	0.42
1:1:131:GLY:HA3	1:2:75:PHE:HE1	1.81	0.42
1:1:224:TYR:CB	1:5:122:VAL:CG2	2.97	0.42
1:1:317:ASP:O	1:1:318:GLY:O	2.37	0.42
1:1:336:ASP:CG	1:1:337:THR:H	2.27	0.42
1:2:180:LYS:HA	1:2:180:LYS:HD3	1.81	0.42
1:2:333:VAL:HG12	1:2:334:TYR:N	2.35	0.42
1:3:266:ILE:N	1:3:266:ILE:HD12	2.35	0.42
1:4:132:THR:HG22	1:4:133:GLN:N	2.35	0.42
1:6:280:LYS:CG	1:6:281:GLY:N	2.82	0.42
1:1:90:VAL:CG2	1:1:91:ALA:H	2.33	0.42
1:1:311:ARG:HH21	1:5:33:GLU:HG2	1.85	0.42
1:2:126:LEU:HD21	1:3:224:TYR:HE2	1.84	0.42
1:2:168:TYR:CD1	1:2:184:VAL:HA	2.55	0.42
1:4:123:THR:HB	1:5:205:VAL:O	2.20	0.42
1:4:325:SER:O	1:4:326:SER:C	2.62	0.42
1:6:34:VAL:C	1:6:36:GLY:N	2.75	0.42
1:6:118:GLU:CD	1:6:236:ILE:HG13	2.45	0.42
1:6:315:ARG:HD2	1:6:315:ARG:C	2.45	0.42
1:6:319:GLN:HA	1:6:320:PRO:HD3	1.48	0.42
1:1:65:LEU:HA	1:1:65:LEU:HD23	1.83	0.42
1:2:98:ILE:HG13	1:2:108:LEU:HB2	2.01	0.42
1:2:340:LEU:HD12	1:2:341:PRO:N	2.35	0.42
1:3:28:ILE:HG12	1:3:34:VAL:HG13	2.01	0.42
1:4:285:TYR:C	1:4:285:TYR:CD1	2.98	0.42
1:5:152:PHE:CD1	1:5:153:ALA:N	2.88	0.42
1:5:322:ILE:CG2	1:5:323:GLY:N	2.83	0.42
1:1:67:LYS:HB2	1:1:83:GLU:HB3	2.01	0.42
1:1:84:GLN:O	1:1:86:PRO:HD3	2.19	0.42
1:1:209:VAL:HG11	1:5:121:GLY:CA	2.45	0.42
1:2:115:VAL:HG13	1:2:242:THR:HB	2.00	0.42
1:3:99:ASN:ND2	1:3:108:LEU:O	2.52	0.42
1:3:130:SER:C	1:3:132:THR:N	2.77	0.42
1:4:63:LYS:HB2	1:5:184:VAL:HG12	2.02	0.42
1:5:334:TYR:N	1:5:334:TYR:CD1	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:51:LEU:HD11	1:6:261:VAL:HG12	2.01	0.42
1:6:221:PHE:CD1	1:6:221:PHE:N	2.88	0.42
1:1:18:LYS:H	1:1:18:LYS:CD	2.27	0.42
1:1:23:VAL:O	1:1:24:PRO:C	2.62	0.42
1:1:88:TYR:CE1	1:1:205:VAL:HG12	2.55	0.42
1:1:152:PHE:HA	1:1:263:ALA:HA	2.02	0.42
1:2:30:GLY:HA3	1:2:34:VAL:HG21	2.02	0.42
1:2:227:GLY:HA3	1:2:230:VAL:CG1	2.50	0.42
1:2:304:LEU:HB2	1:6:304:LEU:HD21	2.02	0.42
1:3:79:SER:HB2	1:3:171:LYS:HB2	2.02	0.42
1:3:86:PRO:HG2	1:3:279:TRP:CD1	2.55	0.42
1:3:146:GLY:O	1:3:147:SER:C	2.62	0.42
1:4:151:PHE:CD1	1:4:152:PHE:N	2.87	0.42
1:2:161:LEU:HD23	1:2:161:LEU:HA	1.72	0.41
1:2:321:MET:HE2	1:2:328:VAL:HG23	1.96	0.41
1:2:340:LEU:HD12	1:2:340:LEU:C	2.45	0.41
1:3:99:ASN:ND2	1:3:108:LEU:N	2.53	0.41
1:3:137:GLU:HB3	1:3:138:ASN:OD1	2.19	0.41
1:4:33:GLU:C	1:4:35:LEU:N	2.78	0.41
1:4:85:LEU:HA	1:4:86:PRO:HD3	1.93	0.41
1:4:303:PHE:CE1	1:4:307:ASP:HB2	2.55	0.41
1:4:326:SER:C	1:4:328:VAL:H	2.27	0.41
1:1:162:GLN:HE21	1:1:194:LYS:HZ2	1.68	0.41
1:2:217:ASN:OD1	1:2:252:PRO:HA	2.19	0.41
1:3:157:GLU:HG3	1:3:217:ASN:HD22	1.84	0.41
1:3:343:ASP:OD1	1:6:255:LYS:HE2	2.20	0.41
1:4:111:GLU:OE2	1:4:250:VAL:HA	2.20	0.41
1:4:158:PRO:HB2	1:4:196:VAL:HG21	2.00	0.41
1:4:160:GLU:C	1:4:161:LEU:HD23	2.44	0.41
1:4:323:GLY:O	1:4:324:MET:C	2.63	0.41
1:5:230:VAL:HA	1:5:231:PRO:HD2	1.76	0.41
1:5:352:GLU:HB2	1:5:353:PHE:CD1	2.56	0.41
