wwPDB EM Map/Model Validation Report (i)

Apr 26, 2016 – 06:28 PM BST

PDB ID	:	5FUA
EMDB ID:	:	EMD-3283
Title	:	Cryo-EM of BK polyomavirus
Authors	:	Hurdiss, D.L.; Morgan, E.L.; Thompson, R.F.; Prescott, E.L.; Panou, M.M.; Macdonald, A.; Ranson, N.A.
Deposited on	:	2016-01-22
Resolution	:	7.60 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

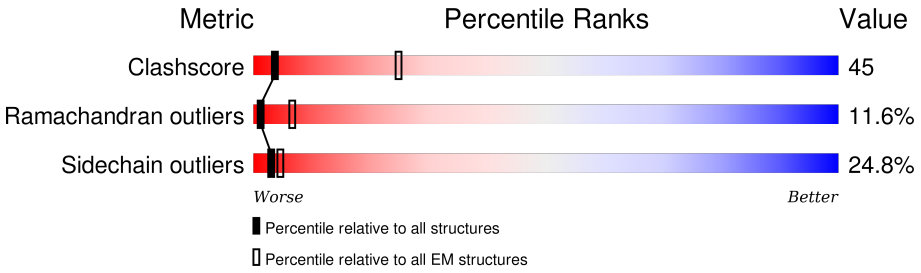
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27461

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.60 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	1	362	22% 38% 25% 12% .
1	2	362	22% 40% 23% 10% .
1	3	362	23% 35% 26% 11% 6%
1	4	362	19% 40% 23% 9% 9%
1	5	362	22% 40% 24% 10% .
1	6	362	23% 39% 24% 9% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 31890 atoms, of which 15848 are hydrogens and 0 are deuteriums.

In the tables below, 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 MAJOR CAPSID PROTEIN VP1.

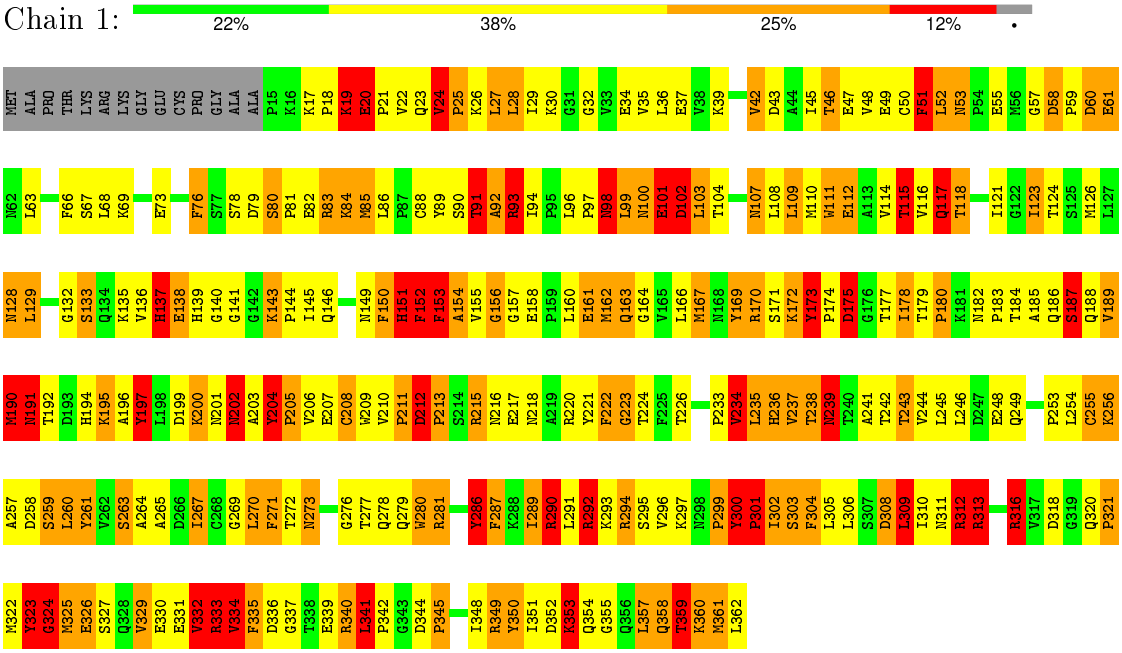
Mol	Chain	Residues	Atoms						AltConf	Trace
1	1	348	Total	C	H	N	O	S	0	0
			5406	1708	2689	470	522	17		
1	2	348	Total	C	H	N	O	S	0	0
			5406	1708	2689	470	522	17		
1	3	342	Total	C	H	N	O	S	0	0
			5297	1676	2630	462	513	16		
1	4	331	Total	C	H	N	O	S	0	0
			5106	1616	2535	445	495	15		
1	5	347	Total	C	H	N	O	S	0	0
			5392	1703	2682	469	521	17		
1	6	341	Total	C	H	N	O	S	0	0
			5283	1671	2623	461	512	16		

3 Residue-property plots (i)

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

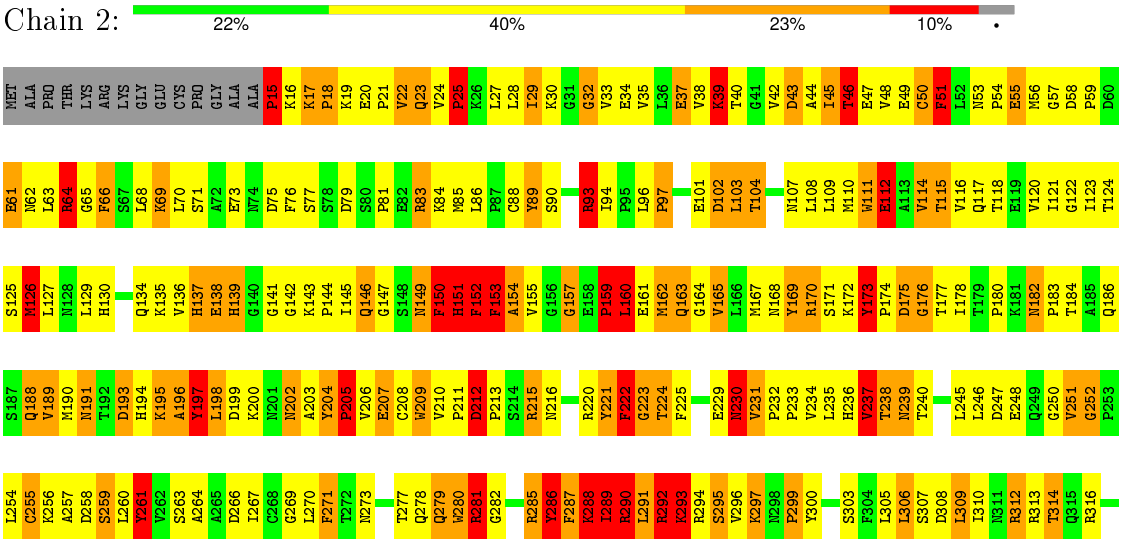
- Molecule 1: MAJOR CAPSID PROTEIN VP1

Chain 1:



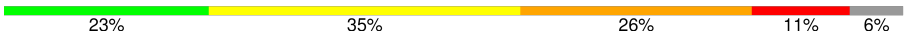
- Molecule 1: MAJOR CAPSID PROTEIN VP1

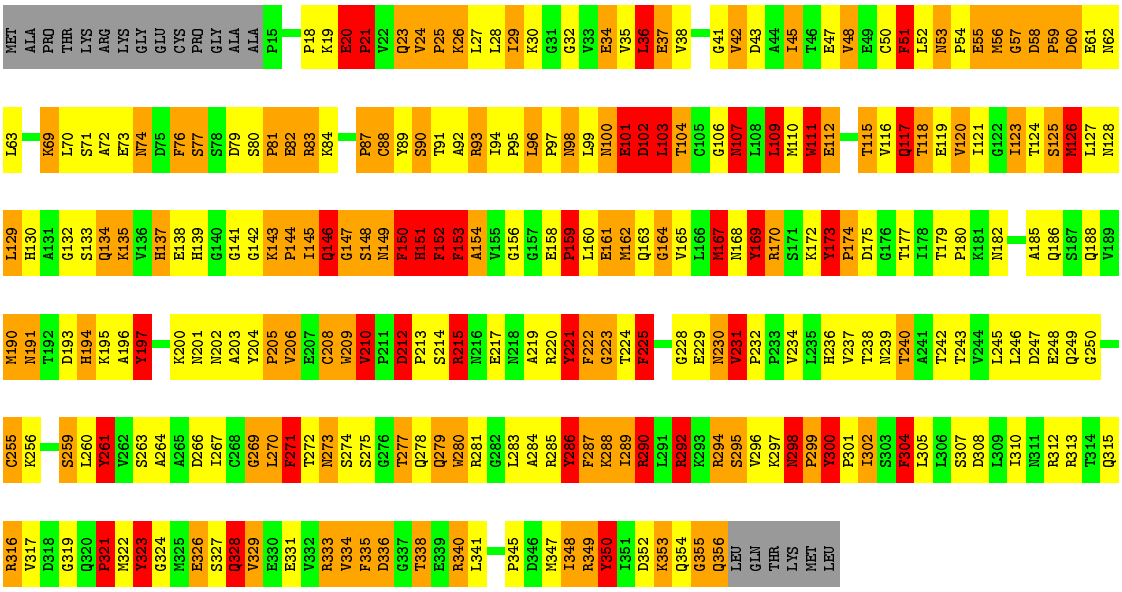
Chain 2:



• Molecule 1: MAJOR CAPSID PROTEIN VP1

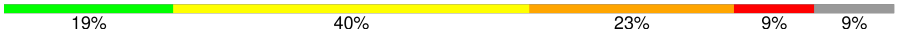
Chain 3:

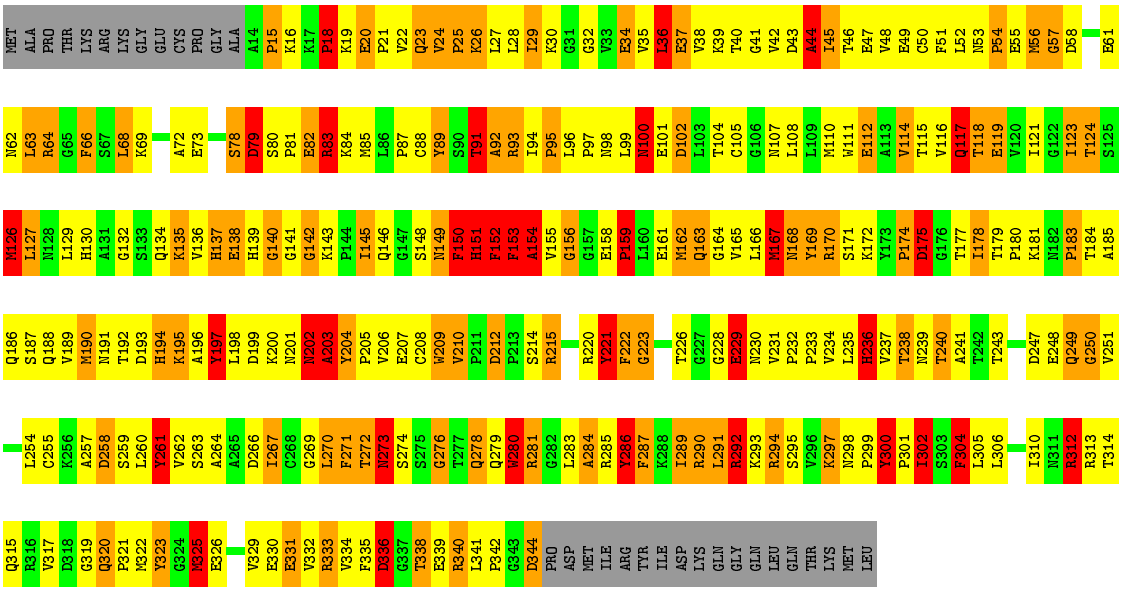




• Molecule 1: MAJOR CAPSID PROTEIN VP1

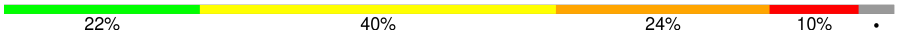
Chain 4:

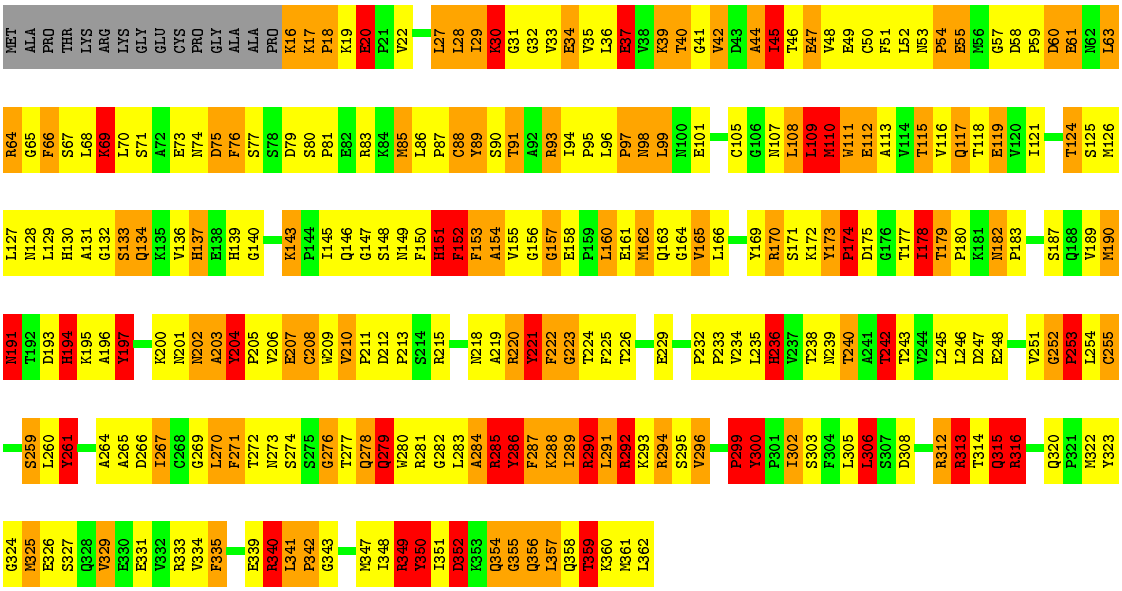




• Molecule 1: MAJOR CAPSID PROTEIN VP1

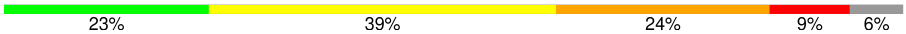
Chain 5:

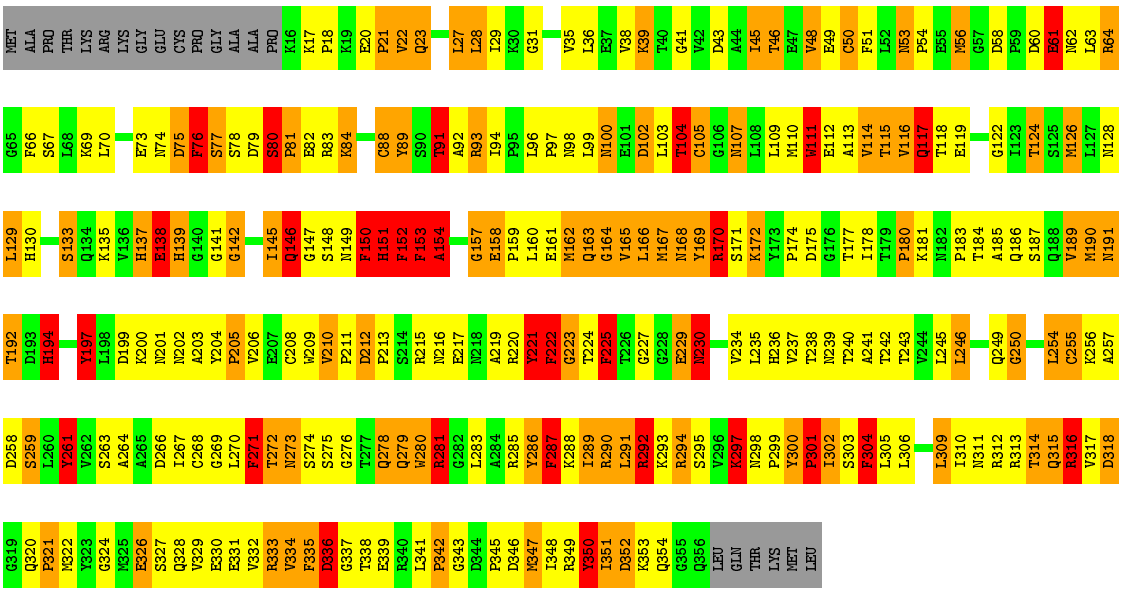




• Molecule 1: MAJOR CAPSID PROTEIN VP1

Chain 6:





4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTFFIND3, Not provided	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	4800	Depositor
Magnification	19000	Depositor
Image detector	GATAN K2 SUMMIT (4K X 4K)	Depositor

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	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	1	1.62	18/2777 (0.6%)	2.15	121/3765 (3.2%)
1	2	1.62	11/2777 (0.4%)	2.02	91/3765 (2.4%)
1	3	1.59	18/2727 (0.7%)	2.05	96/3700 (2.6%)
1	4	1.62	10/2629 (0.4%)	2.16	118/3570 (3.3%)
1	5	1.65	22/2769 (0.8%)	2.10	105/3754 (2.8%)
1	6	1.57	16/2719 (0.6%)	2.04	93/3689 (2.5%)
All	All	1.61	95/16398 (0.6%)	2.08	624/22243 (2.8%)

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	1	0	40
1	2	0	40
1	3	0	37
1	4	0	34
1	5	0	36
1	6	0	33
All	All	0	220

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	31	GLY	CA-C	-8.09	1.39	1.51
1	1	350	TYR	CB-CG	-7.78	1.40	1.51
1	3	197	TYR	CB-CG	-7.47	1.40	1.51
1	4	223	GLY	CA-C	-7.38	1.40	1.51
1	2	223	GLY	CA-C	-7.19	1.40	1.51
1	2	313	ARG	CD-NE	6.98	1.58	1.46
1	1	223	GLY	CA-C	-6.75	1.41	1.51
1	1	173	TYR	CB-CG	-6.68	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	197	TYR	CB-CG	-6.65	1.41	1.51
1	6	164	GLY	CA-C	-6.53	1.41	1.51
1	5	223	GLY	CA-C	-6.47	1.41	1.51
1	3	223	GLY	CA-C	-6.35	1.41	1.51
1	1	361	MET	N-CA	-6.33	1.33	1.46
1	1	205	PRO	CA-C	-6.14	1.40	1.52
1	6	102	ASP	CA-C	-6.11	1.37	1.52
1	1	156	GLY	CA-C	-6.06	1.42	1.51
1	4	261	TYR	CB-CG	-6.05	1.42	1.51
1	1	163	GLN	N-CA	-6.01	1.34	1.46
1	5	350	TYR	N-CA	-5.95	1.34	1.46
1	6	197	TYR	CB-CG	-5.90	1.42	1.51
1	6	31	GLY	CA-C	-5.88	1.42	1.51
1	1	270	LEU	CA-C	-5.85	1.37	1.52
1	1	286	TYR	CB-CG	-5.79	1.43	1.51
1	4	222	PHE	CB-CG	-5.79	1.41	1.51
1	6	152	PHE	N-CA	-5.78	1.34	1.46
1	1	260	LEU	CA-C	-5.77	1.38	1.52
1	5	156	GLY	CA-C	-5.76	1.42	1.51
1	6	210	VAL	C-N	-5.71	1.23	1.34
1	2	313	ARG	NE-CZ	5.67	1.40	1.33
1	1	269	GLY	CA-C	-5.66	1.42	1.51
1	3	25	PRO	CA-C	-5.65	1.41	1.52
1	5	110	MET	CA-C	-5.64	1.38	1.52
1	5	261	TYR	CB-CG	-5.63	1.43	1.51
1	3	269	GLY	CA-C	-5.61	1.42	1.51
1	2	157	GLY	N-CA	-5.57	1.37	1.46
1	5	147	GLY	CA-C	-5.57	1.43	1.51
1	4	156	GLY	CA-C	-5.54	1.43	1.51
1	4	269	GLY	CA-C	-5.53	1.43	1.51
1	1	115	THR	CA-C	-5.52	1.38	1.52
1	3	156	GLY	CA-C	-5.51	1.43	1.51
1	6	41	GLY	CA-C	5.49	1.60	1.51
1	5	109	LEU	CA-C	-5.48	1.38	1.52
1	6	223	GLY	CA-C	-5.48	1.43	1.51
1	5	45	ILE	CA-C	-5.46	1.38	1.52
1	3	270	LEU	CA-C	-5.44	1.38	1.52
1	3	210	VAL	C-N	-5.42	1.24	1.34
1	4	276	GLY	CA-C	-5.42	1.43	1.51
1	3	304	PHE	N-CA	-5.39	1.35	1.46
1	6	146	GLN	N-CA	-5.37	1.35	1.46
1	2	97	PRO	CA-C	-5.35	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	350	TYR	CB-CG	-5.30	1.43	1.51
1	2	351	ILE	N-CA	-5.30	1.35	1.46
1	5	208	CYS	CA-C	-5.30	1.39	1.52
1	5	152	PHE	CA-C	-5.29	1.39	1.52
1	3	87	PRO	CA-C	-5.27	1.42	1.52
1	2	223	GLY	N-CA	-5.27	1.38	1.46
1	5	269	GLY	CA-C	-5.26	1.43	1.51
1	2	215	ARG	N-CA	-5.25	1.35	1.46
1	5	278	GLN	CA-C	-5.25	1.39	1.52
1	2	205	PRO	CA-C	-5.23	1.42	1.52
1	3	222	PHE	CA-C	-5.22	1.39	1.52
1	3	223	GLY	N-CA	-5.21	1.38	1.46
1	1	222	PHE	CA-C	-5.20	1.39	1.52
1	5	279	GLN	CA-C	-5.20	1.39	1.52
1	6	335	PHE	CB-CG	-5.18	1.42	1.51
1	3	88	CYS	CA-C	-5.16	1.39	1.52
1	6	309	LEU	CA-C	-5.16	1.39	1.52
1	2	152	PHE	N-CA	-5.15	1.36	1.46
1	5	47	GLU	CA-C	-5.14	1.39	1.52
1	5	359	THR	N-CA	-5.14	1.36	1.46
1	2	150	PHE	CA-C	-5.13	1.39	1.52
1	5	30	LYS	N-CA	-5.13	1.36	1.46
1	1	180	PRO	N-CD	-5.13	1.40	1.47
1	4	270	LEU	CA-C	-5.12	1.39	1.52
1	1	304	PHE	CB-CG	5.11	1.60	1.51
1	4	278	GLN	CA-C	-5.11	1.39	1.52
1	5	110	MET	N-CA	-5.11	1.36	1.46
1	3	147	GLY	CA-C	-5.11	1.43	1.51
1	6	88	CYS	N-CA	-5.10	1.36	1.46
1	6	46	THR	CA-C	-5.10	1.39	1.52
1	4	150	PHE	CA-C	-5.09	1.39	1.52
1	3	151	HIS	CA-C	-5.09	1.39	1.52
1	4	209	TRP	CA-C	-5.09	1.39	1.52
1	3	150	PHE	CA-C	-5.08	1.39	1.52
1	6	23	GLN	N-CA	-5.08	1.36	1.46
1	5	267	ILE	CA-C	-5.07	1.39	1.52
1	6	221	TYR	CA-C	-5.06	1.39	1.52
1	3	164	GLY	CA-C	-5.05	1.43	1.51
1	5	276	GLY	CA-C	-5.04	1.43	1.51
1	6	49	GLU	N-CA	-5.01	1.36	1.46
1	3	206	VAL	N-CA	-5.01	1.36	1.46
1	1	162	MET	CA-C	-5.01	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	343	GLY	N-CA	-5.01	1.38	1.46
1	1	259	SER	CA-CB	-5.00	1.45	1.52
1	3	209	TRP	CA-C	-5.00	1.40	1.52