1:6:282:LEU:HA	1:6:282:LEU:HD23	1.83	0.41
1:1:211:ASP:OD1	1:1:211:ASP:C	2.63	0.41
1:1:214:LYS:HA	1:1:216:GLU:OE2	2.19	0.41
1:1:259:LEU:HA	1:1:259:LEU:HD12	1.77	0.41
1:3:129:HIS:HD2	1:4:78:ASP:CG	2.27	0.41
1:3:347:ILE:HG22	1:6:303:PHE:CZ	2.55	0.41
1:4:114:THR:HG23	1:4:241:THR:CG2	2.50	0.41
1:4:203:TYR:HA	1:4:204:PRO:HD2	1.86	0.41
1:4:244:LEU:HA	1:4:244:LEU:HD23	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:269:LEU:HD23	1:4:269:LEU:HA	1.88	0.41
1:4:313:THR:CG2	1:4:314:GLN:N	2.83	0.41
1:6:28:ILE:HG12	1:6:29:LYS:N	2.36	0.41
1:6:132:THR:CG2	1:6:141:GLY:CA	2.96	0.41
1:1:177:VAL:HG11	1:1:203:TYR:CE2	2.55	0.41
1:1:220:TYR:C	1:1:221:PHE:CG	2.99	0.41
1:2:128:LEU:HD23	1:2:128:LEU:HA	1.71	0.41
1:2:166:ALA:O	1:2:167:ASN:HB3	2.20	0.41
1:3:114:THR:CG2	1:3:115:VAL:N	2.81	0.41
1:3:129:HIS:HD2	1:4:78:ASP:OD1	2.03	0.41
1:1:74:GLN:OE1	1:1:74:GLN:HA	2.21	0.41
1:1:115:VAL:HG22	1:1:116:LYS:N	2.35	0.41
1:2:28:ILE:CD1	1:2:34:VAL:HG13	2.49	0.41
1:3:128:LEU:HA	1:3:128:LEU:HD23	1.73	0.41
1:3:253:LEU:HD23	1:3:253:LEU:HA	1.60	0.41
1:4:266:ILE:N	1:4:266:ILE:CD1	2.84	0.41
1:4:305:LEU:CD1	1:4:309:ILE:HD11	2.51	0.41
1:5:55:MET:CE	1:5:279:TRP:CB	2.98	0.41
1:5:107:ILE:HB	1:5:295:VAL:HG23	2.01	0.41
1:6:55:MET:HA	1:6:55:MET:CE	2.45	0.41
1:1:23:VAL:HG23	1:1:24:PRO:CG	2.49	0.41
1:1:107:ILE:CG2	1:1:108:LEU:N	2.83	0.41
1:1:270:PHE:HD1	1:1:270:PHE:C	2.28	0.41
1:2:116:LYS:HB2	1:2:287:LYS:HB3	2.02	0.41
1:2:126:LEU:CD2	1:3:224:TYR:HE2	2.34	0.41
1:2:241:THR:HG22	1:2:242:THR:N	2.35	0.41
1:4:245:LEU:HB3	1:4:249:GLY:HA2	2.01	0.41
1:5:81:ASP:O	1:5:84:GLN:HG3	2.21	0.41
1:5:151:PHE:HA	1:5:222:GLY:HA2	2.01	0.41
1:5:245:LEU:N	1:5:245:LEU:HD23	2.33	0.41
1:6:98:ILE:HD11	1:6:110:TRP:CZ2	2.55	0.41
1:1:226:GLY:HA3	1:5:232:PRO:HG2	2.01	0.41
1:2:266:ILE:N	1:2:266:ILE:HD12	2.36	0.41
1:2:321:MET:HE1	1:2:327:GLN:C	2.45	0.41
1:3:107:ILE:C	1:3:108:LEU:HD23	2.45	0.41
1:3:118:GLU:OE1	1:3:237:THR:N	2.52	0.41
1:3:127:ASN:HD21	1:3:129:HIS:CD2	2.39	0.41
1:5:98:ILE:HG22	1:5:108:LEU:HB2	2.03	0.41
1:5:132:THR:HB	1:5:141:GLY:HA3	2.02	0.41
1:5:186:SER:HA	1:5:190:ASN:HB2	2.02	0.41
1:6:243:VAL:CG1	1:6:245:LEU:H	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:206:GLU:OE2	1:5:129:HIS:HE1	2.03	0.41
1:1:245:LEU:HD22	1:1:251:GLY:N	2.36	0.41
1:2:55:MET:HE2	1:2:280:LYS:O	2.20	0.41
1:2:65:LEU:HD23	1:2:65:LEU:HA	1.89	0.41
1:2:146:GLY:C	1:2:230:VAL:HG22	2.46	0.41
1:2:199:LYS:HD2	1:2:200:ASP:N	2.35	0.41
1:5:153:ALA:HB2	1:5:220:TYR:HB2	2.02	0.41
1:6:121:GLY:O	1:6:122:VAL:C	2.62	0.41
1:6:340:LEU:HD12	1:6:341:PRO:HD2	2.02	0.41
1:1:17:PRO:CG	1:2:106:ASN:HB3	2.51	0.41
1:1:52:ASN:OD1	1:2:188:GLN:HG3	2.21	0.41
1:1:58:PRO:HG2	1:1:62:GLN:HB2	2.03	0.41
1:1:297:ASN:HB3	1:1:300:PRO:HB3	2.02	0.41
1:2:125:MET:HE1	1:2:232:PRO:HG3	2.03	0.41
1:2:128:LEU:HD21	1:2:143:PRO:HB3	2.02	0.41
1:2:178:THR:HB	1:2:179:PRO:CD	2.51	0.41
1:3:298:PRO:HD3	1:6:342:GLY:HA3	2.03	0.41
1:3:347:ILE:CG2	1:6:303:PHE:CZ	3.04	0.41
1:4:217:ASN:O	1:4:252:PRO:HB3	2.20	0.41
1:5:16:LYS:C	1:5:17:PRO:O	2.61	0.41
1:2:81:ASP:OD1	1:2:81:ASP:N	2.54	0.41
1:2:92:ARG:CG	1:2:258:SER:HB3	2.51	0.41
1:2:235:HIS:CD2	1:3:223:THR:HB	2.56	0.41
1:4:66:SER:OG	1:4:279:TRP:N	2.53	0.41
1:4:145:GLN:OE1	1:4:229:ASN:HB3	2.21	0.41
1:5:112:ALA:O	1:5:251:GLY:HA3	2.21	0.41
1:6:156:GLY:HA3	1:6:253:LEU:O	2.21	0.41
1:1:296:LYS:HA	1:1:296:LYS:HD2	1.67	0.40
1:1:359:ARG:NH1	1:1:359:ARG:HG2	2.36	0.40
1:3:245:LEU:N	1:3:245:LEU:HD23	2.36	0.40
1:4:98:ILE:CG2	1:4:108:LEU:HB3	2.50	0.40
1:5:16:LYS:CG	1:5:17:PRO:O	2.68	0.40
1:5:53:PRO:HD3	1:5:283:PRO:CA	2.51	0.40
1:6:298:PRO:HG2	1:6:299:TYR:N	2.36	0.40
1:3:66:SER:HB3	1:3:279:TRP:HB2	2.03	0.40
1:3:133:GLN:HB2	1:3:272:ASN:O	2.21	0.40
1:3:280:LYS:CG	1:3:281:GLY:N	2.84	0.40
1:4:125:MET:CB	1:4:144:ILE:HD12	2.50	0.40
1:5:123:THR:O	1:5:124:ALA:C	2.63	0.40
1:5:126:LEU:O	1:5:128:LEU:N	2.55	0.40
1:2:257:ASP:CG	1:3:350:ILE:HD11	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:326:SER:OG	1:2:328:VAL:HB	2.20	0.40
1:3:93:ILE:HG22	1:3:95:LEU:HD21	2.03	0.40
1:3:126:LEU:HA	1:3:126:LEU:HD23	1.80	0.40
1:5:97:ASN:OD1	1:5:99:ASN:N	2.54	0.40
1:5:114:THR:HG23	1:5:241:THR:HG23	2.03	0.40
1:5:127:ASN:HD22	1:5:129:HIS:H	1.67	0.40
1:5:200:ASP:O	1:5:201:ASN:C	2.63	0.40
1:6:109:MET:HE3	1:6:109:MET:HB2	1.73	0.40
1:1:93:ILE:HA	1:1:94:PRO:HD3	1.62	0.40
1:2:168:TYR:CE1	1:2:184:VAL:HA	2.56	0.40
1:2:253:LEU:HA	1:2:253:LEU:HD23	1.84	0.40
1:3:39:THR:HB	1:3:43:SER:CB	2.51	0.40
1:4:53:PRO:HD3	1:4:283:PRO:CA	2.52	0.40
1:4:93:ILE:O	1:4:259:LEU:N	2.51	0.40
1:5:81:ASP:HB2	1:5:84:GLN:HG3	2.03	0.40
1:6:26:LEU:HD21	1:6:29:LYS:HB3	2.03	0.40
1:6:36:GLY:O	1:6:37:VAL:C	2.64	0.40
1:6:65:LEU:HA	1:6:279:TRP:O	2.20	0.40
1:6:339:GLU:O	1:6:340:LEU:C	2.64	0.40
1:1:111:GLU:OE2	1:1:250:VAL:HA	2.21	0.40
1:2:184:VAL:C	1:2:186:SER:H	2.29	0.40
1:2:259:LEU:HD12	1:2:259:LEU:HA	1.61	0.40
1:3:315:ARG:HG2	1:3:315:ARG:HH11	1.86	0.40
1:4:139:GLY:O	1:4:140:ALA:O	2.39	0.40
1:4:256:ALA:O	1:4:258:SER:N	2.54	0.40
1:5:152:PHE:HA	1:5:263:ALA:HA	2.03	0.40
1:5:162:GLN:NE2	1:5:189:MET:HE1	2.37	0.40
1:5:298:PRO:HG2	1:5:299:TYR:H	1.86	0.40
1:5:298:PRO:HG2	1:5:299:TYR:N	2.36	0.40
1:5:352:GLU:HB2	1:5:353:PHE:CE1	2.56	0.40
1:6:212:PRO:C	1:6:214:LYS:N	2.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	346/361 (96%)	276 (80%)	48 (14%)	22 (6%)	1	6
1	2	346/361 (96%)	292 (84%)	40 (12%)	14 (4%)	2	13
1	3	340/361 (94%)	287 (84%)	39 (12%)	14 (4%)	2	13
1	4	329/361 (91%)	267 (81%)	49 (15%)	13 (4%)	2	13
1	5	345/361 (96%)	279 (81%)	54 (16%)	12 (4%)	3	16
1	6	339/361 (94%)	288 (85%)	41 (12%)	10 (3%)	3	19
All	All	2045/2166 (94%)	1689 (83%)	271 (13%)	85 (4%)	2	13