All (624) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	350	TYR	CB-CG-CD1	-19.61	109.24	121.00
1	4	280	TRP	CB-CG-CD2	-15.46	106.50	126.60
1	5	350	TYR	CB-CG-CD2	-14.63	112.22	121.00
1	6	152	PHE	CB-CG-CD1	-13.64	111.25	120.80
1	2	261	TYR	CB-CG-CD1	-13.47	112.92	121.00
1	6	294	ARG	NE-CZ-NH2	-12.77	113.92	120.30
1	1	173	TYR	CB-CG-CD2	-12.39	113.56	121.00
1	1	323	TYR	CB-CG-CD1	12.34	128.40	121.00
1	1	323	TYR	CB-CG-CD2	-12.29	113.62	121.00
1	3	304	PHE	CB-CG-CD2	-11.90	112.47	120.80
1	5	322	MET	CG-SD-CE	-11.42	81.93	100.20
1	5	110	MET	CG-SD-CE	-11.39	81.98	100.20
1	1	173	TYR	CB-CG-CD1	-11.04	114.38	121.00
1	5	261	TYR	CB-CG-CD2	-11.00	114.40	121.00
1	3	304	PHE	CB-CG-CD1	10.94	128.46	120.80
1	1	153	PHE	CB-CG-CD2	-10.86	113.20	120.80
1	3	292	ARG	CD-NE-CZ	-10.64	108.70	123.60
1	2	152	PHE	CB-CG-CD2	-10.62	113.37	120.80
1	1	286	TYR	CB-CG-CD1	-10.56	114.66	121.00
1	2	197	TYR	CB-CG-CD1	-10.54	114.68	121.00
1	6	197	TYR	CB-CG-CD1	-10.52	114.69	121.00
1	4	204	TYR	CB-CG-CD2	-10.23	114.86	121.00
1	1	280	TRP	CB-CG-CD2	-10.19	113.36	126.60
1	2	197	TYR	CB-CG-CD2	9.92	126.95	121.00
1	3	197	TYR	CB-CG-CD2	-9.83	115.10	121.00
1	4	286	TYR	CB-CG-CD1	-9.74	115.16	121.00
1	3	147	GLY	N-CA-C	-9.63	89.03	113.10
1	6	154	ALA	N-CA-CB	9.62	123.57	110.10
1	4	322	MET	CG-SD-CE	-9.49	85.02	100.20
1	4	169	TYR	CB-CG-CD1	-9.37	115.38	121.00
1	1	304	PHE	CB-CG-CD1	9.33	127.33	120.80
1	3	304	PHE	CB-CA-C	9.25	128.89	110.40
1	3	222	PHE	N-CA-CB	9.22	127.20	110.60
1	3	169	TYR	CB-CG-CD1	-9.16	115.50	121.00
1	3	153	PHE	CB-CG-CD1	-9.09	114.43	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	314	THR	C-N-CA	9.07	144.37	121.70
1	2	293	LYS	N-CA-CB	9.06	126.91	110.60
1	3	286	TYR	CB-CG-CD1	-8.94	115.64	121.00
1	5	359	THR	N-CA-C	-8.93	86.88	111.00
1	4	197	TYR	CB-CG-CD2	-8.91	115.65	121.00
1	4	312	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	5	261	TYR	CA-CB-CG	-8.82	96.64	113.40
1	2	93	ARG	N-CA-C	-8.81	87.21	111.00
1	4	222	PHE	CB-CG-CD1	-8.76	114.67	120.80
1	4	154	ALA	N-CA-CB	8.72	122.31	110.10
1	4	257	ALA	N-CA-C	-8.71	87.50	111.00
1	5	151	HIS	CA-CB-CG	-8.59	98.99	113.60
1	4	152	PHE	CB-CG-CD1	-8.56	114.81	120.80
1	4	320	GLN	N-CA-C	-8.55	87.92	111.00
1	5	286	TYR	CB-CG-CD1	-8.51	115.90	121.00
1	4	153	PHE	CB-CG-CD2	-8.45	114.89	120.80
1	5	236	HIS	N-CA-C	-8.44	88.22	111.00
1	3	151	HIS	CA-CB-CG	-8.42	99.29	113.60
1	3	126	MET	CG-SD-CE	8.41	113.65	100.20
1	1	349	ARG	CA-C-N	-8.40	98.71	117.20
1	6	102	ASP	N-CA-CB	8.40	125.72	110.60
1	1	350	TYR	CB-CG-CD1	-8.39	115.97	121.00
1	3	21	PRO	N-CA-C	-8.34	90.43	112.10
1	4	190	MET	CG-SD-CE	-8.33	86.87	100.20
1	6	23	GLN	N-CA-C	-8.27	88.67	111.00
1	1	92	ALA	N-CA-CB	8.26	121.67	110.10
1	6	261	TYR	CB-CG-CD1	-8.25	116.05	121.00
1	2	153	PHE	CB-CG-CD2	-8.22	115.05	120.80
1	6	146	GLN	N-CA-C	-8.19	88.89	111.00
1	1	151	HIS	CA-CB-CG	-8.15	99.74	113.60
1	1	339	GLU	C-N-CA	8.15	142.08	121.70
1	3	162	MET	CG-SD-CE	-8.15	87.16	100.20
1	3	150	PHE	CB-CG-CD1	-8.14	115.11	120.80
1	2	111	TRP	CB-CG-CD2	-8.13	116.04	126.60
1	2	143	LYS	N-CA-CB	8.12	125.21	110.60
1	1	24	VAL	N-CA-CB	8.04	129.18	111.50
1	5	350	TYR	N-CA-C	-8.00	89.41	111.00
1	1	156	GLY	N-CA-C	-7.99	93.12	113.10
1	1	24	VAL	N-CA-C	-7.98	89.45	111.00
1	4	261	TYR	CB-CG-CD2	-7.96	116.22	121.00
1	3	280	TRP	CB-CG-CD2	-7.95	116.27	126.60
1	2	261	TYR	CB-CG-CD2	-7.92	116.25	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	4	92	ALA	N-CA-C	-7.88	89.71	111.00
1	1	167	MET	CG-SD-CE	-7.88	87.60	100.20
1	4	25	PRO	N-CA-C	-7.83	91.75	112.10
1	4	280	TRP	CB-CA-C	-7.82	94.76	110.40
1	2	159	PRO	C-N-CA	7.80	141.21	121.70
1	1	111	TRP	CB-CG-CD2	-7.79	116.47	126.60
1	4	18	PRO	N-CA-C	7.79	132.35	112.10
1	4	335	PHE	C-N-CA	7.74	141.05	121.70
1	6	286	TYR	CB-CG-CD1	-7.74	116.36	121.00
1	6	191	ASN	C-N-CA	7.71	140.97	121.70
1	4	151	HIS	CA-CB-CG	-7.71	100.50	113.60
1	5	356	GLN	N-CA-CB	7.70	124.46	110.60
1	3	74	ASN	N-CA-C	-7.70	90.22	111.00
1	5	153	PHE	CB-CG-CD2	-7.68	115.42	120.80
1	1	20	GLU	CB-CA-C	-7.67	95.05	110.40
1	4	297	LYS	N-CA-CB	7.66	124.38	110.60
1	4	261	TYR	CA-CB-CG	-7.65	98.87	113.40
1	5	178	ILE	N-CA-C	-7.63	90.40	111.00
1	2	322	MET	CG-SD-CE	-7.62	88.01	100.20
1	1	154	ALA	N-CA-CB	7.62	120.76	110.10
1	2	288	LYS	CB-CA-C	-7.62	95.17	110.40
1	5	126	MET	CB-CA-C	-7.62	95.17	110.40
1	3	110	MET	CG-SD-CE	-7.61	88.02	100.20
1	5	197	TYR	CB-CG-CD1	-7.58	116.45	121.00
1	6	153	PHE	CB-CG-CD2	-7.58	115.49	120.80
1	1	292	ARG	CD-NE-CZ	-7.57	113.00	123.60
1	3	338	THR	N-CA-CB	7.57	124.68	110.30
1	4	89	TYR	CB-CG-CD1	-7.56	116.46	121.00
1	4	149	ASN	CB-CA-C	7.56	125.52	110.40
1	1	99	LEU	CB-CG-CD2	7.55	123.83	111.00
1	2	288	LYS	N-CA-CB	7.54	124.18	110.60
1	4	40	THR	N-CA-CB	7.53	124.61	110.30
1	4	93	ARG	N-CA-C	-7.53	90.67	111.00
1	6	107	ASN	C-N-CA	7.53	140.52	121.70
1	4	269	GLY	N-CA-C	-7.51	94.33	113.10
1	1	169	TYR	CB-CG-CD2	-7.48	116.51	121.00
1	4	44	ALA	N-CA-CB	7.47	120.56	110.10
1	4	222	PHE	CB-CA-C	-7.47	95.46	110.40
1	1	20	GLU	CA-CB-CG	7.46	129.80	113.40
1	6	261	TYR	CA-CB-CG	-7.45	99.25	113.40
1	5	32	GLY	N-CA-C	-7.43	94.52	113.10
1	4	19	LYS	C-N-CA	7.42	140.25	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	204	TYR	CB-CG-CD2	-7.40	116.56	121.00
1	2	351	ILE	N-CA-C	-7.39	91.04	111.00
1	3	160	LEU	CB-CA-C	7.38	124.23	110.20
1	6	56	MET	CG-SD-CE	-7.38	88.40	100.20
1	3	167	MET	CG-SD-CE	-7.37	88.42	100.20
1	1	102	ASP	N-CA-C	-7.33	91.22	111.00
1	1	359	THR	N-CA-C	-7.30	91.29	111.00
1	2	93	ARG	N-CA-CB	7.27	123.68	110.60
1	1	256	LYS	N-CA-C	-7.26	91.39	111.00
1	2	154	ALA	N-CA-CB	7.25	120.25	110.10
1	5	45	ILE	N-CA-C	-7.25	91.42	111.00
1	5	349	ARG	CA-C-N	-7.22	101.32	117.20
1	6	77	SER	N-CA-C	-7.21	91.53	111.00
1	3	112	GLU	C-N-CA	7.20	139.69	121.70
1	3	57	GLY	C-N-CA	7.19	139.68	121.70
1	5	169	TYR	CB-CG-CD2	-7.18	116.69	121.00
1	6	294	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	2	151	HIS	CA-CB-CG	-7.16	101.43	113.60
1	1	304	PHE	N-CA-CB	7.16	123.48	110.60
1	2	330	GLU	CB-CA-C	7.15	124.70	110.40
1	1	30	LYS	N-CA-C	-7.13	91.75	111.00
1	2	45	ILE	CA-C-N	-7.13	101.52	117.20
1	1	337	GLY	N-CA-C	-7.12	95.29	113.10
1	5	41	GLY	C-N-CA	7.12	139.51	121.70
1	2	93	ARG	CB-CA-C	-7.11	96.19	110.40
1	2	259	SER	CB-CA-C	7.11	123.60	110.10
1	1	92	ALA	N-CA-C	-7.07	91.91	111.00
1	6	314	THR	C-N-CA	7.06	139.34	121.70
1	3	111	TRP	CB-CG-CD2	-7.04	117.45	126.60
1	6	167	MET	CG-SD-CE	7.01	111.42	100.20
1	6	280	TRP	CB-CG-CD2	-7.00	117.50	126.60
1	5	210	VAL	N-CA-C	-6.98	92.15	111.00
1	6	271	PHE	CB-CG-CD2	-6.98	115.92	120.80
1	4	292	ARG	CD-NE-CZ	-6.97	113.85	123.60
1	6	133	SER	N-CA-CB	6.96	120.94	110.50
1	4	344	ASP	N-CA-C	-6.96	92.21	111.00
1	4	92	ALA	N-CA-CB	6.96	119.84	110.10
1	1	335	PHE	CB-CG-CD2	-6.94	115.94	120.80
1	5	45	ILE	CA-C-N	-6.94	101.93	117.20
1	5	349	ARG	N-CA-C	-6.94	92.26	111.00
1	4	142	GLY	N-CA-C	-6.92	95.79	113.10
1	1	350	TYR	CG-CD1-CE1	-6.91	115.78	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	152	PHE	CB-CG-CD2	6.90	125.63	120.80
1	2	261	TYR	CA-CB-CG	-6.89	100.30	113.40
1	4	19	LYS	CA-C-N	-6.87	102.08	117.20
1	2	344	ASP	N-CA-C	-6.87	92.45	111.00
1	1	238	THR	N-CA-CB	-6.87	97.25	110.30
1	1	20	GLU	N-CA-CB	6.87	122.96	110.60
1	1	109	LEU	N-CA-CB	6.86	124.12	110.40
1	4	100	ASN	CA-C-N	-6.86	102.11	117.20
1	2	350	TYR	CB-CG-CD2	-6.85	116.89	121.00
1	5	253	PRO	N-CA-CB	-6.84	95.07	102.60
1	6	301	PRO	CA-C-N	-6.84	102.14	117.20
1	2	281	ARG	CD-NE-CZ	-6.83	114.04	123.60
1	6	352	ASP	CA-CB-CG	-6.81	98.41	113.40
1	4	107	ASN	C-N-CA	6.80	138.70	121.70
1	5	252	GLY	N-CA-C	-6.80	96.10	113.10
1	6	157	GLY	N-CA-C	-6.80	96.10	113.10
1	5	324	GLY	N-CA-C	-6.80	96.11	113.10
1	1	111	TRP	CB-CG-CD1	6.76	135.78	127.00
1	4	292	ARG	O-C-N	-6.76	111.89	122.70
1	3	335	PHE	CB-CG-CD1	6.74	125.52	120.80
1	1	32	GLY	N-CA-C	-6.71	96.31	113.10
1	2	223	GLY	N-CA-C	-6.71	96.34	113.10
1	4	229	GLU	C-N-CA	6.70	138.44	121.70
1	4	294	ARG	C-N-CA	6.68	138.40	121.70
1	2	89	TYR	CB-CG-CD1	-6.66	117.01	121.00
1	4	169	TYR	CB-CG-CD2	6.65	124.99	121.00
1	3	119	GLU	N-CA-CB	6.64	122.55	110.60
1	2	202	ASN	N-CA-CB	6.64	122.55	110.60
1	3	261	TYR	CA-CB-CG	-6.63	100.81	113.40
1	6	163	GLN	N-CA-C	-6.62	93.13	111.00
1	2	293	LYS	CB-CA-C	-6.59	97.21	110.40
1	1	169	TYR	CB-CG-CD1	6.59	124.95	121.00
1	6	98	ASN	C-N-CA	6.59	138.17	121.70
1	5	75	ASP	N-CA-C	-6.58	93.22	111.00
1	4	162	MET	CG-SD-CE	-6.57	89.69	100.20
1	1	27	LEU	N-CA-C	-6.57	93.27	111.00
1	4	119	GLU	CB-CA-C	-6.56	97.29	110.40
1	1	354	GLN	N-CA-C	-6.54	93.35	111.00
1	2	126	MET	CG-SD-CE	-6.53	89.75	100.20
1	6	107	ASN	N-CA-C	-6.51	93.42	111.00
1	4	36	LEU	CB-CA-C	-6.51	97.83	110.20
1	4	292	ARG	N-CA-CB	-6.51	98.89	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	162	MET	CG-SD-CE	-6.50	89.80	100.20
1	3	169	TYR	CB-CG-CD2	6.49	124.90	121.00
1	4	203	ALA	N-CA-CB	6.49	119.19	110.10
1	5	296	VAL	C-N-CA	6.49	137.94	121.70
1	5	358	GLN	N-CA-CB	6.49	122.27	110.60
1	6	49	GLU	N-CA-CB	-6.48	98.94	110.60
1	5	299	PRO	C-N-CA	6.48	137.90	121.70
1	1	93	ARG	N-CA-C	-6.47	93.53	111.00
1	3	154	ALA	N-CA-CB	6.47	119.16	110.10
1	6	287	PHE	CB-CG-CD1	-6.47	116.27	120.80
1	3	298	ASN	CB-CA-C	-6.46	97.48	110.40
1	6	91	THR	CA-CB-CG2	6.45	121.42	112.40
1	4	28	LEU	CB-CA-C	-6.44	97.96	110.20
1	6	197	TYR	CB-CA-C	-6.43	97.53	110.40
1	6	80	SER	N-CA-CB	6.43	120.14	110.50
1	3	295	SER	N-CA-CB	6.42	120.12	110.50
1	3	177	THR	N-CA-C	-6.41	93.68	111.00
1	1	313	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	1	117	GLN	N-CA-C	-6.40	93.71	111.00
1	1	239	ASN	CB-CA-C	-6.39	97.62	110.40
1	5	165	VAL	CA-CB-CG2	-6.38	101.34	110.90
1	6	76	PHE	CB-CA-C	-6.36	97.69	110.40
1	4	129	LEU	N-CA-C	-6.35	93.84	111.00
1	1	280	TRP	CB-CG-CD1	6.35	135.25	127.00
1	4	89	TYR	CB-CG-CD2	6.34	124.81	121.00
1	4	300	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	3	316	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	1	173	TYR	CA-CB-CG	-6.33	101.38	113.40
1	1	112	GLU	C-N-CA	6.33	137.52	121.70
1	3	173	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	4	163	GLN	N-CA-CB	6.32	121.97	110.60
1	2	43	ASP	C-N-CA	6.32	137.49	121.70
1	3	20	GLU	C-N-CD	-6.32	106.71	120.60
1	1	334	VAL	N-CA-CB	6.30	125.36	111.50
1	1	263	SER	N-CA-C	-6.30	93.99	111.00
1	1	42	VAL	C-N-CA	6.29	137.44	121.70
1	5	354	GLN	N-CA-CB	6.29	121.93	110.60
1	4	159	PRO	N-CA-C	-6.29	95.75	112.10
1	1	163	GLN	N-CA-C	-6.29	94.03	111.00
1	3	228	GLY	N-CA-C	-6.29	97.39	113.10
1	1	197	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	5	360	LYS	N-CA-C	-6.28	94.04	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	259	SER	N-CA-CB	6.28	119.92	110.50
1	4	138	GLU	CA-CB-CG	6.27	127.20	113.40
1	4	291	LEU	CB-CG-CD1	6.26	121.64	111.00
1	4	273	ASN	CB-CA-C	6.25	122.91	110.40
1	5	109	LEU	CA-C-N	-6.25	103.45	117.20
1	1	280	TRP	CB-CA-C	-6.24	97.92	110.40
1	2	289	ILE	N-CA-C	6.24	127.86	111.00
1	1	323	TYR	N-CA-CB	6.24	121.83	110.60
1	5	88	CYS	N-CA-C	-6.23	94.18	111.00
1	1	152	PHE	CB-CA-C	-6.23	97.94	110.40
1	2	269	GLY	N-CA-C	-6.22	97.56	113.10
1	2	307	SER	N-CA-CB	-6.18	101.22	110.50
1	2	350	TYR	CB-CG-CD1	6.18	124.71	121.00
1	3	288	LYS	N-CA-CB	6.18	121.72	110.60
1	4	338	THR	C-N-CA	6.16	137.10	121.70
1	2	306	LEU	CB-CA-C	-6.16	98.51	110.20
1	3	80	SER	N-CA-CB	6.13	119.69	110.50
1	5	357	LEU	N-CA-C	-6.13	94.46	111.00
1	4	325	MET	N-CA-C	-6.12	94.47	111.00
1	1	93	ARG	CD-NE-CZ	-6.11	115.04	123.60
1	5	350	TYR	CG-CD2-CE2	-6.11	116.41	121.30
1	6	314	THR	O-C-N	6.11	132.47	122.70
1	3	328	GLN	CA-CB-CG	6.10	126.83	113.40
1	4	319	GLY	C-N-CA	6.10	136.96	121.70
1	5	27	LEU	N-CA-C	-6.09	94.56	111.00
1	5	105	CYS	CA-CB-SG	6.09	124.96	114.00
1	2	348	ILE	N-CA-C	-6.09	94.57	111.00
1	1	98	ASN	CA-CB-CG	-6.08	100.02	113.40
1	4	304	PHE	CB-CG-CD2	6.07	125.05	120.80
1	5	194	HIS	CA-CB-CG	6.04	123.87	113.60
1	6	145	ILE	N-CA-C	-6.04	94.69	111.00
1	1	28	LEU	N-CA-CB	6.04	122.48	110.40
1	3	109	LEU	CB-CA-C	-6.03	98.74	110.20
1	6	276	GLY	N-CA-C	-6.03	98.02	113.10
1	1	303	SER	N-CA-C	-6.03	94.72	111.00
1	5	124	THR	CA-CB-CG2	-6.03	103.96	112.40
1	2	37	GLU	N-CA-CB	-6.03	99.75	110.60
1	2	286	TYR	CB-CG-CD1	-6.03	117.39	121.00
1	5	112	GLU	CB-CA-C	6.02	122.45	110.40
1	4	127	LEU	CB-CA-C	6.02	121.64	110.20
1	1	301	PRO	N-CA-C	-6.02	96.45	112.10
1	1	173	TYR	CB-CA-C	-6.02	98.36	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	41	GLY	N-CA-C	6.01	128.13	113.10
1	4	45	ILE	CB-CA-C	-6.01	99.58	111.60
1	5	17	LYS	N-CA-C	-6.01	94.78	111.00
1	2	73	GLU	N-CA-C	-6.00	94.79	111.00
1	2	147	GLY	N-CA-C	-6.00	98.10	113.10
1	4	79	ASP	N-CA-CB	6.00	121.39	110.60
1	6	225	PHE	CB-CG-CD2	-5.99	116.60	120.80
1	6	293	LYS	N-CA-CB	5.99	121.39	110.60
1	1	334	VAL	N-CA-C	-5.99	94.83	111.00
1	1	234	VAL	CB-CA-C	-5.99	100.03	111.40
1	3	109	LEU	CB-CG-CD2	5.99	121.18	111.00
1	4	117	GLN	N-CA-C	-5.98	94.86	111.00
1	2	334	VAL	CA-C-N	-5.97	104.07	117.20
1	1	53	ASN	CA-CB-CG	-5.96	100.28	113.40
1	6	222	PHE	N-CA-C	-5.96	94.91	111.00
1	4	314	THR	C-N-CA	5.96	136.59	121.70
1	1	29	ILE	CA-C-N	-5.96	104.10	117.20
1	2	117	GLN	N-CA-C	-5.95	94.93	111.00
1	4	91	THR	N-CA-CB	5.95	121.60	110.30
1	3	205	PRO	N-CA-CB	5.95	110.43	103.30
1	4	57	GLY	N-CA-C	-5.94	98.26	113.10
1	5	347	MET	N-CA-CB	5.94	121.29	110.60
1	1	312	ARG	N-CA-CB	5.93	121.27	110.60
1	2	296	VAL	C-N-CA	5.92	136.50	121.70
1	5	182	ASN	CA-CB-CG	-5.92	100.38	113.40
1	3	259	SER	N-CA-C	-5.91	95.04	111.00
1	4	40	THR	CA-CB-OG1	5.90	121.38	109.00
1	4	210	VAL	CA-CB-CG2	5.89	119.73	110.90
1	6	237	VAL	C-N-CA	5.89	136.42	121.70
1	6	107	ASN	CA-CB-CG	-5.89	100.45	113.40
1	5	314	THR	N-CA-C	5.88	126.89	111.00
1	4	313	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	3	356	GLN	N-CA-CB	-5.88	100.02	110.60
1	2	111	TRP	CA-CB-CG	-5.88	102.54	113.70
1	3	334	VAL	CA-CB-CG1	-5.88	102.09	110.90
1	3	154	ALA	CB-CA-C	-5.87	101.29	110.10
1	5	45	ILE	N-CA-CB	5.87	124.31	110.80
1	6	350	TYR	CB-CG-CD1	-5.87	117.48	121.00
1	1	350	TYR	N-CA-CB	-5.87	100.04	110.60
1	3	92	ALA	N-CA-C	-5.87	95.16	111.00
1	3	152	PHE	CB-CG-CD2	-5.86	116.70	120.80
1	6	93	ARG	N-CA-C	-5.86	95.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	361	MET	N-CA-CB	-5.86	100.05	110.60
1	1	25	PRO	N-CA-C	-5.86	96.87	112.10
1	1	18	PRO	C-N-CA	5.85	136.31	121.70
1	3	24	VAL	CA-CB-CG2	-5.84	102.14	110.90
1	6	117	GLN	N-CA-C	-5.84	95.23	111.00
1	4	107	ASN	CA-CB-CG	-5.84	100.55	113.40
1	5	27	LEU	CB-CA-C	-5.84	99.10	110.20
1	1	335	PHE	CB-CG-CD1	5.84	124.89	120.80
1	6	124	THR	CA-CB-CG2	-5.83	104.23	112.40
1	1	51	PHE	C-N-CA	5.83	136.28	121.70
1	4	163	GLN	N-CA-C	-5.83	95.25	111.00
1	1	212	ASP	N-CA-C	-5.83	95.26	111.00
1	5	109	LEU	N-CA-CB	5.82	122.05	110.40
1	3	36	LEU	CA-CB-CG	5.82	128.68	115.30
1	5	133	SER	N-CA-C	-5.81	95.32	111.00
1	3	292	ARG	CB-CA-C	5.80	122.01	110.40
1	3	60	ASP	C-N-CA	5.79	136.17	121.70
1	3	106	GLY	N-CA-C	-5.79	98.64	113.10
1	1	187	SER	N-CA-CB	5.78	119.17	110.50
1	1	316	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	5	105	CYS	N-CA-CB	5.77	120.98	110.60
1	3	333	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	3	101	GLU	O-C-N	-5.76	113.48	122.70
1	4	115	THR	N-CA-CB	5.76	121.25	110.30
1	5	355	GLY	N-CA-C	-5.76	98.70	113.10
1	1	80	SER	N-CA-CB	5.76	119.14	110.50
1	5	31	GLY	N-CA-C	-5.75	98.72	113.10
1	2	237	VAL	CA-C-N	-5.75	104.56	117.20
1	6	27	LEU	CB-CA-C	-5.75	99.28	110.20
1	6	39	LYS	N-CA-C	-5.74	95.50	111.00
1	4	222	PHE	C-N-CA	-5.74	110.25	122.30
1	5	207	GLU	CA-CB-CG	5.74	126.02	113.40
1	1	24	VAL	CA-C-N	-5.74	101.04	117.10
1	2	195	LYS	N-CA-C	-5.73	95.53	111.00
1	4	155	VAL	C-N-CA	-5.73	110.27	122.30
1	6	113	ALA	CB-CA-C	-5.72	101.52	110.10
1	3	146	GLN	N-CA-CB	5.71	120.88	110.60
1	6	249	GLN	N-CA-C	-5.71	95.59	111.00
1	1	333	ARG	N-CA-CB	5.70	120.86	110.60
1	6	336	ASP	C-N-CA	5.70	134.26	122.30
1	1	332	VAL	O-C-N	-5.69	113.59	122.70
1	6	22	VAL	CA-C-N	-5.68	104.70	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	27	LEU	N-CA-C	-5.67	95.70	111.00
1	2	43	ASP	CA-C-N	-5.67	104.73	117.20
1	3	209	TRP	CA-CB-CG	-5.67	102.93	113.70
1	5	222	PHE	CB-CG-CD1	-5.67	116.83	120.80
1	4	229	GLU	CA-CB-CG	5.66	125.86	113.40
1	1	91	THR	CA-CB-CG2	5.66	120.32	112.40
1	5	261	TYR	CB-CA-C	-5.66	99.09	110.40
1	1	339	GLU	CA-C-N	-5.65	104.78	117.20
1	2	361	MET	N-CA-CB	5.64	120.75	110.60
1	2	350	TYR	CA-C-N	-5.63	104.81	117.20
1	2	50	CYS	CA-CB-SG	-5.63	103.87	114.00
1	3	280	TRP	CA-CB-CG	-5.63	103.01	113.70
1	4	154	ALA	N-CA-C	-5.62	95.83	111.00
1	5	29	ILE	CA-C-N	-5.62	104.84	117.20
1	2	209	TRP	N-CA-CB	-5.62	100.49	110.60
1	4	302	ILE	N-CA-CB	-5.62	97.89	110.80
1	2	340	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	3	147	GLY	C-N-CA	5.61	135.72	121.70
1	4	162	MET	CB-CA-C	-5.61	99.18	110.40
1	6	304	PHE	CA-CB-CG	-5.61	100.44	113.90
1	5	97	PRO	C-N-CA	5.61	135.72	121.70
1	4	45	ILE	O-C-N	5.61	131.67	122.70
1	6	350	TYR	N-CA-CB	5.60	120.69	110.60
1	1	269	GLY	N-CA-C	-5.59	99.12	113.10
1	6	22	VAL	C-N-CA	5.59	135.68	121.70
1	6	316	ARG	CG-CD-NE	-5.59	100.06	111.80
1	4	300	TYR	N-CA-C	5.58	126.08	111.00
1	1	286	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	2	143	LYS	CB-CG-CD	5.58	126.10	111.60
1	5	156	GLY	N-CA-C	-5.58	99.16	113.10
1	1	112	GLU	N-CA-CB	5.57	120.62	110.60
1	6	316	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	4	124	THR	CA-CB-CG2	-5.56	104.61	112.40
1	5	261	TYR	N-CA-CB	5.56	120.60	110.60
1	3	38	VAL	C-N-CA	5.56	135.59	121.70
1	1	197	TYR	CB-CA-C	-5.55	99.29	110.40
1	5	290	ARG	CA-CB-CG	-5.55	101.19	113.40
1	5	292	ARG	O-C-N	-5.55	113.82	122.70
1	6	116	VAL	N-CA-CB	5.55	123.71	111.50
1	1	239	ASN	N-CA-CB	5.54	120.58	110.60
1	2	314	THR	C-N-CA	5.54	135.55	121.70
1	3	197	TYR	CA-CB-CG	-5.53	102.89	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	104	THR	O-C-N	5.53	131.55	122.70
1	3	225	PHE	N-CA-C	-5.53	96.07	111.00
1	5	329	VAL	N-CA-C	-5.53	96.08	111.00
1	6	126	MET	CB-CA-C	-5.52	99.36	110.40
1	2	252	GLY	N-CA-C	-5.52	99.30	113.10
1	4	197	TYR	CB-CA-C	-5.51	99.37	110.40
1	6	73	GLU	N-CA-CB	5.51	120.52	110.60
1	3	338	THR	CA-CB-CG2	-5.51	104.69	112.40
1	4	267	ILE	CB-CA-C	-5.51	100.58	111.60
1	1	293	LYS	CB-CA-C	-5.50	99.40	110.40
1	1	333	ARG	CB-CA-C	-5.50	99.41	110.40
1	2	167	MET	N-CA-C	-5.50	96.15	111.00
1	5	37	GLU	N-CA-C	5.49	125.83	111.00
1	3	167	MET	N-CA-C	-5.49	96.18	111.00
1	5	288	LYS	N-CA-CB	5.49	120.48	110.60
1	2	259	SER	N-CA-C	-5.49	96.19	111.00
1	6	194	HIS	C-N-CA	5.48	135.39	121.70
1	2	112	GLU	C-N-CA	5.47	135.38	121.70
1	1	191	ASN	N-CA-C	-5.46	96.25	111.00
1	3	191	ASN	N-CA-CB	-5.46	100.76	110.60
1	1	51	PHE	CB-CG-CD1	-5.46	116.98	120.80
1	1	358	GLN	CA-C-N	-5.46	105.19	117.20
1	1	109	LEU	CB-CA-C	-5.46	99.83	110.20
1	4	344	ASP	N-CA-CB	5.46	120.42	110.60
1	5	191	ASN	N-CA-C	-5.45	96.27	111.00
1	6	102	ASP	N-CA-C	-5.45	96.28	111.00
1	4	53	ASN	CA-CB-CG	-5.45	101.41	113.40
1	4	126	MET	CG-SD-CE	5.45	108.92	100.20
1	6	21	PRO	N-CA-C	-5.45	97.93	112.10
1	3	159	PRO	N-CA-CB	5.45	109.84	103.30
1	4	56	MET	CB-CA-C	-5.45	99.50	110.40
1	1	286	TYR	N-CA-CB	-5.44	100.81	110.60
1	1	52	LEU	N-CA-CB	5.44	121.28	110.40
1	6	104	THR	C-N-CA	5.44	135.30	121.70
1	4	152	PHE	CB-CG-CD2	5.44	124.61	120.80
1	6	297	LYS	CB-CA-C	-5.44	99.53	110.40
1	2	46	THR	CA-CB-CG2	-5.43	104.79	112.40
1	4	236	HIS	N-CA-C	-5.43	96.33	111.00
1	1	360	LYS	C-N-CA	5.43	135.27	121.70
1	1	361	MET	N-CA-C	-5.43	96.35	111.00
1	3	295	SER	CB-CA-C	-5.42	99.80	110.10
1	5	286	TYR	CB-CG-CD2	-5.42	117.75	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	3	298	ASN	N-CA-CB	5.42	120.35	110.60
1	1	344	ASP	N-CA-CB	5.41	120.33	110.60
1	3	120	VAL	CB-CA-C	-5.41	101.12	111.40
1	6	297	LYS	N-CA-CB	5.41	120.33	110.60
1	3	197	TYR	CB-CA-C	-5.40	99.59	110.40
1	3	53	ASN	CA-CB-CG	-5.40	101.53	113.40
1	5	320	GLN	N-CA-C	-5.39	96.44	111.00
1	1	308	ASP	C-N-CA	5.39	135.18	121.70
1	3	103	LEU	C-N-CA	5.38	135.16	121.70
1	6	111	TRP	CB-CA-C	-5.38	99.63	110.40
1	2	51	PHE	CB-CG-CD1	-5.38	117.03	120.80
1	2	295	SER	N-CA-CB	5.38	118.56	110.50
1	2	176	GLY	C-N-CA	5.37	135.13	121.70
1	3	329	VAL	CB-CA-C	-5.37	101.19	111.40
1	3	336	ASP	N-CA-CB	5.37	120.27	110.60
1	5	110	MET	N-CA-C	-5.37	96.49	111.00
1	5	157	GLY	N-CA-C	-5.37	99.67	113.10
1	6	291	LEU	N-CA-C	5.37	125.50	111.00
1	2	45	ILE	CB-CA-C	-5.37	100.87	111.60
1	4	64	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	4	340	ARG	CA-CB-CG	5.36	125.19	113.40
1	5	306	LEU	CB-CG-CD1	5.35	120.09	111.00
1	6	302	ILE	CB-CA-C	-5.34	100.91	111.60
1	6	334	VAL	CB-CA-C	-5.33	101.26	111.40
1	4	126	MET	CB-CA-C	-5.33	99.74	110.40
1	6	31	GLY	N-CA-C	-5.33	99.78	113.10
1	2	196	ALA	N-CA-CB	5.33	117.56	110.10
1	3	261	TYR	N-CA-C	-5.33	96.61	111.00
1	1	138	GLU	CB-CG-CD	-5.33	99.82	114.20
1	6	304	PHE	CB-CG-CD2	-5.33	117.07	120.80
1	1	316	ARG	CA-C-N	-5.32	105.49	117.20
1	2	165	VAL	CA-CB-CG2	-5.32	102.92	110.90
1	1	349	ARG	CD-NE-CZ	-5.31	116.16	123.60
1	5	316	ARG	C-N-CA	5.31	134.97	121.70
1	2	271	PHE	O-C-N	5.30	131.19	122.70
1	6	102	ASP	C-N-CA	5.30	134.95	121.70
1	6	154	ALA	CA-C-N	-5.30	105.53	117.20
1	3	90	SER	CB-CA-C	-5.30	100.03	110.10
1	3	335	PHE	N-CA-C	-5.30	96.69	111.00
1	4	322	MET	CA-CB-CG	5.30	122.31	113.30
1	3	219	ALA	N-CA-CB	5.30	117.52	110.10
1	5	326	GLU	C-N-CA	5.29	134.93	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	204	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	2	163	GLN	N-CA-C	-5.28	96.75	111.00
1	3	48	VAL	CA-CB-CG2	-5.28	102.98	110.90
1	4	154	ALA	CA-C-N	-5.28	105.58	117.20
1	6	151	HIS	CA-C-N	-5.28	105.58	117.20
1	6	215	ARG	N-CA-C	-5.27	96.76	111.00
1	2	198	LEU	N-CA-CB	5.27	120.93	110.40
1	6	27	LEU	N-CA-CB	5.26	120.92	110.40
1	3	45	ILE	CB-CA-C	-5.26	101.08	111.60
1	4	209	TRP	N-CA-CB	5.25	120.06	110.60
1	4	115	THR	CA-CB-CG2	5.25	119.76	112.40
1	3	350	TYR	N-CA-CB	5.25	120.04	110.60
1	2	333	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	1	154	ALA	CB-CA-C	-5.24	102.23	110.10
1	1	243	THR	CA-CB-CG2	-5.24	105.06	112.40
1	5	197	TYR	CA-CB-CG	-5.24	103.44	113.40
1	2	143	LYS	N-CA-C	-5.24	96.86	111.00
1	5	85	MET	CA-CB-CG	5.24	122.20	113.30
1	1	358	GLN	N-CA-CB	5.23	120.01	110.60
1	2	326	GLU	N-CA-C	-5.23	96.89	111.00
1	2	188	GLN	CA-CB-CG	-5.23	101.90	113.40
1	4	249	GLN	C-N-CA	5.23	133.27	122.30
1	5	88	CYS	CB-CA-C	5.23	120.85	110.40
1	1	301	PRO	C-N-CA	5.22	134.76	121.70
1	2	149	ASN	CB-CA-C	5.22	120.84	110.40
1	6	292	ARG	CB-CA-C	-5.21	99.97	110.40
1	4	312	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	5	108	LEU	CB-CA-C	-5.21	100.30	110.20
1	1	334	VAL	CB-CA-C	-5.21	101.50	111.40
1	3	115	THR	CA-CB-CG2	5.21	119.70	112.40
1	4	140	GLY	N-CA-C	-5.21	100.07	113.10
1	2	349	ARG	CD-NE-CZ	-5.21	116.31	123.60
1	5	117	GLN	CB-CA-C	-5.21	99.98	110.40
1	6	197	TYR	CA-CB-CG	-5.21	103.51	113.40
1	3	45	ILE	O-C-N	5.20	131.03	122.70
1	3	280	TRP	CB-CG-CD1	5.20	133.76	127.00
1	6	151	HIS	CA-CB-CG	-5.20	104.76	113.60
1	2	309	LEU	CB-CA-C	-5.20	100.32	110.20
1	1	261	TYR	CA-CB-CG	-5.20	103.53	113.40
1	3	107	ASN	O-C-N	-5.19	114.39	122.70
1	4	93	ARG	N-CA-CB	5.19	119.95	110.60
1	1	107	ASN	C-N-CA	5.19	134.67	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	146	GLN	CB-CA-C	5.19	120.78	110.40
1	1	261	TYR	N-CA-C	-5.19	96.99	111.00
1	2	155	VAL	CA-CB-CG1	-5.19	103.12	110.90
1	4	25	PRO	C-N-CA	5.19	134.67	121.70
1	2	212	ASP	CA-CB-CG	-5.18	102.00	113.40
1	5	242	THR	CA-CB-CG2	5.18	119.66	112.40
1	3	76	PHE	CA-CB-CG	-5.18	101.47	113.90
1	5	222	PHE	CB-CG-CD2	5.18	124.42	120.80
1	1	215	ARG	N-CA-C	-5.17	97.03	111.00
1	5	146	GLN	N-CA-C	-5.17	97.05	111.00
1	1	276	GLY	N-CA-C	-5.17	100.19	113.10
1	2	75	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	5	74	ASN	N-CA-C	-5.16	97.06	111.00
1	5	152	PHE	CB-CG-CD2	-5.16	117.19	120.80
1	5	259	SER	N-CA-C	-5.16	97.06	111.00
1	1	137	HIS	CB-CA-C	-5.16	100.08	110.40
1	1	309	LEU	N-CA-CB	5.16	120.72	110.40
1	2	139	HIS	CA-CB-CG	-5.16	104.83	113.60
1	5	340	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	5	154	ALA	N-CA-CB	5.15	117.31	110.10
1	3	335	PHE	CB-CG-CD2	-5.15	117.19	120.80
1	1	303	SER	N-CA-CB	5.15	118.22	110.50
1	6	291	LEU	N-CA-CB	-5.14	100.12	110.40
1	5	306	LEU	N-CA-CB	-5.14	100.12	110.40
1	1	151	HIS	N-CA-C	-5.14	97.13	111.00
1	3	80	SER	N-CA-C	-5.14	97.13	111.00
1	1	358	GLN	N-CA-C	-5.14	97.13	111.00
1	5	350	TYR	N-CA-CB	-5.14	101.35	110.60
1	6	150	PHE	N-CA-C	-5.13	97.14	111.00
1	6	272	THR	C-N-CA	5.13	134.53	121.70
1	6	347	MET	CG-SD-CE	-5.13	91.99	100.20
1	4	290	ARG	N-CA-CB	5.13	119.83	110.60
1	4	167	MET	CG-SD-CE	-5.13	92.00	100.20
1	2	154	ALA	N-CA-C	-5.12	97.17	111.00
1	6	48	VAL	CA-CB-CG2	-5.12	103.22	110.90
1	4	95	PRO	N-CA-C	-5.11	98.81	112.10
1	4	100	ASN	N-CA-CB	5.11	119.80	110.60
1	5	64	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	3	134	GLN	N-CA-C	-5.11	97.21	111.00
1	2	75	ASP	CB-CG-OD1	5.11	122.90	118.30
1	2	309	LEU	CA-C-N	-5.10	105.97	117.20
1	5	240	THR	N-CA-C	-5.10	97.22	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	278	GLN	CB-CA-C	5.10	120.61	110.40
1	4	243	THR	CA-CB-CG2	-5.10	105.26	112.40
1	5	285	ARG	C-N-CA	5.10	134.45	121.70
1	5	314	THR	N-CA-CB	-5.10	100.61	110.30
1	4	314	THR	CA-C-N	-5.09	105.99	117.20
1	5	342	PRO	N-CA-CB	5.09	109.41	103.30
1	3	334	VAL	CG1-CB-CG2	5.09	119.05	110.90
1	5	127	LEU	CB-CA-C	5.09	119.87	110.20
1	2	222	PHE	N-CA-C	-5.09	97.26	111.00
1	1	349	ARG	O-C-N	5.09	130.84	122.70
1	4	290	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	2	340	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	5	350	TYR	CG-CD1-CE1	-5.08	117.23	121.30
1	4	229	GLU	N-CA-CB	-5.08	101.46	110.60
1	4	300	TYR	CA-CB-CG	-5.08	103.75	113.40
1	5	57	GLY	C-N-CA	5.08	134.39	121.70
1	5	113	ALA	N-CA-CB	5.08	117.20	110.10
1	2	176	GLY	N-CA-C	-5.07	100.42	113.10
1	4	333	ARG	N-CA-C	-5.07	97.31	111.00
1	1	359	THR	CB-CA-C	5.07	125.28	111.60
1	2	64	ARG	N-CA-C	-5.07	97.32	111.00
1	4	18	PRO	CA-N-CD	-5.07	104.41	111.50
1	1	300	TYR	CA-C-N	-5.06	102.92	117.10
1	2	15	PRO	C-N-CA	5.06	134.35	121.70
1	3	117	GLN	N-CA-CB	5.06	119.71	110.60
1	5	193	ASP	N-CA-C	-5.06	97.35	111.00
1	3	109	LEU	N-CA-CB	5.05	120.51	110.40
1	3	225	PHE	CB-CG-CD1	-5.05	117.26	120.80
1	5	119	GLU	CB-CA-C	-5.05	100.31	110.40
1	2	17	LYS	N-CA-CB	5.04	119.68	110.60
1	3	102	ASP	N-CA-C	-5.04	97.38	111.00
1	6	154	ALA	N-CA-C	-5.04	97.40	111.00
1	5	331	GLU	C-N-CA	5.04	134.29	121.70
1	6	107	ASN	O-C-N	5.04	130.76	122.70
1	4	150	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	4	94	ILE	N-CA-C	-5.03	97.42	111.00
1	5	358	GLN	N-CA-C	-5.03	97.42	111.00
1	3	329	VAL	N-CA-C	-5.02	97.45	111.00
1	4	272	THR	C-N-CA	5.01	134.24	121.70
1	3	279	GLN	N-CA-C	-5.01	97.48	111.00
1	4	44	ALA	CA-C-N	-5.00	106.19	117.20
1	4	297	LYS	N-CA-C	-5.00	97.49	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	329	VAL	CB-CA-C	-5.00	101.90	111.40