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	137	GLU
1	1	174	ALA
1	1	191	THR
1	1	257	ASP
1	1	300	PRO
1	1	313	THR
1	1	318	GLY
1	1	351	ASP
1	2	137	GLU
1	2	351	ASP
1	3	105	GLY
1	3	137	GLU
1	3	257	ASP
1	3	301	ILE
1	4	14	PRO
1	4	132	THR
1	4	137	GLU
1	4	140	ALA
1	4	324	MET
1	4	341	PRO
1	5	102	LEU
1	5	137	GLU
1	5	301	ILE
1	5	351	ASP
1	6	132	THR
1	6	137	GLU
1	6	257	ASP

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Mol	Chain	Res	Type
1	6	346	MET
1	1	147	SER
1	1	306	SER
1	1	309	ILE
1	1	317	ASP
1	1	353	PHE
1	2	18	LYS
1	2	257	ASP
1	2	307	ASP
1	3	100	GLU
1	3	132	THR
1	3	191	THR
1	3	300	PRO
1	4	130	SER
1	4	131	GLY
1	5	127	ASN
1	5	131	GLY
1	6	130	SER
1	6	131	GLY
1	1	131	GLY
1	1	360	MET
1	2	103	THR
1	2	215	ASN
1	2	353	PHE
1	3	346	MET
1	4	72	GLU
1	5	191	THR
1	5	257	ASP
1	5	300	PRO
1	6	18	LYS
1	6	101	ASP
1	1	182	ALA
1	1	255	LYS
1	1	346	MET
1	2	131	GLY
1	2	173	PRO
1	3	136	HIS
1	4	191	THR
1	6	72	GLU
1	1	173	PRO
1	2	181	ASN
1	3	124	ALA