There are no chirality outliers.

All (220) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	100	ASN	Mainchain
1	1	150	PHE	Sidechain
1	1	151	HIS	Sidechain
1	1	152	PHE	Sidechain,Mainchain
1	1	153	PHE	Sidechain
1	1	173	TYR	Sidechain
1	1	192	THR	Mainchain
1	1	197	TYR	Sidechain
1	1	20	GLU	Mainchain,Peptide
1	1	204	TYR	Sidechain,Mainchain
1	1	211	PRO	Mainchain,Peptide
1	1	24	VAL	Mainchain,Peptide
1	1	25	PRO	Mainchain
1	1	271	PHE	Sidechain
1	1	281	ARG	Sidechain
1	1	286	TYR	Sidechain
1	1	287	PHE	Sidechain
1	1	290	ARG	Sidechain
1	1	292	ARG	Sidechain
1	1	294	ARG	Sidechain
1	1	300	TYR	Mainchain
1	1	312	ARG	Sidechain
1	1	313	ARG	Sidechain
1	1	316	ARG	Sidechain
1	1	324	GLY	Mainchain
1	1	329	VAL	Mainchain
1	1	333	ARG	Sidechain
1	1	335	PHE	Mainchain
1	1	349	ARG	Sidechain
1	1	357	LEU	Mainchain
1	1	358	GLN	Mainchain,Peptide
1	1	51	PHE	Sidechain
1	1	76	PHE	Sidechain
1	1	93	ARG	Sidechain
1	2	123	ILE	Mainchain,Peptide
1	2	150	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	2	151	HIS	Sidechain
1	2	152	PHE	Sidechain
1	2	153	PHE	Sidechain
1	2	169	TYR	Sidechain
1	2	173	TYR	Sidechain
1	2	176	GLY	Mainchain
1	2	197	TYR	Sidechain
1	2	222	PHE	Sidechain
1	2	230	ASN	Mainchain
1	2	237	VAL	Mainchain,Peptide
1	2	261	TYR	Sidechain
1	2	281	ARG	Sidechain
1	2	285	ARG	Sidechain
1	2	286	TYR	Sidechain
1	2	290	ARG	Sidechain
1	2	292	ARG	Sidechain
1	2	300	TYR	Sidechain
1	2	312	ARG	Sidechain
1	2	323	TYR	Sidechain
1	2	326	GLU	Mainchain
1	2	328	GLN	Peptide
1	2	334	VAL	Mainchain,Peptide
1	2	335	PHE	Sidechain
1	2	340	ARG	Sidechain
1	2	349	ARG	Sidechain
1	2	350	TYR	Sidechain
1	2	43	ASP	Mainchain
1	2	45	ILE	Mainchain,Peptide
1	2	64	ARG	Sidechain
1	2	66	PHE	Sidechain
1	2	69	LYS	Mainchain
1	2	76	PHE	Sidechain
1	2	83	ARG	Sidechain
1	2	93	ARG	Sidechain
1	3	111	TRP	Mainchain
1	3	133	SER	Peptide
1	3	148	SER	Mainchain
1	3	150	PHE	Sidechain
1	3	151	HIS	Sidechain
1	3	152	PHE	Sidechain
1	3	153	PHE	Sidechain
1	3	159	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	3	169	TYR	Sidechain
1	3	173	TYR	Sidechain
1	3	174	PRO	Mainchain,Peptide
1	3	194	HIS	Sidechain
1	3	197	TYR	Sidechain
1	3	212	ASP	Mainchain
1	3	215	ARG	Sidechain
1	3	221	TYR	Sidechain
1	3	225	PHE	Sidechain,Mainchain
1	3	230	ASN	Mainchain
1	3	261	TYR	Sidechain
1	3	271	PHE	Sidechain
1	3	286	TYR	Sidechain
1	3	290	ARG	Sidechain
1	3	292	ARG	Sidechain
1	3	294	ARG	Sidechain
1	3	300	TYR	Sidechain
1	3	323	TYR	Sidechain
1	3	333	ARG	Sidechain
1	3	340	ARG	Sidechain
1	3	349	ARG	Sidechain
1	3	350	TYR	Sidechain
1	3	36	LEU	Peptide
1	3	51	PHE	Sidechain
1	3	76	PHE	Sidechain
1	3	83	ARG	Sidechain
1	3	93	ARG	Sidechain
1	4	100	ASN	Mainchain,Peptide
1	4	137	HIS	Sidechain
1	4	148	SER	Mainchain
1	4	150	PHE	Sidechain
1	4	151	HIS	Sidechain
1	4	152	PHE	Sidechain
1	4	153	PHE	Sidechain
1	4	154	ALA	Mainchain
1	4	159	PRO	Mainchain
1	4	18	PRO	Mainchain
1	4	194	HIS	Sidechain
1	4	197	TYR	Sidechain
1	4	202	ASN	Mainchain,Peptide
1	4	215	ARG	Sidechain
1	4	221	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	4	24	VAL	Mainchain
1	4	261	TYR	Sidechain
1	4	271	PHE	Sidechain
1	4	280	TRP	Mainchain,Peptide
1	4	281	ARG	Sidechain
1	4	286	TYR	Sidechain
1	4	292	ARG	Sidechain
1	4	298	ASN	Mainchain
1	4	300	TYR	Sidechain
1	4	323	TYR	Sidechain
1	4	36	LEU	Mainchain,Peptide
1	4	44	ALA	Mainchain,Peptide
1	4	66	PHE	Sidechain
1	4	83	ARG	Sidechain
1	5	109	LEU	Mainchain,Peptide
1	5	137	HIS	Sidechain
1	5	148	SER	Mainchain
1	5	151	HIS	Sidechain
1	5	152	PHE	Sidechain,Mainchain
1	5	174	PRO	Mainchain,Peptide
1	5	191	ASN	Peptide
1	5	197	TYR	Sidechain
1	5	204	TYR	Sidechain
1	5	220	ARG	Sidechain
1	5	221	TYR	Sidechain
1	5	261	TYR	Sidechain
1	5	271	PHE	Sidechain
1	5	286	TYR	Sidechain
1	5	290	ARG	Sidechain
1	5	292	ARG	Sidechain
1	5	300	TYR	Sidechain
1	5	312	ARG	Sidechain
1	5	313	ARG	Sidechain,Mainchain,Peptide
1	5	333	ARG	Sidechain
1	5	335	PHE	Sidechain
1	5	340	ARG	Sidechain
1	5	349	ARG	Sidechain
1	5	350	TYR	Sidechain
1	5	361	MET	Mainchain
1	5	45	ILE	Mainchain
1	5	66	PHE	Sidechain
1	5	83	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	5	89	TYR	Sidechain
1	5	93	ARG	Sidechain
1	5	98	ASN	Mainchain
1	6	129	LEU	Mainchain,Peptide
1	6	150	PHE	Sidechain
1	6	151	HIS	Mainchain
1	6	153	PHE	Sidechain
1	6	154	ALA	Mainchain
1	6	170	ARG	Sidechain
1	6	172	LYS	Mainchain
1	6	192	THR	Mainchain
1	6	197	TYR	Sidechain
1	6	205	PRO	Mainchain,Peptide
1	6	221	TYR	Sidechain
1	6	222	PHE	Sidechain
1	6	225	PHE	Sidechain
1	6	230	ASN	Mainchain
1	6	261	TYR	Sidechain
1	6	271	PHE	Sidechain
1	6	281	ARG	Sidechain
1	6	287	PHE	Sidechain
1	6	292	ARG	Sidechain
1	6	300	TYR	Sidechain
1	6	304	PHE	Sidechain
1	6	316	ARG	Sidechain,Mainchain
1	6	333	ARG	Sidechain
1	6	349	ARG	Sidechain
1	6	45	ILE	Mainchain,Peptide
1	6	51	PHE	Sidechain
1	6	64	ARG	Sidechain
1	6	76	PHE	Sidechain
1	6	89	TYR	Sidechain

5.2 Too-close contacts (i)

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	2717	2689	2687	263	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	2717	2689	2687	281	0
1	3	2667	2630	2628	268	0
1	4	2571	2535	2532	253	0
1	5	2710	2682	2679	274	0
1	6	2660	2623	2620	238	0
All	All	16042	15848	15833	1429	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 45.

All (1429) 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)
1:4:99:LEU:HD21	1:4:111:TRP:CH2	2.05	0.91
1:3:89:TYR:CD1	1:3:206:VAL:HG12	2.12	0.85
1:2:114:VAL:HG22	1:2:292:ARG:HH11	1.43	0.83
1:3:109:LEU:HD22	1:3:295:SER:HA	1.62	0.81
1:3:310:ILE:HA	1:3:313:ARG:HE	1.46	0.79
1:3:34:GLU:OE2	1:3:35:VAL:HG23	1.83	0.78
1:4:164:GLY:H	1:4:194:HIS:HB2	1.48	0.77
1:6:301:PRO:HG2	1:6:304:PHE:H	1.48	0.77
1:5:165:VAL:HG21	1:5:210:VAL:HG13	1.66	0.76
1:1:309:LEU:HD12	1:5:29:ILE:HA	1.66	0.76
1:4:202:ASN:HD22	1:4:203:ALA:HA	1.53	0.74
1:2:303:SER:HA	1:2:306:LEU:HD12	1.70	0.74
1:1:88:CYS:HB2	1:1:202:ASN:HD22	1.52	0.74
1:3:29:ILE:HG13	1:3:35:VAL:HG22	1.69	0.73
1:6:302:ILE:HD12	1:6:302:ILE:H	1.53	0.73
1:1:153:PHE:HA	1:1:264:ALA:HA	1.69	0.73
1:5:334:VAL:HG12	1:5:335:PHE:O	1.89	0.73
1:2:178:ILE:HG22	1:2:203:ALA:HB1	1.69	0.73
1:3:109:LEU:HD22	1:3:295:SER:CA	2.19	0.72
1:5:89:TYR:CD1	1:5:206:VAL:HG12	2.24	0.72
1:6:351:ILE:HA	1:6:354:GLN:HG2	1.72	0.72
1:4:16:LYS:HE3	1:5:109:LEU:HD13	1.72	0.71
1:1:212:ASP:CG	1:1:215:ARG:HE	1.94	0.71
1:3:115:THR:HG22	1:3:290:ARG:NH1	2.06	0.71
1:1:289:ILE:HD12	1:1:289:ILE:H	1.55	0.71
1:5:153:PHE:HA	1:5:264:ALA:HA	1.71	0.71
1:4:239:ASN:HA	1:5:221:TYR:CE2	2.25	0.70
1:3:107:ASN:HA	1:3:297:LYS:HA	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:70:LEU:HD22	1:5:280:TRP:CZ3	2.27	0.70
1:3:348:ILE:H	1:3:348:ILE:HD12	1.57	0.70
1:4:112:GLU:HB3	1:4:292:ARG:HH22	1.56	0.70
1:2:114:VAL:HG21	1:2:290:ARG:NH1	2.07	0.69
1:4:52:LEU:HD21	1:4:92:ALA:HB2	1.75	0.69
1:5:42:VAL:HG23	1:5:293:LYS:H	1.57	0.69
1:5:91:THR:HG22	1:5:201:ASN:HA	1.74	0.69
1:4:153:PHE:HA	1:4:264:ALA:HA	1.73	0.69
1:5:27:LEU:HD11	1:5:29:ILE:C	2.13	0.69
1:4:124:THR:HG23	1:5:210:VAL:HG12	1.75	0.68
1:2:196:ALA:HB3	1:2:209:TRP:CH2	2.28	0.68
1:2:149:ASN:HA	1:2:267:ILE:O	1.93	0.68
1:1:45:ILE:HG22	1:1:290:ARG:HH21	1.59	0.68
1:5:350:TYR:CE1	1:5:350:TYR:HA	2.27	0.68
1:6:100:ASN:HD22	1:6:104:THR:HG21	1.59	0.68
1:4:292:ARG:HH21	1:4:292:ARG:HB3	1.59	0.68
1:1:89:TYR:CE1	1:1:206:VAL:HA	2.29	0.68
1:2:239:ASN:HD21	1:3:220:ARG:HA	1.59	0.68
1:5:112:GLU:HB3	1:5:292:ARG:HH12	1.59	0.67
1:2:150:PHE:CE1	1:2:152:PHE:HB2	2.29	0.67
1:5:220:ARG:HB3	1:5:222:PHE:CZ	2.30	0.67
1:2:271:PHE:H	1:2:281:ARG:HD3	1.59	0.67
1:3:121:ILE:HD13	1:3:286:TYR:HB2	1.76	0.67
1:6:89:TYR:CD1	1:6:206:VAL:HG12	2.29	0.67
1:5:54:PRO:HD3	1:5:284:ALA:HA	1.76	0.67
1:4:164:GLY:HA2	1:4:209:TRP:HA	1.78	0.66
1:6:114:VAL:HG23	1:6:291:LEU:HA	1.77	0.66
1:3:137:HIS:CD2	1:3:138:GLU:HB2	2.30	0.66
1:4:20:GLU:CD	1:4:20:GLU:H	1.99	0.66
1:4:89:TYR:CZ	1:4:206:VAL:HA	2.30	0.66
1:4:289:ILE:H	1:4:289:ILE:HD12	1.59	0.66
1:5:150:PHE:CE2	1:5:152:PHE:HB2	2.31	0.66
1:1:98:ASN:HD21	1:1:258:ASP:CG	1.99	0.66
1:6:63:LEU:HD23	1:6:66:PHE:HB2	1.78	0.65
1:3:36:LEU:HD23	1:3:97:PRO:HD3	1.77	0.65
1:4:50:CYS:SG	1:4:289:ILE:HD11	2.37	0.65
1:6:114:VAL:CG2	1:6:291:LEU:HA	2.27	0.65
1:1:295:SER:H	1:5:19:LYS:HE3	1.62	0.65
1:4:99:LEU:HD22	1:4:293:LYS:CE	2.27	0.65
1:1:182:ASN:HB2	1:1:194:HIS:CE1	2.32	0.65
1:6:138:GLU:OE1	1:6:139:HIS:CE1	2.50	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:91:THR:HG22	1:3:201:ASN:HA	1.79	0.65
1:3:89:TYR:CD2	1:3:204:TYR:HB2	2.31	0.64
1:4:114:VAL:HG21	1:4:292:ARG:HB2	1.79	0.64
1:2:18:PRO:HA	1:3:107:ASN:HB2	1.79	0.64
1:1:332:VAL:H	1:1:333:ARG:CZ	2.09	0.64
1:5:29:ILE:HG23	1:5:35:VAL:HG13	1.78	0.64
1:4:42:VAL:HG13	1:4:293:LYS:HB2	1.78	0.64
1:3:89:TYR:CE1	1:3:206:VAL:HG12	2.31	0.64
1:3:117:GLN:HB2	1:3:290:ARG:HH22	1.63	0.64
1:1:299:PRO:O	1:1:306:LEU:HD11	1.97	0.64
1:1:136:VAL:HG13	1:1:137:HIS:CE1	2.32	0.64
1:1:221:TYR:CE2	1:5:239:ASN:HA	2.33	0.64
1:1:180:PRO:HD3	1:1:208:CYS:HB2	1.79	0.64
1:3:103:LEU:HG	1:3:104:THR:H	1.61	0.64
1:1:300:TYR:C	1:1:302:ILE:H	2.01	0.64
1:4:220:ARG:HB3	1:4:222:PHE:CZ	2.33	0.64
1:2:116:VAL:HG23	1:2:289:ILE:HG13	1.79	0.63
1:4:99:LEU:HD21	1:4:111:TRP:CZ3	2.33	0.63
1:2:25:PRO:HA	1:6:338:THR:HA	1.79	0.63
1:6:301:PRO:HB2	1:6:303:SER:H	1.63	0.63
1:2:178:ILE:HG22	1:2:203:ALA:CB	2.29	0.63
1:4:261:TYR:N	1:4:261:TYR:CD2	2.64	0.63
1:4:239:ASN:HA	1:5:221:TYR:CD2	2.33	0.63
1:5:219:ALA:HA	1:5:253:PRO:HB3	1.80	0.63
1:5:39:LYS:O	1:5:40:THR:HG23	1.99	0.63
1:4:149:ASN:HA	1:4:267:ILE:O	1.99	0.62
1:3:36:LEU:HB2	1:3:37:GLU:OE1	2.00	0.62
1:4:212:ASP:HB2	1:4:215:ARG:HE	1.63	0.62
1:1:139:HIS:CE1	1:2:278:GLN:H	2.16	0.62
1:1:166:LEU:CD2	1:1:194:HIS:CE1	2.82	0.62
1:6:96:LEU:HB2	1:6:111:TRP:HE1	1.63	0.62
1:1:221:TYR:CZ	1:5:239:ASN:HA	2.34	0.62
1:2:162:MET:SD	1:2:209:TRP:HB3	2.39	0.62
1:1:68:LEU:HD22	1:1:84:LYS:HZ2	1.65	0.62
1:3:59:PRO:CG	1:3:63:LEU:HD22	2.30	0.62
1:3:96:LEU:HD11	1:3:255:CYS:SG	2.40	0.62
1:3:270:LEU:HG	1:3:280:TRP:CH2	2.34	0.62
1:3:261:TYR:CD2	1:3:261:TYR:N	2.66	0.62
1:1:179:THR:HG22	1:1:208:CYS:SG	2.39	0.62
1:5:162:MET:SD	1:5:209:TRP:HB3	2.40	0.62
1:1:156:GLY:C	1:1:158:GLU:H	2.04	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:115:THR:HG23	1:3:243:THR:O	1.99	0.62
1:3:128:ASN:O	1:3:129:LEU:HD23	1.99	0.62
1:5:27:LEU:HD21	1:5:30:LYS:HB2	1.82	0.61
1:4:233:PRO:O	1:4:234:VAL:HG23	2.00	0.61
1:3:341:LEU:HD21	1:6:295:SER:O	2.00	0.61
1:5:315:GLN:HE21	1:5:316:ARG:H	1.48	0.61
1:2:89:TYR:CZ	1:2:206:VAL:HA	2.35	0.61
1:6:187:SER:HA	1:6:191:ASN:HB2	1.82	0.61
1:1:109:LEU:HA	1:1:295:SER:HA	1.82	0.61
1:2:350:TYR:HE1	1:2:359:THR:H	1.48	0.61
1:6:91:THR:HG22	1:6:201:ASN:HA	1.83	0.61
1:5:165:VAL:HG21	1:5:210:VAL:CG1	2.30	0.61
1:1:173:TYR:CE1	1:1:179:THR:HG21	2.35	0.61
1:3:93:ARG:HG3	1:3:261:TYR:CE1	2.35	0.61
1:6:150:PHE:C	1:6:151:HIS:CD2	2.73	0.61
1:2:151:HIS:CD2	1:2:151:HIS:N	2.69	0.61
1:5:272:THR:HG23	1:5:278:GLN:HE22	1.64	0.61
1:4:93:ARG:HG3	1:4:261:TYR:CE1	2.35	0.60
1:3:124:THR:HB	1:4:207:GLU:HA	1.83	0.60
1:5:238:THR:HG22	1:5:240:THR:H	1.66	0.60
1:3:153:PHE:HA	1:3:264:ALA:HA	1.83	0.60
1:6:271:PHE:CE2	1:6:273:ASN:HA	2.36	0.60
1:6:129:LEU:HB3	1:6:142:GLY:H	1.66	0.60
1:3:270:LEU:HD21	1:3:280:TRP:CE2	2.37	0.60
1:3:143:LYS:HZ1	1:3:146:GLN:HG2	1.67	0.60
1:5:325:MET:C	1:5:327:SER:H	2.04	0.60
1:5:150:PHE:CD2	1:5:152:PHE:HB2	2.36	0.60
1:6:27:LEU:HD11	1:6:29:ILE:O	2.01	0.60
1:2:28:LEU:HD13	1:6:334:VAL:HG12	1.83	0.60
1:3:329:VAL:HG12	1:3:331:GLU:H	1.65	0.60
1:5:153:PHE:CE2	1:5:222:PHE:CD2	2.89	0.60
1:6:100:ASN:HD22	1:6:104:THR:CG2	2.15	0.60
1:2:27:LEU:HD12	1:6:334:VAL:O	2.02	0.60
1:2:145:ILE:HG23	1:2:281:ARG:HG2	1.84	0.60
1:1:280:TRP:CE3	1:1:280:TRP:HA	2.36	0.60
1:3:59:PRO:HG2	1:3:63:LEU:HD22	1.83	0.60
1:1:238:THR:HA	1:2:222:PHE:CD2	2.37	0.60
1:5:351:ILE:HA	1:5:356:GLN:HA	1.83	0.60
1:1:357:LEU:HD23	1:1:362:LEU:O	2.02	0.60
1:4:164:GLY:HA3	1:4:180:PRO:HG3	1.84	0.60
1:5:116:VAL:HG23	1:5:289:ILE:HG13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:129:LEU:HD22	1:3:144:PRO:HA	1.84	0.60
1:6:264:ALA:HB1	1:6:285:ARG:NH1	2.16	0.60
1:6:39:LYS:HD3	1:6:97:PRO:HG2	1.83	0.59
1:1:209:TRP:O	1:5:124:THR:HG21	2.02	0.59
1:1:150:PHE:CE2	1:1:152:PHE:HB2	2.36	0.59
1:5:291:LEU:HG	1:5:292:ARG:N	2.17	0.59
1:1:69:LYS:HZ2	1:1:277:THR:HB	1.67	0.59
1:3:93:ARG:HH12	1:3:95:PRO:N	2.00	0.59
1:4:64:ARG:HE	1:5:189:VAL:HB	1.66	0.59
1:6:83:ARG:HH21	1:6:203:ALA:HA	1.67	0.59
1:6:75:ASP:HA	1:6:76:PHE:CZ	2.37	0.59
1:3:150:PHE:CE2	1:3:152:PHE:HB3	2.36	0.59
1:5:129:LEU:H	1:5:130:HIS:CE1	2.19	0.59
1:3:238:THR:HA	1:4:222:PHE:CD1	2.37	0.59
1:6:162:MET:SD	1:6:209:TRP:HB3	2.43	0.59
1:2:204:TYR:CD2	1:2:209:TRP:CD2	2.90	0.59
1:6:184:THR:H	1:6:187:SER:HB2	1.67	0.59
1:5:158:GLU:HG2	1:5:218:ASN:HD22	1.67	0.59
1:1:169:TYR:H	1:1:170:ARG:NH1	2.00	0.59
1:5:89:TYR:CD2	1:5:204:TYR:HB2	2.37	0.59
1:4:116:VAL:HG23	1:4:289:ILE:HG13	1.84	0.59
1:4:312:ARG:HH11	1:4:312:ARG:HB3	1.68	0.59
1:3:57:GLY:O	1:3:84:LYS:HA	2.03	0.59
1:2:79:ASP:HB3	1:2:168:ASN:HD21	1.68	0.59
1:4:163:GLN:O	1:4:210:VAL:HG22	2.03	0.58
1:4:16:LYS:HB3	1:5:109:LEU:HD22	1.85	0.58
1:5:36:LEU:HD22	1:5:97:PRO:HD2	1.85	0.58
1:1:91:THR:HG22	1:1:201:ASN:HB3	1.85	0.58
1:1:334:VAL:HB	1:1:336:ASP:H	1.66	0.58
1:2:161:GLU:HG3	1:2:197:TYR:CE1	2.38	0.58
1:6:348:ILE:HG23	1:6:354:GLN:HB3	1.84	0.58
1:5:261:TYR:CD2	1:5:261:TYR:N	2.68	0.58
1:4:153:PHE:CE2	1:4:222:PHE:HB2	2.38	0.58
1:6:100:ASN:ND2	1:6:104:THR:HG21	2.18	0.58
1:4:47:GLU:OE2	1:4:290:ARG:HA	2.04	0.58
1:5:69:LYS:HA	1:5:278:GLN:O	2.04	0.58
1:3:61:GLU:H	1:3:61:GLU:CD	2.07	0.58
1:1:212:ASP:CB	1:1:215:ARG:HH21	2.16	0.58
1:5:151:HIS:N	1:5:151:HIS:CD2	2.69	0.58
1:3:23:GLN:CD	1:3:23:GLN:H	2.07	0.58
1:2:211:PRO:HB3	1:2:216:ASN:HD22	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:238:THR:HA	1:5:222:PHE:HA	1.86	0.58
1:1:351:ILE:HA	1:1:357:LEU:H	1.68	0.58
1:6:264:ALA:HB1	1:6:285:ARG:HH11	1.68	0.58
1:5:165:VAL:CG2	1:5:210:VAL:HG22	2.34	0.57
1:1:203:ALA:HB3	1:1:204:TYR:CE1	2.39	0.57
1:3:290:ARG:CD	1:3:290:ARG:N	2.67	0.57
1:1:112:GLU:HB3	1:1:292:ARG:HH11	1.68	0.57
1:6:151:HIS:CE1	1:6:266:ASP:C	2.78	0.57
1:1:175:ASP:HB2	1:1:177:THR:HG23	1.87	0.57
1:1:169:TYR:CD2	1:1:184:THR:O	2.58	0.57
1:3:232:PRO:HA	1:4:228:GLY:HA3	1.86	0.57
1:6:116:VAL:HG23	1:6:289:ILE:HG12	1.86	0.57
1:2:309:LEU:HA	1:2:312:ARG:HH21	1.68	0.57
1:5:171:SER:HB2	1:5:173:TYR:CZ	2.40	0.57
1:1:145:ILE:H	1:1:145:ILE:HD12	1.69	0.57
1:3:89:TYR:CZ	1:3:206:VAL:HA	2.39	0.57
1:2:198:LEU:HD13	1:2:204:TYR:CG	2.40	0.57
1:1:305:LEU:HD11	1:1:313:ARG:HH22	1.68	0.57
1:1:213:PRO:HA	1:1:216:ASN:HB2	1.86	0.57
1:3:294:ARG:CZ	1:3:295:SER:H	2.18	0.57
1:4:270:LEU:HD22	1:4:278:GLN:HB3	1.85	0.57
1:6:149:ASN:HB2	1:6:151:HIS:CD2	2.40	0.57
1:1:124:THR:HB	1:2:207:GLU:HA	1.85	0.57
1:3:167:MET:HA	1:3:188:GLN:HA	1.86	0.57
1:5:108:LEU:O	1:5:295:SER:HA	2.04	0.57
1:1:152:PHE:CG	1:1:153:PHE:N	2.71	0.57
1:5:66:PHE:CE1	1:5:271:PHE:HB2	2.40	0.57
1:2:145:ILE:H	1:2:145:ILE:HD12	1.69	0.57
1:6:91:THR:HG22	1:6:201:ASN:CA	2.35	0.57
1:6:234:VAL:HB	1:6:236:HIS:CE1	2.39	0.57
1:5:157:GLY:HA3	1:5:255:CYS:SG	2.45	0.57
1:4:82:GLU:HG2	1:4:84:LYS:H	1.70	0.56
1:1:52:LEU:HD21	1:1:92:ALA:HB2	1.87	0.56
1:5:94:ILE:O	1:5:259:SER:HA	2.05	0.56
1:1:152:PHE:CZ	1:1:154:ALA:HB2	2.40	0.56
1:4:48:VAL:O	1:4:289:ILE:HD12	2.05	0.56
1:5:66:PHE:CD1	1:5:271:PHE:HB2	2.40	0.56
1:2:150:PHE:CZ	1:2:152:PHE:HB2	2.40	0.56
1:3:272:THR:CA	1:3:278:GLN:HE21	2.18	0.56
1:1:169:TYR:CE2	1:1:185:ALA:HA	2.41	0.56
1:5:157:GLY:HA3	1:5:255:CYS:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:19:LYS:HD2	1:2:295:SER:H	1.69	0.56
1:1:116:VAL:HG22	1:1:117:GLN:O	2.06	0.56
1:1:272:THR:HA	1:1:278:GLN:HG3	1.86	0.56
1:6:350:TYR:HB2	1:6:352:ASP:H	1.69	0.56
1:2:50:CYS:SG	1:2:287:PHE:HB2	2.46	0.56
1:6:89:TYR:CD2	1:6:204:TYR:HB2	2.40	0.56
1:4:116:VAL:HG22	1:4:117:GLN:O	2.05	0.56
1:1:305:LEU:C	1:1:306:LEU:HD22	2.26	0.56
1:3:125:SER:H	1:4:165:VAL:HG12	1.71	0.56
1:3:292:ARG:CZ	1:3:294:ARG:HE	2.19	0.56
1:3:292:ARG:NH2	1:3:294:ARG:HE	2.04	0.56
1:4:192:THR:HG22	1:4:195:LYS:HZ1	1.70	0.56
1:2:154:ALA:HA	1:2:221:TYR:HA	1.87	0.56
1:6:69:LYS:HA	1:6:279:GLN:HA	1.87	0.56
1:5:27:LEU:HD11	1:5:29:ILE:O	2.05	0.56
1:5:164:GLY:HA3	1:5:180:PRO:HB3	1.87	0.56
1:4:91:THR:HG22	1:4:201:ASN:HA	1.88	0.56
1:5:88:CYS:H	1:5:202:ASN:ND2	2.04	0.56
1:5:54:PRO:CD	1:5:284:ALA:HA	2.36	0.56
1:2:254:LEU:HB3	1:2:256:LYS:HG3	1.88	0.56
1:1:101:GLU:CD	1:1:102:ASP:H	2.09	0.56
1:2:30:LYS:HA	1:6:333:ARG:HA	1.88	0.56
1:1:212:ASP:HB3	1:1:215:ARG:HH21	1.70	0.56
1:6:152:PHE:CG	1:6:153:PHE:N	2.74	0.56
1:5:251:VAL:HG22	1:5:252:GLY:H	1.71	0.56
1:1:173:TYR:CD1	1:1:179:THR:HG21	2.40	0.55
1:5:68:LEU:H	1:5:85:MET:HA	1.71	0.55
1:6:89:TYR:CZ	1:6:206:VAL:HA	2.40	0.55
1:2:46:THR:O	1:2:290:ARG:HA	2.07	0.55
1:1:191:ASN:HD22	1:1:194:HIS:CD2	2.25	0.55
1:5:48:VAL:O	1:5:288:LYS:HA	2.06	0.55
1:2:255:CYS:SG	1:2:260:LEU:HA	2.46	0.55
1:4:152:PHE:CD2	1:4:222:PHE:O	2.59	0.55
1:6:116:VAL:C	1:6:117:GLN:HG2	2.26	0.55
1:2:139:HIS:CD2	1:3:275:SER:O	2.60	0.55
1:2:150:PHE:HB3	1:2:267:ILE:HD13	1.89	0.55
1:3:93:ARG:HA	1:3:260:LEU:O	2.05	0.55
1:4:124:THR:HB	1:5:207:GLU:HA	1.88	0.55
1:4:239:ASN:HD22	1:5:221:TYR:H	1.55	0.55
1:2:90:SER:HB3	1:6:320:GLN:HE22	1.71	0.55
1:5:166:LEU:HD11	1:5:183:PRO:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:198:LEU:HD13	1:2:204:TYR:CD1	2.42	0.55
1:2:88:CYS:HB2	1:2:202:ASN:HA	1.88	0.55
1:4:150:PHE:CE1	1:4:152:PHE:HB2	2.41	0.55
1:2:153:PHE:HA	1:2:264:ALA:HA	1.88	0.55
1:6:46:THR:O	1:6:290:ARG:HA	2.06	0.55
1:2:157:GLY:HA2	1:2:255:CYS:SG	2.47	0.55
1:6:150:PHE:CZ	1:6:152:PHE:HB2	2.42	0.55
1:1:261:TYR:CD1	1:1:261:TYR:N	2.73	0.55
1:2:19:LYS:HE3	1:3:109:LEU:HD21	1.89	0.55
1:1:177:THR:HG22	1:1:205:PRO:HG3	1.87	0.55
1:4:150:PHE:CZ	1:4:152:PHE:HB2	2.41	0.55
1:3:150:PHE:CZ	1:3:152:PHE:HB2	2.42	0.55
1:5:340:ARG:HE	1:5:341:LEU:C	2.10	0.55
1:6:211:PRO:HB3	1:6:216:ASN:HD22	1.72	0.55
1:4:124:THR:CG2	1:5:210:VAL:HG12	2.37	0.55
1:4:114:VAL:HB	1:4:290:ARG:HH11	1.71	0.55
1:1:145:ILE:HG23	1:1:270:LEU:O	2.07	0.55
1:4:212:ASP:CB	1:4:215:ARG:HE	2.20	0.54
1:3:89:TYR:CE2	1:3:204:TYR:HB2	2.42	0.54
1:4:271:PHE:CE2	1:4:273:ASN:HA	2.43	0.54
1:1:42:VAL:CG1	1:1:292:ARG:HH21	2.21	0.54
1:1:109:LEU:HD11	1:5:17:LYS:HB2	1.89	0.54
1:3:308:ASP:HB2	1:3:312:ARG:HH21	1.71	0.54
1:1:271:PHE:CZ	1:1:273:ASN:HA	2.43	0.54
1:5:152:PHE:HZ	1:5:154:ALA:HB2	1.71	0.54
1:5:45:ILE:HA	1:5:291:LEU:O	2.08	0.54
1:2:94:ILE:O	1:2:259:SER:HA	2.07	0.54
1:4:287:PHE:N	1:4:287:PHE:CD1	2.74	0.54
1:1:340:ARG:HD2	1:1:341:LEU:C	2.28	0.54
1:5:59:PRO:HG2	1:5:63:LEU:HD23	1.90	0.54
1:2:246:LEU:HB3	1:2:250:GLY:HA2	1.89	0.54
1:2:86:LEU:HB2	1:2:177:THR:HG21	1.90	0.54
1:1:157:GLY:HA3	1:1:255:CYS:SG	2.47	0.54
1:3:116:VAL:HG12	1:3:245:LEU:HD21	1.90	0.54
1:6:122:GLY:HA3	1:6:283:LEU:HD22	1.90	0.54
1:4:99:LEU:HD22	1:4:293:LYS:CD	2.38	0.54
1:1:160:LEU:O	1:1:197:TYR:HA	2.07	0.54
1:5:117:GLN:HB2	1:5:290:ARG:HH22	1.72	0.54
1:5:160:LEU:O	1:5:197:TYR:HA	2.08	0.54
1:4:102:ASP:O	1:4:104:THR:HG23	2.07	0.54
1:4:166:LEU:HD11	1:4:187:SER:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:153:PHE:CD1	1:4:153:PHE:N	2.76	0.54
1:1:310:ILE:HG23	1:1:313:ARG:NH2	2.23	0.54
1:1:68:LEU:HD12	1:1:69:LYS:H	1.73	0.54
1:2:94:ILE:H	1:2:260:LEU:H	1.56	0.54
1:6:80:SER:H	1:6:81:PRO:HD3	1.72	0.54
1:5:87:PRO:HD3	1:5:280:TRP:HE1	1.72	0.54
1:6:61:GLU:C	1:6:63:LEU:H	2.09	0.54
1:4:42:VAL:HG13	1:4:293:LYS:O	2.08	0.53
1:5:150:PHE:C	1:5:151:HIS:CD2	2.82	0.53
1:1:348:ILE:HB	1:1:362:LEU:HA	1.90	0.53
1:5:89:TYR:CE1	1:5:206:VAL:HG12	2.43	0.53
1:3:221:TYR:C	1:3:222:PHE:CD1	2.82	0.53
1:3:272:THR:HA	1:3:278:GLN:HE21	1.73	0.53
1:1:360:LYS:HZ2	1:1:361:MET:HB2	1.73	0.53
1:5:89:TYR:CE1	1:5:206:VAL:HA	2.44	0.53
1:4:238:THR:HG22	1:4:240:THR:H	1.73	0.53
1:1:110:MET:HE2	1:1:258:ASP:HA	1.90	0.53
1:6:162:MET:SD	1:6:210:VAL:O	2.67	0.53
1:6:63:LEU:HD23	1:6:66:PHE:CB	2.38	0.53
1:3:321:PRO:HB2	1:3:326:GLU:HG3	1.91	0.53
1:2:287:PHE:HB2	1:2:289:ILE:HD11	1.89	0.53
1:4:151:HIS:CD2	1:4:151:HIS:N	2.76	0.53
1:2:145:ILE:HG22	1:2:146:GLN:N	2.24	0.53
1:1:26:LYS:HE3	1:1:28:LEU:HA	1.90	0.53
1:2:345:PRO:C	1:2:347:MET:H	2.11	0.53
1:6:104:THR:HG22	1:6:105:CYS:H	1.74	0.53
1:2:153:PHE:C	1:2:153:PHE:CD2	2.79	0.53
1:1:76:PHE:HA	1:5:131:ALA:HB1	1.89	0.53
1:5:352:ASP:H	1:5:357:LEU:HB2	1.73	0.53
1:3:21:PRO:HG2	1:4:297:LYS:CG	2.39	0.53
1:2:18:PRO:HA	1:3:107:ASN:CB	2.37	0.53
1:1:164:GLY:HA3	1:1:180:PRO:HG3	1.90	0.53
1:3:203:ALA:HB3	1:3:204:TYR:CD1	2.43	0.53
1:1:88:CYS:HA	1:1:205:PRO:HA	1.91	0.53
1:1:221:TYR:O	1:5:238:THR:HA	2.09	0.53
1:1:48:VAL:O	1:1:289:ILE:HD12	2.08	0.53
1:2:88:CYS:HB2	1:2:202:ASN:CA	2.39	0.53
1:2:204:TYR:CD2	1:2:209:TRP:CE2	2.97	0.53
1:2:152:PHE:N	1:2:285:ARG:HH22	2.07	0.53
1:4:247:ASP:H	1:4:250:GLY:HA2	1.74	0.53
1:3:88:CYS:HA	1:3:205:PRO:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:213:PRO:C	1:3:215:ARG:H	2.12	0.52
1:2:267:ILE:N	1:2:267:ILE:HD12	2.24	0.52
1:3:150:PHE:CZ	1:3:152:PHE:CB	2.92	0.52
1:5:45:ILE:C	1:5:45:ILE:HD12	2.29	0.52
1:3:89:TYR:CE1	1:3:206:VAL:HA	2.43	0.52
1:1:197:TYR:HB3	1:1:199:ASP:OD1	2.09	0.52
1:1:239:ASN:HB3	1:2:221:TYR:CE2	2.44	0.52
1:5:64:ARG:NH1	1:5:65:GLY:H	2.06	0.52
1:2:135:LYS:HA	1:2:142:GLY:HA2	1.91	0.52
1:4:46:THR:HG22	1:4:47:GLU:N	2.24	0.52
1:5:27:LEU:HD21	1:5:30:LYS:CB	2.39	0.52
1:6:221:TYR:CD1	1:6:221:TYR:N	2.78	0.52
1:5:128:ASN:ND2	1:5:131:ALA:HB2	2.25	0.52
1:2:160:LEU:O	1:2:197:TYR:HA	2.09	0.52
1:3:150:PHE:CE2	1:3:152:PHE:CB	2.92	0.52
1:6:60:ASP:OD1	1:6:63:LEU:HD22	2.08	0.52
1:4:96:LEU:H	1:4:259:SER:HA	1.75	0.52
1:4:23:GLN:H	1:4:23:GLN:CD	2.11	0.52
1:3:126:MET:HE2	1:3:127:LEU:HG	1.91	0.52
1:5:312:ARG:HH11	1:5:312:ARG:HB3	1.74	0.52
1:1:150:PHE:CD2	1:1:152:PHE:HB2	2.45	0.52
1:1:153:PHE:CE2	1:1:222:PHE:CD2	2.97	0.52
1:5:161:GLU:HA	1:5:196:ALA:O	2.09	0.52
1:6:152:PHE:HB2	1:6:223:GLY:HA3	1.91	0.52
1:2:199:ASP:HB3	1:6:317:VAL:HG12	1.92	0.52
1:5:87:PRO:O	1:5:206:VAL:HG22	2.10	0.52
1:6:117:GLN:CD	1:6:242:THR:HA	2.30	0.52
1:1:295:SER:H	1:5:19:LYS:CE	2.22	0.52
1:6:36:LEU:HD22	1:6:97:PRO:CD	2.40	0.52
1:5:340:ARG:NE	1:5:341:LEU:H	2.07	0.52
1:4:99:LEU:HD22	1:4:293:LYS:HD3	1.92	0.52
1:5:70:LEU:HD22	1:5:280:TRP:CE3	2.45	0.52
1:3:135:LYS:HA	1:3:142:GLY:HA2	1.92	0.52
1:1:20:GLU:HB3	1:1:21:PRO:O	2.09	0.52
1:1:150:PHE:CZ	1:1:223:GLY:HA3	2.44	0.52
1:5:218:ASN:HD21	1:5:254:LEU:HB2	1.75	0.52
1:4:83:ARG:HH21	1:4:88:CYS:N	2.07	0.52
1:1:89:TYR:CD2	1:1:204:TYR:O	2.63	0.52
1:5:89:TYR:CZ	1:5:206:VAL:HA	2.45	0.52
1:4:270:LEU:HB3	1:4:278:GLN:OE1	2.10	0.52
1:5:46:THR:O	1:5:290:ARG:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:208:CYS:SG	1:6:209:TRP:CD1	3.03	0.52
1:4:273:ASN:HD21	1:4:279:GLN:HG2	1.75	0.52
1:2:323:TYR:O	1:2:326:GLU:HG2	2.10	0.52
1:3:91:THR:H	1:3:201:ASN:HD22	1.57	0.51
1:1:151:HIS:CD2	1:1:151:HIS:N	2.74	0.51
1:1:47:GLU:HA	1:1:289:ILE:O	2.10	0.51
1:6:91:THR:HG23	1:6:92:ALA:N	2.24	0.51
1:4:139:HIS:HD2	1:5:277:THR:HA	1.75	0.51
1:6:94:ILE:O	1:6:259:SER:HA	2.10	0.51
1:4:306:LEU:O	1:4:310:ILE:HD12	2.10	0.51
1:3:237:VAL:O	1:3:237:VAL:HG22	2.10	0.51
1:3:164:GLY:H	1:3:194:HIS:HB2	1.75	0.51
1:2:145:ILE:HA	1:2:271:PHE:HA	1.92	0.51
1:3:102:ASP:N	1:3:103:LEU:HD23	2.25	0.51
1:6:99:LEU:HD22	1:6:111:TRP:CZ3	2.44	0.51
1:5:212:ASP:CG	1:5:215:ARG:HE	2.13	0.51
1:4:16:LYS:CE	1:5:109:LEU:HD13	2.39	0.51
1:5:109:LEU:HA	1:5:294:ARG:O	2.10	0.51
1:2:261:TYR:N	1:2:261:TYR:CD2	2.76	0.51
1:4:341:LEU:HD23	1:4:342:PRO:HD2	1.93	0.51
1:4:43:ASP:O	1:4:45:ILE:HG23	2.10	0.51
1:2:118:THR:HA	1:2:287:PHE:HA	1.93	0.51
1:2:196:ALA:HB3	1:2:209:TRP:CZ3	2.45	0.51
1:4:63:LEU:HD23	1:4:68:LEU:HA	1.91	0.51
1:2:221:TYR:C	1:2:222:PHE:CD1	2.83	0.51
1:2:108:LEU:HD13	1:2:297:LYS:C	2.31	0.51
1:2:191:ASN:HB3	1:2:194:HIS:CD2	2.45	0.51
1:1:162:MET:H	1:1:196:ALA:H	1.57	0.51
1:5:149:ASN:HB2	1:5:267:ILE:O	2.10	0.51
1:5:289:ILE:HD12	1:5:289:ILE:N	2.25	0.51
1:3:138:GLU:CD	1:3:139:HIS:H	2.13	0.51
1:6:150:PHE:CZ	1:6:152:PHE:CB	2.93	0.51
1:5:36:LEU:HD22	1:5:97:PRO:CD	2.40	0.51
1:1:236:HIS:HA	1:2:224:THR:HA	1.93	0.51
1:2:340:ARG:CG	1:2:341:LEU:H	2.23	0.51
1:2:289:ILE:H	1:2:289:ILE:HD12	1.76	0.51
1:4:178:ILE:HA	1:4:181:LYS:HZ1	1.75	0.51
1:1:166:LEU:HD22	1:1:194:HIS:CE1	2.45	0.51
1:3:302:ILE:HA	1:3:305:LEU:HD12	1.91	0.51
1:6:149:ASN:HA	1:6:267:ILE:HB	1.93	0.51
1:2:321:PRO:HA	1:2:323:TYR:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:48:VAL:O	1:3:288:LYS:HA	2.10	0.51
1:3:62:ASN:HA	1:4:188:GLN:HE22	1.75	0.51
1:6:286:TYR:CE2	1:6:288:LYS:HB2	2.46	0.51
1:2:55:GLU:HB2	1:2:202:ASN:OD1	2.11	0.51
1:5:200:LYS:NZ	1:5:203:ALA:HB2	2.26	0.51
1:5:67:SER:HB3	1:5:280:TRP:CD1	2.45	0.51
1:4:239:ASN:HB3	1:5:221:TYR:CD1	2.46	0.51
1:2:129:LEU:H	1:2:130:HIS:CD2	2.29	0.51
1:2:237:VAL:HG12	1:3:223:GLY:N	2.26	0.51
1:1:100:ASN:HB3	1:1:103:LEU:HD11	1.93	0.51
1:5:136:VAL:HA	1:5:143:LYS:NZ	2.26	0.51
1:3:87:PRO:O	1:3:205:PRO:HA	2.10	0.51
1:4:198:LEU:HD12	1:4:204:TYR:CD1	2.46	0.51
1:1:88:CYS:SG	1:1:205:PRO:HA	2.51	0.51
1:1:238:THR:HG23	1:2:222:PHE:CD2	2.46	0.51
1:3:273:ASN:HD22	1:3:277:THR:HB	1.76	0.51
1:2:230:ASN:HD22	1:2:231:VAL:N	2.08	0.51
1:6:310:ILE:HG23	1:6:313:ARG:HH21	1.76	0.51
1:3:150:PHE:HB2	1:3:267:ILE:HD12	1.93	0.51
1:2:145:ILE:HG22	1:2:146:GLN:H	1.74	0.51
1:6:164:GLY:CA	1:6:209:TRP:CE3	2.94	0.51
1:2:287:PHE:N	1:2:287:PHE:CD1	2.78	0.51
1:1:160:LEU:HD21	1:1:211:PRO:HA	1.91	0.51
1:1:47:GLU:OE2	1:1:290:ARG:HD3	2.11	0.51
1:5:115:THR:C	1:5:245:LEU:HD11	2.31	0.51
1:1:169:TYR:CD1	1:1:170:ARG:HD3	2.46	0.51
1:1:169:TYR:CD1	1:1:183:PRO:HA	2.45	0.51
1:3:55:GLU:CD	1:3:201:ASN:HD21	2.15	0.50
1:2:88:CYS:SG	1:2:177:THR:HG22	2.51	0.50
1:5:66:PHE:CD1	1:5:271:PHE:CB	2.95	0.50
1:4:272:THR:HG22	1:4:276:GLY:HA2	1.92	0.50
1:5:171:SER:HB2	1:5:173:TYR:CE1	2.46	0.50
1:3:168:ASN:H	1:3:188:GLN:HE21	1.58	0.50
1:5:16:LYS:O	1:5:18:PRO:HD3	2.11	0.50
1:4:159:PRO:O	1:4:197:TYR:CE2	2.64	0.50
1:1:164:GLY:CA	1:1:180:PRO:HG3	2.40	0.50