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Mol	Chain	Res	Type
1	3	193	HIS
1	5	58	PRO
1	6	181	ASN
1	2	58	PRO
1	2	319	GLN
1	4	173	PRO
1	5	103	THR
1	5	132	THR
1	4	300	PRO
1	1	58	PRO
1	1	319	GLN
1	3	58	PRO
1	2	309	ILE
1	4	301	ILE
1	1	34	VAL
1	3	320	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	306/314 (98%)	242 (79%)	64 (21%)	1	5
1	2	306/314 (98%)	265 (87%)	41 (13%)	4	17
1	3	300/314 (96%)	251 (84%)	49 (16%)	2	11
1	4	289/314 (92%)	247 (86%)	42 (14%)	3	14
1	5	305/314 (97%)	246 (81%)	59 (19%)	1	7
1	6	299/314 (95%)	260 (87%)	39 (13%)	4	18
All	All	1805/1884 (96%)	1511 (84%)	294 (16%)	2	11

All (294) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	18	LYS
1	1	21	VAL

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Mol	Chain	Res	Type
1	1	23	VAL
1	1	28	ILE
1	1	45	THR
1	1	76	THR
1	1	80	PRO
1	1	92	ARG
1	1	98	ILE
1	1	100	GLU
1	1	103	THR
1	1	104	CYS
1	1	114	THR
1	1	117	THR
1	1	122	VAL
1	1	127	ASN
1	1	128	LEU
1	1	132	THR
1	1	138	ASN
1	1	165	LEU
1	1	175	GLN
1	1	183	THR
1	1	191	THR
1	1	197	LEU
1	1	211	ASP
1	1	214	LYS
1	1	218	THR
1	1	223	THR
1	1	229	ASN
1	1	233	VAL
1	1	239	THR
1	1	245	LEU
1	1	250	VAL
1	1	255	LYS
1	1	262	SER
1	1	276	THR
1	1	284	ARG
1	1	285	TYR
1	1	288	ILE
1	1	289	THR
1	1	294	SER
1	1	295	VAL
1	1	296	LYS
1	1	299	TYR

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Mol	Chain	Res	Type
1	1	304	LEU
1	1	306	SER
1	1	308	LEU
1	1	311	ARG
1	1	312	ARG
1	1	314	GLN
1	1	315	ARG
1	1	317	ASP
1	1	321	MET
1	1	322	ILE
1	1	328	VAL
1	1	329	GLU
1	1	344	PRO
1	1	345	ASP
1	1	346	MET
1	1	352	GLU
1	1	353	PHE
1	1	357	THR
1	1	359	ARG
1	1	361	GLN
1	2	21	VAL
1	2	23	VAL
1	2	32	ILE
1	2	33	GLU
1	2	35	LEU
1	2	76	THR
1	2	81	ASP
1	2	100	GLU
1	2	102	LEU
1	2	107	ILE
1	2	114	THR
1	2	122	VAL
1	2	123	THR
1	2	127	ASN
1	2	132	THR
1	2	165	LEU
1	2	183	THR
1	2	188	GLN
1	2	191	THR
1	2	205	VAL
1	2	214	LYS
1	2	218	THR

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Mol	Chain	Res	Type
1	2	223	THR
1	2	225	THR
1	2	229	ASN
1	2	231	PRO
1	2	233	VAL
1	2	250	VAL
1	2	261	VAL
1	2	262	SER
1	2	273	THR
1	2	276	THR
1	2	280	LYS
1	2	289	THR
1	2	302	SER
1	2	307	ASP
1	2	312	ARG
1	2	353	PHE
1	2	356	THR
1	2	359	ARG
1	2	360	MET
1	3	21	VAL
1	3	41	VAL
1	3	43	SER
1	3	45	THR
1	3	76	THR
1	3	84	GLN
1	3	99	ASN
1	3	101	ASP
1	3	102	LEU
1	3	114	THR
1	3	122	VAL
1	3	127	ASN
1	3	132	THR
1	3	138	ASN
1	3	165	LEU
1	3	169	ARG
1	3	173	PRO
1	3	175	GLN
1	3	191	THR
1	3	209	VAL
1	3	213	SER
1	3	214	LYS
1	3	218	THR

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Mol	Chain	Res	Type
1	3	221	PHE
1	3	223	THR
1	3	229	ASN
1	3	250	VAL
1	3	252	PRO
1	3	258	SER
1	3	262	SER
1	3	273	THR
1	3	274	SER
1	3	278	GLN
1	3	280	LYS
1	3	285	TYR
1	3	304	LEU
1	3	305	LEU
1	3	307	ASP
1	3	308	LEU
1	3	309	ILE
1	3	312	ARG
1	3	315	ARG
1	3	322	ILE
1	3	324	MET
1	3	325	SER
1	3	347	ILE
1	3	348	ARG
1	3	350	ILE
1	3	355	GLN
1	4	14	PRO
1	4	21	VAL
1	4	23	VAL
1	4	27	VAL
1	4	45	THR
1	4	76	THR
1	4	103	THR
1	4	108	LEU
1	4	114	THR
1	4	125	MET
1	4	127	ASN
1	4	135	THR
1	4	137	GLU
1	4	151	PHE
1	4	173	PRO
1	4	183	THR

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Mol	Chain	Res	Type
1	4	184	VAL
1	4	191	THR
1	4	196	VAL
1	4	216	GLU
1	4	218	THR
1	4	229	ASN
1	4	230	VAL
1	4	233	VAL
1	4	245	LEU
1	4	250	VAL
1	4	262	SER
1	4	270	PHE
1	4	273	THR
1	4	274	SER
1	4	276	THR
1	4	280	LYS
1	4	295	VAL
1	4	301	ILE
1	4	305	LEU
1	4	310	ASN
1	4	311	ARG
1	4	312	ARG
1	4	316	VAL
1	4	322	ILE
1	4	334	TYR
1	4	338	GLU
1	5	16	LYS
1	5	28	ILE
1	5	33	GLU
1	5	45	THR
1	5	48	GLU
1	5	65	LEU
1	5	76	THR
1	5	84	GLN
1	5	95	LEU
1	5	114	THR
1	5	117	THR
1	5	122	VAL
1	5	125	MET
1	5	127	ASN
1	5	128	LEU
1	5	132	THR