1:5:151:HIS:CE1	1:5:266:ASP:HA	2.47	0.50
1:4:152:PHE:CG	1:4:153:PHE:N	2.79	0.50
1:3:152:PHE:C	1:3:153:PHE:CD2	2.84	0.50
1:5:28:LEU:HD11	1:5:44:ALA:HB2	1.92	0.50
1:3:208:CYS:HB2	1:3:209:TRP:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:26:LYS:HZ2	1:3:28:LEU:H	1.60	0.50
1:1:205:PRO:HB2	1:1:208:CYS:SG	2.52	0.50
1:2:210:VAL:HB	1:2:211:PRO:HD2	1.94	0.50
1:4:16:LYS:HD2	1:5:109:LEU:HB2	1.93	0.50
1:5:221:TYR:C	1:5:222:PHE:CG	2.85	0.50
1:4:149:ASN:HA	1:4:267:ILE:HB	1.92	0.50
1:4:270:LEU:HD21	1:4:280:TRP:CH2	2.46	0.50
1:1:239:ASN:HD21	1:2:220:ARG:HD3	1.77	0.50
1:6:150:PHE:CE2	1:6:152:PHE:CB	2.94	0.50
1:2:235:LEU:O	1:2:236:HIS:CD2	2.64	0.50
1:2:27:LEU:HA	1:6:334:VAL:O	2.11	0.50
1:3:45:ILE:HG22	1:3:292:ARG:HB2	1.92	0.50
1:1:152:PHE:HZ	1:1:154:ALA:HB2	1.77	0.50
1:6:169:TYR:CE1	1:6:170:ARG:HD3	2.46	0.50
1:1:73:GLU:HA	1:5:132:GLY:HA2	1.93	0.50
1:1:359:THR:HG23	1:1:361:MET:HB3	1.93	0.50
1:1:118:THR:HA	1:1:286:TYR:O	2.11	0.50
1:1:53:ASN:HD21	1:2:190:MET:CG	2.23	0.50
1:2:48:VAL:O	1:2:288:LYS:HA	2.11	0.50
1:3:27:LEU:CD1	1:3:29:ILE:HG22	2.41	0.50
1:1:163:GLN:HE22	1:1:195:LYS:HG2	1.76	0.50
1:5:162:MET:SD	1:5:209:TRP:CB	3.00	0.50
1:6:189:VAL:HG13	1:6:190:MET:H	1.77	0.50
1:1:180:PRO:CD	1:1:208:CYS:HB2	2.41	0.50
1:3:151:HIS:N	1:3:151:HIS:CD2	2.78	0.50
1:2:344:ASP:HB3	1:2:347:MET:SD	2.52	0.50
1:4:281:ARG:HH21	1:4:283:LEU:HD11	1.77	0.50
1:5:89:TYR:CE2	1:5:204:TYR:HB2	2.46	0.50
1:1:287:PHE:HB2	1:1:289:ILE:HD11	1.93	0.50
1:5:152:PHE:CZ	1:5:154:ALA:HB2	2.47	0.50
1:3:301:PRO:O	1:3:304:PHE:CD1	2.64	0.50
1:2:97:PRO:HA	1:3:350:TYR:CE2	2.46	0.50
1:2:288:LYS:HZ1	1:2:290:ARG:N	2.09	0.50
1:5:165:VAL:HG21	1:5:210:VAL:HG22	1.92	0.50
1:6:169:TYR:CD1	1:6:170:ARG:NH1	2.80	0.50
1:6:270:LEU:HB3	1:6:279:GLN:H	1.76	0.50
1:5:352:ASP:H	1:5:357:LEU:CB	2.24	0.50
1:4:51:PHE:CD1	1:5:190:MET:SD	3.05	0.50
1:1:222:PHE:CE1	1:5:238:THR:HG23	2.47	0.49
1:1:157:GLY:O	1:1:257:ALA:HB3	2.12	0.49
1:6:99:LEU:HD21	1:6:111:TRP:CH2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:351:ILE:HG23	1:5:355:GLY:C	2.33	0.49
1:4:132:GLY:HA3	1:5:76:PHE:CE2	2.47	0.49
1:3:169:TYR:CE1	1:3:185:ALA:HA	2.47	0.49
1:1:163:GLN:O	1:1:210:VAL:HG22	2.11	0.49
1:5:327:SER:C	1:5:329:VAL:H	2.14	0.49
1:4:169:TYR:HB2	1:4:183:PRO:HB2	1.94	0.49
1:4:158:GLU:C	1:4:261:TYR:CD2	2.85	0.49
1:6:99:LEU:HD23	1:6:99:LEU:N	2.27	0.49
1:4:41:GLY:H	1:4:44:ALA:HB3	1.77	0.49
1:3:26:LYS:HZ2	1:3:28:LEU:N	2.10	0.49
1:5:152:PHE:CG	1:5:153:PHE:N	2.80	0.49
1:2:154:ALA:HB2	1:2:221:TYR:HB3	1.94	0.49
1:1:58:ASP:HA	1:1:66:PHE:O	2.13	0.49
1:6:153:PHE:C	1:6:153:PHE:CD1	2.83	0.49
1:6:150:PHE:CE2	1:6:152:PHE:HB3	2.48	0.49
1:4:139:HIS:CD2	1:5:277:THR:HA	2.47	0.49
1:4:159:PRO:O	1:4:197:TYR:CD2	2.66	0.49
1:1:292:ARG:HH12	1:1:294:ARG:HD3	1.77	0.49
1:5:234:VAL:HG12	1:5:236:HIS:CE1	2.47	0.49
1:4:111:TRP:NE1	1:4:258:ASP:HB3	2.27	0.49
1:3:104:THR:HG23	1:3:302:ILE:HD11	1.94	0.49
1:6:99:LEU:CD2	1:6:111:TRP:CH2	2.96	0.49
1:3:170:ARG:HH12	1:3:188:GLN:CD	2.15	0.49
1:2:110:MET:SD	1:2:256:LYS:HA	2.52	0.49
1:3:27:LEU:HD12	1:3:29:ILE:HG22	1.94	0.49
1:4:162:MET:N	1:4:215:ARG:HH21	2.10	0.49
1:5:152:PHE:CD1	1:5:222:PHE:O	2.66	0.49
1:5:264:ALA:HB1	1:5:285:ARG:HH11	1.78	0.49
1:5:47:GLU:HA	1:5:289:ILE:O	2.11	0.49
1:6:45:ILE:HD13	1:6:290:ARG:NE	2.27	0.49
1:6:112:GLU:HB3	1:6:292:ARG:HE	1.77	0.49
1:3:77:SER:HA	1:3:170:ARG:HB3	1.95	0.49
1:3:322:MET:SD	1:3:328:GLN:CB	3.01	0.49
1:2:198:LEU:HD11	1:2:200:LYS:O	2.13	0.49
1:6:180:PRO:HB3	1:6:194:HIS:CD2	2.47	0.49
1:6:150:PHE:O	1:6:266:ASP:HA	2.12	0.49
1:1:169:TYR:HB2	1:1:183:PRO:HA	1.95	0.49
1:4:22:VAL:HG12	1:4:23:GLN:O	2.12	0.49
1:1:143:LYS:HE3	1:1:146:GLN:HE21	1.77	0.49
1:3:118:THR:HG23	1:3:285:ARG:HH21	1.78	0.49
1:4:54:PRO:HD3	1:4:284:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:163:GLN:HE22	1:5:195:LYS:HG2	1.78	0.49
1:5:109:LEU:HG	1:5:295:SER:HA	1.95	0.49
1:3:239:ASN:HB3	1:4:221:TYR:CD2	2.48	0.49
1:2:120:VAL:HA	1:2:285:ARG:HA	1.94	0.49
1:6:99:LEU:HD21	1:6:111:TRP:CZ2	2.48	0.49
1:5:70:LEU:HG	1:5:279:GLN:HA	1.94	0.48
1:5:93:ARG:HG3	1:5:261:TYR:CE1	2.47	0.48
1:3:147:GLY:HA2	1:3:230:ASN:HA	1.95	0.48
1:5:79:ASP:O	1:5:171:SER:HA	2.13	0.48
1:6:147:GLY:H	1:6:230:ASN:C	2.17	0.48
1:6:239:ASN:OD1	1:6:240:THR:HG23	2.13	0.48
1:3:310:ILE:HG12	1:3:313:ARG:HH21	1.77	0.48
1:4:16:LYS:HD3	1:5:293:LYS:HD3	1.95	0.48
1:3:152:PHE:HB2	1:3:223:GLY:HA3	1.94	0.48
1:6:164:GLY:HA2	1:6:209:TRP:HA	1.94	0.48
1:6:168:ASN:HA	1:6:170:ARG:HH12	1.79	0.48
1:1:207:GLU:H	1:1:207:GLU:CD	2.15	0.48
1:3:55:GLU:HB2	1:3:202:ASN:OD1	2.13	0.48
1:6:264:ALA:CB	1:6:285:ARG:HH11	2.27	0.48
1:2:199:ASP:CB	1:6:317:VAL:HG12	2.43	0.48
1:6:313:ARG:NH1	1:6:314:THR:HA	2.29	0.48
1:4:96:LEU:HG	1:4:259:SER:HA	1.96	0.48
1:3:162:MET:HA	1:3:212:ASP:H	1.78	0.48
1:4:212:ASP:C	1:4:214:SER:H	2.15	0.48
1:5:96:LEU:HB2	1:5:111:TRP:HE1	1.78	0.48
1:2:279:GLN:HB2	1:2:281:ARG:NH1	2.27	0.48
1:6:89:TYR:CE1	1:6:206:VAL:HA	2.48	0.48
1:6:89:TYR:O	1:6:202:ASN:HA	2.13	0.48
1:1:109:LEU:HD11	1:5:17:LYS:CB	2.43	0.48
1:3:322:MET:SD	1:3:328:GLN:HB2	2.53	0.48
1:6:160:LEU:CD1	1:6:261:TYR:HB3	2.42	0.48
1:3:99:LEU:HD11	1:3:111:TRP:CD2	2.49	0.48
1:4:191:ASN:HB3	1:4:194:HIS:CE1	2.49	0.48
1:2:208:CYS:HB2	1:2:209:TRP:CD1	2.49	0.48
1:3:290:ARG:N	1:3:290:ARG:HD3	2.28	0.48
1:4:154:ALA:HA	1:4:221:TYR:HA	1.95	0.48
1:2:35:VAL:HG13	1:6:334:VAL:HG22	1.96	0.48
1:6:329:VAL:HG12	1:6:330:GLU:N	2.29	0.48
1:2:161:GLU:HG2	1:2:215:ARG:HB3	1.96	0.48
1:2:177:THR:HB	1:2:205:PRO:HG3	1.94	0.48
1:2:237:VAL:C	1:3:222:PHE:HA	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:238:THR:HG23	1:2:222:PHE:HD2	1.78	0.48
1:6:321:PRO:HB2	1:6:326:GLU:HB2	1.96	0.48
1:4:161:GLU:HB3	1:4:215:ARG:CZ	2.44	0.48
1:3:341:LEU:HD22	1:6:294:ARG:CZ	2.43	0.48
1:3:168:ASN:HA	1:3:170:ARG:CZ	2.42	0.48
1:2:114:VAL:HG21	1:2:290:ARG:HH12	1.75	0.48
1:2:211:PRO:O	1:2:213:PRO:HD3	2.14	0.48
1:1:115:THR:C	1:1:245:LEU:HD11	2.34	0.48
1:1:45:ILE:CG2	1:1:290:ARG:HH21	2.24	0.48
1:4:151:HIS:CE1	1:4:267:ILE:O	2.67	0.48
1:6:204:TYR:CD1	1:6:204:TYR:N	2.82	0.48
1:6:107:ASN:OD1	1:6:297:LYS:HA	2.14	0.48
1:1:331:GLU:C	1:1:332:VAL:HG13	2.33	0.48
1:2:77:SER:HA	1:2:170:ARG:HB3	1.94	0.48
1:5:306:LEU:C	1:5:306:LEU:HD12	2.34	0.48
1:4:196:ALA:CB	1:4:209:TRP:CH2	2.96	0.48
1:3:150:PHE:CB	1:3:267:ILE:HD12	2.43	0.48
1:2:56:MET:SD	1:2:282:GLY:HA3	2.54	0.48
1:6:114:VAL:HG21	1:6:292:ARG:HG2	1.96	0.48
1:4:36:LEU:HB2	1:4:37:GLU:OE1	2.14	0.48
1:3:270:LEU:HD22	1:3:278:GLN:HB3	1.95	0.47
1:6:99:LEU:CD2	1:6:111:TRP:CZ3	2.97	0.47
1:4:91:THR:HG22	1:4:201:ASN:CA	2.44	0.47
1:1:224:THR:HG23	1:5:235:LEU:O	2.13	0.47
1:2:169:TYR:CE1	1:2:184:THR:O	2.67	0.47
1:5:203:ALA:HB3	1:5:204:TYR:CZ	2.49	0.47
1:4:152:PHE:HA	1:4:223:GLY:HA2	1.94	0.47
1:4:153:PHE:CZ	1:4:222:PHE:HB2	2.49	0.47
1:1:139:HIS:CE1	1:2:277:THR:HA	2.49	0.47
1:1:189:VAL:HG22	1:1:189:VAL:O	2.14	0.47
1:2:175:ASP:HA	1:2:178:ILE:HA	1.96	0.47
1:5:87:PRO:CD	1:5:280:TRP:HE1	2.28	0.47
1:1:115:THR:O	1:1:289:ILE:HA	2.14	0.47
1:3:152:PHE:CG	1:3:153:PHE:N	2.81	0.47
1:3:51:PHE:CD2	1:3:284:ALA:HB1	2.49	0.47
1:1:109:LEU:HG	1:1:295:SER:HA	1.95	0.47
1:4:341:LEU:HD23	1:4:342:PRO:CD	2.44	0.47
1:3:205:PRO:HB2	1:3:208:CYS:SG	2.54	0.47
1:2:239:ASN:HB3	1:3:221:TYR:CE2	2.49	0.47
1:1:49:GLU:HG3	1:1:286:TYR:OH	2.13	0.47
1:1:94:ILE:HB	1:1:260:LEU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:294:ARG:HD2	1:4:295:SER:H	1.80	0.47
1:5:109:LEU:HB3	1:5:293:LYS:HB3	1.95	0.47
1:6:280:TRP:CE3	1:6:281:ARG:O	2.67	0.47
1:2:255:CYS:SG	1:2:260:LEU:HD12	2.54	0.47
1:4:169:TYR:CE1	1:4:185:ALA:HA	2.50	0.47
1:2:121:ILE:HG21	1:2:286:TYR:HB2	1.96	0.47
1:2:47:GLU:HG2	1:6:333:ARG:HB2	1.95	0.47
1:2:164:GLY:HA3	1:2:180:PRO:CG	2.44	0.47
1:2:89:TYR:CD1	1:2:204:TYR:O	2.68	0.47
1:5:204:TYR:CD2	1:5:204:TYR:N	2.83	0.47
1:1:112:GLU:CB	1:1:292:ARG:HH11	2.28	0.47
1:5:150:PHE:HD1	1:5:225:PHE:HA	1.79	0.47
1:4:152:PHE:C	1:4:153:PHE:CD1	2.88	0.47
1:3:151:HIS:O	1:3:223:GLY:HA2	2.15	0.47
1:5:340:ARG:O	1:5:341:LEU:HD12	2.14	0.47
1:3:162:MET:HB2	1:3:209:TRP:CZ3	2.49	0.47
1:3:99:LEU:HG	1:3:111:TRP:CE2	2.49	0.47
1:1:162:MET:O	1:1:195:LYS:HA	2.15	0.47
1:1:200:LYS:HZ1	1:1:203:ALA:HB2	1.80	0.47
1:2:161:GLU:HB2	1:2:216:ASN:OD1	2.15	0.47
1:5:150:PHE:CZ	1:5:223:GLY:HA3	2.50	0.47
1:2:153:PHE:CD1	1:2:153:PHE:N	2.81	0.47
1:1:239:ASN:HD21	1:2:220:ARG:HA	1.79	0.47
1:3:267:ILE:CG2	1:3:280:TRP:CZ3	2.97	0.47
1:2:70:LEU:HD21	1:2:280:TRP:NE1	2.30	0.47
1:6:89:TYR:HD2	1:6:204:TYR:HB2	1.78	0.47
1:6:225:PHE:C	1:6:225:PHE:CD2	2.87	0.47
1:6:157:GLY:O	1:6:257:ALA:HB3	2.15	0.47
1:2:351:ILE:HA	1:2:356:GLN:HA	1.97	0.47
1:1:51:PHE:CD1	1:1:51:PHE:N	2.82	0.47
1:3:287:PHE:CD1	1:3:287:PHE:N	2.81	0.47
1:1:129:LEU:HD11	1:1:144:PRO:HA	1.96	0.47
1:4:93:ARG:HG3	1:4:261:TYR:CZ	2.50	0.47
1:1:152:PHE:CD1	1:1:222:PHE:O	2.68	0.47
1:2:89:TYR:CD2	1:2:206:VAL:HG12	2.50	0.47
1:2:88:CYS:HA	1:2:205:PRO:HA	1.95	0.47
1:4:278:GLN:HA	1:4:278:GLN:OE1	2.15	0.47
1:1:305:LEU:HD21	1:1:313:ARG:HH12	1.79	0.47
1:4:174:PRO:HB2	1:4:177:THR:HG21	1.96	0.47
1:4:304:PHE:CD2	1:4:305:LEU:HD23	2.49	0.47
1:3:112:GLU:HB3	1:3:292:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:221:TYR:CD1	1:4:221:TYR:N	2.81	0.47
1:3:239:ASN:CG	1:4:221:TYR:H	2.19	0.47
1:5:112:GLU:CB	1:5:292:ARG:HH12	2.28	0.47
1:6:111:TRP:CD1	1:6:258:ASP:HA	2.50	0.47
1:1:273:ASN:H	1:1:278:GLN:HA	1.80	0.47
1:3:299:PRO:C	1:3:301:PRO:HD3	2.35	0.47
1:2:126:MET:SD	1:2:127:LEU:HG	2.55	0.47
1:1:114:VAL:O	1:1:244:VAL:HA	2.15	0.47
1:2:27:LEU:HD23	1:6:347:MET:SD	2.55	0.47
1:3:112:GLU:HB3	1:3:292:ARG:HH11	1.80	0.47
1:1:277:THR:HG22	1:1:278:GLN:N	2.30	0.47
1:3:163:GLN:HB3	1:3:210:VAL:HG22	1.95	0.47
1:3:26:LYS:HG2	1:3:28:LEU:H	1.80	0.46
1:2:101:GLU:HA	1:6:304:PHE:CD1	2.50	0.46
1:5:85:MET:O	1:5:87:PRO:HD3	2.15	0.46
1:4:152:PHE:CD1	1:4:152:PHE:C	2.88	0.46
1:4:68:LEU:HB3	1:4:85:MET:HB3	1.96	0.46
1:3:150:PHE:C	1:3:151:HIS:CD2	2.89	0.46
1:6:292:ARG:HH11	1:6:292:ARG:HB2	1.80	0.46
1:6:152:PHE:CD1	1:6:152:PHE:C	2.85	0.46
1:4:112:GLU:HB3	1:4:294:ARG:HB2	1.97	0.46
1:4:98:ASN:CG	1:4:99:LEU:H	2.19	0.46
1:2:19:LYS:HZ3	1:3:294:ARG:NH2	2.12	0.46
1:2:200:LYS:HG3	1:2:203:ALA:HB2	1.96	0.46
1:2:221:TYR:CD1	1:2:221:TYR:N	2.79	0.46
1:5:352:ASP:CA	1:5:357:LEU:HB2	2.45	0.46
1:3:159:PRO:O	1:3:197:TYR:CE2	2.68	0.46
1:5:137:HIS:CE1	1:5:140:GLY:HA3	2.51	0.46
1:4:80:SER:H	1:4:172:LYS:HZ2	1.64	0.46
1:2:112:GLU:HB3	1:2:292:ARG:CZ	2.45	0.46
1:2:257:ALA:C	1:2:259:SER:H	2.19	0.46
1:4:79:ASP:H	1:4:172:LYS:HE3	1.81	0.46
1:4:27:LEU:HG	1:4:29:ILE:H	1.79	0.46
1:6:84:LYS:NZ	1:6:84:LYS:HA	2.30	0.46
1:2:17:LYS:HD3	1:2:18:PRO:N	2.30	0.46
1:1:153:PHE:CZ	1:1:222:PHE:HB2	2.50	0.46
1:5:145:ILE:HG23	1:5:270:LEU:N	2.31	0.46
1:1:69:LYS:HD3	1:1:277:THR:HG21	1.98	0.46
1:3:59:PRO:HG3	1:3:63:LEU:HD22	1.98	0.46
1:1:169:TYR:CD2	1:1:188:GLN:OE1	2.68	0.46
1:3:322:MET:HA	1:3:326:GLU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:107:ASN:H	1:5:18:PRO:HB3	1.80	0.46
1:3:296:VAL:HB	1:6:343:GLY:HA2	1.95	0.46
1:5:118:THR:HA	1:5:286:TYR:O	2.14	0.46
1:2:54:PRO:HG2	1:2:65:GLY:HA2	1.96	0.46
1:4:153:PHE:CZ	1:4:222:PHE:CB	2.98	0.46
1:3:145:ILE:HG13	1:3:271:PHE:HA	1.96	0.46
1:1:139:HIS:CG	1:2:277:THR:HA	2.50	0.46
1:3:341:LEU:HG	1:3:341:LEU:O	2.16	0.46
1:1:300:TYR:CA	1:1:302:ILE:H	2.28	0.46
1:1:280:TRP:CE3	1:1:280:TRP:CA	2.98	0.46
1:6:309:LEU:N	1:6:312:ARG:HH21	2.13	0.46
1:4:111:TRP:HE1	1:4:258:ASP:HB3	1.80	0.46
1:2:50:CYS:HA	1:6:329:VAL:HA	1.98	0.46
1:4:192:THR:CG2	1:4:195:LYS:HZ1	2.28	0.46
1:2:150:PHE:CZ	1:2:152:PHE:CB	2.99	0.46
1:6:50:CYS:SG	1:6:287:PHE:HB2	2.56	0.46
1:6:79:ASP:HB2	1:6:172:LYS:H	1.79	0.46
1:3:98:ASN:HB3	1:3:100:ASN:H	1.81	0.46
1:4:96:LEU:HD12	1:4:111:TRP:CD1	2.50	0.46
1:2:28:LEU:HD11	1:6:336:ASP:OD1	2.16	0.46
1:3:310:ILE:HA	1:3:313:ARG:NE	2.22	0.46
1:4:166:LEU:HD11	1:4:187:SER:CB	2.45	0.46
1:2:205:PRO:HB2	1:2:208:CYS:SG	2.55	0.46
1:5:115:THR:HB	1:5:290:ARG:HH11	1.80	0.46
1:4:118:THR:HA	1:4:287:PHE:HA	1.97	0.46
1:1:190:MET:SD	1:5:53:ASN:HA	2.56	0.46
1:6:29:ILE:HG23	1:6:35:VAL:HG22	1.98	0.46
1:3:82:GLU:HG2	1:3:84:LYS:H	1.81	0.46
1:6:213:PRO:HA	1:6:216:ASN:HB2	1.97	0.46
1:6:261:TYR:CD2	1:6:261:TYR:N	2.82	0.46
1:1:93:ARG:HA	1:1:260:LEU:O	2.16	0.46
1:2:171:SER:HB3	1:2:173:TYR:CZ	2.51	0.46
1:2:115:THR:HA	1:2:245:LEU:HG	1.98	0.46
1:3:297:LYS:O	1:6:342:PRO:HA	2.15	0.46
1:2:104:THR:HG23	1:6:301:PRO:HB3	1.98	0.46
1:4:89:TYR:CD1	1:4:204:TYR:O	2.68	0.46
1:5:178:ILE:HG22	1:5:203:ALA:HB1	1.98	0.46
1:1:112:GLU:HB2	1:1:294:ARG:HB2	1.96	0.46
1:4:150:PHE:O	1:4:266:ASP:HA	2.16	0.46
1:6:270:LEU:C	1:6:281:ARG:HE	2.19	0.46
1:6:145:ILE:HG12	1:6:271:PHE:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:139:HIS:CG	1:4:139:HIS:O	2.66	0.46
1:3:170:ARG:HH12	1:3:188:GLN:NE2	2.14	0.46
1:6:118:THR:C	1:6:119:GLU:HG3	2.36	0.46
1:3:350:TYR:N	1:3:350:TYR:CD1	2.84	0.46
1:1:353:LYS:NZ	1:1:355:GLY:H	2.14	0.46
1:2:116:VAL:HA	1:2:288:LYS:O	2.16	0.46
1:2:103:LEU:O	1:6:301:PRO:CB	2.63	0.46
1:3:47:GLU:HA	1:3:289:ILE:O	2.16	0.46
1:6:280:TRP:CZ3	1:6:281:ARG:O	2.69	0.46
1:6:66:PHE:CZ	1:6:281:ARG:HB2	2.51	0.46
1:5:158:GLU:C	1:5:261:TYR:CD2	2.89	0.46
1:3:53:ASN:HB3	1:3:54:PRO:HD2	1.98	0.46
1:6:53:ASN:HD22	1:6:54:PRO:HD2	1.80	0.46
1:6:128:ASN:HA	1:6:130:HIS:CD2	2.50	0.46
1:4:164:GLY:HA3	1:4:180:PRO:CG	2.45	0.46
1:5:162:MET:H	1:5:196:ALA:H	1.64	0.46
1:4:145:ILE:HG21	1:4:270:LEU:O	2.16	0.46
1:2:150:PHE:C	1:2:151:HIS:CD2	2.89	0.46
1:1:68:LEU:HD23	1:1:85:MET:SD	2.56	0.46
1:2:350:TYR:CB	1:2:357:LEU:HD23	2.46	0.46
1:2:111:TRP:CZ2	1:2:293:LYS:HD2	2.50	0.45
1:4:162:MET:O	1:4:195:LYS:HA	2.16	0.45
1:4:152:PHE:CZ	1:4:154:ALA:HB2	2.52	0.45
1:3:269:GLY:O	1:3:280:TRP:CE3	2.69	0.45
1:5:166:LEU:HG	1:5:187:SER:HB3	1.98	0.45
1:6:157:GLY:HA3	1:6:255:CYS:HA	1.98	0.45
1:1:55:GLU:OE1	1:1:90:SER:HA	2.16	0.45
1:2:57:GLY:O	1:2:84:LYS:HA	2.16	0.45
1:2:361:MET:SD	1:2:361:MET:O	2.73	0.45
1:1:89:TYR:CZ	1:1:206:VAL:HA	2.52	0.45
1:5:67:SER:HB2	1:5:85:MET:HA	1.98	0.45
1:6:163:GLN:O	1:6:210:VAL:O	2.34	0.45
1:6:271:PHE:N	1:6:279:GLN:O	2.49	0.45
1:5:158:GLU:OE2	1:5:253:PRO:HB2	2.15	0.45
1:5:128:ASN:HA	1:5:130:HIS:CD2	2.51	0.45
1:3:89:TYR:OH	1:3:209:TRP:HB2	2.17	0.45
1:4:89:TYR:CE1	1:4:204:TYR:HB3	2.51	0.45
1:1:290:ARG:HH22	1:1:292:ARG:HB3	1.82	0.45
1:5:153:PHE:CZ	1:5:222:PHE:CB	2.99	0.45
1:3:273:ASN:ND2	1:3:279:GLN:HE21	2.14	0.45
1:4:50:CYS:SG	1:4:287:PHE:HB2	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:348:ILE:HB	1:2:350:TYR:CE1	2.51	0.45
1:1:24:VAL:O	1:1:24:VAL:HG23	2.17	0.45
1:2:35:VAL:HG13	1:6:334:VAL:CG2	2.47	0.45
1:3:99:LEU:HB3	1:3:109:LEU:HB2	1.98	0.45
1:4:184:THR:H	1:4:187:SER:HB2	1.82	0.45
1:5:88:CYS:HB2	1:5:202:ASN:CG	2.36	0.45
1:5:149:ASN:HA	1:5:267:ILE:O	2.15	0.45
1:4:280:TRP:HA	1:4:280:TRP:CE3	2.51	0.45
1:3:150:PHE:O	1:3:266:ASP:HA	2.17	0.45
1:1:299:PRO:HG2	1:1:300:TYR:CD1	2.51	0.45
1:6:152:PHE:CZ	1:6:154:ALA:HB2	2.52	0.45
1:1:19:LYS:HZ2	1:2:109:LEU:HD22	1.82	0.45
1:5:191:ASN:HB3	1:5:194:HIS:CE1	2.52	0.45
1:3:132:GLY:HA3	1:4:73:GLU:HA	1.98	0.45
1:4:42:VAL:O	1:4:292:ARG:HA	2.16	0.45
1:3:124:THR:HG23	1:4:210:VAL:HG12	1.98	0.45
1:2:213:PRO:HA	1:2:216:ASN:HB2	1.97	0.45
1:2:220:ARG:HB3	1:2:222:PHE:HE1	1.82	0.45
1:2:239:ASN:CB	1:3:221:TYR:CE2	3.00	0.45
1:6:289:ILE:HG22	1:6:291:LEU:HD21	1.98	0.45
1:6:70:LEU:HG	1:6:270:LEU:HD21	1.97	0.45
1:6:77:SER:O	1:6:172:LYS:HD2	2.16	0.45
1:1:79:ASP:H	1:1:171:SER:HA	1.80	0.45
1:1:89:TYR:CE2	1:1:162:MET:HE1	2.50	0.45
1:2:178:ILE:HG23	1:2:178:ILE:O	2.15	0.45
1:4:134:GLN:HA	1:5:73:GLU:CD	2.37	0.45
1:2:150:PHE:CD1	1:2:225:PHE:HA	2.52	0.45
1:3:153:PHE:CD2	1:3:153:PHE:N	2.85	0.45
1:3:145:ILE:HG23	1:3:270:LEU:C	2.36	0.45
1:5:289:ILE:HG22	1:5:290:ARG:N	2.31	0.45
1:5:111:TRP:HB3	1:5:291:LEU:HD11	1.98	0.45
1:3:340:ARG:HH21	1:3:341:LEU:HB3	1.80	0.45
1:3:340:ARG:HE	1:3:341:LEU:H	1.65	0.45
1:6:269:GLY:O	1:6:281:ARG:HG2	2.16	0.45
1:1:121:ILE:HG21	1:1:286:TYR:HB2	1.98	0.45
1:6:309:LEU:CA	1:6:312:ARG:HH21	2.29	0.45
1:2:322:MET:HA	1:2:327:SER:HA	1.98	0.45
1:1:80:SER:HB2	1:1:172:LYS:HE2	1.98	0.45
1:1:108:LEU:HB3	1:1:296:VAL:HG23	1.97	0.45
1:4:292:ARG:HB3	1:4:292:ARG:NH2	2.27	0.45
1:2:101:GLU:O	1:6:301:PRO:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:89:TYR:CD2	1:1:204:TYR:HB2	2.52	0.45
1:1:221:TYR:C	1:1:222:PHE:CG	2.89	0.45
1:2:211:PRO:HB3	1:2:216:ASN:ND2	2.32	0.45
1:3:305:LEU:HA	1:3:308:ASP:OD2	2.17	0.45
1:1:69:LYS:HB3	1:1:277:THR:HG21	1.97	0.45
1:3:299:PRO:HD2	1:3:300:TYR:CD2	2.52	0.45
1:6:309:LEU:HA	1:6:312:ARG:HE	1.81	0.45
1:2:49:GLU:HA	1:2:286:TYR:OH	2.17	0.45
1:4:187:SER:HA	1:4:191:ASN:H	1.82	0.45
1:5:29:ILE:HD11	1:5:34:GLU:OE1	2.17	0.45
1:1:88:CYS:HB2	1:1:202:ASN:C	2.37	0.45
1:1:210:VAL:HB	1:1:211:PRO:HD2	1.99	0.45
1:4:153:PHE:CE2	1:4:222:PHE:CB	3.00	0.45
1:2:220:ARG:HB3	1:2:222:PHE:CE1	2.51	0.45
1:3:154:ALA:HB2	1:3:221:TYR:HB3	1.98	0.45
1:6:116:VAL:HG21	1:6:287:PHE:HB3	1.99	0.45
1:1:295:SER:HB3	1:5:19:LYS:HB2	1.98	0.45
1:6:151:HIS:N	1:6:151:HIS:CD2	2.84	0.45
1:2:93:ARG:HA	1:2:261:TYR:CE1	2.52	0.45
1:6:146:GLN:HB2	1:6:230:ASN:O	2.17	0.45
1:6:272:THR:HG23	1:6:278:GLN:HG3	1.99	0.45
1:1:153:PHE:N	1:1:153:PHE:CD1	2.84	0.45
1:4:68:LEU:HG	1:4:69:LYS:H	1.82	0.45
1:5:116:VAL:HG22	1:5:117:GLN:N	2.31	0.45
1:3:340:ARG:NH2	1:3:341:LEU:HD23	2.32	0.45
1:1:67:SER:HB2	1:1:85:MET:HA	1.99	0.45
1:6:135:LYS:HA	1:6:142:GLY:HA2	1.99	0.45
1:5:351:ILE:HD12	1:5:351:ILE:N	2.32	0.45
1:3:349:ARG:HB3	1:3:350:TYR:CE1	2.51	0.45
1:2:102:ASP:HA	1:6:300:TYR:HA	1.99	0.45
1:4:99:LEU:HD11	1:4:111:TRP:CE3	2.52	0.45
1:4:202:ASN:HD22	1:4:203:ALA:CA	2.28	0.45
1:4:55:GLU:HB3	1:4:202:ASN:OD1	2.17	0.45
1:2:198:LEU:CD1	1:2:204:TYR:CD1	2.99	0.45
1:5:112:GLU:HB3	1:5:292:ARG:HH22	1.82	0.45
1:2:271:PHE:O	1:2:278:GLN:HA	2.16	0.45
1:6:114:VAL:HG21	1:6:290:ARG:CZ	2.47	0.45
1:6:45:ILE:HG21	1:6:292:ARG:HB3	1.99	0.45
1:5:36:LEU:HB2	1:5:37:GLU:OE1	2.17	0.45
1:3:307:SER:HB2	1:6:351:ILE:HD12	1.99	0.44
1:4:272:THR:HA	1:4:278:GLN:OE1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:66:PHE:N	1:4:66:PHE:CD1	2.83	0.44
1:2:149:ASN:HB2	1:2:151:HIS:NE2	2.32	0.44
1:2:150:PHE:O	1:2:266:ASP:HA	2.17	0.44
1:5:45:ILE:HD13	1:5:290:ARG:HB3	1.98	0.44
1:3:138:GLU:CG	1:3:139:HIS:H	2.30	0.44
1:3:129:LEU:H	1:3:130:HIS:CD2	2.35	0.44
1:1:26:LYS:CE	1:1:28:LEU:HA	2.46	0.44
1:1:94:ILE:O	1:1:259:SER:HA	2.17	0.44
1:4:42:VAL:O	1:4:292:ARG:HG2	2.17	0.44
1:3:191:ASN:H	1:3:194:HIS:HE2	1.64	0.44
1:4:162:MET:SD	1:4:209:TRP:HB2	2.57	0.44
1:1:99:LEU:HD11	1:1:111:TRP:CZ2	2.52	0.44
1:5:264:ALA:HB1	1:5:285:ARG:NH1	2.32	0.44
1:2:152:PHE:CG	1:2:153:PHE:N	2.86	0.44
1:2:51:PHE:HA	1:2:285:ARG:O	2.18	0.44
1:6:153:PHE:CD1	1:6:153:PHE:O	2.70	0.44
1:4:123:ILE:HB	1:4:126:MET:SD	2.58	0.44
1:2:286:TYR:CD2	1:2:286:TYR:C	2.91	0.44
1:2:27:LEU:HB2	1:6:335:PHE:CZ	2.52	0.44
1:5:70:LEU:CD2	1:5:280:TRP:CE3	3.01	0.44
1:1:331:GLU:O	1:1:332:VAL:HG13	2.18	0.44
1:2:139:HIS:CD2	1:3:275:SER:HB2	2.53	0.44
1:1:21:PRO:HG3	1:2:297:LYS:CA	2.47	0.44
1:2:136:VAL:C	1:2:137:HIS:CD2	2.91	0.44
1:4:134:GLN:OE1	1:4:276:GLY:HA3	2.17	0.44
1:4:221:TYR:C	1:4:222:PHE:CG	2.91	0.44
1:3:221:TYR:O	1:3:222:PHE:CD1	2.70	0.44
1:2:279:GLN:O	1:2:281:ARG:HD3	2.17	0.44
1:2:56:MET:CE	1:2:280:TRP:HB2	2.47	0.44
1:6:66:PHE:CD2	1:6:281:ARG:HA	2.51	0.44
1:5:53:ASN:ND2	1:5:64:ARG:HE	2.16	0.44
1:1:149:ASN:HB2	1:1:267:ILE:O	2.16	0.44
1:5:349:ARG:HA	1:5:356:GLN:OE1	2.17	0.44
1:1:213:PRO:CA	1:1:216:ASN:HB2	2.47	0.44
1:3:20:GLU:HA	1:3:21:PRO:HD3	1.73	0.44
1:5:77:SER:HB2	1:5:170:ARG:HE	1.82	0.44
1:4:96:LEU:HB2	1:4:258:ASP:O	2.18	0.44
1:4:196:ALA:HB3	1:4:209:TRP:CH2	2.53	0.44
1:4:16:LYS:HZ3	1:5:99:LEU:HD13	1.83	0.44
1:3:115:THR:HG22	1:3:290:ARG:HH11	1.80	0.44
1:2:270:LEU:HD12	1:2:270:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:271:PHE:CE2	1:2:273:ASN:HA	2.52	0.44
1:6:183:PRO:HA	1:6:187:SER:HB2	2.00	0.44
1:1:267:ILE:HG23	1:1:280:TRP:CE3	2.52	0.44
1:2:251:VAL:HG22	1:2:252:GLY:O	2.17	0.44
1:4:331:GLU:HA	1:4:333:ARG:HE	1.81	0.44
1:2:16:LYS:HA	1:3:109:LEU:HG	1.99	0.44
1:2:162:MET:SD	1:2:210:VAL:O	2.76	0.44
1:5:162:MET:HA	1:5:211:PRO:HA	1.99	0.44
1:4:220:ARG:HB3	1:4:222:PHE:HZ	1.81	0.44
1:1:149:ASN:HA	1:1:267:ILE:HG22	1.98	0.44
1:6:220:ARG:HB3	1:6:222:PHE:CE2	2.52	0.44
1:4:62:ASN:C	1:4:64:ARG:H	2.21	0.44
1:3:299:PRO:HG3	1:6:343:GLY:H	1.83	0.44
1:6:254:LEU:HB2	1:6:256:LYS:HG3	2.00	0.44
1:4:99:LEU:HD22	1:4:293:LYS:HE2	1.97	0.44
1:4:92:ALA:O	1:4:262:VAL:HG22	2.17	0.44
1:3:43:ASP:CG	1:3:292:ARG:HD2	2.38	0.44
1:1:289:ILE:HB	1:1:291:LEU:HD21	2.00	0.44
1:3:69:LYS:HA	1:3:279:GLN:HB3	1.99	0.44
1:5:245:LEU:C	1:5:246:LEU:HD12	2.38	0.44
1:5:158:GLU:CG	1:5:218:ASN:HD22	2.31	0.44
1:1:169:TYR:CZ	1:1:185:ALA:HA	2.52	0.44
1:4:100:ASN:HD21	1:4:108:LEU:HD22	1.83	0.44
1:4:78:SER:CA	1:4:171:SER:HA	2.48	0.44
1:3:52:LEU:HD22	1:3:90:SER:HB3	2.00	0.44
1:5:152:PHE:HA	1:5:223:GLY:HA2	1.99	0.44
1:2:152:PHE:HA	1:2:223:GLY:HA2	1.99	0.44
1:1:166:LEU:CD2	1:1:194:HIS:HE1	2.29	0.44
1:1:191:ASN:ND2	1:1:194:HIS:CD2	2.86	0.44
1:3:245:LEU:O	1:3:246:LEU:HD23	2.17	0.44
1:3:323:TYR:O	1:3:326:GLU:HG2	2.18	0.44
1:1:129:LEU:HD11	1:1:144:PRO:CA	2.48	0.44
1:4:26:LYS:HD3	1:4:27:LEU:N	2.32	0.44
1:3:132:GLY:HA2	1:4:72:ALA:O	2.17	0.44
1:6:20:GLU:HA	1:6:20:GLU:OE1	2.18	0.44
1:2:290:ARG:HE	1:2:291:LEU:N	2.16	0.44
1:3:42:VAL:HG22	1:3:43:ASP:H	1.83	0.44
1:1:220:ARG:HB3	1:1:222:PHE:CZ	2.53	0.44
1:1:116:VAL:HG23	1:1:289:ILE:HG13	1.99	0.44
1:5:267:ILE:HA	1:5:282:GLY:HA2	2.00	0.44
1:3:152:PHE:CD1	1:3:222:PHE:O	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:260:LEU:HG	1:3:261:TYR:N	2.33	0.44
1:2:168:ASN:HA	1:2:170:ARG:NH2	2.33	0.44
1:6:314:THR:HG22	1:6:315:GLN:H	1.82	0.44
1:4:29:ILE:HD11	1:4:34:GLU:HG2	1.99	0.44
1:2:111:TRP:CZ3	1:2:292:ARG:C	2.92	0.43
1:5:27:LEU:HD21	1:5:30:LYS:CA	2.48	0.43
1:1:57:GLY:HA2	1:1:83:ARG:HH11	1.82	0.43
1:5:205:PRO:HD2	1:5:209:TRP:HE1	1.82	0.43
1:4:237:VAL:HG22	1:4:238:THR:N	2.33	0.43
1:1:137:HIS:O	1:1:137:HIS:CD2	2.71	0.43
1:1:66:PHE:HA	1:1:280:TRP:O	2.17	0.43
1:1:76:PHE:CZ	1:5:132:GLY:HA3	2.54	0.43
1:2:124:THR:CG2	1:3:210:VAL:HG12	2.48	0.43
1:4:164:GLY:N	1:4:194:HIS:O	2.51	0.43
1:4:166:LEU:HD12	1:4:167:MET:O	2.18	0.43
1:4:178:ILE:O	1:4:204:TYR:HA	2.18	0.43
1:1:162:MET:SD	1:1:209:TRP:CE3	3.11	0.43
1:1:89:TYR:CE2	1:1:204:TYR:HB2	2.52	0.43
1:1:154:ALA:HA	1:1:221:TYR:HA	1.99	0.43
1:2:165:VAL:HG21	1:2:210:VAL:HG11	2.00	0.43
1:2:204:TYR:CE2	1:2:209:TRP:CZ2	3.06	0.43
1:2:83:ARG:HA	1:2:86:LEU:HD12	1.99	0.43
1:5:86:LEU:HD12	1:5:177:THR:HG21	2.00	0.43
1:2:69:LYS:C	1:2:70:LEU:HG	2.39	0.43
1:1:272:THR:HA	1:1:278:GLN:CG	2.47	0.43
1:1:68:LEU:H	1:1:85:MET:HA	1.83	0.43
1:2:94:ILE:N	1:2:260:LEU:H	2.16	0.43
1:6:79:ASP:O	1:6:172:LYS:HB2	2.18	0.43
1:6:159:PRO:HB2	1:6:197:TYR:HD1	1.83	0.43
1:5:134:GLN:NE2	1:5:276:GLY:HA3	2.34	0.43
1:4:205:PRO:HB2	1:4:208:CYS:SG	2.58	0.43
1:4:46:THR:HB	1:4:291:LEU:HD22	1.98	0.43
1:6:281:ARG:HB2	1:6:281:ARG:HH11	1.81	0.43
1:1:273:ASN:ND2	1:1:279:GLN:HE21	2.16	0.43
1:1:158:GLU:CD	1:1:218:ASN:HD22	2.21	0.43
1:4:80:SER:H	1:4:172:LYS:NZ	2.16	0.43
1:2:53:ASN:N	1:6:328:GLN:HE22	2.16	0.43
1:4:255:CYS:HB3	1:4:258:ASP:HA	2.00	0.43
1:4:163:GLN:HE22	1:4:195:LYS:CD	2.32	0.43
1:1:200:LYS:NZ	1:1:203:ALA:HB2	2.33	0.43
1:1:160:LEU:HD11	1:1:211:PRO:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:180:PRO:HA	1:2:209:TRP:CZ2	2.53	0.43
1:5:117:GLN:CB	1:5:290:ARG:HH22	2.31	0.43
1:6:165:VAL:HG12	1:6:166:LEU:H	1.83	0.43
1:1:189:VAL:HG13	1:5:53:ASN:HD21	1.82	0.43
1:4:138:GLU:HB3	1:4:139:HIS:H	1.48	0.43
1:5:81:PRO:HB2	1:5:174:PRO:HD3	2.00	0.43
1:1:286:TYR:C	1:1:286:TYR:CD2	2.92	0.43
1:3:191:ASN:O	1:3:194:HIS:CD2	2.72	0.43
1:3:204:TYR:HB3	1:3:209:TRP:CD1	2.53	0.43
1:2:111:TRP:CE3	1:2:292:ARG:O	2.72	0.43
1:2:116:VAL:HG12	1:2:245:LEU:HD21	2.01	0.43
1:2:290:ARG:C	1:2:291:LEU:HD23	2.39	0.43
1:4:162:MET:HB2	1:4:196:ALA:H	1.84	0.43
1:1:255:CYS:HB3	1:1:258:ASP:H	1.84	0.43
1:3:239:ASN:ND2	1:4:220:ARG:HA	2.34	0.43
1:4:63:LEU:HA	1:4:66:PHE:HB2	2.00	0.43
1:3:302:ILE:HA	1:3:305:LEU:CD1	2.48	0.43
1:4:139:HIS:CD2	1:4:139:HIS:O	2.71	0.43
1:1:237:VAL:HG22	1:1:237:VAL:O	2.18	0.43
1:4:179:THR:C	1:4:209:TRP:CZ2	2.91	0.43
1:2:210:VAL:HB	1:2:211:PRO:CD	2.48	0.43
1:5:99:LEU:HD23	1:5:99:LEU:HA	1.85	0.43
1:4:239:ASN:HB3	1:5:221:TYR:H	1.83	0.43
1:2:153:PHE:CZ	1:2:222:PHE:HB2	2.54	0.43
1:3:271:PHE:CD2	1:3:279:GLN:HG2	2.53	0.43
1:3:340:ARG:NH2	1:6:297:LYS:HB2	2.34	0.43
1:3:322:MET:SD	1:3:328:GLN:HB3	2.59	0.43
1:3:123:ILE:O	1:3:126:MET:HG3	2.18	0.43
1:1:128:ASN:O	1:1:129:LEU:HG	2.19	0.43
1:3:81:PRO:HD2	1:3:173:TYR:HA	2.00	0.43
1:1:161:GLU:HA	1:1:196:ALA:O	2.18	0.43
1:1:150:PHE:C	1:1:151:HIS:CD2	2.92	0.43
1:5:110:MET:O	1:5:293:LYS:HA	2.18	0.43
1:6:114:VAL:HG23	1:6:290:ARG:O	2.19	0.43
1:6:153:PHE:CZ	1:6:222:PHE:O	2.71	0.43
1:5:164:GLY:HA3	1:5:180:PRO:CB	2.47	0.43
1:2:53:ASN:H	1:6:328:GLN:HE22	1.65	0.43
1:4:121:ILE:HD13	1:4:286:TYR:HB2	2.01	0.43
1:2:334:VAL:O	1:2:334:VAL:HG12	2.18	0.43
1:3:310:ILE:CA	1:3:313:ARG:HH21	2.32	0.43
1:5:177:THR:HA	1:5:203:ALA:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:70:LEU:HD11	1:3:280:TRP:CD1	2.54	0.43
1:6:149:ASN:O	1:6:225:PHE:HA	2.18	0.43
1:2:96:LEU:HG	1:2:259:SER:N	2.34	0.43
1:2:94:ILE:O	1:2:260:LEU:N	2.52	0.43
1:1:234:VAL:HG12	1:1:236:HIS:CD2	2.54	0.43
1:3:248:GLU:CD	1:3:248:GLU:H	2.21	0.43
1:2:38:VAL:HA	1:2:39:LYS:HZ2	1.82	0.43
1:4:111:TRP:CD1	1:4:258:ASP:OD2	2.72	0.43
1:4:156:GLY:O	1:4:260:LEU:HD12	2.19	0.43
1:4:42:VAL:HG12	1:4:43:ASP:OD1	2.19	0.43
1:3:212:ASP:HB3	1:3:215:ARG:HG3	2.00	0.43
1:3:88:CYS:HB2	1:3:202:ASN:HA	2.01	0.43
1:2:288:LYS:HZ1	1:2:289:ILE:C	2.22	0.43
1:5:109:LEU:HG	1:5:295:SER:CA	2.49	0.43
1:5:153:PHE:CD1	1:5:153:PHE:N	2.83	0.43
1:5:91:THR:HG22	1:5:201:ASN:CA	2.45	0.43
1:3:221:TYR:CD1	1:3:221:TYR:N	2.85	0.43
1:5:219:ALA:HA	1:5:253:PRO:CB	2.48	0.43
1:3:255:CYS:SG	1:3:259:SER:O	2.74	0.43
1:1:185:ALA:HB1	1:5:61:GLU:HA	2.01	0.43
1:4:146:GLN:HB2	1:4:232:PRO:HA	2.01	0.43
1:4:114:VAL:CG2	1:4:292:ARG:HB2	2.47	0.43
1:1:162:MET:SD	1:1:196:ALA:HB3	2.59	0.43
1:1:83:ARG:HB3	1:1:175:ASP:CG	2.39	0.43
1:2:200:LYS:HG3	1:2:203:ALA:CB	2.49	0.43
1:4:267:ILE:HG23	1:4:280:TRP:CZ3	2.54	0.43
1:3:150:PHE:HD1	1:3:224:THR:O	2.02	0.43
1:3:231:VAL:HA	1:3:232:PRO:HD2	1.90	0.43
1:4:260:LEU:HG	1:4:262:VAL:HG13	2.00	0.42
1:3:164:GLY:HA2	1:3:209:TRP:HA	2.01	0.42
1:2:35:VAL:CG1	1:6:334:VAL:HG22	2.49	0.42
1:3:26:LYS:HG2	1:3:27:LEU:N	2.34	0.42
1:1:178:ILE:HD12	1:1:179:THR:O	2.19	0.42
1:3:115:THR:HA	1:3:243:THR:O	2.18	0.42
1:5:151:HIS:CE1	1:5:266:ASP:CA	3.02	0.42
1:2:237:VAL:HG13	1:3:221:TYR:HB2	2.01	0.42
1:1:139:HIS:CD2	1:2:277:THR:HA	2.54	0.42
1:1:187:SER:HA	1:1:191:ASN:HB2	2.01	0.42
1:6:150:PHE:N	1:6:151:HIS:CD2	2.87	0.42
1:6:150:PHE:CE2	1:6:152:PHE:CG	3.07	0.42
1:2:323:TYR:O	1:2:326:GLU:CG	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:122:GLY:O	1:3:165:VAL:HG11	2.18	0.42
1:2:141:GLY:HA2	1:3:72:ALA:HA	2.01	0.42
1:2:29:ILE:HG22	1:6:334:VAL:HG21	2.00	0.42
1:2:162:MET:O	1:2:212:ASP:HB2	2.19	0.42
1:5:149:ASN:HB2	1:5:151:HIS:NE2	2.33	0.42
1:2:170:ARG:HH22	1:2:188:GLN:CD	2.23	0.42
1:2:254:LEU:CB	1:2:256:LYS:HG3	2.49	0.42
1:1:353:LYS:HZ3	1:1:355:GLY:H	1.66	0.42
1:3:109:LEU:HD22	1:3:295:SER:N	2.34	0.42
1:5:178:ILE:CG2	1:5:203:ALA:HB1	2.49	0.42
1:2:37:GLU:HA	1:3:349:ARG:HD3	2.00	0.42
1:1:94:ILE:HD12	1:1:260:LEU:HD23	2.01	0.42
1:1:80:SER:HA	1:1:172:LYS:O	2.18	0.42
1:2:59:PRO:HD2	1:2:63:LEU:HB3	2.01	0.42
1:5:313:ARG:NH1	1:5:313:ARG:HA	2.34	0.42
1:3:179:THR:CA	1:3:209:TRP:HE1	2.32	0.42
1:4:163:GLN:HB2	1:4:212:ASP:HA	2.01	0.42
1:4:162:MET:O	1:4:212:ASP:HB2	2.19	0.42
1:1:110:MET:O	1:1:294:ARG:O	2.37	0.42
1:3:270:LEU:HG	1:3:280:TRP:CZ3	2.55	0.42
1:5:116:VAL:C	1:5:290:ARG:HH12	2.23	0.42
1:1:233:PRO:O	1:1:234:VAL:HG23	2.19	0.42
1:2:39:LYS:HZ3	1:2:39:LYS:HG2	1.76	0.42
1:3:56:MET:C	1:3:58:ASP:H	2.23	0.42
1:5:299:PRO:HG2	1:5:300:TYR:CD1	2.54	0.42
1:3:234:VAL:HG12	1:3:236:HIS:CE1	2.53	0.42
1:5:302:ILE:HB	1:5:303:SER:H	1.65	0.42
1:2:50:CYS:O	1:2:286:TYR:CD1	2.73	0.42
1:4:178:ILE:HG22	1:4:203:ALA:HB1	2.00	0.42
1:1:292:ARG:C	1:1:292:ARG:HE	2.23	0.42
1:3:239:ASN:HD21	1:4:220:ARG:HA	1.85	0.42
1:3:152:PHE:CD2	1:3:152:PHE:C	2.93	0.42
1:3:270:LEU:CD2	1:3:280:TRP:CE2	3.02	0.42
1:6:191:ASN:OD1	1:6:194:HIS:CE1	2.72	0.42
1:6:292:ARG:NH2	1:6:294:ARG:HA	2.35	0.42
1:6:137:HIS:ND1	1:6:138:GLU:HB2	2.34	0.42
1:3:246:LEU:HD22	1:3:250:GLY:O	2.19	0.42
1:2:345:PRO:HD2	1:2:346:ASP:H	1.84	0.42
1:3:300:TYR:HA	1:3:304:PHE:CE2	2.54	0.42
1:2:171:SER:HB3	1:2:173:TYR:CE2	2.54	0.42
1:2:229:GLU:CD	1:2:229:GLU:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:89:TYR:CE1	1:4:204:TYR:O	2.72	0.42
1:1:160:LEU:HD23	1:1:162:MET:HG2	2.02	0.42
1:1:57:GLY:HA3	1:1:83:ARG:O	2.20	0.42
1:1:86:LEU:HD12	1:1:177:THR:HG21	2.01	0.42
1:2:161:GLU:HB3	1:2:215:ARG:CZ	2.50	0.42
1:3:115:THR:HG22	1:3:290:ARG:HH12	1.83	0.42
1:3:47:GLU:OE2	1:3:290:ARG:HA	2.19	0.42
1:1:99:LEU:HD11	1:1:111:TRP:CE2	2.55	0.42
1:1:111:TRP:CE3	1:1:292:ARG:O	2.72	0.42
1:1:42:VAL:HG13	1:1:292:ARG:HH21	1.83	0.42
1:5:152:PHE:HB3	1:5:265:ALA:HB3	2.01	0.42
1:3:153:PHE:HB3	1:3:264:ALA:HB2	2.02	0.42
1:6:112:GLU:HB2	1:6:294:ARG:N	2.35	0.42
1:3:103:LEU:CG	1:3:104:THR:H	2.30	0.42
1:4:139:HIS:CD2	1:5:278:GLN:H	2.38	0.42
1:2:59:PRO:HG2	1:2:63:LEU:HD13	2.01	0.42
1:2:22:VAL:C	1:2:24:VAL:H	2.22	0.42
1:2:286:TYR:CZ	1:2:287:PHE:O	2.73	0.42
1:3:124:THR:CG2	1:4:210:VAL:HG12	2.49	0.42
1:1:161:GLU:OE1	1:1:215:ARG:HB2	2.20	0.42
1:5:88:CYS:HA	1:5:204:TYR:O	2.20	0.42
1:2:70:LEU:HD11	1:2:280:TRP:CE2	2.54	0.42
1:3:341:LEU:HD22	1:6:294:ARG:NH2	2.34	0.42
1:3:312:ARG:HG3	1:3:312:ARG:H	1.52	0.42
1:6:153:PHE:HA	1:6:264:ALA:HA	2.01	0.42
1:3:168:ASN:H	1:3:188:GLN:NE2	2.18	0.42
1:4:57:GLY:CA	1:4:84:LYS:HA	2.49	0.42
1:1:107:ASN:O	1:5:16:LYS:HB3	2.19	0.42
1:2:125:SER:C	1:2:127:LEU:H	2.22	0.42
1:2:62:ASN:C	1:2:64:ARG:H	2.22	0.42
1:1:123:ILE:HG21	1:1:235:LEU:HD13	2.00	0.42
1:2:193:ASP:C	1:2:195:LYS:H	2.23	0.42
1:2:15:PRO:O	1:3:99:LEU:HA	2.20	0.42
1:2:17:LYS:HB3	1:2:19:LYS:HG3	2.01	0.42
1:1:222:PHE:CZ	1:5:239:ASN:OD1	2.73	0.42
1:5:271:PHE:HB3	1:5:279:GLN:O	2.20	0.42
1:3:154:ALA:HA	1:3:220:ARG:O	2.19	0.42
1:3:51:PHE:CD2	1:3:121:ILE:HD11	2.55	0.42
1:4:83:ARG:HH21	1:4:88:CYS:H	1.67	0.42
1:2:29:ILE:HG12	1:2:30:LYS:H	1.85	0.42
1:2:35:VAL:HG11	1:6:332:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:16:LYS:CA	1:3:109:LEU:HG	2.50	0.42
1:3:99:LEU:HG	1:3:111:TRP:CZ2	2.55	0.42
1:2:200:LYS:HD2	1:6:318:ASP:HB3	2.02	0.42
1:5:109:LEU:HD23	1:5:293:LYS:O	2.19	0.42
1:2:267:ILE:N	1:2:267:ILE:CD1	2.83	0.42
1:5:45:ILE:C	1:5:45:ILE:CD1	2.89	0.42
1:6:205:PRO:O	1:6:209:TRP:HB2	2.20	0.42
1:6:45:ILE:HG22	1:6:292:ARG:HA	2.02	0.42
1:1:19:LYS:NZ	1:2:109:LEU:HD22	2.35	0.42
1:4:273:ASN:HD21	1:4:279:GLN:CG	2.32	0.42
1:5:286:TYR:O	1:5:287:PHE:CD1	2.73	0.42
1:4:119:GLU:HB2	1:4:121:ILE:HG23	2.02	0.42
1:2:33:VAL:HG21	1:6:324:GLY:H	1.85	0.42
1:4:135:LYS:HA	1:4:142:GLY:HA2	2.01	0.42
1:1:60:ASP:HB2	1:1:61:GLU:H	1.57	0.42
1:3:52:LEU:HD11	1:3:91:THR:C	2.40	0.42
1:3:310:ILE:CG1	1:3:313:ARG:HH21	2.33	0.42
1:2:178:ILE:HG23	1:2:204:TYR:CE1	2.55	0.42
1:1:96:LEU:HD12	1:1:255:CYS:SG	2.60	0.42
1:4:235:LEU:HB2	1:5:225:PHE:HB3	2.02	0.42
1:2:152:PHE:CD1	1:2:153:PHE:N	2.88	0.42
1:2:130:HIS:CE1	1:3:70:LEU:HB3	2.54	0.42
1:6:169:TYR:HB2	1:6:183:PRO:HB2	2.00	0.42
1:6:290:ARG:NH1	1:6:292:ARG:HB3	2.35	0.42
1:6:290:ARG:HH12	1:6:292:ARG:HB3	1.85	0.42
1:6:46:THR:HG22	1:6:48:VAL:HG23	2.01	0.42
1:3:94:ILE:O	1:3:259:SER:HA	2.19	0.42
1:2:345:PRO:CD	1:2:346:ASP:H	2.33	0.42
1:5:352:ASP:N	1:5:357:LEU:HB2	2.35	0.42
1:6:311:ASN:HA	1:6:314:THR:OG1	2.20	0.42
1:3:213:PRO:HD2	1:3:214:SER:H	1.85	0.41
1:2:159:PRO:O	1:2:197:TYR:CE2	2.73	0.41
1:5:88:CYS:SG	1:5:205:PRO:HA	2.60	0.41
1:5:91:THR:CG2	1:5:201:ASN:HA	2.45	0.41
1:3:149:ASN:HD22	1:3:269:GLY:CA	2.33	0.41
1:5:116:VAL:HG12	1:5:245:LEU:HD21	2.02	0.41
1:3:50:CYS:O	1:3:286:TYR:CE1	2.73	0.41
1:6:116:VAL:HG22	1:6:117:GLN:N	2.34	0.41
1:3:93:ARG:HH12	1:3:94:ILE:C	2.23	0.41
1:5:191:ASN:OD1	1:5:194:HIS:CE1	2.73	0.41
1:1:21:PRO:HB3	1:2:297:LYS:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:257:ALA:C	1:6:259:SER:H	2.22	0.41
1:2:124:THR:H	1:2:124:THR:HG23	1.62	0.41
1:6:115:THR:C	1:6:245:LEU:HD11	2.40	0.41
1:4:96:LEU:HD11	1:4:260:LEU:HB2	2.02	0.41
1:4:163:GLN:O	1:4:210:VAL:O	2.37	0.41
1:1:160:LEU:HD11	1:1:211:PRO:HA	2.02	0.41
1:5:200:LYS:HZ3	1:5:203:ALA:HB2	1.85	0.41
1:5:271:PHE:HB2	1:5:281:ARG:HB2	2.02	0.41
1:5:70:LEU:CD2	1:5:279:GLN:HA	2.51	0.41
1:1:245:LEU:O	1:1:246:LEU:HD23	2.19	0.41
1:1:46:THR:O	1:1:290:ARG:HA	2.20	0.41
1:5:153:PHE:CE2	1:5:222:PHE:CG	3.08	0.41
1:4:153:PHE:HD1	1:4:285:ARG:HH12	1.68	0.41
1:6:50:CYS:HG	1:6:287:PHE:C	2.24	0.41
1:6:60:ASP:CG	1:6:61:GLU:H	2.24	0.41
1:1:308:ASP:HA	1:1:310:ILE:HG22	2.02	0.41
1:3:94:ILE:HB	1:3:260:LEU:HB3	2.02	0.41
1:4:234:VAL:HG12	1:4:236:HIS:CD2	2.55	0.41
1:2:96:LEU:HB2	1:2:258:ASP:HA	2.02	0.41
1:3:322:MET:C	1:3:327:SER:HA	2.40	0.41
1:5:18:PRO:C	1:5:20:GLU:N	2.74	0.41
1:3:298:ASN:CG	1:3:300:TYR:H	2.23	0.41
1:2:171:SER:HB3	1:2:173:TYR:CE1	2.55	0.41
1:3:248:GLU:OE2	1:3:249:GLN:HG2	2.20	0.41
1:3:180:PRO:HD3	1:3:208:CYS:HB3	2.01	0.41
1:4:186:GLN:HG3	1:4:191:ASN:HA	2.03	0.41
1:4:237:VAL:HG22	1:4:238:THR:H	1.85	0.41
1:4:238:THR:HG23	1:5:222:PHE:CD1	2.55	0.41
1:4:221:TYR:C	1:4:222:PHE:CD2	2.93	0.41
1:6:112:GLU:HB2	1:6:294:ARG:CB	2.50	0.41
1:1:277:THR:CG2	1:5:139:HIS:CE1	3.03	0.41
1:6:91:THR:HG22	1:6:201:ASN:CB	2.50	0.41
1:2:94:ILE:HB	1:2:260:LEU:HB3	2.02	0.41
1:2:32:GLY:HA2	1:6:331:GLU:HA	2.02	0.41
1:5:55:GLU:HG2	1:5:90:SER:HA	2.01	0.41
1:4:200:LYS:HG2	1:4:200:LYS:HZ3	1.65	0.41
1:5:232:PRO:HA	1:5:233:PRO:HD2	1.96	0.41
1:4:114:VAL:HG23	1:4:290:ARG:O	2.19	0.41
1:1:39:LYS:HD2	1:1:99:LEU:HA	2.03	0.41
1:2:69:LYS:HA	1:2:278:GLN:O	2.20	0.41
1:6:169:TYR:HB2	1:6:183:PRO:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:116:VAL:HA	1:6:289:ILE:HA	2.02	0.41
1:6:145:ILE:HG21	1:6:270:LEU:O	2.20	0.41
1:6:133:SER:HA	1:6:271:PHE:HZ	1.84	0.41
1:1:301:PRO:O	1:1:302:ILE:HG22	2.20	0.41
1:5:158:GLU:O	1:5:160:LEU:HD13	2.20	0.41
1:3:143:LYS:HZ3	1:3:146:GLN:HE21	1.67	0.41
1:5:187:SER:HA	1:5:191:ASN:CB	2.50	0.41
1:1:103:LEU:HA	1:5:16:LYS:HD2	2.03	0.41
1:5:286:TYR:CD2	1:5:286:TYR:C	2.93	0.41
1:3:281:ARG:HE	1:3:283:LEU:HD21	1.84	0.41
1:3:26:LYS:NZ	1:3:29:ILE:H	2.18	0.41
1:4:191:ASN:O	1:4:194:HIS:CD2	2.73	0.41
1:1:178:ILE:O	1:1:204:TYR:HA	2.20	0.41
1:4:270:LEU:CD2	1:4:280:TRP:CH2	3.03	0.41
1:4:69:LYS:HA	1:4:278:GLN:O	2.21	0.41
1:2:152:PHE:HB2	1:2:223:GLY:HA3	2.02	0.41
1:2:238:THR:HA	1:3:222:PHE:CE2	2.55	0.41
1:5:260:LEU:HG	1:5:261:TYR:N	2.34	0.41
1:5:50:CYS:SG	1:5:287:PHE:HB2	2.61	0.41
1:5:49:GLU:HA	1:5:286:TYR:OH	2.21	0.41
1:4:135:LYS:HG2	1:4:137:HIS:H	1.86	0.41
1:4:156:GLY:C	1:4:158:GLU:H	2.22	0.41
1:4:110:MET:O	1:4:294:ARG:N	2.53	0.41
1:4:95:PRO:HA	1:4:259:SER:CB	2.51	0.41
1:2:46:THR:O	1:2:290:ARG:HD2	2.21	0.41
1:2:290:ARG:HE	1:2:291:LEU:H	1.68	0.41
1:5:163:GLN:O	1:5:210:VAL:O	2.38	0.41
1:1:153:PHE:CZ	1:1:222:PHE:CB	3.03	0.41
1:6:166:LEU:HD11	1:6:169:TYR:HA	2.02	0.41
1:6:45:ILE:HG21	1:6:290:ARG:NH1	2.35	0.41
1:6:270:LEU:HD23	1:6:279:GLN:N	2.36	0.41
1:1:67:SER:HB3	1:1:280:TRP:HB2	2.02	0.41
1:6:254:LEU:HB2	1:6:256:LYS:CG	2.51	0.41
1:6:245:LEU:C	1:6:246:LEU:HD23	2.40	0.41
1:2:234:VAL:HA	1:3:225:PHE:O	2.20	0.41
1:3:186:GLN:HG3	1:3:191:ASN:HA	2.03	0.41
1:2:27:LEU:HD11	1:2:30:LYS:HB3	2.02	0.41
1:5:88:CYS:CA	1:5:206:VAL:HG13	2.50	0.41
1:6:348:ILE:HA	1:6:353:LYS:CG	2.51	0.41
1:3:69:LYS:HA	1:3:278:GLN:O	2.21	0.41
1:5:112:GLU:O	1:5:292:ARG:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:66:PHE:HB3	1:2:281:ARG:NH1	2.35	0.41
1:6:270:LEU:HD23	1:6:279:GLN:CA	2.50	0.41
1:6:58:ASP:OD1	1:6:63:LEU:HB2	2.21	0.41
1:5:158:GLU:N	1:5:261:TYR:CD2	2.89	0.41
1:5:158:GLU:N	1:5:261:TYR:HD2	2.19	0.41
1:5:93:ARG:HE	1:5:95:PRO:HG3	1.86	0.41
1:4:228:GLY:O	1:4:231:VAL:HG13	2.20	0.41
1:2:325:MET:SD	1:2:325:MET:N	2.93	0.41
1:3:19:LYS:O	1:4:295:SER:HB2	2.20	0.41
1:3:162:MET:O	1:3:195:LYS:HA	2.21	0.41
1:4:187:SER:CB	1:4:194:HIS:HE1	2.34	0.41
1:2:162:MET:SD	1:2:209:TRP:CE3	3.14	0.41
1:5:162:MET:C	1:5:212:ASP:H	2.24	0.41
1:1:116:VAL:HG22	1:1:117:GLN:C	2.42	0.41
1:2:152:PHE:C	1:2:152:PHE:CD2	2.94	0.41
1:2:145:ILE:HA	1:2:270:LEU:O	2.21	0.41
1:6:204:TYR:HB3	1:6:209:TRP:CD1	2.55	0.41
1:6:88:CYS:H	1:6:202:ASN:HD21	1.69	0.41
1:1:271:PHE:H	1:1:281:ARG:H	1.68	0.41
1:6:29:ILE:HG23	1:6:35:VAL:HG13	2.03	0.41
1:4:78:SER:H	1:4:168:ASN:HD21	1.69	0.41
1:4:249:GLN:OE1	1:4:249:GLN:HA	2.21	0.41
1:5:51:PHE:N	1:5:51:PHE:CD1	2.88	0.41
1:4:329:VAL:HG12	1:4:330:GLU:N	2.36	0.41
1:2:115:THR:O	1:2:289:ILE:HA	2.21	0.41
1:2:49:GLU:HG2	1:6:333:ARG:HH21	1.85	0.41
1:6:164:GLY:O	1:6:194:HIS:CD2	2.74	0.41
1:6:271:PHE:N	1:6:281:ARG:HE	2.19	0.41
1:1:166:LEU:HD21	1:1:194:HIS:HE1	1.85	0.41
1:1:299:PRO:CG	1:1:300:TYR:H	2.34	0.41
1:6:150:PHE:HB3	1:6:267:ILE:HG13	2.03	0.41
1:6:27:LEU:HD12	1:6:28:LEU:N	2.36	0.41
1:1:91:THR:HG22	1:1:201:ASN:N	2.36	0.41
1:1:334:VAL:C	1:1:336:ASP:H	2.23	0.41
1:6:119:GLU:OE1	1:6:286:TYR:CD2	2.74	0.41
1:3:353:LYS:HZ1	1:6:314:THR:HB	1.86	0.41
1:2:327:SER:HB3	1:2:329:VAL:HB	2.03	0.41
1:6:159:PRO:HB2	1:6:197:TYR:CD1	2.56	0.41
1:1:322:MET:O	1:1:323:TYR:CG	2.73	0.41
1:1:242:THR:HG22	1:1:243:THR:N	2.35	0.41
1:4:334:VAL:HG12	1:4:336:ASP:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:322:MET:C	1:6:327:SER:HA	2.41	0.41
1:2:81:PRO:HB2	1:2:174:PRO:HD2	2.03	0.41
1:3:161:GLU:HA	1:3:196:ALA:O	2.21	0.41
1:5:35:VAL:HG23	1:5:35:VAL:H	1.57	0.41
1:1:179:THR:HB	1:1:180:PRO:HD2	2.03	0.41
1:2:89:TYR:CE1	1:2:204:TYR:HB3	2.56	0.41
1:2:164:GLY:HA2	1:2:209:TRP:CE3	2.56	0.41
1:3:115:THR:HG23	1:3:243:THR:C	2.40	0.41
1:6:270:LEU:HA	1:6:280:TRP:HA	2.02	0.41
1:1:182:ASN:ND2	1:1:191:ASN:HD21	2.19	0.41
1:6:234:VAL:HB	1:6:236:HIS:HE1	1.82	0.41
1:6:216:ASN:HB3	1:6:219:ALA:HB3	2.03	0.41
1:3:323:TYR:CD1	1:3:323:TYR:N	2.89	0.41
1:4:51:PHE:CD1	1:4:51:PHE:C	2.93	0.41
1:4:137:HIS:CE1	1:4:140:GLY:HA3	2.56	0.41
1:1:324:GLY:O	1:1:325:MET:SD	2.79	0.41
1:5:362:LEU:HA	1:5:362:LEU:HD23	1.94	0.41
1:1:23:GLN:NE2	1:1:23:GLN:HA	2.32	0.41
1:1:59:PRO:HG2	1:1:63:LEU:CB	2.51	0.41
1:4:251:VAL:HB	1:4:254:LEU:HD21	2.03	0.41
1:5:242:THR:HG23	1:5:243:THR:N	2.36	0.41
1:2:28:LEU:HD11	1:6:336:ASP:CG	2.41	0.40
1:1:152:PHE:HB3	1:1:265:ALA:HB3	2.03	0.40
1:5:161:GLU:HB3	1:5:215:ARG:NH1	2.37	0.40
1:5:70:LEU:CD1	1:5:270:LEU:HD21	2.51	0.40
1:5:66:PHE:HB3	1:5:279:GLN:HG3	2.02	0.40
1:1:290:ARG:HD2	1:1:291:LEU:N	2.35	0.40
1:3:340:ARG:HE	1:3:341:LEU:N	2.19	0.40
1:3:305:LEU:O	1:3:308:ASP:HB2	2.20	0.40
1:6:234:VAL:HG12	1:6:235:LEU:N	2.35	0.40
1:4:82:GLU:HA	1:4:175:ASP:OD2	2.21	0.40
1:4:341:LEU:CD2	1:4:342:PRO:HD2	2.51	0.40
1:6:246:LEU:HB3	1:6:250:GLY:HA2	2.03	0.40
1:5:80:SER:HA	1:5:172:LYS:H	1.86	0.40
1:4:186:GLN:OE1	1:4:189:VAL:HG23	2.22	0.40
1:3:154:ALA:HA	1:3:221:TYR:HA	2.03	0.40
1:3:270:LEU:HB3	1:3:278:GLN:NE2	2.36	0.40
1:6:112:GLU:HB3	1:6:292:ARG:NE	2.36	0.40
1:6:91:THR:CG2	1:6:92:ALA:N	2.84	0.40
1:2:68:LEU:HB2	1:2:84:LYS:HB3	2.04	0.40
1:1:59:PRO:HG2	1:1:63:LEU:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:36:LEU:HD13	1:1:97:PRO:HD2	2.03	0.40
1:2:232:PRO:HA	1:2:233:PRO:HD2	1.98	0.40
1:3:355:GLY:C	1:6:316:ARG:HG2	2.42	0.40
1:4:46:THR:CG2	1:4:47:GLU:N	2.84	0.40
1:2:18:PRO:HA	1:3:107:ASN:O	2.21	0.40
1:3:310:ILE:HG13	1:3:310:ILE:H	1.69	0.40
1:2:163:GLN:N	1:2:210:VAL:O	2.54	0.40
1:5:281:ARG:HH21	1:5:283:LEU:HD21	1.86	0.40
1:4:150:PHE:C	1:4:151:HIS:CD2	2.95	0.40
1:1:332:VAL:O	1:1:332:VAL:HG23	2.21	0.40
1:6:96:LEU:HB2	1:6:111:TRP:NE1	2.34	0.40
1:5:351:ILE:CD1	1:5:351:ILE:N	2.84	0.40
1:5:81:PRO:HG2	1:5:173:TYR:HA	2.03	0.40
1:2:191:ASN:HA	1:2:191:ASN:HD22	1.71	0.40
1:2:68:LEU:HD22	1:2:84:LYS:HB2	2.04	0.40
1:4:126:MET:HE3	1:4:127:LEU:HD21	2.02	0.40
1:5:134:GLN:HE22	1:5:276:GLY:HA3	1.86	0.40
1:2:61:GLU:H	1:2:61:GLU:CD	2.24	0.40
1:5:119:GLU:HB2	1:5:121:ILE:HG23	2.03	0.40
1:4:18:PRO:HG3	1:5:109:LEU:HD11	2.03	0.40
1:5:116:VAL:CG2	1:5:289:ILE:HG13	2.51	0.40
1:5:289:ILE:CD1	1:5:289:ILE:N	2.85	0.40
1:1:190:MET:O	1:1:191:ASN:HB2	2.20	0.40
1:2:350:TYR:CD1	1:2:357:LEU:HG	2.56	0.40
1:6:221:TYR:O	1:6:222:PHE:CE1	2.75	0.40
1:5:357:LEU:O	1:5:359:THR:HG22	2.22	0.40
1:3:60:ASP:HB3	1:3:62:ASN:H	1.87	0.40
1:3:132:GLY:CA	1:4:73:GLU:HA	2.52	0.40
1:2:38:VAL:HA	1:2:39:LYS:NZ	2.36	0.40
1:3:87:PRO:O	1:3:206:VAL:HG13	2.22	0.40
1:4:190:MET:CE	1:4:192:THR:HA	2.51	0.40
1:1:163:GLN:HE21	1:1:195:LYS:NZ	2.19	0.40
1:5:177:THR:HB	1:5:179:THR:HG23	2.04	0.40
1:5:203:ALA:HB3	1:5:204:TYR:CE2	2.56	0.40
1:5:145:ILE:HG23	1:5:270:LEU:O	2.22	0.40
1:4:239:ASN:ND2	1:5:221:TYR:H	2.20	0.40
1:5:150:PHE:CD1	1:5:224:THR:O	2.75	0.40
1:5:225:PHE:CG	1:5:226:THR:N	2.89	0.40
1:6:169:TYR:CE1	1:6:185:ALA:HA	2.57	0.40
1:5:64:ARG:HH11	1:5:64:ARG:HA	1.86	0.40
1:2:23:GLN:HE22	1:6:338:THR:CB	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:277:THR:HG22	1:1:278:GLN:H	1.87	0.40
1:3:146:GLN:HB2	1:3:230:ASN:O	2.21	0.40
1:6:157:GLY:H	1:6:158:GLU:CD	2.24	0.40
1:4:302:ILE:O	1:4:306:LEU:HG	2.21	0.40
1:4:168:ASN:C	1:4:170:ARG:H	2.25	0.40
1:2:186:GLN:NE2	1:2:189:VAL:HG23	2.36	0.40
1:3:24:VAL:HA	1:3:25:PRO:HD2	1.78	0.40