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Mol	Chain	Res	Type
1	5	133	GLN
1	5	137	GLU
1	5	138	ASN
1	5	151	PHE
1	5	164	VAL
1	5	165	LEU
1	5	169	ARG
1	5	173	PRO
1	5	184	VAL
1	5	189	MET
1	5	191	THR
1	5	205	VAL
1	5	218	THR
1	5	221	PHE
1	5	223	THR
1	5	225	THR
1	5	229	ASN
1	5	236	ILE
1	5	239	THR
1	5	245	LEU
1	5	250	VAL
1	5	255	LYS
1	5	262	SER
1	5	270	PHE
1	5	273	THR
1	5	274	SER
1	5	280	LYS
1	5	284	ARG
1	5	288	ILE
1	5	296	LYS
1	5	297	ASN
1	5	301	ILE
1	5	302	SER
1	5	305	LEU
1	5	316	VAL
1	5	322	ILE
1	5	324	MET
1	5	332	ARG
1	5	346	MET
1	5	353	PHE
1	5	355	GLN
1	5	358	THR

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Mol	Chain	Res	Type
1	5	359	ARG
1	6	15	LYS
1	6	21	VAL
1	6	35	LEU
1	6	55	MET
1	6	68	SER
1	6	76	THR
1	6	98	ILE
1	6	102	LEU
1	6	103	THR
1	6	109	MET
1	6	114	THR
1	6	127	ASN
1	6	134	LYS
1	6	151	PHE
1	6	165	LEU
1	6	173	PRO
1	6	184	VAL
1	6	191	THR
1	6	214	LYS
1	6	218	THR
1	6	223	THR
1	6	229	ASN
1	6	250	VAL
1	6	255	LYS
1	6	262	SER
1	6	273	THR
1	6	274	SER
1	6	276	THR
1	6	278	GLN
1	6	284	ARG
1	6	289	THR
1	6	298	PRO
1	6	301	ILE
1	6	303	PHE
1	6	312	ARG
1	6	315	ARG
1	6	324	MET
1	6	345	ASP
1	6	350	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	HIS
1	1	97	ASN
1	1	99	ASN
1	1	127	ASN
1	1	136	HIS
1	1	162	GLN
1	1	167	ASN
1	1	190	ASN
1	1	201	ASN
1	1	229	ASN
1	1	235	HIS
1	1	272	ASN
1	1	277	GLN
1	1	327	GLN
1	2	22	GLN
1	2	61	HIS
1	2	62	GLN
1	2	99	ASN
1	2	127	ASN
1	2	129	HIS
1	2	150	HIS
1	2	162	GLN
1	2	167	ASN
1	2	175	GLN
1	2	181	ASN
1	2	187	GLN
1	2	190	ASN
1	2	201	ASN
1	2	229	ASN
1	2	235	HIS
1	2	272	ASN
1	2	277	GLN
1	2	278	GLN
1	2	319	GLN
1	2	327	GLN
1	3	22	GLN
1	3	61	HIS
1	3	62	GLN
1	3	99	ASN
1	3	127	ASN
1	3	129	HIS
1	3	162	GLN
1	3	167	ASN

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Mol	Chain	Res	Type
1	3	175	GLN
1	3	181	ASN
1	3	187	GLN
1	3	188	GLN
1	3	190	ASN
1	3	201	ASN
1	3	229	ASN
1	3	235	HIS
1	3	272	ASN
1	3	277	GLN
1	3	319	GLN
1	3	327	GLN
1	4	61	HIS
1	4	62	GLN
1	4	99	ASN
1	4	127	ASN
1	4	129	HIS
1	4	136	HIS
1	4	162	GLN
1	4	167	ASN
1	4	175	GLN
1	4	181	ASN
1	4	201	ASN
1	4	229	ASN
1	4	277	GLN
1	4	319	GLN
1	4	327	GLN
1	5	61	HIS
1	5	62	GLN
1	5	99	ASN
1	5	127	ASN
1	5	129	HIS
1	5	162	GLN
1	5	175	GLN
1	5	190	ASN
1	5	201	ASN
1	5	229	ASN
1	5	272	ASN
1	5	277	GLN
1	5	278	GLN
1	5	297	ASN
1	5	314	GLN

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Mol	Chain	Res	Type
1	5	319	GLN
1	5	327	GLN
1	6	22	GLN
1	6	62	GLN
1	6	99	ASN
1	6	127	ASN
1	6	138	ASN
1	6	150	HIS
1	6	162	GLN
1	6	167	ASN
1	6	175	GLN
1	6	181	ASN
1	6	190	ASN
1	6	201	ASN
1	6	229	ASN
1	6	272	ASN
1	6	278	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.