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	346/362 (96%)	248 (72%)	53 (15%)	45 (13%)	0 7
1	2	346/362 (96%)	247 (71%)	60 (17%)	39 (11%)	0 10
1	3	340/362 (94%)	243 (72%)	54 (16%)	43 (13%)	0 8
1	4	329/362 (91%)	233 (71%)	56 (17%)	40 (12%)	0 8
1	5	345/362 (95%)	261 (76%)	54 (16%)	30 (9%)	1 17
1	6	339/362 (94%)	241 (71%)	58 (17%)	40 (12%)	0 9
All	All	2045/2172 (94%)	1473 (72%)	335 (16%)	237 (12%)	1 9

All (237) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	19	LYS
1	1	78	SER
1	1	81	PRO
1	1	129	LEU
1	1	133	SER

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Mol	Chain	Res	Type
1	1	137	HIS
1	1	175	ASP
1	1	191	ASN
1	1	202	ASN
1	1	234	VAL
1	1	241	ALA
1	1	302	ILE
1	1	303	SER
1	1	309	LEU
1	1	321	PRO
1	1	323	TYR
1	1	327	SER
1	1	345	PRO
1	2	22	VAL
1	2	39	LYS
1	2	44	ALA
1	2	137	HIS
1	2	146	GLN
1	2	160	LEU
1	2	183	PRO
1	2	231	VAL
1	2	238	THR
1	2	239	ASN
1	2	335	PHE
1	2	340	ARG
1	2	345	PRO
1	2	347	MET
1	2	353	LYS
1	3	20	GLU
1	3	21	PRO
1	3	58	ASP
1	3	102	ASP
1	3	104	THR
1	3	137	HIS
1	3	146	GLN
1	3	148	SER
1	3	190	MET
1	3	193	ASP
1	3	231	VAL
1	3	242	THR
1	3	299	PRO
1	3	326	GLU

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Mol	Chain	Res	Type
1	3	338	THR
1	4	15	PRO
1	4	18	PRO
1	4	24	VAL
1	4	26	LYS
1	4	32	GLY
1	4	79	ASP
1	4	81	PRO
1	4	87	PRO
1	4	105	CYS
1	4	130	HIS
1	4	174	PRO
1	4	175	ASP
1	4	203	ALA
1	4	230	ASN
1	4	241	ALA
1	4	273	ASN
1	4	299	PRO
1	4	336	ASP
1	4	339	GLU
1	4	340	ARG
1	5	42	VAL
1	5	99	LEU
1	5	190	MET
1	5	213	PRO
1	5	300	TYR
1	5	302	ILE
1	5	315	GLN
1	5	352	ASP
1	5	354	GLN
1	6	21	PRO
1	6	61	GLU
1	6	80	SER
1	6	102	ASP
1	6	105	CYS
1	6	137	HIS
1	6	169	TYR
1	6	171	SER
1	6	229	GLU
1	6	238	THR
1	6	241	ALA
1	6	254	LEU

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Mol	Chain	Res	Type
1	6	273	ASN
1	6	301	PRO
1	6	337	GLY
1	1	60	ASP
1	1	104	THR
1	1	141	GLY
1	1	312	ARG
1	1	324	GLY
1	1	330	GLU
1	1	332	VAL
1	1	353	LYS
1	2	32	GLY
1	2	42	VAL
1	2	134	GLN
1	2	308	ASP
1	2	329	VAL
1	2	336	ASP
1	3	42	VAL
1	3	74	ASN
1	3	98	ASN
1	3	141	GLY
1	3	274	SER
1	3	319	GLY
1	3	324	GLY
1	3	336	ASP
1	3	345	PRO
1	4	29	ILE
1	4	30	LYS
1	4	38	VAL
1	4	54	PRO
1	4	250	GLY
1	4	325	MET
1	5	40	THR
1	5	44	ALA
1	5	69	LYS
1	5	71	SER
1	5	98	ASN
1	5	284	ALA
1	5	299	PRO
1	5	340	ARG
1	6	103	LEU
1	6	138	GLU

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Mol	Chain	Res	Type
1	6	141	GLY
1	6	168	ASN
1	6	174	PRO
1	6	192	THR
1	6	230	ASN
1	1	174	PRO
1	1	299	PRO
1	1	326	GLU
1	2	103	LEU
1	2	144	PRO
1	2	159	PRO
1	2	175	ASP
1	2	299	PRO
1	3	41	GLY
1	3	59	PRO
1	3	174	PRO
1	3	182	ASN
1	3	315	GLN
1	3	328	GLN
1	3	352	ASP
1	4	25	PRO
1	4	141	GLY
1	4	284	ALA
1	4	300	TYR
1	5	54	PRO
1	5	229	GLU
1	5	236	HIS
1	5	342	PRO
1	6	146	GLN
1	6	148	SER
1	6	180	PRO
1	6	250	GLY
1	6	299	PRO
1	6	336	ASP
1	6	339	GLU
1	6	341	LEU
1	6	345	PRO
1	1	22	VAL
1	1	58	ASP
1	1	98	ASN
1	1	140	GLY
1	1	213	PRO

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Mol	Chain	Res	Type
1	1	253	PRO
1	1	341	LEU
1	2	21	PRO
1	2	58	ASP
1	2	138	GLU
1	2	323	TYR
1	3	18	PRO
1	3	32	GLY
1	3	144	PRO
1	3	321	PRO
1	4	97	PRO
1	4	168	ASN
1	4	236	HIS
1	4	301	PRO
1	5	20	GLU
1	5	60	ASP
1	5	174	PRO
1	5	182	ASN
1	6	81	PRO
1	6	142	GLY
1	6	175	ASP
1	6	189	VAL
1	6	212	ASP
1	6	346	ASP
1	1	190	MET
1	1	342	PRO
1	2	126	MET
1	2	182	ASN
1	2	310	ILE
1	3	81	PRO
1	3	101	GLU
1	3	298	ASN
1	4	58	ASP
1	4	193	ASP
1	4	202	ASN
1	4	229	GLU
1	5	58	ASP
1	5	203	ALA
1	1	101	GLU
1	1	138	GLU
1	1	325	MET
1	2	247	ASP

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Mol	Chain	Res	Type
1	3	240	THR
1	3	247	ASP
1	4	321	PRO
1	5	18	PRO
1	2	25	PRO
1	3	212	ASP
1	3	355	GLY
1	6	227	GLY
1	6	321	PRO
1	1	189	VAL
1	1	301	PRO
1	2	18	PRO
1	3	300	TYR
1	1	132	GLY
1	1	237	VAL
1	2	20	GLU
1	2	189	VAL
1	5	22	VAL
1	5	173	TYR
1	6	18	PRO
1	2	29	ILE
1	4	302	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	304/313 (97%)	221 (73%)	83 (27%)	0 4
1	2	304/313 (97%)	235 (77%)	69 (23%)	1 8
1	3	298/313 (95%)	220 (74%)	78 (26%)	0 5
1	4	287/313 (92%)	220 (77%)	67 (23%)	1 7
1	5	303/313 (97%)	234 (77%)	69 (23%)	1 8
1	6	297/313 (95%)	218 (73%)	79 (27%)	0 5
All	All	1793/1878 (96%)	1348 (75%)	445 (25%)	3 6

All (445) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	17	LYS
1	1	19	LYS
1	1	24	VAL
1	1	27	LEU
1	1	34	GLU
1	1	35	VAL
1	1	37	GLU
1	1	43	ASP
1	1	46	THR
1	1	50	CYS
1	1	61	GLU
1	1	82	GLU
1	1	83	ARG
1	1	84	LYS
1	1	85	MET
1	1	91	THR
1	1	93	ARG
1	1	101	GLU
1	1	102	ASP
1	1	103	LEU
1	1	115	THR
1	1	117	GLN
1	1	118	THR
1	1	123	ILE
1	1	126	MET
1	1	128	ASN
1	1	133	SER
1	1	135	LYS
1	1	143	LYS
1	1	155	VAL
1	1	161	GLU
1	1	167	MET
1	1	170	ARG
1	1	172	LYS
1	1	175	ASP
1	1	178	ILE
1	1	186	GLN
1	1	187	SER
1	1	190	MET
1	1	195	LYS
1	1	200	LYS
1	1	202	ASN

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Mol	Chain	Res	Type
1	1	204	TYR
1	1	208	CYS
1	1	212	ASP
1	1	217	GLU
1	1	226	THR
1	1	235	LEU
1	1	236	HIS
1	1	239	ASN
1	1	248	GLU
1	1	249	GLN
1	1	254	LEU
1	1	255	CYS
1	1	256	LYS
1	1	263	SER
1	1	267	ILE
1	1	273	ASN
1	1	289	ILE
1	1	290	ARG
1	1	292	ARG
1	1	297	LYS
1	1	300	TYR
1	1	304	PHE
1	1	309	LEU
1	1	311	ASN
1	1	313	ARG
1	1	316	ARG
1	1	318	ASP
1	1	320	GLN
1	1	321	PRO
1	1	323	TYR
1	1	326	GLU
1	1	329	VAL
1	1	333	ARG
1	1	334	VAL
1	1	340	ARG
1	1	341	LEU
1	1	345	PRO
1	1	350	TYR
1	1	352	ASP
1	1	353	LYS
1	1	359	THR
1	2	15	PRO

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Mol	Chain	Res	Type
1	2	23	GLN
1	2	25	PRO
1	2	34	GLU
1	2	39	LYS
1	2	40	THR
1	2	46	THR
1	2	51	PHE
1	2	55	GLU
1	2	61	GLU
1	2	64	ARG
1	2	71	SER
1	2	85	MET
1	2	93	ARG
1	2	102	ASP
1	2	104	THR
1	2	107	ASN
1	2	112	GLU
1	2	114	VAL
1	2	115	THR
1	2	126	MET
1	2	138	GLU
1	2	160	LEU
1	2	162	MET
1	2	170	ARG
1	2	172	LYS
1	2	173	TYR
1	2	182	ASN
1	2	191	ASN
1	2	193	ASP
1	2	205	PRO
1	2	207	GLU
1	2	212	ASP
1	2	221	TYR
1	2	224	THR
1	2	230	ASN
1	2	240	THR
1	2	248	GLU
1	2	251	VAL
1	2	255	CYS
1	2	263	SER
1	2	279	GLN
1	2	280	TRP

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Mol	Chain	Res	Type
1	2	281	ARG
1	2	287	PHE
1	2	288	LYS
1	2	289	ILE
1	2	290	ARG
1	2	291	LEU
1	2	292	ARG
1	2	293	LYS
1	2	294	ARG
1	2	297	LYS
1	2	299	PRO
1	2	305	LEU
1	2	314	THR
1	2	316	ARG
1	2	320	GLN
1	2	323	TYR
1	2	325	MET
1	2	332	VAL
1	2	340	ARG
1	2	341	LEU
1	2	345	PRO
1	2	349	ARG
1	2	350	TYR
1	2	352	ASP
1	2	357	LEU
1	2	361	MET
1	3	23	GLN
1	3	26	LYS
1	3	29	ILE
1	3	30	LYS
1	3	34	GLU
1	3	37	GLU
1	3	51	PHE
1	3	55	GLU
1	3	56	MET
1	3	69	LYS
1	3	71	SER
1	3	73	GLU
1	3	77	SER
1	3	79	ASP
1	3	82	GLU
1	3	83	ARG

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Mol	Chain	Res	Type
1	3	96	LEU
1	3	100	ASN
1	3	101	GLU
1	3	103	LEU
1	3	107	ASN
1	3	109	LEU
1	3	117	GLN
1	3	118	THR
1	3	120	VAL
1	3	123	ILE
1	3	125	SER
1	3	126	MET
1	3	129	LEU
1	3	134	GLN
1	3	135	LYS
1	3	143	LYS
1	3	145	ILE
1	3	149	ASN
1	3	153	PHE
1	3	158	GLU
1	3	161	GLU
1	3	167	MET
1	3	170	ARG
1	3	172	LYS
1	3	173	TYR
1	3	175	ASP
1	3	190	MET
1	3	197	TYR
1	3	200	LYS
1	3	208	CYS
1	3	210	VAL
1	3	212	ASP
1	3	215	ARG
1	3	217	GLU
1	3	221	TYR
1	3	229	GLU
1	3	231	VAL
1	3	240	THR
1	3	255	CYS
1	3	256	LYS
1	3	263	SER
1	3	271	PHE

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Mol	Chain	Res	Type
1	3	273	ASN
1	3	277	THR
1	3	287	PHE
1	3	289	ILE
1	3	290	ARG
1	3	292	ARG
1	3	302	ILE
1	3	304	PHE
1	3	316	ARG
1	3	317	VAL
1	3	321	PRO
1	3	323	TYR
1	3	334	VAL
1	3	335	PHE
1	3	347	MET
1	3	348	ILE
1	3	350	TYR
1	3	353	LYS
1	3	354	GLN
1	3	356	GLN
1	4	15	PRO
1	4	18	PRO
1	4	20	GLU
1	4	21	PRO
1	4	23	GLN
1	4	34	GLU
1	4	35	VAL
1	4	37	GLU
1	4	39	LYS
1	4	49	GLU
1	4	56	MET
1	4	61	GLU
1	4	63	LEU
1	4	68	LEU
1	4	78	SER
1	4	79	ASP
1	4	82	GLU
1	4	83	ARG
1	4	91	THR
1	4	101	GLU
1	4	102	ASP
1	4	112	GLU

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Mol	Chain	Res	Type
1	4	114	VAL
1	4	117	GLN
1	4	118	THR
1	4	123	ILE
1	4	126	MET
1	4	135	LYS
1	4	136	VAL
1	4	143	LYS
1	4	145	ILE
1	4	152	PHE
1	4	167	MET
1	4	170	ARG
1	4	175	ASP
1	4	178	ILE
1	4	183	PRO
1	4	195	LYS
1	4	199	ASP
1	4	202	ASN
1	4	212	ASP
1	4	221	TYR
1	4	226	THR
1	4	229	GLU
1	4	236	HIS
1	4	238	THR
1	4	240	THR
1	4	248	GLU
1	4	258	ASP
1	4	263	SER
1	4	274	SER
1	4	287	PHE
1	4	289	ILE
1	4	292	ARG
1	4	304	PHE
1	4	312	ARG
1	4	315	GLN
1	4	317	VAL
1	4	320	GLN
1	4	323	TYR
1	4	325	MET
1	4	326	GLU
1	4	331	GLU
1	4	332	VAL

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Mol	Chain	Res	Type
1	4	336	ASP
1	4	338	THR
1	4	344	ASP
1	5	16	LYS
1	5	20	GLU
1	5	28	LEU
1	5	30	LYS
1	5	33	VAL
1	5	34	GLU
1	5	37	GLU
1	5	39	LYS
1	5	52	LEU
1	5	55	GLU
1	5	60	ASP
1	5	61	GLU
1	5	63	LEU
1	5	69	LYS
1	5	75	ASP
1	5	76	PHE
1	5	91	THR
1	5	101	GLU
1	5	107	ASN
1	5	110	MET
1	5	111	TRP
1	5	115	THR
1	5	125	SER
1	5	133	SER
1	5	134	GLN
1	5	143	LYS
1	5	155	VAL
1	5	160	LEU
1	5	162	MET
1	5	170	ARG
1	5	175	ASP
1	5	178	ILE
1	5	179	THR
1	5	194	HIS
1	5	202	ASN
1	5	208	CYS
1	5	221	TYR
1	5	236	HIS
1	5	242	THR

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Mol	Chain	Res	Type
1	5	247	ASP
1	5	248	GLU
1	5	253	PRO
1	5	255	CYS
1	5	270	LEU
1	5	273	ASN
1	5	274	SER
1	5	279	GLN
1	5	285	ARG
1	5	287	PHE
1	5	289	ILE
1	5	291	LEU
1	5	292	ARG
1	5	294	ARG
1	5	296	VAL
1	5	300	TYR
1	5	305	LEU
1	5	306	LEU
1	5	308	ASP
1	5	313	ARG
1	5	315	GLN
1	5	316	ARG
1	5	323	TYR
1	5	325	MET
1	5	339	GLU
1	5	340	ARG
1	5	341	LEU
1	5	348	ILE
1	5	352	ASP
1	5	359	THR
1	6	17	LYS
1	6	22	VAL
1	6	23	GLN
1	6	28	LEU
1	6	38	VAL
1	6	43	ASP
1	6	50	CYS
1	6	53	ASN
1	6	56	MET
1	6	61	GLU
1	6	62	ASN
1	6	64	ARG

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Mol	Chain	Res	Type
1	6	67	SER
1	6	74	ASN
1	6	75	ASP
1	6	78	SER
1	6	82	GLU
1	6	84	LYS
1	6	91	THR
1	6	93	ARG
1	6	100	ASN
1	6	104	THR
1	6	109	LEU
1	6	110	MET
1	6	111	TRP
1	6	114	VAL
1	6	115	THR
1	6	117	GLN
1	6	124	THR
1	6	126	MET
1	6	138	GLU
1	6	139	HIS
1	6	152	PHE
1	6	153	PHE
1	6	158	GLU
1	6	161	GLU
1	6	162	MET
1	6	165	VAL
1	6	166	LEU
1	6	167	MET
1	6	170	ARG
1	6	177	THR
1	6	178	ILE
1	6	181	LYS
1	6	186	GLN
1	6	190	MET
1	6	194	HIS
1	6	199	ASP
1	6	200	LYS
1	6	212	ASP
1	6	217	GLU
1	6	224	THR
1	6	229	GLU
1	6	243	THR

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Mol	Chain	Res	Type
1	6	246	LEU
1	6	255	CYS
1	6	263	SER
1	6	268	CYS
1	6	274	SER
1	6	275	SER
1	6	279	GLN
1	6	281	ARG
1	6	287	PHE
1	6	289	ILE
1	6	290	ARG
1	6	292	ARG
1	6	297	LYS
1	6	298	ASN
1	6	301	PRO
1	6	305	LEU
1	6	306	LEU
1	6	315	GLN
1	6	316	ARG
1	6	318	ASP
1	6	326	GLU
1	6	336	ASP
1	6	342	PRO
1	6	350	TYR
1	6	351	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	98	ASN
1	1	107	ASN
1	1	117	GLN
1	1	139	HIS
1	1	182	ASN
1	1	194	HIS
1	1	202	ASN
1	1	218	ASN
1	1	236	HIS
1	1	273	ASN
1	1	298	ASN
1	1	328	GLN
1	2	130	HIS

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Mol	Chain	Res	Type
1	2	139	HIS
1	2	216	ASN
1	2	230	ASN
1	2	236	HIS
1	2	358	GLN
1	3	134	GLN
1	3	146	GLN
1	3	163	GLN
1	3	182	ASN
1	3	201	ASN
1	3	236	HIS
1	3	273	ASN
1	3	278	GLN
1	3	315	GLN
1	4	53	ASN
1	4	74	ASN
1	4	100	ASN
1	4	107	ASN
1	4	139	HIS
1	4	202	ASN
1	4	239	ASN
1	4	315	GLN
1	5	202	ASN
1	5	218	ASN
1	5	315	GLN
1	5	320	GLN
1	6	53	ASN
1	6	62	ASN
1	6	74	ASN
1	6	100	ASN
1	6	130	HIS
1	6	194	HIS
1	6	202	ASN
1	6	218	ASN
1	6	320	GLN
1	6	328	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.